



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:30 PM UTC

PDB ID : 6RIN / pdb_00006rin
EMDB ID : EMD-4892
Title : Cryo-EM structure of E. coli RNA polymerase backtracked elongation complex bound to GreB transcription factor
Authors : Abdelkareem, M.; Saint-Andre, C.; Takacs, M.; Papai, G.; Crucifix, C.; Guo, X.; Ortiz, J.; Weixlbaumer, A.
Deposited on : 2019-04-24
Resolution : 3.70 Å (reported)
Based on initial model : 6ALH

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

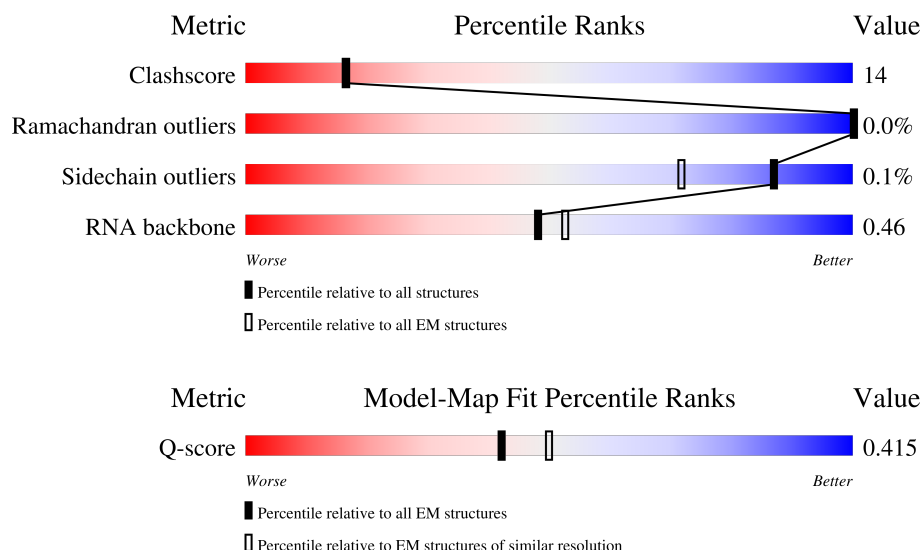
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.

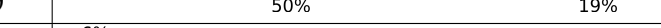


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	39	
2	T	39	
3	F	158	

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Mol	Chain	Length	Quality of chain
4	A	329	 6% 50% 19% 31%
4	B	329	 8% 50% 19% 30%
5	C	1342	 14% 69% 29% 1%
6	D	1407	 14% 64% 32% 4%
7	E	91	 7% 63% 18% 20%
8	R	14	 7% 43% 36% 14% 7%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 27584 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	19	Total	C	N	O	P	0	0
			392	186	72	115	19		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	27	Total	C	N	O	P	0	0
			550	261	102	160	27		

- Molecule 3 is a protein called Transcription elongation factor GreB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	156	Total	C	N	O	S	0	0
			1292	821	225	242	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	228	Total	C	N	O	S	0	0
			1768	1102	312	348	6		
4	B	229	Total	C	N	O	S	0	0
			1772	1104	313	349	6		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1319	Total	C	N	O	S	0	0
			10407	6530	1814	2020	43		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1358	Total	C	N	O	S	0	0
			10545	6620	1883	1992	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 8 is a RNA chain called RNA.

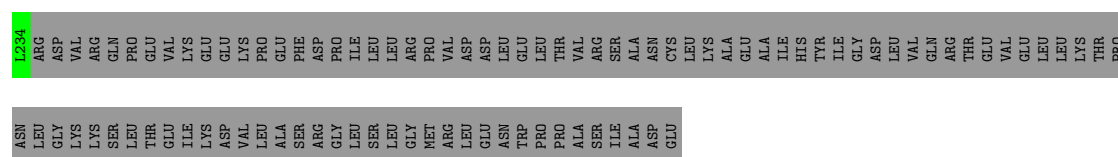
Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	13	Total	C	N	O	P	0	0
			273	123	46	92	12		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

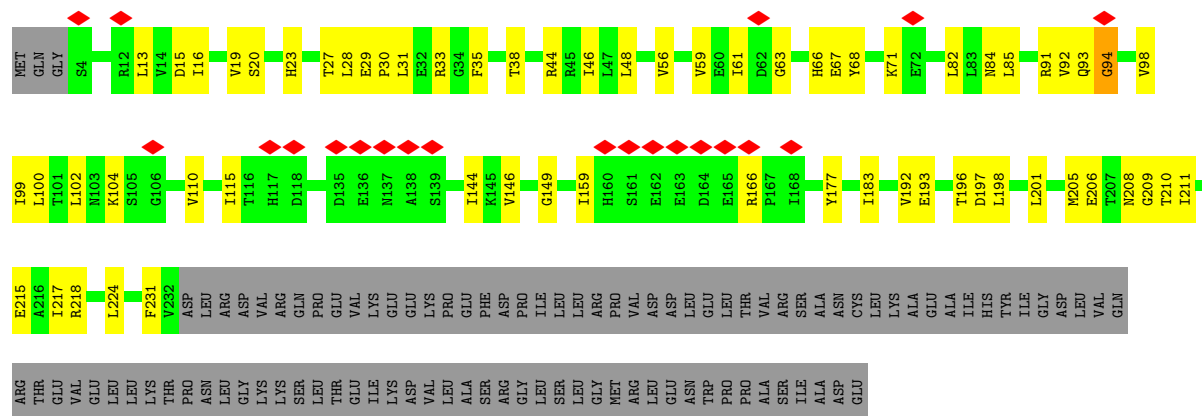
Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

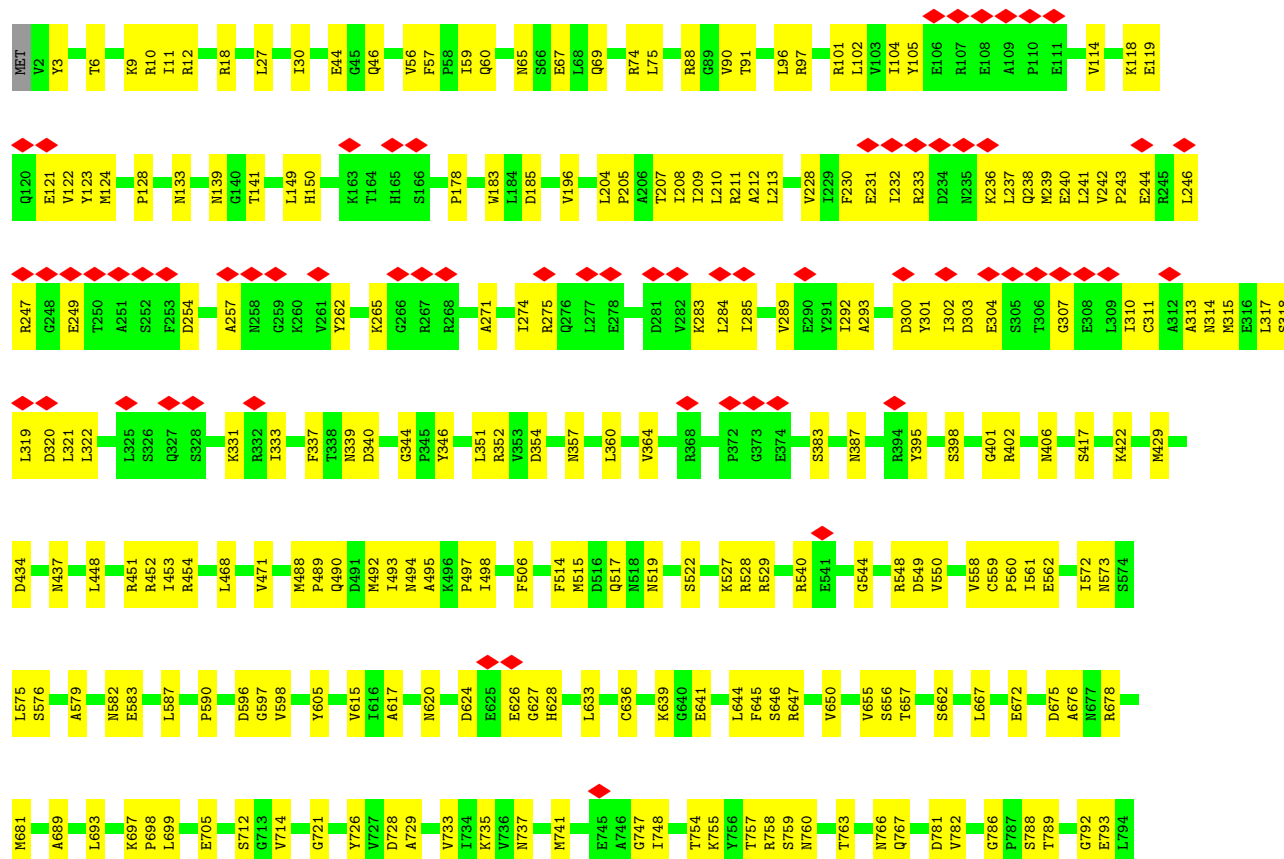
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

