Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:02 AM EDT

PDB ID	:	4AID
Title	:	Crystal structure of C. crescentus PNPase bound to RNase E recognition peptide
Authors	:	Hardwick, S.W.; Gubbey, T.; Hug, I.; Jenal, U.; Luisi, B.F.
Deposited on	:	2012-02-09
Resolution	:	2.60 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 ⓘ) were used in the production of this report:

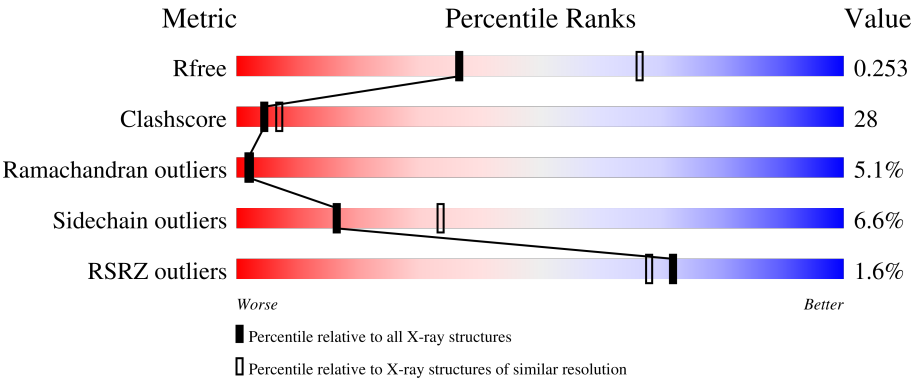
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	726	2% 48% 23% 6% • 21%
1	B	726	47% 23% 6% • 23%
1	C	726	2% 45% 26% • 26%
2	F	14	14% 21% 7% 7% 50%
2	G	14	29% 21% 7% 43%

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Mol	Chain	Length	Quality of chain
2	H	14	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12655 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 POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	1	0
			4248	2686	720	819	23			
1	B	558	Total	C	N	O	S	0	0	0
			4170	2639	706	802	23			
1	C	539	Total	C	N	O	S	0	0	0
			3836	2425	654	735	22			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q9AC32
A	-12	GLY	-	expression tag	UNP Q9AC32
A	-11	SER	-	expression tag	UNP Q9AC32
A	-10	SER	-	expression tag	UNP Q9AC32
A	-9	HIS	-	expression tag	UNP Q9AC32
A	-8	HIS	-	expression tag	UNP Q9AC32
A	-7	HIS	-	expression tag	UNP Q9AC32
A	-6	HIS	-	expression tag	UNP Q9AC32
A	-5	HIS	-	expression tag	UNP Q9AC32
A	-4	HIS	-	expression tag	UNP Q9AC32
A	-3	SER	-	expression tag	UNP Q9AC32
A	-2	GLN	-	expression tag	UNP Q9AC32
A	-1	ASP	-	expression tag	UNP Q9AC32
A	0	PRO	-	expression tag	UNP Q9AC32
B	-13	MET	-	expression tag	UNP Q9AC32
B	-12	GLY	-	expression tag	UNP Q9AC32
B	-11	SER	-	expression tag	UNP Q9AC32
B	-10	SER	-	expression tag	UNP Q9AC32
B	-9	HIS	-	expression tag	UNP Q9AC32
B	-8	HIS	-	expression tag	UNP Q9AC32
B	-7	HIS	-	expression tag	UNP Q9AC32
B	-6	HIS	-	expression tag	UNP Q9AC32

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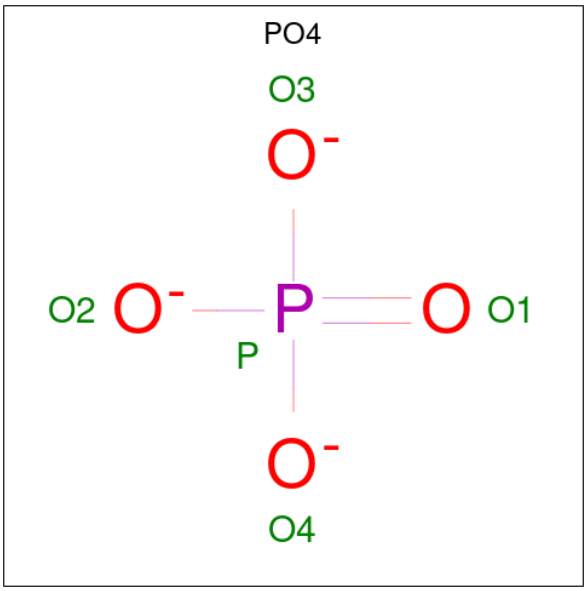
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q9AC32
B	-4	HIS	-	expression tag	UNP Q9AC32
B	-3	SER	-	expression tag	UNP Q9AC32
B	-2	GLN	-	expression tag	UNP Q9AC32
B	-1	ASP	-	expression tag	UNP Q9AC32
B	0	PRO	-	expression tag	UNP Q9AC32
C	-13	MET	-	expression tag	UNP Q9AC32
C	-12	GLY	-	expression tag	UNP Q9AC32
C	-11	SER	-	expression tag	UNP Q9AC32
C	-10	SER	-	expression tag	UNP Q9AC32
C	-9	HIS	-	expression tag	UNP Q9AC32
C	-8	HIS	-	expression tag	UNP Q9AC32
C	-7	HIS	-	expression tag	UNP Q9AC32
C	-6	HIS	-	expression tag	UNP Q9AC32
C	-5	HIS	-	expression tag	UNP Q9AC32
C	-4	HIS	-	expression tag	UNP Q9AC32
C	-3	SER	-	expression tag	UNP Q9AC32
C	-2	GLN	-	expression tag	UNP Q9AC32
C	-1	ASP	-	expression tag	UNP Q9AC32
C	0	PRO	-	expression tag	UNP Q9AC32

- Molecule 2 is a protein called RIBONUCLEASE, RNE/RNG FAMILY PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	0	0	0
			66	44	15	7			
2	G	8	Total	C	N	O	0	0	0
			77	50	19	8			
2	H	5	Total	C	N	O	0	0	0
			42	30	7	5			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

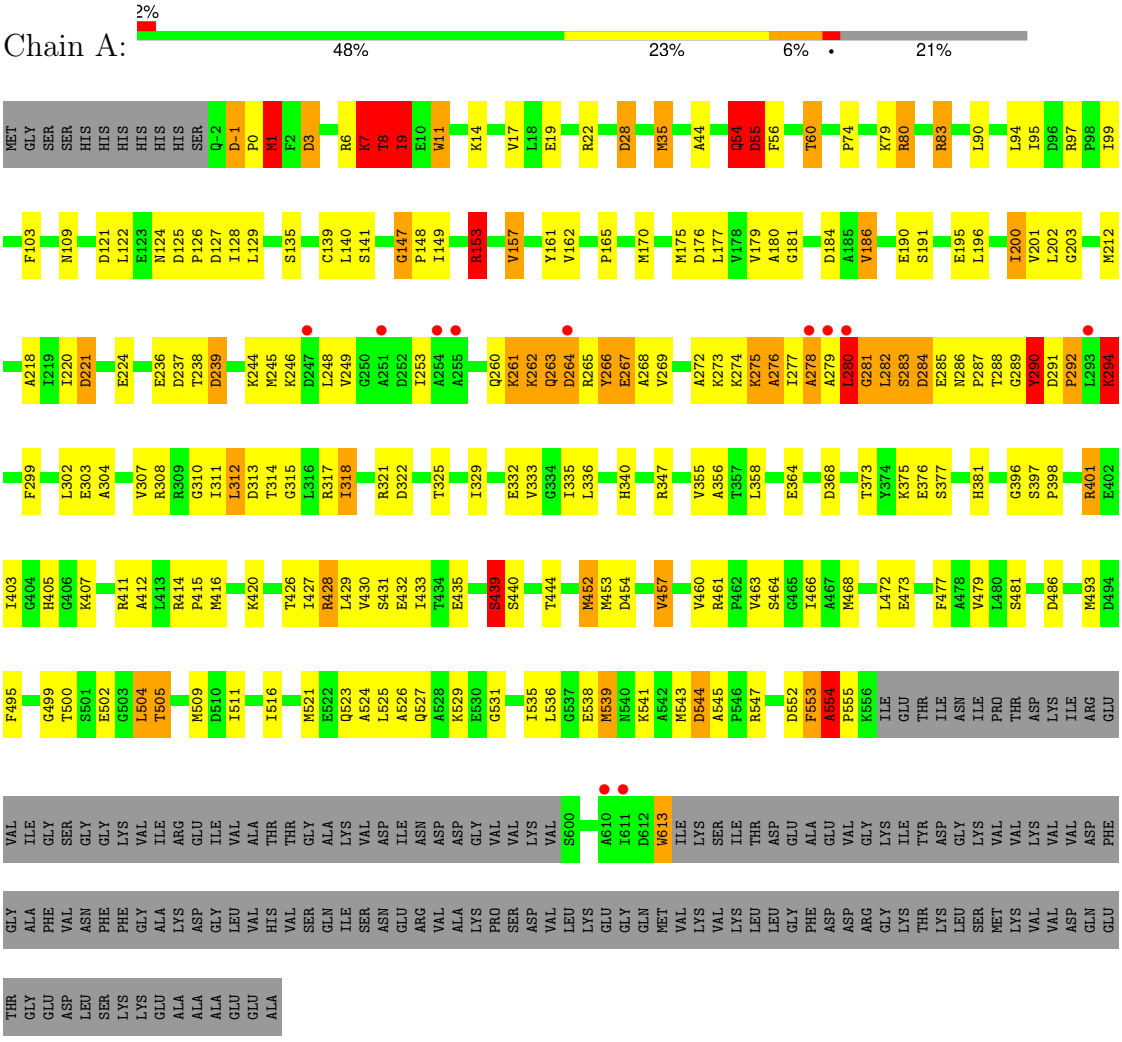
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	96	Total O 96 96	0	0
4	B	80	Total O 80 80	0	0
4	C	24	Total O 24 24	0	0
4	G	1	Total O 1 1	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

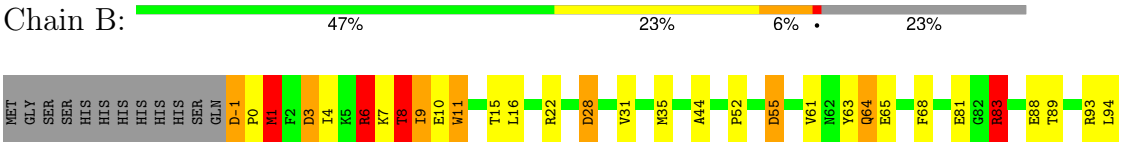
• Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE

