



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:28 PM GMT

PDB ID : 1AWV  
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](mailto: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.

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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

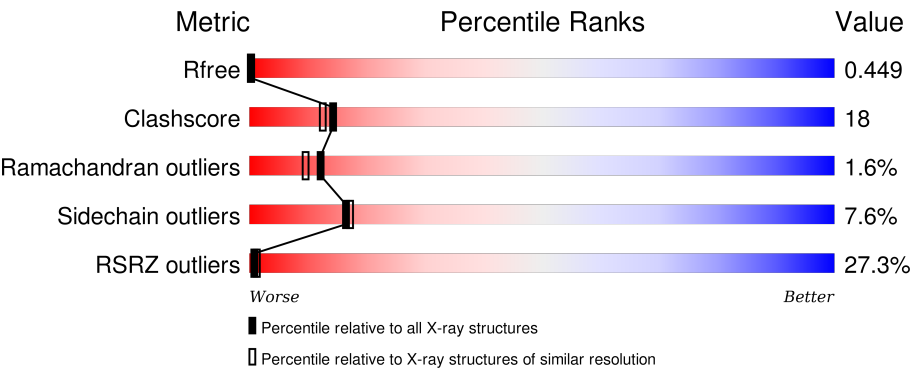
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 <sub>free</sub>	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>8%</div><div><div></div><div></div><div></div><div></div></div><div>71%27%•</div></div>
1	B	164	<div><div>54%</div><div><div></div><div></div><div></div><div></div></div><div>50%42%8%</div></div>
1	C	164	<div><div>18%</div><div><div></div><div></div><div></div><div></div></div><div>62%35%•</div></div>
1	D	164	<div><div>21%</div><div><div></div><div></div><div></div><div></div></div><div>58%39%•</div></div>
1	E	164	<div><div>15%</div><div><div></div><div></div><div></div><div></div></div><div>66%30%•</div></div>

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Mol	Chain	Length	Quality of chain
1	F	164	<div><div></div><div>51%</div><div></div><div>57%</div><div></div><div>40%</div><div></div></div>
2	G	6	<div><div></div><div>67%</div><div></div><div>33%</div><div></div></div>
2	H	6	<div><div></div><div>17%</div><div></div><div>67%</div><div></div><div>33%</div><div></div></div>
2	I	6	<div><div></div><div>50%</div><div></div><div>50%</div><div></div></div>
2	J	6	<div><div></div><div>17%</div><div></div><div>33%</div><div></div><div>67%</div><div></div></div>
2	K	6	<div><div></div><div>17%</div><div></div><div>67%</div><div></div><div>33%</div><div></div></div>
2	L	6	<div><div></div><div>33%</div><div></div><div>83%</div><div></div><div>17%</div><div></div></div>

## 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			

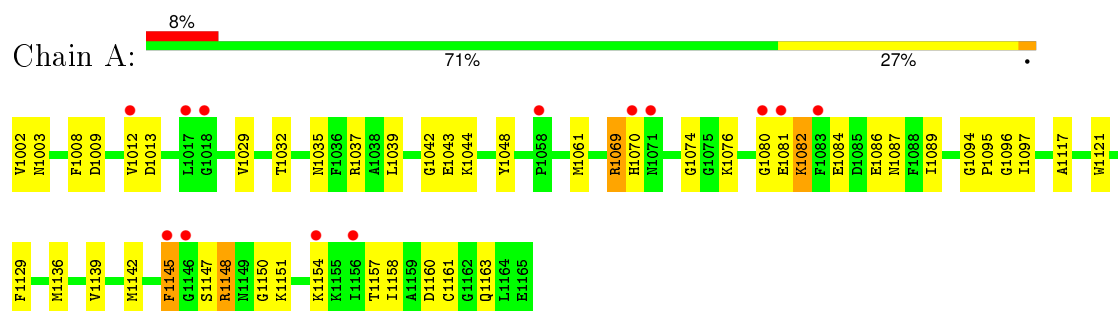
- Molecule 3 is water.

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

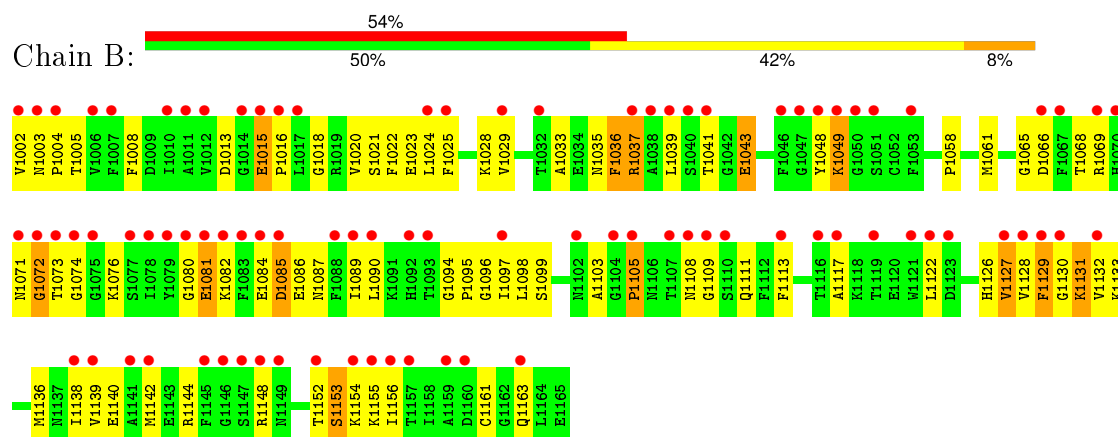
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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 ( $RSRZ > 2$ ). 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.

