



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:47 AM UTC

PDB ID : 7F75 / pdb_00007f75
EMDB ID : EMD-31485
Title : Cryo-EM structure of Spx-dependent transcription activation complex
Authors : Lin, W.; Feng, Y.; Shi, J.
Deposited on : 2021-06-28
Resolution : 4.20 Å(reported)

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:

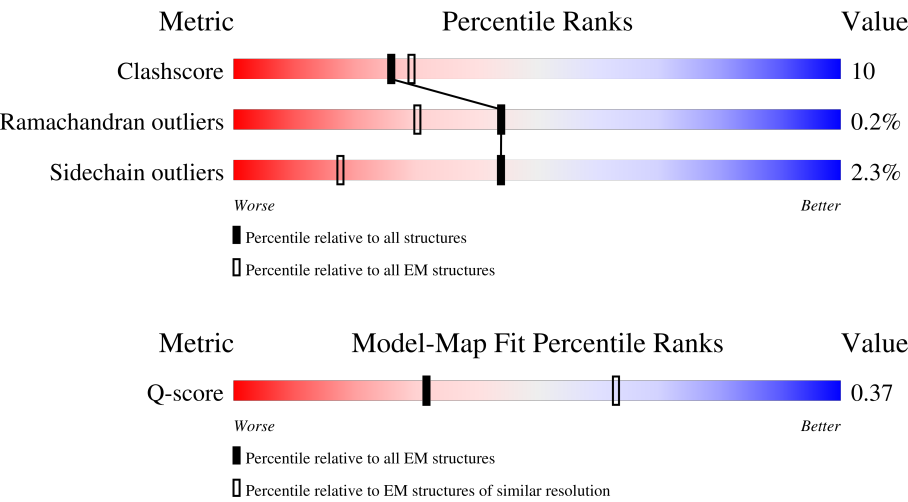
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	-
Q-score	-	25397	5410 (3.70 - 4.70)

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 <=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	A	314	
1	B	314	
1	I	314	
2	C	1193	

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Mol	Chain	Length	Quality of chain
3	D	1199	81%13%5%
4	E	67	9%85%7%7%
5	F	371	61%12%27%
6	H	69	88%12%
7	G	131	66%31%
8	J	68	50%37%13%
9	K	68	56%37%7%
10	L	173	18%36%17%47%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26887 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	224	Total	C	N	O		0	0
			1540	961	266	313			
1	B	220	Total	C	N	O		0	0
			1538	968	263	307			
1	I	67	Total	C	N	O	S	0	0
			530	327	94	105	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1133	Total	C	N	O	S	0	0
			8041	5033	1380	1612	16		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1142	Total	C	N	O	S	0	0
			7891	4972	1391	1501	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	62	Total	C	N	O	S	0	0
			405	253	73	78	1		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	272	Total	C	N	O	S	0	0
			2047	1289	361	391	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	69	Total	C	N	O	S	0	0
			542	348	86	107	1		

- Molecule 7 is a protein called transcriptional regulator Spx.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	129	Total	C	N	O	S	0	0
			1077	679	196	197	5		

- Molecule 8 is a DNA chain called trxA promoter DNA-Non template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	59	Total	C	N	O	P	0	0
			1225	582	240	345	58		

- Molecule 9 is a DNA chain called trxA promoter DNA-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	63	Total	C	N	O	P	0	0
			1285	615	225	382	63		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	92	Total	C	N	O	S	0	0
			763	489	122	150	2		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

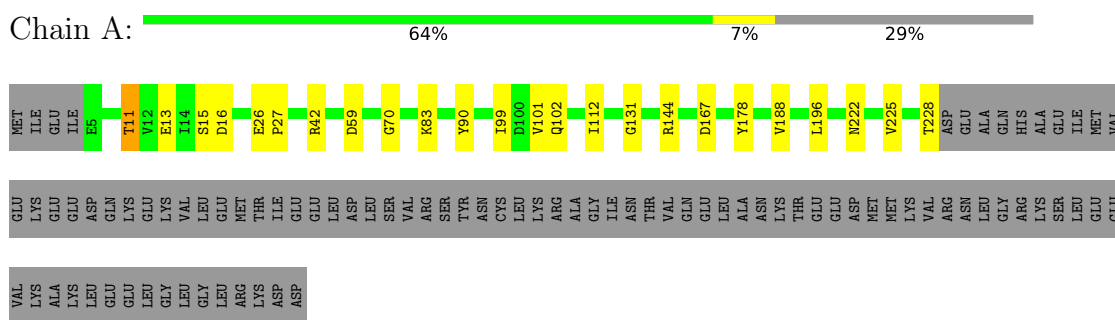
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

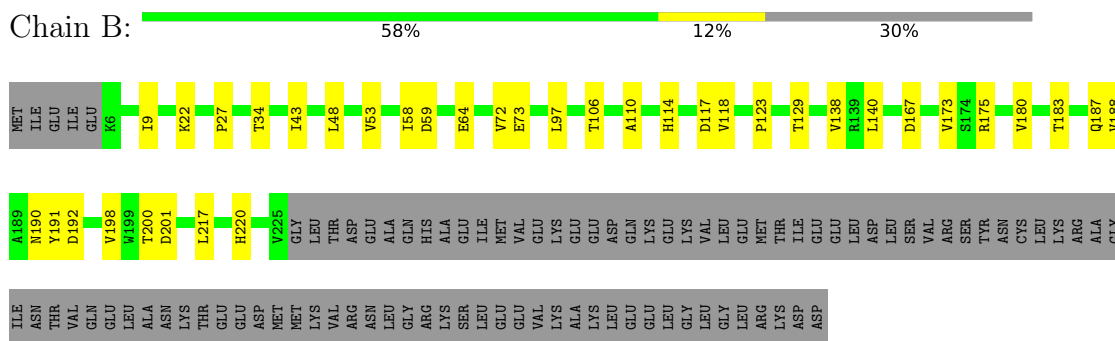
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

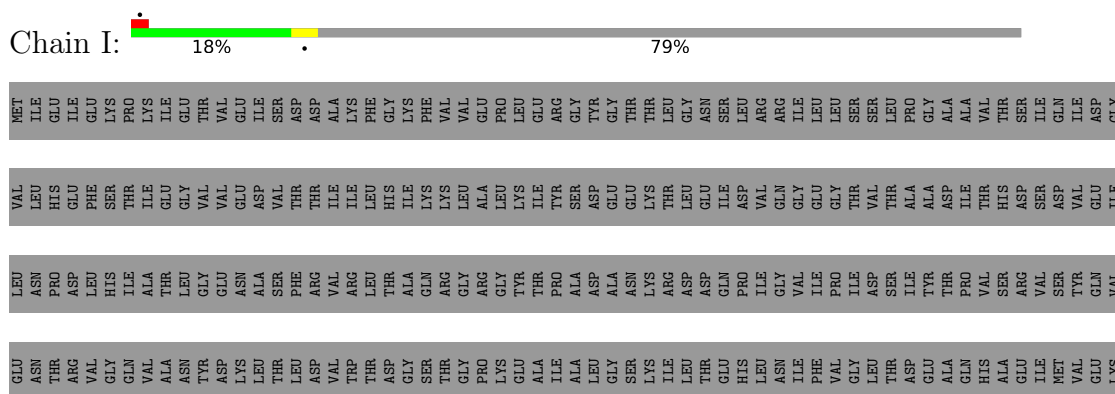
- Molecule 1: DNA-directed RNA polymerase subunit alpha

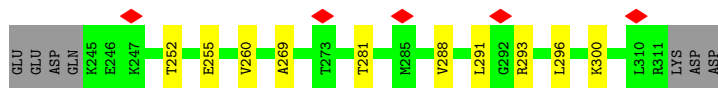


- Molecule 1: DNA-directed RNA polymerase subunit alpha



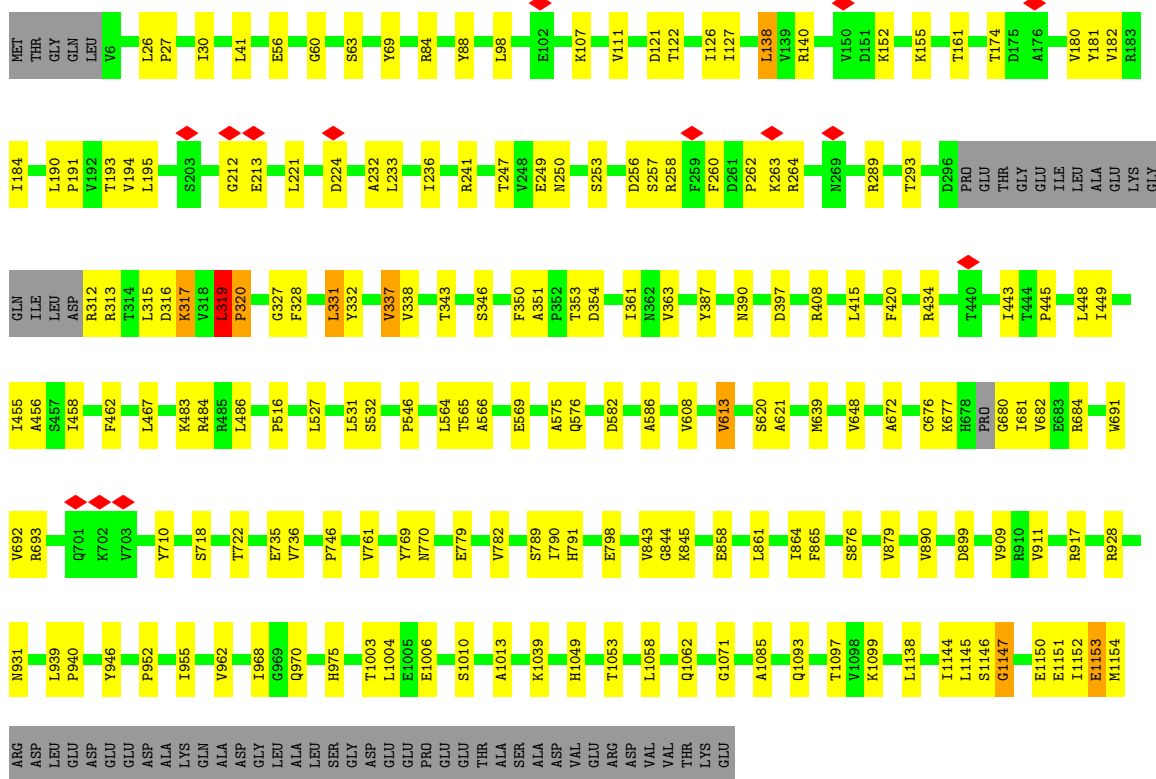
- Molecule 1: DNA-directed RNA polymerase subunit alpha