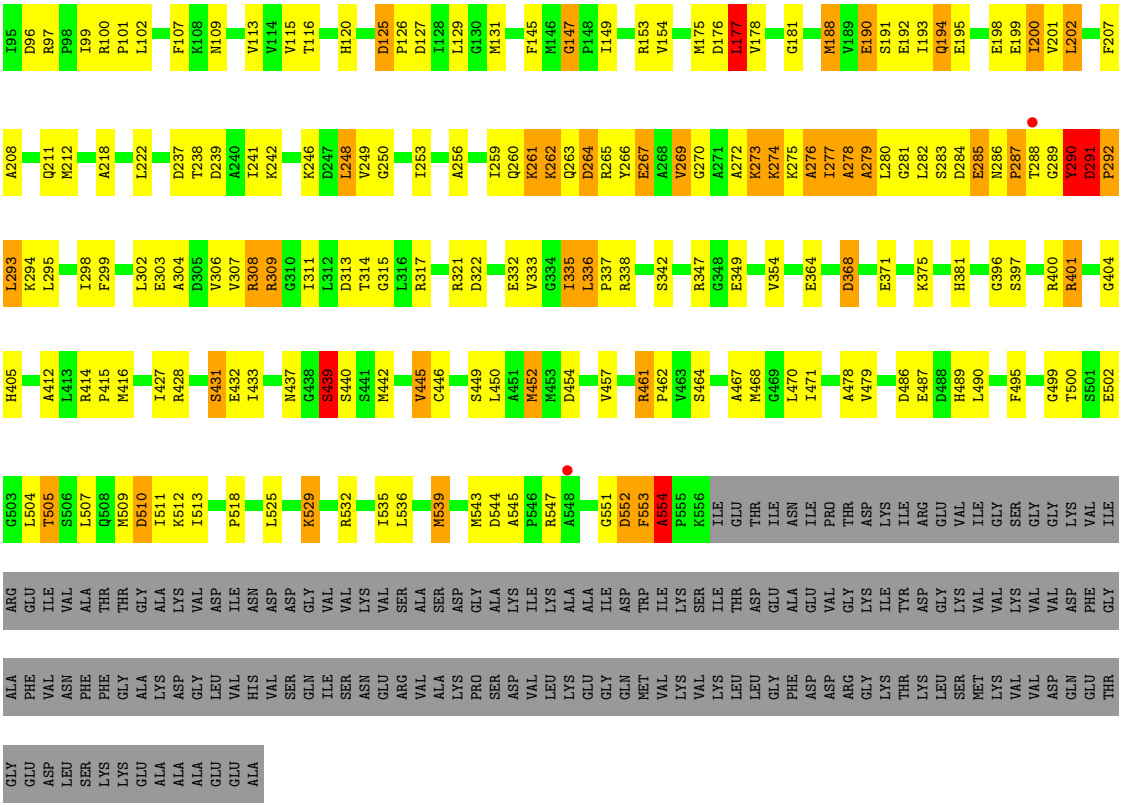
Chain A:



• Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE

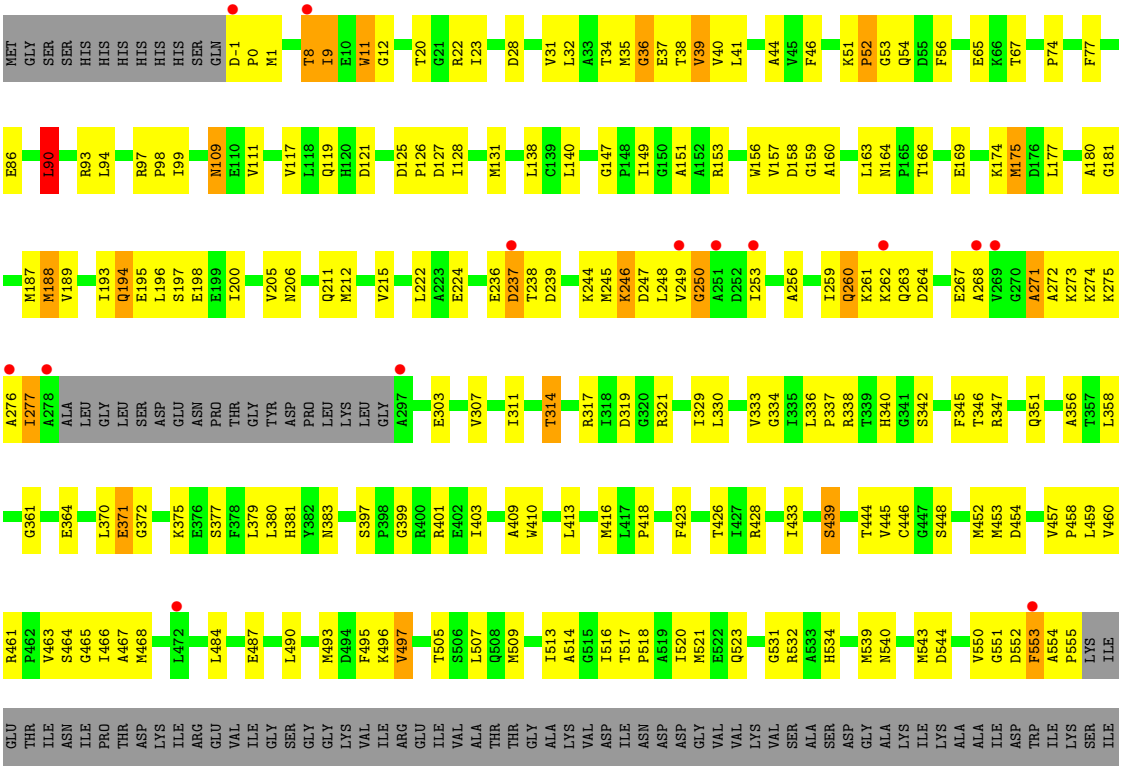
Chain B:

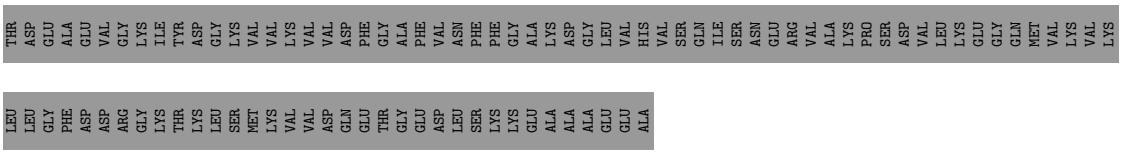




• Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE

Chain C:





• Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN

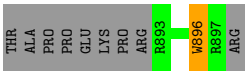
Chain F:

• Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN

Chain G:

• Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	157.44Å 157.44Å 302.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.60) 90.0 (29.75-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.254 0.209 , 0.253	Depositor DCC
R_{free} test set	2319 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 16.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.357 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12655	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	1.01	8/4324 (0.2%)	1.15	27/5859 (0.5%)
1	B	1.03	9/4242 (0.2%)	1.21	33/5744 (0.6%)
1	C	0.66	2/3900 (0.1%)	0.87	3/5305 (0.1%)
2	F	1.59	2/70 (2.9%)	1.32	1/94 (1.1%)
2	G	1.30	1/81 (1.2%)	1.14	0/109
2	H	1.49	1/45 (2.2%)	1.03	0/62
All	All	0.94	23/12662 (0.2%)	1.10	64/17173 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
2	F	0	1
All	All	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	896	TRP	CD2-CE2	7.50	1.50	1.41
1	B	81	GLU	CD-OE1	6.69	1.33	1.25
2	G	896	TRP	CD2-CE2	6.34	1.49	1.41
1	A	432	GLU	CD-OE1	6.33	1.32	1.25
1	A	332	GLU	CD-OE1	6.26	1.32	1.25
1	A	11	TRP	CD2-CE2	6.05	1.48	1.41
1	B	432	GLU	CD-OE1	5.86	1.32	1.25
1	B	332	GLU	CD-OE1	5.74	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLY	N-CA	5.73	1.54	1.46
1	A	376	GLU	CD-OE1	5.72	1.31	1.25
2	F	895	TRP	CD2-CE2	5.68	1.48	1.41
1	A	147	GLY	C-O	-5.62	1.14	1.23
1	B	81	GLU	CD-OE2	5.58	1.31	1.25
1	A	435	GLU	CD-OE1	5.57	1.31	1.25
1	B	11	TRP	CD2-CE2	5.49	1.48	1.41
1	B	199	GLU	CG-CD	5.45	1.60	1.51
1	B	190	GLU	CD-OE1	5.44	1.31	1.25
1	A	190	GLU	CD-OE1	5.40	1.31	1.25
1	A	613	TRP	CD2-CE2	5.37	1.47	1.41
1	C	11	TRP	CD2-CE2	5.34	1.47	1.41
1	B	3	ASP	CB-CG	-5.24	1.40	1.51
1	C	410	TRP	CD2-CE2	5.19	1.47	1.41
2	H	896	TRP	CD2-CE2	5.11	1.47	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177	LEU	CB-CG-CD1	-10.79	92.66	111.00
1	B	28	ASP	CB-CG-OD2	10.72	127.95	118.30
1	B	3	ASP	CB-CG-OD1	-10.37	108.97	118.30
1	B	153	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	B	486	ASP	CB-CG-OD1	-9.45	109.80	118.30
1	A	9	ILE	N-CA-C	-9.45	85.50	111.00
1	B	28	ASP	CB-CG-OD1	-9.40	109.84	118.30
1	A	80	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	80	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	486	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	B	539	MET	CG-SD-CE	-8.26	86.98	100.20
1	A	97	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	55	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	94	LEU	CB-CG-CD1	-7.84	97.67	111.00
1	B	486	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	539	MET	CG-SD-CE	-7.54	88.14	100.20
1	B	532	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	452	MET	CG-SD-CE	-7.31	88.50	100.20
1	A	553	PHE	N-CA-C	-6.56	93.29	111.00
1	B	525	LEU	CA-CB-CG	-6.45	100.46	115.30
1	B	291	ASP	C-N-CD	-6.45	106.42	120.60
1	A	439	SER	N-CA-C	6.40	128.28	111.00
1	B	83	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	8	THR	N-CA-C	-6.20	94.26	111.00
1	B	153	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	3	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	452	MET	CG-SD-CE	-6.05	90.52	100.20
1	A	-1	ASP	C-N-CD	6.05	141.10	128.40
1	A	28	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	B	55	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	96	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	401	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	461	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	153	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	96	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	A	544	ASP	N-CA-CB	-5.67	100.39	110.60
1	A	468	MET	CG-SD-CE	5.63	109.21	100.20
1	B	321	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	7	LYS	N-CA-C	-5.57	95.97	111.00
1	B	510	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	439	SER	N-CA-C	5.50	125.84	111.00
1	A	294	LYS	N-CA-C	-5.49	96.19	111.00
1	A	411	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	125	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	428	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	3	ASP	N-CA-CB	-5.35	100.97	110.60
2	F	894	GLY	N-CA-C	5.34	126.45	113.10
1	C	90	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	504	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	7	LYS	N-CA-C	-5.29	96.71	111.00
1	B	529	LYS	CD-CE-NZ	-5.27	99.59	111.70
1	A	55	ASP	CB-CA-C	-5.25	99.90	110.40
1	B	1	MET	CB-CG-SD	5.23	128.10	112.40
1	A	317	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	194	GLN	CA-CB-CG	5.21	124.87	113.40
1	A	28	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	192	GLU	N-CA-C	-5.20	96.97	111.00
1	A	19	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	A	8	THR	N-CA-C	-5.12	97.18	111.00
1	A	184	ASP	CB-CA-C	-5.10	100.19	110.40
1	B	6	ARG	N-CA-C	-5.10	97.23	111.00
1	A	486	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	463	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	554	ALA	Peptide
1	A	8	THR	Peptide
1	B	554	ALA	Peptide
1	B	6	ARG	Peptide
1	B	9	ILE	Peptide
1	C	35	MET	Peptide
2	F	892	ARG	Peptide

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	4248	0	4212	272	1
1	B	4170	0	4161	260	1
1	C	3836	0	3670	172	2
2	F	66	0	58	2	0
2	G	77	0	70	3	0
2	H	42	0	26	1	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
4	A	96	0	0	6	0
4	B	80	0	0	1	0
4	C	24	0	0	3	0
4	G	1	0	0	0	0
All	All	12655	0	12197	699	2

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 28.

