Full wwPDB X-ray Structure Validation Report

May 25, 2020 – 02:44 pm BST

PDB ID	:	1AWT
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

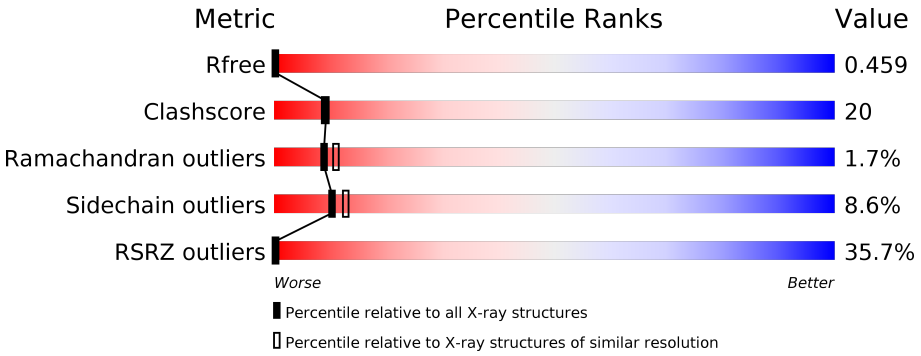
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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 <=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	18% 66% 32% ·
1	B	164	65% 49% 42% 9%
1	C	164	24% 63% 34% ·
1	D	164	30% 59% 35% 6%
1	E	164	14% 72% 26% ·
1	F	164	62% 47% 48% · ·

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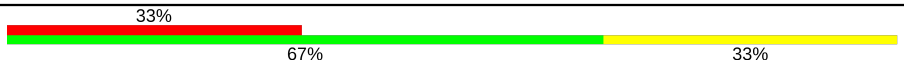
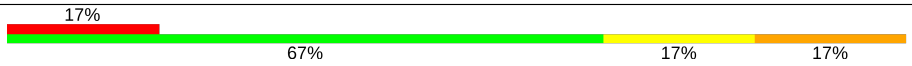
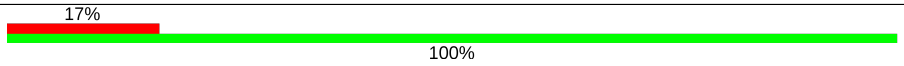
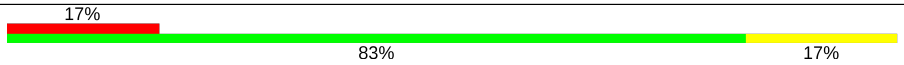
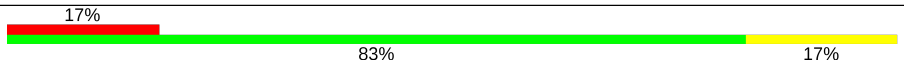
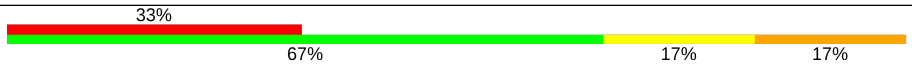
Mol	Chain	Length	Quality of chain
2	G	6	
2	H	6	
2	I	6	
2	J	6	
2	K	6	
2	L	6	

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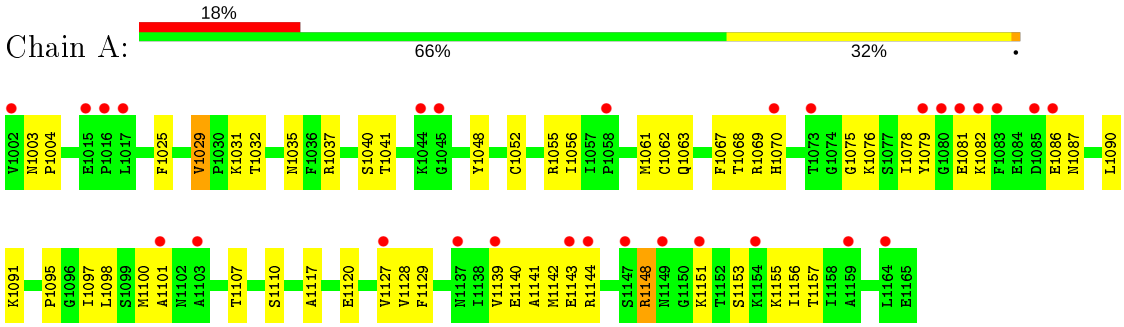
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O 1 1	0	0
3	J	1	Total O 1 1	0	0
3	K	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