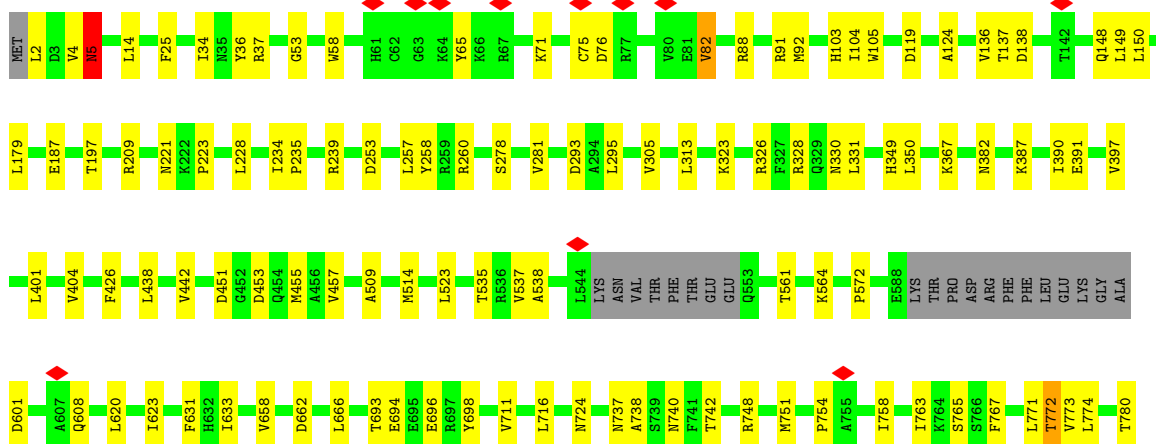
- Molecule 2: DNA-directed RNA polymerase subunit beta

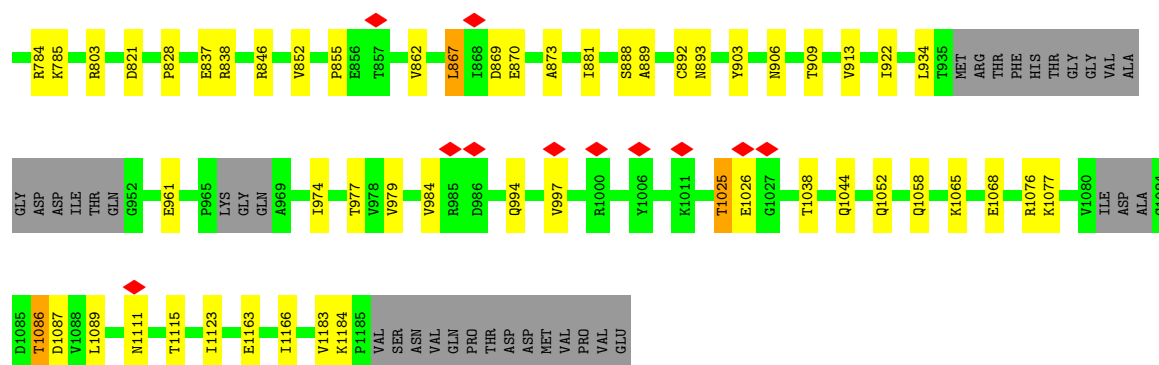
Chain C: 79% 15% 5%



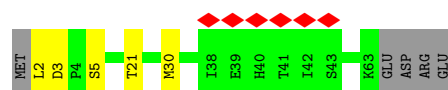
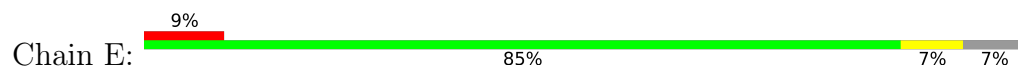
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 81% 13% 5%

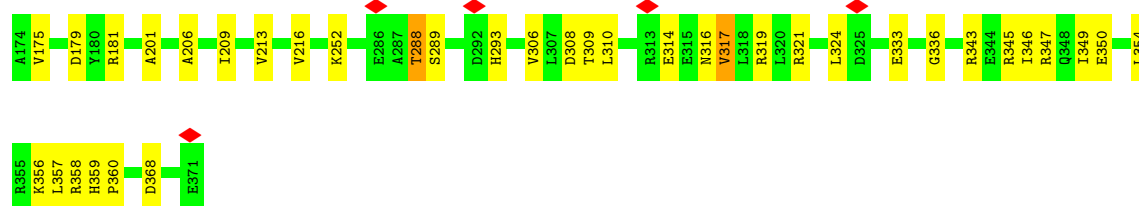
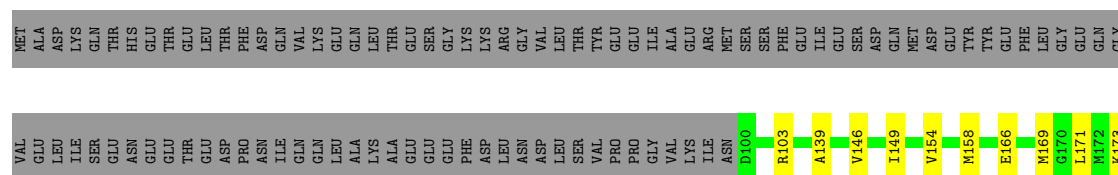




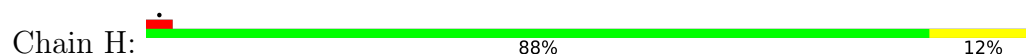
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA-directed RNA polymerase subunit epsilon



- Molecule 7: transcriptional regulator Spx



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	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	0.152	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3069999, 1.3069999, 1.3069999	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	A	0.30	0/1558	0.52	0/2132
1	B	0.26	0/1558	0.52	0/2138
1	I	0.23	0/530	0.54	0/705
2	C	0.33	0/8164	0.61	5/11137 (0.0%)
3	D	0.31	0/7999	0.61	0/10896
4	E	0.35	1/407 (0.2%)	0.56	0/550
5	F	0.26	0/2074	0.58	0/2804
6	H	0.26	0/550	0.66	0/740
7	G	0.30	1/1096 (0.1%)	0.62	0/1478
8	J	0.28	0/1380	0.53	0/2132
9	K	0.32	0/1438	0.56	0/2216
10	L	0.15	0/779	0.41	0/1051
All	All	0.30	2/27533 (0.0%)	0.58	5/37979 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	ASP	C-N	5.54	1.38	1.33
7	G	120	PRO	N-CD	5.05	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1147	GLY	CA-C-N	6.19	133.37	121.54
2	C	1147	GLY	C-N-CA	6.19	133.37	121.54
2	C	319	LEU	CA-C-N	5.21	126.35	119.84
2	C	319	LEU	C-N-CA	5.21	126.35	119.84
2	C	30	ILE	N-CA-C	-5.14	107.33	111.91

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	A	1540	0	1395	12	0
1	B	1538	0	1427	26	0
1	I	530	0	555	7	0
2	C	8041	0	7238	156	0
3	D	7891	0	7094	115	0
4	E	405	0	330	4	0
5	F	2047	0	1937	40	0
6	H	542	0	520	4	0
7	G	1077	0	1103	50	0
8	J	1225	0	664	61	0
9	K	1285	0	714	62	0
10	L	763	0	740	37	0
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	26887	0	23717	511	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 10.

