



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:22 PM UTC

PDB ID : 1AWV / pdb_00001awv
Title : CYPA COMPLEXED WITH HVGPIA
Authors : Vajdos, F.F.
Deposited on : 1997-10-05
Resolution : 2.34 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:

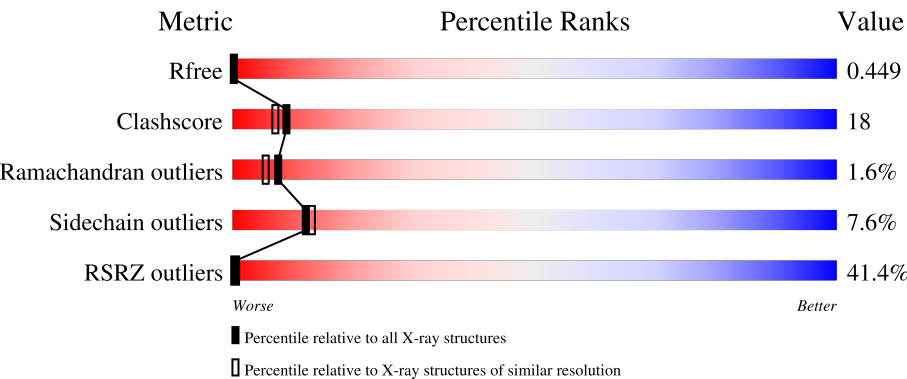
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	23% 67% 27% 5%
1	B	164	65% 50% 41% 7% .
1	C	164	38% 62% 34% .
1	D	164	35% 58% 39% .
1	E	164	30% 66% 30% .

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Mol	Chain	Length	Quality of chain
1	F	164	57% 55% 38% 7%
2	G	6	17% 50% 50%
2	H	6	50% 50%
2	I	6	33% 50% 50%
2	J	6	50% 33% 67%
2	K	6	50% 67% 33%
2	L	6	67% 67% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7975 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	11	0	0
			42	27	8	7			
2	H	6	Total	C	N	O	0	0	0
			42	27	8	7			
2	I	6	Total	C	N	O	0	0	0
			42	27	8	7			
2	J	6	Total	C	N	O	0	0	0
			42	27	8	7			
2	K	6	Total	C	N	O	11	0	0
			42	27	8	7			
2	L	6	Total	C	N	O	0	0	0
			42	27	8	7			

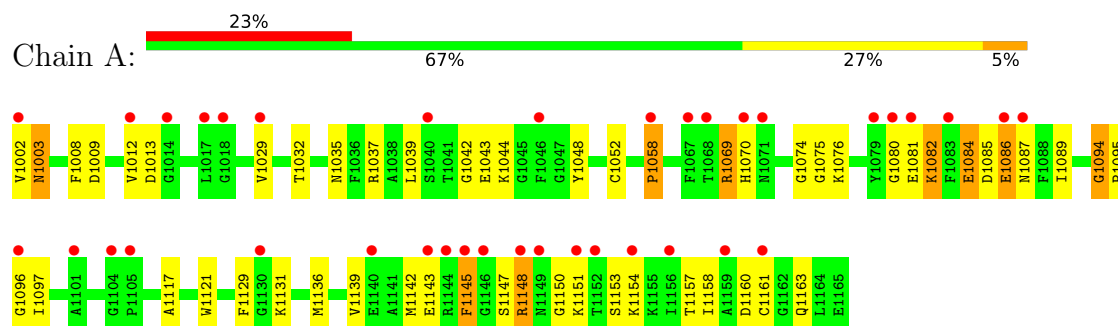
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	22	Total 22	O 22	0	0
3	C	31	Total 31	O 31	0	0
3	D	20	Total 20	O 20	0	0
3	E	28	Total 28	O 28	0	0
3	F	29	Total 29	O 29	0	0
3	G	3	Total 3	O 3	0	0
3	H	1	Total 1	O 1	0	0
3	I	2	Total 2	O 2	0	0
3	J	2	Total 2	O 2	0	0
3	K	3	Total 3	O 3	0	0
3	L	2	Total 2	O 2	0	0

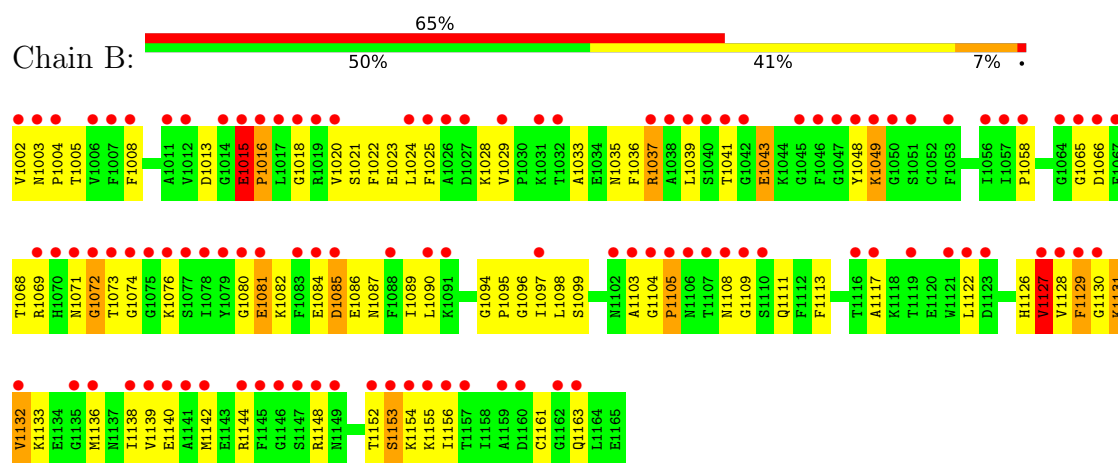
3 Residue-property plots [i](#)

