Full wwPDB X-ray Structure Validation Report

May 29, 2024 – 02:23 PM EDT

PDB ID	:	4RUB
Title	:	A CRYSTAL FORM OF RIBULOSE-1,5-BISPHOSPHATE CARBOXY LASE(SLASH)OXYGENASE FROM NICOTIANA TABACUM IN THE ACTIVATED STATE
Authors	:	Schreuder, H.; Cascio, D.; Curmi, P.M.G.; Eisenberg, D.
Deposited on	:	1990-05-25
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:

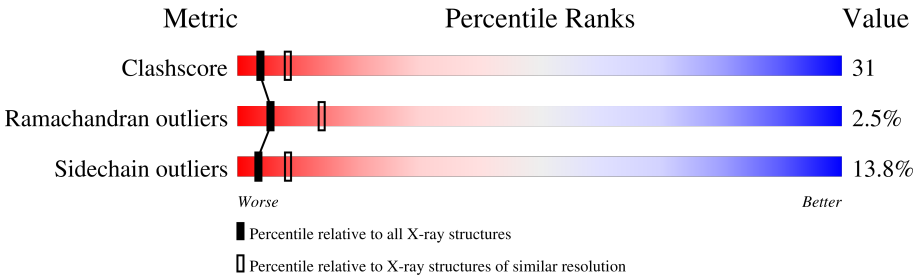
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	477	35% 39% 19% • •
1	B	477	34% 42% 17% 5% •
1	C	477	31% 41% 21% 5% •
1	D	477	36% 38% 18% 5% •
2	S	123	30% 46% 20% 5%
2	T	123	34% 43% 17% 6%
2	U	123	20% 43% 33% 5%
2	V	123	27% 41% 25% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CAP	A	490	-	X	-	-
4	CAP	B	490	-	X	-	-
4	CAP	C	490	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			
1	B	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			
1	C	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			
1	D	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			

- Molecule 2 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			
2	T	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			
2	U	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			
2	V	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			

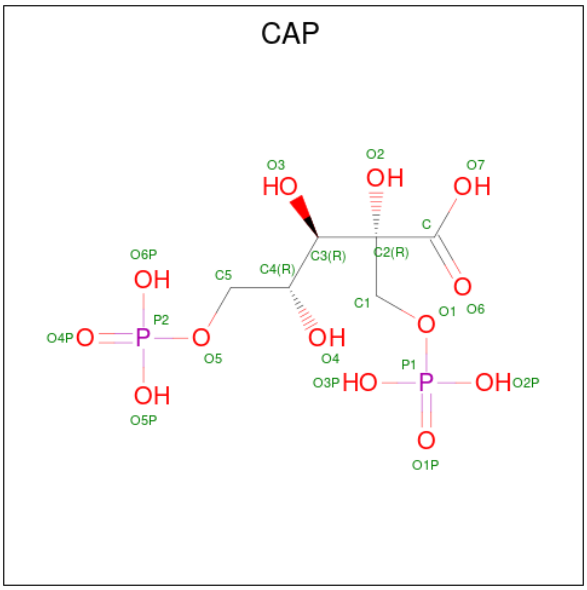
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	88	GLY	GLU	conflict	UNP P69249
T	88	GLY	GLU	conflict	UNP P69249
U	88	GLY	GLU	conflict	UNP P69249
V	88	GLY	GLU	conflict	UNP P69249

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

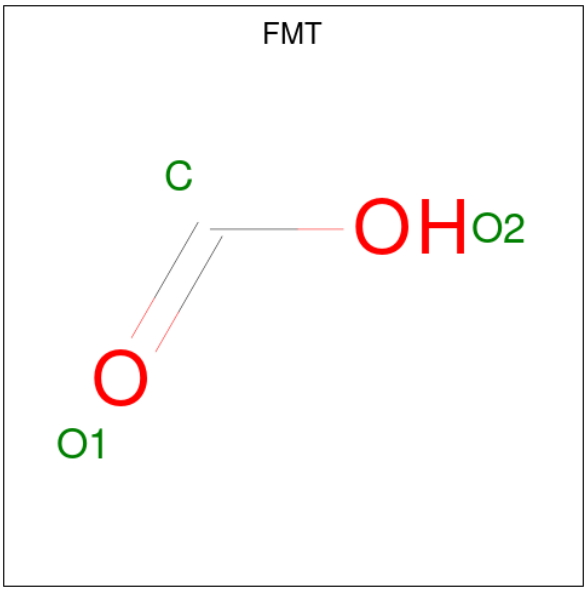
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 21 6 13 2	0	0
4	B	1	Total C O P 21 6 13 2	0	0
4	C	1	Total C O P 21 6 13 2	0	0
4	D	1	Total C O P 21 6 13 2	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		

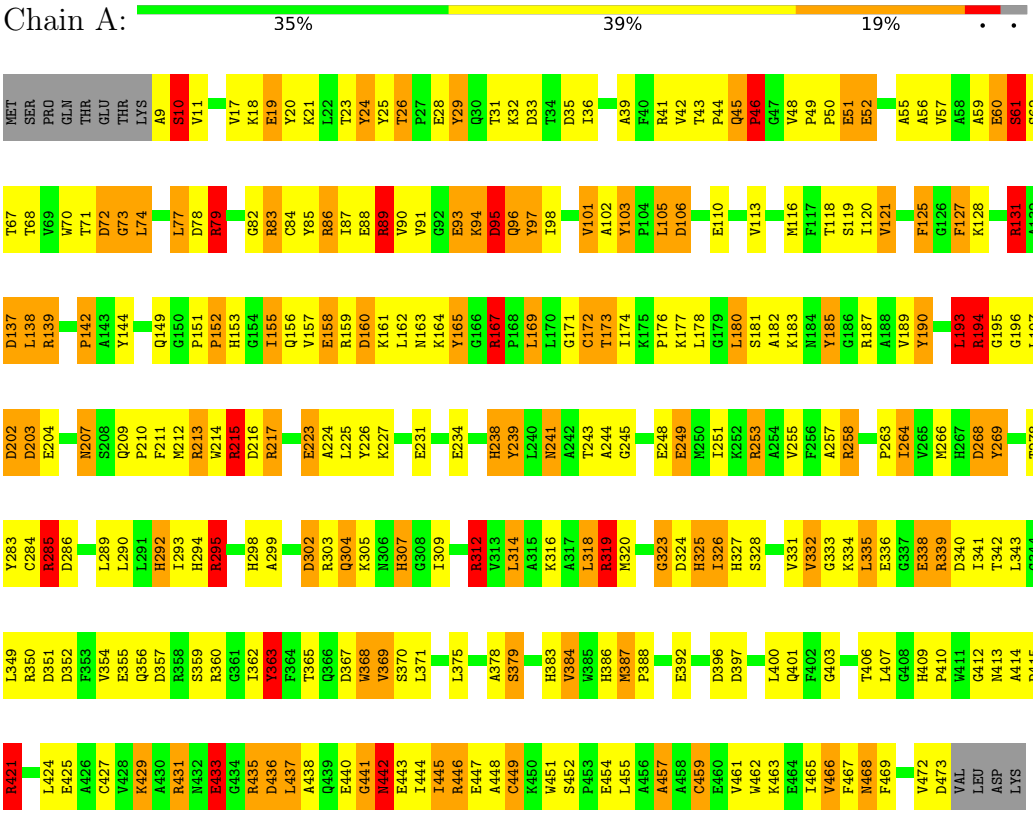
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

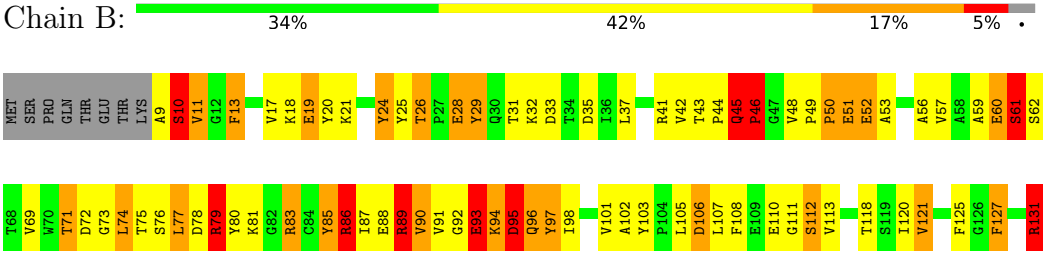
• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

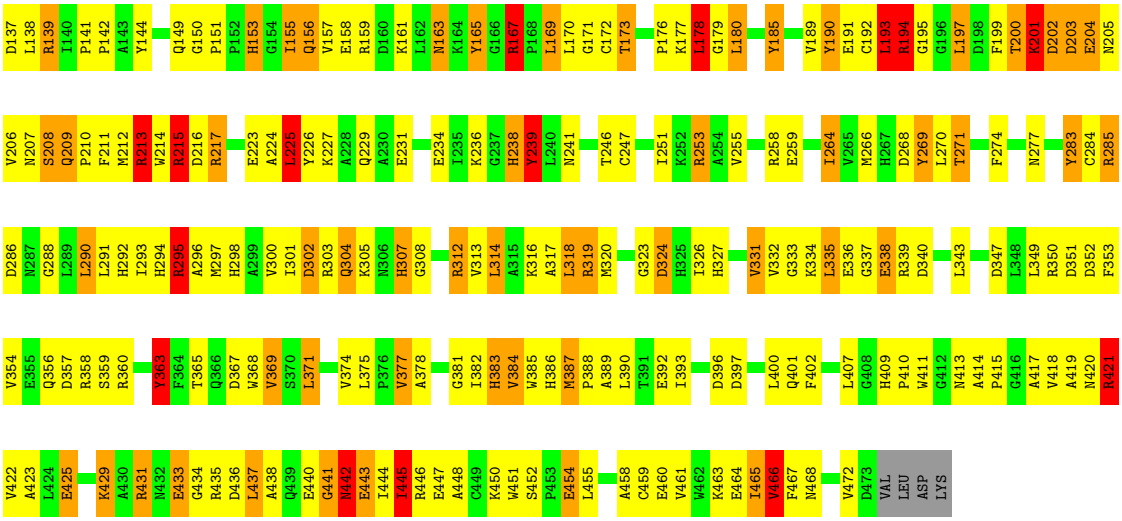
Chain A:



• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

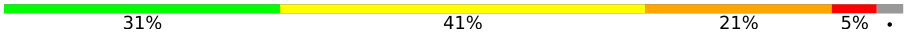
Chain B:

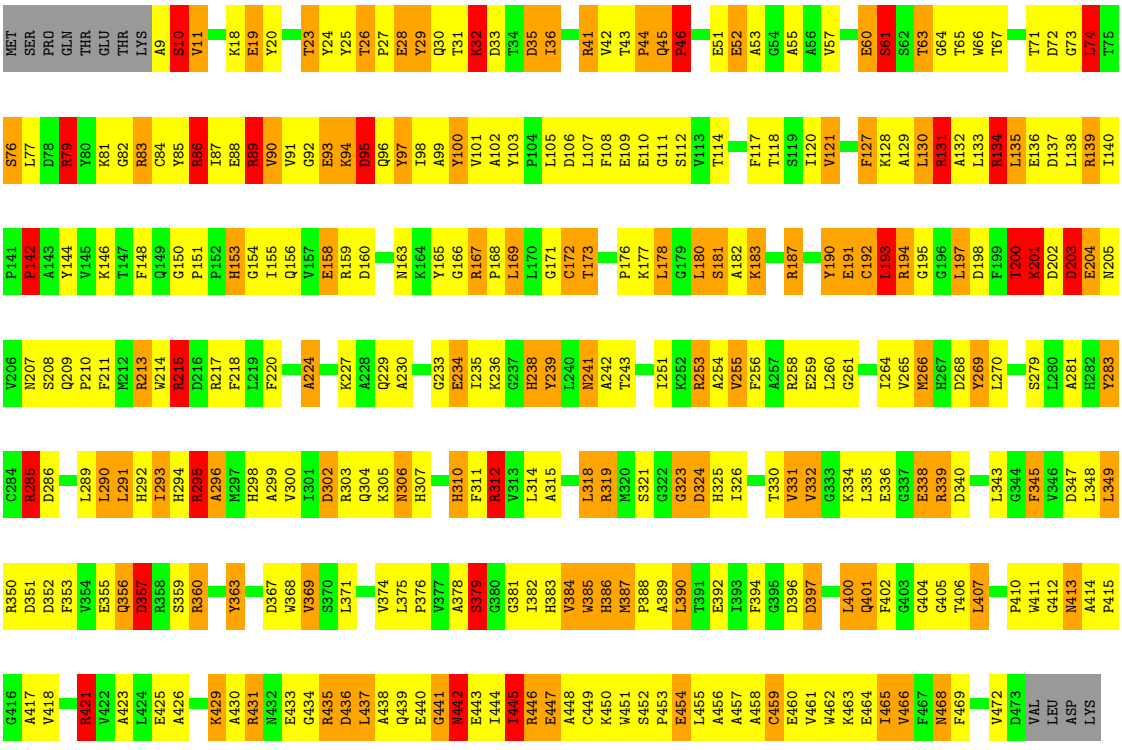




• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

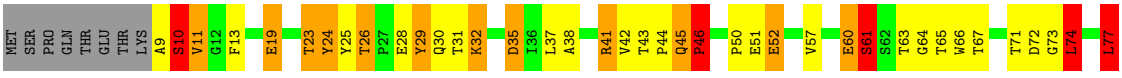
Chain C:

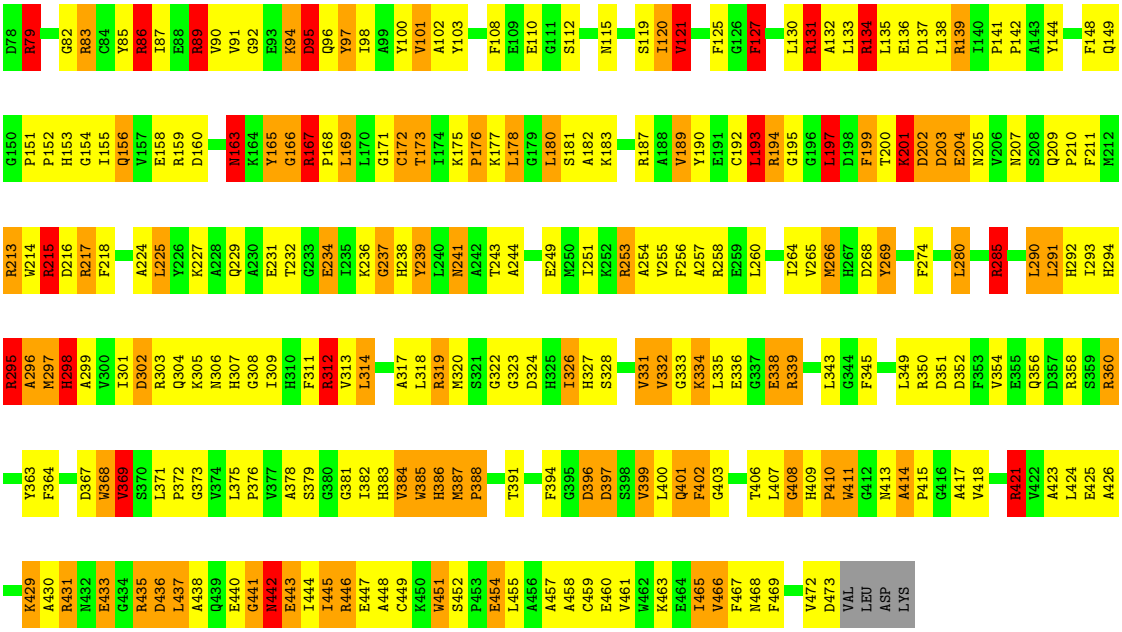




• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

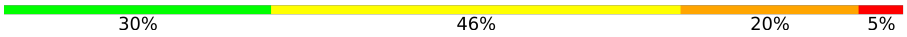
Chain D:

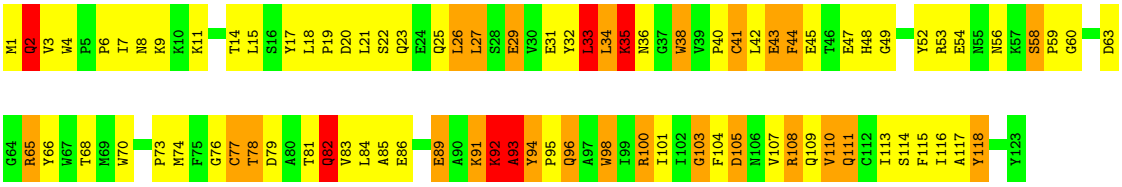




• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

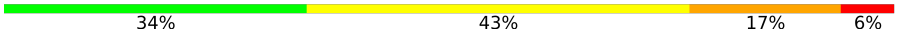
Chain S:

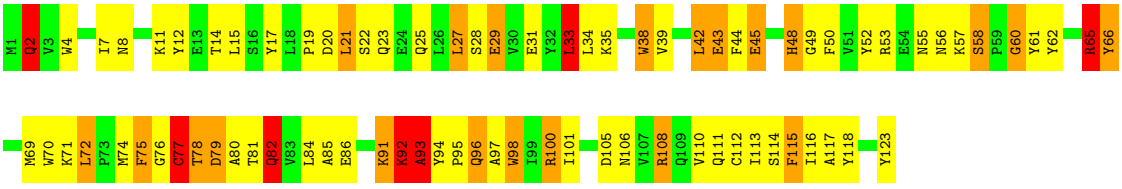




• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

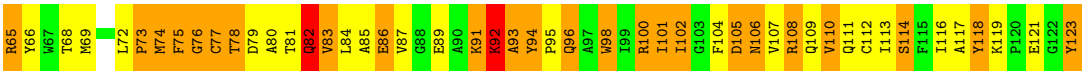
Chain T:





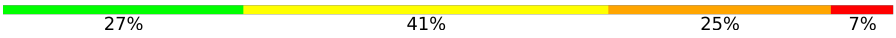
• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain U:



• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain V:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.60Å 204.60Å 117.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18708	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, FMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.69	30/3716 (0.8%)	2.59	253/5038 (5.0%)
1	B	1.66	24/3716 (0.6%)	2.57	227/5038 (4.5%)
1	C	1.75	46/3716 (1.2%)	2.66	253/5038 (5.0%)
1	D	1.69	39/3716 (1.0%)	2.60	235/5038 (4.7%)
2	S	1.57	8/1057 (0.8%)	2.51	71/1435 (4.9%)
2	T	1.48	3/1057 (0.3%)	2.25	56/1435 (3.9%)
2	U	1.79	13/1057 (1.2%)	2.53	70/1435 (4.9%)
2	V	1.70	14/1057 (1.3%)	2.50	80/1435 (5.6%)
All	All	1.68	177/19092 (0.9%)	2.57	1245/25892 (4.8%)

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	58	SER	CB-OG	-9.13	1.30	1.42
1	C	181	SER	CB-OG	8.99	1.53	1.42
1	C	323	GLY	N-CA	8.87	1.59	1.46
1	A	459	CYS	CB-SG	-8.49	1.67	1.82
1	A	134	ARG	CZ-NH1	8.02	1.43	1.33
1	A	234	GLU	CD-OE2	-7.93	1.17	1.25
1	C	110	GLU	CB-CG	-7.78	1.37	1.52
1	C	201	LYS	CA-CB	7.77	1.71	1.53
2	V	7	ILE	C-O	7.74	1.38	1.23
1	C	405	GLY	C-O	7.74	1.36	1.23
1	C	266	MET	C-O	7.70	1.38	1.23
1	C	319	ARG	CD-NE	-7.69	1.33	1.46
1	D	201	LYS	CA-CB	7.43	1.70	1.53
2	U	7	ILE	C-O	7.42	1.37	1.23
1	D	403	GLY	N-CA	7.41	1.57	1.46
1	C	243	THR	CB-OG1	7.37	1.57	1.43
1	C	285	ARG	CZ-NH1	7.25	1.42	1.33
1	D	158	GLU	CD-OE1	7.25	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	SER	CB-OG	7.17	1.51	1.42
1	C	454	GLU	CD-OE2	7.13	1.33	1.25
1	A	319	ARG	NE-CZ	-7.02	1.24	1.33
2	V	82	GLN	C-O	7.02	1.36	1.23
1	B	459	CYS	CB-SG	-6.98	1.70	1.82
1	D	258	ARG	NE-CZ	6.97	1.42	1.33
1	D	231	GLU	CD-OE1	6.97	1.33	1.25
1	A	201	LYS	CA-CB	6.89	1.69	1.53
1	B	223	GLU	CD-OE1	-6.88	1.18	1.25
1	A	319	ARG	CD-NE	-6.77	1.34	1.46
1	A	427	CYS	CB-SG	-6.74	1.70	1.82
1	C	259	GLU	CD-OE2	6.73	1.33	1.25
1	B	201	LYS	CA-CB	6.66	1.68	1.53
1	C	156	GLN	CD-NE2	6.59	1.49	1.32
1	C	253	ARG	CZ-NH1	6.58	1.41	1.33
1	B	110	GLU	CD-OE2	-6.56	1.18	1.25
1	D	290	LEU	C-O	6.55	1.35	1.23
2	S	7	ILE	C-O	6.55	1.35	1.23
1	C	310	HIS	C-O	6.53	1.35	1.23
2	T	62	TYR	CE2-CZ	-6.50	1.30	1.38
1	B	52	GLU	CD-OE1	-6.48	1.18	1.25
1	A	279	SER	CA-CB	-6.47	1.43	1.52
2	U	65	ARG	NE-CZ	6.45	1.41	1.33
1	A	72	ASP	C-O	6.42	1.35	1.23
1	D	201	LYS	CE-NZ	-6.38	1.33	1.49
1	D	388	PRO	N-CD	6.36	1.56	1.47
1	D	364	PHE	CE2-CZ	6.35	1.49	1.37
1	D	172	CYS	CB-SG	-6.29	1.71	1.82
1	A	449	CYS	CB-SG	-6.20	1.71	1.82
1	B	425	GLU	CD-OE1	-6.19	1.18	1.25
1	C	153	HIS	C-O	6.15	1.35	1.23
1	D	217	ARG	CZ-NH2	6.14	1.41	1.33
1	A	61	SER	CA-CB	6.09	1.62	1.52
1	C	127	PHE	C-O	6.04	1.34	1.23
1	D	60	GLU	CD-OE2	-6.02	1.19	1.25
2	V	65	ARG	NE-CZ	6.01	1.40	1.33
1	A	201	LYS	CE-NZ	-6.00	1.34	1.49
1	D	328	SER	CB-OG	5.97	1.50	1.42
1	A	370	SER	C-O	5.94	1.34	1.23
1	A	24	TYR	C-O	5.93	1.34	1.23
1	C	215	ARG	CZ-NH1	5.92	1.40	1.33
2	V	13	GLU	CD-OE2	5.90	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	SER	CB-OG	-5.86	1.34	1.42
1	A	350	ARG	CD-NE	-5.85	1.36	1.46
2	S	8	ASN	N-CA	5.83	1.58	1.46
1	B	284	CYS	CB-SG	-5.82	1.72	1.81
1	D	319	ARG	NE-CZ	-5.81	1.25	1.33
2	U	8	ASN	N-CA	5.80	1.57	1.46
1	D	61	SER	CB-OG	-5.79	1.34	1.42
2	V	69	MET	CG-SD	5.79	1.96	1.81
2	V	43	GLU	CD-OE1	-5.77	1.19	1.25
1	C	111	GLY	C-O	5.77	1.32	1.23
1	B	83	ARG	CZ-NH2	5.76	1.40	1.33
2	S	47	GLU	CD-OE2	5.75	1.31	1.25
1	C	431	ARG	NE-CZ	5.74	1.40	1.33
1	A	119	SER	C-O	5.73	1.34	1.23
1	B	223	GLU	CG-CD	-5.70	1.43	1.51
1	A	217	ARG	CD-NE	-5.68	1.36	1.46
1	D	368	TRP	CG-CD1	5.68	1.44	1.36
2	V	53	ARG	CZ-NH1	5.66	1.40	1.33
1	A	238	HIS	CG-CD2	-5.66	1.26	1.35
1	C	319	ARG	CZ-NH1	5.66	1.40	1.33
1	D	306	ASN	C-O	5.65	1.34	1.23
1	C	256	PHE	C-O	5.64	1.34	1.23
1	D	285	ARG	NE-CZ	5.62	1.40	1.33
2	U	49	GLY	C-O	5.60	1.32	1.23
1	D	148	PHE	CG-CD1	-5.60	1.30	1.38
1	B	201	LYS	N-CA	-5.59	1.35	1.46
1	C	238	HIS	C-O	5.58	1.33	1.23
1	B	433	GLU	CB-CG	-5.57	1.41	1.52
2	T	92	LYS	C-O	5.57	1.33	1.23
2	V	8	ASN	N-CA	5.56	1.57	1.46
1	B	350	ARG	CD-NE	-5.56	1.36	1.46
1	D	411	TRP	C-O	5.55	1.33	1.23
2	V	88	GLY	N-CA	5.55	1.54	1.46
1	D	258	ARG	CG-CD	-5.55	1.38	1.51
2	S	73	PRO	N-CD	-5.51	1.40	1.47
1	C	306	ASN	C-O	5.50	1.33	1.23
1	B	365	THR	C-O	5.49	1.33	1.23
1	C	177	LYS	C-O	5.49	1.33	1.23
2	U	76	GLY	C-O	5.44	1.32	1.23
1	D	291	LEU	C-O	5.42	1.33	1.23
1	C	36	ILE	C-O	5.42	1.33	1.23
2	S	53	ARG	CZ-NH2	-5.42	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	295	ARG	C-O	5.40	1.33	1.23
1	A	359	SER	CA-CB	-5.40	1.44	1.52
1	A	284	CYS	CB-SG	-5.40	1.73	1.81
2	S	65	ARG	CG-CD	-5.40	1.38	1.51
1	D	237	GLY	C-O	5.39	1.32	1.23
2	V	37	GLY	C-O	5.39	1.32	1.23
1	D	408	GLY	C-O	5.37	1.32	1.23
1	D	112	SER	CB-OG	-5.36	1.35	1.42
1	C	445	ILE	N-CA	5.34	1.57	1.46
1	A	362	ILE	C-O	5.32	1.33	1.23
1	C	379	SER	CB-OG	5.32	1.49	1.42
1	B	259	GLU	CD-OE1	5.31	1.31	1.25
1	D	339	ARG	CZ-NH1	5.31	1.40	1.33
1	A	433	GLU	CB-CG	-5.30	1.42	1.52
1	C	321	SER	CA-CB	-5.30	1.45	1.52
2	U	102	ILE	C-O	5.30	1.33	1.23
1	A	103	TYR	C-O	5.29	1.33	1.23
1	C	261	GLY	C-O	5.29	1.32	1.23
1	D	443	GLU	CB-CG	5.29	1.62	1.52
1	A	379	SER	CB-OG	-5.28	1.35	1.42
1	C	201	LYS	CE-NZ	-5.28	1.35	1.49
1	C	406	THR	CB-OG1	5.27	1.53	1.43
2	V	93	ALA	N-CA	5.27	1.56	1.46
1	D	460	GLU	CD-OE1	5.27	1.31	1.25
1	D	176	PRO	C-O	5.27	1.33	1.23
1	D	385	TRP	CA-CB	5.26	1.65	1.53
1	D	421	ARG	C-O	5.25	1.33	1.23
1	B	206	VAL	C-O	-5.25	1.13	1.23
2	U	86	GLU	CB-CG	5.25	1.62	1.52
2	S	100	ARG	CG-CD	-5.25	1.38	1.51
1	C	233	GLY	C-O	5.24	1.32	1.23
1	B	179	GLY	N-CA	-5.22	1.38	1.46
1	C	201	LYS	N-CA	-5.22	1.35	1.46
1	C	435	ARG	N-CA	5.21	1.56	1.46
1	C	114	THR	CB-OG1	5.21	1.53	1.43
1	C	421	ARG	C-O	5.21	1.33	1.23
2	U	54	GLU	C-O	5.21	1.33	1.23
1	B	204	GLU	CD-OE1	-5.21	1.20	1.25
2	V	77	CYS	CB-SG	5.17	1.91	1.82
1	D	332	VAL	C-O	5.17	1.33	1.23
2	U	41	CYS	CB-SG	5.17	1.91	1.82
1	C	293	ILE	C-N	-5.16	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	PHE	CE1-CZ	5.15	1.47	1.37
1	D	290	LEU	N-CA	5.15	1.56	1.46
1	C	204	GLU	CD-OE1	-5.14	1.20	1.25
2	U	74	MET	CG-SD	5.13	1.94	1.81
2	V	62	TYR	CD2-CE2	5.13	1.47	1.39
2	U	98	TRP	C-O	5.12	1.33	1.23
1	D	232	THR	CB-OG1	5.11	1.53	1.43
1	C	217	ARG	CZ-NH2	5.11	1.39	1.33
1	C	459	CYS	CB-SG	-5.11	1.73	1.81
1	C	404	GLY	N-CA	5.10	1.53	1.46
1	A	285	ARG	CD-NE	5.10	1.55	1.46
1	D	167	ARG	CZ-NH1	5.10	1.39	1.33
1	B	201	LYS	CE-NZ	-5.09	1.36	1.49
1	B	247	CYS	CB-SG	-5.09	1.73	1.81
1	C	158	GLU	CB-CG	5.09	1.61	1.52
1	C	110	GLU	CG-CD	-5.09	1.44	1.51
1	D	322	GLY	N-CA	-5.08	1.38	1.46
1	B	190	TYR	CG-CD2	-5.07	1.32	1.39
1	D	197	LEU	C-O	5.07	1.32	1.23
1	C	173	THR	CB-OG1	5.05	1.53	1.43
1	A	368	TRP	C-N	-5.05	1.22	1.34
1	A	342	THR	CB-OG1	5.04	1.53	1.43
2	U	114	SER	CA-CB	-5.04	1.45	1.52
1	A	73	GLY	N-CA	5.04	1.53	1.46
1	A	172	CYS	CB-SG	-5.04	1.73	1.81
1	B	367	ASP	N-CA	5.04	1.56	1.46
1	B	61	SER	CA-CB	5.02	1.60	1.52
2	T	106	ASN	C-O	5.02	1.32	1.23
2	V	62	TYR	N-CA	5.02	1.56	1.46
1	A	253	ARG	CZ-NH1	5.01	1.39	1.33
2	U	59	PRO	C-O	5.01	1.33	1.23
1	D	144	TYR	CG-CD1	-5.01	1.32	1.39
1	B	208	SER	CA-CB	-5.00	1.45	1.52