All (511) 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)
9:K:33:DC:H2''	9:K:34:DC:C5	1.46	1.47
2:C:331:LEU:CD1	2:C:343:THR:HG23	1.64	1.26
8:J:36:DT:C6	8:J:37:DT:H72	1.73	1.24
2:C:681:ILE:CG2	2:C:693:ARG:HB2	1.74	1.16
9:K:21:DA:H2''	9:K:22:DA:OP1	1.44	1.15
2:C:681:ILE:HG21	2:C:693:ARG:CB	1.80	1.11
9:K:33:DC:C2'	9:K:34:DC:C5	2.33	1.10
2:C:331:LEU:HD13	2:C:343:THR:HG23	1.18	1.09
2:C:681:ILE:HG22	2:C:693:ARG:HB2	1.36	1.08
2:C:681:ILE:HB	2:C:693:ARG:O	1.51	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:308:ASP:HA	7:G:119:ARG:HH12	1.15	1.05
3:D:997:VAL:HG21	10:L:84:TYR:HB3	1.38	1.05
2:C:317:LYS:HA	2:C:317:LYS:HE2	1.36	1.05
9:K:17:DG:N2	9:K:17:DG:OP2	1.88	1.05
2:C:681:ILE:CG2	2:C:693:ARG:CB	2.36	1.04
4:E:2:LEU:N	4:E:5:SER:HG	1.57	1.03
9:K:22:DA:C2'	9:K:23:DT:H71	1.88	1.03
9:K:34:DC:H2''	9:K:35:DC:OP1	1.53	1.02
2:C:682:VAL:HG13	2:C:691:TRP:O	1.60	1.02
2:C:681:ILE:HG21	2:C:693:ARG:HB3	1.42	1.01
9:K:22:DA:H2'	9:K:23:DT:H71	1.37	1.01
7:G:118:VAL:HA	7:G:121:PHE:CD2	1.95	1.00
8:J:26:DT:H2''	8:J:27:DG:H5'	1.50	0.93
2:C:456:ALA:HB2	9:K:22:DA:OP1	1.70	0.92
9:K:61:DA:H2''	9:K:62:DC:C6	2.06	0.91
7:G:115:PRO:HB2	7:G:118:VAL:HG23	1.54	0.89
2:C:331:LEU:HD12	2:C:343:THR:HG23	1.53	0.89
8:J:52:DC:C2'	8:J:53:DA:C8	2.57	0.88
3:D:997:VAL:HG23	10:L:83:PRO:O	1.74	0.88
8:J:19:DG:H2''	8:J:20:DA:C8	2.08	0.87
5:F:308:ASP:HA	7:G:119:ARG:NH1	1.89	0.86
8:J:52:DC:H2''	8:J:53:DA:C8	2.09	0.86
5:F:308:ASP:CA	7:G:119:ARG:HH12	1.87	0.86
7:G:116:ARG:HG2	7:G:116:ARG:HH21	1.39	0.85
2:C:682:VAL:HA	2:C:692:VAL:HA	1.58	0.85
2:C:1144:ILE:O	2:C:1152:ILE:HG12	1.75	0.84
2:C:456:ALA:CB	9:K:22:DA:OP1	2.25	0.83
2:C:682:VAL:CG1	2:C:691:TRP:O	2.27	0.83
9:K:33:DC:H2''	9:K:34:DC:H5	1.36	0.83
2:C:293:THR:OG1	2:C:316:ASP:HB3	1.79	0.82
7:G:116:ARG:O	7:G:120:PRO:HD3	1.79	0.82
2:C:331:LEU:HD13	2:C:343:THR:CG2	2.07	0.82
9:K:21:DA:C2'	9:K:22:DA:OP1	2.22	0.81
2:C:1146:SER:HB3	2:C:1150:GLU:HB3	1.63	0.81
3:D:1115:THR:CB	10:L:63:ASN:CG	2.53	0.81
9:K:33:DC:H1'	9:K:34:DC:C6	2.16	0.81
9:K:51:DT:H2''	9:K:52:DT:H5''	1.61	0.81
8:J:39:DT:H2''	8:J:40:DA:C8	2.15	0.81
8:J:36:DT:C4	8:J:37:DT:O4	2.34	0.80
2:C:1145:LEU:HA	2:C:1150:GLU:O	1.82	0.80
2:C:317:LYS:HA	2:C:317:LYS:CE	2.03	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:LYS:O	7:G:120:PRO:HD2	1.82	0.79
8:J:52:DC:H2'	8:J:53:DA:C8	2.18	0.79
8:J:9:DA:H4'	8:J:10:DA:OP1	1.82	0.79
9:K:61:DA:H2''	9:K:62:DC:H6	1.42	0.79
2:C:455:ILE:HA	2:C:458:ILE:CG1	2.13	0.79
7:G:115:PRO:HB2	7:G:118:VAL:CG2	2.13	0.78
8:J:39:DT:H2''	8:J:40:DA:H8	1.48	0.77
8:J:39:DT:H2''	8:J:40:DA:H5'	1.68	0.76
2:C:317:LYS:HE2	2:C:317:LYS:CA	2.15	0.76
8:J:39:DT:C4	8:J:40:DA:N6	2.54	0.75
7:G:116:ARG:HG2	7:G:116:ARG:NH2	1.98	0.75
8:J:39:DT:C2'	8:J:40:DA:C8	2.70	0.75
8:J:36:DT:C6	8:J:37:DT:C7	2.64	0.74
3:D:852:VAL:HG12	3:D:862:VAL:HG22	1.69	0.73
8:J:25:DA:H2''	8:J:26:DT:OP2	1.89	0.73
2:C:138:LEU:HD12	2:C:138:LEU:C	2.14	0.73
10:L:51:LEU:HB3	10:L:54:ARG:HB3	1.71	0.72
8:J:19:DG:H2''	8:J:20:DA:H8	1.53	0.72
3:D:867:LEU:N	3:D:867:LEU:HD23	2.03	0.72
8:J:36:DT:N3	8:J:37:DT:C4	2.58	0.72
2:C:337:VAL:HG13	2:C:338:VAL:N	2.04	0.71
7:G:118:VAL:HA	7:G:121:PHE:CE2	2.26	0.71
9:K:33:DC:H2''	9:K:34:DC:C4	2.23	0.71
8:J:39:DT:C4	8:J:40:DA:C6	2.78	0.71
3:D:821:ASP:HB3	10:L:13:GLU:O	1.91	0.70
2:C:337:VAL:HG22	2:C:338:VAL:H	1.56	0.70
2:C:241:ARG:HH11	5:F:103:ARG:HH12	1.40	0.70
3:D:997:VAL:CG2	10:L:83:PRO:O	2.40	0.69
8:J:37:DT:H2'	8:J:37:DT:OP2	1.92	0.69
2:C:138:LEU:HD12	2:C:138:LEU:O	1.93	0.69
7:G:19:TRP:HH2	7:G:114:LEU:HD21	1.55	0.69
8:J:36:DT:C5	8:J:37:DT:H72	2.26	0.68
7:G:125:GLU:O	7:G:129:LEU:HD23	1.93	0.67
8:J:46:DA:OP1	8:J:48:DC:N4	2.28	0.67
2:C:684:ARG:H	2:C:691:TRP:HB2	1.59	0.67
3:D:561:THR:HG23	3:D:564:LYS:H	1.58	0.67
9:K:33:DC:C2'	9:K:34:DC:C6	2.78	0.67
3:D:1115:THR:CB	10:L:63:ASN:CB	2.73	0.66
7:G:7:SER:OG	7:G:10:CYS:SG	2.54	0.66
8:J:26:DT:C2'	8:J:27:DG:H5'	2.25	0.66
2:C:213:GLU:HB2	2:C:351:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HD2	1:A:167:ASP:HB2	1.76	0.66
3:D:763:ILE:HG22	3:D:765:SER:H	1.60	0.66
3:D:323:LYS:HA	3:D:328:ARG:HD3	1.77	0.66
3:D:997:VAL:CG2	10:L:84:TYR:HB3	2.22	0.65
7:G:120:PRO:O	7:G:123:LEU:N	2.30	0.65
9:K:33:DC:H1'	9:K:34:DC:N1	2.11	0.65
2:C:681:ILE:HB	2:C:693:ARG:C	2.21	0.65
9:K:22:DA:H2'	9:K:23:DT:C7	2.19	0.65
10:L:16:LEU:HD11	10:L:54:ARG:HH11	1.60	0.65
1:B:97:LEU:HB2	1:B:140:LEU:HB2	1.78	0.65
7:G:43:LYS:HD2	1:I:255:GLU:HG2	1.79	0.65
2:C:1097:THR:HG23	2:C:1099:LYS:H	1.60	0.64
2:C:253:SER:HA	2:C:256:ASP:HB2	1.80	0.64
9:K:17:DG:C2'	9:K:18:DG:O5'	2.44	0.64
2:C:680:GLY:N	2:C:736:VAL:HG13	2.13	0.64
3:D:852:VAL:HG12	3:D:862:VAL:CG2	2.28	0.64
2:C:256:ASP:HA	2:C:260:PHE:HB2	1.79	0.64
2:C:680:GLY:HA2	2:C:736:VAL:H	1.64	0.63
1:B:106:THR:HG22	1:B:129:THR:HG23	1.80	0.63
2:C:931:ASN:ND2	2:C:970:GLN:OE1	2.31	0.63
8:J:39:DT:H2''	8:J:40:DA:C5'	2.29	0.62
8:J:39:DT:C2	8:J:40:DA:C5	2.87	0.62
3:D:1115:THR:HA	10:L:63:ASN:HB3	1.82	0.62
10:L:11:LEU:HD22	10:L:43:LEU:HD21	1.82	0.61
3:D:1115:THR:CA	10:L:63:ASN:HB3	2.30	0.61
2:C:516:PRO:HB2	3:D:780:THR:HG21	1.82	0.61
2:C:337:VAL:HG13	2:C:338:VAL:H	1.65	0.61
3:D:1115:THR:CB	10:L:63:ASN:HB3	2.31	0.60
3:D:1115:THR:CB	10:L:63:ASN:OD1	2.48	0.60
8:J:36:DT:C4	8:J:37:DT:C4	2.90	0.60
9:K:33:DC:H2''	9:K:34:DC:C6	2.22	0.60
2:C:798:GLU:O	2:C:845:LYS:NZ	2.34	0.60
9:K:33:DC:O3'	9:K:34:DC:C6	2.54	0.60
1:B:188:VAL:HG12	1:B:190:ASN:H	1.67	0.60
3:D:65:TYR:HB2	3:D:82:VAL:HG11	1.83	0.59
8:J:10:DA:C2	8:J:11:DA:C6	2.90	0.59
8:J:19:DG:C2	8:J:20:DA:C6	2.90	0.59
8:J:46:DA:OP1	8:J:47:DG:N2	2.35	0.59
3:D:119:ASP:OD2	3:D:209:ARG:NH2	2.35	0.59
3:D:1115:THR:HA	10:L:63:ASN:CG	2.27	0.59
9:K:51:DT:H72	9:K:52:DT:H73	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:ARG:O	7:G:114:LEU:HG	2.02	0.59
9:K:33:DC:C1'	9:K:34:DC:C5	2.85	0.59
2:C:194:VAL:HG23	2:C:232:ALA:HB1	1.84	0.59
5:F:181:ARG:HD3	8:J:38:DA:N6	2.18	0.59
7:G:10:CYS:HB3	7:G:13:CYS:HB2	1.85	0.59
9:K:33:DC:C1'	9:K:34:DC:C6	2.85	0.59
5:F:308:ASP:CB	7:G:119:ARG:HH12	2.16	0.58
2:C:1146:SER:HB3	2:C:1150:GLU:CB	2.32	0.58
9:K:51:DT:C2'	9:K:52:DT:H5''	2.31	0.58
8:J:36:DT:H2''	8:J:37:DT:OP2	2.04	0.58
10:L:71:LEU:HB3	10:L:75:THR:HG23	1.86	0.58
8:J:36:DT:C2	8:J:37:DT:C5	2.92	0.58
3:D:837:GLU:HG3	3:D:1052:GLN:HE21	1.69	0.57
4:E:2:LEU:N	4:E:5:SER:OG	2.32	0.57
2:C:1152:ILE:HG22	2:C:1154:MET:CB	2.33	0.57
9:K:61:DA:C2'	9:K:62:DC:C6	2.86	0.57
3:D:234:ILE:O	3:D:239:ARG:NH1	2.38	0.57
5:F:166:GLU:HG2	5:F:201:ALA:HB2	1.86	0.57
2:C:779:GLU:HA	2:C:782:VAL:HG12	1.86	0.57
3:D:426:PHE:HZ	3:D:442:VAL:HG11	1.68	0.57
3:D:754:PRO:HB3	3:D:785:LYS:HB2	1.86	0.57
7:G:44:GLN:OE1	7:G:47:ARG:NH2	2.37	0.57
1:B:34:THR:HG22	1:B:180:VAL:HG21	1.85	0.56
9:K:52:DT:H2''	9:K:53:DT:OP1	2.04	0.56
3:D:892:CYS:SG	3:D:893:ASN:N	2.79	0.56
1:B:53:VAL:HG11	1:B:140:LEU:HD12	1.87	0.56
7:G:5:TYR:HB2	7:G:94:ILE:HB	1.87	0.56
7:G:10:CYS:SG	7:G:92:ARG:HD2	2.45	0.56
9:K:17:DG:H21	9:K:17:DG:P	2.22	0.56
2:C:224:ASP:OD1	2:C:224:ASP:N	2.39	0.56
2:C:484:ARG:NH1	2:C:532:SER:O	2.38	0.56
2:C:843:VAL:HG11	2:C:909:VAL:HG21	1.86	0.56
2:C:213:GLU:HB3	2:C:361:ILE:HB	1.86	0.56
2:C:127:ILE:HD13	2:C:462:PHE:HB3	1.88	0.56
2:C:516:PRO:O	3:D:784:ARG:NH2	2.39	0.56
3:D:888:SER:OG	3:D:889:ALA:N	2.39	0.56
2:C:152:LYS:O	2:C:155:LYS:NZ	2.37	0.55
2:C:258:ARG:HA	2:C:262:PRO:HB3	1.88	0.55
3:D:124:ALA:HB1	3:D:149:LEU:HD21	1.87	0.55
3:D:934:LEU:HD12	3:D:1058:GLN:HG2	1.87	0.55
9:K:53:DT:H1'	9:K:54:DA:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:337:VAL:HG22	2:C:338:VAL:N	2.20	0.55
3:D:828:PRO:HB3	3:D:838:ARG:HA	1.89	0.55
2:C:56:GLU:HG3	2:C:60:GLY:HA2	1.87	0.55
1:B:114:HIS:NE2	1:B:118:VAL:O	2.39	0.55
9:K:33:DC:H1'	9:K:34:DC:C2	2.42	0.55
9:K:58:DC:H2'	9:K:59:DT:H72	1.89	0.55
