



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:28 PM GMT

PDB ID : 1AWR
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

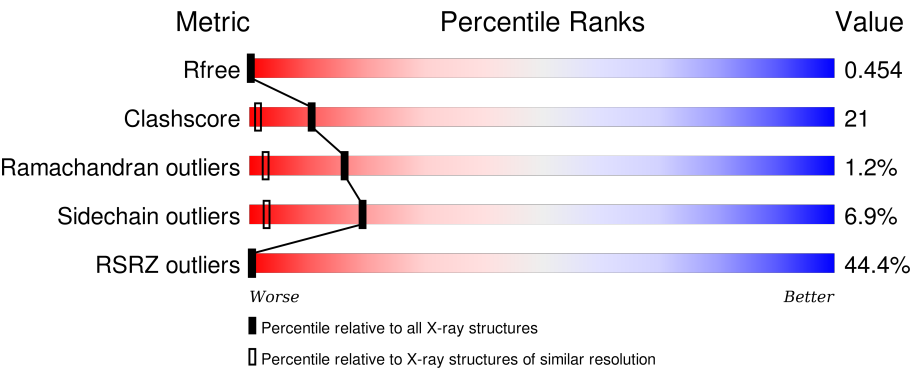
1 Overall quality at a glance i

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}	91344	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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. 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	<div><div>20%</div><div><div>65%</div><div>32%</div><div>.</div></div></div>
1	B	164	<div><div>73%</div><div><div>49%</div><div>45%</div><div>6%</div></div></div>
1	C	164	<div><div>48%</div><div><div>62%</div><div>35%</div><div>.</div></div></div>
1	D	164	<div><div>37%</div><div><div>66%</div><div>30%</div><div>.</div></div></div>
1	E	164	<div><div>22%</div><div><div>70%</div><div>25%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	164	<div><div></div><div>67%</div><div></div><div>57%</div><div></div><div>40%</div><div></div></div>
2	G	6	<div><div></div><div>50%</div><div></div><div>50%</div><div></div><div>33%</div><div></div><div>17%</div></div>
2	H	6	<div><div></div><div>50%</div><div></div><div>83%</div><div></div><div>17%</div></div>
2	I	6	<div><div></div><div>33%</div><div></div><div>83%</div><div></div><div>17%</div></div>
2	J	6	<div><div></div><div>17%</div><div></div><div>67%</div><div></div><div>33%</div></div>
2	K	6	<div><div></div><div>33%</div><div></div><div>100%</div></div>
2	L	6	<div><div></div><div>67%</div><div></div><div>67%</div><div></div><div>33%</div></div>

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			

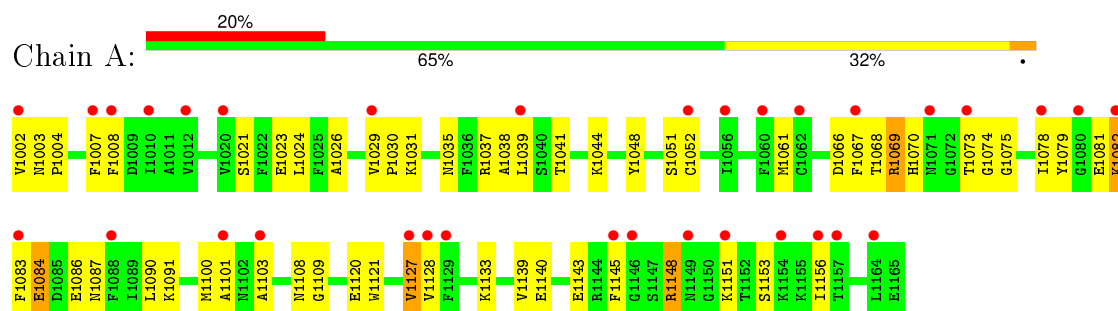
- Molecule 3 is water.

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

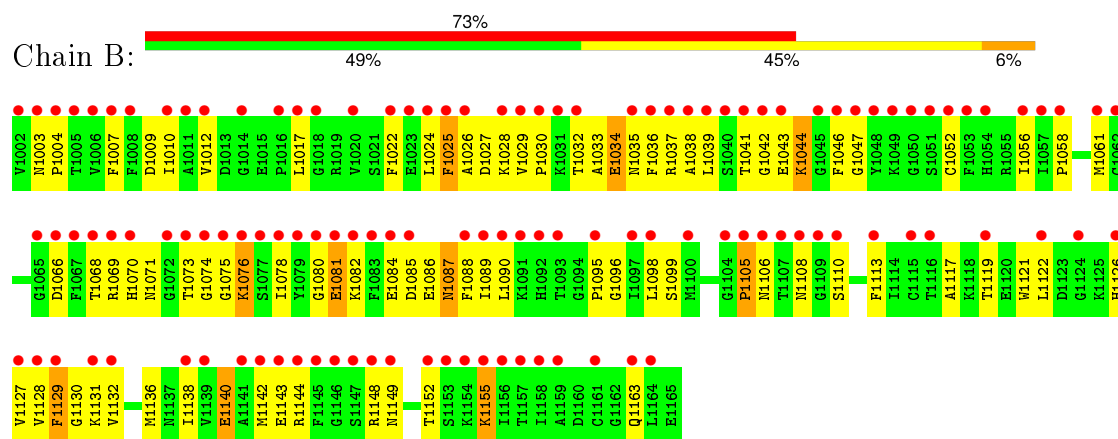
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

