



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:28 PM UTC

PDB ID : 4XMM / pdb_00004xmm
Title : Structure of the yeast coat nucleoporin complex, space group C2
Authors : Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.;
Hoelz, A.
Deposited on : 2015-01-14
Resolution : 7.38 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:

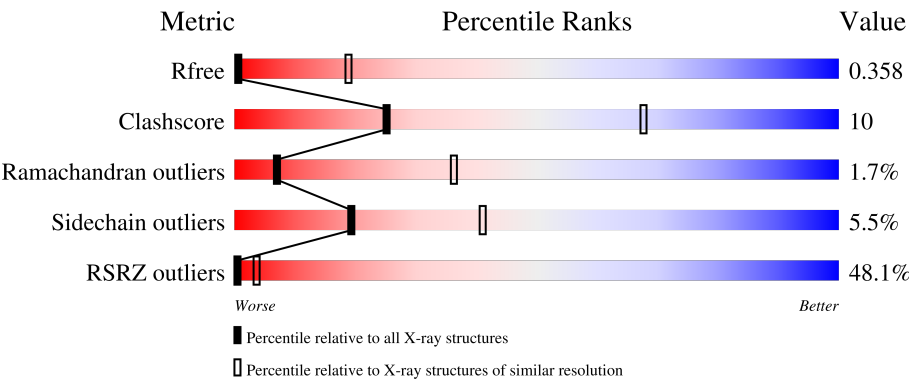
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 7.38 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	297	49% 64%25%8%
2	B	652	38% 54%19%22%
3	C	349	36% 58%29%12%
4	D	715	48% 65%19%13%
5	E	1045	41% 70%15%14%

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Mol	Chain	Length	Quality of chain
6	F	454	51% 66% 22% • 8%
7	H	271	29% 68% 13% 20%
8	L	217	33% 85% 11% • •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26139 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	511	Total	C	N	O	S	0	0	0
			3805	2417	648	730	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MET	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	307	Total	C	N	O	S	0	0	0
			2438	1543	422	462	11			

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	620	Total	C	N	O	S	0	0	0
			4535	2884	753	877	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	MET	-	initiating methionine	UNP P46673
D	31	GLY	-	expression tag	UNP P46673
D	32	SER	-	expression tag	UNP P46673
D	33	SER	-	expression tag	UNP P46673
D	34	HIS	-	expression tag	UNP P46673
D	35	HIS	-	expression tag	UNP P46673
D	36	HIS	-	expression tag	UNP P46673
D	37	HIS	-	expression tag	UNP P46673
D	38	HIS	-	expression tag	UNP P46673
D	39	HIS	-	expression tag	UNP P46673
D	40	SER	-	expression tag	UNP P46673
D	41	ASP	-	expression tag	UNP P46673
D	42	GLN	-	expression tag	UNP P46673
D	43	PRO	-	expression tag	UNP P46673

- Molecule 5 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	896	Total	C	N	O	S	0	0	0
			6622	4232	1099	1275	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729
E	1	THR	-	expression tag	UNP P35729

- Molecule 6 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			

There are 3 discrepancies between the modelled and reference sequences:

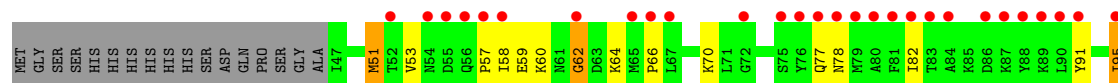
Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891

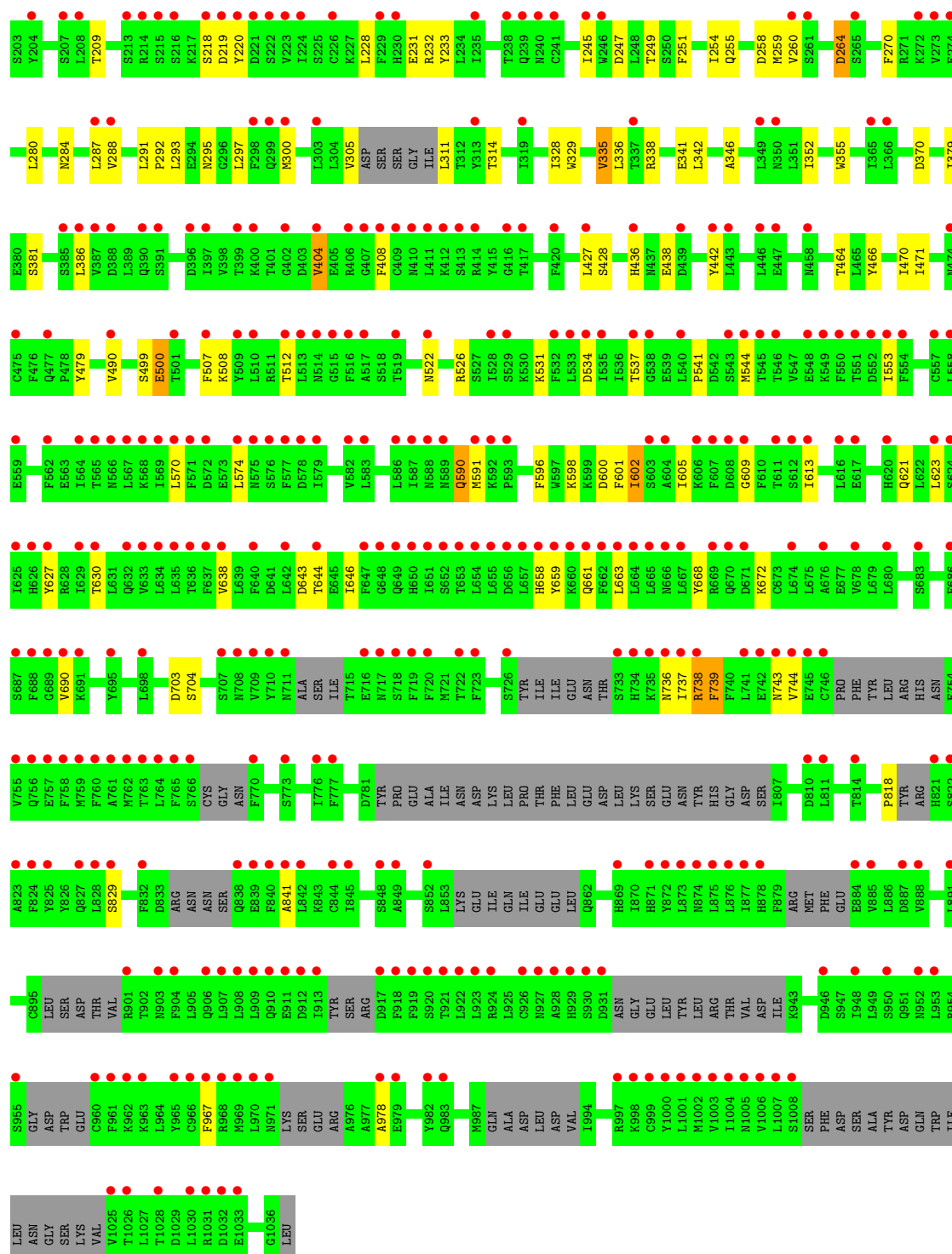
- Molecule 7 is a protein called Antibody 57 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	217	Total	C	N	O	S	0	0	0
			1576	988	267	315	6			

- Molecule 8 is a protein called Antibody 57 light chain.

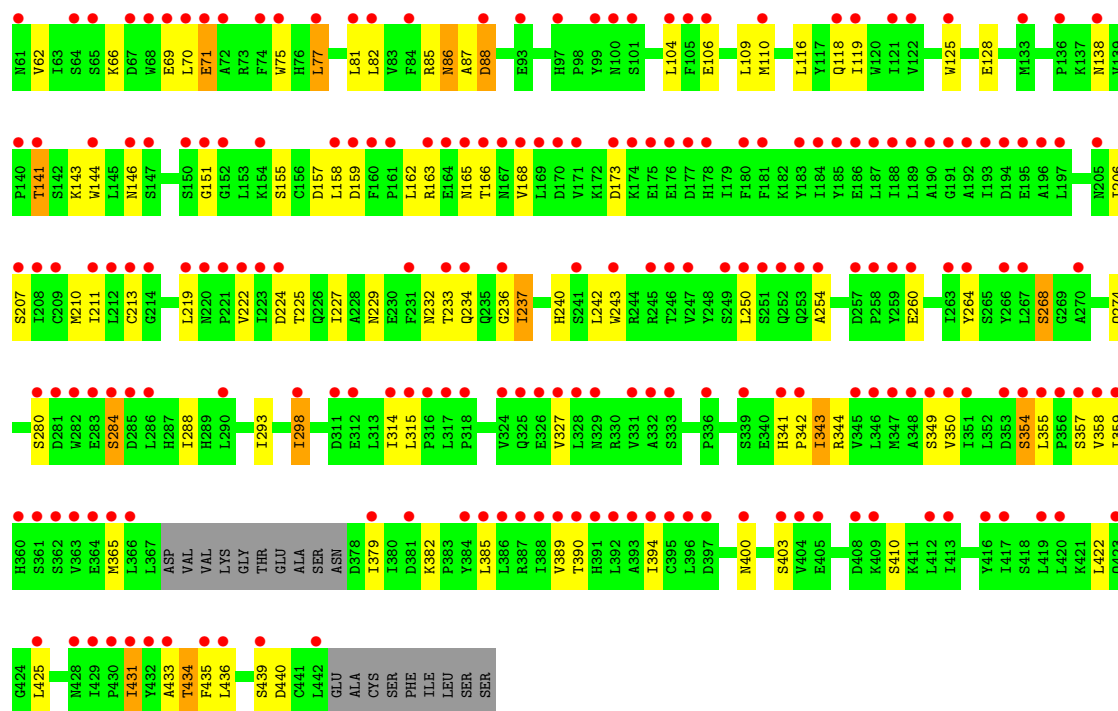
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L	210	Total	C	N	O	S	0	0	0
			1599	996	270	327	6			



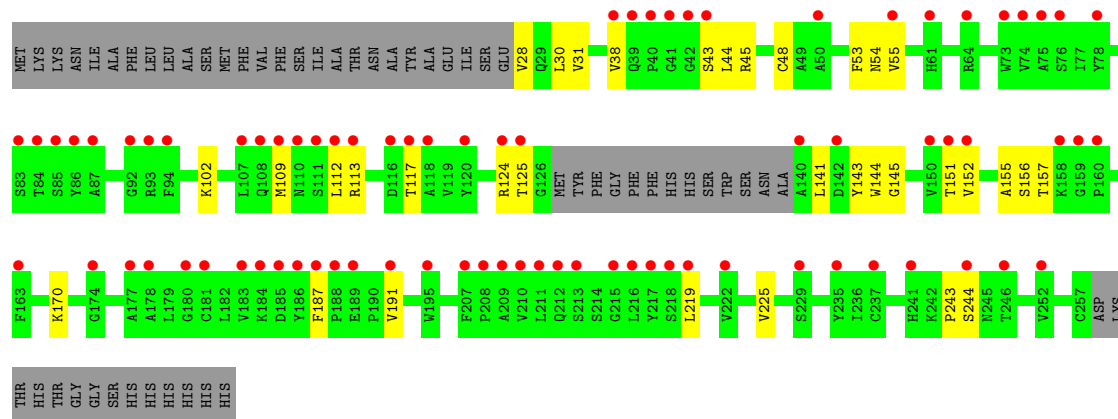


● Molecule 6: Nucleoporin NUP84

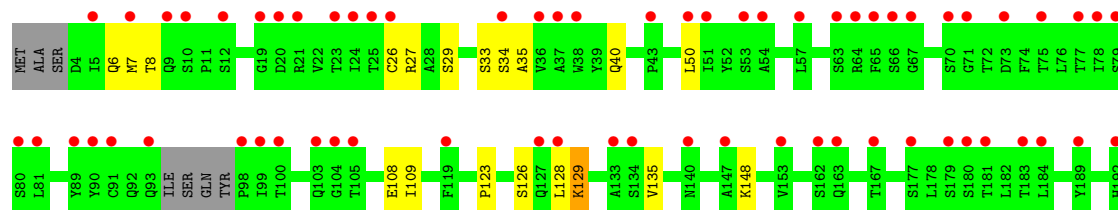
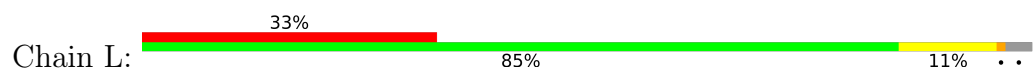




• Molecule 7: Antibody 57 heavy chain



• Molecule 8: Antibody 57 light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.65Å 186.30Å 199.57Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	67.52 – 7.38 67.52 – 7.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (67.52-7.38) 99.5 (67.52-7.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 7.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, R_{free}	0.330 , 0.353 0.335 , 0.358	Depositor DCC
R_{free} test set	1025 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	734.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	26139	wwPDB-VP
Average B, all atoms (Å ²)	716.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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	0.41	0/2220	0.90	4/3028 (0.1%)
2	B	0.49	0/3860	1.01	15/5224 (0.3%)
3	C	0.35	0/2499	0.95	7/3388 (0.2%)
4	D	0.41	0/4602	1.00	16/6246 (0.3%)
5	E	0.40	0/6730	0.86	3/9158 (0.0%)
6	F	0.48	0/3472	0.99	5/4714 (0.1%)
7	H	0.39	0/1610	0.97	9/2194 (0.4%)
8	L	0.38	0/1631	0.91	2/2210 (0.1%)
All	All	0.42	0/26624	0.95	61/36162 (0.2%)

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
2	B	0	2
5	E	0	2
6	F	0	1
All	All	0	5

