



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:23 AM UTC

PDB ID : 1AWT / pdb_00001awt
Title : SECYPA COMPLEXED WITH HAGPIA
Authors : Vajdos, F.F.
Deposited on : 1997-10-05
Resolution : 2.55 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

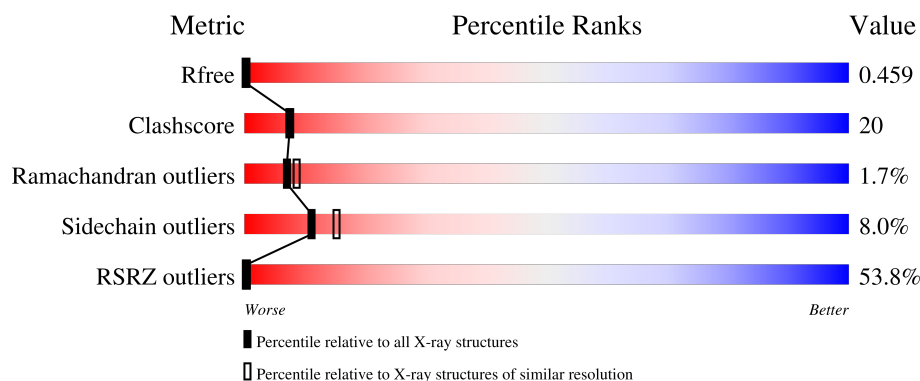
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	164	35% 64% 30% 5%
1	B	164	76% 47% 40% 13% .
1	C	164	48% 59% 37% .
1	D	164	52% 53% 41% 5% .
1	E	164	34% 69% 28% .

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Mol	Chain	Length	Quality of chain
1	F	164	71% 47% 44% 9%
2	G	6	67% 67% 33%
2	H	6	33% 67% 17% 17%
2	I	6	50% 67% 33%
2	J	6	67% 67% 33%
2	K	6	33% 50% 50%
2	L	6	50% 67% 17% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7963 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 CYCLOPHILIN A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	Se	0	0	0
			1258	797	217	236	4	4			
1	B	164	Total	C	N	O	S	Se	0	0	0
			1258	797	217	236	4	4			
1	C	164	Total	C	N	O	S	Se	0	0	0
			1258	797	217	236	4	4			
1	D	164	Total	C	N	O	S	Se	0	0	0
			1258	797	217	236	4	4			
1	E	164	Total	C	N	O	S	Se	0	0	0
			1258	797	217	236	4	4			
1	F	164	Total	C	N	O	S	Se	0	0	0
			1258	797	217	236	4	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1061	MSE	MET	modified residue	UNP P62937
A	1100	MSE	MET	modified residue	UNP P62937
A	1136	MSE	MET	modified residue	UNP P62937
A	1142	MSE	MET	modified residue	UNP P62937
B	1061	MSE	MET	modified residue	UNP P62937
B	1100	MSE	MET	modified residue	UNP P62937
B	1136	MSE	MET	modified residue	UNP P62937
B	1142	MSE	MET	modified residue	UNP P62937
C	1061	MSE	MET	modified residue	UNP P62937
C	1100	MSE	MET	modified residue	UNP P62937
C	1136	MSE	MET	modified residue	UNP P62937
C	1142	MSE	MET	modified residue	UNP P62937
D	1061	MSE	MET	modified residue	UNP P62937
D	1100	MSE	MET	modified residue	UNP P62937
D	1136	MSE	MET	modified residue	UNP P62937
D	1142	MSE	MET	modified residue	UNP P62937
E	1061	MSE	MET	modified residue	UNP P62937

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1100	MSE	MET	modified residue	UNP P62937
E	1136	MSE	MET	modified residue	UNP P62937
E	1142	MSE	MET	modified residue	UNP P62937
F	1061	MSE	MET	modified residue	UNP P62937
F	1100	MSE	MET	modified residue	UNP P62937
F	1136	MSE	MET	modified residue	UNP P62937
F	1142	MSE	MET	modified residue	UNP P62937

- Molecule 2 is a protein called PEPTIDE FROM THE HIV-1 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	0
			40	25	8	7			
2	H	6	Total	C	N	O	0	0	0
			40	25	8	7			
2	I	6	Total	C	N	O	0	0	0
			40	25	8	7			
2	J	6	Total	C	N	O	0	0	0
			40	25	8	7			
2	K	6	Total	C	N	O	0	0	0
			40	25	8	7			
2	L	6	Total	C	N	O	0	0	0
			40	25	8	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	22	Total	O	0	0
			22	22		
3	C	32	Total	O	0	0
			32	32		
3	D	21	Total	O	0	0
			21	21		
3	E	30	Total	O	0	0
			30	30		
3	F	31	Total	O	0	0
			31	31		
3	G	2	Total	O	0	0
			2	2		
3	H	1	Total	O	0	0
			1	1		

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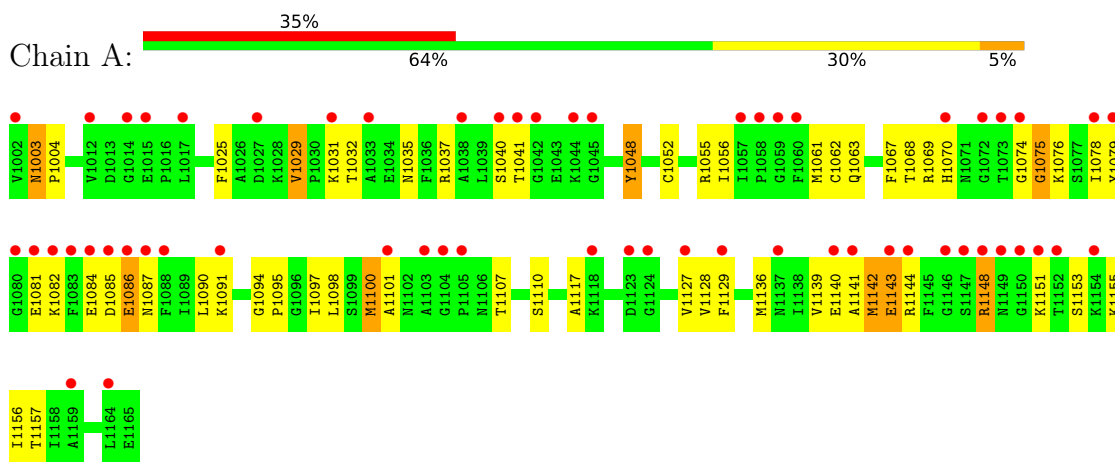
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	O	0	0
			1	1		
3	J	1	Total	O	0	0
			1	1		
3	K	1	Total	O	0	0
			1	1		

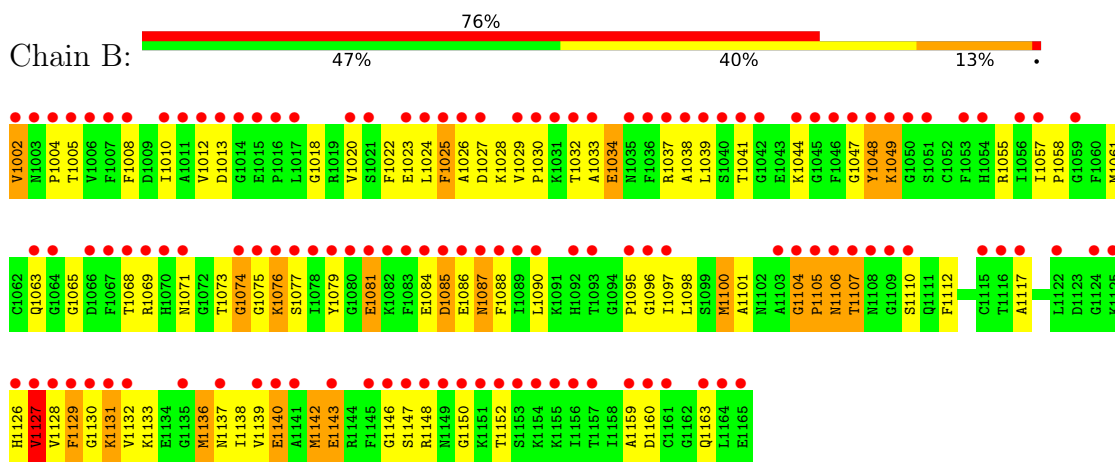
3 Residue-property plots

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.