All (699) 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)
1:A:287:PRO:HB2	1:A:288:THR:CG2	1.29	1.60
1:A:287:PRO:CB	1:A:288:THR:CG2	1.84	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HA	1:A:292:PRO:CG	1.44	1.43
1:A:281:GLY:CA	1:A:289:GLY:O	1.68	1.37
1:B:274:LYS:HA	1:B:277:ILE:CG2	1.57	1.34
1:B:291:ASP:O	1:B:293:LEU:N	1.61	1.29
1:A:282:LEU:CA	1:A:292:PRO:HG3	1.66	1.25
1:A:493:MET:HE3	1:A:509:MET:CE	1.70	1.21
1:A:287:PRO:CB	1:A:288:THR:HG22	1.56	1.21
1:A:493:MET:CE	1:A:509:MET:HE2	1.74	1.18
1:B:278:ALA:O	1:B:282:LEU:HD23	1.37	1.18
1:A:274:LYS:O	1:A:277:ILE:HG22	1.43	1.14
1:A:274:LYS:HE2	1:A:274:LYS:HA	1.29	1.13
1:A:277:ILE:O	1:A:282:LEU:HD12	1.46	1.13
1:B:279:ALA:O	1:B:282:LEU:CD2	1.97	1.13
1:A:287:PRO:CB	1:A:288:THR:HG23	1.57	1.13
1:B:274:LYS:CD	1:B:277:ILE:HG21	1.80	1.12
1:B:274:LYS:CD	1:B:277:ILE:HD13	1.80	1.12
1:A:287:PRO:CA	1:A:288:THR:CG2	2.28	1.10
1:A:277:ILE:C	1:A:282:LEU:HD12	1.71	1.09
1:A:543:MET:O	1:A:544:ASP:HB3	1.36	1.09
1:B:279:ALA:O	1:B:282:LEU:HD21	1.53	1.09
1:B:274:LYS:HA	1:B:277:ILE:HG22	1.30	1.09
1:B:274:LYS:HA	1:B:277:ILE:HG21	1.28	1.08
1:A:281:GLY:HA2	1:A:289:GLY:O	0.90	1.08
1:C:338:ARG:HA	1:C:553:PHE:HE1	1.05	1.07
1:A:493:MET:HE3	1:A:509:MET:HE2	1.16	1.07
1:A:416:MET:HE1	1:A:500:THR:HG21	1.30	1.06
1:A:287:PRO:CA	1:A:288:THR:HG22	1.85	1.06
1:B:287:PRO:HB2	1:B:288:THR:HA	1.08	1.05
1:A:453:MET:HB3	1:A:543:MET:CE	1.86	1.05
1:C:249:VAL:CG1	1:C:272:ALA:HB1	1.87	1.04
1:C:338:ARG:HA	1:C:553:PHE:CE1	1.93	1.02
1:B:279:ALA:O	1:B:282:LEU:CG	2.07	1.02
1:C:52:PRO:O	1:C:54:GLN:N	1.92	1.01
1:B:303:GLU:O	1:B:306:VAL:HG12	1.61	1.00
1:A:493:MET:CE	1:A:509:MET:CE	2.36	0.99
1:C:340:HIS:HD2	1:C:358:LEU:H	1.05	0.98
1:A:381:HIS:HD2	1:A:428:ARG:NH1	1.62	0.98
1:B:287:PRO:CB	1:B:288:THR:HA	1.94	0.98
1:B:354:VAL:HG22	1:B:431:SER:HB2	1.42	0.98
1:B:416:MET:CE	1:B:461:ARG:HB2	1.93	0.97
1:C:128:ILE:HD11	1:C:153:ARG:HB2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:NH2	1:B:190:GLU:OE1	1.96	0.97
1:A:340:HIS:HD2	1:A:358:LEU:H	1.13	0.97
1:B:83:ARG:HB2	1:B:83:ARG:HH11	1.28	0.97
1:B:275:LYS:O	1:B:277:ILE:N	1.97	0.97
1:A:381:HIS:CD2	1:A:428:ARG:HH11	1.82	0.97
1:A:281:GLY:O	1:A:290:TYR:O	1.82	0.97
1:A:54:GLN:O	1:A:55:ASP:HB2	1.62	0.96
1:C:99:ILE:HG22	1:C:149:ILE:HD12	1.47	0.96
1:B:263:GLN:HG3	1:B:264:ASP:H	1.28	0.96
1:A:364:GLU:HG2	1:A:426:THR:HG21	1.47	0.95
1:A:287:PRO:HB3	1:A:288:THR:HG22	1.49	0.93
1:B:364:GLU:OE1	1:B:375:LYS:HE3	1.68	0.93
1:B:263:GLN:O	1:B:266:TYR:N	2.01	0.93
1:B:93:ARG:HH11	1:B:404:GLY:HA3	1.34	0.93
1:A:8:THR:O	1:A:9:ILE:HG12	1.68	0.93
1:B:279:ALA:O	1:B:282:LEU:HG	1.66	0.93
1:A:493:MET:HG3	1:A:511:ILE:HG13	1.52	0.92
1:B:9:ILE:HG13	1:B:218:ALA:HB2	1.50	0.92
1:B:282:LEU:HB3	1:B:287:PRO:O	1.70	0.92
1:C:39:VAL:HG12	1:C:119:GLN:HB3	1.53	0.91
1:B:283:SER:HB2	1:B:287:PRO:HB3	1.52	0.91
1:B:102:LEU:HD12	1:B:149:ILE:HD11	1.51	0.91
1:A:60:THR:HG23	4:A:2012:HOH:O	1.69	0.91
1:A:543:MET:O	1:A:544:ASP:CB	2.11	0.91
1:C:67:THR:HG21	1:C:74:PRO:HG3	1.52	0.91
1:A:276:ALA:O	1:A:280:LEU:CB	2.19	0.91
1:B:287:PRO:HB2	1:B:288:THR:CA	1.99	0.90
1:B:1:MET:HG2	1:B:22:ARG:HA	1.54	0.90
1:C:94:LEU:HD12	1:C:97:ARG:NH2	1.87	0.90
1:A:281:GLY:O	1:A:292:PRO:HD3	1.73	0.89
1:C:249:VAL:HG13	1:C:272:ALA:HB1	1.54	0.89
1:A:416:MET:CE	1:A:500:THR:HG21	2.03	0.89
1:A:282:LEU:CA	1:A:292:PRO:CG	2.38	0.89
1:B:284:ASP:HA	1:B:285:GLU:HB3	1.51	0.89
1:A:274:LYS:HE2	1:A:277:ILE:HG21	1.52	0.89
1:B:274:LYS:CA	1:B:277:ILE:CG2	2.47	0.88
1:A:287:PRO:HB2	1:A:288:THR:HG23	0.89	0.88
1:A:282:LEU:HA	1:A:292:PRO:HG2	1.56	0.88
1:B:470:LEU:HD12	1:B:478:ALA:O	1.72	0.88
1:C:340:HIS:CD2	1:C:358:LEU:H	1.92	0.88
1:B:275:LYS:HG2	1:B:276:ALA:N	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PRO:O	1:C:338:ARG:HB2	1.72	0.87
1:A:287:PRO:HB2	1:A:288:THR:HG21	1.53	0.87
1:B:93:ARG:NH1	1:B:404:GLY:HA3	1.88	0.86
1:A:381:HIS:HD2	1:A:428:ARG:HH11	0.91	0.86
1:A:416:MET:CE	1:A:461:ARG:HB2	2.06	0.86
1:A:464:SER:HB2	1:A:539:MET:HE1	1.55	0.85
1:B:97:ARG:CZ	1:B:188:MET:HE3	2.06	0.85
1:B:274:LYS:CA	1:B:277:ILE:HG22	2.03	0.85
1:C:39:VAL:CG1	1:C:119:GLN:HB3	2.05	0.85
1:A:181:GLY:HA3	1:A:212:MET:HE1	1.57	0.85
1:B:275:LYS:HG2	1:B:276:ALA:H	1.39	0.84
1:C:338:ARG:CA	1:C:553:PHE:HE1	1.87	0.84
1:C:409:ALA:O	1:C:413:LEU:HG	1.77	0.83
1:A:249:VAL:CG2	1:A:276:ALA:HB2	2.08	0.82
1:A:502:GLU:OE2	1:B:529:LYS:HE2	1.78	0.82
1:B:-1:ASP:HB3	1:B:0:PRO:HD3	1.61	0.82
1:B:97:ARG:CZ	1:B:188:MET:CE	2.57	0.82
1:A:245:MET:HE3	1:A:299:PHE:HA	1.62	0.82
1:A:8:THR:HG22	1:A:9:ILE:HD13	1.59	0.82
1:B:263:GLN:HG3	1:B:264:ASP:N	1.95	0.82
1:A:277:ILE:C	1:A:282:LEU:CD1	2.49	0.81
1:A:200:ILE:HD11	1:B:200:ILE:HD11	1.62	0.81
1:A:276:ALA:O	1:A:280:LEU:HB3	1.80	0.81
1:C:125:ASP:OD1	1:C:126:PRO:HD2	1.81	0.81
1:C:268:ALA:O	1:C:271:ALA:HB3	1.81	0.81
1:A:464:SER:HB2	1:A:539:MET:CE	2.10	0.81
1:B:283:SER:HB2	1:B:287:PRO:CB	2.11	0.81
1:A:177:LEU:HD12	1:A:191:SER:HB3	1.62	0.81
1:A:364:GLU:OE1	1:A:375:LYS:HE3	1.80	0.80
1:B:309:ARG:HG3	1:B:309:ARG:HH11	1.46	0.80
1:B:277:ILE:O	1:B:278:ALA:C	2.20	0.80
1:A:274:LYS:HA	1:A:274:LYS:CE	2.10	0.80
1:A:274:LYS:C	1:A:277:ILE:HG22	2.00	0.80
1:B:277:ILE:HG23	1:B:278:ALA:H	1.46	0.80
1:B:291:ASP:C	1:B:293:LEU:N	2.32	0.80
1:A:453:MET:HB3	1:A:543:MET:HE3	1.62	0.80
1:B:-1:ASP:HB3	1:B:0:PRO:CD	2.11	0.80
1:C:338:ARG:HG2	1:C:553:PHE:CZ	2.17	0.80
1:B:433:ILE:HD12	1:B:440:SER:HB2	1.63	0.80
1:B:464:SER:HB2	1:B:539:MET:CE	2.12	0.80
1:A:287:PRO:HA	1:A:288:THR:HG22	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:HIS:HD2	1:C:428:ARG:HH11	1.30	0.79
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.46	0.79
1:A:276:ALA:O	1:A:280:LEU:HB2	1.81	0.79
1:A:95:ILE:O	1:A:99:ILE:HG12	1.82	0.79
1:B:338:ARG:HA	1:B:553:PHE:HE1	1.48	0.79
1:B:249:VAL:O	1:B:253:ILE:HG12	1.82	0.79
1:A:249:VAL:CG1	1:A:272:ALA:HB1	2.11	0.79
1:A:287:PRO:CA	1:A:288:THR:HG23	2.00	0.79
1:A:274:LYS:O	1:A:277:ILE:CG2	2.30	0.78
1:B:278:ALA:O	1:B:282:LEU:CD2	2.28	0.78
1:C:319:ASP:OD2	1:C:321:ARG:NH1	2.16	0.78
1:B:274:LYS:CA	1:B:277:ILE:HG21	2.11	0.77
1:A:277:ILE:HG12	1:A:282:LEU:HD11	1.64	0.77
1:A:284:ASP:OD1	1:A:285:GLU:N	2.18	0.77
1:A:282:LEU:HA	1:A:292:PRO:HG3	0.77	0.77
1:B:97:ARG:NH2	1:B:188:MET:HE1	2.00	0.76
1:C:249:VAL:CG2	1:C:276:ALA:HB2	2.15	0.76
1:B:275:LYS:C	1:B:277:ILE:H	1.87	0.76
1:A:464:SER:CB	1:A:539:MET:CE	2.64	0.76
1:A:236:GLU:HB3	1:A:238:THR:HG23	1.66	0.76
1:B:283:SER:CB	1:B:287:PRO:HB3	2.15	0.76
1:A:83:ARG:HH11	1:A:83:ARG:CG	1.98	0.75
1:C:249:VAL:O	1:C:253:ILE:HG12	1.86	0.75
1:C:383:ASN:O	1:C:433:ILE:HG12	1.86	0.75
1:A:287:PRO:C	1:A:288:THR:HG23	2.07	0.75
1:A:401:ARG:NE	1:A:405:HIS:HE1	1.85	0.75
1:A:308:ARG:O	1:A:312:LEU:HD12	1.87	0.74
1:C:236:GLU:O	1:C:238:THR:N	2.20	0.74
1:A:287:PRO:HB3	1:A:288:THR:CG2	2.07	0.74
1:B:286:ASN:N	1:B:287:PRO:O	2.20	0.74
1:C:99:ILE:HG22	1:C:149:ILE:CD1	2.16	0.74
1:A:7:LYS:O	1:A:8:THR:C	2.26	0.74
1:A:340:HIS:CD2	1:A:358:LEU:H	2.01	0.74
1:C:12:GLY:HA3	1:C:163:LEU:HD23	1.67	0.74
1:A:202:LEU:HD11	1:A:525:LEU:HD12	1.70	0.74
1:B:412:ALA:HA	1:B:505:THR:HG23	1.70	0.74
1:A:281:GLY:O	1:A:292:PRO:CD	2.35	0.74
1:B:290:TYR:O	1:B:292:PRO:N	2.21	0.74
1:B:464:SER:HB2	1:B:539:MET:HE1	1.69	0.73
1:A:249:VAL:HG11	1:A:272:ALA:HB1	1.69	0.73
1:C:67:THR:HG21	1:C:74:PRO:CG	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:OD1	1:A:547:ARG:NH1	2.20	0.73
1:A:303:GLU:O	1:A:307:VAL:HG23	1.88	0.73
1:B:97:ARG:HD2	1:B:510:ASP:OD1	1.88	0.73
1:B:83:ARG:HH11	1:B:83:ARG:CB	1.99	0.73
1:A:464:SER:HB3	1:A:539:MET:HE3	1.69	0.73
1:A:499:GLY:HA2	1:A:505:THR:HB	1.71	0.73