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	454	LEU	N-CA-C	10.15	124.33	111.24
5	E	738	ARG	N-CA-C	-10.02	100.60	113.12
5	E	739	PHE	N-CA-C	-9.95	100.51	111.36
6	F	24	ILE	N-CA-C	8.50	125.83	113.16
7	H	144	TRP	N-CA-C	8.42	122.62	109.07
1	A	154	ALA	CA-C-N	-8.04	112.43	120.31
1	A	154	ALA	C-N-CA	-8.04	112.43	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	152	VAL	N-CA-C	7.83	117.97	106.85
4	D	288	SER	N-CA-C	-7.46	102.30	111.40
7	H	30	LEU	N-CA-C	-7.32	98.39	110.17
3	C	146	ARG	N-CA-C	-6.91	106.05	114.75
3	C	314	LEU	N-CA-C	-6.84	104.75	113.23
4	D	167	GLY	N-CA-C	-6.79	97.09	113.18
6	F	382	LYS	CA-C-N	6.66	128.17	119.84
6	F	382	LYS	C-N-CA	6.66	128.17	119.84
4	D	400	GLY	N-CA-C	6.64	124.03	114.67
4	D	608	PRO	N-CA-CB	6.63	110.62	103.33
5	E	818	PRO	N-CA-CB	6.57	110.23	103.00
7	H	144	TRP	CA-C-N	6.57	126.34	120.10
7	H	144	TRP	C-N-CA	6.57	126.34	120.10
4	D	453	ASP	N-CA-C	6.46	118.03	108.60
8	L	128	LEU	N-CA-C	-6.41	104.30	111.28
2	B	307	ALA	N-CA-C	-6.31	104.32	111.14
3	C	291	ASN	N-CA-C	-6.29	103.65	113.02
4	D	461	MET	N-CA-C	-6.26	105.47	113.23
2	B	319	LEU	N-CA-C	-6.24	104.17	110.97
2	B	516	ILE	N-CA-C	6.23	117.72	110.62
2	B	399	SER	N-CA-C	-6.07	102.36	110.55
8	L	203	GLY	N-CA-C	-6.03	107.43	115.32
4	D	166	ASP	N-CA-C	6.02	118.27	108.76
2	B	369	GLY	N-CA-C	5.99	120.04	111.12
1	A	63	HIS	CA-C-N	5.96	125.64	119.56
1	A	63	HIS	C-N-CA	5.96	125.64	119.56
7	H	225	VAL	CA-C-N	-5.89	113.87	119.76
7	H	225	VAL	C-N-CA	-5.89	113.87	119.76
2	B	305	VAL	N-CA-C	5.72	116.45	110.62
7	H	145	GLY	N-CA-C	-5.68	105.40	111.93
7	H	156	SER	N-CA-C	-5.60	102.19	110.48
4	D	95	ILE	CA-C-N	5.58	126.82	119.84
4	D	95	ILE	C-N-CA	5.58	126.82	119.84
2	B	176	LEU	CA-C-N	5.47	126.33	119.98
2	B	176	LEU	C-N-CA	5.47	126.33	119.98
6	F	168	VAL	N-CA-C	5.41	116.04	110.36
3	C	298	SER	N-CA-C	5.37	117.35	109.24
4	D	320	SER	N-CA-C	5.35	115.30	108.24
2	B	516	ILE	CB-CA-C	-5.29	105.11	112.04
4	D	516	ASN	N-CA-C	-5.29	105.19	111.69
6	F	236	GLY	N-CA-C	-5.29	103.84	112.83
4	D	355	GLU	N-CA-C	-5.23	105.25	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	268	SER	N-CA-C	5.19	119.08	111.34
3	C	165	LEU	N-CA-C	-5.16	106.50	112.89
2	B	152	ALA	N-CA-C	5.13	116.73	108.32
2	B	206	ASN	CA-C-N	-5.13	114.76	120.45
2	B	206	ASN	C-N-CA	-5.13	114.76	120.45
3	C	290	SER	N-CA-C	5.12	117.14	110.53
3	C	59	VAL	N-CA-C	5.08	116.18	111.81
2	B	248	PRO	CA-C-N	-5.07	114.59	122.09
2	B	248	PRO	C-N-CA	-5.07	114.59	122.09
2	B	328	SER	N-CA-C	-5.04	101.49	109.76
4	D	362	LEU	N-CA-C	5.04	117.89	111.69
4	D	534	ILE	N-CA-C	-5.02	106.17	110.74

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide
5	E	190	ASP	Mainchain
5	E	264	ASP	Sidechain
6	F	151	GLY	Mainchain

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	2160	0	2096	62	0
2	B	3805	0	3499	109	0
3	C	2438	0	2378	60	0
4	D	4535	0	4073	110	0
5	E	6622	0	5907	87	0
6	F	3404	0	3378	81	2
7	H	1576	0	1532	15	0
8	L	1599	0	1554	11	2
All	All	26139	0	24417	491	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 10.