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

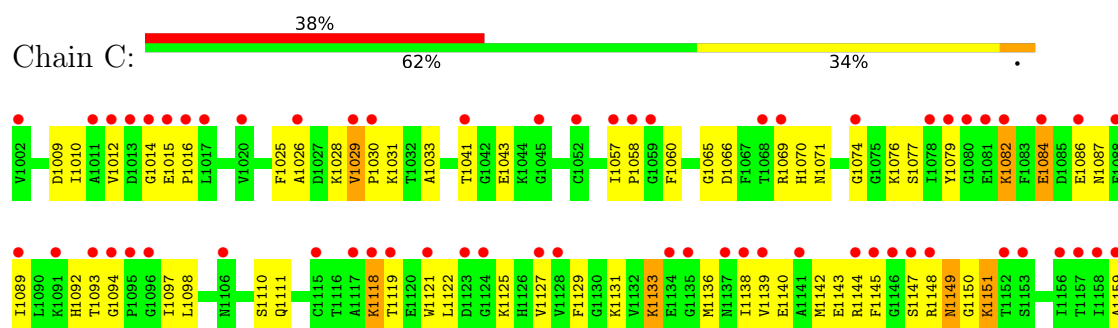
• Molecule 1: CYCLOPHILIN A



• Molecule 1: CYCLOPHILIN A

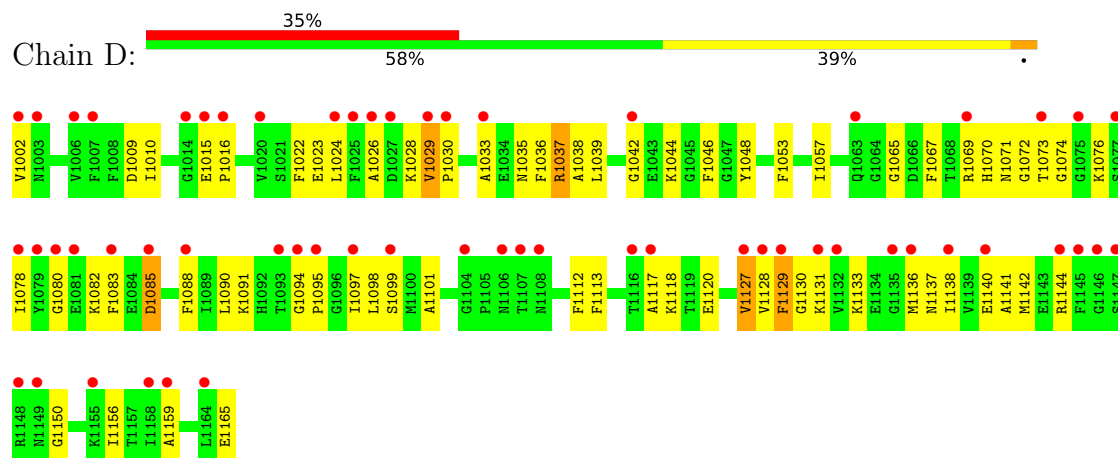


• Molecule 1: CYCLOPHILIN A

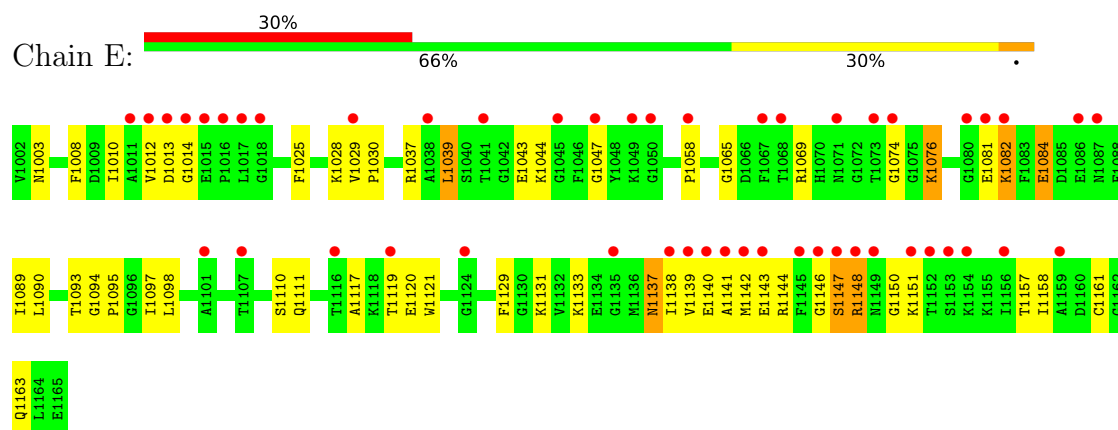




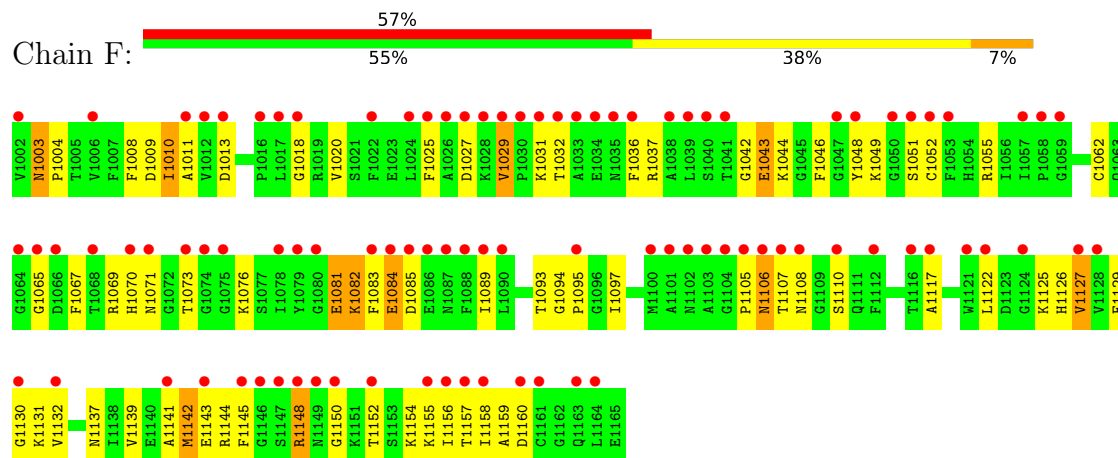
• Molecule 1: CYCLOPHILIN A



• Molecule 1: CYCLOPHILIN A



• Molecule 1: CYCLOPHILIN A

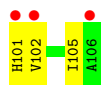


• Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN

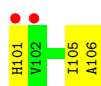




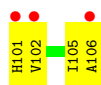
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



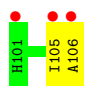
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



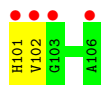
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



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- 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	74.00Å 74.00Å 190.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.34 15.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	83.1 (15.00-2.34) 83.7 (15.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.34Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.358 , 0.460 0.355 , 0.449	Depositor DCC
R_{free} test set	2081 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7975	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 85.32 % 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 1.3041e-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	0.62	0/1286	1.09	7/1723 (0.4%)
1	B	0.61	0/1286	1.08	7/1723 (0.4%)
1	C	0.56	0/1286	1.02	0/1723
1	D	0.55	0/1286	1.01	0/1723
1	E	0.59	0/1286	1.08	5/1723 (0.3%)
1	F	0.61	0/1286	1.12	11/1723 (0.6%)
2	G	0.52	0/43	1.59	2/57 (3.5%)
2	H	0.55	0/43	0.81	0/57
2	I	0.80	0/43	1.53	0/57
2	J	0.83	0/43	1.23	0/57
2	K	0.78	0/43	1.49	0/57
2	L	0.70	0/43	1.48	1/57 (1.8%)
All	All	0.59	0/7974	1.08	33/10680 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1104	GLY	CA-C-N	9.30	131.47	119.84
1	B	1104	GLY	C-N-CA	9.30	131.47	119.84
1	E	1084	GLU	N-CA-C	8.55	120.92	110.41
1	A	1084	GLU	N-CA-C	8.17	120.87	110.33
2	L	102	VAL	N-CA-C	7.34	119.17	108.53
1	F	1003	ASN	CA-C-N	6.71	127.24	119.99
1	F	1003	ASN	C-N-CA	6.71	127.24	119.99
1	B	1015	GLU	CA-C-N	6.56	126.32	119.76
1	B	1015	GLU	C-N-CA	6.56	126.32	119.76
1	F	1003	ASN	N-CA-C	6.25	119.97	109.09
1	F	1084	GLU	N-CA-C	6.17	118.52	110.43
1	E	1148	ARG	N-CA-C	-6.16	104.56	111.28
1	F	1089	ILE	N-CA-C	6.08	116.86	110.72
1	A	1003	ASN	CA-C-N	5.88	125.81	119.76
1	A	1003	ASN	C-N-CA	5.88	125.81	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1081	GLU	N-CA-C	-5.87	103.96	108.78
1	A	1075	GLY	N-CA-C	-5.76	106.48	111.95
1	F	1073	THR	N-CA-C	5.69	120.38	113.38
1	F	1010	ILE	N-CA-C	5.55	116.76	109.21
1	B	1127	VAL	CB-CA-C	-5.41	104.75	111.08
1	F	1093	THR	N-CA-C	5.37	119.45	113.01
1	F	1052	CYS	N-CA-C	5.34	117.39	109.69
1	B	1015	GLU	N-CA-C	5.32	118.01	110.24
1	E	1003	ASN	CA-C-N	5.32	125.23	119.76
1	E	1003	ASN	C-N-CA	5.32	125.23	119.76
1	A	1094	GLY	CA-C-N	5.29	125.54	119.83
1	A	1094	GLY	C-N-CA	5.29	125.54	119.83
2	G	103	GLY	CA-C-N	5.29	125.58	119.92
2	G	103	GLY	C-N-CA	5.29	125.58	119.92
1	B	1016	PRO	N-CA-C	5.27	119.46	111.19
1	A	1052	CYS	N-CA-C	5.13	117.08	109.69
1	E	1093	THR	N-CA-C	5.09	119.25	113.19
1	F	1127	VAL	CB-CA-C	-5.08	105.75	111.23

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	44	0
1	D	1258	0	1225	49	0
1	E	1258	0	1225	39	0
1	F	1258	0	1225	52	0
2	G	42	0	41	1	0
2	H	42	0	41	1	0
2	I	42	0	41	2	0
2	J	42	0	41	3	0
2	K	42	0	41	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	42	0	41	0	0
3	A	32	0	0	1	0
3	B	22	0	0	1	0
3	C	31	0	0	1	0
3	D	20	0	0	2	0
3	E	28	0	0	1	0
3	F	29	0	0	6	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	1	0
3	K	3	0	0	0	0
3	L	2	0	0	0	0
All	All	7975	0	7596	284	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 18.