1:B:304:ALA:O	1:B:308:ARG:HG3	1.89	0.73
1:A:8:THR:O	1:A:9:ILE:CG1	2.37	0.72
1:B:337:PRO:O	1:B:338:ARG:HB2	1.90	0.72
1:C:128:ILE:HD11	1:C:153:ARG:CB	2.17	0.72
1:B:416:MET:CE	1:B:461:ARG:CB	2.67	0.72
1:B:454:ASP:OD1	1:B:547:ARG:NH1	2.22	0.72
1:B:253:ILE:CG2	1:B:306:VAL:HG11	2.20	0.71
1:B:260:GLN:O	1:B:261:LYS:CB	2.35	0.71
1:A:181:GLY:CA	1:A:212:MET:HE1	2.21	0.71
1:B:291:ASP:O	1:B:292:PRO:C	2.27	0.71
1:B:176:ASP:O	1:B:191:SER:HA	1.90	0.71
1:B:97:ARG:NH1	1:B:188:MET:HE3	2.06	0.71
1:A:181:GLY:O	1:A:212:MET:HE3	1.91	0.71
1:A:493:MET:CE	1:A:509:MET:HE3	2.21	0.71
1:A:401:ARG:CZ	1:A:405:HIS:HE1	2.05	0.70
1:B:238:THR:O	1:B:241:ILE:HG22	1.91	0.70
1:C:464:SER:HB3	1:C:539:MET:HE1	1.72	0.70
1:B:175:MET:SD	1:B:177:LEU:HD23	2.32	0.70
1:B:439:SER:HA	3:B:1557:PO4:O4	1.91	0.70
1:A:54:GLN:O	1:A:55:ASP:CB	2.36	0.70
1:A:377:SER:HB2	1:A:426:THR:HG22	1.74	0.69
1:B:416:MET:HE1	1:B:461:ARG:HB2	1.73	0.69
1:A:277:ILE:O	1:A:282:LEU:CD1	2.34	0.69
1:C:249:VAL:HG11	1:C:272:ALA:HB1	1.72	0.69
1:C:333:VAL:HG11	1:C:543:MET:HE2	1.73	0.69
1:A:278:ALA:HA	1:A:282:LEU:HD13	1.74	0.69
1:C:157:VAL:O	1:C:159:GLY:N	2.25	0.69
1:C:452:MET:O	1:C:457:VAL:HG22	1.93	0.69
1:A:464:SER:CB	1:A:539:MET:HE3	2.22	0.69
1:B:277:ILE:O	1:B:279:ALA:N	2.26	0.69
1:B:277:ILE:HG23	1:B:278:ALA:N	2.08	0.69
1:C:177:LEU:HD11	1:C:189:VAL:HG13	1.74	0.69
1:B:181:GLY:HA3	1:B:212:MET:HE1	1.75	0.69
1:B:261:LYS:O	1:B:262:LYS:O	2.11	0.69
1:A:464:SER:CB	1:A:539:MET:HE1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:THR:O	1:C:9:ILE:HB	1.93	0.68
1:C:39:VAL:O	1:C:40:VAL:HG23	1.91	0.68
1:C:109:ASN:N	1:C:109:ASN:HD22	1.91	0.68
1:A:433:ILE:HD12	1:A:440:SER:HB2	1.75	0.68
1:B:275:LYS:CG	1:B:276:ALA:N	2.55	0.68
1:C:364:GLU:OE2	1:C:375:LYS:HE3	1.93	0.68
1:A:181:GLY:CA	1:A:212:MET:CE	2.72	0.68
1:C:94:LEU:HD12	1:C:97:ARG:HH21	1.56	0.68
1:B:291:ASP:OD1	1:B:293:LEU:HB2	1.93	0.68
1:B:364:GLU:OE1	1:B:375:LYS:CE	2.42	0.68
1:A:181:GLY:C	1:A:212:MET:HE3	2.15	0.67
1:A:275:LYS:HG2	1:A:276:ALA:N	2.09	0.67
1:A:453:MET:CB	1:A:543:MET:CE	2.70	0.67
1:A:153:ARG:HD3	1:A:176:ASP:OD1	1.95	0.67
1:B:309:ARG:HG3	1:B:309:ARG:NH1	2.09	0.67
1:C:340:HIS:HB2	1:C:356:ALA:O	1.95	0.67
1:B:274:LYS:C	1:B:277:ILE:HG22	2.15	0.66
1:A:401:ARG:HD2	4:A:2078:HOH:O	1.95	0.66
1:B:263:GLN:O	1:B:267:GLU:N	2.26	0.66
1:A:416:MET:HE1	1:A:500:THR:CG2	2.18	0.66
1:B:9:ILE:HG13	1:B:218:ALA:CB	2.26	0.66
1:B:83:ARG:HB2	1:B:83:ARG:NH1	2.06	0.66
1:A:401:ARG:NE	1:A:405:HIS:CE1	2.63	0.66
1:C:338:ARG:HG2	1:C:553:PHE:HZ	1.60	0.66
1:A:381:HIS:CD2	1:A:428:ARG:NH1	2.54	0.65
1:B:97:ARG:NH1	1:B:188:MET:CE	2.59	0.65
1:B:303:GLU:O	1:B:307:VAL:HG23	1.95	0.65
1:A:249:VAL:HG21	1:A:276:ALA:HB2	1.76	0.65
1:B:9:ILE:HG22	1:B:11:TRP:HB2	1.79	0.65
1:C:249:VAL:HG12	1:C:253:ILE:HG12	1.79	0.65
1:A:265:ARG:HH22	1:A:318:ILE:HA	1.61	0.65
1:C:189:VAL:HG11	1:C:507:LEU:HD12	1.77	0.64
1:A:277:ILE:HG12	1:A:282:LEU:CD1	2.27	0.64
1:B:381:HIS:HD2	1:B:428:ARG:HE	1.45	0.64
1:C:39:VAL:CG1	1:C:119:GLN:CB	2.76	0.64
1:A:266:TYR:O	1:A:267:GLU:C	2.36	0.64
1:A:135:SER:HB2	1:A:149:ILE:HG12	1.80	0.63
1:A:311:ILE:O	1:A:314:THR:O	2.16	0.63
1:A:427:ILE:HD13	1:A:452:MET:CE	2.27	0.63
1:A:502:GLU:O	4:A:2091:HOH:O	2.15	0.63
1:B:286:ASN:HB2	1:B:287:PRO:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG13	1:B:272:ALA:HB1	1.81	0.63
1:B:535:ILE:HG22	1:B:539:MET:CE	2.27	0.63
1:A:479:VAL:HG23	1:A:527:GLN:CD	2.19	0.62
1:A:281:GLY:C	1:A:289:GLY:O	2.36	0.62
1:B:9:ILE:CG1	1:B:218:ALA:HB2	2.24	0.62
1:B:269:VAL:HG12	1:B:270:GLY:N	2.15	0.62
1:B:468:MET:HB2	1:B:495:PHE:CE1	2.35	0.62
1:C:40:VAL:HG22	1:C:117:VAL:HA	1.80	0.62
1:C:175:MET:HB2	1:C:193:ILE:HG23	1.82	0.62
1:C:468:MET:HB2	1:C:495:PHE:CE2	2.34	0.62
1:B:303:GLU:O	1:B:306:VAL:CG1	2.44	0.62
1:B:337:PRO:O	1:B:338:ARG:CB	2.42	0.62
1:C:340:HIS:HD2	1:C:358:LEU:N	1.87	0.61
1:C:381:HIS:CD2	1:C:428:ARG:HD2	2.35	0.61
1:B:442:MET:HA	1:B:445:VAL:HG13	1.81	0.61
1:A:200:ILE:HD11	1:B:200:ILE:CD1	2.31	0.61
1:A:161:TYR:OH	1:A:203:GLY:HA3	2.00	0.61
1:B:381:HIS:CD2	1:B:428:ARG:HE	2.19	0.61
1:C:423:PHE:CZ	1:C:457:VAL:HG12	2.35	0.61
1:B:181:GLY:O	1:B:212:MET:HE3	2.01	0.60
1:C:256:ALA:O	1:C:259:ILE:CB	2.49	0.60
1:B:253:ILE:HG22	1:B:306:VAL:HG11	1.83	0.60
1:A:495:PHE:HB3	1:A:509:MET:HG2	1.83	0.60
1:C:337:PRO:O	1:C:338:ARG:CB	2.41	0.60
1:A:249:VAL:HG23	1:A:276:ALA:HB2	1.83	0.60
1:B:464:SER:HB2	1:B:539:MET:HE3	1.83	0.60
1:B:259:ILE:O	1:B:265:ARG:NH1	2.34	0.60
1:A:245:MET:CE	1:A:299:PHE:HA	2.31	0.60
1:A:340:HIS:CE1	1:A:554:ALA:HB3	2.36	0.60
1:A:238:THR:HG22	1:A:290:TYR:OH	2.02	0.60
1:A:536:LEU:HA	1:A:539:MET:HE3	1.83	0.60
1:A:364:GLU:HG2	1:A:426:THR:CG2	2.28	0.59
1:B:3:ASP:O	1:B:4:ILE:HG13	2.01	0.59
1:C:67:THR:HG21	1:C:74:PRO:CD	2.32	0.59
1:A:304:ALA:O	1:A:308:ARG:HG3	2.03	0.59
1:B:287:PRO:HD2	1:B:288:THR:HG23	1.82	0.59
1:B:284:ASP:CA	1:B:285:GLU:HB3	2.29	0.59
1:A:315:GLY:O	1:A:322:ASP:HA	2.03	0.59
1:A:401:ARG:CZ	1:A:405:HIS:CE1	2.85	0.59
1:C:264:ASP:O	1:C:267:GLU:N	2.36	0.59
1:A:412:ALA:O	1:A:505:THR:HG21	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLN:HE21	1:B:116:THR:HG23	1.68	0.59
1:B:99:ILE:HD13	1:B:149:ILE:CD1	2.32	0.58
1:C:550:VAL:HG21	1:C:555:PRO:HB3	1.85	0.58
1:B:274:LYS:CD	1:B:277:ILE:CG2	2.70	0.58
1:C:509:MET:CE	1:C:521:MET:SD	2.91	0.58
1:B:464:SER:CB	1:B:539:MET:HE1	2.34	0.58
1:B:260:GLN:HA	1:B:265:ARG:NH1	2.18	0.58
1:B:470:LEU:HD13	1:B:479:VAL:HG13	1.85	0.58
1:A:6:ARG:HD3	1:A:221:ASP:HB3	1.85	0.58
1:C:67:THR:HG21	1:C:74:PRO:HD3	1.85	0.58
1:C:531:GLY:HA3	4:C:2020:HOH:O	2.03	0.58
1:A:275:LYS:O	1:A:278:ALA:N	2.36	0.58
1:A:412:ALA:HA	1:A:505:THR:CG2	2.34	0.58
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.12	0.58
1:B:277:ILE:O	1:B:280:LEU:N	2.37	0.58
1:B:253:ILE:HG21	1:B:306:VAL:HG11	1.84	0.58
1:B:303:GLU:HA	1:B:306:VAL:HG12	1.86	0.57
1:A:176:ASP:O	1:A:191:SER:HA	2.04	0.57
1:A:479:VAL:HG23	1:A:527:GLN:NE2	2.19	0.57
1:B:4:ILE:HG22	1:B:222:LEU:HD11	1.87	0.57
2:G:896:TRP:N	2:G:897:ARG:HA	2.19	0.57
1:A:260:GLN:O	1:A:261:LYS:C	2.42	0.57
1:A:262:LYS:O	1:A:263:GLN:C	2.42	0.57
1:B:499:GLY:HA2	1:B:505:THR:HB	1.87	0.57
1:C:317:ARG:HG3	1:C:321:ARG:O	2.04	0.57
1:A:200:ILE:CD1	1:B:200:ILE:HD11	2.32	0.56
1:A:274:LYS:NZ	1:A:277:ILE:HD13	2.20	0.56
1:A:333:VAL:HG11	1:A:543:MET:HG3	1.86	0.56
1:C:93:ARG:HH12	1:C:401:ARG:HA	1.69	0.56
1:A:236:GLU:C	1:A:238:THR:H	2.08	0.56
1:B:303:GLU:C	1:B:306:VAL:HG12	2.23	0.56
1:B:414:ARG:N	1:B:415:PRO:CD	2.67	0.56
1:A:277:ILE:HG23	1:A:278:ALA:N	2.20	0.56
1:A:416:MET:HE3	1:A:461:ARG:HB2	1.83	0.56
1:B:64:GLN:NE2	1:B:116:THR:HG23	2.20	0.56
1:A:535:ILE:HG22	1:A:539:MET:HE2	1.88	0.56
1:B:282:LEU:CB	1:B:287:PRO:O	2.50	0.56
1:B:97:ARG:CZ	1:B:188:MET:HE1	2.35	0.56
1:B:147:GLY:HA2	2:G:896:TRP:O	2.06	0.56
1:A:125:ASP:OD1	1:A:126:PRO:HD2	2.05	0.56
1:A:285:GLU:O	1:A:286:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:HB2	1:B:44:ALA:O	2.07	0.55
1:B:282:LEU:HA	1:B:284:ASP:O	2.05	0.55
1:B:315:GLY:O	1:B:322:ASP:HA	2.07	0.55
1:A:266:TYR:O	1:A:269:VAL:N	2.39	0.55
1:B:291:ASP:O	1:B:293:LEU:CA	2.52	0.55
1:C:333:VAL:HG11	1:C:543:MET:CE	2.37	0.55
1:A:310:GLY:O	1:A:313:ASP:O	2.24	0.55
1:C:246:LYS:O	1:C:247:ASP:C	2.43	0.55
1:C:439:SER:HB2	1:C:467:ALA:HB2	1.88	0.55
1:B:181:GLY:CA	1:B:212:MET:HE1	2.37	0.55
1:C:86:GLU:O	1:C:90:LEU:HB2	2.07	0.55
1:B:284:ASP:HA	1:B:285:GLU:CB	2.16	0.55
1:B:381:HIS:CD2	1:B:428:ARG:HH21	2.25	0.55
1:C:493:MET:SD	1:C:516:ILE:HD13	2.47	0.55
1:A:261:LYS:O	1:A:262:LYS:C	2.45	0.55
1:B:193:ILE:HD13	1:B:201:VAL:HG21	1.89	0.55
