



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:40 PM UTC

PDB ID : 3FKI / pdb_00003fki
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

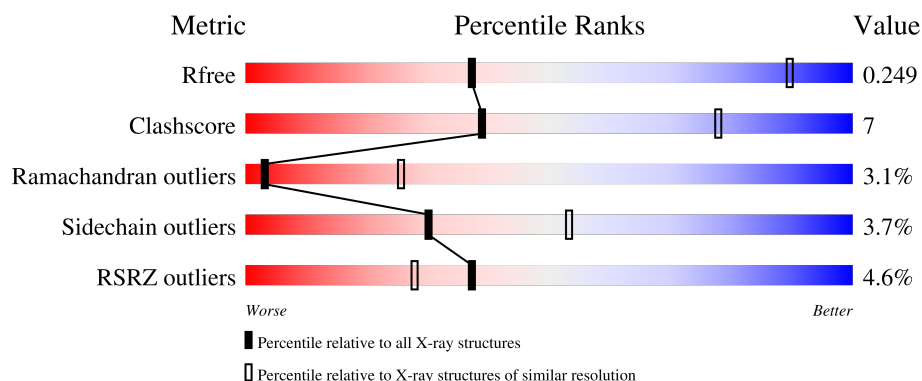
1 Overall quality at a glance

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}	180053	1186 (4.06-3.70)
Clashscore	190562	1012 (4.04-3.72)
Ramachandran outliers	187476	1167 (4.06-3.70)
Sidechain outliers	187428	1160 (4.06-3.70)
RSRZ outliers	180081	1185 (4.06-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	4% 65% 15% • 18%
2	B	1224	6% 72% 18% • 8%
3	C	318	• 64% 17% • 16%
4	D	221	3% 65% 13% • 19%
5	E	215	2% 88% 12%

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

2 Entry composition [i](#)

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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		

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

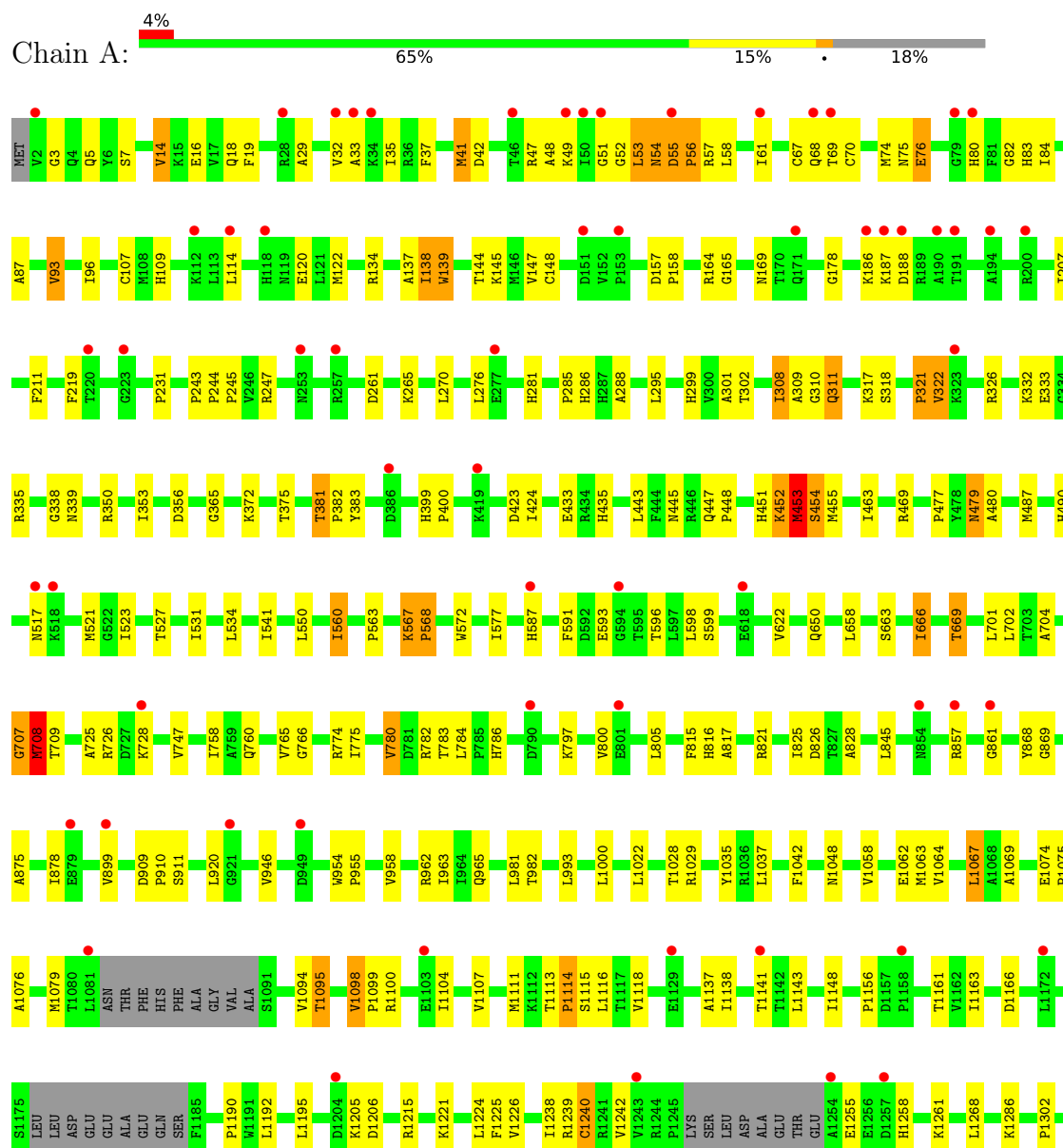
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