All (491) 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)
5:E:537:THR:HG22	5:E:743:ASN:HA	1.54	0.86
5:E:293:LEU:HD13	5:E:297:LEU:HD12	1.59	0.85
4:D:517:ASP:OD1	7:H:54:ASN:N	2.10	0.85
4:D:159:ILE:HG12	4:D:175:LEU:HB3	1.59	0.84
4:D:156:GLU:OE2	4:D:214:ARG:NH1	2.13	0.81
6:F:314:ILE:HG22	6:F:315:LEU:HG	1.64	0.80
4:D:155:LEU:O	4:D:159:ILE:HG13	1.82	0.80
1:A:18:ASP:OD2	2:B:548:TYR:OH	2.01	0.78
5:E:113:VAL:HG23	5:E:114:GLU:H	1.49	0.77
4:D:141:ASN:O	4:D:145:ASN:ND2	2.18	0.76
2:B:416:ASP:HA	2:B:443:THR:HG21	1.66	0.76
2:B:292:ILE:HD12	2:B:292:ILE:H	1.52	0.75
2:B:317:GLY:HA3	6:F:250:LEU:HD13	1.70	0.74
6:F:70:LEU:HD22	6:F:343:ILE:HD11	1.68	0.74
2:B:483:GLU:CD	2:B:514:ARG:HH22	1.96	0.73
3:C:329:ARG:HG2	3:C:344:VAL:HG22	1.70	0.73
4:D:152:LEU:HD21	4:D:182:LEU:HB3	1.70	0.72
4:D:241:GLU:HG2	4:D:328:LEU:HD13	1.71	0.71
1:A:12:ILE:HD12	2:B:170:GLY:HA3	1.73	0.71
6:F:62:VAL:HG12	6:F:66:LYS:HE3	1.73	0.71
8:L:126:SER:O	8:L:129:LYS:HB3	1.91	0.70
5:E:404:VAL:HG11	5:E:438:GLU:HA	1.74	0.70
2:B:315:LYS:HG3	6:F:162:LEU:HB3	1.74	0.70
2:B:367:PHE:O	2:B:369:GLY:N	2.26	0.69
6:F:8:GLN:C	6:F:10:GLU:H	1.99	0.69
4:D:454:LEU:O	4:D:456:SER:N	2.26	0.69
4:D:163:LYS:HB2	4:D:172:PHE:CD1	2.29	0.68
3:C:220:TRP:HA	3:C:231:ILE:HG22	1.76	0.67
3:C:102:CYS:SG	3:C:103:THR:N	2.67	0.67
3:C:161:PRO:HB2	3:C:164:HIS:CD2	2.30	0.67
8:L:193:LYS:HE3	8:L:213:ASN:HB3	1.76	0.67
3:C:306:GLU:N	3:C:324:ASP:OD2	2.27	0.66
2:B:152:ALA:HB1	2:B:160:LEU:HD11	1.78	0.66
5:E:335:VAL:HG13	5:E:352:ILE:HB	1.77	0.66
2:B:209:PRO:HB3	2:B:532:LYS:HB2	1.78	0.66
8:L:33:SER:O	8:L:35:ALA:N	2.29	0.65
4:D:119:GLY:O	4:D:122:ARG:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:MET:HE1	4:D:182:LEU:HD22	1.78	0.65
2:B:305:VAL:HG22	6:F:242:LEU:HD22	1.78	0.65
3:C:221:ALA:HB2	3:C:312:TRP:CE2	2.31	0.65
5:E:63:SER:OG	5:E:112:GLU:OE1	2.15	0.64
6:F:13:THR:O	6:F:17:ASP:N	2.24	0.64
6:F:20:LYS:O	6:F:24:ILE:HG12	1.97	0.64
5:E:55:GLU:HB2	5:E:74:SER:HA	1.78	0.64
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.79	0.63
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.79	0.63
7:H:109:MET:HB3	7:H:112:LEU:HD21	1.79	0.63
3:C:85:GLU:HB2	3:C:101:LEU:HD11	1.80	0.63
2:B:318:HIS:NE2	6:F:260:GLU:OE2	2.29	0.63
3:C:313:ASN:HB2	3:C:318:ILE:H	1.61	0.63
5:E:829:SER:HA	5:E:841:ALA:HB1	1.81	0.62
3:C:81:VAL:HG23	3:C:111:LEU:HD13	1.81	0.62
4:D:265:ILE:HG21	4:D:289:ILE:HD11	1.81	0.61
2:B:300:LEU:HD23	2:B:388:LEU:HD21	1.82	0.61
4:D:170:ASN:O	4:D:174:GLU:HG3	2.00	0.61
8:L:216:GLU:O	8:L:217:CYS:HB2	1.98	0.61
2:B:332:ARG:NH1	6:F:213:CYS:SG	2.73	0.61
3:C:42:THR:O	3:C:44:ASN:N	2.31	0.61
3:C:219:SER:HG	3:C:312:TRP:CD1	2.19	0.61
5:E:119:VAL:HB	5:E:131:LEU:HB2	1.82	0.61
4:D:515:THR:HG22	4:D:516:ASN:H	1.65	0.61
8:L:33:SER:C	8:L:35:ALA:H	2.09	0.60
4:D:240:PHE:O	4:D:241:GLU:HG3	2.01	0.60
2:B:297:LEU:HD23	2:B:300:LEU:HD12	1.84	0.60
2:B:519:LEU:O	2:B:529:ASN:ND2	2.34	0.60
4:D:244:TYR:O	4:D:248:LEU:HG	2.02	0.59
2:B:525:ASP:O	2:B:528:LEU:HB2	2.02	0.59
5:E:609:GLY:O	5:E:613:ILE:HG22	2.02	0.59
2:B:426:TYR:O	2:B:464:ARG:NH2	2.36	0.59
5:E:596:PHE:CZ	5:E:704:SER:HA	2.38	0.59
4:D:162:VAL:O	4:D:166:ASP:HB3	2.03	0.59
2:B:152:ALA:HB1	2:B:160:LEU:CD1	2.32	0.59
1:A:217:LEU:HD22	1:A:218:LEU:H	1.69	0.58
2:B:433:GLU:OE1	2:B:467:SER:OG	2.20	0.58
4:D:258:LEU:HD22	4:D:292:LEU:HD22	1.85	0.58
4:D:534:ILE:O	4:D:538:ILE:HG12	2.02	0.58
3:C:123:LEU:HB2	3:C:139:ALA:HB3	1.86	0.58
4:D:163:LYS:HD2	4:D:172:PHE:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:VAL:HG11	6:F:211:ILE:HG23	1.85	0.58
4:D:265:ILE:C	4:D:267:ARG:H	2.12	0.58
4:D:520:GLU:OE2	7:H:54:ASN:ND2	2.37	0.58
5:E:185:GLY:O	5:E:196:PRO:HA	2.04	0.58
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.85	0.57
2:B:180:LEU:HD21	2:B:185:LEU:HD13	1.85	0.57
5:E:245:ILE:HB	5:E:255:GLN:HB2	1.84	0.57
6:F:280:SER:HB2	6:F:284:SER:HB3	1.86	0.57
3:C:225:GLY:O	4:D:453:ASP:HB3	2.04	0.57
6:F:433:ALA:HB1	6:F:439:SER:OG	2.05	0.57
5:E:329:TRP:HB3	5:E:355:TRP:HB3	1.85	0.57
3:C:238:GLY:HA2	3:C:305:GLY:O	2.05	0.57
5:E:342:LEU:HD13	5:E:379:ILE:HD12	1.86	0.57
5:E:101:SER:HA	5:E:123:LEU:HA	1.87	0.57
6:F:71:GLU:OE1	6:F:75:TRP:NE1	2.36	0.57
6:F:343:ILE:HD13	6:F:344:ARG:N	2.19	0.57
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.20	0.56
4:D:227:VAL:C	4:D:229:SER:H	2.12	0.56
2:B:199:THR:HB	2:B:213:GLU:HB2	1.87	0.56
4:D:145:ASN:OD1	4:D:190:PHE:HA	2.04	0.56
4:D:159:ILE:HG22	4:D:172:PHE:CE1	2.39	0.56
4:D:271:LEU:O	4:D:275:SER:HB3	2.04	0.56
5:E:659:TYR:OH	5:E:744:VAL:HA	2.05	0.56
4:D:517:ASP:CG	7:H:53:PHE:HA	2.31	0.56
5:E:288:VAL:HG12	5:E:300:MET:HB3	1.88	0.56
2:B:156:THR:HG22	2:B:514:ARG:HD2	1.88	0.56
3:C:29:SER:C	3:C:31:GLN:H	2.13	0.56
5:E:537:THR:CG2	5:E:743:ASN:HA	2.31	0.56
4:D:536:LYS:O	4:D:540:THR:OG1	2.20	0.56
7:H:157:THR:HG22	7:H:244:SER:HB3	1.87	0.56
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.42	0.56
6:F:34:ASP:HB3	6:F:35:PRO:HD3	1.88	0.55
2:B:256:VAL:HA	6:F:222:VAL:CG1	2.36	0.55
4:D:159:ILE:HG21	4:D:176:GLU:HG2	1.87	0.55
2:B:359:TYR:HA	2:B:362:LEU:HD12	1.86	0.55
6:F:237:ILE:HD11	6:F:240:HIS:HA	1.87	0.55
6:F:410:SER:HA	6:F:436:LEU:HD11	1.88	0.55
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.41	0.55
2:B:180:LEU:HD11	2:B:478:PHE:HE1	1.71	0.55
2:B:292:ILE:HD11	6:F:163:ARG:HD3	1.88	0.55
5:E:245:ILE:HG21	5:E:311:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.42	0.55
3:C:15:VAL:O	4:D:70:LYS:HD2	2.07	0.55
4:D:163:LYS:HB2	4:D:172:PHE:CE1	2.41	0.55
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.42	0.55
2:B:322:LEU:HD22	6:F:210:MET:HE3	1.88	0.55
4:D:461:MET:O	4:D:465:MET:HG3	2.07	0.55
6:F:350:VAL:HG22	6:F:355:LEU:HD22	1.90	0.54
4:D:328:LEU:O	4:D:332:ILE:HG13	2.08	0.54
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.08	0.54
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.90	0.54
2:B:351:ILE:HA	6:F:155:SER:HA	1.88	0.54
5:E:91:LYS:NZ	5:E:142:ALA:O	2.30	0.54
2:B:525:ASP:HA	2:B:528:LEU:HD12	1.90	0.54
4:D:186:ARG:HA	4:D:190:PHE:HB2	1.90	0.54
4:D:280:VAL:HG21	4:D:321:ALA:HB3	1.89	0.54
2:B:520:ARG:NH2	2:B:542:GLN:HE21	2.06	0.54
5:E:102:MET:HB3	5:E:107:THR:HG21	1.89	0.54
1:A:64:PRO:HB3	2:B:548:TYR:HB2	1.90	0.54
4:D:60:LYS:C	4:D:62:GLY:H	2.14	0.54
1:A:275:ASP:OD1	1:A:275:ASP:N	2.41	0.53
6:F:341:HIS:CE1	6:F:343:ILE:HD12	2.43	0.53
5:E:125:ASP:OD1	5:E:127:SER:OG	2.17	0.53
2:B:186:PHE:HD1	2:B:487:LEU:HD11	1.74	0.53
3:C:128:LEU:HD23	3:C:169:PHE:HB3	1.89	0.53
3:C:53:ALA:HB1	3:C:84:TRP:CZ2	2.44	0.52
2:B:336:LEU:HB3	6:F:206:ILE:HG23	1.91	0.52
2:B:345:SER:HB3	2:B:371:PHE:CE2	2.43	0.52
2:B:520:ARG:HH21	2:B:542:GLN:HE21	1.58	0.52
2:B:256:VAL:HA	6:F:222:VAL:HG12	1.90	0.52
5:E:232:ARG:NE	5:E:249:THR:OG1	2.39	0.52
3:C:324:ASP:HB3	4:D:64:LYS:HB3	1.90	0.52
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.44	0.52
1:A:178:ALA:HB1	1:A:206:TRP:CE2	2.44	0.52
6:F:431:ILE:HD12	6:F:431:ILE:H	1.74	0.52
6:F:8:GLN:C	6:F:10:GLU:N	2.68	0.52
2:B:355:ILE:HG21	6:F:157:ASP:HB3	1.92	0.52
2:B:524:ASN:O	2:B:528:LEU:HG	2.10	0.52
2:B:178:THR:HG21	2:B:485:ALA:HB2	1.91	0.51
5:E:739:PHE:O	5:E:743:ASN:N	2.36	0.51
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.75	0.51
1:A:214:PRO:HG2	1:A:264:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:SER:CB	2:B:153:LYS:HA	2.41	0.51
5:E:258:ASP:OD1	5:E:260:VAL:HG22	2.11	0.51
5:E:500:GLU:HB2	5:E:507:PHE:CZ	2.45	0.51
5:E:531:LYS:HB3	5:E:553:ILE:HG12	1.93	0.51
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.46	0.51
2:B:315:LYS:NZ	6:F:254:ALA:O	2.40	0.51
5:E:58:ASN:HB3	5:E:70:TYR:CZ	2.46	0.51
4:D:152:LEU:O	4:D:156:GLU:HG3	2.11	0.51
1:A:259:ARG:HB2	1:A:272:SER:HB2	1.93	0.51
2:B:281:ILE:HB	2:B:301:LEU:HD21	1.93	0.51
2:B:435:LEU:O	2:B:439:VAL:HG23	2.11	0.51
5:E:70:TYR:HA	5:E:80:THR:O	2.10	0.51
3:C:308:TRP:CD1	4:D:66:PRO:HA	2.46	0.51
5:E:190:ASP:OD2	5:E:191:GLY:N	2.44	0.51
8:L:7:MET:HE3	8:L:26:CYS:SG	2.51	0.51
2:B:186:PHE:CD1	2:B:487:LEU:HD11	2.46	0.50
4:D:156:GLU:HG2	4:D:179:LEU:CD2	2.41	0.50
6:F:50:ALA:HB1	6:F:69:GLU:HG3	1.93	0.50
2:B:397:GLU:OE1	2:B:397:GLU:N	2.40	0.50
2:B:526:HIS:C	2:B:528:LEU:N	2.68	0.50
3:C:117:ALA:HB3	3:C:124:LYS:HB3	1.93	0.50
4:D:107:TYR:CZ	4:D:111:LEU:HD11	2.47	0.50
5:E:288:VAL:HG13	5:E:336:LEU:HD22	1.94	0.50
2:B:374:LYS:O	2:B:377:GLU:HB2	2.11	0.50
2:B:526:HIS:C	2:B:530:ARG:HD2	2.36	0.50
6:F:354:SER:O	6:F:358:VAL:HG23	2.11	0.50
2:B:389:THR:O	2:B:393:GLY:HA3	2.10	0.50
3:C:10:ASP:HB3	3:C:29:SER:HB2	1.92	0.50
3:C:218:ILE:HG22	3:C:233:THR:HG22	1.94	0.50
4:D:218:GLU:HA	4:D:220:ASP:N	2.27	0.50
4:D:306:TRP:O	4:D:310:VAL:HG23	2.12	0.50
5:E:466:TYR:HB3	5:E:470:ILE:HB	1.92	0.50
1:A:57:TRP:HD1	1:A:102:VAL:O	1.94	0.50
3:C:67:GLU:OE1	3:C:119:ALA:HB1	2.12	0.49
4:D:110:GLY:O	4:D:114:ILE:HG13	2.12	0.49
4:D:158:PHE:O	4:D:162:VAL:HG23	2.12	0.49
6:F:233:THR:HG22	6:F:234:GLN:O	2.12	0.49
8:L:40:GLN:HB2	8:L:50:LEU:HD11	1.93	0.49
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.93	0.49
5:E:591:MET:HE1	5:E:630:THR:OG1	2.12	0.49
6:F:379:ILE:HG13	6:F:385:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:THR:HA	2:B:526:HIS:HB2	1.95	0.49
1:A:174:VAL:HA	1:A:183:LYS:O	2.13	0.49
4:D:278:CYS:SG	4:D:323:ASP:HB2	2.53	0.49
5:E:53:GLY:HA2	5:E:73:SER:HA	1.94	0.49
5:E:102:MET:HE3	5:E:163:PRO:HD2	1.95	0.49
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.95	0.49
2:B:317:GLY:O	2:B:320:SER:HB3	2.13	0.49
2:B:483:GLU:OE2	2:B:514:ARG:NH2	2.35	0.49
1:A:229:ARG:HH11	1:A:229:ARG:HB2	1.78	0.48
1:A:272:SER:OG	2:B:152:ALA:HB3	2.13	0.48
3:C:77:TYR:HA	3:C:110:SER:HB3	1.95	0.48
3:C:219:SER:HG	3:C:312:TRP:HD1	1.59	0.48
1:A:118:VAL:O	1:A:125:VAL:HA	2.14	0.48
2:B:182:ARG:HD2	2:B:449:GLN:OE1	2.13	0.48
5:E:160:VAL:HG23	5:E:161:ARG:N	2.28	0.48
5:E:522:ASN:O	5:E:526:ARG:HG3	2.12	0.48
2:B:173:ILE:HD12	2:B:173:ILE:H	1.78	0.48
4:D:417:ALA:HB1	4:D:465:MET:HE1	1.96	0.48
5:E:967:PHE:HA	5:E:978:ALA:HB2	1.95	0.48
6:F:349:SER:OG	6:F:358:VAL:HG21	2.13	0.48
3:C:30:ASP:OD1	3:C:32:HIS:HB2	2.13	0.48
4:D:228:PHE:HE2	4:D:267:ARG:HB3	1.77	0.48
6:F:227:ILE:C	6:F:229:ASN:H	2.22	0.48
3:C:311:SER:O	3:C:319:LEU:HD12	2.13	0.48
3:C:312:TRP:CZ3	3:C:319:LEU:HB2	2.48	0.48
1:A:38:VAL:O	1:A:39:GLU:HG3	2.14	0.48
4:D:262:ILE:HG12	4:D:289:ILE:HG23	1.96	0.48
5:E:24:VAL:HG11	5:E:143:ASN:HA	1.95	0.48
5:E:736:ASN:C	5:E:738:ARG:H	2.21	0.48
5:E:233:TYR:CG	5:E:311:LEU:HD22	2.49	0.47
5:E:541:PRO:HD2	5:E:544:MET:HE2	1.96	0.47
5:E:188:LYS:HE2	5:E:191:GLY:HA2	1.95	0.47
5:E:247:ASP:O	5:E:251:PHE:N	2.47	0.47
3:C:324:ASP:HB3	4:D:64:LYS:HD3	1.95	0.47
1:A:43:HIS:CD2	2:B:173:ILE:HD11	2.50	0.47
3:C:34:LYS:HG2	3:C:50:SER:HB2	1.95	0.47
4:D:152:LEU:HD22	4:D:179:LEU:HD12	1.97	0.47
6:F:86:ASN:C	6:F:88:ASP:H	2.23	0.47
3:C:159:ILE:O	3:C:161:PRO:HD3	2.15	0.47
4:D:390:TRP:C	4:D:393:PRO:HD2	2.39	0.47
5:E:24:VAL:HG23	5:E:93:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:VAL:HG23	5:E:161:ARG:H	1.79	0.47
6:F:431:ILE:HD12	6:F:431:ILE:N	2.30	0.47
3:C:312:TRP:CE2	3:C:319:LEU:HD13	2.50	0.47
4:D:186:ARG:HG3	4:D:190:PHE:HB2	1.97	0.47
4:D:392:GLN:HB3	4:D:393:PRO:HD3	1.96	0.47
5:E:163:PRO:HA	5:E:178:LEU:HA	1.95	0.47
6:F:293:ILE:HD11	6:F:327:VAL:HG21	1.97	0.47
7:H:31:VAL:O	7:H:48:CYS:HA	2.14	0.47
2:B:270:THR:OG1	2:B:391:CYS:SG	2.72	0.47
6:F:157:ASP:OD1	6:F:163:ARG:NH2	2.46	0.47
4:D:249:LEU:O	4:D:253:VAL:HG23	2.15	0.47
6:F:86:ASN:OD1	6:F:400:ASN:ND2	2.48	0.47
2:B:304:VAL:HG13	2:B:323:ILE:HG22	1.97	0.47
5:E:570:LEU:O	5:E:574:LEU:HB2	2.15	0.47
6:F:207:SER:O	6:F:211:ILE:HG13	2.15	0.47
6:F:431:ILE:H	6:F:431:ILE:CD1	2.28	0.47
3:C:140:LEU:O	3:C:142:PRO:HD3	2.15	0.46
1:A:227:GLN:OE1	1:A:256:VAL:HG11	2.15	0.46
2:B:256:VAL:HG13	6:F:222:VAL:O	2.15	0.46
2:B:309:LYS:HE3	6:F:314:ILE:HD12	1.98	0.46
3:C:236:LYS:HG3	3:C:306:GLU:OE1	2.15	0.46
1:A:12:ILE:HA	1:A:28:SER:HA	1.96	0.46
2:B:319:LEU:HB2	6:F:159:ASP:OD2	2.15	0.46
3:C:16:VAL:HG12	3:C:63:TRP:HD1	1.81	0.46
3:C:196:ARG:HH11	3:C:202:LEU:HD21	1.78	0.46
1:A:191:ALA:C	1:A:193:THR:H	2.23	0.46
2:B:431:ASN:HB2	2:B:434:LYS:HB3	1.96	0.46
4:D:226:GLN:O	4:D:230:VAL:HG23	2.15	0.46
1:A:12:ILE:HG23	1:A:27:CYS:O	2.15	0.46
4:D:223:TYR:HA	4:D:226:GLN:HB2	1.96	0.46
6:F:8:GLN:O	6:F:10:GLU:N	2.48	0.46
2:B:156:THR:HG22	2:B:514:ARG:CD	2.45	0.46
3:C:79:LYS:HG2	3:C:109:GLY:C	2.41	0.46
5:E:490:VAL:HG22	5:E:590:GLN:HG3	1.97	0.46
1:A:16:VAL:HG21	1:A:59:VAL:O	2.16	0.46
1:A:259:ARG:NH1	2:B:151:PHE:HB2	2.30	0.46
5:E:177:PHE:CD1	5:E:183:LEU:HD22	2.51	0.46
4:D:141:ASN:C	4:D:145:ASN:HD22	2.24	0.46
1:A:95:HIS:NE2	1:A:138:PRO:HB3	2.31	0.46
1:A:116:LEU:O	1:A:127:VAL:HA	2.16	0.46
2:B:360:LYS:HG3	2:B:366:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:ASP:C	3:C:146:ARG:H	2.24	0.46
3:C:208:LEU:HD11	3:C:231:ILE:CD1	2.46	0.46
4:D:141:ASN:C	4:D:145:ASN:ND2	2.74	0.46
2:B:325:TYR:OH	6:F:210:MET:O	2.21	0.45
4:D:97:ARG:HB3	4:D:97:ARG:NH1	2.32	0.45
4:D:268:SER:HB2	4:D:269:ASP:OD1	2.17	0.45
6:F:433:ALA:O	6:F:435:PHE:N	2.44	0.45
6:F:219:LEU:HD22	6:F:227:ILE:HG12	1.98	0.45
4:D:97:ARG:NH2	4:D:411:SER:O	2.50	0.45
5:E:232:ARG:HE	5:E:249:THR:HG1	1.62	0.45
8:L:123:PRO:HD3	8:L:135:VAL:HG22	1.98	0.45
2:B:492:LEU:HD12	2:B:508:ILE:HD13	1.96	0.45
4:D:152:LEU:CD2	4:D:182:LEU:HB3	2.44	0.45
4:D:453:ASP:OD1	4:D:499:ALA:HB1	2.17	0.45
7:H:43:SER:HA	7:H:109:MET:O	2.16	0.45
2:B:178:THR:HG22	2:B:180:LEU:H	1.81	0.45
2:B:352:ASP:HB3	2:B:355:ILE:HD13	1.98	0.45
3:C:124:LYS:HG3	3:C:138:ASP:OD1	2.17	0.45
5:E:291:LEU:HA	5:E:292:PRO:HD3	1.76	0.45
5:E:643:ASP:OD2	5:E:646:ILE:HG13	2.17	0.45
6:F:144:TRP:CH2	6:F:158:LEU:HA	2.51	0.45
1:A:16:VAL:HG23	1:A:59:VAL:HG23	1.98	0.45
4:D:153:ASN:HA	4:D:156:GLU:OE1	2.16	0.45
5:E:4:LEU:HB2	5:E:381:SER:HB2	1.96	0.45
2:B:187:ASP:C	2:B:187:ASP:OD1	2.60	0.45
2:B:375:GLU:C	2:B:377:GLU:H	2.24	0.45
2:B:393:GLY:O	2:B:394:GLN:HB2	2.17	0.45
3:C:346:THR:C	4:D:51:MET:HB3	2.41	0.45
3:C:208:LEU:HD11	3:C:231:ILE:HD11	1.97	0.45
4:D:522:MET:HE1	4:D:538:ILE:HD12	1.98	0.45
6:F:284:SER:O	6:F:288:ILE:HG12	2.16	0.45
7:H:157:THR:HG21	7:H:243:PRO:C	2.42	0.45
2:B:513:MET:HG2	2:B:541:ALA:HB2	1.99	0.45
4:D:198:GLU:HG2	4:D:300:SER:CB	2.47	0.45
4:D:268:SER:O	4:D:272:PRO:HG2	2.16	0.45
5:E:436:HIS:NE2	5:E:438:GLU:HB2	2.31	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.46	0.45
3:C:7:GLY:C	3:C:34:LYS:HE3	2.42	0.45
3:C:119:ALA:C	3:C:121:LEU:H	2.25	0.45
5:E:130:THR:O	5:E:150:PHE:HA	2.17	0.45
6:F:143:LYS:HG3	6:F:144:TRP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:322:THR:HG23	4:D:329:ARG:HD3	1.97	0.44
1:A:43:HIS:HD2	2:B:173:ILE:HD11	1.82	0.44
3:C:296:LEU:HD21	3:C:299:GLU:HG3	1.98	0.44
7:H:155:ALA:HB3	7:H:187:PHE:CE1	2.52	0.44
5:E:623:LEU:HD23	5:E:623:LEU:HA	1.74	0.44
6:F:81:LEU:HD13	6:F:85:ARG:NH2	2.32	0.44
6:F:116:LEU:O	6:F:119:ILE:HB	2.17	0.44
6:F:264:TYR:O	6:F:268:SER:OG	2.34	0.44
1:A:273:GLY:C	1:A:275:ASP:H	2.25	0.44
4:D:285:VAL:O	4:D:289:ILE:HG13	2.18	0.44
4:D:406:LEU:HB2	4:D:407:PRO:HD3	1.98	0.44
7:H:28:VAL:HG11	7:H:143:TYR:CE1	2.53	0.44
3:C:31:GLN:OE1	3:C:52:ARG:NH1	2.50	0.44
4:D:202:SER:HA	4:D:297:LYS:O	2.18	0.44
5:E:247:ASP:HB2	5:E:254:ILE:HG13	1.98	0.44
1:A:257:LEU:HA	1:A:273:GLY:HA2	1.98	0.44
5:E:352:ILE:HD13	5:E:471:ILE:HG12	1.99	0.44
5:E:658:HIS:HA	5:E:661:GLN:OE1	2.18	0.44
1:A:35:ILE:HB	1:A:47:ASP:HB2	2.00	0.44
2:B:391:CYS:O	2:B:395:ILE:HD11	2.17	0.44
5:E:534:ASP:HA	5:E:537:THR:OG1	2.18	0.44
4:D:141:ASN:N	4:D:141:ASN:HD22	2.16	0.44
5:E:499:SER:O	5:E:500:GLU:C	2.60	0.44
5:E:668:TYR:CZ	5:E:672:LYS:HE3	2.53	0.44
7:H:44:LEU:HB2	7:H:109:MET:HE3	2.00	0.44
7:H:125:THR:HG23	7:H:141:LEU:HD23	1.99	0.44
2:B:256:VAL:HG22	6:F:222:VAL:O	2.18	0.44
2:B:392:TYR:O	2:B:394:GLN:N	2.44	0.44
3:C:107:SER:HA	3:C:135:ARG:HH21	1.83	0.44
4:D:148:MET:HE3	4:D:152:LEU:HG	2.00	0.44
5:E:218:SER:OG	5:E:219:ASP:N	2.50	0.44
5:E:427:LEU:HD13	5:E:442:TYR:CE1	2.53	0.44
2:B:311:ALA:HB1	2:B:316:ASN:O	2.18	0.43
4:D:328:LEU:HA	4:D:331:TYR:HB2	2.00	0.43
6:F:106:GLU:O	6:F:110:MET:HG2	2.18	0.43
2:B:394:GLN:HG2	2:B:397:GLU:HB2	2.00	0.43
6:F:385:LEU:O	6:F:389:VAL:HG23	2.18	0.43
2:B:333:ILE:HG23	6:F:210:MET:SD	2.59	0.43
5:E:297:LEU:HD23	5:E:297:LEU:HA	1.88	0.43
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.53	0.43
2:B:319:LEU:N	6:F:159:ASP:OD2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:390:THR:O	6:F:394:ILE:HG12	2.19	0.43
2:B:309:LYS:CE	6:F:314:ILE:HD12	2.48	0.43
2:B:344:TRP:C	2:B:346:THR:H	2.27	0.43
4:D:58:ILE:HG22	4:D:59:GLU:N	2.33	0.43
4:D:221:GLU:HA	4:D:224:ILE:HG13	2.00	0.43
8:L:6:GLN:HB2	8:L:29:SER:HB3	2.01	0.43
1:A:63:HIS:CD2	1:A:64:PRO:HD2	2.53	0.43
2:B:400:LEU:HB3	2:B:426:TYR:OH	2.18	0.43
3:C:303:HIS:HA	3:C:325:ASP:OD2	2.19	0.43
5:E:508:LYS:O	5:E:512:THR:HG23	2.19	0.43
6:F:109:LEU:HD23	6:F:298:ILE:HG13	2.00	0.43
4:D:243:GLN:O	4:D:247:LYS:HG3	2.19	0.43
6:F:82:LEU:HD23	6:F:82:LEU:HA	1.87	0.43
8:L:194:VAL:HG22	8:L:213:ASN:ND2	2.34	0.43
3:C:131:ASP:OD2	3:C:135:ARG:NH2	2.51	0.43
4:D:511:TYR:HA	4:D:512:PRO:HD3	1.73	0.43
6:F:77:LEU:HG	6:F:125:TRP:CD2	2.54	0.43
7:H:117:THR:HG23	7:H:151:THR:HA	2.01	0.43
4:D:215:SER:HB2	4:D:390:TRP:CH2	2.54	0.43
4:D:215:SER:HB2	4:D:390:TRP:CZ2	2.53	0.43
4:D:335:PHE:O	4:D:339:ILE:HG13	2.19	0.43
5:E:627:TYR:HA	5:E:661:GLN:OE1	2.19	0.43
1:A:45:LEU:HB2	2:B:168:LYS:HE2	2.01	0.42
1:A:261:SER:HB2	2:B:153:LYS:HA	2.01	0.42
1:A:280:LEU:HB2	1:A:292:ALA:O	2.19	0.42
2:B:345:SER:HB3	2:B:371:PHE:HE2	1.84	0.42
2:B:531:LEU:O	2:B:532:LYS:HG2	2.19	0.42
4:D:508:LEU:HG	4:D:522:MET:HE3	2.01	0.42
5:E:601:PHE:O	5:E:602:ILE:C	2.61	0.42
6:F:293:ILE:HD11	6:F:327:VAL:CG2	2.49	0.42
2:B:208:TYR:CE2	2:B:505:GLU:HG3	2.54	0.42
2:B:247:TYR:CE2	2:B:260:LEU:HD13	2.54	0.42
2:B:513:MET:HA	2:B:541:ALA:HB1	2.02	0.42
3:C:313:ASN:HD22	3:C:313:ASN:HA	1.61	0.42
4:D:454:LEU:HD21	4:D:503:VAL:HG21	2.01	0.42
2:B:418:PRO:HB3	2:B:445:ALA:HB1	2.02	0.42
5:E:295:ASN:ND2	5:E:329:TRP:O	2.52	0.42
6:F:341:HIS:HA	6:F:342:PRO:HD3	1.89	0.42
5:E:177:PHE:HD1	5:E:183:LEU:HD22	1.84	0.42
5:E:180:ASP:HA	5:E:220:TYR:CD1	2.55	0.42
2:B:203:ARG:NE	2:B:210:GLN:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:HIS:C	2:B:528:LEU:H	2.26	0.42
4:D:168:ARG:HD3	4:D:170:ASN:HB3	2.02	0.42
5:E:53:GLY:HA3	5:E:71:HIS:HB3	2.02	0.42
5:E:92:THR:HG21	5:E:479:TYR:OH	2.19	0.42
3:C:76:SER:HB3	3:C:78:ASP:OD1	2.19	0.42
4:D:149:GLU:HG3	4:D:186:ARG:NE	2.34	0.42
4:D:159:ILE:HD13	4:D:176:GLU:HA	2.01	0.42
5:E:386:LEU:HD23	5:E:621:GLN:HA	2.01	0.42
2:B:365:SER:HB3	2:B:368:GLU:HB2	2.01	0.42
2:B:452:TRP:CD1	2:B:475:THR:HA	2.54	0.42
3:C:189:GLU:HA	3:C:213:SER:O	2.20	0.42
4:D:57:PRO:HB3	4:D:91:TYR:OH	2.19	0.42
5:E:111:GLN:HG3	5:E:168:TYR:CG	2.55	0.42
1:A:222:LEU:O	1:A:233:ILE:HA	2.20	0.42
3:C:192:ILE:HG22	3:C:207:LYS:HG2	2.02	0.42
5:E:436:HIS:CD2	5:E:438:GLU:H	2.37	0.42
6:F:23:LYS:HD2	6:F:434:THR:HG21	2.01	0.42
1:A:60:ASP:H	1:A:70:LEU:CD1	2.33	0.42
5:E:59:CYS:HB2	5:E:464:THR:OG1	2.19	0.42
5:E:153:GLN:OE1	5:E:193:HIS:HA	2.20	0.42
3:C:29:SER:C	3:C:31:GLN:N	2.78	0.41
5:E:287:LEU:O	5:E:300:MET:HA	2.20	0.41
6:F:22:PHE:CG	6:F:38:ILE:HD11	2.54	0.41
8:L:126:SER:C	8:L:129:LYS:HB3	2.44	0.41
2:B:539:PHE:CD1	2:B:539:PHE:C	2.98	0.41
4:D:78:ASN:HD21	4:D:95:ILE:HG13	1.85	0.41
4:D:269:ASP:OD1	4:D:269:ASP:N	2.53	0.41
6:F:104:LEU:HG	6:F:224:ASP:HB3	2.02	0.41
6:F:359:ILE:HD13	6:F:389:VAL:HG13	2.02	0.41
7:H:102:LYS:HE2	7:H:102:LYS:HB3	1.87	0.41
6:F:146:ASN:HB2	6:F:173:ASP:CG	2.46	0.41
2:B:216:LEU:O	2:B:217:LEU:HD23	2.19	0.41
3:C:77:TYR:HD1	3:C:110:SER:HB3	1.86	0.41
3:C:131:ASP:O	3:C:133:ILE:HG13	2.20	0.41
3:C:175:PRO:HD3	3:C:220:TRP:HB3	2.02	0.41
5:E:117:LEU:HD23	5:E:117:LEU:HA	1.90	0.41
6:F:242:LEU:O	6:F:243:TRP:C	2.64	0.41
7:H:38:VAL:HG11	7:H:112:LEU:HD13	2.02	0.41
2:B:162:THR:HG22	2:B:163:LYS:N	2.35	0.41
2:B:373:LEU:HB3	2:B:376:LEU:HD12	2.02	0.41
1:A:227:GLN:C	1:A:229:ARG:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD22	2:B:440:ARG:HB3	2.02	0.41
2:B:155:SER:HB3	2:B:159:MET:H	1.85	0.41
4:D:152:LEU:HD23	4:D:152:LEU:HA	1.85	0.41
5:E:186:LEU:HD12	5:E:186:LEU:HA	1.91	0.41
5:E:659:TYR:OH	5:E:743:ASN:C	2.64	0.41
6:F:81:LEU:HD12	6:F:350:VAL:HG12	2.00	0.41
4:D:396:ASP:OD1	4:D:401:LYS:HE3	2.20	0.41
2:B:263:LYS:HD3	2:B:263:LYS:HA	1.75	0.41
4:D:57:PRO:HB2	4:D:82:ILE:HD11	2.03	0.41
4:D:373:GLU:O	4:D:377:MET:HG3	2.21	0.41
5:E:167:PHE:O	5:E:174:SER:HB2	2.21	0.41
1:A:223:ALA:HB2	1:A:262:TRP:CZ2	2.55	0.41
2:B:247:TYR:CZ	2:B:260:LEU:HD13	2.56	0.41
4:D:265:ILE:C	4:D:267:ARG:N	2.77	0.41
4:D:403:HIS:O	4:D:405:ILE:HG23	2.20	0.41
1:A:63:HIS:HD2	1:A:65:LYS:H	1.68	0.41
4:D:240:PHE:CD1	4:D:268:SER:HB3	2.56	0.41
5:E:169:VAL:HG13	5:E:228:LEU:HD22	2.03	0.41
1:A:261:SER:HB2	2:B:153:LYS:HG2	2.03	0.40
3:C:86:GLU:HB2	3:C:98:TRP:CZ2	2.56	0.40
4:D:145:ASN:OD1	4:D:190:PHE:CA	2.69	0.40
4:D:159:ILE:HG12	4:D:175:LEU:CB	2.40	0.40
4:D:531:LEU:HB3	4:D:534:ILE:CG1	2.51	0.40
6:F:13:THR:O	6:F:17:ASP:HB2	2.21	0.40
1:A:217:LEU:HD13	1:A:218:LEU:N	2.36	0.40
1:A:225:VAL:CG2	1:A:271:LEU:HD22	2.51	0.40
4:D:246:TRP:CD1	4:D:331:TYR:CD2	3.09	0.40
4:D:291:LEU:HD13	4:D:310:VAL:HG22	2.03	0.40
6:F:206:ILE:HG22	6:F:210:MET:HE2	2.02	0.40
6:F:425:LEU:HD23	6:F:425:LEU:HA	1.90	0.40
1:A:17:LEU:HG	2:B:161:LEU:HD11	2.03	0.40
3:C:16:VAL:HG12	3:C:63:TRP:CD1	2.55	0.40
4:D:97:ARG:HB3	4:D:97:ARG:HH11	1.86	0.40
4:D:105:SER:HB2	4:D:481:LEU:HD21	2.03	0.40
5:E:19:GLU:HA	5:E:20:PRO:HD3	1.99	0.40
1:A:23:ARG:NH1	1:A:84:GLU:OE1	2.54	0.40
1:A:59:VAL:HB	1:A:70:LEU:HD11	2.03	0.40
4:D:352:THR:OG1	4:D:355:GLU:HG3	2.21	0.40
6:F:237:ILE:C	6:F:237:ILE:HD12	2.47	0.40
2:B:492:LEU:HD11	2:B:508:ILE:HG23	2.04	0.40
4:D:60:LYS:C	4:D:62:GLY:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:227:VAL:C	4:D:229:SER:N	2.79	0.40
4:D:334:ASP:HB3	4:D:349:TYR:HE2	1.86	0.40
6:F:343:ILE:HD13	6:F:344:ARG:H	1.85	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)
6:F:233:THR:OG1	8:L:203:GLY:O[4_455]	2.05	0.15
6:F:232:ASN:O	8:L:205:SER:N[4_455]	2.08	0.12

