



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 7BW2 / pdb_00007bw2
Title : Crystal Structure of Cyanobacterial PSI Monomer from T.elongatus at 6.5 Å Resolution
Authors : Kurisu, G.; Coruh, O.; Tanaka, H.; Eithar, E.M.; Mian, Y.
Deposited on : 2020-04-13
Resolution : 6.50 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:

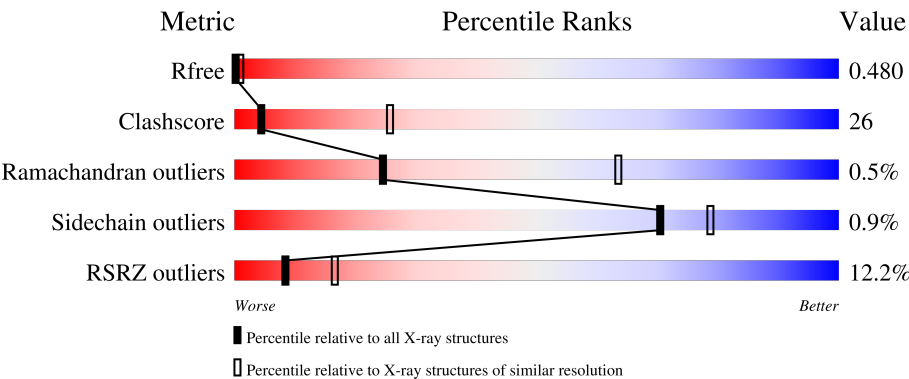
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 6.50 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}	180053	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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 $\leq 5\%$. 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	755	12% 71% 26% ..
2	B	740	14% 71% 27% .
3	C	81	19% 46% 48% 5% .
4	D	139	6% 58% 40% ..
5	E	76	12% 61% 30% 9%

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Mol	Chain	Length	Quality of chain
6	F	164	9% 43% 41% 14%
7	I	38	5% 55% 37% 5%
8	J	41	12% 78% 20%
9	K	83	2% 51% 6% 43%
10	L	155	10% 75% 6% 17%
11	M	31	10% 81% 19%
12	X	39	13% 64% 10% 26%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17345 atoms, of which 111 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	743	Total	C	H	N	O	S	0	0	0
			5914	3807	111	991	979	26			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	47	Total	C	N	O	S	0	0	0
			227	133	47	47				

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	128	Total	C	N	O	S	0	0	0
			936	609	154	170	3			

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

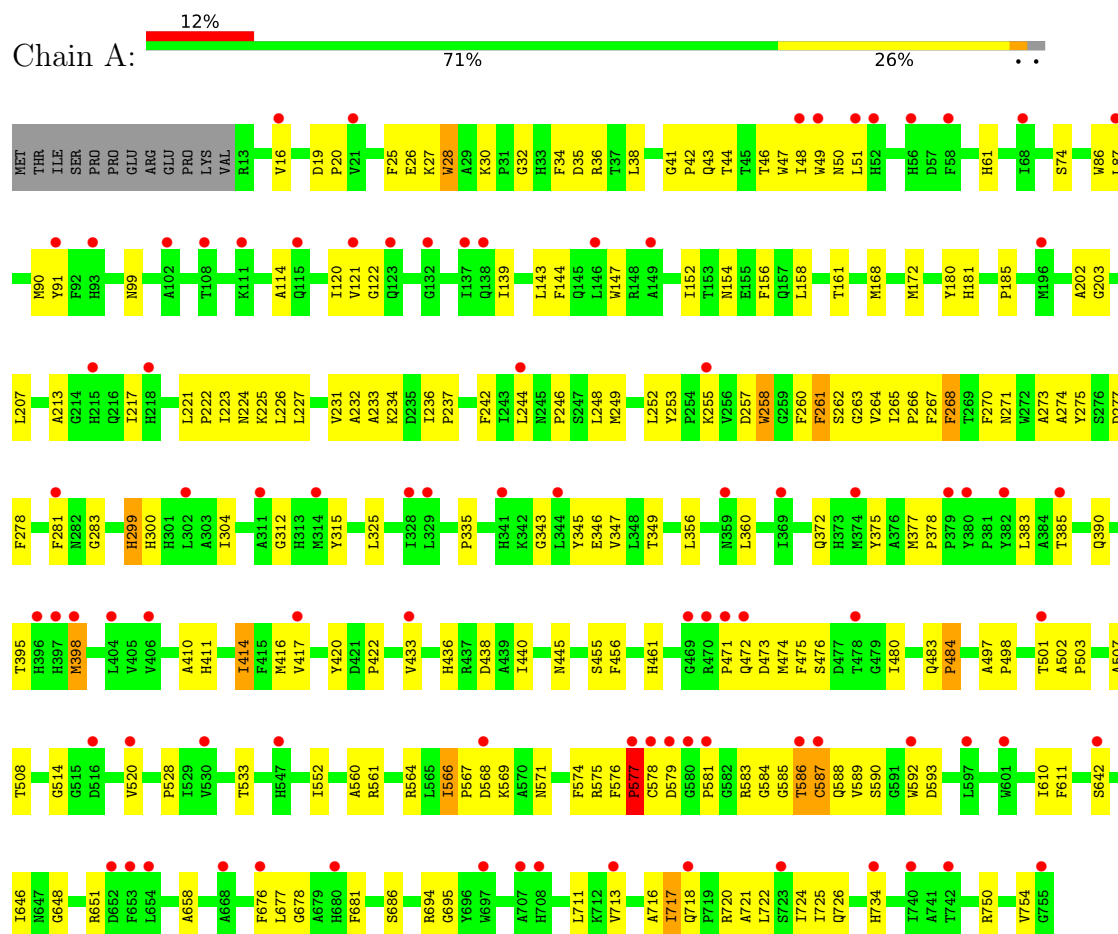
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	S	0	0	0
			232	163	34	35				

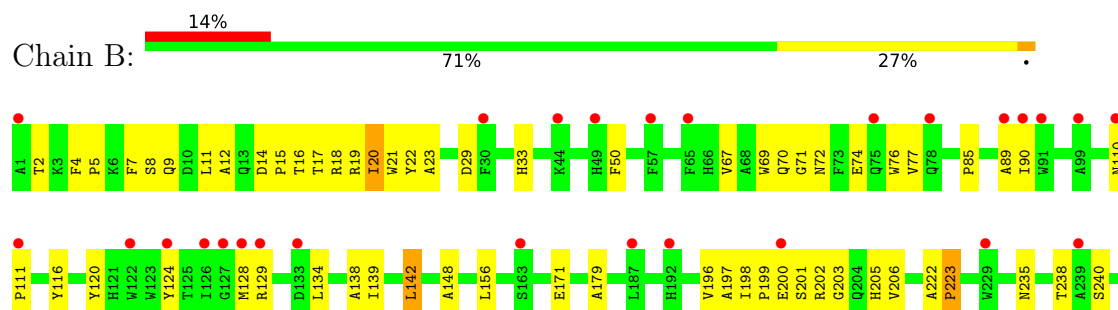
3 Residue-property plots [i](#)

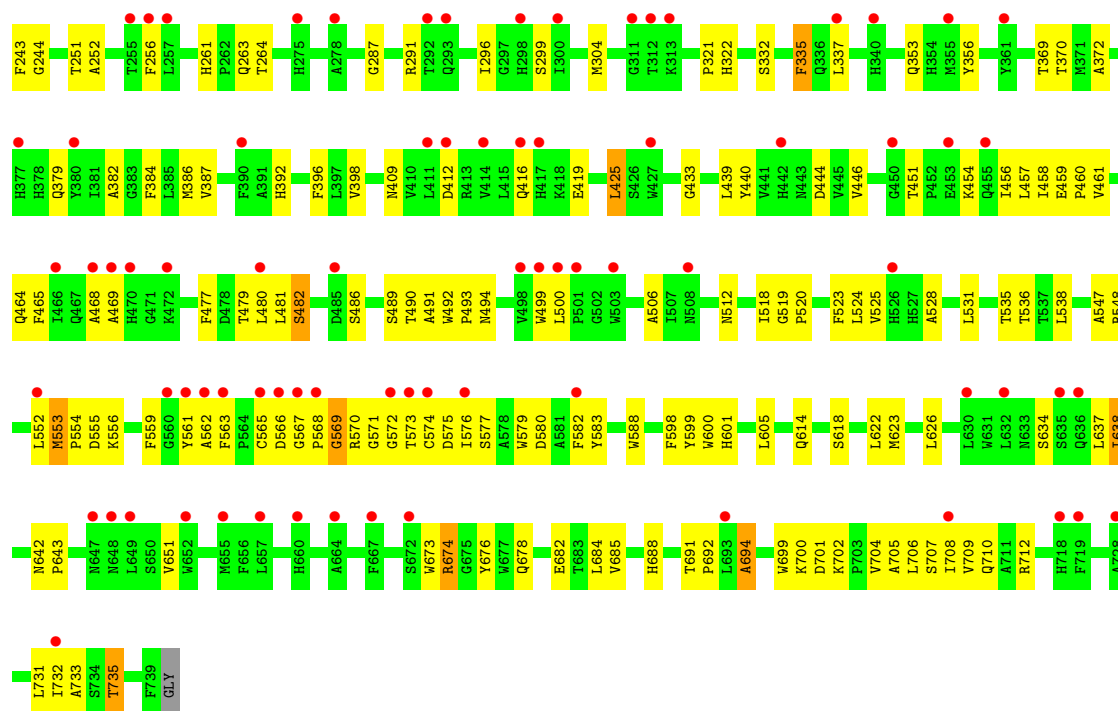
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Photosystem I P700 chlorophyll a apoprotein A1

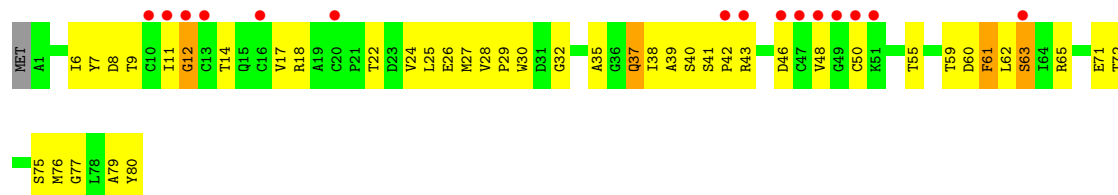


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

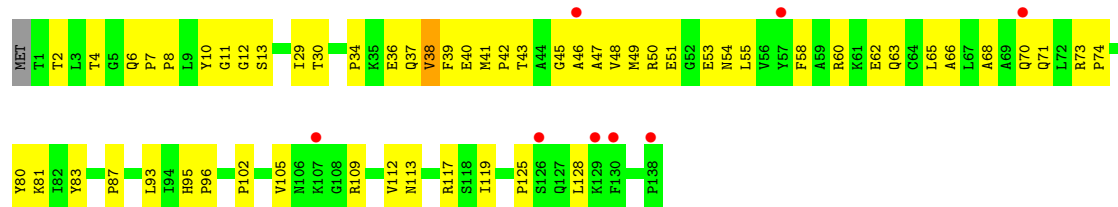




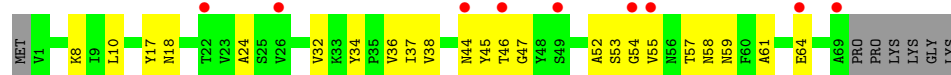
• Molecule 3: Photosystem I iron-sulfur center



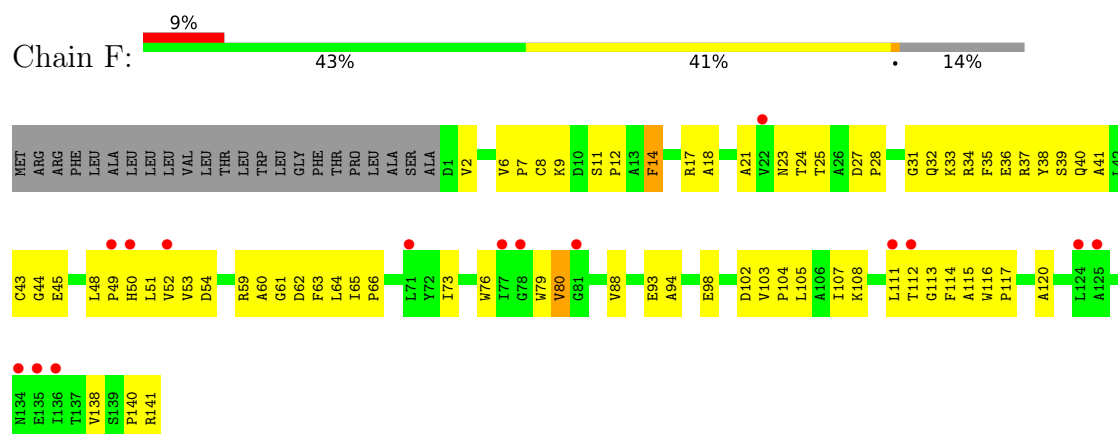
• Molecule 4: Photosystem I reaction center subunit II



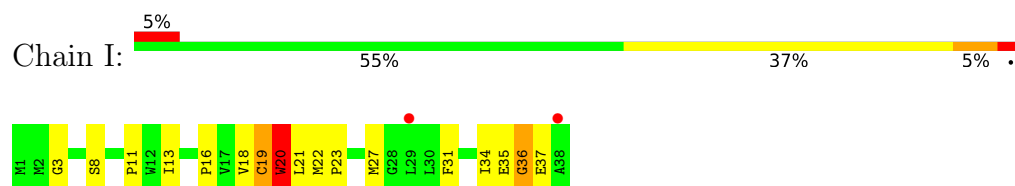
• Molecule 5: Photosystem I reaction center subunit IV