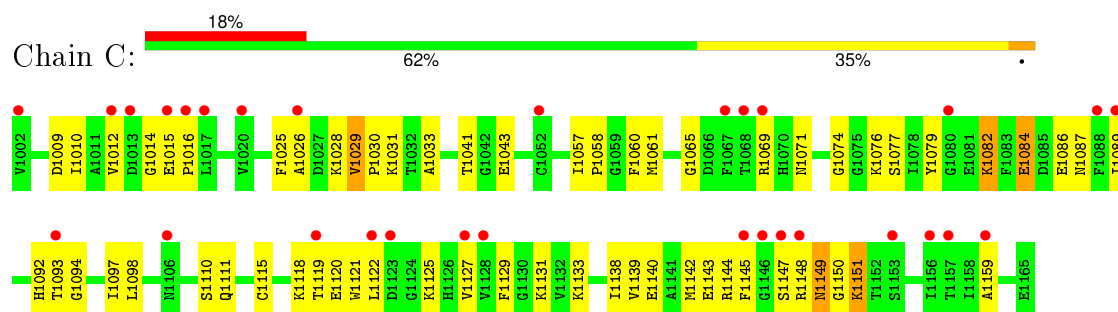
#### • Molecule 1: CYCLOPHILIN A



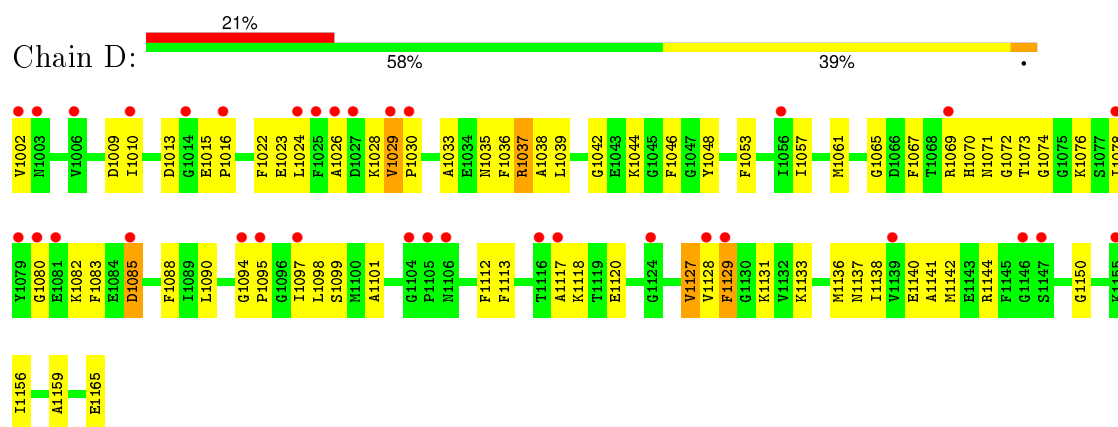
#### • Molecule 1: CYCLOPHILIN A



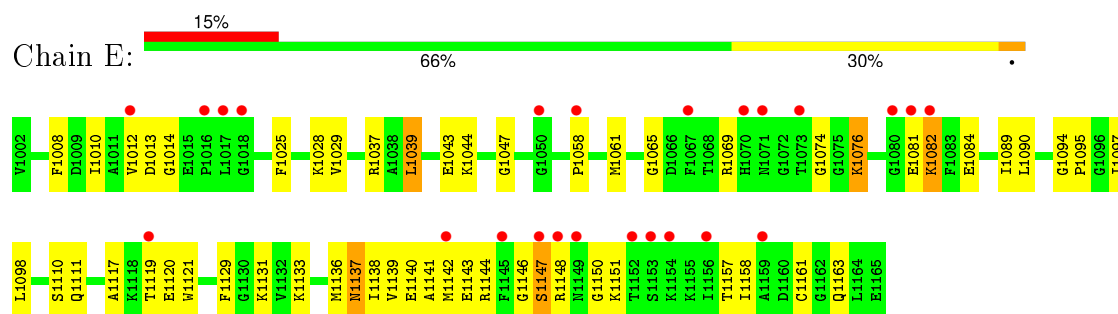
#### • Molecule 1: CYCLOPHILIN A



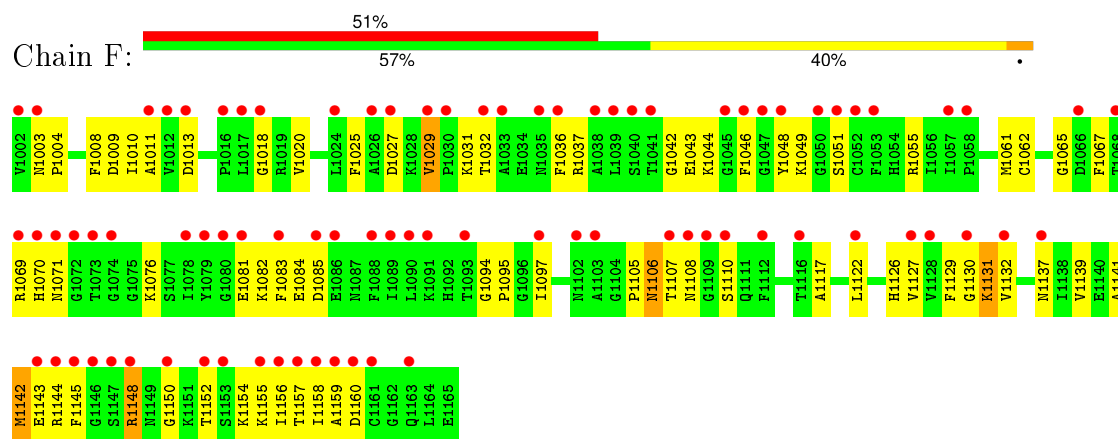
#### • Molecule 1: CYCLOPHILIN A



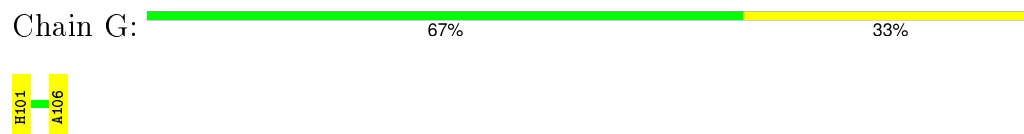
• Molecule 1: CYCLOPHILIN A



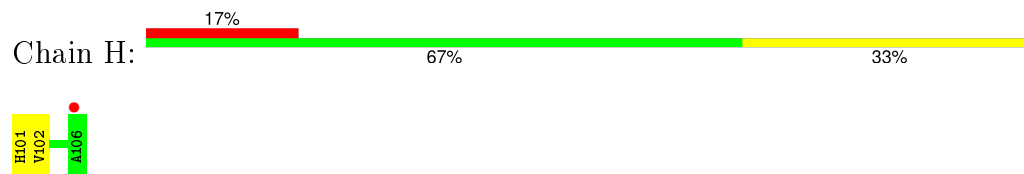
• Molecule 1: CYCLOPHILIN A



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



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



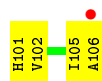
- Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.00 Å 74.00 Å 190.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.34 14.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	83.1 (15.00-2.34) 84.1 (14.98-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 2.34 Å)	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	1781 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 63.0	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 41416 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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	0.49	0/1286	0.69	0/1723
1	B	0.51	0/1286	0.71	0/1723
1	C	0.50	1/1286 (0.1%)	0.68	0/1723
1	D	0.48	0/1286	0.67	0/1723
1	E	0.51	0/1286	0.70	0/1723
1	F	0.49	0/1286	0.71	0/1723
2	G	0.45	0/43	0.80	0/57
2	H	0.50	0/43	0.58	0/57
2	I	0.61	0/43	0.92	0/57
2	J	0.67	0/43	0.86	0/57
2	K	0.60	0/43	0.78	0/57
2	L	0.53	0/43	0.76	0/57
All	All	0.50	1/7974 (0.0%)	0.70	0/10680

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1115	CYS	CB-SG	-5.18	1.73	1.81