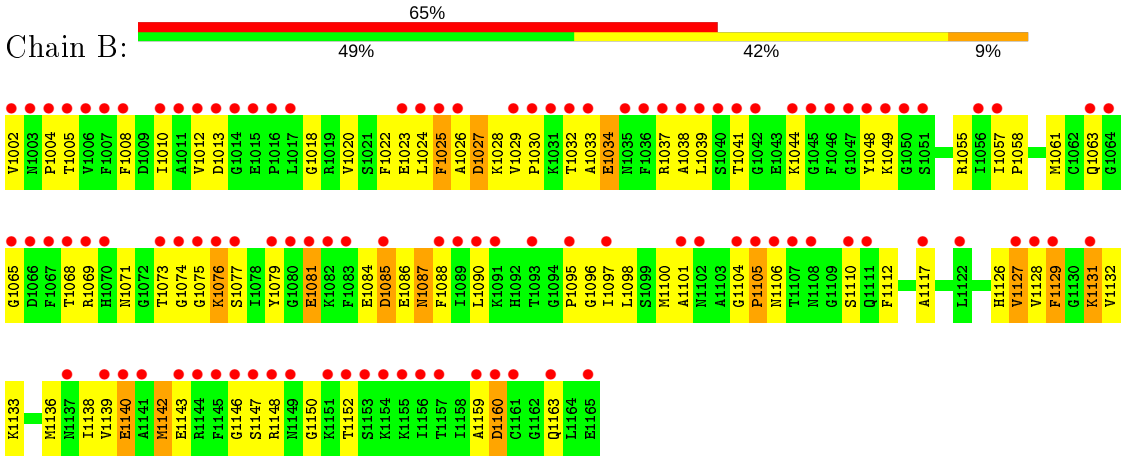
- Molecule 1: CYCLOPHILIN A

Chain A:



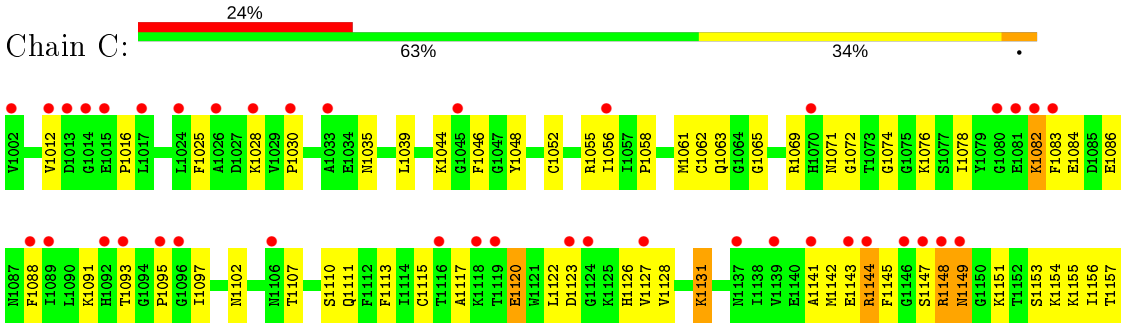
- Molecule 1: CYCLOPHILIN A

Chain B:



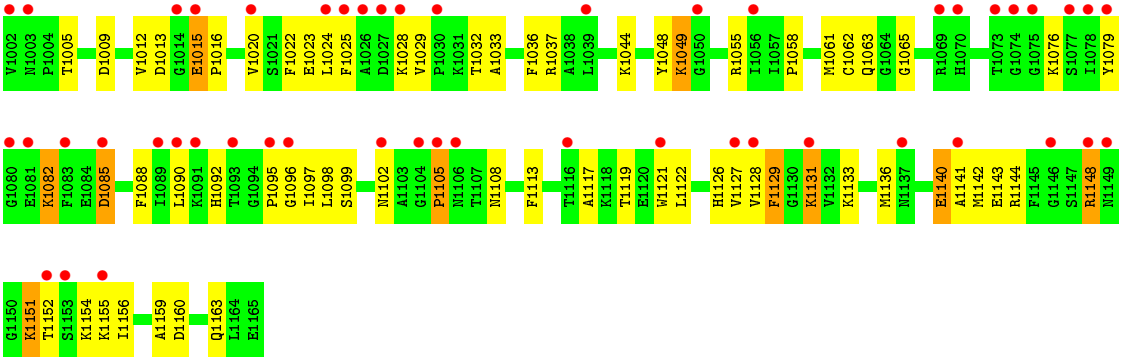
- Molecule 1: CYCLOPHILIN A

Chain C:



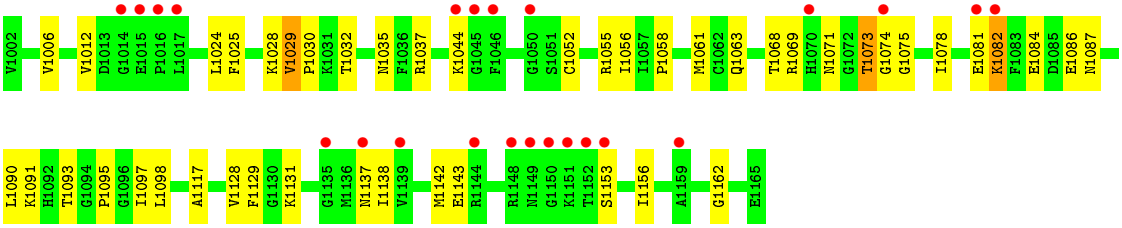
• Molecule 1: CYCLOPHILIN A

Chain D:



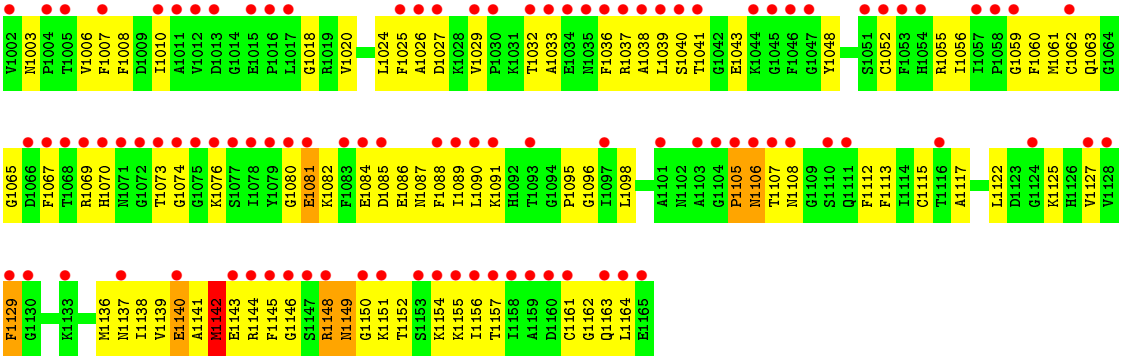
• Molecule 1: CYCLOPHILIN A

Chain E:



• Molecule 1: CYCLOPHILIN A

Chain F:



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

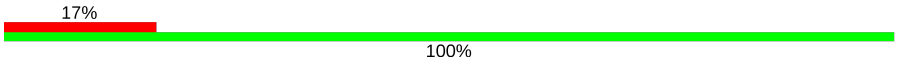
Chain G:

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

Chain H:

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

Chain I:



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

Chain J:

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

Chain K:

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

Chain L:

4 Data and refinement statistics (i)

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 14.85 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.3 (15.00-2.55) 93.2 (14.85-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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)	0.43 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/1282	0.72	0/1711
1	B	0.67	1/1282 (0.1%)	0.70	0/1711
1	C	0.63	0/1282	0.70	0/1711
1	D	0.60	1/1282 (0.1%)	0.71	0/1711
1	E	0.62	0/1282	0.71	0/1711
1	F	0.62	0/1282	0.72	0/1711
2	G	0.51	0/41	0.73	0/54
2	H	0.57	0/41	0.64	0/54
2	I	0.65	0/41	0.97	0/54
2	J	0.74	0/41	0.74	0/54
2	K	0.64	0/41	1.00	0/54
2	L	0.57	0/41	0.68	0/54
All	All	0.63	2/7938 (0.0%)	0.71	0/10590

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1142	MSE	CG-SE	-5.72	1.76	1.95
1	D	1142	MSE	CG-SE	-5.05	1.78	1.95

There are no bond angle outliers.

