



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 1AWR / pdb_00001awr
Title : CYPA COMPLEXED WITH HAGPIA
Authors : Vajdos, F.F.
Deposited on : 1997-10-04
Resolution : 1.58 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

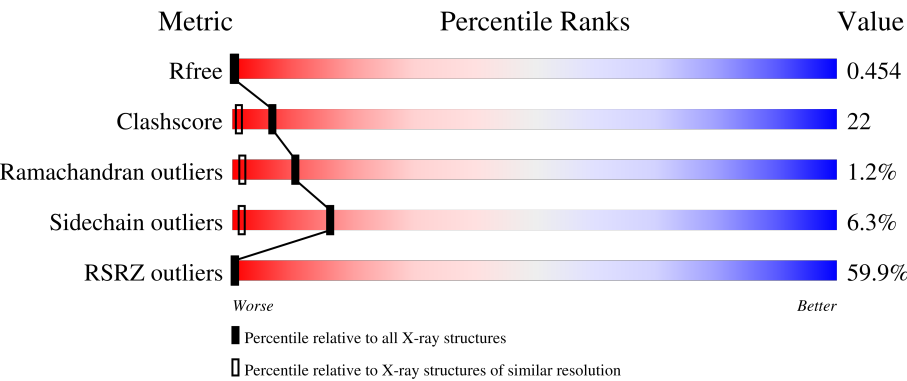
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	33% 64%32% . .
1	B	164	85% 47%45%7% .
1	C	164	68% 60%35% . .
1	D	164	60% 62%34% .
1	E	164	37% 68%25%7%

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Mol	Chain	Length	Quality of chain
1	F	164	77% 57% 38% 5%
2	G	6	67% 50% 17% 33%
2	H	6	67% 67% 33%
2	I	6	33% 50% 50%
2	J	6	50% 67% 33%
2	K	6	50% 67% 33%
2	L	6	83% 83% 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	0	0	0
			1258	797	217	236	8			
1	B	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			
1	C	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			
1	D	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			
1	E	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			
1	F	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			

- 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			

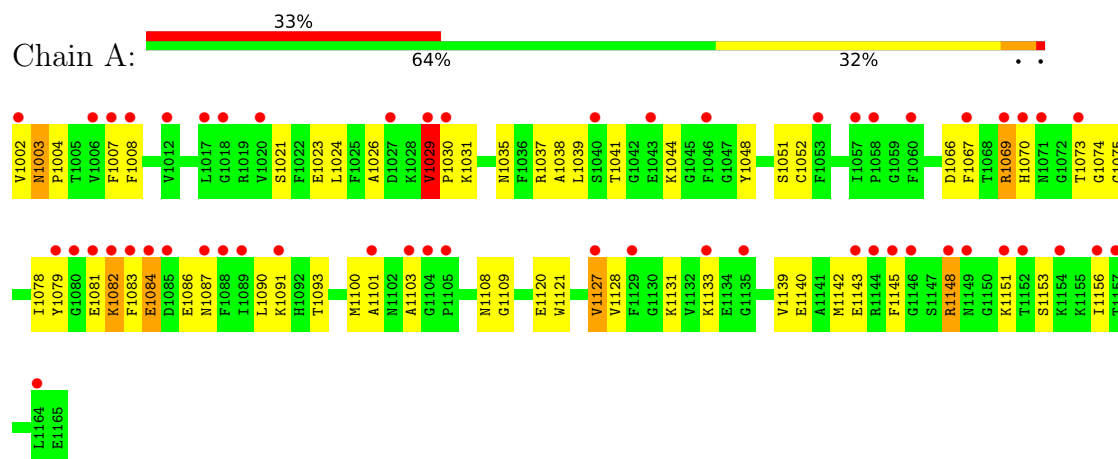
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total 33	O 33	0	0
3	B	22	Total 22	O 22	0	0
3	C	32	Total 32	O 32	0	0
3	D	20	Total 20	O 20	0	0
3	E	29	Total 29	O 29	0	0
3	F	30	Total 30	O 30	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	J	2	Total 2	O 2	0	0
3	K	2	Total 2	O 2	0	0
3	L	1	Total 1	O 1	0	0

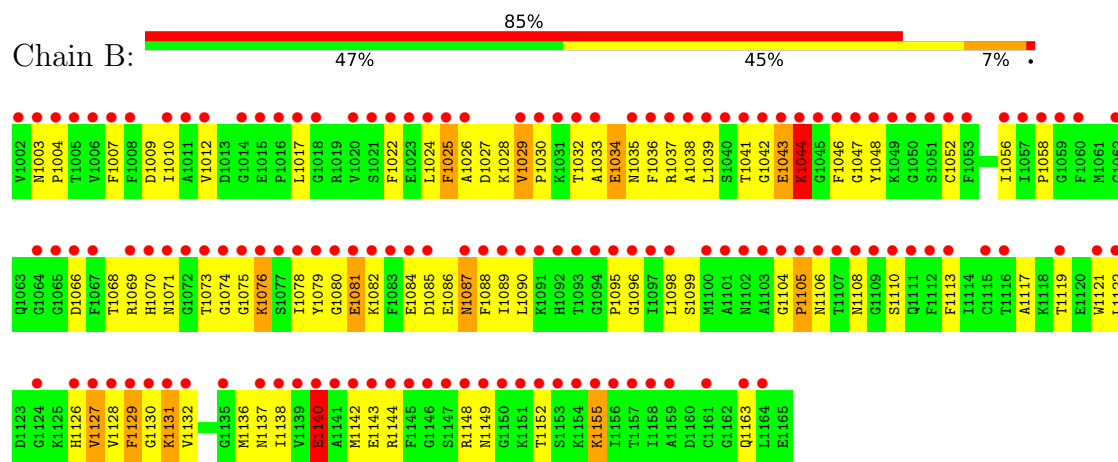
3 Residue-property plots

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.