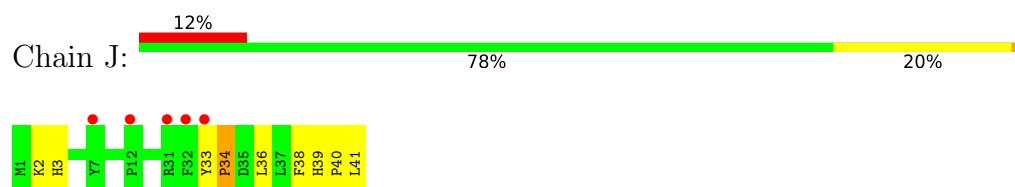
- Molecule 6: Photosystem I reaction center subunit III



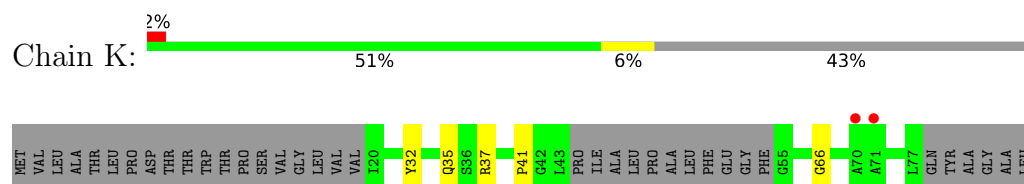
- Molecule 7: Photosystem I reaction center subunit VIII



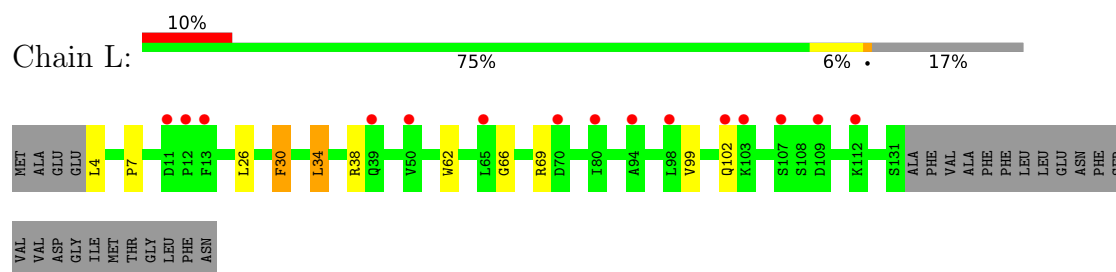
- Molecule 8: Photosystem I reaction center subunit IX



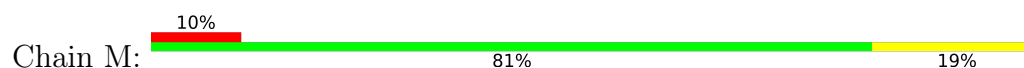
- Molecule 9: Photosystem I reaction center subunit PsaK

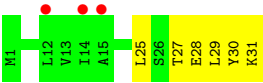


- Molecule 10: Photosystem I reaction center subunit XI

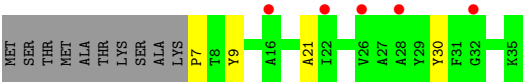


- Molecule 11: Photosystem I reaction center subunit XII





● Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.03Å 187.03Å 233.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.57 – 6.50 49.57 – 6.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.57-6.50) 98.6 (49.57-6.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.76 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.409 , 0.486 0.408 , 0.480	Depositor DCC
R_{free} test set	479 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	296.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 230.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	17345	wwPDB-VP
Average B, all atoms (Å ²)	274.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.81	1/6003 (0.0%)	1.12	17/8188 (0.2%)
2	B	0.81	2/6096 (0.0%)	1.11	16/8332 (0.2%)
3	C	1.01	1/608 (0.2%)	1.34	2/824 (0.2%)
4	D	0.86	0/1101	1.17	2/1492 (0.1%)
5	E	0.95	0/551	1.20	1/750 (0.1%)
6	F	0.94	0/1087	1.24	0/1476
7	I	0.83	0/312	1.40	5/425 (1.2%)
8	J	0.69	0/350	1.12	2/477 (0.4%)
9	K	1.22	1/225 (0.4%)	1.76	2/307 (0.7%)
10	L	0.83	0/960	1.10	2/1304 (0.2%)
11	M	0.76	0/244	1.05	0/332
12	X	0.76	0/241	1.22	1/330 (0.3%)
All	All	0.84	5/17778 (0.0%)	1.15	50/24237 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ARG	C-O	6.88	1.32	1.24
2	B	29	ASP	C-O	6.14	1.30	1.23
2	B	735	THR	C-O	5.44	1.30	1.24
3	C	12	GLY	C-O	5.11	1.30	1.23
9	K	66	GLY	C-O	5.09	1.30	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	CYS	N-CA-CB	11.10	126.81	110.06
2	B	482	SER	N-CA-C	-9.38	101.85	113.38
7	I	20	TRP	CA-C-N	-8.50	108.07	120.82
7	I	20	TRP	C-N-CA	-8.50	108.07	120.82
8	J	2	LYS	N-CA-C	-7.00	103.73	111.36
3	C	63	SER	N-CA-C	-6.57	105.23	113.18
2	B	694	ALA	N-CA-C	-6.55	105.91	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	674	ARG	N-CA-C	6.26	118.63	111.11
1	A	611	PHE	N-CA-C	-6.21	104.59	111.36
2	B	553	MET	CA-C-N	6.20	126.09	119.28
2	B	553	MET	C-N-CA	6.20	126.09	119.28
1	A	213	ALA	N-CA-C	-6.14	104.65	111.71
7	I	27	MET	N-CA-C	-6.06	104.75	111.36
7	I	19	CYS	CA-C-N	-6.04	110.00	121.54
7	I	19	CYS	C-N-CA	-6.04	110.00	121.54
2	B	528	ALA	N-CA-C	-5.96	104.86	111.36
10	L	34	LEU	N-CA-C	-5.96	101.55	110.24
1	A	658	ALA	N-CA-C	-5.90	105.84	113.16
1	A	577	PRO	N-CA-CB	-5.82	97.14	103.25
9	K	37	ARG	CA-C-N	5.81	126.77	121.31
9	K	37	ARG	C-N-CA	5.81	126.77	121.31
1	A	587	CYS	CB-CA-C	-5.75	99.81	109.53
2	B	156	LEU	N-CA-C	-5.75	106.25	113.72
2	B	694	ALA	CA-C-N	5.70	129.37	120.82
2	B	694	ALA	C-N-CA	5.70	129.37	120.82
2	B	569	GLY	CA-C-O	-5.68	116.41	121.41
1	A	234	LYS	N-CA-C	-5.64	105.21	111.36
1	A	461	HIS	N-CA-C	-5.60	105.08	111.07
2	B	142	LEU	N-CA-C	-5.58	105.20	111.28
2	B	425	LEU	N-CA-C	-5.50	105.29	111.28
1	A	28	TRP	N-CA-C	-5.49	104.69	111.33
4	D	87	PRO	CA-C-N	5.45	127.90	120.54
4	D	87	PRO	C-N-CA	5.45	127.90	120.54
1	A	99	ASN	N-CA-C	-5.43	106.44	112.57
1	A	586	THR	CA-C-N	-5.42	113.66	121.42
1	A	586	THR	C-N-CA	-5.42	113.66	121.42
3	C	79	ALA	N-CA-C	-5.39	106.48	113.16
5	E	24	ALA	N-CA-C	-5.34	106.93	113.50
1	A	484	PRO	N-CA-CB	5.27	106.09	102.35
1	A	299	HIS	N-CA-C	-5.21	105.67	111.36
2	B	598	PHE	N-CA-C	-5.20	105.61	111.28
1	A	398	MET	N-CA-C	-5.19	105.53	111.14
2	B	335	PHE	N-CA-C	-5.17	105.55	111.14
12	X	21	ALA	N-CA-C	-5.15	105.56	111.07
2	B	223	PRO	CA-C-N	5.11	127.09	120.44
2	B	223	PRO	C-N-CA	5.11	127.09	120.44
8	J	34	PRO	N-CA-C	5.11	119.51	111.38
10	L	30	PHE	N-CA-C	-5.10	105.62	111.07
1	A	646	ILE	N-CA-C	-5.08	105.59	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ILE	O-C-N	5.06	126.78	121.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5803	111	5664	280	0
2	B	5879	0	5634	331	0
3	C	598	0	588	101	0
4	D	1075	0	1077	78	0
5	E	539	0	527	40	0
6	F	1065	0	1076	136	0
7	I	301	0	306	57	0
8	J	338	0	347	10	0
9	K	227	0	116	1	0
10	L	936	0	944	19	0
11	M	241	0	264	3	0
12	X	232	0	220	2	0
All	All	17234	111	16763	901	0

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 26.