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	30	0
1	B	1258	0	1225	63	0
1	C	1258	0	1225	47	0
1	D	1258	0	1225	50	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
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	306	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 (306) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:1086:GLU:HG2	1:E:1087:ASN:ND2	2.14	0.63
1:D:1126:HIS:NE2	2:J:104:PRO:HB3	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:C:1069:ARG:HB3	1:C:1071:ASN:OD1	2.01	0.61
1:C:1149:ASN:C	1:C:1149:ASN:HD22	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:F:1037:ARG:HG2	1.67	0.58
1:B:1048:TYR:CE1	1:B:1065:GLY:HA2	2.38	0.58
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:C:1028:LYS:C	1:C:1030:PRO:HD3	2.25	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:F:1141:ALA:C	1:F:1143:GLU:H	2.08	0.56
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:E:1097:ILE:HG23	1:E:1128:VAL:HG13	1.90	0.54
1:D:1126:HIS:CD2	2:J:104:PRO:HB3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1069:ARG:HE	1:C:1074:GLY:HA3	1.72	0.54
1:C:1082:LYS:HB3	1:C:1082:LYS:NZ	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
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:1082:LYS:H	1:E:1082:LYS:HD3	1.75	0.52
1:B:1075:GLY:HA3	1:B:1110:SER:OG	2.09	0.52
1:B:1018:GLY:HA3	1:B:1138:ILE:HD12	1.91	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:NE	1:A:1148:ARG:HA	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
1:E:1068:THR:HG1	1:E:1075:GLY:H	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:F:1091:LYS:HA	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:O	1:A:1127:VAL:HG23	2.11	0.49
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: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: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: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:NH1	1:F:1037:ARG:HG2	2.28	0.47
1:F:1040:SER:HA	1:F:1048:TYR:HD2	1.80	0.47
1:F:1082:LYS:HZ2	1:F:1107:THR:HG22	1.78	0.47
1:F:1048:TYR:CE1	1:F:1112:PHE:HE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1146:GLY:HA2	1:F:1152:THR:HA	1.97	0.47
1:C:1088:PHE:HA	3:C:7133:HOH:O	2.14	0.47
1:F:1152:THR:HB	1:F:1154:LYS:O	2.14	0.47
1:A:1031:LYS:HE3	1:A:1079:TYR:CD2	2.50	0.47
1:D:1009:ASP:O	1:D:1159:ALA:N	2.47	0.47
1:F:1136:MSE:HG2	3:F:7149:HOH:O	2.15	0.47
1:F:1041:THR:HG22	1:F:1162:GLY:HA2	1.97	0.47
1:F:1149:ASN:ND2	1:F:1149:ASN:H	2.13	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: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:NE	1:F:1148:ARG:HA	2.31	0.45
1:D:1058:PRO:HA	1:D:1143:GLU:HG3	1.97	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:F:1080:GLY:O	1:F:1081:GLU:O	2.35	0.45
1:F:1090:LEU:C	1:F:1091:LYS:HD2	2.37	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:E:1044:LYS:NZ	1:E:1078:ILE:HB	2.32	0.44
1:F:1007:PHE:CD2	1:F:1164:LEU:HG	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1140:GLU:O	1:F:1143:GLU:HB2	2.18	0.44
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:B:1076:LYS:HZ2	1:B:1081:GLU:HB3	1.83	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: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:C:1072:GLY:HA2	1:C:1111:GLN:OE1	2.18	0.43
1:C:1012:VAL:HG11	1:C:1154:LYS:HD3	1.99	0.43
1:A:1141:ALA:HA	1:A:1144:ARG:HH21	1.84	0.43
1:B:1140:GLU:C	1:B:1143:GLU:HB2	2.39	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:F:1024:LEU:CD1	1:F:1037:ARG:HB2	2.48	0.42
1:B:1129:PHE:CD1	1:B:1129:PHE:N	2.88	0.42
1:B:1012:VAL:O	1:B:1013:ASP:HB2	2.19	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:E:1028:LYS:C	1:E:1030:PRO:HD3	2.39	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