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	270/297 (91%)	228 (84%)	36 (13%)	6 (2%)	5	29
2	B	491/652 (75%)	451 (92%)	30 (6%)	10 (2%)	6	31
3	C	303/349 (87%)	266 (88%)	31 (10%)	6 (2%)	6	31
4	D	592/715 (83%)	532 (90%)	50 (8%)	10 (2%)	7	36
5	E	858/1045 (82%)	798 (93%)	49 (6%)	11 (1%)	9	42
6	F	413/454 (91%)	368 (89%)	34 (8%)	11 (3%)	4	25
7	H	213/271 (79%)	206 (97%)	7 (3%)	0	100	100
8	L	206/217 (95%)	198 (96%)	6 (3%)	2 (1%)	12	48
All	All	3346/4000 (84%)	3047 (91%)	243 (7%)	56 (2%)	7	36

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER

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Mol	Chain	Res	Type
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	C	43	SER
4	D	272	PRO
4	D	403	HIS
4	D	455	PHE
6	F	9	THR
6	F	11	ARG
6	F	138	ASN
6	F	165	ASN
8	L	34	SER
1	A	218	LEU
2	B	180	LEU
2	B	348	GLY
2	B	429	ASN
2	B	527	ILE
3	C	162	ALA
3	C	302	ASP
4	D	62	GLY
4	D	239	VAL
5	E	113	VAL
5	E	598	LYS
5	E	602	ILE
6	F	8	GLN
6	F	55	ASN
6	F	141	THR
6	F	354	SER
8	L	129	LYS
3	C	120	HIS
4	D	404	SER
5	E	264	ASP
6	F	434	THR
6	F	440	ASP
2	B	531	LEU
3	C	213	SER
5	E	284	ASN
5	E	346	ALA
6	F	87	ALA
1	A	114	PRO
1	A	131	LYS
4	D	53	VAL

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Mol	Chain	Res	Type
4	D	200	ASN
4	D	364	TYR
5	E	190	ASP
5	E	600	ASP
1	A	247	LEU
3	C	188	LEU
5	E	231	GLU
5	E	500	GLU
2	B	393	GLY
5	E	737	ILE
1	A	202	GLY
4	D	191	ILE
1	A	97	VAL

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	233/252 (92%)	223 (96%)	10 (4%)	26	47
2	B	367/594 (62%)	321 (88%)	46 (12%)	4	16
3	C	269/305 (88%)	258 (96%)	11 (4%)	27	48
4	D	424/642 (66%)	408 (96%)	16 (4%)	29	50
5	E	639/980 (65%)	611 (96%)	28 (4%)	25	47
6	F	387/418 (93%)	363 (94%)	24 (6%)	16	38
7	H	175/224 (78%)	168 (96%)	7 (4%)	28	49
8	L	184/191 (96%)	179 (97%)	5 (3%)	39	61
All	All	2678/3606 (74%)	2531 (94%)	147 (6%)	19	41