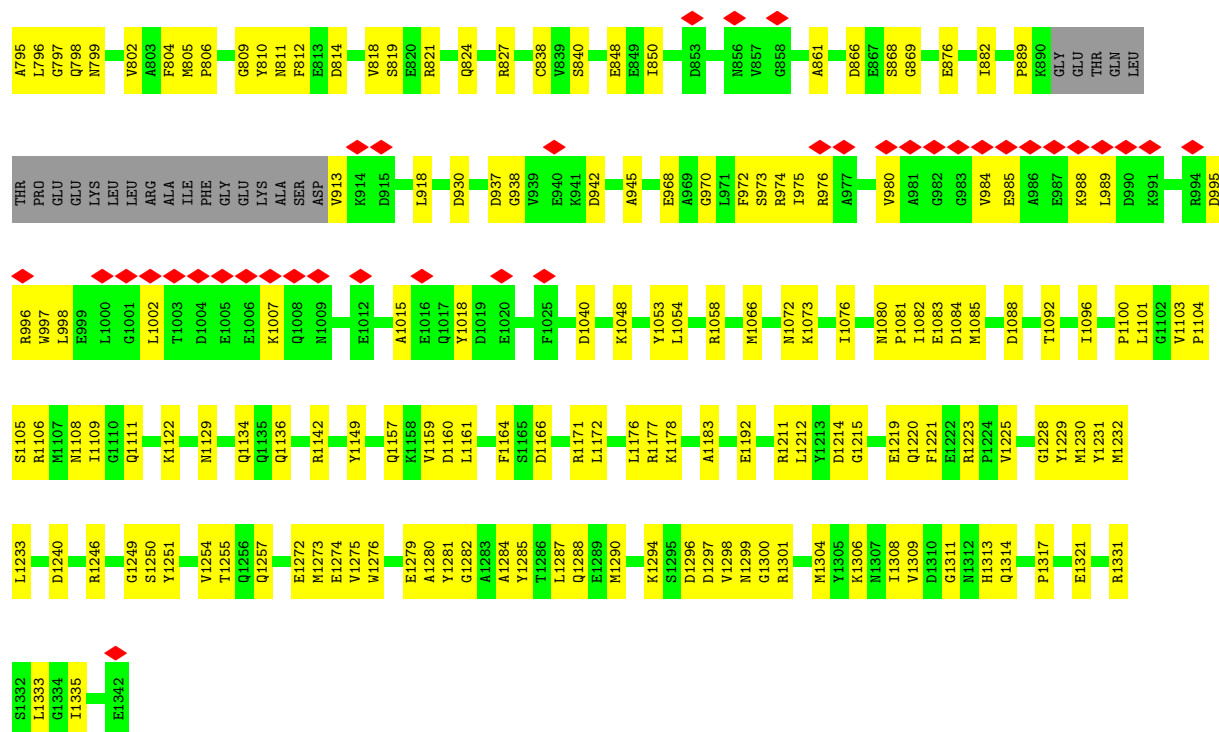


• Molecule 4: DNA-directed RNA polymerase subunit alpha

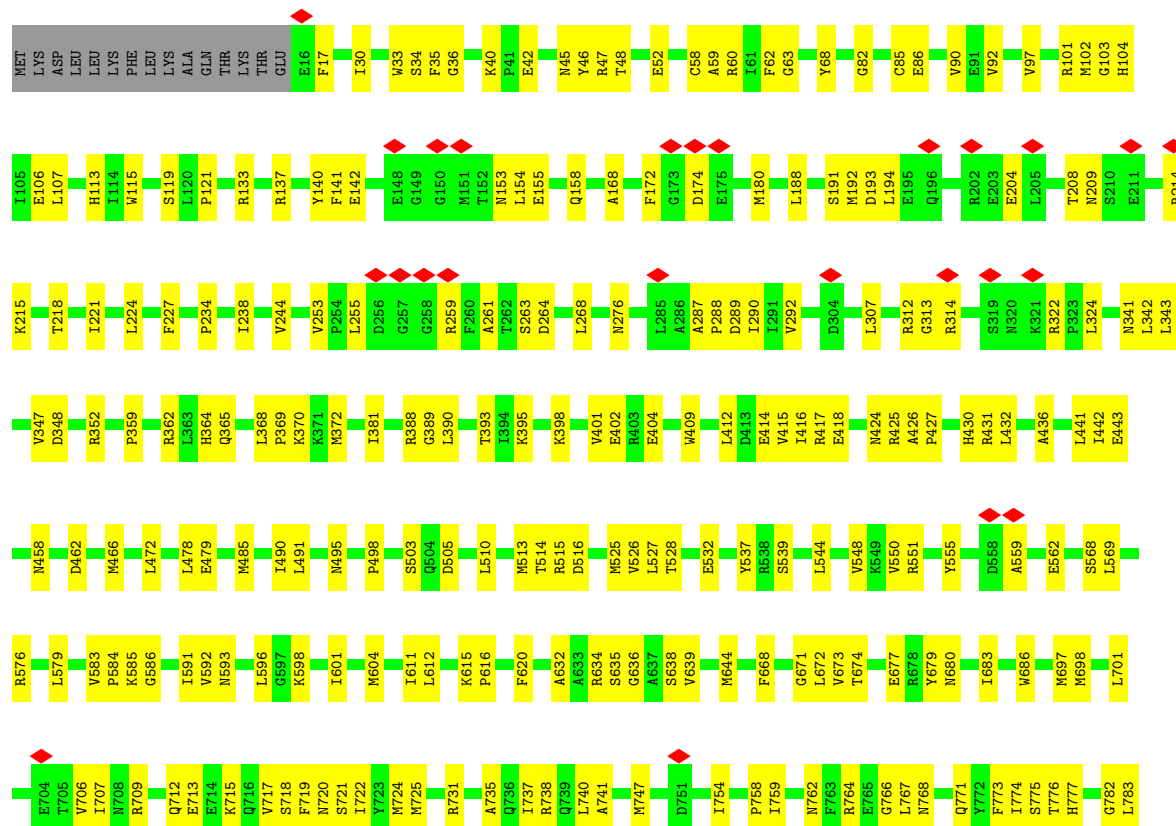


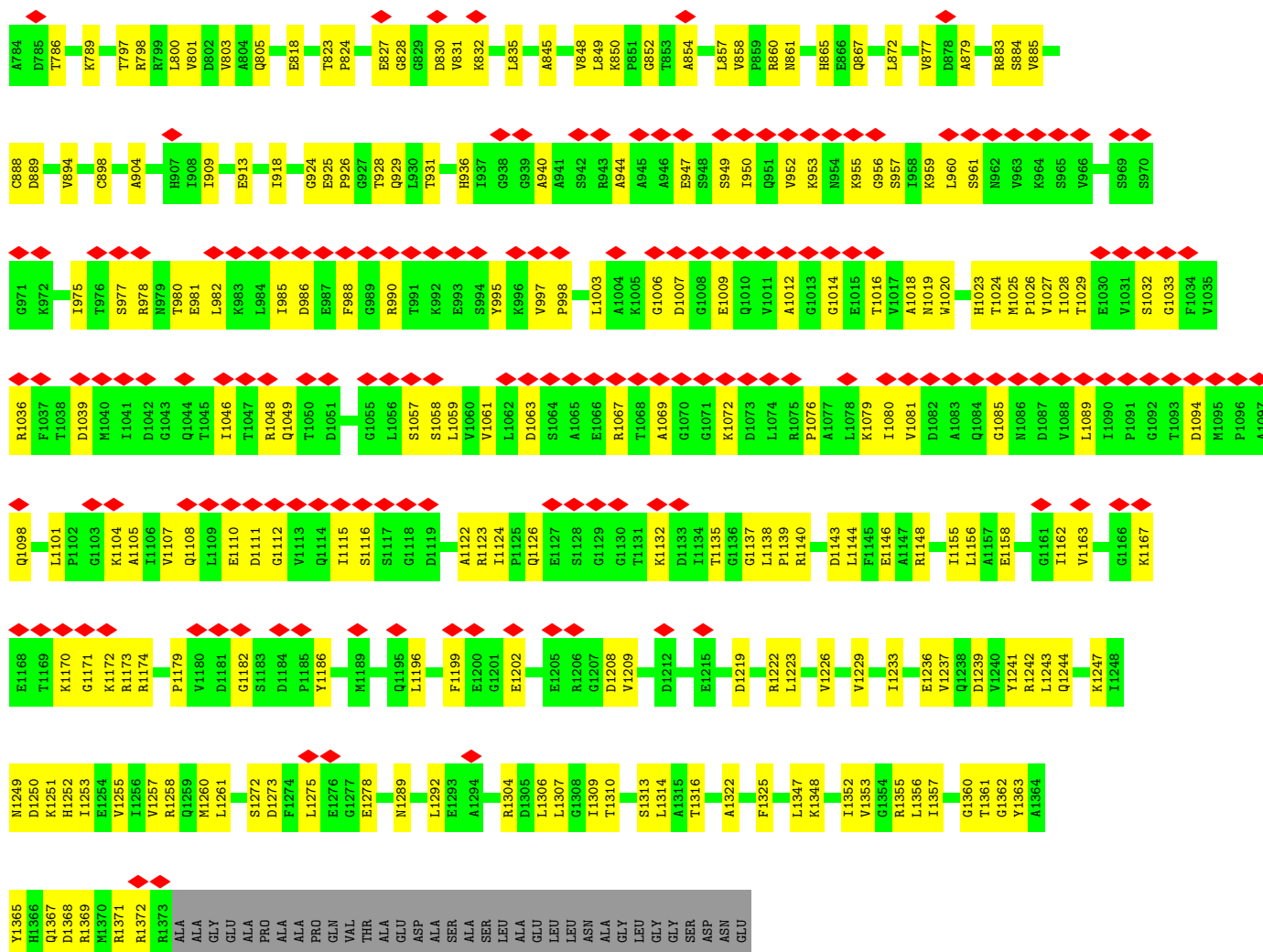
• Molecule 5: DNA-directed RNA polymerase subunit beta





• Molecule 6: DNA-directed RNA polymerase subunit beta'





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	574584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.136	Depositor
Minimum map value	-1.072	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	N	0.30	0/438	0.41	0/672
2	T	0.40	0/616	0.60	2/947 (0.2%)
3	F	0.27	0/1319	0.48	0/1780
4	A	0.47	1/1790 (0.1%)	0.60	0/2426
4	B	0.39	0/1794	0.61	0/2432
5	C	0.45	1/10573 (0.0%)	0.58	0/14265
6	D	0.41	0/10706	0.61	4/14456 (0.0%)
7	E	0.39	0/584	0.59	0/786
8	R	0.37	0/304	0.35	0/472
All	All	0.42	2/28124 (0.0%)	0.59	6/38236 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	178	SER	C-N	-6.78	1.28	1.33
5	C	448	LEU	CA-C	-5.55	1.45	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2	DC	OP2-P-O3'	-8.88	81.34	108.00
2	T	2	DC	OP1-P-O3'	-7.83	84.53	108.00
6	D	586	GLY	CA-C-N	-6.99	111.17	122.48
6	D	586	GLY	C-N-CA	-6.99	111.17	122.48
6	D	503	SER	CA-C-N	-6.92	108.42	121.63
6	D	503	SER	C-N-CA	-6.92	108.42	121.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	392	0	216	8	0
2	T	550	0	303	31	0
3	F	1292	0	1281	39	0
4	A	1768	0	1793	50	0
4	B	1772	0	1799	52	0
5	C	10407	0	10420	309	0
6	D	10545	0	10760	336	0
7	E	582	0	593	15	0
8	R	273	0	140	10	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	27584	0	27305	773	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 14.