All (1245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	350	ARG	NE-CZ-NH2	-35.79	102.40	120.30
1	A	319	ARG	CD-NE-CZ	25.36	159.11	123.60
1	C	319	ARG	CD-NE-CZ	23.95	157.13	123.60
1	D	139	ARG	NE-CZ-NH1	-23.24	108.68	120.30
1	A	139	ARG	NE-CZ-NH2	23.20	131.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	217	ARG	NE-CZ-NH2	-21.79	109.41	120.30
2	U	65	ARG	NE-CZ-NH2	-20.93	109.83	120.30
1	D	139	ARG	NE-CZ-NH2	20.81	130.71	120.30
1	B	350	ARG	NE-CZ-NH2	-20.56	110.02	120.30
1	D	350	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	C	215	ARG	NE-CZ-NH1	-19.88	110.36	120.30
1	D	215	ARG	NE-CZ-NH2	19.77	130.19	120.30
1	B	215	ARG	NE-CZ-NH1	-19.20	110.70	120.30
1	A	134	ARG	NE-CZ-NH1	-18.79	110.90	120.30
1	B	139	ARG	NE-CZ-NH2	18.71	129.65	120.30
2	S	65	ARG	NE-CZ-NH2	-18.54	111.03	120.30
1	C	217	ARG	NE-CZ-NH1	18.11	129.35	120.30
1	D	319	ARG	CD-NE-CZ	18.00	148.80	123.60
2	S	53	ARG	NE-CZ-NH2	17.98	129.29	120.30
1	B	319	ARG	CD-NE-CZ	17.68	148.35	123.60
1	D	194	ARG	NE-CZ-NH1	17.60	129.10	120.30
1	B	139	ARG	NE-CZ-NH1	-17.49	111.56	120.30
1	B	217	ARG	NE-CZ-NH1	17.46	129.03	120.30
1	C	79	ARG	NE-CZ-NH1	-16.98	111.81	120.30
1	B	215	ARG	NE-CZ-NH2	16.97	128.78	120.30
2	S	66	TYR	CB-CG-CD2	16.71	131.03	121.00
1	A	217	ARG	CD-NE-CZ	16.66	146.93	123.60
1	A	295	ARG	NE-CZ-NH1	16.55	128.58	120.30
1	A	350	ARG	CD-NE-CZ	16.47	146.65	123.60
1	D	79	ARG	NE-CZ-NH1	-16.43	112.08	120.30
1	C	360	ARG	NE-CZ-NH1	-16.38	112.11	120.30
1	C	258	ARG	NE-CZ-NH1	16.18	128.39	120.30
1	D	421	ARG	NE-CZ-NH1	-16.15	112.22	120.30
1	A	258	ARG	NE-CZ-NH1	16.12	128.36	120.30
1	A	213	ARG	NE-CZ-NH2	16.12	128.36	120.30
1	B	217	ARG	CD-NE-CZ	15.98	145.97	123.60
1	A	89	ARG	CD-NE-CZ	15.91	145.87	123.60
1	A	139	ARG	NE-CZ-NH1	-15.73	112.44	120.30
1	B	319	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	C	350	ARG	NE-CZ-NH1	15.65	128.12	120.30
1	C	89	ARG	NE-CZ-NH1	14.89	127.75	120.30
1	D	86	ARG	NE-CZ-NH2	14.80	127.70	120.30
1	D	350	ARG	NE-CZ-NH1	14.63	127.62	120.30
1	B	201	LYS	CA-CB-CG	14.62	145.55	113.40
1	C	41	ARG	NE-CZ-NH2	14.56	127.58	120.30
2	U	105	ASP	CB-CG-OD1	14.52	131.37	118.30
1	B	283	TYR	CB-CG-CD1	14.50	129.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	431	ARG	NE-CZ-NH2	-14.35	113.12	120.30
2	S	53	ARG	NE-CZ-NH1	-14.05	113.28	120.30
1	D	367	ASP	CB-CG-OD1	13.75	130.68	118.30
1	B	360	ARG	NE-CZ-NH1	-13.56	113.52	120.30
1	C	269	TYR	CB-CG-CD1	13.47	129.08	121.00
1	C	41	ARG	NE-CZ-NH1	-13.45	113.57	120.30
1	D	217	ARG	CD-NE-CZ	13.23	142.12	123.60
1	B	89	ARG	CD-NE-CZ	13.21	142.09	123.60
1	C	253	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	D	83	ARG	NE-CZ-NH1	-13.10	113.75	120.30
1	C	89	ARG	CD-NE-CZ	13.06	141.89	123.60
1	A	367	ASP	CB-CG-OD1	13.06	130.05	118.30
1	C	134	ARG	NE-CZ-NH1	-13.01	113.80	120.30
1	D	89	ARG	CD-NE-CZ	13.00	141.79	123.60
1	A	312	ARG	NE-CZ-NH1	-12.97	113.82	120.30
1	A	215	ARG	NE-CZ-NH1	-12.84	113.88	120.30
1	C	160	ASP	CB-CG-OD1	-12.80	106.78	118.30
1	B	351	ASP	CB-CG-OD2	-12.62	106.94	118.30
1	A	367	ASP	CB-CG-OD2	-12.61	106.95	118.30
1	A	167	ARG	NE-CZ-NH1	-12.54	114.03	120.30
1	C	367	ASP	CB-CG-OD1	12.34	129.41	118.30
1	C	339	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	A	324	ASP	CB-CG-OD1	12.03	129.12	118.30
1	A	347	ASP	CB-CG-OD1	11.99	129.09	118.30
1	B	167	ARG	NE-CZ-NH2	11.85	126.23	120.30
1	C	72	ASP	CB-CG-OD1	11.84	128.95	118.30
1	A	33	ASP	CB-CG-OD2	-11.66	107.81	118.30
1	D	253	ARG	NE-CZ-NH2	-11.65	114.47	120.30
1	B	25	TYR	CB-CG-CD1	-11.63	114.02	121.00
2	T	20	ASP	CB-CG-OD2	-11.57	107.89	118.30
1	D	41	ARG	NE-CZ-NH1	-11.52	114.54	120.30
1	C	217	ARG	CD-NE-CZ	11.46	139.65	123.60
1	C	295	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	285	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	C	285	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	C	431	ARG	NE-CZ-NH1	11.25	125.93	120.30
1	A	319	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	D	352	ASP	CB-CG-OD2	11.18	128.36	118.30
1	A	433	GLU	CA-CB-CG	11.16	137.95	113.40
2	V	105	ASP	CB-CG-OD1	11.09	128.28	118.30
1	C	295	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	D	360	ARG	NE-CZ-NH1	-11.00	114.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	25	TYR	CB-CG-CD1	-10.90	114.46	121.00
1	D	160	ASP	CB-CG-OD2	10.78	128.00	118.30
2	V	62	TYR	CB-CG-CD1	-10.75	114.55	121.00
1	A	25	TYR	CB-CG-CD2	10.72	127.43	121.00
1	A	190	TYR	CB-CG-CD2	10.69	127.42	121.00
1	C	46	PRO	N-CA-CB	-10.68	90.49	103.30
1	D	396	ASP	CB-CG-OD1	-10.68	108.69	118.30
2	V	62	TYR	CB-CG-CD2	10.66	127.39	121.00
1	B	89	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	A	216	ASP	CB-CG-OD2	10.58	127.82	118.30
1	D	319	ARG	NE-CZ-NH1	-10.56	115.02	120.30
1	A	25	TYR	CB-CG-CD1	-10.54	114.68	121.00
1	D	324	ASP	CB-CG-OD1	10.54	127.78	118.30
2	U	66	TYR	CB-CG-CD2	10.52	127.31	121.00
1	B	79	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	41	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	A	286	ASP	CB-CG-OD2	-10.49	108.86	118.30
1	B	350	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	B	131	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	72	ASP	CA-CB-CG	10.44	136.36	113.40
1	A	169	LEU	CA-CB-CG	10.44	139.30	115.30
1	A	217	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	B	421	ARG	NE-CZ-NH1	-10.37	115.11	120.30
1	B	312	ARG	NE-CZ-NH2	-10.35	115.13	120.30
1	D	446	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	D	433	GLU	CA-CB-CG	10.33	136.12	113.40
1	B	269	TYR	CB-CG-CD1	10.32	127.19	121.00
1	B	156	GLN	CG-CD-OE1	10.31	142.23	121.60
1	C	79	ARG	NH1-CZ-NH2	10.28	130.71	119.40
2	S	43	GLU	OE1-CD-OE2	-10.20	111.06	123.30
1	D	397	ASP	O-C-N	10.20	139.03	122.70
1	C	110	GLU	OE1-CD-OE2	-10.13	111.15	123.30
1	B	433	GLU	CA-CB-CG	10.09	135.60	113.40
1	D	167	ARG	NE-CZ-NH2	10.07	125.34	120.30
1	D	25	TYR	CB-CG-CD1	-10.06	114.96	121.00
1	B	217	ARG	NH1-CZ-NH2	-10.02	108.38	119.40
1	A	83	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	A	83	ARG	NE-CZ-NH2	10.00	125.30	120.30
2	S	66	TYR	CB-CG-CD1	-9.98	115.01	121.00
1	D	165	TYR	CB-CG-CD1	-9.98	115.01	121.00
1	B	283	TYR	CB-CG-CD2	-9.94	115.04	121.00
1	A	216	ASP	CB-CG-OD1	-9.90	109.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	347	ASP	CB-CG-OD1	9.89	127.20	118.30
1	D	350	ARG	CD-NE-CZ	9.86	137.41	123.60
1	D	258	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	D	360	ARG	CD-NE-CZ	-9.84	109.83	123.60
1	A	421	ARG	NE-CZ-NH1	-9.83	115.39	120.30
1	B	72	ASP	CB-CG-OD1	9.79	127.11	118.30
1	B	33	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	D	79	ARG	NH1-CZ-NH2	9.75	130.13	119.40
1	D	358	ARG	NE-CZ-NH1	-9.72	115.44	120.30
2	S	7	ILE	CA-C-O	-9.67	99.79	120.10
2	V	65	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	D	446	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	D	202	ASP	CB-CG-OD1	9.60	126.94	118.30
1	D	134	ARG	NE-CZ-NH1	-9.59	115.50	120.30
1	B	88	GLU	CA-CB-CG	9.58	134.48	113.40
1	C	367	ASP	CB-CG-OD2	-9.54	109.71	118.30
2	U	66	TYR	CB-CG-CD1	-9.54	115.27	121.00
1	D	72	ASP	CA-CB-CG	9.52	134.35	113.40
1	B	46	PRO	N-CA-CB	-9.52	91.88	103.30
1	C	218	PHE	CB-CG-CD2	-9.52	114.14	120.80
2	S	82	GLN	CB-CG-CD	9.50	136.31	111.60
2	T	110	VAL	CA-CB-CG1	9.50	125.15	110.90
1	B	86	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	D	352	ASP	CB-CG-OD1	-9.47	109.77	118.30
1	C	131	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	B	25	TYR	CB-CG-CD2	9.44	126.66	121.00
1	B	139	ARG	CD-NE-CZ	-9.43	110.40	123.60
1	B	72	ASP	CA-CB-CG	9.42	134.13	113.40
1	C	85	TYR	CB-CG-CD1	9.42	126.65	121.00
1	A	339	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	185	TYR	CB-CG-CD2	9.31	126.59	121.00
2	S	100	ARG	N-CA-CB	-9.30	93.86	110.60
1	C	110	GLU	CG-CD-OE2	9.30	136.89	118.30
1	D	285	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	D	72	ASP	CB-CG-OD1	9.29	126.66	118.30
2	U	105	ASP	CB-CG-OD2	-9.27	109.96	118.30
1	C	433	GLU	CA-CB-CG	9.27	133.79	113.40
2	T	53	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	C	269	TYR	CB-CG-CD2	-9.22	115.47	121.00
1	B	33	ASP	CB-CG-OD1	9.19	126.57	118.30
1	B	24	TYR	CB-CG-CD1	9.17	126.50	121.00
1	C	350	ARG	NH1-CZ-NH2	9.15	129.47	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	108	ARG	NE-CZ-NH1	-9.15	115.72	120.30
1	A	312	ARG	NH1-CZ-NH2	9.15	129.46	119.40
1	C	72	ASP	CA-CB-CG	9.15	133.53	113.40
1	A	79	ARG	NE-CZ-NH1	-9.13	115.73	120.30
1	D	201	LYS	CG-CD-CE	-9.13	84.52	111.90
1	A	33	ASP	CB-CG-OD1	9.12	126.51	118.30
1	A	193	LEU	CA-CB-CG	9.09	136.21	115.30
1	D	86	ARG	NE-CZ-NH1	-9.07	115.76	120.30
1	D	386	HIS	CA-CB-CG	9.07	129.01	113.60
1	B	347	ASP	CB-CG-OD1	9.06	126.45	118.30
1	D	83	ARG	CD-NE-CZ	9.03	136.24	123.60
1	A	258	ARG	NH1-CZ-NH2	-9.01	109.49	119.40
1	A	144	TYR	CB-CG-CD1	-9.00	115.60	121.00
1	C	243	THR	O-C-N	8.98	137.07	122.70
1	D	213	ARG	NE-CZ-NH2	8.98	124.79	120.30
1	B	295	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	C	86	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	D	89	ARG	CA-CB-CG	8.93	133.04	113.40
1	C	266	MET	N-CA-CB	-8.92	94.55	110.60
1	D	201	LYS	CA-CB-CG	8.90	132.98	113.40
1	A	156	GLN	CG-CD-OE1	8.86	139.33	121.60
1	D	19	GLU	CA-CB-CG	8.85	132.87	113.40
1	C	187	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	T	7	ILE	CA-C-O	-8.80	101.63	120.10
1	C	397	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	C	190	TYR	CB-CG-CD1	-8.77	115.74	121.00
2	U	65	ARG	CD-NE-CZ	-8.76	111.34	123.60
1	D	41	ARG	NH1-CZ-NH2	8.76	129.04	119.40
1	D	266	MET	N-CA-CB	-8.76	94.84	110.60
1	C	83	ARG	NE-CZ-NH1	-8.75	115.93	120.30
1	B	350	ARG	CD-NE-CZ	8.74	135.84	123.60
1	C	156	GLN	CG-CD-OE1	8.71	139.03	121.60
1	C	347	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	D	156	GLN	CG-CD-OE1	8.69	138.97	121.60
1	B	97	TYR	CB-CG-CD1	-8.67	115.80	121.00
1	D	225	LEU	CB-CG-CD2	-8.66	96.28	111.00
1	A	46	PRO	N-CA-CB	-8.59	93.00	103.30
1	C	387	MET	CA-CB-CG	-8.59	98.71	113.30
1	D	46	PRO	N-CA-CB	-8.58	93.01	103.30
1	C	435	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	C	258	ARG	NH1-CZ-NH2	-8.51	110.04	119.40
1	D	231	GLU	OE1-CD-OE2	8.50	133.50	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	194	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	360	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	201	LYS	CB-CA-C	-8.48	93.44	110.40
1	C	173	THR	CA-CB-CG2	8.48	124.27	112.40
1	B	203	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	A	187	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	D	302	ASP	CB-CG-OD2	8.42	125.88	118.30
2	U	20	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	B	216	ASP	CB-CG-OD1	-8.38	110.76	118.30
2	V	66	TYR	CB-CG-CD1	-8.38	115.97	121.00
1	D	338	GLU	OE1-CD-OE2	-8.37	113.26	123.30
1	A	190	TYR	CB-CG-CD1	-8.35	115.99	121.00
1	A	121	VAL	N-CA-CB	-8.33	93.17	111.50
1	B	83	ARG	NE-CZ-NH1	-8.33	116.13	120.30
1	A	435	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	C	160	ASP	CB-CG-OD2	8.31	125.78	118.30
1	A	435	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	215	ARG	CD-NE-CZ	-8.28	112.01	123.60
1	A	201	LYS	CA-CB-CG	8.26	131.57	113.40
1	C	311	PHE	CB-CG-CD2	8.26	126.58	120.80
1	C	60	GLU	CG-CD-OE2	8.26	134.82	118.30
2	U	12	TYR	CB-CG-CD1	8.22	125.93	121.00
2	U	65	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	T	7	ILE	CA-C-N	8.21	135.27	117.20
1	C	138	LEU	CA-CB-CG	8.19	134.13	115.30
1	A	156	GLN	CB-CG-CD	8.18	132.85	111.60
2	U	61	TYR	CB-CG-CD2	-8.17	116.09	121.00
1	A	302	ASP	CB-CG-OD2	8.14	125.63	118.30
1	C	312	ARG	NE-CZ-NH1	-8.12	116.24	120.30
2	V	7	ILE	CA-C-O	-8.12	103.05	120.10
1	C	253	ARG	NH1-CZ-NH2	8.12	128.33	119.40
2	V	66	TYR	CB-CG-CD2	8.10	125.86	121.00
2	V	61	TYR	CG-CD2-CE2	-8.10	114.82	121.30
1	A	360	ARG	CD-NE-CZ	-8.07	112.30	123.60
1	C	340	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	D	312	ARG	NE-CZ-NH2	-8.04	116.28	120.30
2	U	100	ARG	N-CA-CB	-8.03	96.14	110.60
1	B	91	VAL	CA-C-N	-8.00	100.20	116.20
1	B	41	ARG	NE-CZ-NH1	-7.99	116.30	120.30
2	V	52	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	C	10	SER	N-CA-CB	7.98	122.47	110.50
2	U	2	GLN	N-CA-CB	7.97	124.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	108	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	B	269	TYR	CA-CB-CG	7.94	128.49	113.40
1	C	295	ARG	CD-NE-CZ	-7.91	112.52	123.60
2	S	21	LEU	CA-CB-CG	7.90	133.47	115.30
1	A	324	ASP	CB-CG-OD2	-7.90	111.19	118.30
2	V	98	TRP	N-CA-CB	7.89	124.80	110.60
1	B	358	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	C	386	HIS	CA-CB-CG	7.87	126.97	113.60
1	B	26	THR	N-CA-CB	-7.83	95.41	110.30
1	B	216	ASP	CB-CG-OD2	7.83	125.35	118.30
2	U	58	SER	CB-CA-C	7.83	124.98	110.10
1	B	137	ASP	CB-CG-OD1	-7.82	111.26	118.30
1	D	256	PHE	CB-CG-CD2	-7.81	115.33	120.80
1	B	144	TYR	CB-CG-CD2	7.81	125.68	121.00
2	V	2	GLN	N-CA-CB	7.80	124.64	110.60
1	C	90	VAL	O-C-N	7.80	135.18	122.70
1	C	213	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	185	TYR	CB-CG-CD1	-7.79	116.33	121.00
2	S	65	ARG	CG-CD-NE	7.78	128.15	111.80
1	D	41	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	201	LYS	CG-CD-CE	-7.76	88.60	111.90
1	C	351	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	C	33	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	A	253	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	D	303	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	216	ASP	O-C-N	7.72	135.06	122.70
1	D	435	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	201	LYS	CA-CB-CG	7.69	130.33	113.40
1	C	91	VAL	CA-C-N	-7.69	100.82	116.20
1	B	302	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	339	ARG	NH1-CZ-NH2	7.66	127.82	119.40
1	B	45	GLN	CA-CB-CG	7.65	130.23	113.40
1	A	436	ASP	O-C-N	7.65	134.94	122.70
1	B	156	GLN	CB-CG-CD	7.64	131.47	111.60
2	T	53	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	C	79	ARG	O-C-N	7.63	134.90	122.70
1	D	258	ARG	CB-CG-CD	7.62	131.42	111.60
2	U	33	LEU	CB-CA-C	7.61	124.66	110.20
1	A	149	GLN	O-C-N	7.61	136.13	123.20
2	S	100	ARG	CG-CD-NE	7.60	127.75	111.80
1	A	269	TYR	CB-CG-CD1	7.59	125.56	121.00
1	D	110	GLU	OE1-CD-OE2	-7.59	114.19	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	GLN	CA-CB-CG	7.56	130.03	113.40
1	B	180	LEU	N-CA-CB	-7.55	95.29	110.40
1	D	269	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	C	169	LEU	CA-CB-CG	7.52	132.59	115.30
1	C	72	ASP	OD1-CG-OD2	-7.51	109.03	123.30
1	D	431	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	226	TYR	CG-CD1-CE1	-7.51	115.29	121.30
2	V	26	LEU	CB-CA-C	7.51	124.47	110.20
1	C	201	LYS	N-CA-CB	-7.50	97.09	110.60
1	A	35	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	A	339	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	D	28	GLU	CG-CD-OE2	-7.49	103.32	118.30
1	D	351	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	110	GLU	CA-CB-CG	7.49	129.87	113.40
1	D	290	LEU	CB-CG-CD1	-7.48	98.29	111.00
1	A	134	ARG	NH1-CZ-NH2	7.47	127.62	119.40
1	D	339	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	D	121	VAL	N-CA-CB	-7.47	95.07	111.50
1	D	201	LYS	CB-CA-C	-7.47	95.47	110.40
1	A	61	SER	CB-CA-C	-7.46	95.93	110.10
1	C	319	ARG	CA-CB-CG	7.46	129.80	113.40
1	A	245	GLY	CA-C-O	-7.45	107.19	120.60
1	B	352	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	A	159	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	C	215	ARG	NE-CZ-NH2	7.44	124.02	120.30
2	S	7	ILE	CA-C-N	7.44	133.57	117.20
1	B	127	PHE	CA-CB-CG	-7.44	96.05	113.90
1	B	194	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	C	193	LEU	CB-CG-CD1	7.43	123.63	111.00
1	C	360	ARG	CD-NE-CZ	-7.43	113.20	123.60
2	S	47	GLU	OE1-CD-OE2	7.43	132.21	123.30
2	V	114	SER	CB-CA-C	7.43	124.21	110.10
1	A	137	ASP	CB-CG-OD1	-7.42	111.62	118.30
2	V	47	GLU	OE1-CD-OE2	7.42	132.20	123.30
1	A	312	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	D	108	PHE	O-C-N	7.40	134.55	122.70
1	A	85	TYR	CB-CG-CD1	7.40	125.44	121.00
2	U	121	GLU	CA-CB-CG	7.40	129.68	113.40
1	A	10	SER	N-CA-CB	7.39	121.59	110.50
1	D	131	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	225	LEU	CB-CG-CD1	7.38	123.55	111.00
1	B	60	GLU	CG-CD-OE2	7.37	133.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	TYR	CB-CG-CD2	-7.37	116.58	121.00
1	D	217	ARG	NE-CZ-NH2	-7.37	116.62	120.30
2	S	63	ASP	CA-CB-CG	7.36	129.59	113.40
2	S	89	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	D	213	ARG	CA-CB-CG	-7.35	97.22	113.40
1	B	85	TYR	CB-CG-CD1	7.34	125.40	121.00
2	V	59	PRO	O-C-N	7.34	135.68	123.20
2	U	21	LEU	CA-CB-CG	7.32	132.13	115.30
2	V	7	ILE	CA-C-N	7.32	133.29	117.20
1	D	215	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	C	200	THR	CA-CB-CG2	-7.30	102.18	112.40
2	V	104	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	D	136	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	D	24	TYR	CB-CA-C	7.28	124.97	110.40
2	V	53	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	291	LEU	CA-CB-CG	7.27	132.03	115.30
2	V	99	ILE	O-C-N	7.26	134.32	122.70
1	C	338	GLU	OE1-CD-OE2	-7.26	114.59	123.30
1	C	302	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	60	GLU	CG-CD-OE2	7.25	132.79	118.30
1	B	169	LEU	CA-CB-CG	7.25	131.97	115.30
1	A	28	GLU	OE1-CD-OE2	7.24	131.98	123.30
1	D	294	HIS	CA-C-O	-7.24	104.91	120.10
1	A	213	ARG	CB-CG-CD	7.23	130.40	111.60
1	D	202	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	A	204	GLU	CG-CD-OE1	7.22	132.74	118.30
2	V	48	HIS	O-C-N	7.21	135.45	123.20
2	V	82	GLN	CB-CA-C	7.21	124.81	110.40
1	D	394	PHE	CB-CG-CD1	-7.20	115.76	120.80
1	B	363	TYR	CB-CG-CD1	-7.20	116.68	121.00
2	V	57	LYS	N-CA-CB	7.20	123.55	110.60
1	D	127	PHE	CB-CG-CD1	-7.19	115.77	120.80
2	V	115	PHE	O-C-N	7.19	134.21	122.70
1	B	215	ARG	CD-NE-CZ	-7.19	113.53	123.60
1	C	103	TYR	N-CA-CB	-7.19	97.67	110.60
2	U	53	ARG	CD-NE-CZ	-7.18	113.55	123.60
1	B	212	MET	O-C-N	7.18	134.19	122.70
1	D	156	GLN	CB-CG-CD	7.17	130.24	111.60
1	B	108	PHE	CB-CG-CD2	7.17	125.82	120.80
1	A	95	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	C	360	ARG	NH1-CZ-NH2	7.16	127.28	119.40
2	T	65	ARG	CG-CD-NE	7.16	126.83	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	79	ARG	CB-CA-C	-7.15	96.09	110.40
1	A	396	ASP	CB-CG-OD1	7.15	124.74	118.30
2	V	58	SER	CB-CA-C	7.15	123.68	110.10
2	S	32	TYR	CB-CG-CD2	7.14	125.28	121.00
1	A	249	GLU	N-CA-CB	7.14	123.45	110.60
1	C	198	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	B	110	GLU	OE1-CD-OE2	7.13	131.85	123.30
1	D	194	ARG	CD-NE-CZ	7.13	133.58	123.60
1	D	172	CYS	N-CA-CB	-7.11	97.80	110.60
1	A	89	ARG	CA-CB-CG	7.11	129.04	113.40
1	D	91	VAL	CA-C-N	-7.11	101.99	116.20
2	S	43	GLU	CG-CD-OE2	7.09	132.49	118.30
1	C	130	LEU	O-C-N	7.09	134.05	122.70
2	S	118	TYR	CB-CG-CD1	7.09	125.25	121.00
1	A	165	TYR	C-N-CA	7.07	137.16	122.30
2	S	98	TRP	N-CA-C	-7.07	91.91	111.00
1	C	435	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	137	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	19	GLU	N-CA-CB	7.06	123.30	110.60
1	A	131	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	192	CYS	CA-CB-SG	-7.06	101.30	114.00
1	D	257	ALA	CB-CA-C	7.05	120.68	110.10
2	S	34	LEU	CB-CA-C	7.05	123.60	110.20
1	C	33	ASP	CB-CG-OD1	7.04	124.63	118.30
1	D	79	ARG	CG-CD-NE	7.04	126.58	111.80
2	S	100	ARG	CB-CG-CD	7.03	129.89	111.60
1	B	95	ASP	CB-CG-OD1	-7.03	111.97	118.30
2	V	53	ARG	O-C-N	7.03	133.95	122.70
2	U	7	ILE	N-CA-C	7.03	129.97	111.00
1	B	149	GLN	O-C-N	7.02	135.14	123.20
1	B	125	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	D	324	ASP	CB-CA-C	7.00	124.40	110.40
1	B	61	SER	CB-CA-C	-6.99	96.81	110.10
1	D	204	GLU	CG-CD-OE2	-6.99	104.33	118.30
1	D	194	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	295	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	A	180	LEU	CB-CA-C	6.96	123.43	110.20
2	S	105	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	226	TYR	CB-CG-CD2	6.95	125.17	121.00
1	C	35	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	B	270	LEU	CA-C-O	-6.93	105.54	120.10
2	U	75	PHE	CA-C-O	-6.93	105.54	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	10	SER	N-CA-CB	6.91	120.87	110.50
1	C	25	TYR	CB-CG-CD2	6.91	125.14	121.00
1	A	204	GLU	CG-CD-OE2	-6.91	104.49	118.30
1	D	358	ARG	NE-CZ-NH2	6.90	123.75	120.30
2	V	75	PHE	CB-CG-CD1	-6.89	115.98	120.80
1	A	332	VAL	N-CA-CB	-6.88	96.36	111.50
1	A	110	GLU	OE1-CD-OE2	-6.87	115.06	123.30
2	S	65	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	24	TYR	N-CA-CB	-6.86	98.25	110.60
1	C	99	ALA	CB-CA-C	6.86	120.39	110.10
1	D	213	ARG	CB-CA-C	6.86	124.11	110.40
1	A	84	CYS	CA-CB-SG	-6.84	101.69	114.00
2	T	100	ARG	N-CA-CB	-6.83	98.31	110.60
2	T	66	TYR	CB-CG-CD2	6.83	125.10	121.00
1	D	213	ARG	NH1-CZ-NH2	-6.82	111.90	119.40
1	B	204	GLU	CG-CD-OE2	-6.82	104.66	118.30
1	A	341	ILE	O-C-N	6.81	133.60	122.70
1	A	454	GLU	OE1-CD-OE2	6.81	131.47	123.30
1	B	89	ARG	CA-CB-CG	6.81	128.38	113.40
1	D	25	TYR	CB-CG-CD2	6.81	125.08	121.00
2	U	109	GLN	CB-CG-CD	6.79	129.25	111.60
1	A	292	HIS	CA-C-O	-6.78	105.85	120.10
1	A	95	ASP	CB-CG-OD2	6.78	124.40	118.30
1	C	339	ARG	NH1-CZ-NH2	6.78	126.85	119.40
1	D	165	TYR	CB-CG-CD2	6.77	125.06	121.00
1	D	64	GLY	N-CA-C	6.77	130.02	113.10
1	A	200	THR	CA-C-N	6.76	132.07	117.20
1	C	121	VAL	N-CA-CB	-6.76	96.63	111.50
2	S	107	VAL	O-C-N	6.76	133.51	122.70
1	A	125	PHE	CA-C-N	6.75	129.70	116.20
1	A	101	VAL	CG1-CB-CG2	6.75	121.69	110.90
1	C	74	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	207	ASN	OD1-CG-ND2	6.74	137.40	121.90
1	C	153	HIS	CA-CB-CG	-6.74	102.14	113.60
2	S	48	HIS	CA-C-N	-6.74	102.73	116.20
2	U	98	TRP	N-CA-CB	6.73	122.72	110.60
2	S	1	MET	CG-SD-CE	6.72	110.95	100.20
2	V	21	LEU	CA-CB-CG	6.72	130.76	115.30
2	V	7	ILE	N-CA-C	6.71	129.13	111.00
1	D	110	GLU	CG-CD-OE2	6.71	131.72	118.30
2	T	79	ASP	CB-CG-OD1	-6.71	112.26	118.30
2	U	7	ILE	CA-C-N	6.70	131.94	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	60	GLU	CG-CD-OE1	-6.70	104.91	118.30
2	V	61	TYR	O-C-N	6.69	133.41	122.70
1	A	106	ASP	CB-CG-OD1	6.69	124.32	118.30
2	V	42	LEU	CB-CG-CD1	6.69	122.37	111.00
1	D	454	GLU	OE1-CD-OE2	6.68	131.32	123.30
2	U	36	ASN	OD1-CG-ND2	6.67	137.25	121.90
1	C	431	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	92	GLY	O-C-N	6.66	133.36	122.70
1	A	173	THR	CA-CB-CG2	6.66	121.72	112.40
1	B	377	VAL	CA-C-O	6.66	134.08	120.10
2	V	13	GLU	CG-CD-OE2	-6.66	104.99	118.30
1	C	200	THR	CA-C-O	-6.65	106.13	120.10
1	C	89	ARG	CA-CB-CG	6.65	128.03	113.40
2	S	89	GLU	CA-CB-CG	6.64	128.01	113.40
2	V	34	LEU	CB-CA-C	6.64	122.82	110.20
2	S	26	LEU	CB-CA-C	6.64	122.81	110.20
1	B	204	GLU	CG-CD-OE1	6.64	131.57	118.30
1	B	238	HIS	CA-C-N	6.63	131.78	117.20
1	C	26	THR	CA-CB-CG2	6.63	121.68	112.40
1	B	96	GLN	CA-CB-CG	6.63	127.98	113.40
1	A	86	ARG	N-CA-CB	6.62	122.52	110.60
1	B	360	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	D	387	MET	CA-CB-CG	-6.62	102.06	113.30
2	V	98	TRP	N-CA-C	-6.61	93.15	111.00
1	A	24	TYR	CB-CA-C	6.61	123.62	110.40
1	B	153	HIS	CA-CB-CG	-6.60	102.38	113.60
2	V	44	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	C	52	GLU	N-CA-CB	6.59	122.46	110.60
1	A	97	TYR	CB-CA-C	-6.59	97.23	110.40
1	B	203	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	278	THR	CA-CB-OG1	-6.58	95.17	109.00
1	B	91	VAL	O-C-N	6.58	134.39	123.20
1	D	10	SER	N-CA-CB	6.58	120.37	110.50
2	S	52	TYR	CA-CB-CG	6.58	125.89	113.40
1	B	247	CYS	CA-CB-SG	6.58	125.84	114.00
1	B	52	GLU	N-CA-CB	6.57	122.43	110.60
1	C	218	PHE	CB-CG-CD1	6.57	125.40	120.80
2	T	60	GLY	O-C-N	-6.57	112.19	122.70
2	T	108	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	B	24	TYR	CB-CA-C	6.55	123.51	110.40
1	D	158	GLU	CG-CD-OE2	6.55	131.41	118.30
2	V	86	GLU	OE1-CD-OE2	6.55	131.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	105	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	C	324	ASP	CB-CG-OD1	6.54	124.19	118.30
1	B	288	GLY	C-N-CA	6.53	138.01	121.70
1	C	431	ARG	CG-CD-NE	6.53	125.51	111.80
1	B	259	GLU	CB-CG-CD	6.52	131.81	114.20
1	D	467	PHE	CB-CG-CD1	-6.52	116.23	120.80
1	D	280	LEU	CB-CA-C	6.51	122.58	110.20
2	T	21	LEU	CA-CB-CG	6.51	130.27	115.30
1	B	360	ARG	CD-NE-CZ	-6.51	114.49	123.60
1	D	431	ARG	CD-NE-CZ	-6.50	114.49	123.60
1	B	319	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
1	B	13	PHE	O-C-N	6.50	133.10	122.70
1	D	144	TYR	CG-CD1-CE1	6.50	126.50	121.30
2	T	82	GLN	CB-CA-C	6.49	123.38	110.40
2	T	50	PHE	O-C-N	-6.48	112.33	122.70
1	C	183	LYS	CA-CB-CG	-6.47	99.17	113.40
2	T	45	GLU	CA-CB-CG	6.47	127.63	113.40
1	A	110	GLU	CG-CD-OE2	6.47	131.23	118.30
2	U	75	PHE	O-C-N	6.47	134.19	123.20
2	V	57	LYS	CA-C-O	-6.47	106.52	120.10
1	C	110	GLU	CA-CB-CG	6.46	127.62	113.40
1	B	239	TYR	CB-CG-CD1	6.46	124.88	121.00
1	A	212	MET	O-C-N	6.45	133.03	122.70
1	C	135	LEU	CB-CA-C	6.45	122.45	110.20
1	D	139	ARG	CD-NE-CZ	-6.45	114.58	123.60
1	A	203	ASP	N-CA-CB	6.44	122.19	110.60
1	C	468	ASN	N-CA-CB	6.44	122.19	110.60
1	D	436	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	180	LEU	N-CA-CB	-6.42	97.55	110.40
1	D	189	VAL	CA-CB-CG1	6.42	120.53	110.90
2	T	33	LEU	CA-CB-CG	6.42	130.06	115.30
1	D	332	VAL	N-CA-CB	-6.41	97.40	111.50
1	B	347	ASP	CA-CB-CG	6.41	127.50	113.40
1	C	156	GLN	CB-CG-CD	6.41	128.26	111.60
1	A	215	ARG	CB-CG-CD	6.41	128.25	111.60
1	B	159	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	B	225	LEU	CB-CG-CD2	-6.39	100.13	111.00
1	D	95	ASP	CB-CG-OD1	-6.39	112.54	118.30
1	C	89	ARG	O-C-N	6.39	132.92	122.70
1	C	220	PHE	O-C-N	6.39	132.92	122.70
1	C	357	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	C	19	GLU	CA-CB-CG	6.38	127.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	281	ALA	N-CA-CB	6.38	119.03	110.10
1	B	226	TYR	CA-C-O	-6.38	106.71	120.10
2	T	112	CYS	CA-CB-SG	-6.37	102.54	114.00
2	S	38	TRP	CB-CG-CD2	-6.36	118.33	126.60
1	D	326	ILE	N-CA-CB	6.36	125.44	110.80
1	C	79	ARG	CG-CD-NE	6.36	125.16	111.80
2	S	100	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	292	HIS	O-C-N	6.35	132.86	122.70
1	B	159	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	B	194	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	D	60	GLU	CG-CD-OE2	6.35	131.00	118.30
2	U	82	GLN	CB-CG-CD	6.34	128.08	111.60
1	D	296	ALA	N-CA-CB	-6.34	101.23	110.10
1	B	201	LYS	N-CA-CB	-6.33	99.21	110.60
1	D	291	LEU	O-C-N	6.33	132.83	122.70
2	U	111	GLN	N-CA-C	-6.32	93.93	111.00
1	D	350	ARG	CB-CG-CD	-6.32	95.17	111.60
1	D	92	GLY	O-C-N	6.32	132.81	122.70
1	C	160	ASP	O-C-N	6.31	132.80	122.70
1	D	41	ARG	CD-NE-CZ	-6.31	114.77	123.60
2	V	63	ASP	CA-CB-CG	6.31	127.28	113.40
1	A	24	TYR	N-CA-CB	-6.31	99.25	110.60
1	D	159	ARG	CD-NE-CZ	-6.30	114.78	123.60
2	T	66	TYR	CB-CG-CD1	-6.30	117.22	121.00
2	V	100	ARG	CA-CB-CG	6.30	127.27	113.40
1	D	328	SER	CA-C-O	-6.29	106.88	120.10
1	B	331	VAL	C-N-CA	6.29	137.41	121.70
2	U	40	PRO	O-C-N	6.28	132.75	122.70
1	A	194	ARG	N-CA-CB	6.28	121.90	110.60
2	V	48	HIS	CA-CB-CG	-6.28	102.92	113.60
2	U	43	GLU	CA-CB-CG	6.28	127.21	113.40
1	B	383	HIS	O-C-N	6.28	132.74	122.70
1	B	88	GLU	O-C-N	6.27	132.73	122.70
1	B	202	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	194	ARG	NH1-CZ-NH2	-6.27	112.51	119.40
2	U	55	ASN	CA-CB-CG	-6.26	99.62	113.40
2	V	20	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	D	193	LEU	CA-CB-CG	6.26	129.69	115.30
2	U	7	ILE	CA-C-O	-6.26	106.96	120.10
1	D	269	TYR	CB-CG-CD1	6.26	124.75	121.00
2	S	89	GLU	CG-CD-OE1	-6.25	105.79	118.30
2	U	94	TYR	CB-CG-CD1	-6.25	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	93	GLU	CA-C-N	-6.25	103.45	117.20
1	A	433	GLU	CB-CG-CD	6.25	131.06	114.20
1	D	30	GLN	O-C-N	6.24	132.69	122.70
1	D	394	PHE	CA-C-N	6.23	128.67	116.20
1	C	447	GLU	CG-CD-OE1	-6.22	105.86	118.30
1	D	253	ARG	NH1-CZ-NH2	6.22	126.25	119.40
2	V	94	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	T	98	TRP	N-CA-CB	6.22	121.79	110.60
1	C	445	ILE	CB-CA-C	6.21	124.03	111.60
1	C	324	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	88	GLU	CG-CD-OE1	-6.21	105.88	118.30
2	U	54	GLU	CG-CD-OE1	-6.20	105.89	118.30
1	A	213	ARG	CD-NE-CZ	6.20	132.28	123.60
2	U	111	GLN	N-CA-CB	6.20	121.76	110.60
1	D	319	ARG	NH1-CZ-NH2	6.20	126.21	119.40
1	A	196	GLY	C-N-CA	6.19	137.18	121.70
1	C	61	SER	CA-CB-OG	-6.19	94.48	111.20
1	A	469	PHE	N-CA-CB	6.19	121.75	110.60
1	C	110	GLU	N-CA-CB	-6.19	99.46	110.60
1	D	334	LYS	CA-CB-CG	6.19	127.02	113.40
1	A	409	HIS	CA-CB-CG	6.19	124.12	113.60
1	D	294	HIS	O-C-N	6.18	132.60	122.70
1	D	165	TYR	C-N-CA	6.18	135.28	122.30
1	A	248	GLU	CA-CB-CG	6.18	126.99	113.40
1	B	300	VAL	CG1-CB-CG2	6.17	120.78	110.90
1	A	360	ARG	NH1-CZ-NH2	6.17	126.19	119.40
1	A	135	LEU	CB-CA-C	6.17	121.92	110.20
2	T	82	GLN	CA-CB-CG	6.17	126.96	113.40
2	S	110	VAL	CA-CB-CG1	6.16	120.14	110.90
2	V	43	GLU	CG-CD-OE1	6.16	130.63	118.30
1	B	246	THR	O-C-N	6.16	132.56	122.70
1	C	19	GLU	N-CA-CB	6.16	121.69	110.60
1	D	296	ALA	CB-CA-C	6.16	119.34	110.10
1	D	298	HIS	CA-CB-CG	6.16	124.07	113.60
1	C	413	ASN	CA-CB-CG	6.16	126.94	113.40
1	B	26	THR	CA-CB-CG2	6.15	121.01	112.40
1	D	199	PHE	CB-CG-CD1	-6.15	116.50	120.80
1	C	187	ARG	CD-NE-CZ	6.14	132.20	123.60
1	A	201	LYS	CB-CA-C	-6.14	98.12	110.40
2	V	20	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	S	111	GLN	N-CA-C	-6.14	94.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	44	PHE	CB-CG-CD2	-6.14	116.50	120.80
2	U	110	VAL	CG1-CB-CG2	-6.13	101.08	110.90
2	U	118	TYR	CB-CG-CD1	6.13	124.68	121.00
1	C	281	ALA	CB-CA-C	-6.13	100.90	110.10
1	C	61	SER	CB-CA-C	-6.12	98.46	110.10
1	B	213	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	U	110	VAL	O-C-N	6.12	132.50	122.70
1	B	396	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	89	ARG	N-CA-CB	6.12	121.61	110.60
1	D	136	GLU	CG-CD-OE2	-6.12	106.06	118.30
1	D	402	PHE	CA-C-O	6.12	132.95	120.10
1	A	160	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	C	159	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	C	435	ARG	CD-NE-CZ	-6.10	115.05	123.60
1	C	144	TYR	CB-CG-CD2	6.10	124.66	121.00
2	T	100	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	207	ASN	CA-CB-CG	6.09	126.81	113.40
1	A	217	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	B	165	TYR	CB-CG-CD2	6.09	124.65	121.00
1	D	103	TYR	CG-CD1-CE1	6.09	126.17	121.30
2	T	75	PHE	CB-CG-CD1	-6.08	116.54	120.80
2	S	66	TYR	CG-CD2-CE2	6.08	126.16	121.30
1	D	406	THR	CA-CB-CG2	6.08	120.91	112.40
1	B	460	GLU	CG-CD-OE2	6.08	130.45	118.30
1	C	326	ILE	N-CA-CB	6.08	124.77	110.80
2	S	98	TRP	N-CA-CB	6.07	121.52	110.60
1	D	201	LYS	N-CA-CB	-6.06	99.70	110.60
2	S	74	MET	CG-SD-CE	6.06	109.89	100.20
1	B	303	ARG	CG-CD-NE	-6.06	99.08	111.80
1	C	201	LYS	CB-CA-C	-6.06	98.29	110.40
1	C	97	TYR	CB-CG-CD1	6.05	124.63	121.00
1	C	321	SER	O-C-N	-6.05	112.91	123.20
2	U	82	GLN	CB-CA-C	6.05	122.51	110.40
2	V	56	ASN	O-C-N	6.05	132.39	122.70
2	V	47	GLU	CG-CD-OE2	-6.05	106.19	118.30
1	A	257	ALA	CB-CA-C	6.05	119.17	110.10
1	D	469	PHE	N-CA-CB	6.05	121.49	110.60
1	D	421	ARG	NH1-CZ-NH2	6.05	126.05	119.40
1	B	19	GLU	CA-CB-CG	6.05	126.70	113.40
1	A	201	LYS	N-CA-CB	-6.04	99.72	110.60
1	A	217	ARG	N-CA-CB	6.04	121.48	110.60
1	C	355	GLU	N-CA-CB	-6.03	99.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	139	ARG	CD-NE-CZ	-6.03	115.16	123.60
1	B	466	VAL	O-C-N	6.03	132.34	122.70
1	B	133	LEU	O-C-N	6.02	132.33	122.70
1	C	256	PHE	CB-CG-CD2	-6.02	116.59	120.80
1	C	265	VAL	O-C-N	6.02	132.33	122.70
1	B	211	PHE	CB-CG-CD2	6.01	125.01	120.80
1	C	190	TYR	CB-CG-CD2	6.01	124.61	121.00
1	C	303	ARG	CG-CD-NE	-6.01	99.18	111.80
1	D	213	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	V	85	ALA	CA-C-N	-6.00	103.99	117.20
1	D	285	ARG	CD-NE-CZ	-6.00	115.20	123.60
1	A	167	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	138	LEU	CA-CB-CG	5.99	129.09	115.30
1	A	431	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	350	ARG	CA-CB-CG	5.99	126.57	113.40
1	A	357	ASP	CB-CG-OD2	5.98	123.69	118.30
2	T	100	ARG	CA-CB-CG	5.98	126.56	113.40
1	B	307	HIS	CB-CA-C	-5.98	98.44	110.40
1	D	32	LYS	N-CA-CB	5.98	121.36	110.60
1	D	89	ARG	N-CA-CB	5.97	121.35	110.60
1	D	244	ALA	O-C-N	-5.97	113.06	123.20
1	A	355	GLU	CG-CD-OE2	-5.96	106.37	118.30
1	B	97	TYR	CB-CA-C	-5.96	98.47	110.40
1	A	347	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	203	ASP	N-CA-C	-5.96	94.92	111.00
1	A	194	ARG	CD-NE-CZ	5.95	131.93	123.60
1	C	321	SER	CB-CA-C	5.95	121.40	110.10
1	D	244	ALA	CA-C-O	5.95	132.59	120.10
2	S	9	LYS	CA-CB-CG	5.94	126.47	113.40
1	A	44	PRO	CA-C-N	-5.94	104.14	117.20
2	V	2	GLN	CA-CB-CG	5.93	126.45	113.40
1	C	334	LYS	CA-CB-CG	5.93	126.44	113.40
1	A	285	ARG	CG-CD-NE	-5.93	99.36	111.80
1	B	217	ARG	N-CA-CB	5.92	121.26	110.60
1	B	409	HIS	CA-CB-CG	5.92	123.67	113.60
1	C	52	GLU	N-CA-C	-5.92	95.00	111.00
1	C	311	PHE	CB-CG-CD1	-5.92	116.65	120.80
1	A	26	THR	CA-CB-CG2	5.92	120.69	112.40
1	A	351	ASP	CB-CG-OD2	-5.92	112.97	118.30
2	V	20	ASP	OD1-CG-OD2	5.92	134.54	123.30
1	B	347	ASP	OD1-CG-OD2	-5.92	112.06	123.30
1	B	340	ASP	O-C-N	5.92	132.16	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	2	GLN	CA-C-N	-5.92	104.19	117.20
2	S	49	GLY	CA-C-O	-5.91	109.95	120.60
2	S	109	GLN	CB-CG-CD	5.91	126.98	111.60
1	D	217	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	C	350	ARG	CB-CG-CD	-5.91	96.25	111.60
1	C	293	ILE	C-N-CA	5.90	136.46	121.70
1	B	29	TYR	CA-C-N	-5.90	104.22	117.20
2	V	105	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	D	203	ASP	N-CA-C	-5.90	95.07	111.00
1	B	454	GLU	CG-CD-OE2	-5.90	106.51	118.30
1	A	93	GLU	CG-CD-OE2	5.90	130.09	118.30
1	A	213	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	A	202	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	79	ARG	CB-CA-C	-5.89	98.62	110.40
1	D	391	THR	N-CA-CB	5.89	121.49	110.30
1	B	253	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	D	406	THR	N-CA-CB	5.89	121.48	110.30
1	A	194	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
1	B	37	LEU	O-C-N	5.88	132.11	122.70
1	C	469	PHE	N-CA-CB	5.88	121.19	110.60
1	A	283	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	B	121	VAL	N-CA-CB	-5.88	98.56	111.50
1	C	295	ARG	O-C-N	5.88	132.11	122.70
2	V	77	CYS	CA-CB-SG	-5.88	103.41	114.00
1	C	165	TYR	C-N-CA	5.88	134.64	122.30
2	U	65	ARG	CG-CD-NE	5.88	124.14	111.80
1	D	204	GLU	CG-CD-OE1	5.88	130.06	118.30
1	B	431	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	100	TYR	N-CA-CB	5.87	121.17	110.60
2	U	98	TRP	N-CA-C	-5.87	95.14	111.00
2	V	32	TYR	CA-C-O	5.87	132.43	120.10
1	C	234	GLU	OE1-CD-OE2	5.87	130.34	123.30
1	B	357	ASP	CB-CG-OD1	-5.87	113.02	118.30
2	S	93	ALA	N-CA-CB	5.86	118.30	110.10
2	V	93	ALA	N-CA-CB	5.86	118.30	110.10
1	A	335	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	86	ARG	O-C-N	5.86	132.07	122.70
1	D	203	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	338	GLU	CA-C-O	5.85	132.39	120.10
1	B	110	GLU	CG-CD-OE1	-5.85	106.61	118.30
2	T	2	GLN	N-CA-CB	5.85	121.12	110.60
2	S	48	HIS	O-C-N	5.85	133.14	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	53	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	A	187	ARG	CD-NE-CZ	5.84	131.78	123.60
1	C	153	HIS	CB-CA-C	-5.84	98.72	110.40
1	D	258	ARG	NH1-CZ-NH2	-5.84	112.98	119.40
1	A	338	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	B	443	GLU	OE1-CD-OE2	-5.84	116.30	123.30
2	V	90	ALA	CB-CA-C	5.84	118.86	110.10
1	A	82	GLY	N-CA-C	-5.83	98.51	113.10
1	C	93	GLU	CA-C-N	-5.83	104.37	117.20
1	D	433	GLU	OE1-CD-OE2	5.83	130.30	123.30
1	B	193	LEU	CB-CG-CD1	5.83	120.91	111.00
2	S	7	ILE	C-N-CA	-5.83	107.13	121.70
