Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:48 PM EDT

PDB ID	:	1W91
Title	:	crystal structure of 1,4-BETA-D-XYLAN XYLOHYDROLASE solve using anomalous signal from Seleniomethionine
Authors	:	Jakoncic, J.; Shoham, G.; Stojanoff, V.
Deposited on	:	2004-10-05
Resolution	:	2.20 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:

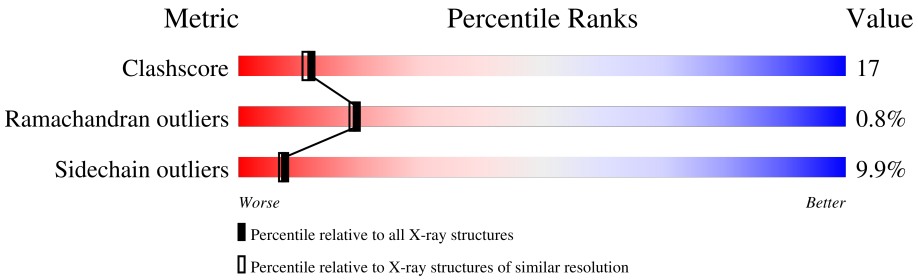
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	503	66% 26% 6% ••
1	B	503	70% 23% 5% ••
1	C	503	67% 25% 6% ••
1	D	503	69% 23% 6% ••
1	E	503	70% 23% 5% ••
1	F	503	72% 21% 5% ••
1	G	503	70% 23% 5% ••
1	H	503	72% 21% 6% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 35545 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 BETA-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	B	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	C	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	D	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	E	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	F	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	G	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	H	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	ARG	PRO	conflict	UNP Q9ZFM2
A	446	GLN	SER	conflict	UNP Q9ZFM2
B	445	ARG	PRO	conflict	UNP Q9ZFM2
B	446	GLN	SER	conflict	UNP Q9ZFM2
C	445	ARG	PRO	conflict	UNP Q9ZFM2
C	446	GLN	SER	conflict	UNP Q9ZFM2
D	445	ARG	PRO	conflict	UNP Q9ZFM2
D	446	GLN	SER	conflict	UNP Q9ZFM2
E	445	ARG	PRO	conflict	UNP Q9ZFM2
E	446	GLN	SER	conflict	UNP Q9ZFM2
F	445	ARG	PRO	conflict	UNP Q9ZFM2
F	446	GLN	SER	conflict	UNP Q9ZFM2
G	445	ARG	PRO	conflict	UNP Q9ZFM2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	446	GLN	SER	conflict	UNP Q9ZFM2
H	445	ARG	PRO	conflict	UNP Q9ZFM2
H	446	GLN	SER	conflict	UNP Q9ZFM2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	363	Total O 363 363	0	0
2	B	317	Total O 317 317	0	0
2	C	371	Total O 371 371	0	0
2	D	340	Total O 340 340	0	0
2	E	347	Total O 347 347	0	0
2	F	414	Total O 414 414	0	0
2	G	340	Total O 340 340	0	0
2	H	397	Total O 397 397	0	0

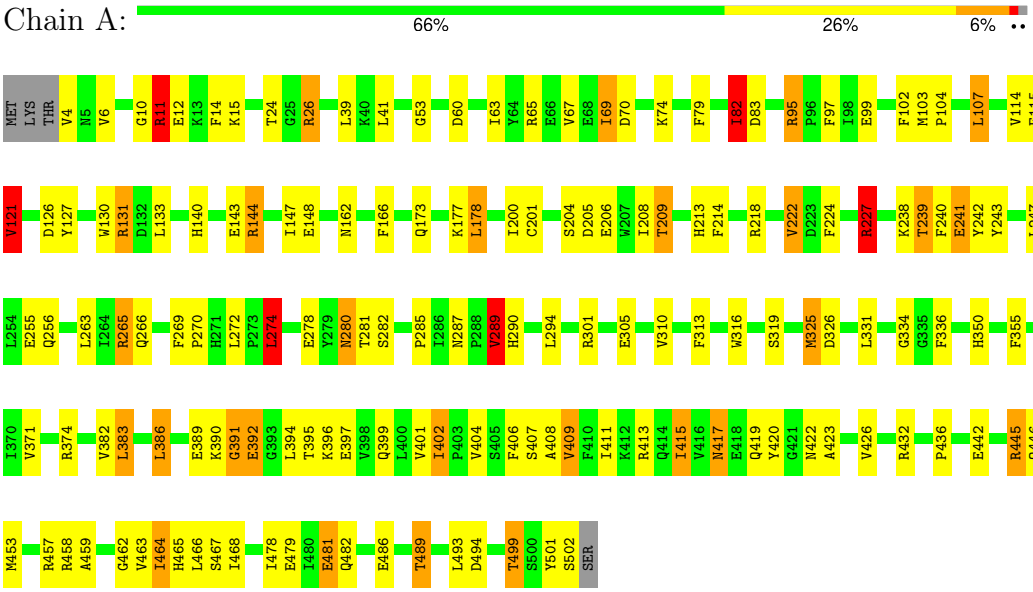
3 Residue-property plots (i)

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. 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.

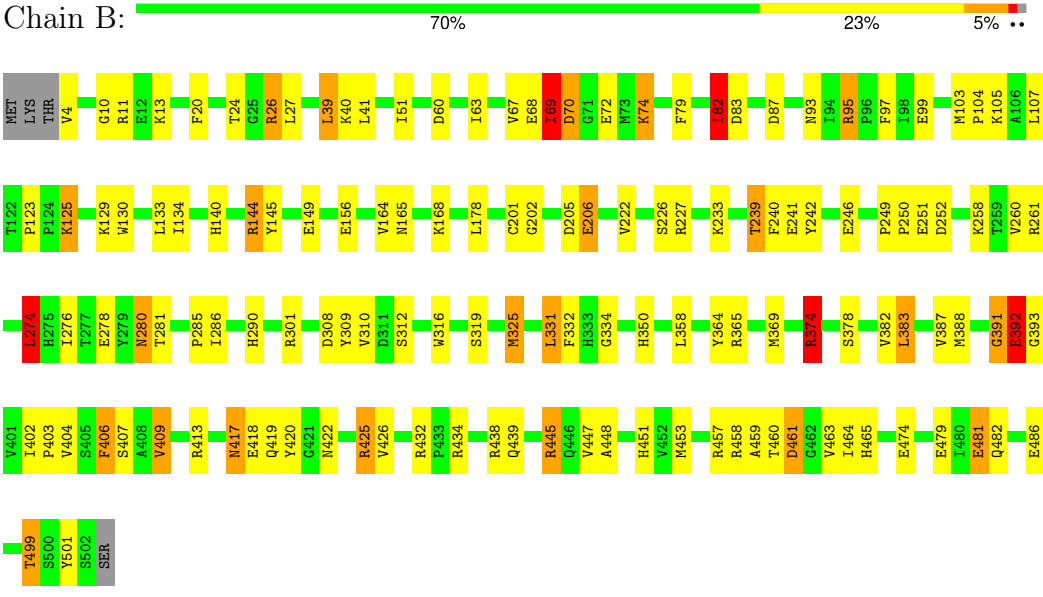
• Molecule 1: BETA-XYLOSIDASE

Chain A:



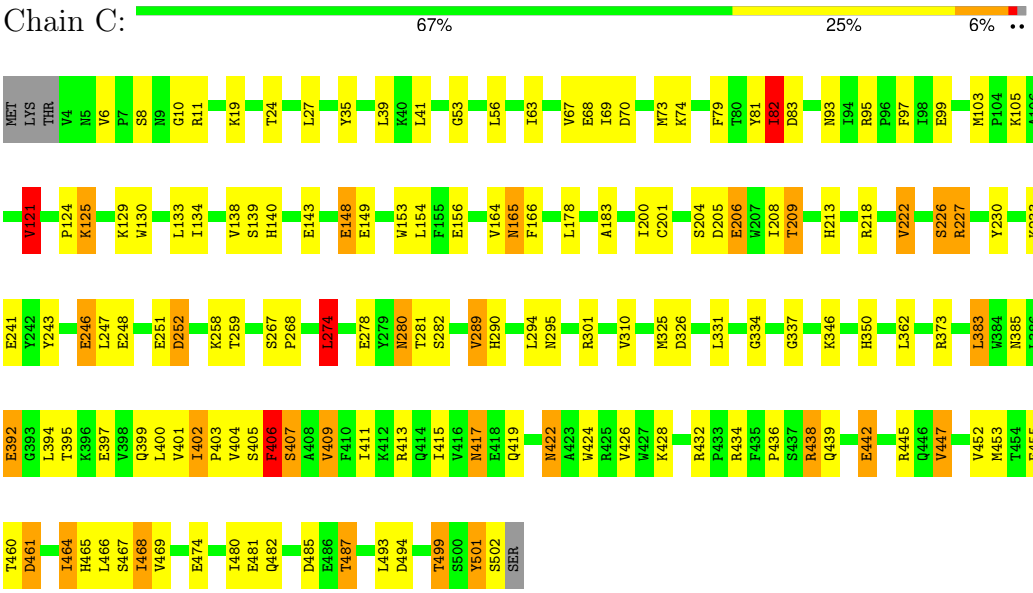
• Molecule 1: BETA-XYLOSIDASE

Chain B:



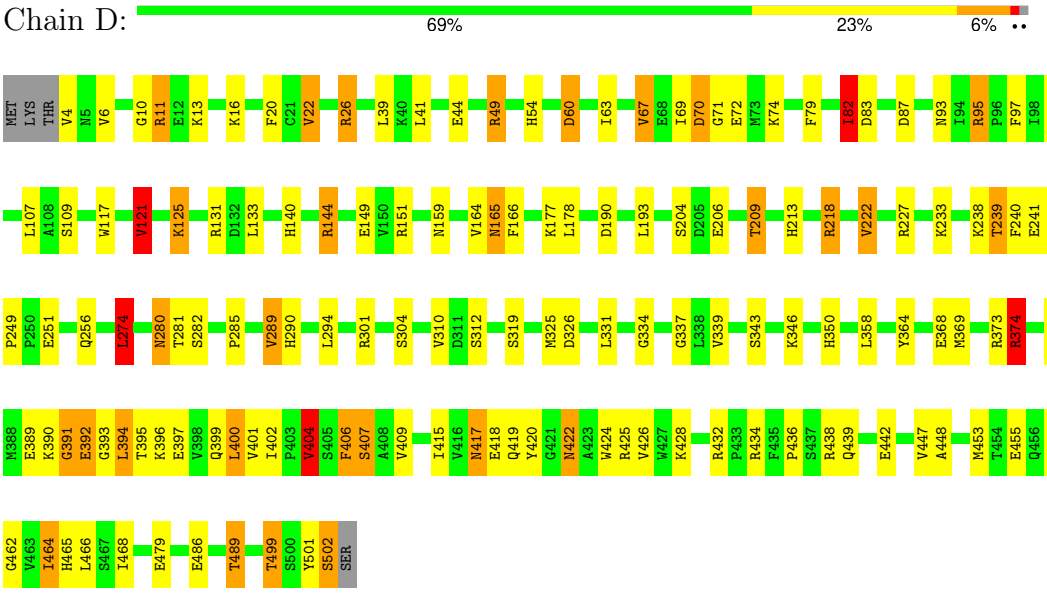
• Molecule 1: BETA-XYLOSIDASE

Chain C:



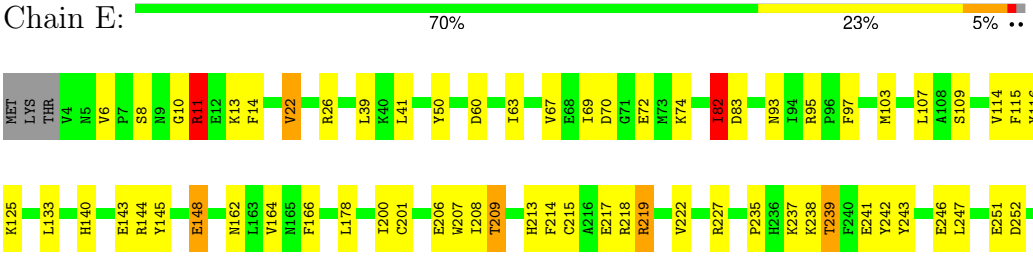
• Molecule 1: BETA-XYLOSIDASE

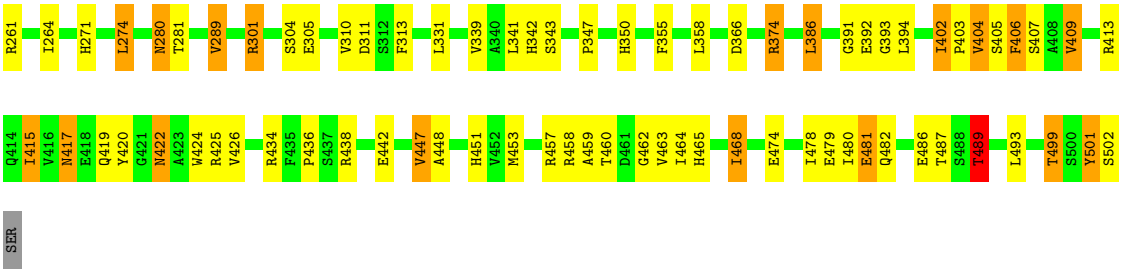
Chain D:



• Molecule 1: BETA-XYLOSIDASE

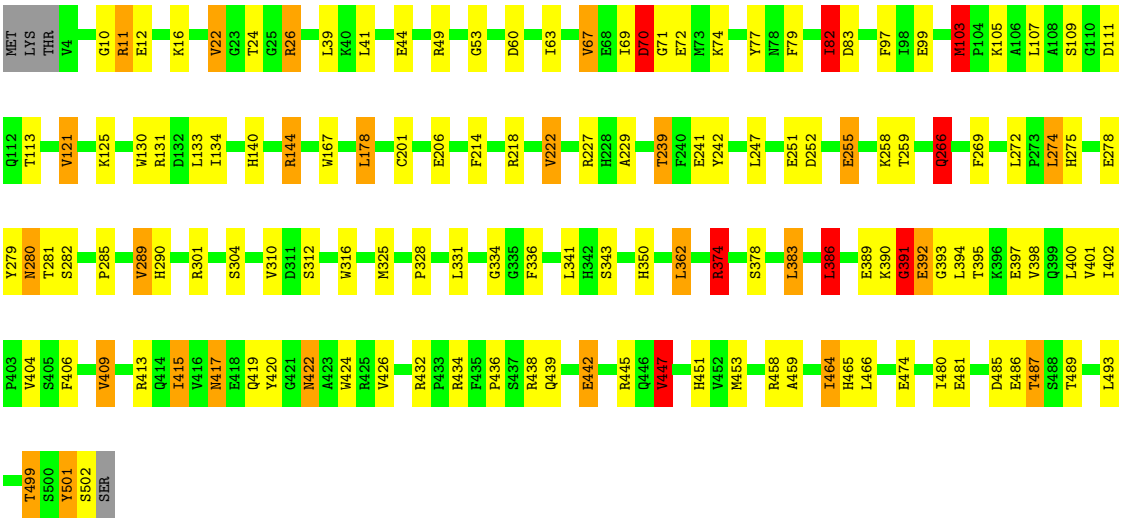
Chain E:





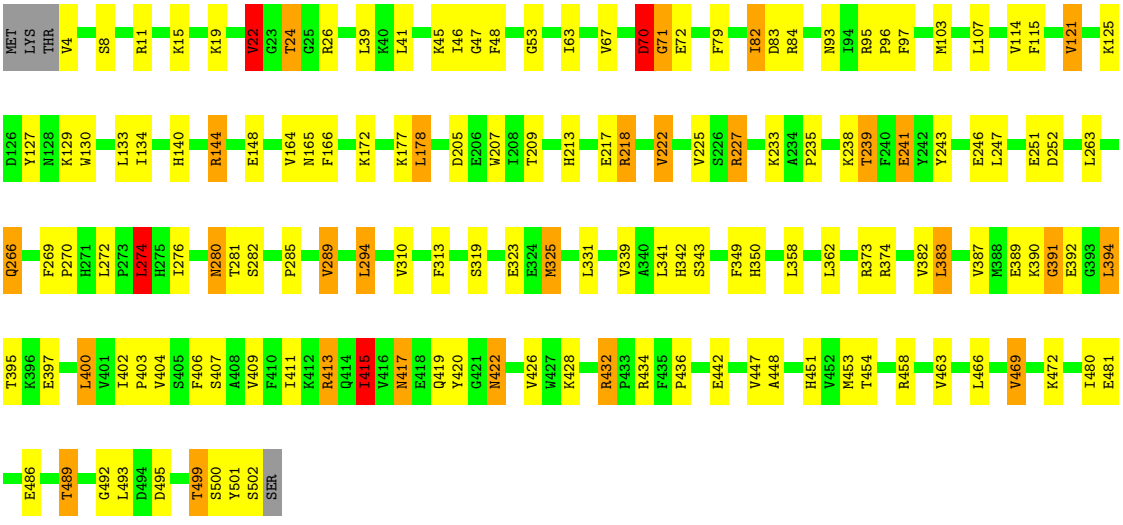
• Molecule 1: BETA-XYLOSIDASE

Chain F:



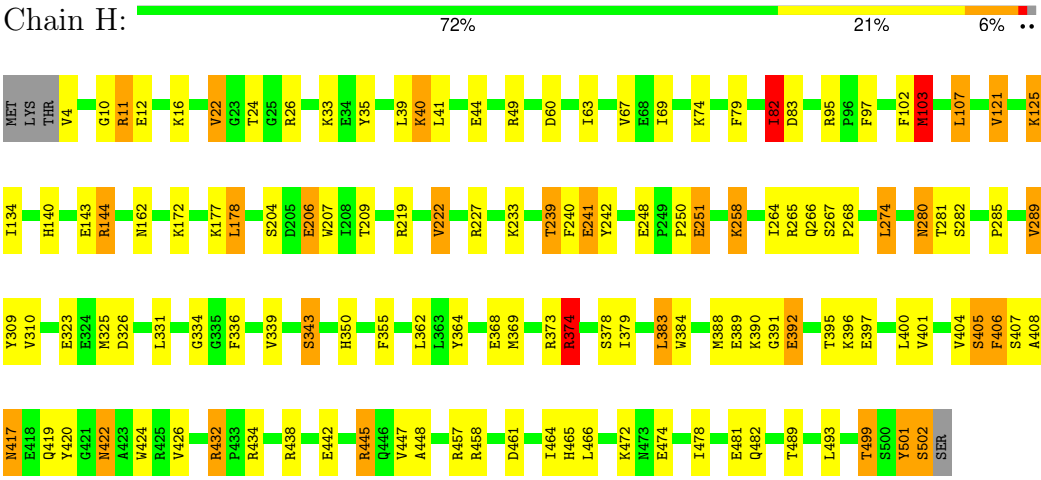
• Molecule 1: BETA-XYLOSIDASE

Chain G:



• Molecule 1: BETA-XYLOSIDASE

Chain H:


72%
21%
6%
MET LYS THR V4 G10 R11 E12 K16 V22 G23 T24 G25 R26 K33 E34 Y35 L39 K40 L41 E44 R49 D60 I63 V67 E68 I69 K74 F79 I82 D83 R95 P96 F97 F102 M103 L107 V121 K125 W130 L133
I134 H140 E143 R144 N162 K172 K177 L178 S204 D205 E206 W207 I208 T209 R219 V222 R227 K233 T239 F240 E241 Y242 E248 P249 P250 E251 K258 I264 R265 Q266 S267 P268 L274 N280 T281 S282 P285 V289 H290 L294
Y309 V310 E323 E324 M325 D326 L331 G334 G335 F336 V339 S343 H350 F355 L362 L363 Y364 E368 M369 R373 R374 S378 I379 L383 W384 M388 E389 K390 G391 E392 T395 K396 E397 L400 V401 V404 S405 F406 S407 A408 V409 I415 V416
N417 E418 Q419 Y420 G421 N422 A423 W424 R425 V426 R432 P433 R434 R438 E442 R445 Q446 V447 A448 R457 R458 D461 I464 H465 L466 K472 N473 E474 I478 E481 Q482 T489 L493 T499 S500 Y501 S502 SER

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.70Å 166.02Å 313.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (8.00-2.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35545	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.05	6/4198 (0.1%)	1.04	23/5699 (0.4%)
1	B	1.04	4/4198 (0.1%)	1.00	18/5699 (0.3%)
1	C	1.09	9/4198 (0.2%)	1.03	19/5699 (0.3%)
1	D	1.07	1/4197 (0.0%)	1.01	19/5696 (0.3%)
1	E	1.10	9/4198 (0.2%)	1.06	14/5699 (0.2%)
1	F	1.11	8/4198 (0.2%)	1.09	27/5699 (0.5%)
1	G	1.03	3/4198 (0.1%)	1.05	22/5699 (0.4%)
1	H	1.13	6/4198 (0.1%)	1.08	24/5699 (0.4%)
All	All	1.08	46/33583 (0.1%)	1.05	166/45589 (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	B	0	1
1	F	0	3
1	H	0	2
All	All	0	6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	TYR	C-N	15.40	1.69	1.34
1	E	501	TYR	C-N	15.16	1.69	1.34
1	F	501	TYR	C-N	11.59	1.60	1.34
1	F	442	GLU	CG-CD	10.00	1.67	1.51
1	A	501	TYR	C-N	9.61	1.56	1.34
1	G	442	GLU	CG-CD	9.25	1.65	1.51
1	A	442	GLU	CG-CD	8.78	1.65	1.51
1	D	442	GLU	CG-CD	8.59	1.64	1.51
1	H	103	MET	CB-CG	7.94	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	442	GLU	CG-CD	7.93	1.63	1.51
1	B	501	TYR	C-N	7.77	1.51	1.34
1	F	103	MET	CB-CG	7.72	1.76	1.51
1	E	148	GLU	CG-CD	7.63	1.63	1.51
1	E	246	GLU	CG-CD	6.81	1.62	1.51
1	H	355	PHE	CE1-CZ	6.81	1.50	1.37
1	E	442	GLU	CG-CD	6.75	1.62	1.51
1	E	447	VAL	CB-CG1	-6.04	1.40	1.52
1	F	255	GLU	CG-CD	5.95	1.60	1.51
1	C	442	GLU	CG-CD	5.94	1.60	1.51
1	F	266	GLN	CG-CD	5.87	1.64	1.51
1	H	501	TYR	C-N	5.86	1.47	1.34
1	B	156	GLU	CG-CD	5.81	1.60	1.51
1	C	206	GLU	CG-CD	5.78	1.60	1.51
1	H	241	GLU	CB-CG	-5.75	1.41	1.52
1	C	82	ILE	CB-CG2	5.65	1.70	1.52
1	C	252	ASP	CB-CG	5.61	1.63	1.51
1	F	77	TYR	CD1-CE1	5.49	1.47	1.39
1	G	241	GLU	CB-CG	-5.44	1.41	1.52
1	A	255	GLU	CG-CD	5.40	1.60	1.51
1	E	116	TYR	CE1-CZ	5.38	1.45	1.38
1	B	206	GLU	CB-CG	5.37	1.62	1.52
1	C	81	TYR	CD2-CE2	5.30	1.47	1.39
1	C	138	VAL	CB-CG1	5.30	1.64	1.52
1	E	481	GLU	CG-CD	5.30	1.59	1.51
1	F	432	ARG	CZ-NH1	5.30	1.40	1.33
1	C	183	ALA	CA-CB	5.29	1.63	1.52
1	G	432	ARG	CZ-NH1	5.29	1.40	1.33
1	A	131	ARG	CB-CG	-5.23	1.38	1.52
1	B	206	GLU	CG-CD	5.23	1.59	1.51
1	A	355	PHE	CE1-CZ	5.21	1.47	1.37
1	F	167	TRP	CB-CG	5.18	1.59	1.50
1	A	241	GLU	CB-CG	-5.12	1.42	1.52
1	E	481	GLU	CB-CG	5.12	1.61	1.52
1	H	44	GLU	CG-CD	5.06	1.59	1.51
1	C	148	GLU	CB-CG	5.03	1.61	1.52
1	E	235	PRO	C-O	5.01	1.33	1.23

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	501	TYR	O-C-N	-20.19	90.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	501	TYR	O-C-N	-18.79	92.63	122.70
1	C	501	TYR	O-C-N	-18.28	93.45	122.70
1	B	501	TYR	C-N-CA	17.61	165.72	121.70
1	H	501	TYR	C-N-CA	17.18	164.65	121.70
1	G	501	TYR	C-N-CA	16.61	163.22	121.70
1	E	501	TYR	CA-C-N	16.10	152.62	117.20
1	E	144	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	F	501	TYR	CA-C-N	13.69	147.31	117.20
1	G	144	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	144	ARG	NE-CZ-NH2	-12.53	114.03	120.30
1	H	144	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	G	432	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	26	ARG	NE-CZ-NH1	-12.05	114.28	120.30
1	C	501	TYR	CA-C-N	11.84	143.25	117.20
1	C	432	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	D	144	ARG	NE-CZ-NH2	-11.25	114.68	120.30
1	F	386	LEU	CA-CB-CG	10.87	140.30	115.30
1	H	144	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	H	432	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	B	144	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	A	432	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	144	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	D	432	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	F	103	MET	CG-SD-CE	-10.05	84.11	100.20
1	H	374	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	F	432	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	E	144	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	C	438	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	G	415	ILE	CG1-CB-CG2	-9.52	90.46	111.40
1	B	26	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	H	415	ILE	CG1-CB-CG2	-9.22	91.11	111.40
1	D	432	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	A	445	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	222	VAL	CB-CA-C	-8.93	94.43	111.40
1	A	26	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	F	222	VAL	CB-CA-C	-8.81	94.65	111.40
1	G	501	TYR	O-C-N	-8.71	108.76	122.70
1	G	144	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	C	383	LEU	CA-CB-CG	8.54	134.95	115.30
1	C	501	TYR	C-N-CA	8.49	142.92	121.70
1	H	103	MET	CG-SD-CE	-8.20	87.08	100.20
1	H	222	VAL	CB-CA-C	-8.15	95.92	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	438	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	F	144	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	G	501	TYR	CA-C-N	8.05	134.91	117.20
1	A	432	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	F	22	VAL	CG1-CB-CG2	8.02	123.73	110.90
1	B	82	ILE	CG1-CB-CG2	8.02	129.04	111.40
1	B	501	TYR	O-C-N	-8.01	109.89	122.70
1	G	222	VAL	CB-CA-C	-8.00	96.21	111.40
1	C	289	VAL	CG1-CB-CG2	8.00	123.69	110.90
1	D	22	VAL	CG1-CB-CG2	7.98	123.67	110.90
1	D	144	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	H	289	VAL	CB-CA-C	-7.90	96.39	111.40
1	E	22	VAL	CB-CA-C	-7.89	96.41	111.40
1	D	289	VAL	CB-CA-C	-7.89	96.41	111.40
1	A	289	VAL	CG1-CB-CG2	7.81	123.39	110.90
1	E	289	VAL	CG1-CB-CG2	7.81	123.39	110.90
1	H	22	VAL	CB-CA-C	-7.75	96.68	111.40
1	G	22	VAL	CB-CA-C	-7.75	96.68	111.40
1	G	289	VAL	CB-CA-C	-7.70	96.77	111.40
1	H	22	VAL	CG1-CB-CG2	7.67	123.17	110.90
1	H	103	MET	CB-CG-SD	-7.66	89.41	112.40
1	C	289	VAL	CB-CA-C	-7.50	97.15	111.40
1	G	289	VAL	CG1-CB-CG2	7.41	122.75	110.90
1	F	121	VAL	CG1-CB-CG2	7.40	122.74	110.90
1	C	432	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	F	103	MET	CB-CG-SD	-7.30	90.50	112.40
1	F	49	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	445	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	F	289	VAL	CB-CA-C	-7.24	97.64	111.40
1	F	82	ILE	CG1-CB-CG2	7.20	127.24	111.40
1	F	289	VAL	CG1-CB-CG2	7.11	122.28	110.90
1	F	22	VAL	CB-CA-C	-7.09	97.92	111.40
1	G	22	VAL	CG1-CB-CG2	7.07	122.20	110.90
1	H	40	LYS	CD-CE-NZ	7.00	127.80	111.70
1	F	374	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	289	VAL	CB-CA-C	-7.00	98.11	111.40
1	E	289	VAL	CB-CA-C	-6.99	98.11	111.40
1	E	82	ILE	CG1-CB-CG2	6.96	126.72	111.40
1	F	144	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	289	VAL	CG1-CB-CG2	6.88	121.90	110.90
1	B	222	VAL	CB-CA-C	-6.82	98.44	111.40
1	H	289	VAL	CG1-CB-CG2	6.81	121.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	LEU	CA-CB-CG	6.81	130.96	115.30
1	D	383	LEU	CA-CB-CG	6.71	130.74	115.30
1	B	501	TYR	CA-C-N	6.69	131.93	117.20
1	D	26	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	B	432	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	E	22	VAL	CG1-CB-CG2	6.58	121.43	110.90
1	G	413	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	B	274	LEU	CB-CG-CD2	6.55	122.14	111.00
1	D	22	VAL	CB-CA-C	-6.55	98.95	111.40
1	A	227	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	274	LEU	CB-CG-CD2	6.48	122.01	111.00
1	E	374	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	D	82	ILE	CG1-CB-CG2	6.44	125.56	111.40
1	D	121	VAL	CG1-CB-CG2	6.41	121.15	110.90
1	F	447	VAL	CG1-CB-CG2	6.39	121.12	110.90
1	H	49	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	H	383	LEU	CA-CB-CG	6.35	129.90	115.30
1	C	227	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	F	26	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	C	445	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	445	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	B	383	LEU	CA-CB-CG	6.25	129.69	115.30
1	B	144	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	274	LEU	CB-CG-CD2	6.22	121.57	111.00
1	B	445	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	445	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	F	383	LEU	CA-CB-CG	6.18	129.52	115.30
1	D	274	LEU	CB-CG-CD2	6.16	121.47	111.00
1	D	222	VAL	CB-CA-C	-6.15	99.71	111.40
1	G	274	LEU	CB-CG-CD2	6.14	121.43	111.00
1	E	121	VAL	CG1-CB-CG2	6.13	120.70	110.90
1	C	121	VAL	CG1-CB-CG2	6.12	120.69	110.90
1	C	222	VAL	CB-CA-C	-6.08	99.85	111.40
1	G	144	ARG	CG-CD-NE	-6.04	99.12	111.80
1	B	26	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	H	82	ILE	CG1-CB-CG2	5.92	124.43	111.40
1	A	121	VAL	CG1-CB-CG2	5.89	120.32	110.90
1	B	39	LEU	CB-CG-CD2	5.89	121.01	111.00
1	D	374	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	374	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	131	ARG	CG-CD-NE	-5.82	99.57	111.80
1	A	386	LEU	CB-CG-CD2	5.80	120.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	432	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	H	49	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	82	ILE	CG1-CB-CG2	5.76	124.07	111.40
1	F	49	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	131	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	253	MET	CG-SD-CE	5.70	109.33	100.20
1	E	289	VAL	CA-CB-CG2	5.63	119.35	110.90
1	G	383	LEU	CA-CB-CG	5.62	128.24	115.30
1	D	131	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	489	THR	N-CA-CB	-5.61	99.64	110.30
1	D	49	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	G	495	ASP	CB-CG-OD1	5.52	123.27	118.30
1	H	241	GLU	CB-CA-C	-5.45	99.50	110.40
1	G	84	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	178	LEU	CA-CB-CG	5.44	127.80	115.30
1	F	178	LEU	CB-CG-CD1	5.41	120.19	111.00
1	H	445	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	G	178	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	501	TYR	C-N-CA	5.32	135.00	121.70
1	F	131	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	G	400	LEU	CA-CB-CG	5.29	127.46	115.30
1	H	432	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	60	ASP	CB-CG-OD1	5.28	123.05	118.30
1	H	82	ILE	CB-CA-C	-5.28	101.03	111.60
1	C	19	LYS	CD-CE-NZ	-5.26	99.60	111.70
1	C	383	LEU	CB-CG-CD2	5.20	119.84	111.00
1	F	383	LEU	CB-CG-CD2	5.18	119.80	111.00
1	H	178	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	95	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	82	ILE	CG1-CB-CG2	5.15	122.73	111.40
1	A	336	PHE	CB-CA-C	-5.13	100.15	110.40
1	H	222	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	82	ILE	CB-CA-C	-5.10	101.39	111.60
1	A	82	ILE	CG1-CB-CG2	5.08	122.58	111.40
1	F	22	VAL	CA-CB-CG2	5.08	118.52	110.90
1	D	87	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	386	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	82	ILE	CB-CA-C	-5.04	101.53	111.60
1	F	362	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	69	ILE	Peptide
1	F	391	GLY	Peptide
1	F	501	TYR	Mainchain
1	F	71	GLY	Peptide
1	H	390	LYS	Peptide
1	H	501	TYR	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	4082	0	3992	157	0
1	B	4082	0	3992	138	0
1	C	4082	0	3992	165	0
1	D	4082	0	3991	159	0
1	E	4082	0	3992	142	0
1	F	4082	0	3992	139	0
1	G	4082	0	3991	115	0
1	H	4082	0	3992	140	0
2	A	363	0	0	43	1
2	B	317	0	0	26	0
2	C	371	0	0	37	0
2	D	340	0	0	37	1
2	E	347	0	0	41	0
2	F	414	0	0	48	1
2	G	340	0	0	25	1
2	H	397	0	0	41	0
All	All	35545	0	31934	1109	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 17.