1:B:416:MET:HE3	1:B:461:ARG:HB2	1.83	0.55
1:A:277:ILE:CG2	1:A:278:ALA:N	2.70	0.54
1:C:490:LEU:O	1:C:490:LEU:HG	2.06	0.54
1:B:263:GLN:O	1:B:265:ARG:N	2.41	0.54
1:B:439:SER:HB2	1:B:467:ALA:HB2	1.90	0.54
1:A:275:LYS:O	1:A:277:ILE:N	2.40	0.54
1:B:464:SER:CB	1:B:539:MET:CE	2.85	0.54
1:A:261:LYS:O	1:A:262:LYS:O	2.25	0.54
1:B:102:LEU:CD1	1:B:149:ILE:HD11	2.33	0.54
1:A:249:VAL:HG21	1:A:276:ALA:CB	2.38	0.54
1:A:368:ASP:N	1:A:368:ASP:OD1	2.37	0.54
1:C:36:GLY:O	1:C:37:GLU:HB2	2.08	0.54
1:C:98:PRO:HD3	1:C:188:MET:HG2	1.89	0.54
1:A:281:GLY:N	1:A:289:GLY:O	2.39	0.54
1:A:431:SER:OG	1:A:444:THR:CG2	2.56	0.54
1:C:377:SER:HA	1:C:426:THR:HG23	1.89	0.54
1:B:100:ARG:HB3	1:B:101:PRO:HD3	1.90	0.54
1:C:20:THR:HG21	1:C:140:LEU:HD21	1.89	0.54
1:C:416:MET:HE3	1:C:460:VAL:HB	1.90	0.54
1:A:127:ASP:OD1	1:A:128:ILE:N	2.41	0.54
1:C:509:MET:HE3	1:C:521:MET:SD	2.48	0.54
1:C:330:LEU:O	1:C:346:THR:HG22	2.09	0.53
1:A:274:LYS:HA	1:A:277:ILE:HG21	1.91	0.53
1:A:464:SER:HB3	1:A:539:MET:CE	2.33	0.53
1:A:529:LYS:HE2	1:B:502:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ARG:HG2	1:C:23:ILE:HG13	1.91	0.53
1:B:246:LYS:O	1:B:250:GLY:N	2.41	0.53
1:C:93:ARG:NH1	1:C:401:ARG:HA	2.24	0.53
1:B:181:GLY:CA	1:B:212:MET:CE	2.87	0.53
1:B:145:PHE:HZ	1:B:149:ILE:HD12	1.74	0.53
1:B:470:LEU:HD13	1:B:479:VAL:CG1	2.39	0.53
1:C:32:LEU:HD11	1:C:39:VAL:CG2	2.39	0.53
1:A:195:GLU:HA	1:A:504:LEU:O	2.09	0.53
1:A:287:PRO:HA	1:A:288:THR:CG2	2.25	0.53
1:A:175:MET:CE	1:A:196:LEU:HD12	2.39	0.53
1:A:401:ARG:CD	4:A:2078:HOH:O	2.55	0.53
1:A:329:ILE:CG1	1:A:347:ARG:HG3	2.39	0.52
1:C:259:ILE:O	1:C:260:GLN:O	2.27	0.52
1:A:157:VAL:HG13	1:A:162:VAL:HG11	1.90	0.52
1:B:313:ASP:O	1:B:314:THR:OG1	2.13	0.52
1:C:531:GLY:O	1:C:534:HIS:HB3	2.09	0.52
1:A:274:LYS:CE	1:A:277:ILE:HG21	2.34	0.52
1:B:193:ILE:HD13	1:B:201:VAL:CG2	2.39	0.52
1:B:416:MET:HE2	1:B:461:ARG:CB	2.39	0.52
1:C:163:LEU:HD13	1:C:211:GLN:HG2	1.91	0.52
1:A:253:ILE:HD11	1:A:299:PHE:HE1	1.75	0.52
1:A:440:SER:O	1:A:444:THR:HG23	2.10	0.52
1:A:493:MET:HE1	1:A:509:MET:CE	2.33	0.52
1:A:412:ALA:O	1:A:505:THR:CG2	2.58	0.52
1:B:280:LEU:N	1:B:280:LEU:HD12	2.24	0.51
1:B:317:ARG:HD2	1:B:487:GLU:OE2	2.11	0.51
1:C:249:VAL:CG2	1:C:276:ALA:CB	2.88	0.51
1:A:181:GLY:CA	1:A:212:MET:HE3	2.40	0.51
1:A:479:VAL:CG2	1:A:527:GLN:OE1	2.58	0.51
1:B:263:GLN:O	1:B:266:TYR:CA	2.58	0.51
1:A:427:ILE:HD13	1:A:452:MET:HE3	1.91	0.51
1:A:35:MET:HB2	1:A:129:LEU:HD13	1.92	0.51
1:A:157:VAL:CG1	1:A:162:VAL:HG11	2.40	0.51
1:A:175:MET:HE2	1:A:196:LEU:HD12	1.92	0.51
1:A:429:LEU:HD21	1:A:452:MET:HG3	1.92	0.51
1:A:502:GLU:OE2	1:B:529:LYS:CE	2.55	0.51
1:A:453:MET:CB	1:A:543:MET:HE2	2.41	0.51
1:B:89:THR:HG23	1:B:400:ARG:HG2	1.93	0.51
1:A:479:VAL:HG23	1:A:527:GLN:OE1	2.11	0.51
1:B:298:ILE:N	1:B:298:ILE:HD13	2.25	0.51
1:C:416:MET:HE2	1:C:461:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HB3	1:A:325:THR:HB	1.91	0.51
1:C:416:MET:CE	1:C:461:ARG:HB2	2.41	0.51
1:A:28:ASP:HB2	1:A:44:ALA:O	2.10	0.51
1:A:260:GLN:O	1:A:261:LYS:O	2.28	0.51
1:A:453:MET:HB3	1:A:543:MET:HE1	1.88	0.50
1:A:265:ARG:O	1:A:266:TYR:O	2.29	0.50
1:B:256:ALA:O	1:B:259:ILE:HB	2.11	0.50
1:B:274:LYS:CD	1:B:277:ILE:CD1	2.72	0.50
1:B:293:LEU:C	1:B:295:LEU:H	2.14	0.50
1:C:358:LEU:HD21	1:C:457:VAL:HG11	1.94	0.50
1:C:39:VAL:HG13	1:C:119:GLN:HB3	1.90	0.50
1:A:236:GLU:CB	1:A:238:THR:HG23	2.38	0.50
1:B:311:ILE:O	1:B:314:THR:O	2.29	0.50
1:B:416:MET:CE	1:B:500:THR:HG21	2.41	0.50
1:C:249:VAL:HG22	1:C:276:ALA:HB2	1.91	0.50
1:B:154:VAL:CG2	1:B:208:ALA:HB2	2.42	0.50
1:C:329:ILE:CG1	1:C:347:ARG:HG3	2.41	0.50
1:B:99:ILE:HD13	1:B:149:ILE:HD12	1.94	0.50
1:C:340:HIS:HE1	1:C:554:ALA:H	1.59	0.50
1:A:523:GLN:O	1:A:526:ALA:N	2.44	0.50
1:B:381:HIS:HD2	1:B:428:ARG:HH21	1.59	0.50
1:C:439:SER:HA	3:C:1556:PO4:P	2.51	0.50
1:A:401:ARG:HE	1:A:405:HIS:HE1	1.59	0.50
1:A:535:ILE:HG22	1:A:539:MET:CE	2.42	0.50
1:C:131:MET:HE1	1:C:151:ALA:HB1	1.93	0.50
1:B:97:ARG:NH2	1:B:188:MET:CE	2.68	0.50
1:C:38:THR:OG1	1:C:121:ASP:N	2.34	0.49
1:C:181:GLY:O	1:C:212:MET:HE3	2.12	0.49
1:C:416:MET:CE	1:C:460:VAL:HB	2.42	0.49
1:B:308:ARG:HB3	1:B:471:ILE:HG21	1.93	0.49
1:C:39:VAL:HG13	1:C:119:GLN:CB	2.42	0.49
1:C:370:LEU:C	1:C:372:GLY:H	2.15	0.49
1:B:286:ASN:H	1:B:287:PRO:C	2.14	0.49
1:A:493:MET:HE1	1:A:509:MET:HE3	1.92	0.49
1:B:275:LYS:C	1:B:277:ILE:N	2.53	0.49
1:C:-1:ASP:O	1:C:0:PRO:C	2.49	0.49
1:B:9:ILE:HG21	1:B:16:LEU:HD23	1.93	0.49
1:B:264:ASP:HA	1:B:267:GLU:CB	2.42	0.49
1:A:274:LYS:HA	1:A:277:ILE:CG2	2.43	0.49
1:A:278:ALA:CA	1:A:282:LEU:HD13	2.42	0.49
1:A:403:ILE:HA	4:A:2080:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:MET:HE1	1:C:521:MET:SD	2.51	0.49
1:A:263:GLN:O	1:A:264:ASP:C	2.52	0.48
1:A:340:HIS:HB2	1:A:356:ALA:O	2.13	0.48
1:A:99:ILE:CG2	1:A:103:PHE:HE1	2.26	0.48
1:A:460:VAL:O	1:A:461:ARG:HG3	2.13	0.48
1:B:181:GLY:C	1:B:212:MET:HE3	2.34	0.48
1:B:237:ASP:OD1	1:B:239:ASP:HB2	2.12	0.48
1:C:330:LEU:O	1:C:346:THR:CG2	2.61	0.48
1:B:281:GLY:O	1:B:289:GLY:O	2.32	0.48
1:B:427:ILE:HG21	1:B:452:MET:HE2	1.95	0.48
1:C:193:ILE:CG2	1:C:196:LEU:HB2	2.43	0.48
1:B:551:GLY:O	1:B:552:ASP:C	2.51	0.48
1:C:531:GLY:CA	4:C:2020:HOH:O	2.58	0.48
1:A:335:ILE:HG13	1:A:336:LEU:N	2.28	0.48
1:A:452:MET:HE1	1:A:457:VAL:HG21	1.95	0.48
1:B:8:THR:O	1:B:9:ILE:C	2.48	0.48
1:A:377:SER:CB	1:A:426:THR:HG22	2.41	0.48
1:B:535:ILE:HG22	1:B:539:MET:HE2	1.93	0.48
1:A:165:PRO:HG2	1:A:170:MET:SD	2.53	0.48
1:C:333:VAL:HG12	1:C:334:GLY:N	2.28	0.48
1:A:414:ARG:N	1:A:415:PRO:HD2	2.28	0.48
1:C:370:LEU:O	1:C:372:GLY:N	2.47	0.48
1:C:468:MET:HB2	1:C:495:PHE:CZ	2.48	0.48
1:C:195:GLU:OE2	1:C:461:ARG:NH1	2.47	0.48
1:A:181:GLY:C	1:A:212:MET:CE	2.82	0.47
1:A:282:LEU:N	1:A:292:PRO:HG3	2.25	0.47
1:B:468:MET:HB2	1:B:495:PHE:CZ	2.48	0.47
1:A:220:ILE:HG12	2:F:896:TRP:CD1	2.50	0.47
1:A:263:GLN:O	1:A:265:ARG:N	2.47	0.47
1:B:4:ILE:HG22	1:B:222:LEU:CD1	2.43	0.47
1:A:273:LYS:HB2	1:A:299:PHE:CE2	2.50	0.47
1:B:303:GLU:CA	1:B:306:VAL:HG12	2.43	0.47
1:C:109:ASN:N	1:C:109:ASN:ND2	2.61	0.47
1:C:336:LEU:HB2	1:C:342:SER:HB3	1.97	0.47
1:C:516:ILE:HG22	1:C:521:MET:HG3	1.96	0.47
1:A:401:ARG:NH2	1:A:405:HIS:HE1	2.12	0.47
1:B:414:ARG:N	1:B:415:PRO:HD2	2.29	0.47
1:C:346:THR:HB	1:C:351:GLN:HG3	1.96	0.47
1:C:513:ILE:HD12	1:C:514:ALA:O	2.13	0.47
1:A:277:ILE:HG23	1:A:282:LEU:HD11	1.96	0.47
1:B:125:ASP:OD1	1:B:126:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HA	1:B:298:ILE:HG12	1.97	0.47
1:B:543:MET:O	1:B:545:ALA:N	2.45	0.47
1:C:54:GLN:NE2	1:C:56:PHE:CE1	2.82	0.47
1:C:197:SER:H	1:C:200:ILE:HD12	1.79	0.47
1:C:338:ARG:HG2	1:C:553:PHE:CE1	2.50	0.47
1:C:8:THR:O	1:C:9:ILE:CB	2.63	0.47
1:C:65:GLU:HB3	1:C:370:LEU:HD11	1.95	0.47
1:A:8:THR:C	1:A:9:ILE:HD13	2.35	0.47
1:B:8:THR:HG23	1:B:9:ILE:H	1.80	0.47
1:B:279:ALA:C	1:B:282:LEU:HD21	2.26	0.46
1:C:446:CYS:SG	4:C:2015:HOH:O	2.50	0.46
1:A:0:PRO:O	1:A:1:MET:HB2	2.15	0.46
1:B:274:LYS:CB	1:B:277:ILE:HG21	2.44	0.46
1:C:381:HIS:CD2	1:C:428:ARG:HH11	2.22	0.46
1:C:418:PRO:HG3	1:C:458:PRO:HD2	1.96	0.46
1:C:466:ILE:HG12	1:C:467:ALA:N	2.31	0.46
1:A:9:ILE:HG22	1:A:11:TRP:HB2	1.98	0.46
1:A:139:CYS:HA	4:A:2030:HOH:O	2.15	0.46
1:B:89:THR:CG2	1:B:400:ARG:HG2	2.46	0.46
1:B:207:PHE:O	1:B:211:GLN:HG2	2.15	0.46
1:B:261:LYS:C	1:B:262:LYS:O	2.52	0.46
1:B:266:TYR:CD1	1:B:266:TYR:C	2.89	0.46
1:B:280:LEU:N	1:B:280:LEU:CD1	2.79	0.46
1:C:131:MET:HE2	1:C:151:ALA:HB2	1.97	0.46
1:C:237:ASP:C	1:C:239:ASP:H	2.19	0.46
1:A:109:ASN:N	1:A:109:ASN:HD22	2.14	0.46
1:A:265:ARG:O	1:A:266:TYR:C	2.52	0.46
1:A:299:PHE:O	1:A:302:LEU:N	2.48	0.46
1:C:551:GLY:O	1:C:552:ASP:C	2.52	0.46