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	43	HIS
1	A	46	ILE
1	A	47	ASP
1	A	139	ILE
1	A	225	VAL
1	A	227	GLN
1	A	229	ARG
1	A	275	ASP
2	B	160	LEU
2	B	175	ARG
2	B	195	ILE
2	B	198	VAL
2	B	201	GLU
2	B	210	GLN
2	B	214	SER
2	B	216	LEU
2	B	225	MET
2	B	234	LEU
2	B	251	THR
2	B	283	GLU
2	B	292	ILE
2	B	308	SER
2	B	319	LEU
2	B	328	SER
2	B	336	LEU
2	B	341	LEU
2	B	346	THR
2	B	349	CYS
2	B	351	ILE
2	B	355	ILE
2	B	368	GLU
2	B	370	LEU
2	B	371	PHE
2	B	400	LEU
2	B	402	SER
2	B	406	SER
2	B	408	LEU
2	B	412	SER
2	B	419	ILE
2	B	440	ARG
2	B	443	THR
2	B	456	GLN

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Mol	Chain	Res	Type
2	B	464	ARG
2	B	465	VAL
2	B	467	SER
2	B	469	GLU
2	B	508	ILE
2	B	516	ILE
2	B	522	SER
2	B	524	ASN
2	B	530	ARG
2	B	531	LEU
2	B	539	PHE
2	B	547	ARG
3	C	61	ILE
3	C	80	THR
3	C	125	LEU
3	C	154	MET
3	C	168	ASP
3	C	183	LEU
3	C	226	ARG
3	C	301	ASP
3	C	313	ASN
3	C	314	LEU
3	C	334	THR
4	D	51	MET
4	D	77	GLN
4	D	141	ASN
4	D	143	THR
4	D	239	VAL
4	D	269	ASP
4	D	280	VAL
4	D	324	ILE
4	D	384	VAL
4	D	387	THR
4	D	453	ASP
4	D	488	LEU
4	D	496	THR
4	D	514	VAL
4	D	525	ILE
4	D	539	TYR
5	E	63	SER
5	E	127	SER
5	E	162	VAL

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Mol	Chain	Res	Type
5	E	172	GLN
5	E	175	VAL
5	E	183	LEU
5	E	188	LYS
5	E	209	THR
5	E	259	MET
5	E	270	PHE
5	E	280	LEU
5	E	305	VAL
5	E	314	THR
5	E	328	ILE
5	E	335	VAL
5	E	338	ARG
5	E	341	GLU
5	E	370	ASP
5	E	404	VAL
5	E	408	PHE
5	E	428	SER
5	E	590	GLN
5	E	605	ILE
5	E	638	VAL
5	E	644	THR
5	E	663	LEU
5	E	690	VAL
5	E	703	ASP
6	F	13	THR
6	F	17	ASP
6	F	26	GLN
6	F	58	ASP
6	F	71	GLU
6	F	77	LEU
6	F	86	ASN
6	F	88	ASP
6	F	118	GLN
6	F	128	GLU
6	F	141	THR
6	F	166	THR
6	F	225	THR
6	F	237	ILE
6	F	268	SER
6	F	274	GLN
6	F	284	SER

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Mol	Chain	Res	Type
6	F	298	ILE
6	F	343	ILE
6	F	357	SER
6	F	365	MET
6	F	403	SER
6	F	422	LEU
6	F	431	ILE
7	H	45	ARG
7	H	55	VAL
7	H	113	ARG
7	H	124	ARG
7	H	170	LYS
7	H	191	VAL
7	H	219	LEU
8	L	8	THR
8	L	27	ARG
8	L	108	GLU
8	L	109	ILE
8	L	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	43	HIS
1	A	63	HIS
1	A	91	GLN
1	A	103	ASN
1	A	188	ASN
2	B	210	GLN
2	B	329	ASN
2	B	354	ASN
2	B	405	GLN
2	B	461	ASN
2	B	488	HIS
2	B	490	HIS
2	B	536	GLN
2	B	542	GLN
3	C	90	GLN
3	C	99	ASN
4	D	170	ASN
4	D	260	GLN

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Mol	Chain	Res	Type
4	D	308	ASN
4	D	315	GLN
4	D	342	ASN
4	D	403	HIS
4	D	467	ASN
4	D	510	HIS
5	E	10	ASN
5	E	116	GLN
5	E	154	ASN
5	E	255	GLN
5	E	295	ASN
5	E	393	HIS
5	E	575	ASN
5	E	584	ASN
5	E	588	ASN
6	F	300	ASN
6	F	360	HIS
6	F	423	GLN
7	H	65	GLN
7	H	205	HIS
8	L	41	GLN
8	L	202	GLN
8	L	213	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	274/297 (92%)	4.45	146 (53%) 0 3	629, 712, 763, 800	0
2	B	511/652 (78%)	3.04	245 (47%) 0 4	374, 655, 746, 784	0
3	C	307/349 (87%)	2.07	127 (41%) 0 4	631, 756, 814, 905	0
4	D	620/715 (86%)	3.68	340 (54%) 0 3	388, 746, 989, 1000	0
5	E	896/1045 (85%)	3.06	424 (47%) 0 4	422, 725, 816, 883	0
6	F	419/454 (92%)	3.73	230 (54%) 0 3	545, 699, 803, 877	0
7	H	217/271 (80%)	2.22	79 (36%) 1 5	528, 677, 821, 884	0
8	L	210/217 (96%)	1.81	71 (33%) 1 6	526, 676, 756, 791	0
All	All	3454/4000 (86%)	3.14	1662 (48%) 0 4	374, 711, 890, 1000	0

All (1662) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	SER	52.2
2	B	403	LEU	44.7
1	A	27	CYS	40.1
6	F	49	LEU	38.2
6	F	46	ALA	38.1
2	B	400	LEU	38.0
6	F	68	TRP	37.5
1	A	230	THR	36.3
6	F	65	SER	35.5
1	A	12	ILE	32.7
6	F	45	ALA	30.7
1	A	120	SER	30.3
4	D	390	TRP	30.2
6	F	15	PHE	29.7
1	A	148	VAL	29.2
4	D	219	PRO	28.8

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Mol	Chain	Res	Type	RSRZ
4	D	172	PHE	28.3
4	D	180	THR	27.8
4	D	176	GLU	27.8
1	A	104	SER	27.3
2	B	404	VAL	26.6
4	D	177	GLU	26.2
1	A	119	ALA	25.6
5	E	918	PHE	25.1
5	E	971	ASN	25.1
4	D	216	ASP	24.4
5	E	912	ASP	23.9
7	H	218	SER	23.4
1	A	13	HIS	23.3
1	A	14	ASP	23.0
4	D	215	SER	23.0
6	F	16	SER	22.9
5	E	970	LEU	22.8
7	H	212	GLN	22.8
5	E	841	ALA	22.6
5	E	689	GLY	22.4
1	A	73	CYS	22.3
4	D	220	ASP	21.7
6	F	50	ALA	21.7
2	B	406	SER	21.7
5	E	653	THR	21.2
1	A	231	CYS	21.1
4	D	251	GLN	21.0
1	A	28	SER	21.0
5	E	516	PHE	20.2
6	F	52	ASP	20.0
4	D	352	THR	19.9
7	H	186	TYR	19.7
7	H	112	LEU	19.5
6	F	8	GLN	19.3
4	D	327	GLU	19.3
7	H	111	SER	19.1
4	D	173	TYR	18.7
6	F	12	PHE	18.6
5	E	670	GLN	18.4
4	D	605	VAL	18.3
6	F	170	ASP	18.2
2	B	706	MET	18.1

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Mol	Chain	Res	Type	RSRZ
2	B	261	LEU	18.0
2	B	151	PHE	17.7
2	B	251	THR	17.7
2	B	170	GLY	17.7
1	A	149	ASN	17.6
6	F	171	VAL	17.5
2	B	710	TYR	17.1
2	B	427	ALA	17.1
1	A	102	VAL	17.0
5	E	410	ASN	17.0
5	E	838	GLN	16.9
1	A	118	VAL	16.8
4	D	218	GLU	16.7
5	E	180	ASP	16.5
5	E	213	SER	16.5
5	E	763	THR	16.5
6	F	420	LEU	16.3
6	F	333	SER	16.3
2	B	262	LYS	16.3
5	E	574	LEU	16.3
4	D	171	ARG	16.2
2	B	704	ASP	16.1
6	F	71	GLU	16.0
4	D	174	GLU	15.9
1	A	56	VAL	15.9
1	A	207	VAL	15.9
6	F	416	TYR	15.9
2	B	407	HIS	15.8
4	D	394	CYS	15.5
6	F	358	VAL	15.3
1	A	225	VAL	15.3
1	A	257	LEU	15.2
4	D	217	GLY	15.2
1	A	177	GLY	15.1
6	F	355	LEU	15.1
4	D	350	SER	14.9
4	D	242	THR	14.8
4	D	241	GLU	14.8
2	B	408	LEU	14.7
4	D	351	ARG	14.7
1	A	58	ARG	14.5
6	F	387	ARG	14.5

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Mol	Chain	Res	Type	RSRZ
5	E	687	SER	14.4
1	A	103	ASN	14.4
6	F	147	SER	14.3
2	B	401	GLU	14.3
3	C	202	LEU	14.3
1	A	147	GLY	14.3
1	A	228	ASP	13.8
5	E	198	LEU	13.5
5	E	624	SER	13.4
1	A	227	GLN	13.4
4	D	328	LEU	13.3
2	B	149	TYR	13.2
6	F	53	LEU	13.2
1	A	32	THR	13.2
4	D	388	ASN	13.1
4	D	160	GLY	13.1
3	C	203	HIS	13.1
5	E	743	ASN	13.0
4	D	355	GLU	13.0
5	E	406	ARG	12.9
5	E	962	LYS	12.9
4	D	543	GLY	12.9
5	E	930	SER	12.8
5	E	90	GLY	12.8
6	F	349	SER	12.7
5	E	764	LEU	12.7
5	E	239	GLN	12.6
4	D	246	TRP	12.6
4	D	252	LEU	12.5
4	D	163	LYS	12.4
6	F	361	SER	12.4
2	B	471	SER	12.4
4	D	629	VAL	12.3
4	D	585	LYS	12.3
1	A	74	SER	12.2
6	F	391	HIS	12.2
6	F	362	SER	12.1
4	D	332	ILE	12.1
4	D	554	GLU	12.1
2	B	395	ILE	12.0
2	B	411	PHE	12.0
1	A	26	THR	12.0

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Mol	Chain	Res	Type	RSRZ
5	E	575	ASN	12.0
5	E	978	ALA	11.9
5	E	927	ASN	11.8
6	F	417	ILE	11.7
5	E	952	ASN	11.7
5	E	570	LEU	11.6
5	E	572	ASP	11.6
5	E	222	SER	11.6
5	E	735	LYS	11.6
1	A	33	ILE	11.5
2	B	393	GLY	11.5
1	A	105	VAL	11.4
4	D	555	SER	11.4
2	B	256	VAL	11.3
3	C	195	GLN	11.3
4	D	502	MET	11.2
4	D	179	LEU	11.2
5	E	220	TYR	11.2
6	F	396	LEU	11.1
4	D	169	VAL	11.1
5	E	910	GLN	11.1
4	D	255	ARG	11.0
6	F	42	PHE	10.9
5	E	161	ARG	10.9
4	D	227	VAL	10.9
5	E	920	SER	10.9
8	L	9	GLN	10.8
4	D	221	GLU	10.8
4	D	157	VAL	10.7
6	F	339	SER	10.7
5	E	967	PHE	10.6
5	E	875	LEU	10.6
4	D	213	ASN	10.6
4	D	710	TYR	10.5
6	F	354	SER	10.5
4	D	240	PHE	10.4
2	B	414	PRO	10.4
2	B	657	CYS	10.4
5	E	654	LEU	10.4
5	E	565	THR	10.3
7	H	210	VAL	10.3
5	E	407	GLY	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	TRP	10.2
2	B	382	TRP	10.2
4	D	331	TYR	10.2
4	D	159	ILE	10.2
3	C	174	CYS	10.2
6	F	175	GLU	10.1
5	E	848	SER	10.1
5	E	840	PHE	10.0
5	E	178	LEU	10.0
5	E	571	PHE	10.0
5	E	612	SER	9.9
5	E	650	HIS	9.9
6	F	100	ASN	9.9
1	A	176	GLY	9.9
4	D	412	LEU	9.9
4	D	154	GLU	9.9
4	D	245	PHE	9.8
8	L	79	SER	9.8
5	E	919	PHE	9.8
4	D	281	SER	9.8
5	E	89	HIS	9.7
5	E	647	PHE	9.7
6	F	326	GLU	9.7
6	F	429	ILE	9.6
5	E	550	PHE	9.6
6	F	168	VAL	9.6
5	E	661	GLN	9.6
2	B	399	SER	9.6
5	E	651	ILE	9.6
4	D	391	GLU	9.5
5	E	913	ILE	9.5
5	E	736	ASN	9.5
4	D	248	LEU	9.5
5	E	906	GLN	9.4
6	F	18	THR	9.4
2	B	413	LEU	9.4
5	E	413	SER	9.4
5	E	745	GLU	9.4
2	B	210	GLN	9.4
4	D	467	ASN	9.3
4	D	730	ASN	9.3
1	A	150	SER	9.3

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Mol	Chain	Res	Type	RSRZ
2	B	270	THR	9.3
4	D	644	GLN	9.3
2	B	266	HIS	9.3
2	B	410	LYS	9.3
5	E	955	SER	9.3
6	F	390	THR	9.3
5	E	517	ALA	9.3
4	D	162	VAL	9.2
4	D	156	GLU	9.2
1	A	208	ARG	9.2
2	B	329	ASN	9.1
5	E	636	THR	9.1
2	B	573	VAL	9.1
1	A	79	VAL	9.1
5	E	568	LYS	9.1
1	A	57	TRP	9.1
7	H	158	LYS	9.0
2	B	463	THR	9.0
5	E	150	PHE	9.0
4	D	269	ASP	9.0
2	B	150	THR	9.0
6	F	432	TYR	9.0
2	B	377	GLU	9.0
3	C	238	GLY	9.0
4	D	726	THR	9.0
4	D	499	ALA	8.9
5	E	657	LEU	8.9
4	D	526	CYS	8.9
4	D	249	LEU	8.9
2	B	597	GLU	8.8
5	E	537	THR	8.8
5	E	553	ILE	8.8
4	D	453	ASP	8.7
2	B	426	TYR	8.7
5	E	1025	VAL	8.7
4	D	356	SER	8.7
5	E	917	ASP	8.7
5	E	156	TYR	8.7
5	E	688	PHE	8.6
5	E	966	CYS	8.6
3	C	289	GLN	8.6
4	D	229	SER	8.6