All (773) 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)
6:D:961:SER:O	6:D:980:THR:HA	1.62	0.99
1:N:38:DG:N2	2:T:2:DC:O2	1.99	0.94
5:C:69:GLN:HE21	5:C:101:ARG:HD2	1.40	0.86
5:C:747:GLY:O	5:C:974:ARG:NH2	2.09	0.85
3:F:42:ARG:NH1	6:D:929:GLN:HE21	1.76	0.83
3:F:92:GLU:OE2	3:F:102:ARG:NH2	2.12	0.83
6:D:1076:PRO:HG2	6:D:1101:LEU:HB2	1.60	0.83
5:C:133:ASN:O	5:C:527:LYS:NZ	2.14	0.81
6:D:425:ARG:NH1	6:D:458:ASN:O	2.14	0.80
5:C:233:ARG:HD3	5:C:238:GLN:HB2	1.61	0.80
4:A:45:ARG:HD3	4:B:38:THR:HB	1.64	0.79
6:D:576:ARG:HD3	6:D:593:ASN:HA	1.63	0.79
6:D:1025:MET:HB3	6:D:1124:ILE:HD12	1.65	0.78
5:C:211:ARG:NH2	5:C:357:ASN:O	2.17	0.78
6:D:591:ILE:HG23	6:D:592:VAL:HG13	1.66	0.78
6:D:1036:ARG:HE	6:D:1081:VAL:HG11	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:741:MET:SD	5:C:974:ARG:NH1	2.58	0.77
5:C:9:LYS:HG2	5:C:1171:ARG:HH12	1.50	0.77
4:A:207:THR:HG22	4:A:209:GLY:H	1.48	0.77
6:D:936:HIS:HB3	6:D:1135:THR:HB	1.66	0.76
4:A:45:ARG:NH2	5:C:1084:ASP:OD1	2.19	0.76
6:D:1143:ASP:OD1	6:D:1148:ARG:NH1	2.19	0.75
4:B:23:HIS:ND1	4:B:206:GLU:OE2	2.18	0.75
4:B:205:MET:HE1	4:B:217:ILE:HG13	1.68	0.75
2:T:18:DT:H4'	6:D:352:ARG:HH22	1.52	0.74
5:C:1223:ARG:NH2	6:D:721:SER:OG	2.20	0.74
6:D:709:ARG:NH2	6:D:712:GLN:OE1	2.19	0.73
4:A:190:ALA:HB2	4:A:200:LYS:HB2	1.71	0.73
5:C:1142:ARG:NH2	5:C:1166:ASP:OD1	2.21	0.73
6:D:322:ARG:NH1	8:R:4:G:O3'	2.22	0.73
4:A:70:THR:HG21	5:C:755:LYS:HE2	1.69	0.73
2:T:13:DG:H2'	2:T:14:DC:C6	2.24	0.72
5:C:3:TYR:OH	5:C:1157:GLN:NE2	2.22	0.72
3:F:52:LYS:NZ	6:D:1244:GLN:OE1	2.23	0.72
4:A:228:LEU:HD21	4:B:224:LEU:HD23	1.71	0.72
5:C:1296:ASP:CG	5:C:1321:GLU:H	1.98	0.72
2:T:16:DC:H2'	2:T:17:DA:H8	1.54	0.71
5:C:232:ILE:HA	5:C:237:LEU:HG	1.72	0.71
5:C:590:PRO:HB2	5:C:655:VAL:HG21	1.70	0.71
4:B:93:GLN:HG3	4:B:94:GLY:H	1.56	0.71
4:B:15:ASP:OD1	4:B:16:ILE:N	2.24	0.71
5:C:1073:LYS:NZ	8:R:10:G:OP1	2.24	0.71
5:C:1072:ASN:ND2	5:C:1111:GLN:OE1	2.23	0.70
5:C:633:LEU:HD13	5:C:644:LEU:HD23	1.73	0.70
4:B:23:HIS:HA	4:B:206:GLU:HG2	1.72	0.70
6:D:789:LYS:NZ	8:R:13:U:O3'	2.24	0.70
5:C:402:ARG:NH2	5:C:417:SER:O	2.25	0.69
6:D:955:LYS:HG3	6:D:1012:ALA:HA	1.74	0.69
6:D:741:ALA:O	6:D:762:ASN:ND2	2.21	0.69
5:C:18:ARG:HE	5:C:620:ASN:HA	1.58	0.68
3:F:6:VAL:HG21	3:F:72:LEU:HD22	1.74	0.68
6:D:417:ARG:NH1	7:E:43:ASN:O	2.27	0.68
5:C:453:ILE:HD12	5:C:587:LEU:HD21	1.75	0.68
5:C:383:SER:O	5:C:387:ASN:ND2	2.26	0.68
6:D:959:LYS:NZ	6:D:960:LEU:O	2.26	0.68
6:D:1076:PRO:HB2	6:D:1101:LEU:HD12	1.75	0.68
4:A:58:GLU:OE1	4:A:170:ARG:NH2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1311:GLY:O	7:E:31:GLN:NE2	2.27	0.68
6:D:978:ARG:NH1	6:D:997:VAL:O	2.27	0.68
6:D:515:ARG:NH2	6:D:718:SER:O	2.26	0.68
5:C:10:ARG:NH1	5:C:697:LYS:HD3	2.08	0.67
5:C:101:ARG:HE	5:C:118:LYS:HD3	1.58	0.67
5:C:318:SER:OG	5:C:320:ASP:OD1	2.10	0.67
6:D:312:ARG:HG3	6:D:313:GLY:H	1.61	0.66
5:C:766:ASN:OD1	5:C:767:GLN:N	2.28	0.66
6:D:576:ARG:NH1	6:D:593:ASN:OD1	2.28	0.66
5:C:985:GLU:HB3	5:C:988:LYS:HB2	1.76	0.66
4:A:166:ARG:NH2	5:C:876:GLU:OE1	2.28	0.66
2:T:16:DC:H2'	2:T:17:DA:C8	2.31	0.66
4:A:135:ASP:OD1	4:A:136:GLU:N	2.28	0.66
5:C:814:ASP:OD2	5:C:1106:ARG:NH2	2.25	0.66
6:D:686:TRP:CD2	6:D:758:PRO:HG2	2.31	0.66
5:C:549:ASP:OD1	5:C:550:VAL:N	2.28	0.65
6:D:393:THR:HG23	6:D:395:LYS:H	1.61	0.65
6:D:883:ARG:NH2	6:D:898:CYS:SG	2.66	0.65
2:T:18:DT:H4'	6:D:352:ARG:HH12	1.62	0.65
4:B:44:ARG:HA	4:B:183:ILE:HD11	1.77	0.65
5:C:289:VAL:HA	5:C:292:ILE:HD12	1.79	0.65
5:C:302:ILE:HA	5:C:310:ILE:HD12	1.79	0.65
5:C:1314:GLN:HB2	7:E:28:ARG:HH12	1.61	0.65
5:C:244:GLU:OE2	5:C:247:ARG:NH2	2.29	0.64
6:D:514:THR:HG21	6:D:596:LEU:HD12	1.78	0.64
6:D:824:PRO:HD3	6:D:835:LEU:HD12	1.79	0.64
6:D:85:CYS:SG	6:D:86:GLU:N	2.70	0.64
6:D:425:ARG:HG2	6:D:426:ALA:H	1.62	0.64
6:D:527:LEU:HD13	6:D:548:VAL:HG11	1.80	0.64
5:C:65:ASN:O	5:C:105:TYR:N	2.21	0.64
5:C:1251:TYR:CZ	5:C:1301:ARG:NE	2.66	0.63
6:D:82:GLY:H	6:D:92:VAL:HG13	1.63	0.63
6:D:679:TYR:OH	6:D:754:ILE:O	2.12	0.63
4:A:23:HIS:HB2	4:A:205:MET:O	1.98	0.63
5:C:1255:THR:O	5:C:1257:GLN:N	2.30	0.63
6:D:140:TYR:OH	6:D:312:ARG:NE	2.31	0.63
6:D:632:ALA:O	6:D:635:SER:OG	2.13	0.63
6:D:1067:ARG:HD2	6:D:1072:LYS:HA	1.81	0.63
5:C:699:LEU:HG	5:C:799:ASN:HD22	1.63	0.63
6:D:59:ALA:HA	6:D:63:GLY:H	1.63	0.62
6:D:1239:ASP:OD1	6:D:1242:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:ARG:NH1	3:F:55:LEU:HD22	2.14	0.62
4:A:100:LEU:HD23	4:A:115:ILE:HG21	1.82	0.62
5:C:12:ARG:NH2	5:C:793:GLU:OE1	2.31	0.62
5:C:97:ARG:HB3	5:C:121:GLU:HB2	1.82	0.62
6:D:528:THR:N	6:D:532:GLU:OE2	2.28	0.62
6:D:888:CYS:SG	6:D:889:ASP:N	2.69	0.62
5:C:786:GLY:N	5:C:789:THR:OG1	2.31	0.62
5:C:689:ALA:HB2	5:C:1233:LEU:HD23	1.82	0.61
5:C:1088:ASP:OD1	5:C:1092:THR:N	2.33	0.61
5:C:1246:ARG:HH21	5:C:1249:GLY:H	1.48	0.61
6:D:527:LEU:HB2	6:D:550:VAL:HG12	1.81	0.61
5:C:11:ILE:HG23	5:C:1149:TYR:OH	2.00	0.61
6:D:155:GLU:HB2	6:D:158:GLN:HB2	1.82	0.61
2:T:13:DG:H2'	2:T:14:DC:H6	1.62	0.61
4:A:218:ARG:NH1	4:B:231:PHE:O	2.33	0.61
4:A:18:GLN:NE2	4:A:20:SER:O	2.29	0.61
6:D:1026:PRO:HB2	6:D:1028:ILE:HG23	1.82	0.61
6:D:1158:GLU:HG3	6:D:1186:TYR:CZ	2.35	0.61
5:C:398:SER:OG	5:C:401:GLY:N	2.25	0.61
5:C:320:ASP:OD1	5:C:321:LEU:N	2.34	0.60
6:D:113:HIS:HE1	6:D:115:TRP:HB2	1.66	0.60
6:D:141:PHE:HD1	6:D:180:MET:HE2	1.66	0.60
5:C:615:VAL:HG13	5:C:650:VAL:HA	1.83	0.60
5:C:210:LEU:HD11	5:C:429:MET:HE1	1.82	0.60
6:D:884:SER:OG	6:D:885:VAL:N	2.34	0.60
5:C:995:ASP:OD1	5:C:996:ARG:N	2.31	0.60
2:T:18:DT:H4'	6:D:352:ARG:NH2	2.16	0.60
3:F:68:CYS:O	3:F:72:LEU:HG	2.02	0.60
6:D:986:ASP:OD2	6:D:990:ARG:HG2	2.00	0.60
5:C:1219:GLU:OE2	6:D:634:ARG:NH2	2.35	0.60
4:A:75:GLN:HG3	4:A:76:GLU:HG3	1.83	0.59
6:D:638:SER:OG	6:D:639:VAL:N	2.32	0.59
3:F:95:ASN:OD1	3:F:96:ASP:N	2.35	0.59
2:T:11:DA:H5'	2:T:11:DA:H8	1.68	0.59
5:C:207:THR:HA	5:C:210:LEU:HD12	1.82	0.59
5:C:243:PRO:HB2	5:C:274:ILE:HG23	1.85	0.59
6:D:425:ARG:HG2	6:D:426:ALA:N	2.15	0.59
5:C:1296:ASP:OD2	5:C:1321:GLU:N	2.29	0.59
6:D:832:LYS:HD3	6:D:1242:ARG:HH12	1.68	0.59
6:D:978:ARG:HH12	6:D:998:PRO:HA	1.67	0.59
1:N:24:DA:H2'	5:C:183:TRP:CZ2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:838:CYS:HB2	5:C:918:LEU:HD22	1.84	0.59
5:C:1157:GLN:HG3	5:C:1159:VAL:HG13	1.83	0.59
6:D:783:LEU:O	6:D:786:THR:OG1	2.16	0.59
2:T:19:DC:H2'	2:T:20:DG:C8	2.38	0.59
5:C:300:ASP:OD1	5:C:313:ALA:N	2.36	0.59
5:C:866:ASP:OD1	5:C:869:GLY:N	2.19	0.59
6:D:528:THR:HG22	6:D:532:GLU:CD	2.28	0.59
4:B:91:ARG:NH2	4:B:210:THR:O	2.36	0.59
6:D:193:ASP:OD1	6:D:194:LEU:N	2.32	0.59
5:C:930:ASP:HB3	5:C:1053:TYR:HD2	1.68	0.58
2:T:20:DG:H2'	2:T:21:DC:H6	1.68	0.58
4:B:59:VAL:HG22	4:B:144:ILE:HG13	1.84	0.58
5:C:1313:HIS:CD2	7:E:31:GLN:HE22	2.20	0.58
6:D:515:ARG:HG2	6:D:516:ASP:H	1.68	0.58
5:C:1285:TYR:N	6:D:479:GLU:OE2	2.36	0.58
6:D:949:SER:HB3	6:D:1016:THR:HG23	1.85	0.58
2:T:20:DG:H2'	2:T:21:DC:C6	2.39	0.58
4:B:56:VAL:HG22	4:B:146:VAL:HG12	1.86	0.58
6:D:58:CYS:SG	6:D:60:ARG:HG2	2.42	0.58
6:D:827:GLU:HB2	6:D:832:LYS:HE2	1.84	0.58
3:F:42:ARG:NH2	6:D:928:THR:OG1	2.37	0.58
5:C:88:ARG:NE	5:C:1040:ASP:OD2	2.36	0.58
5:C:515:MET:HE3	5:C:517:GLN:HB2	1.86	0.58
5:C:1287:LEU:HD22	6:D:1357:ILE:HD11	1.85	0.58
6:D:1089:LEU:HD13	6:D:1094:ASP:HA	1.85	0.58
4:B:208:ASN:OD1	4:B:209:GLY:N	2.37	0.57
5:C:698:PRO:HG3	5:C:1231:TYR:CZ	2.39	0.57
3:F:47:ASP:OD1	3:F:51:ASN:ND2	2.36	0.57
2:T:19:DC:H2'	2:T:20:DG:H8	1.69	0.57
5:C:12:ARG:HH21	5:C:793:GLU:CD	2.12	0.57
5:C:1246:ARG:NH2	5:C:1250:SER:O	2.35	0.57
5:C:1296:ASP:OD1	5:C:1321:GLU:HB3	2.05	0.57
6:D:805:GLN:HE22	6:D:1348:LYS:HB2	1.69	0.57
5:C:559:CYS:SG	5:C:561:ILE:N	2.77	0.57
6:D:583:VAL:HA	6:D:620:PHE:CE1	2.40	0.57
6:D:644:MET:SD	6:D:740:LEU:HD23	2.44	0.57
6:D:909:ILE:HD11	6:D:913:GLU:HB3	1.86	0.57
3:F:117:TYR:O	3:F:118:ILE:HG13	2.05	0.57
5:C:231:GLU:O	5:C:237:LEU:C	2.48	0.57
5:C:728:ASP:OD1	5:C:729:ALA:N	2.37	0.57
6:D:584:PRO:HD3	6:D:620:PHE:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:850:LYS:C	6:D:852:GLY:H	2.13	0.56
5:C:398:SER:HG	5:C:401:GLY:H	1.53	0.56
6:D:982:LEU:HB3	6:D:995:TYR:HB2	1.87	0.56
4:B:19:VAL:HB	4:B:23:HIS:HB3	1.87	0.56
5:C:6:THR:OG1	5:C:781:ASP:OD1	2.21	0.56
5:C:624:ASP:O	5:C:626:GLU:N	2.37	0.56
5:C:806:PRO:HD3	5:C:1100:PRO:HG2	1.87	0.56
6:D:172:PHE:C	6:D:174:ASP:H	2.14	0.56
4:B:28:LEU:HD12	4:B:201:LEU:HD23	1.85	0.56
6:D:68:TYR:HA	6:D:92:VAL:HG23	1.86	0.56
2:T:21:DC:H2'	2:T:22:DC:H6	1.71	0.56
3:F:77:TYR:OH	3:F:81:GLN:N	2.38	0.56
4:A:91:ARG:NH1	4:A:210:THR:O	2.38	0.56
3:F:63:ARG:NH2	3:F:67:LYS:HZ1	2.04	0.56
3:F:84:LYS:HD3	3:F:130:LYS:HB2	1.87	0.56
5:C:254:ASP:HB2	5:C:265:LYS:HB2	1.86	0.56
2:T:10:DC:H2''	2:T:11:DA:C8	2.41	0.56
6:D:1208:ASP:OD1	6:D:1209:VAL:N	2.37	0.56
4:A:57:THR:HG22	4:A:58:GLU:HG3	1.87	0.56
5:C:1122:LYS:NZ	5:C:1229:TYR:OH	2.37	0.56
6:D:113:HIS:CE1	6:D:115:TRP:HB2	2.40	0.56
6:D:583:VAL:HA	6:D:620:PHE:HE1	1.70	0.56
5:C:232:ILE:HD12	5:C:331:LYS:HD3	1.87	0.56
6:D:848:VAL:HB	6:D:858:VAL:HG22	1.87	0.56
5:C:238:GLN:HB3	5:C:285:ILE:O	2.06	0.55
5:C:102:LEU:HD22	5:C:492:MET:HE1	1.88	0.55
5:C:1273:MET:HG2	5:C:1276:TRP:CZ3	2.41	0.55
7:E:25:ARG:HH21	7:E:68:GLU:CD	2.14	0.55
5:C:1254:VAL:HG13	5:C:1255:THR:H	1.72	0.55
3:F:35:TRP:HE1	6:D:598:LYS:HD3	1.71	0.55
5:C:582:ASN:OD1	5:C:583:GLU:N	2.39	0.55
5:C:1220:GLN:HG2	5:C:1221:PHE:O	2.06	0.55
5:C:797:GLY:N	5:C:1231:TYR:OH	2.35	0.55
6:D:956:GLY:HA3	6:D:985:ILE:O	2.06	0.55
4:B:98:VAL:HG22	4:B:99:ILE:H	1.72	0.55
5:C:1058:ARG:NE	5:C:1240:ASP:OD2	2.29	0.55
5:C:1080:ASN:HB2	5:C:1085:MET:HE3	1.89	0.55
5:C:1142:ARG:NH1	5:C:1161:LEU:O	2.40	0.55
4:A:82:LEU:HD11	4:A:171:LEU:HD23	1.89	0.54
5:C:1101:LEU:HD12	6:D:505:ASP:OD1	2.07	0.54
6:D:119:SER:OG	6:D:121:PRO:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:707:ILE:O	6:D:713:GLU:HA	2.07	0.54
6:D:978:ARG:NH1	6:D:998:PRO:HA	2.21	0.54
3:F:3:THR:HG22	3:F:5:LEU:H	1.73	0.54
5:C:351:LEU:HA	5:C:354:ASP:OD2	2.06	0.54
5:C:598:VAL:HA	5:C:627:GLY:HA3	1.88	0.54
6:D:774:ILE:HA	6:D:777:HIS:HD2	1.72	0.54
3:F:92:GLU:HB2	3:F:151:ASN:HB3	1.90	0.54
6:D:322:ARG:HH12	8:R:5:G:P	2.30	0.54
4:A:231:PHE:CZ	4:B:28:LEU:HD11	2.42	0.54
4:B:149:GLY:HA3	4:B:177:TYR:CZ	2.43	0.54
5:C:1129:ASN:OD1	5:C:1177:ARG:NH2	2.41	0.54
6:D:1069:ALA:HA	6:D:1072:LYS:HB2	1.89	0.54
6:D:1081:VAL:HB	6:D:1085:GLY:HA2	1.88	0.54
5:C:560:PRO:HB2	5:C:561:ILE:HG23	1.89	0.54
5:C:575:LEU:HD21	5:C:579:ALA:HB3	1.90	0.54
1:N:33:DT:H2"	1:N:34:DA:C8	2.43	0.54
5:C:1106:ARG:O	5:C:1108:ASN:N	2.40	0.54
5:C:178:PRO:HG3	5:C:395:TYR:CE1	2.43	0.54
5:C:759:SER:OG	5:C:763:THR:N	2.26	0.54
6:D:674:THR:N	6:D:677:GLU:OE1	2.38	0.54
6:D:986:ASP:OD2	6:D:988:PHE:HB2	2.08	0.54
6:D:1199:PHE:HB2	6:D:1202:GLU:HG2	1.90	0.54
3:F:42:ARG:NH1	6:D:929:GLN:NE2	2.53	0.54
5:C:726:TYR:HB3	5:C:733:VAL:HB	1.89	0.54
5:C:596:ASP:OD1	5:C:597:GLY:N	2.38	0.53
6:D:35:PHE:CE2	6:D:101:ARG:HG2	2.43	0.53
6:D:668:PHE:HD1	6:D:673:VAL:HG23	1.72	0.53
6:D:1063:ASP:OD2	6:D:1104:LYS:HE3	2.08	0.53
5:C:942:ASP:OD1	5:C:945:ALA:N	2.28	0.53
6:D:805:GLN:NE2	6:D:1348:LYS:HB2	2.22	0.53
4:A:55:ALA:O	4:A:146:VAL:HG13	2.09	0.53
5:C:672:GLU:N	5:C:672:GLU:OE1	2.41	0.53
5:C:11:ILE:O	5:C:1149:TYR:OH	2.27	0.53
5:C:104:ILE:O	5:C:114:VAL:N	2.39	0.53
6:D:209:ASN:HA	6:D:214:ARG:HH21	1.73	0.53
6:D:388:ARG:NH2	6:D:414:GLU:OE1	2.42	0.53
6:D:1137:GLY:O	6:D:1140:ARG:HB3	2.09	0.53
5:C:69:GLN:NE2	5:C:101:ARG:HD2	2.17	0.52