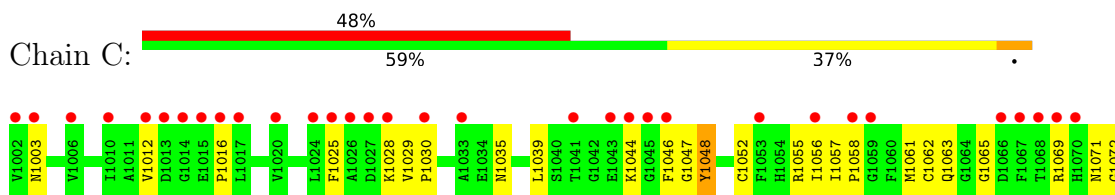
• Molecule 1: CYCLOPHILIN A

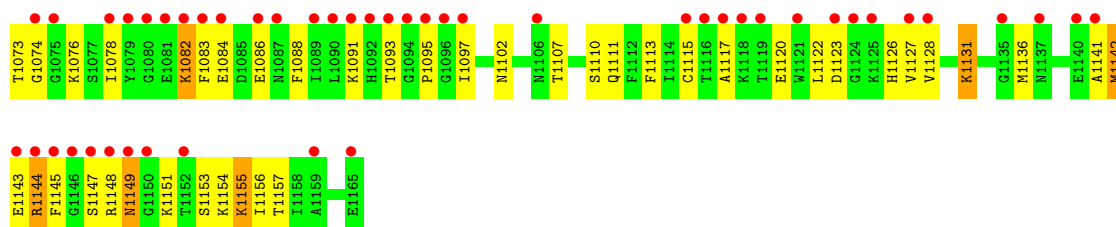


• Molecule 1: CYCLOPHILIN A

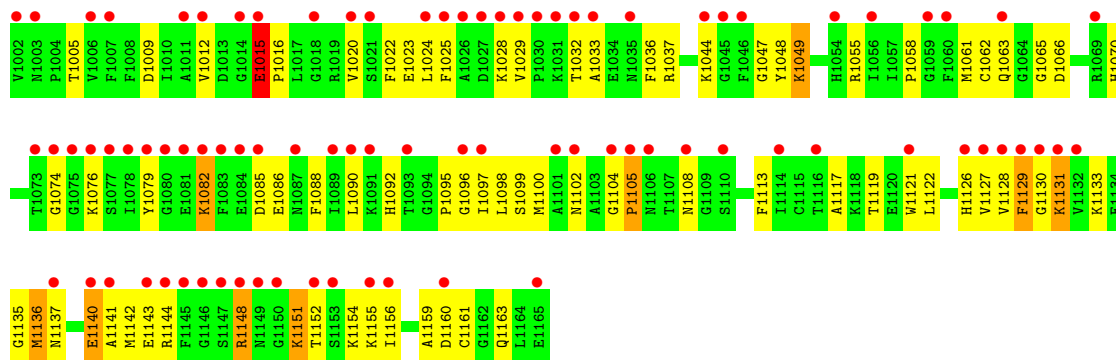


• Molecule 1: CYCLOPHILIN A

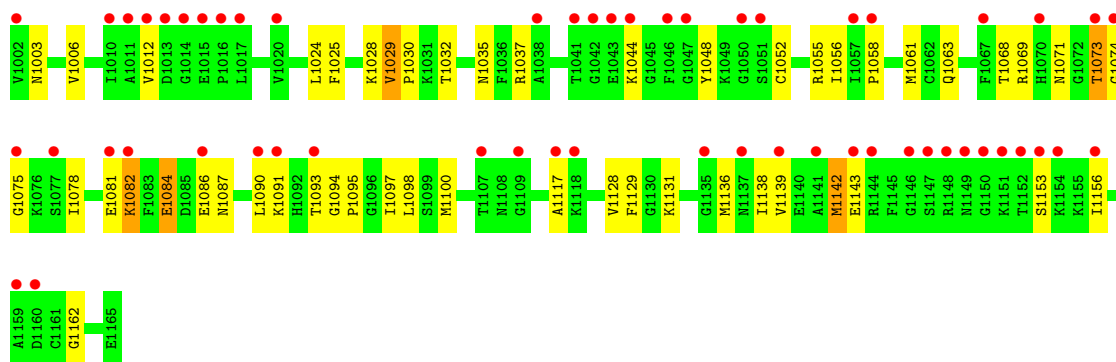




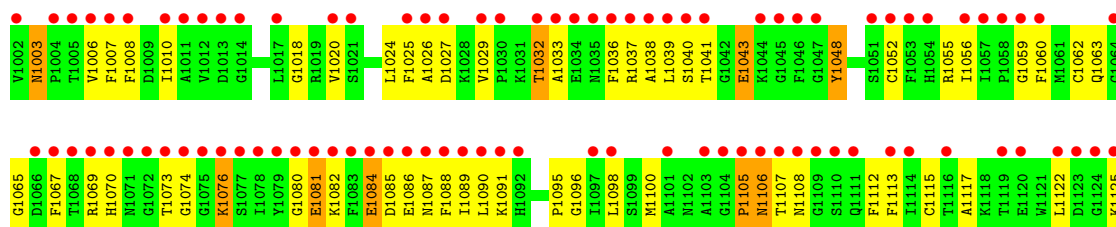
• Molecule 1: CYCLOPHILIN A

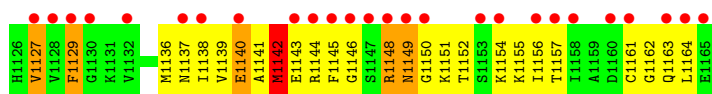


• Molecule 1: CYCLOPHILIN A

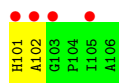


• Molecule 1: CYCLOPHILIN A

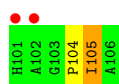




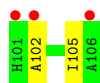
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



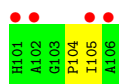
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



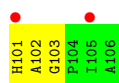
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



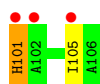
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	73.20Å 73.20Å 189.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.55 15.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.3 (15.00-2.55) 92.8 (15.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.54Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.378 , 0.465 0.384 , 0.459	Depositor DCC
R_{free} test set	1592 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7963	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 84.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5492e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.77	4/1282 (0.3%)	1.12	9/1711 (0.5%)
1	B	0.85	6/1282 (0.5%)	1.06	7/1711 (0.4%)
1	C	0.75	3/1282 (0.2%)	1.04	6/1711 (0.4%)
1	D	0.76	5/1282 (0.4%)	1.11	9/1711 (0.5%)
1	E	0.78	5/1282 (0.4%)	1.05	7/1711 (0.4%)
1	F	0.78	2/1282 (0.2%)	1.11	8/1711 (0.5%)
2	G	0.73	0/41	1.46	0/54
2	H	0.72	0/41	0.95	0/54
2	I	0.98	0/41	1.75	1/54 (1.9%)
2	J	0.86	0/41	1.20	0/54
2	K	0.74	0/41	1.87	3/54 (5.6%)
2	L	0.80	0/41	1.11	0/54
All	All	0.78	25/7938 (0.3%)	1.10	50/10590 (0.5%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1136	MSE	SE-CE	-9.23	1.67	1.95
1	D	1100	MSE	SE-CE	-8.84	1.69	1.95
1	F	1100	MSE	SE-CE	-8.81	1.69	1.95
1	E	1061	MSE	SE-CE	-7.76	1.72	1.95
1	B	1142	MSE	SE-CE	-7.59	1.72	1.95
1	D	1142	MSE	SE-CE	-7.29	1.73	1.95
1	D	1136	MSE	SE-CE	-6.72	1.75	1.95
1	B	1142	MSE	CG-SE	-6.48	1.76	1.95
1	A	1142	MSE	SE-CE	-6.35	1.76	1.95
1	C	1136	MSE	SE-CE	-6.27	1.76	1.95
1	A	1136	MSE	SE-CE	-6.16	1.76	1.95
1	E	1136	MSE	SE-CE	-6.10	1.77	1.95
1	E	1142	MSE	SE-CE	-5.92	1.77	1.95
1	D	1142	MSE	CG-SE	-5.72	1.78	1.95
1	B	1061	MSE	SE-CE	-5.42	1.79	1.95
1	B	1107	THR	CA-CB	5.40	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1061	MSE	CG-SE	-5.38	1.79	1.95
1	C	1142	MSE	SE-CE	-5.34	1.79	1.95
1	A	1061	MSE	CG-SE	-5.23	1.79	1.95
1	D	1061	MSE	SE-CE	-5.21	1.79	1.95
1	C	1061	MSE	SE-CE	-5.20	1.79	1.95
1	E	1100	MSE	SE-CE	-5.14	1.80	1.95
1	F	1142	MSE	CG-SE	-5.08	1.80	1.95
1	A	1100	MSE	SE-CE	-5.06	1.80	1.95
1	B	1100	MSE	SE-CE	-5.06	1.80	1.95