All (284) 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:B:1028:LYS:HD3	1:B:1090:LEU:HD21	1.63	0.80
1:F:1067:PHE:HB3	3:F:7016:HOH:O	1.84	0.78
1:D:1095:PRO:HG3	1:D:1117:ALA:HA	1.67	0.77
1:D:1028:LYS:O	1:D:1030:PRO:HD3	1.87	0.74
1:D:1028:LYS:HD3	1:D:1090:LEU:HD21	1.69	0.74
1:C:1140:GLU:O	1:C:1144:ARG:HG3	1.86	0.74
1:E:1028:LYS:HD3	1:E:1090:LEU:HD21	1.69	0.73
1:B:1024:LEU:HB3	1:B:1033:ALA:HB1	1.71	0.73
1:C:1148:ARG:HH11	1:C:1148:ARG:HA	1.54	0.73
1:E:1141:ALA:HA	1:E:1144:ARG:HE	1.53	0.72
1:B:1095:PRO:HG3	1:B:1117:ALA:HA	1.73	0.70
1:B:1103:ALA:HB2	2:H:102:VAL:HG12	1.72	0.70
1:C:1069:ARG:HB3	1:C:1071:ASN:OD1	1.93	0.69
1:D:1085:ASP:HB3	1:D:1127:VAL:CG2	2.23	0.69
1:B:1069:ARG:HD2	1:B:1073:THR:HB	1.74	0.69
1:B:1090:LEU:HB2	1:B:1128:VAL:HB	1.75	0.68
1:E:1058:PRO:CD	1:E:1147:SER:H	2.07	0.67
1:B:1068:THR:OG1	1:B:1074:GLY:HA3	1.95	0.66
1:C:1136:MET:HE3	1:C:1139:VAL:HB	1.77	0.66
1:B:1025:PHE:CE1	1:B:1130:GLY:HA2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:GLY:HA3	3:B:7017:HOH:O	1.96	0.66
1:A:1082:LYS:H	1:A:1082:LYS:HD3	1.61	0.66
1:B:1018:GLY:HA3	1:B:1138:ILE:HD12	1.76	0.66
1:A:1145:PHE:HE2	1:A:1154:LYS:HD2	1.60	0.65
1:B:1140:GLU:O	1:B:1144:ARG:HG3	1.97	0.65
1:E:1039:LEU:HD23	1:E:1047:GLY:HA2	1.78	0.65
1:D:1024:LEU:HB3	1:D:1033:ALA:HB1	1.80	0.64
1:D:1023:GLU:HB2	1:D:1133:LYS:HE2	1.78	0.63
1:A:1148:ARG:HA	1:A:1148:ARG:NE	2.13	0.63
1:D:1026:ALA:O	1:D:1030:PRO:HG3	1.98	0.63
1:F:1009:ASP:HB2	1:F:1160:ASP:HB3	1.81	0.63
1:B:1085:ASP:CB	1:B:1108:ASN:HD21	2.12	0.62
1:C:1093:THR:HA	1:C:1118:LYS:HE3	1.81	0.62
1:D:1036:PHE:HB2	1:D:1129:PHE:HE2	1.64	0.62
1:D:1138:ILE:O	1:D:1142:MET:HG2	1.99	0.62
1:B:1041:THR:OG1	1:B:1043:GLU:HB3	2.00	0.62
1:B:1085:ASP:HB3	1:B:1127:VAL:CG2	2.30	0.62
1:C:1092:HIS:O	1:C:1118:LYS:HD3	2.01	0.61
1:F:1127:VAL:HA	3:F:7029:HOH:O	2.00	0.61
1:F:1095:PRO:HG3	1:F:1117:ALA:HA	1.83	0.61
1:D:1085:ASP:HB3	1:D:1127:VAL:HG22	1.82	0.61
1:F:1044:LYS:HB2	3:F:7004:HOH:O	2.00	0.60
1:B:1122:LEU:HD22	1:B:1126:HIS:CD2	2.36	0.60
1:B:1025:PHE:CD2	1:B:1028:LYS:HD2	2.36	0.60
1:E:1069:ARG:HD3	1:E:1074:GLY:HA3	1.83	0.60
1:D:1057:ILE:HG12	1:D:1150:GLY:HA2	1.82	0.60
1:E:1058:PRO:HD3	1:E:1147:SER:H	1.65	0.60
1:B:1025:PHE:HD2	1:B:1028:LYS:HD2	1.66	0.60
1:B:1153:SER:O	1:B:1154:LYS:HG3	2.01	0.60
1:C:1058:PRO:HA	1:C:1143:GLU:HG3	1.82	0.60
1:F:1048:TYR:HA	3:F:7016:HOH:O	2.01	0.60
1:E:1029:VAL:HG21	1:E:1129:PHE:HB2	1.84	0.59
1:F:1152:THR:HB	1:F:1154:LYS:O	2.03	0.59
1:E:1043:GLU:O	1:E:1044:LYS:HD3	2.03	0.58
1:C:1077:SER:HB2	1:C:1079:TYR:HD2	1.69	0.58
1:F:1029:VAL:HG21	1:F:1129:PHE:CB	2.33	0.57
1:F:1085:ASP:HA	1:F:1108:ASN:HD21	1.67	0.57
1:B:1058:PRO:HB2	1:B:1148:ARG:HH22	1.69	0.57
1:D:1038:ALA:HB3	1:D:1078:ILE:HD13	1.85	0.57
1:B:1136:MET:O	1:B:1140:GLU:HG2	2.04	0.57
1:C:1057:ILE:HG12	1:C:1150:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1085:ASP:HA	1:F:1108:ASN:ND2	2.19	0.57
1:C:1077:SER:HB2	1:C:1079:TYR:CD2	2.40	0.57
1:C:1139:VAL:HA	1:C:1142:MET:HE3	1.85	0.57
1:D:1044:LYS:HB2	3:D:7103:HOH:O	2.05	0.57
1:E:1058:PRO:HG3	1:E:1143:GLU:O	2.04	0.56
1:D:1023:GLU:HB2	1:D:1133:LYS:CE	2.35	0.56
1:B:1058:PRO:HB2	1:B:1148:ARG:NH2	2.20	0.56
1:A:1087:ASN:ND2	1:A:1089:ILE:HD12	2.20	0.56
1:F:1036:PHE:HB2	1:F:1129:PHE:HE2	1.71	0.56
1:D:1028:LYS:C	1:D:1030:PRO:HD3	2.30	0.56
1:F:1037:ARG:HG2	1:F:1037:ARG:HH11	1.70	0.56
1:F:1062:CYS:SG	1:F:1143:GLU:OE2	2.64	0.56
1:F:1048:TYR:CE1	1:F:1065:GLY:HA2	2.41	0.56
1:B:1022:PHE:CD2	1:B:1098:LEU:HD22	2.41	0.55
1:C:1069:ARG:HB2	1:C:1074:GLY:HA3	1.88	0.55
1:F:1031:LYS:HB2	1:F:1031:LYS:HZ3	1.72	0.55
1:E:1147:SER:HB3	1:E:1150:GLY:H	1.72	0.54
1:F:1145:PHE:HB2	1:F:1156:ILE:HD11	1.88	0.54
1:E:1137:ASN:OD1	1:E:1138:ILE:HD13	2.08	0.54
1:B:1002:VAL:C	1:B:1003:ASN:HD22	2.16	0.54
1:B:1023:GLU:HB2	1:B:1133:LYS:HE2	1.88	0.54
1:D:1035:ASN:O	1:D:1039:LEU:HG	2.07	0.54
1:A:1044:LYS:HB2	3:A:7013:HOH:O	2.07	0.53
1:B:1008:PHE:HB2	1:B:1020:VAL:CG1	2.38	0.53
1:F:1029:VAL:HG21	1:F:1129:PHE:HB2	1.89	0.53
1:F:1051:SER:HA	1:F:1070:HIS:NE2	2.23	0.53
1:B:1085:ASP:HB3	1:B:1127:VAL:HG22	1.89	0.53
1:D:1137:ASN:O	1:D:1141:ALA:HB2	2.08	0.53
1:F:1139:VAL:O	1:F:1143:GLU:HG2	2.09	0.53
1:C:1030:PRO:HD2	1:C:1086:GLU:OE2	2.09	0.52
1:F:1069:ARG:HB3	1:F:1071:ASN:OD1	2.08	0.52
1:D:1069:ARG:HG2	1:D:1074:GLY:HA3	1.92	0.52
1:A:1037:ARG:HD2	1:A:1163:GLN:NE2	2.23	0.52
1:A:1042:GLY:O	1:A:1044:LYS:N	2.41	0.52
1:E:1029:VAL:HG23	1:E:1029:VAL:O	2.10	0.51
1:B:1008:PHE:HB2	1:B:1020:VAL:HG13	1.92	0.51
1:A:1029:VAL:HG21	1:A:1129:PHE:CB	2.40	0.51
1:B:1071:ASN:OD1	1:B:1072:GLY:N	2.44	0.51
1:B:1085:ASP:HB3	1:B:1127:VAL:HG21	1.93	0.51