All (901) 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)
3:C:26:GLU:C	4:D:109:ARG:HH22	1.07	1.56
2:B:562:ALA:HB2	2:B:579:TRP:CB	1.34	1.53
1:A:44:THR:CG2	1:A:717:ILE:HB	1.33	1.52
1:A:264:VAL:HG23	1:A:268:PHE:CE1	1.48	1.48
7:I:20:TRP:HA	7:I:23:PRO:CG	1.44	1.47
6:F:6:VAL:HG13	6:F:12:PRO:CD	1.44	1.44
1:A:49:TRP:CE3	1:A:726:GLN:OE1	1.70	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:THR:CG2	2:B:702:LYS:HB2	1.47	1.41
2:B:562:ALA:CB	2:B:579:TRP:HB3	1.54	1.38
2:B:11:LEU:HD13	2:B:23:ALA:CB	1.56	1.35
3:C:26:GLU:C	4:D:109:ARG:NH2	1.82	1.34
1:A:44:THR:CB	1:A:717:ILE:HB	1.58	1.34
2:B:4:PHE:CG	2:B:5:PRO:HD3	1.65	1.32
2:B:16:THR:HG22	2:B:702:LYS:CB	1.59	1.32
1:A:122:GLY:HA2	6:F:24:THR:OG1	1.31	1.31
2:B:4:PHE:CD2	2:B:5:PRO:HD3	1.64	1.30
5:E:36:VAL:O	5:E:59:ASN:HB2	1.12	1.29
1:A:122:GLY:CA	6:F:24:THR:OG1	1.83	1.26
1:A:578:CYS:SG	1:A:724:ILE:HG21	1.76	1.25
1:A:44:THR:CG2	1:A:717:ILE:CB	2.14	1.24
1:A:578:CYS:SG	1:A:724:ILE:HD13	1.78	1.24
2:B:674:ARG:HD2	2:B:707:SER:C	1.63	1.24
1:A:44:THR:HB	1:A:717:ILE:CD1	1.67	1.22
1:A:44:THR:HG21	1:A:717:ILE:CA	1.71	1.21
7:I:19:CYS:O	7:I:23:PRO:HG3	1.39	1.21
3:C:22:THR:HA	4:D:65:LEU:HD13	1.23	1.19
1:A:414:ILE:HG12	1:A:574:PHE:CZ	1.77	1.18
3:C:26:GLU:HB3	4:D:109:ARG:NH2	1.58	1.18
3:C:26:GLU:CA	4:D:109:ARG:HH22	1.59	1.16
2:B:16:THR:HB	2:B:702:LYS:O	1.46	1.16
1:A:44:THR:HB	1:A:717:ILE:HD12	1.19	1.16
1:A:49:TRP:CZ3	1:A:726:GLN:OE1	2.00	1.14
1:A:246:PRO:HB3	1:A:258:TRP:O	1.46	1.14
7:I:20:TRP:C	7:I:23:PRO:HD2	1.72	1.14
2:B:568:PRO:HA	2:B:572:GLY:HA2	1.30	1.14
1:A:44:THR:HB	1:A:717:ILE:CG1	1.80	1.12
1:A:578:CYS:SG	1:A:724:ILE:CD1	2.38	1.11
6:F:6:VAL:CG1	6:F:12:PRO:HD2	1.81	1.11
7:I:20:TRP:CA	7:I:23:PRO:HG2	1.80	1.11
1:A:44:THR:HG22	1:A:717:ILE:HB	1.25	1.11
1:A:49:TRP:CE3	1:A:726:GLN:CD	2.29	1.10
1:A:267:PHE:HB2	1:A:275:TYR:OH	1.49	1.10
2:B:11:LEU:HD13	2:B:23:ALA:HB2	1.17	1.10
2:B:4:PHE:CE1	2:B:12:ALA:HA	1.87	1.09
1:A:414:ILE:HG12	1:A:574:PHE:CE2	1.87	1.09
7:I:35:GLU:HB3	10:L:99:VAL:HB	1.27	1.08
2:B:570:ARG:N	5:E:47:GLY:O	1.85	1.08
2:B:11:LEU:HD13	2:B:23:ALA:CA	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:CG2	1:A:268:PHE:CE1	2.36	1.08
5:E:36:VAL:O	5:E:59:ASN:CB	2.00	1.08
2:B:709:VAL:HG22	2:B:712:ARG:NH2	1.69	1.07
1:A:43:GLN:HG3	1:A:47:TRP:HB2	1.32	1.06
6:F:6:VAL:HG13	6:F:12:PRO:HD3	1.36	1.06
7:I:20:TRP:CA	7:I:23:PRO:CG	2.34	1.06
3:C:26:GLU:O	4:D:109:ARG:NH2	1.88	1.04
6:F:6:VAL:HG13	6:F:12:PRO:HD2	1.08	1.04
1:A:44:THR:HB	1:A:717:ILE:CB	1.88	1.04
2:B:568:PRO:HA	2:B:572:GLY:CA	1.87	1.03
2:B:563:PHE:O	2:B:577:SER:HB3	1.58	1.03
6:F:33:LYS:O	6:F:37:ARG:N	1.91	1.03
3:C:26:GLU:CB	4:D:109:ARG:NH2	2.21	1.02
1:A:44:THR:CB	1:A:717:ILE:HD12	1.90	1.02
1:A:264:VAL:CG2	1:A:268:PHE:HE1	1.71	1.02
2:B:4:PHE:CG	2:B:5:PRO:CD	2.42	1.02
2:B:11:LEU:CD1	2:B:23:ALA:HA	1.90	1.02
2:B:568:PRO:CA	2:B:572:GLY:HA2	1.91	1.01
1:A:44:THR:HB	1:A:717:ILE:HB	1.37	1.00
2:B:570:ARG:HD2	5:E:45:TYR:O	1.62	1.00
2:B:566:ASP:HB3	2:B:573:THR:HG21	1.42	1.00
1:A:122:GLY:H	6:F:24:THR:HG21	1.28	0.98
2:B:15:PRO:HD2	3:C:72:THR:HA	1.45	0.98
6:F:6:VAL:CG1	6:F:12:PRO:CD	2.39	0.97
1:A:122:GLY:H	6:F:24:THR:CG2	1.77	0.97
1:A:586:THR:O	1:A:589:VAL:HG12	1.63	0.97
1:A:122:GLY:N	6:F:24:THR:OG1	1.98	0.97
1:A:578:CYS:HG	1:A:724:ILE:HD13	1.17	0.96
3:C:25:LEU:O	3:C:42:PRO:CD	2.14	0.96
1:A:49:TRP:HE3	1:A:726:GLN:OE1	1.40	0.96
2:B:11:LEU:CD1	2:B:23:ALA:CB	2.44	0.95
2:B:569:GLY:HA2	3:C:55:THR:HG23	1.47	0.95
1:A:49:TRP:CZ3	1:A:726:GLN:CD	2.44	0.95
5:E:10:LEU:HB3	5:E:64:GLU:O	1.66	0.94
1:A:44:THR:CG2	1:A:717:ILE:CA	2.44	0.94
1:A:122:GLY:H	6:F:24:THR:CB	1.80	0.94
3:C:17:VAL:HA	3:C:25:LEU:HD12	1.47	0.93
1:A:720:ARG:HH21	5:E:45:TYR:HA	1.30	0.93
7:I:20:TRP:HA	7:I:23:PRO:HG2	0.94	0.93
2:B:4:PHE:CD1	2:B:5:PRO:HD3	2.04	0.93
7:I:20:TRP:O	7:I:23:PRO:HD2	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG23	1:A:268:PHE:HE1	1.13	0.92
1:A:46:THR:HG22	1:A:50:ASN:ND2	1.83	0.92
2:B:562:ALA:HB2	2:B:579:TRP:HB2	1.48	0.92
2:B:566:ASP:HB3	2:B:573:THR:CG2	2.00	0.92
5:E:37:ILE:HA	5:E:59:ASN:HB3	1.52	0.91
2:B:481:LEU:HD11	2:B:500:LEU:HD11	1.52	0.91
1:A:44:THR:HG21	1:A:718:GLN:N	1.86	0.91
2:B:4:PHE:HZ	2:B:11:LEU:O	1.53	0.91
7:I:20:TRP:O	7:I:23:PRO:CD	2.18	0.91
2:B:709:VAL:HG22	2:B:712:ARG:HH22	1.29	0.91
3:C:8:ASP:O	3:C:9:THR:HG22	1.69	0.91
1:A:414:ILE:CG1	1:A:574:PHE:CZ	2.54	0.91
2:B:4:PHE:CD2	2:B:5:PRO:CD	2.53	0.90
1:A:44:THR:CB	1:A:717:ILE:CB	2.39	0.90
2:B:4:PHE:CE2	2:B:5:PRO:HD3	2.07	0.90
6:F:61:GLY:O	6:F:66:PRO:HD3	1.71	0.90
3:C:71:GLU:O	3:C:75:SER:HB2	1.72	0.89
1:A:122:GLY:N	6:F:24:THR:HG21	1.88	0.89
2:B:116:TYR:HA	2:B:370:THR:HG22	1.52	0.89
2:B:700:LYS:HE2	7:I:37:GLU:HG3	1.55	0.89
1:A:44:THR:HG21	1:A:717:ILE:C	1.97	0.88
1:A:44:THR:HG21	1:A:717:ILE:HA	1.54	0.88
2:B:562:ALA:CB	2:B:579:TRP:CB	2.29	0.88
1:A:720:ARG:HH21	5:E:45:TYR:CA	1.87	0.88
2:B:674:ARG:HD2	2:B:708:ILE:N	1.87	0.87
1:A:43:GLN:HE21	1:A:47:TRP:CD1	1.93	0.87
1:A:268:PHE:HD1	1:A:268:PHE:H	1.22	0.87
2:B:566:ASP:HB3	2:B:573:THR:CB	2.06	0.86
2:B:566:ASP:CB	2:B:573:THR:HG21	2.05	0.86
7:I:37:GLU:O	10:L:102:GLN:CB	2.23	0.86
4:D:10:TYR:CE1	4:D:12:GLY:CA	2.58	0.86
4:D:10:TYR:HE1	4:D:12:GLY:CA	1.89	0.85
2:B:562:ALA:HB2	2:B:579:TRP:CG	2.12	0.85
3:C:26:GLU:HB3	4:D:109:ARG:CZ	2.06	0.84
2:B:353:GLN:HA	2:B:356:TYR:CE2	2.12	0.84
4:D:10:TYR:HE1	4:D:12:GLY:HA2	1.43	0.84
7:I:35:GLU:CB	10:L:99:VAL:HB	2.05	0.84
2:B:11:LEU:CD1	2:B:23:ALA:HB2	2.06	0.83
3:C:22:THR:CA	4:D:65:LEU:HD13	2.06	0.83
1:A:27:LYS:O	1:A:30:LYS:N	2.13	0.82
2:B:562:ALA:HB2	2:B:579:TRP:HB3	0.83	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:ARG:CA	5:E:47:GLY:O	2.26	0.82
7:I:35:GLU:O	7:I:37:GLU:HG2	1.80	0.82
6:F:60:ALA:O	6:F:64:LEU:HB3	1.79	0.82
2:B:457:LEU:O	6:F:50:HIS:HA	1.78	0.81
1:A:583:ARG:NE	3:C:48:VAL:HG11	1.96	0.81
2:B:573:THR:CG2	2:B:576:ILE:HG12	2.11	0.81
7:I:20:TRP:O	7:I:21:LEU:C	2.16	0.81
2:B:691:THR:HG23	2:B:694:ALA:HB3	1.60	0.81
3:C:6:ILE:HG21	3:C:39:ALA:HB3	1.63	0.81
7:I:20:TRP:C	7:I:23:PRO:CD	2.52	0.81
3:C:27:MET:O	4:D:109:ARG:CZ	2.30	0.80
2:B:16:THR:HG22	2:B:702:LYS:HB2	0.81	0.80
1:A:576:PHE:HE2	1:A:579:ASP:HB2	1.47	0.80
6:F:31:GLY:O	6:F:35:PHE:HD2	1.64	0.80
1:A:44:THR:CB	1:A:717:ILE:CG1	2.60	0.80
1:A:122:GLY:N	6:F:24:THR:CG2	2.44	0.80
7:I:37:GLU:O	10:L:102:GLN:HB3	1.82	0.80
1:A:122:GLY:N	6:F:24:THR:CB	2.44	0.79
1:A:264:VAL:HB	1:A:267:PHE:HB3	1.65	0.79
2:B:15:PRO:CD	3:C:72:THR:HA	2.13	0.79
2:B:22:TYR:CE1	2:B:707:SER:HB3	2.17	0.79
1:A:578:CYS:SG	1:A:724:ILE:HD12	2.21	0.79
6:F:23:ASN:OD1	6:F:23:ASN:O	2.00	0.79
4:D:36:GLU:HA	4:D:49:MET:O	1.83	0.78
6:F:23:ASN:HD22	6:F:31:GLY:H	1.31	0.78
1:A:246:PRO:CB	1:A:258:TRP:O	2.29	0.78
1:A:43:GLN:CG	1:A:47:TRP:HB2	2.13	0.78
2:B:674:ARG:CZ	2:B:707:SER:HA	2.14	0.78
2:B:332:SER:HG	2:B:396:PHE:HD1	1.31	0.78
6:F:60:ALA:O	6:F:64:LEU:N	2.16	0.78
3:C:9:THR:HB	5:E:34:TYR:CE1	2.18	0.77
1:A:414:ILE:CG1	1:A:574:PHE:CE2	2.66	0.77
7:I:37:GLU:O	10:L:102:GLN:HB2	1.84	0.77
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.64	0.77
7:I:20:TRP:CA	7:I:23:PRO:CD	2.63	0.77
1:A:122:GLY:HA2	6:F:24:THR:CB	2.15	0.77
6:F:8:CYS:HB3	6:F:41:ALA:O	1.84	0.77
2:B:200:GLU:OE1	2:B:205:HIS:HA	1.85	0.76
2:B:11:LEU:HD11	2:B:23:ALA:HA	1.65	0.76
2:B:16:THR:HG21	2:B:702:LYS:HB2	1.63	0.76
2:B:461:VAL:HG11	6:F:52:VAL:CG2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ALA:HA	2:B:480:LEU:O	1.85	0.76
7:I:20:TRP:HA	7:I:23:PRO:CD	2.16	0.76
1:A:414:ILE:HG12	1:A:574:PHE:CE1	2.19	0.76
3:C:25:LEU:O	3:C:42:PRO:HD2	1.82	0.76
2:B:4:PHE:CZ	2:B:11:LEU:O	2.38	0.76
1:A:416:MET:CE	1:A:561:ARG:HB2	2.15	0.76
2:B:708:ILE:HG22	2:B:712:ARG:HH12	1.49	0.76
8:J:38:PHE:HE1	8:J:40:PRO:HA	1.50	0.76
2:B:552:LEU:HD23	2:B:576:ILE:HG21	1.68	0.75
2:B:562:ALA:HA	2:B:577:SER:HB2	1.68	0.75
1:A:265:ILE:N	1:A:266:PRO:HD2	2.01	0.75
3:C:32:GLY:O	5:E:32:VAL:HA	1.87	0.75
2:B:4:PHE:HE1	2:B:12:ALA:HA	1.50	0.75