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1003	ASN	CA-C-N	9.72	129.77	119.76
1	F	1003	ASN	C-N-CA	9.72	129.77	119.76
1	D	1104	GLY	CA-C-N	8.45	130.41	119.84
1	D	1104	GLY	C-N-CA	8.45	130.41	119.84
1	B	1104	GLY	CA-C-N	8.41	130.35	119.84
1	B	1104	GLY	C-N-CA	8.41	130.35	119.84
1	B	1048	TYR	N-CA-C	8.17	122.51	112.54
2	I	102	ALA	N-CA-C	7.88	122.63	110.42
1	A	1048	TYR	N-CA-C	7.85	120.92	111.82
1	A	1075	GLY	N-CA-C	-7.60	103.77	112.29
1	F	1084	GLU	N-CA-C	7.54	120.04	110.24
1	F	1048	TYR	N-CA-C	7.38	121.87	113.01
1	B	1047	GLY	N-CA-C	7.38	119.67	111.85
1	E	1003	ASN	CA-C-N	7.30	127.28	119.76
1	E	1003	ASN	C-N-CA	7.30	127.28	119.76
1	F	1043	GLU	N-CA-C	7.30	119.13	111.03
1	A	1003	ASN	CA-C-N	7.14	126.90	119.76
1	A	1003	ASN	C-N-CA	7.14	126.90	119.76
1	D	1047	GLY	N-CA-C	7.09	120.44	110.38
1	D	1015	GLU	N-CA-C	6.87	117.50	109.60
1	B	1074	GLY	N-CA-C	6.64	120.75	112.79
1	D	1015	GLU	CA-C-N	6.63	128.13	119.84
1	D	1015	GLU	C-N-CA	6.63	128.13	119.84
2	K	102	ALA	N-CA-C	6.49	120.87	109.96
1	A	1074	GLY	N-CA-C	6.37	121.70	112.60
1	C	1048	TYR	N-CA-C	6.30	120.70	112.89
1	E	1048	TYR	N-CA-C	6.29	120.22	112.54
1	D	1161	CYS	N-CA-C	6.00	117.66	108.42
2	K	103	GLY	CA-C-N	5.83	127.01	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	103	GLY	C-N-CA	5.83	127.01	120.66
1	D	1061	MSE	N-CA-C	5.73	116.11	108.38
1	C	1003	ASN	CA-C-N	5.65	125.66	119.90
1	C	1003	ASN	C-N-CA	5.65	125.66	119.90
1	F	1003	ASN	N-CA-C	5.64	118.84	110.32
1	D	1074	GLY	N-CA-C	5.53	120.14	112.57
1	C	1047	GLY	N-CA-C	5.45	117.53	110.45
1	A	1084	GLU	N-CA-C	5.37	117.02	110.41
1	A	1094	GLY	CA-C-N	5.30	125.22	119.76
1	A	1094	GLY	C-N-CA	5.30	125.22	119.76
1	E	1139	VAL	N-CA-C	-5.29	104.35	111.44
1	A	1143	GLU	N-CA-C	5.21	117.38	111.02
1	B	1137	ASN	N-CA-C	-5.21	106.43	112.89
1	B	1127	VAL	CB-CA-C	-5.15	105.66	111.23
1	E	1084	GLU	N-CA-C	5.14	118.13	110.52
1	E	1094	GLY	CA-C-N	5.12	125.03	119.76
1	E	1094	GLY	C-N-CA	5.12	125.03	119.76
1	C	1057	ILE	CA-C-N	5.10	126.21	119.84
1	C	1057	ILE	C-N-CA	5.10	126.21	119.84
1	F	1076	LYS	N-CA-C	5.04	117.96	109.95
1	F	1032	THR	N-CA-C	-5.02	105.52	111.69