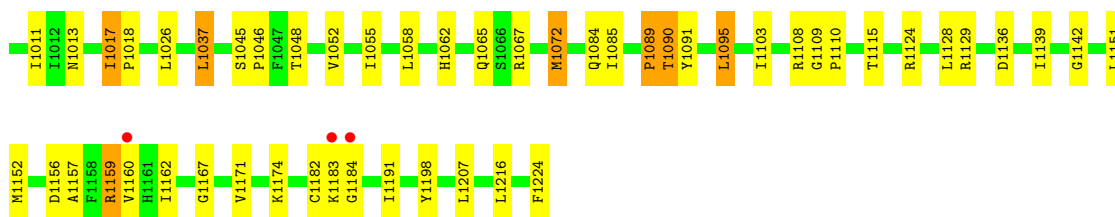
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

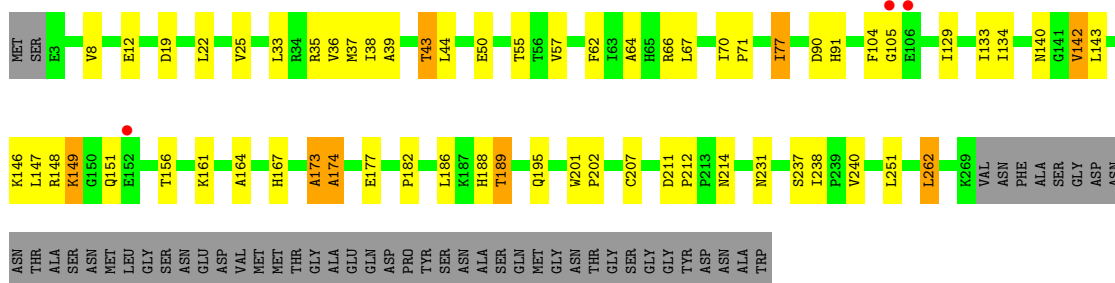
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

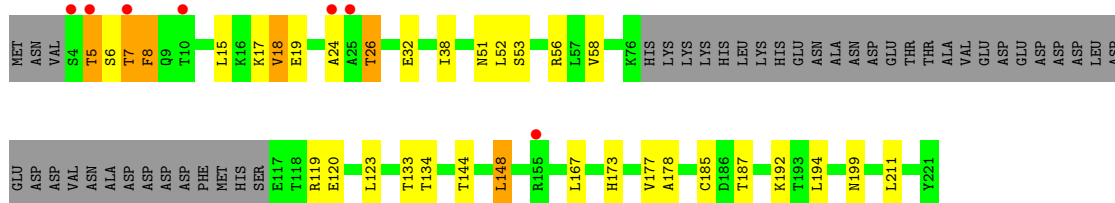




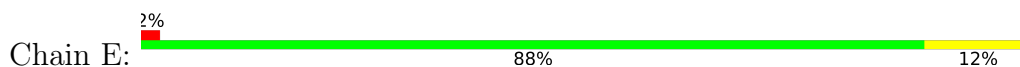
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