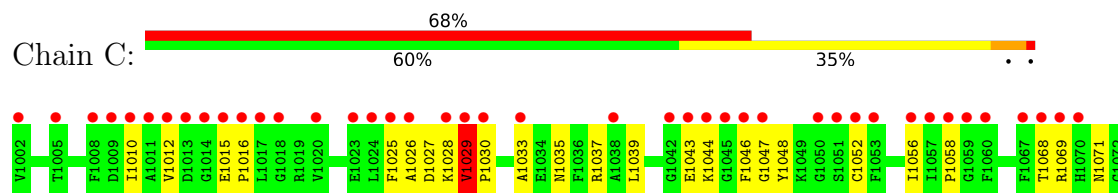
• Molecule 1: CYCLOPHILIN A

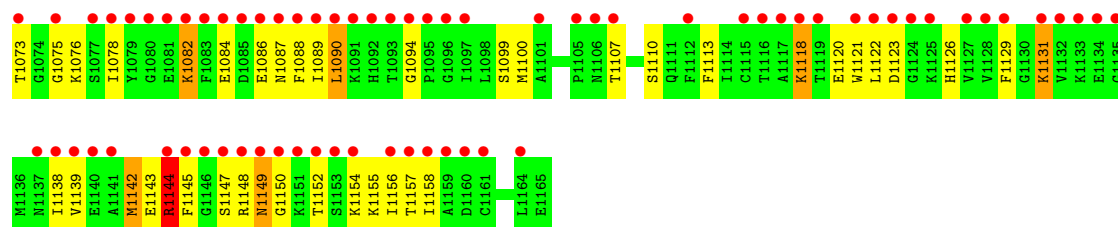


• Molecule 1: CYCLOPHILIN A

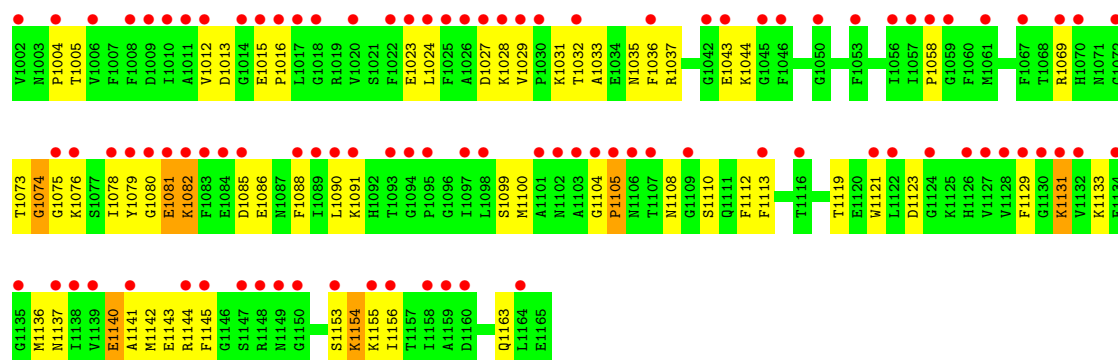


• Molecule 1: CYCLOPHILIN A

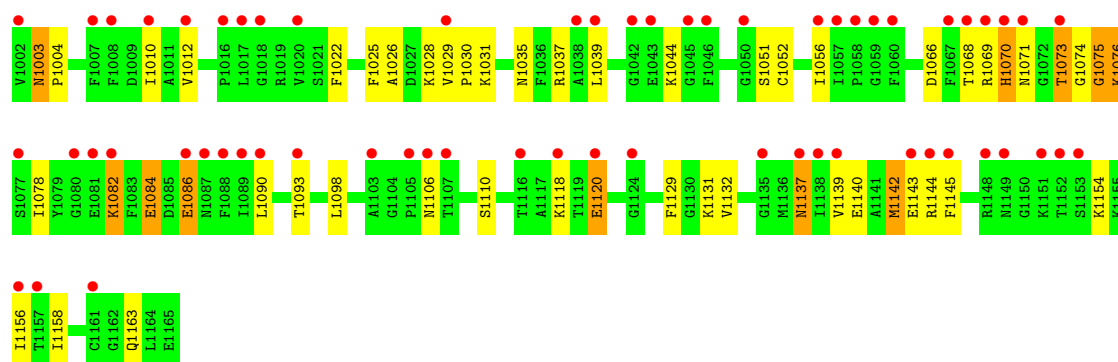




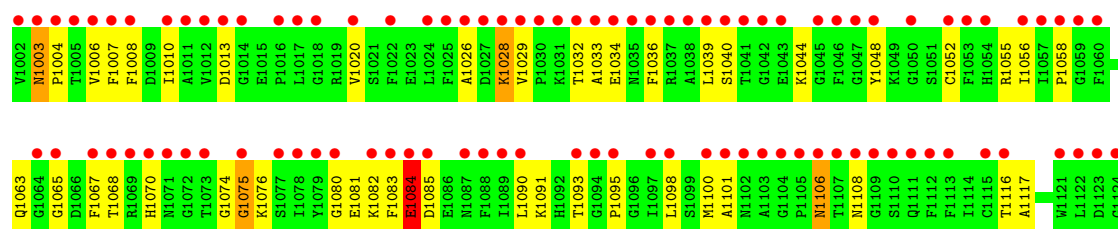
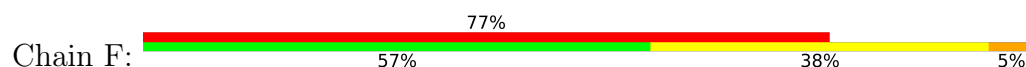
• Molecule 1: CYCLOPHILIN A



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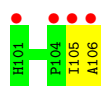




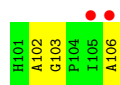
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



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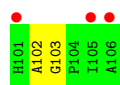
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



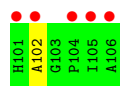
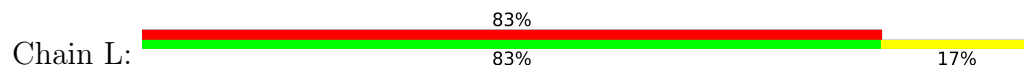
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	72.91Å 72.91Å 188.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.58 15.00 – 1.58	Depositor EDS
% Data completeness (in resolution range)	88.3 (15.00-1.58) 84.0 (15.00-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.53Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.394 , 0.461 0.391 , 0.454	Depositor DCC
R_{free} test set	6255 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	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 82.07 % 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 3.0506e-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 [i](#)

