



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:46 am BST

PDB ID : 3FKI  
Title : 12-Subunit RNA Polymerase II Refined with Zn-SAD data  
Authors : Meyer, P.A.; Ye, P.; Suh, M.H.; Zhang, M.; Fu, J.  
Deposited on : 2008-12-16  
Resolution : 3.88 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

<https://www.wwpdb.org/validation/2017/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
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

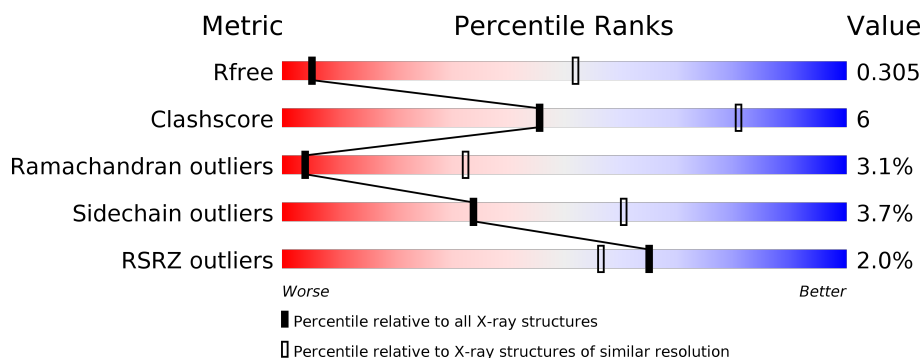
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.88 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	1026 (4.12-3.64)
Clashscore	141614	1045 (4.10-3.66)
Ramachandran outliers	138981	1008 (4.10-3.66)
Sidechain outliers	138945	1001 (4.10-3.66)
RSRZ outliers	127900	1213 (4.16-3.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>2%</div> <div>66% 15% 18%</div> </div>
2	B	1224	<div> <div>2%</div> <div>73% 17% 8%</div> </div>
3	C	318	<div> <div>0%</div> <div>65% 16% 16%</div> </div>
4	D	221	<div> <div>2%</div> <div>66% 13% 19%</div> </div>
5	E	215	<div> <div>2%</div> <div>88% 12%</div> </div>
6	F	155	<div> <div>0%</div> <div>46% 10% 44%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	MG	A	1736	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31412 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1427	Total	C	N	O	S	0	0	0
			11225	7069	1964	2130	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8947	5662	1568	1661	56			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2104	1323	350	418	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1436	887	257	290	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			704	451	119	131	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	136	Total	C	N	O	S	0	0	0
			1089	685	184	215	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	66	Total	C	N	O	S	0	0	0
			540	345	94	95	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			371	228	73	66	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

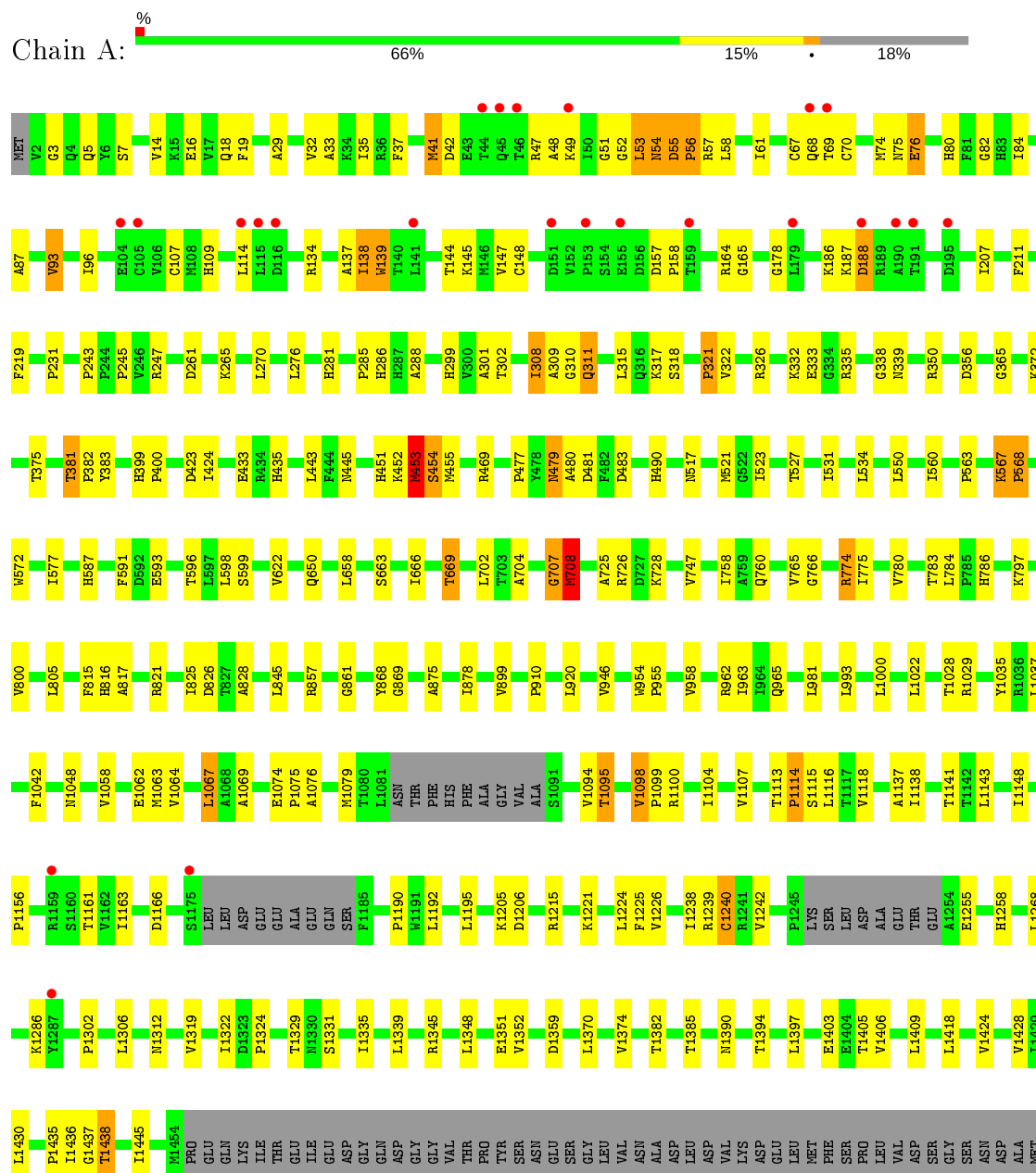
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