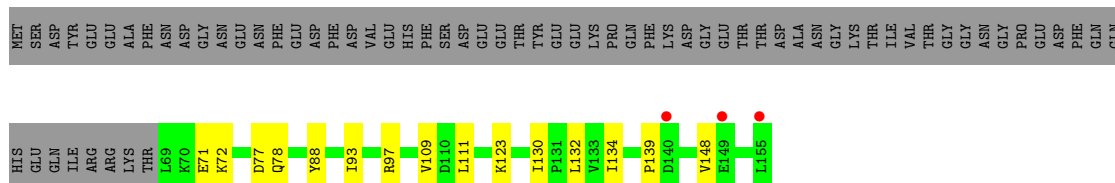
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



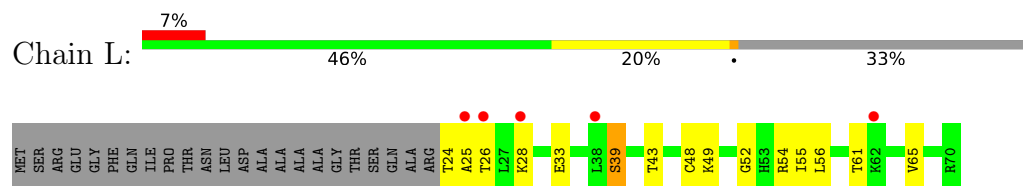
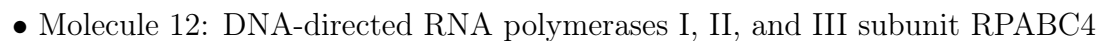
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.58Å 391.54Å 280.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.22 – 3.88 20.22 – 3.88	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.22-3.88) 94.8 (20.22-3.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5D	Depositor
R, R_{free}	0.282 , 0.301 (Not available) , 0.249	Depositor DCC
R_{free} test set	5355 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 10.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	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	0.86	EDS
Total number of atoms	31412	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/11426	0.79	1/15451 (0.0%)
2	B	0.41	0/9122	0.76	2/12300 (0.0%)
3	C	0.39	0/2142	0.75	0/2902
4	D	0.39	0/1446	0.80	2/1937 (0.1%)
5	E	0.40	0/1788	0.76	1/2406 (0.0%)
6	F	0.39	0/716	0.79	0/967
7	G	0.41	0/1368	0.73	0/1844
8	H	0.44	0/1107	0.71	0/1498
9	I	0.42	0/989	0.71	0/1331
10	J	0.38	0/549	0.78	0/738
11	K	0.38	0/942	0.78	1/1272 (0.1%)
12	L	0.47	0/373	0.75	0/495
All	All	0.41	0/31968	0.77	7/43141 (0.0%)

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.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	509	ALA	N-CA-C	-7.70	102.46	108.78
2	B	508	LEU	N-CA-C	5.98	118.14	107.80
1	A	244	PRO	N-CA-C	5.78	117.75	110.70
4	D	173	HIS	CA-C-N	5.66	125.13	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	173	HIS	C-N-CA	5.66	125.13	119.24
11	K	6	ARG	N-CA-C	5.66	118.22	111.71
5	E	127	ILE	N-CA-C	5.45	113.55	108.15

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	178	0
2	B	8947	0	8975	146	0
3	C	2104	0	2064	34	0
4	D	1436	0	1457	22	0
5	E	1752	0	1776	14	0
6	F	704	0	731	13	0
7	G	1340	0	1357	18	0
8	H	1089	0	1063	20	0
9	I	971	0	932	8	0
10	J	540	0	554	12	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	427	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 7.