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	1258	0	1225	31	0
1	B	1258	0	1225	64	0
1	C	1258	0	1225	47	0
1	D	1258	0	1225	55	0
1	E	1258	0	1225	34	0
1	F	1258	0	1225	78	0
2	G	40	0	37	1	0
2	H	40	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	40	0	37	0	0
2	J	40	0	37	4	0
2	K	40	0	37	0	0
2	L	40	0	37	2	0
3	A	33	0	0	2	0
3	B	22	0	0	3	0
3	C	32	0	0	4	0
3	D	21	0	0	4	0
3	E	30	0	0	1	0
3	F	31	0	0	9	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
All	All	7963	0	7572	313	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 20.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1025:PHE:HZ	1:C:1131:LYS:HD2	1.40	0.87
1:D:1023:GLU:HB2	1:D:1133:LYS:HE2	1.61	0.82
1:B:1029:VAL:HG22	1:B:1087:ASN:HD21	1.44	0.80
1:D:1028:LYS:HD2	1:D:1090:LEU:HD21	1.64	0.79
1:F:1003:ASN:ND2	1:F:1025:PHE:HA	1.97	0.79
1:F:1085:ASP:HA	1:F:1108:ASN:ND2	1.99	0.78
1:C:1148:ARG:HH11	1:C:1148:ARG:HA	1.49	0.77
1:D:1148:ARG:HE	1:D:1148:ARG:HA	1.50	0.77
1:D:1024:LEU:HB3	1:D:1033:ALA:HB1	1.68	0.76
1:C:1025:PHE:CZ	1:C:1131:LYS:HD2	2.19	0.76
1:C:1044:LYS:HG2	1:C:1078:ILE:HB	1.68	0.74
1:E:1028:LYS:HD3	1:E:1090:LEU:HD21	1.69	0.74
1:F:1082:LYS:NZ	1:F:1107:THR:HG22	2.02	0.74
1:F:1127:VAL:HA	3:F:7029:HOH:O	1.89	0.73
1:F:1048:TYR:HA	3:F:7016:HOH:O	1.87	0.73
1:B:1024:LEU:HB3	1:B:1033:ALA:HB1	1.70	0.71
1:E:1098:LEU:HG	1:E:1129:PHE:CZ	2.26	0.71
1:B:1022:PHE:CD1	1:B:1098:LEU:HD22	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1052:CYS:HB2	1:F:1156:ILE:O	1.90	0.70
1:D:1095:PRO:HG3	1:D:1117:ALA:HA	1.72	0.70
1:C:1141:ALA:O	1:C:1144:ARG:HG2	1.90	0.69
1:F:1048:TYR:CD1	1:F:1065:GLY:HA2	2.28	0.69
1:D:1141:ALA:O	1:D:1144:ARG:HG2	1.93	0.69
1:F:1082:LYS:HZ3	1:F:1107:THR:HG22	1.57	0.68
1:A:1067:PHE:HB3	3:A:7165:HOH:O	1.94	0.68
1:E:1069:ARG:HG2	1:E:1073:THR:HG22	1.76	0.67
1:C:1082:LYS:HG3	1:C:1107:THR:HA	1.77	0.67
1:F:1139:VAL:O	1:F:1143:GLU:HG2	1.95	0.67
1:D:1090:LEU:HB2	1:D:1128:VAL:HB	1.78	0.66
1:C:1149:ASN:C	1:C:1149:ASN:HD22	2.05	0.65
1:D:1025:PHE:HZ	1:D:1131:LYS:HD2	1.61	0.64
1:F:1067:PHE:HB3	3:F:7016:HOH:O	1.98	0.64
1:C:1142:MSE:SE	1:C:1156:ILE:HG21	2.47	0.64
1:F:1062:CYS:O	1:F:1113:PHE:HA	1.98	0.64
1:D:1029:VAL:HG12	1:D:1032:THR:HB	1.80	0.64
1:C:1058:PRO:HA	1:C:1143:GLU:HG3	1.79	0.63
1:D:1126:HIS:NE2	2:J:104:PRO:HB3	2.14	0.63
1:E:1086:GLU:HG2	1:E:1087:ASN:ND2	2.14	0.63
1:D:1102:ASN:ND2	1:D:1126:HIS:ND1	2.48	0.62
1:B:1085:ASP:HB3	1:B:1127:VAL:HG13	1.82	0.61
1:B:1023:GLU:HB2	1:B:1133:LYS:HE2	1.81	0.61
1:F:1141:ALA:C	1:F:1143:GLU:H	2.08	0.61
1:C:1069:ARG:HB3	1:C:1071:ASN:OD1	2.01	0.61
1:C:1028:LYS:C	1:C:1030:PRO:HD3	2.25	0.61
1:E:1082:LYS:HD3	1:E:1082:LYS:N	2.16	0.61
1:A:1098:LEU:HG	1:A:1129:PHE:CZ	2.37	0.60
1:E:1035:ASN:OD1	1:E:1078:ILE:HG12	2.01	0.60
1:A:1082:LYS:HD2	1:A:1107:THR:HA	1.83	0.60
1:B:1100:MSE:HB2	1:B:1127:VAL:HG23	1.82	0.60
1:A:1095:PRO:HG3	1:A:1117:ALA:HA	1.84	0.59
1:F:1098:LEU:HG	1:F:1129:PHE:CE1	2.37	0.59
1:B:1028:LYS:HD3	1:B:1090:LEU:HD21	1.82	0.59
1:D:1151:LYS:HG3	1:D:1152:THR:N	2.16	0.59
1:D:1096:GLY:HA2	1:D:1136:MSE:SE	2.52	0.59
1:B:1087:ASN:HD22	1:B:1087:ASN:N	2.00	0.59
1:E:1069:ARG:HD3	1:E:1074:GLY:HA3	1.85	0.58
1:F:1037:ARG:HG2	1:F:1037:ARG:HH11	1.67	0.58
1:B:1048:TYR:CE1	1:B:1065:GLY:HA2	2.38	0.58
1:B:1076:LYS:HZ2	1:B:1081:GLU:HB3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:THR:O	1:B:1163:GLN:HG3	2.03	0.58
1:A:1048:TYR:HA	3:A:7165:HOH:O	2.03	0.58
1:D:1126:HIS:HE2	2:J:104:PRO:HB3	1.69	0.58
1:B:1037:ARG:O	1:B:1041:THR:HG23	2.03	0.57
1:A:1052:CYS:HB2	1:A:1156:ILE:O	2.04	0.57
1:B:1004:PRO:CD	1:B:1026:ALA:HB2	2.35	0.57
1:B:1034:GLU:HB3	1:B:1079:TYR:OH	2.04	0.57
1:B:1126:HIS:CE1	2:H:104:PRO:HB3	2.39	0.57
1:B:1139:VAL:HA	1:B:1142:MSE:HE3	1.86	0.57
1:E:1056:ILE:HG21	1:E:1143:GLU:HA	1.85	0.57
1:E:1069:ARG:HD3	1:E:1074:GLY:CA	2.34	0.57
1:B:1010:ILE:HG13	1:B:1142:MSE:HE1	1.87	0.57
1:C:1058:PRO:HD2	1:C:1147:SER:O	2.05	0.57
1:D:1029:VAL:CG1	1:D:1032:THR:HB	2.35	0.57
1:B:1024:LEU:HD13	1:B:1033:ALA:O	2.05	0.57
1:A:1100:MSE:HB2	1:A:1127:VAL:HG22	1.86	0.56
1:F:1048:TYR:HD1	1:F:1065:GLY:HA2	1.69	0.56
1:B:1049:LYS:HE3	1:B:1159:ALA:O	2.06	0.56
1:F:1082:LYS:HD2	1:F:1107:THR:HA	1.88	0.56
1:B:1090:LEU:HB2	1:B:1128:VAL:HB	1.86	0.56
1:E:1030:PRO:HD2	1:E:1086:GLU:OE2	2.06	0.55
1:B:1095:PRO:HG3	1:B:1117:ALA:HA	1.88	0.55
1:D:1025:PHE:CZ	1:D:1131:LYS:HD2	2.39	0.55
1:B:1004:PRO:HD3	1:B:1026:ALA:HB2	1.88	0.55
1:D:1023:GLU:CB	1:D:1133:LYS:HE2	2.36	0.55
1:C:1012:VAL:HG21	1:C:1145:PHE:HE2	1.72	0.55
1:C:1028:LYS:HG3	3:C:7062:HOH:O	2.07	0.54
1:D:1082:LYS:HD3	1:D:1082:LYS:N	2.21	0.54
1:F:1025:PHE:HD2	1:F:1090:LEU:HD13	1.71	0.54
1:A:1076:LYS:O	1:A:1110:SER:HB3	2.08	0.54
1:D:1126:HIS:CD2	2:J:104:PRO:HB3	2.42	0.54
1:E:1097:ILE:HG23	1:E:1128:VAL:HG13	1.90	0.54
1:B:1024:LEU:CD1	1:B:1037:ARG:HB2	2.38	0.54
1:B:1057:ILE:HG12	1:B:1150:GLY:HA2	1.89	0.54
1:F:1145:PHE:CE2	1:F:1154:LYS:HD2	2.43	0.54
1:C:1069:ARG:HE	1:C:1074:GLY:HA3	1.72	0.54
1:C:1082:LYS:NZ	1:C:1082:LYS:HB3	2.23	0.53
1:C:1122:LEU:HD22	1:C:1126:HIS:CD2	2.44	0.53
1:A:1139:VAL:HA	1:A:1142:MSE:SE	2.58	0.53
1:F:1085:ASP:HA	1:F:1108:ASN:HD22	1.71	0.53
1:C:1120:GLU:O	1:C:1123:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1148:ARG:HA	1:C:1148:ARG:NH1	2.21	0.53
1:F:1145:PHE:N	1:F:1145:PHE:CD1	2.76	0.53
1:E:1081:GLU:HB3	1:E:1082:LYS:HD3	1.91	0.53
1:F:1036:PHE:HB2	1:F:1129:PHE:HE2	1.73	0.53
1:E:1044:LYS:HZ1	1:E:1078:ILE:HB	1.74	0.53
1:E:1082:LYS:HD3	1:E:1082:LYS:H	1.75	0.52