3:C:28:VAL:HG12	4:D:109:ARG:CB	2.16	0.74
4:D:10:TYR:CE1	4:D:12:GLY:HA2	2.23	0.74
1:A:217:ILE:HA	1:A:221:LEU:HD12	1.69	0.74
7:I:20:TRP:CA	7:I:23:PRO:HD2	2.17	0.74
2:B:458:ILE:HA	6:F:50:HIS:HB2	1.69	0.73
5:E:46:THR:HB	5:E:54:GLY:HA3	1.69	0.73
2:B:568:PRO:C	2:B:572:GLY:HA2	2.12	0.73
6:F:60:ALA:O	6:F:64:LEU:CB	2.36	0.73
6:F:31:GLY:O	6:F:35:PHE:CD2	2.42	0.73
3:C:14:THR:O	3:C:18:ARG:HB2	1.89	0.73
3:C:62:LEU:HB2	3:C:65:ARG:NE	2.04	0.73
5:E:37:ILE:HA	5:E:59:ASN:CB	2.18	0.72
6:F:61:GLY:HA2	6:F:65:ILE:CG1	2.18	0.72
2:B:4:PHE:CD1	2:B:5:PRO:CD	2.69	0.72
2:B:8:SER:OG	2:B:11:LEU:HG	1.88	0.72
2:B:17:THR:O	2:B:20:ILE:HG22	1.89	0.72
4:D:10:TYR:CE1	4:D:12:GLY:N	2.57	0.72
1:A:44:THR:HG22	1:A:717:ILE:CB	2.00	0.72
1:A:583:ARG:CZ	3:C:48:VAL:HG11	2.18	0.72
1:A:46:THR:HG22	1:A:50:ASN:HD21	1.50	0.72
2:B:16:THR:HG22	2:B:702:LYS:CG	2.19	0.72
3:C:26:GLU:CA	4:D:109:ARG:NH2	2.33	0.72
1:A:144:PHE:HA	1:A:147:TRP:HD1	1.53	0.72
1:A:420:TYR:CE2	1:A:561:ARG:NE	2.58	0.72
1:A:583:ARG:HG2	3:C:77:GLY:HA3	1.70	0.72
3:C:17:VAL:CA	3:C:25:LEU:HD12	2.20	0.71
1:A:20:PRO:HD2	1:A:181:HIS:O	1.90	0.71
1:A:561:ARG:NH2	4:D:40:GLU:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:VAL:CG1	3:C:46:ASP:HB2	2.19	0.71
1:A:471:PRO:O	1:A:474:MET:HG2	1.90	0.71
2:B:353:GLN:HA	2:B:356:TYR:HE2	1.51	0.71
1:A:44:THR:HG21	1:A:717:ILE:CB	1.93	0.71
1:A:49:TRP:CE3	1:A:726:GLN:NE2	2.58	0.71
2:B:17:THR:HB	2:B:701:ASP:CB	2.20	0.71
2:B:674:ARG:HH11	2:B:708:ILE:H	1.38	0.71
2:B:457:LEU:O	6:F:50:HIS:CA	2.39	0.71
2:B:570:ARG:HA	5:E:47:GLY:O	1.91	0.71
2:B:486:SER:O	2:B:490:THR:HG23	1.90	0.70
6:F:61:GLY:O	6:F:66:PRO:CD	2.39	0.70
1:A:44:THR:CG2	1:A:717:ILE:HA	2.15	0.70
1:A:44:THR:HG21	1:A:718:GLN:H	1.53	0.70
2:B:573:THR:HG23	2:B:576:ILE:HG12	1.73	0.70
2:B:461:VAL:CG1	6:F:52:VAL:CG2	2.70	0.70
1:A:586:THR:O	1:A:589:VAL:CG1	2.37	0.70
2:B:553:MET:HE1	2:B:566:ASP:OD1	1.91	0.70
1:A:34:PHE:HB3	1:A:61:HIS:CG	2.27	0.70
2:B:570:ARG:CD	5:E:45:TYR:O	2.38	0.70
3:C:25:LEU:O	3:C:42:PRO:CG	2.40	0.70
11:M:25:LEU:O	11:M:29:LEU:HG	1.92	0.70
1:A:47:TRP:CH2	1:A:51:LEU:HD22	2.26	0.69
2:B:569:GLY:CA	3:C:55:THR:HG23	2.22	0.69
3:C:59:THR:HB	3:C:61:PHE:CE2	2.27	0.69
2:B:11:LEU:CD1	2:B:23:ALA:CA	2.52	0.69
3:C:27:MET:O	4:D:109:ARG:NH1	2.25	0.69
2:B:481:LEU:HA	2:B:489:SER:OG	1.91	0.69
2:B:579:TRP:HZ3	2:B:712:ARG:HE	1.39	0.69
1:A:718:GLN:HG3	5:E:44:ASN:HB2	1.74	0.69
2:B:461:VAL:HA	2:B:464:GLN:HG2	1.72	0.69
7:I:19:CYS:HB2	7:I:20:TRP:CD1	2.27	0.69
6:F:14:PHE:HA	6:F:17:ARG:HD2	1.75	0.69
9:K:32:TYR:HA	9:K:35:GLN:CB	2.22	0.69
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.75	0.69
1:A:695:GLY:CA	2:B:576:ILE:CG2	2.71	0.69
2:B:674:ARG:CD	2:B:708:ILE:N	2.56	0.69
3:C:26:GLU:HG2	4:D:102:PRO:HB3	1.75	0.69
2:B:457:LEU:O	6:F:50:HIS:CB	2.41	0.68
2:B:197:ALA:O	2:B:201:SER:HB2	1.93	0.68
2:B:553:MET:CE	2:B:566:ASP:HB2	2.23	0.68
2:B:461:VAL:HG21	6:F:54:ASP:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:MET:O	1:A:172:MET:HG2	1.94	0.68
3:C:22:THR:HA	4:D:65:LEU:CD1	2.14	0.68
6:F:60:ALA:C	6:F:64:LEU:HB3	2.18	0.68
1:A:122:GLY:CA	6:F:24:THR:CB	2.71	0.67
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.76	0.67
2:B:16:THR:HA	2:B:702:LYS:H	1.59	0.67
4:D:6:GLN:O	4:D:55:LEU:HG	1.93	0.67
2:B:2:THR:HG23	7:I:37:GLU:H	1.60	0.67
3:C:71:GLU:O	3:C:75:SER:CB	2.42	0.67
6:F:43:CYS:HB3	6:F:48:LEU:O	1.95	0.67
2:B:674:ARG:CD	2:B:707:SER:C	2.57	0.67
3:C:9:THR:HB	5:E:34:TYR:CD1	2.29	0.67
1:A:261:PHE:O	1:A:268:PHE:HZ	1.76	0.67
6:F:32:GLN:O	6:F:36:GLU:N	2.25	0.67
7:I:35:GLU:HG3	10:L:99:VAL:HG21	1.77	0.67
1:A:576:PHE:O	1:A:590:SER:HB2	1.95	0.67
2:B:568:PRO:HA	2:B:572:GLY:HA3	1.75	0.67
1:A:576:PHE:HE2	1:A:579:ASP:CB	2.07	0.67
1:A:385:THR:HG21	1:A:520:VAL:HB	1.76	0.66
1:A:578:CYS:O	2:B:568:PRO:HB3	1.96	0.66
2:B:16:THR:HA	2:B:702:LYS:N	2.09	0.66
2:B:7:PHE:HZ	2:B:23:ALA:O	1.79	0.66
6:F:53:VAL:HG11	6:F:63:PHE:HB3	1.76	0.66
1:A:472:GLN:CD	1:A:472:GLN:H	2.04	0.66
1:A:695:GLY:CA	2:B:576:ILE:HG22	2.26	0.66
6:F:34:ARG:O	6:F:38:TYR:CD2	2.49	0.65
1:A:583:ARG:HG3	3:C:48:VAL:HB	1.79	0.65
3:C:27:MET:CE	3:C:37:GLN:HB2	2.26	0.65
6:F:21:ALA:HB3	6:F:35:PHE:CZ	2.31	0.65
1:A:471:PRO:HA	1:A:474:MET:CE	2.26	0.65
4:D:11:GLY:O	10:L:7:PRO:HD3	1.96	0.65
6:F:107:ILE:O	6:F:111:LEU:HG	1.96	0.65
1:A:43:GLN:HG3	1:A:47:TRP:CB	2.19	0.65
1:A:560:ALA:O	1:A:569:LYS:CG	2.45	0.65
1:A:281:PHE:CZ	1:A:299:HIS:CE1	2.84	0.65
1:A:143:LEU:HD22	1:A:147:TRP:CZ2	2.31	0.65
1:A:695:GLY:HA3	2:B:576:ILE:HG23	1.78	0.65
3:C:17:VAL:HA	3:C:25:LEU:CD1	2.25	0.65
3:C:25:LEU:O	3:C:42:PRO:HG2	1.97	0.65
2:B:562:ALA:CA	2:B:579:TRP:HB3	2.26	0.65
3:C:62:LEU:HD12	3:C:65:ARG:NH1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:VAL:C	5:E:59:ASN:HB2	2.13	0.65
2:B:304:MET:HG3	2:B:322:HIS:O	1.97	0.64
2:B:457:LEU:O	6:F:50:HIS:HB2	1.96	0.64
2:B:700:LYS:HE3	7:I:37:GLU:CD	2.22	0.64
4:D:60:ARG:HG3	4:D:62:GLU:H	1.63	0.64
4:D:68:ALA:HB1	4:D:80:TYR:CZ	2.32	0.64
6:F:6:VAL:N	6:F:7:PRO:CD	2.59	0.64
2:B:22:TYR:HE1	2:B:707:SER:HB3	1.63	0.64
1:A:120:ILE:HG12	1:A:121:VAL:HG13	1.79	0.64
1:A:564:ARG:HD2	2:B:682:GLU:HB3	1.79	0.64
2:B:4:PHE:HZ	2:B:11:LEU:C	2.05	0.64
3:C:17:VAL:HG23	3:C:25:LEU:HB2	1.80	0.64
3:C:28:VAL:O	3:C:38:ILE:HG22	1.98	0.64
1:A:249:MET:O	1:A:252:LEU:O	2.17	0.63
2:B:461:VAL:CG1	6:F:52:VAL:HG21	2.27	0.63
1:A:264:VAL:CB	1:A:268:PHE:HE1	2.11	0.63
6:F:18:ALA:HA	6:F:35:PHE:CD1	2.34	0.63
2:B:569:GLY:HA3	3:C:55:THR:HA	1.79	0.63
6:F:60:ALA:HB1	6:F:64:LEU:HD13	1.79	0.63
7:I:35:GLU:O	7:I:37:GLU:N	2.32	0.63
2:B:439:LEU:HD22	2:B:456:ILE:HG21	1.81	0.63
1:A:41:GLY:N	1:A:42:PRO:HD2	2.13	0.63
1:A:471:PRO:HA	1:A:474:MET:HE3	1.80	0.63
2:B:444:ASP:OD2	2:B:622:LEU:N	2.26	0.63
1:A:16:VAL:HG12	1:A:185:PRO:HA	1.81	0.62
6:F:21:ALA:HB3	6:F:35:PHE:HZ	1.64	0.62
1:A:224:ASN:HA	1:A:227:LEU:HD12	1.81	0.62
2:B:553:MET:HE1	2:B:566:ASP:CG	2.23	0.62
2:B:699:TRP:HE1	2:B:702:LYS:HD3	1.65	0.62
1:A:122:GLY:CA	6:F:24:THR:CG2	2.77	0.62
2:B:4:PHE:CZ	2:B:11:LEU:C	2.77	0.62
2:B:458:ILE:HD11	6:F:52:VAL:HA	1.82	0.62
1:A:583:ARG:HG2	3:C:77:GLY:CA	2.29	0.62
2:B:456:ILE:O	2:B:457:LEU:HD23	1.98	0.62
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.81	0.62
6:F:61:GLY:HA2	6:F:65:ILE:HG12	1.81	0.62
1:A:43:GLN:CB	5:E:52:ALA:HB3	2.30	0.62
2:B:235:ASN:O	2:B:252:ALA:CB	2.47	0.62
1:A:414:ILE:CD1	1:A:574:PHE:CE2	2.83	0.62
2:B:459:GLU:HG2	2:B:519:GLY:HA2	1.81	0.61
2:B:506:ALA:O	2:B:512:ASN:ND2	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:ILE:HG22	2:B:712:ARG:NH1	2.14	0.61
1:A:577:PRO:HB3	1:A:725:ILE:HD11	1.83	0.61
3:C:27:MET:HE3	3:C:37:GLN:HB2	1.81	0.61
4:D:10:TYR:CD1	4:D:12:GLY:N	2.69	0.61
2:B:22:TYR:CE1	2:B:707:SER:CB	2.84	0.60
3:C:6:ILE:HD13	3:C:39:ALA:HB1	1.82	0.60
8:J:38:PHE:CE1	8:J:40:PRO:HA	2.34	0.60
2:B:21:TRP:CE3	2:B:710:GLN:NE2	2.70	0.60
3:C:9:THR:HG23	3:C:61:PHE:CZ	2.35	0.60
6:F:8:CYS:CB	6:F:41:ALA:O	2.49	0.60
1:A:417:VAL:HG11	1:A:574:PHE:N	2.15	0.60
2:B:674:ARG:HD3	2:B:708:ILE:HG13	1.82	0.60
2:B:384:PHE:O	2:B:387:VAL:HG12	2.01	0.60
7:I:35:GLU:O	7:I:36:GLY:C	2.45	0.60
1:A:695:GLY:HA3	2:B:576:ILE:CG2	2.32	0.60
3:C:14:THR:HG22	3:C:27:MET:HG3	1.81	0.60
5:E:46:THR:HB	5:E:54:GLY:CA	2.31	0.60
2:B:198:ILE:O	2:B:202:ARG:HG3	2.02	0.60
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.82	0.60
2:B:461:VAL:HB	12:X:30:TYR:OH	2.02	0.60
2:B:491:ALA:HB1	2:B:494:ASN:HB3	1.83	0.60
2:B:461:VAL:HG11	6:F:52:VAL:HG21	1.83	0.60
2:B:567:GLY:O	2:B:573:THR:N	2.34	0.60
2:B:22:TYR:CZ	2:B:707:SER:HB3	2.37	0.60
2:B:22:TYR:OH	2:B:707:SER:HB3	2.01	0.60
1:A:576:PHE:CE2	1:A:579:ASP:HB2	2.33	0.59
1:A:718:GLN:HB3	5:E:44:ASN:ND2	2.17	0.59
2:B:14:ASP:HB2	2:B:19:ARG:HG3	1.84	0.59
8:J:39:HIS:CG	8:J:41:LEU:HG	2.37	0.59
1:A:420:TYR:CD2	1:A:561:ARG:CZ	2.85	0.59
2:B:459:GLU:OE1	2:B:464:GLN:OE1	2.20	0.59
8:J:33:TYR:HB3	8:J:36:LEU:HD11	1.85	0.59
2:B:678:GLN:OE1	2:B:704:VAL:HG13	2.03	0.59
6:F:14:PHE:HE2	6:F:39:SER:HA	1.67	0.59
1:A:25:PHE:HA	1:A:28:TRP:CD1	2.38	0.59