All (427) 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
1:A:137:ALA:HA	1:A:138:ILE:C	1.89	0.96
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:453:MET:C	1:A:455:MET:H	2.03	0.65
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.78	0.65
1:A:75:ASN:O	1:A:76:GLU:HB3	1.95	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
1:A:54:ASN:O	1:A:55:ASP:HB2	1.97	0.63
1:A:821:ARG:HH21	2:B:534:GLY:HA2	1.64	0.63
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.62	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:372:LYS:HA	1:A:435:HIS:CD2	2.34	0.62
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.30	0.62
4:D:18:VAL:HG13	4:D:19:GLU:N	2.15	0.62
8:H:91:ASP:C	8:H:93:TYR:H	2.08	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:774:ARG:HG3	1:A:797:LYS:HD2	1.84	0.60
4:D:32:GLU:HG3	7:G:5:LYS:HZ2	1.66	0.60
8:H:82:PRO:C	8:H:84:ALA:H	2.09	0.59
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.85	0.59
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
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.86	0.58
2:B:494:HIS:HA	2:B:497:ARG:HE	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.87	0.57
3:C:104:PHE:HD2	3:C:105:GLY:H	1.51	0.57
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.87	0.57
1:A:1116:LEU:HB3	1:A:1329:THR:HG23	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
2:B:444:MET:CB	2:B:445:LYS:HA	2.17	0.56
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.88	0.56
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.70	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
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
2:B:713:ALA:O	2:B:714:GLU:HB2	2.05	0.55
4:D:18:VAL:HG13	4:D:19:GLU:H	1.71	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:350:ARG:HB2	2:B:1128:LEU:HD11	1.91	0.53
1:A:1143:LEU:HB3	1:A:1268:LEU:HA	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
3:C:33:LEU:HG	3:C:37:MET:HE2	1.90	0.52
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:33:ALA:HB2	1:A:82:GLY:CA	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.91	0.52
1:A:68:GLN:C	1:A:70:CYS:H	2.17	0.52
2:B:500:THR:O	2:B:501:PRO:C	2.53	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
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
1:A:1111:MET:HE2	1:A:1331:SER:HA	1.93	0.51
2:B:453:ILE:HD12	2:B:453:ILE:H	1.76	0.51
1:A:479:ASN:CA	1:A:480:ALA:HB3	2.41	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
8:H:40:LEU:HD13	8:H:123:MET:HE3	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
1:A:1094:VAL:O	1:A:1095:THR:C	2.55	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
10:J:47:ARG:C	10:J:49:MET:H	2.19	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:705:MET:HE2	2:B:745:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:453:MET:C	1:A:455:MET:N	2.72	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
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
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:49:LYS:HZ2	1:A:61:ILE:HG13	1.78	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
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	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
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: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
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:LEU:HD12	6:F:111:LEU:H	1.80	0.47
1:A:452:LYS:HD3	1:A:1067:LEU:HD21	1.96	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
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.97	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:663:SER:OG	2:B:1085:ILE:HA	2.15	0.47
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.46	0.47
1:A:1035:TYR:HB2	1:A:1037:LEU:HD12	1.97	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
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.98	0.46
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.79	0.46
2:B:1002:THR:HG22	2:B:1072:MET:HG3	1.98	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:7:SER:HB2	2:B:1159:ARG:HH21	1.80	0.46
1:A:1114:PRO:HB2	1:A:1115:SER:H	1.56	0.46
5:E:156:LEU:HD23	5:E:160:GLU:HB3	1.97	0.46
1:A:825:ILE:HD13	2:B:513:GLN:HB3	1.96	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.98	0.46
1:A:381:THR:C	1:A:383:TYR:H	2.24	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
2:B:789:MET:HE1	2:B:967:ARG:HB2	1.96	0.46
2:B:792:MET:HE2	2:B:857:ARG:HH12	1.80	0.46
1:A:527:THR:HG21	1:A:650:GLN:HA	1.98	0.46
1:A:1224:LEU:HD12	1:A:1242:VAL:HG22	1.97	0.46
2:B:542:MET:HE3	2:B:636:PRO:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.99	0.45
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.99	0.45