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Mol	Chain	Res	Type	RSRZ
5	E	637	PHE	8.5
6	F	363	VAL	8.5
5	E	656	ASP	8.5
2	B	703	GLN	8.5
5	E	757	GLU	8.5
5	E	845	ILE	8.4
2	B	475	THR	8.4
5	E	922	LEU	8.4
5	E	686	PHE	8.4
5	E	627	TYR	8.4
5	E	216	SER	8.4
7	H	85	SER	8.4
5	E	135	LEU	8.3
2	B	405	GLN	8.3
5	E	136	SER	8.3
6	F	173	ASP	8.3
4	D	731	LEU	8.3
5	E	22	ASN	8.3
5	E	969	MET	8.3
5	E	8	ASP	8.3
5	E	872	TYR	8.3
2	B	265	ARG	8.2
4	D	237	LYS	8.2
5	E	409	CYS	8.2
5	E	181	GLY	8.1
6	F	167	ASN	8.1
4	D	463	SER	8.0
5	E	579	ILE	8.0
5	E	760	PHE	8.0
6	F	393	ALA	8.0
5	E	101	SER	8.0
5	E	829	SER	8.0
6	F	356	PRO	8.0
6	F	403	SER	8.0
5	E	734	HIS	8.0
4	D	250	ASN	7.9
6	F	224	ASP	7.9
6	F	329	ASN	7.9
5	E	924	ARG	7.9
8	L	51	ILE	7.9
1	A	15	ALA	7.9
7	H	244	SER	7.9