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

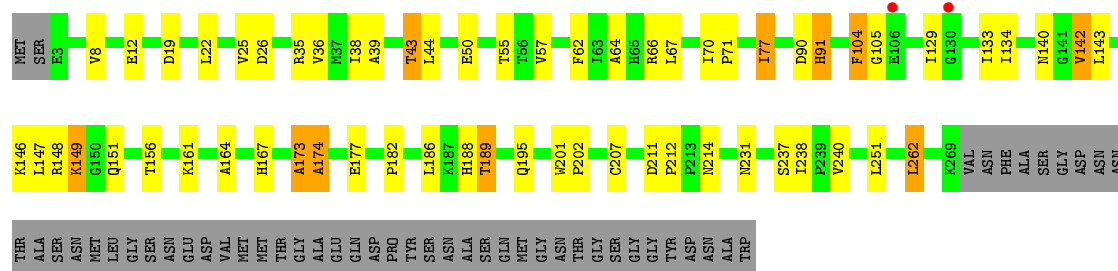
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA-directed RNA polymerase II subunit RPB1





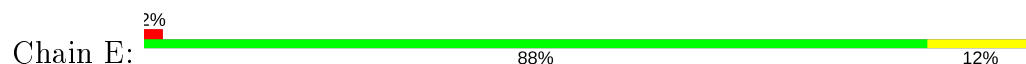




- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



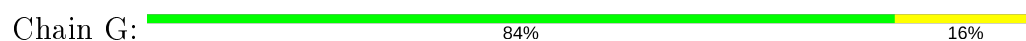
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



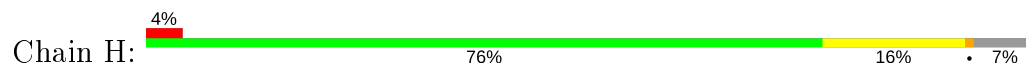
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

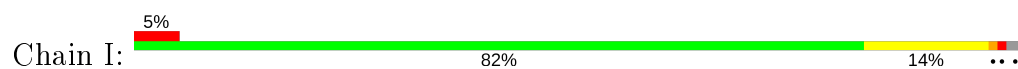


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

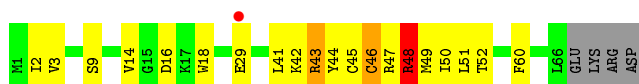




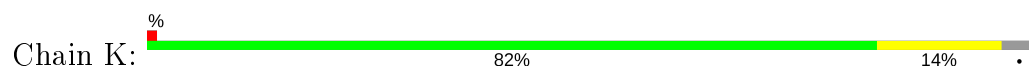
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.58Å 391.54Å 280.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.22 – 3.88 50.07 – 3.88	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.22-3.88) 95.5 (50.07-3.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5D	Depositor
R, $R_{free}$	0.282 , 0.301 0.284 , 0.305	Depositor DCC
$R_{free}$ test set	5355 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.3	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 21.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.098 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.105 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	31412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.30	0/11426	0.47	0/15451
2	B	0.31	0/9122	0.48	0/12300
3	C	0.29	0/2142	0.45	0/2902
4	D	0.31	0/1446	0.49	0/1937
5	E	0.31	0/1788	0.44	0/2406
6	F	0.28	0/716	0.47	0/967
7	G	0.31	0/1368	0.45	0/1844
8	H	0.33	0/1107	0.48	0/1498
9	I	0.33	0/989	0.48	0/1331
10	J	0.30	0/549	0.49	0/738
11	K	0.31	0/942	0.47	0/1272
12	L	0.34	0/373	0.54	0/495
All	All	0.31	0/31968	0.47	0/43141

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	508	LEU	Peptide

## 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	11225	0	11293	170	0
2	B	8947	0	8975	135	0
3	C	2104	0	2064	33	0
4	D	1436	0	1457	20	0
5	E	1752	0	1776	14	0
6	F	704	0	731	13	0
7	G	1340	0	1357	17	0
8	H	1089	0	1063	16	0
9	I	971	0	932	8	0
10	J	540	0	554	11	0
11	K	924	0	934	12	0
12	L	371	0	394	4	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	31412	0	31530	401	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 6.