1:B:1018:GLY:HA3	1:B:1138:ILE:HD12	1.91	0.52
1:B:1075:GLY:HA3	1:B:1110:SER:OG	2.09	0.52
1:E:1058:PRO:HG3	1:E:1143:GLU:O	2.09	0.52
1:F:1006:VAL:HA	1:F:1163:GLN:HA	1.91	0.52
2:L:105:ILE:HD12	2:L:105:ILE:O	2.09	0.52
1:D:1062:CYS:O	1:D:1113:PHE:HA	2.09	0.52
1:A:1148:ARG:HA	1:A:1148:ARG:NE	2.24	0.52
2:H:105:ILE:HD12	2:H:105:ILE:H	1.75	0.52
1:A:1037:ARG:O	1:A:1041:THR:HG23	2.10	0.52
1:D:1096:GLY:CA	1:D:1136:MSE:SE	3.08	0.52
1:F:1055:ARG:HB3	1:F:1063:GLN:HB3	1.92	0.52
2:H:105:ILE:HD12	2:H:105:ILE:O	2.10	0.52
1:B:1148:ARG:HA	1:B:1148:ARG:NE	2.25	0.51
1:C:1082:LYS:HG2	1:C:1083:PHE:N	2.24	0.51
1:E:1095:PRO:HG3	1:E:1117:ALA:HA	1.92	0.51
1:B:1002:VAL:O	1:B:1004:PRO:HD3	2.11	0.51
1:C:1035:ASN:O	1:C:1039:LEU:HG	2.11	0.51
1:F:1048:TYR:CE1	1:F:1065:GLY:HA2	2.45	0.51
1:B:1088:PHE:HA	3:B:7001:HOH:O	2.11	0.51
1:F:1076:LYS:HA	3:F:7002:HOH:O	2.10	0.51
1:D:1022:PHE:CD1	1:D:1098:LEU:HD22	2.46	0.51
1:F:1008:PHE:HB2	1:F:1020:VAL:HG13	1.93	0.51
1:F:1091:LYS:N	1:F:1091:LYS:HD2	2.26	0.51
1:A:1101:ALA:O	2:G:102:ALA:HB1	2.11	0.50
1:B:1055:ARG:HB3	1:B:1063:GLN:HB3	1.93	0.50
1:C:1123:ASP:HA	3:C:7028:HOH:O	2.11	0.50
1:E:1025:PHE:HZ	1:E:1131:LYS:HE3	1.76	0.50
1:E:1025:PHE:CZ	1:E:1131:LYS:HE3	2.46	0.50
1:F:1085:ASP:HA	1:F:1108:ASN:HD21	1.75	0.50
1:D:1012:VAL:HA	1:D:1155:LYS:O	2.12	0.50
1:B:1146:GLY:HA2	1:B:1152:THR:HA	1.94	0.50
1:F:1091:LYS:HA	1:F:1091:LYS:HE3	1.93	0.50
1:B:1026:ALA:O	1:B:1030:PRO:HB3	2.11	0.50
1:F:1096:GLY:HA2	1:F:1136:MSE:SE	2.61	0.49
1:A:1127:VAL:HG23	1:A:1127:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1023:GLU:CB	1:B:1133:LYS:HE2	2.41	0.49
2:L:101:HIS:ND1	2:L:101:HIS:N	2.60	0.49
1:B:1025:PHE:HZ	1:B:1131:LYS:HG2	1.77	0.49
1:B:1101:ALA:H	1:B:1112:PHE:HA	1.77	0.49
1:F:1090:LEU:C	1:F:1091:LYS:HD2	2.37	0.49
1:F:1105:PRO:O	1:F:1107:THR:HG23	2.11	0.49
1:C:1155:LYS:HE2	1:C:1157:THR:OG1	2.13	0.49
1:D:1049:LYS:HE2	1:D:1160:ASP:OD1	2.13	0.49
1:A:1040:SER:HA	1:A:1048:TYR:HD2	1.77	0.48
1:D:1085:ASP:HA	1:D:1108:ASN:ND2	2.29	0.48
1:B:1023:GLU:CA	1:B:1133:LYS:HE2	2.43	0.48
1:E:1068:THR:HG1	1:E:1075:GLY:H	1.56	0.48
1:A:1055:ARG:HB3	1:A:1063:GLN:HB3	1.94	0.48
1:C:1030:PRO:HD2	1:C:1086:GLU:OE2	2.14	0.48
1:C:1076:LYS:O	1:C:1110:SER:HB3	2.13	0.48
1:F:1052:CYS:HB3	1:F:1155:LYS:HE3	1.94	0.48
1:B:1160:ASP:HB2	3:B:7021:HOH:O	2.12	0.48
1:C:1044:LYS:HE2	1:C:1078:ILE:HD12	1.96	0.48
1:D:1044:LYS:HB2	3:D:7103:HOH:O	2.12	0.48
1:A:1141:ALA:HA	1:A:1144:ARG:NH2	2.29	0.48
1:B:1139:VAL:HA	1:B:1142:MSE:HG2	1.95	0.48
1:E:1052:CYS:HB2	1:E:1156:ILE:O	2.14	0.48
1:B:1037:ARG:HD3	1:B:1163:GLN:OE1	2.13	0.48
1:C:1145:PHE:HD2	1:C:1156:ILE:HD11	1.78	0.48
1:D:1099:SER:HB3	1:D:1113:PHE:CZ	2.48	0.48
1:F:1038:ALA:HA	1:F:1043:GLU:HG3	1.95	0.48
1:E:1086:GLU:HG2	1:E:1087:ASN:HD22	1.79	0.48
1:E:1090:LEU:HB3	3:E:7075:HOH:O	2.13	0.47
1:B:1058:PRO:HD2	1:B:1147:SER:O	2.14	0.47
1:B:1140:GLU:C	1:B:1143:GLU:HB2	2.39	0.47
1:B:1030:PRO:O	1:B:1034:GLU:HB2	2.14	0.47
1:B:1129:PHE:HD1	1:B:1129:PHE:H	1.62	0.47
1:E:1056:ILE:CG2	1:E:1143:GLU:HA	2.44	0.47
1:F:1070:HIS:CD2	3:F:7161:HOH:O	2.67	0.47
1:F:1037:ARG:HG2	1:F:1037:ARG:NH1	2.28	0.47
1:F:1040:SER:HA	1:F:1048:TYR:HD2	1.80	0.47
1:F:1048:TYR:CE1	1:F:1112:PHE:HE2	2.32	0.47
1:F:1082:LYS:HZ2	1:F:1107:THR:HG22	1.78	0.47
1:F:1146:GLY:HA2	1:F:1152:THR:HA	1.97	0.47
1:A:1031:LYS:HE3	1:A:1079:TYR:CD2	2.50	0.47
1:C:1088:PHE:HA	3:C:7133:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1009:ASP:O	1:D:1159:ALA:N	2.47	0.47
1:F:1152:THR:HB	1:F:1154:LYS:O	2.14	0.47
1:F:1136:MSE:HG2	3:F:7149:HOH:O	2.15	0.47
1:E:1028:LYS:C	1:E:1030:PRO:HD3	2.39	0.47
1:F:1041:THR:HG22	1:F:1162:GLY:HA2	1.97	0.47
1:F:1041:THR:HG22	1:F:1163:GLN:N	2.30	0.47
1:B:1029:VAL:HG13	1:B:1086:GLU:HB3	1.97	0.47
1:D:1088:PHE:HA	3:D:7060:HOH:O	2.15	0.47
1:F:1106:ASN:OD1	1:F:1106:ASN:N	2.49	0.47
1:C:1127:VAL:HG11	3:C:7148:HOH:O	2.15	0.46
1:D:1024:LEU:CD1	1:D:1037:ARG:HB2	2.46	0.46
1:D:1085:ASP:HB3	1:D:1127:VAL:CG2	2.45	0.46
1:F:1149:ASN:H	1:F:1149:ASN:ND2	2.13	0.46
1:F:1008:PHE:HB2	1:F:1020:VAL:CG1	2.46	0.46
1:B:1096:GLY:HA2	1:B:1136:MSE:SE	2.66	0.46
1:F:1056:ILE:HG23	1:F:1062:CYS:SG	2.56	0.46
1:F:1129:PHE:H	1:F:1129:PHE:HD1	1.62	0.46
1:F:1148:ARG:HA	1:F:1148:ARG:NE	2.31	0.45
1:D:1058:PRO:HA	1:D:1143:GLU:HG3	1.97	0.45
1:A:1090:LEU:C	1:A:1091:LYS:HD2	2.41	0.45
1:B:1048:TYR:HE1	1:B:1065:GLY:HA2	1.79	0.45
1:D:1015:GLU:HA	1:D:1016:PRO:HD3	1.61	0.45
1:D:1085:ASP:CG	1:D:1108:ASN:HD21	2.24	0.45
1:F:1080:GLY:O	1:F:1081:GLU:O	2.35	0.45
1:C:1062:CYS:O	1:C:1113:PHE:HA	2.16	0.45
1:A:1035:ASN:OD1	1:A:1078:ILE:HG23	2.16	0.45
1:A:1068:THR:HG1	1:A:1075:GLY:N	2.15	0.45
1:B:1027:ASP:OD1	1:B:1028:LYS:HG3	2.17	0.44
1:A:1097:ILE:HG23	1:A:1128:VAL:HG13	1.99	0.44
1:B:1127:VAL:HG22	3:B:7118:HOH:O	2.17	0.44
1:C:1095:PRO:HG3	1:C:1117:ALA:HA	1.98	0.44
1:B:1048:TYR:CD1	1:B:1065:GLY:HA2	2.52	0.44
1:B:1097:ILE:HG23	1:B:1128:VAL:HG13	1.98	0.44
1:F:1026:ALA:HA	1:F:1033:ALA:CB	2.48	0.44
1:F:1155:LYS:HE3	1:F:1157:THR:OG1	2.17	0.44
1:C:1091:LYS:O	1:C:1093:THR:N	2.49	0.44
1:F:1007:PHE:CD2	1:F:1164:LEU:HG	2.53	0.44
1:A:1085:ASP:O	1:A:1086:GLU:C	2.60	0.44
1:F:1059:GLY:O	1:F:1117:ALA:HB3	2.18	0.44
1:F:1087:ASN:OD1	1:F:1089:ILE:HG13	2.18	0.44
1:F:1140:GLU:O	1:F:1143:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:LEU:HB3	1:B:1048:TYR:CE2	2.52	0.44
1:B:1069:ARG:HD2	1:B:1073:THR:HB	2.00	0.44
1:C:1097:ILE:HB	1:C:1115:CYS:HB2	1.99	0.44
1:A:1068:THR:HG1	1:A:1075:GLY:H	1.65	0.44