2:C:1093:GLN:O	2:C:1097:THR:HB	2.07	0.55
10:L:10:GLU:O	10:L:14:MET:N	2.38	0.55
3:D:631:PHE:HB3	3:D:633:ILE:HG12	1.88	0.55
3:D:803:ARG:NH1	3:D:961:GLU:OE2	2.40	0.55
2:C:456:ALA:HB1	9:K:22:DA:OP1	2.05	0.54
3:D:326:ARG:HD2	3:D:330:ASN:HD22	1.72	0.54
3:D:234:ILE:HG22	3:D:258:TYR:HE2	1.72	0.54
3:D:997:VAL:HG21	10:L:84:TYR:CB	2.25	0.54
7:G:118:VAL:O	7:G:121:PHE:HB2	2.06	0.54
3:D:4:VAL:HG23	3:D:5:ASN:OD1	2.07	0.54
3:D:453:ASP:OD2	3:D:453:ASP:N	2.37	0.54
2:C:582:ASP:OD1	2:C:586:ALA:N	2.40	0.54
2:C:890:VAL:HG22	2:C:911:VAL:HG12	1.90	0.54
3:D:438:LEU:HD11	3:D:455:MET:HE1	1.90	0.54
8:J:36:DT:C2	8:J:37:DT:C4	2.96	0.54
2:C:26:LEU:HD12	2:C:27:PRO:HD2	1.89	0.54
5:F:310:LEU:HD13	5:F:314:GLU:HG2	1.90	0.54
8:J:39:DT:N3	8:J:40:DA:C6	2.76	0.54
2:C:190:LEU:HG	2:C:194:VAL:HG11	1.89	0.54
2:C:680:GLY:N	2:C:736:VAL:CG1	2.71	0.54
9:K:34:DC:P	9:K:34:DC:H6	2.31	0.54
2:C:681:ILE:HG21	2:C:693:ARG:HB2	1.50	0.53
8:J:19:DG:N2	8:J:20:DA:C2	2.75	0.53
2:C:98:LEU:HB3	2:C:107:LYS:HB3	1.89	0.53
2:C:257:SER:O	2:C:264:ARG:NH2	2.33	0.53
3:D:1115:THR:HA	10:L:63:ASN:CB	2.37	0.53
7:G:10:CYS:CB	7:G:13:CYS:SG	2.97	0.53
3:D:1111:ASN:CG	10:L:74:GLN:HE21	2.15	0.53
8:J:39:DT:N3	8:J:40:DA:C5	2.76	0.53
2:C:247:THR:OG1	2:C:249:GLU:OE1	2.24	0.53
3:D:738:ALA:O	3:D:742:THR:OG1	2.26	0.53
7:G:47:ARG:NH1	7:G:48:MET:SD	2.82	0.53
8:J:36:DT:H2'	8:J:37:DT:C7	2.39	0.53
2:C:1144:ILE:HG13	2:C:1152:ILE:HB	1.90	0.53
7:G:56:ILE:HG13	7:G:90:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:18:DT:H2''	8:J:19:DG:C8	2.44	0.53
2:C:684:ARG:N	2:C:691:TRP:HB2	2.24	0.53
3:D:75:CYS:SG	3:D:76:ASP:N	2.82	0.53
3:D:260:ARG:HH12	3:D:305:VAL:HG11	1.74	0.53
3:D:1076:ARG:HD3	3:D:1077:LYS:HZ2	1.73	0.53
2:C:212:GLY:HA2	2:C:361:ILE:HG13	1.90	0.52
5:F:181:ARG:HD3	8:J:38:DA:C6	2.44	0.52
3:D:1115:THR:CA	10:L:63:ASN:CG	2.82	0.52
2:C:434:ARG:NH2	2:C:434:ARG:O	2.43	0.52
3:D:257:LEU:HD13	3:D:295:LEU:HA	1.90	0.52
1:A:178:TYR:HB3	1:A:196:LEU:HD23	1.91	0.52
2:C:680:GLY:HA2	2:C:735:GLU:HA	1.92	0.52
10:L:28:LYS:HA	10:L:81:TRP:HZ2	1.75	0.52
2:C:546:PRO:HG2	2:C:613:VAL:HG11	1.90	0.52
2:C:331:LEU:HD12	2:C:343:THR:CG2	2.34	0.52
2:C:565:THR:OG1	2:C:566:ALA:N	2.43	0.52
5:F:309:THR:O	5:F:356:LYS:NZ	2.43	0.52
5:F:347:ARG:NH1	5:F:350:GLU:OE1	2.42	0.52
5:F:336:GLY:O	5:F:343:ARG:NH2	2.43	0.52
8:J:26:DT:H2''	8:J:27:DG:H2'	1.92	0.52
1:I:296:LEU:HG	1:I:300:LYS:HE2	1.93	0.51
8:J:52:DC:C2'	8:J:53:DA:H8	2.16	0.51
3:D:666:LEU:HD11	3:D:716:LEU:HD13	1.92	0.51
3:D:855:PRO:HG3	3:D:881:ILE:HG23	1.92	0.51
2:C:769:TYR:OH	3:D:349:HIS:NE2	2.44	0.51
3:D:870:GLU:O	3:D:873:ALA:HB3	2.10	0.51
9:K:22:DA:H2''	9:K:23:DT:H71	1.89	0.51
2:C:247:THR:HG23	2:C:250:ASN:H	1.76	0.51
5:F:308:ASP:CB	7:G:119:ARG:NH1	2.73	0.51
8:J:36:DT:C5	8:J:37:DT:C7	2.92	0.51
5:F:345:ARG:O	5:F:345:ARG:NH1	2.44	0.51
8:J:36:DT:N1	8:J:37:DT:H72	2.20	0.51
2:C:387:TYR:HA	2:C:390:ASN:HD22	1.75	0.51
7:G:118:VAL:HA	7:G:121:PHE:HD2	1.67	0.51
2:C:121:ASP:N	2:C:121:ASP:OD1	2.44	0.51
2:C:486:LEU:HD11	2:C:531:LEU:HD12	1.92	0.50
5:F:308:ASP:CG	7:G:119:ARG:NH1	2.69	0.50
2:C:620:SER:OG	2:C:621:ALA:N	2.43	0.50
3:D:977:THR:O	3:D:994:GLN:N	2.44	0.50
2:C:233:LEU:HA	2:C:236:ILE:HD12	1.93	0.50
2:C:676:CYS:CB	2:C:710:TYR:CZ	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:443:ILE:HD11	2:C:448:LEU:HD21	1.94	0.50
7:G:116:ARG:HH21	7:G:116:ARG:CG	2.14	0.50
5:F:359:HIS:HD2	5:F:360:PRO:HD2	1.75	0.50
7:G:70:ASN:O	7:G:74:MET:HB2	2.12	0.50
10:L:59:TYR:CE2	10:L:63:ASN:ND2	2.80	0.50
1:B:110:ALA:HB2	1:B:123:PRO:HB2	1.94	0.49
3:D:148:GLN:HE22	3:D:150:LEU:HB2	1.77	0.49
9:K:51:DT:C6	9:K:52:DT:H71	2.47	0.49
10:L:87:LEU:O	10:L:91:THR:HG23	2.13	0.49
3:D:331:LEU:HD22	3:D:1166:ILE:HG13	1.93	0.49
2:C:363:VAL:HG23	2:C:390:ASN:HD21	1.77	0.49
2:C:791:HIS:CE1	2:C:917:ARG:HH11	2.31	0.49
3:D:103:HIS:HD2	3:D:228:LEU:HD22	1.78	0.49
9:K:53:DT:C4	9:K:54:DA:C5	3.01	0.49
2:C:289:ARG:HB2	2:C:350:PHE:HB2	1.95	0.49
3:D:36:TYR:OH	3:D:37:ARG:NH1	2.46	0.49
8:J:39:DT:C2	8:J:40:DA:N7	2.81	0.49
10:L:72:SER:OG	10:L:73:ASP:N	2.45	0.49
1:B:167:ASP:OD1	1:B:167:ASP:N	2.46	0.49
2:C:41:LEU:O	2:C:69:TYR:OH	2.24	0.49
5:F:317:VAL:O	5:F:321:ARG:HB2	2.12	0.49
7:G:19:TRP:CH2	7:G:114:LEU:HD21	2.43	0.49
7:G:76:LEU:HD23	1:I:260:VAL:HG22	1.93	0.49
1:B:64:GLU:OE2	3:D:601:ASP:N	2.46	0.48
2:C:789:SER:OG	2:C:790:ILE:N	2.46	0.48
2:C:1006:GLU:HA	6:H:31:ARG:HG3	1.95	0.48
3:D:693:THR:HG23	3:D:696:GLU:H	1.78	0.48
9:K:17:DG:H2'	9:K:18:DG:O5'	2.12	0.48
3:D:253:ASP:HB2	3:D:313:LEU:HD22	1.94	0.48
2:C:575:ALA:HB2	2:C:608:VAL:HG21	1.95	0.48
9:K:33:DC:H1'	9:K:34:DC:C5	2.48	0.48
2:C:1146:SER:OG	2:C:1147:GLY:N	2.46	0.48
3:D:278:SER:HA	3:D:281:VAL:HG22	1.94	0.48
1:I:291:LEU:HD21	1:I:296:LEU:HB2	1.95	0.48
2:C:181:TYR:HA	2:C:191:PRO:HA	1.95	0.48
7:G:60:ARG:HD3	9:K:57:DG:H5''	1.93	0.48
8:J:11:DA:H1'	8:J:12:DA:H5'	1.94	0.48
2:C:975:HIS:HB3	2:C:1004:LEU:HD11	1.95	0.48
3:D:451:ASP:OD1	3:D:451:ASP:N	2.47	0.48
3:D:772:THR:OG1	3:D:773:VAL:N	2.46	0.48
3:D:1163:GLU:HA	3:D:1166:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:28:LYS:HA	10:L:81:TRP:CZ2	2.49	0.48
2:C:397:ASP:OD1	2:C:397:ASP:N	2.47	0.48
3:D:903:TYR:O	3:D:1065:LYS:NZ	2.37	0.48
10:L:6:TYR:HB3	10:L:11:LEU:HG	1.95	0.48
2:C:180:VAL:H	2:C:221:LEU:HD21	1.79	0.48
2:C:184:ILE:HD11	2:C:195:LEU:HD21	1.96	0.48
3:D:53:GLY:H	3:D:88:ARG:HG3	1.79	0.48
5:F:158:MET:HG3	5:F:206:ALA:HB2	1.96	0.48
7:G:19:TRP:HH2	7:G:114:LEU:CD2	2.24	0.48
2:C:332:TYR:HD2	2:C:346:SER:H	1.62	0.47
2:C:962:VAL:HG11	3:D:658:VAL:HG11	1.96	0.47
3:D:1044:GLN:NE2	3:D:1068:GLU:OE2	2.47	0.47
4:E:2:LEU:N	4:E:5:SER:O	2.47	0.47
2:C:770:ASN:OD1	2:C:770:ASN:N	2.43	0.47
3:D:5:ASN:OD1	3:D:5:ASN:N	2.45	0.47
9:K:51:DT:C7	9:K:52:DT:H73	2.44	0.47
8:J:18:DT:H2''	8:J:19:DG:H8	1.79	0.47
10:L:57:GLN:HA	10:L:60:THR:HG22	1.96	0.47
2:C:682:VAL:HG22	2:C:692:VAL:HG12	1.97	0.47
3:D:34:ILE:HG22	5:F:209:ILE:HD12	1.95	0.47
3:D:136:VAL:HG12	3:D:148:GLN:HE21	1.79	0.47
9:K:33:DC:C2'	9:K:34:DC:C4	2.92	0.47
10:L:71:LEU:HD23	10:L:71:LEU:HA	1.82	0.47
8:J:53:DA:H2	9:K:9:DT:H3	1.63	0.47
10:L:73:ASP:OD1	10:L:74:GLN:N	2.46	0.47
1:B:110:ALA:N	1:B:123:PRO:O	2.48	0.47
2:C:182:VAL:N	2:C:190:LEU:O	2.39	0.46
2:C:319:LEU:HA	2:C:320:PRO:HD3	1.50	0.46
3:D:92:MET:HG2	3:D:235:PRO:HD3	1.95	0.46
2:C:672:ALA:HB1	2:C:746:PRO:HD2	1.97	0.46
2:C:680:GLY:HA2	2:C:736:VAL:N	2.31	0.46
1:A:11:THR:OG1	1:A:13:GLU:OE2	2.33	0.46
2:C:639:MET:HE3	2:C:639:MET:HB3	1.81	0.46
2:C:864:ILE:HD11	5:F:357:LEU:HB3	1.97	0.46
3:D:906:ASN:HB2	3:D:913:VAL:HG22	1.96	0.46
1:B:175:ARG:HG3	3:D:523:LEU:HD22	1.98	0.46
8:J:10:DA:N1	8:J:11:DA:N6	2.64	0.46
2:C:864:ILE:HA	5:F:354:LEU:HD11	1.98	0.46
6:H:10:LYS:O	6:H:41:LYS:NZ	2.47	0.46
8:J:39:DT:C2'	8:J:40:DA:H5'	2.42	0.46
2:C:858:GLU:HA	2:C:861:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1025:THR:OG1	3:D:1026:GLU:N	2.48	0.46
1:B:27:PRO:HB2	1:B:191:TYR:HD2	1.81	0.45
5:F:146:VAL:HA	5:F:149:ILE:HG22	1.97	0.45
2:C:1151:GLU:N	2:C:1151:GLU:CD	2.73	0.45
3:D:253:ASP:N	3:D:253:ASP:OD1	2.46	0.45
8:J:36:DT:H2''	8:J:37:DT:C6	2.50	0.45
1:A:99:ILE:HG12	1:A:112:ILE:HG12	1.99	0.45
2:C:1138:LEU:HD21	3:D:105:TRP:CZ2	2.52	0.45
2:C:455:ILE:CA	2:C:458:ILE:CG1	2.89	0.45
3:D:179:LEU:HD12	3:D:223:PRO:HB2	1.98	0.45
1:A:15:SER:OG	1:A:16:ASP:N	2.50	0.45
1:B:58:ILE:HG13	1:B:138:VAL:HG13	1.98	0.45
3:D:137:THR:OG1	3:D:138:ASP:N	2.50	0.45
7:G:64:PHE:HB2	7:G:89:LEU:HD13	1.98	0.45
2:C:328:PHE:O	2:C:332:TYR:OH	2.28	0.45
3:D:187:GLU:OE1	3:D:209:ARG:NH1	2.50	0.45
3:D:514:MET:HB2	3:D:537:VAL:HG13	1.97	0.45
5:F:213:VAL:HA	5:F:216:VAL:HG12	1.99	0.45
7:G:62:LYS:NZ	9:K:59:DT:H72	2.31	0.45
9:K:32:DT:H2''	9:K:33:DC:C5	2.51	0.45
2:C:865:PHE:HA	5:F:358:ARG:HD3	1.99	0.45
1:B:59:ASP:OD1	1:B:59:ASP:N	2.50	0.45
1:B:72:VAL:HG23	1:B:73:GLU:HG3	1.99	0.45