All (401) 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)
4:D:17:LYS:HA	4:D:18:VAL:HB	1.30	1.11
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.30	1.10
6:F:71:GLU:HA	6:F:72:LYS:HB3	1.08	1.07
2:B:471:LYS:HB3	2:B:472:ALA:HA	1.37	1.04
1:A:187:LYS:HB3	1:A:188:ASP:HA	1.36	1.03
2:B:444:MET:HB3	2:B:445:LYS:HA	1.41	1.01
1:A:707:GLY:CA	1:A:708:MET:HB2	1.93	0.97
1:A:567:LYS:HB3	1:A:568:PRO:CD	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:GLY:HA3	1:A:708:MET:HB2	1.46	0.94
2:B:471:LYS:HB3	2:B:472:ALA:CA	1.96	0.94
1:A:567:LYS:CB	1:A:568:PRO:HD3	1.98	0.93
2:B:714:GLU:HB2	2:B:715:ALA:HA	1.51	0.92
1:A:137:ALA:HA	1:A:138:ILE:C	1.89	0.92
6:F:71:GLU:CA	6:F:72:LYS:HB3	1.99	0.91
2:B:714:GLU:CB	2:B:715:ALA:HA	2.03	0.88
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.56	0.85
1:A:707:GLY:HA3	1:A:708:MET:CB	2.07	0.83
4:D:17:LYS:HA	4:D:18:VAL:CB	2.07	0.83
4:D:17:LYS:CA	4:D:18:VAL:HB	2.09	0.83
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.61	0.83
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.62	0.82
1:A:144:THR:HB	1:A:145:LYS:HA	1.60	0.82
6:F:71:GLU:HA	6:F:72:LYS:CB	1.96	0.81
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.61	0.81
2:B:843:GLN:HB2	2:B:993:THR:HB	1.64	0.78
3:C:142:VAL:H	10:J:16:ASP:HB3	1.49	0.76
1:A:187:LYS:HB3	1:A:188:ASP:CA	2.18	0.74
1:A:187:LYS:CB	1:A:188:ASP:HA	2.09	0.74
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.53	0.72
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.54	0.72
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.72	0.71
2:B:444:MET:HB3	2:B:445:LYS:CA	2.19	0.69
1:A:707:GLY:N	1:A:708:MET:HB2	2.07	0.69
1:A:825:ILE:CD1	2:B:513:GLN:HB3	2.23	0.68
1:A:75:ASN:O	1:A:76:GLU:HB3	1.95	0.67
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.76	0.67
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.26	0.66
12:L:28:LYS:HB2	12:L:39:SER:HA	1.78	0.66
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.60	0.66
2:B:471:LYS:HB3	2:B:472:ALA:CB	2.25	0.65
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.61	0.65
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.79	0.65
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.77	0.65
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.78	0.65
1:A:54:ASN:O	1:A:55:ASP:HB2	1.97	0.64
4:D:7:THR:O	4:D:8:PHE:HB3	1.97	0.64
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.78	0.64
2:B:471:LYS:CB	2:B:472:ALA:HA	2.15	0.64
1:A:857:ARG:HD2	1:A:861:GLY:HA2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.62	0.63
1:A:821:ARG:HH21	2:B:534:GLY:HA2	1.64	0.63
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.81	0.62
2:B:512:ARG:O	2:B:534:GLY:HA3	1.99	0.62
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.30	0.62
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.34	0.62
4:D:18:VAL:HG13	4:D:19:GLU:N	2.15	0.62
7:G:46:LEU:HD21	7:G:105:PRO:HG3	1.82	0.62
2:B:843:GLN:HG2	11:K:6:ARG:NH2	2.14	0.62
1:A:663:SER:HB2	2:B:827:ILE:O	2.00	0.61
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.82	0.61
1:A:164:ARG:HG3	1:A:165:GLY:H	1.66	0.60
1:A:453:MET:C	1:A:455:MET:H	2.03	0.60
1:A:774:ARG:HG3	1:A:797:LYS:HD2	1.84	0.60
5:E:176:PRO:HG2	5:E:211:TYR:O	2.03	0.59
1:A:669:THR:HB	1:A:805:LEU:HD13	1.85	0.58
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.85	0.58
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.85	0.58
2:B:494:HIS:HA	2:B:497:ARG:HE	1.68	0.58
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.86	0.58
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.86	0.58
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.85	0.58
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.67	0.58
7:G:15:PRO:HA	7:G:18:PHE:HD1	1.68	0.58
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	1.85	0.57
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.85	0.57
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.86	0.57
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.39	0.57
3:C:104:PHE:HD2	3:C:105:GLY:H	1.51	0.57
1:A:1116:LEU:HB3	1:A:1329:THR:HG23	1.87	0.57
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.87	0.57
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.87	0.57
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.87	0.57
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.85	0.57
8:H:82:PRO:O	8:H:84:ALA:N	2.37	0.56
8:H:91:ASP:C	8:H:93:TYR:H	2.08	0.56
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.70	0.56
2:B:444:MET:CB	2:B:445:LYS:HA	2.17	0.56
2:B:713:ALA:O	2:B:714:GLU:HB2	2.05	0.56
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.87	0.56
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:LEU:HD12	7:G:67:SER:HB3	1.88	0.55
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.89	0.55
1:A:144:THR:N	1:A:145:LYS:HB2	2.22	0.55
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.89	0.55
4:D:18:VAL:HG13	4:D:19:GLU:H	1.71	0.55
8:H:82:PRO:C	8:H:84:ALA:H	2.09	0.55
1:A:33:ALA:HB2	1:A:82:GLY:HA2	1.89	0.54
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.72	0.54
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.89	0.54
1:A:567:LYS:HD2	8:H:95:TYR:HA	1.90	0.54
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.89	0.54
8:H:58:THR:HB	8:H:143:LEU:HB2	1.90	0.53
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.90	0.53
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.89	0.53
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.90	0.53
1:A:1143:LEU:HB3	1:A:1268:LEU:HA	1.91	0.53
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.91	0.53
2:B:335:GLY:HA2	2:B:336:ARG:HB3	1.90	0.53
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.91	0.53
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.90	0.53
2:B:997:GLU:HB3	3:C:35:ARG:HG2	1.90	0.53
3:C:43:THR:HG22	3:C:44:LEU:H	1.73	0.53
12:L:48:CYS:SG	12:L:49:LYS:N	2.82	0.53
1:A:479:ASN:N	1:A:480:ALA:HB3	2.24	0.52
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.91	0.52
3:C:12:GLU:H	3:C:19:ASP:HB3	1.73	0.52
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.91	0.52
1:A:33:ALA:HB2	1:A:82:GLY:CA	2.38	0.52
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.74	0.52
1:A:14:VAL:HG21	1:A:1430:LEU:HD22	1.92	0.52
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.91	0.52
1:A:707:GLY:HA3	1:A:708:MET:CG	2.39	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.51
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.91	0.51
2:B:424:LEU:HD11	2:B:448:ILE:HG23	1.92	0.51
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.91	0.51
1:A:35:ILE:HD11	1:A:53:LEU:HG	1.92	0.51
1:A:53:LEU:HD23	1:A:54:ASN:H	1.76	0.51
1:A:598:LEU:HD11	8:H:124:ARG:HD2	1.93	0.51
4:D:120:GLU:HA	4:D:123:LEU:HD12	1.92	0.51
5:E:47:CYS:HB3	5:E:51:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.92	0.51
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.92	0.51
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.93	0.51