5.1 Standard geometry [i](#)

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	0.74	0/1286	1.14	6/1723 (0.3%)
1	B	0.72	0/1286	1.15	9/1723 (0.5%)
1	C	0.71	0/1286	1.13	10/1723 (0.6%)
1	D	0.68	0/1286	1.08	5/1723 (0.3%)
1	E	0.77	0/1286	1.13	7/1723 (0.4%)
1	F	0.76	0/1286	1.18	9/1723 (0.5%)
2	G	0.84	0/41	1.43	1/54 (1.9%)
2	H	0.78	0/41	0.99	0/54
2	I	0.85	0/41	1.89	3/54 (5.6%)
2	J	0.85	0/41	1.44	0/54
2	K	1.05	0/41	1.66	3/54 (5.6%)
2	L	0.78	0/41	0.78	0/54
All	All	0.73	0/7962	1.15	53/10662 (0.5%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1075	GLY	N-CA-C	-8.41	103.96	111.95
1	F	1147	SER	N-CA-C	8.30	122.74	109.79
1	A	1003	ASN	CA-C-N	8.25	128.18	119.85
1	A	1003	ASN	C-N-CA	8.25	128.18	119.85
1	B	1048	TYR	N-CA-C	7.55	121.75	112.54
1	E	1075	GLY	N-CA-C	-7.19	103.31	112.65
1	D	1074	GLY	N-CA-C	7.14	121.12	111.20
1	D	1081	GLU	N-CA-C	-6.95	103.93	113.18
1	C	1138	ILE	N-CA-C	-6.92	105.01	111.45
1	F	1003	ASN	CA-C-N	6.68	126.60	119.85
1	F	1003	ASN	C-N-CA	6.68	126.60	119.85
1	E	1084	GLU	N-CA-C	6.64	119.52	110.55
1	B	1044	LYS	N-CA-C	-6.59	105.16	113.72
1	D	1104	GLY	CA-C-N	6.50	127.97	119.84
1	D	1104	GLY	C-N-CA	6.50	127.97	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1142	MET	N-CA-C	-6.42	105.10	113.12
2	I	102	ALA	N-CA-C	6.38	120.03	110.14
1	C	1084	GLU	N-CA-C	6.17	119.60	110.46
1	B	1104	GLY	CA-C-N	6.16	127.54	119.84
1	B	1104	GLY	C-N-CA	6.16	127.54	119.84
1	F	1155	LYS	N-CA-C	6.06	118.06	108.67
2	I	103	GLY	CA-C-N	6.00	126.19	120.31
2	I	103	GLY	C-N-CA	6.00	126.19	120.31
1	C	1029	VAL	CA-C-N	5.93	125.40	119.24
1	C	1029	VAL	C-N-CA	5.93	125.40	119.24
2	G	102	ALA	N-CA-C	5.91	119.34	109.95
1	A	1093	THR	N-CA-C	5.88	120.18	112.89
1	E	1093	THR	N-CA-C	5.88	119.71	112.54
1	C	1047	GLY	N-CA-C	5.85	118.76	110.74
1	B	1079	TYR	N-CA-C	-5.83	106.50	113.21
1	E	1003	ASN	CA-C-N	5.70	125.63	119.76
1	E	1003	ASN	C-N-CA	5.70	125.63	119.76
1	C	1048	TYR	N-CA-C	5.58	119.25	112.23
2	K	102	ALA	N-CA-C	5.52	119.06	110.17
1	B	1155	LYS	N-CA-C	5.51	118.34	107.98
1	B	1137	ASN	N-CA-C	-5.50	106.41	113.23
1	F	1040	SER	N-CA-C	-5.50	106.70	113.41
1	A	1075	GLY	N-CA-C	-5.46	105.80	112.68
1	B	1127	VAL	CB-CA-C	-5.46	105.40	111.35
1	F	1093	THR	N-CA-C	5.41	119.60	112.89
1	A	1029	VAL	CA-C-N	5.39	126.57	119.84
1	A	1029	VAL	C-N-CA	5.39	126.57	119.84
1	C	1094	GLY	CA-C-N	5.36	125.28	119.76
1	C	1094	GLY	C-N-CA	5.36	125.28	119.76
1	E	1106	ASN	N-CA-C	5.33	119.06	112.24
1	B	1140	GLU	N-CA-C	-5.31	106.75	113.18
1	F	1032	THR	N-CA-C	-5.21	105.68	111.36
2	K	103	GLY	CA-C-N	5.21	127.07	120.51
2	K	103	GLY	C-N-CA	5.21	127.07	120.51
1	F	1084	GLU	N-CA-C	5.19	117.23	110.43
1	D	1137	ASN	N-CA-C	-5.13	107.02	113.28
1	C	1118	LYS	N-CA-C	-5.02	101.57	109.25
1	E	1144	ARG	N-CA-C	-5.00	106.86	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1258	0	1225	42	0
1	B	1258	0	1225	72	0
1	C	1258	0	1225	63	0
1	D	1258	0	1225	51	0
1	E	1258	0	1225	41	0
1	F	1258	0	1225	64	0
2	G	40	0	37	3	0
2	H	40	0	37	1	0
2	I	40	0	37	1	0
2	J	40	0	37	2	0
2	K	40	0	37	0	0
2	L	40	0	37	1	0
3	A	33	0	0	7	0
3	B	22	0	0	6	0
3	C	32	0	0	4	0
3	D	20	0	0	3	0
3	E	29	0	0	0	0
3	F	30	0	0	12	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	1	0	0	0	0
All	All	7963	0	7572	333	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 22.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1100:MET:HB2	1:F:1127:VAL:HG23	1.39	1.02
1:E:1069:ARG:HG2	1:E:1073:THR:HG22	1.48	0.93
1:F:1052:CYS:HB3	1:F:1155:LYS:HE2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1148:ARG:HH11	1:C:1148:ARG:HA	1.36	0.90
1:F:1048:TYR:HA	3:F:7016:HOH:O	1.70	0.90
1:E:1137:ASN:HD22	1:E:1137:ASN:H	1.13	0.90
1:A:1048:TYR:HA	3:A:7165:HOH:O	1.69	0.89
1:F:1010:ILE:HG13	1:F:1142:MET:HE1	1.52	0.89
1:D:1023:GLU:HB2	1:D:1133:LYS:HE2	1.58	0.85
1:C:1090:LEU:HD12	1:C:1090:LEU:H	1.47	0.78
1:A:1127:VAL:HG11	3:A:7142:HOH:O	1.85	0.77
1:B:1024:LEU:HB3	1:B:1033:ALA:HB1	1.65	0.77
1:A:1067:PHE:HB3	3:A:7165:HOH:O	1.86	0.76
1:A:1100:MET:HB2	1:A:1127:VAL:HG23	1.66	0.75
1:D:1029:VAL:HG12	1:D:1032:THR:HB	1.69	0.75
1:C:1155:LYS:NZ	1:C:1155:LYS:HB3	2.01	0.74
1:C:1025:PHE:HZ	1:C:1131:LYS:HD2	1.53	0.73
1:B:1138:ILE:O	1:B:1142:MET:HE3	1.87	0.73
1:B:1041:THR:OG1	1:B:1043:GLU:HG2	1.89	0.73
1:B:1038:ALA:HB1	1:B:1044:LYS:HD3	1.70	0.72
1:B:1044:LYS:HG2	1:B:1078:ILE:HG21	1.71	0.72
1:E:1137:ASN:HD22	1:E:1137:ASN:N	1.84	0.72
1:C:1148:ARG:HA	1:C:1148:ARG:NH1	2.05	0.72
1:F:1058:PRO:HD3	1:F:1146:GLY:O	1.92	0.70
1:D:1023:GLU:CB	1:D:1133:LYS:HE2	2.22	0.70
1:F:1052:CYS:CB	1:F:1155:LYS:HE2	2.20	0.70
1:C:1090:LEU:HD12	1:C:1090:LEU:N	2.04	0.70
1:C:1035:ASN:O	1:C:1039:LEU:HG	1.92	0.69
1:F:1084:GLU:HA	1:F:1106:ASN:HA	1.74	0.69
1:E:1044:LYS:HZ2	1:E:1078:ILE:HB	1.58	0.69
1:B:1032:THR:HG22	1:B:1129:PHE:CD2	2.28	0.69
1:D:1024:LEU:HB3	1:D:1033:ALA:HB1	1.75	0.69
1:E:1137:ASN:H	1:E:1137:ASN:ND2	1.90	0.69
1:C:1044:LYS:HG2	1:C:1078:ILE:HB	1.75	0.69
1:F:1146:GLY:HA2	1:F:1152:THR:HA	1.74	0.68
1:F:1127:VAL:HA	3:F:7029:HOH:O	1.94	0.68
1:F:1145:PHE:HB2	1:F:1156:ILE:HD11	1.75	0.68
1:B:1044:LYS:HB2	3:B:7163:HOH:O	1.94	0.68
1:A:1148:ARG:HA	1:A:1148:ARG:NE	2.09	0.68
1:D:1036:PHE:HB2	1:D:1129:PHE:HE2	1.58	0.68
1:D:1028:LYS:HD3	1:D:1090:LEU:HD21	1.75	0.67
1:D:1029:VAL:CG1	1:D:1032:THR:HB	2.25	0.67
1:D:1121:TRP:NE1	2:J:106:ALA:HB3	2.10	0.67
1:F:1074:GLY:HA2	3:F:7065:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:VAL:HG12	1:B:1032:THR:HB	1.78	0.66
1:B:1149:ASN:ND2	1:B:1149:ASN:H	1.95	0.65
1:B:1090:LEU:HB2	1:B:1128:VAL:HB	1.80	0.64
1:C:1144:ARG:C	1:C:1145:PHE:HD1	2.06	0.64
1:A:1026:ALA:O	1:A:1030:PRO:HG3	1.98	0.63
1:B:1030:PRO:O	1:B:1034:GLU:HB2	1.99	0.63
1:F:1076:LYS:HA	3:F:7002:HOH:O	1.97	0.63
1:E:1056:ILE:HG21	1:E:1143:GLU:HA	1.81	0.63
1:E:1082:LYS:H	1:E:1082:LYS:HD3	1.63	0.62
1:E:1118:LYS:HZ2	1:E:1120:GLU:HB3	1.64	0.62
1:B:1087:ASN:HD22	1:B:1087:ASN:N	1.96	0.62
1:D:1012:VAL:CG1	1:D:1154:LYS:HD3	2.30	0.62
1:B:1089:ILE:HG22	1:B:1090:LEU:HD23	1.82	0.62
1:C:1012:VAL:HG21	1:C:1145:PHE:HE2	1.64	0.62
1:B:1044:LYS:HG2	1:B:1078:ILE:CG2	2.30	0.61
1:B:1037:ARG:O	1:B:1041:THR:HG23	2.01	0.61
1:B:1096:GLY:HA2	1:B:1136:MET:SD	2.41	0.61
1:C:1139:VAL:HA	1:C:1142:MET:HE2	1.81	0.60
1:E:1118:LYS:NZ	1:E:1120:GLU:HB3	2.17	0.60
1:A:1073:THR:HG22	1:A:1073:THR:O	2.01	0.60
1:A:1035:ASN:O	1:A:1039:LEU:HG	2.02	0.59
1:B:1127:VAL:HG23	3:B:7118:HOH:O	2.02	0.59
1:D:1058:PRO:HA	1:D:1143:GLU:HG3	1.84	0.59