All (1109) 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:F:103:MET:CG	1:F:103:MET:CB	1.76	1.60
1:H:103:MET:HE3	1:H:103:MET:CB	1.11	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:MET:CB	1:H:103:MET:CG	1.76	1.54
1:H:103:MET:HB3	1:H:103:MET:CE	1.02	1.47
1:E:501:TYR:C	1:E:502:SER:N	1.68	1.46
1:A:103:MET:CE	1:A:104:PRO:HD2	1.45	1.46
1:F:103:MET:HB3	1:F:103:MET:CE	0.95	1.42
1:C:501:TYR:C	1:C:502:SER:N	1.69	1.40
1:F:103:MET:CB	1:F:103:MET:HE2	0.92	1.38
1:F:386:LEU:HB2	2:F:2385:HOH:O	1.32	1.26
1:E:201:CYS:HB2	2:E:2185:HOH:O	1.39	1.19
1:E:358:LEU:HD12	2:E:2259:HOH:O	1.43	1.18
1:A:272:LEU:HB3	2:A:2226:HOH:O	1.44	1.14
1:C:205:ASP:OD1	1:C:227:ARG:NH1	1.82	1.13
1:A:26:ARG:NH1	1:A:60:ASP:OD2	1.82	1.12
1:C:439:GLN:HG3	2:C:2331:HOH:O	1.47	1.11
1:E:415:ILE:HD11	1:E:420:TYR:HD1	1.14	1.11
1:F:415:ILE:CD1	1:F:451:HIS:HB3	1.79	1.11
1:B:392:GLU:HG2	1:B:393:GLY:H	1.06	1.09
1:F:252:ASP:HB3	2:F:2254:HOH:O	1.50	1.08
1:B:392:GLU:HG2	1:B:393:GLY:N	1.67	1.08
1:F:103:MET:CB	1:F:103:MET:CE	1.74	1.08
1:H:405:SER:HA	2:H:2313:HOH:O	1.55	1.07
1:G:252:ASP:HB3	2:G:2206:HOH:O	1.53	1.07
1:G:103:MET:CE	1:G:107:LEU:HB3	1.85	1.06
1:A:103:MET:CE	1:A:104:PRO:CD	2.33	1.06
1:G:274:LEU:HD13	1:G:310:VAL:HG12	1.33	1.06
1:H:392:GLU:HA	2:H:2305:HOH:O	1.55	1.05
1:B:274:LEU:HD13	1:B:310:VAL:HG12	1.32	1.05
1:E:219:ARG:HG2	1:E:219:ARG:HH11	1.13	1.04
1:H:103:MET:CB	1:H:103:MET:SD	2.45	1.04
1:A:103:MET:HE3	1:A:104:PRO:HD2	1.39	1.04
1:H:10:GLY:O	1:H:11:ARG:HB3	1.52	1.04
1:A:103:MET:HE2	1:A:104:PRO:HD2	1.07	1.04
1:D:238:LYS:HE2	1:D:243:TYR:CZ	1.94	1.03
1:F:103:MET:HE2	1:F:103:MET:HB2	1.40	1.02
1:C:148:GLU:HB2	2:C:2162:HOH:O	1.57	1.02
1:F:103:MET:CB	1:F:103:MET:SD	2.48	1.02
1:A:10:GLY:O	1:A:11:ARG:HB3	1.57	1.02
1:D:274:LEU:HD13	1:D:310:VAL:HG12	1.41	1.02
1:F:26:ARG:NH1	1:F:60:ASP:OD2	1.93	1.01
1:D:103:MET:CE	1:D:104:PRO:HD2	1.91	1.01
1:B:26:ARG:NH1	1:B:60:ASP:OD2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:VAL:HG11	1:H:369:MET:CE	1.91	1.01
1:D:238:LYS:HE2	1:D:243:TYR:CE1	1.96	1.01
1:H:83:ASP:OD1	1:H:140:HIS:HE1	1.44	1.00
1:B:252:ASP:HB3	2:B:2192:HOH:O	1.58	1.00
1:D:69:ILE:HD12	1:D:69:ILE:O	1.61	1.00
1:F:201:CYS:HB3	2:F:2180:HOH:O	1.58	1.00
1:E:103:MET:HE3	1:E:107:LEU:CB	1.92	1.00
1:F:350:HIS:HD2	2:F:2315:HOH:O	1.45	0.99
1:A:15:LYS:HD2	2:A:2240:HOH:O	1.60	0.99
1:E:103:MET:CE	1:E:107:LEU:HB3	1.92	0.99
1:B:103:MET:CE	1:B:104:PRO:HD2	1.92	0.99
1:A:103:MET:SD	2:A:2121:HOH:O	2.20	0.99
1:H:4:VAL:HG11	1:H:369:MET:HE1	1.43	0.98
1:F:415:ILE:HD13	1:F:451:HIS:HB3	1.40	0.98
1:D:280:ASN:HD22	1:D:281:THR:H	1.05	0.98
1:E:259:THR:HG22	2:E:2187:HOH:O	1.62	0.97
1:G:266:GLN:HG3	2:G:2213:HOH:O	1.65	0.97
1:E:103:MET:HE3	1:E:107:LEU:HB2	1.42	0.97
1:G:239:THR:HG22	1:G:241:GLU:H	1.24	0.96
1:A:103:MET:HE2	1:A:104:PRO:CD	1.95	0.96
1:E:274:LEU:HD13	1:E:310:VAL:HG12	1.47	0.96
1:F:12:GLU:HG2	2:F:2015:HOH:O	1.66	0.96
1:D:103:MET:HE3	1:D:104:PRO:HD2	1.43	0.95
1:F:406:PHE:HE2	1:F:409:VAL:HG23	1.31	0.95
1:C:274:LEU:HD13	1:C:310:VAL:HG12	1.47	0.95
1:C:103:MET:CE	1:C:107:LEU:HB3	1.96	0.95
1:A:239:THR:HG22	1:A:241:GLU:H	1.30	0.94
1:H:103:MET:CB	1:H:103:MET:CE	1.83	0.94
1:C:205:ASP:CG	1:C:227:ARG:HH12	1.68	0.94
1:E:426:VAL:HG21	1:E:447:VAL:HG11	1.49	0.94
1:B:103:MET:HE3	1:B:104:PRO:HD2	1.46	0.94
1:B:350:HIS:HD2	2:B:2233:HOH:O	1.50	0.94
1:E:415:ILE:HD11	1:E:420:TYR:CD1	2.02	0.93
1:H:206:GLU:HB2	2:H:2196:HOH:O	1.67	0.93
1:H:395:THR:HG22	2:H:2309:HOH:O	1.67	0.93
1:F:274:LEU:HD13	1:F:310:VAL:HG12	1.49	0.93
1:D:239:THR:HG22	1:D:242:TYR:H	1.33	0.93
1:E:239:THR:HG22	1:E:242:TYR:H	1.30	0.93
1:B:239:THR:HG22	1:B:242:TYR:H	1.34	0.93
1:A:103:MET:HE3	1:A:104:PRO:CD	1.96	0.93
1:B:280:ASN:HD22	1:B:281:THR:H	1.14	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:MET:HB3	1:F:103:MET:HE3	1.47	0.92
1:H:364:TYR:CE2	1:H:369:MET:HE2	2.05	0.92
1:F:69:ILE:HD12	1:F:69:ILE:O	1.70	0.91
1:G:390:LYS:O	1:G:391:GLY:O	1.84	0.91
1:B:364:TYR:CE2	1:B:369:MET:HE2	2.05	0.91
1:D:501:TYR:C	1:D:502:SER:N	2.24	0.91
1:H:274:LEU:HD13	1:H:310:VAL:HG12	1.50	0.91
1:D:26:ARG:NH1	1:D:60:ASP:OD2	2.04	0.91
1:C:390:LYS:O	1:C:391:GLY:O	1.87	0.91
1:D:301:ARG:HB2	2:D:2230:HOH:O	1.70	0.91
1:G:4:VAL:N	2:G:2001:HOH:O	2.05	0.90
1:C:239:THR:HG22	1:C:241:GLU:H	1.33	0.90
1:H:107:LEU:HD23	2:H:2136:HOH:O	1.71	0.90
1:F:481:GLU:HG3	2:F:2388:HOH:O	1.72	0.90
1:G:26:ARG:NH2	1:G:323:GLU:OE1	2.05	0.90
1:A:280:ASN:HD22	1:A:281:THR:H	1.19	0.89
1:A:413:ARG:HD3	1:A:453:MET:HE2	1.55	0.89
1:C:485:ASP:OD1	1:C:487:THR:HG23	1.73	0.89
1:A:413:ARG:HD3	1:A:453:MET:CE	2.02	0.89
1:E:280:ASN:HD22	1:E:281:THR:H	1.21	0.88
1:C:280:ASN:HD22	1:C:281:THR:H	1.21	0.88
1:F:415:ILE:HD11	1:F:451:HIS:HB3	1.55	0.88
1:H:389:GLU:HG2	2:H:2299:HOH:O	1.73	0.88
1:D:439:GLN:HG3	2:D:2296:HOH:O	1.74	0.88
1:F:390:LYS:O	1:F:391:GLY:O	1.92	0.87
1:F:445:ARG:NH1	2:F:2368:HOH:O	2.07	0.87
1:H:368:GLU:OE2	1:H:396:LYS:NZ	2.08	0.87
1:C:69:ILE:HB	1:C:74:LYS:HD2	1.55	0.86
1:F:280:ASN:HD22	1:F:281:THR:H	1.20	0.86
1:D:415:ILE:HD11	1:D:453:MET:HE1	1.55	0.86
1:E:218:ARG:HG2	2:E:2191:HOH:O	1.76	0.86
1:A:12:GLU:HG2	2:A:2008:HOH:O	1.74	0.86
1:B:489:THR:CG2	1:D:434:ARG:HE	1.86	0.86
1:E:255:GLU:HG2	2:E:2214:HOH:O	1.73	0.86
1:H:350:HIS:HD2	2:H:2282:HOH:O	1.58	0.85
1:E:93:ASN:HB3	2:E:2092:HOH:O	1.75	0.85
1:F:485:ASP:OD1	1:F:487:THR:HG23	1.75	0.85
1:B:392:GLU:CG	1:B:393:GLY:H	1.90	0.85
1:E:301:ARG:HB2	2:E:2229:HOH:O	1.74	0.85
1:C:274:LEU:CD1	1:C:310:VAL:HG12	2.06	0.85
1:F:10:GLY:O	1:F:11:ARG:HB3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:MET:HE1	1:D:107:LEU:HB3	1.56	0.84
1:E:350:HIS:HD2	2:E:2257:HOH:O	1.60	0.84
1:F:105:LYS:HE2	2:F:2078:HOH:O	1.74	0.84
1:E:501:TYR:O	1:E:502:SER:N	2.10	0.84
1:F:439:GLN:HG3	2:F:2364:HOH:O	1.77	0.84
1:F:489:THR:CG2	1:H:434:ARG:HE	1.91	0.84
1:E:26:ARG:NH1	1:E:60:ASP:OD2	2.10	0.84
1:E:434:ARG:HE	1:G:489:THR:CG2	1.89	0.84
1:A:4:VAL:N	2:A:2001:HOH:O	2.09	0.84
1:E:481:GLU:HG3	2:E:2328:HOH:O	1.76	0.84
1:A:489:THR:CG2	1:C:434:ARG:HE	1.90	0.84
1:F:438:ARG:CD	2:F:2363:HOH:O	2.26	0.84
1:H:408:ALA:HB1	2:H:2356:HOH:O	1.79	0.83
1:E:219:ARG:HH11	1:E:219:ARG:CG	1.91	0.83
1:A:69:ILE:O	1:A:69:ILE:HG13	1.79	0.82
1:H:280:ASN:HD22	1:H:281:THR:H	1.26	0.82
1:B:489:THR:HG21	1:D:434:ARG:HE	1.43	0.82
1:D:213:HIS:HD2	2:D:2191:HOH:O	1.61	0.82
1:E:403:PRO:HA	1:E:462:GLY:O	1.80	0.81
1:C:238:LYS:HD3	1:C:243:TYR:CE1	2.14	0.81
1:C:103:MET:HE2	1:C:107:LEU:HB3	1.62	0.81
1:F:406:PHE:CE2	1:F:409:VAL:HG23	2.15	0.81
1:C:399:GLN:HE21	1:C:467:SER:HB3	1.43	0.81
1:E:103:MET:CE	1:E:107:LEU:CB	2.53	0.81
1:E:239:THR:HG22	1:E:242:TYR:N	1.95	0.81
1:G:103:MET:HE3	1:G:107:LEU:HB3	1.63	0.81
1:A:350:HIS:HD2	2:A:2271:HOH:O	1.62	0.81
1:A:274:LEU:HD13	1:A:310:VAL:HG12	1.63	0.80
1:D:4:VAL:HG11	1:D:369:MET:HE2	1.63	0.80
1:A:270:PRO:HG2	2:A:2224:HOH:O	1.82	0.80
1:G:280:ASN:HD22	1:G:281:THR:H	1.28	0.80
1:F:386:LEU:HD13	2:F:2331:HOH:O	1.81	0.80
1:H:103:MET:HE3	1:H:103:MET:CA	2.11	0.80
1:A:209:THR:HG21	2:A:2178:HOH:O	1.81	0.80
1:A:426:VAL:HG21	1:A:447:VAL:HG11	1.62	0.80
1:F:259:THR:HG22	2:F:2220:HOH:O	1.83	0.80
1:C:201:CYS:HB2	2:C:2206:HOH:O	1.81	0.79
1:F:390:LYS:O	1:F:391:GLY:C	2.18	0.79
1:H:239:THR:HG22	1:H:241:GLU:H	1.47	0.79
1:D:69:ILE:HD11	1:D:74:LYS:NZ	1.97	0.79
1:C:501:TYR:O	1:C:502:SER:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:PHE:HD2	1:F:82:ILE:HD11	1.47	0.79
1:D:93:ASN:HB3	2:D:2105:HOH:O	1.82	0.78
1:H:438:ARG:NE	2:H:2330:HOH:O	2.06	0.78
1:B:125:LYS:HD2	2:B:2111:HOH:O	1.82	0.78
1:A:468:ILE:HD13	1:A:478:ILE:HD13	1.65	0.78
1:D:103:MET:CE	1:D:107:LEU:HB3	2.13	0.77
1:H:374:ARG:HD3	1:H:378:SER:OG	1.84	0.77
1:F:130:TRP:NE1	1:F:134:ILE:HD11	1.99	0.77
1:F:391:GLY:HA3	1:F:394:LEU:HD11	1.67	0.77
1:A:224:PHE:HA	2:A:2226:HOH:O	1.83	0.77
1:H:265:ARG:HD2	2:H:2236:HOH:O	1.85	0.77
1:E:404:VAL:O	1:E:462:GLY:HA2	1.84	0.77
1:D:280:ASN:HD22	1:D:281:THR:N	1.83	0.76
1:F:83:ASP:OD1	1:F:140:HIS:HE1	1.66	0.76
1:D:390:LYS:O	1:D:391:GLY:O	2.03	0.76
1:E:271:HIS:HB2	2:E:2220:HOH:O	1.83	0.76
1:E:493:LEU:HD22	2:G:2284:HOH:O	1.84	0.76
1:H:407:SER:O	1:H:458:ARG:HG3	1.85	0.76
1:F:239:THR:HG22	1:F:241:GLU:H	1.48	0.76
1:D:69:ILE:CD1	1:D:74:LYS:HZ3	1.98	0.76
1:F:434:ARG:HH21	1:H:489:THR:HG22	1.50	0.76
1:D:239:THR:HG22	1:D:241:GLU:H	1.51	0.76
1:C:205:ASP:CG	1:C:227:ARG:NH1	2.34	0.76
1:B:103:MET:HE1	1:B:107:LEU:HD13	1.67	0.76
1:G:238:LYS:HD3	1:G:243:TYR:CE1	2.19	0.76
1:A:239:THR:CG2	1:A:241:GLU:H	1.99	0.75
1:C:148:GLU:CB	2:C:2162:HOH:O	2.24	0.75
1:F:438:ARG:HD2	2:F:2363:HOH:O	1.87	0.75
1:A:399:GLN:HG3	1:A:467:SER:HB3	1.68	0.74
1:B:486:GLU:O	1:B:489:THR:HB	1.86	0.74
1:F:397:GLU:HB3	2:F:2380:HOH:O	1.87	0.74
1:G:285:PRO:HG2	1:G:325:MET:HG3	1.70	0.74
1:B:130:TRP:CE2	1:B:134:ILE:HD11	2.22	0.74
1:D:69:ILE:O	1:D:69:ILE:CD1	2.35	0.73
1:C:233:LYS:HD2	1:C:246:GLU:HG2	1.70	0.73
1:E:239:THR:CG2	1:E:241:GLU:H	2.01	0.73
1:F:144:ARG:NH2	1:G:436:PRO:O	2.22	0.73
1:H:266:GLN:HB2	2:H:2234:HOH:O	1.88	0.73
1:B:438:ARG:CZ	2:B:2264:HOH:O	2.36	0.73
1:D:69:ILE:HG12	1:D:74:LYS:HG3	1.70	0.73
1:D:280:ASN:ND2	1:D:281:THR:H	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASP:OD1	1:C:140:HIS:HE1	1.72	0.73
1:B:103:MET:HE2	1:B:104:PRO:HD2	1.69	0.73
1:E:219:ARG:HG2	1:E:219:ARG:NH1	1.89	0.72
1:F:206:GLU:HB2	2:F:2221:HOH:O	1.89	0.72
1:A:489:THR:HG21	1:C:434:ARG:HE	1.52	0.72
1:B:434:ARG:HE	1:D:489:THR:CG2	2.02	0.72
1:C:99:GLU:OE1	2:C:2121:HOH:O	2.06	0.72
1:C:103:MET:HE3	1:C:107:LEU:HB3	1.70	0.72
1:D:404:VAL:O	1:D:462:GLY:HA2	1.88	0.72
1:E:10:GLY:O	1:E:11:ARG:HB2	1.88	0.72
1:D:69:ILE:CG1	1:D:74:LYS:HG3	2.19	0.72
1:G:426:VAL:HG21	1:G:447:VAL:HG11	1.70	0.72
1:A:83:ASP:OD1	1:A:140:HIS:HE1	1.73	0.71
2:A:2205:HOH:O	1:C:499:THR:CG2	2.37	0.71
2:F:2252:HOH:O	1:H:499:THR:HB	1.89	0.71
1:G:350:HIS:HD2	2:G:2255:HOH:O	1.71	0.71
1:B:239:THR:HG22	1:B:242:TYR:N	2.05	0.71
1:E:215:CYS:SG	1:E:222:VAL:CG2	2.78	0.71
1:E:434:ARG:HE	1:G:489:THR:HG21	1.55	0.71
1:F:63:ILE:HD11	1:F:82:ILE:HG12	1.71	0.71
1:A:99:GLU:OE1	2:A:2104:HOH:O	2.09	0.71
2:A:2207:HOH:O	1:C:499:THR:HB	1.89	0.71
1:C:200:ILE:HD11	1:C:208:ILE:CD1	2.20	0.71
1:H:438:ARG:NH2	2:H:2330:HOH:O	2.24	0.71
1:D:240:PHE:CE2	1:D:241:GLU:HG3	2.27	0.70
1:G:125:LYS:O	1:G:125:LYS:HG3	1.91	0.70
1:A:148:GLU:HG3	2:A:2146:HOH:O	1.90	0.70
1:D:501:TYR:O	1:D:502:SER:N	2.24	0.70
1:F:391:GLY:HA3	1:F:394:LEU:CD1	2.21	0.70
1:B:364:TYR:CD2	1:B:369:MET:HE2	2.27	0.70
1:F:350:HIS:CD2	2:F:2315:HOH:O	2.31	0.70
1:D:400:LEU:HD23	1:D:468:ILE:HD12	1.74	0.69
1:H:16:LYS:HD2	2:H:2286:HOH:O	1.92	0.69
1:D:426:VAL:HG21	1:D:447:VAL:HG11	1.74	0.69
1:D:49:ARG:HD2	2:D:2056:HOH:O	1.91	0.69
1:E:415:ILE:CD1	1:E:420:TYR:CD1	2.75	0.69
1:F:474:GLU:OE1	2:F:2386:HOH:O	2.09	0.69
1:E:215:CYS:SG	1:E:222:VAL:HG21	2.33	0.69
2:F:2248:HOH:O	1:H:499:THR:HG22	1.92	0.69
1:G:107:LEU:HD22	2:G:2112:HOH:O	1.91	0.69
1:D:350:HIS:HD2	2:D:2261:HOH:O	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:MET:HE3	1:G:107:LEU:CB	2.21	0.69
1:B:130:TRP:NE1	1:B:134:ILE:HD11	2.07	0.69
1:C:426:VAL:HG21	1:C:447:VAL:HG11	1.75	0.69
1:D:227:ARG:NH2	1:D:256:GLN:HE21	1.91	0.69
1:H:69:ILE:HD11	1:H:74:LYS:HE2	1.75	0.69
1:H:103:MET:HB3	1:H:103:MET:HE2	1.56	0.69
1:C:474:GLU:OE1	2:C:2358:HOH:O	2.09	0.69
1:D:213:HIS:CD2	2:D:2191:HOH:O	2.39	0.69
1:A:486:GLU:O	1:A:489:THR:HB	1.91	0.69
1:B:201:CYS:HB2	2:B:2162:HOH:O	1.93	0.69
1:H:177:LYS:HE3	2:H:2180:HOH:O	1.93	0.69
1:D:400:LEU:HD23	1:D:468:ILE:CD1	2.23	0.68
1:D:44:GLU:HG3	2:D:2050:HOH:O	1.91	0.68
1:D:103:MET:HE2	1:D:104:PRO:HD2	1.71	0.68
1:E:438:ARG:HD3	2:E:2304:HOH:O	1.92	0.68
1:F:125:LYS:HD2	2:F:2150:HOH:O	1.94	0.68
2:A:2205:HOH:O	1:C:499:THR:HG23	1.92	0.68
1:B:285:PRO:HG2	1:B:325:MET:HG3	1.74	0.68
1:D:121:VAL:HG22	1:D:166:PHE:O	1.93	0.68
1:E:489:THR:CG2	1:G:434:ARG:HE	2.06	0.68
1:A:417:ASN:ND2	1:A:420:TYR:H	1.92	0.68
1:C:259:THR:HG22	2:C:2210:HOH:O	1.94	0.68
1:H:121:VAL:O	1:H:121:VAL:CG1	2.40	0.68
1:A:282:SER:HB3	1:A:290:HIS:CE1	2.28	0.68
1:B:145:TYR:HE2	1:C:438:ARG:HH22	1.40	0.68
1:B:239:THR:HG22	1:B:241:GLU:H	1.57	0.67
1:H:83:ASP:OD1	1:H:140:HIS:CE1	2.36	0.67
1:A:449:GLN:HG3	2:A:2324:HOH:O	1.93	0.67