2:C:467:LEU:HD23	2:C:467:LEU:HA	1.83	0.45
2:C:648:VAL:HG11	2:C:1039:LYS:HD2	1.99	0.45
3:D:1111:ASN:CG	10:L:74:GLN:NE2	2.74	0.45
5:F:179:ASP:OD1	5:F:179:ASP:N	2.38	0.45
5:F:308:ASP:OD1	5:F:308:ASP:O	2.35	0.45
1:I:293:ARG:HE	1:I:293:ARG:HB2	1.58	0.45
9:K:44:DA:H2''	9:K:45:DC:H5''	2.00	0.45
2:C:1010:SER:OG	2:C:1013:ALA:N	2.48	0.44
7:G:115:PRO:HG2	7:G:118:VAL:HG21	1.99	0.44
9:K:51:DT:C6	9:K:52:DT:C7	3.01	0.44
1:A:222:ASN:HA	1:A:225:VAL:HG12	2.00	0.44
2:C:861:LEU:HA	2:C:864:ILE:HG22	2.00	0.44
3:D:58:TRP:HZ3	3:D:71:LYS:HA	1.82	0.44
8:J:39:DT:H2'	8:J:40:DA:C8	2.52	0.44
1:B:22:LYS:HB2	1:B:22:LYS:HE3	1.78	0.44
1:B:173:VAL:HA	1:B:200:THR:HA	1.98	0.44
8:J:19:DG:N2	9:K:43:DC:N3	2.52	0.44
1:B:200:THR:OG1	1:B:201:ASP:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:84:ARG:NH1	2:C:899:ASP:OD2	2.51	0.44
2:C:312:ARG:NH2	2:C:327:GLY:O	2.45	0.44
3:D:1115:THR:HA	10:L:63:ASN:ND2	2.32	0.44
2:C:88:TYR:HB3	2:C:126:ILE:HG23	1.99	0.44
2:C:98:LEU:N	2:C:107:LYS:O	2.42	0.44
10:L:71:LEU:CB	10:L:75:THR:HG23	2.46	0.44
1:A:70:GLY:O	1:A:131:GLY:N	2.46	0.44
3:D:1086:THR:OG1	3:D:1087:ASP:N	2.51	0.44
5:F:316:ASN:HD21	7:G:123:LEU:HB3	1.81	0.44
5:F:319:ARG:HA	5:F:324:LEU:HB2	1.98	0.44
8:J:19:DG:C2'	8:J:20:DA:C8	2.93	0.44
9:K:34:DC:C2'	9:K:35:DC:OP1	2.40	0.44
2:C:576:GLN:HE22	3:D:774:LEU:HD22	1.82	0.44
3:D:608:GLN:HE21	3:D:608:GLN:HB2	1.60	0.44
3:D:1123:ILE:HD13	3:D:1123:ILE:HA	1.88	0.44
3:D:1183:VAL:HG12	3:D:1184:LYS:H	1.82	0.44
10:L:78:LEU:HB2	10:L:81:TRP:CZ3	2.52	0.44
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.87	0.43
2:C:56:GLU:OE2	2:C:63:SER:OG	2.35	0.43
3:D:694:GLU:O	3:D:698:TYR:HB2	2.18	0.43
3:D:257:LEU:HB3	3:D:295:LEU:HD12	2.00	0.43
9:K:39:DC:H2''	9:K:40:DG:C8	2.53	0.43
2:C:262:PRO:HB2	2:C:264:ARG:H	1.83	0.43
3:D:387:LYS:O	3:D:391:GLU:HB3	2.18	0.43
8:J:52:DC:H2'	8:J:53:DA:N7	2.33	0.43
2:C:138:LEU:C	2:C:138:LEU:CD1	2.86	0.43
3:D:737:ASN:OD1	3:D:740:ASN:N	2.50	0.43
5:F:345:ARG:HD3	8:J:12:DA:H2'	2.00	0.43
1:B:192:ASP:OD1	1:B:192:ASP:N	2.52	0.43
2:C:293:THR:HG1	2:C:316:ASP:HB3	1.79	0.43
2:C:445:PRO:HA	2:C:448:LEU:HB2	2.01	0.43
3:D:620:LEU:HA	3:D:623:ILE:HG22	1.99	0.43
10:L:37:LEU:HA	10:L:40:ILE:HG22	2.00	0.43
1:A:90:TYR:O	1:A:144:ARG:NH2	2.52	0.43
8:J:19:DG:H1	9:K:43:DC:H42	1.67	0.43
3:D:455:MET:HB2	3:D:455:MET:HE3	1.79	0.43
1:A:42:ARG:NH2	1:B:34:THR:OG1	2.51	0.43
3:D:509:ALA:HB1	3:D:535:THR:HA	2.01	0.43
7:G:99:LYS:HD3	7:G:100:ARG:HG2	2.00	0.43
2:C:718:SER:HG	2:C:722:THR:H	1.60	0.43
3:D:14:LEU:H	3:D:221:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:748:ARG:HB2	3:D:763:ILE:HB	2.00	0.43
9:K:61:DA:H2"	9:K:62:DC:C5	2.51	0.43
3:D:104:ILE:HB	3:D:293:ASP:HB2	2.01	0.42
2:C:353:THR:HG22	2:C:354:ASP:H	1.83	0.42
2:C:213:GLU:HG2	2:C:361:ILE:HD12	2.01	0.42
2:C:681:ILE:HG22	2:C:693:ARG:CB	2.16	0.42
5:F:333:GLU:O	5:F:343:ARG:NH1	2.52	0.42
10:L:34:GLN:OE1	10:L:74:GLN:NE2	2.47	0.42
2:C:1049:HIS:NE2	2:C:1071:GLY:O	2.44	0.42
2:C:1062:GLN:NE2	3:D:330:ASN:OD1	2.52	0.42
7:G:74:MET:HA	7:G:75:PRO:HD3	1.89	0.42
9:K:53:DT:C5	9:K:54:DA:N7	2.87	0.42
2:C:939:LEU:HD13	2:C:940:PRO:HD2	2.00	0.42
2:C:1152:ILE:O	2:C:1153:GLU:C	2.62	0.42
7:G:32:ILE:HG22	7:G:37:LEU:HD21	2.00	0.42
8:J:36:DT:C2'	8:J:37:DT:OP2	2.68	0.42
2:C:180:VAL:HB	2:C:221:LEU:HD11	2.02	0.42
4:E:30:MET:HE2	4:E:30:MET:HB2	1.90	0.42
7:G:100:ARG:HE	7:G:100:ARG:HB3	1.51	0.42
9:K:61:DA:C2'	9:K:62:DC:C5	3.02	0.42
1:A:101:VAL:O	1:A:102:GLN:NE2	2.53	0.42
2:C:415:LEU:HD23	2:C:415:LEU:HA	1.90	0.42
3:D:390:ILE:HG22	3:D:397:VAL:HG21	2.00	0.42
7:G:47:ARG:HD3	1:I:252:THR:HG21	2.02	0.42
7:G:92:ARG:NH2	9:K:57:DG:N7	2.67	0.42
8:J:22:DC:H42	9:K:40:DG:H22	1.66	0.42
2:C:946:TYR:HA	2:C:952:PRO:HA	2.02	0.42
2:C:1152:ILE:HG22	2:C:1154:MET:H	1.84	0.42
7:G:120:PRO:O	7:G:121:PHE:C	2.63	0.42
1:I:269:ALA:HB2	1:I:288:VAL:HG13	2.00	0.42
1:B:187:GLN:HG2	1:B:188:VAL:HG23	2.01	0.42
2:C:111:VAL:HG21	2:C:449:ILE:HD11	2.01	0.42
2:C:576:GLN:HE22	3:D:774:LEU:HD13	1.84	0.42
2:C:1152:ILE:HG22	2:C:1154:MET:N	2.35	0.42
3:D:401:LEU:HA	3:D:404:VAL:HG12	2.02	0.42
2:C:761:VAL:HG23	2:C:955:ILE:HB	2.02	0.42
3:D:228:LEU:HD12	3:D:228:LEU:HA	1.81	0.42
3:D:846:ARG:HH22	3:D:888:SER:HB2	1.84	0.42
5:F:345:ARG:HH22	5:F:349:ILE:HD13	1.85	0.41
1:B:43:ILE:HG13	1:B:217:LEU:HD13	2.01	0.41
2:C:564:LEU:HD23	2:C:569:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:SER:HB3	8:J:3:DA:N7	2.35	0.41
8:J:24:DA:H2''	8:J:25:DA:H8	1.85	0.41
2:C:263:LYS:H	2:C:264:ARG:NH2	2.18	0.41
2:C:680:GLY:N	2:C:736:VAL:O	2.54	0.41
5:F:139:ALA:HA	5:F:171:LEU:HD21	2.00	0.41
5:F:288:THR:OG1	5:F:289:SER:N	2.53	0.41
6:H:5:VAL:HG11	6:H:37:LEU:HD21	2.02	0.41
8:J:36:DT:H2'	8:J:37:DT:H72	2.01	0.41
2:C:122:THR:O	2:C:483:LYS:NZ	2.42	0.41
3:D:326:ARG:HA	3:D:326:ARG:HD3	1.78	0.41
9:K:51:DT:H6	9:K:52:DT:H71	1.85	0.41
2:C:313:ARG:NE	2:C:315:LEU:O	2.47	0.41
3:D:601:ASP:N	3:D:601:ASP:OD1	2.51	0.41
6:H:4:LYS:NZ	6:H:58:GLU:OE1	2.37	0.41
9:K:33:DC:O3'	9:K:34:DC:H6	2.01	0.41
9:K:52:DT:H2'	9:K:53:DT:C2	2.56	0.41
1:A:59:ASP:N	1:A:59:ASP:OD1	2.54	0.41
7:G:62:LYS:HZ3	9:K:59:DT:C7	2.33	0.41
2:C:1152:ILE:CG2	2:C:1154:MET:CB	2.98	0.41
5:F:169:MET:HE3	5:F:173:LYS:HG2	2.03	0.41
5:F:252:LYS:HE2	5:F:252:LYS:HB2	1.82	0.41
5:F:333:GLU:HA	5:F:343:ARG:HE	1.86	0.41
9:K:54:DA:C2	9:K:55:DA:C6	3.09	0.41
3:D:25:PHE:CZ	3:D:91:ARG:HG2	2.56	0.41
3:D:382:ASN:HD21	5:F:368:ASP:HB2	1.86	0.41
3:D:537:VAL:HG12	3:D:538:ALA:H	1.85	0.41
1:B:183:THR:H	1:B:192:ASP:HA	1.84	0.41
2:C:140:ARG:HE	2:C:140:ARG:HB2	1.69	0.41
2:C:527:LEU:HD12	2:C:527:LEU:HA	1.90	0.41
2:C:1085:ALA:HB1	3:D:922:ILE:HG12	2.03	0.41
5:F:308:ASP:HB2	7:G:119:ARG:HH22	1.86	0.41
2:C:408:ARG:HE	2:C:408:ARG:HB2	1.72	0.40
8:J:58:DT:H2''	8:J:59:DG:C8	2.56	0.40
1:B:43:ILE:HD13	1:B:43:ILE:HA	1.91	0.40
1:B:117:ASP:OD1	1:B:117:ASP:N	2.53	0.40
2:C:968:ILE:HD12	2:C:968:ILE:HA	1.95	0.40
3:D:367:LYS:HE2	3:D:367:LYS:HB3	1.81	0.40
3:D:662:ASP:OD2	3:D:724:ASN:ND2	2.55	0.40
5:F:336:GLY:HA2	5:F:346:ILE:HD12	2.02	0.40
9:K:34:DC:C6	9:K:34:DC:P	3.13	0.40
10:L:59:TYR:O	10:L:62:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:HA	1:A:27:PRO:HA	1.91	0.40
3:D:767:PHE:HE1	3:D:771:LEU:HD11	1.86	0.40
7:G:51:ASP:N	7:G:55:GLU:OE2	2.42	0.40
3:D:751:MET:HE2	3:D:751:MET:HB3	1.85	0.40
5:F:319:ARG:O	5:F:324:LEU:N	2.42	0.40
2:C:434:ARG:HA	2:C:434:ARG:HD2	1.97	0.40
2:C:844:GLY:HA2	2:C:876:SER:HB3	2.03	0.40
2:C:928:ARG:HH11	2:C:928:ARG:HD3	1.74	0.40
3:D:974:ILE:HD12	3:D:974:ILE:HA	1.90	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	
1	A	222/314 (71%)	207 (93%)	15 (7%)	0	100	100
1	B	218/314 (69%)	197 (90%)	21 (10%)	0	100	100
1	I	65/314 (21%)	65 (100%)	0	0	100	100
2	C	1127/1193 (94%)	1025 (91%)	99 (9%)	3 (0%)	36	71
3	D	1130/1199 (94%)	1014 (90%)	113 (10%)	3 (0%)	36	71
4	E	60/67 (90%)	55 (92%)	5 (8%)	0	100	100
5	F	270/371 (73%)	242 (90%)	28 (10%)	0	100	100
6	H	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
7	G	127/131 (97%)	123 (97%)	4 (3%)	0	100	100
10	L	90/173 (52%)	78 (87%)	12 (13%)	0	100	100
All	All	3376/4145 (81%)	3067 (91%)	303 (9%)	6 (0%)	44	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1153	GLU
3	D	5	ASN
3	D	869	ASP
3	D	572	PRO
2	C	337	VAL
2	C	320	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 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	
1	A	145/273 (53%)	142 (98%)	3 (2%)	47	65
1	B	146/273 (54%)	143 (98%)	3 (2%)	47	65
1	I	59/273 (22%)	58 (98%)	1 (2%)	53	67
2	C	752/1026 (73%)	738 (98%)	14 (2%)	50	66
3	D	679/1027 (66%)	662 (98%)	17 (2%)	42	62
4	E	28/61 (46%)	27 (96%)	1 (4%)	31	52
5	F	192/329 (58%)	186 (97%)	6 (3%)	35	56
6	H	56/65 (86%)	55 (98%)	1 (2%)	51	66
7	G	123/124 (99%)	118 (96%)	5 (4%)	27	49
10	L	82/159 (52%)	82 (100%)	0	100	100
All	All	2262/3610 (63%)	2211 (98%)	51 (2%)	44	64