2:B:453:ILE:H	2:B:453:ILE:HD12	1.76	0.51
1:A:479:ASN:CA	1:A:480:ALA:HB3	2.41	0.51
1:A:707:GLY:CA	1:A:708:MET:CB	2.70	0.51
2:B:511:PRO:O	2:B:512:ARG:HB2	2.11	0.51
3:C:35:ARG:HB3	11:K:41:THR:HG22	1.93	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.92	0.50
2:B:296:GLU:HA	2:B:299:GLU:HB2	1.93	0.50
3:C:173:ALA:O	3:C:174:ALA:CB	2.59	0.50
3:C:262:LEU:HD22	11:K:88:LYS:HE3	1.93	0.50
2:B:471:LYS:HB3	2:B:472:ALA:HB2	1.93	0.50
4:D:51:ASN:HB3	4:D:178:ALA:HA	1.94	0.50
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.92	0.50
1:A:55:ASP:N	1:A:56:PRO:CD	2.74	0.49
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.93	0.49
4:D:52:LEU:O	4:D:53:SER:HB3	2.11	0.49
1:A:54:ASN:O	1:A:55:ASP:CB	2.60	0.49
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.42	0.49
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.93	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.93	0.49
1:A:550:LEU:HD13	1:A:560:ILE:HG22	1.94	0.49
1:A:57:ARG:HB3	1:A:68:GLN:HB2	1.95	0.49
2:B:655:LYS:HA	2:B:658:ILE:HD12	1.95	0.49
7:G:91:VAL:HG22	7:G:101:VAL:HG22	1.94	0.49
1:A:857:ARG:HD3	6:F:139:PRO:HB3	1.95	0.49
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.93	0.49
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.76	0.49
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.78	0.49
4:D:18:VAL:CG1	4:D:19:GLU:H	2.26	0.48
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.78	0.48
1:A:479:ASN:HA	1:A:480:ALA:HB3	1.94	0.48
2:B:60:GLN:O	2:B:63:ILE:HG22	2.14	0.48
7:G:26:LEU:HD13	7:G:56:ILE:HG21	1.95	0.48
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.94	0.48
2:B:216:GLU:HB3	2:B:500:THR:HA	1.95	0.48
2:B:955:THR:HG23	12:L:54:ARG:O	2.13	0.48
1:A:469:ARG:NH2	2:B:991:GLY:O	2.46	0.48
1:A:1148:ILE:HG23	9:I:49:ILE:HB	1.96	0.48
2:B:1037:LEU:HD22	2:B:1062:HIS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:THR:HG21	1:A:433:GLU:HB3	1.95	0.48
2:B:120:ARG:HG2	2:B:955:THR:CG2	2.37	0.48
1:A:49:LYS:HZ2	1:A:61:ILE:HG13	1.78	0.48
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.78	0.48
3:C:71:PRO:HB2	3:C:133:ILE:HD12	1.96	0.48
4:D:7:THR:O	4:D:8:PHE:CB	2.60	0.48
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.95	0.48
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.95	0.48
3:C:148:ARG:HG2	3:C:149:LYS:N	2.29	0.48
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.96	0.47
1:A:144:THR:HB	1:A:145:LYS:CA	2.39	0.47
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.96	0.47
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.49	0.47
4:D:5:THR:HG23	4:D:6:SER:H	1.79	0.47
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.95	0.47
2:B:500:THR:O	2:B:501:PRO:C	2.53	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.95	0.47
1:A:1329:THR:HG22	1:A:1331:SER:H	1.79	0.47
1:A:219:PHE:CD1	1:A:231:PRO:HD2	2.50	0.47
1:A:567:LYS:HG2	1:A:568:PRO:HD3	1.97	0.47
1:A:68:GLN:C	1:A:70:CYS:H	2.17	0.47
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.97	0.47
6:F:111:LEU:H	6:F:111:LEU:HD12	1.80	0.47
1:A:452:LYS:HD3	1:A:1067:LEU:HD21	1.96	0.47
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.97	0.47
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.97	0.47
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.95	0.47
4:D:18:VAL:CG1	4:D:19:GLU:N	2.77	0.47
2:B:215:GLN:HB2	2:B:407:ASP:HB2	1.95	0.47
12:L:24:THR:HA	12:L:25:ALA:HA	1.69	0.47
1:A:1035:TYR:HB2	1:A:1037:LEU:HD12	1.97	0.47
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.46	0.47
1:A:663:SER:OG	2:B:1085:ILE:HA	2.15	0.47
1:A:598:LEU:HD21	8:H:124:ARG:HB2	1.97	0.47
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.27	0.47
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.96	0.46
1:A:137:ALA:HA	1:A:139:TRP:N	2.29	0.46
1:A:825:ILE:HD11	2:B:513:GLN:HB3	1.96	0.46
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.97	0.46
3:C:173:ALA:O	3:C:174:ALA:HB3	2.16	0.46
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.98	0.46
2:B:1002:THR:HG22	2:B:1072:MET:HG3	1.98	0.46
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.79	0.46
3:C:133:ILE:HD11	3:C:237:SER:HA	1.98	0.46
1:A:1436:ILE:O	1:A:1438:THR:N	2.48	0.46
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.97	0.46
1:A:1114:PRO:HB2	1:A:1115:SER:H	1.56	0.46
1:A:7:SER:HB2	2:B:1159:ARG:HH21	1.80	0.46
5:E:156:LEU:HD23	5:E:160:GLU:HB3	1.97	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.98	0.46
1:A:825:ILE:HD13	2:B:513:GLN:HB3	1.96	0.46
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.98	0.46
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.80	0.46
2:B:475:SER:O	2:B:476:ARG:HG3	2.16	0.46
1:A:1224:LEU:HD12	1:A:1242:VAL:HG22	1.97	0.46
1:A:527:THR:HG21	1:A:650:GLN:HA	1.98	0.46
1:A:531:ILE:HD13	1:A:622:VAL:HG11	1.97	0.45
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.97	0.45
1:A:375:THR:CG2	1:A:433:GLU:HB3	2.46	0.45
1:A:55:ASP:H	1:A:58:LEU:HD12	1.80	0.45
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.64	0.45
2:B:531:GLN:HG3	2:B:532:ALA:H	1.80	0.45
3:C:147:LEU:HD22	3:C:151:GLN:HB3	1.99	0.45
1:A:1094:VAL:O	1:A:1095:THR:C	2.55	0.45
1:A:75:ASN:O	1:A:76:GLU:CB	2.64	0.45
2:B:763:GLN:O	2:B:764:SER:HB3	2.16	0.45
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.80	0.45
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.98	0.45
10:J:47:ARG:C	10:J:49:MET:H	2.19	0.45
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.99	0.45
2:B:1089:PRO:HB2	2:B:1090:THR:H	1.58	0.45
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.99	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.98	0.45
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.98	0.45
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.99	0.45
9:I:53:GLY:O	9:I:89:GLN:HB2	2.16	0.45
1:A:567:LYS:H	8:H:96:VAL:HB	1.82	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.17	0.45
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.99	0.45
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.99	0.45
1:A:1141:THR:HG22	1:A:1205:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.98	0.45
2:B:615:MET:HG2	2:B:626:ILE:HG12	1.99	0.45
5:E:56:LYS:HG3	5:E:84:ASP:HB2	1.98	0.45
9:I:8:ARG:O	9:I:10:CYS:N	2.50	0.45
1:A:453:MET:O	1:A:455:MET:N	2.49	0.44
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.99	0.44
2:B:444:MET:H	2:B:445:LYS:HG2	1.82	0.44
2:B:714:GLU:CB	2:B:715:ALA:CA	2.83	0.44
1:A:19:PHE:HZ	1:A:1397:LEU:HG	1.82	0.44
6:F:77:ASP:O	6:F:78:GLN:HB2	2.18	0.44
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.52	0.44
1:A:658:LEU:HD13	2:B:831:SER:H	1.82	0.44
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.33	0.44
1:A:981:LEU:HD11	1:A:1042:PHE:HB2	2.00	0.44
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.44
2:B:442:PHE:O	2:B:443:ASN:HB3	2.18	0.44
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.99	0.44
1:A:445:ASN:HA	1:A:454:SER:O	2.18	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HG3	2.00	0.44