1:D:390:LYS:O	1:D:391:GLY:C	2.33	0.67
1:E:206:GLU:HB2	2:E:2188:HOH:O	1.93	0.67
1:B:4:VAL:HG11	1:B:369:MET:CE	2.24	0.67
1:B:227:ARG:CD	1:B:260:VAL:HG21	2.24	0.67
1:E:486:GLU:O	1:E:489:THR:HB	1.95	0.67
1:F:406:PHE:HE2	1:F:409:VAL:CG2	2.05	0.67
1:D:364:TYR:CE2	1:D:369:MET:HE2	2.30	0.67
1:G:103:MET:HE2	1:G:107:LEU:HB3	1.75	0.67
1:H:143:GLU:HG3	2:H:2145:HOH:O	1.95	0.67
1:C:239:THR:HG21	2:C:2236:HOH:O	1.95	0.67
1:C:125:LYS:HD2	2:C:2138:HOH:O	1.95	0.67
1:C:373:ARG:HD2	2:C:2005:HOH:O	1.94	0.67
1:C:415:ILE:HD11	1:C:453:MET:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ILE:HD11	1:E:82:ILE:HG12	1.76	0.67
1:G:130:TRP:NE1	1:G:134:ILE:HD11	2.10	0.66
1:B:400:LEU:HB3	1:B:402:ILE:HD11	1.77	0.66
1:H:69:ILE:HG12	1:H:74:LYS:HG2	1.78	0.66
1:C:280:ASN:HD22	1:C:281:THR:N	1.94	0.66
1:F:11:ARG:HG2	2:F:2013:HOH:O	1.96	0.66
1:D:71:GLY:N	2:D:2086:HOH:O	2.19	0.66
1:E:274:LEU:CD1	1:E:310:VAL:HG12	2.24	0.66
1:F:386:LEU:CD1	2:F:2331:HOH:O	2.39	0.66
1:F:417:ASN:ND2	1:F:419:GLN:H	1.94	0.66
1:B:239:THR:CG2	1:B:241:GLU:H	2.09	0.66
1:C:301:ARG:HB2	2:C:2264:HOH:O	1.95	0.66
1:D:239:THR:CG2	1:D:241:GLU:H	2.08	0.65
1:G:413:ARG:HD3	1:G:453:MET:CE	2.25	0.65
1:C:10:GLY:O	1:C:11:ARG:HB3	1.95	0.65
1:F:436:PRO:O	1:G:144:ARG:NH2	2.27	0.65
1:E:355:PHE:HD2	2:E:2259:HOH:O	1.79	0.65
1:F:239:THR:HG22	1:F:242:TYR:H	1.59	0.65
1:C:417:ASN:HD22	1:C:419:GLN:H	1.44	0.65
1:G:24:THR:HG23	1:G:53:GLY:HA3	1.79	0.65
1:D:70:ASP:O	2:D:2084:HOH:O	2.14	0.65
1:F:99:GLU:OE1	2:F:2123:HOH:O	2.15	0.65
1:A:209:THR:CG2	2:A:2178:HOH:O	2.41	0.65
1:E:355:PHE:CD2	2:E:2259:HOH:O	2.49	0.65
1:A:239:THR:HG22	1:A:241:GLU:N	2.07	0.65
1:E:402:ILE:HD12	1:E:480:ILE:HD13	1.79	0.65
1:C:259:THR:CG2	2:C:2210:HOH:O	2.45	0.64
1:D:79:PHE:HD2	1:D:82:ILE:HD11	1.62	0.64
1:H:26:ARG:NH2	1:H:323:GLU:OE1	2.31	0.64
1:F:301:ARG:HB2	2:F:2283:HOH:O	1.97	0.64
1:G:8:SER:HB3	1:G:403:PRO:CB	2.27	0.64
1:G:8:SER:O	1:G:373:ARG:NH2	2.29	0.64
1:A:209:THR:HB	2:A:2216:HOH:O	1.96	0.64
1:C:455:GLU:OE2	1:C:457:ARG:NH2	2.28	0.64
1:C:417:ASN:ND2	1:C:419:GLN:H	1.94	0.64
1:D:93:ASN:CB	2:D:2105:HOH:O	2.40	0.64
1:A:392:GLU:O	1:A:392:GLU:HG2	1.98	0.64
1:D:406:PHE:O	1:D:407:SER:CB	2.45	0.64
1:C:206:GLU:HB2	2:C:2213:HOH:O	1.97	0.64
1:E:145:TYR:HE2	1:H:438:ARG:HH21	1.46	0.64
1:F:392:GLU:H	1:F:394:LEU:HD12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HE3	2:B:2139:HOH:O	1.98	0.63
1:H:474:GLU:OE1	2:H:2370:HOH:O	2.15	0.63
1:E:413:ARG:HD3	1:E:453:MET:CE	2.27	0.63
1:A:280:ASN:HD22	1:A:281:THR:N	1.95	0.63
1:F:341:LEU:CD1	2:F:2179:HOH:O	2.47	0.63
1:G:103:MET:CE	1:G:107:LEU:CB	2.70	0.63
1:A:103:MET:HE1	1:A:107:LEU:CD1	2.29	0.63
1:G:481:GLU:HG2	2:G:2315:HOH:O	1.97	0.63
1:H:69:ILE:HD11	1:H:74:LYS:CE	2.28	0.63
1:D:204:SER:CB	2:D:2184:HOH:O	2.46	0.63
1:A:63:ILE:HD11	1:A:82:ILE:HG12	1.80	0.63
1:A:404:VAL:HG11	1:A:459:ALA:CB	2.29	0.63
1:G:339:VAL:CG1	1:G:343:SER:HA	2.29	0.63
1:G:407:SER:O	1:G:458:ARG:HG3	1.99	0.63
1:C:205:ASP:OD2	1:C:227:ARG:NH1	2.27	0.63
1:E:109:SER:HA	1:E:125:LYS:HG3	1.81	0.63
1:B:99:GLU:OE1	2:B:2087:HOH:O	2.16	0.62
1:H:4:VAL:HG11	1:H:369:MET:HE2	1.79	0.62
1:A:408:ALA:HB2	1:A:458:ARG:HE	1.64	0.62
1:D:364:TYR:CD2	1:D:369:MET:HE3	2.34	0.62
1:F:301:ARG:CB	2:F:2283:HOH:O	2.46	0.62
1:C:93:ASN:HB3	2:C:2114:HOH:O	1.98	0.62
1:D:165:ASN:H	1:D:165:ASN:ND2	1.96	0.62
1:E:13:LYS:HE3	2:E:2003:HOH:O	1.97	0.62
1:G:82:ILE:HD12	1:G:83:ASP:N	2.14	0.62
1:G:83:ASP:OD1	1:G:140:HIS:HE1	1.82	0.62
1:G:274:LEU:HD13	1:G:310:VAL:CG1	2.21	0.62
1:D:417:ASN:ND2	1:D:419:GLN:H	1.98	0.62
1:H:406:PHE:CD1	1:H:482:GLN:NE2	2.68	0.62
1:F:103:MET:CG	1:F:103:MET:CA	2.71	0.62
1:E:70:ASP:HB3	2:E:2073:HOH:O	2.00	0.62
1:A:79:PHE:HD2	1:A:82:ILE:HD11	1.65	0.62
1:A:103:MET:HE3	1:A:104:PRO:HD3	1.82	0.62
1:B:426:VAL:HG21	1:B:447:VAL:HG11	1.81	0.62
1:C:415:ILE:HD11	1:C:453:MET:CE	2.30	0.62
1:F:415:ILE:HD11	1:F:420:TYR:CD1	2.35	0.62
1:F:499:THR:HG22	2:H:2223:HOH:O	2.00	0.61
1:D:103:MET:CE	1:D:107:LEU:CB	2.78	0.61
1:F:130:TRP:CE2	1:F:134:ILE:HD11	2.35	0.61
1:F:247:LEU:HG	1:H:499:THR:HG21	1.80	0.61
1:A:205:ASP:HB3	1:A:263:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASN:HD22	1:B:281:THR:N	1.92	0.61
1:E:493:LEU:HD13	2:G:2284:HOH:O	1.99	0.61
1:H:445:ARG:NH1	2:H:2338:HOH:O	2.11	0.61
1:A:144:ARG:NH2	1:D:436:PRO:O	2.33	0.61
1:A:213:HIS:ND1	2:A:2182:HOH:O	2.31	0.61
1:B:227:ARG:NE	1:B:260:VAL:HG21	2.15	0.61
1:F:417:ASN:ND2	1:F:420:TYR:H	1.98	0.61
1:H:404:VAL:CG2	1:H:406:PHE:CE2	2.83	0.61
1:A:6:VAL:HG21	1:A:402:ILE:HD13	1.82	0.61
1:C:411:ILE:HD13	1:C:466:LEU:HD21	1.83	0.61
1:D:239:THR:HG22	1:D:242:TYR:N	2.11	0.61
1:E:438:ARG:CD	2:E:2304:HOH:O	2.46	0.61
1:F:489:THR:HG21	1:H:434:ARG:HE	1.66	0.61
1:D:103:MET:HE1	1:D:107:LEU:CD1	2.31	0.61
1:D:501:TYR:C	1:D:502:SER:CA	2.69	0.61
1:G:417:ASN:ND2	1:G:420:TYR:H	1.98	0.61
1:H:290:HIS:HD2	1:H:334:GLY:O	1.84	0.61
1:D:457:ARG:HD2	1:D:464:ILE:HD11	1.82	0.60
1:E:213:HIS:NE2	1:E:217:GLU:OE2	2.33	0.60
1:H:417:ASN:ND2	1:H:419:GLN:H	1.98	0.60
1:G:8:SER:HB3	1:G:403:PRO:HB2	1.82	0.60
1:A:95:ARG:NH1	2:A:2103:HOH:O	2.35	0.60
1:C:238:LYS:HD3	1:C:243:TYR:HE1	1.61	0.60
1:E:280:ASN:HD22	1:E:281:THR:N	1.97	0.60
1:F:398:VAL:HG12	1:F:400:LEU:HD13	1.83	0.60
1:G:213:HIS:HE1	2:G:2175:HOH:O	1.83	0.60
1:A:251:GLU:HG2	1:A:301:ARG:HH12	1.67	0.60
1:C:406:PHE:O	1:C:407:SER:HB3	2.00	0.60
1:D:165:ASN:H	1:D:165:ASN:HD22	1.50	0.60
1:D:248:GLU:HG3	1:D:249:PRO:HD2	1.83	0.60
1:H:392:GLU:HG3	2:H:2304:HOH:O	2.01	0.60
1:E:239:THR:HG22	1:E:241:GLU:H	1.66	0.60
1:E:417:ASN:ND2	1:E:419:GLN:H	2.00	0.60
1:F:255:GLU:HG2	2:F:2258:HOH:O	2.01	0.60
1:E:239:THR:HG23	1:E:241:GLU:H	1.65	0.60
1:H:369:MET:HE1	1:H:400:LEU:CD1	2.32	0.60
1:C:130:TRP:CE2	1:C:134:ILE:HD11	2.36	0.59
1:F:275:HIS:HD1	1:F:312:SER:CB	2.16	0.59
1:F:280:ASN:HD22	1:F:281:THR:N	1.97	0.59
1:G:130:TRP:CE2	1:G:134:ILE:HD11	2.37	0.59
1:B:439:GLN:NE2	2:B:2265:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:LEU:HD12	2:F:2179:HOH:O	2.03	0.59
1:A:391:GLY:HA3	1:A:394:LEU:HD11	1.83	0.59
1:D:63:ILE:HD11	1:D:82:ILE:HG12	1.83	0.59
1:E:145:TYR:HE2	1:H:438:ARG:NH2	2.00	0.59
1:C:103:MET:HE1	1:C:124:PRO:HB3	1.85	0.59
1:D:6:VAL:HG21	1:D:402:ILE:HD13	1.84	0.59
1:B:4:VAL:HG11	1:B:369:MET:HE2	1.83	0.59
1:E:436:PRO:O	1:H:144:ARG:NH2	2.35	0.59
1:D:69:ILE:HD11	1:D:74:LYS:HZ2	1.67	0.59
1:H:364:TYR:CE2	1:H:369:MET:CE	2.85	0.59
1:H:438:ARG:CZ	2:H:2330:HOH:O	2.43	0.59
1:A:399:GLN:NE2	2:A:2289:HOH:O	2.36	0.59
1:F:426:VAL:HG21	1:F:447:VAL:HG11	1.84	0.59
1:C:464:ILE:CD1	1:C:466:LEU:HG	2.33	0.59
1:A:426:VAL:CG2	1:A:447:VAL:HG11	2.33	0.59
1:B:438:ARG:NH2	2:B:2263:HOH:O	2.36	0.59
1:D:10:GLY:O	1:D:11:ARG:HB3	2.02	0.59
1:D:103:MET:HE1	1:D:107:LEU:HD13	1.84	0.59
1:D:391:GLY:O	1:D:392:GLU:HB2	2.02	0.59
1:F:402:ILE:HB	1:F:464:ILE:CD1	2.32	0.59
1:F:486:GLU:O	1:F:489:THR:HB	2.02	0.59
1:C:103:MET:HE1	1:C:107:LEU:HD13	1.85	0.58
1:C:350:HIS:ND1	2:C:2292:HOH:O	2.32	0.58
1:E:499:THR:CG2	2:G:2199:HOH:O	2.50	0.58
1:A:10:GLY:O	1:A:11:ARG:CB	2.40	0.58
1:C:502:SER:HA	2:C:2371:HOH:O	2.03	0.58
1:G:274:LEU:CD1	1:G:310:VAL:HG12	2.22	0.58
1:H:391:GLY:HA3	1:H:472:LYS:HZ2	1.67	0.58
1:A:417:ASN:ND2	1:A:419:GLN:H	2.01	0.58
1:D:238:LYS:CE	1:D:243:TYR:CE1	2.80	0.58
1:A:4:VAL:HG11	1:A:369:MET:HE1	1.84	0.58
1:C:301:ARG:CB	2:C:2264:HOH:O	2.50	0.58
1:D:103:MET:HE1	1:D:107:LEU:CB	2.29	0.58
1:A:404:VAL:N	1:A:462:GLY:O	2.36	0.58
1:C:240:PHE:CE2	1:C:241:GLU:HG3	2.38	0.58
1:D:4:VAL:HG11	1:D:369:MET:CE	2.33	0.58
1:C:165:ASN:ND2	1:C:165:ASN:H	2.01	0.58
1:D:364:TYR:CD2	1:D:369:MET:CE	2.87	0.58
1:E:214:PHE:CE1	1:E:218:ARG:HD3	2.39	0.58
1:E:499:THR:HG21	1:G:247:LEU:HG	1.86	0.58
1:F:417:ASN:HD22	1:F:417:ASN:C	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:ASN:C	1:F:422:ASN:HD22	2.06	0.58
1:F:109:SER:HA	1:F:125:LYS:HG2	1.84	0.57
1:E:417:ASN:ND2	1:E:420:TYR:H	2.02	0.57
1:G:107:LEU:CD2	2:G:2112:HOH:O	2.51	0.57
1:A:489:THR:CG2	1:C:434:ARG:HH21	2.17	0.57
1:E:413:ARG:HD3	1:E:453:MET:HE2	1.85	0.57
1:H:69:ILE:CD1	1:H:74:LYS:HG3	2.34	0.57
1:H:63:ILE:HD11	1:H:82:ILE:HG12	1.85	0.57
2:E:2341:HOH:O	1:G:239:THR:HG21	2.03	0.57
1:D:274:LEU:CD1	1:D:310:VAL:HG12	2.26	0.57
1:C:121:VAL:HG22	1:C:166:PHE:O	2.05	0.57
1:G:481:GLU:CG	2:G:2315:HOH:O	2.50	0.57
1:B:107:LEU:HD21	1:B:129:LYS:HB3	1.86	0.57
1:E:474:GLU:OE1	2:E:2325:HOH:O	2.17	0.57
1:E:487:THR:HG23	2:G:2284:HOH:O	2.03	0.57
1:E:426:VAL:HG21	1:E:447:VAL:CG1	2.30	0.57
1:F:393:GLY:C	1:F:394:LEU:HG	2.25	0.57
1:F:398:VAL:CG1	1:F:400:LEU:CD1	2.83	0.57
1:C:267:SER:HB2	1:C:268:PRO:HD2	1.85	0.56
1:D:16:LYS:HE3	2:D:2023:HOH:O	2.05	0.56
1:H:482:GLN:CD	2:H:2377:HOH:O	2.44	0.56
1:A:368:GLU:OE1	1:A:396:LYS:HE2	2.05	0.56
1:A:411:ILE:HD11	1:A:464:ILE:HD11	1.88	0.56
1:F:398:VAL:HG12	1:F:400:LEU:CD1	2.35	0.56
1:H:432:ARG:NE	2:H:2324:HOH:O	2.03	0.56
1:C:83:ASP:OD1	1:C:140:HIS:CE1	2.57	0.56
1:E:409:VAL:HG11	1:E:464:ILE:HD13	1.87	0.56
1:A:239:THR:HG22	1:A:242:TYR:H	1.68	0.56
1:B:434:ARG:HE	1:D:489:THR:HG23	1.70	0.56
1:F:386:LEU:CD2	2:F:2385:HOH:O	2.54	0.56
1:B:144:ARG:HB2	2:B:2123:HOH:O	2.04	0.56
1:C:401:VAL:HG22	1:C:465:HIS:CD2	2.40	0.56
1:E:227:ARG:HD2	1:E:260:VAL:HG21	1.88	0.56
1:H:404:VAL:HG22	1:H:406:PHE:CE2	2.41	0.56
1:H:422:ASN:HD21	1:H:424:TRP:HB3	1.70	0.56
1:A:200:ILE:HD11	1:A:208:ILE:HG13	1.88	0.56
1:C:252:ASP:HB3	2:C:2243:HOH:O	2.04	0.56
1:D:69:ILE:CD1	1:D:74:LYS:NZ	2.62	0.56
1:E:10:GLY:O	1:E:11:ARG:CB	2.54	0.56
1:H:130:TRP:NE1	1:H:134:ILE:HD11	2.21	0.56
1:H:417:ASN:ND2	1:H:420:TYR:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:HG2	1:A:325:MET:HG3	1.88	0.56
1:B:205:ASP:OD1	1:B:227:ARG:NH1	2.39	0.56
1:B:250:PRO:HD3	1:B:388:MET:HE2	1.88	0.56
1:H:481:GLU:HG2	2:H:2374:HOH:O	2.05	0.56
1:A:227:ARG:NH2	1:A:256:GLN:OE1	2.37	0.55
1:E:350:HIS:CD2	2:E:2257:HOH:O	2.45	0.55
1:B:103:MET:HE3	1:B:104:PRO:CD	2.27	0.55
1:F:79:PHE:CD2	1:F:82:ILE:HD11	2.35	0.55
1:B:4:VAL:HG11	1:B:369:MET:HE1	1.88	0.55
1:C:82:ILE:HD12	1:C:83:ASP:N	2.22	0.55
1:D:501:TYR:C	1:D:502:SER:HA	2.27	0.55
1:A:369:MET:HE2	1:A:371:VAL:HG23	1.88	0.55
1:E:407:SER:O	1:E:458:ARG:HD3	2.06	0.55
1:F:438:ARG:O	1:F:442:GLU:HG3	2.06	0.55
1:H:266:GLN:CB	2:H:2234:HOH:O	2.51	0.55
1:E:350:HIS:HE1	1:E:448:ALA:O	1.89	0.55
1:A:290:HIS:HD2	1:A:334:GLY:O	1.89	0.55
1:B:105:LYS:HG3	2:B:2053:HOH:O	2.06	0.55
1:C:413:ARG:NH2	1:C:468:ILE:HD12	2.21	0.55
1:H:426:VAL:HG21	1:H:447:VAL:HG11	1.89	0.55
1:C:206:GLU:HG3	2:C:2212:HOH:O	2.05	0.55
1:F:105:LYS:HG3	2:F:2079:HOH:O	2.07	0.55
1:F:325:MET:HE2	2:F:2277:HOH:O	2.07	0.55
1:G:387:VAL:HG11	1:G:394:LEU:HD13	1.89	0.55
1:B:392:GLU:CG	1:B:393:GLY:N	2.52	0.55
1:C:413:ARG:CZ	1:C:468:ILE:HD12	2.36	0.55
1:G:63:ILE:HD11	1:G:82:ILE:HG12	1.89	0.55
1:H:233:LYS:HE3	1:H:248:GLU:OE2	2.07	0.55
1:H:250:PRO:HD3	1:H:388:MET:HE1	1.89	0.54
1:B:325:MET:HE2	2:B:2203:HOH:O	2.06	0.54
1:B:499:THR:HG23	2:D:2209:HOH:O	2.06	0.54
1:G:19:LYS:HE3	1:G:46:ILE:O	2.07	0.54
1:H:264:ILE:CD1	1:H:274:LEU:HG	2.38	0.54
1:C:466:LEU:HD11	1:C:480:ILE:HD11	1.89	0.54
1:D:374:ARG:NH2	1:D:479:GLU:OE1	2.36	0.54
1:E:103:MET:HE2	1:E:107:LEU:HB3	1.81	0.54
1:F:266:GLN:HG3	2:F:2265:HOH:O	2.07	0.54
1:B:417:ASN:ND2	1:B:419:GLN:H	2.05	0.54
1:B:418:GLU:O	1:B:425:ARG:HD2	2.08	0.54
1:E:238:LYS:HD3	1:E:243:TYR:CE1	2.43	0.54
1:F:269:PHE:HB3	1:F:272:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:391:GLY:HA3	1:H:472:LYS:NZ	2.22	0.54
1:C:399:GLN:NE2	1:C:467:SER:HB3	2.19	0.54
1:D:417:ASN:HD22	1:D:419:GLN:H	1.56	0.54
1:G:15:LYS:HD2	2:G:2223:HOH:O	2.08	0.54
1:A:409:VAL:HG11	1:A:464:ILE:HD12	1.90	0.54
1:B:130:TRP:NE1	1:B:134:ILE:CD1	2.71	0.54
1:A:489:THR:CG2	1:C:434:ARG:NE	2.67	0.54
1:F:214:PHE:CE1	1:F:218:ARG:HD3	2.43	0.54
1:A:24:THR:HG23	1:A:53:GLY:HA3	1.90	0.53
1:D:213:HIS:HB3	2:D:2192:HOH:O	2.07	0.53
1:G:397:GLU:HG3	1:G:469:VAL:HG13	1.90	0.53
1:H:69:ILE:HG12	1:H:74:LYS:CG	2.38	0.53
1:B:387:VAL:HG11	1:B:394:LEU:HD13	1.90	0.53
1:C:103:MET:HE3	1:C:107:LEU:CB	2.37	0.53
1:E:350:HIS:CE1	1:E:448:ALA:O	2.61	0.53
1:G:406:PHE:HE2	1:G:409:VAL:HG22	1.74	0.53
1:A:489:THR:HG23	1:C:434:ARG:HH21	1.73	0.53
1:B:79:PHE:HD2	1:B:82:ILE:HD11	1.72	0.53
1:G:93:ASN:HB3	2:G:2089:HOH:O	2.07	0.53