1:A:43:GLN:HB3	5:E:52:ALA:HB3	1.84	0.59
1:A:120:ILE:C	6:F:24:THR:HG21	2.28	0.59
6:F:9:LYS:CA	6:F:39:SER:O	2.50	0.59
1:A:695:GLY:CA	2:B:576:ILE:HG23	2.33	0.59
12:X:7:PRO:N	12:X:9:TYR:HH	1.99	0.59
1:A:223:ILE:O	1:A:227:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:VAL:HG12	3:C:46:ASP:HB2	1.84	0.59
6:F:7:PRO:O	6:F:11:SER:N	2.35	0.59
6:F:60:ALA:O	6:F:64:LEU:CA	2.50	0.59
1:A:144:PHE:HA	1:A:147:TRP:CD1	2.37	0.58
6:F:14:PHE:CE2	6:F:39:SER:HA	2.38	0.58
7:I:19:CYS:CB	7:I:20:TRP:CD1	2.86	0.58
1:A:414:ILE:HG12	1:A:574:PHE:CD2	2.38	0.58
1:A:19:ASP:HA	1:A:181:HIS:O	2.04	0.58
1:A:260:PHE:O	1:A:262:SER:N	2.36	0.58
2:B:702:LYS:CE	3:C:80:TYR:OXT	2.51	0.58
6:F:33:LYS:O	6:F:37:ARG:HB2	2.03	0.58
2:B:256:PHE:CD1	2:B:499:TRP:HB3	2.39	0.58
1:A:577:PRO:HB3	1:A:725:ILE:CD1	2.33	0.58
1:A:577:PRO:HG3	1:A:725:ILE:HG12	1.86	0.58
1:A:264:VAL:HG23	1:A:268:PHE:CZ	2.29	0.58
2:B:17:THR:N	2:B:701:ASP:HB3	2.18	0.58
6:F:23:ASN:HB3	6:F:31:GLY:CA	2.34	0.58
1:A:46:THR:CG2	1:A:50:ASN:HD21	2.15	0.58
1:A:237:PRO:HG2	1:A:248:LEU:HD21	1.86	0.58
2:B:481:LEU:O	2:B:481:LEU:HG	2.03	0.58
2:B:481:LEU:CD1	2:B:500:LEU:HD11	2.31	0.58
2:B:568:PRO:O	2:B:572:GLY:N	2.37	0.58
1:A:35:ASP:HB3	1:A:38:LEU:HB2	1.86	0.57
3:C:14:THR:O	3:C:18:ARG:CB	2.51	0.57
6:F:60:ALA:CB	6:F:64:LEU:HD13	2.33	0.57
2:B:197:ALA:O	2:B:201:SER:CB	2.52	0.57
1:A:372:GLN:HE21	1:A:398:MET:HE3	1.69	0.57
1:A:560:ALA:O	1:A:569:LYS:HG3	2.04	0.57
1:A:583:ARG:HA	3:C:76:MET:C	2.30	0.57
1:A:265:ILE:N	1:A:266:PRO:CD	2.68	0.57
1:A:383:LEU:HG	1:A:390:GLN:OE1	2.05	0.57
2:B:4:PHE:CE1	2:B:5:PRO:HD3	2.40	0.57
2:B:688:HIS:O	2:B:691:THR:HG22	2.04	0.57
7:I:31:PHE:CZ	10:L:99:VAL:HG21	2.40	0.57
2:B:67:VAL:O	2:B:71:GLY:O	2.23	0.57
2:B:456:ILE:C	2:B:457:LEU:HD23	2.30	0.57
2:B:446:VAL:HG13	2:B:454:LYS:HB2	1.85	0.57
2:B:553:MET:HE1	2:B:566:ASP:HB2	1.85	0.57
4:D:37:GLN:O	4:D:38:VAL:HB	2.04	0.56
2:B:171:GLU:OE2	2:B:299:SER:HA	2.05	0.56
1:A:237:PRO:CG	1:A:248:LEU:HD21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:HB2	1:A:275:TYR:HH	1.67	0.56
2:B:469:ALA:O	2:B:480:LEU:O	2.23	0.56
2:B:674:ARG:NH1	2:B:708:ILE:H	2.04	0.56
4:D:10:TYR:CE1	4:D:12:GLY:C	2.84	0.56
3:C:37:GLN:HB3	4:D:105:VAL:CG2	2.36	0.56
1:A:49:TRP:CD2	1:A:726:GLN:NE2	2.74	0.56
1:A:750:ARG:O	1:A:754:VAL:HG22	2.05	0.56
1:A:86:TRP:O	1:A:90:MET:HG2	2.04	0.56
1:A:578:CYS:CB	1:A:724:ILE:HD12	2.36	0.56
10:L:62:TRP:O	10:L:66:GLY:N	2.36	0.56
2:B:567:GLY:O	2:B:572:GLY:HA2	2.06	0.55
2:B:702:LYS:HD2	3:C:80:TYR:OXT	2.07	0.55
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.89	0.55
1:A:552:ILE:HG12	2:B:676:TYR:OH	2.07	0.55
2:B:67:VAL:O	2:B:71:GLY:N	2.38	0.55
2:B:461:VAL:HA	2:B:464:GLN:CG	2.36	0.55
1:A:43:GLN:CB	5:E:52:ALA:CB	2.84	0.55
1:A:583:ARG:NH2	4:D:62:GLU:OE1	2.40	0.55
6:F:111:LEU:O	6:F:114:PHE:CE2	2.59	0.55
2:B:4:PHE:N	2:B:5:PRO:HD2	2.21	0.55
5:E:36:VAL:O	5:E:59:ASN:CA	2.55	0.55
6:F:59:ARG:NE	6:F:59:ARG:HA	2.22	0.55
1:A:47:TRP:CZ3	1:A:51:LEU:HD22	2.41	0.55
7:I:20:TRP:CD1	7:I:20:TRP:N	2.74	0.55
7:I:35:GLU:CB	10:L:99:VAL:CB	2.81	0.55
4:D:10:TYR:OH	4:D:13:SER:HB3	2.07	0.55
1:A:560:ALA:O	1:A:569:LYS:HG2	2.07	0.55
2:B:700:LYS:HE2	7:I:37:GLU:CG	2.35	0.55
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.88	0.55
2:B:562:ALA:CA	2:B:577:SER:HB2	2.35	0.55
4:D:41:MET:HB3	4:D:42:PRO:HD2	1.89	0.55
2:B:4:PHE:CZ	2:B:5:PRO:HD3	2.42	0.54
2:B:731:LEU:O	2:B:735:THR:HG22	2.07	0.54
3:C:17:VAL:CB	3:C:25:LEU:HD12	2.36	0.54
2:B:67:VAL:O	2:B:71:GLY:CA	2.56	0.54
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.38	0.54
7:I:19:CYS:C	7:I:23:PRO:HG3	2.26	0.54
2:B:568:PRO:CA	2:B:572:GLY:CA	2.67	0.54
3:C:14:THR:HA	3:C:17:VAL:HG12	1.90	0.54
1:A:43:GLN:HB3	5:E:52:ALA:CB	2.37	0.54
1:A:566:ILE:CG2	1:A:568:ASP:OD1	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:O	1:A:360:LEU:HG	2.08	0.54
2:B:566:ASP:HB3	2:B:573:THR:HB	1.89	0.54
2:B:700:LYS:CE	7:I:37:GLU:HG3	2.33	0.54
4:D:40:GLU:HG2	4:D:71:GLN:OE1	2.07	0.54
7:I:19:CYS:CB	7:I:20:TRP:HD1	2.20	0.54
2:B:7:PHE:O	2:B:33:HIS:CD2	2.61	0.54
3:C:28:VAL:HG12	4:D:109:ARG:HB2	1.90	0.54
7:I:22:MET:N	7:I:23:PRO:HD2	2.22	0.54
2:B:562:ALA:C	2:B:577:SER:HB2	2.33	0.54
2:B:563:PHE:CE1	2:B:565:CYS:O	2.61	0.54
4:D:55:LEU:O	4:D:55:LEU:HD12	2.08	0.54
2:B:4:PHE:CD2	2:B:20:ILE:HG13	2.43	0.54
2:B:461:VAL:HG21	6:F:54:ASP:CB	2.38	0.54
1:A:43:GLN:HE21	1:A:47:TRP:CG	2.24	0.53
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.44	0.53
1:A:584:GLY:O	2:B:674:ARG:NH2	2.41	0.53
2:B:461:VAL:HA	2:B:464:GLN:CD	2.33	0.53
3:C:41:SER:HB2	4:D:113:ASN:HD22	1.72	0.53
2:B:14:ASP:CB	2:B:19:ARG:HG3	2.37	0.53
2:B:468:ALA:HB1	2:B:477:PHE:HB3	1.89	0.53
1:A:567:PRO:HB2	4:D:66:ALA:CB	2.38	0.53
1:A:676:PHE:HE2	2:B:626:LEU:HD21	1.73	0.53
1:A:44:THR:CG2	1:A:718:GLN:H	2.20	0.53
2:B:520:PRO:O	2:B:523:PHE:HB3	2.08	0.53
3:C:24:VAL:HG11	3:C:46:ASP:HB2	1.88	0.53
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.89	0.53
2:B:9:GLN:OE1	2:B:9:GLN:HA	2.08	0.53
2:B:568:PRO:C	2:B:572:GLY:CA	2.80	0.53
1:A:253:TYR:CE1	1:A:278:PHE:HB3	2.44	0.53
1:A:590:SER:HB3	1:A:593:ASP:OD2	2.09	0.53
4:D:6:GLN:HG2	4:D:53:GLU:HB2	1.91	0.53
1:A:244:LEU:O	1:A:246:PRO:HD3	2.09	0.53
2:B:22:TYR:OH	2:B:707:SER:CB	2.57	0.53
4:D:10:TYR:OH	4:D:13:SER:CB	2.56	0.53
2:B:461:VAL:CA	2:B:464:GLN:HG2	2.39	0.53
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.90	0.53
6:F:61:GLY:HA2	6:F:65:ILE:HB	1.90	0.53
1:A:260:PHE:C	1:A:261:PHE:CD1	2.87	0.53
2:B:674:ARG:NE	2:B:707:SER:HA	2.23	0.53
2:B:382:ALA:O	2:B:386:MET:HG2	2.09	0.52
3:C:11:ILE:O	3:C:35:ALA:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB3	1:A:139:ILE:HG21	1.91	0.52
1:A:265:ILE:H	1:A:266:PRO:HD2	1.73	0.52
1:A:283:GLY:O	1:A:508:THR:O	2.28	0.52
2:B:555:ASP:OD2	2:B:559:PHE:CE2	2.62	0.52
2:B:2:THR:OG1	7:I:37:GLU:CD	2.53	0.52
4:D:41:MET:HB3	4:D:42:PRO:CD	2.40	0.52
5:E:61:ALA:HB3	5:E:64:GLU:HG2	1.91	0.52
7:I:20:TRP:O	7:I:23:PRO:N	2.43	0.52
1:A:577:PRO:CB	1:A:725:ILE:HG12	2.40	0.52
1:A:268:PHE:CD1	1:A:268:PHE:N	2.71	0.52
2:B:138:ALA:O	2:B:142:LEU:HG	2.09	0.52
2:B:553:MET:HE1	2:B:566:ASP:CB	2.39	0.52
4:D:50:ARG:HB3	4:D:54:ASN:OD1	2.10	0.52
4:D:125:PRO:HA	4:D:128:LEU:HD12	1.90	0.52
6:F:6:VAL:HG12	6:F:6:VAL:O	2.10	0.52
1:A:577:PRO:HB3	1:A:725:ILE:HG12	1.91	0.52
2:B:235:ASN:O	2:B:252:ALA:HB2	2.10	0.52
6:F:33:LYS:O	6:F:37:ARG:CB	2.57	0.52
6:F:60:ALA:HB1	6:F:64:LEU:HB3	1.92	0.52
3:C:30:TRP:CZ2	3:C:32:GLY:HA3	2.45	0.52
7:I:20:TRP:O	7:I:23:PRO:CG	2.58	0.52
2:B:18:ARG:HD3	2:B:705:ALA:O	2.10	0.51
7:I:18:VAL:O	7:I:22:MET:HE2	2.10	0.51
2:B:20:ILE:HD11	7:I:34:ILE:HG22	1.91	0.51
2:B:553:MET:CE	2:B:566:ASP:CG	2.84	0.51
4:D:2:THR:O	4:D:4:THR:HG23	2.10	0.51
5:E:55:VAL:HG22	5:E:57:THR:HG22	1.92	0.51
7:I:13:ILE:O	7:I:16:PRO:HD2	2.10	0.51
1:A:35:ASP:HB3	1:A:38:LEU:HD22	1.92	0.51
4:D:10:TYR:HE1	4:D:12:GLY:C	2.19	0.51
5:E:10:LEU:HG	5:E:10:LEU:O	2.10	0.51
2:B:702:LYS:NZ	3:C:80:TYR:OXT	2.43	0.51
7:I:13:ILE:C	7:I:16:PRO:HD2	2.36	0.51
1:A:257:ASP:O	1:A:258:TRP:HB2	2.10	0.51
1:A:416:MET:HE3	1:A:561:ARG:HB2	1.92	0.51
2:B:461:VAL:O	2:B:464:GLN:HG2	2.10	0.51
2:B:458:ILE:CD1	6:F:52:VAL:HA	2.40	0.51
6:F:6:VAL:HG11	6:F:45:GLU:O	2.11	0.51
6:F:53:VAL:HG23	6:F:59:ARG:O	2.11	0.51
1:A:420:TYR:CD2	1:A:561:ARG:NE	2.78	0.51
2:B:563:PHE:N	2:B:577:SER:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:ARG:HH21	8:J:34:PRO:HB2	1.76	0.51
6:F:51:LEU:HB3	6:F:62:ASP:HB3	1.93	0.51
1:A:583:ARG:HG3	3:C:48:VAL:CG1	2.41	0.50
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.46	0.50
2:B:674:ARG:HH11	2:B:708:ILE:N	2.05	0.50
3:C:71:GLU:C	3:C:75:SER:HB2	2.36	0.50
4:D:30:THR:O	4:D:80:TYR:HA	2.11	0.50
6:F:34:ARG:O	6:F:38:TYR:CG	2.65	0.50
1:A:44:THR:CB	1:A:717:ILE:CD1	2.58	0.50
1:A:91:TYR:CE2	1:A:147:TRP:HZ3	2.30	0.50
1:A:410:ALA:O	1:A:414:ILE:HG13	2.12	0.50
1:A:695:GLY:HA2	2:B:576:ILE:CG2	2.40	0.50
2:B:335:PHE:HB2	2:B:396:PHE:CD1	2.46	0.50
7:I:20:TRP:C	7:I:23:PRO:HG2	2.36	0.50