1:A:1155:LYS:HE2	1:A:1157:THR:OG1	2.17	0.44
1:C:1056:ILE:HG21	1:C:1143:GLU:HA	1.98	0.44
1:E:1138:ILE:O	1:E:1142:MSE:HB2	2.18	0.44
1:F:1040:SER:O	1:F:1161:CYS:SG	2.74	0.44
1:B:1034:GLU:OE1	1:B:1037:ARG:HB3	2.17	0.43
1:F:1032:THR:HG22	1:F:1129:PHE:CD2	2.53	0.43
1:E:1091:LYS:O	1:E:1093:THR:HG23	2.18	0.43
1:D:1048:TYR:CE1	1:D:1065:GLY:HA2	2.54	0.43
1:D:1126:HIS:HE2	2:J:104:PRO:CB	2.31	0.43
1:E:1044:LYS:NZ	1:E:1078:ILE:HB	2.32	0.43
1:D:1036:PHE:HB2	1:D:1129:PHE:HE2	1.82	0.43
1:D:1122:LEU:HD13	1:D:1126:HIS:HD2	1.83	0.43
1:F:1145:PHE:HD2	1:F:1154:LYS:HB2	1.84	0.43
1:C:1052:CYS:HB2	1:C:1156:ILE:O	2.19	0.43
1:F:1010:ILE:HG21	1:F:1142:MSE:HE2	1.99	0.43
1:C:1012:VAL:HG21	1:C:1145:PHE:CE2	2.53	0.43
1:F:1095:PRO:HA	1:F:1115:CYS:O	2.19	0.43
1:F:1003:ASN:HB3	1:F:1024:LEU:O	2.18	0.43
1:B:1098:LEU:HB3	1:B:1130:GLY:C	2.43	0.43
1:C:1012:VAL:HG11	1:C:1154:LYS:HD3	1.99	0.43
1:C:1072:GLY:HA2	1:C:1111:GLN:OE1	2.18	0.43
1:A:1141:ALA:HA	1:A:1144:ARG:HH21	1.84	0.43
1:B:1106:ASN:C	1:B:1107:THR:HG23	2.44	0.43
1:F:1055:ARG:HA	1:F:1150:GLY:O	2.19	0.43
1:D:1119:THR:HA	1:D:1121:TRP:CZ3	2.54	0.42
1:F:1090:LEU:HD12	3:F:7048:HOH:O	2.19	0.42
1:C:1046:PHE:CD1	1:C:1046:PHE:N	2.87	0.42
1:B:1024:LEU:HD12	1:B:1037:ARG:HB2	2.00	0.42
1:C:1025:PHE:CZ	1:C:1131:LYS:CD	2.98	0.42
1:D:1135:GLY:C	1:D:1137:ASN:N	2.76	0.42
1:F:1024:LEU:CD1	1:F:1037:ARG:HB2	2.48	0.42
1:B:1129:PHE:N	1:B:1129:PHE:CD1	2.88	0.42
1:E:1071:ASN:OD1	1:E:1073:THR:HB	2.19	0.42
1:A:1037:ARG:HG2	1:A:1037:ARG:HH11	1.84	0.42
1:D:1025:PHE:HB3	1:D:1028:LYS:HE3	2.01	0.42
1:A:1056:ILE:HG23	1:A:1062:CYS:SG	2.60	0.42
1:D:1135:GLY:C	1:D:1137:ASN:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1136:MSE:HE3	1:D:1140:GLU:OE1	2.20	0.42
1:C:1149:ASN:C	1:C:1149:ASN:ND2	2.76	0.42
1:D:1090:LEU:HG	3:D:7137:HOH:O	2.20	0.42
1:E:1012:VAL:HG22	1:E:1156:ILE:HD12	2.02	0.42
1:F:1039:LEU:O	1:F:1048:TYR:CD2	2.73	0.42
1:A:1029:VAL:HG13	1:A:1087:ASN:ND2	2.35	0.41
1:A:1140:GLU:O	1:A:1143:GLU:HB2	2.20	0.41
1:B:1037:ARG:NH1	1:B:1038:ALA:HA	2.35	0.41
1:D:1055:ARG:HB3	1:D:1063:GLN:HB3	2.01	0.41
1:D:1098:LEU:HB3	1:D:1130:GLY:C	2.44	0.41
1:C:1149:ASN:ND2	1:C:1151:LYS:H	2.17	0.41
1:D:1085:ASP:O	1:D:1086:GLU:C	2.62	0.41
1:F:1048:TYR:CE1	1:F:1112:PHE:CE2	3.08	0.41
1:D:1097:ILE:HG23	1:D:1128:VAL:HG13	2.01	0.41
1:F:1029:VAL:HB	1:F:1086:GLU:OE1	2.20	0.41
1:F:1060:PHE:HE1	1:F:1122:LEU:HD11	1.85	0.41
1:B:1140:GLU:O	1:B:1143:GLU:HB2	2.20	0.41
1:B:1068:THR:OG1	1:B:1074:GLY:HA3	2.20	0.41
1:D:1005:THR:O	1:D:1163:GLN:HG3	2.20	0.41
1:F:1145:PHE:HE2	1:F:1154:LYS:HD2	1.84	0.41
1:C:1055:ARG:HB3	1:C:1063:GLN:HB3	2.02	0.41
1:D:1066:ASP:CG	1:D:1070:HIS:H	2.28	0.41
1:F:1018:GLY:HA3	1:F:1138:ILE:HD12	2.02	0.41
1:A:1025:PHE:CD2	1:A:1090:LEU:HD13	2.56	0.41
1:B:1012:VAL:O	1:B:1013:ASP:HB2	2.19	0.41
1:B:1068:THR:HG1	1:B:1074:GLY:HA3	1.86	0.41
1:C:1097:ILE:HG23	1:C:1128:VAL:HG13	2.02	0.41
1:C:1056:ILE:CG2	1:C:1143:GLU:HA	2.51	0.41
1:D:1020:VAL:O	1:D:1020:VAL:HG13	2.21	0.41
1:D:1023:GLU:HB2	1:D:1133:LYS:CE	2.42	0.41
1:D:1092:HIS:HB2	1:D:1119:THR:O	2.20	0.41
1:D:1129:PHE:N	1:D:1129:PHE:CD1	2.88	0.41
1:F:1037:ARG:HD2	1:F:1163:GLN:NE2	2.36	0.41
1:F:1069:ARG:HG2	1:F:1074:GLY:HA3	2.03	0.41
1:E:1024:LEU:HD12	1:E:1037:ARG:HB2	2.03	0.41
1:F:1029:VAL:HG13	3:F:7048:HOH:O	2.21	0.41
1:A:1003:ASN:HA	1:A:1004:PRO:HD3	1.78	0.40
1:E:1142:MSE:CG	1:E:1156:ILE:HG21	2.51	0.40
1:F:1088:PHE:HA	3:F:7029:HOH:O	2.21	0.40
1:F:1141:ALA:O	1:F:1143:GLU:N	2.54	0.40
1:B:1008:PHE:HB2	1:B:1020:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1006:VAL:HA	1:E:1162:GLY:O	2.19	0.40
1:E:1055:ARG:HB3	1:E:1063:GLN:HB3	2.02	0.40
1:F:1052:CYS:HA	1:F:1157:THR:HA	2.03	0.40
1:C:1048:TYR:CE1	1:C:1065:GLY:HA2	2.56	0.40
1:C:1102:ASN:ND2	1:C:1126:HIS:ND1	2.69	0.40
1:D:1156:ILE:HG12	3:D:7150:HOH:O	2.20	0.40
1:B:1029:VAL:HG12	1:B:1032:THR:HB	2.02	0.40
1:E:1029:VAL:HG12	1:E:1032:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	147 (91%)	12 (7%)	3 (2%)	6	7
1	B	162/164 (99%)	136 (84%)	20 (12%)	6 (4%)	2	1
1	C	162/164 (99%)	140 (86%)	21 (13%)	1 (1%)	21	29
1	D	162/164 (99%)	140 (86%)	18 (11%)	4 (2%)	4	4
1	E	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	F	162/164 (99%)	146 (90%)	13 (8%)	3 (2%)	6	7
2	G	4/6 (67%)	4 (100%)	0	0	100	100
2	H	4/6 (67%)	4 (100%)	0	0	100	100
2	I	4/6 (67%)	4 (100%)	0	0	100	100
2	J	4/6 (67%)	4 (100%)	0	0	100	100
2	K	4/6 (67%)	4 (100%)	0	0	100	100
2	L	4/6 (67%)	4 (100%)	0	0	100	100
All	All	996/1020 (98%)	879 (88%)	100 (10%)	17 (2%)	7	8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1070	HIS
1	A	1081	GLU
1	B	1025	PHE
1	B	1105	PRO
1	D	1105	PRO
1	F	1081	GLU
1	D	1049	LYS
1	D	1154	LYS
1	F	1142	MSE
1	B	1071	ASN
1	B	1077	SER
1	F	1148	ARG
1	A	1086	GLU
1	D	1079	TYR
1	B	1104	GLY
1	B	1132	VAL
1	C	1016	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	132/128 (103%)	126 (96%)	6 (4%)	24	38
1	B	132/128 (103%)	116 (88%)	16 (12%)	5	5
1	C	132/128 (103%)	123 (93%)	9 (7%)	14	20
1	D	132/128 (103%)	123 (93%)	9 (7%)	14	20
1	E	132/128 (103%)	127 (96%)	5 (4%)	29	44
1	F	132/128 (103%)	118 (89%)	14 (11%)	6	7
2	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	H	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	I	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	J	3/3 (100%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	L	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	810/786 (103%)	745 (92%)	65 (8%)	11	15