1:D:1136:MET:HG3	1:D:1140:GLU:OE2	2.09	0.51
1:E:1082:LYS:H	1:E:1082:LYS:HD3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1089:ILE:HG22	1:E:1090:LEU:HD23	1.93	0.51
1:E:1147:SER:HB2	1:E:1151:LYS:O	2.11	0.51
1:B:1043:GLU:O	1:B:1043:GLU:HG3	2.09	0.51
1:B:1131:LYS:O	1:B:1131:LYS:HD3	2.11	0.51
1:C:1143:GLU:C	1:C:1145:PHE:H	2.18	0.51
1:F:1029:VAL:HB	1:F:1032:THR:HB	1.92	0.51
1:B:1048:TYR:CE1	1:B:1065:GLY:HA2	2.46	0.51
1:A:1095:PRO:HG3	1:A:1117:ALA:HA	1.91	0.51
1:B:1085:ASP:O	1:B:1087:ASN:N	2.45	0.50
1:C:1065:GLY:HA3	1:C:1111:GLN:HA	1.93	0.50
1:E:1146:GLY:O	1:E:1147:SER:HB2	2.10	0.50
1:F:1081:GLU:HG2	1:F:1082:LYS:H	1.75	0.50
1:F:1008:PHE:HB2	1:F:1020:VAL:HG13	1.94	0.50
1:C:1082:LYS:HD2	1:C:1082:LYS:C	2.37	0.50
1:F:1018:GLY:HA2	3:F:7005:HOH:O	2.11	0.50
1:A:1008:PHE:HD1	1:A:1161:CYS:HB3	1.77	0.50
1:E:1058:PRO:HD2	1:E:1147:SER:O	2.12	0.50
1:B:1087:ASN:HD22	1:B:1089:ILE:HD12	1.75	0.50
1:B:1085:ASP:HB3	1:B:1108:ASN:HD21	1.77	0.49
1:F:1141:ALA:C	1:F:1143:GLU:H	2.20	0.49
1:F:1083:PHE:CD1	1:F:1108:ASN:O	2.65	0.49
1:A:1009:ASP:N	1:A:1160:ASP:O	2.39	0.49
1:B:1005:THR:O	1:B:1163:GLN:HG3	2.12	0.49
1:B:1025:PHE:HE1	1:B:1130:GLY:HA2	1.75	0.49
1:B:1024:LEU:HD22	1:B:1036:PHE:HB3	1.94	0.49
1:E:1010:ILE:HG13	1:E:1142:MET:CE	2.42	0.49
1:D:1057:ILE:HG12	1:D:1150:GLY:CA	2.43	0.49
1:C:1127:VAL:HG11	3:C:7148:HOH:O	2.13	0.49
1:D:1029:VAL:HG21	1:D:1129:PHE:HA	1.95	0.48
1:D:1067:PHE:CZ	1:D:1076:LYS:HG2	2.49	0.48
1:F:1155:LYS:HG2	1:F:1157:THR:OG1	2.14	0.48
1:C:1138:ILE:O	1:C:1142:MET:HG3	2.14	0.48
1:F:1037:ARG:HG2	1:F:1037:ARG:NH1	2.28	0.48
1:C:1026:ALA:HA	1:C:1033:ALA:CB	2.44	0.47
1:C:1076:LYS:O	1:C:1110:SER:HB3	2.14	0.47
1:B:1065:GLY:HA3	1:B:1111:GLN:HA	1.96	0.47
1:E:1029:VAL:HG21	1:E:1129:PHE:CB	2.44	0.47
1:A:1139:VAL:HA	1:A:1142:MET:HB3	1.96	0.47
1:D:1088:PHE:HA	3:D:7060:HOH:O	2.14	0.47
1:F:1029:VAL:HG13	3:F:7048:HOH:O	2.14	0.47
1:F:1076:LYS:O	1:F:1110:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:PHE:N	1:A:1145:PHE:CD1	2.83	0.47
1:E:1098:LEU:HG	1:E:1129:PHE:CZ	2.50	0.47
1:F:1025:PHE:CE2	1:F:1130:GLY:HA2	2.50	0.47
1:C:1058:PRO:HD2	1:C:1147:SER:O	2.15	0.47
1:B:1013:ASP:OD1	1:B:1154:LYS:HB3	2.14	0.47
1:B:1004:PRO:HB2	1:B:1024:LEU:HB2	1.96	0.47
1:C:1087:ASN:HB2	1:C:1089:ILE:HG13	1.97	0.47
1:C:1094:GLY:O	1:C:1097:ILE:HG12	2.15	0.47
1:D:1129:PHE:CD1	1:D:1129:PHE:N	2.82	0.47
1:F:1011:ALA:HB2	1:F:1159:ALA:HB2	1.97	0.46
1:D:1044:LYS:HG3	1:D:1078:ILE:CG2	2.46	0.46
1:D:1085:ASP:HB3	1:D:1127:VAL:HG21	1.98	0.46
1:E:1010:ILE:HG13	1:E:1142:MET:HE3	1.97	0.46
1:D:1099:SER:HB3	1:D:1113:PHE:CZ	2.51	0.46
1:F:1105:PRO:O	1:F:1107:THR:HG23	2.14	0.46
1:A:1002:VAL:HG23	1:A:1003:ASN:H	1.81	0.46
1:C:1012:VAL:C	1:C:1014:GLY:H	2.23	0.46
1:D:1071:ASN:OD1	1:D:1072:GLY:N	2.48	0.46
1:F:1010:ILE:HG13	1:F:1142:MET:CE	2.45	0.46
1:F:1094:GLY:O	1:F:1097:ILE:HG12	2.16	0.46
1:B:1069:ARG:CD	1:B:1073:THR:HB	2.44	0.46
1:E:1025:PHE:HZ	1:E:1131:LYS:HE2	1.80	0.46
1:B:1099:SER:HB3	1:B:1113:PHE:CZ	2.51	0.46
1:C:1015:GLU:HA	1:C:1016:PRO:HD3	1.79	0.46
1:C:1147:SER:HB3	1:C:1151:LYS:HB3	1.98	0.46
1:E:1037:ARG:HD3	1:E:1163:GLN:CD	2.41	0.46
1:A:1048:TYR:HB3	1:A:1158:ILE:HD12	1.98	0.46
1:A:1096:GLY:HA2	1:A:1136:MET:SD	2.55	0.46
1:F:1049:LYS:CD	1:F:1160:ASP:HA	2.46	0.46
1:B:1037:ARG:O	1:B:1041:THR:HG23	2.15	0.45
1:E:1065:GLY:HA3	1:E:1111:GLN:HA	1.98	0.45
1:F:1048:TYR:HE1	1:F:1065:GLY:HA2	1.78	0.45
1:A:1042:GLY:C	1:A:1044:LYS:H	2.25	0.45
1:A:1048:TYR:HB3	1:A:1158:ILE:CD1	2.46	0.45
1:B:1035:ASN:O	1:B:1039:LEU:HB2	2.16	0.45
1:B:1015:GLU:HA	1:B:1016:PRO:HD3	1.74	0.45
1:F:1027:ASP:OD1	1:F:1027:ASP:N	2.48	0.45
1:B:1087:ASN:HD22	1:B:1089:ILE:CD1	2.30	0.45
1:E:1137:ASN:ND2	1:E:1137:ASN:H	2.14	0.45
1:F:1145:PHE:CB	1:F:1156:ILE:HD11	2.45	0.45
1:A:1012:VAL:O	1:A:1013:ASP:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1095:PRO:HG3	1:E:1117:ALA:HA	1.98	0.45
2:I:105:ILE:O	2:I:106:ALA:HB3	2.17	0.45
1:C:1069:ARG:HB3	1:C:1071:ASN:CG	2.42	0.45
1:A:1076:LYS:HB2	1:A:1080:GLY:O	2.17	0.45
1:C:1029:VAL:N	1:C:1030:PRO:HD3	2.31	0.45
1:C:1058:PRO:HG3	1:C:1143:GLU:O	2.16	0.45
1:C:1098:LEU:HG	1:C:1129:PHE:CZ	2.51	0.45
1:A:1035:ASN:O	1:A:1039:LEU:HD23	2.17	0.45
1:F:1008:PHE:HB2	1:F:1020:VAL:CG1	2.47	0.45
1:A:1145:PHE:HD2	1:A:1154:LYS:HB2	1.82	0.45
1:C:1025:PHE:CZ	1:C:1131:LYS:HG2	2.52	0.45
1:C:1066:ASP:CG	1:C:1070:HIS:H	2.25	0.45
1:A:1058:PRO:HA	1:A:1143:GLU:CD	2.42	0.44
1:A:1069:ARG:HD2	1:A:1074:GLY:HA3	1.99	0.44
1:D:1082:LYS:O	1:D:1083:PHE:HB3	2.17	0.44
1:F:1010:ILE:HG13	1:F:1142:MET:HE1	1.98	0.44
1:D:1129:PHE:N	1:D:1129:PHE:HD1	2.15	0.44