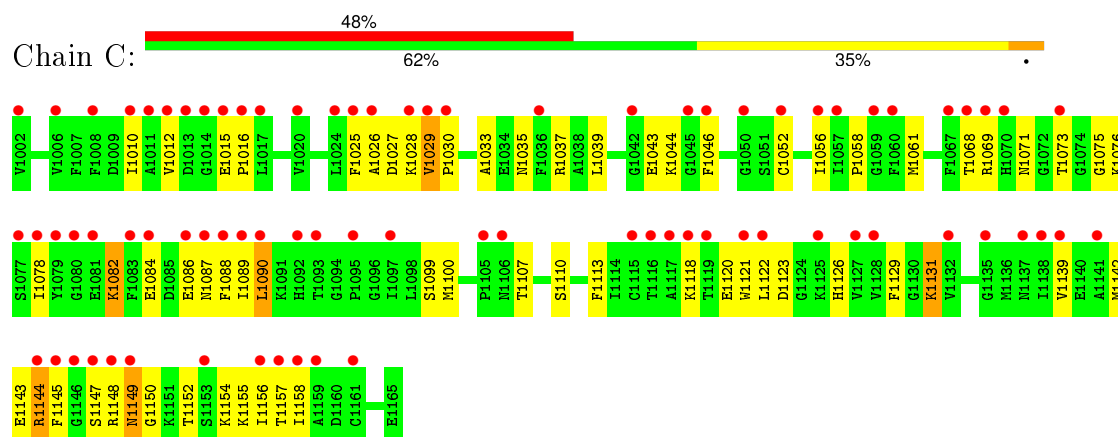
• Molecule 1: CYCLOPHILIN A



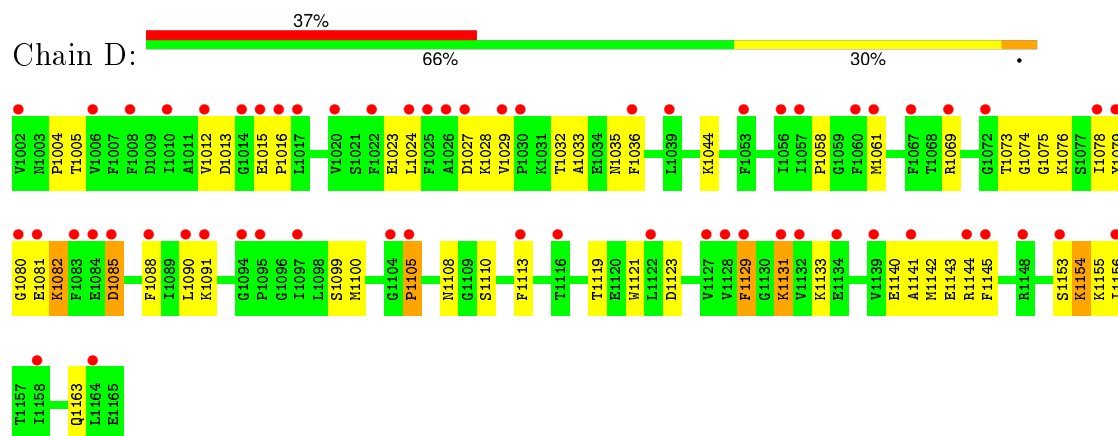
• Molecule 1: CYCLOPHILIN A



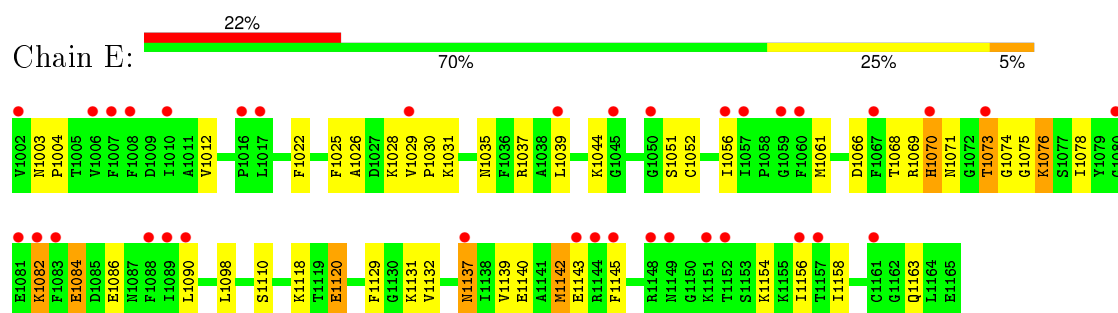
• Molecule 1: CYCLOPHILIN A



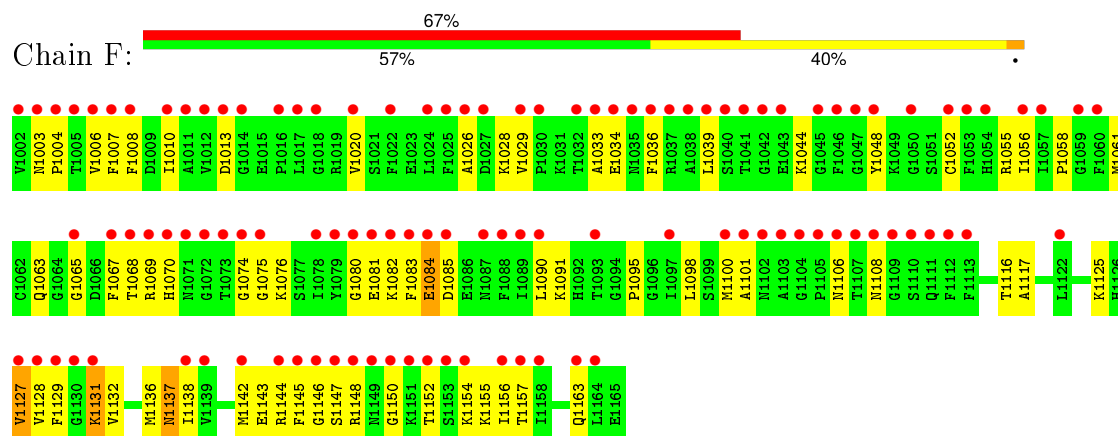
- Molecule 1: CYCLOPHILIN A



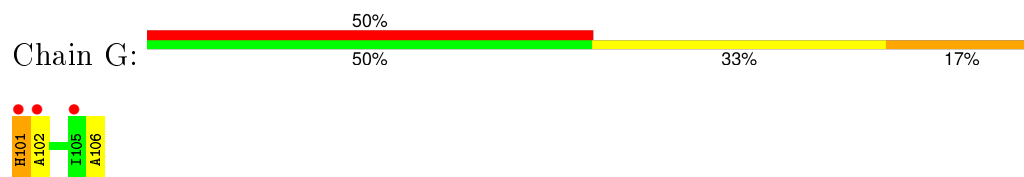
- Molecule 1: CYCLOPHILIN A



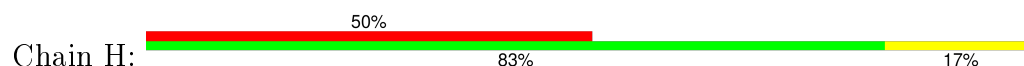
- Molecule 1: CYCLOPHILIN A



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

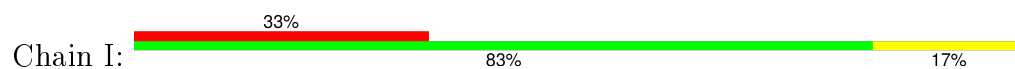


- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN





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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	72.91Å 72.91Å 188.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.58 14.96 – 1.53	Depositor EDS
% Data completeness (in resolution range)	88.3 (15.00-1.58) 79.5 (14.96-1.53)	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	5691 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 123869 reflections (0.003%)	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.62	0/1286	0.76	0/1723
1	B	0.63	0/1286	0.77	0/1723
1	C	0.64	0/1286	0.77	0/1723
1	D	0.58	0/1286	0.73	0/1723
1	E	0.64	0/1286	0.76	0/1723
1	F	0.60	0/1286	0.79	0/1723
2	G	0.63	0/41	0.89	0/54
2	H	0.65	0/41	0.72	0/54
2	I	0.74	0/41	0.90	0/54
2	J	0.78	0/41	0.91	0/54
2	K	0.76	0/41	0.92	0/54
2	L	0.57	0/41	0.62	0/54
All	All	0.62	0/7962	0.76	0/10662

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1258	0	1225	41	0
1	B	1258	0	1225	73	0
1	C	1258	0	1225	62	0
1	D	1258	0	1225	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1258	0	1225	39	0
1	F	1258	0	1225	65	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	327	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 21.