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	28	0
1	B	1258	0	1225	65	0
1	C	1258	0	1225	42	0
1	D	1258	0	1225	48	0
1	E	1258	0	1225	39	0
1	F	1258	0	1225	51	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
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	278	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 (278) 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:C:1148:ARG:HH11	1:C:1148:ARG:HA	1.54	0.73
1:B:1024:LEU:HB3	1:B:1033:ALA:HB1	1.71	0.73
1:E:1141:ALA:HA	1:E:1144:ARG:HE	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1025:PHE:CE1	1:B:1130:GLY:HA2	2.30	0.66
1:B:1109:GLY:HA3	3:B:7017:HOH:O	1.96	0.66
1:A:1082:LYS:HD3	1:A:1082:LYS:H	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:E:1039:LEU:HD23	1:E:1047:GLY:HA2	1.78	0.65
1:B:1140:GLU:O	1:B:1144:ARG:HG3	1.97	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:NE	1:A:1148:ARG:HA	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:1138:ILE:O	1:D:1142:MET:HG2	1.99	0.62
1:D:1036:PHE:HB2	1:D:1129:PHE:HE2	1.64	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:E:1058:PRO:HD3	1:E:1147:SER:H	1.65	0.60
1:D:1057:ILE:HG12	1:D:1150:GLY:HA2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1038:ALA:HB3	1:D:1078:ILE:HD13	1.85	0.57
1:B:1058:PRO:HB2	1:B:1148:ARG:HH22	1.69	0.57
1:B:1136:MET:O	1:B:1140:GLU:HG2	2.04	0.57
1:F:1085:ASP:HA	1:F:1108:ASN:ND2	2.19	0.57
1:C:1057:ILE:HG12	1:C:1150:GLY:HA2	1.86	0.57
1:C:1077:SER:HB2	1:C:1079:TYR:CD2	2.40	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:F:1037:ARG:HH11	1:F:1037:ARG:HG2	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:C:1069:ARG:HB2	1:C:1074:GLY:HA3	1.88	0.55
1:B:1022:PHE:CD2	1:B:1098:LEU:HD22	2.41	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: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:F:1029:VAL:HG21	1:F:1129:PHE:HB2	1.89	0.53
1:B:1008:PHE:HB2	1:B:1020:VAL:CG1	2.38	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:F:1069:ARG:HB3	1:F:1071:ASN:OD1	2.08	0.52
1:C:1030:PRO:HD2	1:C:1086:GLU:OE2	2.09	0.52
1:D:1069:ARG:HG2	1:D:1074:GLY:HA3	1.92	0.52
1:A:1042:GLY:O	1:A:1044:LYS:N	2.41	0.52
1:A:1037:ARG:HD2	1:A:1163:GLN:NE2	2.23	0.52
1:E:1029:VAL:O	1:E:1029:VAL:HG23	2.10	0.51
1:B:1008:PHE:HB2	1:B:1020:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1029:VAL:HG21	1:A:1129:PHE:CB	2.40	0.51
1:E:1082:LYS:H	1:E:1082:LYS:HD3	1.76	0.51
1:D:1028:LYS:C	1:D:1030:PRO:HD3	2.30	0.51
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:F:1029:VAL:HB	1:F:1032:THR:HB	1.92	0.51
1:B:1131:LYS:O	1:B:1131:LYS:HD3	2.11	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:E:1146:GLY:O	1:E:1147:SER:HB2	2.10	0.50
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: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:F:1018:GLY:HA2	3:F:7005:HOH:O	2.11	0.50
1:E:1058:PRO:HD2	1:E:1147:SER:O	2.12	0.50
1:A:1008:PHE:HD1	1:A:1161:CYS:HB3	1.77	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:1083:PHE:CD1	1:F:1108:ASN:O	2.65	0.49
1:B:1002:VAL:C	1:B:1003:ASN:HD22	2.16	0.49