1:B:1049:LYS:HB2	1:B:1161:CYS:SG	2.57	0.44
1:E:1076:LYS:O	1:E:1110:SER:HB3	2.18	0.44
1:D:1042:GLY:HA2	1:D:1046:PHE:O	2.17	0.44
1:D:1002:VAL:HG21	1:D:1165:GLU:HG2	2.00	0.44
1:D:1090:LEU:HB2	1:D:1128:VAL:HB	2.00	0.44
1:B:1129:PHE:HD1	1:B:1129:PHE:H	1.66	0.44
1:C:1122:LEU:HA	1:C:1125:LYS:HD3	2.00	0.44
2:J:105:ILE:O	2:J:106:ALA:HB3	2.18	0.44
2:K:105:ILE:O	2:K:106:ALA:HB3	2.18	0.44
1:B:1081:GLU:HG3	1:B:1082:LYS:NZ	2.33	0.44
1:C:1010:ILE:HG21	1:C:1142:MET:SD	2.58	0.44
1:A:1121:TRP:NE1	2:G:106:ALA:HB3	2.32	0.43
1:F:1003:ASN:HA	1:F:1004:PRO:HD3	1.76	0.43
1:B:1048:TYR:CD1	1:B:1065:GLY:HA2	2.52	0.43
1:B:1096:GLY:HA2	1:B:1136:MET:SD	2.59	0.43
1:D:1118:LYS:HE2	1:D:1120:GLU:OE1	2.17	0.43
1:D:1073:THR:O	1:D:1073:THR:HG22	2.17	0.43
1:D:1101:ALA:H	1:D:1112:PHE:HA	1.83	0.43
1:F:1131:LYS:HE3	1:F:1131:LYS:HB3	1.72	0.43
1:B:1139:VAL:HA	1:B:1142:MET:HG2	2.00	0.43
1:C:1142:MET:O	1:C:1145:PHE:HB2	2.19	0.43
1:E:1025:PHE:O	1:E:1029:VAL:HG22	2.18	0.43
1:D:1069:ARG:O	1:D:1070:HIS:HB2	2.17	0.43
1:B:1066:ASP:OD2	1:B:1073:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1133:LYS:HB3	1:C:1133:LYS:HE2	1.72	0.43
1:E:1139:VAL:HA	1:E:1142:MET:HB3	2.01	0.43
1:F:1055:ARG:HA	1:F:1150:GLY:O	2.19	0.43
1:A:1029:VAL:HB	1:A:1032:THR:HB	2.01	0.42
1:D:1033:ALA:O	1:D:1037:ARG:HB2	2.19	0.42
1:F:1013:ASP:OD1	1:F:1154:LYS:HB3	2.19	0.42
1:A:1094:GLY:O	1:A:1097:ILE:HG12	2.19	0.42
1:C:1139:VAL:O	1:C:1142:MET:HB2	2.18	0.42
1:E:1008:PHE:HD1	1:E:1161:CYS:HB3	1.84	0.42
1:E:1121:TRP:NE1	2:K:106:ALA:HB3	2.35	0.42
1:B:1020:VAL:HG23	1:B:1132:VAL:HG22	2.00	0.42
1:C:1139:VAL:HA	1:C:1142:MET:CE	2.49	0.42
1:F:1131:LYS:HG2	1:F:1132:VAL:N	2.34	0.42
1:B:1155:LYS:HD3	1:B:1156:ILE:N	2.35	0.42
1:D:1015:GLU:HA	1:D:1016:PRO:HD3	1.71	0.42
1:C:1119:THR:HA	1:C:1121:TRP:CZ3	2.55	0.42
1:F:1048:TYR:HB3	1:F:1158:ILE:HD12	2.01	0.42
1:E:1012:VAL:O	1:E:1013:ASP:HB2	2.18	0.42
1:E:1029:VAL:O	1:E:1030:PRO:C	2.63	0.42
1:E:1069:ARG:HD2	1:E:1069:ARG:N	2.34	0.42
1:B:1069:ARG:HB3	1:B:1071:ASN:ND2	2.35	0.42
1:B:1087:ASN:O	1:B:1127:VAL:HG13	2.20	0.41
1:D:1094:GLY:O	1:D:1097:ILE:HG12	2.19	0.41
1:F:1044:LYS:HA	1:F:1044:LYS:HD3	1.86	0.41
1:D:1022:PHE:CD2	1:D:1098:LEU:HD22	2.55	0.41
1:F:1122:LEU:HD22	1:F:1126:HIS:CD2	2.55	0.41
1:B:1129:PHE:N	1:B:1129:PHE:CD1	2.88	0.41
1:F:1037:ARG:HH22	1:F:1043:GLU:CD	2.28	0.41
1:B:1025:PHE:CD1	1:B:1025:PHE:N	2.87	0.41
1:D:1010:ILE:HG21	1:D:1142:MET:SD	2.60	0.41
1:D:1129:PHE:HD1	1:D:1129:PHE:H	1.67	0.41
1:C:1009:ASP:O	1:C:1159:ALA:N	2.51	0.41
1:D:1053:PHE:HB2	1:D:1156:ILE:HB	2.01	0.41
1:B:1018:GLY:HA3	1:B:1138:ILE:CD1	2.48	0.41
1:A:1157:THR:HG22	1:A:1158:ILE:N	2.36	0.41
1:B:1129:PHE:HD1	1:B:1129:PHE:N	2.19	0.41
1:D:1098:LEU:HB3	1:D:1130:GLY:C	2.46	0.41
1:B:1094:GLY:O	1:B:1097:ILE:HG12	2.20	0.41
1:C:1031:LYS:HE2	1:C:1084:GLU:OE2	2.20	0.41
1:E:1014:GLY:HA3	3:E:7175:HOH:O	2.21	0.41
2:J:105:ILE:O	2:J:106:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1041:THR:OG1	1:C:1043:GLU:HG2	2.20	0.41
1:E:1094:GLY:O	1:E:1097:ILE:HG12	2.20	0.41
1:E:1119:THR:HA	1:E:1121:TRP:CZ3	2.55	0.41
1:A:1002:VAL:HG23	1:A:1003:ASN:N	2.36	0.41
1:E:1131:LYS:HE2	1:E:1131:LYS:HB3	1.65	0.41
1:D:1009:ASP:O	1:D:1159:ALA:N	2.51	0.40
1:D:1141:ALA:O	1:D:1144:ARG:HG2	2.21	0.40
1:A:1147:SER:O	1:A:1150:GLY:N	2.53	0.40
1:D:1048:TYR:CE1	1:D:1065:GLY:HA2	2.56	0.40
1:F:1085:ASP:H	1:F:1106:ASN:HA	1.86	0.40
1:A:1085:ASP:O	1:A:1086:GLU:C	2.64	0.40
1:B:1021:SER:OG	1:B:1133:LYS:HB2	2.20	0.40
1:C:1060:PHE:CZ	2:I:105:ILE:O	2.74	0.40
2:J:106:ALA:HB2	3:J:7041:HOH:O	2.21	0.40
1:C:1149:ASN:HD21	1:C:1151:LYS:HB2	1.87	0.40
1:E:1157:THR:HG22	1:E:1158:ILE:N	2.36	0.40
1:D:1069:ARG:HG2	1:D:1074:GLY:CA	2.51	0.40
1:F:1042:GLY:HA2	1:F:1046:PHE:O	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%)	143 (88%)	15 (9%)	4 (2%)	4	2
1	B	162/164 (99%)	134 (83%)	21 (13%)	7 (4%)	2	0
1	C	162/164 (99%)	141 (87%)	20 (12%)	1 (1%)	21	22
1	D	162/164 (99%)	134 (83%)	27 (17%)	1 (1%)	21	22
1	E	162/164 (99%)	143 (88%)	18 (11%)	1 (1%)	21	22
1	F	162/164 (99%)	138 (85%)	22 (14%)	2 (1%)	10	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	3 (75%)	1 (25%)	0	100	100
2	J	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	K	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	L	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	996/1020 (98%)	851 (85%)	129 (13%)	16 (2%)	7	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1043	GLU
1	B	1086	GLU
1	B	1105	PRO
1	B	1081	GLU
1	C	1151	LYS
1	D	1080	GLY
1	A	1081	GLU
1	F	1043	GLU
1	F	1148	ARG
1	E	1147	SER
1	A	1086	GLU
1	B	1049	LYS
1	B	1072	GLY
1	A	1070	HIS
1	B	1037	ARG
1	B	1080	GLY