All (327) 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
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:H	1:E:1137:ASN:HD22	1.13	0.90
1:A:1048:TYR:HA	3:A:7165:HOH:O	1.69	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:B:1024:LEU:HB3	1:B:1033:ALA:HB1	1.65	0.77
1:A:1127:VAL:HG11	3:A:7142:HOH:O	1.85	0.77
1:A:1067:PHE:HB3	3:A:7165:HOH:O	1.86	0.76
1:B:1010:ILE:HG13	1:B:1142:MET:HE1	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:E:1137:ASN:HD22	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:F:1052:CYS:CB	1:F:1155:LYS:HE2	2.20	0.70
1:D:1023:GLU:CB	1:D:1133:LYS:HE2	2.22	0.70
1:C:1090:LEU:N	1:C:1090:LEU:HD12	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:NE	1:A:1148:ARG:HA	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
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:F:1010:ILE:HG21	1:F:1142:MET:HE1	1.79	0.64
1:A:1026:ALA:O	1:A:1030:PRO:HG3	1.98	0.63
1:C:1139:VAL:HA	1:C:1142:MET:HE2	1.78	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:B:1087:ASN:HD22	1:B:1087:ASN:N	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1118:LYS:NZ	1:E:1120:GLU:HB3	2.17	0.60
1:A:1073:THR:O	1:A:1073:THR:HG22	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:F:1145:PHE:CB	1:F:1156:ILE:HD11	2.32	0.59
1:D:1058:PRO:HA	1:D:1143:GLU:HG3	1.84	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:C:1144:ARG:C	1:C:1145:PHE:HD1	2.06	0.58
1:D:1131:LYS:HD3	1:D:1131:LYS:O	2.02	0.58
1:C:1121:TRP:NE1	2:I:106:ALA:HB3	2.18	0.58
1:B:1056:ILE:HD12	1:B:1152:THR:HG21	1.85	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:D:1012:VAL:HG11	1:D:1154:LYS:HD3	1.87	0.57
1:A:1029:VAL:HG12	1:A:1086:GLU:OE1	2.05	0.57
1:F:1148:ARG:NE	1:F:1148:ARG:HA	2.20	0.57
1:D:1085:ASP:HA	1:D:1108:ASN:HD21	1.70	0.56
1:F:1136:MET:HG2	3:F:7149:HOH:O	2.04	0.56
1:B:1121:TRP:NE1	2:H:106:ALA:HB3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1012:VAL:HA	1:D:1155:LYS:O	2.06	0.54
1:A:1109:GLY:HA3	3:A:7113:HOH:O	2.06	0.54
1:A:1083:PHE:O	1:A:1108:ASN:HB2	2.07	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:E:1044:LYS:NZ	1:E:1078:ILE:HB	2.23	0.54
1:B:1132:VAL:HG21	1:B:1136:MET:SD	2.48	0.54
1:F:1029:VAL:HG13	3:F:7048:HOH:O	2.07	0.54
1:B:1136:MET:HG2	3:B:7094:HOH:O	2.06	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:D:1073:THR:O	1:D:1073:THR:HG22	2.08	0.53
1:B:1052:CYS:CB	1:B:1155:LYS:HE3	2.39	0.53
1:C:1143:GLU:C	1:C:1145:PHE:H	2.12	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:C:1155:LYS:HZ3	1:C:1155:LYS:HB3	1.73	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:C:1149:ASN:C	1:C:1149:ASN:HD22	2.13	0.52
1:C:1025:PHE:HB2	1:C:1029:VAL:HG23	1.92	0.52
1:A:1052:CYS:HB2	1:A:1156:ILE:O	2.10	0.52
1:F:1138:ILE:HG22	1:F:1142:MET:CE	2.39	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
1:D:1044:LYS:HB2	3:D:7103:HOH:O	2.09	0.51
1:E:1118:LYS:HZ2	1:E:1120:GLU:HB3	1.75	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:D:1023:GLU:CA	1:D:1133:LYS:HE2	2.41	0.51
1:C:1123:ASP:HA	3:C:7028:HOH:O	2.10	0.51
1:B:1012:VAL:CG2	1:B:1017:LEU:HD22	2.41	0.51
1:C:1030:PRO:HD2	1:C:1086:GLU:OE2	2.10	0.51
1:B:1024:LEU:HD13	1:B:1033:ALA:O	2.11	0.51
1:F:1010:ILE:HG13	1:F:1142:MET:CE	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1090:LEU:HD12	3:F:7048:HOH:O	2.11	0.50
1:E:1052:CYS:HB2	1:E:1156:ILE:O	2.12	0.50
1:F:1056:ILE:HB	1:F:1146:GLY:HA3	1.94	0.50
1:A:1066:ASP:O	1:A:1070:HIS:HA	2.12	0.50
1:B:1149:ASN:HD22	1:B:1149:ASN:H	1.58	0.50
1:F:1138:ILE:HG22	1:F:1142:MET:HE2	1.92	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:F:1055:ARG:HA	1:F:1150:GLY:O	2.13	0.49
1:A:1090:LEU:HB2	1:A:1128:VAL:HB	1.94	0.49
1:C:1028:LYS:C	1:C:1030:PRO:HD3	2.33	0.49
1:B:1028:LYS:HD3	1:B:1090:LEU:HD21	1.93	0.49
1:B:1073:THR:O	1:B:1073:THR:HG22	2.13	0.49
1:F:1137:ASN:N	1:F:1137:ASN:HD22	2.10	0.49
1:B:1121:TRP:HH2	3:B:7036:HOH:O	1.94	0.49
1:A:1082:LYS:HD3	1:A:1082:LYS:H	1.78	0.49
1:B:1025:PHE:CD2	1:B:1130:GLY:HA2	2.48	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:F:1137:ASN:H	1:F:1137:ASN:HD22	1.61	0.49
1:F:1076:LYS:HB2	1:F:1080:GLY:O	2.12	0.49
1:F:1007:PHE:O	1:F:1008:PHE:HD1	1.96	0.49
1:F:1090:LEU:C	1:F:1091:LYS:HD2	2.33	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
1:F:1048:TYR:CE1	1:F:1065:GLY:HA2	2.49	0.48
1:B:1081:GLU:N	1:B:1081:GLU:OE1	2.46	0.48
1:C:1147:SER:OG	1:C:1148:ARG:N	2.47	0.48
1:B:1140:GLU:O	1:B:1143:GLU:HB2	2.13	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:D:1075:GLY:HA3	1:D:1110:SER:OG	2.13	0.48
1:C:1118:LYS:HE2	1:C:1120:GLU:HB3	1.96	0.48
1:C:1029:VAL:HG13	1:C:1087:ASN:HD21	1.79	0.48
1:B:1026:ALA:O	1:B:1030:PRO:HB3	2.14	0.48
1:A:1145:PHE:HB2	1:A:1156:ILE:HD11	1.96	0.47
1:C:1088:PHE:HA	3:C:7133:HOH:O	2.15	0.47
1:B:1088:PHE:HA	3:B:7001:HOH:O	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:VAL:HA	3:A:7044:HOH:O	2.14	0.47
1:B:1138:ILE:O	1:B:1142:MET:HE3	2.14	0.47
1:B:1066:ASP:O	1:B:1070:HIS:HA	2.15	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:B:1119:THR:HA	1:B:1121:TRP:CZ3	2.50	0.47
1:D:1145:PHE:HD2	1:D:1156:ILE:HD11	1.79	0.46
1:D:1085:ASP:HA	1:D:1108:ASN:ND2	2.29	0.46
1:E:1068:THR:HG1	1:E:1075:GLY:H	1.59	0.46
1:C:1099:SER:HB3	1:C:1113:PHE:CZ	2.50	0.46