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	188	VAL
1	A	228	THR
1	B	9	ILE
1	B	198	VAL
1	B	220	HIS
2	C	138	LEU
2	C	161	THR

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Mol	Chain	Res	Type
2	C	174	THR
2	C	193	THR
2	C	317	LYS
2	C	319	LEU
2	C	331	LEU
2	C	420	PHE
2	C	613	VAL
2	C	677	LYS
2	C	879	VAL
2	C	1003	THR
2	C	1053	THR
2	C	1058	LEU
3	D	2	LEU
3	D	5	ASN
3	D	82	VAL
3	D	197	THR
3	D	350	LEU
3	D	457	VAL
3	D	711	VAL
3	D	758	ILE
3	D	772	THR
3	D	867	LEU
3	D	909	THR
3	D	979	VAL
3	D	984	VAL
3	D	1025	THR
3	D	1038	THR
3	D	1086	THR
3	D	1089	LEU
4	E	21	THR
5	F	154	VAL
5	F	175	VAL
5	F	288	THR
5	F	293	HIS
5	F	306	VAL
5	F	317	VAL
6	H	50	VAL
7	G	12	SER
7	G	25	ILE
7	G	116	ARG
7	G	122	GLN
7	G	129	LEU

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Mol	Chain	Res	Type
1	I	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	B	220	HIS
2	C	280	HIS
2	C	287	ASN
2	C	390	ASN
2	C	473	GLN
2	C	576	GLN
2	C	644	GLN
2	C	815	ASN
2	C	1062	GLN
2	C	1069	GLN
3	D	148	GLN
3	D	221	ASN
3	D	283	ASN
3	D	478	ASN
3	D	608	GLN
3	D	740	ASN
3	D	1044	GLN
3	D	1052	GLN
3	D	1058	GLN
3	D	1066	HIS
3	D	1164	ASN
5	F	142	ASN
5	F	316	ASN
7	G	70	ASN
7	G	86	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

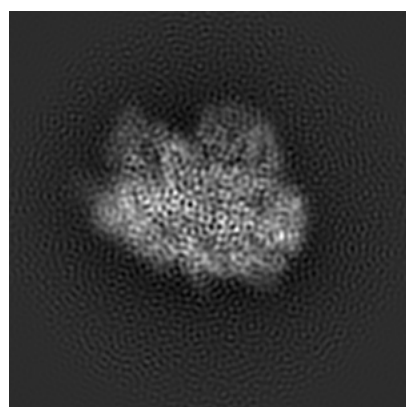
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31485. These allow visual inspection of the internal detail of the map and identification of artifacts.

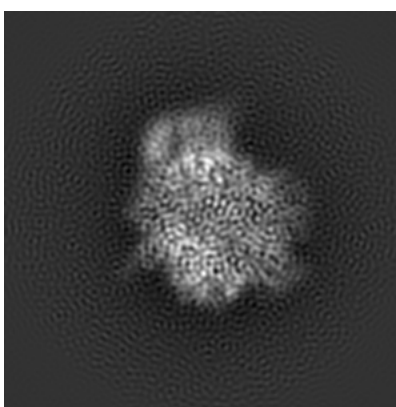
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

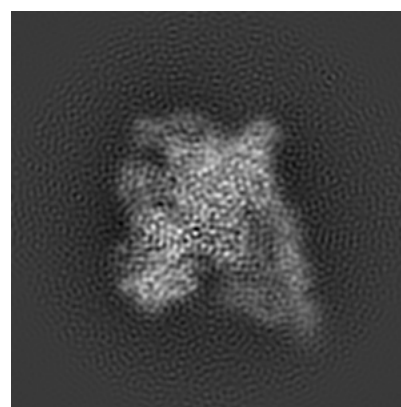
6.1.1 Primary map



X



Y

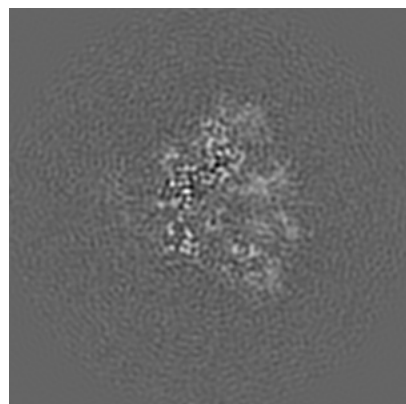


Z

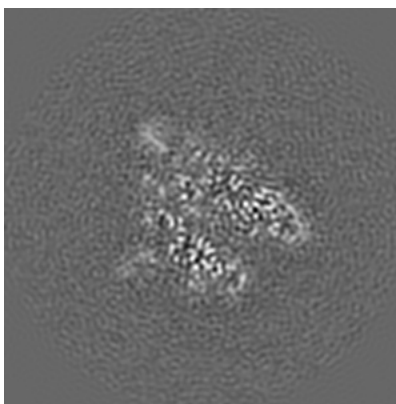
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