6:D:364:HIS:O	6:D:364:HIS:ND1	2.43	0.52
6:D:1140:ARG:HH21	6:D:1236:GLU:CD	2.16	0.52
5:C:204:LEU:HD13	5:C:208:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:319:LEU:HA	5:C:322:LEU:HD12	1.90	0.52
5:C:210:LEU:HD21	5:C:429:MET:SD	2.49	0.52
6:D:204:GLU:O	6:D:208:THR:HG23	2.09	0.52
5:C:866:ASP:CG	5:C:868:SER:H	2.18	0.52
5:C:976:ARG:HB2	5:C:997:TRP:HZ3	1.75	0.52
6:D:491:LEU:HB2	6:D:904:ALA:HA	1.90	0.52
2:T:18:DT:H4'	6:D:352:ARG:NH1	2.22	0.52
5:C:1282:GLY:HA3	7:E:17:PHE:CZ	2.44	0.52
6:D:1108:GLN:HE21	6:D:1123:ARG:HH22	1.58	0.52
4:A:52:PRO:HG2	4:A:219:ARG:NH1	2.25	0.52
5:C:1304:MET:HE2	6:D:472:LEU:HB3	1.92	0.52
3:F:111:ILE:HD12	3:F:111:ILE:O	2.10	0.52
4:B:66:HIS:CD2	4:B:68:TYR:H	2.27	0.52
5:C:60:GLN:HA	5:C:67:GLU:HG3	1.90	0.52
7:E:8:ASP:HB2	7:E:55:GLU:CD	2.34	0.52
5:C:802:VAL:HG12	5:C:1228:GLY:O	2.10	0.52
6:D:352:ARG:HG3	6:D:466:MET:O	2.09	0.52
6:D:362:ARG:H	6:D:365:GLN:HE21	1.56	0.52
6:D:513:MET:HE1	6:D:579:LEU:HD13	1.90	0.52
6:D:818:GLU:OE1	6:D:818:GLU:N	2.43	0.52
5:C:562:GLU:OE1	5:C:662:SER:OG	2.24	0.52
6:D:45:ASN:ND2	6:D:48:THR:H	2.08	0.52
6:D:1173:ARG:NH2	6:D:1196:LEU:HD21	2.25	0.52
6:D:1363:TYR:OH	6:D:1367:GLN:NE2	2.43	0.52
4:B:99:ILE:C	4:B:100:LEU:HD12	2.35	0.51
5:C:128:PRO:HG2	5:C:506:PHE:CD2	2.46	0.51
6:D:789:LYS:HZ3	6:D:931:THR:HA	1.76	0.51
6:D:1289:ASN:HA	6:D:1292:LEU:HD12	1.91	0.51
5:C:1297:ASP:CG	5:C:1300:GLY:H	2.19	0.51
6:D:42:GLU:HB2	6:D:52:GLU:HG2	1.91	0.51
4:B:33:ARG:HH11	5:C:1081:PRO:HG3	1.74	0.51
4:A:102:LEU:HD12	4:A:115:ILE:HG12	1.93	0.51
5:C:1083:GLU:CD	5:C:1083:GLU:H	2.17	0.51
4:A:102:LEU:HD22	4:A:142:MET:HG2	1.93	0.51
6:D:342:LEU:HD23	6:D:1352:ILE:HG23	1.93	0.51
5:C:626:GLU:HB2	5:C:628:HIS:HD2	1.75	0.51
5:C:810:TYR:CE1	6:D:359:PRO:HD2	2.45	0.51
4:B:15:ASP:HB3	4:B:27:THR:OG1	2.11	0.51
6:D:97:VAL:HG11	6:D:101:ARG:HE	1.76	0.51
6:D:774:ILE:O	6:D:777:HIS:HB2	2.11	0.51
6:D:1023:HIS:C	6:D:1126:GLN:HB3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1222:ARG:HG3	6:D:1223:LEU:HG	1.92	0.51
5:C:231:GLU:O	5:C:237:LEU:CA	2.59	0.51
5:C:540:ARG:O	5:C:548:ARG:NH2	2.43	0.51
5:C:1272:GLU:OE2	6:D:798:ARG:NH1	2.44	0.51
6:D:709:ARG:NH1	6:D:712:GLN:H	2.09	0.51
6:D:1067:ARG:NH1	6:D:1072:LYS:O	2.44	0.51
5:C:804:PHE:HZ	5:C:1230:MET:HE1	1.76	0.50
6:D:218:THR:HA	6:D:221:ILE:HG22	1.92	0.50
6:D:706:VAL:HG12	6:D:715:LYS:HB3	1.92	0.50
6:D:782:GLY:O	6:D:786:THR:HG23	2.11	0.50
5:C:301:TYR:H	5:C:311:CYS:HG	1.56	0.50
5:C:818:VAL:HG21	5:C:1066:MET:HE1	1.92	0.50
5:C:1279:GLU:CD	6:D:1347:LEU:HD23	2.36	0.50
2:T:16:DC:H4'	5:C:1273:MET:HE2	1.94	0.50
4:A:28:LEU:HD22	4:A:201:LEU:HD23	1.92	0.50
5:C:1214:ASP:OD1	5:C:1215:GLY:N	2.45	0.50
6:D:1249:ASN:HD21	6:D:1251:LYS:NZ	2.10	0.50
6:D:1322:ALA:O	6:D:1325:PHE:N	2.43	0.50
2:T:11:DA:H5'	2:T:11:DA:C8	2.45	0.50
5:C:236:LYS:HE2	5:C:289:VAL:HB	1.93	0.50
5:C:840:SER:HA	5:C:848:GLU:OE1	2.12	0.50
6:D:747:MET:HE2	6:D:775:SER:HA	1.93	0.50
4:B:19:VAL:HG12	4:B:20:SER:H	1.77	0.50
5:C:656:SER:OG	5:C:657:THR:N	2.44	0.50
7:E:46:THR:HA	7:E:49:ILE:HD12	1.92	0.50
6:D:106:GLU:O	6:D:276:ASN:ND2	2.32	0.50
6:D:1249:ASN:OD1	6:D:1250:ASP:N	2.45	0.50
6:D:1368:ASP:OD1	6:D:1371:ARG:NH2	2.45	0.50
3:F:56:ARG:HH22	8:R:13:U:H2'	1.77	0.50
7:E:58:LEU:HD12	7:E:59:ILE:HG12	1.93	0.50
5:C:840:SER:HB3	5:C:1048:LYS:H	1.77	0.50
5:C:1282:GLY:HA3	7:E:17:PHE:HZ	1.77	0.50
6:D:709:ARG:NH1	6:D:713:GLU:H	2.09	0.50
2:T:7:DA:H2''	2:T:8:DG:H8	1.76	0.50
5:C:1284:ALA:N	6:D:479:GLU:OE2	2.42	0.50
6:D:1029:THR:HG21	6:D:1115:ILE:HD13	1.94	0.50
6:D:1272:SER:OG	6:D:1273:ASP:N	2.43	0.50
5:C:128:PRO:HG2	5:C:506:PHE:HD2	1.77	0.49
5:C:972:PHE:HD1	5:C:975:ILE:HD12	1.76	0.49
5:C:1176:LEU:O	5:C:1178:LYS:N	2.45	0.49
6:D:491:LEU:HD23	6:D:498:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1275:LEU:N	6:D:1278:GLU:OE1	2.41	0.49
4:B:92:VAL:HG12	4:B:93:GLN:O	2.13	0.49
5:C:149:LEU:HD21	5:C:451:ARG:HD3	1.94	0.49
6:D:1179:PRO:HB2	6:D:1182:GLY:H	1.76	0.49
6:D:1249:ASN:HD21	6:D:1251:LYS:HZ2	1.59	0.49
3:F:68:CYS:O	3:F:71:ASN:N	2.45	0.49
4:A:28:LEU:HB2	4:A:201:LEU:HB3	1.94	0.49
5:C:633:LEU:HA	5:C:645:PHE:O	2.12	0.49
5:C:788:SER:HB3	5:C:795:ALA:O	2.13	0.49
6:D:559:ALA:HB3	6:D:562:GLU:HB3	1.95	0.49
5:C:1082:ILE:H	5:C:1082:ILE:HD12	1.78	0.49
5:C:1274:GLU:N	5:C:1274:GLU:OE1	2.44	0.49
6:D:1029:THR:OG1	6:D:1116:SER:O	2.31	0.49
6:D:1049:GLN:O	6:D:1057:SER:HB2	2.12	0.49
6:D:1252:HIS:O	6:D:1255:VAL:HG12	2.13	0.49
4:B:102:LEU:HD13	4:B:115:ILE:HG12	1.95	0.49
3:F:45:ASN:OD1	3:F:46:ALA:N	2.46	0.49
4:A:66:HIS:CE1	4:A:68:TYR:HB2	2.48	0.49
5:C:850:ILE:HG13	5:C:1048:LYS:HD2	1.95	0.49
6:D:188:LEU:O	6:D:191:SER:OG	2.29	0.49
6:D:722:ILE:HA	6:D:725:MET:HE3	1.93	0.49
4:A:66:HIS:HE1	4:A:68:TYR:HB2	1.77	0.49
3:F:63:ARG:NH1	3:F:67:LYS:HZ2	2.11	0.48
5:C:257:ALA:HB3	5:C:262:TYR:HE2	1.78	0.48
5:C:810:TYR:CD1	6:D:359:PRO:HD2	2.47	0.48
5:C:1103:VAL:HG22	5:C:1111:GLN:HE21	1.78	0.48
5:C:1298:VAL:HG13	5:C:1299:ASN:H	1.78	0.48
6:D:789:LYS:NZ	6:D:931:THR:HA	2.27	0.48
4:A:152:TYR:CD1	5:C:824:GLN:HG2	2.48	0.48
6:D:1173:ARG:HG2	6:D:1174:ARG:H	1.78	0.48
6:D:1357:ILE:O	6:D:1362:GLY:HA3	2.13	0.48
6:D:312:ARG:CG	6:D:313:GLY:H	2.26	0.48
6:D:950:ILE:HG13	6:D:1020:TRP:HH2	1.79	0.48
6:D:1356:LEU:HD12	6:D:1365:TYR:CD2	2.48	0.48
3:F:103:PHE:CD1	3:F:118:ILE:HD12	2.48	0.48
3:F:108:TYR:OH	6:D:680:ASN:ND2	2.47	0.48
4:A:170:ARG:C	4:A:171:LEU:HD12	2.39	0.48
5:C:980:VAL:O	5:C:984:VAL:HB	2.13	0.48
6:D:525:MET:O	6:D:548:VAL:HG13	2.14	0.48
6:D:526:VAL:C	6:D:527:LEU:HD12	2.38	0.48
5:C:119:GLU:HB2	5:C:489:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:LYS:NZ	3:F:108:TYR:CG	2.82	0.48
5:C:231:GLU:O	5:C:237:LEU:HA	2.14	0.48
5:C:519:ASN:O	5:C:522:SER:N	2.47	0.48
6:D:555:TYR:HE2	6:D:585:LYS:HD2	1.79	0.48
2:T:21:DC:H2'	2:T:22:DC:C6	2.47	0.48
3:F:87:PHE:CE1	3:F:120:ILE:HD11	2.48	0.48
2:T:18:DT:H2'	2:T:19:DC:C6	2.48	0.48
5:C:303:ASP:H	5:C:307:GLY:HA2	1.78	0.48
5:C:239:MET:HE2	5:C:241:LEU:HB2	1.96	0.48
5:C:315:MET:HA	5:C:352:ARG:HH22	1.79	0.48
6:D:426:ALA:HB3	6:D:427:PRO:HD3	1.96	0.48
5:C:590:PRO:HG3	5:C:605:TYR:CE1	2.49	0.47
6:D:495:ASN:HD22	6:D:1247:LYS:HB2	1.78	0.47
5:C:178:PRO:HG3	5:C:395:TYR:HE1	1.77	0.47
5:C:230:PHE:HB2	5:C:333:ILE:HB	1.96	0.47
5:C:712:SER:O	5:C:714:VAL:N	2.42	0.47
5:C:1192:GLU:OE1	6:D:764:ARG:NH2	2.47	0.47
6:D:255:LEU:HD11	6:D:259:ARG:HB2	1.94	0.47
6:D:701:LEU:HD22	6:D:720:ASN:HD22	1.78	0.47
5:C:242:VAL:HG12	5:C:244:GLU:H	1.78	0.47
5:C:1250:SER:OG	5:C:1251:TYR:N	2.47	0.47
6:D:555:TYR:CE2	6:D:585:LYS:HD2	2.49	0.47
5:C:819:SER:HB3	5:C:1085:MET:HG3	1.96	0.47
5:C:968:GLU:HG3	5:C:1018:TYR:HE1	1.79	0.47
6:D:568:SER:OG	6:D:569:LEU:N	2.48	0.47
5:C:149:LEU:HD12	5:C:452:ARG:O	2.14	0.47
5:C:705:GLU:OE1	5:C:705:GLU:N	2.47	0.47
6:D:611:ILE:HG22	6:D:612:LEU:HD12	1.97	0.47
3:F:44:GLU:HG2	5:C:678:ARG:HH22	1.78	0.47
4:A:183:ILE:HD13	4:A:205:MET:HA	1.96	0.47
4:B:23:HIS:HD1	4:B:206:GLU:CD	2.20	0.47
6:D:263:SER:OG	6:D:264:ASP:N	2.47	0.47
4:A:79:LEU:HD21	5:C:693:LEU:HD21	1.96	0.47
4:A:182:ARG:HB3	4:A:206:GLU:HB3	1.97	0.47
5:C:213:LEU:HD13	5:C:422:LYS:HG2	1.97	0.47
5:C:303:ASP:OD1	5:C:304:GLU:N	2.44	0.47
5:C:514:PHE:CE2	5:C:760:ASN:HB3	2.50	0.47
5:C:1275:VAL:HG13	5:C:1287:LEU:HD11	1.97	0.47
4:B:35:PHE:HA	4:B:38:THR:HG22	1.97	0.47
5:C:1331:ARG:HG3	6:D:33:TRP:CH2	2.49	0.47
6:D:424:ASN:OD1	6:D:425:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:510:LEU:HD22	6:D:601:ILE:HD12	1.95	0.47
6:D:1314:LEU:O	6:D:1316:THR:N	2.48	0.47
5:C:139:ASN:C	5:C:141:THR:H	2.23	0.46
6:D:398:LYS:HA	6:D:401:VAL:HG22	1.97	0.46
2:T:12:DT:H2''	2:T:13:DG:H8	1.80	0.46
2:T:22:DC:H2''	2:T:23:DT:H5'	1.96	0.46
5:C:1276:TRP:CZ2	6:D:801:VAL:HG21	2.50	0.46
6:D:478:LEU:HD23	6:D:478:LEU:HA	1.71	0.46
6:D:615:LYS:HB2	6:D:616:PRO:HD3	1.97	0.46
6:D:830:ASP:OD1	6:D:831:VAL:N	2.48	0.46
5:C:1254:VAL:HG13	5:C:1255:THR:N	2.30	0.46
6:D:34:SER:OG	6:D:103:GLY:HA2	2.16	0.46
2:T:22:DC:H2'	2:T:23:DT:H71	1.97	0.46
4:A:19:VAL:HG11	4:A:23:HIS:NE2	2.31	0.46
5:C:302:ILE:HB	5:C:307:GLY:HA2	1.98	0.46
6:D:370:LYS:HD3	6:D:409:TRP:CZ3	2.51	0.46
2:T:10:DC:H2''	2:T:11:DA:H8	1.78	0.46
5:C:754:THR:N	5:C:767:GLN:OE1	2.43	0.46
5:C:798:GLN:OE1	5:C:827:ARG:HB2	2.16	0.46
5:C:1288:GLN:NE2	5:C:1317:PRO:HB3	2.30	0.46
6:D:805:GLN:OE1	6:D:1348:LYS:HB2	2.15	0.46
5:C:10:ARG:NH2	5:C:793:GLU:OE1	2.49	0.46
5:C:759:SER:HG	5:C:763:THR:H	1.54	0.46
6:D:1006:GLY:N	6:D:1009:GLU:OE1	2.48	0.46
1:N:30:DG:H2''	1:N:31:DG:H8	1.80	0.46
5:C:639:LYS:O	5:C:641:GLU:HG2	2.14	0.46
6:D:153:ASN:HB3	6:D:154:LEU:HD12	1.97	0.46
6:D:686:TRP:CG	6:D:758:PRO:HG2	2.51	0.46
6:D:805:GLN:OE1	6:D:1348:LYS:HE2	2.16	0.46
5:C:205:PRO:O	5:C:208:ILE:HG22	2.16	0.46
5:C:230:PHE:CE1	5:C:239:MET:HB2	2.50	0.46
5:C:233:ARG:NH1	5:C:284:LEU:HB3	2.30	0.46
5:C:675:ASP:CG	5:C:676:ALA:N	2.73	0.46
5:C:805:MET:HE1	5:C:1221:PHE:CZ	2.51	0.46
5:C:1081:PRO:HB2	5:C:1083:GLU:OE1	2.16	0.46
6:D:1306:LEU:C	6:D:1307:LEU:HD12	2.40	0.46
1:N:13:DT:H2''	1:N:14:DT:H5'	1.98	0.46
4:A:105:SER:HB3	4:A:139:SER:HB2	1.98	0.46
4:A:135:ASP:CG	4:A:137:ASN:H	2.24	0.46
6:D:952:VAL:HG13	6:D:1014:GLY:H	1.81	0.46
6:D:1018:ALA:HB1	6:D:1020:TRP:HZ3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1309:ILE:HG13	6:D:1310:THR:N	2.32	0.46
4:B:84:ASN:ND2	6:D:551:ARG:HH22	2.14	0.45
5:C:646:SER:OG	5:C:647:ARG:N	2.48	0.45
5:C:675:ASP:CG	5:C:676:ALA:H	2.24	0.45
6:D:800:LEU:O	6:D:803:VAL:HG12	2.16	0.45
6:D:1162:ILE:HG13	6:D:1163:VAL:H	1.80	0.45
8:R:6:C:H2'	8:R:7:G:C8	2.51	0.45
6:D:472:LEU:HD23	6:D:472:LEU:HA	1.60	0.45
5:C:237:LEU:HD23	5:C:333:ILE:HD11	1.98	0.45
6:D:537:TYR:CE1	6:D:544:LEU:HD13	2.52	0.45
4:A:52:PRO:O	4:A:179:PRO:HG3	2.16	0.45
6:D:683:ILE:HD11	6:D:754:ILE:HD13	1.97	0.45
6:D:940:ALA:N	6:D:1132:LYS:NZ	2.65	0.45
6:D:1111:ASP:OD1	6:D:1112:GLY:N	2.50	0.45
4:A:164:ASP:OD1	4:A:165:GLU:N	2.50	0.45
5:C:314:ASN:ND2	5:C:351:LEU:HB2	2.32	0.45
5:C:488:MET:HB2	5:C:490:GLN:HE22	1.81	0.45
8:R:7:G:H2'	8:R:8:A:H8	1.82	0.45
5:C:56:VAL:HG13	5:C:57:PHE:H	1.81	0.45
5:C:1251:TYR:OH	5:C:1301:ARG:NE	2.49	0.45
6:D:1033:GLY:HA3	6:D:1080:ILE:HG23	1.97	0.45
4:A:52:PRO:HG2	4:A:219:ARG:HH11	1.81	0.45
5:C:228:VAL:HG23	5:C:337:PHE:HB2	1.98	0.45
5:C:1103:VAL:HB	5:C:1104:PRO:HD3	1.99	0.45
6:D:417:ARG:HH12	7:E:43:ASN:HB2	1.82	0.45
6:D:611:ILE:C	6:D:612:LEU:HD12	2.41	0.45
6:D:766:GLY:C	6:D:767:LEU:HD12	2.41	0.45
6:D:828:GLY:HA2	6:D:953:LYS:HG2	1.98	0.45
6:D:1039:ASP:O	6:D:1076:PRO:HA	2.16	0.45
4:A:70:THR:CG2	5:C:755:LYS:HE2	2.43	0.45
5:C:976:ARG:HB2	5:C:997:TRP:CZ3	2.51	0.45
5:C:1285:TYR:HE2	6:D:1361:THR:HG21	1.81	0.45
6:D:36:GLY:O	6:D:104:HIS:ND1	2.49	0.45
6:D:845:ALA:HA	6:D:883:ARG:HG3	1.98	0.45
1:N:14:DT:H2''	1:N:15:DC:C5	2.52	0.45
5:C:56:VAL:HG13	5:C:57:PHE:N	2.32	0.45
5:C:468:LEU:HA	5:C:471:VAL:HG12	1.99	0.45
5:C:678:ARG:NH1	5:C:681:MET:SD	2.90	0.45
6:D:368:LEU:HA	6:D:369:PRO:HD3	1.78	0.45
3:F:141:THR:OG1	3:F:144:GLY:O	2.32	0.45
4:A:181:GLU:OE1	5:C:821:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1211:ARG:C	5:C:1212:LEU:HD12	2.42	0.45
6:D:341:ASN:C	6:D:342:LEU:HD12	2.43	0.45
6:D:513:MET:HE3	6:D:579:LEU:HB2	1.99	0.45
5:C:1134:GLN:O	5:C:1136:GLN:HG2	2.17	0.44
6:D:823:THR:HG22	6:D:879:ALA:HB2	2.00	0.44
6:D:961:SER:HB2	6:D:981:GLU:HB3	1.98	0.44
6:D:1061:VAL:HB	6:D:1105:ALA:H	1.80	0.44
6:D:1170:LYS:HD2	6:D:1174:ARG:HH21	1.82	0.44
5:C:339:ASN:OD1	5:C:340:ASP:N	2.44	0.44