1:A:272:LEU:HD13	2:A:2226:HOH:O	2.06	0.53
1:B:369:MET:HE1	1:B:400:LEU:CD1	2.38	0.53
1:C:68:GLU:HG3	1:C:73:MET:SD	2.48	0.53
1:E:209:THR:HB	2:E:2218:HOH:O	2.09	0.53
1:F:70:ASP:HB2	2:F:2097:HOH:O	2.09	0.53
1:F:325:MET:CE	2:F:2277:HOH:O	2.56	0.53
1:B:489:THR:CG2	1:D:434:ARG:HH21	2.22	0.53
1:D:95:ARG:CZ	2:D:2108:HOH:O	2.57	0.53
1:E:83:ASP:OD1	1:E:140:HIS:HE1	1.92	0.53
1:E:252:ASP:HB3	2:E:2210:HOH:O	2.08	0.53
1:A:449:GLN:CD	2:A:2324:HOH:O	2.47	0.53
1:D:70:ASP:HA	2:D:2084:HOH:O	2.07	0.53
1:B:481:GLU:HG3	2:B:2286:HOH:O	2.09	0.53
1:E:391:GLY:CA	2:E:2279:HOH:O	2.57	0.53
1:F:312:SER:OG	2:F:2292:HOH:O	2.18	0.53
1:A:103:MET:HE1	1:A:107:LEU:HD13	1.89	0.53
1:A:481:GLU:HG3	2:A:2292:HOH:O	2.09	0.53
1:A:499:THR:CG2	2:C:2240:HOH:O	2.55	0.53
1:D:369:MET:HE1	1:D:400:LEU:HD11	1.89	0.53
1:D:387:VAL:HG11	1:D:394:LEU:HD13	1.90	0.53
1:G:417:ASN:HD22	1:G:420:TYR:H	1.56	0.53
1:H:11:ARG:HG2	1:H:12:GLU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:OE1	1:G:270:PRO:HG3	2.09	0.52
1:G:172:LYS:HA	1:G:207:TRP:CH2	2.43	0.52
1:H:121:VAL:O	1:H:121:VAL:HG13	2.09	0.52
1:G:125:LYS:HE2	2:G:2097:HOH:O	2.10	0.52
1:H:285:PRO:HG2	1:H:325:MET:HG3	1.90	0.52
1:B:144:ARG:NH2	1:C:436:PRO:O	2.41	0.52
1:B:202:GLY:HA2	1:B:227:ARG:HH12	1.74	0.52
1:B:481:GLU:CG	2:B:2286:HOH:O	2.57	0.52
1:A:426:VAL:HG21	1:A:447:VAL:CG1	2.37	0.52
1:B:40:LYS:HE3	2:B:2037:HOH:O	2.09	0.52
1:C:8:SER:OG	1:C:403:PRO:HB2	2.10	0.52
1:C:70:ASP:CG	1:C:70:ASP:O	2.48	0.52
2:E:2208:HOH:O	1:G:499:THR:HB	2.07	0.52
1:F:11:ARG:CG	2:F:2013:HOH:O	2.55	0.52
1:G:269:PHE:HB3	1:G:272:LEU:HG	1.90	0.52
1:H:239:THR:HG21	2:H:2217:HOH:O	2.08	0.52
1:B:10:GLY:O	1:B:11:ARG:HB2	2.09	0.52
1:C:233:LYS:CD	1:C:246:GLU:HG2	2.38	0.52
1:E:264:ILE:CD1	1:E:274:LEU:HG	2.39	0.52
2:E:2206:HOH:O	1:G:499:THR:CG2	2.57	0.52
1:D:70:ASP:HB2	2:D:2085:HOH:O	2.10	0.52
1:E:301:ARG:HH21	1:E:305:GLU:CD	2.13	0.52
1:G:422:ASN:HD22	1:G:422:ASN:C	2.13	0.52
1:H:432:ARG:NH2	2:H:2324:HOH:O	2.38	0.52
1:A:390:LYS:HD3	1:C:501:TYR:O	2.10	0.52
1:C:465:HIS:HB3	2:C:2311:HOH:O	2.09	0.52
1:D:415:ILE:HD11	1:D:453:MET:CE	2.36	0.52
1:H:121:VAL:O	1:H:121:VAL:HG12	2.09	0.52
1:A:239:THR:HG21	2:A:2201:HOH:O	2.09	0.52
1:D:392:GLU:CD	1:D:393:GLY:H	2.13	0.52
1:E:415:ILE:HD13	1:E:451:HIS:HB3	1.91	0.52
1:B:103:MET:HE1	1:B:107:LEU:CD1	2.40	0.51
1:C:56:LEU:CD1	1:C:82:ILE:HG21	2.39	0.51
1:E:339:VAL:CG1	1:E:343:SER:HA	2.40	0.51
1:A:103:MET:HE1	1:A:107:LEU:HD12	1.92	0.51
1:A:127:TYR:CE1	1:A:177:LYS:HE3	2.44	0.51
1:D:72:GLU:HG2	1:D:74:LYS:HG2	1.92	0.51
1:D:422:ASN:ND2	2:D:2282:HOH:O	2.43	0.51
1:D:486:GLU:O	1:D:489:THR:HB	2.10	0.51
1:B:489:THR:CG2	1:D:434:ARG:NE	2.66	0.51
1:C:290:HIS:HD2	1:C:334:GLY:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:CD2	1:D:468:ILE:HD12	2.39	0.51
1:A:214:PHE:CE1	1:A:218:ARG:HD3	2.45	0.51
1:B:331:LEU:HD13	1:B:332:PHE:CE1	2.45	0.51
1:E:252:ASP:CG	2:E:2210:HOH:O	2.49	0.51
2:F:2248:HOH:O	1:H:499:THR:CG2	2.52	0.51
1:B:350:HIS:CD2	2:B:2233:HOH:O	2.39	0.51
1:B:451:HIS:HD2	2:D:2157:HOH:O	1.94	0.51
1:F:290:HIS:HD2	1:F:334:GLY:O	1.93	0.51
1:F:415:ILE:CD1	1:F:451:HIS:CB	2.72	0.51
1:H:350:HIS:CD2	2:H:2282:HOH:O	2.45	0.51
1:A:499:THR:HG21	1:C:247:LEU:HG	1.91	0.51
1:C:251:GLU:HB2	2:C:2242:HOH:O	2.09	0.51
1:A:240:PHE:CD2	1:D:67:VAL:HG11	2.46	0.51
1:D:71:GLY:CA	2:D:2086:HOH:O	2.56	0.51
1:E:69:ILE:HG12	1:E:74:LYS:HG3	1.92	0.51
1:E:457:ARG:NH1	1:E:465:HIS:O	2.42	0.51
1:G:8:SER:HB3	1:G:403:PRO:CG	2.41	0.51
1:G:82:ILE:HD12	1:G:83:ASP:H	1.73	0.51
1:C:415:ILE:CD1	1:C:453:MET:CE	2.88	0.51
1:E:280:ASN:ND2	1:E:281:THR:H	2.01	0.51
1:F:44:GLU:HG3	2:F:2052:HOH:O	2.10	0.51
1:F:493:LEU:C	1:F:493:LEU:HD23	2.31	0.51
1:G:247:LEU:HD21	2:G:2198:HOH:O	2.11	0.51
1:H:481:GLU:CG	2:H:2374:HOH:O	2.59	0.51
1:A:265:ARG:HD2	2:A:2217:HOH:O	2.12	0.51
1:E:374:ARG:NH2	1:E:479:GLU:OE1	2.36	0.51
1:H:69:ILE:HD11	1:H:74:LYS:HG3	1.93	0.50
1:B:240:PHE:CD1	1:C:69:ILE:HD11	2.46	0.50
2:B:2187:HOH:O	1:D:499:THR:HG23	2.10	0.50
1:C:424:TRP:CH2	1:C:428:LYS:HE2	2.46	0.50
1:D:70:ASP:N	2:D:2085:HOH:O	2.43	0.50
1:F:16:LYS:HE2	2:F:2318:HOH:O	2.11	0.50
1:G:426:VAL:HG21	1:G:447:VAL:CG1	2.41	0.50
1:A:173:GLN:HG2	2:A:2168:HOH:O	2.11	0.50
1:A:350:HIS:HE1	1:A:448:ALA:O	1.94	0.50
1:A:404:VAL:CG1	1:A:459:ALA:HB1	2.42	0.50
1:C:200:ILE:HD11	1:C:208:ILE:HD12	1.93	0.50
1:D:82:ILE:HD12	1:D:83:ASP:N	2.26	0.50
1:A:14:PHE:HE2	2:A:2020:HOH:O	1.94	0.50
1:A:266:GLN:NE2	2:A:2218:HOH:O	2.43	0.50
1:A:499:THR:HG22	2:C:2240:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:HG2	1:B:316:TRP:CE3	2.46	0.50
1:C:103:MET:CE	1:C:107:LEU:HD13	2.41	0.50
1:G:70:ASP:O	1:G:71:GLY:O	2.29	0.50
1:E:14:PHE:HE2	2:E:2259:HOH:O	1.94	0.50
1:E:404:VAL:N	1:E:462:GLY:O	2.43	0.50
1:H:4:VAL:CG1	1:H:369:MET:HE1	2.30	0.50
1:H:103:MET:CG	1:H:103:MET:CA	2.80	0.50
1:C:63:ILE:HD11	1:C:82:ILE:HG12	1.94	0.50
1:D:373:ARG:HG2	2:D:2264:HOH:O	2.12	0.50
1:D:415:ILE:CD1	1:D:453:MET:HE1	2.36	0.50
1:H:26:ARG:NH1	2:H:2034:HOH:O	2.37	0.50
2:B:2187:HOH:O	1:D:499:THR:CG2	2.59	0.50
1:C:218:ARG:HD2	2:C:2217:HOH:O	2.11	0.50
1:C:413:ARG:CZ	1:C:468:ILE:CD1	2.89	0.50
1:E:145:TYR:CE2	1:H:438:ARG:NH2	2.79	0.50
1:F:499:THR:HB	2:H:2228:HOH:O	2.11	0.50
1:H:239:THR:CG2	2:H:2217:HOH:O	2.59	0.50
1:A:305:GLU:HB3	2:A:2238:HOH:O	2.11	0.50
1:F:393:GLY:O	1:F:394:LEU:HG	2.12	0.50
1:C:415:ILE:CD1	1:C:453:MET:HE1	2.41	0.50
1:E:402:ILE:HD12	1:E:480:ILE:CD1	2.40	0.50
1:G:205:ASP:HB3	1:G:263:LEU:HD11	1.94	0.50
1:H:364:TYR:CD2	1:H:369:MET:CE	2.95	0.50
1:A:413:ARG:HD3	1:A:453:MET:HE1	1.88	0.49
1:E:499:THR:HG23	2:G:2199:HOH:O	2.12	0.49
1:A:436:PRO:O	1:D:144:ARG:NH2	2.45	0.49
1:A:499:THR:HB	2:C:2241:HOH:O	2.13	0.49
1:E:392:GLU:HG2	1:E:393:GLY:H	1.76	0.49
1:E:404:VAL:H	1:E:462:GLY:C	2.15	0.49
1:E:422:ASN:ND2	1:E:425:ARG:H	2.11	0.49
1:E:426:VAL:CG2	1:E:447:VAL:HG11	2.31	0.49
1:G:404:VAL:HG12	1:G:406:PHE:H	1.77	0.49
1:H:422:ASN:C	1:H:422:ASN:HD22	2.15	0.49
1:B:417:ASN:ND2	1:B:420:TYR:H	2.10	0.49
1:D:209:THR:CG2	2:D:2185:HOH:O	2.60	0.49
1:F:374:ARG:HD3	1:F:378:SER:OG	2.12	0.49
1:G:239:THR:HG22	1:G:241:GLU:N	2.09	0.49
1:C:82:ILE:HD12	1:C:83:ASP:H	1.77	0.49
1:C:93:ASN:CB	2:C:2114:HOH:O	2.57	0.49
1:E:200:ILE:HD11	1:E:208:ILE:HG13	1.95	0.49
1:E:341:LEU:O	1:E:342:HIS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:TRP:O	1:G:134:ILE:HD12	2.12	0.49
1:A:402:ILE:HB	1:A:464:ILE:CG2	2.43	0.49
1:B:286:ILE:HG12	1:B:325:MET:HE3	1.93	0.49
1:B:457:ARG:NH1	1:B:465:HIS:O	2.43	0.49
1:A:269:PHE:HB3	1:A:272:LEU:HG	1.95	0.49
1:A:369:MET:CE	1:A:371:VAL:CG2	2.91	0.49
1:A:493:LEU:C	1:A:493:LEU:HD23	2.33	0.49
1:H:79:PHE:HD2	1:H:82:ILE:HD11	1.78	0.49
1:C:246:GLU:HG3	1:C:247:LEU:N	2.28	0.49
1:E:366:ASP:OD1	1:E:366:ASP:C	2.50	0.49
1:B:83:ASP:OD1	1:B:140:HIS:HE1	1.95	0.49
1:C:442:GLU:HG2	2:C:2336:HOH:O	2.11	0.49
1:F:489:THR:HG22	1:H:434:ARG:HE	1.71	0.49
1:G:114:VAL:O	1:G:115:PHE:HB2	2.13	0.49
1:C:485:ASP:OD1	1:C:487:THR:CG2	2.55	0.49
1:E:114:VAL:O	1:E:115:PHE:HB2	2.12	0.49
1:E:264:ILE:HD11	1:E:274:LEU:HG	1.95	0.49
1:A:389:GLU:CD	1:A:389:GLU:H	2.15	0.49
1:C:24:THR:HG23	1:C:53:GLY:HA3	1.94	0.49
1:D:125:LYS:HD3	2:D:2129:HOH:O	2.12	0.49
1:F:434:ARG:HE	1:H:489:THR:HG21	1.77	0.49
1:A:401:VAL:HG22	1:A:465:HIS:HD2	1.78	0.48
1:A:411:ILE:HD13	1:A:466:LEU:HD21	1.94	0.48
1:B:369:MET:HE1	1:B:400:LEU:HD11	1.95	0.48
1:B:417:ASN:HD22	1:B:419:GLN:H	1.61	0.48
1:C:213:HIS:HB3	2:C:2216:HOH:O	2.13	0.48
1:C:413:ARG:NH2	1:C:474:GLU:OE2	2.47	0.48
1:D:103:MET:HE2	1:D:107:LEU:CB	2.43	0.48
1:A:126:ASP:N	2:A:2122:HOH:O	2.45	0.48
1:E:417:ASN:C	1:E:417:ASN:HD22	2.16	0.48
1:G:22:VAL:HG13	1:G:48:PHE:CZ	2.49	0.48
1:A:83:ASP:OD1	1:A:140:HIS:CE1	2.60	0.48
1:C:391:GLY:HA3	1:C:394:LEU:HD11	1.94	0.48
1:C:413:ARG:NH2	1:C:468:ILE:CD1	2.76	0.48
1:E:402:ILE:CD1	1:E:480:ILE:HD13	2.44	0.48
1:C:406:PHE:HB3	1:C:482:GLN:HG3	1.95	0.48
1:D:438:ARG:NE	2:D:2295:HOH:O	2.43	0.48
1:E:391:GLY:C	2:E:2279:HOH:O	2.51	0.48
1:D:109:SER:HA	1:D:125:LYS:HG2	1.95	0.48
1:D:239:THR:HG22	1:D:241:GLU:N	2.26	0.48
1:F:422:ASN:HD21	1:F:424:TRP:HB3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLU:HG2	2:A:2289:HOH:O	2.14	0.48
1:C:130:TRP:NE1	1:C:134:ILE:HD11	2.29	0.48
1:D:20:PHE:HB3	1:D:312:SER:HB2	1.96	0.48
1:H:415:ILE:HG21	1:H:415:ILE:HD12	1.39	0.48
1:A:69:ILE:HD11	1:A:74:LYS:NZ	2.29	0.48
1:A:103:MET:HE3	1:A:130:TRP:HZ3	1.77	0.48
1:A:401:VAL:HG22	1:A:465:HIS:CD2	2.48	0.48
1:E:489:THR:HG21	1:G:434:ARG:HE	1.78	0.48
1:F:402:ILE:HB	1:F:464:ILE:HD11	1.95	0.48
1:F:415:ILE:HD13	1:F:451:HIS:CB	2.28	0.48
1:H:417:ASN:HD22	1:H:419:GLN:H	1.62	0.48
1:B:406:PHE:HD2	1:B:409:VAL:CG2	2.26	0.47
1:E:140:HIS:HD2	2:E:2135:HOH:O	1.96	0.47
1:E:143:GLU:HG3	2:E:2133:HOH:O	2.14	0.47
1:F:130:TRP:NE1	1:F:134:ILE:CD1	2.74	0.47
1:G:451:HIS:HD2	2:G:2136:HOH:O	1.97	0.47
1:H:373:ARG:NH1	1:H:379:ILE:HD11	2.29	0.47
1:E:422:ASN:HD21	1:E:424:TRP:HB3	1.79	0.47
1:H:458:ARG:HG2	2:H:2361:HOH:O	2.13	0.47
1:B:301:ARG:CB	2:B:2209:HOH:O	2.61	0.47
1:C:238:LYS:CD	1:C:243:TYR:CE1	2.94	0.47
1:C:405:SER:O	1:C:406:PHE:O	2.32	0.47
1:E:501:TYR:C	1:E:502:SER:CA	2.74	0.47
1:F:402:ILE:HB	1:F:464:ILE:HD13	1.95	0.47
1:G:341:LEU:O	1:G:342:HIS:HB2	2.14	0.47
1:G:387:VAL:HB	1:G:472:LYS:HG3	1.95	0.47
1:G:79:PHE:HD2	1:G:82:ILE:HD11	1.78	0.47
1:B:63:ILE:HD11	1:B:82:ILE:HG12	1.96	0.47
1:H:69:ILE:O	1:H:69:ILE:HG13	2.13	0.47
1:A:489:THR:HG23	1:C:434:ARG:HE	1.74	0.47
1:B:82:ILE:HD12	1:B:83:ASP:N	2.28	0.47
1:B:233:LYS:HD3	1:B:246:GLU:HG2	1.97	0.47
1:C:233:LYS:CE	1:C:246:GLU:HG2	2.44	0.47
1:C:274:LEU:HD13	1:C:310:VAL:CG1	2.31	0.47
1:D:453:MET:HE3	1:D:453:MET:HB2	1.77	0.47
1:F:239:THR:CG2	2:F:2244:HOH:O	2.62	0.47
1:H:239:THR:CG2	1:H:241:GLU:H	2.22	0.47
1:H:373:ARG:CZ	1:H:379:ILE:HD11	2.44	0.47
1:A:201:CYS:HB2	2:A:2176:HOH:O	2.13	0.47
1:A:404:VAL:CG1	1:A:459:ALA:CB	2.92	0.47
1:A:446:GLN:HG2	1:C:452:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:THR:HG23	1:G:53:GLY:CA	2.45	0.47
1:H:364:TYR:CD2	1:H:369:MET:HE3	2.49	0.47
1:C:129:LYS:HE3	2:C:2078:HOH:O	2.15	0.47
1:D:394:LEU:HD12	2:D:2276:HOH:O	2.14	0.47
1:G:233:LYS:HD3	1:G:246:GLU:OE1	2.14	0.47
1:G:415:ILE:HG23	1:G:415:ILE:HD13	1.29	0.47
1:C:6:VAL:HG21	1:C:402:ILE:HD13	1.97	0.47
1:G:486:GLU:O	1:G:489:THR:HB	2.15	0.47
1:C:6:VAL:O	1:C:403:PRO:HD3	2.15	0.47
1:H:384:TRP:HA	1:H:474:GLU:O	2.14	0.47
1:A:404:VAL:HG11	1:A:459:ALA:HB1	1.96	0.46
1:D:140:HIS:HD2	2:D:2144:HOH:O	1.98	0.46
1:D:406:PHE:O	1:D:407:SER:HB3	2.14	0.46
1:E:164:VAL:HG13	2:E:2107:HOH:O	2.15	0.46
1:E:261:ARG:NH2	1:E:311:ASP:OD2	2.44	0.46
1:G:428:LYS:HD3	1:G:432:ARG:NH1	2.31	0.46
1:B:406:PHE:HB3	1:B:482:GLN:HG3	1.97	0.46
2:B:2305:HOH:O	1:D:239:THR:HG21	2.15	0.46
1:G:45:LYS:HD3	2:G:2041:HOH:O	2.14	0.46
1:A:457:ARG:HH11	1:A:466:LEU:HD23	1.81	0.46
1:B:364:TYR:CD2	1:B:369:MET:CE	2.97	0.46
1:F:434:ARG:HE	1:H:489:THR:CG2	2.29	0.46
1:H:364:TYR:HE2	1:H:369:MET:HE2	1.70	0.46
1:E:438:ARG:NE	2:E:2302:HOH:O	2.48	0.46
1:G:107:LEU:HD21	1:G:129:LYS:HB3	1.97	0.46
1:G:426:VAL:CG2	1:G:447:VAL:HG11	2.43	0.46
1:C:24:THR:OG1	1:C:35:TYR:OH	2.29	0.46
1:D:339:VAL:CG1	1:D:343:SER:HA	2.45	0.46
1:F:398:VAL:CG1	1:F:400:LEU:HD13	2.42	0.46
1:B:402:ILE:HA	1:B:403:PRO:HD2	1.80	0.46
1:D:337:GLY:O	1:D:346:LYS:HD2	2.15	0.46
1:D:426:VAL:HG21	1:D:447:VAL:CG1	2.44	0.46
1:E:69:ILE:CG1	1:E:74:LYS:HG3	2.46	0.46
1:E:342:HIS:HD2	2:E:2007:HOH:O	1.98	0.46
1:H:339:VAL:CG1	1:H:343:SER:HA	2.46	0.46
1:H:389:GLU:OE2	2:H:2301:HOH:O	2.20	0.46
1:A:238:LYS:HD3	1:A:243:TYR:CE1	2.51	0.46
1:D:394:LEU:HD23	2:D:2277:HOH:O	2.16	0.46
1:G:93:ASN:CB	2:G:2089:HOH:O	2.63	0.46
1:G:417:ASN:ND2	1:G:419:GLN:H	2.14	0.46
1:H:162:ASN:ND2	1:H:204:SER:OG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:CG	2:A:2008:HOH:O	2.47	0.46
1:B:24:THR:HB	1:B:51:ILE:HD11	1.98	0.46
1:C:95:ARG:HD3	1:C:149:GLU:OE2	2.16	0.46
1:C:325:MET:O	1:C:326:ASP:CB	2.63	0.46
1:C:406:PHE:HD2	1:C:409:VAL:HG23	1.81	0.46
1:C:460:THR:O	1:C:461:ASP:HB2	2.16	0.46
1:H:239:THR:HG22	1:H:241:GLU:N	2.23	0.46
1:B:87:ASP:OD1	1:C:438:ARG:NH2	2.49	0.45
1:B:459:ALA:HA	1:B:464:ILE:HG22	1.98	0.45
1:C:143:GLU:HG3	2:C:2151:HOH:O	2.16	0.45
1:D:364:TYR:CE2	1:D:369:MET:CE	2.97	0.45