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.99	0.44
2:B:654:ARG:H	2:B:657:HIS:HD2	1.66	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.00	0.44
1:A:1104:ILE:HG23	1:A:1348:LEU:HD11	2.00	0.44
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.18	0.44
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.58	0.44
5:E:3:GLN:HG3	5:E:5:ASN:H	1.83	0.44
10:J:14:VAL:HG22	10:J:50:ILE:HD11	2.00	0.44
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.82	0.43
2:B:1171:VAL:HG12	2:B:1182:CYS:HB2	2.00	0.43
2:B:600:LEU:HB3	2:B:615:MET:SD	2.58	0.43
2:B:763:GLN:O	2:B:765:PRO:HD2	2.18	0.43
3:C:77:ILE:HG12	3:C:129:ILE:HD11	2.01	0.43
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.00	0.43
4:D:32:GLU:HG3	7:G:5:LYS:NZ	2.33	0.43
9:I:105:SER:O	9:I:106:CYS:HB3	2.17	0.43
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.84	0.43
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.99	0.43
2:B:806:THR:HG23	2:B:1045:SER:HA	2.01	0.43
2:B:459:TYR:HE2	2:B:469:GLN:HA	1.84	0.43
1:A:899:VAL:HG21	1:A:1028:THR:HB	2.00	0.43
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ALA:O	1:A:821:ARG:HB2	2.18	0.43
7:G:83:LYS:HE3	7:G:150:CYS:H	1.83	0.43
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.01	0.43
6:F:130:ILE:HB	6:F:148:VAL:HG21	2.01	0.43
1:A:310:GLY:O	1:A:311:GLN:CB	2.66	0.43
4:D:185:CYS:HB2	4:D:211:LEU:HD22	2.01	0.43
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.59	0.43
1:A:207:ILE:O	1:A:211:PHE:HD2	2.00	0.43
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.01	0.43
4:D:58:VAL:HG13	7:G:49:LEU:HD21	2.01	0.43
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	2.01	0.43
2:B:270:LYS:HA	2:B:281:PRO:HA	2.01	0.43
2:B:42:GLY:O	2:B:44:VAL:N	2.52	0.43
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.01	0.42
2:B:512:ARG:O	2:B:534:GLY:CA	2.66	0.42
1:A:816:HIS:NE2	2:B:763:GLN:O	2.51	0.42
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.01	0.42
1:A:47:ARG:O	1:A:48:ALA:HB3	2.19	0.42
2:B:1052:VAL:HA	2:B:1055:ILE:HD12	2.01	0.42
9:I:65:ASP:HA	9:I:66:PRO:HD3	1.83	0.42
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.84	0.42
2:B:1110:PRO:HG3	2:B:1124:ARG:O	2.19	0.42
2:B:1167:GLY:CA	2:B:1216:LEU:H	2.31	0.42
2:B:992:ILE:HD13	11:K:67:PHE:CE2	2.54	0.42
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.20	0.42
1:A:783:THR:HG21	1:A:815:PHE:HE1	1.84	0.42
2:B:259:TYR:HB2	2:B:268:THR:HG23	2.01	0.42
2:B:843:GLN:HG2	11:K:6:ARG:HH21	1.85	0.42
7:G:85:GLU:HB3	7:G:147:ILE:HD12	2.01	0.42
1:A:869:GLY:O	5:E:204:THR:HG21	2.20	0.42
1:A:962:ARG:HA	1:A:965:GLN:HE21	1.84	0.42
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.53	0.42
2:B:577:ALA:HB1	2:B:589:VAL:HG11	2.01	0.42
2:B:830:TYR:O	2:B:832:GLY:N	2.53	0.42
2:B:976:ILE:HG12	2:B:993:THR:HG23	2.01	0.42
2:B:1089:PRO:O	2:B:1090:THR:CB	2.67	0.42
6:F:109:VAL:HG11	6:F:123:LYS:HG2	2.02	0.42
9:I:8:ARG:HB2	9:I:9:ASP:H	1.70	0.42
10:J:9:SER:OG	10:J:45:CYS:HB2	2.18	0.42
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.85	0.42
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:H	2:B:619:ILE:HG13	1.70	0.42
3:C:50:GLU:HB2	3:C:156:THR:HB	2.02	0.42
5:E:177:ARG:HD3	5:E:215:MET:HB2	2.01	0.42
10:J:41:LEU:HD22	10:J:46:CYS:HB2	2.02	0.42
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.20	0.42
1:A:299:HIS:HA	1:A:302:THR:HG22	2.01	0.42
2:B:1167:GLY:HA3	2:B:1216:LEU:N	2.34	0.42
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.84	0.42
2:B:473:MET:HA	2:B:474:SER:HA	1.61	0.42
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.91	0.41
2:B:283:VAL:HG21	2:B:318:VAL:HA	2.02	0.41
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	2.02	0.41
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.20	0.41
1:A:321:PRO:HB2	1:A:322:VAL:H	1.60	0.41
2:B:444:MET:H	2:B:445:LYS:CG	2.33	0.41
3:C:22:LEU:HD11	11:K:101:LEU:HD11	2.02	0.41
2:B:843:GLN:CG	11:K:6:ARG:NH2	2.82	0.41
1:A:1138:ILE:HG12	1:A:1319:VAL:HG21	2.02	0.41
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.02	0.41
2:B:916:THR:HA	2:B:917:PRO:HD3	1.95	0.41
10:J:42:LYS:HG3	10:J:43:ARG:HD3	2.01	0.41
2:B:282:ILE:HA	2:B:285:ILE:HD12	2.01	0.41
2:B:559:SER:HA	2:B:563:MET:HB3	2.01	0.41
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.03	0.41
3:C:36:VAL:HG21	3:C:251:LEU:HD13	2.03	0.41
1:A:477:PRO:HG2	1:A:521:MET:HG2	2.02	0.41
6:F:132:LEU:HD22	7:G:61:ILE:HD11	2.01	0.41
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.02	0.41
3:C:133:ILE:CD1	3:C:237:SER:HA	2.50	0.41
1:A:114:LEU:HB3	1:A:145:LYS:HZ3	1.86	0.41
1:A:308:ILE:HG22	1:A:309:ALA:H	1.85	0.41
1:A:381:THR:HG22	1:A:382:PRO:HD2	2.03	0.41
2:B:637:LEU:HD12	2:B:693:ILE:HD12	2.03	0.41
1:A:1226:VAL:HG12	1:A:1240:CYS:HB3	2.03	0.41
1:A:946:VAL:HG22	5:E:201:LYS:HB3	2.03	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
2:B:292:ILE:N	2:B:293:PRO:CD	2.84	0.41
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.56	0.41
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.03	0.41
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.50	0.40
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.36	0.40
1:A:1076:ALA:HA	1:A:1079:MET:SD	2.61	0.40
1:A:962:ARG:HA	1:A:965:GLN:HB2	2.02	0.40
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.96	0.40
2:B:468:GLU:H	2:B:471:LYS:HB2	1.86	0.40
2:B:590:HIS:CG	2:B:596:LEU:HD22	2.56	0.40
2:B:638:PHE:HB2	2:B:741:CYS:HB3	2.03	0.40
9:I:52:ILE:H	9:I:52:ILE:HG13	1.74	0.40
1:A:1062:GLU:HG2	6:F:88:TYR:HE1	1.86	0.40
2:B:769:TYR:O	2:B:773:MET:HB2	2.22	0.40
4:D:144:THR:HG21	7:G:46:LEU:HD13	2.03	0.40
1:A:381:THR:C	1:A:383:TYR:H	2.24	0.40
1:A:596:THR:C	1:A:598:LEU:H	2.24	0.40
1:A:725:ALA:HA	1:A:728:LYS:HE2	2.03	0.40
7:G:56:ILE:HG13	7:G:56:ILE:H	1.68	0.40
1:A:134:ARG:O	1:A:138:ILE:HG12	2.21	0.40
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.57	0.40
2:B:572:HIS:O	2:B:574:SER:N	2.51	0.40
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.22	0.40
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.95	0.40
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.02	0.40
7:G:147:ILE:HG23	7:G:159:ALA:HB1	2.04	0.40
8:H:100:THR:HG23	8:H:138:GLU:HA	2.04	0.40
11:K:49:GLU:HG3	11:K:94:ILE:HG12	2.04	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	1419/1733 (82%)	1228 (86%)	141 (10%)	50 (4%)	<b>3</b> 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1111/1224 (91%)	957 (86%)	117 (10%)	37 (3%)	4	31
3	C	265/318 (83%)	236 (89%)	20 (8%)	9 (3%)	3	31
4	D	174/221 (79%)	148 (85%)	21 (12%)	5 (3%)	4	33
5	E	212/215 (99%)	193 (91%)	19 (9%)	0	100	100
6	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
7	G	169/171 (99%)	146 (86%)	21 (12%)	2 (1%)	13	49
8	H	132/146 (90%)	106 (80%)	19 (14%)	7 (5%)	2	23
9	I	117/122 (96%)	99 (85%)	15 (13%)	3 (3%)	5	35
10	J	64/70 (91%)	57 (89%)	4 (6%)	3 (5%)	2	25
11	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
12	L	45/70 (64%)	33 (73%)	7 (16%)	5 (11%)	0	8
All	All	3906/4565 (86%)	3390 (87%)	395 (10%)	121 (3%)	4	32