1:F:1090:LEU:CB	1:F:1128:VAL:HB	2.45	0.46
1:B:1099:SER:HB3	1:B:1113:PHE:CZ	2.51	0.46
1:A:1023:GLU:HB2	1:A:1133:LYS:HD2	1.96	0.46
1:E:1028:LYS:C	1:E:1030:PRO:HD3	2.36	0.46
1:C:1142:MET:SD	1:C:1156:ILE:HG21	2.56	0.46
1:F:1090:LEU:HB3	1:F:1128:VAL:CG1	2.46	0.46
1:C:1037:ARG:NH2	1:C:1043:GLU:OE2	2.48	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:E:1071:ASN:OD1	1:E:1073:THR:HB	2.16	0.46
1:E:1069:ARG:N	1:E:1069:ARG:HD2	2.31	0.46
1:D:1121:TRP:HE1	2:J:106:ALA:HB3	1.79	0.46
1:B:1058:PRO:HB2	1:B:1148:ARG:NH2	2.31	0.46
1:D:1028:LYS:CD	1:D:1090:LEU:HD21	2.42	0.46
1:B:1131:LYS:HD2	1:B:1132:VAL:O	2.14	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:E:1143:GLU:C	1:E:1145:PHE:H	2.20	0.45
1:F:1008:PHE:HB2	1:F:1020:VAL:HG13	1.98	0.45
1:C:1076:LYS:O	1:C:1110:SER:HB3	2.16	0.45
1:F:1010:ILE:HG13	1:F:1142:MET:HE1	1.97	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:D:1142:MET:HE2	1:D:1142:MET:HB2	1.86	0.44
1:A:1073:THR:O	1:A:1073:THR:CG2	2.65	0.44
1:E:1073:THR:CG2	1:E:1073:THR:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1148:ARG:HE	1:F:1148:ARG:HA	1.83	0.44
1:D:1012:VAL:O	1:D:1013:ASP:HB2	2.18	0.44
1:F:1058:PRO:HG3	1:F:1143:GLU:O	2.17	0.44
1:B:1036:PHE:HB2	1:B:1129:PHE:HE2	1.82	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:F:1116:THR:HG21	1:F:1143:GLU:CD	2.38	0.43
1:E:1143:GLU:C	1:E:1145:PHE:N	2.71	0.43
1:B:1012:VAL:HG23	1:B:1017:LEU:HD22	2.00	0.43
1:D:1005:THR:O	1:D:1163:GLN:HG3	2.18	0.43
1:C:1026:ALA:HA	1:C:1033:ALA:HB3	1.99	0.43
1:E:1131:LYS:HB3	1:E:1131:LYS:HE3	1.82	0.43
1:E:1044:LYS:NZ	1:E:1078:ILE:HD12	2.34	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:C:1087:ASN:CG	1:C:1089:ILE:HD12	2.37	0.43
1:C:1056:ILE:HG21	1:C:1143:GLU:HA	2.00	0.43
1:F:1145:PHE:O	1:F:1152:THR:HG22	2.18	0.43
1:A:1139:VAL:O	1:A:1143:GLU:HG2	2.18	0.43
1:A:1007:PHE:O	1:A:1008:PHE:HD1	2.02	0.43
1:F:1100:MET:HB2	1:F:1127:VAL:CG2	2.30	0.43
1:F:1013:ASP:OD2	1:F:1154:LYS:HD3	2.17	0.43
1:D:1032:THR:HG22	1:D:1129:PHE:CD2	2.54	0.43
1:A:1083:PHE:N	1:A:1108:ASN:O	2.45	0.43
1:F:1039:LEU:HD23	1:F:1039:LEU:HA	1.79	0.43
1:B:1035:ASN:ND2	1:B:1039:LEU:HD12	2.33	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
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:C:1044:LYS:HE2	1:C:1078:ILE:HD12	2.01	0.42
1:B:1075:GLY:HA3	1:B:1110:SER:OG	2.19	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:E:1037:ARG:HD2	1:E:1163:GLN:NE2	2.34	0.42
1:C:1100:MET:SD	1:C:1129:PHE:CE1	3.12	0.42
1:D:1119:THR:HA	1:D:1121:TRP:CH2	2.54	0.42
1:D:1044:LYS:HG3	1:D:1078:ILE:HG21	2.00	0.42
1:F:1008:PHE:HB2	1:F:1020:VAL:CG1	2.48	0.42
1:A:1038:ALA:HB3	1:A:1078:ILE:HG21	2.01	0.42
1:F:1052:CYS:HA	1:F:1157:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1056:ILE:O	1:C:1150:GLY:HA2	2.19	0.42
1:E:1044:LYS:HZ2	1:E:1078:ILE:HD12	1.85	0.42
1:C:1027:ASP:N	1:C:1027:ASP:OD1	2.48	0.42
1:D:1141:ALA:HA	1:D:1144:ARG:HE	1.84	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:C:1068:THR:HG1	1:C:1075:GLY:H	1.64	0.42
1:D:1091:LYS:HE2	1:D:1123:ASP:OD2	2.20	0.42
1:C:1010:ILE:HG21	1:C:1142:MET:SD	2.60	0.42
1:A:1090:LEU:CB	1:A:1128:VAL:HB	2.49	0.42
1:C:1122:LEU:HB3	1:C:1126:HIS:HD2	1.84	0.42
1:C:1155:LYS:HZ2	1:C:1155:LYS:HB3	1.84	0.42
1:C:1143:GLU:C	1:C:1145:PHE:N	2.73	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:B:1078:ILE:C	1:B:1080:GLY:H	2.24	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:B:1046:PHE:HE2	1:B:1076:LYS:O	2.03	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:D:1090:LEU:HG	3:D:7137:HOH:O	2.21	0.41
1:C:1052:CYS:HB2	1:C:1156:ILE:O	2.20	0.41
1:B:1087:ASN:ND2	1:B:1087:ASN:N	2.67	0.41
1:F:1116:THR:HG21	1:F:1143:GLU:OE2	2.20	0.41
1:D:1027:ASP:OD1	1:D:1028:LYS:HG3	2.19	0.41
1:C:1145:PHE:N	1:C:1145:PHE:HD1	2.18	0.41
1:E:1012:VAL:HG12	1:E:1154:LYS:HD3	2.03	0.41
1:C:1082:LYS:HG3	1:C:1107:THR:HA	2.01	0.41
1:C:1071:ASN:OD1	1:C:1073:THR:HB	2.20	0.41
1:D:1119:THR:HG22	1:D:1121:TRP:CZ2	2.56	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:A:1121:TRP:CD1	2:G:106:ALA:HB3	2.55	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:D:1004:PRO:HB3	1:D:1163:GLN:NE2	2.36	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:A:1003:ASN:HA	1:A:1004:PRO:HD3	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1026:ALA:HA	1:F:1033:ALA:CB	2.50	0.41
1:E:1051:SER:OG	1:E:1158:ILE:HD12	2.20	0.41
1:B:1028:LYS:HD2	1:B:1090:LEU:HD11	2.02	0.41
1:F:1091:LYS:N	1:F:1091:LYS:HD2	2.35	0.41
1:B:1042:GLY:HA2	1:B:1046:PHE:O	2.21	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:C:1152:THR:HG21	3:C:7092:HOH:O	2.21	0.41
1:C:1012:VAL:CG2	1:C:1145:PHE:HE2	2.33	0.41
1:D:1082:LYS:O	1:D:1082:LYS:HG2	2.20	0.41
1:C:1157:THR:CG2	1:C:1158:ILE:N	2.84	0.41
1:F:1137:ASN:ND2	1:F:1138:ILE:HG12	2.36	0.40
1:B:1086:GLU:HG2	1:B:1087:ASN:ND2	2.36	0.40
1:F:1028:LYS:CB	3:F:7048:HOH:O	2.68	0.40
1:B:1144:ARG:HB2	1:B:1144:ARG:HE	1.73	0.40
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: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:1068:THR:HG1	1:A:1075:GLY:H	1.66	0.40
1:A:1007:PHE:HA	1:A:1021:SER:HA	2.03	0.40
1:E:1066:ASP:O	1:E:1070:HIS:HA	2.21	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