1:A:1009:ASP:N	1:A:1160:ASP:O	2.39	0.49
1:B:1025:PHE:HE1	1:B:1130:GLY:HA2	1.75	0.49
1:B:1005:THR:O	1:B:1163:GLN:HG3	2.12	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:E:1010:ILE:HG13	1:E:1142:MET:HE3	1.96	0.48
1:F:1037:ARG:NH1	1:F:1037:ARG:HG2	2.28	0.48
1:C:1076:LYS:O	1:C:1110:SER:HB3	2.14	0.47
1:C:1026:ALA:HA	1:C:1033:ALA:CB	2.44	0.47
1:E:1029:VAL:HG21	1:E:1129:PHE:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:GLY:HA3	1:B:1111:GLN:HA	1.96	0.47
1:F:1029:VAL:HG13	3:F:7048:HOH:O	2.14	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:1076:LYS:O	1:F:1110:SER:HB3	2.14	0.47
1:A:1145:PHE:CD1	1:A:1145:PHE:N	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:D:1129:PHE:N	1:D:1129:PHE:CD1	2.82	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:F:1011:ALA:HB2	1:F:1159:ALA:HB2	1.97	0.46
1:D:1085:ASP:HB3	1:D:1127:VAL:HG21	1.98	0.46
1:C:1143:GLU:C	1:C:1145:PHE:H	2.18	0.46
1:D:1044:LYS:HG3	1:D:1078:ILE:CG2	2.46	0.46
1:F:1105:PRO:O	1:F:1107:THR:HG23	2.14	0.46
1:D:1099:SER:HB3	1:D:1113:PHE:CZ	2.51	0.46
1:F:1010:ILE:HG13	1:F:1142:MET:CE	2.45	0.46
1:A:1002:VAL:HG23	1:A:1003:ASN:H	1.81	0.46
1:A:1012:VAL:O	1:A:1013:ASP:HB2	2.15	0.46
1:D:1071:ASN:OD1	1:D:1072:GLY:N	2.48	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:C:1147:SER:HB3	1:C:1151:LYS:HB3	1.98	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:F:1049:LYS:CD	1:F:1160:ASP:HA	2.46	0.46
1:A:1096:GLY:HA2	1:A:1136:MET:SD	2.55	0.46
1:A:1048:TYR:HB3	1:A:1158:ILE:HD12	1.98	0.46
1:F:1048:TYR:HE1	1:F:1065:GLY:HA2	1.78	0.45
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: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:F:1027:ASP:OD1	1:F:1027:ASP:N	2.48	0.45
1:C:1082:LYS:HD2	1:C:1082:LYS:C	2.37	0.45
1:B:1015:GLU:HA	1:B:1016:PRO:HD3	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1087:ASN:HD22	1:B:1089:ILE:CD1	2.30	0.45
1:F:1145:PHE:CB	1:F:1156:ILE:HD11	2.45	0.45
1:E:1137:ASN:H	1:E:1137:ASN:ND2	2.14	0.45
1:B:1025:PHE:HE2	1:B:1028:LYS:HZ2	1.63	0.45
2:I:105:ILE:O	2:I:106:ALA:HB3	2.17	0.45
1:E:1095:PRO:HG3	1:E:1117:ALA:HA	1.98	0.45
1:C:1058:PRO:HG3	1:C:1143:GLU:O	2.16	0.45
1:C:1029:VAL:N	1:C:1030:PRO:HD3	2.31	0.45
1:C:1098:LEU:HG	1:C:1129:PHE:CZ	2.51	0.45
1:A:1076:LYS:HB2	1:A:1080:GLY:O	2.17	0.45
1:F:1008:PHE:HB2	1:F:1020:VAL:CG1	2.47	0.45
1:A:1035:ASN:O	1:A:1039:LEU:HD23	2.17	0.45
1:A:1145:PHE:HD2	1:A:1154:LYS:HB2	1.82	0.45
1:F:1141:ALA:C	1:F:1143:GLU:H	2.20	0.45
1:D:1082:LYS:O	1:D:1083:PHE:HB3	2.17	0.45
1:C:1025:PHE:CZ	1:C:1131:LYS:HG2	2.52	0.45
1:A:1069:ARG:HD2	1:A:1074:GLY:HA3	1.99	0.44
1:D:1129:PHE:HD1	1:D:1129:PHE:N	2.15	0.44
1:F:1031:LYS:HB2	1:F:1031:LYS:HZ3	1.82	0.44
1:E:1076:LYS:O	1:E:1110:SER:HB3	2.18	0.44
1:B:1049:LYS:HB2	1:B:1161:CYS:SG	2.57	0.44
1:D:1042:GLY:HA2	1:D:1046:PHE:O	2.17	0.44
1:D:1090:LEU:HB2	1:D:1128:VAL:HB	2.00	0.44
1:D:1002:VAL:HG21	1:D:1165:GLU:HG2	2.00	0.44
1:B:1129:PHE:HD1	1:B:1129:PHE:H	1.66	0.44
2:J:105:ILE:O	2:J:106:ALA:HB3	2.18	0.44
1:C:1122:LEU:HA	1:C:1125:LYS:HD3	2.00	0.44