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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: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:C:1149:ASN:ND2	1:C:1151:LYS:H	2.17	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:B:1076:LYS:HZ2	1:B:1076:LYS:HB2	1.85	0.41
1:C:1055:ARG:HB3	1:C:1063:GLN:HB3	2.02	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:C:1097:ILE:HG23	1:C:1128:VAL:HG13	2.02	0.41
1:D:1020:VAL:HG13	1:D:1020:VAL:O	2.21	0.41
1:D:1092:HIS:HB2	1:D:1119:THR:O	2.20	0.41
1:F:1069:ARG:HG2	1:F:1074:GLY:HA3	2.03	0.41
1:F:1037:ARG:HD2	1:F:1163:GLN:NE2	2.36	0.41
1:C:1056:ILE:CG2	1:C:1143:GLU:HA	2.51	0.41
1:D:1023:GLU:HB2	1:D:1133:LYS:CE	2.42	0.41
1:D:1129:PHE:N	1:D:1129:PHE:CD1	2.88	0.41
1:C:1147:SER:OG	1:C:1148:ARG:N	2.45	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:A:1090:LEU:C	1:A:1091:LYS:HD2	2.41	0.40
1:B:1008:PHE:HB2	1:B:1020:VAL:HG13	2.03	0.40
1:B:1076:LYS:HZ2	1:B:1076:LYS:CB	2.34	0.40
1:D:1085:ASP:CG	1:D:1108:ASN:HD21	2.24	0.40
1:E:1006:VAL:HA	1:E:1162:GLY:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1044:LYS:HZ1	1:E:1078:ILE:HB	1.86	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%)	8 9
1	B	162/164 (99%)	136 (84%)	20 (12%)	6 (4%)	3 2
1	C	162/164 (99%)	140 (86%)	21 (13%)	1 (1%)	25 34
1	D	162/164 (99%)	140 (86%)	18 (11%)	4 (2%)	5 5
1	E	162/164 (99%)	146 (90%)	16 (10%)	0	100 100
1	F	162/164 (99%)	146 (90%)	13 (8%)	3 (2%)	8 9
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%)	9 11

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 (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	132/128 (103%)	124 (94%)	8 (6%)	18 24
1	B	132/128 (103%)	116 (88%)	16 (12%)	5 4
1	C	132/128 (103%)	123 (93%)	9 (7%)	16 20
1	D	132/128 (103%)	120 (91%)	12 (9%)	9 11
1	E	132/128 (103%)	125 (95%)	7 (5%)	22 30
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%)	3 (100%)	0	100 100
2	J	3/3 (100%)	3 (100%)	0	100 100

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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%)	740 (91%)	70 (9%)	10 13

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1029	VAL
1	A	1032	THR
1	A	1061	MSE
1	A	1069	ARG
1	A	1120	GLU
1	A	1148	ARG
1	A	1151	LYS
1	A	1153	SER
1	B	1027	ASP
1	B	1034	GLU
1	B	1044	LYS
1	B	1061	MSE
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	1160	ASP
1	C	1061	MSE
1	C	1082	LYS
1	C	1084	GLU
1	C	1120	GLU
1	C	1131	LYS
1	C	1144	ARG
1	C	1148	ARG
1	C	1149	ASN
1	C	1153	SER
1	D	1013	ASP

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Mol	Chain	Res	Type
1	D	1015	GLU
1	D	1061	MSE
1	D	1076	LYS
1	D	1082	LYS
1	D	1085	ASP
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	1061	MSE
1	E	1073	THR
1	E	1082	LYS
1	E	1084	GLU
1	E	1137	ASN
1	E	1153	SER
1	F	1027	ASP
1	F	1061	MSE
1	F	1073	THR
1	F	1084	GLU
1	F	1105	PRO
1	F	1106	ASN
1	F	1125	LYS
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	K	101	HIS
2	L	101	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1003	ASN
1	B	1087	ASN