1	C	323	GLY	N-CA-C	-5.83	98.53	113.10
1	D	35	ASP	CB-CG-OD2	5.83	123.54	118.30
1	C	108	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	C	255	VAL	CG1-CB-CG2	5.82	120.22	110.90
1	D	274	PHE	CB-CG-CD2	-5.82	116.73	120.80
1	C	220	PHE	CA-C-O	-5.81	107.90	120.10
1	A	253	ARG	NE-CZ-NH2	5.81	123.20	120.30
2	S	82	GLN	CA-CB-CG	5.81	126.18	113.40
1	A	355	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	63	THR	CA-C-O	-5.80	107.91	120.10
2	U	27	LEU	CA-CB-CG	-5.80	101.96	115.30
1	B	178	LEU	C-N-CA	5.80	134.48	122.30
1	B	285	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	D	86	ARG	N-CA-CB	5.80	121.03	110.60
2	U	114	SER	CB-CA-C	5.79	121.11	110.10
1	C	332	VAL	N-CA-CB	-5.79	98.75	111.50
1	C	215	ARG	CD-NE-CZ	-5.79	115.49	123.60
2	S	2	GLN	N-CA-CB	5.79	121.02	110.60
2	T	38	TRP	CD1-NE1-CE2	-5.78	103.80	109.00
1	C	289	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	D	199	PHE	CG-CD1-CE1	-5.78	114.44	120.80
1	D	216	ASP	CB-CG-OD2	5.78	123.50	118.30
2	U	65	ARG	NH1-CZ-NH2	5.78	125.75	119.40
1	C	79	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	S	18	LEU	O-C-N	5.77	132.07	121.10
2	T	7	ILE	N-CA-C	5.77	126.59	111.00
1	C	460	GLU	CG-CD-OE2	5.77	129.84	118.30
2	V	48	HIS	CA-C-N	-5.77	104.66	116.20
2	S	45	GLU	CG-CD-OE1	5.77	129.84	118.30
1	A	89	ARG	NE-CZ-NH2	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	20	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	215	ARG	NH1-CZ-NH2	5.75	125.73	119.40
2	T	82	GLN	CB-CG-CD	5.75	126.55	111.60
1	B	377	VAL	O-C-N	-5.75	113.50	122.70
1	A	199	PHE	CB-CG-CD1	5.75	124.82	120.80
1	A	359	SER	CB-CA-C	5.75	121.02	110.10
1	D	312	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	B	180	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	D	85	TYR	CB-CG-CD1	5.74	124.45	121.00
2	S	105	ASP	CA-C-N	5.74	129.83	117.20
1	C	168	PRO	N-CD-CG	-5.74	94.60	103.20
1	C	238	HIS	CG-ND1-CE1	5.73	116.23	108.20
1	B	173	THR	CA-CB-CG2	5.73	120.42	112.40
1	B	90	VAL	O-C-N	5.72	131.86	122.70
1	B	155	ILE	CA-C-O	-5.72	108.08	120.10
1	C	259	GLU	CB-CG-CD	5.72	129.66	114.20
2	T	33	LEU	CB-CA-C	5.72	121.07	110.20
2	S	92	LYS	CA-C-O	-5.71	108.10	120.10
1	C	201	LYS	CG-CD-CE	-5.71	94.76	111.90
1	C	260	LEU	O-C-N	-5.71	113.48	123.20
2	U	12	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	D	215	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	A	350	ARG	CG-CD-NE	5.70	123.77	111.80
1	C	29	TYR	C-N-CA	5.70	135.94	121.70
2	V	120	PRO	N-CA-C	-5.70	97.29	112.10
1	A	286	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	75	THR	O-C-N	5.69	131.81	122.70
1	C	74	LEU	CB-CA-C	5.69	121.01	110.20
1	C	91	VAL	CA-CB-CG1	5.69	119.43	110.90
1	A	340	ASP	CB-CG-OD1	5.69	123.42	118.30
2	T	34	LEU	CB-CA-C	5.68	121.00	110.20
2	S	44	PHE	CB-CG-CD1	-5.68	116.82	120.80
2	U	26	LEU	CB-CA-C	5.68	120.99	110.20
1	B	286	ASP	O-C-N	5.68	131.78	122.70
1	C	239	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	C	352	ASP	O-C-N	5.67	131.77	122.70
1	A	283	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
1	A	35	ASP	CB-CA-C	-5.66	99.08	110.40
1	C	340	ASP	CB-CG-OD1	5.66	123.39	118.30
2	S	82	GLN	CB-CA-C	5.66	121.71	110.40
1	B	71	THR	O-C-N	5.66	131.75	122.70
1	C	215	ARG	NH1-CZ-NH2	5.65	125.62	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	93	GLU	CA-C-N	-5.65	104.77	117.20
1	C	136	GLU	CG-CD-OE1	5.65	129.61	118.30
1	D	280	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	D	29	TYR	CA-C-N	-5.65	104.77	117.20
1	B	312	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	C	84	CYS	CA-CB-SG	-5.65	103.83	114.00
1	C	44	PRO	N-CA-CB	5.64	110.07	103.30
1	A	354	VAL	CA-C-N	-5.64	104.79	117.20
2	V	82	GLN	CB-CG-CD	5.64	126.26	111.60
1	B	89	ARG	O-C-N	5.64	131.72	122.70
1	B	231	GLU	OE1-CD-OE2	5.64	130.06	123.30
1	D	89	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	89	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	A	314	LEU	CB-CA-C	5.63	120.90	110.20
1	C	286	ASP	O-C-N	5.63	131.71	122.70
1	B	270	LEU	O-C-N	5.62	131.70	122.70
2	T	110	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	C	454	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	C	180	LEU	N-CA-CB	-5.62	99.17	110.40
1	C	144	TYR	CB-CG-CD1	-5.61	117.63	121.00
2	T	98	TRP	N-CA-C	-5.61	95.85	111.00
1	B	445	ILE	CB-CA-C	5.61	122.82	111.60
1	C	454	GLU	CG-CD-OE2	-5.61	107.09	118.30
1	A	193	LEU	N-CA-CB	-5.60	99.19	110.40
1	B	13	PHE	N-CA-CB	5.60	120.68	110.60
1	A	116	MET	CG-SD-CE	-5.60	91.24	100.20
1	B	193	LEU	CA-C-O	-5.60	108.34	120.10
1	C	356	GLN	CA-C-N	5.60	129.52	117.20
1	A	333	GLY	CA-C-O	-5.60	110.52	120.60
2	T	65	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	110	GLU	C-N-CA	5.60	134.05	122.30
2	T	118	TYR	CB-CG-CD1	5.60	124.36	121.00
1	D	401	GLN	CA-C-O	5.59	131.85	120.10
1	A	88	GLU	CA-CB-CG	5.59	125.70	113.40
2	V	55	ASN	CB-CG-OD1	-5.59	110.41	121.60
1	C	82	GLY	N-CA-C	-5.59	99.12	113.10
1	D	51	GLU	CA-CB-CG	5.59	125.70	113.40
2	T	74	MET	CB-CA-C	5.59	121.58	110.40
1	A	193	LEU	CA-C-N	5.59	129.49	117.20
1	B	258	ARG	CB-CG-CD	5.59	126.12	111.60
2	T	108	ARG	NE-CZ-NH1	-5.59	117.51	120.30
2	S	108	ARG	NE-CZ-NH1	-5.58	117.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	32	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	266	MET	N-CA-CB	-5.57	100.57	110.60
1	A	334	LYS	CA-CB-CG	5.57	125.66	113.40
1	D	79	ARG	CA-CB-CG	5.57	125.65	113.40
1	A	160	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	319	ARG	CB-CG-CD	5.57	126.07	111.60
1	B	52	GLU	CG-CD-OE1	5.57	129.43	118.30
1	A	264	ILE	CA-CB-CG2	5.56	122.02	110.90
1	B	44	PRO	CA-C-N	-5.55	104.99	117.20
1	C	28	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	C	211	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	C	194	ARG	CD-NE-CZ	5.54	131.36	123.60
1	D	396	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	86	ARG	N-CA-CB	5.54	120.57	110.60
1	C	406	THR	N-CA-CB	5.54	120.82	110.30
1	D	120	ILE	CA-CB-CG1	-5.53	100.49	111.00
1	C	142	PRO	N-CD-CG	-5.52	94.92	103.20
1	D	328	SER	O-C-N	5.52	132.58	123.20
1	D	218	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	A	326	ILE	N-CA-CB	5.52	123.49	110.80
2	S	45	GLU	O-C-N	5.51	131.52	122.70
1	C	134	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	D	77	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	169	LEU	CB-CA-C	5.51	120.66	110.20
1	B	167	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
1	C	64	GLY	N-CA-C	5.51	126.87	113.10
1	B	91	VAL	N-CA-CB	5.50	123.61	111.50
1	A	52	GLU	CG-CD-OE1	5.50	129.30	118.30
1	B	314	LEU	CB-CA-C	5.50	120.65	110.20
1	D	338	GLU	CA-C-O	5.49	131.63	120.10
2	V	52	TYR	CG-CD1-CE1	-5.49	116.91	121.30
2	S	43	GLU	CA-CB-CG	5.49	125.48	113.40
2	T	57	LYS	CA-C-O	-5.49	108.57	120.10
1	A	457	ALA	CB-CA-C	5.49	118.33	110.10
1	D	319	ARG	CB-CA-C	5.48	121.36	110.40
2	S	118	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	C	394	PHE	CA-C-N	5.48	127.16	116.20
1	A	319	ARG	NH1-CZ-NH2	-5.48	113.38	119.40
1	C	345	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	D	137	ASP	N-CA-CB	-5.47	100.75	110.60
1	D	265	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	D	137	ASP	CB-CG-OD1	-5.47	113.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	32	LYS	N-CA-CB	5.47	120.45	110.60
1	B	290	LEU	O-C-N	5.47	131.44	122.70
1	D	268	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	340	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	371	LEU	CB-CG-CD1	-5.46	101.72	111.00
2	S	65	ARG	CD-NE-CZ	-5.46	115.96	123.60
1	B	78	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	B	374	VAL	N-CA-CB	-5.46	99.49	111.50
1	D	52	GLU	N-CA-CB	5.46	120.43	110.60
2	V	53	ARG	CA-C-O	-5.46	108.64	120.10
1	B	191	GLU	O-C-N	-5.46	113.97	122.70
2	T	93	ALA	N-CA-CB	5.45	117.73	110.10
1	A	328	SER	CA-C-O	-5.45	108.65	120.10
1	B	296	ALA	CB-CA-C	5.45	118.28	110.10
1	B	209	GLN	CA-CB-CG	5.45	125.39	113.40
2	U	123	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	B	238	HIS	CA-C-O	-5.45	108.66	120.10
1	A	216	ASP	CA-C-O	-5.45	108.66	120.10
1	A	268	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	283	TYR	CZ-CE2-CD2	-5.44	114.90	119.80
1	B	326	ILE	N-CA-CB	5.44	123.31	110.80
1	A	234	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	C	129	ALA	CA-C-N	5.44	129.17	117.20
1	D	173	THR	CA-CB-CG2	5.44	120.02	112.40
1	A	286	ASP	CA-C-O	-5.44	108.68	120.10
2	U	34	LEU	CB-CA-C	5.44	120.53	110.20
1	B	277	ASN	CA-CB-CG	-5.44	101.44	113.40
1	D	160	ASP	CB-CG-OD1	-5.43	113.41	118.30
2	T	60	GLY	CA-C-O	5.43	130.38	120.60
1	C	400	LEU	O-C-N	5.43	131.39	122.70
1	C	268	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	91	VAL	O-C-N	5.42	132.42	123.20
2	U	106	ASN	CA-CB-CG	-5.42	101.47	113.40
1	D	82	GLY	N-CA-C	-5.42	99.54	113.10
2	S	7	ILE	N-CA-C	5.42	125.64	111.00
1	B	271	THR	CA-CB-CG2	-5.42	104.81	112.40
2	V	98	TRP	O-C-N	5.42	131.37	122.70
1	D	249	GLU	O-C-N	5.42	131.37	122.70
1	A	307	HIS	CB-CA-C	-5.42	99.57	110.40
1	B	92	GLY	O-C-N	5.42	131.37	122.70
2	V	121	GLU	CA-CB-CG	5.42	125.32	113.40
1	A	442	ASN	CA-CB-CG	-5.41	101.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	61	TYR	O-C-N	5.41	131.35	122.70
1	A	39	ALA	CA-C-N	5.40	129.09	117.20
2	T	49	GLY	CA-C-O	-5.40	110.87	120.60
1	C	283	TYR	CA-CB-CG	-5.40	103.13	113.40
1	A	113	VAL	O-C-N	-5.40	114.06	122.70
1	C	138	LEU	O-C-N	5.40	131.34	122.70
1	D	28	GLU	CG-CD-OE1	5.40	129.10	118.30
1	B	392	GLU	CA-CB-CG	5.40	125.27	113.40
1	B	213	ARG	CD-NE-CZ	-5.40	116.05	123.60
1	C	401	GLN	N-CA-C	5.39	125.56	111.00
1	A	26	THR	N-CA-CB	-5.39	100.06	110.30
2	T	7	ILE	CB-CA-C	-5.39	100.81	111.60
1	D	187	ARG	NE-CZ-NH2	5.39	123.00	120.30
2	V	63	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	352	ASP	N-CA-CB	5.39	120.30	110.60
1	D	410	PRO	O-C-N	5.38	131.32	122.70
1	A	239	TYR	CA-CB-CG	5.38	123.63	113.40
2	U	48	HIS	CA-CB-CG	-5.38	104.45	113.60
2	U	65	ARG	CB-CG-CD	-5.38	97.61	111.60
1	D	197	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	A	60	GLU	CG-CD-OE1	-5.37	107.55	118.30
1	D	183	LYS	CA-CB-CG	-5.37	101.58	113.40
1	A	85	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	234	GLU	CA-CB-CG	5.37	125.22	113.40
1	D	319	ARG	CA-CB-CG	5.37	125.22	113.40
1	D	331	VAL	C-N-CA	5.37	135.13	121.70
1	A	72	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	201	LYS	CG-CD-CE	-5.37	95.80	111.90
1	C	165	TYR	CB-CG-CD1	-5.36	117.78	121.00
2	V	2	GLN	O-C-N	5.36	131.28	122.70
1	D	399	VAL	CA-CB-CG1	5.36	118.94	110.90
2	U	36	ASN	CB-CG-OD1	-5.36	110.89	121.60
1	D	163	ASN	O-C-N	5.36	131.27	122.70
2	U	45	GLU	O-C-N	5.35	131.26	122.70
1	B	50	PRO	O-C-N	5.35	131.26	122.70
1	B	319	ARG	CA-CB-CG	5.35	125.17	113.40
1	C	110	GLU	CB-CG-CD	5.35	128.65	114.20
2	U	29	GLU	CG-CD-OE2	5.35	129.00	118.30
1	A	363	TYR	CB-CG-CD2	5.35	124.21	121.00
1	B	111	GLY	CA-C-O	-5.35	110.97	120.60
2	V	55	ASN	CA-CB-CG	-5.35	101.64	113.40
1	B	156	GLN	CG-CD-NE2	-5.34	103.87	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	390	LEU	O-C-N	5.34	131.25	122.70
2	U	32	TYR	CA-C-N	-5.34	105.44	117.20
1	C	20	TYR	CB-CG-CD1	5.34	124.20	121.00
1	D	95	ASP	CA-CB-CG	-5.34	101.65	113.40
1	D	203	ASP	O-C-N	5.34	131.24	122.70
2	U	48	HIS	O-C-N	5.34	132.27	123.20
1	B	51	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	D	115	ASN	CB-CG-OD1	5.33	132.27	121.60
1	B	79	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	89	ARG	N-CA-CB	5.33	120.19	110.60
1	A	446	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	B	363	TYR	CB-CG-CD2	5.32	124.19	121.00
2	T	8	ASN	O-C-N	5.32	131.22	122.70
2	T	115	PHE	CG-CD1-CE1	5.32	126.65	120.80
2	U	92	LYS	N-CA-C	-5.32	96.63	111.00
1	A	70	TRP	CD1-CG-CD2	5.32	110.56	106.30
1	B	264	ILE	CA-CB-CG2	5.32	121.54	110.90
1	D	183	LYS	O-C-N	-5.32	114.19	122.70
1	A	268	ASP	CB-CG-OD1	-5.32	113.52	118.30
2	U	8	ASN	O-C-N	5.31	131.20	122.70
1	B	259	GLU	CA-CB-CG	5.31	125.09	113.40
2	U	100	ARG	NE-CZ-NH1	-5.31	117.64	120.30
2	V	42	LEU	CA-CB-CG	5.31	127.52	115.30
1	D	254	ALA	N-CA-CB	5.31	117.53	110.10
1	B	170	LEU	N-CA-CB	-5.31	99.78	110.40
1	A	406	THR	N-CA-CB	5.30	120.38	110.30
2	S	65	ARG	NH1-CZ-NH2	5.30	125.23	119.40
1	C	270	LEU	CA-C-O	-5.30	108.96	120.10
1	B	89	ARG	N-CA-CB	5.30	120.14	110.60
1	C	88	GLU	CA-CB-CG	5.30	125.07	113.40
2	V	111	GLN	N-CA-C	-5.30	96.69	111.00
1	C	396	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	T	34	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	C	172	CYS	N-CA-CB	-5.30	101.06	110.60
1	D	345	PHE	O-C-N	5.30	131.17	122.70
1	A	136	GLU	CA-CB-CG	5.29	125.04	113.40
2	S	92	LYS	N-CA-C	-5.29	96.71	111.00
1	B	158	GLU	CG-CD-OE2	5.29	128.88	118.30
1	D	127	PHE	CA-CB-CG	-5.29	101.20	113.90
1	A	211	PHE	CA-C-O	-5.29	108.99	120.10
1	B	334	LYS	CA-CB-CG	5.29	125.04	113.40
2	S	94	TYR	CB-CA-C	5.29	120.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	100	ARG	CA-CB-CG	5.29	125.04	113.40
1	A	281	ALA	N-CA-CB	-5.29	102.70	110.10
1	B	274	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	C	401	GLN	N-CA-CB	-5.28	101.09	110.60
2	U	28	SER	N-CA-CB	-5.28	102.57	110.50
1	B	83	ARG	CG-CD-NE	-5.28	100.71	111.80
1	C	208	SER	CB-CA-C	5.28	120.13	110.10
1	D	125	PHE	CA-C-N	5.28	126.75	116.20
2	S	118	TYR	N-CA-CB	-5.28	101.10	110.60
1	A	127	PHE	CA-CB-CG	-5.27	101.25	113.90
1	A	91	VAL	CA-CB-CG1	5.27	118.81	110.90
2	U	123	TYR	CA-C-O	-5.27	109.03	120.10
1	C	24	TYR	CB-CA-C	5.27	120.94	110.40
1	C	254	ALA	N-CA-CB	5.27	117.47	110.10
1	D	211	PHE	CB-CG-CD2	-5.27	117.11	120.80
2	V	66	TYR	O-C-N	5.26	131.12	122.70
1	A	445	ILE	CB-CA-C	5.26	122.12	111.60
2	T	105	ASP	CA-C-O	-5.26	109.05	120.10
1	A	238	HIS	CG-ND1-CE1	5.26	115.57	108.20
1	B	324	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	338	GLU	CA-C-O	5.26	131.15	120.10
1	A	365	THR	O-C-N	5.26	131.12	122.70
1	C	353	PHE	O-C-N	5.25	131.10	122.70
1	B	178	LEU	CA-C-N	5.25	126.70	116.20
1	A	93	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	B	217	ARG	CA-CB-CG	5.25	124.94	113.40
1	D	119	SER	O-C-N	5.25	131.09	122.70
1	B	211	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	C	140	ILE	CA-CB-CG1	5.24	120.96	111.00
2	T	115	PHE	CD1-CE1-CZ	-5.24	113.81	120.10
2	T	38	TRP	CB-CA-C	5.24	120.88	110.40
1	C	338	GLU	CA-C-O	5.24	131.11	120.10
2	V	54	GLU	CG-CD-OE1	-5.24	107.82	118.30
1	B	167	ARG	O-C-N	5.24	131.06	121.10
1	B	191	GLU	CB-CA-C	5.24	120.87	110.40
1	D	324	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	D	451	TRP	CB-CG-CD2	-5.24	119.79	126.60
1	A	79	ARG	CG-CD-NE	5.23	122.79	111.80
1	A	174	ILE	CA-C-N	5.23	128.71	117.20
1	B	259	GLU	N-CA-CB	5.23	120.01	110.60
1	A	36	ILE	CA-C-O	-5.23	109.12	120.10
2	T	48	HIS	N-CA-CB	5.23	120.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	291	LEU	CA-C-O	-5.23	109.13	120.10
1	B	434	GLY	CA-C-O	-5.22	111.19	120.60
1	C	63	THR	CA-C-N	5.22	126.64	116.20
1	D	291	LEU	N-CA-CB	-5.22	99.96	110.40
2	T	77	CYS	CA-CB-SG	-5.22	104.61	114.00
2	T	100	ARG	CB-CG-CD	5.21	125.16	111.60
2	V	37	GLY	C-N-CA	-5.21	108.66	121.70
1	D	132	ALA	CB-CA-C	5.21	117.92	110.10
1	D	371	LEU	N-CA-C	-5.21	96.92	111.00
1	D	199	PHE	CB-CA-C	-5.21	99.98	110.40
1	B	353	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	C	290	LEU	N-CA-C	-5.21	96.94	111.00
2	V	79	ASP	CA-CB-CG	-5.21	101.94	113.40
1	A	289	LEU	CA-C-O	-5.20	109.17	120.10
1	A	203	ASP	N-CA-C	-5.20	96.96	111.00
1	D	367	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	350	ARG	CA-C-N	5.20	128.64	117.20
1	A	134	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	D	149	GLN	O-C-N	5.20	132.03	123.20
1	B	62	SER	O-C-N	5.19	131.01	122.70
1	B	112	SER	N-CA-CB	-5.19	102.71	110.50
1	C	32	LYS	CA-C-N	-5.19	105.78	117.20
2	V	33	LEU	CB-CA-C	5.19	120.06	110.20
1	A	269	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	C	191	GLU	CA-C-O	-5.18	109.21	120.10
2	S	41	CYS	CA-CB-SG	-5.18	104.67	114.00
1	C	296	ALA	N-CA-CB	-5.18	102.85	110.10
2	V	59	PRO	CA-C-O	-5.18	107.77	120.20
1	C	95	ASP	CA-CB-CG	-5.18	102.01	113.40
1	D	79	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	131	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	A	387	MET	CA-CB-CG	-5.17	104.52	113.30
1	C	79	ARG	CB-CA-C	-5.17	100.06	110.40
1	D	319	ARG	CG-CD-NE	-5.17	100.95	111.80
2	S	2	GLN	OE1-CD-NE2	5.16	133.77	121.90
2	S	104	PHE	CB-CA-C	-5.16	100.08	110.40
1	B	354	VAL	CA-C-N	-5.16	105.84	117.20
1	A	263	PRO	CA-C-N	5.16	128.55	117.20
1	A	351	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	244	ALA	CB-CA-C	5.16	117.84	110.10
1	A	88	GLU	O-C-N	5.16	130.95	122.70
1	C	324	ASP	CB-CA-C	5.16	120.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	414	ALA	CB-CA-C	5.16	117.83	110.10
1	B	268	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	C	230	ALA	O-C-N	5.15	130.94	122.70
2	V	111	GLN	N-CA-CB	5.15	119.88	110.60
1	A	158	GLU	N-CA-CB	5.15	119.87	110.60
1	C	434	GLY	CA-C-O	-5.15	111.33	120.60
2	V	92	LYS	N-CA-C	-5.15	97.09	111.00
1	D	354	VAL	O-C-N	5.15	130.94	122.70
1	A	78	ASP	CB-CA-C	5.15	120.69	110.40
1	A	245	GLY	CA-C-N	5.15	128.53	117.20
1	A	319	ARG	CA-CB-CG	5.15	124.72	113.40
1	A	325	HIS	CA-CB-CG	5.15	122.35	113.60
1	D	234	GLU	N-CA-CB	5.14	119.86	110.60
1	B	340	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	S	40	PRO	O-C-N	5.13	130.91	122.70
1	A	283	TYR	CA-CB-CG	-5.13	103.65	113.40
1	C	180	LEU	CA-C-N	5.13	128.49	117.20
1	B	200	THR	N-CA-C	-5.13	97.16	111.00
1	B	442	ASN	CA-CB-CG	-5.12	102.13	113.40
2	U	101	ILE	CA-C-O	-5.12	109.34	120.10
1	D	61	SER	CA-CB-OG	-5.12	97.37	111.20
1	A	304	GLN	CB-CA-C	5.12	120.64	110.40
1	A	468	ASN	N-CA-CB	5.12	119.81	110.60
1	A	231	GLU	CG-CD-OE1	-5.11	108.08	118.30
1	A	436	ASP	CB-CG-OD1	5.11	122.90	118.30
2	S	33	LEU	CB-CA-C	5.11	119.91	110.20
1	B	295	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	260	LEU	O-C-N	-5.11	114.51	123.20
2	U	41	CYS	CA-CB-SG	-5.11	104.80	114.00
1	A	355	GLU	N-CA-CB	-5.11	101.41	110.60
2	T	52	TYR	CA-CB-CG	5.11	123.10	113.40
1	D	10	SER	O-C-N	5.11	130.87	122.70
1	D	26	THR	CA-CB-CG2	5.11	119.55	112.40
1	D	239	TYR	CZ-CE2-CD2	-5.11	115.20	119.80
1	C	18	LYS	CD-CE-NZ	5.10	123.44	111.70
1	B	385	TRP	CA-C-N	5.10	128.42	117.20
1	C	134	ARG	CD-NE-CZ	-5.10	116.46	123.60
1	B	80	TYR	CB-CG-CD2	5.10	124.06	121.00
1	A	52	GLU	N-CA-CB	5.09	119.76	110.60
1	A	207	ASN	CB-CG-OD1	-5.09	111.42	121.60
1	C	132	ALA	O-C-N	5.09	130.84	122.70
2	U	48	HIS	CA-C-N	-5.09	106.02	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	301	ILE	CB-CG1-CD1	-5.09	99.65	113.90
1	C	446	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	B	178	LEU	CA-CB-CG	5.08	127.00	115.30
1	B	264	ILE	CB-CG1-CD1	-5.08	99.66	113.90
1	C	207	ASN	CB-CA-C	5.08	120.57	110.40
1	D	101	VAL	O-C-N	5.08	130.84	122.70
1	A	309	ILE	O-C-N	5.08	130.83	122.70
2	T	55	ASN	CA-CB-CG	-5.08	102.22	113.40
1	C	436	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	45	GLN	CA-CB-CG	5.08	124.57	113.40
1	D	119	SER	N-CA-CB	5.08	118.12	110.50
2	U	2	GLN	CA-C-N	-5.08	106.03	117.20
1	A	223	GLU	CG-CD-OE2	-5.08	108.15	118.30
1	B	158	GLU	N-CA-CB	5.08	119.74	110.60
1	D	97	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	28	GLU	CG-CD-OE2	-5.07	108.17	118.30
1	D	44	PRO	CA-C-N	-5.07	106.05	117.20
1	C	258	ARG	CB-CG-CD	5.07	124.77	111.60
1	D	327	HIS	CA-CB-CG	5.07	122.21	113.60
2	S	103	GLY	CA-C-O	-5.06	111.49	120.60
1	C	468	ASN	O-C-N	5.06	130.80	122.70
1	A	323	GLY	CA-C-O	-5.06	111.49	120.60
1	C	447	GLU	OE1-CD-OE2	5.06	129.37	123.30
2	U	58	SER	N-CA-CB	-5.06	102.92	110.50
1	D	312	ARG	CD-NE-CZ	-5.06	116.52	123.60
2	T	58	SER	CB-CA-C	5.05	119.70	110.10
2	U	83	VAL	CA-CB-CG2	5.05	118.48	110.90
2	S	104	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	A	32	LYS	N-CA-CB	5.05	119.68	110.60
1	A	190	TYR	CA-C-O	5.05	130.70	120.10
1	B	288	GLY	N-CA-C	5.05	125.71	113.10
1	C	433	GLU	CB-CA-C	-5.05	100.31	110.40
1	B	387	MET	CA-CB-CG	-5.04	104.73	113.30
1	C	93	GLU	CG-CD-OE2	5.04	128.39	118.30
1	B	83	ARG	CD-NE-CZ	5.04	130.66	123.60
2	T	43	GLU	CG-CD-OE1	-5.04	108.22	118.30
1	C	224	ALA	CB-CA-C	5.04	117.66	110.10
1	A	303	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	392	GLU	CA-CB-CG	5.04	124.48	113.40
1	A	29	TYR	CA-C-N	-5.03	106.12	117.20
1	C	374	VAL	N-CA-CB	-5.03	100.43	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	369	VAL	CA-C-O	5.03	130.67	120.10
2	V	37	GLY	O-C-N	5.03	130.75	122.70
1	D	386	HIS	CG-ND1-CE1	5.03	115.24	108.20
1	C	117	PHE	N-CA-CB	5.03	119.65	110.60
1	A	352	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	465	ILE	CB-CA-C	-5.02	101.55	111.60
1	D	74	LEU	CB-CG-CD1	5.02	119.54	111.00
1	C	376	PRO	N-CD-CG	-5.02	95.67	103.20
1	B	303	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	148	PHE	CD1-CE1-CZ	-5.02	114.08	120.10
2	U	73	PRO	N-CA-C	-5.02	99.06	112.10
1	A	88	GLU	CA-C-O	-5.02	109.57	120.10
1	A	431	ARG	CD-NE-CZ	-5.01	116.58	123.60
1	A	105	LEU	CB-CG-CD2	5.01	119.52	111.00
1	B	420	ASN	CB-CG-OD1	-5.01	111.58	121.60
1	C	407	LEU	N-CA-CB	-5.01	100.38	110.40
2	V	96	GLN	O-C-N	5.01	130.72	122.70
1	D	297	MET	CA-CB-CG	-5.01	104.79	113.30
1	B	425	GLU	CG-CD-OE1	5.01	128.31	118.30
2	V	55	ASN	OD1-CG-ND2	5.01	133.42	121.90
1	B	200	THR	CA-C-O	-5.00	109.59	120.10
2	U	92	LYS	CA-C-O	-5.00	109.60	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	3559	200	0
1	B	3628	0	3558	225	1
1	C	3628	0	3556	246	1
1	D	3628	0	3557	242	0
2	S	1024	0	991	67	0
2	T	1024	0	991	85	0
2	U	1024	0	991	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	1024	0	991	93	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	6	2	0
4	B	21	0	5	0	0
4	C	21	0	6	1	0
4	D	21	0	6	3	0
5	A	3	0	0	1	0
5	B	3	0	0	0	0
5	C	3	0	0	1	0
5	D	3	0	0	1	0
All	All	18708	0	18217	1145	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:79:ASP:HB3	2:U:82:GLN:HE21	1.13	1.10
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.18	1.09
2:V:79:ASP:HB3	2:V:82:GLN:HE21	1.14	1.09
1:D:79:ARG:HG2	1:D:79:ARG:HH11	1.15	1.06
1:C:26:THR:HG22	1:C:29:TYR:HB2	1.37	1.05
1:C:79:ARG:HH11	1:C:79:ARG:HG2	1.18	1.04
1:C:90:VAL:HG21	1:C:96:GLN:HG2	1.37	1.02
2:T:79:ASP:HB3	2:T:82:GLN:HE21	1.18	1.02
1:D:176:PRO:HD2	1:D:180:LEU:HD22	1.43	1.01
1:A:26:THR:HG22	1:A:29:TYR:HB2	1.43	0.98
1:C:452:SER:HB3	1:C:455:LEU:HB3	1.48	0.96
2:S:27:LEU:HD23	2:S:31:GLU:OE2	1.65	0.96
2:S:79:ASP:HB3	2:S:82:GLN:HE21	1.32	0.94
1:B:304:GLN:HA	1:B:304:GLN:HE21	1.34	0.93
1:A:89:ARG:HH11	1:A:89:ARG:HB2	1.35	0.92
2:V:79:ASP:CB	2:V:82:GLN:HE21	1.82	0.92
2:S:56:ASN:ND2	2:S:58:SER:H	1.68	0.92
1:B:29:TYR:OH	1:B:32:LYS:NZ	2.01	0.92
1:B:155:ILE:HG12	1:B:375:LEU:HD13	1.51	0.92
1:C:89:ARG:HB2	1:C:89:ARG:HH11	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HG22	1:D:29:TYR:HB2	1.53	0.91
1:D:293:ILE:HG21	1:D:318:LEU:CD1	2.00	0.91
1:D:383:HIS:H	1:D:386:HIS:CD2	1.88	0.91
1:D:452:SER:HB3	1:D:455:LEU:HB3	1.53	0.91
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.53	0.90
2:V:22:SER:H	2:V:25:GLN:HE21	1.18	0.90
1:D:89:ARG:HH11	1:D:89:ARG:HB2	1.37	0.90
1:D:383:HIS:H	1:D:386:HIS:HD2	1.13	0.88
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.54	0.88
2:U:11:LYS:HG3	2:U:17:TYR:CE1	2.09	0.88
2:U:79:ASP:CB	2:U:82:GLN:HE21	1.87	0.87
2:T:75:PHE:HD1	1:D:9:ALA:HB1	1.39	0.87
1:C:431:ARG:HB2	1:C:437:LEU:HD21	1.57	0.86
2:V:33:LEU:HD13	2:V:38:TRP:HB2	1.54	0.86
1:D:457:ALA:O	1:D:461:VAL:HG23	1.74	0.86
2:V:82:GLN:O	2:V:85:ALA:HB3	1.76	0.86
1:C:26:THR:CG2	1:C:29:TYR:HB2	2.06	0.86
2:T:60:GLY:O	2:T:65:ARG:NH2	2.09	0.85
1:B:304:GLN:HA	1:B:304:GLN:NE2	1.89	0.85
2:U:56:ASN:ND2	2:U:58:SER:H	1.73	0.85
1:A:26:THR:HG22	1:A:26:THR:O	1.77	0.85
1:C:455:LEU:HD12	1:C:455:LEU:O	1.77	0.85
1:A:293:ILE:HG21	1:A:318:LEU:CD1	2.06	0.84
2:S:22:SER:H	2:S:25:GLN:HE21	1.25	0.84
2:S:82:GLN:O	2:S:85:ALA:HB3	1.76	0.84
1:B:383:HIS:H	1:B:386:HIS:HD2	1.20	0.84
2:U:33:LEU:HD13	2:U:38:TRP:HB2	1.58	0.84
1:C:176:PRO:HD2	1:C:180:LEU:HD22	1.58	0.84
1:C:293:ILE:HG21	1:C:318:LEU:CD1	2.08	0.84
2:U:79:ASP:HB3	2:U:82:GLN:NE2	1.93	0.83
2:T:92:LYS:O	2:T:93:ALA:HB3	1.78	0.83
1:C:448:ALA:HA	1:C:451:TRP:CD1	2.12	0.83
1:D:26:THR:CG2	1:D:29:TYR:HB2	2.08	0.83
1:A:29:TYR:CD1	1:A:83:ARG:HD2	2.13	0.83
1:D:448:ALA:HA	1:D:451:TRP:CD1	2.12	0.83
1:A:26:THR:CG2	1:A:29:TYR:HB2	2.09	0.83
1:C:155:ILE:HG12	1:C:375:LEU:HD13	1.58	0.83
1:C:332:VAL:HG13	1:C:386:HIS:ND1	1.94	0.82
2:V:56:ASN:HB3	2:V:61:TYR:CD2	2.13	0.82
1:D:295:ARG:HG3	1:D:298:HIS:CD2	2.15	0.82
2:T:79:ASP:CB	2:T:82:GLN:HE21	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:HG2	1:D:79:ARG:NH1	1.92	0.82
1:A:155:ILE:HG12	1:A:375:LEU:HD13	1.63	0.81
2:T:77:CYS:HB2	2:T:82:GLN:OE1	1.81	0.80
1:D:414:ALA:O	1:D:418:VAL:HG23	1.81	0.80
1:B:293:ILE:HG21	1:B:318:LEU:CD1	2.11	0.80
1:B:178:LEU:HD21	1:B:205:ASN:ND2	1.97	0.80
1:D:201:LYS:HE2	1:D:202:ASP:O	1.81	0.80
1:D:29:TYR:OH	1:D:32:LYS:NZ	2.13	0.79
1:B:89:ARG:HH11	1:B:89:ARG:HB2	1.47	0.79
1:C:79:ARG:HG2	1:C:79:ARG:NH1	1.96	0.79
1:B:9:ALA:HB1	2:V:75:PHE:HD1	1.47	0.79
1:C:195:GLY:HA3	1:C:417:ALA:HB3	1.65	0.79
2:T:56:ASN:ND2	2:T:58:SER:H	1.81	0.78
2:V:56:ASN:ND2	2:V:58:SER:H	1.81	0.78
2:S:27:LEU:CD2	2:S:31:GLU:OE2	2.32	0.78
2:T:39:VAL:HG21	1:D:9:ALA:CB	2.13	0.78
1:A:79:ARG:HG2	1:A:79:ARG:NH1	1.95	0.78
1:A:90:VAL:HG21	1:A:96:GLN:HG2	1.65	0.78
1:B:383:HIS:H	1:B:386:HIS:CD2	2.02	0.78
1:B:26:THR:HG21	1:B:83:ARG:HD3	1.63	0.78
1:B:26:THR:HG22	1:B:29:TYR:HB2	1.64	0.78
1:B:79:ARG:HG2	1:B:79:ARG:HH11	1.47	0.77
1:A:293:ILE:HG21	1:A:318:LEU:HD13	1.65	0.77
2:T:92:LYS:O	2:T:93:ALA:CB	2.32	0.77
2:T:11:LYS:HG3	2:T:17:TYR:CE1	2.19	0.77
1:B:452:SER:HB3	1:B:455:LEU:HB3	1.67	0.77
1:D:293:ILE:HG13	1:D:318:LEU:HD11	1.67	0.76
1:B:9:ALA:CB	2:V:39:VAL:HG21	2.15	0.76
2:S:77:CYS:HB2	2:S:82:GLN:OE1	1.84	0.76
1:C:181:SER:HB2	1:D:156:GLN:HE22	1.49	0.76
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.67	0.76
1:B:293:ILE:HG21	1:B:318:LEU:HD13	1.67	0.76
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.69	0.75
1:D:171:GLY:O	1:D:402:PHE:N	2.18	0.75
1:C:387:MET:HB3	1:C:388:PRO:HD3	1.68	0.75
2:U:33:LEU:HD12	2:U:33:LEU:C	2.07	0.75
1:D:57:VAL:O	1:D:61:SER:HB2	1.85	0.75
1:B:71:THR:O	1:B:74:LEU:HB2	1.85	0.75
1:B:332:VAL:HG13	1:B:386:HIS:ND1	2.01	0.75
1:C:435:ARG:HD2	1:C:440:GLU:OE1	1.87	0.75
2:U:98:TRP:HD1	2:U:116:ILE:HD11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ALA:HA	1:A:451:TRP:CD1	2.22	0.74
1:A:71:THR:O	1:A:74:LEU:HB2	1.87	0.74
2:U:22:SER:H	2:U:25:GLN:HE21	1.33	0.74
1:A:43:THR:HG22	1:A:131:ARG:HG3	1.68	0.74
1:D:332:VAL:O	1:D:332:VAL:HG13	1.86	0.74
1:A:251:ILE:O	1:A:255:VAL:HG23	1.87	0.74
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.70	0.73
2:S:92:LYS:O	2:S:93:ALA:HB3	1.88	0.73
1:D:26:THR:HG21	1:D:83:ARG:HD3	1.67	0.73
1:C:43:THR:HG22	1:C:131:ARG:HG3	1.70	0.73
2:U:93:ALA:C	2:U:95:PRO:HD3	2.09	0.73
1:B:77:LEU:O	1:B:81:LYS:HG2	1.89	0.73
1:C:29:TYR:CD1	1:C:83:ARG:HD2	2.23	0.73
1:B:155:ILE:HG12	1:B:375:LEU:CD1	2.18	0.73
1:B:193:LEU:HD13	1:B:200:THR:HG23	1.70	0.73
1:C:26:THR:HG22	1:C:26:THR:O	1.89	0.73
2:S:33:LEU:HD13	2:S:38:TRP:HB2	1.70	0.73
1:A:383:HIS:H	1:A:386:HIS:HD2	1.36	0.73
2:U:82:GLN:O	2:U:85:ALA:HB3	1.89	0.73
2:S:93:ALA:C	2:S:95:PRO:HD3	2.10	0.72
1:A:455:LEU:O	1:A:455:LEU:HD12	1.89	0.72
2:T:75:PHE:HD1	1:D:9:ALA:CB	2.01	0.72
2:V:94:TYR:HB3	2:V:97:ALA:HB2	1.71	0.72
1:A:26:THR:HG21	1:A:83:ARG:HD3	1.70	0.72
2:T:93:ALA:C	2:T:95:PRO:HD3	2.09	0.72
1:C:304:GLN:HA	1:C:304:GLN:NE2	2.05	0.71
1:D:171:GLY:O	1:D:401:GLN:HA	1.90	0.71
2:V:93:ALA:C	2:V:95:PRO:HD3	2.09	0.71
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.72	0.71
1:A:19:GLU:HB3	1:A:52:GLU:OE1	1.90	0.71
1:B:332:VAL:HG13	1:B:332:VAL:O	1.91	0.71
1:B:448:ALA:HA	1:B:451:TRP:CD1	2.25	0.71
1:C:181:SER:CB	1:D:156:GLN:HE22	2.03	0.71
2:U:86:GLU:HA	2:U:86:GLU:OE1	1.90	0.71
2:S:79:ASP:CB	2:S:82:GLN:HE21	2.03	0.70
1:A:29:TYR:CE2	1:A:31:THR:HA	2.25	0.70
2:U:3:VAL:HG21	2:V:70:TRP:CE3	2.27	0.70
1:C:120:ILE:HG22	1:C:121:VAL:HG23	1.73	0.70
1:C:383:HIS:H	1:C:386:HIS:CD2	2.10	0.70
1:A:293:ILE:HG13	1:A:318:LEU:HD11	1.73	0.70
2:T:75:PHE:CD1	1:D:9:ALA:CB	2.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:HA	1:C:201:LYS:HG2	1.73	0.70
1:C:414:ALA:O	1:C:418:VAL:HG23	1.91	0.70
1:D:29:TYR:CD1	1:D:83:ARG:HD2	2.27	0.70
1:C:79:ARG:HH11	1:C:79:ARG:CG	1.91	0.70
2:V:77:CYS:HB2	2:V:82:GLN:OE1	1.92	0.70
1:C:171:GLY:O	1:C:401:GLN:HA	1.91	0.69
1:C:26:THR:HG21	1:C:83:ARG:HD3	1.74	0.69
2:V:79:ASP:HB3	2:V:82:GLN:NE2	1.98	0.69
1:D:26:THR:HG22	1:D:26:THR:O	1.92	0.69
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.74	0.69
2:U:77:CYS:HB2	2:U:82:GLN:OE1	1.93	0.69
1:B:332:VAL:O	1:B:332:VAL:CG1	2.40	0.69
1:D:431:ARG:HB2	1:D:437:LEU:HD21	1.75	0.69
1:C:293:ILE:HG21	1:C:318:LEU:HD13	1.73	0.69
2:S:84:LEU:O	2:S:84:LEU:HD23	1.93	0.68
1:C:412:GLY:HA3	2:V:72:LEU:HD11	1.75	0.68
1:D:305:LYS:O	1:D:305:LYS:HG2	1.91	0.68
1:B:29:TYR:CD1	1:B:83:ARG:HD2	2.29	0.68
1:B:387:MET:HB3	1:B:388:PRO:HD3	1.74	0.68
1:B:431:ARG:HB2	1:B:437:LEU:HD21	1.75	0.68
1:C:383:HIS:H	1:C:386:HIS:HD2	1.39	0.68
1:B:19:GLU:HB3	1:B:52:GLU:OE1	1.94	0.68
2:U:92:LYS:O	2:U:93:ALA:HB3	1.93	0.68
2:V:79:ASP:H	2:V:82:GLN:NE2	1.91	0.68
1:B:178:LEU:CD2	1:B:205:ASN:ND2	2.57	0.68
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.28	0.68
1:D:293:ILE:HG21	1:D:318:LEU:HD13	1.72	0.68
1:A:332:VAL:HG13	1:A:386:HIS:ND1	2.08	0.67
1:A:443:GLU:O	1:A:447:GLU:HG3	1.94	0.67
1:B:194:ARG:NH2	2:T:4:TRP:O	2.26	0.67
2:T:94:TYR:N	2:T:95:PRO:HD3	2.09	0.67
1:A:26:THR:O	1:A:26:THR:CG2	2.40	0.67
2:S:43:GLU:OE1	2:S:100:ARG:NH1	2.27	0.67
1:D:32:LYS:NZ	1:D:35:ASP:OD1	2.25	0.67
1:B:414:ALA:O	1:B:418:VAL:HG23	1.94	0.67
1:A:431:ARG:HB2	1:A:437:LEU:HD21	1.75	0.67
1:D:293:ILE:HG21	1:D:318:LEU:HD11	1.77	0.67
1:D:90:VAL:HG21	1:D:96:GLN:HG2	1.75	0.67
1:C:209:GLN:HB3	1:C:210:PRO:CD	2.24	0.67
1:D:435:ARG:HD2	1:D:440:GLU:OE1	1.95	0.67
2:S:33:LEU:CD1	2:S:38:TRP:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ARG:O	1:C:343:LEU:HG	1.95	0.66
1:D:176:PRO:HD2	1:D:180:LEU:CD2	2.23	0.66
1:D:466:VAL:HG23	1:D:468:ASN:H	1.59	0.66
1:A:194:ARG:NH2	2:S:4:TRP:O	2.27	0.66
1:A:436:ASP:OD1	1:A:438:ALA:N	2.28	0.66
2:S:92:LYS:O	2:S:93:ALA:CB	2.43	0.66
1:B:195:GLY:HA3	1:B:417:ALA:HB3	1.76	0.66
1:C:89:ARG:HB2	1:C:89:ARG:NH1	2.09	0.66
2:U:43:GLU:OE1	2:U:100:ARG:NH1	2.26	0.66
1:C:293:ILE:HG21	1:C:318:LEU:HD11	1.76	0.66
1:B:202:ASP:OD2	1:B:217:ARG:NH2	2.29	0.66
2:T:33:LEU:HD13	2:T:38:TRP:HB2	1.78	0.66
1:D:151:PRO:HG2	1:D:372:PRO:HB2	1.78	0.65
1:B:466:VAL:HG23	1:B:467:PHE:N	2.11	0.65
1:A:293:ILE:HG21	1:A:318:LEU:HD11	1.78	0.65
1:D:332:VAL:O	1:D:332:VAL:CG1	2.44	0.65
1:A:440:GLU:O	1:A:444:ILE:HG13	1.96	0.65
1:B:383:HIS:O	1:B:386:HIS:N	2.25	0.65
1:A:89:ARG:HB2	1:A:89:ARG:NH1	2.10	0.65
1:D:451:TRP:CH2	2:V:19:PRO:HD3	2.31	0.65
1:D:383:HIS:N	1:D:386:HIS:HD2	1.92	0.65
1:C:71:THR:O	1:C:74:LEU:HB2	1.96	0.64
1:D:455:LEU:O	1:D:455:LEU:HD12	1.96	0.64
1:A:383:HIS:H	1:A:386:HIS:CD2	2.13	0.64
1:B:142:PRO:HB3	1:B:369:VAL:HG11	1.79	0.64
2:V:43:GLU:HA	2:V:68:THR:O	1.96	0.64
2:T:22:SER:H	2:T:25:GLN:HE21	1.45	0.64
1:C:436:ASP:OD1	1:C:438:ALA:N	2.30	0.64
1:D:193:LEU:HD13	1:D:200:THR:HG23	1.79	0.64
1:C:457:ALA:O	1:C:461:VAL:HG23	1.98	0.64
2:U:56:ASN:HB3	2:U:61:TYR:CD1	2.33	0.64
1:D:79:ARG:HH11	1:D:79:ARG:CG	1.85	0.64
1:B:176:PRO:HD2	1:B:180:LEU:HD22	1.78	0.64
1:B:304:GLN:NE2	1:B:304:GLN:CA	2.60	0.64
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.81	0.64
1:C:292:HIS:HA	1:C:325:HIS:HB2	1.80	0.64
1:C:440:GLU:O	1:C:444:ILE:HG13	1.96	0.64
1:B:297:MET:CG	1:B:297:MET:O	2.46	0.64
1:B:79:ARG:HG2	1:B:79:ARG:NH1	2.13	0.64
2:T:79:ASP:HB3	2:T:82:GLN:NE2	2.02	0.64
2:U:27:LEU:O	2:U:31:GLU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:TYR:OH	1:D:35:ASP:OD2	2.14	0.64
1:D:443:GLU:O	1:D:446:ARG:HB3	1.97	0.64
2:T:56:ASN:HB3	2:T:61:TYR:CD1	2.33	0.64
1:D:195:GLY:HA3	1:D:417:ALA:HB3	1.80	0.64
1:B:29:TYR:CE2	1:B:31:THR:HA	2.33	0.63
2:T:75:PHE:CD1	1:D:9:ALA:HB1	2.27	0.63
1:C:52:GLU:O	1:C:53:ALA:C	2.36	0.63
1:D:251:ILE:O	1:D:255:VAL:HG23	1.98	0.63
2:U:98:TRP:HD1	2:U:116:ILE:CD1	2.10	0.63
2:S:23:GLN:O	2:S:27:LEU:HB2	1.98	0.63
2:T:43:GLU:OE1	2:T:100:ARG:NH1	2.31	0.63
1:C:19:GLU:HB3	1:C:52:GLU:OE1	1.98	0.63
2:V:99:ILE:O	2:V:116:ILE:HG13	1.98	0.63
1:B:305:LYS:HG2	1:B:305:LYS:O	1.99	0.63
1:A:29:TYR:CG	1:A:83:ARG:HD2	2.32	0.63
1:B:9:ALA:CB	2:V:75:PHE:HD1	2.12	0.63
2:U:98:TRP:CD1	2:U:116:ILE:HD11	2.32	0.63
2:V:71:LYS:O	2:V:72:LEU:HD12	1.98	0.63
1:C:414:ALA:HB3	1:C:415:PRO:CD	2.28	0.63
2:U:33:LEU:CD1	2:U:38:TRP:HB2	2.29	0.63
1:D:43:THR:HG22	1:D:131:ARG:HG3	1.81	0.63
1:A:435:ARG:HD2	1:A:440:GLU:OE1	1.99	0.63
1:C:379:SER:OG	1:C:401:GLN:HB2	1.99	0.63
1:C:90:VAL:HG23	1:C:96:GLN:O	1.99	0.62
1:C:425:GLU:OE1	2:U:17:TYR:HB2	1.99	0.62
1:A:176:PRO:HD2	1:A:180:LEU:HD22	1.79	0.62
1:C:332:VAL:HG13	1:C:332:VAL:O	1.99	0.62
1:C:382:ILE:HD12	1:C:390:LEU:CD1	2.29	0.62
1:C:23:THR:HG22	1:C:81:LYS:NZ	2.14	0.62
1:A:62:SER:O	1:D:178:LEU:HD22	2.00	0.62
1:B:151:PRO:HB3	1:B:323:GLY:O	1.99	0.62
1:B:435:ARG:HD2	1:B:440:GLU:OE1	2.00	0.62
1:C:51:GLU:HA	1:C:87:ILE:HD11	1.81	0.62
1:C:379:SER:HB3	4:C:490:CAP:O3	2.00	0.62
2:S:96:GLN:OE1	2:S:96:GLN:N	2.28	0.62
1:A:429:LYS:NZ	2:S:29:GLU:OE1	2.33	0.62
1:B:363:TYR:CD1	1:B:363:TYR:N	2.67	0.62
1:C:192:CYS:HB3	1:C:197:LEU:HD23	1.82	0.62
1:A:207:ASN:O	1:A:217:ARG:NH2	2.26	0.61
1:B:443:GLU:OE1	1:B:446:ARG:NH2	2.33	0.61
1:C:305:LYS:O	1:C:305:LYS:HG2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ASN:O	1:B:217:ARG:NH1	2.27	0.61
1:C:269:TYR:CD1	1:C:293:ILE:CG2	2.84	0.61
1:A:195:GLY:HA3	1:A:417:ALA:HB3	1.81	0.61
2:U:60:GLY:O	2:U:65:ARG:NH2	2.33	0.61
2:U:117:ALA:O	2:U:118:TYR:HB2	2.00	0.61
1:D:166:GLY:O	1:D:167:ARG:HB3	1.99	0.61
1:A:134:ARG:HG3	1:A:135:LEU:N	2.15	0.61
1:B:440:GLU:O	1:B:444:ILE:HG13	2.00	0.61
1:B:90:VAL:HG21	1:B:96:GLN:HG2	1.82	0.61
2:U:84:LEU:HD23	2:U:84:LEU:O	2.00	0.61
1:B:297:MET:O	1:B:297:MET:HG3	1.99	0.61
2:T:75:PHE:CE1	1:D:9:ALA:HB2	2.36	0.61
1:D:387:MET:N	1:D:388:PRO:HD2	2.16	0.61
2:T:77:CYS:CB	2:T:82:GLN:OE1	2.48	0.61
1:C:158:GLU:OE2	1:C:325:HIS:NE2	2.28	0.61
1:D:199:PHE:HA	1:D:237:GLY:O	2.00	0.61
1:A:449:CYS:CB	1:A:459:CYS:SG	2.88	0.61
1:D:430:ALA:HB1	1:D:444:ILE:HD13	1.81	0.61
1:C:304:GLN:HA	1:C:304:GLN:HE21	1.65	0.61
1:D:38:ALA:HB2	1:D:138:LEU:HD23	1.82	0.61
1:A:45:GLN:OE1	1:A:131:ARG:HB3	2.01	0.60
1:B:368:TRP:O	1:B:369:VAL:C	2.38	0.60
1:C:382:ILE:HD12	1:C:390:LEU:HD13	1.83	0.60
1:D:430:ALA:CB	1:D:444:ILE:HD13	2.30	0.60
1:C:90:VAL:CG2	1:C:96:GLN:HG2	2.24	0.60
1:C:193:LEU:HD13	1:C:200:THR:HG23	1.82	0.60
2:V:11:LYS:HG3	2:V:17:TYR:CE1	2.37	0.60
1:B:57:VAL:O	1:B:61:SER:HB2	2.02	0.60
2:T:79:ASP:H	2:T:82:GLN:NE2	2.00	0.60
1:C:66:TRP:CE3	1:C:67:THR:HB	2.36	0.60
1:A:429:LYS:CE	2:S:29:GLU:OE1	2.50	0.60
1:D:26:THR:CG2	1:D:26:THR:O	2.49	0.60
1:A:181:SER:HB2	1:B:156:GLN:HE22	1.67	0.60
1:A:425:GLU:OE1	2:S:17:TYR:HB2	2.02	0.60
2:S:83:VAL:O	2:S:86:GLU:HB2	2.02	0.60
1:B:271:THR:HG1	1:C:118:THR:HG1	1.50	0.60
1:B:363:TYR:N	1:B:363:TYR:HD1	2.00	0.60
2:U:79:ASP:H	2:U:82:GLN:NE2	1.99	0.60
1:D:120:ILE:HG22	1:D:121:VAL:HG23	1.84	0.60
2:V:113:ILE:O	2:V:114:SER:HB2	2.02	0.60
2:S:60:GLY:O	2:S:65:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:HIS:NE2	1:C:465:ILE:HB	2.17	0.59
1:D:155:ILE:HG12	1:D:375:LEU:HD13	1.84	0.59
1:C:385:TRP:CZ2	1:C:459:CYS:HB3	2.37	0.59
2:U:6:PRO:HG3	2:V:44:PHE:CE2	2.37	0.59
2:U:79:ASP:H	2:U:82:GLN:HE22	1.50	0.59
2:U:92:LYS:O	2:U:93:ALA:CB	2.49	0.59
1:D:190:TYR:O	1:D:194:ARG:HG2	2.02	0.59
1:D:295:ARG:O	1:D:298:HIS:HB3	2.01	0.59
1:B:9:ALA:CB	2:V:75:PHE:CD1	2.84	0.59
1:B:381:GLY:HA2	1:C:66:TRP:CD1	2.37	0.59