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1029	VAL
1	A	1032	THR
1	A	1069	ARG
1	A	1148	ARG
1	A	1151	LYS
1	A	1153	SER
1	B	1002	VAL
1	B	1034	GLU
1	B	1044	LYS
1	B	1049	LYS
1	B	1076	LYS
1	B	1081	GLU
1	B	1084	GLU
1	B	1085	ASP
1	B	1087	ASN
1	B	1105	PRO
1	B	1106	ASN
1	B	1127	VAL
1	B	1129	PHE
1	B	1131	LYS
1	B	1140	GLU
1	B	1143	GLU
1	C	1029	VAL
1	C	1073	THR
1	C	1082	LYS
1	C	1084	GLU
1	C	1131	LYS
1	C	1144	ARG
1	C	1149	ASN
1	C	1153	SER
1	C	1155	LYS
1	D	1015	GLU
1	D	1076	LYS
1	D	1082	LYS

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Mol	Chain	Res	Type
1	D	1105	PRO
1	D	1129	PHE
1	D	1131	LYS
1	D	1140	GLU
1	D	1148	ARG
1	D	1151	LYS
1	E	1029	VAL
1	E	1073	THR
1	E	1082	LYS
1	E	1084	GLU
1	E	1153	SER
1	F	1027	ASP
1	F	1073	THR
1	F	1084	GLU
1	F	1105	PRO
1	F	1106	ASN
1	F	1125	LYS
1	F	1127	VAL
1	F	1129	PHE
1	F	1137	ASN
1	F	1140	GLU
1	F	1142	MSE
1	F	1144	ARG
1	F	1149	ASN
1	F	1151	LYS
2	G	101	HIS
2	H	105	ILE
2	I	105	ILE
2	J	105	ILE
2	K	101	HIS
2	L	101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1163	GLN
1	B	1087	ASN
1	B	1108	ASN
1	C	1087	ASN
1	C	1106	ASN
1	C	1149	ASN
1	D	1003	ASN

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Mol	Chain	Res	Type
1	D	1035	ASN
1	D	1108	ASN
1	E	1070	HIS
1	E	1137	ASN
1	E	1149	ASN
1	F	1003	ASN
1	F	1070	HIS
1	F	1108	ASN
2	K	101	HIS

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 [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	160/164 (97%)	1.86	58 (36%) 1 0	5, 13, 21, 23	0
1	B	160/164 (97%)	3.02	124 (77%) 0 0	11, 20, 28, 34	0
1	C	160/164 (97%)	2.25	79 (49%) 0 0	5, 16, 26, 35	0
1	D	160/164 (97%)	2.24	85 (53%) 0 0	7, 18, 25, 33	0
1	E	160/164 (97%)	1.90	55 (34%) 1 0	4, 12, 22, 27	0
1	F	160/164 (97%)	2.84	117 (73%) 0 0	10, 18, 26, 30	0
2	G	6/6 (100%)	2.53	4 (66%) 0 0	13, 17, 21, 29	0
2	H	6/6 (100%)	2.09	2 (33%) 1 0	11, 14, 22, 24	0
2	I	6/6 (100%)	2.41	3 (50%) 0 0	6, 8, 11, 26	0
2	J	6/6 (100%)	2.93	4 (66%) 0 0	9, 10, 12, 18	0
2	K	6/6 (100%)	1.71	2 (33%) 1 0	7, 9, 20, 23	0
2	L	6/6 (100%)	2.61	3 (50%) 0 0	16, 19, 24, 24	0
All	All	996/1020 (97%)	2.35	536 (53%) 0 0	4, 17, 26, 35	0