1:F:1145:PHE:CB	1:F:1156:ILE:HD11	2.32	0.59
1:F:1044:LYS:HB2	3:F:7004:HOH:O	2.02	0.59
1:A:1103:ALA:CB	2:G:101:HIS:CE1	2.85	0.59
1:F:1052:CYS:HB2	1:F:1156:ILE:O	2.03	0.59
1:B:1085:ASP:HA	1:B:1108:ASN:ND2	2.19	0.58
1:D:1131:LYS:O	1:D:1131:LYS:HD3	2.02	0.58
1:B:1056:ILE:HD12	1:B:1152:THR:HG21	1.85	0.58
1:C:1121:TRP:NE1	2:I:106:ALA:HB3	2.18	0.58
1:F:1036:PHE:HB2	1:F:1129:PHE:HE2	1.68	0.58
1:B:1085:ASP:HA	1:B:1108:ASN:HD21	1.69	0.58
1:B:1084:GLU:HB2	1:B:1106:ASN:OD1	2.03	0.57
1:C:1025:PHE:CD2	1:C:1090:LEU:HD22	2.40	0.57
1:D:1076:LYS:O	1:D:1110:SER:HB3	2.03	0.57
1:A:1029:VAL:HG12	1:A:1086:GLU:OE1	2.05	0.57
1:D:1012:VAL:HG11	1:D:1154:LYS:HD3	1.87	0.57
1:C:1143:GLU:C	1:C:1145:PHE:H	2.12	0.57
1:F:1148:ARG:HA	1:F:1148:ARG:NE	2.20	0.57
1:D:1085:ASP:HA	1:D:1108:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1149:ASN:C	1:C:1149:ASN:HD22	2.13	0.56
1:C:1155:LYS:HB3	1:C:1155:LYS:HZ3	1.69	0.56
1:B:1121:TRP:NE1	2:H:106:ALA:HB3	2.21	0.56
1:F:1136:MET:HG2	3:F:7149:HOH:O	2.04	0.56
1:A:1002:VAL:HG23	1:A:1003:ASN:H	1.70	0.56
1:C:1012:VAL:HG21	1:C:1145:PHE:CE2	2.41	0.55
1:C:1012:VAL:HG11	1:C:1145:PHE:CE2	2.42	0.55
1:C:1025:PHE:CZ	1:C:1131:LYS:HD2	2.38	0.55
1:F:1068:THR:HG23	1:F:1075:GLY:HA2	1.87	0.55
1:C:1058:PRO:HA	1:C:1143:GLU:HG3	1.87	0.55
1:D:1035:ASN:HB2	1:D:1079:TYR:HE2	1.71	0.55
1:B:1010:ILE:HG13	1:B:1142:MET:CE	2.36	0.55
1:E:1069:ARG:HD3	1:E:1074:GLY:HA3	1.88	0.55
1:F:1028:LYS:HB3	3:F:7048:HOH:O	2.07	0.55
1:A:1083:PHE:O	1:A:1108:ASN:HB2	2.07	0.54
1:A:1109:GLY:HA3	3:A:7113:HOH:O	2.06	0.54
1:D:1012:VAL:HA	1:D:1155:LYS:O	2.06	0.54
1:D:1088:PHE:HA	3:D:7060:HOH:O	2.06	0.54
1:F:1101:ALA:O	2:L:102:ALA:HB1	2.07	0.54
1:C:1028:LYS:C	1:C:1030:PRO:HD3	2.33	0.54
1:B:1132:VAL:HG21	1:B:1136:MET:SD	2.48	0.54
1:E:1044:LYS:NZ	1:E:1078:ILE:HB	2.23	0.54
1:F:1029:VAL:HG13	3:F:7048:HOH:O	2.07	0.54
1:A:1142:MET:HE3	1:A:1156:ILE:HG21	1.89	0.54
1:B:1136:MET:HG2	3:B:7094:HOH:O	2.06	0.53
1:F:1090:LEU:C	1:F:1091:LYS:HD2	2.33	0.53
1:E:1026:ALA:O	1:E:1030:PRO:HG3	2.08	0.53
1:E:1035:ASN:O	1:E:1039:LEU:HG	2.09	0.53
1:B:1052:CYS:CB	1:B:1155:LYS:HE3	2.39	0.53
1:D:1073:THR:HG22	1:D:1073:THR:O	2.08	0.53
1:E:1139:VAL:O	1:E:1142:MET:HB2	2.08	0.52
1:B:1122:LEU:HD22	1:B:1126:HIS:CD2	2.44	0.52
1:E:1076:LYS:O	1:E:1110:SER:HB3	2.09	0.52
1:B:1037:ARG:NH1	1:B:1038:ALA:HA	2.25	0.52
1:D:1119:THR:HA	1:D:1121:TRP:CZ3	2.45	0.52
1:D:1153:SER:O	1:D:1154:LYS:HG3	2.10	0.52
1:C:1145:PHE:CD2	1:C:1156:ILE:HD11	2.45	0.52
1:A:1052:CYS:HB2	1:A:1156:ILE:O	2.10	0.52
1:C:1025:PHE:HB2	1:C:1029:VAL:HG23	1.92	0.52
1:B:1022:PHE:CD1	1:B:1098:LEU:HD22	2.45	0.52
1:D:1099:SER:HB3	1:D:1113:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1138:ILE:HG22	1:F:1142:MET:CE	2.39	0.52
1:D:1044:LYS:HB2	3:D:7103:HOH:O	2.09	0.51
1:F:1067:PHE:HB3	3:F:7016:HOH:O	2.11	0.51
1:F:1098:LEU:HG	1:F:1129:PHE:CE1	2.45	0.51
1:F:1131:LYS:HG2	1:F:1132:VAL:N	2.25	0.51
1:B:1012:VAL:CG2	1:B:1017:LEU:HD22	2.41	0.51
1:C:1123:ASP:HA	3:C:7028:HOH:O	2.10	0.51
1:D:1023:GLU:CA	1:D:1133:LYS:HE2	2.41	0.51
1:B:1024:LEU:HD13	1:B:1033:ALA:O	2.11	0.51
1:C:1030:PRO:HD2	1:C:1086:GLU:OE2	2.10	0.51
1:D:1069:ARG:HG2	1:D:1074:GLY:HA3	1.92	0.51
1:C:1012:VAL:HG11	1:C:1145:PHE:HE2	1.76	0.50
1:E:1028:LYS:C	1:E:1030:PRO:HD3	2.36	0.50
1:E:1052:CYS:HB2	1:E:1156:ILE:O	2.12	0.50
1:F:1090:LEU:HD12	3:F:7048:HOH:O	2.11	0.50
1:A:1066:ASP:O	1:A:1070:HIS:HA	2.12	0.50
1:E:1143:GLU:C	1:E:1145:PHE:H	2.20	0.50
1:F:1056:ILE:HB	1:F:1146:GLY:HA3	1.94	0.50
1:B:1149:ASN:H	1:B:1149:ASN:HD22	1.58	0.50
1:C:1058:PRO:HG2	3:C:7108:HOH:O	2.12	0.50
1:B:1029:VAL:CG1	1:B:1032:THR:HB	2.40	0.49
1:C:1145:PHE:HD2	1:C:1156:ILE:HD11	1.77	0.49
1:A:1090:LEU:HB2	1:A:1128:VAL:HB	1.94	0.49
1:F:1055:ARG:HA	1:F:1150:GLY:O	2.13	0.49
1:B:1028:LYS:HD3	1:B:1090:LEU:HD21	1.93	0.49
1:B:1073:THR:HG22	1:B:1073:THR:O	2.13	0.49
1:F:1137:ASN:N	1:F:1137:ASN:HD22	2.10	0.49
1:E:1143:GLU:C	1:E:1145:PHE:N	2.71	0.49
1:A:1082:LYS:H	1:A:1082:LYS:HD3	1.78	0.49
1:B:1025:PHE:CD2	1:B:1130:GLY:HA2	2.48	0.49
1:B:1121:TRP:HH2	3:B:7036:HOH:O	1.94	0.49
1:E:1068:THR:HG1	1:E:1075:GLY:H	1.57	0.49
1:B:1027:ASP:OD1	1:B:1028:LYS:HG3	2.12	0.49
1:B:1029:VAL:HG21	1:B:1128:VAL:O	2.12	0.49
1:E:1142:MET:HE2	1:E:1156:ILE:HG21	1.95	0.49
1:F:1007:PHE:O	1:F:1008:PHE:HD1	1.96	0.49
1:F:1076:LYS:HB2	1:F:1080:GLY:O	2.12	0.49
1:F:1137:ASN:HD22	1:F:1137:ASN:H	1.61	0.49
1:C:1087:ASN:CG	1:C:1089:ILE:HD12	2.37	0.48
1:D:1081:GLU:HB3	1:D:1082:LYS:NZ	2.28	0.48
1:F:1085:ASP:HA	1:F:1108:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1048:TYR:CE1	1:F:1065:GLY:HA2	2.49	0.48
1:F:1116:THR:HG21	1:F:1143:GLU:CD	2.38	0.48
1:B:1081:GLU:OE1	1:B:1081:GLU:N	2.46	0.48
1:B:1140:GLU:O	1:B:1143:GLU:HB2	2.13	0.48
1:C:1147:SER:OG	1:C:1148:ARG:N	2.47	0.48
1:B:1082:LYS:HB2	3:B:7032:HOH:O	2.14	0.48
1:B:1038:ALA:HB3	1:B:1078:ILE:HD13	1.95	0.48
1:C:1118:LYS:HE2	1:C:1120:GLU:HB3	1.96	0.48
1:D:1075:GLY:HA3	1:D:1110:SER:OG	2.13	0.48
1:B:1026:ALA:O	1:B:1030:PRO:HB3	2.14	0.48
1:C:1029:VAL:HG13	1:C:1087:ASN:HD21	1.79	0.48
1:A:1145:PHE:HB2	1:A:1156:ILE:HD11	1.96	0.47
1:B:1088:PHE:HA	3:B:7001:HOH:O	2.14	0.47
1:C:1088:PHE:HA	3:C:7133:HOH:O	2.15	0.47
1:A:1069:ARG:HE	1:A:1074:GLY:HA3	1.78	0.47
1:F:1132:VAL:HG21	1:F:1136:MET:SD	2.55	0.47
1:A:1127:VAL:HA	3:A:7044:HOH:O	2.14	0.47
1:B:1066:ASP:O	1:B:1070:HIS:HA	2.15	0.47
1:B:1119:THR:HA	1:B:1121:TRP:CZ3	2.50	0.47
1:C:1028:LYS:NZ	1:C:1090:LEU:HG	2.29	0.47
1:D:1100:MET:SD	1:D:1129:PHE:CZ	3.07	0.47
1:C:1143:GLU:C	1:C:1145:PHE:N	2.73	0.47
1:C:1099:SER:HB3	1:C:1113:PHE:CZ	2.50	0.46
1:D:1085:ASP:HA	1:D:1108:ASN:ND2	2.29	0.46
1:D:1145:PHE:HD2	1:D:1156:ILE:HD11	1.79	0.46
1:A:1023:GLU:HB2	1:A:1133:LYS:HD2	1.96	0.46
1:B:1099:SER:HB3	1:B:1113:PHE:CZ	2.51	0.46
1:F:1090:LEU:CB	1:F:1128:VAL:HB	2.45	0.46
1:B:1078:ILE:C	1:B:1080:GLY:H	2.24	0.46
1:C:1037:ARG:NH2	1:C:1043:GLU:OE2	2.48	0.46
1:C:1142:MET:SD	1:C:1156:ILE:HG21	2.56	0.46
1:E:1012:VAL:CG1	1:E:1154:LYS:HD3	2.46	0.46
1:F:1006:VAL:HA	1:F:1163:GLN:HA	1.97	0.46
1:F:1090:LEU:HB3	1:F:1128:VAL:CG1	2.46	0.46
1:E:1010:ILE:HD12	1:E:1142:MET:HE3	1.98	0.46
1:E:1071:ASN:OD1	1:E:1073:THR:HB	2.16	0.46
1:B:1058:PRO:HB2	1:B:1148:ARG:NH2	2.31	0.46
1:D:1121:TRP:HE1	2:J:106:ALA:HB3	1.79	0.46
1:D:1142:MET:HE2	1:D:1142:MET:HB2	1.81	0.46
1:E:1069:ARG:HD2	1:E:1069:ARG:N	2.31	0.46