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Mol	Chain	Res	Type	RSRZ
7	H	116	ASP	7.9
5	E	566	ASN	7.9
2	B	402	SER	7.9
4	D	239	VAL	7.9
6	F	221	PRO	7.9
5	E	240	ASN	7.8
2	B	271	SER	7.8
5	E	182	GLY	7.8
2	B	412	SER	7.8
1	A	126	SER	7.8
5	E	885	VAL	7.8
5	E	710	TYR	7.7
1	A	253	PHE	7.7
4	D	608	PRO	7.7
4	D	175	LEU	7.7
5	E	832	PHE	7.7
4	D	604	ASP	7.7
6	F	381	ASP	7.7
1	A	224	SER	7.6
4	D	734	LYS	7.6
1	A	95	HIS	7.6
5	E	921	THR	7.6
2	B	260	LEU	7.6
2	B	656	ALA	7.6
5	E	221	ASP	7.6
4	D	214	ARG	7.6
7	H	217	TYR	7.5
4	D	354	TYR	7.5
8	L	98	PRO	7.5
5	E	746	CYS	7.5
5	E	1005	ASN	7.5
5	E	926	CYS	7.5
7	H	76	SER	7.5
4	D	714	ILE	7.5
4	D	382	ASN	7.5
5	E	968	ARG	7.5
5	E	658	HIS	7.4
4	D	153	ASN	7.4
6	F	13	THR	7.4
4	D	228	PHE	7.4
5	E	842	LEU	7.4
1	A	59	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
4	D	211	TRP	7.3
5	E	200	ASN	7.3
4	D	623	THR	7.3
5	E	57	SER	7.3
1	A	259	ARG	7.2
2	B	274	VAL	7.2
4	D	222	GLU	7.2
4	D	713	ILE	7.2
6	F	223	ILE	7.2
3	C	152	SER	7.2
3	C	291	ASN	7.2
2	B	557	GLN	7.1
4	D	583	GLY	7.1
5	E	907	LEU	7.1
6	F	72	ALA	7.1
4	D	75	SER	7.1
5	E	608	ASP	7.1
1	A	77	GLY	7.0
3	C	290	SER	7.0
2	B	661	MET	7.0
6	F	7	TYR	7.0
2	B	428	ALA	6.9
5	E	607	PHE	6.9
2	B	290	ASN	6.9
5	E	587	ILE	6.9
2	B	254	ASP	6.9
5	E	707	SER	6.9
4	D	183	ASN	6.9
6	F	169	LEU	6.9
7	H	184	LYS	6.9
3	C	307	VAL	6.9
2	B	257	LYS	6.9
5	E	877	ILE	6.9
4	D	693	GLU	6.9
1	A	151	ALA	6.9
4	D	668	ALA	6.9
5	E	873	LEU	6.9
5	E	207	SER	6.8
2	B	705	LEU	6.8
2	B	654	VAL	6.8
5	E	201	ASP	6.8
8	L	21	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
2	B	381	SER	6.8
4	D	265	ILE	6.8
8	L	91	CYS	6.8
4	D	110	GLY	6.8
4	D	288	SER	6.7
4	D	465	MET	6.7
8	L	25	THR	6.7
6	F	11	ARG	6.7
4	D	274	LEU	6.7
5	E	961	PHE	6.7
4	D	97	ARG	6.7
6	F	9	THR	6.6
4	D	466	LEU	6.6
5	E	583	LEU	6.6
2	B	396	ASP	6.6
5	E	671	ASP	6.6
1	A	236	GLN	6.6
1	A	232	ILE	6.6
5	E	76	SER	6.6
5	E	513	LEU	6.6
1	A	235	THR	6.6
4	D	627	TYR	6.6
2	B	498	LEU	6.6
5	E	179	GLU	6.5
6	F	67	ASP	6.5
5	E	1006	VAL	6.5
3	C	118	PRO	6.5
2	B	259	ALA	6.5
5	E	660	LYS	6.4
4	D	84	ALA	6.4
4	D	335	PHE	6.4
5	E	544	MET	6.4
2	B	539	PHE	6.4
6	F	19	LEU	6.4
4	D	626	PRO	6.4
5	E	551	THR	6.4
5	E	604	ALA	6.4
5	E	642	LEU	6.4
6	F	404	VAL	6.4
4	D	264	CYS	6.4
5	E	215	SER	6.4
7	H	159	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
8	L	7	MET	6.3
4	D	224	ILE	6.3
6	F	188	ILE	6.3
4	D	261	ALA	6.3
4	D	645	ALA	6.3
7	H	140	ALA	6.3
6	F	220	ASN	6.3
6	F	99	TYR	6.2
3	C	324	ASP	6.2
6	F	164	GLU	6.2
2	B	352	ASP	6.2
5	E	756	GLN	6.2
5	E	738	ARG	6.2
1	A	9	ASN	6.2
8	L	73	ASP	6.2
5	E	623	LEU	6.1
4	D	105	SER	6.1
6	F	47	GLY	6.1
3	C	323	GLY	6.1
4	D	56	GLN	6.1
7	H	237	CYS	6.1
4	D	733	LYS	6.1
2	B	194	GLU	6.1
6	F	163	ARG	6.1
4	D	620	MET	6.1
5	E	515	GLY	6.1
6	F	394	ILE	6.0
5	E	214	ARG	6.0
5	E	91	LYS	6.0
5	E	744	VAL	6.0
6	F	234	GLN	6.0
4	D	285	VAL	6.0
4	D	540	THR	6.0
4	D	738	LYS	6.0
5	E	638	VAL	6.0
2	B	493	PHE	6.0
6	F	332	ALA	6.0
6	F	69	GLU	6.0
4	D	717	ASP	6.0
2	B	389	THR	6.0
5	E	999	CYS	6.0
5	E	549	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
8	L	66	SER	6.0
8	L	163	GLN	5.9
4	D	692	ILE	5.9
5	E	814	THR	5.9
5	E	659	TYR	5.9
4	D	462	ALA	5.9
4	D	260	GLN	5.9
4	D	212	ILE	5.9
8	L	63	SER	5.9
4	D	628	ALA	5.9
4	D	671	LEU	5.9
4	D	741	GLN	5.9
5	E	876	LEU	5.8
5	E	509	TYR	5.8
2	B	643	ILE	5.8
4	D	413	ASP	5.8
7	H	215	GLY	5.8
1	A	85	GLU	5.8
2	B	496	CYS	5.8
3	C	343	SER	5.8
3	C	173	TRP	5.7
5	E	1028	THR	5.7
4	D	689	ALA	5.7
4	D	742	ALA	5.7
4	D	618	ASN	5.7
5	E	1001	LEU	5.7
2	B	554	SER	5.7
6	F	433	ALA	5.7
2	B	575	SER	5.6
3	C	223	SER	5.6
4	D	624	LEU	5.6
5	E	844	CYS	5.6
5	E	1003	VAL	5.6
4	D	164	ASP	5.6
4	D	582	GLU	5.6
1	A	203	HIS	5.6
1	A	220	SER	5.6
5	E	683	SER	5.6
2	B	267	CYS	5.5
2	B	546	ASP	5.5
8	L	77	THR	5.5
5	E	593	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
8	L	20	ASP	5.5
6	F	61	ASN	5.5
5	E	399	THR	5.5
6	F	413	ILE	5.5
4	D	310	VAL	5.5
4	D	456	SER	5.5
2	B	280	GLU	5.4
3	C	196	ARG	5.4
7	H	83	SER	5.4
6	F	185	TYR	5.4
4	D	719	SER	5.4
2	B	529	ASN	5.4
5	E	711	ASN	5.4
5	E	1000	TYR	5.4
4	D	378	SER	5.4
7	H	151	THR	5.4
6	F	184	ILE	5.4
4	D	99	ASP	5.4
5	E	558	LEU	5.4
4	D	181	VAL	5.3
6	F	88	ASP	5.3
5	E	741	LEU	5.3
3	C	117	ALA	5.3
5	E	100	ALA	5.3
1	A	128	VAL	5.3
4	D	284	ALA	5.3
4	D	270	LEU	5.3
5	E	1004	ILE	5.3
8	L	100	THR	5.3
3	C	182	LYS	5.2
3	C	338	GLU	5.2
5	E	149	TRP	5.2
5	E	901	ARG	5.2
4	D	649	LEU	5.2
6	F	357	SER	5.2
4	D	667	VAL	5.2
5	E	979	GLU	5.2
6	F	14	LYS	5.2
1	A	30	ASP	5.2
3	C	154	MET	5.2
4	D	98	LEU	5.2
4	D	695	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
6	F	430	PRO	5.2
5	E	640	PHE	5.2
4	D	737	PHE	5.1
6	F	150	SER	5.1
2	B	464	ARG	5.1
4	D	170	ASN	5.1
5	E	655	LEU	5.1
5	E	141	SER	5.1
4	D	505	ALA	5.1
2	B	169	SER	5.1
5	E	151	HIS	5.1
2	B	171	VAL	5.1
4	D	631	SER	5.0
5	E	908	LEU	5.0
4	D	336	LEU	5.0
7	H	216	LEU	5.0
8	L	133	ALA	5.0
4	D	313	LEU	5.0
5	E	265	SER	5.0
2	B	264	GLU	5.0
1	A	238	ASN	5.0
5	E	633	VAL	5.0
5	E	592	LYS	5.0
5	E	557	CYS	5.0
6	F	412	LEU	5.0
4	D	88	TYR	5.0
5	E	272	LYS	5.0
2	B	374	LYS	5.0
8	L	99	ILE	4.9
4	D	735	LEU	4.9
6	F	439	SER	4.9
1	A	178	ALA	4.9
2	B	474	ALA	4.9
1	A	115	LEU	4.9
1	A	265	SER	4.9
2	B	472	ASP	4.9
5	E	726	SER	4.9
7	H	185	ASP	4.9
5	E	545	THR	4.9
5	E	559	GLU	4.9
1	A	125	VAL	4.9
5	E	665	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
5	E	765	PHE	4.9
4	D	669	LYS	4.9
5	E	140	SER	4.9
5	E	761	ALA	4.9
2	B	497	PHE	4.9
4	D	86	ASP	4.9
3	C	226	ARG	4.9
7	H	93	ARG	4.9
1	A	98	HIS	4.8
5	E	86	ASP	4.8
5	E	71	HIS	4.8
7	H	188	PRO	4.8
3	C	80	THR	4.8
4	D	82	ILE	4.8
5	E	64	ASN	4.8
5	E	770	PHE	4.8
8	L	93	GLN	4.8
2	B	571	ALA	4.8
4	D	516	ASN	4.8
1	A	123	GLY	4.8
3	C	103	THR	4.8
5	E	514	ASN	4.8
1	A	237	ASP	4.8
5	E	208	LEU	4.8
4	D	662	TYR	4.7
8	L	34	SER	4.7
5	E	690	VAL	4.7
4	D	95	ILE	4.7
6	F	364	GLU	4.7
5	E	577	PHE	4.7
1	A	117	LEU	4.7
2	B	409	ASP	4.7
4	D	691	VAL	4.7
5	E	589	ASN	4.7
2	B	709	THR	4.7
3	C	181	GLU	4.7
7	H	152	VAL	4.7
5	E	528	ILE	4.7
5	E	634	LEU	4.7
3	C	199	ASP	4.7
5	E	630	THR	4.7
2	B	195	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
6	F	93	GLU	4.7
4	D	210	ASN	4.6
5	E	261	SER	4.6
6	F	192	ALA	4.6
4	D	665	LEU	4.6
6	F	187	LEU	4.6
6	F	379	ILE	4.6
7	H	125	THR	4.6
5	E	204	TYR	4.6
3	C	306	GLU	4.6
1	A	256	VAL	4.6
6	F	359	ILE	4.6
2	B	591	GLU	4.6
4	D	317	PHE	4.6
5	E	219	ASP	4.6
8	L	181	THR	4.6
3	C	232	ALA	4.6
3	C	322	ALA	4.6
8	L	36	VAL	4.6
6	F	84	PHE	4.6
3	C	137	TYR	4.5
4	D	254	LEU	4.5
3	C	305	GLY	4.5
3	C	78	ASP	4.5
1	A	175	THR	4.5
2	B	235	TRP	4.5
5	E	669	ARG	4.5
6	F	408	ASP	4.5
8	L	167	THR	4.5
5	E	723	PHE	4.5
6	F	196	ALA	4.5
5	E	635	LEU	4.5
2	B	273	ILE	4.5
5	E	408	PHE	4.5
6	F	282	TRP	4.5
5	E	184	LEU	4.5
6	F	348	ALA	4.5
3	C	225	GLY	4.5
8	L	38	TRP	4.5
4	D	542	LEU	4.4
5	E	953	LEU	4.4
4	D	289	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
4	D	346	ILE	4.4
8	L	5	ILE	4.4
2	B	253	ASN	4.4
2	B	490	HIS	4.4
4	D	235	ALA	4.4
3	C	201	LYS	4.4
4	D	257	LEU	4.4
6	F	350	VAL	4.4
2	B	209	PRO	4.4
1	A	72	SER	4.4
4	D	325	SER	4.4
4	D	619	SER	4.4
6	F	122	VAL	4.4
6	F	181	PHE	4.4
4	D	504	ILE	4.4
4	D	238	LYS	4.4
6	F	212	LEU	4.4
3	C	26	THR	4.4
2	B	380	PHE	4.4
5	E	950	SER	4.3
5	E	66	GLU	4.3
2	B	492	LEU	4.3
6	F	351	ILE	4.3
5	E	238	THR	4.3
7	H	178	ALA	4.3
5	E	742	GLU	4.3
4	D	385	ASP	4.3
5	E	199	PHE	4.3
6	F	189	LEU	4.3
6	F	64	SER	4.3
5	E	644	THR	4.3
3	C	191	ALA	4.3
2	B	242	PHE	4.3
5	E	54	SER	4.3
2	B	655	ALA	4.3
3	C	243	PHE	4.3
4	D	273	TYR	4.3
4	D	641	ASP	4.3
5	E	14	TYR	4.3
5	E	53	GLY	4.3
3	C	59	VAL	4.2
8	L	199	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
4	D	223	TYR	4.2
5	E	652	SER	4.2
7	H	38	VAL	4.2
1	A	218	LEU	4.2
1	A	215	THR	4.2
8	L	127	GLN	4.2
8	L	180	SER	4.2
2	B	417	ASP	4.2
4	D	57	PRO	4.2
3	C	330	LEU	4.2
4	D	531	LEU	4.2
5	E	404	VAL	4.2
2	B	658	CYS	4.2
5	E	532	PHE	4.2
4	D	707	SER	4.2
5	E	839	GLU	4.2
7	H	109	MET	4.2
6	F	249	SER	4.2
2	B	598	ILE	4.2
4	D	87	LYS	4.2
2	B	461	ASN	4.2
6	F	146	ASN	4.2
5	E	825	TYR	4.2
4	D	519	ILE	4.1
5	E	718	SER	4.1
8	L	57	LEU	4.1
5	E	24	VAL	4.1
6	F	285	ASP	4.1
1	A	219	ARG	4.1
5	E	648	GLY	4.1
6	F	193	ILE	4.1
6	F	360	HIS	4.1
1	A	90	SER	4.1
5	E	411	LEU	4.1
5	E	923	LEU	4.1
5	E	810	ASP	4.1
4	D	670	PHE	4.1
7	H	42	GLY	4.1
6	F	260	GLU	4.1
2	B	495	SER	4.1
2	B	574	THR	4.1
3	C	233	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	127	VAL	4.1
2	B	424	GLN	4.0
1	A	121	SER	4.0
4	D	184	CYS	4.0
4	D	278	CYS	4.0
6	F	388	ILE	4.0
5	E	982	TYR	4.0
1	A	243	TRP	4.0
5	E	680	LEU	4.0
5	E	737	ILE	4.0
2	B	429	ASN	4.0
8	L	195	TYR	4.0
4	D	518	ASP	4.0
6	F	425	LEU	4.0
5	E	529	SER	4.0
4	D	106	ALA	4.0
5	E	613	ILE	4.0
6	F	208	ILE	4.0
4	D	507	LEU	4.0
4	D	621	ARG	4.0
2	B	489	GLY	4.0
2	B	528	LEU	4.0
3	C	304	ASN	4.0
6	F	395	CYS	4.0
5	E	766	SER	4.0
4	D	253	VAL	4.0
7	H	208	PRO	4.0
4	D	696	GLU	3.9
2	B	190	TYR	3.9
2	B	436	TYR	3.9
3	C	231	ILE	3.9
2	B	184	PHE	3.9
2	B	378	SER	3.9
2	B	221	ALA	3.9
2	B	494	VAL	3.9
5	E	260	VAL	3.9
3	C	298	SER	3.9
4	D	411	SER	3.9
6	F	174	LYS	3.9
2	B	292	ILE	3.9
6	F	431	ILE	3.9
2	B	376	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
5	E	567	LEU	3.9
5	E	1002	MET	3.9
5	E	385	SER	3.9
3	C	235	CYS	3.9
6	F	183	TYR	3.9
5	E	649	GLN	3.9
7	H	219	LEU	3.9
3	C	200	GLY	3.9
2	B	452	TRP	3.9
4	D	715	GLU	3.9
8	L	119	PHE	3.9
3	C	345	ILE	3.9
2	B	288	SER	3.9
3	C	242	ILE	3.8
3	C	68	TYR	3.8
4	D	161	ARG	3.8
4	D	727	LEU	3.8
6	F	386	LEU	3.8
4	D	596	SER	3.8
5	E	400	LYS	3.8
7	H	73	TRP	3.8
8	L	26	CYS	3.8
4	D	111	LEU	3.8
4	D	481	LEU	3.8
4	D	661	HIS	3.8
4	D	286	SER	3.8
1	A	134	GLY	3.8
4	D	699	TRP	3.8
4	D	104	PHE	3.8
4	D	640	GLU	3.8
5	E	965	TYR	3.8
2	B	543	ALA	3.8
3	C	25	ALA	3.8
2	B	533	ILE	3.8
6	F	165	ASN	3.8
1	A	247	LEU	3.8
2	B	662	SER	3.8
4	D	622	GLN	3.8
1	A	64	PRO	3.8
1	A	135	THR	3.8
5	E	540	LEU	3.8
6	F	328	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
4	D	96	PRO	3.8
8	L	54	ALA	3.8
3	C	192	ILE	3.8
5	E	929	HIS	3.8
1	A	217	LEU	3.8
5	E	586	LEU	3.8
4	D	535	ALA	3.7
5	E	447	GLU	3.7
8	L	65	PHE	3.7
6	F	48	GLN	3.7
4	D	414	SER	3.7
8	L	134	SER	3.7
6	F	263	ILE	3.7
2	B	587	VAL	3.7
5	E	157	ASP	3.7
5	E	554	PHE	3.7
4	D	107	TYR	3.7
1	A	25	ALA	3.7
2	B	432	THR	3.7
3	C	151	THR	3.7
5	E	223	VAL	3.7
5	E	582	VAL	3.7
5	E	821	HIS	3.7
3	C	237	ASP	3.7
4	D	393	PRO	3.7
1	A	213	SER	3.7
4	D	534	ILE	3.7
8	L	75	THR	3.7
1	A	229	ARG	3.7
5	E	512	THR	3.7
2	B	450	PHE	3.7
6	F	345	VAL	3.7
4	D	478	ASP	3.7
6	F	211	ILE	3.7
3	C	100	LYS	3.7
2	B	162	THR	3.7
2	B	470	THR	3.7
3	C	208	LEU	3.7
4	D	666	LEU	3.7
2	B	272	TRP	3.7
5	E	439	ASP	3.7
5	E	904	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	266	GLY	3.6
4	D	476	LEU	3.6
8	L	104	GLY	3.6
6	F	54	ALA	3.6
4	D	664	VAL	3.6
1	A	29	SER	3.6
2	B	216	LEU	3.6
5	E	588	ASN	3.6
6	F	178	HIS	3.6
6	F	186	GLU	3.6
1	A	86	ASN	3.6
3	C	315	THR	3.6
6	F	97	HIS	3.6
4	D	65	MET	3.6
3	C	224	ILE	3.6
2	B	289	SER	3.6
5	E	548	GLU	3.6
5	E	709	VAL	3.6
6	F	286	LEU	3.6
3	C	197	GLY	3.6
4	D	544	ASN	3.6
5	E	874	ASN	3.6
2	B	318	HIS	3.6
2	B	185	LEU	3.6
2	B	531	LEU	3.6
4	D	739	LEU	3.6
3	C	318	ILE	3.6
8	L	78	ILE	3.6
4	D	603	ASP	3.6
4	D	314	SER	3.6
5	E	164	HIS	3.6
5	E	620	HIS	3.6
6	F	44	SER	3.6
5	E	617	GLU	3.6
1	A	205	ASP	3.5
3	C	180	PRO	3.5
6	F	264	TYR	3.5
5	E	827	GLN	3.5
5	E	26	LEU	3.5
5	E	303	LEU	3.5
1	A	69	ILE	3.5
8	L	162	SER	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	227	TRP	3.5
7	H	113	ARG	3.5
8	L	64	ARG	3.5
4	D	389	ASP	3.5
1	A	184	ILE	3.5
2	B	250	LYS	3.5
4	D	688	VAL	3.5
5	E	387	VAL	3.5
4	D	151	ILE	3.5
6	F	397	ASP	3.5
6	F	75	TRP	3.5
5	E	666	ASN	3.5
5	E	719	PHE	3.5
5	E	475	CYS	3.5
1	A	221	TYR	3.5
4	D	90	LEU	3.4
2	B	243	ASP	3.4
5	E	412	LYS	3.4
1	A	101	SER	3.4
1	A	263	SER	3.4
2	B	364	GLY	3.4
5	E	609	GLY	3.4
3	C	49	ASP	3.4
5	E	852	SER	3.4
6	F	266	TYR	3.4
4	D	424	CYS	3.4
2	B	252	ASP	3.4
8	L	37	ALA	3.4
3	C	104	LEU	3.4
8	L	205	SER	3.4
5	E	522	ASN	3.4
6	F	331	VAL	3.4
6	F	243	TRP	3.4
4	D	150	ALA	3.4
5	E	388	ASP	3.4
4	D	632	GLN	3.4
4	D	672	TYR	3.4
8	L	10	SER	3.4
5	E	162	VAL	3.4
5	E	998	LYS	3.4
4	D	236	GLY	3.4
6	F	191	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	306	TRP	3.4
1	A	155	PRO	3.4