7:I:35:GLU:HB2	10:L:99:VAL:CG1	2.41	0.50
1:A:27:LYS:O	1:A:28:TRP:C	2.53	0.50
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.92	0.50
6:F:61:GLY:HA2	6:F:65:ILE:CB	2.42	0.50
8:J:38:PHE:CD1	8:J:38:PHE:C	2.88	0.50
6:F:113:GLY:O	6:F:116:TRP:HB3	2.11	0.50
1:A:416:MET:HE2	1:A:561:ARG:HB2	1.90	0.50
2:B:580:ASP:O	2:B:583:TYR:HB3	2.12	0.50
3:C:30:TRP:CH2	3:C:32:GLY:HA3	2.46	0.50
6:F:88:VAL:CG1	6:F:94:ALA:HA	2.42	0.50
5:E:37:ILE:HG12	5:E:59:ASN:HD22	1.77	0.50
1:A:44:THR:CA	1:A:717:ILE:HD12	2.41	0.50
3:C:27:MET:N	4:D:109:ARG:NH2	2.54	0.50
5:E:38:VAL:N	5:E:58:ASN:O	2.45	0.50
6:F:23:ASN:OD1	6:F:25:THR:O	2.30	0.50
6:F:53:VAL:HG23	6:F:59:ARG:C	2.36	0.50
6:F:53:VAL:CG1	6:F:63:PHE:HB3	2.41	0.50
2:B:425:LEU:HB3	2:B:538:LEU:HD13	1.92	0.49
1:A:471:PRO:CA	1:A:474:MET:HE3	2.41	0.49
1:A:694:ARG:HD3	2:B:571:GLY:O	2.12	0.49
3:C:6:ILE:HD13	3:C:39:ALA:CB	2.41	0.49
6:F:52:VAL:HG22	6:F:54:ASP:OD2	2.12	0.49
3:C:11:ILE:O	3:C:35:ALA:HB2	2.12	0.49
1:A:237:PRO:CB	1:A:248:LEU:HD21	2.42	0.49
2:B:116:TYR:CA	2:B:370:THR:HG22	2.34	0.49
1:A:677:LEU:HD11	2:B:623:MET:HB2	1.93	0.49
6:F:6:VAL:N	6:F:7:PRO:HD3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:LYS:N	6:F:39:SER:O	2.45	0.49
8:J:39:HIS:ND1	8:J:41:LEU:HG	2.28	0.49
1:A:253:TYR:CD1	1:A:277:ASP:HB3	2.47	0.49
1:A:25:PHE:HA	1:A:28:TRP:HD1	1.78	0.49
2:B:477:PHE:CZ	2:B:479:THR:HB	2.47	0.49
1:A:257:ASP:HB2	1:A:263:GLY:O	2.12	0.49
2:B:674:ARG:HG2	2:B:706:LEU:O	2.13	0.49
10:L:62:TRP:O	10:L:66:GLY:HA3	2.13	0.49
1:A:576:PHE:O	1:A:590:SER:CB	2.60	0.49
2:B:548:ARG:HB2	6:F:141:ARG:O	2.13	0.49
2:B:566:ASP:HB2	2:B:573:THR:HG21	1.93	0.49
1:A:578:CYS:HB2	1:A:724:ILE:HD12	1.94	0.49
3:C:62:LEU:HD12	3:C:65:ARG:CZ	2.43	0.49
7:I:35:GLU:O	7:I:37:GLU:CG	2.58	0.49
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.48	0.48
2:B:491:ALA:O	2:B:494:ASN:N	2.45	0.48
2:B:553:MET:HE2	2:B:566:ASP:HB2	1.94	0.48
6:F:6:VAL:CG1	6:F:12:PRO:HD3	2.23	0.48
2:B:465:PHE:CE1	2:B:477:PHE:CZ	3.01	0.48
2:B:642:ASN:HB2	2:B:643:PRO:HD2	1.95	0.48
1:A:44:THR:C	1:A:717:ILE:HD12	2.38	0.48
1:A:583:ARG:HG3	3:C:48:VAL:CB	2.43	0.48
2:B:468:ALA:CB	2:B:477:PHE:HB3	2.44	0.48
4:D:40:GLU:CG	4:D:71:GLN:NE2	2.77	0.48
4:D:42:PRO:HG2	4:D:58:PHE:CE1	2.48	0.48
6:F:14:PHE:HE2	6:F:39:SER:CA	2.25	0.48
6:F:114:PHE:CD1	6:F:115:ALA:N	2.81	0.48
3:C:12:GLY:HA3	3:C:37:GLN:HG3	1.94	0.48
1:A:255:LYS:HD3	1:A:274:ALA:HA	1.94	0.48
2:B:412:ASP:O	2:B:416:GLN:HG2	2.14	0.48
2:B:525:VAL:HG11	2:B:599:TYR:HB2	1.94	0.48
3:C:27:MET:N	4:D:109:ARG:HH22	1.91	0.48
6:F:9:LYS:HA	6:F:39:SER:O	2.12	0.48
1:A:43:GLN:HB2	5:E:52:ALA:CB	2.43	0.48
1:A:475:PHE:HA	1:A:480:ILE:O	2.14	0.48
1:A:695:GLY:C	2:B:576:ILE:HG22	2.37	0.48
2:B:4:PHE:HD2	2:B:20:ILE:HG13	1.78	0.48
2:B:17:THR:HB	2:B:701:ASP:HB2	1.92	0.48
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.96	0.48
2:B:199:PRO:O	2:B:202:ARG:HB2	2.14	0.48
1:A:711:LEU:O	1:A:713:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:HIS:HB3	4:D:96:PRO:HD3	1.95	0.48
10:L:34:LEU:O	10:L:38:ARG:N	2.47	0.48
2:B:461:VAL:HG13	6:F:52:VAL:HG23	1.96	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.77	0.48
2:B:433:GLY:HA2	2:B:531:LEU:HD22	1.96	0.48
2:B:460:PRO:HG2	2:B:518:ILE:HD12	1.95	0.48
3:C:22:THR:CB	4:D:65:LEU:CD1	2.92	0.48
6:F:9:LYS:HA	6:F:39:SER:OG	2.14	0.48
2:B:199:PRO:HB2	2:B:206:VAL:HG21	1.96	0.47
4:D:43:THR:HG22	4:D:45:GLY:H	1.78	0.47
1:A:242:PHE:HB3	1:A:249:MET:SD	2.54	0.47
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.96	0.47
2:B:559:PHE:HB3	2:B:563:PHE:CD2	2.49	0.47
4:D:37:GLN:O	4:D:38:VAL:CB	2.61	0.47
2:B:709:VAL:CG2	2:B:712:ARG:HH22	2.15	0.47
3:C:25:LEU:HA	3:C:42:PRO:HD2	1.97	0.47
1:A:143:LEU:HB3	1:A:147:TRP:NE1	2.29	0.47
1:A:567:PRO:HG2	4:D:63:GLN:HA	1.95	0.47
1:A:577:PRO:HB3	1:A:725:ILE:CG1	2.43	0.47
2:B:8:SER:CB	2:B:11:LEU:HD12	2.44	0.47
2:B:17:THR:HB	2:B:701:ASP:HB3	1.93	0.47
6:F:108:LYS:HA	6:F:111:LEU:HD12	1.95	0.47
1:A:47:TRP:CE3	1:A:47:TRP:C	2.93	0.47
2:B:7:PHE:HA	2:B:33:HIS:NE2	2.29	0.47
2:B:479:THR:HG22	2:B:480:LEU:N	2.29	0.47
1:A:203:GLY:O	1:A:207:LEU:HB2	2.15	0.47
1:A:345:TYR:O	1:A:349:THR:HG23	2.15	0.47
1:A:372:GLN:HA	1:A:375:TYR:CE2	2.50	0.47
1:A:433:VAL:HG13	1:A:440:ILE:HD12	1.97	0.47
2:B:439:LEU:HD22	2:B:456:ILE:CG2	2.44	0.47
7:I:19:CYS:O	7:I:23:PRO:CG	2.28	0.47
8:J:39:HIS:CE1	8:J:41:LEU:HG	2.50	0.47
1:A:420:TYR:CE2	1:A:561:ARG:CZ	2.97	0.47
1:A:414:ILE:CD1	1:A:574:PHE:CZ	2.97	0.47
1:A:568:ASP:HB2	1:A:571:ASN:HB2	1.97	0.47
1:A:445:ASN:ND2	2:B:684:LEU:HD21	2.30	0.47
1:A:578:CYS:SG	1:A:724:ILE:CG2	2.72	0.47
2:B:16:THR:HB	2:B:702:LYS:C	2.33	0.47
2:B:22:TYR:CZ	2:B:707:SER:CB	2.98	0.47
1:A:253:TYR:HD1	1:A:277:ASP:HB3	1.78	0.46
3:C:17:VAL:HG23	3:C:25:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:PHE:HE2	6:F:39:SER:CB	2.28	0.46
1:A:642:SER:O	1:A:648:GLY:HA3	2.15	0.46
2:B:674:ARG:HH11	2:B:708:ILE:HG13	1.79	0.46
1:A:335:PRO:O	10:L:4:LEU:N	2.48	0.46
2:B:4:PHE:CD1	2:B:5:PRO:HD2	2.49	0.46
5:E:10:LEU:CB	5:E:64:GLU:O	2.50	0.46
6:F:8:CYS:HB2	6:F:43:CYS:N	2.30	0.46
6:F:2:VAL:HG12	6:F:2:VAL:O	2.16	0.46
6:F:14:PHE:HZ	6:F:35:PHE:O	1.99	0.46
1:A:564:ARG:HB2	2:B:682:GLU:OE1	2.16	0.46
2:B:479:THR:HG22	2:B:480:LEU:HG	1.97	0.46
3:C:60:ASP:HB3	5:E:58:ASN:ND2	2.31	0.46
6:F:65:ILE:HG21	8:J:39:HIS:HB3	1.97	0.46
1:A:356:LEU:HD23	1:A:411:HIS:CE1	2.51	0.46
2:B:387:VAL:HG22	2:B:582:PHE:CE2	2.50	0.46
7:I:36:GLY:O	7:I:37:GLU:C	2.59	0.46
2:B:18:ARG:CD	2:B:705:ALA:O	2.64	0.46
2:B:461:VAL:HG13	6:F:52:VAL:CG2	2.45	0.46
3:C:40:SER:HB2	4:D:112:VAL:H	1.79	0.46
6:F:112:THR:O	6:F:112:THR:HG22	2.15	0.46
1:A:471:PRO:HA	1:A:474:MET:HE2	1.97	0.46
1:A:581:PRO:HA	1:A:585:GLY:HA2	1.98	0.46
3:C:24:VAL:HB	3:C:43:ARG:O	2.16	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
1:A:473:ASP:HA	10:L:69:ARG:HH22	1.80	0.46
2:B:332:SER:OG	2:B:396:PHE:HD1	1.94	0.46
2:B:553:MET:CE	2:B:566:ASP:CB	2.92	0.46
2:B:685:VAL:HG21	3:C:80:TYR:CE2	2.51	0.46
2:B:4:PHE:CE2	2:B:5:PRO:CD	2.92	0.46
2:B:469:ALA:O	2:B:481:LEU:HB3	2.15	0.46
2:B:601:HIS:O	2:B:605:LEU:HD13	2.16	0.46
2:B:465:PHE:HE1	2:B:477:PHE:CZ	2.33	0.45
6:F:60:ALA:CA	6:F:64:LEU:HB3	2.45	0.45
1:A:686:SER:HB3	1:A:734:HIS:CB	2.46	0.45
2:B:536:THR:OG1	2:B:588:TRP:HB3	2.16	0.45
2:B:700:LYS:CE	7:I:37:GLU:CD	2.88	0.45
3:C:29:PRO:HG3	4:D:105:VAL:CG1	2.47	0.45
4:D:40:GLU:HG3	4:D:40:GLU:O	2.16	0.45
6:F:53:VAL:CG2	6:F:60:ALA:HA	2.46	0.45
1:A:43:GLN:HB2	5:E:52:ALA:HB3	1.98	0.45
1:A:261:PHE:O	1:A:268:PHE:CZ	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PRO:HB3	4:D:46:ALA:HB2	1.98	0.45
2:B:8:SER:HB3	2:B:11:LEU:HD12	1.98	0.45
2:B:110:ASN:HB3	7:I:3:GLY:HA2	1.99	0.45
2:B:369:THR:HG23	2:B:735:THR:HG23	1.98	0.45
4:D:39:PHE:CD1	4:D:47:ALA:O	2.69	0.45
4:D:55:LEU:HD12	4:D:55:LEU:C	2.42	0.45
6:F:23:ASN:HD21	6:F:28:PRO:HA	1.80	0.45
10:L:26:LEU:O	10:L:30:PHE:CD2	2.70	0.45
1:A:91:TYR:CD2	1:A:147:TRP:HZ3	2.34	0.45
2:B:563:PHE:HE1	2:B:565:CYS:O	2.00	0.45
6:F:51:LEU:HD23	6:F:62:ASP:HB3	1.98	0.45
1:A:583:ARG:CG	3:C:77:GLY:HA3	2.45	0.45
6:F:63:PHE:C	6:F:66:PRO:HD2	2.42	0.45
1:A:244:LEU:C	1:A:246:PRO:HD3	2.41	0.45
1:A:577:PRO:CG	1:A:725:ILE:HG12	2.46	0.45
2:B:692:PRO:C	2:B:694:ALA:H	2.24	0.45
1:A:226:LEU:HD13	1:A:236:ILE:HG23	1.99	0.45
1:A:686:SER:CB	1:A:734:HIS:HB2	2.47	0.45
2:B:129:ARG:HG3	2:B:200:GLU:OE2	2.16	0.45
2:B:634:SER:O	2:B:638:ILE:HB	2.17	0.45
6:F:93:GLU:OE1	6:F:93:GLU:HA	2.16	0.45
2:B:425:LEU:CB	2:B:538:LEU:HD13	2.46	0.45
2:B:556:LYS:HE2	2:B:576:ILE:HD12	1.99	0.45
1:A:253:TYR:CD1	1:A:278:PHE:HB3	2.52	0.45
2:B:2:THR:HG21	7:I:34:ILE:O	2.16	0.45
2:B:7:PHE:CZ	2:B:23:ALA:O	2.65	0.45
2:B:291:ARG:HA	2:B:296:ILE:O	2.17	0.45
2:B:554:PRO:HB3	6:F:140:PRO:HG2	1.99	0.45
3:C:61:PHE:CD1	3:C:61:PHE:C	2.95	0.45
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.98	0.45
2:B:15:PRO:HD2	3:C:72:THR:CA	2.30	0.44
2:B:446:VAL:CG1	2:B:454:LYS:HB2	2.46	0.44