1:A:596:THR:C	1:A:598:LEU:H	2.24	0.45
2:B:1089:PRO:HB2	2:B:1090:THR:H	1.58	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.98	0.45
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.99	0.45
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.98	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
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
4:D:24:ALA:C	4:D:26:THR:H	2.26	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
1:A:780:VAL:C	1:A:782:ARG:H	2.25	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
10:J:8:PHE:H	10:J:49:MET:HE3	1.83	0.44
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:C	1:A:122:MET:H	2.25	0.44
1:A:445:ASN:HA	1:A:454:SER:O	2.18	0.44
8:H:97:MET:HE3	8:H:142:LEU:HD23	2.00	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:32:GLU:HG3	7:G:5:LYS:NZ	2.33	0.43
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.00	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:459:TYR:HE2	2:B:469:GLN:HA	1.84	0.43
2:B:806:THR:HG23	2:B:1045:SER:HA	2.01	0.43
1:A:817:ALA:O	1:A:821:ARG:HB2	2.18	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
7:G:83:LYS:HE3	7:G:150:CYS:H	1.83	0.43
8:H:82:PRO:C	8:H:84:ALA:N	2.77	0.43
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.01	0.43
1:A:1400:CYS:C	1:A:1402:PHE:H	2.27	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
2:B:466:TRP:O	2:B:467:GLY:C	2.62	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:42:GLY:O	2:B:44:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LYS:HA	2:B:281:PRO:HA	2.01	0.43
1:A:816:HIS:NE2	2:B:763:GLN:O	2.51	0.42
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
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:992:ILE:HD13	11:K:67:PHE:CE2	2.54	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:597:MET:HE1	2:B:615:MET:HB3	2.01	0.42
1:A:783:THR:HG21	1:A:815:PHE:HE1	1.84	0.42
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.20	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: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:1084:GLN:HG2	3:C:201:TRP:CZ2	2.53	0.42
1:A:909:ASP:C	1:A:911:SER:H	2.28	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
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:299:HIS:HA	1:A:302:THR:HG22	2.01	0.42
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.20	0.42
1:A:1431:GLY:HA3	2:B:1152:MET:HE2	2.01	0.42
2:B:473:MET:HA	2:B:474:SER:HA	1.61	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
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:VAL:HG21	2:B:318:VAL:HA	2.02	0.41
1:A:321:PRO:HB2	1:A:322:VAL:H	1.60	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
2:B:444:MET:H	2:B:445:LYS:CG	2.33	0.41
2:B:843:GLN:CG	11:K:6:ARG:NH2	2.82	0.41
3:C:22:LEU:HD11	11:K:101:LEU:HD11	2.02	0.41
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.02	0.41
1:A:1138:ILE:HG12	1:A:1319:VAL:HG21	2.02	0.41
2:B:246:LYS:HA	2:B:418:LYS:HZ1	1.85	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
2:B:1089:PRO:O	2:B:1090:THR:CB	2.67	0.41
3:C:36:VAL:HG21	3:C:251:LEU:HD13	2.03	0.41
1:A:114:LEU:HB3	1:A:145:LYS:HZ3	1.85	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: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:447:GLN:HA	1:A:448:PRO:C	2.45	0.41
1:A:946:VAL:HG22	5:E:201:LYS:HB3	2.03	0.41
1:A:1226:VAL:HG12	1:A:1240:CYS:HB3	2.03	0.41
2:B:44:VAL:O	2:B:45:SER:C	2.64	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:604:ARG:C	2:B:606:LYS:H	2.28	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:356:ASP:HB2	1:A:469:ARG:HH11	1.85	0.40
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.50	0.40
2:B:408:LEU:O	2:B:409:ALA:C	2.64	0.40
1:A:962:ARG:HA	1:A:965:GLN:HB2	2.02	0.40
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
2:B:468:GLU:H	2:B:471:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.96	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:725:ALA:HA	1:A:728:LYS:HE2	2.03	0.40
7:G:56:ILE:H	7:G:56:ILE:HG13	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%)	3	23
2	B	1111/1224 (91%)	957 (86%)	117 (10%)	37 (3%)	3	24
3	C	265/318 (83%)	236 (89%)	20 (8%)	9 (3%)	3	24
4	D	174/221 (79%)	148 (85%)	21 (12%)	5 (3%)	3	26
5	E	212/215 (99%)	193 (91%)	19 (9%)	0	100	100
6	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/171 (99%)	146 (86%)	21 (12%)	2 (1%)	10	41
8	H	132/146 (90%)	106 (80%)	19 (14%)	7 (5%)	1	17
9	I	117/122 (96%)	99 (85%)	15 (13%)	3 (3%)	4	28
10	J	64/70 (91%)	57 (89%)	4 (6%)	3 (5%)	2	19
11	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
12	L	45/70 (64%)	33 (73%)	7 (16%)	5 (11%)	0	6
All	All	3906/4565 (86%)	3390 (87%)	395 (10%)	121 (3%)	3	25