1:D:190:TYR:CE1	1:D:227:LYS:HD3	2.38	0.59
1:A:101:VAL:HG12	1:A:102:ALA:N	2.16	0.59
1:C:462:TRP:O	1:C:465:ILE:HG12	2.02	0.59
1:B:208:SER:O	1:C:109:GLU:HB2	2.02	0.59
1:C:387:MET:HB3	1:C:388:PRO:CD	2.31	0.59
2:V:60:GLY:O	2:V:65:ARG:NH2	2.36	0.59
1:B:443:GLU:O	1:B:447:GLU:HG3	2.01	0.59
2:V:27:LEU:O	2:V:31:GLU:HB2	2.03	0.59
1:A:452:SER:HB3	1:A:455:LEU:HB3	1.84	0.59
2:S:79:ASP:H	2:S:82:GLN:NE2	2.01	0.59
2:T:77:CYS:SG	2:T:78:THR:N	2.75	0.59
2:T:96:GLN:OE1	2:T:96:GLN:N	2.28	0.58
1:C:19:GLU:HB3	1:C:52:GLU:CD	2.23	0.58
1:D:234:GLU:O	1:D:236:LYS:HG2	2.03	0.58
1:D:440:GLU:O	1:D:444:ILE:HG13	2.02	0.58
2:V:56:ASN:ND2	2:V:58:SER:OG	2.36	0.58
1:B:171:GLY:O	1:B:401:GLN:HA	2.03	0.58
1:D:385:TRP:CZ2	1:D:459:CYS:HB3	2.38	0.58
1:B:378:ALA:HB3	1:B:400:LEU:HD23	1.86	0.58
1:D:436:ASP:OD1	1:D:438:ALA:N	2.36	0.58
1:B:66:TRP:CE3	1:B:67:THR:HB	2.38	0.58
1:B:79:ARG:HH11	1:B:79:ARG:CG	2.15	0.58
1:C:448:ALA:HA	1:C:451:TRP:HD1	1.65	0.58
2:V:27:LEU:HD12	2:V:84:LEU:CD1	2.33	0.58
1:A:137:ASP:OD1	1:A:138:LEU:N	2.35	0.58
1:D:97:TYR:O	1:D:98:ILE:HD13	2.03	0.58
2:U:23:GLN:O	2:U:27:LEU:HB2	2.04	0.58
2:V:33:LEU:CD1	2:V:38:TRP:HB2	2.31	0.58
1:C:10:SER:O	1:C:11:VAL:HB	2.04	0.58
1:C:459:CYS:O	1:C:463:LYS:HB2	2.04	0.58
1:B:209:GLN:HB3	1:B:210:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:56:ASN:HB3	2:V:61:TYR:CG	2.39	0.58
1:C:443:GLU:O	1:C:447:GLU:N	2.32	0.58
1:D:429:LYS:NZ	2:V:29:GLU:OE1	2.37	0.58
1:A:19:GLU:HB3	1:A:52:GLU:CD	2.23	0.57
1:A:414:ALA:O	1:A:418:VAL:HG23	2.04	0.57
2:S:77:CYS:SG	2:S:82:GLN:NE2	2.77	0.57
1:C:209:GLN:HB3	1:C:210:PRO:HD2	1.86	0.57
1:D:332:VAL:HG13	1:D:386:HIS:ND1	2.19	0.57
1:A:466:VAL:HG23	1:A:468:ASN:H	1.69	0.57
2:T:39:VAL:HG21	1:D:9:ALA:HB2	1.85	0.57
1:C:19:GLU:HB3	1:C:52:GLU:OE2	2.04	0.57
1:C:26:THR:HG22	1:C:29:TYR:CB	2.25	0.57
1:C:32:LYS:NZ	1:C:35:ASP:OD1	2.35	0.57
1:C:443:GLU:O	1:C:446:ARG:HB3	2.04	0.57
2:U:96:GLN:OE1	2:U:96:GLN:N	2.31	0.57
1:D:23:THR:HB	1:D:24:TYR:CD1	2.39	0.57
1:D:71:THR:O	1:D:74:LEU:HB2	2.05	0.57
1:D:133:LEU:O	1:D:307:HIS:HA	2.04	0.57
1:A:443:GLU:O	1:A:447:GLU:N	2.37	0.57
1:B:127:PHE:CE1	1:C:335:LEU:HD21	2.40	0.57
1:D:378:ALA:HB3	1:D:400:LEU:HD23	1.85	0.57
2:V:92:LYS:O	2:V:93:ALA:HB3	2.05	0.57
2:T:27:LEU:HD12	2:T:84:LEU:CD1	2.35	0.57
1:C:57:VAL:O	1:C:61:SER:HB2	2.04	0.57
1:C:94:LYS:O	1:C:96:GLN:N	2.38	0.57
2:U:43:GLU:HA	2:U:68:THR:O	2.04	0.57
1:D:202:ASP:OD1	1:D:238:HIS:CE1	2.55	0.57
1:B:429:LYS:HE3	2:T:21:LEU:HD22	1.87	0.57
1:D:89:ARG:HB2	1:D:89:ARG:NH1	2.16	0.57
1:D:304:GLN:HA	1:D:304:GLN:NE2	2.19	0.57
2:T:94:TYR:HB3	2:T:97:ALA:HB2	1.85	0.57
1:C:155:ILE:HG12	1:C:375:LEU:CD1	2.31	0.57
1:C:293:ILE:HG13	1:C:318:LEU:HD11	1.85	0.56
1:A:120:ILE:HD13	1:A:138:LEU:HD21	1.86	0.56
1:A:193:LEU:HD13	1:A:200:THR:HG23	1.87	0.56
1:B:387:MET:HB3	1:B:388:PRO:CD	2.35	0.56
1:C:264:ILE:HG13	1:C:290:LEU:O	2.05	0.56
2:U:94:TYR:N	2:U:95:PRO:HD3	2.20	0.56
1:D:383:HIS:NE2	1:D:465:ILE:HB	2.20	0.56
1:A:449:CYS:HB3	1:A:459:CYS:SG	2.45	0.56
1:B:425:GLU:OE1	2:T:17:TYR:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:86:GLU:OE1	2:T:86:GLU:HA	2.05	0.56
1:C:332:VAL:O	1:C:332:VAL:CG1	2.53	0.56
2:V:94:TYR:N	2:V:95:PRO:HD3	2.20	0.56
2:T:77:CYS:SG	2:T:82:GLN:NE2	2.79	0.56
1:C:26:THR:CG2	1:C:26:THR:O	2.51	0.56
2:V:33:LEU:C	2:V:33:LEU:HD12	2.25	0.56
1:A:305:LYS:O	1:A:305:LYS:HG2	2.06	0.56
2:T:101:ILE:HG13	2:T:117:ALA:HB2	1.87	0.56
1:C:447:GLU:O	1:C:450:LYS:HB2	2.06	0.56
1:A:181:SER:CB	1:B:156:GLN:HE22	2.18	0.56
2:S:94:TYR:N	2:S:95:PRO:HD3	2.21	0.56
1:B:466:VAL:HG23	1:B:468:ASN:H	1.71	0.56
1:C:431:ARG:CB	1:C:437:LEU:HD21	2.34	0.56
1:B:387:MET:N	1:B:388:PRO:HD2	2.21	0.55
1:D:90:VAL:HG23	1:D:97:TYR:HA	1.87	0.55
1:D:331:VAL:HG12	1:D:332:VAL:N	2.20	0.55
1:C:45:GLN:OE1	1:C:131:ARG:HB3	2.07	0.55
1:C:306:ASN:OD1	1:C:306:ASN:N	2.33	0.55
1:C:383:HIS:O	1:C:386:HIS:N	2.36	0.55
1:C:443:GLU:O	1:C:447:GLU:HG3	2.06	0.55
1:A:209:GLN:HB3	1:A:210:PRO:HD2	1.88	0.55
1:C:378:ALA:HB3	1:C:400:LEU:HD23	1.87	0.55
1:D:94:LYS:O	1:D:95:ASP:C	2.45	0.55
1:A:63:THR:HA	1:D:177:LYS:HB2	1.89	0.55
2:S:103:GLY:HA3	2:S:113:ILE:HG22	1.88	0.55
1:B:173:THR:HA	1:B:201:LYS:HG2	1.88	0.55
1:C:466:VAL:HG23	1:C:468:ASN:H	1.72	0.55
2:U:83:VAL:O	2:U:86:GLU:HB2	2.06	0.55
1:B:60:GLU:OE2	1:B:65:THR:HA	2.07	0.55
2:T:42:LEU:HB3	2:T:70:TRP:HB3	1.88	0.55
1:C:214:TRP:CD2	1:C:253:ARG:HG2	2.42	0.55
1:D:304:GLN:HA	1:D:304:GLN:HE21	1.72	0.55
1:B:293:ILE:HG21	1:B:318:LEU:HD11	1.88	0.55
1:C:234:GLU:OE2	1:C:421:ARG:NH2	2.38	0.55
1:D:166:GLY:O	1:D:167:ARG:CB	2.54	0.55
1:A:94:LYS:O	1:A:96:GLN:N	2.40	0.55
1:C:298:HIS:CG	1:C:299:ALA:N	2.75	0.55
1:D:173:THR:HA	1:D:201:LYS:HG2	1.88	0.55
1:D:448:ALA:HA	1:D:451:TRP:HD1	1.70	0.55
1:A:190:TYR:O	1:A:194:ARG:HG2	2.06	0.54
1:B:445:ILE:HG13	1:B:446:ARG:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:56:ASN:HD21	2:U:58:SER:CB	2.19	0.54
1:A:42:VAL:HG13	1:A:97:TYR:HB2	1.90	0.54
1:B:201:LYS:HE2	1:B:202:ASP:O	2.07	0.54
1:A:295:ARG:O	1:A:298:HIS:HB3	2.08	0.54
2:T:39:VAL:CG2	1:D:9:ALA:CB	2.85	0.54
2:V:77:CYS:SG	2:V:78:THR:N	2.80	0.54
2:U:6:PRO:HG3	2:V:44:PHE:HE2	1.72	0.54
1:A:138:LEU:O	1:A:316:LYS:NZ	2.40	0.54
1:B:425:GLU:OE1	2:T:17:TYR:HB2	2.07	0.54
1:D:94:LYS:O	1:D:96:GLN:N	2.40	0.54
1:C:201:LYS:HE2	1:C:202:ASP:O	2.08	0.54
1:D:29:TYR:CG	1:D:83:ARG:HD2	2.43	0.54
1:D:190:TYR:CZ	1:D:194:ARG:HD2	2.43	0.54
1:C:454:GLU:CD	1:C:454:GLU:H	2.10	0.54
2:U:79:ASP:CB	2:U:82:GLN:NE2	2.61	0.54
1:C:382:ILE:HG13	1:C:402:PHE:CE1	2.43	0.54
1:D:449:CYS:HA	1:D:455:LEU:HG	1.89	0.54
1:D:298:HIS:ND1	1:D:302:ASP:OD2	2.21	0.54
1:D:368:TRP:O	1:D:369:VAL:C	2.46	0.54
2:T:69:MET:CE	2:T:72:LEU:HD12	2.38	0.54
2:U:56:ASN:ND2	2:U:58:SER:OG	2.41	0.53
1:D:45:GLN:OE1	1:D:131:ARG:HB3	2.09	0.53
2:S:77:CYS:CB	2:S:82:GLN:OE1	2.55	0.53
2:U:3:VAL:HG22	2:V:71:LYS:H	1.74	0.53
1:A:79:ARG:HH11	1:A:79:ARG:CG	1.97	0.53
1:A:319:ARG:HD2	1:A:371:LEU:HD23	1.89	0.53
1:B:9:ALA:HB3	2:V:39:VAL:HG21	1.91	0.53
1:B:43:THR:O	1:B:43:THR:HG22	2.06	0.53
1:C:29:TYR:CE2	1:C:31:THR:HA	2.43	0.53
1:C:251:ILE:O	1:C:255:VAL:HG23	2.09	0.53
1:D:101:VAL:HG12	1:D:102:ALA:N	2.24	0.53
1:D:214:TRP:CD2	1:D:253:ARG:HG2	2.44	0.53
1:D:383:HIS:O	1:D:386:HIS:N	2.41	0.53
2:V:79:ASP:HB3	2:V:82:GLN:HB3	1.89	0.53
1:B:190:TYR:CE1	1:B:227:LYS:HD3	2.44	0.53
1:B:443:GLU:O	1:B:447:GLU:N	2.39	0.53
2:U:79:ASP:O	2:U:82:GLN:N	2.42	0.53
1:B:298:HIS:ND1	1:B:302:ASP:OD2	2.33	0.53
2:V:113:ILE:HG13	2:V:114:SER:N	2.23	0.53
2:V:84:LEU:O	2:V:84:LEU:HD23	2.09	0.53
1:A:383:HIS:NE2	1:A:465:ILE:HB	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:THR:HG22	1:C:81:LYS:HZ3	1.74	0.53
1:C:411:TRP:CH2	2:U:2:GLN:OE1	2.62	0.53
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.92	0.53
1:A:209:GLN:HB3	1:A:210:PRO:CD	2.39	0.53
1:B:397:ASP:OD2	2:T:108:ARG:NH2	2.42	0.53
1:A:9:ALA:N	1:A:73:GLY:O	2.42	0.52
1:C:29:TYR:CG	1:C:83:ARG:HD2	2.44	0.52
1:C:133:LEU:O	1:C:307:HIS:HA	2.10	0.52
1:C:429:LYS:HE3	2:U:21:LEU:HD22	1.90	0.52
2:U:107:VAL:HG12	2:U:107:VAL:O	2.08	0.52
1:C:429:LYS:NZ	2:U:29:GLU:OE1	2.42	0.52
1:D:178:LEU:HD21	1:D:205:ASN:ND2	2.25	0.52
1:A:94:LYS:O	1:A:95:ASP:C	2.47	0.52
1:B:69:VAL:HA	1:C:407:LEU:O	2.09	0.52
1:C:332:VAL:CG1	1:C:386:HIS:ND1	2.71	0.52
2:S:86:GLU:OE1	2:S:86:GLU:HA	2.08	0.52
1:C:76:SER:O	1:C:76:SER:OG	2.23	0.52
1:C:430:ALA:CB	1:C:444:ILE:HD13	2.39	0.52
2:U:119:LYS:HD2	2:U:123:TYR:C	2.29	0.52
1:D:134:ARG:HA	1:D:308:GLY:O	2.10	0.52
2:V:89:GLU:O	2:V:92:LYS:NZ	2.35	0.52
2:V:113:ILE:HG13	2:V:114:SER:H	1.73	0.52
2:S:34:LEU:O	2:S:36:ASN:N	2.42	0.52
1:B:214:TRP:CD2	1:B:253:ARG:HG2	2.44	0.52
1:B:410:PRO:HD3	1:B:461:VAL:HG21	1.90	0.52
2:T:75:PHE:CD1	1:D:9:ALA:HB2	2.43	0.52
1:D:192:CYS:SG	1:D:413:ASN:ND2	2.83	0.52
1:A:155:ILE:HG12	1:A:375:LEU:CD1	2.38	0.52
1:B:335:LEU:HD21	1:C:127:PHE:CE1	2.45	0.52
1:B:466:VAL:HG23	1:B:468:ASN:N	2.25	0.52
1:D:190:TYR:HB2	1:D:224:ALA:HB1	1.92	0.52
1:A:397:ASP:OD2	2:S:108:ARG:NH2	2.43	0.52
2:S:27:LEU:O	2:S:31:GLU:HB2	2.10	0.52
1:B:32:LYS:O	1:B:35:ASP:HB2	2.10	0.52
2:T:22:SER:OG	2:T:25:GLN:HB2	2.09	0.52
1:C:214:TRP:CE3	1:C:253:ARG:HG2	2.45	0.52
1:C:227:LYS:HE2	2:V:66:TYR:O	2.10	0.52
1:A:50:PRO:HG3	1:A:97:TYR:CZ	2.45	0.52
1:A:241:ASN:ND2	1:A:243:THR:H	2.08	0.52
1:A:387:MET:HB3	1:A:388:PRO:HD3	1.92	0.52
2:T:77:CYS:SG	2:T:82:GLN:CD	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:HIS:N	1:C:324:ASP:OD1	2.41	0.52
1:D:10:SER:O	1:D:11:VAL:HB	2.09	0.52
2:S:56:ASN:ND2	2:S:58:SER:OG	2.42	0.52
1:C:94:LYS:O	1:C:95:ASP:C	2.49	0.52
1:C:449:CYS:HA	1:C:455:LEU:HG	1.92	0.52
1:D:19:GLU:HB3	1:D:52:GLU:CD	2.31	0.52
2:S:98:TRP:HD1	2:S:116:ILE:HD11	1.74	0.51
1:B:9:ALA:HB2	2:V:75:PHE:CE1	2.45	0.51
1:C:60:GLU:OE2	1:C:65:THR:HA	2.09	0.51
1:C:166:GLY:O	1:C:167:ARG:HB3	2.09	0.51
1:D:214:TRP:CE3	1:D:253:ARG:HG2	2.45	0.51
2:V:27:LEU:HD12	2:V:84:LEU:HD12	1.92	0.51
2:V:77:CYS:CB	2:V:82:GLN:OE1	2.58	0.51
1:C:153:HIS:CD2	1:C:290:LEU:HD23	2.45	0.51
1:C:178:LEU:HD21	1:C:205:ASN:ND2	2.26	0.51
1:D:181:SER:O	1:D:182:ALA:C	2.49	0.51
1:C:90:VAL:HG23	1:C:96:GLN:C	2.31	0.51
2:U:89:GLU:O	2:U:92:LYS:HB3	2.09	0.51
1:A:21:LYS:HB2	1:A:52:GLU:OE1	2.10	0.51
1:A:24:TYR:HB2	1:A:55:ALA:HB1	1.93	0.51
1:B:442:ASN:OD1	1:B:446:ARG:NH1	2.40	0.51
1:B:443:GLU:OE2	1:B:446:ARG:NE	2.42	0.51
2:T:23:GLN:O	2:T:27:LEU:HB2	2.09	0.51
1:C:269:TYR:CD1	1:C:293:ILE:HG21	2.46	0.51
2:S:26:LEU:C	2:S:26:LEU:HD23	2.31	0.51
1:B:93:GLU:OE1	1:B:93:GLU:HA	2.10	0.51
1:C:331:VAL:HG12	1:C:332:VAL:N	2.24	0.51
1:A:440:GLU:O	1:A:441:GLY:C	2.49	0.51
1:B:411:TRP:CH2	2:T:2:GLN:OE1	2.63	0.51
1:A:43:THR:HG22	1:A:131:ARG:CG	2.38	0.51
2:S:34:LEU:O	2:S:35:LYS:C	2.48	0.51
1:B:133:LEU:O	1:B:307:HIS:HA	2.11	0.51
1:D:209:GLN:HB3	1:D:210:PRO:HD2	1.93	0.51
1:D:459:CYS:O	1:D:463:LYS:HB2	2.11	0.51
2:U:35:LYS:HD2	2:U:35:LYS:O	2.11	0.51
1:D:446:ARG:HG3	1:D:446:ARG:O	2.11	0.51
2:V:25:GLN:O	2:V:28:SER:HB2	2.11	0.51
1:D:189:VAL:HG13	1:D:200:THR:OG1	2.10	0.51
1:D:269:TYR:CD1	1:D:293:ILE:CG2	2.94	0.51
2:V:86:GLU:O	2:V:89:GLU:HB3	2.11	0.51
1:A:412:GLY:HA3	2:T:72:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ALA:HA	1:D:320:MET:CE	2.41	0.50
1:D:385:TRP:HZ2	1:D:459:CYS:HB3	1.75	0.50
1:B:17:VAL:HG12	1:B:18:LYS:N	2.27	0.50
1:B:26:THR:HG22	1:B:26:THR:O	2.11	0.50
1:B:190:TYR:HB2	1:B:224:ALA:HB1	1.94	0.50
1:B:229:GLN:HE21	1:B:236:LYS:H	1.58	0.50
1:C:241:ASN:HD22	1:C:242:ALA:N	2.09	0.50
1:C:330:THR:O	1:C:331:VAL:HB	2.11	0.50
1:A:72:ASP:HB3	1:A:77:LEU:HD21	1.94	0.50
1:B:19:GLU:HB3	1:B:52:GLU:CD	2.31	0.50
1:B:363:TYR:HD1	1:B:363:TYR:H	1.57	0.50
1:B:422:VAL:O	1:B:423:ALA:C	2.48	0.50
2:U:11:LYS:HG3	2:U:17:TYR:HE1	1.73	0.50
1:D:299:ALA:HA	1:D:302:ASP:OD1	2.12	0.50
1:A:26:THR:HG22	1:A:29:TYR:CB	2.29	0.50
1:B:455:LEU:HD12	1:B:455:LEU:O	2.12	0.50
1:C:190:TYR:CE1	1:C:227:LYS:HD3	2.46	0.50
2:U:26:LEU:C	2:U:26:LEU:HD23	2.32	0.50
1:A:60:GLU:OE1	1:D:334:LYS:HE3	2.12	0.50
1:B:138:LEU:O	1:B:316:LYS:NZ	2.44	0.50
1:C:43:THR:HG22	1:C:43:THR:O	2.10	0.50
1:C:336:GLU:OE2	1:C:472:VAL:HB	2.12	0.50
1:D:9:ALA:N	1:D:73:GLY:O	2.45	0.50
2:V:83:VAL:O	2:V:86:GLU:HB2	2.12	0.50
1:B:436:ASP:OD1	1:B:436:ASP:C	2.50	0.50
2:T:12:TYR:HE2	2:T:98:TRP:NE1	2.10	0.50
1:C:304:GLN:NE2	1:C:304:GLN:CA	2.73	0.50
1:D:19:GLU:HB3	1:D:52:GLU:OE2	2.12	0.50
1:A:60:GLU:O	1:D:177:LYS:HE3	2.11	0.50
1:A:151:PRO:O	1:A:285:ARG:NH1	2.45	0.50
2:S:44:PHE:HA	2:S:98:TRP:O	2.11	0.50
1:B:127:PHE:CD1	1:C:335:LEU:HD23	2.47	0.50
1:B:436:ASP:OD1	1:B:438:ALA:N	2.44	0.50
1:C:9:ALA:N	1:C:73:GLY:O	2.45	0.50
1:C:345:PHE:HA	1:C:348:LEU:HB2	1.92	0.50
2:S:33:LEU:C	2:S:33:LEU:HD12	2.32	0.50
2:S:77:CYS:SG	2:S:78:THR:N	2.84	0.50
1:B:120:ILE:HG22	1:B:121:VAL:HG23	1.94	0.50
1:C:442:ASN:O	1:C:446:ARG:HB2	2.12	0.50
2:U:33:LEU:C	2:U:33:LEU:CD1	2.79	0.50
1:A:60:GLU:OE2	1:A:65:THR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:31:GLU:OE2	2:T:80:ALA:HB2	2.12	0.50
1:A:151:PRO:HB3	1:A:323:GLY:O	2.11	0.49
1:A:190:TYR:CZ	1:A:194:ARG:HD2	2.47	0.49
1:A:378:ALA:HB3	1:A:400:LEU:HD23	1.92	0.49
1:C:41:ARG:O	1:C:41:ARG:HG2	2.12	0.49
2:V:86:GLU:OE1	2:V:86:GLU:HA	2.12	0.49
1:A:181:SER:O	1:A:182:ALA:C	2.51	0.49
1:B:157:VAL:O	1:B:161:LYS:HG2	2.13	0.49
1:A:336:GLU:OE2	1:A:472:VAL:HB	2.12	0.49
1:C:194:ARG:NH2	2:U:4:TRP:O	2.39	0.49
2:U:72:LEU:HG	2:U:73:PRO:HD2	1.94	0.49
1:A:51:GLU:HA	1:A:87:ILE:HD11	1.95	0.49
1:A:127:PHE:HA	1:D:335:LEU:HD23	1.94	0.49
1:D:98:ILE:HG22	1:D:100:TYR:CE1	2.47	0.49
1:D:317:ALA:HA	1:D:320:MET:HE3	1.94	0.49
1:A:185:TYR:O	1:A:189:VAL:HG23	2.12	0.49
1:C:423:ALA:O	1:C:426:ALA:HB3	2.11	0.49
1:C:429:LYS:CE	2:U:29:GLU:OE1	2.61	0.49
1:D:207:ASN:O	1:D:217:ARG:NH2	2.30	0.49
2:V:26:LEU:O	2:V:29:GLU:HB2	2.12	0.49
2:V:56:ASN:HD21	2:V:58:SER:CB	2.25	0.49
2:V:79:ASP:CB	2:V:82:GLN:NE2	2.65	0.49
1:A:60:GLU:HG3	1:A:127:PHE:CZ	2.47	0.49
1:B:134:ARG:HA	1:B:308:GLY:O	2.12	0.49
1:B:332:VAL:CG1	1:B:386:HIS:ND1	2.73	0.49
1:C:43:THR:HG22	1:C:131:ARG:CG	2.40	0.49
1:D:26:THR:HG22	1:D:29:TYR:CB	2.34	0.49
1:D:29:TYR:CE2	1:D:31:THR:HA	2.48	0.49
2:V:23:GLN:O	2:V:27:LEU:HB2	2.13	0.49
1:A:298:HIS:CG	1:A:299:ALA:N	2.81	0.49
1:A:466:VAL:HG23	1:A:467:PHE:N	2.28	0.49
2:T:56:ASN:HD21	2:T:58:SER:CB	2.25	0.49
1:D:86:ARG:HG3	1:D:86:ARG:HH11	1.78	0.49
1:A:66:TRP:CE3	1:A:67:THR:HB	2.48	0.49
2:S:91:LYS:HD2	2:S:118:TYR:CD2	2.48	0.49
1:B:317:ALA:HA	1:B:320:MET:CE	2.43	0.49
1:C:142:PRO:HB3	1:C:369:VAL:HG11	1.94	0.49
1:D:455:LEU:O	1:D:458:ALA:HB3	2.13	0.49
1:A:142:PRO:HB3	1:A:369:VAL:HG11	1.94	0.49
1:A:190:TYR:HB2	1:A:224:ALA:HB1	1.95	0.49
1:B:190:TYR:CZ	1:B:227:LYS:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:O	1:D:167:ARG:HG3	2.12	0.49
1:D:193:LEU:CD1	1:D:200:THR:HG23	2.43	0.49
1:D:339:ARG:O	1:D:343:LEU:HG	2.12	0.49
1:A:118:THR:HG21	1:D:204:GLU:O	2.13	0.49
1:A:190:TYR:CE1	1:A:227:LYS:HD3	2.48	0.49
1:A:202:ASP:OD2	1:A:217:ARG:NH1	2.46	0.49
1:B:24:TYR:CD2	1:B:59:ALA:HB2	2.48	0.49
1:B:26:THR:CG2	1:B:29:TYR:HB2	2.38	0.49
1:B:42:VAL:HG13	1:B:97:TYR:HB2	1.95	0.49
1:B:251:ILE:O	1:B:255:VAL:HG23	2.13	0.49
1:D:60:GLU:OE2	1:D:65:THR:HA	2.13	0.49
1:D:331:VAL:HG21	1:D:339:ARG:HA	1.95	0.49
2:V:79:ASP:N	2:V:82:GLN:NE2	2.61	0.49
1:A:97:TYR:O	1:A:98:ILE:HD13	2.12	0.48
1:A:336:GLU:OE2	1:A:473:ASP:N	2.46	0.48
1:A:436:ASP:O	1:A:440:GLU:HB2	2.12	0.48
1:B:317:ALA:HA	1:B:320:MET:HE2	1.94	0.48
1:B:454:GLU:H	1:B:454:GLU:CD	2.16	0.48
2:V:33:LEU:HD22	2:V:113:ILE:HG21	1.94	0.48
1:A:223:GLU:OE1	2:T:65:ARG:HD3	2.12	0.48
1:A:368:TRP:O	1:A:369:VAL:C	2.49	0.48
1:A:61:SER:HB3	1:A:103:TYR:HE1	1.78	0.48
1:B:429:LYS:NZ	2:T:29:GLU:OE1	2.46	0.48
1:C:202:ASP:OD1	1:C:238:HIS:CE1	2.64	0.48
1:C:229:GLN:HE21	1:C:236:LYS:H	1.60	0.48
2:U:86:GLU:O	2:U:89:GLU:HB3	2.12	0.48
1:D:203:ASP:HA	5:D:492:FMT:O1	2.13	0.48
1:C:454:GLU:CD	1:C:454:GLU:N	2.66	0.48
1:D:42:VAL:HG23	1:D:130:LEU:HD22	1.95	0.48
2:V:11:LYS:HE3	2:V:17:TYR:CZ	2.48	0.48
1:A:153:HIS:CD2	1:A:290:LEU:HD23	2.48	0.48
1:A:414:ALA:O	1:A:417:ALA:HB3	2.13	0.48
1:A:462:TRP:O	1:A:465:ILE:HG12	2.13	0.48
1:B:295:ARG:O	1:B:298:HIS:HB3	2.14	0.48
1:A:97:TYR:C	1:A:98:ILE:HD13	2.33	0.48
1:B:177:LYS:HB2	1:C:63:THR:HA	1.95	0.48
1:B:192:CYS:HB3	1:B:197:LEU:HD23	1.96	0.48
1:D:23:THR:HB	1:D:24:TYR:CE1	2.49	0.48
1:A:162:LEU:O	1:A:164:LYS:HG3	2.13	0.48
1:A:339:ARG:O	1:A:343:LEU:HG	2.14	0.48
1:B:167:ARG:O	1:B:167:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:44:PHE:HA	2:T:98:TRP:O	2.14	0.48
1:D:387:MET:HB3	1:D:388:PRO:HD3	1.95	0.48
2:V:22:SER:H	2:V:25:GLN:NE2	1.98	0.48
1:B:86:ARG:NH1	1:B:86:ARG:HG3	2.29	0.48
1:B:331:VAL:HG12	1:B:332:VAL:N	2.29	0.48
1:D:202:ASP:OD2	1:D:217:ARG:NH1	2.46	0.48
2:S:77:CYS:SG	2:S:82:GLN:CD	2.92	0.48
1:B:48:VAL:HA	1:B:49:PRO:HD2	1.78	0.48
1:B:120:ILE:HD13	1:B:138:LEU:CD2	2.44	0.48
2:T:98:TRP:HD1	2:T:116:ILE:HD11	1.78	0.48
2:U:73:PRO:HG2	2:U:75:PHE:CE2	2.49	0.48
2:U:77:CYS:SG	2:U:78:THR:N	2.86	0.48
1:D:175:LYS:NZ	4:D:490:CAP:O1	2.41	0.48
1:A:90:VAL:HG23	1:A:97:TYR:HA	1.96	0.48
2:U:84:LEU:HD23	2:U:84:LEU:C	2.34	0.48
1:D:239:TYR:CE2	1:D:292:HIS:CD2	3.02	0.48
1:A:133:LEU:O	1:A:307:HIS:HA	2.14	0.47
1:B:94:LYS:O	1:B:95:ASP:C	2.50	0.47
1:C:445:ILE:HD12	1:C:449:CYS:SG	2.53	0.47
2:T:39:VAL:CG2	1:D:9:ALA:HB3	2.44	0.47
2:V:92:LYS:O	2:V:93:ALA:CB	2.62	0.47
1:C:389:ALA:O	1:C:392:GLU:HB3	2.13	0.47
1:B:43:THR:HG22	1:B:131:ARG:HG3	1.96	0.47
1:B:327:HIS:HA	1:B:377:VAL:HB	1.97	0.47
2:T:82:GLN:O	2:T:85:ALA:HB3	2.15	0.47
1:C:181:SER:HB2	1:D:156:GLN:NE2	2.23	0.47
1:C:414:ALA:O	1:C:417:ALA:HB3	2.14	0.47
1:D:19:GLU:HB3	1:D:52:GLU:OE1	2.13	0.47
1:D:50:PRO:HB2	1:D:87:ILE:HG21	1.96	0.47
1:A:158:GLU:OE2	1:A:325:HIS:NE2	2.29	0.47
1:A:332:VAL:HG13	1:A:332:VAL:O	2.14	0.47
1:D:41:ARG:NH1	1:D:96:GLN:OE1	2.44	0.47
1:B:440:GLU:O	1:B:441:GLY:C	2.52	0.47
1:C:52:GLU:O	1:C:55:ALA:N	2.48	0.47
1:C:154:GLY:N	1:C:324:ASP:OD1	2.45	0.47
1:D:425:GLU:OE1	2:V:17:TYR:N	2.43	0.47
1:D:429:LYS:CE	2:V:29:GLU:OE1	2.63	0.47
1:A:165:TYR:CD1	2:S:111:GLN:HB2	2.50	0.47
1:A:443:GLU:OE1	1:A:446:ARG:NH2	2.48	0.47
1:B:293:ILE:HG13	1:B:318:LEU:HD11	1.97	0.47
1:C:98:ILE:HG22	1:C:100:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ARG:NH2	2:V:111:GLN:OE1	2.39	0.47
1:C:190:TYR:HB2	1:C:224:ALA:HB1	1.95	0.47
1:C:363:TYR:CD1	1:C:363:TYR:N	2.82	0.47
1:C:411:TRP:O	1:C:415:PRO:HG2	2.15	0.47
2:U:106:ASN:OD1	2:U:106:ASN:C	2.52	0.47
1:D:43:THR:HG22	1:D:43:THR:O	2.13	0.47
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.98	0.47
1:D:410:PRO:HD3	1:D:461:VAL:HG21	1.97	0.47
1:A:71:THR:HA	1:A:74:LEU:HD22	1.97	0.47
1:A:93:GLU:HG2	1:A:96:GLN:OE1	2.15	0.47
1:A:295:ARG:HG3	1:A:298:HIS:CD2	2.49	0.47
2:S:2:GLN:OE1	2:S:2:GLN:N	2.47	0.47
1:C:151:PRO:HB3	1:C:323:GLY:O	2.14	0.47
1:C:204:GLU:HB3	1:C:294:HIS:CD2	2.50	0.47
1:B:382:ILE:HG13	1:B:402:PHE:CE1	2.49	0.47
1:C:298:HIS:ND1	1:C:302:ASP:OD2	2.38	0.47
1:C:436:ASP:OD1	1:C:436:ASP:C	2.53	0.47
1:D:97:TYR:C	1:D:98:ILE:HD13	2.34	0.47
1:D:167:ARG:H	1:D:396:ASP:HB3	1.80	0.47
1:A:121:VAL:HG22	1:A:125:PHE:CE1	2.50	0.47
1:A:60:GLU:OE1	1:A:127:PHE:HZ	1.97	0.46
1:A:101:VAL:CG1	1:A:102:ALA:N	2.78	0.46
2:T:12:TYR:CE2	2:T:98:TRP:NE1	2.83	0.46
2:T:77:CYS:SG	2:T:82:GLN:OE1	2.74	0.46
1:D:229:GLN:HE21	1:D:236:LYS:H	1.62	0.46
1:D:397:ASP:OD2	2:V:108:ARG:NH2	2.48	0.46
2:V:108:ARG:HB3	2:V:110:VAL:HG13	1.96	0.46
1:A:19:GLU:HB3	1:A:52:GLU:OE2	2.15	0.46
2:S:22:SER:H	2:S:25:GLN:NE2	2.04	0.46
1:B:239:TYR:HE2	1:B:292:HIS:CE1	2.33	0.46
1:B:239:TYR:CE2	1:B:292:HIS:CE1	3.03	0.46
1:B:418:VAL:O	1:B:419:ALA:C	2.52	0.46
1:C:385:TRP:HZ2	1:C:459:CYS:HB3	1.80	0.46
1:B:214:TRP:CE3	1:B:253:ARG:HG2	2.50	0.46
1:B:269:TYR:CD1	1:B:293:ILE:CG2	2.98	0.46
2:U:77:CYS:CB	2:U:82:GLN:OE1	2.61	0.46
1:D:407:LEU:HG	1:D:413:ASN:OD1	2.16	0.46
1:C:90:VAL:HG23	1:C:97:TYR:HA	1.98	0.46
1:C:105:LEU:O	1:C:107:LEU:N	2.48	0.46
1:C:291:LEU:HG	1:C:293:ILE:HD11	1.97	0.46
1:D:336:GLU:OE2	1:D:472:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:26:LEU:C	2:V:26:LEU:HD23	2.36	0.46
1:A:41:ARG:HA	1:A:97:TYR:O	2.15	0.46
1:B:90:VAL:HG23	1:B:97:TYR:HA	1.96	0.46
1:B:333:GLY:O	1:C:128:LYS:NZ	2.26	0.46
1:C:315:ALA:HB1	1:C:349:LEU:CD1	2.46	0.46
1:D:414:ALA:HB3	1:D:415:PRO:CD	2.35	0.46
2:S:19:PRO:O	2:S:20:ASP:C	2.53	0.46
2:S:42:LEU:HB3	2:S:70:TRP:HB3	1.98	0.46
1:B:50:PRO:HB2	1:B:87:ILE:HG21	1.97	0.46
1:B:59:ALA:C	1:B:61:SER:H	2.19	0.46
1:B:204:GLU:HB3	1:B:294:HIS:CD2	2.50	0.46
1:B:331:VAL:HG21	1:B:339:ARG:HA	1.96	0.46
1:B:387:MET:CB	1:B:388:PRO:CD	2.91	0.46
1:D:296:ALA:O	1:D:297:MET:HB3	2.15	0.46
1:D:376:PRO:O	1:D:376:PRO:HG2	2.14	0.46
2:V:101:ILE:O	2:V:114:SER:HA	2.15	0.46
1:B:178:LEU:HD22	1:B:205:ASN:HD21	1.79	0.46
1:C:134:ARG:HG3	1:C:135:LEU:N	2.27	0.46
1:C:425:GLU:OE1	2:U:17:TYR:N	2.47	0.46
1:A:331:VAL:HG12	1:A:332:VAL:N	2.31	0.46
1:A:429:LYS:HE2	2:S:29:GLU:OE1	2.15	0.46
1:A:466:VAL:HG23	1:A:468:ASN:N	2.31	0.46
1:B:381:GLY:HA2	1:C:66:TRP:NE1	2.31	0.46
2:T:33:LEU:HD22	2:T:113:ILE:HG21	1.97	0.46
1:C:388:PRO:HD3	1:C:445:ILE:HG21	1.97	0.46
1:D:436:ASP:OD1	1:D:436:ASP:C	2.53	0.46
2:V:105:ASP:HB2	2:V:112:CYS:SG	2.56	0.46
1:A:312:ARG:HH11	1:A:312:ARG:HD3	1.55	0.46
1:D:295:ARG:HD3	4:D:490:CAP:O6P	2.16	0.46
1:D:466:VAL:HG23	1:D:468:ASN:N	2.28	0.46
1:A:239:TYR:HB3	1:A:266:MET:HB2	1.98	0.46
2:S:84:LEU:HD23	2:S:84:LEU:C	2.36	0.46
1:B:283:TYR:CD1	1:B:283:TYR:C	2.88	0.46
1:B:463:LYS:HE2	1:B:463:LYS:HB3	1.44	0.46
1:D:41:ARG:HD3	1:D:96:GLN:OE1	2.15	0.46
1:A:57:VAL:O	1:A:61:SER:HB2	2.15	0.45
1:B:383:HIS:N	1:B:386:HIS:HD2	2.01	0.45
1:C:195:GLY:HA3	1:C:417:ALA:CB	2.41	0.45
1:D:192:CYS:HB3	1:D:197:LEU:HD23	1.97	0.45
1:A:244:ALA:HB1	1:A:249:GLU:HB3	1.98	0.45
1:A:269:TYR:CD1	1:A:293:ILE:CG2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:C	1:B:320:MET:N	2.66	0.45
1:C:463:LYS:HE2	1:C:463:LYS:HB3	1.39	0.45
2:T:79:ASP:HB3	2:T:82:GLN:HB3	1.98	0.45
1:C:203:ASP:HA	5:C:492:FMT:O1	2.16	0.45
1:C:455:LEU:O	1:C:458:ALA:HB3	2.16	0.45
2:U:79:ASP:O	2:U:80:ALA:C	2.54	0.45
1:D:153:HIS:CD2	1:D:290:LEU:HD23	2.50	0.45
1:A:120:ILE:HG22	1:A:121:VAL:HG23	1.99	0.45
1:B:200:THR:OG1	1:B:238:HIS:CD2	2.63	0.45
1:C:97:TYR:O	1:C:98:ILE:HD13	2.16	0.45
2:U:91:LYS:HD2	2:U:118:TYR:CD2	2.52	0.45
1:D:291:LEU:HG	1:D:293:ILE:HD11	1.98	0.45
1:C:363:TYR:N	1:C:363:TYR:HD1	2.14	0.45
1:D:151:PRO:HB3	1:D:323:GLY:O	2.16	0.45
1:B:20:TYR:CD2	1:B:56:ALA:HA	2.51	0.45
2:T:12:TYR:OH	2:T:123:TYR:HB3	2.16	0.45
2:T:69:MET:HE2	2:T:72:LEU:HD12	1.98	0.45
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.18	0.45
1:C:383:HIS:N	1:C:386:HIS:HD2	2.12	0.45
1:A:20:TYR:CD2	1:A:56:ALA:HA	2.51	0.45
1:B:429:LYS:CE	2:T:29:GLU:OE1	2.65	0.45
2:T:91:LYS:H	2:T:91:LYS:HG2	1.63	0.45
1:A:120:ILE:HD13	1:A:138:LEU:CD2	2.47	0.45
1:B:451:TRP:CH2	2:T:19:PRO:HD3	2.52	0.45
2:T:75:PHE:HE1	1:D:9:ALA:HB2	1.82	0.45
1:D:301:ILE:CG2	1:D:309:ILE:HB	2.46	0.45
1:D:313:VAL:O	1:D:314:LEU:C	2.55	0.45
1:C:183:LYS:O	2:V:66:TYR:OH	2.30	0.45
1:D:421:ARG:NH1	1:D:425:GLU:OE2	2.50	0.45
1:A:335:LEU:HD23	1:D:127:PHE:CD1	2.51	0.45
1:B:66:TRP:CZ3	1:B:67:THR:HB	2.51	0.45
1:B:215:ARG:HH11	1:B:215:ARG:HD2	1.34	0.45
1:B:455:LEU:O	1:B:458:ALA:HB3	2.17	0.45
1:C:190:TYR:CZ	1:C:194:ARG:HD2	2.52	0.45
2:U:2:GLN:OE1	2:U:2:GLN:N	2.50	0.45
2:U:68:THR:HG22	2:U:69:MET:O	2.17	0.45
1:D:169:LEU:HB2	1:D:399:VAL:HG22	1.99	0.45
2:U:44:PHE:HA	2:U:98:TRP:O	2.17	0.44
1:D:334:LYS:HB3	1:D:381:GLY:HA3	1.98	0.44
1:A:105:LEU:HA	1:A:105:LEU:HD12	1.79	0.44
1:A:407:LEU:HG	1:A:413:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ASP:OD1	1:A:436:ASP:C	2.55	0.44
4:A:490:CAP:O4	5:A:492:FMT:O2	2.35	0.44
1:B:66:TRP:CD1	1:C:381:GLY:HA2	2.53	0.44
1:B:76:SER:O	1:B:76:SER:OG	2.36	0.44
2:T:27:LEU:HD12	2:T:84:LEU:HD12	1.99	0.44
2:T:45:GLU:OE2	2:T:48:HIS:N	2.44	0.44
1:C:451:TRP:CH2	2:U:19:PRO:HD3	2.52	0.44
1:D:141:PRO:HA	1:D:142:PRO:HD3	1.87	0.44
1:A:239:TYR:CE2	1:A:292:HIS:CE1	3.05	0.44
1:A:318:LEU:C	1:A:320:MET:N	2.70	0.44
1:B:10:SER:OG	1:B:11:VAL:HG23	2.17	0.44
1:B:61:SER:HB3	1:B:103:TYR:HE1	1.82	0.44
1:B:239:TYR:CE2	1:B:292:HIS:CD2	3.06	0.44
1:B:264:ILE:HD13	1:B:264:ILE:HG21	1.52	0.44
2:U:12:TYR:OH	2:U:123:TYR:HB3	2.18	0.44
1:D:90:VAL:HG23	1:D:97:TYR:CA	2.48	0.44
1:D:165:TYR:CD1	2:V:111:GLN:HB2	2.52	0.44
1:D:194:ARG:NH2	2:V:4:TRP:O	2.45	0.44
1:D:387:MET:HE2	1:D:424:LEU:N	2.32	0.44
1:D:414:ALA:CB	1:D:415:PRO:HD3	2.34	0.44
4:D:490:CAP:O2	4:D:490:CAP:O4	2.33	0.44
1:A:157:VAL:O	1:A:161:LYS:HG2	2.18	0.44
1:A:387:MET:HG2	1:A:424:LEU:HA	1.99	0.44
1:B:421:ARG:HH11	1:B:421:ARG:HD2	1.58	0.44
1:C:204:GLU:HG3	1:C:294:HIS:CE1	2.53	0.44
1:D:452:SER:CB	1:D:455:LEU:HB3	2.35	0.44
1:B:45:GLN:OE1	1:B:131:ARG:HB3	2.18	0.44
1:C:387:MET:CB	1:C:388:PRO:CD	2.93	0.44
1:A:127:PHE:CE1	1:D:335:LEU:HD21	2.52	0.44
1:B:150:GLY:HA3	1:B:371:LEU:HD11	1.99	0.44
1:C:191:GLU:O	1:C:194:ARG:HG2	2.18	0.44
2:U:41:CYS:HB3	2:U:102:ILE:HD11	2.00	0.44
1:D:90:VAL:HG23	1:D:96:GLN:O	2.18	0.44
1:A:173:THR:HA	1:A:201:LYS:HG2	1.99	0.44
1:A:214:TRP:CD2	1:A:253:ARG:HG2	2.52	0.44
2:S:41:CYS:SG	2:S:42:LEU:N	2.90	0.44
1:B:118:THR:HG21	1:C:204:GLU:O	2.17	0.44
1:C:239:TYR:HB3	1:C:266:MET:HB2	2.00	0.44
1:A:214:TRP:CD2	1:A:215:ARG:N	2.86	0.44
1:B:291:LEU:HG	1:B:293:ILE:HD11	2.00	0.44
1:C:23:THR:CG2	1:C:81:LYS:HZ3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ASN:ND2	1:D:243:THR:H	2.16	0.44
1:D:318:LEU:HD22	1:D:326:ILE:HD12	2.00	0.44
1:A:177:LYS:HB2	1:D:63:THR:HA	2.00	0.44
1:B:239:TYR:CE2	1:B:292:HIS:CG	3.06	0.44
1:C:414:ALA:CB	1:C:415:PRO:HD3	2.37	0.44
2:U:84:LEU:O	2:U:87:VAL:HB	2.17	0.44
1:D:142:PRO:HB3	1:D:369:VAL:HG11	2.00	0.44
1:A:227:LYS:HE2	2:T:66:TYR:O	2.18	0.43
1:A:331:VAL:HG21	1:A:339:ARG:HA	2.00	0.43
1:B:52:GLU:O	1:B:53:ALA:C	2.56	0.43
1:B:101:VAL:HG12	1:B:102:ALA:N	2.32	0.43
1:B:127:PHE:CD1	1:C:335:LEU:CD2	3.01	0.43
1:B:138:LEU:HD12	1:B:313:VAL:HG13	1.99	0.43
1:B:382:ILE:HD12	1:B:390:LEU:HD13	1.99	0.43
1:C:10:SER:OG	1:C:11:VAL:HG23	2.17	0.43
1:C:101:VAL:HG12	1:C:102:ALA:N	2.33	0.43
1:C:310:HIS:CE1	1:C:312:ARG:CZ	3.00	0.43
2:U:56:ASN:ND2	2:U:58:SER:N	2.55	0.43
2:U:102:ILE:HG22	2:U:114:SER:HB2	2.00	0.43
1:D:63:THR:OG1	1:D:77:LEU:HD13	2.17	0.43
1:D:411:TRP:CH2	2:V:2:GLN:OE1	2.70	0.43
1:D:443:GLU:O	1:D:447:GLU:N	2.48	0.43
2:S:43:GLU:HA	2:S:68:THR:O	2.18	0.43
1:B:86:ARG:HG3	1:B:86:ARG:HH11	1.83	0.43
1:B:264:ILE:HG13	1:B:290:LEU:O	2.17	0.43
1:B:336:GLU:OE2	1:B:472:VAL:HB	2.18	0.43
2:T:101:ILE:O	2:T:114:SER:HA	2.17	0.43
2:U:79:ASP:N	2:U:82:GLN:NE2	2.64	0.43
1:D:151:PRO:O	1:D:285:ARG:NH1	2.51	0.43
1:D:311:PHE:O	1:D:312:ARG:C	2.55	0.43
1:D:443:GLU:OE2	1:D:446:ARG:NE	2.50	0.43
1:A:41:ARG:O	1:A:41:ARG:HG2	2.18	0.43
1:A:183:LYS:O	2:T:66:TYR:OH	2.33	0.43
2:S:58:SER:O	2:S:59:PRO:C	2.55	0.43
1:B:331:VAL:HA	1:B:337:GLY:O	2.18	0.43
1:B:343:LEU:HD21	1:B:393:ILE:HG23	2.00	0.43
1:D:440:GLU:O	1:D:441:GLY:C	2.56	0.43
2:V:44:PHE:HA	2:V:98:TRP:O	2.18	0.43
2:V:113:ILE:CG1	2:V:114:SER:N	2.81	0.43
1:B:97:TYR:C	1:B:98:ILE:HD13	2.38	0.43
2:T:39:VAL:HG21	1:D:9:ALA:HB3	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:79:ASP:H	2:T:82:GLN:HE22	1.64	0.43
1:C:23:THR:CG2	1:C:81:LYS:NZ	2.80	0.43
1:D:264:ILE:HG13	1:D:290:LEU:O	2.19	0.43
1:B:454:GLU:CD	1:B:454:GLU:N	2.72	0.43
2:T:29:GLU:HB3	2:T:115:PHE:CZ	2.53	0.43
2:U:10:LYS:HB3	2:U:50:PHE:CZ	2.53	0.43
2:U:11:LYS:HG3	2:U:17:TYR:CZ	2.53	0.43
1:B:24:TYR:CG	1:B:59:ALA:HB2	2.54	0.43
1:B:153:HIS:N	1:B:324:ASP:OD1	2.38	0.43
1:B:389:ALA:O	1:B:393:ILE:HG13	2.19	0.43
1:C:215:ARG:HH11	1:C:215:ARG:HD2	1.30	0.43
1:D:190:TYR:CZ	1:D:227:LYS:HD3	2.52	0.43
1:D:269:TYR:CD1	1:D:293:ILE:HG21	2.53	0.43
1:A:421:ARG:HH11	1:A:421:ARG:HD2	1.58	0.43
1:C:295:ARG:O	1:C:296:ALA:C	2.56	0.43
1:C:375:LEU:HD12	1:C:375:LEU:HA	1.80	0.43
2:U:41:CYS:HB2	2:U:104:PHE:HE2	1.82	0.43
1:D:383:HIS:N	1:D:386:HIS:CD2	2.71	0.43
1:D:463:LYS:HB3	1:D:463:LYS:HE2	1.40	0.43
2:V:30:VAL:O	2:V:34:LEU:HB2	2.19	0.43
1:A:298:HIS:ND1	1:A:302:ASP:OD2	2.35	0.43
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.72	0.43
2:S:86:GLU:O	2:S:89:GLU:HB3	2.18	0.43
1:D:86:ARG:HG3	1:D:86:ARG:NH1	2.34	0.43
1:D:387:MET:HB3	1:D:388:PRO:CD	2.48	0.43
2:V:103:GLY:HA3	2:V:113:ILE:HG22	2.00	0.43
1:A:410:PRO:HD3	1:A:461:VAL:HG21	2.01	0.43
1:B:29:TYR:CG	1:B:83:ARG:HD2	2.54	0.43
1:B:94:LYS:HB2	1:B:94:LYS:NZ	2.34	0.43
1:B:185:TYR:O	1:B:189:VAL:HG23	2.18	0.43
1:B:293:ILE:HA	1:B:293:ILE:HD13	1.79	0.43
1:C:42:VAL:HG23	1:C:130:LEU:HD22	2.00	0.43
1:C:167:ARG:HG2	2:U:14:THR:OG1	2.18	0.43
1:C:178:LEU:CD2	1:C:205:ASN:ND2	2.81	0.43
1:C:410:PRO:HD3	1:C:461:VAL:HG21	2.00	0.43
2:U:117:ALA:O	2:U:118:TYR:CB	2.60	0.43
1:D:193:LEU:HD13	1:D:200:THR:CG2	2.47	0.43
2:V:11:LYS:HE3	2:V:17:TYR:CE1	2.54	0.43
2:V:82:GLN:O	2:V:85:ALA:CB	2.59	0.43
2:V:98:TRP:HD1	2:V:116:ILE:CD1	2.32	0.43
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:HE2	1:A:463:LYS:HB3	1.36	0.43
1:B:190:TYR:O	1:B:194:ARG:HG2	2.19	0.43
1:C:36:ILE:N	1:C:36:ILE:HD12	2.34	0.43
1:C:44:PRO:O	1:C:131:ARG:HG2	2.19	0.43
2:U:15:LEU:C	2:U:17:TYR:H	2.22	0.43
1:D:163:ASN:HD22	1:D:163:ASN:HA	1.61	0.43
1:D:293:ILE:CG1	1:D:318:LEU:HD11	2.42	0.43
1:A:457:ALA:O	1:A:461:VAL:HG23	2.18	0.42
2:T:14:THR:HG22	2:T:15:LEU:HG	2.01	0.42
2:U:89:GLU:O	2:U:92:LYS:O	2.37	0.42
1:D:280:LEU:HA	1:D:280:LEU:HD12	1.81	0.42
1:D:336:GLU:OE2	1:D:473:ASP:N	2.52	0.42
2:V:42:LEU:HB3	2:V:70:TRP:HB3	2.01	0.42
1:A:268:ASP:HA	1:A:294:HIS:O	2.19	0.42
1:A:332:VAL:O	1:A:332:VAL:CG1	2.66	0.42
1:B:141:PRO:O	1:B:142:PRO:C	2.56	0.42
1:B:239:TYR:CD2	1:B:292:HIS:CD2	3.07	0.42
1:C:86:ARG:HG3	1:C:86:ARG:NH1	2.33	0.42
1:C:315:ALA:HB1	1:C:349:LEU:HD11	2.01	0.42
2:U:101:ILE:O	2:U:114:SER:HA	2.19	0.42
1:A:45:GLN:HA	1:A:46:PRO:HD2	1.78	0.42
2:S:98:TRP:CD1	2:S:116:ILE:HD11	2.54	0.42
1:B:112:SER:O	1:B:113:VAL:C	2.57	0.42
1:B:435:ARG:HD2	1:B:435:ARG:HH11	1.61	0.42
2:U:41:CYS:SG	2:U:42:LEU:N	2.92	0.42
2:U:79:ASP:HB3	2:U:82:GLN:HB3	2.01	0.42
2:V:29:GLU:HB3	2:V:115:PHE:CZ	2.53	0.42
2:V:43:GLU:OE2	2:V:100:ARG:NH1	2.45	0.42
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.34	0.42
1:B:106:ASP:O	1:C:210:PRO:HD2	2.19	0.42
1:B:190:TYR:CZ	1:B:194:ARG:HD2	2.55	0.42
2:T:33:LEU:HD22	2:T:113:ILE:CG2	2.49	0.42
1:D:264:ILE:HA	1:D:290:LEU:O	2.19	0.42
1:D:454:GLU:H	1:D:454:GLU:CD	2.23	0.42
1:A:425:GLU:OE1	2:S:17:TYR:N	2.47	0.42
1:B:73:GLY:HA3	2:V:75:PHE:CE1	2.55	0.42
1:B:94:LYS:O	1:B:96:GLN:N	2.52	0.42
1:C:234:GLU:O	1:C:235:ILE:C	2.58	0.42
1:C:295:ARG:CZ	1:C:298:HIS:CE1	3.03	0.42
2:U:1:MET:SD	2:V:71:LYS:HB3	2.59	0.42
1:D:293:ILE:CG2	1:D:318:LEU:HD11	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:113:ILE:O	2:V:114:SER:CB	2.66	0.42
1:A:318:LEU:HD22	1:A:326:ILE:HB	2.01	0.42
1:A:345:PHE:O	1:A:348:LEU:HB2	2.18	0.42
2:T:2:GLN:OE1	2:T:2:GLN:N	2.52	0.42
2:T:56:ASN:ND2	2:T:58:SER:OG	2.49	0.42
1:C:41:ARG:NH1	1:C:96:GLN:OE1	2.52	0.42
1:C:192:CYS:SG	1:C:413:ASN:ND2	2.93	0.42
1:D:443:GLU:O	1:D:447:GLU:HG3	2.19	0.42
1:A:292:HIS:NE2	1:A:327:HIS:NE2	2.68	0.42
1:A:318:LEU:HD22	1:A:326:ILE:HD12	2.00	0.42
2:S:3:VAL:HG22	2:T:71:LYS:H	1.84	0.42
1:B:85:TYR:O	1:B:86:ARG:HB3	2.19	0.42
1:C:442:ASN:O	1:C:446:ARG:CB	2.68	0.42
1:D:66:TRP:CE3	1:D:67:THR:HB	2.54	0.42
1:D:134:ARG:HG3	1:D:135:LEU:N	2.33	0.42
1:D:154:GLY:HA2	1:D:373:GLY:O	2.20	0.42
2:S:113:ILE:O	2:S:114:SER:HB2	2.20	0.42
1:B:89:ARG:HB2	1:B:89:ARG:NH1	2.25	0.42
2:T:84:LEU:HD23	2:T:84:LEU:O	2.20	0.42
1:C:150:GLY:HA3	1:C:371:LEU:HD11	2.01	0.42
1:D:167:ARG:HA	1:D:168:PRO:HD3	1.79	0.42
1:D:421:ARG:O	1:D:425:GLU:HG3	2.19	0.42
1:A:167:ARG:HG2	2:S:14:THR:OG1	2.20	0.42
2:S:26:LEU:O	2:S:29:GLU:HB2	2.20	0.42
1:B:9:ALA:N	1:B:73:GLY:O	2.53	0.42
1:C:151:PRO:O	1:C:285:ARG:NH1	2.53	0.42
1:C:190:TYR:CZ	1:C:227:LYS:HD3	2.55	0.42
1:C:357:ASP:C	1:C:359:SER:N	2.73	0.42
1:C:436:ASP:O	1:C:437:LEU:C	2.57	0.42
1:C:441:GLY:O	1:C:444:ILE:HB	2.19	0.42
1:D:239:TYR:HB3	1:D:266:MET:HB2	2.02	0.42
1:A:465:ILE:HG12	1:A:465:ILE:H	1.37	0.42
1:C:330:THR:HG21	1:C:382:ILE:HG23	2.01	0.42
1:A:17:VAL:C	1:A:18:LYS:HG3	2.39	0.41
1:A:68:THR:O	1:D:408:GLY:HA2	2.19	0.41
1:A:429:LYS:NZ	1:A:433:GLU:OE1	2.53	0.41
2:S:3:VAL:HG21	2:T:70:TRP:CE3	2.55	0.41
1:C:41:ARG:HH11	1:C:41:ARG:HD3	1.43	0.41
2:U:30:VAL:O	2:U:34:LEU:HD12	2.20	0.41
1:D:423:ALA:O	1:D:426:ALA:HB3	2.20	0.41
1:A:77:LEU:N	1:A:77:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.82	0.41
2:S:22:SER:OG	2:S:25:GLN:HB2	2.20	0.41
2:S:33:LEU:HD13	2:S:38:TRP:CB	2.45	0.41
1:B:225:LEU:HD12	1:B:225:LEU:C	2.40	0.41
1:B:229:GLN:HG3	1:B:234:GLU:O	2.20	0.41
1:B:411:TRP:CZ3	2:T:2:GLN:OE1	2.74	0.41
1:C:269:TYR:CD1	1:C:293:ILE:HG22	2.55	0.41
2:U:105:ASP:HB2	2:U:112:CYS:SG	2.59	0.41
1:D:409:HIS:HA	1:D:410:PRO:HD2	1.74	0.41
1:B:251:ILE:HD13	1:B:251:ILE:HA	1.73	0.41
1:C:440:GLU:O	1:C:441:GLY:C	2.59	0.41
1:A:304:GLN:NE2	1:A:304:GLN:HA	2.35	0.41
1:B:295:ARG:HG3	1:B:298:HIS:CD2	2.55	0.41
1:C:27:PRO:HD2	1:C:28:GLU:OE2	2.20	0.41
1:C:452:SER:HA	1:C:453:PRO:HD3	1.91	0.41
2:U:3:VAL:HG21	2:V:70:TRP:CZ3	2.55	0.41
1:D:465:ILE:H	1:D:465:ILE:HG12	1.67	0.41
2:V:96:GLN:OE1	2:V:96:GLN:N	2.41	0.41
2:S:101:ILE:HG13	2:S:117:ALA:HB2	2.01	0.41
1:B:407:LEU:HG	1:B:413:ASN:OD1	2.20	0.41
1:C:45:GLN:HA	1:C:46:PRO:HD2	1.80	0.41
1:C:436:ASP:CG	1:C:439:GLN:H	2.23	0.41
1:D:360:ARG:HE	1:D:360:ARG:HB2	1.59	0.41
1:D:363:TYR:N	1:D:363:TYR:CD1	2.89	0.41
2:V:55:ASN:N	2:V:63:ASP:OD2	2.45	0.41
1:A:24:TYR:CD2	1:A:59:ALA:HB2	2.55	0.41
1:A:304:GLN:HA	1:A:304:GLN:HE21	1.84	0.41
1:A:363:TYR:CD1	1:A:363:TYR:N	2.88	0.41
1:A:435:ARG:HH22	1:A:447:GLU:CD	2.24	0.41
1:A:451:TRP:CH2	2:S:19:PRO:HD3	2.56	0.41
2:U:30:VAL:HG11	2:U:83:VAL:HG22	2.01	0.41
2:U:113:ILE:CG1	2:U:114:SER:N	2.83	0.41
1:D:382:ILE:HG13	1:D:402:PHE:CE1	2.56	0.41
2:V:19:PRO:O	2:V:20:ASP:C	2.58	0.41
2:S:29:GLU:HB3	2:S:115:PHE:CZ	2.56	0.41
1:C:312:ARG:HH11	1:C:312:ARG:HD3	1.55	0.41
1:C:397:ASP:OD2	2:U:108:ARG:NH2	2.53	0.41
1:C:449:CYS:HB3	1:C:456:ALA:HA	2.01	0.41
2:U:35:LYS:NZ	2:U:36:ASN:ND2	2.69	0.41
1:D:442:ASN:O	1:D:446:ARG:HB2	2.20	0.41
1:A:128:LYS:HD2	1:D:333:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HD13	1:A:264:ILE:HG21	1.88	0.41
1:A:335:LEU:HD21	1:D:127:PHE:CE1	2.55	0.41
1:A:387:MET:N	1:A:388:PRO:HD2	2.36	0.41
1:C:71:THR:HA	1:C:74:LEU:HD22	2.02	0.41
1:C:181:SER:O	1:C:182:ALA:C	2.59	0.41
1:D:388:PRO:HD3	1:D:445:ILE:HG21	2.03	0.41
1:A:171:GLY:O	1:A:401:GLN:HA	2.21	0.41
1:B:17:VAL:O	1:B:18:LYS:HG3	2.21	0.41
1:B:105:LEU:O	1:B:107:LEU:N	2.54	0.41
1:B:213:ARG:HH11	1:B:213:ARG:HD2	1.60	0.41
1:B:447:GLU:O	1:B:450:LYS:HB2	2.21	0.41
2:T:98:TRP:HD1	2:T:116:ILE:CD1	2.34	0.41
1:C:192:CYS:HB2	1:C:200:THR:HG21	2.03	0.41
1:C:201:LYS:HG3	1:C:202:ASP:O	2.21	0.41
1:C:310:HIS:ND1	1:C:312:ARG:CZ	2.84	0.41
1:C:388:PRO:O	1:C:392:GLU:HB2	2.21	0.41
2:U:11:LYS:HE3	2:U:17:TYR:CZ	2.56	0.41
2:U:13:GLU:HB3	2:U:14:THR:H	1.67	0.41
2:U:119:LYS:HD2	2:U:123:TYR:OXT	2.20	0.41
1:D:431:ARG:HG3	1:D:437:LEU:CD2	2.51	0.41
1:A:239:TYR:HE2	1:A:292:HIS:CE1	2.39	0.41
1:B:171:GLY:HA2	1:B:199:PHE:O	2.20	0.41
2:T:11:LYS:HG3	2:T:17:TYR:CZ	2.56	0.41
1:C:200:THR:OG1	1:C:238:HIS:HD2	2.04	0.41
2:U:15:LEU:O	2:U:17:TYR:N	2.54	0.41
1:D:215:ARG:HH11	1:D:215:ARG:HD2	1.66	0.41
1:D:304:GLN:NE2	1:D:304:GLN:CA	2.84	0.41
1:D:451:TRP:CZ2	2:V:19:PRO:HD3	2.56	0.41
1:B:121:VAL:HG13	1:C:300:VAL:HG21	2.01	0.40
2:T:33:LEU:HD12	2:T:33:LEU:C	2.41	0.40
1:C:283:TYR:CD2	1:C:283:TYR:C	2.94	0.40
1:C:371:LEU:HD12	1:C:371:LEU:HA	1.94	0.40
1:D:343:LEU:HD23	1:D:343:LEU:HA	1.70	0.40
1:A:440:GLU:O	1:A:441:GLY:O	2.39	0.40
1:B:26:THR:C	1:B:28:GLU:H	2.24	0.40
1:C:51:GLU:HA	1:C:87:ILE:CD1	2.48	0.40
1:D:152:PRO:O	1:D:285:ARG:NH1	2.51	0.40
1:A:173:THR:HG21	4:A:490:CAP:O2	2.21	0.40
1:B:9:ALA:HB2	2:V:75:PHE:CD1	2.56	0.40
1:A:48:VAL:HA	1:A:49:PRO:HD2	1.71	0.40
1:A:152:PRO:HA	1:A:285:ARG:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ALA:HA	1:A:451:TRP:HD1	1.82	0.40
2:S:105:ASP:OD2	2:S:108:ARG:HD3	2.21	0.40
1:B:51:GLU:HA	1:B:87:ILE:CD1	2.51	0.40
1:B:105:LEU:HA	1:B:105:LEU:HD12	1.75	0.40
1:B:163:ASN:HD22	1:B:163:ASN:HA	1.53	0.40
1:B:165:TYR:CD1	2:T:111:GLN:HB2	2.56	0.40
1:B:429:LYS:HE2	2:T:29:GLU:OE1	2.22	0.40
1:C:146:LYS:HA	1:C:146:LYS:HD2	1.83	0.40
2:U:53:ARG:HD3	2:U:57:LYS:HG2	2.03	0.40
2:V:107:VAL:O	2:V:107:VAL:HG12	2.21	0.40
1:A:17:VAL:HG21	1:D:465:ILE:HD12	2.03	0.40
1:A:157:VAL:HA	1:A:160:ASP:HB2	2.04	0.40
2:S:14:THR:HG22	2:S:15:LEU:HG	2.04	0.40
1:C:357:ASP:OD2	1:C:360:ARG:HB2	2.21	0.40
1:C:368:TRP:O	1:C:369:VAL:C	2.59	0.40
1:C:466:VAL:HG23	1:C:468:ASN:N	2.37	0.40
1:D:86:ARG:HH11	1:D:86:ARG:CG	2.33	0.40
1:D:305:LYS:O	1:D:305:LYS:CG	2.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:NH2	1:C:30:GLN:NE2[3_654]	2.00	0.20