6:D:402:GLU:O	6:D:404:GLU:HG3	2.17	0.44
6:D:680:ASN:HA	6:D:683:ILE:HG22	1.98	0.44
5:C:11:ILE:HG22	5:C:1172:LEU:HD11	1.98	0.44
5:C:27:LEU:O	5:C:528:ARG:NH1	2.48	0.44
5:C:30:ILE:HD12	5:C:30:ILE:H	1.82	0.44
5:C:697:LYS:HG3	5:C:697:LYS:O	2.18	0.44
5:C:796:LEU:N	5:C:1231:TYR:OH	2.41	0.44
5:C:1002:LEU:HD21	5:C:1007:LYS:HB2	1.98	0.44
4:B:196:THR:HG23	6:D:443:GLU:HG3	1.98	0.44
5:C:12:ARG:HD3	5:C:1183:ALA:HB2	1.99	0.44
5:C:558:VAL:HG13	5:C:573:ASN:HB3	1.98	0.44
5:C:624:ASP:C	5:C:626:GLU:H	2.24	0.44
5:C:1212:LEU:HD13	5:C:1225:VAL:HG22	1.99	0.44
6:D:290:ILE:HD12	6:D:290:ILE:H	1.83	0.44
6:D:312:ARG:HG3	6:D:313:GLY:N	2.29	0.44
6:D:555:TYR:HB2	6:D:585:LYS:O	2.17	0.44
6:D:718:SER:OG	6:D:719:PHE:N	2.51	0.44
6:D:1058:SER:OG	6:D:1108:GLN:NE2	2.50	0.44
5:C:617:ALA:HA	5:C:636:CYS:SG	2.58	0.44
5:C:818:VAL:HG22	5:C:1096:ILE:HG12	2.00	0.44
5:C:1314:GLN:HG3	7:E:28:ARG:HH22	1.82	0.44
6:D:1079:LYS:HB2	6:D:1098:GLN:HB3	1.99	0.44
5:C:67:GLU:O	5:C:102:LEU:HD12	2.18	0.44
5:C:998:LEU:CD2	5:C:1015:ALA:HB2	2.48	0.44
5:C:1053:TYR:C	5:C:1054:LEU:HD12	2.43	0.44
5:C:1274:GLU:HG2	6:D:424:ASN:ND2	2.33	0.44
6:D:592:VAL:HG12	6:D:604:MET:HE2	1.98	0.44
6:D:697:MET:HE1	6:D:737:ILE:HG12	2.00	0.44
2:T:7:DA:H2"	2:T:8:DG:C8	2.53	0.44
3:F:2:LYS:NZ	3:F:108:TYR:CD2	2.86	0.44
4:B:59:VAL:HG21	4:B:85:LEU:HD13	1.99	0.44
4:B:61:ILE:HG22	4:B:63:GLY:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:699:LEU:HA	5:C:699:LEU:HD23	1.73	0.44
5:C:721:GLY:O	5:C:737:ASN:ND2	2.50	0.44
6:D:40:LYS:HB3	6:D:42:GLU:OE1	2.17	0.44
6:D:1355:ARG:HH11	6:D:1369:ARG:HH12	1.64	0.44
4:B:100:LEU:HB2	4:B:144:ILE:CG2	2.48	0.44
5:C:185:ASP:O	5:C:196:VAL:HG23	2.18	0.44
5:C:575:LEU:HD23	5:C:576:SER:O	2.18	0.44
5:C:1223:ARG:NH1	6:D:724:MET:HE1	2.32	0.44
8:R:4:G:H2'	8:R:5:G:C8	2.53	0.44
5:C:271:ALA:O	5:C:275:ARG:HG3	2.18	0.44
5:C:293:ALA:HA	5:C:317:LEU:HB2	2.00	0.44
5:C:861:ALA:HB1	5:C:882:ILE:HD13	2.00	0.44
6:D:133:ARG:O	6:D:137:ARG:HG3	2.18	0.44
6:D:1167:LYS:HB3	6:D:1174:ARG:HD2	2.00	0.44
4:B:183:ILE:HG22	4:B:205:MET:HG3	2.00	0.43
5:C:1111:GLN:HB2	5:C:1230:MET:HE2	2.00	0.43
6:D:417:ARG:HG2	6:D:418:GLU:HG2	2.00	0.43
6:D:701:LEU:HD23	6:D:701:LEU:HA	1.81	0.43
6:D:1241:TYR:O	6:D:1244:GLN:N	2.48	0.43
4:B:30:PRO:C	4:B:31:LEU:HD12	2.43	0.43
6:D:97:VAL:HG12	6:D:101:ARG:HG3	2.00	0.43
6:D:381:ILE:HD11	6:D:412:LEU:HD12	2.00	0.43
6:D:944:ALA:HA	6:D:947:GLU:HG2	2.00	0.43
6:D:1369:ARG:O	6:D:1372:ARG:HB2	2.18	0.43
4:B:61:ILE:HG21	4:B:71:LYS:HE3	2.00	0.43
6:D:416:ILE:HD13	6:D:416:ILE:HA	1.81	0.43
6:D:1261:LEU:CD1	6:D:1304:ARG:HH21	2.30	0.43
3:F:87:PHE:CD1	3:F:120:ILE:HD11	2.52	0.43
4:A:57:THR:O	4:A:173:VAL:HG22	2.18	0.43
5:C:74:ARG:HH21	5:C:121:GLU:CD	2.25	0.43
5:C:544:GLY:O	5:C:548:ARG:NH1	2.52	0.43
5:C:1161:LEU:HG	5:C:1164:PHE:CD2	2.53	0.43
6:D:62:PHE:O	6:D:101:ARG:HD2	2.19	0.43
6:D:107:LEU:HD23	6:D:276:ASN:ND2	2.33	0.43
3:F:92:GLU:OE2	3:F:102:ARG:CZ	2.64	0.43
5:C:74:ARG:HG2	5:C:75:LEU:O	2.18	0.43
5:C:149:LEU:HA	5:C:452:ARG:O	2.19	0.43
5:C:490:GLN:N	5:C:490:GLN:OE1	2.51	0.43
5:C:498:ILE:HD12	5:C:498:ILE:H	1.83	0.43
5:C:1101:LEU:HD23	5:C:1101:LEU:HA	1.73	0.43
6:D:957:SER:HB3	6:D:985:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1138:LEU:HB3	6:D:1139:PRO:HD3	1.99	0.43
7:E:30:MET:SD	7:E:37:PRO:HB3	2.59	0.43
4:A:29:GLU:HA	4:A:30:PRO:HA	1.75	0.43
4:B:19:VAL:HG12	4:B:20:SER:N	2.33	0.43
5:C:976:ARG:HG3	5:C:989:LEU:HD21	2.00	0.43
6:D:85:CYS:HB3	6:D:90:VAL:H	1.84	0.43
6:D:137:ARG:HG2	6:D:142:GLU:OE2	2.18	0.43
6:D:1024:THR:HG23	6:D:1124:ILE:H	1.83	0.43
4:A:231:PHE:HZ	4:B:28:LEU:HD11	1.84	0.43
5:C:434:ASP:HA	5:C:437:ASN:HD22	1.83	0.43
5:C:889:PRO:HA	5:C:913:VAL:HG23	1.99	0.43
4:B:46:ILE:HD11	4:B:224:LEU:HD13	2.00	0.43
5:C:246:LEU:HA	5:C:249:GLU:OE1	2.19	0.43
5:C:798:GLN:HE22	5:C:827:ARG:HB2	1.84	0.43
5:C:970:GLY:O	5:C:973:SER:OG	2.27	0.43
6:D:227:PHE:CE2	6:D:234:PRO:HG3	2.54	0.43
6:D:362:ARG:O	6:D:365:GLN:HG2	2.18	0.43
3:F:44:GLU:OE2	6:D:462:ASP:OD2	2.36	0.43
4:A:102:LEU:O	4:A:141:SER:HA	2.19	0.43
5:C:620:ASN:HD21	6:D:768:ASN:CB	2.32	0.43
6:D:287:ALA:HB1	6:D:288:PRO:HD2	2.00	0.43
4:B:149:GLY:HA3	4:B:177:TYR:CE2	2.54	0.43
5:C:97:ARG:NH1	5:C:123:TYR:HB2	2.34	0.43
5:C:1285:TYR:CE2	6:D:1361:THR:HG21	2.54	0.43
6:D:215:LYS:O	6:D:218:THR:HG22	2.19	0.43
6:D:735:ALA:O	6:D:738:ARG:HB3	2.19	0.43
5:C:529:ARG:HH11	5:C:572:ILE:HG22	1.83	0.42
6:D:805:GLN:CD	6:D:1348:LYS:HB2	2.44	0.42
1:N:29:DT:H4'	6:D:1148:ARG:HH21	1.84	0.42
6:D:773:PHE:O	6:D:776:THR:HB	2.19	0.42
6:D:1289:ASN:HA	6:D:1292:LEU:HB2	2.02	0.42
8:R:4:G:H2'	8:R:5:G:H8	1.83	0.42
3:F:77:TYR:OH	3:F:80:GLN:HB3	2.19	0.42
5:C:1274:GLU:HG2	6:D:424:ASN:HD21	1.84	0.42
6:D:168:ALA:O	6:D:172:PHE:N	2.36	0.42
6:D:430:HIS:O	6:D:432:LEU:N	2.53	0.42
6:D:1146:GLU:HG2	6:D:1148:ARG:CZ	2.48	0.42
4:B:33:ARG:NH1	5:C:1081:PRO:HG3	2.35	0.42
4:B:215:GLU:HA	4:B:218:ARG:HD2	2.01	0.42
5:C:96:LEU:HB3	5:C:124:MET:O	2.20	0.42
5:C:402:ARG:HD2	5:C:406:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:494:ASN:O	5:C:497:PRO:HD2	2.19	0.42
5:C:975:ILE:HD13	5:C:998:LEU:HD11	2.02	0.42
5:C:1280:ALA:HB1	6:D:918:ILE:HG22	2.02	0.42
5:C:1306:LYS:O	5:C:1309:VAL:HG22	2.19	0.42
6:D:347:VAL:HG12	6:D:348:ASP:O	2.19	0.42
6:D:1027:VAL:HB	6:D:1122:ALA:H	1.85	0.42
7:E:54:ILE:HD13	7:E:59:ILE:HB	2.01	0.42
2:T:13:DG:C6	2:T:14:DC:N4	2.88	0.42
2:T:16:DC:C2	2:T:17:DA:C8	3.07	0.42
5:C:209:ILE:HA	5:C:212:ALA:HB3	2.01	0.42
5:C:1331:ARG:HG2	6:D:102:MET:HE1	2.01	0.42
6:D:192:MET:HG2	6:D:193:ASP:O	2.19	0.42
6:D:372:MET:HE2	6:D:372:MET:HB3	1.95	0.42
6:D:894:VAL:HG22	6:D:1258:ARG:NH1	2.35	0.42
6:D:1032:SER:HA	6:D:1115:ILE:HD12	2.02	0.42
6:D:1171:GLY:C	6:D:1172:LYS:HD2	2.43	0.42
6:D:1313:SER:O	6:D:1316:THR:OG1	2.34	0.42
4:B:48:LEU:HD21	6:D:539:SER:HB3	2.01	0.42
5:C:735:LYS:HA	5:C:748:ILE:HG22	2.02	0.42
6:D:436:ALA:HB3	6:D:485:MET:HA	2.01	0.42
6:D:1144:LEU:HD23	6:D:1144:LEU:HA	1.65	0.42
4:A:32:GLU:HB2	4:A:35:PHE:CD2	2.55	0.42
5:C:150:HIS:CE1	5:C:454:ARG:NE	2.88	0.42
5:C:1105:SER:OG	6:D:731:ARG:NH2	2.53	0.42
5:C:1282:GLY:O	6:D:1360:GLY:HA3	2.19	0.42
5:C:1308:ILE:HD13	5:C:1308:ILE:HA	1.93	0.42
6:D:45:ASN:O	6:D:46:TYR:HB2	2.20	0.42
6:D:268:LEU:HD21	6:D:324:LEU:HD11	2.01	0.42
5:C:59:ILE:O	5:C:67:GLU:HG3	2.19	0.42
5:C:90:VAL:HG12	5:C:91:THR:N	2.35	0.42
5:C:806:PRO:HA	5:C:811:ASN:HD21	1.85	0.42
5:C:809:GLY:O	5:C:811:ASN:N	2.53	0.42
6:D:103:GLY:C	6:D:244:VAL:HG22	2.45	0.42
6:D:412:LEU:HD22	6:D:441:LEU:HD21	2.02	0.42
6:D:759:ILE:HD12	6:D:771:GLN:HG2	2.01	0.42
6:D:872:LEU:HD22	6:D:877:VAL:HG21	2.00	0.42
6:D:975:ILE:HG22	6:D:977:SER:H	1.85	0.42
4:B:13:LEU:HD21	4:B:29:GLU:HG3	2.00	0.42
5:C:559:CYS:SG	5:C:562:GLU:N	2.93	0.42
6:D:17:PHE:HZ	6:D:1353:VAL:HG21	1.85	0.42
6:D:253:VAL:HG23	6:D:261:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1107:VAL:HG22	6:D:1122:ALA:HB2	2.02	0.42
6:D:1257:VAL:O	6:D:1260:MET:HB2	2.20	0.42
5:C:18:ARG:HH21	5:C:620:ASN:C	2.27	0.42
5:C:344:GLY:HA3	5:C:346:TYR:CE2	2.54	0.42
5:C:758:ARG:HG2	5:C:759:SER:O	2.20	0.42
5:C:1230:MET:O	5:C:1232:MET:HG3	2.20	0.42
6:D:45:ASN:C	6:D:47:ARG:H	2.28	0.42
6:D:975:ILE:HD11	6:D:1003:LEU:HD11	2.02	0.42
6:D:1219:ASP:HA	6:D:1222:ARG:HG2	2.02	0.42
3:F:78:SER:HB2	3:F:79:PRO:HD2	2.01	0.41
3:F:85:VAL:HG22	3:F:153:ILE:HG12	2.00	0.41
5:C:10:ARG:HH21	5:C:793:GLU:CD	2.27	0.41
5:C:1160:ASP:OD1	5:C:1160:ASP:N	2.52	0.41
6:D:45:ASN:CG	6:D:47:ARG:HB3	2.45	0.41
6:D:865:HIS:CE1	6:D:867:GLN:HB2	2.55	0.41
2:T:15:DA:H2'	2:T:16:DC:H6	1.85	0.41
3:F:104:ARG:HD3	3:F:116:ASP:HB3	2.01	0.41
4:A:47:LEU:HD23	4:A:47:LEU:HA	1.82	0.41
5:C:558:VAL:N	5:C:576:SER:OG	2.54	0.41
6:D:103:GLY:O	6:D:244:VAL:HG22	2.20	0.41
4:B:192:VAL:HG12	4:B:193:GLU:N	2.36	0.41
4:B:224:LEU:HD12	4:B:224:LEU:HA	1.83	0.41
6:D:209:ASN:HA	6:D:214:ARG:NH2	2.36	0.41
6:D:1237:VAL:HG13	6:D:1253:ILE:HD13	2.02	0.41
2:T:18:DT:H4'	6:D:352:ARG:CZ	2.50	0.41
4:A:231:PHE:CE1	4:B:28:LEU:HD11	2.55	0.41
5:C:1333:LEU:C	5:C:1335:ILE:H	2.28	0.41
6:D:515:ARG:HH21	6:D:717:VAL:CG2	2.34	0.41
6:D:1019:ASN:OD1	6:D:1020:TRP:N	2.54	0.41
4:B:67:GLU:H	4:B:67:GLU:CD	2.27	0.41
4:B:159:ILE:HD11	4:B:166:ARG:HH21	1.86	0.41
5:C:1109:ILE:HD12	5:C:1109:ILE:HA	1.94	0.41
6:D:30:ILE:O	6:D:33:TRP:N	2.53	0.41
6:D:313:GLY:O	6:D:314:ARG:C	2.64	0.41
3:F:26:ARG:HH21	6:D:1243:LEU:HG	1.85	0.41
4:B:82:LEU:HA	4:B:82:LEU:HD23	1.80	0.41
5:C:620:ASN:HD21	6:D:768:ASN:HB3	1.85	0.41
6:D:959:LYS:HB2	6:D:985:ILE:HG12	2.03	0.41
6:D:1048:ARG:NH2	6:D:1110:GLU:OE2	2.53	0.41
5:C:402:ARG:HH21	5:C:417:SER:C	2.22	0.41
5:C:1298:VAL:HG13	5:C:1299:ASN:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1333:LEU:HD22	6:D:307:LEU:HD22	2.02	0.41
1:N:27:DC:H2''	1:N:28:DA:H5'	2.02	0.41
5:C:228:VAL:HG13	5:C:239:MET:HE3	2.03	0.41
5:C:495:ALA:HA	5:C:498:ILE:HD13	2.02	0.41
5:C:667:LEU:HA	5:C:667:LEU:HD23	1.81	0.41
6:D:515:ARG:HH21	6:D:717:VAL:HG23	1.86	0.41
6:D:849:LEU:HD23	6:D:854:ALA:H	1.86	0.41
3:F:59:ASP:HA	3:F:62:VAL:HG12	2.03	0.41
4:A:20:SER:OG	4:A:21:SER:N	2.54	0.41
4:A:73:GLY:O	4:A:134:THR:HG22	2.20	0.41
5:C:207:THR:O	5:C:211:ARG:HG2	2.21	0.41
5:C:930:ASP:HB3	5:C:1053:TYR:CD2	2.53	0.41
5:C:998:LEU:HD22	5:C:1015:ALA:HB2	2.03	0.41
6:D:238:ILE:HD13	6:D:238:ILE:HA	1.87	0.41
6:D:343:LEU:HA	6:D:343:LEU:HD23	1.88	0.41
6:D:515:ARG:HG2	6:D:516:ASP:N	2.34	0.41
6:D:635:SER:OG	6:D:636:GLY:N	2.54	0.41
6:D:697:MET:HG3	6:D:698:MET:N	2.36	0.41
6:D:925:GLU:HB3	6:D:926:PRO:HD3	2.02	0.41
5:C:122:VAL:HG21	5:C:493:ILE:HG21	2.03	0.41
5:C:809:GLY:O	5:C:812:PHE:N	2.53	0.41
6:D:960:LEU:HD13	6:D:1007:ASP:HB2	2.02	0.41
8:R:7:G:H2'	8:R:8:A:C8	2.56	0.41
4:B:104:LYS:NZ	4:B:110:VAL:HA	2.36	0.40
5:C:360:LEU:O	5:C:364:VAL:HG23	2.21	0.40
5:C:587:LEU:HD23	5:C:587:LEU:HA	1.80	0.40
5:C:1281:TYR:CE1	6:D:431:ARG:HD3	2.57	0.40
6:D:224:LEU:HD23	6:D:224:LEU:HA	1.85	0.40
6:D:1046:ILE:HD12	6:D:1059:LEU:HD22	2.03	0.40
6:D:1155:ILE:C	6:D:1156:LEU:HD12	2.46	0.40
6:D:1313:SER:OG	6:D:1314:LEU:N	2.53	0.40
2:T:18:DT:C4'	6:D:352:ARG:HH22	2.29	0.40
4:B:211:ILE:HD12	4:B:211:ILE:HA	1.92	0.40
5:C:805:MET:HE1	5:C:1221:PHE:CE1	2.56	0.40
6:D:107:LEU:HD23	6:D:107:LEU:HA	1.88	0.40
6:D:442:ILE:HG22	6:D:443:GLU:N	2.36	0.40
6:D:797:THR:HG22	6:D:924:GLY:HA3	2.03	0.40
6:D:860:ARG:HG3	6:D:861:ASN:CG	2.46	0.40
6:D:1226:VAL:HA	6:D:1229:VAL:HG12	2.02	0.40
4:B:197:ASP:C	4:B:198:LEU:HD12	2.45	0.40
5:C:44:GLU:O	5:C:46:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:757:THR:OG1	5:C:758:ARG:N	2.52	0.40
6:D:671:GLY:C	6:D:672:LEU:HD12	2.47	0.40
6:D:857:LEU:HG	6:D:858:VAL:HG13	2.03	0.40
7:E:15:ASN:C	7:E:17:PHE:H	2.29	0.40
3:F:7:THR:HG22	3:F:9:GLU:OE1	2.22	0.40
4:A:57:THR:HG23	4:A:158:ARG:HH21	1.86	0.40
4:A:197:ASP:C	4:A:198:LEU:HD12	2.47	0.40
5:C:208:ILE:HG23	5:C:209:ILE:N	2.37	0.40
5:C:782:VAL:HG11	5:C:792:GLY:HA2	2.03	0.40
6:D:289:ASP:HA	6:D:292:VAL:HG22	2.03	0.40
6:D:389:GLY:C	6:D:390:LEU:HD12	2.46	0.40
6:D:776:THR:O	6:D:777:HIS:C	2.65	0.40
5:C:240:GLU:HA	5:C:283:LYS:O	2.22	0.40
5:C:795:ALA:C	5:C:796:LEU:HD12	2.46	0.40
5:C:937:ASP:OD1	5:C:938:GLY:N	2.55	0.40
5:C:1066:MET:HE1	5:C:1076:ILE:HD12	2.03	0.40
5:C:1290:MET:SD	5:C:1294:LYS:NZ	2.90	0.40
6:D:412:LEU:HA	6:D:415:VAL:HG22	2.04	0.40
6:D:490:ILE:HG13	6:D:491:LEU:HG	2.02	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 PDB entries followed by that with respect to all EM entries.