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	1199 (96%)	48 (4%)	29	52
2	B	976/1061 (92%)	940 (96%)	36 (4%)	30	53
3	C	235/274 (86%)	224 (95%)	11 (5%)	23	48
4	D	160/200 (80%)	151 (94%)	9 (6%)	19	45
5	E	196/197 (100%)	195 (100%)	1 (0%)	81	81
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	147 (97%)	5 (3%)	33	56
8	H	119/128 (93%)	116 (98%)	3 (2%)	42	62
9	I	113/116 (97%)	108 (96%)	5 (4%)	25	49
10	J	61/65 (94%)	57 (93%)	4 (7%)	15	41
11	K	99/102 (97%)	97 (98%)	2 (2%)	48	65
12	L	41/57 (72%)	37 (90%)	4 (10%)	7	28
All	All	3476/4009 (87%)	3348 (96%)	128 (4%)	30	53

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	32	VAL

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Mol	Chain	Res	Type
1	A	41	MET
1	A	42	ASP
1	A	53	LEU
1	A	80	HIS
1	A	83	HIS
1	A	93	VAL
1	A	96	ILE
1	A	169	ASN
1	A	186	LYS
1	A	261	ASP
1	A	265	LYS
1	A	281	HIS
1	A	295	LEU
1	A	308	ILE
1	A	322	VAL
1	A	381	THR
1	A	451	HIS
1	A	452	LYS
1	A	453	MET
1	A	463	ILE
1	A	517	ASN
1	A	541	ILE
1	A	560	ILE
1	A	587	HIS
1	A	666	ILE
1	A	669	THR
1	A	701	LEU
1	A	702	LEU
1	A	708	MET
1	A	709	THR
1	A	800	VAL
1	A	826	ASP
1	A	982	THR
1	A	1000	LEU
1	A	1067	LEU
1	A	1215	ARG
1	A	1240	CYS
1	A	1258	HIS
1	A	1261	LYS
1	A	1312	ASN
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	108	VAL
2	B	178	ASN
2	B	192	LEU
2	B	225	VAL
2	B	294	ASP
2	B	329	THR
2	B	365	THR
2	B	387	LEU
2	B	479	VAL
2	B	485	ARG
2	B	549	THR
2	B	570	VAL
2	B	603	LEU
2	B	604	ARG
2	B	618	ASP
2	B	646	LEU
2	B	731	VAL
2	B	743	ILE
2	B	773	MET
2	B	839	MET
2	B	956	THR
2	B	999	MET
2	B	1007	VAL
2	B	1037	LEU
2	B	1048	THR
2	B	1058	LEU
2	B	1072	MET
2	B	1095	LEU
2	B	1103	ILE
2	B	1115	THR
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1183	LYS
2	B	1191	ILE
3	C	25	VAL
3	C	43	THR