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	463/477 (97%)	402 (87%)	48 (10%)	13 (3%)	5 11
1	B	463/477 (97%)	399 (86%)	52 (11%)	12 (3%)	5 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	463/477 (97%)	388 (84%)	63 (14%)	12 (3%)	5 13
1	D	463/477 (97%)	400 (86%)	52 (11%)	11 (2%)	6 15
2	S	121/123 (98%)	104 (86%)	14 (12%)	3 (2%)	5 14
2	T	121/123 (98%)	102 (84%)	17 (14%)	2 (2%)	9 23
2	U	121/123 (98%)	99 (82%)	19 (16%)	3 (2%)	5 14
2	V	121/123 (98%)	100 (83%)	19 (16%)	2 (2%)	9 23
All	All	2336/2400 (97%)	1994 (85%)	284 (12%)	58 (2%)	5 14

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	95	ASP
1	A	167	ARG
2	S	93	ALA
1	B	46	PRO
1	B	95	ASP
1	B	167	ARG
2	T	93	ALA
1	C	46	PRO
1	C	95	ASP
1	C	167	ARG
2	U	93	ALA
1	D	46	PRO
1	D	95	ASP
1	D	167	ARG
2	V	93	ALA
1	A	106	ASP
1	A	441	GLY
1	A	442	ASN
1	B	10	SER
1	B	106	ASP
1	B	441	GLY
1	B	442	ASN
1	C	86	ARG
1	C	106	ASP
1	C	441	GLY
1	C	442	ASN
2	U	16	SER
1	D	369	VAL