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Mol	Chain	Res	Type
1	B	1108	ASN
1	C	1149	ASN
1	D	1102	ASN
1	D	1108	ASN
1	E	1137	ASN
1	F	1070	HIS
1	F	1108	ASN
2	K	101	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.22	29 (18%)	1 1	5, 13, 21, 23	0
1	B	160/164 (97%)	2.71	106 (66%)	0 0	11, 20, 28, 34	0
1	C	160/164 (97%)	1.44	40 (25%)	0 0	5, 16, 26, 35	0
1	D	160/164 (97%)	1.59	49 (30%)	0 0	7, 18, 25, 33	0
1	E	160/164 (97%)	1.17	23 (14%)	2 3	4, 12, 22, 27	0
1	F	160/164 (97%)	2.70	101 (63%)	0 0	10, 18, 26, 30	0
2	G	6/6 (100%)	1.37	2 (33%)	0 0	13, 17, 21, 29	0
2	H	6/6 (100%)	1.18	1 (16%)	1 1	11, 14, 22, 24	0
2	I	6/6 (100%)	1.53	1 (16%)	1 1	6, 8, 11, 26	0
2	J	6/6 (100%)	1.78	1 (16%)	1 1	9, 10, 12, 18	0
2	K	6/6 (100%)	1.16	1 (16%)	1 1	7, 9, 20, 23	0
2	L	6/6 (100%)	1.85	2 (33%)	0 0	16, 19, 24, 24	0
All	All	996/1020 (97%)	1.79	356 (35%)	0 0	4, 17, 26, 35	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1107	THR	9.5
1	F	1070	HIS	7.1
1	F	1083	PHE	6.8
1	B	1074	GLY	6.6
1	F	1069	ARG	6.0
1	B	1141	ALA	6.0
1	B	1025	PHE	5.8
1	B	1002	VAL	5.5
1	B	1003	ASN	5.5
1	C	1002	VAL	5.3
1	B	1049	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	1046	PHE	5.1
1	B	1105	PRO	5.1
1	F	1012	VAL	5.1
1	F	1030	PRO	5.0
1	F	1080	GLY	4.9
1	F	1103	ALA	4.8
1	F	1090	LEU	4.7
1	B	1080	GLY	4.7
1	F	1017	LEU	4.7
1	F	1085	ASP	4.7
1	F	1078	ILE	4.7
1	F	1081	GLU	4.6
1	F	1105	PRO	4.6
1	F	1163	GLN	4.6
1	F	1032	THR	4.6
1	B	1067	PHE	4.6
1	F	1052	CYS	4.6
1	B	1079	TYR	4.6
1	B	1104	GLY	4.5
1	B	1024	LEU	4.5
1	F	1033	ALA	4.5
1	B	1090	LEU	4.5
1	B	1066	ASP	4.4
1	B	1160	ASP	4.4
1	E	1017	LEU	4.4
1	D	1105	PRO	4.4
1	B	1016	PRO	4.4
1	D	1080	GLY	4.4
1	B	1069	ARG	4.4
1	A	1080	GLY	4.3
1	F	1068	THR	4.3
1	B	1038	ALA	4.3
1	B	1089	ILE	4.3
2	L	101	HIS	4.3
1	B	1088	PHE	4.3
1	F	1041	THR	4.3
1	F	1039	LEU	4.2
1	F	1127	VAL	4.2
1	C	1148	ARG	4.2
1	B	1081	GLU	4.2
1	B	1093	THR	4.2
1	F	1026	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	1030	PRO	4.2
1	C	1095	PRO	4.1
1	F	1046	PHE	4.1
1	C	1017	LEU	4.1
1	B	1037	ARG	4.1
1	B	1159	ALA	4.1
1	F	1104	GLY	4.1
1	B	1106	ASN	4.1
1	B	1026	ALA	4.1
1	F	1144	ARG	4.0
1	D	1030	PRO	4.0
1	F	1074	GLY	4.0
1	F	1038	ALA	4.0
1	F	1071	ASN	4.0
1	F	1010	ILE	4.0
1	F	1089	ILE	4.0
1	C	1093	THR	4.0
1	B	1085	ASP	4.0
1	B	1128	VAL	4.0
1	B	1032	THR	4.0
1	B	1039	LEU	4.0
1	E	1014	GLY	4.0
1	B	1161	CYS	4.0
1	F	1029	VAL	3.9
1	D	1155	LYS	3.9
1	B	1041	THR	3.9
1	F	1013	ASP	3.8
1	F	1045	GLY	3.8
1	F	1157	THR	3.8
1	C	1015	GLU	3.8
2	K	101	HIS	3.8
1	E	1137	ASN	3.8
1	B	1050	GLY	3.7
2	G	101	HIS	3.7