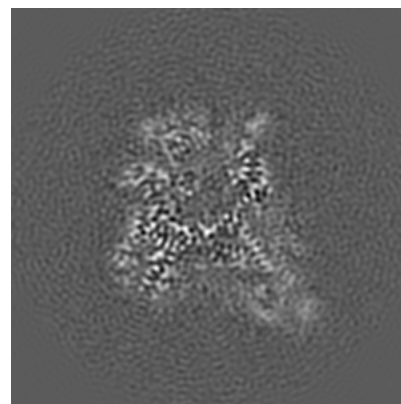
6.2.1 Primary map



X Index: 100



Y Index: 100

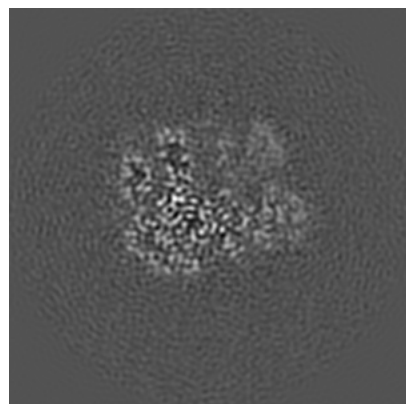


Z Index: 100

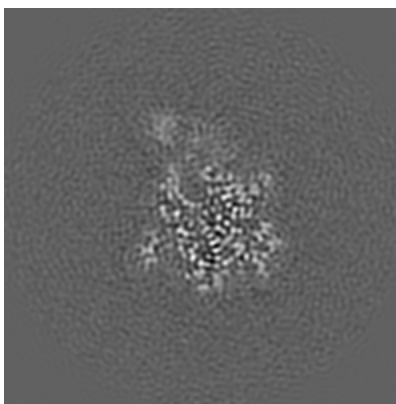
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

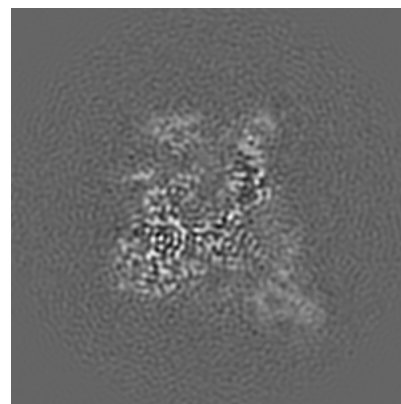
6.3.1 Primary map



X Index: 82



Y Index: 86

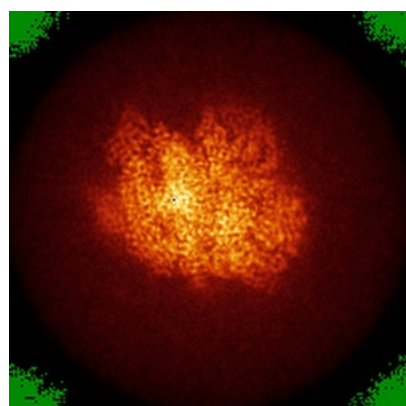


Z Index: 103

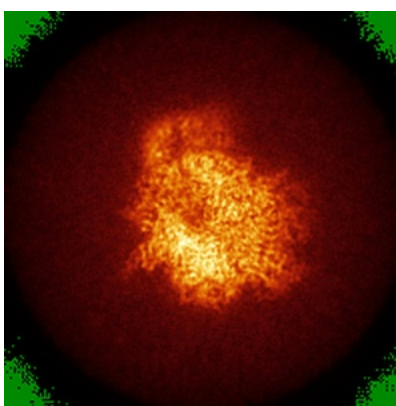
The images above show the largest variance slices of the map in three orthogonal directions.

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

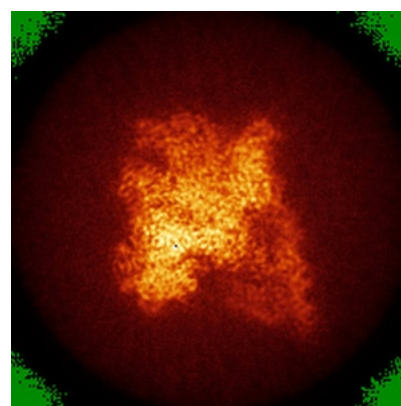
6.4.1 Primary map



X



Y

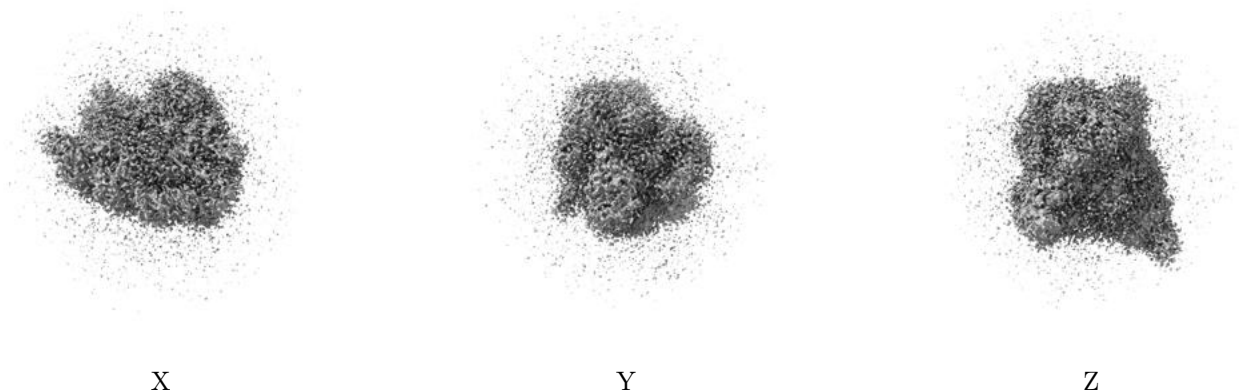


Z

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 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

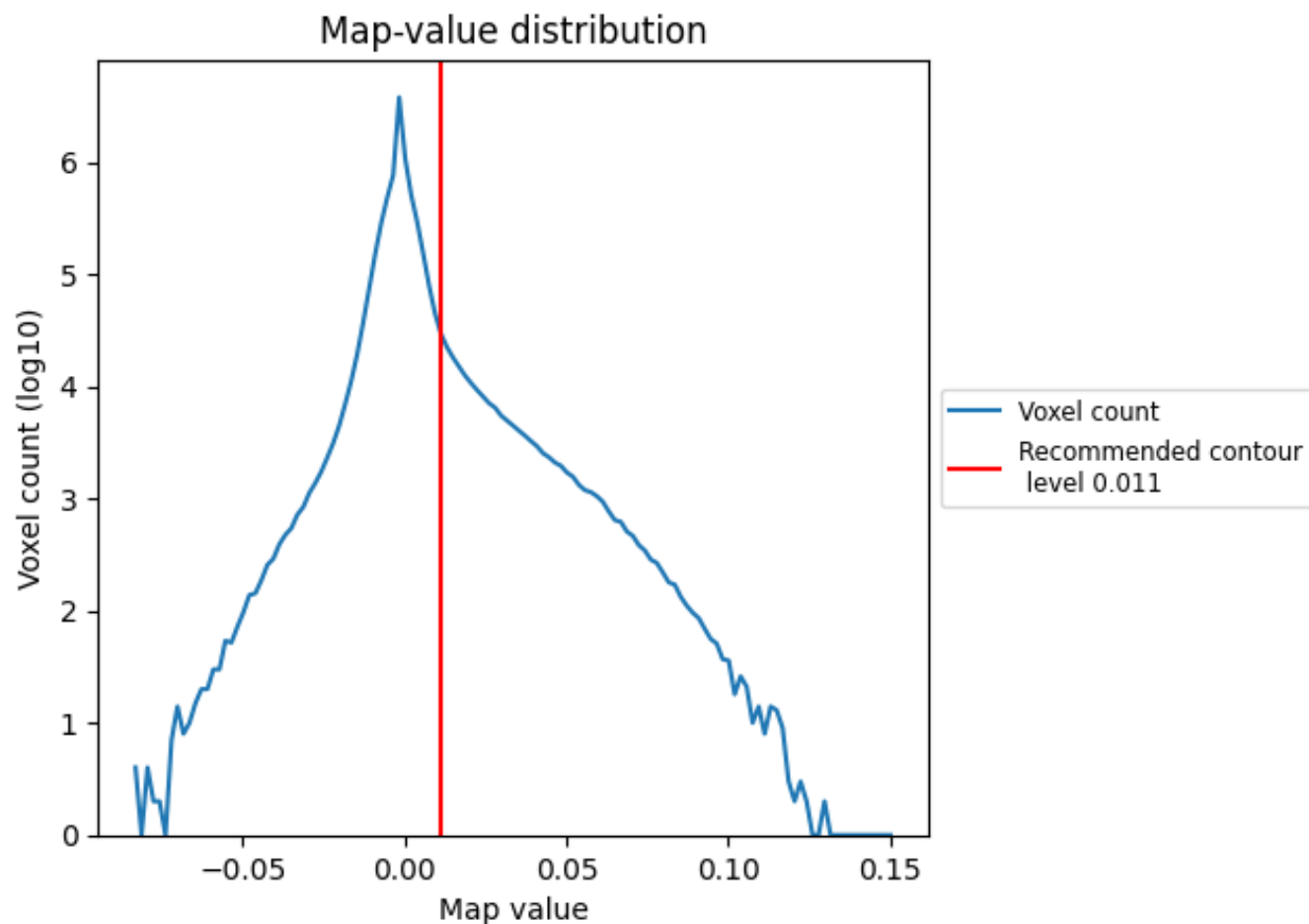
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

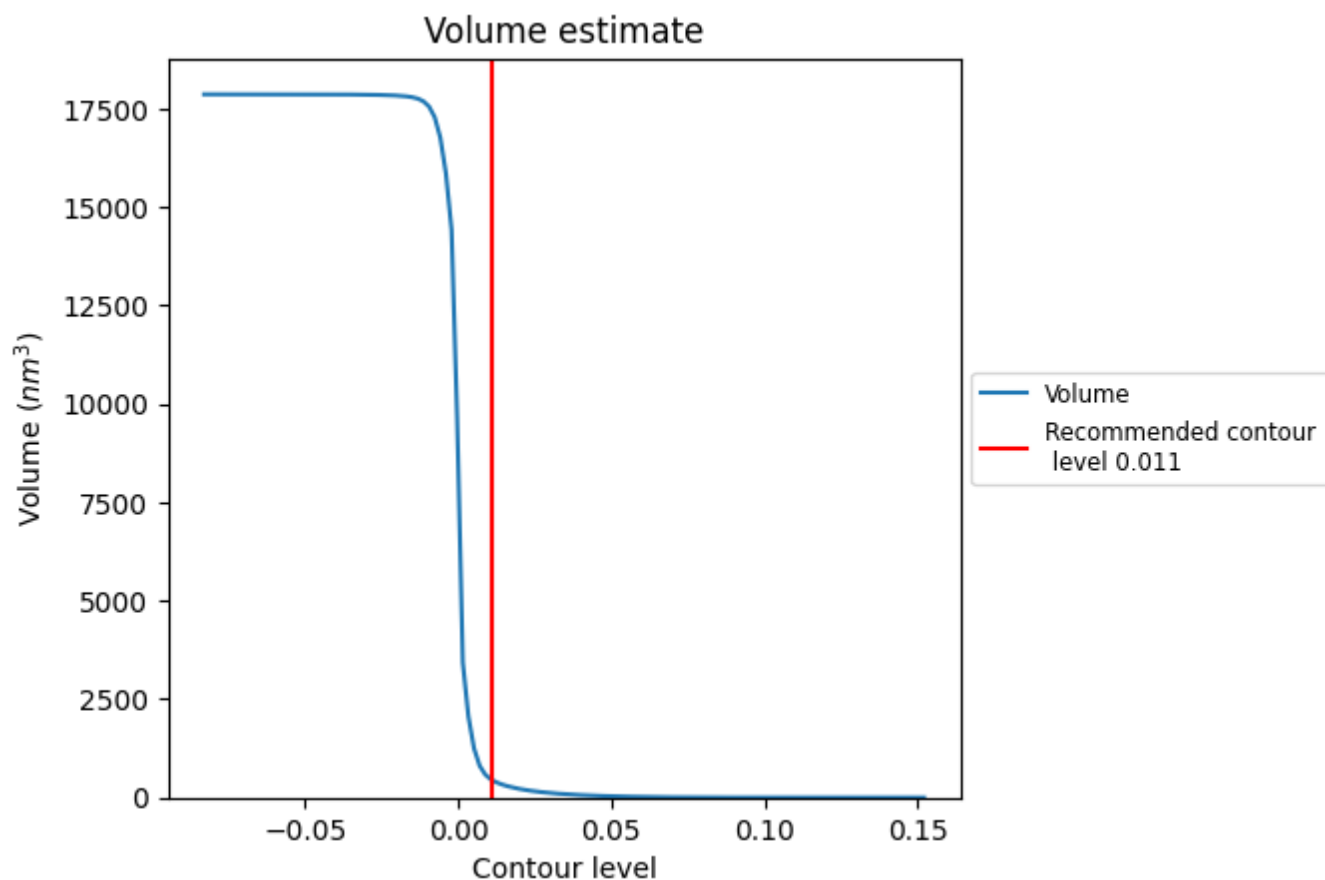
This section contains the results of statistical analysis of the map.