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	
3	F	154/158 (98%)	139 (90%)	15 (10%)	0	100	100
4	A	226/329 (69%)	198 (88%)	28 (12%)	0	100	100
4	B	227/329 (69%)	196 (86%)	30 (13%)	1 (0%)	30	60
5	C	1315/1342 (98%)	1125 (86%)	190 (14%)	0	100	100
6	D	1356/1407 (96%)	1173 (86%)	183 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	E	71/91 (78%)	60 (84%)	11 (16%)	0	100	100
All	All	3349/3656 (92%)	2891 (86%)	457 (14%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	94	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 PDB entries followed by that with respect to all EM entries.

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	
3	F	137/139 (99%)	136 (99%)	1 (1%)	76	77
4	A	196/286 (68%)	196 (100%)	0	100	100
4	B	197/286 (69%)	197 (100%)	0	100	100
5	C	1138/1157 (98%)	1138 (100%)	0	100	100
6	D	1134/1168 (97%)	1133 (100%)	1 (0%)	88	88
7	E	63/75 (84%)	63 (100%)	0	100	100
All	All	2865/3111 (92%)	2863 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	111	ILE
6	D	1233	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	80	GLN
4	A	37	HIS
4	B	37	HIS

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Mol	Chain	Res	Type
4	B	66	HIS
4	B	84	ASN
5	C	69	GLN
5	C	150	HIS
5	C	327	GLN
5	C	330	HIS
5	C	343	HIS
5	C	406	ASN
5	C	580	GLN
5	C	628	HIS
5	C	761	GLN
5	C	1072	ASN
5	C	1080	ASN
5	C	1111	GLN
5	C	1116	HIS
5	C	1157	GLN
5	C	1209	GLN
5	C	1237	HIS
5	C	1257	GLN
5	C	1268	GLN
5	C	1313	HIS
6	D	45	ASN
6	D	80	HIS
6	D	341	ASN
6	D	365	GLN
6	D	435	GLN
6	D	665	GLN
6	D	736	GLN
6	D	777	HIS
6	D	929	GLN
6	D	1108	GLN
6	D	1238	GLN
6	D	1366	HIS
6	D	1367	GLN
7	E	15	ASN
7	E	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	12/14 (85%)	2 (16%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	10	G
8	R	13	U

There are no RNA pucker outliers to report.