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%)	30	8
1	B	162/164 (99%)	141 (87%)	18 (11%)	3 (2%)	10	1
1	C	162/164 (99%)	147 (91%)	12 (7%)	3 (2%)	10	1
1	D	162/164 (99%)	146 (90%)	13 (8%)	3 (2%)	10	1
1	E	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	30	8
1	F	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	30	8
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%)	16	3

All (12) Ramachandran outliers are listed below:

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

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%)	20	3
1	B	132/132 (100%)	122 (92%)	10 (8%)	16	2
1	C	132/132 (100%)	125 (95%)	7 (5%)	28	6
1	D	132/132 (100%)	125 (95%)	7 (5%)	28	6
1	E	132/132 (100%)	122 (92%)	10 (8%)	16	2
1	F	132/132 (100%)	122 (92%)	10 (8%)	16	2
2	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	H	3/3 (100%)	3 (100%)	0	100	100
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%)	2 (67%)	1 (33%)	0	0
All	All	810/810 (100%)	754 (93%)	56 (7%)	19	3

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1061	MET
1	A	1069	ARG
1	A	1082	LYS
1	A	1084	GLU
1	A	1120	GLU
1	A	1127	VAL
1	A	1148	ARG
1	A	1151	LYS
1	A	1153	SER
1	B	1034	GLU
1	B	1044	LYS
1	B	1061	MET
1	B	1076	LYS
1	B	1081	GLU
1	B	1087	ASN
1	B	1105	PRO
1	B	1129	PHE
1	B	1140	GLU
1	B	1155	LYS
1	C	1029	VAL
1	C	1061	MET
1	C	1082	LYS