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Mol	Chain	Res	Type
3	C	55	THR
3	C	77	ILE
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	133	THR
4	D	134	THR
4	D	148	LEU
4	D	187	THR
4	D	192	LYS
5	E	196	VAL
7	G	13	LEU
7	G	49	LEU
7	G	56	ILE
7	G	87	VAL
7	G	138	THR
8	H	31	THR
8	H	76	THR
8	H	89	LEU
9	I	28	GLU
9	I	58	VAL
9	I	75	CYS
9	I	78	CYS
9	I	111	THR
10	J	27	GLU
10	J	46	CYS
10	J	48	ARG
10	J	51	LEU
11	K	29	ASN
11	K	47	ARG
12	L	43	THR
12	L	55	ILE
12	L	61	THR
12	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	394	ASN
1	A	576	GLN
1	A	611	GLN
1	A	736	ASN
1	A	994	GLN
1	A	1171	GLN
2	B	178	ASN
2	B	255	GLN
2	B	433	GLN
2	B	499	ASN
2	B	770	GLN
2	B	794	ASN
2	B	822	ASN
2	B	1093	GLN
3	C	65	HIS
3	C	131	HIS
3	C	135	GLN
4	D	41	GLN
4	D	51	ASN
4	D	150	ASN
5	E	63	ASN
7	G	53	ASN
7	G	102	GLN
8	H	134	ASN
9	I	90	GLN
12	L	53	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1427/1733 (82%)	0.51	65 (4%) 37 28	78, 111, 134, 158	0
2	B	1125/1224 (91%)	0.55	68 (6%) 27 23	79, 107, 133, 155	0
3	C	267/318 (83%)	0.27	3 (1%) 78 57	87, 103, 117, 127	0
4	D	178/221 (80%)	0.58	7 (3%) 43 31	114, 120, 129, 135	0
5	E	214/215 (99%)	0.44	4 (1%) 66 46	93, 122, 143, 152	0
6	F	87/155 (56%)	0.50	3 (3%) 48 33	89, 97, 104, 106	0
7	G	171/171 (100%)	0.60	5 (2%) 53 37	113, 116, 127, 137	0
8	H	136/146 (93%)	0.73	11 (8%) 18 18	107, 126, 142, 151	0
9	I	119/122 (97%)	0.81	6 (5%) 34 26	109, 126, 143, 152	0
10	J	66/70 (94%)	0.28	2 (3%) 52 36	91, 104, 117, 123	0
11	K	115/120 (95%)	0.14	2 (1%) 69 48	80, 93, 117, 125	0
12	L	47/70 (67%)	0.92	5 (10%) 11 14	88, 112, 121, 127	0
All	All	3952/4565 (86%)	0.51	181 (4%) 37 28	78, 112, 135, 158	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	6.2
1	A	34	LYS	6.1
1	A	79	GLY	5.9
1	A	171	GLN	5.5
2	B	470	LYS	5.2
1	A	68	GLN	4.9
4	D	10	THR	4.9
1	A	1081	LEU	4.7
2	B	708	GLU	4.4
2	B	71	LEU	4.3
1	A	187	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	723	VAL	4.2
9	I	76	PRO	4.1
1	A	49	LYS	4.1
1	A	188	ASP	4.1
4	D	4	SER	4.1
7	G	1	MET	3.9
2	B	246	LYS	3.9
8	H	132	LEU	3.8
2	B	164	LYS	3.8
1	A	153	PRO	3.8
1	A	69	THR	3.7
2	B	505	ASP	3.7
10	J	66	LEU	3.7
1	A	190	ALA	3.6
2	B	735	ALA	3.6
2	B	347	LYS	3.5
2	B	472	ALA	3.3
2	B	265	SER	3.3
1	A	857	ARG	3.3
11	K	115	ALA	3.3
1	A	50	ILE	3.3
2	B	710	LEU	3.3
4	D	24	ALA	3.3
2	B	934	LYS	3.3
2	B	443	ASN	3.2
1	A	618	GLU	3.2
2	B	513	GLN	3.2
1	A	2	VAL	3.2
9	I	119	THR	3.2
12	L	25	ALA	3.2
2	B	721	LEU	3.2
1	A	1204	ASP	3.1
8	H	130	ARG	3.1
2	B	577	ALA	3.1
2	B	511	PRO	3.1
7	G	94	CYS	3.1
2	B	715	ALA	3.0
6	F	155	LEU	3.0
2	B	709	ASP	3.0
1	A	112	LYS	3.0
2	B	440	HIS	3.0
1	A	151	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	729	ILE	2.9
4	D	5	THR	2.9
9	I	120	GLN	2.8