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 3 ligands modelled in this entry, 3 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.

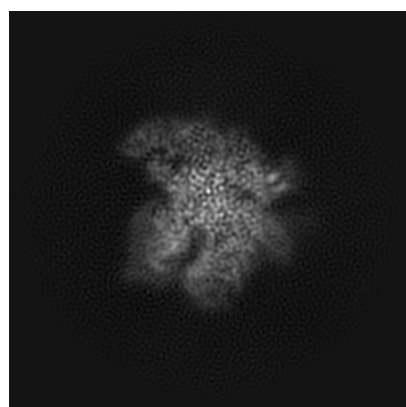
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4892. These allow visual inspection of the internal detail of the map and identification of artifacts.

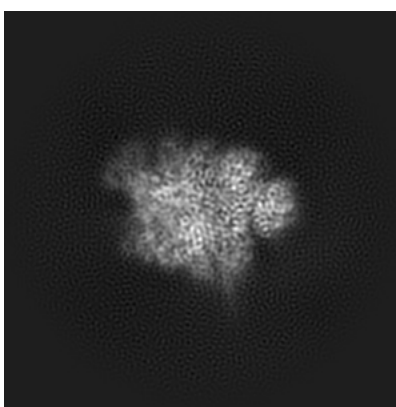
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

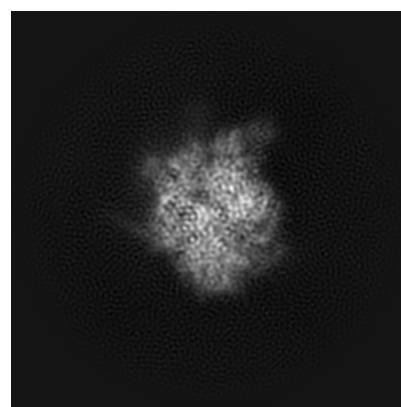
6.1.1 Primary map



X



Y

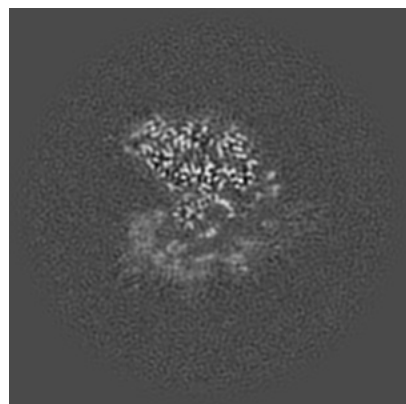


Z

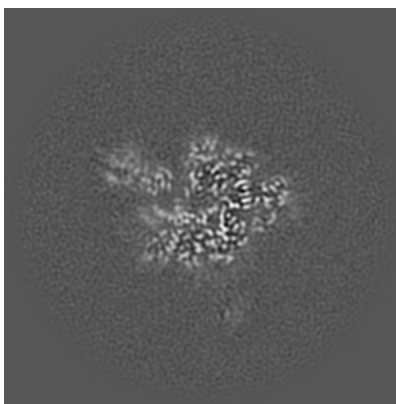
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

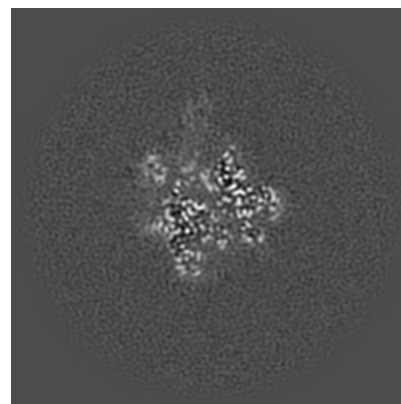
6.2.1 Primary map



X Index: 140



Y Index: 140

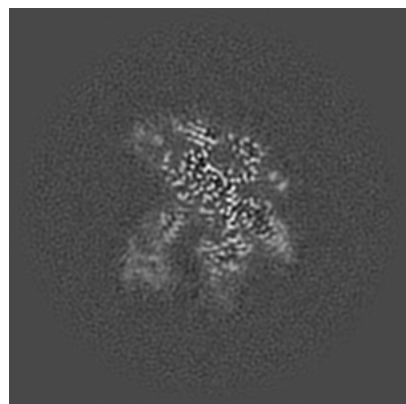


Z Index: 140

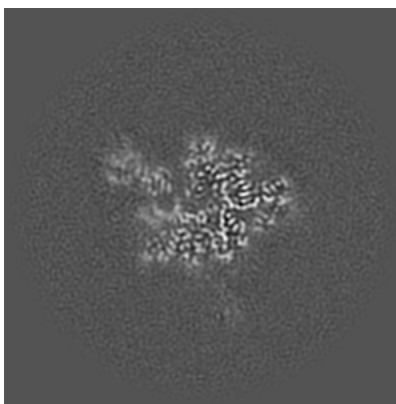
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

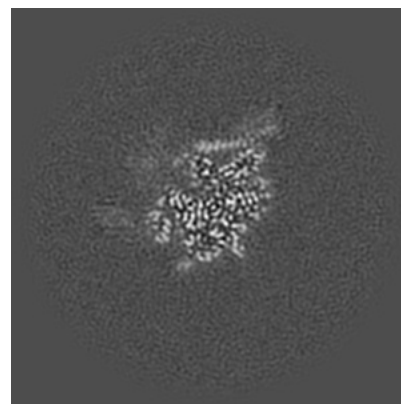
6.3.1 Primary map



X Index: 154



Y Index: 139

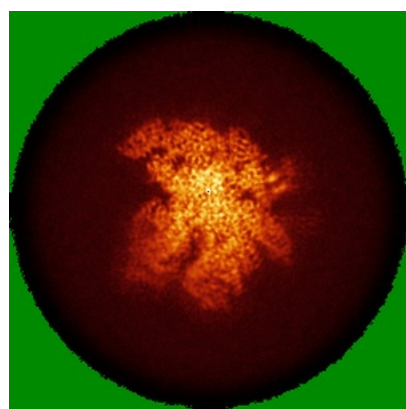


Z Index: 161

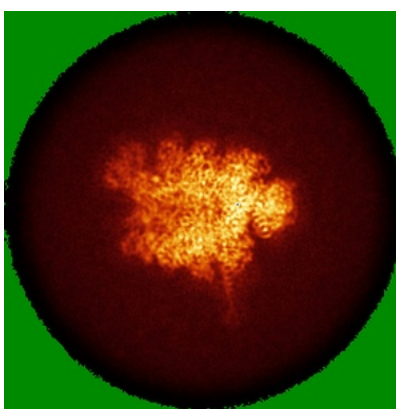
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

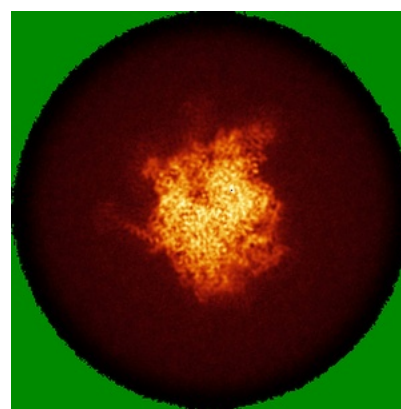
6.4.1 Primary map



X



Y

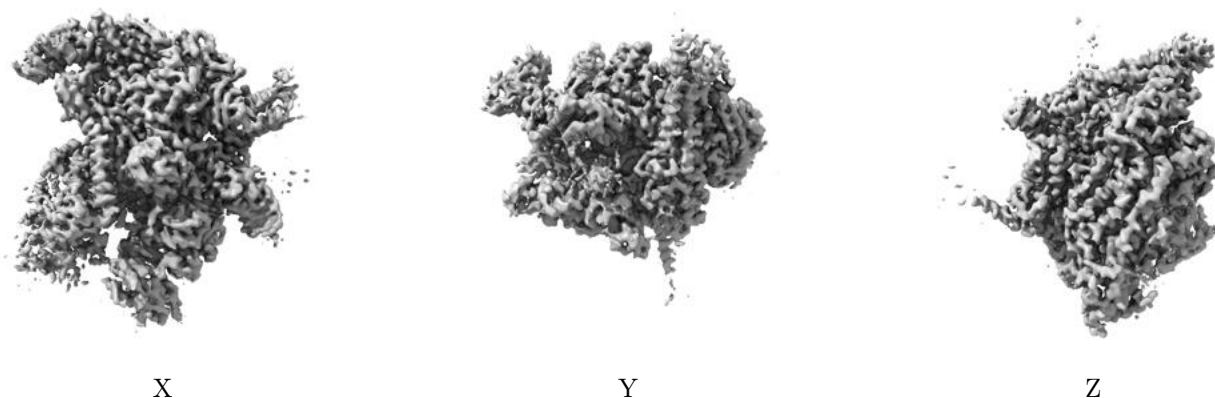


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

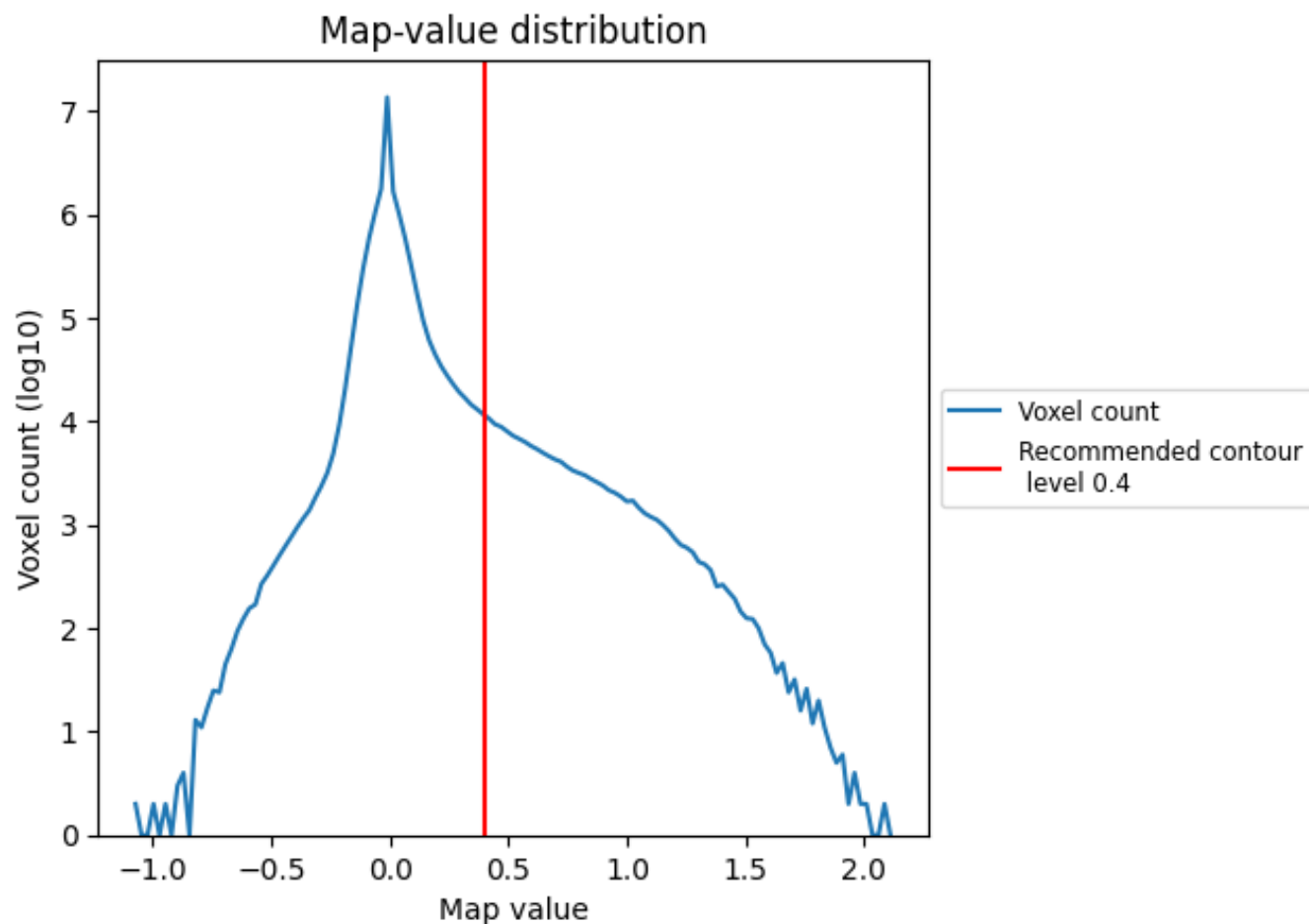
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