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.

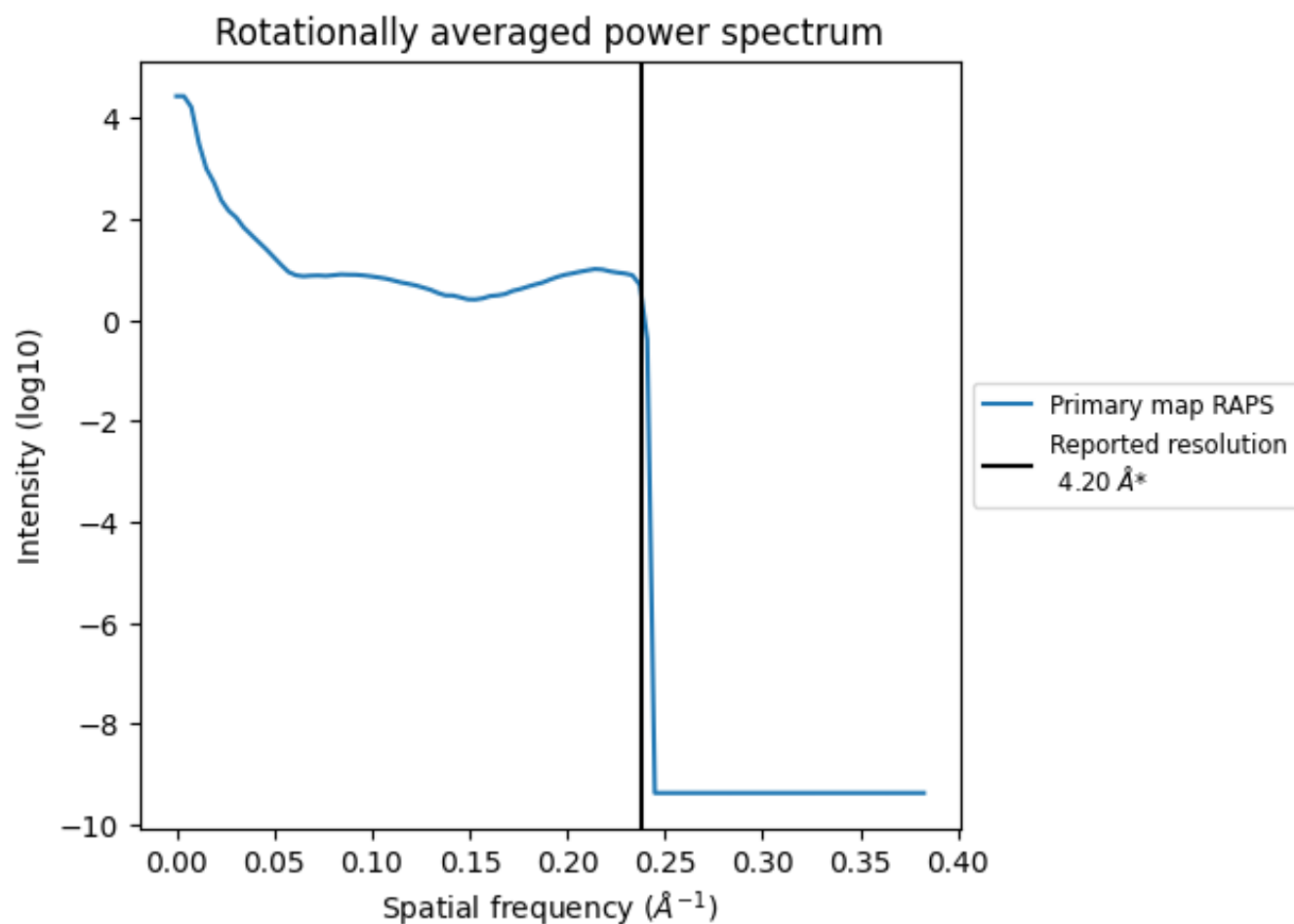
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 446 nm³; this corresponds to an approximate mass of 403 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 0.238 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

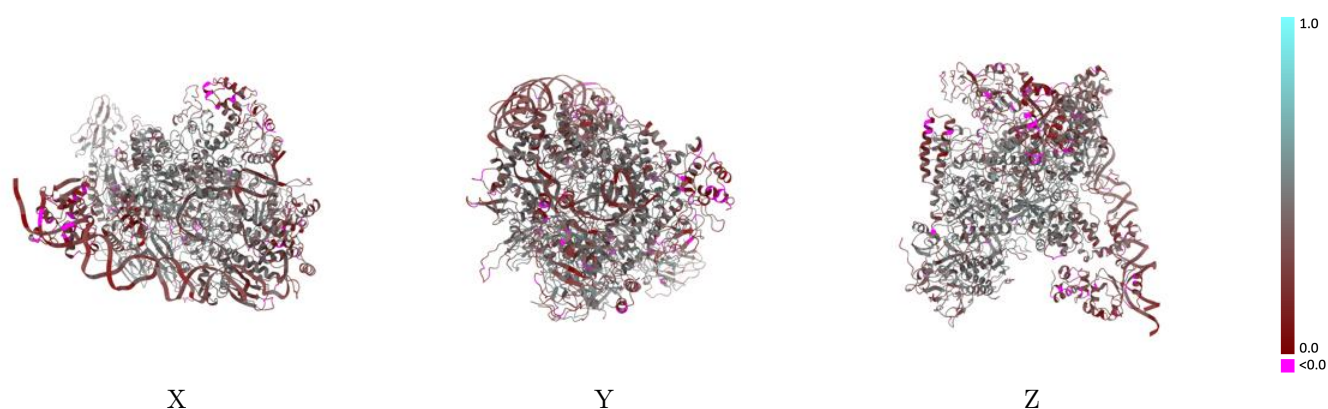
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31485 and PDB model 7F75. 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](#)

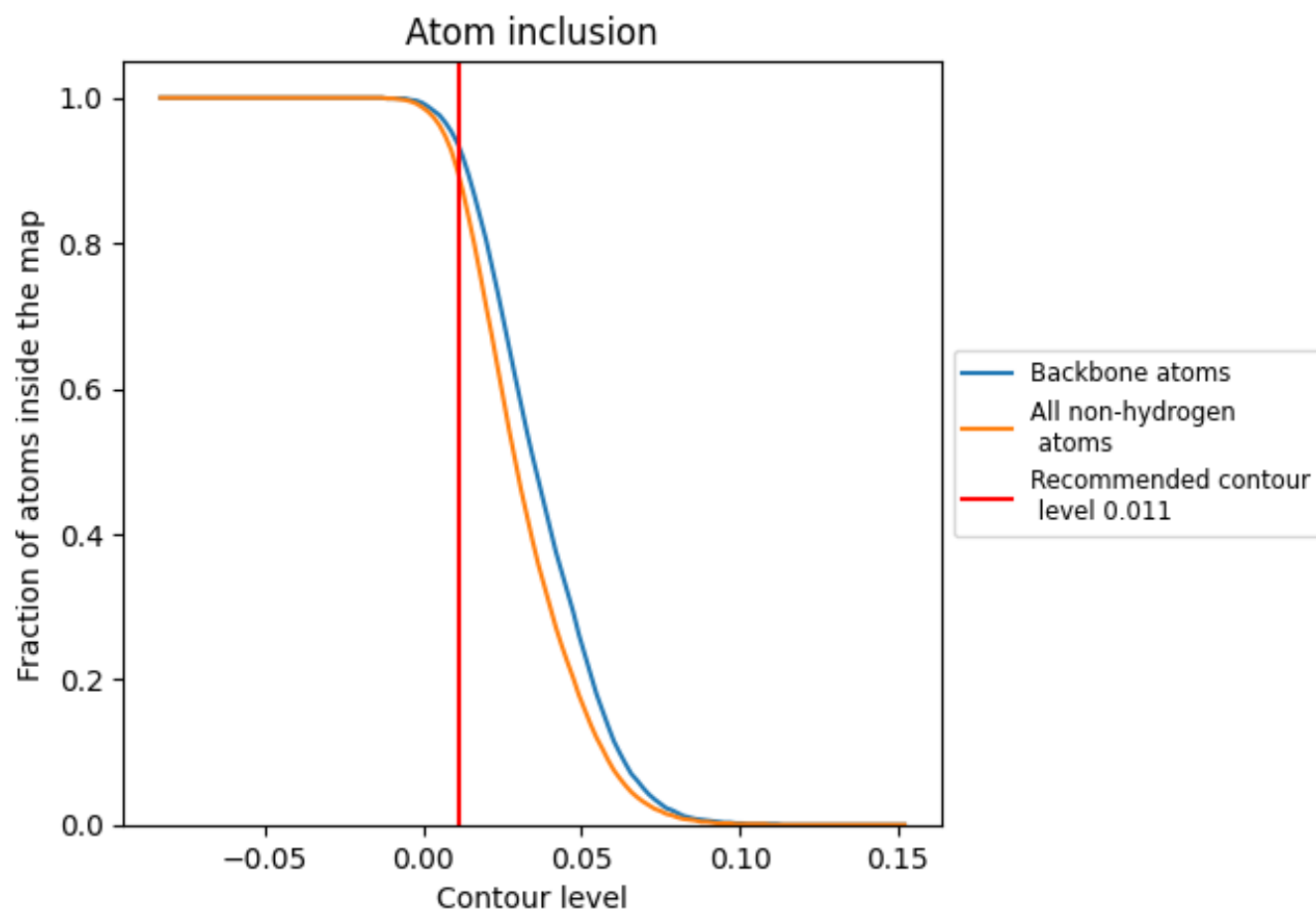


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.3700
A	0.9460	0.4510
B	0.9430	0.4160
C	0.9120	0.4100
D	0.9060	0.3980
E	0.8770	0.3780
F	0.9000	0.3450
G	0.8690	0.2240
H	0.8820	0.4080
I	0.7360	0.1760
J	0.9150	0.2490
K	0.9140	0.2700
L	0.5550	0.1310

1.0

0.0

<0.0