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	132/132 (100%)	123 (93%)	9 (7%)	14	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	132/132 (100%)	119 (90%)	13 (10%)	7	7
1	C	132/132 (100%)	125 (95%)	7 (5%)	20	25
1	D	132/132 (100%)	125 (95%)	7 (5%)	20	25
1	E	132/132 (100%)	122 (92%)	10 (8%)	12	13
1	F	132/132 (100%)	123 (93%)	9 (7%)	14	16
2	G	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	H	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	I	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	J	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	K	4/4 (100%)	4 (100%)	0	100	100
2	L	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	816/816 (100%)	754 (92%)	62 (8%)	12	13

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1058	PRO
1	A	1069	ARG
1	A	1082	LYS
1	A	1084	GLU
1	A	1131	LYS
1	A	1145	PHE
1	A	1148	ARG
1	A	1151	LYS
1	A	1153	SER
1	B	1015	GLU
1	B	1029	VAL
1	B	1043	GLU
1	B	1076	LYS
1	B	1084	GLU
1	B	1085	ASP
1	B	1105	PRO
1	B	1127	VAL
1	B	1129	PHE
1	B	1131	LYS
1	B	1132	VAL
1	B	1152	THR
1	B	1153	SER

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Mol	Chain	Res	Type
1	C	1028	LYS
1	C	1029	VAL
1	C	1082	LYS
1	C	1084	GLU
1	C	1118	LYS
1	C	1133	LYS
1	C	1149	ASN
1	D	1029	VAL
1	D	1037	ARG
1	D	1085	ASP
1	D	1091	LYS
1	D	1127	VAL
1	D	1129	PHE
1	D	1131	LYS
1	E	1039	LEU
1	E	1076	LYS
1	E	1081	GLU
1	E	1082	LYS
1	E	1084	GLU
1	E	1120	GLU
1	E	1133	LYS
1	E	1137	ASN
1	E	1140	GLU
1	E	1148	ARG
1	F	1029	VAL
1	F	1082	LYS
1	F	1084	GLU
1	F	1106	ASN
1	F	1125	LYS
1	F	1137	ASN
1	F	1142	MET
1	F	1144	ARG
1	F	1148	ARG
2	G	101	HIS
2	H	101	HIS
2	H	105	ILE
2	I	101	HIS
2	J	101	HIS
2	J	102	VAL
2	L	101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1035	ASN
1	A	1070	HIS
1	A	1087	ASN
1	B	1003	ASN
1	B	1108	ASN
1	B	1126	HIS
1	B	1137	ASN
1	B	1149	ASN
1	C	1106	ASN
1	C	1149	ASN
1	E	1035	ASN
1	F	1108	ASN
1	F	1137	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	1.46	37 (22%) 2 2	5, 13, 20, 23	0
1	B	164/164 (100%)	2.59	106 (64%) 0 0	11, 20, 28, 34	0
1	C	164/164 (100%)	1.79	62 (37%) 1 0	5, 16, 25, 35	0
1	D	164/164 (100%)	1.84	58 (35%) 1 0	7, 18, 25, 33	0
1	E	164/164 (100%)	1.55	49 (29%) 1 1	3, 12, 21, 27	0
1	F	164/164 (100%)	2.43	93 (56%) 0 0	10, 18, 26, 30	0
2	G	4/6 (66%)	1.85	1 (25%) 2 1	17, 19, 21, 29	0
2	H	6/6 (100%)	2.17	3 (50%) 0 0	11, 16, 22, 24	0
2	I	6/6 (100%)	1.68	2 (33%) 1 1	7, 10, 11, 26	0
2	J	6/6 (100%)	2.10	3 (50%) 0 0	9, 10, 12, 18	0
2	K	4/6 (66%)	2.57	3 (75%) 0 0	12, 13, 20, 23	0
2	L	6/6 (100%)	2.51	4 (66%) 0 0	16, 19, 24, 24	0
All	All	1016/1020 (99%)	1.95	421 (41%) 0 0	3, 17, 26, 35	0