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	139	TRP
1	A	311	GLN
1	A	321	PRO
1	A	479	ASN
1	A	567	LYS
1	A	568	PRO
1	A	708	MET
1	A	1098	VAL
1	A	1437	GLY
2	B	43	LEU
2	B	45	SER
2	B	504	ARG
2	B	714	GLU
2	B	764	SER
2	B	1089	PRO
3	C	174	ALA
4	D	8	PHE
4	D	18	VAL
4	D	199	ASN
8	H	82	PRO

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Mol	Chain	Res	Type
9	I	9	ASP
1	A	74	MET
1	A	76	GLU
1	A	138	ILE
1	A	286	HIS
1	A	318	SER
1	A	593	GLU
1	A	1095	THR
1	A	1114	PRO
1	A	1405	THR
2	B	108	VAL
2	B	467	GLY
2	B	469	GLN
2	B	501	PRO
2	B	503	GLY
2	B	512	ARG
2	B	531	GLN
2	B	1090	THR
3	C	161	LYS
4	D	119	ARG
8	H	83	GLN
8	H	129	TYR
12	L	56	LEU
1	A	147	VAL
1	A	332	LYS
1	A	453	MET
1	A	454	SER
1	A	704	ALA
1	A	1221	LYS
2	B	367	LEU
2	B	466	TRP
2	B	511	PRO
2	B	711	GLU
2	B	713	ALA
2	B	751	VAL
2	B	831	SER
2	B	1157	ALA
3	C	91	HIS
3	C	149	LYS
3	C	173	ALA
8	H	63	LEU
9	I	47	GLU