2	J	106	ALA	3.7
1	D	1002	VAL	3.7
1	F	1108	ASN	3.7
1	C	1141	ALA	3.7
1	B	1143	GLU	3.7
1	B	1011	ALA	3.7
1	B	1013	ASP	3.7
1	B	1151	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	1151	LYS	3.6
1	B	1075	GLY	3.6
1	F	1075	GLY	3.6
1	B	1012	VAL	3.6
1	F	1025	PHE	3.6
1	A	1017	LEU	3.6
1	F	1110	SER	3.6
1	F	1153	SER	3.6
1	F	1091	LYS	3.6
1	B	1007	PHE	3.6
1	B	1051	SER	3.6
1	B	1077	SER	3.6
1	F	1154	LYS	3.6
1	A	1144	ARG	3.5
1	F	1053	PHE	3.5
1	B	1147	SER	3.5
1	B	1155	LYS	3.5
1	F	1036	PHE	3.5
1	B	1065	GLY	3.5
1	B	1156	ILE	3.5
1	F	1129	PHE	3.5
1	B	1107	THR	3.5
1	E	1081	GLU	3.5
1	F	1088	PHE	3.4
1	B	1023	GLU	3.4
1	B	1068	THR	3.4
1	D	1116	THR	3.4
1	B	1047	GLY	3.4
1	F	1059	GLY	3.4
1	F	1160	ASP	3.4
1	C	1144	ARG	3.4
1	D	1104	GLY	3.3
1	B	1152	THR	3.3
1	D	1028	LYS	3.3
1	B	1108	ASN	3.3
1	F	1161	CYS	3.3
1	C	1082	LYS	3.3
1	B	1083	PHE	3.3
1	D	1027	ASP	3.3
1	D	1069	ARG	3.3
1	B	1006	VAL	3.3
1	F	1011	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	1145	PHE	3.3
1	D	1106	ASN	3.3
1	F	1106	ASN	3.3
1	B	1110	SER	3.3
1	C	1070	HIS	3.2
1	A	1045	GLY	3.2
1	B	1045	GLY	3.2
1	E	1045	GLY	3.2
1	F	1027	ASP	3.2
1	A	1081	GLU	3.2
1	B	1029	VAL	3.2
1	B	1127	VAL	3.2
1	F	1158	ILE	3.2
1	F	1156	ILE	3.2
1	F	1093	THR	3.2
1	F	1040	SER	3.2
1	D	1014	GLY	3.2
1	B	1129	PHE	3.1
1	F	1051	SER	3.1
1	E	1150	GLY	3.1
1	D	1085	ASP	3.1
1	C	1081	GLU	3.1
1	C	1118	LYS	3.1
1	F	1150	GLY	3.1
1	B	1097	ILE	3.1
1	B	1015	GLU	3.1
1	E	1144	ARG	3.1
1	B	1033	ALA	3.1
1	D	1081	GLU	3.1
1	B	1044	LYS	3.1
1	F	1005	THR	3.1
1	D	1078	ILE	3.0
1	B	1010	ILE	3.0
1	F	1137	ASN	3.0
1	F	1143	GLU	3.0
1	F	1077	SER	3.0
1	A	1143	GLU	3.0
1	F	1079	TYR	3.0
1	F	1147	SER	3.0
2	I	106	ALA	3.0
1	E	1149	ASN	3.0
1	B	1145	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	1148	ARG	2.9
1	F	1146	GLY	2.9
1	A	1002	VAL	2.9
1	A	1154	LYS	2.9
1	D	1128	VAL	2.9
1	D	1079	TYR	2.9
1	B	1144	ARG	2.9
1	D	1121	TRP	2.9
1	F	1066	ASP	2.8
1	B	1005	THR	2.8
1	C	1026	ALA	2.8
1	B	1035	ASN	2.8
1	D	1127	VAL	2.8
1	D	1089	ILE	2.8
1	D	1141	ALA	2.8
1	F	1164	LEU	2.8
1	D	1003	ASN	2.8
1	A	1147	SER	2.8
1	B	1095	PRO	2.8
1	C	1116	THR	2.8
1	B	1149	ASN	2.8
1	D	1075	GLY	2.8
1	D	1152	THR	2.8
1	E	1153	SER	2.8
1	E	1050	GLY	2.8
1	E	1074	GLY	2.8
1	E	1135	GLY	2.8
1	C	1127	VAL	2.7
1	D	1026	ALA	2.7
1	A	1164	LEU	2.7
1	B	1122	LEU	2.7
1	E	1016	PRO	2.7
1	F	1116	THR	2.7
1	B	1165	GLU	2.7
1	F	1034	GLU	2.7
1	F	1002	VAL	2.7
1	A	1159	ALA	2.7
1	F	1151	LYS	2.7
1	F	1054	HIS	2.7
1	D	1146	GLY	2.7
1	F	1058	PRO	2.7
1	F	1084	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	1159	ALA	2.7
1	B	1017	LEU	2.7
1	B	1056	ILE	2.7