1:A:90:LEU:HD13	1:A:407:LYS:HG2	1.97	0.46
1:A:373:THR:O	1:A:373:THR:CG2	2.63	0.46
1:C:127:ASP:OD1	1:C:128:ILE:N	2.47	0.46
1:C:31:VAL:O	1:C:41:LEU:HD12	2.16	0.46
1:B:55:ASP:OD1	1:B:55:ASP:N	2.48	0.46
1:C:311:ILE:O	1:C:314:THR:O	2.33	0.46
1:C:330:LEU:HB3	1:C:346:THR:HG23	1.98	0.46
1:B:83:ARG:HH11	1:B:83:ARG:CG	2.28	0.45
1:B:286:ASN:N	1:B:287:PRO:CA	2.79	0.45
1:B:127:ASP:O	1:B:131:MET:HG3	2.16	0.45
1:A:74:PRO:O	1:A:79:LYS:HD3	2.16	0.45
1:A:224:GLU:O	2:F:892:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLY:CA	1:C:212:MET:HE1	2.46	0.45
1:A:9:ILE:HG13	1:A:218:ALA:HB2	1.98	0.45
1:B:295:LEU:HG	1:B:295:LEU:O	2.16	0.45
1:C:174:LYS:O	1:C:194:GLN:HG3	2.16	0.45
1:B:61:VAL:HG22	1:B:113:VAL:CG1	2.47	0.45
1:B:462:PRO:HB2	1:B:536:LEU:HD11	1.99	0.45
1:A:466:ILE:HD12	1:A:531:GLY:HA3	1.99	0.45
1:B:3:ASP:HB2	4:B:2002:HOH:O	2.17	0.45
1:B:260:GLN:HA	1:B:265:ARG:HH12	1.82	0.45
1:B:279:ALA:C	1:B:280:LEU:HD12	2.37	0.45
1:A:14:LYS:HD3	1:A:124:ASN:OD1	2.17	0.45
1:A:416:MET:HE1	1:A:461:ARG:HB2	1.92	0.45
1:A:543:MET:HE3	1:A:543:MET:HB3	1.92	0.45
1:C:484:LEU:HB2	1:C:487:GLU:HG3	1.98	0.45
1:A:175:MET:HE3	1:A:196:LEU:CD1	2.47	0.45
1:A:179:VAL:HG12	1:A:180:ALA:N	2.32	0.45
1:A:275:LYS:C	1:A:277:ILE:N	2.70	0.45
1:B:147:GLY:HA2	2:G:896:TRP:CA	2.47	0.45
1:B:198:GLU:O	1:B:202:LEU:HB2	2.17	0.45
1:B:273:LYS:O	1:B:275:LYS:N	2.50	0.45
1:C:147:GLY:H	2:H:896:TRP:HA	1.82	0.45
1:C:189:VAL:HB	1:C:509:MET:HB2	1.99	0.45
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.82	0.45
1:A:414:ARG:N	1:A:415:PRO:CD	2.80	0.45
1:A:7:LYS:C	1:A:8:THR:O	2.50	0.44
1:A:236:GLU:O	1:A:238:THR:N	2.49	0.44
1:A:452:MET:CE	1:A:457:VAL:HG21	2.46	0.44
1:B:68:PHE:CD1	1:B:68:PHE:C	2.90	0.44
1:B:286:ASN:N	1:B:287:PRO:HA	2.31	0.44
1:C:44:ALA:HB1	1:C:138:LEU:HD23	1.99	0.44
1:B:274:LYS:CG	1:B:277:ILE:HG21	2.46	0.44
1:C:206:ASN:OD1	1:C:518:PRO:HG3	2.18	0.44
1:A:284:ASP:C	1:A:286:ASN:H	2.20	0.44
1:A:420:LYS:HA	1:A:420:LYS:HD3	1.77	0.44
1:C:166:THR:HG23	1:C:169:GLU:OE2	2.18	0.44
1:A:3:ASP:N	1:A:3:ASP:OD1	2.50	0.44
1:A:266:TYR:O	1:A:268:ALA:N	2.51	0.44
1:B:368:ASP:OD1	1:B:368:ASP:N	2.50	0.44
1:B:63:TYR:HD2	1:B:115:VAL:HG22	1.82	0.44
1:B:401:ARG:HH21	1:B:405:HIS:HE1	1.65	0.44
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ARG:NH2	1:B:405:HIS:HE1	2.14	0.44
1:B:509:MET:HE2	1:B:511:ILE:HD11	1.99	0.44
1:B:303:GLU:HA	1:B:306:VAL:CG1	2.48	0.44
1:B:347:ARG:NH2	1:B:439:SER:O	2.51	0.44
1:B:535:ILE:HG22	1:B:539:MET:HE3	1.96	0.44
1:B:283:SER:N	1:B:284:ASP:C	2.71	0.44
1:B:427:ILE:HD13	1:B:452:MET:CE	2.48	0.44
1:A:1:MET:HG2	1:A:22:ARG:HA	1.99	0.44
1:A:7:LYS:O	1:A:9:ILE:N	2.50	0.44
1:A:472:LEU:HD12	1:A:477:PHE:HB3	1.99	0.43
1:B:246:LYS:HA	1:B:302:LEU:HD21	2.00	0.43
1:B:307:VAL:O	1:B:311:ILE:HG13	2.18	0.43
1:A:55:ASP:HB3	1:A:56:PHE:HD1	1.83	0.43
1:A:177:LEU:CD1	1:A:191:SER:HB3	2.40	0.43
1:C:553:PHE:O	1:C:553:PHE:CD1	2.71	0.43
1:B:35:MET:HE3	1:B:129:LEU:HB2	2.00	0.43
1:B:248:LEU:HG	1:B:249:VAL:HG23	1.99	0.43
1:C:246:LYS:O	1:C:250:GLY:N	2.50	0.43
1:C:198:GLU:OE2	1:C:532:ARG:NH2	2.47	0.43
1:A:516:ILE:HG22	1:A:521:MET:HG2	2.01	0.43
1:A:275:LYS:CG	1:A:276:ALA:N	2.76	0.43
1:B:263:GLN:CG	1:B:264:ASP:H	2.04	0.43
1:C:256:ALA:O	1:C:259:ILE:N	2.50	0.43
1:C:345:PHE:O	1:C:351:GLN:HA	2.19	0.43
1:B:551:GLY:O	1:B:552:ASP:O	2.37	0.43
1:C:131:MET:CE	1:C:151:ALA:CB	2.97	0.43
1:C:329:ILE:HG13	1:C:347:ARG:HG3	2.00	0.43
1:B:107:PHE:CZ	1:B:109:ASN:HB2	2.54	0.43
1:B:283:SER:N	1:B:285:GLU:N	2.67	0.43
1:B:338:ARG:HA	1:B:553:PHE:CE1	2.38	0.43
1:C:180:ALA:O	1:C:187:MET:N	2.42	0.43
1:C:303:GLU:O	1:C:307:VAL:HG12	2.18	0.43
1:A:7:LYS:HG2	1:A:17:VAL:HG13	2.01	0.42
1:B:65:GLU:HG3	1:B:88:GLU:HG2	2.01	0.42
1:A:543:MET:O	1:A:545:ALA:N	2.44	0.42
1:C:329:ILE:HG12	1:C:347:ARG:HG3	2.01	0.42
1:C:466:ILE:CG1	1:C:467:ALA:N	2.83	0.42
1:A:249:VAL:HG12	1:A:253:ILE:HG13	2.00	0.42
1:B:145:PHE:CZ	1:B:149:ILE:HD12	2.54	0.42
1:B:381:HIS:HD2	1:B:428:ARG:NE	2.12	0.42
1:B:490:LEU:HG	1:B:490:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LEU:HD12	1:C:97:ARG:HH22	1.80	0.42
1:B:109:ASN:N	1:B:109:ASN:HD22	2.17	0.42
1:B:195:GLU:HA	1:B:504:LEU:O	2.19	0.42
1:A:201:VAL:HG21	1:A:504:LEU:HD12	2.02	0.42
1:B:273:LYS:C	1:B:275:LYS:H	2.23	0.42
1:B:286:ASN:CA	1:B:287:PRO:O	2.68	0.42
1:C:177:LEU:HD21	1:C:205:VAL:HG23	2.01	0.42
1:C:361:GLY:O	1:C:364:GLU:HG2	2.20	0.42
1:C:465:GLY:HA2	1:C:497:VAL:O	2.20	0.42
1:A:265:ARG:HH22	1:A:318:ILE:CA	2.32	0.42
1:A:274:LYS:CE	1:A:274:LYS:CA	2.92	0.42
1:B:99:ILE:O	1:B:100:ARG:C	2.58	0.42
1:C:128:ILE:CD1	1:C:153:ARG:CB	2.95	0.42
1:A:121:ASP:O	1:A:122:LEU:HB2	2.20	0.41
1:B:468:MET:CB	1:B:495:PHE:CZ	3.03	0.41
1:C:189:VAL:HB	1:C:509:MET:CB	2.50	0.41
1:A:274:LYS:HZ3	1:A:277:ILE:HD13	1.84	0.41
1:C:11:TRP:CZ3	1:C:215:VAL:HG21	2.56	0.41
1:C:28:ASP:HB2	1:C:44:ALA:O	2.20	0.41
1:C:453:MET:HG3	1:C:459:LEU:HD12	2.02	0.41
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.81	0.41
1:B:279:ALA:C	1:B:282:LEU:CD2	2.79	0.41
1:C:156:TRP:HA	1:C:160:ALA:O	2.19	0.41
1:C:317:ARG:NH2	1:C:321:ARG:NH2	2.67	0.41
1:A:8:THR:C	1:A:9:ILE:CG1	2.89	0.41
1:B:286:ASN:H	1:B:287:PRO:HA	1.85	0.41
1:C:163:LEU:HD22	1:C:211:GLN:HG2	2.02	0.41
1:C:193:ILE:O	1:C:505:THR:HG22	2.20	0.41
1:C:380:LEU:HD21	1:C:444:THR:HG21	2.01	0.41
1:C:399:GLY:O	1:C:403:ILE:HG13	2.20	0.41
1:A:135:SER:HB2	1:A:149:ILE:CG1	2.48	0.41
1:B:35:MET:HB2	1:B:129:LEU:HD13	2.01	0.41
1:B:287:PRO:CB	1:B:288:THR:CA	2.77	0.41
1:B:427:ILE:HG21	1:B:452:MET:CE	2.51	0.41
1:B:544:ASP:OD1	1:B:544:ASP:C	2.59	0.41
1:B:553:PHE:HA	1:B:554:ALA:HA	1.72	0.41
1:C:163:LEU:O	1:C:164:ASN:C	2.59	0.41
1:C:553:PHE:O	1:C:553:PHE:HD1	2.03	0.41
1:C:334:GLY:HA2	1:C:342:SER:OG	2.20	0.41
1:A:127:ASP:OD1	1:A:128:ILE:HG12	2.21	0.41
1:A:277:ILE:CG2	1:A:278:ALA:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:NH2	1:A:405:HIS:CE1	2.87	0.41
1:A:253:ILE:HD11	1:A:299:PHE:CE1	2.53	0.41
1:A:281:GLY:O	1:A:292:PRO:CG	2.69	0.41
1:A:397[A]:SER:HA	1:A:398:PRO:HD2	1.93	0.41
1:B:336:LEU:C	1:B:337:PRO:O	2.59	0.41
1:B:450:LEU:HD23	1:B:450:LEU:HA	1.94	0.41
1:A:181:GLY:N	1:A:212:MET:CE	2.84	0.41
1:A:186:VAL:O	1:A:511:ILE:HD13	2.20	0.41
1:A:281:GLY:O	1:A:292:PRO:HG3	2.21	0.41
1:B:273:LYS:HD2	1:B:299:PHE:CD2	2.55	0.41
1:B:512:LYS:C	1:B:513:ILE:HG23	2.41	0.41
1:C:493:MET:CE	1:C:495:PHE:CD1	3.04	0.41
1:A:28:ASP:HB3	1:A:141:SER:HB2	2.03	0.41
1:A:147:GLY:HA3	1:A:148:PRO:HA	1.86	0.41
1:A:245:MET:CE	1:A:299:PHE:CA	2.98	0.41
1:A:538:GLU:HA	1:A:541:LYS:HD2	2.03	0.41
1:B:286:ASN:H	1:B:287:PRO:CA	2.34	0.41
1:C:46:PHE:CB	1:C:111:VAL:HG22	2.51	0.41
1:C:177:LEU:HD21	1:C:205:VAL:CG2	2.51	0.41
1:C:381:HIS:HD2	1:C:428:ARG:HD2	1.80	0.41
1:A:495:PHE:CZ	1:A:524:ALA:HB1	2.56	0.40
1:B:263:GLN:CG	1:B:264:ASP:N	2.70	0.40
1:A:308:ARG:NH2	1:A:473:GLU:OE2	2.55	0.40
1:B:191:SER:OG	1:B:507:LEU:O	2.40	0.40
1:B:269:VAL:CG1	1:B:270:GLY:N	2.83	0.40
1:B:308:ARG:CZ	1:B:471:ILE:HG23	2.51	0.40
1:C:256:ALA:HB1	1:C:268:ALA:HB3	2.02	0.40
1:B:99:ILE:HD13	1:B:99:ILE:HA	1.91	0.40
1:C:256:ALA:HB2	1:C:268:ALA:HB1	2.03	0.40
1:A:279:ALA:O	1:A:280:LEU:HD22	2.21	0.40
1:A:439:SER:HA	3:A:1614:PO4:O1	2.22	0.40
1:B:15:THR:O	1:B:35:MET:HA	2.21	0.40
1:B:238:THR:HG22	1:B:290:TYR:OH	2.22	0.40
1:C:256:ALA:CB	1:C:268:ALA:HB1	2.51	0.40
1:C:274:LYS:O	1:C:277:ILE:CB	2.70	0.40
1:A:291:ASP:O	1:A:294:LYS:HB3	2.21	0.40
1:B:335:ILE:HG13	1:B:342:SER:OG	2.21	0.40
1:B:349:GLU:OE1	1:B:437:ASN:ND2	2.54	0.40
1:B:446:CYS:SG	1:B:539:MET:HE1	2.62	0.40
1:C:333:VAL:HG13	1:C:454:ASP:HB2	2.03	0.40
1:C:517:THR:OG1	1:C:520:ILE:HG12	2.21	0.40