1:B:1131:LYS:HD2	1:B:1132:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1028:LYS:CD	1:D:1090:LEU:HD21	2.42	0.46
1:C:1143:GLU:O	1:C:1145:PHE:N	2.49	0.45
1:C:1145:PHE:N	1:C:1145:PHE:CD1	2.82	0.45
1:D:1145:PHE:CD1	1:D:1154:LYS:HD2	2.51	0.45
1:A:1101:ALA:O	2:G:102:ALA:HB1	2.16	0.45
1:C:1076:LYS:O	1:C:1110:SER:HB3	2.16	0.45
1:F:1008:PHE:HB2	1:F:1020:VAL:HG13	1.98	0.45
1:A:1044:LYS:HB2	3:A:7013:HOH:O	2.16	0.45
1:B:1095:PRO:HG3	1:B:1117:ALA:HA	1.98	0.45
1:B:1056:ILE:HB	1:B:1152:THR:CG2	2.47	0.45
1:F:1003:ASN:HA	1:F:1004:PRO:HD3	1.78	0.45
1:C:1145:PHE:CD2	1:C:1154:LYS:HD2	2.51	0.44
1:A:1073:THR:O	1:A:1073:THR:CG2	2.65	0.44
1:D:1031:LYS:HB3	1:D:1086:GLU:CD	2.42	0.44
1:E:1073:THR:O	1:E:1073:THR:CG2	2.64	0.44
1:F:1148:ARG:HA	1:F:1148:ARG:HE	1.83	0.44
1:B:1036:PHE:HB2	1:B:1129:PHE:HE2	1.82	0.44
1:F:1058:PRO:HG3	1:F:1143:GLU:O	2.17	0.44
1:F:1055:ARG:HB3	1:F:1063:GLN:HB3	2.00	0.44
1:A:1140:GLU:O	1:A:1143:GLU:HB2	2.18	0.44
1:B:1012:VAL:HG23	1:B:1017:LEU:HD22	2.00	0.43
1:C:1026:ALA:HA	1:C:1033:ALA:HB3	1.99	0.43
1:D:1005:THR:O	1:D:1163:GLN:HG3	2.18	0.43
1:E:1131:LYS:HE3	1:E:1131:LYS:HB3	1.82	0.43
1:B:1132:VAL:HG11	1:B:1136:MET:HA	2.00	0.43
1:E:1025:PHE:CD2	1:E:1090:LEU:HD13	2.53	0.43
1:E:1044:LYS:NZ	1:E:1078:ILE:HD12	2.34	0.43
1:C:1056:ILE:HG21	1:C:1143:GLU:HA	2.00	0.43
1:A:1007:PHE:O	1:A:1008:PHE:HD1	2.02	0.43
1:A:1139:VAL:O	1:A:1143:GLU:HG2	2.18	0.43
1:D:1037:ARG:HH22	1:D:1043:GLU:CD	2.26	0.43
1:F:1145:PHE:O	1:F:1152:THR:HG22	2.18	0.43
1:A:1083:PHE:N	1:A:1108:ASN:O	2.45	0.43
1:B:1035:ASN:ND2	1:B:1039:LEU:HD12	2.33	0.43
1:D:1032:THR:HG22	1:D:1129:PHE:CD2	2.54	0.43
1:F:1013:ASP:OD2	1:F:1154:LYS:HD3	2.17	0.43
1:F:1039:LEU:HD23	1:F:1039:LEU:HA	1.79	0.43
1:F:1100:MET:HB2	1:F:1127:VAL:CG2	2.30	0.43
1:C:1028:LYS:HZ3	1:C:1090:LEU:HD11	1.83	0.43
1:E:1070:HIS:ND1	1:E:1070:HIS:N	2.67	0.43
1:A:1087:ASN:O	1:A:1127:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:PRO:HB3	1:B:1163:GLN:NE2	2.33	0.43
1:E:1029:VAL:HG21	1:E:1129:PHE:HA	2.00	0.42
1:B:1075:GLY:HA3	1:B:1110:SER:OG	2.19	0.42
1:C:1044:LYS:HE2	1:C:1078:ILE:HD12	2.01	0.42
1:F:1095:PRO:HG3	1:F:1117:ALA:HA	2.01	0.42
1:C:1046:PHE:HZ	1:C:1078:ILE:HA	1.84	0.42
1:C:1100:MET:SD	1:C:1129:PHE:CE1	3.12	0.42
1:D:1012:VAL:O	1:D:1013:ASP:HB2	2.18	0.42
1:E:1037:ARG:HD2	1:E:1163:GLN:NE2	2.34	0.42
1:A:1038:ALA:HB3	1:A:1078:ILE:HG21	2.01	0.42
1:D:1044:LYS:HG3	1:D:1078:ILE:HG21	2.00	0.42
1:D:1119:THR:HA	1:D:1121:TRP:CH2	2.54	0.42
1:F:1008:PHE:HB2	1:F:1020:VAL:CG1	2.48	0.42
1:C:1056:ILE:O	1:C:1150:GLY:HA2	2.19	0.42
1:F:1052:CYS:HA	1:F:1157:THR:HA	2.01	0.42
1:E:1044:LYS:HZ2	1:E:1078:ILE:HD12	1.85	0.42
1:C:1027:ASP:OD1	1:C:1027:ASP:N	2.48	0.42
1:D:1141:ALA:HA	1:D:1144:ARG:HE	1.84	0.42
1:D:1091:LYS:HE2	1:D:1123:ASP:OD2	2.20	0.42
1:D:1145:PHE:CD2	1:D:1156:ILE:HD11	2.54	0.42
1:E:1098:LEU:HG	1:E:1129:PHE:CZ	2.55	0.42
1:A:1090:LEU:CB	1:A:1128:VAL:HB	2.49	0.42
1:C:1010:ILE:HG21	1:C:1142:MET:SD	2.60	0.42
1:C:1122:LEU:HB3	1:C:1126:HIS:HD2	1.84	0.42
1:B:1003:ASN:HD22	1:B:1026:ALA:H	1.67	0.42
1:B:1007:PHE:HE2	1:B:1009:ASP:OD2	2.02	0.42
1:C:1028:LYS:HZ3	1:C:1090:LEU:CG	2.33	0.42
1:F:1139:VAL:HA	1:F:1142:MET:HE3	2.02	0.42
1:B:1046:PHE:HE2	1:B:1076:LYS:O	2.03	0.41
1:B:1148:ARG:HE	1:B:1148:ARG:HA	1.85	0.41
1:F:1070:HIS:CD2	3:F:7161:HOH:O	2.73	0.41
1:A:1051:SER:N	3:A:7151:HOH:O	2.53	0.41
1:E:1003:ASN:HA	1:E:1004:PRO:HD3	1.73	0.41
1:E:1031:LYS:HE2	1:E:1084:GLU:OE2	2.21	0.41
1:B:1087:ASN:N	1:B:1087:ASN:ND2	2.67	0.41
1:C:1052:CYS:HB2	1:C:1156:ILE:O	2.20	0.41
1:D:1090:LEU:HG	3:D:7137:HOH:O	2.21	0.41
1:C:1071:ASN:OD1	1:C:1073:THR:HB	2.20	0.41
1:C:1082:LYS:HG3	1:C:1107:THR:HA	2.01	0.41
1:C:1145:PHE:HD1	1:C:1145:PHE:N	2.18	0.41
1:D:1027:ASP:OD1	1:D:1028:LYS:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1012:VAL:HG12	1:E:1154:LYS:HD3	2.03	0.41
1:F:1116:THR:HG21	1:F:1143:GLU:OE2	2.20	0.41
1:A:1121:TRP:CD1	2:G:106:ALA:HB3	2.55	0.41
1:B:1003:ASN:ND2	1:B:1026:ALA:H	2.18	0.41
1:C:1069:ARG:HB3	1:C:1071:ASN:OD1	2.20	0.41
1:D:1119:THR:HG22	1:D:1121:TRP:CZ2	2.56	0.41
1:B:1039:LEU:O	1:B:1047:GLY:HA3	2.21	0.41
1:B:1068:THR:OG1	1:B:1074:GLY:HA3	2.21	0.41
1:D:1004:PRO:HB3	1:D:1163:GLN:NE2	2.36	0.41
1:E:1073:THR:O	1:E:1073:THR:HG23	2.21	0.41
1:F:1145:PHE:CE1	1:F:1154:LYS:HD2	2.56	0.41
1:A:1003:ASN:HA	1:A:1004:PRO:HD3	1.63	0.41
1:E:1051:SER:OG	1:E:1158:ILE:HD12	2.20	0.41
1:F:1026:ALA:HA	1:F:1033:ALA:CB	2.50	0.41
1:A:1024:LEU:HD12	1:A:1037:ARG:HB2	2.03	0.41
1:A:1031:LYS:HE3	1:A:1079:TYR:CD2	2.56	0.41
1:B:1028:LYS:HD2	1:B:1090:LEU:HD11	2.02	0.41
1:B:1042:GLY:HA2	1:B:1046:PHE:O	2.21	0.41
1:C:1068:THR:HG1	1:C:1075:GLY:H	1.65	0.41
1:C:1152:THR:HG21	3:C:7092:HOH:O	2.21	0.41
1:D:1136:MET:HE3	1:D:1140:GLU:OE1	2.20	0.41
1:F:1091:LYS:HD2	1:F:1091:LYS:N	2.35	0.41
1:F:1138:ILE:HG22	1:F:1142:MET:HE2	2.02	0.41
1:A:1090:LEU:C	1:A:1091:LYS:HD2	2.45	0.41
1:C:1012:VAL:CG2	1:C:1145:PHE:HE2	2.33	0.41
1:C:1157:THR:CG2	1:C:1158:ILE:N	2.84	0.41
1:D:1082:LYS:O	1:D:1082:LYS:HG2	2.20	0.41
1:A:1084:GLU:OE1	1:A:1084:GLU:N	2.54	0.40
1:A:1091:LYS:HD2	1:A:1091:LYS:N	2.36	0.40
1:B:1086:GLU:HG2	1:B:1087:ASN:ND2	2.36	0.40
1:B:1144:ARG:HE	1:B:1144:ARG:HB2	1.73	0.40
1:F:1028:LYS:CB	3:F:7048:HOH:O	2.68	0.40
1:F:1137:ASN:ND2	1:F:1138:ILE:HG12	2.36	0.40
1:E:1022:PHE:CE1	1:E:1132:VAL:HG22	2.57	0.40
1:F:1147:SER:HB2	1:F:1148:ARG:H	1.78	0.40
1:C:1145:PHE:CE2	1:C:1154:LYS:HD2	2.56	0.40
1:F:1083:PHE:CD1	1:F:1108:ASN:O	2.75	0.40
1:A:1007:PHE:HA	1:A:1021:SER:HA	2.03	0.40
1:A:1037:ARG:O	1:A:1041:THR:HG23	2.21	0.40
1:B:1069:ARG:HH11	1:B:1069:ARG:HG3	1.86	0.40
1:D:1015:GLU:HA	1:D:1016:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1112:PHE:CD1	1:D:1112:PHE:C	3.00	0.40
1:E:1066:ASP:O	1:E:1070:HIS:HA	2.21	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%)	14 (9%)	1 (1%)	21	7
1	B	162/164 (99%)	141 (87%)	18 (11%)	3 (2%)	6	0
1	C	162/164 (99%)	147 (91%)	12 (7%)	3 (2%)	6	0
1	D	162/164 (99%)	146 (90%)	13 (8%)	3 (2%)	6	0
1	E	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	21	7
1	F	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	21	7
2	G	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	H	4/6 (67%)	3 (75%)	1 (25%)	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%)	3 (75%)	1 (25%)	0	100	100
All	All	996/1020 (98%)	897 (90%)	87 (9%)	12 (1%)	10	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1025	PHE
1	B	1105	PRO