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Mol	Chain	Res	Type
1	C	1084	GLU
1	C	1090	LEU
1	C	1131	LYS
1	C	1149	ASN
1	D	1061	MET
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	E	1061	MET
1	E	1070	HIS
1	E	1073	THR
1	E	1076	LYS
1	E	1082	LYS
1	E	1084	GLU
1	E	1120	GLU
1	E	1137	ASN
1	E	1140	GLU
1	E	1142	MET
1	F	1034	GLU
1	F	1061	MET
1	F	1069	ARG
1	F	1082	LYS
1	F	1084	GLU
1	F	1125	LYS
1	F	1127	VAL
1	F	1131	LYS
1	F	1137	ASN
1	F	1144	ARG
2	G	101	HIS
2	J	101	HIS
2	L	101	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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

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Mol	Chain	Res	Type
1	C	1149	ASN
1	D	1108	ASN
1	D	1163	GLN
1	E	1137	ASN
1	F	1070	HIS
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 carbohydrates 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%)	1.40	33 (20%) 1 1	5, 13, 20, 23	0
1	B	164/164 (100%)	3.15	120 (73%) 0 0	11, 20, 28, 34	0
1	C	164/164 (100%)	2.21	79 (48%) 0 0	5, 16, 25, 35	0
1	D	164/164 (100%)	1.89	60 (36%) 0 0	7, 18, 25, 33	0
1	E	164/164 (100%)	1.48	36 (21%) 1 1	3, 12, 21, 27	0
1	F	164/164 (100%)	2.83	110 (67%) 0 0	10, 18, 26, 30	0
2	G	6/6 (100%)	2.34	3 (50%) 0 0	13, 17, 21, 29	0
2	H	6/6 (100%)	2.38	3 (50%) 0 0	11, 14, 22, 24	0
2	I	6/6 (100%)	2.04	2 (33%) 0 0	6, 8, 11, 26	0
2	J	6/6 (100%)	1.65	1 (16%) 2 2	9, 10, 12, 18	0
2	K	6/6 (100%)	1.83	2 (33%) 0 0	7, 9, 20, 23	0
2	L	6/6 (100%)	2.83	4 (66%) 0 0	16, 19, 24, 24	0
All	All	1020/1020 (100%)	2.16	453 (44%) 0 0	3, 17, 26, 35	0

All (453) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1080	GLY	12.1
1	B	1024	LEU	11.0
1	B	1025	PHE	10.1
1	F	1029	VAL	8.9
1	B	1104	GLY	8.3
1	F	1078	ILE	8.1
1	B	1067	PHE	8.1
1	F	1083	PHE	7.5
1	B	1046	PHE	7.5
1	C	1002	VAL	7.3
1	B	1074	GLY	7.3