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Mol	Chain	Res	Type
1	D	441	GLY
1	D	442	ASN
1	A	86	ARG
1	B	86	ARG
2	T	76	GLY
2	U	76	GLY
1	D	10	SER
1	D	86	ARG
1	A	10	SER
2	S	35	LYS
2	S	76	GLY
1	B	21	LYS
1	C	10	SER
1	A	11	VAL
1	B	11	VAL
1	B	369	VAL
1	C	11	VAL
1	C	384	VAL
1	C	385	TRP
1	D	11	VAL
1	D	166	GLY
2	V	16	SER
1	A	155	ILE
1	D	384	VAL
1	A	384	VAL
1	B	384	VAL
1	A	403	GLY
1	C	369	VAL
1	A	369	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	373/386 (97%)	326 (87%)	47 (13%)	4 10
1	B	373/386 (97%)	321 (86%)	52 (14%)	3 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	373/386 (97%)	322 (86%)	51 (14%)	3 8
1	D	373/386 (97%)	325 (87%)	48 (13%)	4 10
2	S	109/109 (100%)	94 (86%)	15 (14%)	3 8
2	T	109/109 (100%)	93 (85%)	16 (15%)	3 7
2	U	109/109 (100%)	91 (84%)	18 (16%)	2 5
2	V	109/109 (100%)	90 (83%)	19 (17%)	2 5
All	All	1928/1980 (97%)	1662 (86%)	266 (14%)	3 8