1:B:261:ARG:O	1:B:265:ARG:HG3	2.16	0.45
1:B:445:ARG:NH1	2:B:2269:HOH:O	2.03	0.45
1:D:227:ARG:NH2	1:D:256:GLN:NE2	2.62	0.45
1:D:350:HIS:HE1	1:D:448:ALA:O	2.00	0.45
1:D:404:VAL:O	1:D:462:GLY:CA	2.61	0.45
1:E:252:ASP:CB	2:E:2210:HOH:O	2.64	0.45
1:F:413:ARG:NH2	1:F:474:GLU:OE2	2.46	0.45
1:H:24:THR:HG1	1:H:35:TYR:HH	1.61	0.45
1:A:383:LEU:HD23	1:A:383:LEU:N	2.31	0.45
1:A:397:GLU:HB3	2:A:2289:HOH:O	2.16	0.45
1:C:417:ASN:HD22	1:C:417:ASN:C	2.20	0.45
1:D:325:MET:O	1:D:326:ASP:CB	2.64	0.45
1:G:83:ASP:OD1	1:G:140:HIS:CE1	2.68	0.45
1:B:406:PHE:CE1	1:B:482:GLN:HB2	2.52	0.45
1:C:406:PHE:HB2	1:C:407:SER:H	1.51	0.45
1:A:148:GLU:CG	2:A:2146:HOH:O	2.57	0.45
1:D:151:ARG:HD2	2:D:2153:HOH:O	2.15	0.45
1:E:13:LYS:NZ	2:E:2003:HOH:O	2.50	0.45
1:H:438:ARG:HD2	2:H:2331:HOH:O	2.16	0.45
1:A:114:VAL:O	1:A:115:PHE:HB2	2.17	0.45
1:B:350:HIS:CE1	1:B:448:ALA:O	2.69	0.45
1:C:407:SER:HA	1:C:459:ALA:HB3	1.99	0.45
1:C:426:VAL:HG21	1:C:447:VAL:CG1	2.43	0.45
1:D:350:HIS:CE1	1:D:448:ALA:O	2.69	0.45
1:D:406:PHE:O	1:D:407:SER:OG	2.34	0.45
1:F:10:GLY:O	1:F:11:ARG:CB	2.50	0.45
1:A:406:PHE:CG	1:A:482:GLN:HG3	2.52	0.45
1:A:417:ASN:HD22	1:A:420:TYR:H	1.61	0.45
1:B:95:ARG:HD3	1:B:149:GLU:OE2	2.17	0.45
1:E:121:VAL:HG22	1:E:166:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:THR:CG2	1:F:241:GLU:H	2.24	0.45
1:G:294:LEU:O	1:G:294:LEU:HG	2.16	0.45
1:H:26:ARG:NH1	1:H:60:ASP:OD2	2.48	0.45
1:H:280:ASN:HD22	1:H:281:THR:N	2.04	0.45
1:B:69:ILE:HG13	1:B:74:LYS:HG3	1.99	0.45
1:C:280:ASN:ND2	1:C:281:THR:H	2.02	0.45
1:E:69:ILE:HD11	1:E:74:LYS:NZ	2.32	0.45
1:H:240:PHE:CE2	1:H:241:GLU:HG3	2.52	0.45
1:A:121:VAL:HG22	1:A:166:PHE:O	2.17	0.45
1:B:206:GLU:HB2	2:B:2165:HOH:O	2.16	0.45
1:G:350:HIS:CE1	1:G:448:ALA:O	2.70	0.45
1:D:417:ASN:ND2	1:D:420:TYR:H	2.15	0.45
1:A:408:ALA:HB2	1:A:458:ARG:NE	2.30	0.44
1:B:417:ASN:HD22	1:B:420:TYR:H	1.64	0.44
1:B:438:ARG:NH2	2:B:2264:HOH:O	2.47	0.44
1:D:285:PRO:HG2	1:D:325:MET:HG3	2.00	0.44
1:E:239:THR:HG22	1:E:241:GLU:N	2.30	0.44
1:G:502:SER:HB2	2:G:2339:HOH:O	2.16	0.44
1:E:162:ASN:HA	1:E:207:TRP:CZ2	2.52	0.44
1:E:438:ARG:NH1	2:E:2304:HOH:O	2.50	0.44
1:F:415:ILE:HD11	1:F:451:HIS:CB	2.37	0.44
1:G:225:VAL:HG23	1:G:272:LEU:HD13	1.99	0.44
1:C:79:PHE:HD2	1:C:82:ILE:HD11	1.82	0.44
1:C:426:VAL:CG2	1:C:447:VAL:HG11	2.46	0.44
1:D:99:GLU:OE1	2:D:2111:HOH:O	2.21	0.44
1:D:368:GLU:OE2	1:D:396:LYS:HE3	2.17	0.44
1:E:14:PHE:CE2	2:E:2259:HOH:O	2.57	0.44
1:E:103:MET:HE2	1:E:124:PRO:HA	2.00	0.44
1:F:285:PRO:HB3	1:F:336:PHE:CE1	2.52	0.44
1:A:102:PHE:HB3	1:A:120:ASN:O	2.18	0.44
1:D:177:LYS:HE3	2:D:2172:HOH:O	2.16	0.44
1:G:148:GLU:HB3	2:G:2126:HOH:O	2.16	0.44
1:G:411:ILE:O	1:G:454:THR:HA	2.17	0.44
1:A:247:LEU:HG	1:C:499:THR:HG21	2.00	0.44
1:B:285:PRO:CG	1:B:325:MET:HG3	2.45	0.44
1:C:406:PHE:O	1:C:407:SER:CB	2.66	0.44
1:D:95:ARG:NH2	2:D:2108:HOH:O	2.51	0.44
1:D:301:ARG:O	1:D:304:SER:HB3	2.17	0.44
1:E:468:ILE:HD12	1:E:478:ILE:HD13	2.00	0.44
1:F:258:LYS:HE2	2:F:2258:HOH:O	2.17	0.44
1:H:417:ASN:HD22	1:H:420:TYR:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:457:ARG:NH1	1:H:465:HIS:O	2.47	0.44
1:B:499:THR:CG2	2:D:2209:HOH:O	2.64	0.44
1:C:464:ILE:HD13	1:C:466:LEU:HG	2.00	0.44
1:G:235:PRO:HG2	1:G:238:LYS:HE2	1.99	0.44
1:A:103:MET:HE3	1:A:130:TRP:CZ3	2.53	0.44
1:B:205:ASP:HB3	1:B:263:LEU:HD11	1.99	0.44
1:B:374:ARG:HD3	1:B:378:SER:OG	2.17	0.44
1:B:426:VAL:CG2	1:B:447:VAL:HG11	2.46	0.44
1:C:413:ARG:HD3	1:C:453:MET:HE3	2.00	0.44
1:C:438:ARG:HD3	2:C:2327:HOH:O	2.17	0.44
1:D:422:ASN:C	1:D:422:ASN:HD22	2.21	0.44
1:B:400:LEU:HB3	1:B:402:ILE:CD1	2.46	0.44
1:C:385:ASN:ND2	1:C:394:LEU:O	2.49	0.44
1:C:406:PHE:CD1	1:C:406:PHE:N	2.85	0.44
1:D:209:THR:HB	2:D:2218:HOH:O	2.17	0.44
1:E:392:GLU:HG2	1:E:393:GLY:N	2.32	0.44
1:F:275:HIS:HD1	1:F:312:SER:HB3	1.80	0.44
1:F:466:LEU:HD11	1:F:480:ILE:HD11	1.99	0.44
1:F:485:ASP:OD1	1:F:487:THR:CG2	2.55	0.44
1:H:392:GLU:CA	2:H:2305:HOH:O	2.36	0.44
1:B:350:HIS:HE1	1:B:448:ALA:O	2.01	0.44
1:C:204:SER:CB	2:C:2207:HOH:O	2.66	0.44
1:E:208:ILE:HD13	1:E:260:VAL:HG13	1.99	0.44
1:G:121:VAL:HG22	1:G:166:PHE:O	2.17	0.44
1:G:406:PHE:CE2	1:G:409:VAL:CG2	3.01	0.44
1:A:26:ARG:HD3	1:A:117:TRP:CE2	2.53	0.43
1:F:459:ALA:HA	1:F:464:ILE:HG22	2.00	0.43
1:G:213:HIS:NE2	1:G:217:GLU:OE2	2.51	0.43
1:A:24:THR:CG2	1:A:53:GLY:HA3	2.47	0.43
1:D:424:TRP:O	1:D:428:LYS:HG3	2.19	0.43
1:D:426:VAL:CG2	1:D:447:VAL:HG11	2.47	0.43
1:E:237:LYS:NZ	1:G:492:GLY:O	2.44	0.43
1:E:247:LEU:HG	1:G:499:THR:HG21	2.00	0.43
1:G:406:PHE:HE2	1:G:409:VAL:CG2	2.31	0.43
1:A:239:THR:HG22	1:A:242:TYR:N	2.33	0.43
1:A:350:HIS:CE1	1:A:448:ALA:O	2.71	0.43
1:B:290:HIS:HD2	1:B:334:GLY:O	2.00	0.43
1:B:391:GLY:HA3	1:B:394:LEU:HD11	2.00	0.43
1:B:460:THR:O	1:B:461:ASP:C	2.57	0.43
1:C:397:GLU:HG2	1:C:469:VAL:HG22	2.01	0.43
1:D:290:HIS:HD2	1:D:334:GLY:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HD3	1:B:117:TRP:CE2	2.54	0.43
1:C:422:ASN:C	1:C:422:ASN:HD22	2.22	0.43
1:D:26:ARG:HD3	1:D:117:TRP:CE2	2.53	0.43
1:D:218:ARG:HE	1:D:218:ARG:HB3	1.46	0.43
1:E:13:LYS:CE	2:E:2003:HOH:O	2.62	0.43
1:E:404:VAL:HG11	1:E:459:ALA:CB	2.48	0.43
1:E:422:ASN:HD22	1:E:422:ASN:C	2.22	0.43
1:H:79:PHE:HA	1:H:82:ILE:HD11	2.00	0.43
1:A:493:LEU:HD23	1:A:494:ASP:N	2.33	0.43
1:B:20:PHE:HB3	1:B:312:SER:HB2	1.99	0.43
1:B:489:THR:HG22	1:D:434:ARG:HH21	1.82	0.43
1:D:227:ARG:HH21	1:D:256:GLN:HE21	1.65	0.43
1:F:285:PRO:HG2	1:F:325:MET:HG3	2.00	0.43
1:H:125:LYS:HA	1:H:125:LYS:HD3	1.71	0.43
1:H:239:THR:HG22	1:H:242:TYR:H	1.84	0.43
1:B:417:ASN:HB3	1:B:474:GLU:HG3	2.01	0.43
1:C:209:THR:HB	2:C:2252:HOH:O	2.19	0.43
1:F:266:GLN:NE2	2:F:2265:HOH:O	2.51	0.43
1:F:389:GLU:HG3	2:F:2334:HOH:O	2.17	0.43
1:F:392:GLU:N	1:F:394:LEU:HD12	2.32	0.43
1:G:103:MET:HE1	1:G:107:LEU:HD13	2.01	0.43
1:B:93:ASN:HB3	2:B:2085:HOH:O	2.17	0.43
1:D:457:ARG:NH1	1:D:466:LEU:HD23	2.34	0.43
1:E:69:ILE:HG13	1:E:69:ILE:O	2.19	0.43
1:G:218:ARG:HE	1:G:218:ARG:HB3	1.34	0.43
1:H:172:LYS:HA	1:H:207:TRP:CH2	2.54	0.43
1:D:82:ILE:HD12	1:D:83:ASP:H	1.83	0.43
1:D:165:ASN:ND2	1:D:165:ASN:N	2.66	0.43
1:E:499:THR:HG22	2:G:2199:HOH:O	2.17	0.43
1:F:125:LYS:CD	2:F:2150:HOH:O	2.59	0.43
1:B:258:LYS:HD3	1:B:309:TYR:CE2	2.53	0.43
1:B:445:ARG:HH11	1:B:445:ARG:HD2	1.58	0.43
1:D:16:LYS:HD2	2:D:2263:HOH:O	2.19	0.43
1:F:502:SER:HA	2:H:2158:HOH:O	2.18	0.43
1:B:434:ARG:HE	1:D:489:THR:HG21	1.82	0.43
1:C:125:LYS:HD3	1:C:125:LYS:HA	1.88	0.43
1:B:458:ARG:HD3	1:B:458:ARG:HA	1.62	0.42
1:F:239:THR:HG23	2:F:2244:HOH:O	2.19	0.42
1:H:502:SER:HA	2:H:2397:HOH:O	2.19	0.42
1:A:26:ARG:HH11	1:A:26:ARG:HD2	1.53	0.42
1:A:162:ASN:ND2	1:A:204:SER:OG	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HB2	2:B:2209:HOH:O	2.19	0.42
1:B:404:VAL:HG13	1:B:406:PHE:HB2	2.01	0.42
1:C:130:TRP:NE1	1:C:134:ILE:CD1	2.82	0.42
1:C:230:TYR:OH	1:C:278:GLU:OE1	2.20	0.42
1:G:415:ILE:HG21	1:G:415:ILE:HD12	1.43	0.42
1:H:285:PRO:HB3	1:H:336:PHE:CE1	2.54	0.42
1:B:107:LEU:HD21	1:B:129:LYS:CB	2.48	0.42
1:E:50:TYR:HA	1:E:95:ARG:O	2.18	0.42
1:A:301:ARG:CB	2:A:2235:HOH:O	2.67	0.42
1:B:308:ASP:OD2	1:B:365:ARG:NH2	2.53	0.42
1:C:103:MET:HE2	1:C:124:PRO:HA	2.01	0.42
1:A:369:MET:HE2	1:A:371:VAL:CG2	2.48	0.42
1:D:418:GLU:O	1:D:425:ARG:HD3	2.18	0.42
1:H:82:ILE:HD12	1:H:83:ASP:N	2.34	0.42
1:A:79:PHE:CD2	1:A:82:ILE:HD11	2.51	0.42
1:A:415:ILE:HG23	1:A:415:ILE:HD13	1.73	0.42
1:B:227:ARG:O	1:B:276:ILE:HA	2.19	0.42
1:C:281:THR:OG1	1:C:295:ASN:ND2	2.47	0.42
1:E:392:GLU:CG	1:E:393:GLY:H	2.31	0.42
2:E:2341:HOH:O	1:G:239:THR:CG2	2.66	0.42
1:F:438:ARG:HD3	2:F:2361:HOH:O	2.18	0.42
1:H:325:MET:O	1:H:326:ASP:CB	2.67	0.42
1:A:374:ARG:NH2	1:A:479:GLU:OE1	2.33	0.42
1:C:156:GLU:OE1	1:C:226:SER:OG	2.29	0.42
1:F:438:ARG:HD3	2:F:2363:HOH:O	2.09	0.42
1:B:227:ARG:HD3	1:B:260:VAL:HG21	2.01	0.42
1:C:493:LEU:HD23	1:C:494:ASP:N	2.35	0.42
1:D:358:LEU:HD21	1:D:382:VAL:HG23	2.01	0.42
1:F:278:GLU:HG2	1:F:316:TRP:CE3	2.54	0.42
1:B:123:PRO:CD	1:B:168:LYS:HE2	2.50	0.42
1:H:267:SER:HB2	1:H:268:PRO:HD2	2.02	0.42
1:H:415:ILE:HG23	1:H:415:ILE:HD13	1.24	0.42
1:A:26:ARG:NH1	1:A:60:ASP:CG	2.65	0.42
1:B:123:PRO:HD2	1:B:168:LYS:HE2	2.01	0.42
1:D:392:GLU:O	1:D:394:LEU:N	2.49	0.42
2:E:2206:HOH:O	1:G:499:THR:HG23	2.19	0.42
1:F:401:VAL:HG22	1:F:465:HIS:CD2	2.55	0.42
1:G:466:LEU:HD11	1:G:480:ILE:HD11	2.01	0.42
1:B:103:MET:HE2	1:B:107:LEU:HB3	2.02	0.41
1:C:125:LYS:CG	2:C:2123:HOH:O	2.67	0.41
1:C:438:ARG:CD	2:C:2327:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:SER:HB3	1:F:290:HIS:CE1	2.55	0.41
1:H:33:LYS:HD2	2:H:2048:HOH:O	2.19	0.41
1:B:274:LEU:CD1	1:B:310:VAL:HG12	2.24	0.41
1:C:8:SER:OG	1:C:403:PRO:CB	2.68	0.41
1:F:451:HIS:HD2	2:H:2165:HOH:O	2.03	0.41
1:A:449:GLN:NE2	2:A:2324:HOH:O	2.53	0.41
1:E:251:GLU:HG2	1:E:301:ARG:NH1	2.36	0.41
1:H:251:GLU:HB2	2:H:2229:HOH:O	2.20	0.41
1:A:287:ASN:OD1	1:A:289:VAL:HG22	2.21	0.41
1:B:374:ARG:NH2	1:B:479:GLU:OE1	2.44	0.41
1:C:107:LEU:HD21	1:C:129:LYS:HB3	2.03	0.41
1:G:19:LYS:HE2	1:G:47:GLY:O	2.20	0.41
1:G:121:VAL:HG13	1:G:121:VAL:O	2.20	0.41
1:G:164:VAL:HG12	2:G:2103:HOH:O	2.20	0.41
1:A:325:MET:O	1:A:326:ASP:CB	2.69	0.41
1:A:449:GLN:CG	2:A:2324:HOH:O	2.57	0.41
1:B:205:ASP:HB3	1:B:263:LEU:CD1	2.50	0.41
1:B:493:LEU:HD23	1:B:493:LEU:C	2.40	0.41
1:C:457:ARG:NH1	1:C:465:HIS:O	2.54	0.41
1:H:401:VAL:HG22	1:H:465:HIS:CD2	2.56	0.41
1:A:369:MET:HE3	1:A:371:VAL:HG21	2.03	0.41
1:A:445:ARG:HD2	2:A:2316:HOH:O	2.20	0.41
1:B:358:LEU:HD21	1:B:382:VAL:HG23	2.03	0.41
1:C:153:TRP:O	1:C:154:LEU:HD23	2.20	0.41
1:C:337:GLY:O	1:C:346:LYS:HD2	2.20	0.41
1:D:190:ASP:HB3	1:D:193:LEU:HG	2.03	0.41
1:D:417:ASN:HD22	1:D:417:ASN:C	2.24	0.41
1:H:264:ILE:HD11	1:H:274:LEU:HG	2.03	0.41
1:H:369:MET:HE1	1:H:400:LEU:HD13	2.02	0.41
1:C:267:SER:HB2	1:C:268:PRO:CD	2.49	0.41
1:C:424:TRP:CZ2	1:C:428:LYS:HE2	2.55	0.41
1:D:206:GLU:HG3	2:D:2187:HOH:O	2.20	0.41
1:D:401:VAL:HG22	1:D:465:HIS:CD2	2.56	0.41
1:E:425:ARG:HG3	2:E:2293:HOH:O	2.19	0.41
1:G:79:PHE:CD2	1:G:82:ILE:HD11	2.55	0.41
1:C:415:ILE:CD1	1:C:453:MET:HE2	2.50	0.41
1:F:111:ASP:O	1:F:113:THR:HG23	2.19	0.41
1:G:227:ARG:O	1:G:276:ILE:HA	2.20	0.41
1:A:143:GLU:OE1	2:A:2137:HOH:O	2.22	0.41
1:A:369:MET:HE3	1:A:371:VAL:CG2	2.50	0.41
1:B:103:MET:HE2	1:B:107:LEU:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASN:H	1:B:165:ASN:ND2	2.18	0.41
1:B:249:PRO:HA	1:B:388:MET:CE	2.51	0.41
1:D:227:ARG:HH21	1:D:256:GLN:NE2	2.19	0.41
1:F:67:VAL:HG13	1:F:69:ILE:HG23	2.03	0.41
1:G:127:TYR:CE1	1:G:177:LYS:HE3	2.56	0.41
1:G:165:ASN:H	1:G:165:ASN:ND2	2.19	0.41
1:H:40:LYS:HE3	2:H:2047:HOH:O	2.20	0.41
1:H:258:LYS:HG3	1:H:309:TYR:CD2	2.55	0.41
1:C:395:THR:HG23	2:C:2309:HOH:O	2.20	0.41
1:F:229:ALA:O	1:F:279:TYR:HA	2.21	0.41
1:G:45:LYS:HD2	1:G:349:PHE:CZ	2.55	0.41
1:A:65:ARG:HG2	2:A:2071:HOH:O	2.19	0.40
1:A:423:ALA:HB2	1:A:448:ALA:HB2	2.03	0.40
1:B:239:THR:HG21	2:B:2183:HOH:O	2.22	0.40
1:C:399:GLN:HE21	1:C:467:SER:CB	2.25	0.40
1:D:95:ARG:HD3	1:D:149:GLU:OE2	2.21	0.40
1:F:481:GLU:CD	2:F:2390:HOH:O	2.60	0.40
1:G:358:LEU:HD21	1:G:382:VAL:HG23	2.01	0.40
1:H:493:LEU:C	1:H:493:LEU:HD23	2.41	0.40
1:A:382:VAL:C	1:A:383:LEU:HD23	2.42	0.40
1:A:417:ASN:HD22	1:A:417:ASN:C	2.24	0.40
1:A:481:GLU:CG	2:A:2292:HOH:O	2.68	0.40
1:B:69:ILE:CG1	1:B:74:LYS:HG3	2.50	0.40
1:C:387:VAL:HG11	1:C:394:LEU:HD13	2.03	0.40
1:H:350:HIS:CE1	1:H:448:ALA:O	2.74	0.40
1:C:114:VAL:O	1:C:115:PHE:HB2	2.22	0.40
1:C:387:VAL:HG13	1:C:394:LEU:HD22	2.04	0.40
1:D:54:HIS:HE1	1:D:159:ASN:OD1	2.04	0.40
1:B:413:ARG:HD3	1:B:453:MET:HE2	2.04	0.40
1:E:6:VAL:HB	1:E:402:ILE:HG22	2.03	0.40
1:F:24:THR:HG23	1:F:53:GLY:HA3	2.04	0.40
1:H:464:ILE:HD12	1:H:466:LEU:HD21	2.04	0.40
1:A:65:ARG:CG	2:A:2071:HOH:O	2.69	0.40
1:A:278:GLU:HG2	1:A:316:TRP:CE3	2.57	0.40
1:B:103:MET:CE	1:B:107:LEU:HB3	2.52	0.40
1:C:239:THR:CG2	2:C:2236:HOH:O	2.60	0.40
1:D:455:GLU:CD	1:D:457:ARG:HH21	2.25	0.40
1:E:406:PHE:CD1	1:E:406:PHE:N	2.89	0.40
1:F:280:ASN:ND2	1:F:281:THR:H	2.01	0.40
1:G:493:LEU:C	1:G:493:LEU:HD23	2.41	0.40
1:H:69:ILE:CG1	1:H:74:LYS:HG2	2.47	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)
2:D:2193:HOH:O	2:G:2069:HOH:O[3_645]	1.99	0.21
2:A:2007:HOH:O	2:F:2015:HOH:O[4_556]	2.18	0.02