2:K:105:ILE:O	2:K:106:ALA:HB3	2.18	0.44
1:C:1010:ILE:HG21	1:C:1142:MET:SD	2.58	0.44
1:B:1081:GLU:HG3	1:B:1082:LYS:NZ	2.33	0.44
1:D:1073:THR:O	1:D:1073:THR:HG22	2.17	0.44
1:E:1012:VAL:O	1:E:1013:ASP:HB2	2.18	0.43
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:1096:GLY:HA2	1:B:1136:MET:SD	2.59	0.43
1:B:1048:TYR:CD1	1:B:1065:GLY:HA2	2.52	0.43
1:D:1118:LYS:HE2	1:D:1120:GLU:OE1	2.17	0.43
1:F:1131:LYS:HE3	1:F:1131:LYS:HB3	1.72	0.43
1:D:1101:ALA:H	1:D:1112:PHE:HA	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1139:VAL:HA	1:B:1142:MET:HG2	2.00	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
1:E:1139:VAL:HA	1:E:1142:MET:HB3	2.01	0.43
1:C:1133:LYS:HE2	1:C:1133:LYS:HB3	1.72	0.43
1:F:1055:ARG:HA	1:F:1150:GLY:O	2.19	0.43
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:1029:VAL:HB	1:A:1032:THR:HB	2.01	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:C:1139:VAL:HA	1:C:1142:MET:CE	2.49	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:F:1131:LYS:HG2	1:F:1132:VAL:N	2.34	0.42
1:D:1015:GLU:HA	1:D:1016:PRO:HD3	1.71	0.42
1:B:1155:LYS:HD3	1:B:1156:ILE:N	2.35	0.42
1:F:1048:TYR:HB3	1:F:1158:ILE:HD12	2.01	0.42
1:C:1119:THR:HA	1:C:1121:TRP:CZ3	2.55	0.42
1:E:1069:ARG:N	1:E:1069:ARG:HD2	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:F:1044:LYS:HD3	1:F:1044:LYS:HA	1.86	0.41
1:F:1031:LYS:HB2	1:F:1031:LYS:NZ	2.35	0.41
1:D:1094:GLY:O	1:D:1097:ILE:HG12	2.19	0.41
1:C:1012:VAL:C	1:C:1014:GLY:H	2.23	0.41
1:F:1122:LEU:HD22	1:F:1126:HIS:CD2	2.55	0.41
1:D:1022:PHE:CD2	1:D:1098:LEU:HD22	2.55	0.41
1:B:1129:PHE:CD1	1:B:1129:PHE:N	2.88	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:H	1:D:1129:PHE:HD1	1.67	0.41
1:C:1139:VAL:HA	1:C:1142:MET:HE3	2.02	0.41
1:E:1136:MET:HE1	1:E:1139:VAL:HG11	2.02	0.41
1:D:1053:PHE:HB2	1:D:1156:ILE:HB	2.01	0.41
1:C:1009:ASP:O	1:C:1159:ALA:N	2.51	0.41
1:B:1018:GLY:HA3	1:B:1138:ILE:CD1	2.48	0.41
1:E:1037:ARG:HD3	1:E:1163:GLN:CD	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:105:ILE:O	2:J:106:ALA:CB	2.69	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
1:E:1119:THR:HA	1:E:1121:TRP:CZ3	2.55	0.41
1:E:1094:GLY:O	1:E:1097:ILE:HG12	2.20	0.41
1:C:1041:THR:OG1	1:C:1043:GLU:HG2	2.20	0.41
1:E:1131:LYS:HB3	1:E:1131:LYS:HE2	1.65	0.41
1:A:1002:VAL:HG23	1:A:1003:ASN:N	2.36	0.41
1:D:1141:ALA:O	1:D:1144:ARG:HG2	2.21	0.40
1:D:1009:ASP:O	1:D:1159:ALA:N	2.51	0.40
1:F:1085:ASP:H	1:F:1106:ASN:HA	1.86	0.40
1:D:1048:TYR:CE1	1:D:1065:GLY:HA2	2.56	0.40
1:A:1147:SER:O	1:A:1150:GLY:N	2.53	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:1069:ARG:HB3	1:C:1071:ASN:CG	2.42	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%)	7	4
1	B	162/164 (99%)	134 (83%)	21 (13%)	7 (4%)	3	1
1	C	162/164 (99%)	141 (87%)	20 (12%)	1 (1%)	30	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	162/164 (99%)	134 (83%)	27 (17%)	1 (1%)	30	32
1	E	162/164 (99%)	143 (88%)	18 (11%)	1 (1%)	30	32
1	F	162/164 (99%)	138 (85%)	22 (14%)	2 (1%)	16	14
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%)	12	9