3	C	106	GLU	2.8
2	B	250	PHE	2.8
2	B	476	ARG	2.8
2	B	469	GLN	2.8
8	H	90	ALA	2.8
2	B	1183	LYS	2.8
12	L	26	THR	2.8
2	B	574	SER	2.7
1	A	277	GLU	2.7
1	A	801	GLU	2.7
1	A	518	LYS	2.7
1	A	51	GLY	2.7
8	H	84	ALA	2.7
2	B	134	LYS	2.7
2	B	883	LEU	2.7
1	A	46	THR	2.7
2	B	665	GLU	2.7
3	C	152	GLU	2.7
2	B	509	ALA	2.7
1	A	55	ASP	2.6
1	A	1257	ASP	2.6
2	B	248	SER	2.6
2	B	731	VAL	2.6
2	B	502	ILE	2.6
12	L	38	LEU	2.6
1	A	728	LYS	2.6
1	A	594	GLY	2.6
4	D	25	ALA	2.6
2	B	113	TYR	2.5
1	A	191	THR	2.5
9	I	34	TYR	2.5
2	B	326	ASP	2.5
2	B	251	ILE	2.5
10	J	29	GLU	2.5
5	E	83	CYS	2.5
4	D	155	ARG	2.5
1	A	879	GLU	2.5
8	H	108	SER	2.5
1	A	194	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	517	ASN	2.4
1	A	1378	GLN	2.4
1	A	921	GLY	2.4
1	A	790	ASP	2.4
1	A	419	LYS	2.4
2	B	475	SER	2.4
1	A	33	ALA	2.4
2	B	441	ASP	2.4
2	B	646	LEU	2.4
7	G	85	GLU	2.4
8	H	136	LYS	2.4
2	B	643	ASP	2.4
2	B	996	ARG	2.4
7	G	21	ARG	2.4
1	A	80	HIS	2.4
1	A	32	VAL	2.4
8	H	89	LEU	2.3
11	K	14	GLU	2.3
2	B	478	GLY	2.3
8	H	63	LEU	2.3
2	B	716	ASN	2.3
1	A	200	ARG	2.3
1	A	1129	GLU	2.3
1	A	61	ILE	2.3
2	B	669	ILE	2.3
6	F	140	ASP	2.3
2	B	503	GLY	2.3
1	A	587	HIS	2.3
9	I	27	PHE	2.3
2	B	919	SER	2.3
1	A	1141	THR	2.3
2	B	325	GLN	2.3
1	A	1243	VAL	2.3
2	B	436	VAL	2.3
2	B	360	PHE	2.2
2	B	266	ALA	2.2
1	A	1103	GLU	2.2
2	B	935	ARG	2.2
2	B	733	HIS	2.2
2	B	652	LYS	2.2
5	E	93	MET	2.2
1	A	223	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	442	PHE	2.2
2	B	668	ASP	2.2
1	A	1403	GLU	2.2
2	B	804	GLY	2.2
4	D	7	THR	2.2
1	A	854	ASN	2.2
1	A	118	HIS	2.2
2	B	1160	VAL	2.2
1	A	220	THR	2.2
1	A	323	LYS	2.2
2	B	507	LYS	2.2
1	A	114	LEU	2.2
2	B	880	THR	2.2
2	B	1006	ILE	2.1
2	B	1184	GLY	2.1
3	C	105	GLY	2.1
1	A	1172	LEU	2.1
2	B	473	MET	2.1
8	H	131	ASN	2.1
2	B	642	ASP	2.1
7	G	96	GLN	2.1
1	A	386	ASP	2.1
12	L	28	LYS	2.1
1	A	1386	ARG	2.1
1	A	186	LYS	2.1
1	A	861	GLY	2.1
1	A	1158	PRO	2.1
1	A	28	ARG	2.1
8	H	109	LYS	2.1
1	A	253	ASN	2.1
5	E	37	LEU	2.1
2	B	615	MET	2.1
1	A	949	ASP	2.0
2	B	70	ILE	2.0
1	A	1364	ASN	2.0
8	H	64	ASN	2.0
1	A	257	ARG	2.0
6	F	149	GLU	2.0
2	B	267	ARG	2.0
9	I	77	LYS	2.0
12	L	62	LYS	2.0
5	E	134	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1254	ALA	2.0
1	A	899	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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	0.67	0.28	114,114,114,114	0
13	ZN	A	1735	1/1	0.87	0.18	114,114,114,114	0
13	ZN	L	71	1/1	0.92	0.09	114,114,114,114	0
13	ZN	I	124	1/1	0.95	0.15	114,114,114,114	0
13	ZN	J	71	1/1	0.96	0.05	114,114,114,114	0
13	ZN	I	123	1/1	0.97	0.08	114,114,114,114	0
13	ZN	C	319	1/1	0.98	0.07	114,114,114,114	0
13	ZN	A	1734	1/1	0.98	0.03	114,114,114,114	0
13	ZN	B	1225	1/1	0.99	0.08	114,114,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.