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.52	0.44
2:B:70:GLN:NE2	2:B:89:ALA:HB3	2.32	0.44
3:C:28:VAL:CG1	4:D:109:ARG:HB3	2.39	0.44
4:D:39:PHE:CE1	4:D:47:ALA:O	2.70	0.44
2:B:16:THR:CG2	2:B:702:LYS:CB	2.42	0.44
2:B:461:VAL:C	2:B:464:GLN:HG2	2.41	0.44
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.47	0.44
6:F:52:VAL:HG13	6:F:52:VAL:O	2.18	0.44
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TYR:HD2	1:A:561:ARG:CZ	2.27	0.44
2:B:77:VAL:HG13	2:B:124:TYR:CE1	2.52	0.44
2:B:547:ALA:O	2:B:556:LYS:HD2	2.17	0.44
4:D:73:ARG:HB2	4:D:74:PRO:HD3	1.99	0.44
1:A:372:GLN:HE21	1:A:398:MET:CE	2.30	0.44
1:A:377:MET:N	1:A:378:PRO:HD3	2.33	0.44
1:A:716:ALA:HB3	6:F:98:GLU:OE1	2.18	0.44
1:A:718:GLN:CG	5:E:44:ASN:HB2	2.47	0.44
2:B:492:TRP:HB3	2:B:493:PRO:HD3	1.99	0.44
5:E:55:VAL:HG13	5:E:57:THR:H	1.83	0.44
6:F:60:ALA:HB1	6:F:64:LEU:CB	2.46	0.44
2:B:128:MET:HE3	2:B:134:LEU:HD23	2.00	0.44
7:I:35:GLU:HB2	10:L:99:VAL:HG11	1.99	0.44
2:B:69:TRP:CD1	2:B:69:TRP:C	2.95	0.44
2:B:72:ASN:N	2:B:72:ASN:HD22	2.16	0.44
1:A:695:GLY:O	2:B:576:ILE:HG22	2.18	0.44
2:B:74:GLU:HA	2:B:77:VAL:HB	1.99	0.43
3:C:26:GLU:CG	4:D:102:PRO:HB3	2.47	0.43
2:B:561:TYR:CE2	2:B:579:TRP:HB2	2.53	0.43
2:B:702:LYS:CD	3:C:80:TYR:OXT	2.65	0.43
2:B:235:ASN:HB3	2:B:251:THR:H	1.83	0.43
4:D:83:TYR:CE2	4:D:93:LEU:HG	2.53	0.43
6:F:40:GLN:C	6:F:40:GLN:CD	2.86	0.43
1:A:264:VAL:CA	1:A:268:PHE:HE1	2.10	0.43
4:D:40:GLU:HG2	4:D:71:GLN:CD	2.44	0.43
4:D:10:TYR:OH	4:D:13:SER:OG	2.37	0.43
5:E:8:LYS:HE3	5:E:18:ASN:HA	1.99	0.43
10:L:62:TRP:O	10:L:66:GLY:CA	2.66	0.43
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.18	0.43
1:A:315:TYR:HE2	1:A:325:LEU:HD21	1.84	0.43
1:A:575:ARG:HG2	1:A:592:TRP:HB2	2.00	0.43
2:B:479:THR:O	2:B:482:SER:HB3	2.19	0.43
7:I:8:SER:O	7:I:11:PRO:HD2	2.19	0.43
7:I:31:PHE:CE2	10:L:99:VAL:HG21	2.54	0.43
4:D:40:GLU:O	4:D:71:GLN:HG3	2.19	0.43
6:F:34:ARG:HB3	6:F:38:TYR:CE2	2.54	0.43
2:B:709:VAL:CG2	2:B:712:ARG:NH2	2.61	0.43
6:F:23:ASN:O	6:F:24:THR:C	2.61	0.43
1:A:114:ALA:HB3	1:A:139:ILE:CG2	2.49	0.42
2:B:203:GLY:HA2	2:B:244:GLY:O	2.19	0.42
2:B:479:THR:HG22	2:B:480:LEU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:VAL:HG23	3:C:50:CYS:H	1.84	0.42
3:C:59:THR:CB	3:C:61:PHE:CE2	3.00	0.42
2:B:11:LEU:HD23	2:B:19:ARG:CZ	2.48	0.42
2:B:235:ASN:O	2:B:252:ALA:HB3	2.18	0.42
1:A:34:PHE:HB3	1:A:61:HIS:CB	2.49	0.42
1:A:41:GLY:N	1:A:42:PRO:CD	2.80	0.42
1:A:74:SER:OG	1:A:180:TYR:HB2	2.18	0.42
1:A:231:VAL:O	1:A:232:ALA:HB3	2.18	0.42
2:B:637:LEU:HD13	2:B:733:ALA:HB3	2.01	0.42
11:M:27:THR:O	11:M:31:LYS:N	2.52	0.42
1:A:300:HIS:O	1:A:304:ILE:HG12	2.19	0.42
2:B:479:THR:CG2	2:B:480:LEU:H	2.32	0.42
1:A:43:GLN:HG3	1:A:47:TRP:CD1	2.55	0.42
6:F:32:GLN:O	6:F:36:GLU:CB	2.68	0.42
1:A:44:THR:CG2	1:A:718:GLN:N	2.70	0.42
1:A:233:ALA:HA	1:A:236:ILE:HB	2.01	0.42
1:A:476:SER:HA	1:A:533:THR:HG21	2.00	0.42
3:C:9:THR:CB	5:E:34:TYR:CD1	2.99	0.42
4:D:38:VAL:HA	4:D:48:VAL:HA	2.01	0.42
6:F:111:LEU:O	6:F:114:PHE:CD2	2.73	0.42
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.90	0.42
2:B:614:GLN:O	2:B:618:SER:HB2	2.19	0.42
6:F:6:VAL:HG13	6:F:12:PRO:CG	2.34	0.42
2:B:11:LEU:HD23	2:B:19:ARG:NE	2.35	0.42
2:B:469:ALA:CA	2:B:480:LEU:O	2.60	0.42
4:D:70:GLN:HG2	4:D:71:GLN:NE2	2.35	0.42
1:A:472:GLN:CD	1:A:472:GLN:N	2.76	0.42
1:A:721:ALA:O	1:A:722:LEU:C	2.63	0.42
2:B:459:GLU:CG	2:B:519:GLY:HA2	2.49	0.42
3:C:28:VAL:HG23	3:C:38:ILE:CG2	2.50	0.42
4:D:29:ILE:HA	4:D:81:LYS:O	2.20	0.42
7:I:19:CYS:HB3	7:I:20:TRP:HD1	1.83	0.42
1:A:122:GLY:HA2	6:F:24:THR:CG2	2.49	0.41
1:A:395:THR:HG22	1:A:610:ILE:HB	2.01	0.41
1:A:417:VAL:HG11	1:A:574:PHE:CA	2.51	0.41
1:A:438:ASP:CG	1:A:564:ARG:HH21	2.28	0.41
1:A:724:ILE:CD1	2:B:574:CYS:HB2	2.49	0.41
2:B:18:ARG:HH21	3:C:76:MET:HE3	1.85	0.41
4:D:68:ALA:HB1	4:D:80:TYR:CE1	2.55	0.41
6:F:62:ASP:O	6:F:66:PRO:HG2	2.20	0.41
1:A:26:GLU:HA	8:J:3:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:O	1:A:147:TRP:CD1	2.73	0.41
2:B:50:PHE:HB3	2:B:148:ALA:O	2.20	0.41
3:C:17:VAL:CG2	3:C:25:LEU:HB2	2.48	0.41
3:C:71:GLU:HB3	3:C:76:MET:HG3	2.01	0.41
1:A:343:GLY:O	1:A:347:VAL:HG23	2.20	0.41
2:B:196:VAL:C	2:B:199:PRO:HD2	2.45	0.41
2:B:561:TYR:CZ	2:B:579:TRP:HA	2.55	0.41
6:F:23:ASN:ND2	6:F:27:ASP:O	2.53	0.41
6:F:53:VAL:HG13	6:F:54:ASP:N	2.36	0.41
5:E:8:LYS:CE	5:E:18:ASN:HA	2.50	0.41
6:F:73:ILE:O	6:F:76:TRP:HB3	2.20	0.41
1:A:501:THR:C	1:A:503:PRO:HD3	2.45	0.41
2:B:76:TRP:CH2	2:B:120:TYR:C	2.99	0.41
2:B:479:THR:H	2:B:482:SER:HB3	1.85	0.41
6:F:44:GLY:N	6:F:48:LEU:O	2.42	0.41
1:A:154:ASN:OD1	1:A:156:PHE:HB3	2.21	0.41
1:A:588:GLN:HB2	2:B:673:TRP:HB2	2.03	0.41
2:B:7:PHE:O	2:B:33:HIS:NE2	2.54	0.41
2:B:460:PRO:HD3	2:B:523:PHE:HB2	2.01	0.41
2:B:565:CYS:SG	2:B:574:CYS:HA	2.61	0.41
3:C:61:PHE:CE1	3:C:63:SER:OG	2.74	0.41
5:E:17:TYR:CD2	6:F:138:VAL:HG22	2.55	0.41
6:F:80:VAL:HG23	6:F:113:GLY:HA2	2.03	0.41
1:A:32:GLY:HA3	1:A:51:LEU:CD1	2.50	0.41
1:A:225:LYS:CE	1:A:252:LEU:HD22	2.51	0.41
1:A:281:PHE:CE2	1:A:299:HIS:CE1	3.09	0.41
2:B:446:VAL:HG13	2:B:451:THR:O	2.20	0.41
3:C:14:THR:HG22	3:C:27:MET:CG	2.50	0.41
6:F:60:ALA:HA	6:F:64:LEU:HB2	2.02	0.41
7:I:19:CYS:C	7:I:20:TRP:CD1	2.99	0.41
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.55	0.41
2:B:76:TRP:CZ3	2:B:120:TYR:HB3	2.56	0.41
2:B:243:PHE:CD2	2:B:264:THR:HG21	2.55	0.41
2:B:535:THR:HG21	2:B:588:TRP:CE2	2.56	0.41
4:D:8:PRO:HG3	4:D:54:ASN:HB3	2.02	0.41
11:M:28:GLU:O	11:M:30:TYR:N	2.48	0.41
1:A:47:TRP:HE3	1:A:48:ILE:N	2.18	0.41
1:A:502:ALA:N	1:A:503:PRO:HD3	2.36	0.41
1:A:720:ARG:HH22	2:B:570:ARG:HB2	1.86	0.41
2:B:7:PHE:HA	2:B:33:HIS:HE2	1.85	0.41
2:B:238:THR:C	2:B:240:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:LEU:O	3:C:42:PRO:HD3	2.12	0.41
6:F:60:ALA:O	6:F:65:ILE:N	2.52	0.41
7:I:20:TRP:O	7:I:23:PRO:HG2	2.19	0.41
1:A:283:GLY:O	1:A:507:ALA:HB3	2.21	0.41
2:B:70:GLN:CD	2:B:89:ALA:HB3	2.45	0.41
6:F:102:ASP:OD2	6:F:105:LEU:HD12	2.20	0.41
1:A:87:LEU:O	1:A:91:TYR:HD1	2.03	0.40
1:A:514:GLY:HA2	1:A:528:PRO:HB3	2.03	0.40
2:B:261:HIS:CE1	2:B:263:GLN:HB2	2.57	0.40
2:B:732:ILE:O	2:B:735:THR:HG22	2.21	0.40
1:A:152:ILE:HG21	1:A:158:LEU:CD2	2.51	0.40
1:A:346:GLU:HA	1:A:349:THR:OG1	2.20	0.40
2:B:4:PHE:N	2:B:5:PRO:CD	2.83	0.40
2:B:337:LEU:HD23	2:B:392:HIS:CE1	2.56	0.40
6:F:76:TRP:CZ3	6:F:114:PHE:HB3	2.56	0.40
1:A:43:GLN:NE2	1:A:47:TRP:HA	2.37	0.40
2:B:535:THR:HG21	2:B:588:TRP:CZ2	2.56	0.40
2:B:580:ASP:O	2:B:583:TYR:N	2.55	0.40
6:F:27:ASP:OD1	6:F:28:PRO:HD2	2.21	0.40
7:I:20:TRP:O	7:I:22:MET:N	2.51	0.40
1:A:686:SER:HB3	1:A:734:HIS:HB3	2.03	0.40
2:B:22:TYR:CE1	2:B:710:GLN:HB2	2.57	0.40
2:B:85:PRO:HB3	2:B:120:TYR:CD2	2.56	0.40
2:B:139:ILE:HD13	2:B:142:LEU:HD12	2.03	0.40
2:B:199:PRO:HA	2:B:202:ARG:HD3	2.03	0.40
2:B:461:VAL:CG1	6:F:52:VAL:HG23	2.47	0.40
2:B:674:ARG:HD3	2:B:708:ILE:CG1	2.49	0.40
3:C:7:TYR:HD2	4:D:117:ARG:O	2.04	0.40
4:D:40:GLU:CG	4:D:71:GLN:CD	2.95	0.40
6:F:138:VAL:HG21	6:F:141:ARG:HH12	1.85	0.40
1:A:455:SER:OG	1:A:456:PHE:N	2.55	0.40
1:A:678:GLY:O	1:A:681:PHE:HB3	2.21	0.40
2:B:479:THR:CG2	2:B:480:LEU:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	741/755 (98%)	697 (94%)	40 (5%)	4 (0%)	24	63
2	B	737/740 (100%)	703 (95%)	34 (5%)	0	100	100
3	C	78/81 (96%)	71 (91%)	6 (8%)	1 (1%)	9	42
4	D	136/139 (98%)	124 (91%)	10 (7%)	2 (2%)	8	40
5	E	67/76 (88%)	60 (90%)	6 (9%)	1 (2%)	8	40
6	F	139/164 (85%)	128 (92%)	9 (6%)	2 (1%)	9	40
7	I	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	24
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	43/83 (52%)	39 (91%)	3 (7%)	1 (2%)	5	28
10	L	126/155 (81%)	121 (96%)	5 (4%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	27/39 (69%)	24 (89%)	3 (11%)	0	100	100
All	All	2198/2342 (94%)	2063 (94%)	123 (6%)	12 (0%)	24	63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PHE
4	D	38	VAL
7	I	36	GLY
9	K	41	PRO
3	C	61	PHE
6	F	14	PHE
4	D	7	PRO
1	A	258	TRP
1	A	273	ALA
1	A	577	PRO
5	E	53	SER
6	F	49	PRO