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%)	125 (95%)	7 (5%)	28	34
1	B	132/132 (100%)	118 (89%)	14 (11%)	8	8
1	C	132/132 (100%)	125 (95%)	7 (5%)	28	34
1	D	132/132 (100%)	124 (94%)	8 (6%)	23	27
1	E	132/132 (100%)	121 (92%)	11 (8%)	14	14
1	F	132/132 (100%)	123 (93%)	9 (7%)	20	22
2	G	4/4 (100%)	3 (75%)	1 (25%)	1	0
2	H	4/4 (100%)	3 (75%)	1 (25%)	1	0
2	I	4/4 (100%)	3 (75%)	1 (25%)	1	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%)	1	0
All	All	816/816 (100%)	754 (92%)	62 (8%)	16	17

All (62) 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	1145	PHE
1	A	1148	ARG
1	A	1151	LYS
1	B	1015	GLU
1	B	1029	VAL
1	B	1036	PHE
1	B	1043	GLU
1	B	1061	MET
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	1152	THR
1	B	1153	SER
1	C	1028	LYS

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Mol	Chain	Res	Type
1	C	1029	VAL
1	C	1061	MET
1	C	1082	LYS
1	C	1084	GLU
1	C	1120	GLU
1	C	1149	ASN
1	D	1013	ASP
1	D	1029	VAL
1	D	1037	ARG
1	D	1061	MET
1	D	1085	ASP
1	D	1127	VAL
1	D	1129	PHE
1	D	1131	LYS
1	E	1039	LEU
1	E	1061	MET
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	1061	MET
1	F	1084	GLU
1	F	1106	ASN
1	F	1131	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	I	101	HIS
2	J	101	HIS
2	J	102	VAL
2	L	101	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1087	ASN
1	A	1163	GLN
1	B	1003	ASN
1	B	1108	ASN
1	B	1126	HIS
1	B	1149	ASN
1	C	1149	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	0.99	13 (7%) 15 23	5, 13, 20, 23	0
1	B	164/164 (100%)	2.28	88 (53%) 0 0	11, 20, 28, 34	0
1	C	164/164 (100%)	1.26	30 (18%) 2 3	5, 16, 25, 35	0
1	D	164/164 (100%)	1.40	34 (20%) 1 2	7, 18, 25, 33	0
1	E	164/164 (100%)	1.04	24 (14%) 3 6	3, 12, 21, 27	0
1	F	164/164 (100%)	2.14	83 (50%) 0 0	10, 18, 26, 30	0
2	G	4/6 (66%)	1.24	0 100 100	17, 19, 21, 29	0
2	H	6/6 (100%)	1.40	1 (16%) 2 4	11, 16, 22, 24	0
2	I	6/6 (100%)	1.20	0 100 100	7, 10, 11, 26	0
2	J	6/6 (100%)	1.61	1 (16%) 2 4	9, 10, 12, 18	0
2	K	4/6 (66%)	2.25	1 (25%) 1 2	12, 13, 20, 23	0
2	L	6/6 (100%)	1.72	2 (33%) 0 0	16, 19, 24, 24	0
All	All	1016/1020 (99%)	1.52	277 (27%) 1 1	3, 17, 26, 35	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1104	GLY	12.2
1	F	1107	THR	7.3
1	F	1080	GLY	6.1
1	F	1127	VAL	5.9
1	D	1080	GLY	5.8
1	F	1078	ILE	5.7
1	B	1024	LEU	5.5
1	C	1016	PRO	5.5
1	F	1026	ALA	5.3
1	D	1104	GLY	5.1
1	B	1070	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	1070	HIS	5.0
1	F	1150	GLY	5.0