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	23	THR
1	A	46	PRO
1	A	51	GLU
1	A	61	SER
1	A	74	LEU
1	A	77	LEU
1	A	79	ARG
1	A	89	ARG
1	A	94	LYS
1	A	131	ARG
1	A	134	ARG
1	A	139	ARG
1	A	142	PRO
1	A	152	PRO
1	A	163	ASN
1	A	169	LEU
1	A	172	CYS
1	A	178	LEU
1	A	193	LEU
1	A	194	ARG
1	A	197	LEU
1	A	201	LYS
1	A	203	ASP
1	A	213	ARG
1	A	215	ARG
1	A	241	ASN
1	A	258	ARG
1	A	285	ARG

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Mol	Chain	Res	Type
1	A	295	ARG
1	A	312	ARG
1	A	314	LEU
1	A	318	LEU
1	A	319	ARG
1	A	338	GLU
1	A	349	LEU
1	A	356	GLN
1	A	363	TYR
1	A	379	SER
1	A	384	VAL
1	A	421	ARG
1	A	429	LYS
1	A	433	GLU
1	A	437	LEU
1	A	442	ASN
1	A	445	ILE
1	A	466	VAL
2	S	2	GLN
2	S	6	PRO
2	S	27	LEU
2	S	29	GLU
2	S	33	LEU
2	S	35	LYS
2	S	54	GLU
2	S	77	CYS
2	S	78	THR
2	S	81	THR
2	S	82	GLN
2	S	91	LYS
2	S	92	LYS
2	S	96	GLN
2	S	110	VAL
1	B	10	SER
1	B	13	PHE
1	B	45	GLN
1	B	46	PRO
1	B	61	SER
1	B	74	LEU
1	B	77	LEU
1	B	79	ARG
1	B	89	ARG