5.3.2 Protein sidechains ⓘ

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	591/603 (98%)	585 (99%)	6 (1%)	68	78
2	B	595/597 (100%)	590 (99%)	5 (1%)	73	80
3	C	67/68 (98%)	66 (98%)	1 (2%)	57	72
4	D	115/116 (99%)	114 (99%)	1 (1%)	70	79
5	E	59/65 (91%)	59 (100%)	0	100	100
6	F	109/128 (85%)	108 (99%)	1 (1%)	70	79
7	I	32/32 (100%)	31 (97%)	1 (3%)	35	56
8	J	36/36 (100%)	36 (100%)	0	100	100
10	L	98/120 (82%)	98 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	20/31 (64%)	20 (100%)	0	100	100
All	All	1748/1822 (96%)	1733 (99%)	15 (1%)	70	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	PHE
1	A	270	PHE
1	A	271	ASN
1	A	566	ILE
1	A	587	CYS
1	A	717	ILE
2	B	20	ILE
2	B	419	GLU
2	B	575	ASP
2	B	638	ILE
2	B	651	VAL
3	C	37	GLN
4	D	119	ILE
6	F	80	VAL
7	I	20	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	181	HIS
1	A	200	HIS
1	A	313	HIS
1	A	426	GLN
1	A	494	HIS
1	A	588	GLN
2	B	52	HIS
2	B	72	ASN
2	B	82	ASN
2	B	131	ASN
2	B	217	HIS
2	B	276	HIS
2	B	336	GLN
2	B	497	ASN
2	B	534	HIS
4	D	113	ASN
6	F	23	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	743/755 (98%)	0.75	88 (11%) 9 17	120, 234, 334, 449	0
2	B	739/740 (99%)	0.96	104 (14%) 6 15	138, 283, 382, 480	0
3	C	80/81 (98%)	1.16	15 (18%) 3 11	172, 259, 413, 481	0
4	D	138/139 (99%)	0.41	8 (5%) 29 33	152, 275, 362, 380	0
5	E	69/76 (90%)	0.85	9 (13%) 7 15	206, 290, 382, 410	0
6	F	141/164 (85%)	0.65	15 (10%) 11 19	178, 275, 373, 446	0
7	I	38/38 (100%)	0.96	2 (5%) 32 34	274, 349, 476, 481	0
8	J	41/41 (100%)	0.65	5 (12%) 8 16	165, 241, 310, 358	0
9	K	47/83 (56%)	0.32	2 (4%) 40 40	184, 298, 338, 354	0
10	L	128/155 (82%)	0.68	15 (11%) 9 17	259, 361, 556, 628	0
11	M	31/31 (100%)	0.78	3 (9%) 13 21	210, 350, 450, 487	0
12	X	29/39 (74%)	1.13	5 (17%) 4 12	166, 262, 394, 411	0
All	All	2224/2342 (94%)	0.80	271 (12%) 8 16	120, 268, 391, 628	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	573	THR	12.1
2	B	576	ILE	9.2
1	A	380	TYR	8.5
2	B	566	ASP	8.2
3	C	10	CYS	8.0
3	C	47	CYS	7.8
5	E	64	GLU	7.7
1	A	579	ASP	7.4
7	I	38	ALA	6.9
6	F	71	LEU	6.9
1	A	654	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
2	B	565	CYS	6.4
3	C	50	CYS	6.3
2	B	470	HIS	6.3
2	B	567	GLY	6.1
10	L	12	PRO	6.1
1	A	244	LEU	6.0
2	B	129	ARG	5.8
2	B	311	GLY	5.6
1	A	580	GLY	5.4
2	B	110	ASN	5.4
2	B	503	TRP	5.4
4	D	129	LYS	5.3
2	B	632	LEU	5.2
3	C	49	GLY	5.2
1	A	385	THR	5.1
2	B	499	TRP	5.1
6	F	78	GLY	5.1
6	F	49	PRO	5.0
1	A	21	VAL	5.0
1	A	578	CYS	4.9
1	A	471	PRO	4.9
2	B	256	PHE	4.8
3	C	13	CYS	4.8
6	F	125	ALA	4.7
2	B	133	ASP	4.6
1	A	587	CYS	4.5
2	B	501	PRO	4.5
1	A	396	HIS	4.5
2	B	187	LEU	4.4
2	B	563	PHE	4.4
6	F	77	ILE	4.3
2	B	90	ILE	4.3
5	E	44	ASN	4.3
1	A	592	TRP	4.3
1	A	581	PRO	4.2
8	J	33	TYR	4.1
3	C	12	GLY	4.0
5	E	26	VAL	4.0
8	J	32	PHE	4.0
3	C	16	CYS	4.0
2	B	122	TRP	4.0
2	B	561	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	128	MET	3.9
2	B	508	ASN	3.9
10	L	65	LEU	3.9
1	A	374	MET	3.9
11	M	15	ALA	3.8
2	B	574	CYS	3.8
7	I	29	LEU	3.8
2	B	572	GLY	3.8
2	B	239	ALA	3.8
1	A	379	PRO	3.8
4	D	130	PHE	3.7
2	B	498	VAL	3.7
9	K	71	ALA	3.7
2	B	414	VAL	3.7
1	A	58	PHE	3.6
12	X	28	ALA	3.6
1	A	48	ILE	3.6
1	A	52	HIS	3.6
1	A	652	ASP	3.6
2	B	293	GLN	3.6
3	C	11	ILE	3.6
2	B	275	HIS	3.6
2	B	126	ILE	3.5
2	B	127	GLY	3.5
2	B	111	PRO	3.5
2	B	124	TYR	3.5
2	B	718	HIS	3.4
6	F	81	GLY	3.4
2	B	44	LYS	3.4
2	B	312	THR	3.4
2	B	568	PRO	3.3
3	C	48	VAL	3.3
2	B	652	TRP	3.3
2	B	99	ALA	3.3
12	X	16	ALA	3.3
1	A	469	GLY	3.3
2	B	257	LEU	3.3
1	A	755	GLY	3.3
2	B	582	PHE	3.3
2	B	30	PHE	3.3
3	C	43	ARG	3.3
1	A	577	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	455	GLN	3.2
1	A	586	THR	3.2
2	B	526	HIS	3.2
3	C	63	SER	3.2
1	A	433	VAL	3.2
1	A	302	LEU	3.2
2	B	278	ALA	3.2
2	B	411	LEU	3.2
10	L	107	SER	3.2
3	C	20	CYS	3.2
1	A	597	LEU	3.2
10	L	13	PHE	3.2
9	K	70	ALA	3.2
10	L	80	ILE	3.1
8	J	12	PRO	3.1
1	A	734	HIS	3.1
10	L	11	ASP	3.0
1	A	676	PHE	3.0
6	F	52	VAL	3.0
2	B	450	GLY	3.0
1	A	547	HIS	3.0
1	A	341	HIS	3.0
2	B	78	GLN	3.0
2	B	89	ALA	3.0
1	A	601	TRP	3.0
2	B	377	HIS	3.0
3	C	51	LYS	3.0
1	A	653	PHE	3.0
1	A	138	GLN	3.0
2	B	91	TRP	2.9
1	A	102	ALA	2.9
2	B	552	LEU	2.9
6	F	111	LEU	2.9
1	A	397	HIS	2.9
10	L	102	GLN	2.9
12	X	22	ILE	2.8
2	B	693	LEU	2.8
2	B	65	PHE	2.8
1	A	406	VAL	2.8
6	F	134	ASN	2.8
4	D	126	SER	2.8
1	A	16	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	1	ALA	2.8
10	L	50	VAL	2.8
1	A	132	GLY	2.8
1	A	680	HIS	2.8
8	J	7	TYR	2.8
2	B	719	PHE	2.8
1	A	713	VAL	2.7
1	A	49	TRP	2.7
1	A	121	VAL	2.7
2	B	49	HIS	2.7
2	B	732	ILE	2.7
2	B	468	ALA	2.7
1	A	708	HIS	2.7
2	B	427	TRP	2.7
4	D	107	LYS	2.7
1	A	314	MET	2.7
1	A	501	THR	2.7
1	A	723	SER	2.7
1	A	93	HIS	2.6
10	L	39	GLN	2.6
2	B	412	ASP	2.6
5	E	22	THR	2.6
1	A	382	TYR	2.6
2	B	562	ALA	2.6
1	A	56	HIS	2.6
1	A	115	GLN	2.6
10	L	70	ASP	2.6
1	A	87	LEU	2.6
1	A	108	THR	2.6
1	A	123	GLN	2.5
4	D	57	TYR	2.5
1	A	369	ILE	2.5
5	E	54	GLY	2.5
5	E	55	VAL	2.5
1	A	329	LEU	2.5
1	A	530	VAL	2.5
2	B	163	SER	2.5
10	L	94	ALA	2.5
1	A	137	ILE	2.5
4	D	138	PRO	2.5
2	B	355	MET	2.5
1	A	707	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	416	GLN	2.5
1	A	255	LYS	2.5
8	J	31	ARG	2.5
1	A	215	HIS	2.5
2	B	664	ALA	2.4
2	B	417	HIS	2.4
2	B	660	HIS	2.4
2	B	560	GLY	2.4
10	L	103	LYS	2.4
1	A	281	PHE	2.4
1	A	68	ILE	2.4
2	B	361	TYR	2.4
1	A	742	THR	2.4
1	A	668	ALA	2.4
2	B	380	TYR	2.4
2	B	466	ILE	2.4
1	A	417	VAL	2.4
4	D	70	GLN	2.4
5	E	69	ALA	2.4
6	F	136	ILE	2.4
1	A	520	VAL	2.4
1	A	398	MET	2.4
2	B	75	GLN	2.3
1	A	146	LEU	2.3
2	B	708	ILE	2.3
2	B	229	TRP	2.3
6	F	50	HIS	2.3
2	B	469	ALA	2.3
2	B	648	ASN	2.3
5	E	46	THR	2.3
2	B	630	LEU	2.3
1	A	472	GLN	2.3
1	A	359	ASN	2.3
2	B	500	LEU	2.3
11	M	14	ILE	2.3
2	B	485	ASP	2.3
1	A	344	LEU	2.3
2	B	313	LYS	2.3
2	B	337	LEU	2.3
2	B	655	MET	2.3
11	M	12	LEU	2.2
2	B	292	THR	2.2

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Mol	Chain	Res	Type	RSRZ
10	L	112	LYS	2.2
12	X	26	VAL	2.2
2	B	442	HIS	2.2
2	B	340	HIS	2.2
1	A	642	SER	2.2
2	B	298	HIS	2.2
2	B	635	SER	2.2
2	B	300	ILE	2.2
2	B	472	LYS	2.2
2	B	200	GLU	2.2
2	B	480	LEU	2.2
2	B	649	LEU	2.2
1	A	478	THR	2.2
2	B	453	GLU	2.2
2	B	728	ALA	2.2
2	B	636	GLN	2.2
2	B	647	ASN	2.1
6	F	135	GLU	2.1
1	A	111	LYS	2.1
1	A	328	ILE	2.1
2	B	390	PHE	2.1
1	A	697	TRP	2.1
3	C	42	PRO	2.1
2	B	57	PHE	2.1
1	A	516	ASP	2.1
3	C	46	ASP	2.1
6	F	112	THR	2.1
4	D	46	ALA	2.1
1	A	218	HIS	2.1
2	B	255	THR	2.1
1	A	311	ALA	2.1
2	B	667	PHE	2.1
6	F	124	LEU	2.1
10	L	109	ASP	2.1
1	A	404	LEU	2.1
12	X	32	GLY	2.1
2	B	672	SER	2.1
1	A	568	ASP	2.1
1	A	51	LEU	2.1
1	A	91	TYR	2.1
1	A	718	GLN	2.1
1	A	196	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	470	ARG	2.0
2	B	657	LEU	2.0
1	A	740	ILE	2.0
10	L	98	LEU	2.0
1	A	149	ALA	2.0
2	B	192	HIS	2.0
6	F	22	VAL	2.0
5	E	49	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.