6	F	336	PRO	3.4
7	H	142	ASP	3.4
1	A	212	TRP	3.4
4	D	83	THR	3.4
4	D	178	SER	3.3
5	E	674	LEU	3.3
4	D	690	THR	3.3
6	F	138	ASN	3.3
5	E	137	PHE	3.3
5	E	420	PHE	3.3
2	B	569	GLU	3.3
2	B	596	ARG	3.3
6	F	152	GLY	3.3
2	B	457	THR	3.3
1	A	144	HIS	3.3
4	D	647	ARG	3.3
5	E	510	LEU	3.3
4	D	740	CYS	3.3
6	F	190	ALA	3.3
6	F	316	PRO	3.3
5	E	300	MET	3.3
5	E	458	ASN	3.3
7	H	92	GLY	3.3
7	H	75	ALA	3.3
1	A	268	VAL	3.3
3	C	48	SER	3.3
3	C	76	SER	3.3
4	D	492	SER	3.3
2	B	391	CYS	3.3
4	D	358	CYS	3.3
5	E	722	THR	3.3
2	B	163	LYS	3.3
4	D	584	GLN	3.3
1	A	154	ALA	3.3
2	B	538	ILE	3.3
5	E	960	CYS	3.2
5	E	849	ALA	3.2
6	F	389	VAL	3.2
7	H	183	VAL	3.2
2	B	211	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	625	ILE	3.2
2	B	392	TYR	3.2
5	E	143	ASN	3.2
4	D	353	TRP	3.2
3	C	10	ASP	3.2
3	C	186	SER	3.2
8	L	53	SER	3.2
8	L	206	SER	3.2
6	F	315	LEU	3.2
3	C	63	TRP	3.2
5	E	313	TYR	3.2
6	F	384	TYR	3.2
3	C	110	SER	3.2
4	D	329	ARG	3.2
5	E	138	LEU	3.2
5	E	273	VAL	3.2
4	D	243	GLN	3.2
3	C	45	TRP	3.2
4	D	291	LEU	3.2
1	A	136	THR	3.2
4	D	230	VAL	3.2
4	D	529	TRP	3.2
5	E	145	LEU	3.2
7	H	124	ARG	3.2
8	L	23	THR	3.2
8	L	80	SER	3.2
1	A	267	ASN	3.2
2	B	451	CYS	3.2
4	D	62	GLY	3.2
4	D	360	PHE	3.2
3	C	185	VAL	3.2
4	D	503	VAL	3.2
7	H	209	ALA	3.2
4	D	268	SER	3.1
5	E	911	GLU	3.1
2	B	222	LEU	3.1
2	B	548	TYR	3.1
5	E	552	ASP	3.1
3	C	346	THR	3.1
2	B	394	GLN	3.1
1	A	248	LEU	3.1
8	L	189	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	305	VAL	3.1
7	H	181	CYS	3.1
2	B	269	LEU	3.1
4	D	652	LEU	3.1
2	B	449	GLN	3.1
2	B	423	PHE	3.1
3	C	119	ALA	3.1
6	F	341	HIS	3.1
5	E	229	PHE	3.1
2	B	247	TYR	3.1
3	C	24	VAL	3.1
1	A	234	TRP	3.1
3	C	313	ASN	3.1
4	D	736	ASN	3.1
2	B	664	GLU	3.1
5	E	85	SER	3.1
5	E	534	ASP	3.1
5	E	997	ARG	3.1
7	H	74	VAL	3.1
1	A	287	GLY	3.1
6	F	428	ASN	3.1
2	B	390	LEU	3.1
6	F	176	GLU	3.1
6	F	312	GLU	3.1
2	B	214	SER	3.1
3	C	176	SER	3.1
1	A	216	VAL	3.1
2	B	500	ASP	3.0
5	E	183	LEU	3.0
7	H	43	SER	3.0
4	D	158	PHE	3.0
5	E	762	MET	3.0
4	D	152	LEU	3.0
2	B	330	ASP	3.0
5	E	25	ASP	3.0
5	E	144	THR	3.0
5	E	773	SER	3.0
4	D	729	LYS	3.0
5	E	869	HIS	3.0
6	F	365	MET	3.0
5	E	134	PRO	3.0
2	B	491	SER	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	331	TRP	3.0
6	F	160	PHE	3.0
7	H	252	VAL	3.0
5	E	626	HIS	3.0
5	E	828	LEU	3.0
4	D	347	LEU	3.0
6	F	419	LEU	3.0
7	H	211	LEU	3.0
7	H	41	GLY	3.0
1	A	68	THR	3.0
5	E	948	ILE	3.0
1	A	116	LEU	3.0
3	C	17	TYR	3.0
2	B	469	GLU	3.0
1	A	206	TRP	3.0
2	B	512	VAL	3.0
3	C	344	VAL	3.0
5	E	576	SER	3.0
6	F	151	GLY	3.0
3	C	67	GLU	3.0
4	D	103	GLU	3.0
4	D	506	GLU	3.0
7	H	50	ALA	3.0
7	H	207	PHE	3.0
5	E	337	THR	2.9
8	L	70	SER	2.9
5	E	562	PHE	2.9
7	H	187	PHE	2.9
5	E	903	ASN	2.9
2	B	369	GLY	2.9
3	C	132	GLY	2.9
4	D	81	PHE	2.9
8	L	90	TYR	2.9
1	A	182	VAL	2.9
4	D	339	ILE	2.9
5	E	124	LYS	2.9
2	B	425	LEU	2.9
7	H	110	ASN	2.9
5	E	507	PHE	2.9
1	A	214	PRO	2.9
2	B	268	ARG	2.9
3	C	6	SER	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	651	LEU	2.9
5	E	1007	LEU	2.9
5	E	578	ASP	2.9
5	E	887	ASP	2.9
6	F	194	ASP	2.9
2	B	456	GLN	2.9
5	E	350	ASN	2.9
5	E	474	ASN	2.9
5	E	632	GLN	2.9
2	B	245	VAL	2.9
2	B	556	VAL	2.9
5	E	235	ILE	2.9
3	C	317	THR	2.9
1	A	251	GLU	2.9
4	D	592	ASN	2.9
1	A	273	GLY	2.9
4	D	326	GLY	2.9
7	H	120	TYR	2.9
1	A	272	SER	2.9
5	E	822	SER	2.9
5	E	824	PHE	2.9
6	F	180	PHE	2.9
4	D	155	LEU	2.9
5	E	287	LEU	2.9
4	D	349	TYR	2.8
1	A	156	ALA	2.8
4	D	287	ASP	2.8
6	F	436	LEU	2.8
2	B	462	GLY	2.8
8	L	19	GLY	2.8
2	B	212	SER	2.8
4	D	468	SER	2.8
5	E	909	LEU	2.8
6	F	251	SER	2.8
4	D	580	CYS	2.8
5	E	224	ILE	2.8
3	C	44	ASN	2.8
5	E	717	ASN	2.8
1	A	34	LYS	2.8
2	B	544	LEU	2.8
3	C	13	HIS	2.8
4	D	633	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
6	F	442	LEU	2.8
2	B	314	SER	2.8
3	C	234	GLY	2.8
5	E	396	ASP	2.8
6	F	236	GLY	2.8
3	C	102	CYS	2.8
4	D	464	TYR	2.8
5	E	676	ALA	2.8
6	F	270	ALA	2.8
6	F	366	LEU	2.8
1	A	107	TRP	2.8
5	E	546	THR	2.8
5	E	611	THR	2.8
1	A	209	ASP	2.8
1	A	11	LEU	2.8
1	A	133	ASN	2.8
2	B	354	ASN	2.8
4	D	362	LEU	2.8
5	E	103	ASN	2.8
3	C	12	VAL	2.8
4	D	122	ARG	2.8
6	F	247	VAL	2.8
4	D	579	SER	2.8
5	E	716	GLU	2.8
6	F	106	GLU	2.8
5	E	695	TYR	2.8
6	F	177	ASP	2.8
4	D	454	LEU	2.8
4	D	558	ASN	2.8
5	E	319	ILE	2.8
5	E	629	ILE	2.8
1	A	63	HIS	2.8
6	F	214	GLY	2.8
6	F	253	GLN	2.8
5	E	196	PRO	2.8
6	F	136	PRO	2.8
2	B	263	LYS	2.7
2	B	488	HIS	2.7
5	E	606	LYS	2.7
1	A	240	GLN	2.7
6	F	70	LEU	2.7
6	F	207	SER	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	455	PHE	2.7
7	H	163	PHE	2.7
4	D	556	ILE	2.7
5	E	776	ILE	2.7
3	C	228	TYR	2.7
4	D	91	TYR	2.7
7	H	78	TYR	2.7
4	D	520	GLU	2.7
8	L	12	SER	2.7
4	D	166	ASP	2.7
1	A	241	GLY	2.7
3	C	136	LEU	2.7
4	D	359	GLY	2.7
4	D	643	GLY	2.7
8	L	196	ALA	2.7
2	B	368	GLU	2.7
3	C	193	ILE	2.7
2	B	198	VAL	2.7
4	D	523	LEU	2.7
2	B	645	TYR	2.7
5	E	662	PHE	2.7
6	F	259	TYR	2.7
7	H	195	TRP	2.7
8	L	89	TYR	2.7
2	B	422	ILE	2.7
5	E	274	GLU	2.7
6	F	324	VAL	2.7
6	F	280	SER	2.7
2	B	458	LEU	2.7
4	D	648	LEU	2.7
6	F	290	LEU	2.7
3	C	194	TYR	2.7
5	E	298	PHE	2.7
5	E	436	HIS	2.7
5	E	720	PHE	2.7
6	F	161	PRO	2.7
1	A	172	LYS	2.7
2	B	618	GLU	2.7
6	F	222	VAL	2.7
4	D	67	LEU	2.7
2	B	550	GLY	2.7
3	C	316	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
8	L	71	GLY	2.7
5	E	9	ALA	2.7
5	E	230	HIS	2.7
5	E	163	PRO	2.7
5	E	963	LYS	2.7
6	F	140	PRO	2.7
8	L	184	LEU	2.7
3	C	122	GLY	2.7
7	H	213	SER	2.7
2	B	644	PHE	2.7
4	D	80	ALA	2.6
4	D	426	ALA	2.6
6	F	74	PHE	2.7
7	H	87	ALA	2.6
7	H	94	PHE	2.7
4	D	114	ILE	2.6
2	B	570	MET	2.6
6	F	342	PRO	2.6
4	D	78	ASN	2.6
5	E	114	GLU	2.6
5	E	443	LEU	2.6
2	B	467	SER	2.6
2	B	708	CYS	2.6
3	C	36	PHE	2.6
5	E	218	SER	2.6
5	E	664	LEU	2.6
6	F	346	LEU	2.6
8	L	81	LEU	2.6
4	D	54	ASN	2.6
2	B	420	GLY	2.6
2	B	152	ALA	2.6
2	B	503	ALA	2.6
3	C	82	LYS	2.6
3	C	179	SER	2.6
5	E	414	ARG	2.6
1	A	76	ASP	2.6
1	A	122	ASP	2.6
3	C	9	ASP	2.6
3	C	131	ASP	2.6
6	F	110	MET	2.6
1	A	67	GLY	2.6
2	B	502	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	373	LEU	2.6
5	E	189	VAL	2.6
7	H	84	THR	2.6
8	L	183	THR	2.6
3	C	27	CYS	2.6
4	D	482	TRP	2.6
2	B	508	ILE	2.6
4	D	500	LYS	2.6
6	F	121	ILE	2.6
8	L	24	ILE	2.6
5	E	823	ALA	2.6
3	C	11	LEU	2.6
2	B	453	TYR	2.6
6	F	133	MET	2.6
8	L	177	SER	2.6
5	E	1032	ASP	2.6
4	D	477	GLY	2.6
6	F	283	GLU	2.6
5	E	7	ILE	2.6
6	F	314	ILE	2.6
6	F	77	LEU	2.6
6	F	233	THR	2.6
5	E	543	SER	2.6
2	B	483	GLU	2.6
6	F	267	LEU	2.6
4	D	76	TYR	2.6
4	D	387	THR	2.6
6	F	258	PRO	2.6
7	H	160	PRO	2.6
2	B	484	PHE	2.5
2	B	187	ASP	2.5
3	C	138	ASP	2.5
3	C	240	ILE	2.5
5	E	538	GLY	2.5
5	E	616	LEU	2.5
5	E	931	ASP	2.5
2	B	663	GLN	2.5
1	A	112	TYR	2.5
4	D	112	PHE	2.5
7	H	229	SER	2.5
3	C	35	VAL	2.5
3	C	205	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	545	LYS	2.5
5	E	113	VAL	2.5
6	F	241	SER	2.5
1	A	71	ALA	2.5
2	B	588	GLN	2.5
5	E	708	ASN	2.5
6	F	250	LEU	2.5
5	E	888	VAL	2.5
5	E	1026	THR	2.5
5	E	946	ASP	2.5
2	B	665	ILE	2.5
4	D	397	ILE	2.5
6	F	119	ILE	2.5
3	C	342	MET	2.5
6	F	347	MET	2.5
7	H	177	ALA	2.5
8	L	192	HIS	2.5
6	F	195	GLU	2.5
5	E	564	ILE	2.5
6	F	400	ASN	2.5
5	E	80	THR	2.5
6	F	141	THR	2.5
4	D	570	SER	2.5
5	E	1008	SER	2.5
1	A	130	PHE	2.5
1	A	271	LEU	2.5
3	C	92	GLU	2.5
5	E	811	LEU	2.5
7	H	189	GLU	2.5
8	L	128	LEU	2.5
1	A	82	TRP	2.5
3	C	187	ALA	2.5
1	A	52	HIS	2.5
2	B	218	PHE	2.4
4	D	58	ILE	2.4
4	D	363	TYR	2.4
5	E	397	ILE	2.4
5	E	733	SER	2.4
4	D	197	VAL	2.4
8	L	153	VAL	2.4
5	E	202	ASN	2.4
6	F	82	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	139	PHE	2.4
7	H	241	HIS	2.4
5	E	417	THR	2.4
4	D	77	GLN	2.4
5	E	299	GLN	2.4
6	F	56	SER	2.4
7	H	39	GLN	2.4
8	L	103	GLN	2.4
4	D	79	MET	2.4
5	E	402	GLY	2.4
4	D	490	ALA	2.4
5	E	891	LEU	2.4
6	F	205	ASN	2.4
4	D	489	ILE	2.4
4	D	374	TYR	2.4
2	B	203	ARG	2.4
4	D	376	GLN	2.4
6	F	118	GLN	2.4
7	H	117	THR	2.4
5	E	20	PRO	2.4
2	B	191	LEU	2.4
3	C	30	ASP	2.4
3	C	39	ASP	2.4
4	D	610	ASP	2.4
4	D	728	LEU	2.4
6	F	385	LEU	2.4
6	F	435	PHE	2.4
2	B	387	ASN	2.4
5	E	490	VAL	2.4
2	B	213	GLU	2.4
4	D	52	THR	2.4
5	E	603	SER	2.4
4	D	72	GLY	2.4
6	F	392	LEU	2.4
1	A	143	ALA	2.4
6	F	125	TRP	2.4
5	E	288	VAL	2.4
5	E	755	VAL	2.4
2	B	225	MET	2.4
6	F	405	GLU	2.4
2	B	234	LEU	2.4
2	B	363	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	446	LEU	2.4
2	B	519	LEU	2.4
4	D	340	GLY	2.4
4	D	557	ALA	2.4
2	B	398	TYR	2.4
2	B	421	VAL	2.4
2	B	439	VAL	2.4
5	E	27	TYR	2.4
4	D	673	PRO	2.4
2	B	282	GLU	2.4
2	B	433	GLU	2.4
2	B	435	LEU	2.4
5	E	1030	LEU	2.4
4	D	725	ALA	2.4
4	D	743	PHE	2.4
5	E	69	CYS	2.4
4	D	686	ASP	2.4
4	D	295	TYR	2.4
2	B	590	ASN	2.4
5	E	698	LEU	2.4
8	L	50	LEU	2.4
7	H	40	PRO	2.3
3	C	184	ALA	2.3
3	C	339	PHE	2.3
4	D	593	ALA	2.3
7	H	118	ALA	2.3
8	L	105	THR	2.3
8	L	179	SER	2.3
3	C	239	ARG	2.3
7	H	150	VAL	2.3
2	B	319	LEU	2.3
6	F	197	LEU	2.3
5	E	132	GLN	2.3
4	D	109	SER	2.3
5	E	28	VAL	2.3
2	B	437	LYS	2.3
1	A	194	TYR	2.3
6	F	219	LEU	2.3
1	A	292	ALA	2.3
4	D	373	GLU	2.3
5	E	94	ASN	2.3
5	E	928	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	691	LYS	2.3
1	A	137	SER	2.3
5	E	663	LEU	2.3
4	D	55	ASP	2.3
5	E	122	ILE	2.3
6	F	213	CYS	2.3
7	H	180	GLY	2.3
4	D	718	LYS	2.3
3	C	246	THR	2.3
7	H	86	TYR	2.3
4	D	205	ILE	2.3
5	E	365	ILE	2.3
5	E	535	ILE	2.3
2	B	96	GLN	2.3
2	B	309	LYS	2.3
5	E	1033	GLU	2.3
4	D	642	TRP	2.3
5	E	519	THR	2.3
6	F	144	TRP	2.3
4	D	115	TYR	2.3
6	F	60	SER	2.3
4	D	204	PHE	2.3
2	B	192	ASP	2.3
3	C	328	VAL	2.3
5	E	386	LEU	2.3
6	F	245	ARG	2.3
4	D	711	GLU	2.3
5	E	148	GLU	2.3
6	F	423	GLN	2.3
2	B	558	ASN	2.3
5	E	81	PHE	2.3
1	A	109	PRO	2.3
1	A	114	PRO	2.3
6	F	318	PRO	2.3
3	C	156	VAL	2.3
7	H	222	VAL	2.3
2	B	201	GLU	2.2
6	F	166	THR	2.2
2	B	328	SER	2.2
2	B	372	SER	2.2
6	F	101	SER	2.2
1	A	62	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	142	ALA	2.2
6	F	158	LEU	2.2
6	F	317	LEU	2.2
2	B	287	ASN	2.2
5	E	245	ILE	2.2
5	E	477	GLN	2.2
4	D	471	PHE	2.2
6	F	159	ASP	2.2
6	F	281	ASP	2.2
7	H	108	GLN	2.2
4	D	486	ILE	2.2
1	A	49	LEU	2.2
5	E	446	LEU	2.2
7	H	55	VAL	2.2
8	L	67	GLY	2.2
2	B	182	ARG	2.2
2	B	275	SER	2.2
3	C	321	SER	2.2
6	F	311	ASP	2.2
6	F	353	ASP	2.2
5	E	667	LEU	2.2
4	D	595	VAL	2.2
5	E	759	MET	2.2
6	F	254	ALA	2.2
4	D	100	THR	2.2
8	L	200	THR	2.2
4	D	415	CYS	2.2
5	E	390	GLN	2.2
2	B	397	GLU	2.2
5	E	884	GLU	2.2
6	F	327	VAL	2.2
5	E	416	GLY	2.2
7	H	246	THR	2.2
1	A	198	SER	2.2
2	B	527	ILE	2.2
6	F	209	CYS	2.2
6	F	409	LYS	2.2
4	D	457	TYR	2.2
6	F	252	GLN	2.2
1	A	157	THR	2.2
2	B	367	PHE	2.2
6	F	105	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	154	LYS	2.2
6	F	298	ILE	2.2
2	B	232	TYR	2.2
5	E	241	CYS	2.2
4	D	66	PRO	2.1
6	F	257	ASP	2.1
7	H	174	GLY	2.1
3	C	215	ILE	2.1
4	D	510	HIS	2.1
5	E	678	VAL	2.1
5	E	983	GLN	2.1
7	H	235	TYR	2.1
2	B	541	ALA	2.1
4	D	508	LEU	2.1
6	F	104	LEU	2.1
2	B	431	ASN	2.1
5	E	1031	ARG	2.1
5	E	117	LEU	2.1
5	E	533	LEU	2.1
2	B	589	ASN	2.1
2	B	659	ASN	2.1
8	L	140	ASN	2.1
5	E	501	THR	2.1
5	E	591	MET	2.1
1	A	261	SER	2.1
2	B	639	SER	2.1
1	A	108	ALA	2.1
2	B	386	LEU	2.1
2	B	454	LEU	2.1
4	D	501	LYS	2.1
2	B	612	VAL	2.1
7	H	64	ARG	2.1
6	F	246	THR	2.1
4	D	89	LYS	2.1
4	D	488	LEU	2.1
4	D	575	LEU	2.1
1	A	81	ILE	2.1
2	B	476	PHE	2.1
6	F	284	SER	2.1
3	C	175	PRO	2.1
1	A	222	LEU	2.1
5	E	58	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	119	GLY	2.1
5	E	427	LEU	2.1
3	C	58	ILE	2.1
4	D	470	ALA	2.1
4	D	553	ILE	2.1
5	E	569	ILE	2.1
3	C	15	VAL	2.1
3	C	81	VAL	2.1
2	B	487	LEU	2.1
3	C	297	LEU	2.1
5	E	226	CYS	2.1
2	B	504	ALA	2.1
2	B	93	TRP	2.1
5	E	169	VAL	2.1
7	H	191	VAL	2.1
2	B	559	LEU	2.0
5	E	442	TYR	2.0
1	A	202	GLY	2.0
3	C	300	HIS	2.0
5	E	871	HIS	2.0
7	H	61	HIS	2.0
8	L	147	ALA	2.0
2	B	499	ASN	2.0
3	C	220	TRP	2.0
5	E	171	PRO	2.0
5	E	391	SER	2.0
1	A	280	LEU	2.0
5	E	366	LEU	2.0
6	F	81	LEU	2.0
4	D	262	ILE	2.0
5	E	758	PHE	2.0
6	F	231	PHE	2.0
4	D	509	PRO	2.0
2	B	555	GLU	2.0
3	C	241	ARG	2.0
4	D	410	GLU	2.0
4	D	541	THR	2.0
5	E	777	PHE	2.0
3	C	129	GLY	2.0
1	A	110	HIS	2.0
5	E	878	HIS	2.0
8	L	43	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	229	GLN	2.0
5	E	246	TRP	2.0
6	F	325	GLN	2.0
5	E	118	LEU	2.0
5	E	349	LEU	2.0
7	H	107	LEU	2.0
2	B	238	SER	2.0
5	E	128	PHE	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.