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1104	GLY	11.4
1	F	1127	VAL	7.0
1	D	1029	VAL	6.6
1	F	1107	THR	6.4
1	D	1080	GLY	6.4
1	C	1016	PRO	6.2
1	D	1104	GLY	6.0
1	F	1026	ALA	5.8
1	B	1146	GLY	5.7
1	F	1030	PRO	5.5
1	F	1029	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	1039	LEU	5.5
1	B	1003	ASN	5.4
1	B	1070	HIS	5.3
1	D	1026	ALA	5.2
1	A	1080	GLY	4.9
1	E	1152	THR	4.9
1	E	1159	ALA	4.8
1	B	1067	PHE	4.8
1	A	1146	GLY	4.7
1	C	1013	ASP	4.7
1	F	1032	THR	4.7
1	C	1012	VAL	4.7
1	B	1109	GLY	4.7
1	F	1156	ILE	4.6
1	C	1068	THR	4.6
1	B	1108	ASN	4.6
1	B	1024	LEU	4.5
1	F	1103	ALA	4.5
1	B	1130	GLY	4.4
1	F	1088	PHE	4.4
1	F	1038	ALA	4.3
1	E	1073	THR	4.3
1	B	1012	VAL	4.2
1	F	1150	GLY	4.2
1	F	1078	ILE	4.2
1	B	1073	THR	4.2
1	F	1012	VAL	4.1
1	D	1003	ASN	4.1
1	E	1012	VAL	4.1
1	B	1083	PHE	4.0
1	F	1080	GLY	4.0
1	B	1127	VAL	4.0
1	C	1146	GLY	4.0
1	F	1085	ASP	4.0
1	C	1081	GLU	4.0
1	E	1081	GLU	4.0
1	B	1105	PRO	4.0
1	F	1070	HIS	4.0
1	C	1148	ARG	4.0
1	B	1159	ALA	4.0
2	L	101	HIS	3.9
1	B	1148	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	1027	ASP	3.9
1	D	1081	GLU	3.9
1	B	1141	ALA	3.9
1	F	1143	GLU	3.9
1	B	1085	ASP	3.8
1	D	1147	SER	3.8
1	B	1080	GLY	3.8
1	F	1146	GLY	3.8
1	F	1040	SER	3.8
1	B	1079	TYR	3.8
1	F	1035	ASN	3.8
1	A	1012	VAL	3.8
1	C	1002	VAL	3.8
2	H	106	ALA	3.7
1	D	1079	TYR	3.7
2	K	106	ALA	3.7
1	C	1093	THR	3.7
1	B	1016	PRO	3.7
1	D	1078	ILE	3.7
1	F	1002	VAL	3.7
1	C	1159	ALA	3.7
1	C	1145	PHE	3.6
1	E	1148	ARG	3.6
1	B	1032	THR	3.6
1	F	1073	THR	3.6
1	B	1129	PHE	3.6
1	C	1080	GLY	3.6
1	B	1102	ASN	3.6
1	C	1089	ILE	3.6
1	B	1050	GLY	3.6
1	B	1088	PHE	3.6
1	D	1030	PRO	3.6
1	C	1015	GLU	3.6
1	E	1080	GLY	3.5
1	A	1154	LYS	3.5
1	D	1085	ASP	3.5
1	A	1143	GLU	3.5
1	B	1152	THR	3.5
1	A	1081	GLU	3.5
1	F	1036	PHE	3.5
1	B	1077	SER	3.4
1	B	1084	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	1034	GLU	3.4
1	B	1066	ASP	3.4
1	C	1017	LEU	3.4
1	F	1071	ASN	3.4
1	E	1145	PHE	3.4
1	C	1123	ASP	3.4
1	F	1083	PHE	3.4
1	E	1154	LYS	3.4
1	E	1156	ILE	3.3
1	B	1041	THR	3.3
1	B	1119	THR	3.3
2	J	106	ALA	3.3
1	F	1130	GLY	3.3
1	B	1147	SER	3.3
1	D	1002	VAL	3.3
2	L	102	VAL	3.3
1	B	1097	ILE	3.3
1	F	1068	THR	3.3
1	B	1071	ASN	3.3
1	B	1123	ASP	3.3
1	F	1087	ASN	3.3
1	F	1116	THR	3.3
1	C	1127	VAL	3.3
1	F	1152	THR	3.2
1	D	1135	GLY	3.2
2	G	101	HIS	3.2
1	F	1163	GLN	3.2
1	B	1051	SER	3.2
1	A	1029	VAL	3.2
1	B	1006	VAL	3.2
1	B	1048	TYR	3.2
1	B	1075	GLY	3.2
1	C	1128	VAL	3.2
1	E	1016	PRO	3.2
1	C	1106	ASN	3.2
1	E	1082	LYS	3.1
1	B	1025	PHE	3.1
1	D	1025	PHE	3.1
1	B	1029	VAL	3.1
1	B	1138	ILE	3.1
1	C	1157	THR	3.1
1	F	1161	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	1071	ASN	3.1
1	F	1124	GLY	3.1
1	B	1038	ALA	3.1
1	B	1132	VAL	3.1
1	C	1020	VAL	3.1
1	D	1024	LEU	3.1
1	C	1134	GLU	3.1
1	C	1147	SER	3.1
1	F	1051	SER	3.1
1	C	1026	ALA	3.1
1	F	1058	PRO	3.1
1	B	1135	GLY	3.1
1	B	1149	ASN	3.1
1	C	1156	ILE	3.0
1	B	1107	THR	3.0
1	F	1066	ASP	3.0
1	D	1016	PRO	3.0
1	E	1018	GLY	3.0
1	C	1088	PHE	3.0
1	D	1128	VAL	3.0
1	A	1156	ILE	3.0
1	E	1119	THR	3.0
1	F	1155	LYS	3.0
1	D	1075	GLY	3.0
1	F	1013	ASP	3.0
1	B	1139	VAL	3.0
1	A	1040	SER	3.0
1	F	1047	GLY	3.0
1	F	1074	GLY	3.0
1	B	1081	GLU	3.0
1	A	1058	PRO	3.0
1	B	1090	LEU	2.9
1	B	1155	LYS	2.9
1	A	1148	ARG	2.9
1	F	1148	ARG	2.9
1	B	1110	SER	2.9
1	B	1042	GLY	2.9
1	C	1137	ASN	2.9
1	D	1094	GLY	2.9
1	B	1026	ALA	2.9
1	E	1017	LEU	2.9
1	F	1117	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1031	LYS	2.9
1	C	1069	ARG	2.9
1	B	1027	ASP	2.9
1	B	1117	ALA	2.9
1	B	1002	VAL	2.9
1	F	1128	VAL	2.9
1	C	1084	GLU	2.9
1	D	1015	GLU	2.9
1	F	1079	TYR	2.9
1	B	1103	ALA	2.9
1	B	1122	LEU	2.9
1	B	1145	PHE	2.9
1	B	1047	GLY	2.8
1	F	1075	GLY	2.8
1	A	1145	PHE	2.8
1	B	1046	PHE	2.8
1	E	1087	ASN	2.8
1	B	1040	SER	2.8
1	B	1074	GLY	2.8
1	C	1045	GLY	2.8
1	E	1101	ALA	2.8
1	C	1014	GLY	2.8
1	E	1147	SER	2.8
1	F	1017	LEU	2.8
1	F	1011	ALA	2.8
1	B	1007	PHE	2.8
1	B	1020	VAL	2.8
1	D	1020	VAL	2.8
1	F	1132	VAL	2.8
1	D	1027	ASP	2.8
1	F	1102	ASN	2.8