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Mol	Chain	Res	Type
1	B	93	GLU
1	B	94	LYS
1	B	131	ARG
1	B	134	ARG
1	B	139	ARG
1	B	163	ASN
1	B	169	LEU
1	B	172	CYS
1	B	178	LEU
1	B	185	TYR
1	B	193	LEU
1	B	194	ARG
1	B	197	LEU
1	B	201	LYS
1	B	203	ASP
1	B	213	ARG
1	B	215	ARG
1	B	225	LEU
1	B	239	TYR
1	B	241	ASN
1	B	285	ARG
1	B	295	ARG
1	B	304	GLN
1	B	312	ARG
1	B	314	LEU
1	B	318	LEU
1	B	319	ARG
1	B	335	LEU
1	B	338	GLU
1	B	349	LEU
1	B	356	GLN
1	B	359	SER
1	B	363	TYR
1	B	384	VAL
1	B	421	ARG
1	B	429	LYS
1	B	433	GLU
1	B	437	LEU
1	B	442	ASN
1	B	445	ILE
1	B	464	GLU
1	B	465	ILE

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Mol	Chain	Res	Type
1	B	466	VAL
2	T	2	GLN
2	T	27	LEU
2	T	28	SER
2	T	29	GLU
2	T	33	LEU
2	T	35	LYS
2	T	42	LEU
2	T	65	ARG
2	T	72	LEU
2	T	77	CYS
2	T	78	THR
2	T	81	THR
2	T	82	GLN
2	T	91	LYS
2	T	92	LYS
2	T	96	GLN
1	C	10	SER
1	C	23	THR
1	C	32	LYS
1	C	45	GLN
1	C	46	PRO
1	C	61	SER
1	C	74	LEU
1	C	76	SER
1	C	77	LEU
1	C	79	ARG
1	C	89	ARG
1	C	93	GLU
1	C	94	LYS
1	C	131	ARG
1	C	134	ARG
1	C	139	ARG
1	C	142	PRO
1	C	163	ASN
1	C	169	LEU
1	C	172	CYS
1	C	178	LEU
1	C	193	LEU
1	C	197	LEU
1	C	200	THR
1	C	201	LYS

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Mol	Chain	Res	Type
1	C	203	ASP
1	C	213	ARG
1	C	215	ARG
1	C	241	ASN
1	C	285	ARG
1	C	295	ARG
1	C	312	ARG
1	C	314	LEU
1	C	318	LEU
1	C	319	ARG
1	C	331	VAL
1	C	338	GLU
1	C	349	LEU
1	C	356	GLN
1	C	357	ASP
1	C	363	TYR
1	C	379	SER
1	C	384	VAL
1	C	421	ARG
1	C	429	LYS
1	C	437	LEU
1	C	442	ASN
1	C	445	ILE
1	C	464	GLU
1	C	465	ILE
1	C	466	VAL
2	U	2	GLN
2	U	6	PRO
2	U	23	GLN
2	U	27	LEU
2	U	28	SER
2	U	29	GLU
2	U	33	LEU
2	U	35	LYS
2	U	42	LEU
2	U	74	MET
2	U	77	CYS
2	U	78	THR
2	U	81	THR
2	U	82	GLN
2	U	91	LYS
2	U	92	LYS

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Mol	Chain	Res	Type
2	U	96	GLN
2	U	110	VAL
1	D	10	SER
1	D	13	PHE
1	D	23	THR
1	D	37	LEU
1	D	45	GLN
1	D	46	PRO
1	D	61	SER
1	D	74	LEU
1	D	77	LEU
1	D	79	ARG
1	D	89	ARG
1	D	94	LYS
1	D	121	VAL
1	D	127	PHE
1	D	131	ARG
1	D	134	ARG
1	D	139	ARG
1	D	163	ASN
1	D	169	LEU
1	D	172	CYS
1	D	178	LEU
1	D	180	LEU
1	D	193	LEU
1	D	197	LEU
1	D	201	LYS
1	D	213	ARG
1	D	215	ARG
1	D	225	LEU
1	D	241	ASN
1	D	285	ARG
1	D	295	ARG
1	D	298	HIS
1	D	312	ARG
1	D	314	LEU
1	D	319	ARG
1	D	338	GLU
1	D	349	LEU
1	D	356	GLN
1	D	379	SER
1	D	384	VAL

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Mol	Chain	Res	Type
1	D	421	ARG
1	D	429	LYS
1	D	433	GLU
1	D	437	LEU
1	D	442	ASN
1	D	445	ILE
1	D	465	ILE
1	D	466	VAL
2	V	2	GLN
2	V	6	PRO
2	V	23	GLN
2	V	27	LEU
2	V	29	GLU
2	V	33	LEU
2	V	35	LYS
2	V	52	TYR
2	V	65	ARG
2	V	77	CYS
2	V	78	THR
2	V	81	THR
2	V	82	GLN
2	V	91	LYS
2	V	92	LYS
2	V	96	GLN
2	V	100	ARG
2	V	110	VAL
2	V	121	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	163	ASN
1	A	238	HIS
1	A	241	ASN
1	A	304	GLN
1	A	356	GLN
2	S	25	GLN
2	S	36	ASN
2	S	55	ASN
2	S	56	ASN
2	S	82	GLN

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Mol	Chain	Res	Type
2	S	111	GLN
1	B	153	HIS
1	B	156	GLN
1	B	163	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	304	GLN
1	B	356	GLN
1	B	420	ASN
1	B	439	GLN
2	T	23	GLN
2	T	25	GLN
2	T	36	ASN
2	T	56	ASN
2	T	82	GLN
1	C	163	ASN
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	304	GLN
1	C	356	GLN
1	C	420	ASN
2	U	25	GLN
2	U	36	ASN
2	U	55	ASN
2	U	56	ASN
2	U	82	GLN
2	U	111	GLN
1	D	156	GLN
1	D	163	ASN
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	304	GLN
1	D	386	HIS
1	D	420	ASN
2	V	23	GLN
2	V	25	GLN
2	V	36	ASN
2	V	56	ASN
2	V	82	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FMT	B	492	3,1	2,2,2	0.46	0	1,1,1	0.27	0
4	CAP	D	490	3	17,20,20	1.85	4 (23%)	22,31,31	5.42	12 (54%)
5	FMT	A	492	3,1	2,2,2	0.78	0	1,1,1	1.51	0
4	CAP	C	490	3	17,20,20	2.44	9 (52%)	22,31,31	6.52	13 (59%)
5	FMT	C	492	3,1	2,2,2	1.30	0	1,1,1	0.67	0
4	CAP	B	490	3	17,20,20	3.07	7 (41%)	22,31,31	5.53	12 (54%)
4	CAP	A	490	3	17,20,20	2.93	10 (58%)	22,31,31	5.14	12 (54%)
5	FMT	D	492	3,1	2,2,2	1.11	0	1,1,1	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	A	490	3	-	16/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	B	490	3	-	17/29/29/29	-
4	CAP	C	490	3	-	12/29/29/29	-
4	CAP	D	490	3	-	13/29/29/29	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	490	CAP	C5-C4	-7.22	1.41	1.51
4	A	490	CAP	C4-C3	-6.23	1.48	1.54
4	C	490	CAP	C4-C3	-5.96	1.48	1.54
4	B	490	CAP	O2-C2	-4.80	1.32	1.42
4	B	490	CAP	P1-O1P	4.47	1.65	1.50
4	A	490	CAP	O2-C2	-4.32	1.33	1.42
4	B	490	CAP	C4-C3	-4.18	1.50	1.54
4	D	490	CAP	P1-O1P	4.14	1.63	1.50
4	A	490	CAP	P1-O1P	4.11	1.63	1.50
4	A	490	CAP	C5-C4	-3.75	1.46	1.51
4	B	490	CAP	O5-C5	-3.67	1.30	1.44
4	B	490	CAP	O3-C3	-3.31	1.36	1.42
4	D	490	CAP	O2-C2	-3.25	1.36	1.42
4	A	490	CAP	P2-O5P	3.09	1.66	1.54
4	C	490	CAP	P1-O1P	3.03	1.60	1.50
4	D	490	CAP	P2-O5P	2.96	1.66	1.54
4	C	490	CAP	O2-C2	-2.80	1.37	1.42
4	C	490	CAP	C5-C4	-2.76	1.47	1.51
4	D	490	CAP	O5-C5	-2.73	1.34	1.44
4	A	490	CAP	O1-C1	-2.70	1.35	1.43
4	A	490	CAP	O5-C5	-2.69	1.34	1.44
4	C	490	CAP	O5-C5	-2.69	1.34	1.44
4	A	490	CAP	P1-O3P	-2.60	1.44	1.54
4	C	490	CAP	P1-O2P	-2.53	1.45	1.54
4	A	490	CAP	P1-O2P	-2.53	1.45	1.54
4	C	490	CAP	P2-O4P	-2.47	1.42	1.50
4	C	490	CAP	P2-O5P	2.37	1.64	1.54
4	B	490	CAP	P2-O5P	2.25	1.63	1.54
4	A	490	CAP	O7-C	-2.23	1.22	1.30
4	C	490	CAP	O7-C	-2.17	1.22	1.30

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	490	CAP	O3-C3-C4	-15.43	76.08	109.13
4	C	490	CAP	C5-C4-C3	-14.67	81.95	111.94
4	C	490	CAP	O2-C2-C	-14.36	82.72	108.97
4	D	490	CAP	C5-C4-C3	-13.08	85.20	111.94
4	A	490	CAP	O2-C2-C	-12.84	85.51	108.97
4	B	490	CAP	O3-C3-C4	-11.88	83.68	109.13
4	B	490	CAP	C5-C4-C3	-11.73	87.95	111.94
4	A	490	CAP	C5-C4-C3	-11.47	88.49	111.94
4	D	490	CAP	O3-C3-C4	-11.25	85.02	109.13
4	B	490	CAP	O2-C2-C	-11.03	88.81	108.97
4	D	490	CAP	P2-O5-C5	10.80	148.05	118.30
4	C	490	CAP	P2-O5-C5	10.56	147.39	118.30
4	A	490	CAP	O3-C3-C4	-9.62	88.52	109.13
4	B	490	CAP	P2-O5-C5	9.05	143.22	118.30
4	D	490	CAP	O2-C2-C	-8.92	92.68	108.97
4	A	490	CAP	P2-O5-C5	8.14	140.73	118.30
4	B	490	CAP	O4-C4-C5	7.95	127.78	109.92
4	D	490	CAP	O4-C4-C5	7.34	126.42	109.92
4	C	490	CAP	O4-C4-C5	6.88	125.39	109.92
4	C	490	CAP	O4-C4-C3	-6.32	96.16	108.78
4	B	490	CAP	O4-C4-C3	-6.22	96.35	108.78
4	A	490	CAP	O4-C4-C5	6.06	123.53	109.92
4	A	490	CAP	O3P-P1-O2P	5.60	129.05	107.64
4	D	490	CAP	O4-C4-C3	-5.07	98.65	108.78
4	B	490	CAP	P1-O1-C1	-4.83	104.98	118.30
4	B	490	CAP	O3P-P1-O2P	4.49	124.79	107.64
4	C	490	CAP	O3P-P1-O1	-4.48	94.82	106.73
4	C	490	CAP	O6P-P2-O5P	-3.89	92.75	107.64
4	D	490	CAP	P1-O1-C1	-3.85	107.70	118.30
4	D	490	CAP	O3P-P1-O2P	3.71	121.83	107.64
4	B	490	CAP	O6P-P2-O4P	3.36	123.85	110.68
4	C	490	CAP	P1-O1-C1	-3.36	109.03	118.30
4	A	490	CAP	O6P-P2-O4P	3.30	123.59	110.68
4	D	490	CAP	O6P-P2-O5P	-3.18	95.49	107.64
4	A	490	CAP	P1-O1-C1	-2.88	110.35	118.30
4	C	490	CAP	O3P-P1-O2P	2.87	118.59	107.64
4	D	490	CAP	O2P-P1-O1	-2.82	99.23	106.73
4	A	490	CAP	O4-C4-C3	-2.82	103.15	108.78
4	B	490	CAP	O5-C5-C4	2.80	116.84	109.36
4	D	490	CAP	O6P-P2-O4P	2.61	120.91	110.68
4	C	490	CAP	O5P-P2-O4P	2.60	120.87	110.68
4	A	490	CAP	O5P-P2-O4P	-2.54	100.73	110.68
4	A	490	CAP	O6P-P2-O5	-2.50	100.07	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	490	CAP	O5-P2-O4P	2.50	113.48	106.47
4	C	490	CAP	O2P-P1-O1P	2.24	119.46	110.68
4	D	490	CAP	O7-C-O6	-2.22	116.74	123.82
4	B	490	CAP	O6P-P2-O5P	-2.19	99.26	107.64
4	B	490	CAP	O3P-P1-O1	-2.19	100.91	106.73
4	C	490	CAP	O5-P2-O4P	2.03	112.17	106.47

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	490	CAP	C1-C2-C3-O3
4	A	490	CAP	O2-C2-C3-C4
4	A	490	CAP	O2-C2-C3-O3
4	A	490	CAP	O6-C-C2-O2
4	A	490	CAP	C2-C3-C4-C5
4	A	490	CAP	C2-C3-C4-O4
4	A	490	CAP	O3-C3-C4-O4
4	A	490	CAP	O4-C4-C5-O5
4	B	490	CAP	O1-C1-C2-C
4	B	490	CAP	C1-C2-C3-C4
4	B	490	CAP	O2-C2-C3-C4
4	B	490	CAP	O2-C2-C3-O3
4	B	490	CAP	O6-C-C2-C3
4	B	490	CAP	C2-C3-C4-O4
4	B	490	CAP	O3-C3-C4-O4
4	B	490	CAP	O4-C4-C5-O5
4	B	490	CAP	C5-O5-P2-O4P
4	B	490	CAP	C5-O5-P2-O5P
4	B	490	CAP	C5-O5-P2-O6P
4	C	490	CAP	C1-C2-C3-C4
4	C	490	CAP	O2-C2-C3-C4
4	C	490	CAP	C2-C3-C4-C5
4	C	490	CAP	C2-C3-C4-O4
4	C	490	CAP	O3-C3-C4-O4
4	C	490	CAP	O4-C4-C5-O5
4	C	490	CAP	C4-C5-O5-P2
4	C	490	CAP	C5-O5-P2-O5P
4	D	490	CAP	C1-C2-C3-C4
4	D	490	CAP	C1-C2-C3-O3
4	D	490	CAP	O2-C2-C3-C4
4	D	490	CAP	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	490	CAP	C2-C3-C4-O4
4	D	490	CAP	O3-C3-C4-O4
4	D	490	CAP	C3-C4-C5-O5
4	D	490	CAP	O4-C4-C5-O5
4	D	490	CAP	C5-O5-P2-O5P
4	A	490	CAP	C4-C5-O5-P2
4	B	490	CAP	C4-C5-O5-P2
4	D	490	CAP	C4-C5-O5-P2
4	A	490	CAP	C3-C4-C5-O5
4	B	490	CAP	C3-C4-C5-O5
4	C	490	CAP	C3-C4-C5-O5
4	A	490	CAP	O7-C-C2-O2
4	C	490	CAP	C5-O5-P2-O6P
4	C	490	CAP	O3-C3-C4-C5
4	A	490	CAP	O6-C-C2-C1
4	A	490	CAP	O7-C-C2-C1
4	B	490	CAP	O1-C1-C2-C3
4	B	490	CAP	C1-C2-C3-O3
4	B	490	CAP	C2-C3-C4-C5
4	D	490	CAP	C2-C3-C4-C5
4	A	490	CAP	C5-O5-P2-O6P
4	C	490	CAP	O6-C-C2-O2
4	D	490	CAP	O6-C-C2-C3
4	A	490	CAP	C5-O5-P2-O4P
4	A	490	CAP	O3-C3-C4-C5
4	B	490	CAP	O3-C3-C4-C5
4	D	490	CAP	O3-C3-C4-C5

There are no ring outliers.

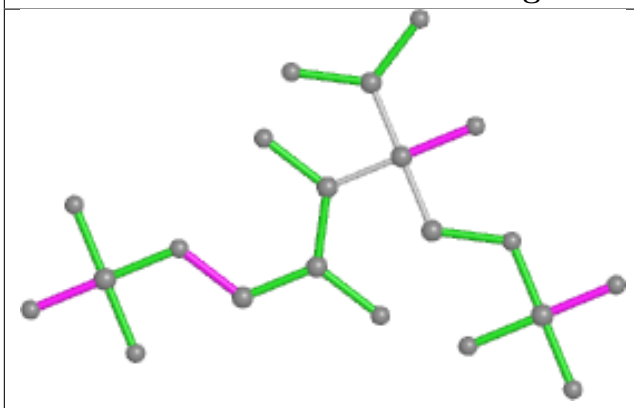
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	490	CAP	3	0
5	A	492	FMT	1	0
4	C	490	CAP	1	0
5	C	492	FMT	1	0
4	A	490	CAP	2	0
5	D	492	FMT	1	0

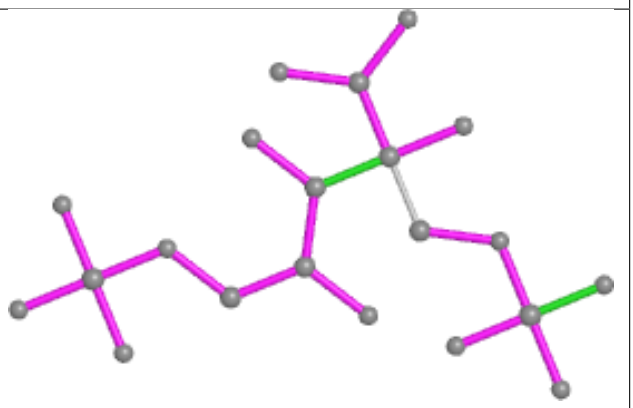
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

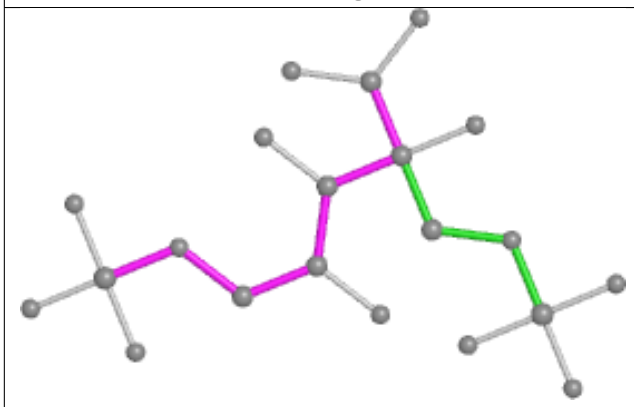
Ligand CAP D 490



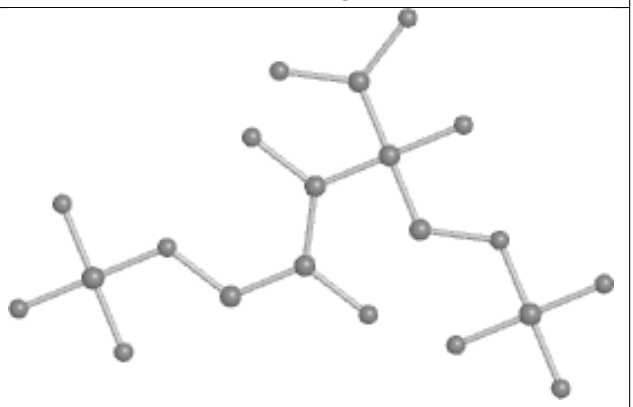
Bond lengths



Bond angles

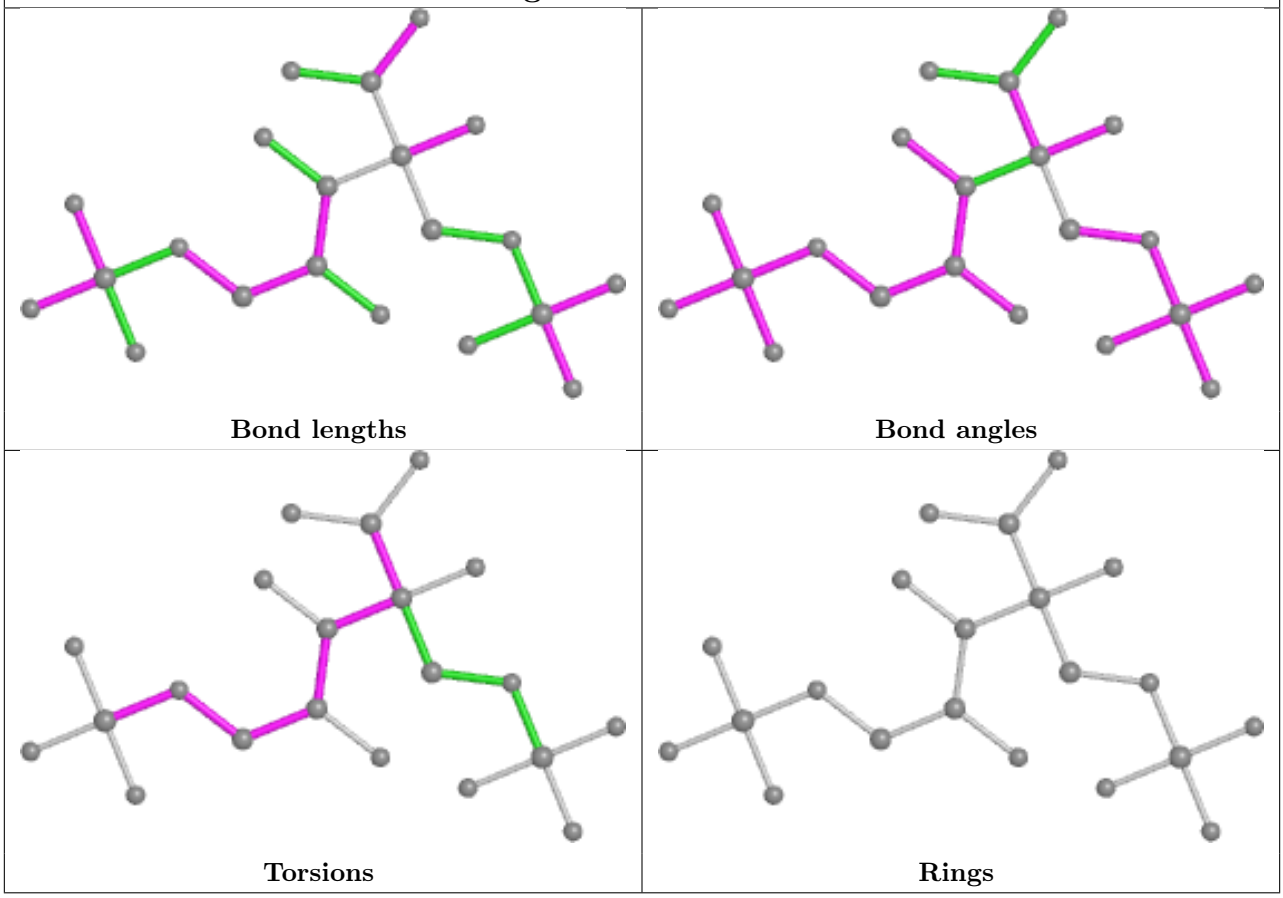


Torsions

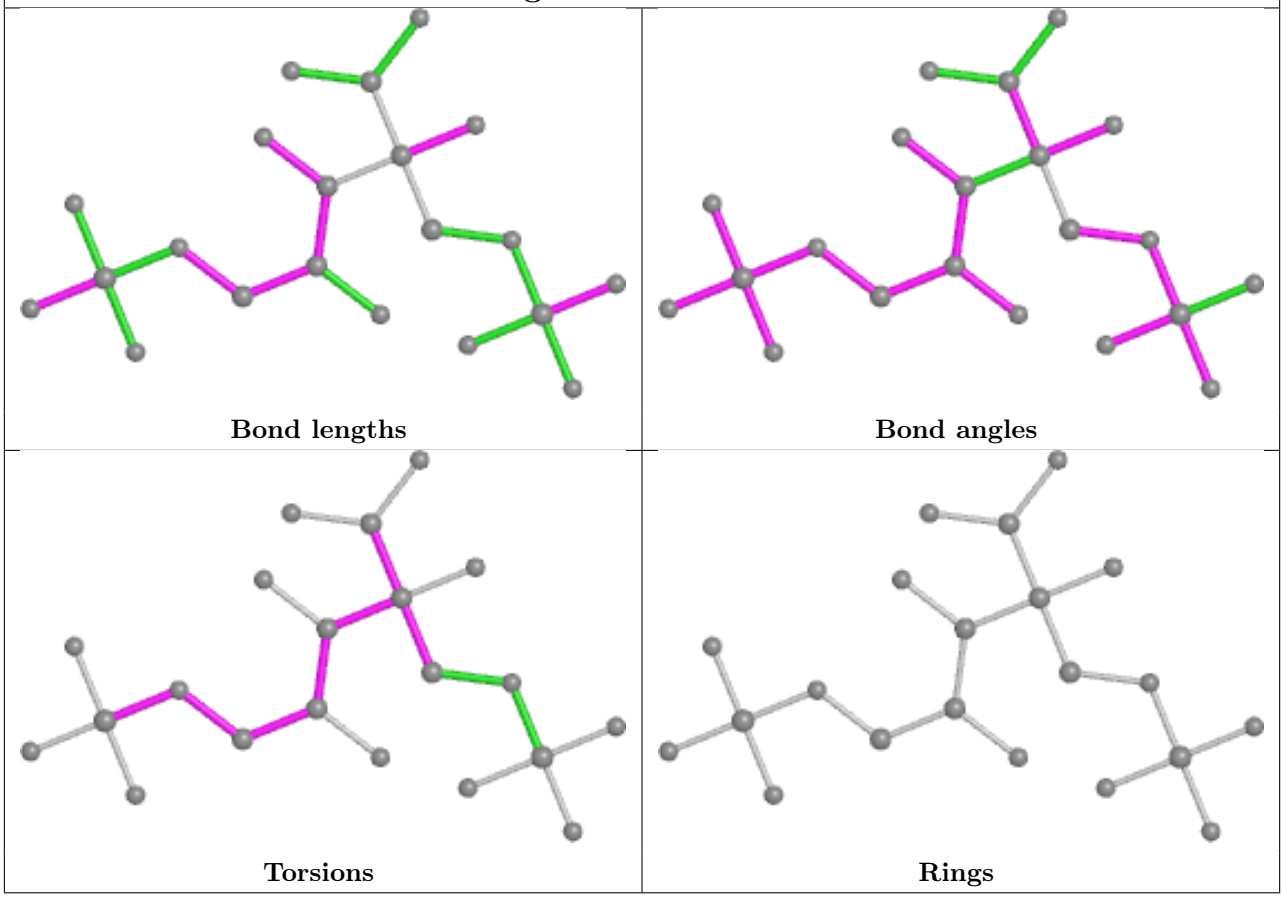


Rings

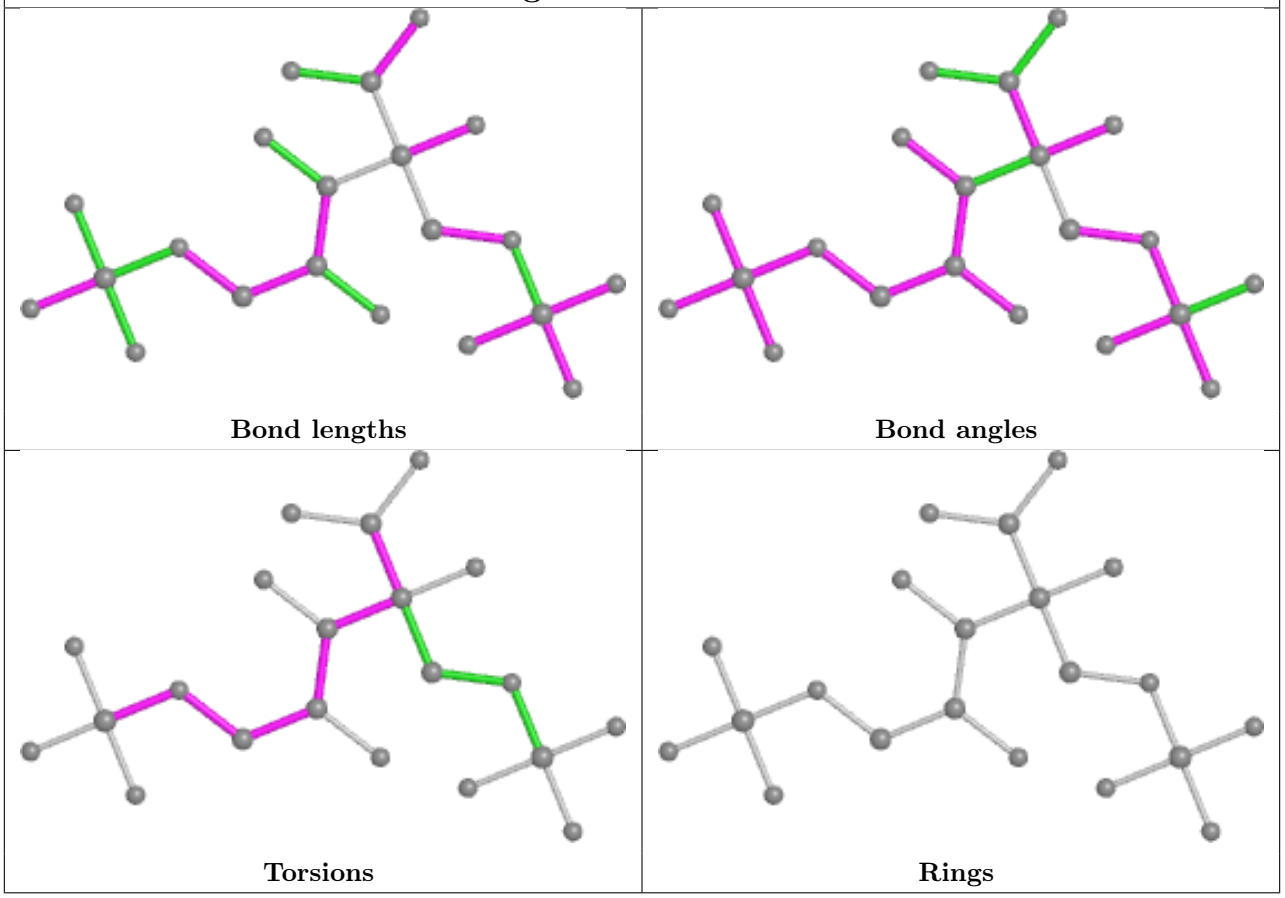
Ligand CAP C 490



Ligand CAP B 490



Ligand CAP A 490



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.