1	F	1156	ILE	4.9
1	F	1030	PRO	4.8
1	B	1046	PHE	4.7
1	B	1014	GLY	4.7
1	F	1012	VAL	4.6
1	F	1032	THR	4.5
1	B	1079	TYR	4.4
1	D	1029	VAL	4.4
1	F	1039	LEU	4.3
1	F	1029	VAL	4.3
2	K	106	ALA	4.3
1	F	1071	ASN	4.3
1	B	1109	GLY	4.3
1	F	1017	LEU	4.3
1	B	1146	GLY	4.2
1	B	1067	PHE	4.2
1	F	1103	ALA	4.1
1	F	1016	PRO	4.0
1	B	1080	GLY	4.0
1	C	1012	VAL	4.0
1	B	1003	ASN	4.0
1	B	1016	PRO	3.9
1	F	1146	GLY	3.9
1	F	1090	LEU	3.9
1	B	1049	LYS	3.9
1	D	1026	ALA	3.8
1	E	1159	ALA	3.8
1	B	1071	ASN	3.7
1	B	1012	VAL	3.7
1	F	1002	VAL	3.6
1	B	1108	ASN	3.6
1	B	1074	GLY	3.6
1	F	1038	ALA	3.6
1	B	1090	LEU	3.6
1	D	1024	LEU	3.6
1	C	1153	SER	3.5
1	B	1072	GLY	3.5
1	B	1088	PHE	3.5
1	F	1036	PHE	3.5
1	B	1152	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1032	THR	3.5
1	B	1119	THR	3.5
1	D	1095	PRO	3.5
1	B	1038	ALA	3.5
1	D	1079	TYR	3.5
1	B	1139	VAL	3.4
1	C	1002	VAL	3.4
1	B	1129	PHE	3.4
1	B	1041	THR	3.4
1	F	1088	PHE	3.4
1	B	1138	ILE	3.4
1	B	1017	LEU	3.4
1	E	1152	THR	3.4
1	C	1093	THR	3.3
2	L	101	HIS	3.3
1	B	1127	VAL	3.3
1	C	1013	ASP	3.3
1	C	1145	PHE	3.3
1	C	1068	THR	3.3
1	F	1155	LYS	3.2
1	B	1089	ILE	3.2
1	C	1089	ILE	3.2
1	B	1110	SER	3.2
1	C	1017	LEU	3.2
1	A	1012	VAL	3.2
1	F	1068	THR	3.2
1	B	1117	ALA	3.2
1	B	1141	ALA	3.2
1	E	1017	LEU	3.2
1	F	1035	ASN	3.2
1	F	1143	GLU	3.2
1	F	1040	SER	3.2
1	D	1016	PRO	3.2
1	F	1052	CYS	3.1
1	B	1097	ILE	3.1
1	B	1102	ASN	3.1
1	C	1052	CYS	3.1
1	A	1080	GLY	3.1
1	F	1083	PHE	3.1
1	B	1105	PRO	3.1
1	B	1048	TYR	3.1
1	B	1128	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1073	THR	3.0
1	B	1147	SER	3.0
1	F	1013	ASP	3.0
1	B	1083	PHE	3.0
1	D	1085	ASP	3.0
1	F	1148	ARG	3.0
1	B	1077	SER	3.0
1	A	1156	ILE	3.0
1	B	1084	GLU	3.0
1	B	1037	ARG	3.0
1	B	1159	ALA	3.0
1	D	1025	PHE	3.0
1	F	1157	THR	3.0
1	E	1119	THR	2.9
1	B	1025	PHE	2.9
1	F	1069	ARG	2.9
1	B	1148	ARG	2.9
1	A	1017	LEU	2.9
1	B	1051	SER	2.9
1	F	1053	PHE	2.9
1	D	1003	ASN	2.9
1	B	1085	ASP	2.9
1	E	1018	GLY	2.8
1	B	1123	ASP	2.8
1	C	1146	GLY	2.8
1	B	1069	ARG	2.8
1	B	1011	ALA	2.8
1	C	1148	ARG	2.8
1	F	1158	ILE	2.8
1	F	1152	THR	2.8
1	E	1153	SER	2.8
1	B	1122	LEU	2.8
1	B	1116	THR	2.7
1	B	1130	GLY	2.7
1	B	1053	PHE	2.7
1	D	1081	GLU	2.7
1	F	1163	GLN	2.7
1	C	1128	VAL	2.7
1	E	1012	VAL	2.7
1	D	1097	ILE	2.7
1	B	1157	THR	2.7
1	F	1073	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1006	VAL	2.7
1	E	1016	PRO	2.7
1	F	1018	GLY	2.7
1	F	1027	ASP	2.7
1	F	1116	THR	2.7
1	F	1130	GLY	2.7
1	C	1106	ASN	2.6
1	E	1156	ILE	2.6
1	E	1148	ARG	2.6
2	L	102	VAL	2.6