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Mol	Chain	Res	Type
10	J	2	ILE
12	L	26	THR
12	L	39	SER
1	A	41	MET
1	A	67	CYS
1	A	317	LYS
1	A	423	ASP
1	A	424	ILE
1	A	591	PHE
1	A	775	ILE
1	A	780	VAL
1	A	958	VAL
1	A	1403	GLU
2	B	409	ALA
2	B	724	ASP
2	B	880	THR
2	B	881	ASN
2	B	1017	ILE
3	C	214	ASN
7	G	84	GLY
8	H	52	GLN
8	H	92	ASP
9	I	8	ARG
12	L	33	GLU
1	A	5	GLN
1	A	109	HIS
1	A	920	LEU
1	A	1206	ASP
1	A	1255	GLU
2	B	735	ALA
2	B	1046	PRO
2	B	1108	ARG
3	C	90	ASP
3	C	142	VAL
3	C	202	PRO
4	D	7	THR
10	J	29	GLU
10	J	48	ARG
12	L	52	GLY
1	A	3	GLY
1	A	1137	ALA
2	B	249	ARG

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Mol	Chain	Res	Type
1	A	56	PRO
2	B	506	GLY
2	B	575	PRO
1	A	178	GLY
1	A	599	SER
2	B	364	ILE
2	B	832	GLY
1	A	1435	PRO
1	A	707	GLY
1	A	910	PRO
1	A	1107	VAL
2	B	295	GLY
2	B	977	GLY
7	G	154	VAL
8	H	81	PRO

### 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	1247/1520 (82%)	1206 (97%)	41 (3%)	38	63
2	B	976/1061 (92%)	937 (96%)	39 (4%)	31	58
3	C	235/274 (86%)	221 (94%)	14 (6%)	19	49
4	D	160/200 (80%)	150 (94%)	10 (6%)	18	47
5	E	196/197 (100%)	194 (99%)	2 (1%)	76	86
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	148 (97%)	4 (3%)	46	68
8	H	119/128 (93%)	117 (98%)	2 (2%)	60	78
9	I	113/116 (97%)	107 (95%)	6 (5%)	22	52
10	J	61/65 (94%)	57 (93%)	4 (7%)	16	46
11	K	99/102 (97%)	96 (97%)	3 (3%)	41	64
12	L	41/57 (72%)	37 (90%)	4 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3476/4009 (87%)	3347 (96%)	129 (4%)	34 60

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	41	MET
1	A	42	ASP
1	A	53	LEU
1	A	80	HIS
1	A	93	VAL
1	A	96	ILE
1	A	186	LYS
1	A	188	ASP
1	A	261	ASP
1	A	265	LYS
1	A	281	HIS
1	A	308	ILE
1	A	315	LEU
1	A	381	THR
1	A	451	HIS
1	A	453	MET
1	A	481	ASP
1	A	483	ASP
1	A	517	ASN
1	A	587	HIS
1	A	669	THR
1	A	702	LEU
1	A	708	MET
1	A	774	ARG
1	A	800	VAL
1	A	826	ASP
1	A	1000	LEU
1	A	1067	LEU
1	A	1215	ARG
1	A	1240	CYS
1	A	1258	HIS
1	A	1312	ASN
1	A	1345	ARG
1	A	1359	ASP
1	A	1382	THR
1	A	1385	THR

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Mol	Chain	Res	Type
1	A	1390	ASN
1	A	1394	THR
1	A	1438	THR
1	A	1445	ILE
2	B	63	ILE
2	B	175	ARG
2	B	178	ASN
2	B	192	LEU
2	B	225	VAL
2	B	246	LYS
2	B	261	ARG
2	B	294	ASP
2	B	329	THR
2	B	365	THR
2	B	387	LEU
2	B	429	PHE
2	B	444	MET
2	B	466	TRP
2	B	485	ARG
2	B	549	THR
2	B	570	VAL
2	B	576	ASP
2	B	603	LEU
2	B	604	ARG
2	B	618	ASP
2	B	646	LEU
2	B	830	TYR
2	B	837	ASP
2	B	839	MET
2	B	953	LEU
2	B	956	THR
2	B	999	MET
2	B	1048	THR
2	B	1058	LEU
2	B	1060	ARG
2	B	1095	LEU
2	B	1104	HIS
2	B	1115	THR
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1183	LYS