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Mol	Chain	Res	Type	RSRZ
1	C	1012	VAL	7.1
1	B	1079	TYR	7.1
1	F	1012	VAL	6.8
1	F	1080	GLY	6.8
1	B	1011	ALA	6.7
1	B	1017	LEU	6.7
1	F	1107	THR	6.2
1	C	1029	VAL	6.1
1	B	1129	PHE	6.1
1	D	1002	VAL	6.1
2	L	101	HIS	6.1
1	F	1088	PHE	6.0
1	F	1039	LEU	5.9
1	C	1017	LEU	5.8
1	B	1090	LEU	5.7
1	B	1016	PRO	5.6
1	B	1147	SER	5.6
1	F	1127	VAL	5.5
1	D	1026	ALA	5.5
1	B	1080	GLY	5.5
1	F	1103	ALA	5.4
1	D	1078	ILE	5.4
1	F	1128	VAL	5.4
1	B	1002	VAL	5.3
1	D	1079	TYR	5.3
1	C	1145	PHE	5.3
1	C	1089	ILE	5.3
1	B	1007	PHE	5.2
2	I	106	ALA	5.2
1	F	1030	PRO	5.2
1	B	1083	PHE	5.2
1	B	1088	PHE	5.2
1	B	1077	SER	5.1
2	H	106	ALA	5.1
1	F	1153	SER	5.0
1	F	1038	ALA	5.0
1	B	1156	ILE	5.0
1	B	1139	VAL	5.0
1	B	1003	ASN	5.0
1	B	1048	TYR	5.0
2	G	101	HIS	4.9
1	F	1089	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	1030	PRO	4.8
1	F	1026	ALA	4.8
1	F	1090	LEU	4.8
1	F	1027	ASP	4.8
1	B	1032	THR	4.8
1	C	1011	ALA	4.8
1	F	1156	ILE	4.8
1	B	1084	GLU	4.7
1	B	1035	ASN	4.7
1	F	1129	PHE	4.7
1	D	1024	LEU	4.7
1	B	1010	ILE	4.7
1	F	1145	PHE	4.6
1	C	1024	LEU	4.6
1	F	1079	TYR	4.6
1	A	1002	VAL	4.6
1	E	1002	VAL	4.6
1	D	1104	GLY	4.5
1	F	1002	VAL	4.5
1	D	1156	ILE	4.5
1	F	1010	ILE	4.5
1	F	1032	THR	4.5
1	F	1147	SER	4.5
1	F	1050	GLY	4.5
1	D	1025	PHE	4.5
1	F	1013	ASP	4.4
1	B	1036	PHE	4.4
1	B	1012	VAL	4.4
1	F	1033	ALA	4.4
1	B	1075	GLY	4.4
2	K	101	HIS	4.3
1	F	1025	PHE	4.3
1	B	1020	VAL	4.2
1	C	1028	LYS	4.2
1	B	1152	THR	4.2
1	B	1109	GLY	4.2
1	F	1070	HIS	4.2
1	F	1164	LEU	4.2
1	E	1152	THR	4.2
1	F	1068	THR	4.2
1	B	1041	THR	4.2
1	D	1129	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	1050	GLY	4.1
1	F	1069	ARG	4.1
1	F	1146	GLY	4.1
1	C	1014	GLY	4.1
1	F	1150	GLY	4.1
1	C	1069	ARG	4.1
1	C	1127	VAL	4.1
1	A	1080	GLY	4.0
1	F	1052	CYS	4.0
1	B	1029	VAL	4.0
1	F	1045	GLY	4.0
1	B	1161	CYS	4.0
1	F	1071	ASN	4.0
1	B	1069	ARG	4.0
1	B	1052	CYS	4.0
1	B	1138	ILE	4.0
1	C	1156	ILE	4.0
1	B	1040	SER	3.9
1	A	1127	VAL	3.9
1	B	1076	LYS	3.9
1	B	1037	ARG	3.9
1	B	1127	VAL	3.9
1	B	1153	SER	3.9
1	F	1101	ALA	3.9
1	C	1046	PHE	3.9
1	E	1067	PHE	3.9
1	F	1041	THR	3.9
1	D	1083	PHE	3.8
1	D	1081	GLU	3.8
1	C	1088	PHE	3.8
1	F	1073	THR	3.8
1	C	1148	ARG	3.8
1	C	1093	THR	3.8
1	B	1097	ILE	3.8
1	B	1105	PRO	3.8
2	L	105	ILE	3.7
1	B	1155	LYS	3.7
1	A	1029	VAL	3.7
1	C	1153	SER	3.7
1	C	1067	PHE	3.7
1	E	1010	ILE	3.7
1	B	1141	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	1015	GLU	3.7
1	B	1072	GLY	3.7
1	B	1049	LYS	3.6
1	C	1119	THR	3.6
1	B	1050	GLY	3.6
1	F	1110	SER	3.6
1	C	1083	PHE	3.6
1	F	1007	PHE	3.6
1	F	1024	LEU	3.6
1	B	1038	ALA	3.6
1	B	1089	ILE	3.6
1	B	1144	ARG	3.6
1	F	1105	PRO	3.6
1	F	1157	THR	3.6
1	C	1077	SER	3.6
1	B	1122	LEU	3.6
1	A	1012	VAL	3.6
1	A	1145	PHE	3.5
1	F	1163	GLN	3.5
1	E	1148	ARG	3.5
1	D	1084	GLU	3.5
1	D	1017	LEU	3.5
1	C	1010	ILE	3.5
1	E	1156	ILE	3.5
1	B	1154	LYS	3.4
1	E	1145	PHE	3.4
1	B	1078	ILE	3.4
1	B	1039	LEU	3.4
1	A	1060	PHE	3.4
1	B	1142	MET	3.4
1	D	1036	PHE	3.4
1	F	1085	ASP	3.4
1	B	1132	VAL	3.4
1	A	1129	PHE	3.4
1	B	1053	PHE	3.4
1	B	1082	LYS	3.4
1	C	1132	VAL	3.3
1	D	1128	VAL	3.3
1	B	1107	THR	3.3
1	B	1070	HIS	3.3
1	D	1127	VAL	3.3
1	A	1007	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	1158	ILE	3.3
1	F	1017	LEU	3.3
1	C	1137	ASN	3.3
1	E	1080	GLY	3.2
1	F	1018	GLY	3.2
1	B	1022	PHE	3.2
1	B	1145	PHE	3.2
1	F	1112	PHE	3.2
1	F	1011	ALA	3.2
1	D	1067	PHE	3.2
1	F	1122	LEU	3.2
1	B	1128	VAL	3.2
1	B	1085	ASP	3.2
1	C	1116	THR	3.2
1	C	1056	ILE	3.2
1	B	1164	LEU	3.2
1	B	1030	PRO	3.2
1	B	1047	GLY	3.2
1	D	1012	VAL	3.2
1	B	1143	GLU	3.2
1	A	1083	PHE	3.1
1	E	1088	PHE	3.1
1	A	1146	GLY	3.1
1	D	1020	VAL	3.1
1	B	1018	GLY	3.1
1	F	1046	PHE	3.1
1	F	1042	GLY	3.1
1	B	1081	GLU	3.1
1	A	1128	VAL	3.1
1	D	1010	ILE	3.1
2	L	106	ALA	3.0
1	F	1003	ASN	3.0
1	B	1148	ARG	3.0
1	D	1069	ARG	3.0
1	B	1045	GLY	3.0
1	B	1073	THR	3.0
1	C	1095	PRO	3.0
1	B	1108	ASN	3.0
2	H	101	HIS	3.0
2	K	106	ALA	3.0
1	B	1056	ILE	3.0
1	B	1113	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1078	ILE	3.0
1	C	1013	ASP	3.0
1	C	1117	ALA	3.0
1	B	1066	ASP	3.0
1	C	1068	THR	3.0
1	D	1053	PHE	3.0
1	E	1089	ILE	3.0
1	B	1042	GLY	3.0
1	C	1141	ALA	3.0
1	B	1023	GLU	3.0