All (536) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1107	THR	7.2
1	C	1148	ARG	7.2
1	F	1085	ASP	6.7
1	A	1080	GLY	6.7
1	C	1141	ALA	6.7
1	F	1083	PHE	6.6
1	F	1070	HIS	6.4
1	F	1030	PRO	6.4
1	B	1141	ALA	6.0
1	C	1014	GLY	5.9
1	A	1143	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	1003	ASN	5.7
2	J	106	ALA	5.6
1	C	1002	VAL	5.6
1	B	1032	THR	5.5
1	B	1074	GLY	5.5
1	D	1080	GLY	5.5
1	E	1074	GLY	5.5
1	D	1030	PRO	5.5
1	F	1029	VAL	5.4
1	E	1081	GLU	5.4
1	D	1085	ASP	5.4
1	B	1066	ASP	5.3
1	F	1163	GLN	5.3
1	C	1093	THR	5.1
1	B	1143	GLU	5.1
1	C	1095	PRO	5.1
1	F	1103	ALA	5.1
2	G	101	HIS	5.0
1	B	1067	PHE	5.0
1	D	1128	VAL	5.0
1	B	1025	PHE	5.0
1	B	1081	GLU	5.0
1	D	1002	VAL	5.0
1	B	1049	LYS	4.9
1	B	1105	PRO	4.9
1	B	1080	GLY	4.9
1	B	1085	ASP	4.9
1	C	1015	GLU	4.9
1	B	1047	GLY	4.9
1	E	1014	GLY	4.9
1	B	1024	LEU	4.8
1	B	1046	PHE	4.8
1	B	1006	VAL	4.8
1	B	1012	VAL	4.8
1	B	1104	GLY	4.8
1	D	1104	GLY	4.8
1	C	1123	ASP	4.8
2	L	101	HIS	4.8
1	B	1077	SER	4.7
1	F	1068	THR	4.7
1	B	1002	VAL	4.6
1	E	1082	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	1088	PHE	4.6
1	B	1007	PHE	4.6
1	C	1146	GLY	4.6
1	B	1016	PRO	4.6
2	K	101	HIS	4.6
1	E	1149	ASN	4.5
1	F	1069	ARG	4.5
1	D	1027	ASP	4.5
1	F	1013	ASP	4.5
1	C	1017	LEU	4.4
1	F	1105	PRO	4.4
1	E	1137	ASN	4.4
1	D	1079	TYR	4.4
1	B	1128	VAL	4.4
1	F	1127	VAL	4.4
1	F	1071	ASN	4.4
1	B	1159	ALA	4.4
2	I	106	ALA	4.4
1	B	1044	LYS	4.4
1	C	1082	LYS	4.4
1	F	1078	ILE	4.4
1	F	1038	ALA	4.4
1	D	1069	ARG	4.3
1	D	1003	ASN	4.3
1	B	1041	THR	4.3
1	D	1116	THR	4.3
1	F	1012	VAL	4.3
1	B	1050	GLY	4.3
1	F	1074	GLY	4.3
1	D	1078	ILE	4.3
1	F	1033	ALA	4.3
1	F	1040	SER	4.3
2	H	101	HIS	4.2
1	F	1116	THR	4.2
1	F	1157	THR	4.2
1	B	1153	SER	4.2
1	F	1041	THR	4.2
1	E	1086	GLU	4.2
1	E	1143	GLU	4.2
1	B	1045	GLY	4.1
1	F	1124	GLY	4.1
1	B	1015	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	1152	THR	4.1
1	F	1052	CYS	4.1
1	C	1144	ARG	4.1
1	B	1106	ASN	4.1
1	A	1081	GLU	4.1
1	B	1160	ASP	4.1
1	C	1116	THR	4.1
1	B	1079	TYR	4.0
1	C	1081	GLU	4.0
1	D	1127	VAL	4.0
1	E	1044	LYS	4.0
1	E	1151	LYS	4.0
1	F	1032	THR	4.0
1	F	1011	ALA	3.9
1	B	1023	GLU	3.9
1	B	1088	PHE	3.9
1	B	1107	THR	3.9
1	F	1059	GLY	3.9
1	B	1140	GLU	3.9
1	B	1026	ALA	3.9
1	C	1026	ALA	3.9
1	F	1039	LEU	3.9
1	A	1086	GLU	3.9
1	C	1147	SER	3.9
1	B	1030	PRO	3.9
1	C	1127	VAL	3.9
1	B	1083	PHE	3.8
1	F	1010	ILE	3.8
1	F	1081	GLU	3.8
1	F	1104	GLY	3.8
1	D	1152	THR	3.8
1	C	1020	VAL	3.8
1	B	1011	ALA	3.8
1	F	1154	LYS	3.8
1	B	1035	ASN	3.8
1	B	1108	ASN	3.8
1	E	1050	GLY	3.8
1	E	1017	LEU	3.8
1	F	1027	ASP	3.8
1	C	1124	GLY	3.7
1	F	1034	GLU	3.7
1	C	1149	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	1089	ILE	3.7
2	L	105	ILE	3.7
1	D	1105	PRO	3.7
1	B	1033	ALA	3.7
1	C	1159	ALA	3.7
1	C	1118	LYS	3.7
1	E	1148	ARG	3.7
1	F	1073	THR	3.7
1	A	1147	SER	3.7
1	C	1079	TYR	3.6
1	B	1082	LYS	3.6
1	B	1097	ILE	3.6
1	B	1165	GLU	3.6
1	B	1110	SER	3.6
1	B	1037	ARG	3.6
1	B	1069	ARG	3.6
1	E	1150	GLY	3.6
1	A	1058	PRO	3.6
1	D	1093	THR	3.6
1	C	1028	LYS	3.6
1	B	1127	VAL	3.5
1	B	1051	SER	3.5
1	F	1110	SER	3.5
1	D	1096	GLY	3.5
1	A	1044	LYS	3.5
1	F	1084	GLU	3.5
1	B	1132	VAL	3.5
1	F	1072	GLY	3.5
1	B	1010	ILE	3.5
1	A	1085	ASP	3.5
1	D	1077	SER	3.5
1	F	1026	ALA	3.5
1	D	1025	PHE	3.5
1	F	1161	CYS	3.4
1	F	1025	PHE	3.4
1	E	1015	GLU	3.4
1	E	1043	GLU	3.4
1	F	1132	VAL	3.4
1	A	1154	LYS	3.4
1	B	1042	GLY	3.4
1	D	1075	GLY	3.4
1	A	1103	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1038	ALA	3.4
1	D	1081	GLU	3.4
1	D	1020	VAL	3.4
1	C	1070	HIS	3.4
1	F	1150	GLY	3.4
1	A	1144	ARG	3.4
1	B	1156	ILE	3.4
1	B	1161	CYS	3.3
1	A	1002	VAL	3.3
1	F	1005	THR	3.3
1	B	1146	GLY	3.3
1	C	1045	GLY	3.3
1	D	1026	ALA	3.3
1	C	1092	HIS	3.3
1	E	1070	HIS	3.3
1	C	1084	GLU	3.3
1	A	1137	ASN	3.3
1	F	1058	PRO	3.3
1	A	1101	ALA	3.3
1	B	1048	TYR	3.3
1	D	1106	ASN	3.3
1	D	1149	ASN	3.3
1	E	1144	ARG	3.3
1	A	1073	THR	3.3
1	C	1087	ASN	3.2
1	A	1070	HIS	3.2
1	C	1080	GLY	3.2
1	A	1082	LYS	3.2
1	F	1158	ILE	3.2
1	B	1149	ASN	3.2
1	D	1108	ASN	3.2
1	F	1143	GLU	3.2
1	B	1152	THR	3.2
1	D	1146	GLY	3.2
1	B	1145	PHE	3.2
1	F	1129	PHE	3.2
1	F	1066	ASP	3.2
1	F	1160	ASP	3.2
1	B	1039	LEU	3.2
1	C	1143	GLU	3.2
1	B	1103	ALA	3.2
1	B	1163	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1151	LYS	3.2
1	B	1004	PRO	3.2
1	F	1140	GLU	3.2
1	A	1079	TYR	3.2
1	A	1074	GLY	3.2
1	E	1020	VAL	3.2
1	D	1089	ILE	3.2
1	F	1156	ILE	3.2
1	E	1077	SER	3.1
1	B	1129	PHE	3.1
1	D	1132	VAL	3.1
1	A	1084	GLU	3.1
1	C	1030	PRO	3.1
1	B	1090	LEU	3.1
1	F	1090	LEU	3.1
1	C	1119	THR	3.1
1	F	1082	LYS	3.1
1	D	1084	GLU	3.1
1	F	1144	ARG	3.1
1	F	1079	TYR	3.0
1	F	1153	SER	3.0
1	B	1075	GLY	3.0
1	F	1075	GLY	3.0
1	B	1029	VAL	3.0
1	F	1097	ILE	3.0
1	E	1153	SER	3.0
1	B	1109	GLY	3.0
1	C	1089	ILE	3.0
1	F	1138	ILE	3.0
1	D	1090	LEU	3.0
1	A	1083	PHE	3.0
1	F	1067	PHE	3.0
1	F	1145	PHE	3.0
1	D	1028	LYS	3.0
1	B	1139	VAL	3.0
1	F	1101	ALA	3.0
1	F	1091	LYS	3.0
1	A	1149	ASN	3.0
1	F	1080	GLY	3.0
1	E	1012	VAL	2.9
1	C	1117	ALA	2.9
1	B	1008	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	1025	PHE	2.9
1	D	1083	PHE	2.9
1	F	1046	PHE	2.9
1	B	1040	SER	2.9
1	C	1165	GLU	2.9
1	E	1041	THR	2.9
1	F	1054	HIS	2.9
2	J	102	ALA	2.9
1	B	1095	PRO	2.9
1	A	1146	GLY	2.9
1	B	1157	THR	2.9
1	B	1154	LYS	2.9
1	D	1014	GLY	2.9
1	E	1109	GLY	2.9
1	D	1012	VAL	2.9
1	C	1091	LYS	2.9
1	E	1118	LYS	2.9
1	D	1073	THR	2.9
1	A	1159	ALA	2.9
1	D	1141	ALA	2.9
1	E	1135	GLY	2.9
1	F	1051	SER	2.8
1	F	1137	ASN	2.8
1	A	1127	VAL	2.8
1	B	1020	VAL	2.8
1	F	1128	VAL	2.8
1	E	1016	PRO	2.8
2	G	102	ALA	2.8
1	F	1111	GLN	2.8
1	F	1053	PHE	2.8
1	D	1155	LYS	2.8
1	F	1077	SER	2.8
1	C	1041	THR	2.8
1	A	1015	GLU	2.8
1	B	1031	LYS	2.8
1	D	1044	LYS	2.8
1	C	1096	GLY	2.8
1	F	1017	LEU	2.8
1	F	1122	LEU	2.8
2	L	102	ALA	2.8
1	B	1063	GLN	2.8
1	D	1148	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	1044	LYS	2.8
1	E	1160	ASP	2.8
1	F	1130	GLY	2.8
1	C	1106	ASN	2.8
1	D	1153	SER	2.8
1	A	1012	VAL	2.8
1	A	1164	LEU	2.8
1	D	1024	LEU	2.7
1	B	1130	GLY	2.7
1	D	1097	ILE	2.7
1	D	1087	ASN	2.7
1	F	1108	ASN	2.7
1	B	1147	SER	2.7
1	E	1154	LYS	2.7
1	A	1104	GLY	2.7
1	C	1094	GLY	2.7
1	C	1135	GLY	2.7
1	F	1036	PHE	2.7
1	C	1121	TRP	2.7
1	D	1131	LYS	2.7
1	B	1093	THR	2.7
1	F	1037	ARG	2.7
1	C	1140	GLU	2.7
1	C	1075	GLY	2.7
1	D	1130	GLY	2.7
1	D	1150	GLY	2.7
1	F	1064	GLY	2.7
1	E	1057	ILE	2.7
1	C	1137	ASN	2.7
1	D	1102	ASN	2.7
1	A	1017	LEU	2.7
1	D	1006	VAL	2.7
1	F	1147	SER	2.7
1	A	1141	ALA	2.7
1	B	1005	THR	2.7
1	B	1014	GLY	2.6
1	C	1059	GLY	2.6
1	B	1131	LYS	2.6
1	C	1033	ALA	2.6
1	D	1121	TRP	2.6
2	J	101	HIS	2.6
1	C	1013	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	1146	GLY	2.6
1	F	1164	LEU	2.6
1	B	1086	GLU	2.6
1	C	1012	VAL	2.6
1	F	1002	VAL	2.6
1	B	1021	SER	2.6
1	B	1116	THR	2.6
1	B	1117	ALA	2.6
1	B	1135	GLY	2.6
1	F	1123	ASP	2.6
1	A	1140	GLU	2.6
1	D	1015	GLU	2.6
1	B	1126	HIS	2.6
1	B	1155	LYS	2.6
2	G	105	ILE	2.6
2	J	105	ILE	2.6
1	B	1122	LEU	2.6
1	C	1024	LEU	2.6
1	C	1043	GLU	2.6
1	E	1002	VAL	2.6
1	E	1038	ALA	2.6
1	E	1159	ALA	2.6
1	C	1069	ARG	2.5
1	B	1056	ILE	2.5
1	B	1078	ILE	2.5
1	F	1020	VAL	2.5
1	C	1044	LYS	2.5
1	D	1031	LYS	2.5
1	A	1152	THR	2.5
1	F	1119	THR	2.5
1	A	1150	GLY	2.5
1	D	1063	GLN	2.5
1	B	1125	LYS	2.5
1	D	1082	LYS	2.5
1	D	1126	HIS	2.5
1	D	1137	ASN	2.5
1	E	1156	ILE	2.5
1	F	1056	ILE	2.5
1	D	1091	LYS	2.5
1	F	1006	VAL	2.5
1	B	1148	ARG	2.5
1	C	1086	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1083	PHE	2.5
1	D	1060	PHE	2.5
1	B	1059	GLY	2.4
1	D	1007	PHE	2.4
1	B	1071	ASN	2.4
1	B	1096	GLY	2.4
1	B	1124	GLY	2.4
1	F	1047	GLY	2.4
1	C	1010	ILE	2.4
1	C	1027	ASP	2.4
1	F	1114	ILE	2.4
1	E	1046	PHE	2.4
1	F	1008	PHE	2.4
1	F	1035	ASN	2.4
1	D	1011	ALA	2.4
1	E	1141	ALA	2.4
1	A	1091	LYS	2.4
1	E	1047	GLY	2.4
1	A	1027	ASP	2.4
1	F	1098	LEU	2.4
1	B	1092	HIS	2.4
1	F	1086	GLU	2.4
1	F	1014	GLY	2.4
1	C	1066	ASP	2.4
1	C	1067	PHE	2.4
1	C	1145	PHE	2.4
1	D	1046	PHE	2.4
2	H	102	ALA	2.4
1	F	1021	SER	2.3
1	D	1114	ILE	2.3
1	A	1060	PHE	2.3
1	A	1129	PHE	2.3
1	A	1031	LYS	2.3
1	B	1076	LYS	2.3
1	E	1117	ALA	2.3
1	D	1144	ARG	2.3
1	D	1147	SER	2.3
1	E	1042	GLY	2.3
1	C	1056	ILE	2.3
1	D	1056	ILE	2.3
1	C	1115	CYS	2.3
1	F	1076	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1087	ASN	2.3
1	D	1033	ALA	2.3
1	E	1011	ALA	2.3
1	D	1018	GLY	2.3
1	E	1051	SER	2.3
1	B	1070	HIS	2.3
1	B	1164	LEU	2.3
1	B	1151	LYS	2.3
1	B	1053	PHE	2.3
1	C	1128	VAL	2.3
1	D	1140	GLU	2.3
1	B	1137	ASN	2.3
1	F	1148	ARG	2.3
1	A	1014	GLY	2.3
1	B	1017	LEU	2.3
1	C	1090	LEU	2.3
1	E	1090	LEU	2.3
1	D	1076	LYS	2.3
1	A	1088	PHE	2.3
1	B	1036	PHE	2.3
1	D	1165	GLU	2.3
1	F	1060	PHE	2.3
1	C	1003	ASN	2.2
1	F	1106	ASN	2.2
1	E	1073	THR	2.2
1	E	1107	THR	2.2
1	A	1045	GLY	2.2
1	A	1118	LYS	2.2
2	K	105	ILE	2.2
1	C	1016	PRO	2.2
1	A	1033	ALA	2.2
1	B	1115	CYS	2.2
1	A	1042	GLY	2.2
1	A	1124	GLY	2.2
1	B	1150	GLY	2.2
2	G	103	GLY	2.2
1	E	1013	ASP	2.2
1	B	1084	GLU	2.2
1	C	1053	PHE	2.2
1	C	1058	PRO	2.2
1	B	1087	ASN	2.2
1	F	1087	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	1149	ASN	2.2
1	B	1054	HIS	2.2
1	D	1054	HIS	2.2
1	F	1092	HIS	2.2
2	I	101	HIS	2.2
1	C	1152	THR	2.2
1	A	1057	ILE	2.2
1	A	1040	SER	2.2
1	A	1105	PRO	2.2
1	C	1046	PHE	2.2
1	B	1068	THR	2.2
1	D	1059	GLY	2.2
1	B	1057	ILE	2.2
1	E	1010	ILE	2.2
1	E	1147	SER	2.2
1	E	1058	PRO	2.2
1	C	1125	LYS	2.2
1	D	1129	PHE	2.2
1	A	1041	THR	2.1
1	B	1064	GLY	2.1
1	E	1075	GLY	2.1
1	A	1078	ILE	2.1
1	B	1089	ILE	2.1
1	C	1078	ILE	2.1
1	C	1097	ILE	2.1
1	D	1156	ILE	2.1
1	D	1110	SER	2.1
1	E	1091	LYS	2.1
1	F	1125	LYS	2.1
1	C	1006	VAL	2.1
2	I	102	ALA	2.1
1	A	1059	GLY	2.1
1	C	1074	GLY	2.1
1	D	1074	GLY	2.1
1	E	1146	GLY	2.1
1	F	1109	GLY	2.1
1	A	1148	ARG	2.1
1	B	1013	ASP	2.1
1	D	1021	SER	2.1
1	D	1160	ASP	2.1
1	E	1139	VAL	2.1
1	D	1101	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1150	GLY	2.1
1	E	1093	THR	2.1
1	F	1165	GLU	2.1
1	B	1027	ASP	2.1
1	F	1007	PHE	2.1
1	A	1072	GLY	2.1
1	F	1045	GLY	2.1
1	C	1068	THR	2.1
1	D	1032	THR	2.1
1	D	1143	GLU	2.1
1	F	1120	GLU	2.1
1	F	1057	ILE	2.1
1	D	1145	PHE	2.0
1	F	1113	PHE	2.0
1	A	1038	ALA	2.0
1	D	1035	ASN	2.0
1	D	1045	GLY	2.0
1	F	1004	PRO	2.0
1	D	1029	VAL	2.0
1	E	1067	PHE	2.0
1	A	1123	ASP	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.