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	497/503 (99%)	467 (94%)	27 (5%)	3 (1%)	25	26
1	B	497/503 (99%)	473 (95%)	18 (4%)	6 (1%)	13	10
1	C	497/503 (99%)	469 (94%)	24 (5%)	4 (1%)	19	19
1	D	496/503 (99%)	468 (94%)	22 (4%)	6 (1%)	13	10
1	E	497/503 (99%)	475 (96%)	21 (4%)	1 (0%)	47	55
1	F	497/503 (99%)	468 (94%)	25 (5%)	4 (1%)	19	19
1	G	497/503 (99%)	474 (95%)	20 (4%)	3 (1%)	25	26
1	H	497/503 (99%)	476 (96%)	18 (4%)	3 (1%)	25	26
All	All	3975/4024 (99%)	3770 (95%)	175 (4%)	30 (1%)	19	19

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	GLY
1	B	406	PHE
1	B	461	ASP
1	C	391	GLY
1	C	406	PHE
1	C	407	SER
1	D	70	ASP
1	D	392	GLU

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Mol	Chain	Res	Type
1	D	407	SER
1	F	392	GLU
1	G	391	GLY
1	H	392	GLU
1	A	11	ARG
1	B	391	GLY
1	C	392	GLU
1	D	391	GLY
1	E	11	ARG
1	F	11	ARG
1	F	391	GLY
1	G	70	ASP
1	G	71	GLY
1	H	11	ARG
1	B	70	ASP
1	B	392	GLU
1	B	407	SER
1	D	406	PHE
1	F	70	ASP
1	A	70	ASP
1	H	102	PHE
1	D	404	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	439/443 (99%)	392 (89%)	47 (11%)	6 6
1	B	439/443 (99%)	402 (92%)	37 (8%)	11 11
1	C	439/443 (99%)	394 (90%)	45 (10%)	7 6
1	D	439/443 (99%)	392 (89%)	47 (11%)	6 6
1	E	439/443 (99%)	399 (91%)	40 (9%)	9 9
1	F	439/443 (99%)	397 (90%)	42 (10%)	8 8
1	G	439/443 (99%)	392 (89%)	47 (11%)	6 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	439/443 (99%)	397 (90%)	42 (10%)	8 8
All	All	3512/3544 (99%)	3165 (90%)	347 (10%)	8 7