1	C	1122	LEU	3.0
1	B	1043	GLU	3.0
1	F	1008	PHE	3.0
1	F	1067	PHE	3.0
1	F	1037	ARG	2.9
1	D	1006	VAL	2.9
1	F	1084	GLU	2.9
1	F	1082	LYS	2.9
1	B	1146	GLY	2.9
1	F	1065	GLY	2.9
1	D	1116	THR	2.9
1	C	1042	GLY	2.9
1	C	1118	LYS	2.9
1	F	1148	ARG	2.9
1	B	1159	ALA	2.9
1	E	1137	ASN	2.9
1	C	1079	TYR	2.9
1	C	1149	ASN	2.9
1	F	1144	ARG	2.9
1	A	1062	CYS	2.8
1	B	1006	VAL	2.8
1	C	1016	PRO	2.8
1	C	1025	PHE	2.8
1	E	1007	PHE	2.8
1	C	1073	THR	2.8
1	E	1082	LYS	2.8
1	F	1081	GLU	2.8
2	G	102	ALA	2.8
1	C	1157	THR	2.8
1	A	1010	ILE	2.8
2	G	105	ILE	2.8
1	B	1157	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	1039	LEU	2.8
1	F	1154	LYS	2.8
1	D	1057	ILE	2.8
1	F	1036	PHE	2.8
1	A	1103	ALA	2.8
1	C	1121	TRP	2.8
1	D	1029	VAL	2.7
1	B	1158	ILE	2.7
1	F	1016	PRO	2.7
1	F	1048	TYR	2.7
1	A	1056	ILE	2.7
1	C	1158	ILE	2.7
1	F	1057	ILE	2.7
1	D	1145	PHE	2.7
1	B	1091	LYS	2.7
1	D	1132	VAL	2.7
1	F	1108	ASN	2.7
1	C	1144	ARG	2.7
1	F	1138	ILE	2.7
1	B	1008	PHE	2.7
1	D	1008	PHE	2.7
1	F	1053	PHE	2.7
1	C	1147	SER	2.7
1	F	1087	ASN	2.7
1	B	1093	THR	2.7
1	C	1086	GLU	2.7
1	E	1081	GLU	2.7
1	E	1157	THR	2.7
1	C	1159	ALA	2.7
1	C	1070	HIS	2.7
1	F	1149	ASN	2.6
2	I	105	ILE	2.6
1	E	1008	PHE	2.6
1	C	1081	GLU	2.6
1	C	1020	VAL	2.6
1	B	1028	LYS	2.6
1	C	1045	GLY	2.6
1	C	1115	CYS	2.6
1	C	1106	ASN	2.6
1	A	1039	LEU	2.6
1	C	1090	LEU	2.6
1	B	1026	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1052	CYS	2.6
1	B	1057	ILE	2.6
1	C	1057	ILE	2.6
1	F	1113	PHE	2.6
1	B	1124	GLY	2.6
1	C	1146	GLY	2.6
1	B	1095	PRO	2.6
1	B	1068	THR	2.6
1	C	1084	GLU	2.6
1	F	1139	VAL	2.6
1	B	1149	ASN	2.5
1	F	1035	ASN	2.5
1	D	1061	MET	2.5
1	A	1020	VAL	2.5
1	F	1006	VAL	2.5
1	D	1164	LEU	2.5
1	B	1163	GLN	2.5
1	E	1149	ASN	2.5
1	F	1014	GLY	2.5
1	F	1072	GLY	2.5
1	B	1126	HIS	2.5
2	L	102	ALA	2.5
1	D	1014	GLY	2.5
1	C	1006	VAL	2.5
1	D	1027	ASP	2.5
1	D	1030	PRO	2.5
1	F	1004	PRO	2.5
1	F	1040	SER	2.5
1	D	1148	ARG	2.5
1	A	1156	ILE	2.5
1	F	1100	MET	2.5
1	A	1164	LEU	2.5
1	A	1151	LYS	2.5
1	B	1116	THR	2.5
1	B	1014	GLY	2.5
1	D	1016	PRO	2.5
1	D	1131	LYS	2.5
1	C	1059	GLY	2.4
1	D	1122	LEU	2.4
1	B	1110	SER	2.4
1	B	1058	PRO	2.4
1	A	1052	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	1161	CYS	2.4
1	F	1054	HIS	2.4
1	F	1097	ILE	2.4
1	C	1128	VAL	2.4
1	C	1139	VAL	2.4
1	E	1016	PRO	2.4
1	D	1022	PHE	2.4
1	F	1109	GLY	2.4
1	F	1142	MET	2.4
1	D	1097	ILE	2.4
1	D	1060	PHE	2.4
1	F	1034	GLU	2.4
1	D	1094	GLY	2.4
1	F	1104	GLY	2.4
1	B	1131	LYS	2.4
1	D	1158	ILE	2.4
1	A	1073	THR	2.4
1	A	1008	PHE	2.4
1	C	1008	PHE	2.4
1	E	1060	PHE	2.4
1	D	1091	LYS	2.3
1	D	1085	ASP	2.3
1	D	1105	PRO	2.3
1	A	1082	LYS	2.3
1	B	1065	GLY	2.3
1	F	1060	PHE	2.3
1	F	1152	THR	2.3
1	D	1095	PRO	2.3
1	E	1151	LYS	2.3
1	D	1015	GLU	2.3
1	E	1143	GLU	2.3
1	B	1098	LEU	2.3
1	E	1090	LEU	2.3
1	C	1097	ILE	2.3
1	D	1141	ALA	2.3
1	E	1050	GLY	2.3
1	B	1062	CYS	2.3
1	E	1006	VAL	2.3
1	E	1144	ARG	2.3
1	D	1090	LEU	2.3
1	A	1078	ILE	2.3
1	B	1004	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	1106	ASN	2.3
1	C	1060	PHE	2.3
1	A	1071	ASN	2.2
1	C	1026	ALA	2.2
2	J	106	ALA	2.2
1	F	1005	THR	2.2
1	C	1161	CYS	2.2
1	F	1059	GLY	2.2
1	E	1056	ILE	2.2
1	F	1056	ILE	2.2
2	H	105	ILE	2.2
1	B	1092	HIS	2.2
1	C	1105	PRO	2.2
1	F	1093	THR	2.2
1	E	1070	HIS	2.2
1	B	1061	MET	2.2
1	F	1102	ASN	2.2
1	D	1153	SER	2.2
1	E	1057	ILE	2.2
1	A	1088	PHE	2.2
1	D	1113	PHE	2.2
1	D	1139	VAL	2.2
1	B	1031	LYS	2.2
1	D	1039	LEU	2.2
1	B	1115	CYS	2.2
1	F	1074	GLY	2.2
1	C	1138	ILE	2.2
1	D	1056	ILE	2.2
1	D	1088	PHE	2.2
1	C	1092	HIS	2.1
1	C	1080	GLY	2.1
1	F	1020	VAL	2.1
1	B	1100	MET	2.1
1	D	1144	ARG	2.1
1	A	1067	PHE	2.1
1	E	1045	GLY	2.1
1	E	1029	VAL	2.1
1	E	1073	THR	2.1
1	A	1154	LYS	2.1
1	C	1125	LYS	2.1
1	F	1130	GLY	2.1
1	F	1111	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1157	THR	2.1
1	A	1101	ALA	2.1
1	F	1022	PHE	2.1
1	F	1151	LYS	2.1
1	B	1106	ASN	2.1
1	B	1051	SER	2.1
1	F	1043	GLU	2.1
1	C	1036	PHE	2.1
1	D	1072	GLY	2.1
1	F	1075	GLY	2.1
1	E	1017	LEU	2.1
1	A	1149	ASN	2.1
1	B	1054	HIS	2.1
1	C	1087	ASN	2.1
1	F	1131	LYS	2.0
1	E	1083	PHE	2.0
1	B	1005	THR	2.0
1	B	1119	THR	2.0
1	D	1134	GLU	2.0
1	C	1135	GLY	2.0
1	E	1059	GLY	2.0
1	F	1047	GLY	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.