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Mol	Chain	Res	Type
2	B	1187	ASN
3	C	25	VAL
3	C	26	ASP
3	C	43	THR
3	C	55	THR
3	C	77	ILE
3	C	91	HIS
3	C	104	PHE
3	C	134	ILE
3	C	140	ASN
3	C	189	THR
3	C	195	GLN
3	C	238	ILE
3	C	240	VAL
3	C	262	LEU
4	D	5	THR
4	D	15	LEU
4	D	26	THR
4	D	38	ILE
4	D	70	PHE
4	D	134	THR
4	D	148	LEU
4	D	187	THR
4	D	204	ASP
4	D	221	TYR
5	E	2	ASP
5	E	196	VAL
7	G	13	LEU
7	G	24	GLN
7	G	87	VAL
7	G	138	THR
8	H	76	THR
8	H	89	LEU
9	I	8	ARG
9	I	28	GLU
9	I	58	VAL
9	I	75	CYS
9	I	78	CYS
9	I	111	THR
10	J	43	ARG
10	J	46	CYS
10	J	48	ARG

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Mol	Chain	Res	Type
10	J	51	LEU
11	K	29	ASN
11	K	47	ARG
11	K	85	ASP
12	L	43	THR
12	L	60	ARG
12	L	61	THR
12	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	12	ASN

### 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 ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	1427/1733 (82%)	0.12	24 (1%) 70 61	78, 111, 134, 158	0
2	B	1125/1224 (91%)	0.08	28 (2%) 57 47	79, 107, 133, 155	0
3	C	267/318 (83%)	0.00	2 (0%) 87 82	87, 103, 117, 127	0
4	D	178/221 (80%)	0.14	4 (2%) 62 52	114, 120, 129, 135	0
5	E	214/215 (99%)	0.17	4 (1%) 66 58	93, 122, 143, 152	0
6	F	87/155 (56%)	-0.10	0 100 100	89, 97, 104, 106	0
7	G	171/171 (100%)	0.25	0 100 100	113, 116, 127, 137	0
8	H	136/146 (93%)	0.40	6 (4%) 34 28	107, 126, 142, 151	0
9	I	119/122 (97%)	0.24	6 (5%) 28 24	109, 126, 143, 152	0
10	J	66/70 (94%)	-0.17	1 (1%) 73 65	91, 104, 117, 123	0
11	K	115/120 (95%)	-0.01	1 (0%) 84 78	80, 93, 117, 125	0
12	L	47/70 (67%)	0.26	3 (6%) 19 14	88, 112, 121, 127	0
All	All	3952/4565 (86%)	0.11	79 (1%) 65 56	78, 112, 135, 158	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	505	ASP	5.3
9	I	119	THR	4.5
2	B	443	ASN	4.2
8	H	108	SER	4.0
2	B	716	ASN	3.8
2	B	919	SER	3.7
1	A	115	LEU	3.6
2	B	504	ARG	3.6
2	B	643	ASP	3.5
2	B	642	ASP	3.5
9	I	120	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
4	D	4	SER	3.5
9	I	76	PRO	3.2
2	B	444	MET	3.2
1	A	69	THR	3.2
1	A	116	ASP	3.1
2	B	882	THR	3.0
1	A	141	LEU	3.0
5	E	50	MET	2.9
2	B	503	GLY	2.9
1	A	44	THR	2.9
1	A	188	ASP	2.9
2	B	476	ARG	2.8
1	A	190	ALA	2.8
2	B	441	ASP	2.8
4	D	10	THR	2.8
4	D	35	LEU	2.8
1	A	1175	SER	2.7
12	L	50	ASP	2.7
2	B	475	SER	2.7
2	B	506	GLY	2.7
3	C	130	GLY	2.7
5	E	49	SER	2.7
1	A	114	LEU	2.6
2	B	132	VAL	2.6
2	B	715	ALA	2.6
1	A	191	THR	2.6
1	A	45	GLN	2.5
2	B	720	ASP	2.5
8	H	86	ASP	2.5
9	I	116	ASN	2.5
8	H	83	GLN	2.5
2	B	346	GLU	2.5
2	B	92	PHE	2.5
11	K	115	ALA	2.4
1	A	179	LEU	2.4
3	C	106	GLU	2.4
1	A	153	PRO	2.4
4	D	76	LYS	2.4
5	E	93	MET	2.4
5	E	40	GLU	2.4
1	A	49	LYS	2.4
1	A	151	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	591	ARG	2.3
2	B	325	GLN	2.3
1	A	104	GLU	2.3
1	A	159	THR	2.3
2	B	360	PHE	2.3
2	B	448	ILE	2.3
2	B	356	LEU	2.2
1	A	68	GLN	2.2
12	L	26	THR	2.2
1	A	195	ASP	2.2
10	J	29	GLU	2.2
8	H	107	VAL	2.1
8	H	50	ALA	2.1
9	I	117	LYS	2.1
1	A	155	GLU	2.1
1	A	105	CYS	2.1
1	A	1159	ARG	2.1
2	B	721	LEU	2.1
1	A	1287	TYR	2.1
12	L	25	ALA	2.1
2	B	439	ALA	2.1
1	A	46	THR	2.1
8	H	109	LYS	2.1
2	B	512	ARG	2.0
9	I	77	LYS	2.0
2	B	917	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	MG	A	1736	1/1	0.75	0.84	114,114,114,114	0
13	ZN	A	1735	1/1	0.88	0.14	114,114,114,114	0
13	ZN	I	123	1/1	0.92	0.09	114,114,114,114	0
13	ZN	J	71	1/1	0.94	0.14	114,114,114,114	0
13	ZN	I	124	1/1	0.94	0.05	114,114,114,114	0
13	ZN	L	71	1/1	0.97	0.08	114,114,114,114	0
13	ZN	A	1734	1/1	0.97	0.07	114,114,114,114	0
13	ZN	B	1225	1/1	0.99	0.17	114,114,114,114	0
13	ZN	C	319	1/1	0.99	0.12	114,114,114,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.