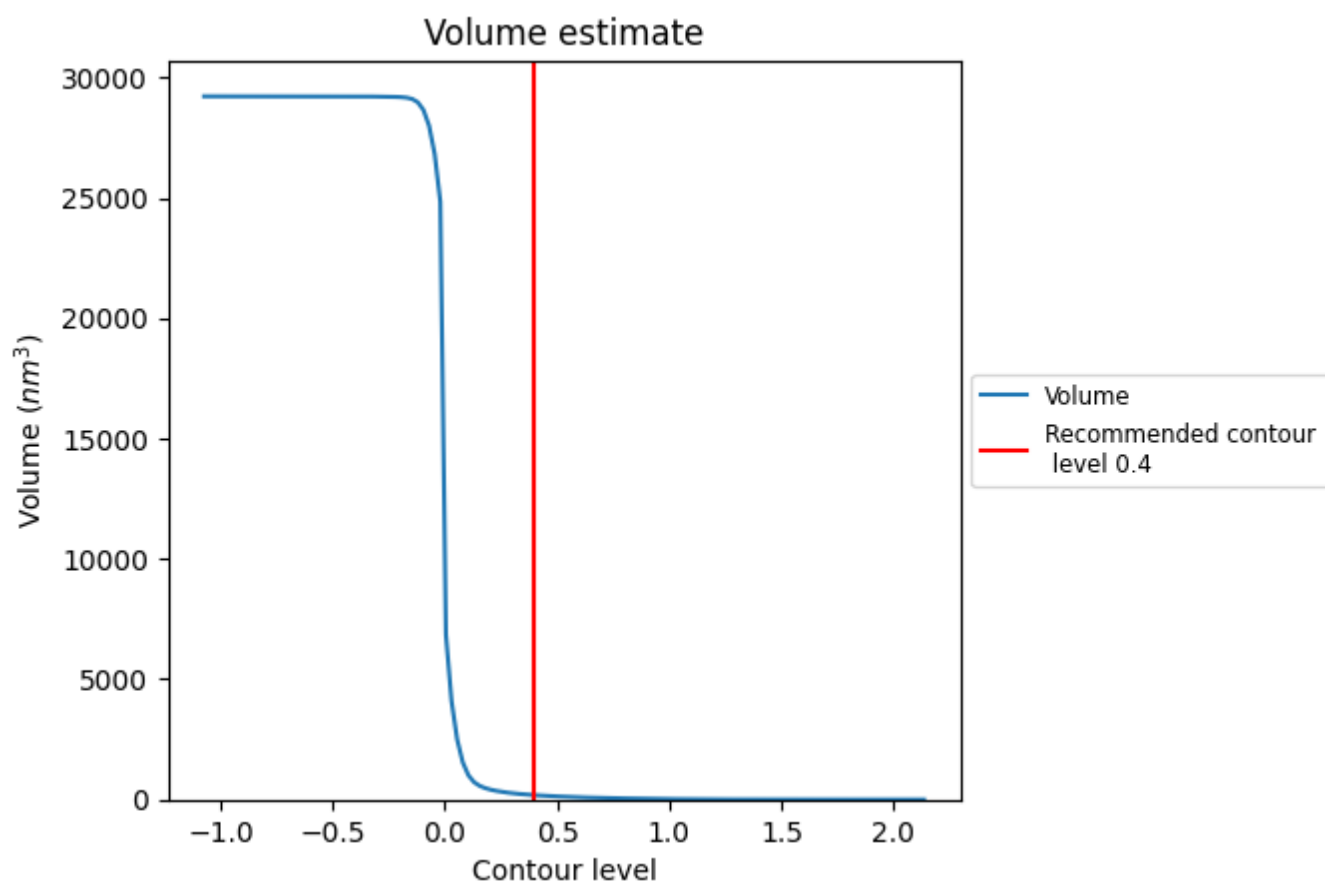
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

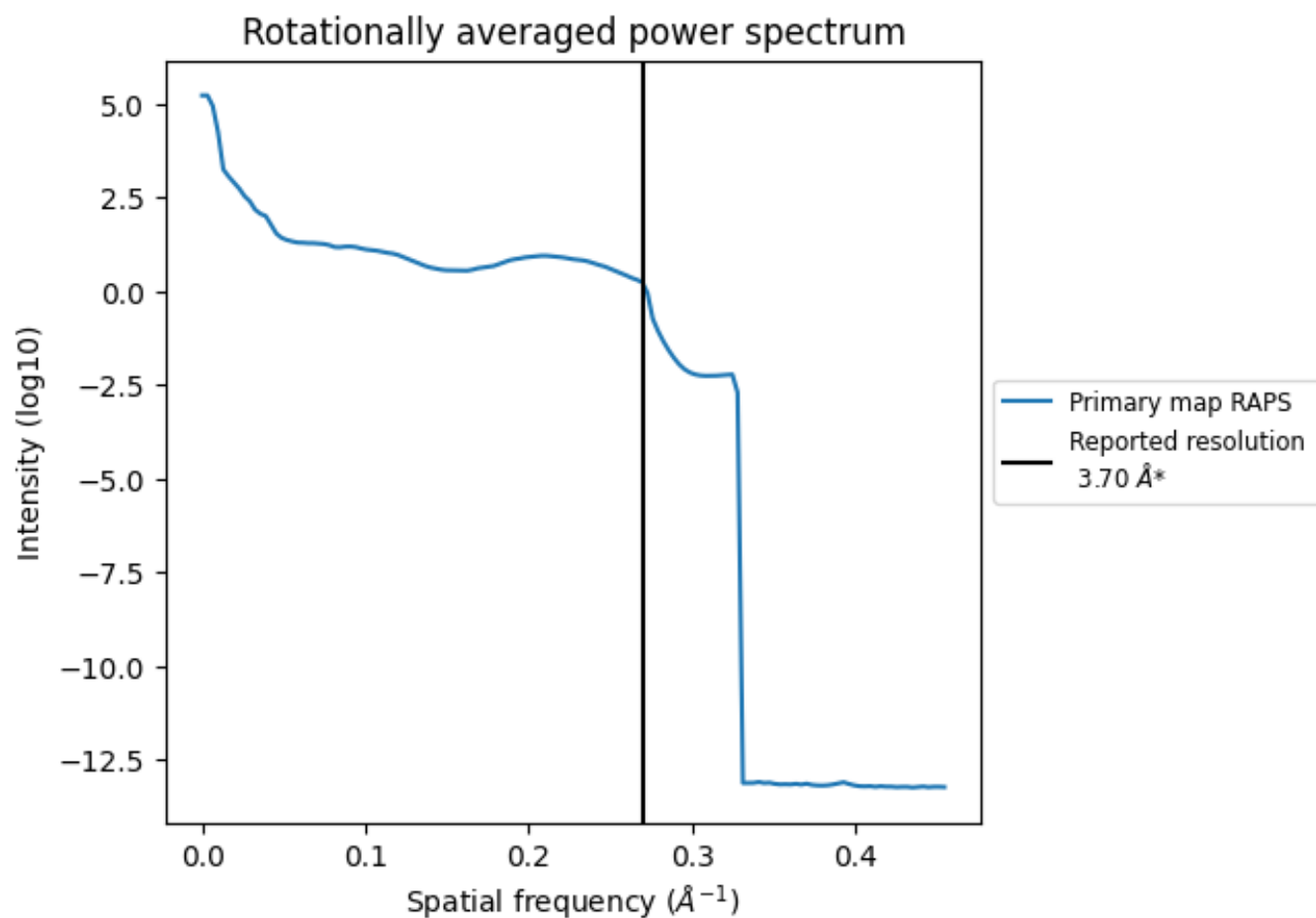
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

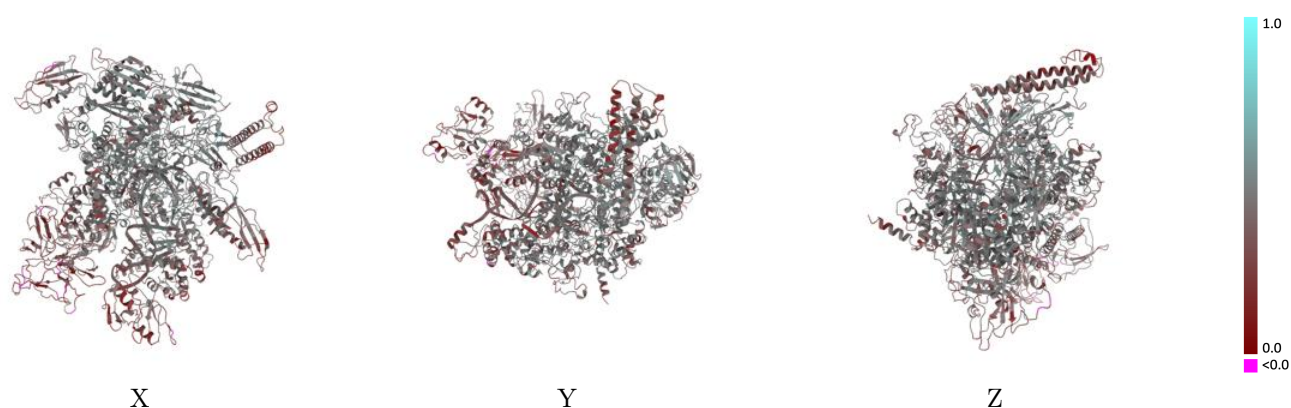
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4892 and PDB model 6RIN. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

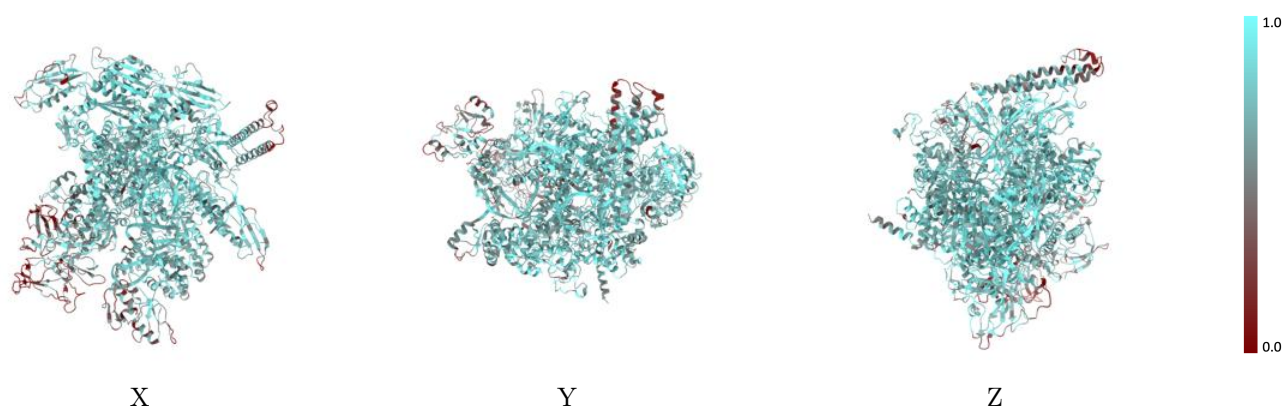
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



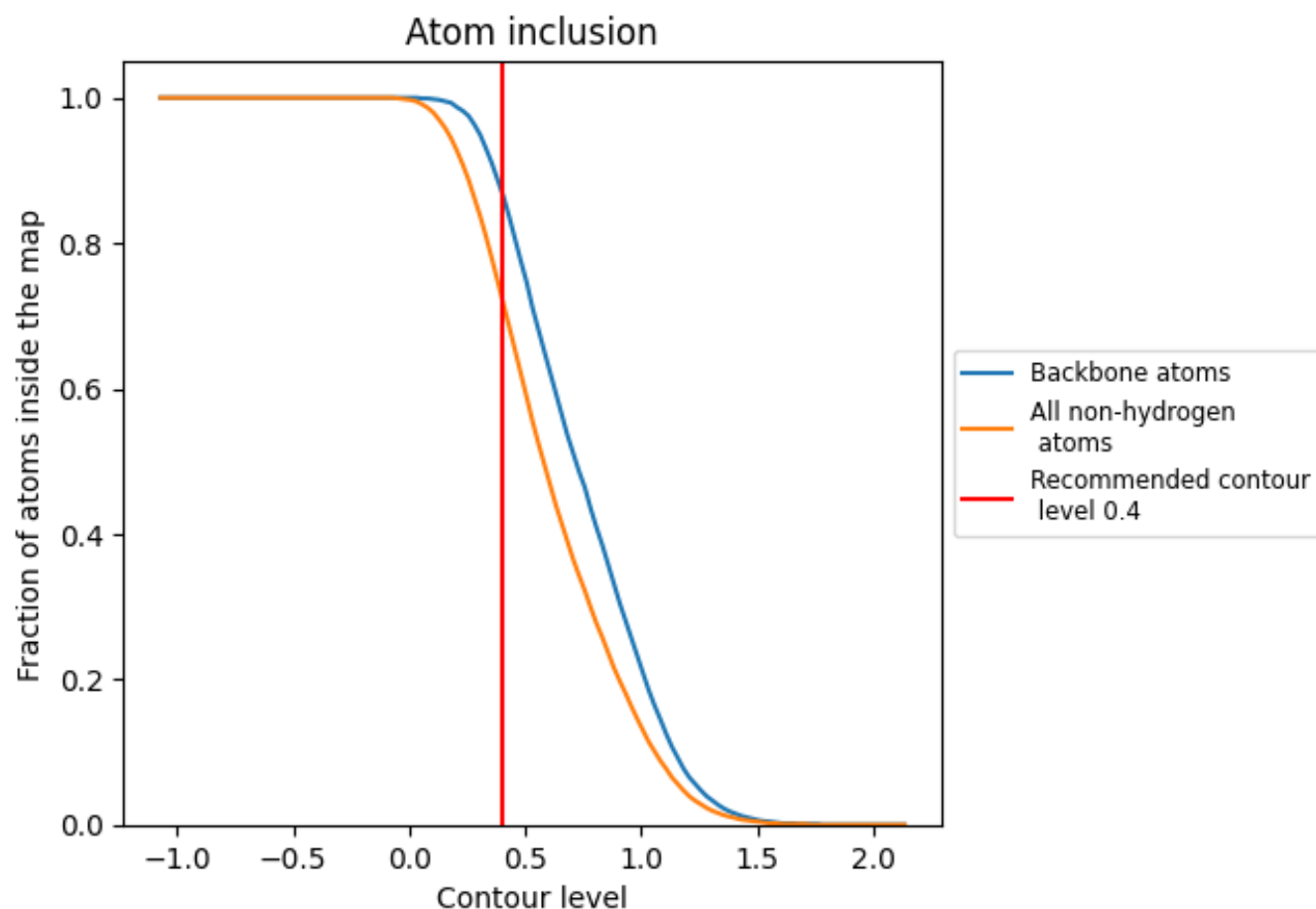
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.4150
A	0.7830	0.4520
B	0.7070	0.4090
C	0.7430	0.4280
D	0.6960	0.4040
E	0.7540	0.4120
F	0.6450	0.3910
N	0.7730	0.3410
R	0.8210	0.4290
T	0.8620	0.4060

1.0

0.0

<0.0