1	B	1045	GLY	2.8
1	D	1014	GLY	2.8
1	A	1140	GLU	2.8
1	E	1015	GLU	2.8
1	B	1154	LYS	2.8
1	A	1149	ASN	2.7
1	F	1057	ILE	2.7
1	C	1121	TRP	2.7
1	F	1064	GLY	2.7
1	A	1105	PRO	2.7
1	C	1052	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	1086	GLU	2.7
1	E	1143	GLU	2.7
1	F	1028	LYS	2.7
1	A	1101	ALA	2.7
1	B	1011	ALA	2.7
1	E	1067	PHE	2.7
1	A	1087	ASN	2.7
1	B	1157	THR	2.7
1	C	1119	THR	2.7
1	B	1078	ILE	2.7
1	F	1160	ASP	2.7
1	E	1050	GLY	2.7
1	F	1108	ASN	2.7
1	F	1018	GLY	2.7
1	B	1140	GLU	2.7
1	E	1151	LYS	2.7
1	F	1110	SER	2.7
1	F	1052	CYS	2.7
1	F	1164	LEU	2.7
1	B	1053	PHE	2.7
1	B	1116	THR	2.7
1	A	1104	GLY	2.7
1	E	1146	GLY	2.7
1	F	1016	PRO	2.7
1	D	1117	ALA	2.6
1	E	1141	ALA	2.6
1	D	1129	PHE	2.6
1	B	1160	ASP	2.6
2	J	102	VAL	2.6
1	F	1065	GLY	2.6
1	B	1017	LEU	2.6
1	F	1084	GLU	2.6
1	F	1086	GLU	2.6
1	D	1145	PHE	2.6
1	A	1002	VAL	2.6
2	H	102	VAL	2.6
1	E	1047	GLY	2.6
1	B	1156	ILE	2.6
2	K	101	HIS	2.6
1	A	1151	LYS	2.6
1	D	1155	LYS	2.6
1	F	1053	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1029	VAL	2.6
1	F	1050	GLY	2.6
2	L	103	GLY	2.6
1	A	1071	ASN	2.6
1	C	1094	GLY	2.6
1	D	1006	VAL	2.6
1	C	1118	LYS	2.6
1	D	1131	LYS	2.6
1	B	1065	GLY	2.5
1	C	1059	GLY	2.5
1	D	1095	PRO	2.5
1	E	1135	GLY	2.5
1	C	1139	VAL	2.5
1	B	1163	GLN	2.5
1	C	1086	GLU	2.5
1	B	1069	ARG	2.5
1	F	1090	LEU	2.5
1	E	1142	MET	2.5
1	F	1101	ALA	2.5
1	F	1141	ALA	2.5
1	B	1014	GLY	2.5
1	B	1049	LYS	2.5
1	F	1145	PHE	2.5
1	B	1015	GLU	2.5
1	C	1079	TYR	2.5
1	C	1011	ALA	2.5
1	B	1072	GLY	2.5
1	F	1157	THR	2.5
1	D	1083	PHE	2.5
1	B	1106	ASN	2.5
1	F	1149	ASN	2.5
1	D	1069	ARG	2.4
1	D	1099	SER	2.4
1	D	1132	VAL	2.4
1	E	1139	VAL	2.4
1	A	1159	ALA	2.4
1	B	1037	ARG	2.4
1	B	1144	ARG	2.4
1	C	1141	ALA	2.4
1	D	1146	GLY	2.4
1	D	1148	ARG	2.4
1	F	1147	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	1089	ILE	2.4
1	E	1138	ILE	2.4
1	D	1106	ASN	2.4
1	E	1140	GLU	2.4
1	E	1074	GLY	2.4
1	F	1059	GLY	2.4
1	D	1116	THR	2.4
1	E	1068	THR	2.4
1	A	1046	PHE	2.4
1	B	1128	VAL	2.4
1	B	1142	MET	2.4
2	I	101	HIS	2.4
1	C	1058	PRO	2.3
1	C	1138	ILE	2.3
1	E	1029	VAL	2.3
1	C	1144	ARG	2.3
2	J	101	HIS	2.3
1	B	1039	LEU	2.3
1	A	1079	TYR	2.3
1	B	1076	LYS	2.3
1	B	1121	TRP	2.3
1	F	1048	TYR	2.3
1	F	1095	PRO	2.3
1	C	1096	GLY	2.3
1	F	1033	ALA	2.3
1	E	1116	THR	2.3
1	D	1138	ILE	2.3
1	C	1095	PRO	2.3
1	C	1124	GLY	2.3
1	D	1033	ALA	2.3
1	A	1152	THR	2.3
1	D	1093	THR	2.3
1	D	1127	VAL	2.3
1	D	1164	LEU	2.3
1	F	1024	LEU	2.3
1	B	1162	GLY	2.3
1	D	1042	GLY	2.3
1	E	1045	GLY	2.3
1	F	1104	GLY	2.3
1	B	1153	SER	2.3
1	E	1153	SER	2.3
1	B	1008	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	1106	ASN	2.2
1	E	1058	PRO	2.2
1	A	1014	GLY	2.2
1	A	1086	GLU	2.2
1	D	1159	ALA	2.2
1	E	1011	ALA	2.2
1	C	1152	THR	2.2
2	H	101	HIS	2.2
1	E	1049	LYS	2.2
1	D	1097	ILE	2.2
1	D	1007	PHE	2.2
1	E	1149	ASN	2.2
1	D	1073	THR	2.2
1	D	1158	ILE	2.2
1	A	1017	LEU	2.2
1	F	1122	LEU	2.2
1	A	1067	PHE	2.2
1	A	1144	ARG	2.2
1	A	1070	HIS	2.2
1	C	1153	SER	2.2
1	F	1041	THR	2.2
1	B	1057	ILE	2.2
1	D	1108	ASN	2.2
1	F	1006	VAL	2.2
2	I	102	VAL	2.2
1	F	1100	MET	2.2
1	F	1112	PHE	2.2
1	A	1018	GLY	2.2
1	C	1135	GLY	2.2
1	A	1068	THR	2.2
2	L	106	ALA	2.2
1	D	1149	ASN	2.1
1	A	1083	PHE	2.1
1	F	1025	PHE	2.1
1	F	1031	LYS	2.1
1	B	1058	PRO	2.1
1	A	1130	GLY	2.1
1	E	1014	GLY	2.1
1	E	1041	THR	2.1
1	C	1057	ILE	2.1
1	C	1082	LYS	2.1
1	C	1158	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	105	ILE	2.1
1	F	1022	PHE	2.1
1	B	1018	GLY	2.1
1	E	1124	GLY	2.1
1	C	1041	THR	2.1
1	B	1136	MET	2.1
1	C	1091	LYS	2.1
1	D	1136	MET	2.1
1	E	1013	ASP	2.1
1	F	1158	ILE	2.1
1	F	1105	PRO	2.1
1	D	1088	PHE	2.1
1	F	1121	TRP	2.1
1	B	1064	GLY	2.1
1	C	1074	GLY	2.1
1	C	1115	CYS	2.1
1	E	1107	THR	2.1
1	C	1117	ALA	2.1
1	D	1140	GLU	2.1
1	A	1096	GLY	2.1
1	B	1019	ARG	2.1
1	D	1077	SER	2.0
1	A	1161	CYS	2.0
1	E	1038	ALA	2.0
1	D	1063	GLN	2.0
1	B	1056	ILE	2.0
1	B	1004	PRO	2.0
1	C	1030	PRO	2.0
1	D	1107	THR	2.0
1	C	1078	ILE	2.0
1	D	1144	ARG	2.0
1	B	1091	LYS	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.