1	C	1123	ASP	2.7
1	F	1044	LYS	2.7
1	B	1157	THR	2.6
1	B	1064	GLY	2.6
1	D	1096	GLY	2.6
1	B	1111	GLN	2.6
1	E	1015	GLU	2.6
1	C	1092	HIS	2.6
1	C	1106	ASN	2.6
1	C	1137	ASN	2.6
1	D	1025	PHE	2.6
1	F	1007	PHE	2.6
1	F	1037	ARG	2.6
1	A	1137	ASN	2.6
1	A	1044	LYS	2.6
1	B	1154	LYS	2.6
1	A	1070	HIS	2.6
1	B	1040	SER	2.6
1	F	1124	GLY	2.6
1	F	1073	THR	2.6
1	F	1047	GLY	2.6
1	A	1103	ALA	2.5
1	B	1008	PHE	2.5
1	C	1056	ILE	2.5
1	B	1070	HIS	2.5
1	C	1147	SER	2.5
1	D	1056	ILE	2.5
1	B	1139	VAL	2.5
1	C	1014	GLY	2.5
1	D	1093	THR	2.5
1	D	1153	SER	2.5
1	F	1067	PHE	2.5
1	B	1101	ALA	2.5
1	C	1089	ILE	2.4
1	B	1073	THR	2.4
1	F	1057	ILE	2.4
1	D	1090	LEU	2.4
1	B	1091	LYS	2.4
1	C	1013	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1102	ASN	2.4
1	B	1031	LYS	2.4
1	D	1039	LEU	2.4
1	C	1080	GLY	2.4
1	D	1149	ASN	2.4
1	A	1082	LYS	2.4
1	C	1028	LYS	2.4
1	B	1117	ALA	2.4
1	B	1137	ASN	2.3
1	E	1082	LYS	2.3
1	B	1004	PRO	2.3
1	B	1102	ASN	2.3
2	H	101	HIS	2.3
1	F	1016	PRO	2.3
1	F	1101	ALA	2.3
1	C	1149	ASN	2.3
1	A	1139	VAL	2.3
1	B	1082	LYS	2.3
1	B	1048	TYR	2.3
1	C	1124	GLY	2.3
2	L	102	ALA	2.3
1	D	1095	PRO	2.3
1	F	1004	PRO	2.3
1	A	1086	GLU	2.3
1	D	1077	SER	2.3
1	F	1155	LYS	2.3
1	F	1111	GLN	2.3
1	A	1073	THR	2.3
1	C	1139	VAL	2.2
1	A	1151	LYS	2.2
1	E	1139	VAL	2.2
1	D	1015	GLU	2.2
1	F	1165	GLU	2.2
1	F	1072	GLY	2.2
1	C	1033	ALA	2.2
1	E	1152	THR	2.2
1	A	1015	GLU	2.2
1	A	1058	PRO	2.2
1	D	1137	ASN	2.2
1	A	1127	VAL	2.2
1	C	1119	THR	2.2
1	D	1073	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	1140	GLU	2.2
1	A	1149	ASN	2.2
1	C	1030	PRO	2.2
1	D	1074	GLY	2.2
1	D	1148	ARG	2.2
1	B	1153	SER	2.2
1	B	1163	GLN	2.2
1	E	1159	ALA	2.2
1	D	1083	PHE	2.2
1	C	1024	LEU	2.2
1	B	1063	GLN	2.1
1	B	1131	LYS	2.1
1	A	1079	TYR	2.1
1	F	1035	ASN	2.1
1	C	1045	GLY	2.1
1	B	1036	PHE	2.1
1	B	1148	ARG	2.1
1	A	1016	PRO	2.1
1	B	1076	LYS	2.1
1	E	1046	PHE	2.1
1	F	1128	VAL	2.1
1	B	1057	ILE	2.1
1	C	1088	PHE	2.1
1	C	1143	GLU	2.1
1	D	1070	HIS	2.1
1	B	1014	GLY	2.1
1	B	1042	GLY	2.1
1	F	1130	GLY	2.1
2	G	102	ALA	2.1
1	F	1015	GLU	2.1
1	C	1012	VAL	2.1
1	E	1044	LYS	2.1
1	D	1131	LYS	2.1
1	D	1050	GLY	2.1
1	F	1148	ARG	2.1
1	A	1085	ASP	2.0
1	B	1146	GLY	2.0
1	C	1083	PHE	2.0
1	F	1076	LYS	2.0
1	F	1133	LYS	2.0
1	F	1062	CYS	2.0
1	C	1096	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1146	GLY	2.0
1	F	1097	ILE	2.0
1	B	1140	GLU	2.0
1	A	1101	ALA	2.0
1	E	1070	HIS	2.0
1	D	1020	VAL	2.0
1	D	1024	LEU	2.0
1	A	1083	PHE	2.0
1	D	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 carbohydrates 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.