All (2) 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:A:8:THR:OG1	1:C:540:ASN:O[2_555]	1.87	0.33
1:B:6:ARG:NH2	1:C:224:GLU:OE2[3_565]	2.10	0.10

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	570/726 (78%)	502 (88%)	37 (6%)	31 (5%)	2 2
1	B	556/726 (77%)	490 (88%)	41 (7%)	25 (4%)	2 3
1	C	535/726 (74%)	476 (89%)	32 (6%)	27 (5%)	2 2
2	F	5/14 (36%)	4 (80%)	0	1 (20%)	0 0
2	G	6/14 (43%)	5 (83%)	0	1 (17%)	0 0
2	H	3/14 (21%)	2 (67%)	1 (33%)	0	100 100
All	All	1675/2220 (76%)	1479 (88%)	111 (7%)	85 (5%)	2 2

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	55	ASP
1	A	239	ASP
1	A	248	LEU
1	A	262	LYS
1	A	263	GLN
1	A	266	TYR
1	A	275	LYS
1	A	294	LYS
1	A	554	ALA
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	264	ASP
1	B	276	ALA
1	B	278	ALA
1	B	287	PRO
1	B	290	TYR
1	B	291	ASP
1	B	292	PRO
1	B	552	ASP
1	B	554	ALA
1	C	8	THR
1	C	53	GLY
1	C	158	ASP
1	C	237	ASP
1	C	244	LYS
1	C	248	LEU
1	C	262	LYS
1	C	271	ALA
1	C	275	LYS
1	C	277	ILE
1	C	397	SER
1	C	544	ASP
1	A	54	GLN
1	A	246	LYS
1	A	261	LYS
1	A	264	ASP
1	A	267	GLU
1	A	276	ALA
1	A	278	ALA
1	A	284	ASP
1	A	318	ILE
1	A	396	GLY
1	B	261	LYS
1	B	262	LYS
1	B	269	VAL
1	B	273	LYS
1	B	274	LYS
1	B	277	ILE
1	B	396	GLY
1	B	439	SER
1	C	1	MET
1	C	9	ILE
1	C	36	GLY