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Mol	Chain	Res	Type
1	D	1105	PRO
1	B	1071	ASN
1	D	1080	GLY
1	F	1081	GLU
1	A	1081	GLU
1	C	1016	PRO
1	C	1144	ARG
1	D	1154	LYS
1	E	1086	GLU
1	C	1015	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/132 (100%)	122 (92%)	10 (8%)	12	1
1	B	132/132 (100%)	121 (92%)	11 (8%)	10	0
1	C	132/132 (100%)	126 (96%)	6 (4%)	24	3
1	D	132/132 (100%)	128 (97%)	4 (3%)	36	8
1	E	132/132 (100%)	123 (93%)	9 (7%)	14	1
1	F	132/132 (100%)	124 (94%)	8 (6%)	17	1
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%)	3 (100%)	0	100	100
2	J	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	K	3/3 (100%)	3 (100%)	0	100	100
2	L	3/3 (100%)	3 (100%)	0	100	100
All	All	810/810 (100%)	759 (94%)	51 (6%)	16	1

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1029	VAL
1	A	1069	ARG
1	A	1082	LYS
1	A	1084	GLU
1	A	1120	GLU
1	A	1127	VAL
1	A	1131	LYS
1	A	1148	ARG
1	A	1151	LYS
1	A	1153	SER
1	B	1029	VAL
1	B	1034	GLU
1	B	1043	GLU
1	B	1044	LYS
1	B	1076	LYS
1	B	1081	GLU
1	B	1087	ASN
1	B	1105	PRO
1	B	1129	PHE
1	B	1131	LYS
1	B	1140	GLU
1	C	1029	VAL
1	C	1082	LYS
1	C	1090	LEU
1	C	1131	LYS
1	C	1144	ARG
1	C	1149	ASN
1	D	1082	LYS
1	D	1105	PRO
1	D	1131	LYS
1	D	1140	GLU
1	E	1070	HIS
1	E	1073	THR
1	E	1076	LYS
1	E	1082	LYS
1	E	1086	GLU
1	E	1120	GLU
1	E	1137	ASN
1	E	1140	GLU
1	E	1142	MET
1	F	1028	LYS
1	F	1034	GLU
1	F	1082	LYS

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Mol	Chain	Res	Type
1	F	1084	GLU
1	F	1106	ASN
1	F	1125	LYS
1	F	1127	VAL
1	F	1137	ASN
2	G	101	HIS
2	H	105	ILE
2	J	101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1003	ASN
1	B	1087	ASN
1	B	1108	ASN
1	B	1149	ASN
1	C	1106	ASN
1	C	1149	ASN
1	D	1035	ASN
1	D	1108	ASN
1	D	1137	ASN
1	D	1163	GLN
1	E	1137	ASN
1	F	1003	ASN
1	F	1108	ASN
1	F	1137	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	164/164 (100%)	1.76	54 (32%) 1 1	5, 13, 20, 23	0
1	B	164/164 (100%)	3.39	139 (84%) 0 0	11, 20, 28, 34	0
1	C	164/164 (100%)	2.78	111 (67%) 0 0	5, 16, 25, 35	0
1	D	164/164 (100%)	2.41	98 (59%) 0 0	7, 18, 25, 33	0
1	E	164/164 (100%)	1.84	61 (37%) 1 1	3, 12, 21, 27	0
1	F	164/164 (100%)	3.12	127 (77%) 0 0	10, 18, 26, 30	0
2	G	6/6 (100%)	3.54	4 (66%) 0 0	13, 17, 21, 29	0
2	H	6/6 (100%)	3.07	4 (66%) 0 0	11, 14, 22, 24	0
2	I	6/6 (100%)	2.39	2 (33%) 1 1	6, 8, 11, 26	0
2	J	6/6 (100%)	1.92	3 (50%) 0 0	9, 10, 12, 18	0
2	K	6/6 (100%)	2.38	3 (50%) 0 0	7, 9, 20, 23	0
2	L	6/6 (100%)	3.53	5 (83%) 0 0	16, 19, 24, 24	0
All	All	1020/1020 (100%)	2.56	611 (59%) 0 0	3, 17, 26, 35	0