1	C	1119	THR	2.6
1	E	1147	SER	2.6
1	E	1142	MET	2.6
1	F	1110	SER	2.6
1	F	1093	THR	2.6
1	F	1085	ASP	2.6
1	F	1128	VAL	2.6
2	J	106	ALA	2.6
1	C	1069	ARG	2.6
1	B	1154	LYS	2.6
1	F	1145	PHE	2.6
1	C	1015	GLU	2.6
1	D	1124	GLY	2.6
1	B	1093	THR	2.6
1	F	1161	CYS	2.6
1	B	1156	ILE	2.5
1	B	1039	LEU	2.5
1	B	1029	VAL	2.5
1	B	1047	GLY	2.5
1	F	1033	ALA	2.5
1	D	1147	SER	2.5
1	A	1058	PRO	2.5
1	D	1078	ILE	2.5
1	C	1088	PHE	2.5
1	F	1041	THR	2.5
1	C	1157	THR	2.5
1	F	1051	SER	2.5
1	F	1147	SER	2.5
1	F	1091	LYS	2.5
1	F	1057	ILE	2.5
1	F	1160	ASP	2.5
1	C	1123	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	1097	ILE	2.4
1	A	1154	LYS	2.4
1	D	1014	GLY	2.4
1	B	1081	GLU	2.4
1	B	1149	ASN	2.4
1	B	1078	ILE	2.4
1	B	1145	PHE	2.4
1	F	1045	GLY	2.4
1	F	1046	PHE	2.4
1	E	1073	THR	2.4
1	F	1079	TYR	2.4
1	D	1006	VAL	2.4
1	E	1082	LYS	2.4
1	B	1163	GLN	2.4
1	E	1067	PHE	2.4
1	F	1050	GLY	2.4
1	E	1071	ASN	2.3
1	F	1153	SER	2.3
1	A	1071	ASN	2.3
1	E	1080	GLY	2.3
1	B	1075	GLY	2.3
1	B	1004	PRO	2.3
1	E	1149	ASN	2.3
1	F	1122	LEU	2.3
1	C	1020	VAL	2.3
1	D	1002	VAL	2.3
1	D	1117	ALA	2.3
1	E	1050	GLY	2.3
1	E	1145	PHE	2.3
1	A	1081	GLU	2.3
1	D	1105	PRO	2.3
1	B	1107	THR	2.3
1	F	1047	GLY	2.3
1	C	1147	SER	2.3
1	F	1086	GLU	2.3
1	B	1007	PHE	2.2
1	D	1069	ARG	2.2
1	F	1072	GLY	2.2
1	C	1159	ALA	2.2
1	B	1015	GLU	2.2
1	F	1108	ASN	2.2
1	B	1142	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1030	PRO	2.2
1	D	1094	GLY	2.2
1	B	1160	ASP	2.2
1	B	1040	SER	2.2
1	D	1056	ILE	2.2
1	B	1132	VAL	2.2
1	D	1128	VAL	2.2
1	F	1109	GLY	2.2
1	C	1122	LEU	2.2
1	B	1092	HIS	2.2
2	H	106	ALA	2.2
1	D	1129	PHE	2.2
1	F	1144	ARG	2.2
1	F	1011	ALA	2.2
1	C	1156	ILE	2.2
1	D	1010	ILE	2.2
1	B	1002	VAL	2.2
1	D	1139	VAL	2.2
1	F	1074	GLY	2.2
1	F	1159	ALA	2.2
1	B	1050	GLY	2.1
1	F	1132	VAL	2.1
1	F	1081	GLU	2.1
1	C	1026	ALA	2.1
1	A	1146	GLY	2.1
1	A	1083	PHE	2.1
1	A	1145	PHE	2.1
1	E	1070	HIS	2.1
1	B	1082	LYS	2.1
1	C	1127	VAL	2.1
1	D	1155	LYS	2.1
1	E	1058	PRO	2.1
1	F	1058	PRO	2.1
1	C	1067	PHE	2.1
1	F	1112	PHE	2.1
1	F	1048	TYR	2.1
1	F	1137	ASN	2.1
1	A	1018	GLY	2.1
1	D	1146	GLY	2.1
1	F	1003	ASN	2.1
1	E	1081	GLU	2.1
1	B	1010	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1155	LYS	2.1
1	B	1113	PHE	2.1
1	D	1116	THR	2.1
1	F	1024	LEU	2.1
1	F	1102	ASN	2.1
1	B	1121	TRP	2.1
1	E	1154	LYS	2.1
1	D	1106	ASN	2.0
1	F	1066	ASP	2.0
1	C	1080	GLY	2.0
1	D	1027	ASP	2.0
1	A	1070	HIS	2.0
1	F	1089	ILE	2.0
1	B	1066	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.