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	39	LEU
1	A	41	LEU
1	A	67	VAL
1	A	69	ILE
1	A	82	ILE
1	A	95	ARG
1	A	97	PHE
1	A	107	LEU
1	A	121	VAL
1	A	131	ARG
1	A	133	LEU
1	A	147	ILE
1	A	178	LEU
1	A	206	GLU
1	A	209	THR
1	A	222	VAL
1	A	227	ARG
1	A	239	THR
1	A	251	GLU
1	A	265	ARG
1	A	274	LEU
1	A	280	ASN
1	A	289	VAL
1	A	294	LEU
1	A	313	PHE
1	A	319	SER
1	A	325	MET
1	A	331	LEU
1	A	362	LEU
1	A	383	LEU
1	A	386	LEU
1	A	392	GLU
1	A	395	THR
1	A	402	ILE
1	A	407	SER

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Mol	Chain	Res	Type
1	A	409	VAL
1	A	415	ILE
1	A	417	ASN
1	A	422	ASN
1	A	447	VAL
1	A	463	VAL
1	A	464	ILE
1	A	481	GLU
1	A	489	THR
1	A	499	THR
1	A	502	SER
1	B	13	LYS
1	B	27	LEU
1	B	39	LEU
1	B	41	LEU
1	B	67	VAL
1	B	68	GLU
1	B	69	ILE
1	B	70	ASP
1	B	74	LYS
1	B	82	ILE
1	B	97	PHE
1	B	121	VAL
1	B	125	LYS
1	B	133	LEU
1	B	164	VAL
1	B	178	LEU
1	B	226	SER
1	B	239	THR
1	B	251	GLU
1	B	265	ARG
1	B	274	LEU
1	B	280	ASN
1	B	319	SER
1	B	325	MET
1	B	331	LEU
1	B	374	ARG
1	B	383	LEU
1	B	392	GLU
1	B	395	THR
1	B	409	VAL
1	B	417	ASN

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Mol	Chain	Res	Type
1	B	422	ASN
1	B	425	ARG
1	B	463	VAL
1	B	481	GLU
1	B	489	THR
1	B	499	THR
1	C	27	LEU
1	C	39	LEU
1	C	41	LEU
1	C	67	VAL
1	C	82	ILE
1	C	97	PHE
1	C	105	LYS
1	C	121	VAL
1	C	125	LYS
1	C	133	LEU
1	C	139	SER
1	C	164	VAL
1	C	165	ASN
1	C	178	LEU
1	C	209	THR
1	C	222	VAL
1	C	226	SER
1	C	239	THR
1	C	246	GLU
1	C	248	GLU
1	C	258	LYS
1	C	274	LEU
1	C	280	ASN
1	C	282	SER
1	C	289	VAL
1	C	294	LEU
1	C	331	LEU
1	C	362	LEU
1	C	383	LEU
1	C	392	GLU
1	C	400	LEU
1	C	402	ILE
1	C	404	VAL
1	C	406	PHE
1	C	409	VAL
1	C	417	ASN

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Mol	Chain	Res	Type
1	C	422	ASN
1	C	447	VAL
1	C	458	ARG
1	C	461	ASP
1	C	464	ILE
1	C	468	ILE
1	C	481	GLU
1	C	487	THR
1	C	499	THR
1	D	11	ARG
1	D	13	LYS
1	D	22	VAL
1	D	39	LEU
1	D	41	LEU
1	D	67	VAL
1	D	82	ILE
1	D	95	ARG
1	D	97	PHE
1	D	121	VAL
1	D	125	LYS
1	D	133	LEU
1	D	164	VAL
1	D	165	ASN
1	D	178	LEU
1	D	209	THR
1	D	218	ARG
1	D	222	VAL
1	D	233	LYS
1	D	239	THR
1	D	248	GLU
1	D	251	GLU
1	D	274	LEU
1	D	280	ASN
1	D	282	SER
1	D	289	VAL
1	D	294	LEU
1	D	319	SER
1	D	331	LEU
1	D	374	ARG
1	D	383	LEU
1	D	389	GLU
1	D	394	LEU

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Mol	Chain	Res	Type
1	D	395	THR
1	D	397	GLU
1	D	399	GLN
1	D	400	LEU
1	D	404	VAL
1	D	409	VAL
1	D	417	ASN
1	D	422	ASN
1	D	458	ARG
1	D	461	ASP
1	D	464	ILE
1	D	489	THR
1	D	499	THR
1	D	502	SER
1	E	8	SER
1	E	11	ARG
1	E	22	VAL
1	E	39	LEU
1	E	41	LEU
1	E	67	VAL
1	E	72	GLU
1	E	82	ILE
1	E	97	PHE
1	E	121	VAL
1	E	133	LEU
1	E	148	GLU
1	E	178	LEU
1	E	209	THR
1	E	219	ARG
1	E	239	THR
1	E	274	LEU
1	E	280	ASN
1	E	289	VAL
1	E	301	ARG
1	E	304	SER
1	E	313	PHE
1	E	331	LEU
1	E	347	PRO
1	E	386	LEU
1	E	394	LEU
1	E	402	ILE
1	E	404	VAL

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Mol	Chain	Res	Type
1	E	405	SER
1	E	406	PHE
1	E	409	VAL
1	E	415	ILE
1	E	417	ASN
1	E	422	ASN
1	E	460	THR
1	E	463	VAL
1	E	468	ILE
1	E	482	GLN
1	E	489	THR
1	E	499	THR
1	F	22	VAL
1	F	39	LEU
1	F	41	LEU
1	F	67	VAL
1	F	70	ASP
1	F	72	GLU
1	F	74	LYS
1	F	82	ILE
1	F	97	PHE
1	F	103	MET
1	F	107	LEU
1	F	121	VAL
1	F	133	LEU
1	F	178	LEU
1	F	222	VAL
1	F	227	ARG
1	F	239	THR
1	F	251	GLU
1	F	266	GLN
1	F	274	LEU
1	F	280	ASN
1	F	289	VAL
1	F	304	SER
1	F	328	PRO
1	F	331	LEU
1	F	343	SER
1	F	362	LEU
1	F	374	ARG
1	F	383	LEU
1	F	386	LEU

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Mol	Chain	Res	Type
1	F	395	THR
1	F	404	VAL
1	F	409	VAL
1	F	415	ILE
1	F	417	ASN
1	F	422	ASN
1	F	447	VAL
1	F	453	MET
1	F	458	ARG
1	F	464	ILE
1	F	487	THR
1	F	499	THR
1	G	11	ARG
1	G	22	VAL
1	G	24	THR
1	G	39	LEU
1	G	41	LEU
1	G	67	VAL
1	G	70	ASP
1	G	72	GLU
1	G	95	ARG
1	G	96	PRO
1	G	97	PHE
1	G	121	VAL
1	G	133	LEU
1	G	178	LEU
1	G	209	THR
1	G	218	ARG
1	G	222	VAL
1	G	227	ARG
1	G	239	THR
1	G	251	GLU
1	G	266	GLN
1	G	274	LEU
1	G	280	ASN
1	G	282	SER
1	G	289	VAL
1	G	294	LEU
1	G	313	PHE
1	G	319	SER
1	G	325	MET
1	G	331	LEU

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Mol	Chain	Res	Type
1	G	362	LEU
1	G	374	ARG
1	G	383	LEU
1	G	389	GLU
1	G	392	GLU
1	G	394	LEU
1	G	395	THR
1	G	400	LEU
1	G	402	ILE
1	G	415	ILE
1	G	417	ASN
1	G	422	ASN
1	G	463	VAL
1	G	469	VAL
1	G	489	THR
1	G	499	THR
1	G	500	SER
1	H	22	VAL
1	H	39	LEU
1	H	41	LEU
1	H	67	VAL
1	H	82	ILE
1	H	95	ARG
1	H	97	PHE
1	H	103	MET
1	H	107	LEU
1	H	121	VAL
1	H	125	LYS
1	H	133	LEU
1	H	178	LEU
1	H	206	GLU
1	H	209	THR
1	H	219	ARG
1	H	222	VAL
1	H	227	ARG
1	H	239	THR
1	H	251	GLU
1	H	258	LYS
1	H	274	LEU
1	H	280	ASN
1	H	282	SER
1	H	289	VAL

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Mol	Chain	Res	Type
1	H	294	LEU
1	H	331	LEU
1	H	343	SER
1	H	362	LEU
1	H	374	ARG
1	H	383	LEU
1	H	397	GLU
1	H	405	SER
1	H	406	PHE
1	H	409	VAL
1	H	415	ILE
1	H	417	ASN
1	H	422	ASN
1	H	461	ASP
1	H	478	ILE
1	H	499	THR
1	H	502	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	165	ASN
1	A	194	GLN
1	A	280	ASN
1	A	290	HIS
1	A	295	ASN
1	A	342	HIS
1	A	350	HIS
1	A	385	ASN
1	A	399	GLN
1	A	417	ASN
1	A	422	ASN
1	A	451	HIS
1	A	465	HIS
1	B	140	HIS
1	B	165	ASN
1	B	280	ASN
1	B	290	HIS
1	B	295	ASN
1	B	350	HIS
1	B	385	ASN

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Mol	Chain	Res	Type
1	B	414	GLN
1	B	417	ASN
1	B	422	ASN
1	B	451	HIS
1	B	482	GLN
1	C	140	HIS
1	C	165	ASN
1	C	194	GLN
1	C	280	ASN
1	C	290	HIS
1	C	295	ASN
1	C	342	HIS
1	C	399	GLN
1	C	417	ASN
1	C	422	ASN
1	C	451	HIS
1	C	456	GLN
1	C	465	HIS
1	C	482	GLN
1	D	140	HIS
1	D	165	ASN
1	D	256	GLN
1	D	280	ASN
1	D	290	HIS
1	D	295	ASN
1	D	342	HIS
1	D	350	HIS
1	D	385	ASN
1	D	417	ASN
1	D	422	ASN
1	D	465	HIS
1	D	482	GLN
1	E	140	HIS
1	E	280	ASN
1	E	290	HIS
1	E	295	ASN
1	E	350	HIS
1	E	385	ASN
1	E	417	ASN
1	E	422	ASN
1	E	439	GLN
1	E	451	HIS

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Mol	Chain	Res	Type
1	E	456	GLN
1	E	465	HIS
1	F	9	ASN
1	F	140	HIS
1	F	165	ASN
1	F	280	ASN
1	F	290	HIS
1	F	295	ASN
1	F	350	HIS
1	F	385	ASN
1	F	417	ASN
1	F	422	ASN
1	F	456	GLN
1	F	465	HIS
1	F	482	GLN
1	G	140	HIS
1	G	165	ASN
1	G	266	GLN
1	G	280	ASN
1	G	290	HIS
1	G	295	ASN
1	G	350	HIS
1	G	385	ASN
1	G	417	ASN
1	G	422	ASN
1	G	439	GLN
1	G	451	HIS
1	G	456	GLN
1	G	482	GLN
1	H	140	HIS
1	H	165	ASN
1	H	194	GLN
1	H	280	ASN
1	H	290	HIS
1	H	295	ASN
1	H	350	HIS
1	H	385	ASN
1	H	417	ASN
1	H	422	ASN
1	H	451	HIS
1	H	456	GLN
1	H	465	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	C	1
1	E	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	501:TYR	C	502:SER	N	2.24
1	C	501:TYR	C	502:SER	N	1.69
1	E	501:TYR	C	502:SER	N	1.68
1	F	501:TYR	C	502:SER	N	1.60

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.