All (611) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1080	GLY	9.7
1	F	1029	VAL	9.0
1	B	1024	LEU	8.9
1	B	1104	GLY	8.3
1	C	1012	VAL	7.4
1	D	1026	ALA	7.4
1	F	1027	ASP	7.2
1	B	1025	PHE	7.1
1	F	1083	PHE	7.0
1	C	1029	VAL	7.0
2	I	106	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
2	G	101	HIS	6.5
1	D	1002	VAL	6.4
1	C	1014	GLY	6.3
1	B	1067	PHE	6.3
1	C	1030	PRO	6.3
2	H	106	ALA	6.3
1	F	1088	PHE	6.2
1	C	1017	LEU	6.2
1	F	1127	VAL	6.2
1	E	1152	THR	6.1
1	A	1002	VAL	6.0
1	B	1129	PHE	6.0
1	C	1002	VAL	6.0
1	F	1033	ALA	6.0
1	F	1026	ALA	6.0
2	K	101	HIS	6.0
1	B	1075	GLY	5.9
1	B	1046	PHE	5.9
1	F	1012	VAL	5.8
1	B	1016	PRO	5.8
2	L	101	HIS	5.7
1	B	1156	ILE	5.6
1	F	1030	PRO	5.6
1	B	1079	TYR	5.6
1	C	1011	ALA	5.6
1	B	1011	ALA	5.6
1	B	1050	GLY	5.4
1	D	1079	TYR	5.3
1	F	1145	PHE	5.3
1	B	1045	GLY	5.3
1	F	1078	ILE	5.3
1	B	1020	VAL	5.3
1	C	1046	PHE	5.3
1	C	1089	ILE	5.3
1	B	1035	ASN	5.2
1	D	1078	ILE	5.2
1	C	1028	LYS	5.2
1	B	1002	VAL	5.2
1	B	1083	PHE	5.1
1	D	1081	GLU	5.1
1	B	1012	VAL	5.1
1	C	1145	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	1107	THR	5.1
1	F	1039	LEU	5.1
1	B	1007	PHE	5.0
1	B	1026	ALA	5.0
1	F	1164	LEU	5.0
1	B	1145	PHE	5.0
1	F	1025	PHE	4.9
1	F	1105	PRO	4.9
1	B	1153	SER	4.9
1	A	1029	VAL	4.8
1	D	1083	PHE	4.8
1	E	1002	VAL	4.8
1	C	1093	THR	4.8
1	B	1038	ALA	4.8
1	B	1127	VAL	4.7
1	F	1128	VAL	4.7
1	B	1138	ILE	4.7
1	F	1129	PHE	4.7
1	C	1077	SER	4.7
1	F	1146	GLY	4.7
1	C	1042	GLY	4.6
1	F	1038	ALA	4.6
1	B	1036	PHE	4.6
1	D	1129	PHE	4.6
1	C	1118	LYS	4.6
1	C	1159	ALA	4.6
1	C	1086	GLU	4.6
1	A	1080	GLY	4.6
1	C	1016	PRO	4.6
1	D	1025	PHE	4.5
1	B	1090	LEU	4.5
1	A	1012	VAL	4.5
1	D	1012	VAL	4.5
1	F	1150	GLY	4.5
1	B	1029	VAL	4.5
1	B	1047	GLY	4.5
1	B	1052	CYS	4.5
1	C	1059	GLY	4.5
1	C	1116	THR	4.5
2	L	105	ILE	4.5
1	B	1017	LEU	4.5
1	B	1074	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	1029	VAL	4.4
1	E	1089	ILE	4.4
1	C	1121	TRP	4.4
1	C	1067	PHE	4.4
1	D	1104	GLY	4.4
1	B	1105	PRO	4.4
1	D	1156	ILE	4.4
1	B	1018	GLY	4.4
1	B	1109	GLY	4.4
1	F	1070	HIS	4.4
1	B	1030	PRO	4.4
1	B	1003	ASN	4.4
1	C	1153	SER	4.4
1	F	1080	GLY	4.3
1	B	1037	ARG	4.3
1	B	1147	SER	4.3
1	A	1073	THR	4.3
1	C	1015	GLU	4.3
1	D	1084	GLU	4.3
1	B	1097	ILE	4.3
1	C	1056	ILE	4.3
1	D	1027	ASP	4.3
1	B	1159	ALA	4.3
2	G	102	ALA	4.3
1	C	1050	GLY	4.2
1	E	1088	PHE	4.2
1	A	1103	ALA	4.2
1	B	1077	SER	4.2
1	F	1156	ILE	4.2
1	E	1067	PHE	4.2
1	F	1013	ASP	4.2
1	B	1084	GLU	4.2
1	B	1139	VAL	4.2
1	E	1081	GLU	4.2
1	B	1146	GLY	4.2
1	F	1071	ASN	4.1
1	B	1076	LYS	4.1
1	E	1145	PHE	4.1
1	A	1127	VAL	4.1
1	F	1002	VAL	4.1
1	F	1068	THR	4.1
1	D	1017	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	1011	ALA	4.1
1	C	1146	GLY	4.1
1	B	1058	PRO	4.1
1	C	1117	ALA	4.1
1	C	1025	PHE	4.0
1	F	1052	CYS	4.0
1	B	1089	ILE	4.0
1	C	1148	ARG	4.0
1	B	1048	TYR	4.0
1	F	1087	ASN	4.0
1	F	1007	PHE	4.0
1	C	1127	VAL	4.0
1	D	1020	VAL	4.0
1	B	1056	ILE	4.0
1	F	1110	SER	4.0
1	D	1024	LEU	4.0
1	B	1103	ALA	4.0
1	B	1015	GLU	4.0
1	E	1143	GLU	4.0
1	A	1146	GLY	4.0
1	F	1059	GLY	4.0
1	B	1088	PHE	4.0
1	F	1089	ILE	4.0
1	F	1085	ASP	4.0
1	C	1068	THR	4.0
1	A	1105	PRO	3.9
1	B	1132	VAL	3.9
1	C	1058	PRO	3.9
1	F	1103	ALA	3.9
1	E	1070	HIS	3.9
1	F	1079	TYR	3.9
1	F	1163	GLN	3.9
1	F	1008	PHE	3.9
1	B	1032	THR	3.9
1	C	1141	ALA	3.9
1	F	1090	LEU	3.9
1	B	1043	GLU	3.9
1	B	1143	GLU	3.9
1	F	1084	GLU	3.9
1	C	1083	PHE	3.9
2	L	106	ALA	3.9
1	C	1079	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	1042	GLY	3.8
1	B	1057	ILE	3.8
1	F	1010	ILE	3.8
1	C	1069	ARG	3.8
1	D	1069	ARG	3.8
1	E	1137	ASN	3.8
1	C	1057	ILE	3.8
1	E	1156	ILE	3.8
1	F	1035	ASN	3.8
1	E	1082	LYS	3.8
1	B	1144	ARG	3.8
1	A	1145	PHE	3.7
1	F	1122	LEU	3.7
1	F	1138	ILE	3.7
2	G	105	ILE	3.7
1	E	1016	PRO	3.7
1	F	1157	THR	3.7
2	H	101	HIS	3.7
1	B	1081	GLU	3.7
1	F	1034	GLU	3.7
1	D	1067	PHE	3.7
1	F	1073	THR	3.7
1	C	1087	ASN	3.7
1	F	1101	ALA	3.7
1	F	1042	GLY	3.7
1	F	1153	SER	3.7
1	B	1041	THR	3.7
1	F	1032	THR	3.7
1	F	1003	ASN	3.7
1	C	1144	ARG	3.7
1	B	1141	ALA	3.7
1	B	1070	HIS	3.6
1	B	1152	THR	3.6
1	B	1066	ASP	3.6
1	C	1137	ASN	3.6
1	C	1088	PHE	3.6
1	B	1040	SER	3.6
1	C	1147	SER	3.6
1	D	1085	ASP	3.6
1	D	1148	ARG	3.6
1	B	1107	THR	3.6
1	B	1039	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	1104	GLY	3.6
1	A	1060	PHE	3.6
1	B	1108	ASN	3.6
1	B	1082	LYS	3.6
1	D	1082	LYS	3.6
2	K	106	ALA	3.6
1	C	1084	GLU	3.5
1	C	1119	THR	3.5
1	F	1147	SER	3.5
1	D	1127	VAL	3.5
1	D	1016	PRO	3.5
1	B	1073	THR	3.5
1	C	1106	ASN	3.5
1	F	1108	ASN	3.5
1	B	1078	ILE	3.5
1	C	1156	ILE	3.5
1	F	1158	ILE	3.5
1	B	1085	ASP	3.5
1	E	1157	THR	3.5
1	F	1005	THR	3.5
1	C	1149	ASN	3.5
1	F	1072	GLY	3.5
1	A	1164	LEU	3.5
1	C	1070	HIS	3.5
2	H	105	ILE	3.5
1	B	1031	LYS	3.5
1	F	1050	GLY	3.4
1	B	1069	ARG	3.4
1	C	1085	ASP	3.4
1	B	1140	GLU	3.4
1	C	1045	GLY	3.4
1	C	1075	GLY	3.4
1	F	1141	ALA	3.4
1	C	1132	VAL	3.4
1	D	1128	VAL	3.4
1	C	1160	ASP	3.4
1	A	1154	LYS	3.4
1	B	1161	CYS	3.4
1	B	1098	LEU	3.4
1	F	1109	GLY	3.4
1	C	1078	ILE	3.4
1	B	1008	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1053	PHE	3.4
1	B	1113	PHE	3.4
1	F	1036	PHE	3.4
1	B	1116	THR	3.4
1	C	1080	GLY	3.4
1	E	1080	GLY	3.4
1	F	1116	THR	3.4
1	D	1030	PRO	3.4
1	B	1142	MET	3.4
1	C	1024	LEU	3.4
1	F	1031	LYS	3.3
1	A	1156	ILE	3.3
1	D	1057	ILE	3.3
1	F	1069	ARG	3.3
1	B	1157	THR	3.3
1	F	1041	THR	3.3
1	F	1121	TRP	3.3
1	C	1013	ASP	3.3
1	B	1154	LYS	3.3
2	L	102	ALA	3.3
1	A	1149	ASN	3.3
1	A	1082	LYS	3.3
1	A	1151	LYS	3.3
1	D	1015	GLU	3.3
1	E	1090	LEU	3.3
2	G	106	ALA	3.3
1	C	1010	ILE	3.3
1	B	1080	GLY	3.3
1	F	1075	GLY	3.3
1	E	1073	THR	3.3
1	F	1020	VAL	3.3
1	F	1004	PRO	3.3
1	D	1141	ALA	3.3
1	B	1126	HIS	3.2
1	E	1148	ARG	3.2
1	F	1014	GLY	3.2
1	C	1140	GLU	3.2
1	E	1149	ASN	3.2
1	B	1006	VAL	3.2
1	C	1139	VAL	3.2
1	D	1132	VAL	3.2
1	C	1122	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	1024	LEU	3.2