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Mol	Chain	Res	Type
1	C	52	PRO
1	C	260	GLN
1	C	261	LYS
1	C	263	GLN
1	C	371	GLU
1	C	439	SER
1	A	244	LYS
1	A	280	LEU
1	A	283	SER
1	A	290	TYR
1	B	279	ALA
1	B	285	GLU
1	B	371	GLU
1	C	246	LYS
1	B	294	LYS
1	C	245	MET
1	C	273	LYS
1	C	314	THR
2	G	894	GLY
1	A	237	ASP
1	A	292	PRO
1	A	439	SER
1	A	552	ASP
1	B	267	GLU
1	B	397	SER
2	F	892	ARG
1	A	1	MET
1	A	281	GLY
1	B	52	PRO
1	C	51	LYS
1	C	250	GLY
1	A	555	PRO

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	432/578 (75%)	401 (93%)	31 (7%)	14 29
1	B	428/578 (74%)	397 (93%)	31 (7%)	14 29
1	C	364/578 (63%)	348 (96%)	16 (4%)	28 53
2	F	5/12 (42%)	3 (60%)	2 (40%)	0 0
2	G	6/12 (50%)	5 (83%)	1 (17%)	2 3
2	H	2/12 (17%)	2 (100%)	0	100 100
All	All	1237/1770 (70%)	1156 (94%)	81 (6%)	16 34

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASP
1	A	1	MET
1	A	3	ASP
1	A	7	LYS
1	A	35	MET
1	A	54	GLN
1	A	55	ASP
1	A	60	THR
1	A	80	ARG
1	A	83	ARG
1	A	140	LEU
1	A	153	ARG
1	A	157	VAL
1	A	186	VAL
1	A	200	ILE
1	A	221	ASP
1	A	239	ASP
1	A	280	LEU
1	A	282	LEU
1	A	283	SER
1	A	290	TYR
1	A	312	LEU
1	A	355	VAL
1	A	401	ARG
1	A	430	VAL
1	A	457	VAL
1	A	463	VAL
1	A	481	SER
1	A	505	THR
1	A	553	PHE

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Mol	Chain	Res	Type
1	A	613	TRP
1	B	-1	ASP
1	B	1	MET
1	B	8	THR
1	B	10	GLU
1	B	31	VAL
1	B	64	GLN
1	B	83	ARG
1	B	120	HIS
1	B	177	LEU
1	B	178	VAL
1	B	188	MET
1	B	194	GLN
1	B	200	ILE
1	B	202	LEU
1	B	242	LYS
1	B	290	TYR
1	B	293	LEU
1	B	308	ARG
1	B	309	ARG
1	B	333	VAL
1	B	335	ILE
1	B	336	LEU
1	B	368	ASP
1	B	431	SER
1	B	445	VAL
1	B	449	SER
1	B	457	VAL
1	B	489	HIS
1	B	505	THR
1	B	518	PRO
1	B	553	PHE
1	C	34	THR
1	C	39	VAL
1	C	77	PHE
1	C	90	LEU
1	C	109	ASN
1	C	175	MET
1	C	188	MET
1	C	194	GLN
1	C	371	GLU
1	C	379	LEU

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Mol	Chain	Res	Type
1	C	445	VAL
1	C	448	SER
1	C	496	LYS
1	C	497	VAL
1	C	523	GLN
1	C	553	PHE
2	F	892	ARG
2	F	897	ARG
2	G	892	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	109	ASN
1	A	112	GLN
1	A	119	GLN
1	A	209	HIS
1	A	225	HIS
1	A	286	ASN
1	A	340	HIS
1	A	381	HIS
1	A	405	HIS
1	A	508	GLN
1	B	26	GLN
1	B	62	ASN
1	B	64	GLN
1	B	109	ASN
1	B	112	GLN
1	B	119	GLN
1	B	206	ASN
1	B	209	HIS
1	B	381	HIS
1	B	405	HIS
1	B	489	HIS
1	C	62	ASN
1	C	109	ASN
1	C	112	GLN
1	C	119	GLN
1	C	225	HIS
1	C	340	HIS
1	C	381	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	PO4	B	1557	-	4,4,4	0.73	0	6,6,6	0.81	0
3	PO4	C	1556	-	4,4,4	0.81	0	6,6,6	1.02	1 (16%)
3	PO4	A	1614	-	4,4,4	0.92	0	6,6,6	1.37	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1614	PO4	O4-P-O3	2.38	115.30	107.91
3	C	1556	PO4	O4-P-O2	2.26	114.96	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1557	PO4	1	0
3	C	1556	PO4	1	0
3	A	1614	PO4	1	0

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	573/726 (78%)	-0.42	11 (1%) 66 62	24, 34, 123, 161	0
1	B	558/726 (76%)	-0.47	2 (0%) 92 91	24, 33, 109, 147	0
1	C	539/726 (74%)	-0.11	14 (2%) 56 50	53, 87, 184, 253	0
2	F	7/14 (50%)	-0.23	0 100 100	40, 67, 84, 94	0
2	G	8/14 (57%)	-0.22	0 100 100	37, 68, 86, 93	0
2	H	5/14 (35%)	-0.07	0 100 100	82, 97, 103, 107	0
All	All	1690/2220 (76%)	-0.33	27 (1%) 72 68	24, 49, 135, 253	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	ALA	5.4
1	A	278	ALA	4.4
1	C	268	ALA	3.7
1	C	278	ALA	3.7
1	C	269	VAL	3.5
1	A	254	ALA	3.4
1	A	247	ASP	3.3
1	A	251	ALA	3.2
1	C	276	ALA	3.1
1	A	279	ALA	3.1
1	C	472	LEU	3.1
1	C	297	ALA	3.1
1	A	611	ILE	2.9
1	C	-1	ASP	2.6
1	A	293	LEU	2.5
1	C	249	VAL	2.5
1	C	553	PHE	2.5
1	A	255	ALA	2.4
1	C	237	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	253	ILE	2.4
1	B	548	ALA	2.4
1	B	288	THR	2.3
1	C	262	LYS	2.3
1	C	8	THR	2.3
1	A	264	ASP	2.3
1	A	610	ALA	2.1
1	A	280	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	C	1556	5/5	0.88	0.19	86,89,109,117	0
3	PO4	B	1557	5/5	0.97	0.10	76,82,92,104	0
3	PO4	A	1614	5/5	0.98	0.10	58,60,69,75	0

6.5 Other polymers (i)

There are no such residues in this entry.