1	B	1149	ASN	3.2
1	E	1135	GLY	3.2
1	D	1097	ILE	3.2
1	A	1058	PRO	3.2
1	C	1033	ALA	3.2
1	B	1106	ASN	3.2
1	A	1083	PHE	3.2
1	F	1046	PHE	3.2
1	C	1073	THR	3.2
1	D	1160	ASP	3.2
1	E	1151	LYS	3.2
1	F	1057	ILE	3.2
1	C	1020	VAL	3.2
1	B	1065	GLY	3.2
1	F	1112	PHE	3.1
1	C	1138	ILE	3.1
2	I	105	ILE	3.1
1	E	1086	GLU	3.1
1	F	1139	VAL	3.1
1	B	1022	PHE	3.1
1	C	1095	PRO	3.1
1	A	1089	ILE	3.1
1	B	1010	ILE	3.1
1	E	1057	ILE	3.1
1	F	1130	GLY	3.1
1	A	1020	VAL	3.1
1	B	1093	THR	3.1
1	D	1116	THR	3.1
1	F	1102	ASN	3.1
1	B	1110	SER	3.1
1	D	1105	PRO	3.1
1	F	1043	GLU	3.1
1	A	1129	PHE	3.1
1	D	1050	GLY	3.1
1	D	1094	GLY	3.1
1	D	1149	ASN	3.0
1	D	1042	GLY	3.0
1	D	1059	GLY	3.0
1	C	1128	VAL	3.0
1	B	1059	GLY	3.0
1	B	1135	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1121	TRP	3.0
1	B	1122	LEU	3.0
1	B	1023	GLU	3.0
1	C	1081	GLU	3.0
1	E	1043	GLU	3.0
1	F	1149	ASN	3.0
1	A	1067	PHE	3.0
1	D	1145	PHE	3.0
1	F	1067	PHE	3.0
1	F	1113	PHE	3.0
1	B	1072	GLY	3.0
1	C	1047	GLY	3.0
1	A	1070	HIS	3.0
1	F	1054	HIS	3.0
1	F	1133	LYS	3.0
1	B	1005	THR	3.0
1	D	1006	VAL	2.9
1	D	1076	LYS	2.9
1	D	1036	PHE	2.9
1	E	1038	ALA	2.9
1	F	1060	PHE	2.9
1	F	1045	GLY	2.9
1	D	1131	LYS	2.9
1	A	1069	ARG	2.9
1	C	1157	THR	2.9
1	F	1106	ASN	2.9
1	C	1026	ALA	2.9
1	B	1155	LYS	2.9
1	F	1154	LYS	2.9
1	F	1053	PHE	2.9
1	B	1014	GLY	2.9
1	C	1096	GLY	2.9
1	D	1014	GLY	2.9
1	D	1155	LYS	2.9
1	D	1103	ALA	2.8
1	D	1053	PHE	2.8
1	C	1097	ILE	2.8
1	C	1134	GLU	2.8
1	F	1028	LYS	2.8
1	F	1093	THR	2.8
1	D	1153	SER	2.8
1	E	1018	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1007	PHE	2.8
1	F	1155	LYS	2.8
1	B	1148	ARG	2.8
1	B	1158	ILE	2.8
1	B	1124	GLY	2.8
2	J	106	ALA	2.8
1	D	1126	HIS	2.8
1	F	1047	GLY	2.8
1	D	1138	ILE	2.8
1	E	1010	ILE	2.8
1	C	1090	LEU	2.8
1	C	1082	LYS	2.8
1	B	1128	VAL	2.7
1	A	1040	SER	2.7
1	A	1135	GLY	2.7
1	F	1065	GLY	2.7
1	F	1094	GLY	2.7
1	D	1089	ILE	2.7
1	A	1079	TYR	2.7
1	E	1058	PRO	2.7
1	B	1164	LEU	2.7
1	F	1040	SER	2.7
1	B	1163	GLN	2.7
1	A	1018	GLY	2.7
1	D	1075	GLY	2.7
1	F	1124	GLY	2.7
1	D	1144	ARG	2.7
1	B	1131	LYS	2.7
1	B	1130	GLY	2.7
1	B	1119	THR	2.7
1	F	1048	TYR	2.6
1	E	1017	LEU	2.6
1	A	1157	THR	2.6
1	E	1069	ARG	2.6
1	E	1105	PRO	2.6
1	D	1106	ASN	2.6
1	A	1088	PHE	2.6
1	D	1008	PHE	2.6
1	D	1088	PHE	2.6
1	D	1090	LEU	2.6
1	D	1164	LEU	2.6
1	C	1154	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	1118	LYS	2.6
1	B	1101	ALA	2.6
1	F	1097	ILE	2.6
1	A	1071	ASN	2.6
1	A	1084	GLU	2.6
1	E	1029	VAL	2.6
1	D	1018	GLY	2.6
1	D	1072	GLY	2.6
1	E	1042	GLY	2.6
1	E	1045	GLY	2.6
1	E	1059	GLY	2.6
1	B	1033	ALA	2.5
1	C	1038	ALA	2.5
1	C	1133	LYS	2.5
1	C	1151	LYS	2.5
1	B	1102	ASN	2.5
1	F	1111	GLN	2.5
1	A	1148	ARG	2.5
1	F	1037	ARG	2.5
1	D	1058	PRO	2.5
1	D	1095	PRO	2.5
1	C	1125	LYS	2.5
1	C	1052	CYS	2.5
1	E	1056	ILE	2.5
1	C	1150	GLY	2.5
1	F	1058	PRO	2.5
1	E	1020	VAL	2.5
1	A	1087	ASN	2.5
1	D	1093	THR	2.5
2	J	102	ALA	2.5
1	A	1104	GLY	2.5
1	C	1094	GLY	2.5
1	C	1124	GLY	2.5
1	D	1045	GLY	2.5
1	F	1064	GLY	2.5
1	D	1122	LEU	2.5
1	F	1017	LEU	2.5
1	B	1004	PRO	2.5
1	E	1046	PHE	2.5
1	B	1071	ASN	2.5
1	E	1071	ASN	2.5
1	F	1142	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1107	THR	2.5
1	C	1115	CYS	2.4
1	D	1011	ALA	2.4
1	D	1134	GLU	2.4
1	E	1120	GLU	2.4
1	F	1077	SER	2.4
1	F	1148	ARG	2.4
1	E	1008	PHE	2.4
1	F	1022	PHE	2.4
1	A	1152	THR	2.4
1	E	1012	VAL	2.4
1	E	1139	VAL	2.4
1	F	1006	VAL	2.4
1	C	1101	ALA	2.4
1	E	1103	ALA	2.4
1	B	1044	LYS	2.4
1	D	1135	GLY	2.4
1	F	1018	GLY	2.4
1	F	1144	ARG	2.4
1	F	1100	MET	2.4
1	E	1087	ASN	2.4
2	J	105	ILE	2.4
1	C	1043	GLU	2.4
1	C	1060	PHE	2.4
1	C	1091	LYS	2.4
1	C	1158	ILE	2.4
1	D	1028	LYS	2.4
1	E	1039	LEU	2.4
1	C	1135	GLY	2.4
1	D	1046	PHE	2.4
1	F	1137	ASN	2.4
1	A	1101	ALA	2.3
1	D	1070	HIS	2.3
1	B	1095	PRO	2.3
1	F	1016	PRO	2.3
2	L	104	PRO	2.3
1	D	1091	LYS	2.3
1	D	1010	ILE	2.3
1	B	1094	GLY	2.3
1	B	1096	GLY	2.3
1	E	1007	PHE	2.3
1	F	1161	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	1139	VAL	2.3
1	A	1143	GLU	2.3
1	E	1107	THR	2.3
1	D	1109	GLY	2.3
1	B	1091	LYS	2.3
1	F	1082	LYS	2.3
1	B	1112	PHE	2.3
1	C	1008	PHE	2.3
1	E	1093	THR	2.3
1	B	1049	LYS	2.3
1	B	1151	LYS	2.3
1	C	1023	GLU	2.3
1	D	1043	GLU	2.3
1	E	1138	ILE	2.3
1	D	1102	ASN	2.2
1	B	1150	GLY	2.2
1	C	1018	GLY	2.2
1	C	1092	HIS	2.2
1	C	1044	LYS	2.2
1	F	1098	LEU	2.2
1	A	1057	ILE	2.2
1	D	1056	ILE	2.2
1	D	1158	ILE	2.2
1	B	1111	GLN	2.2
1	E	1116	THR	2.2
1	B	1064	GLY	2.2
1	A	1046	PHE	2.2
1	C	1009	ASP	2.2
1	C	1123	ASP	2.2
1	A	1017	LEU	2.2
1	A	1081	GLU	2.2
1	F	1056	ILE	2.2
1	D	1101	ALA	2.2
1	D	1004	PRO	2.2
1	F	1095	PRO	2.2
1	F	1125	LYS	2.2
2	H	104	PRO	2.2
1	C	1152	THR	2.2
1	D	1107	THR	2.2
1	D	1147	SER	2.2
1	B	1087	ASN	2.2
1	D	1137	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1133	LYS	2.2
1	C	1105	PRO	2.1
1	D	1130	GLY	2.1
1	B	1115	CYS	2.1
1	C	1161	CYS	2.1
1	E	1077	SER	2.1
1	D	1009	ASP	2.1
1	A	1053	PHE	2.1
1	D	1022	PHE	2.1
1	E	1060	PHE	2.1
1	D	1032	THR	2.1
1	E	1161	CYS	2.1
1	F	1115	CYS	2.1
2	K	105	ILE	2.1
1	B	1100	MET	2.1
1	D	1121	TRP	2.1
1	B	1051	SER	2.1
1	C	1053	PHE	2.1
1	C	1129	PHE	2.1
1	D	1113	PHE	2.1
1	A	1006	VAL	2.1
1	D	1124	GLY	2.1
1	E	1106	ASN	2.1
1	F	1136	MET	2.1
1	C	1005	THR	2.1
1	E	1068	THR	2.1
1	C	1164	LEU	2.1
1	D	1098	LEU	2.1
1	B	1062	CYS	2.1
1	C	1131	LYS	2.1
1	E	1144	ARG	2.1
1	B	1021	SER	2.1
1	E	1153	SER	2.1
1	E	1050	GLY	2.1
1	F	1123	ASP	2.1
1	A	1030	PRO	2.1
1	A	1008	PHE	2.0
1	F	1159	ALA	2.0
1	A	1027	ASP	2.0
1	A	1085	ASP	2.0
1	D	1150	GLY	2.0
1	E	1124	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1091	LYS	2.0
1	A	1144	ARG	2.0
1	B	1092	HIS	2.0
1	A	1043	GLU	2.0
1	D	1023	GLU	2.0
1	D	1159	ALA	2.0
1	B	1060	PHE	2.0
1	C	1112	PHE	2.0
1	D	1061	MET	2.0
1	C	1051	SER	2.0
1	B	1137	ASN	2.0
1	F	1160	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.