



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:53 PM UTC

PDB ID : 8OEU / pdb_00008oeu
EMDB ID : EMD-16835
Title : Structure of the mammalian Pol II-SPT6 complex (composite structure, Structure 4)
Authors : Chen, Y.; Kokic, G.; Dienemann, C.; Dybkov, O.; Urlaub, H.; Cramer, P.
Deposited on : 2023-03-13
Resolution : 3.04 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:

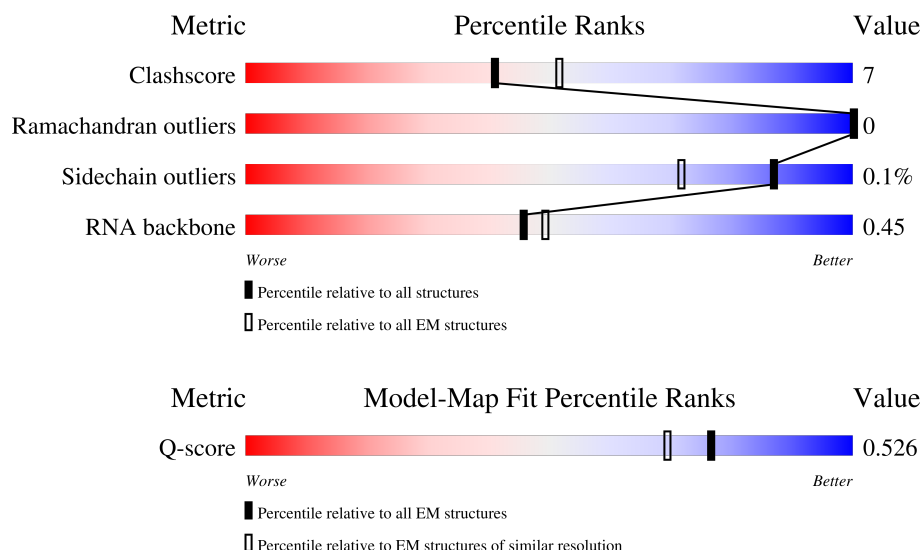
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.04 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	13952 (2.54 - 3.54)

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	A	1970	
2	B	1251	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	184	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	48	
14	P	46	
15	T	48	
16	S	1729	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 39178 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0
			11159	7024	2000	2064	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9047	5721	1592	1670	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	118	Total	C	N	O	S	0	0
			967	608	167	188	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1347	872	218	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			932	577	165	179	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			367	228	69	64	6		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	26	Total	C	N	O	P	0	0
			549	255	117	151	26		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	13	Total	C	N	O	P	0	0
			280	125	54	88	13		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	38	Total	C	N	O	P	0	0
			769	365	130	236	38		

- Molecule 16 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	819	Total	C	N	O	S	0	0
			6703	4260	1164	1246	33		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP Q7KZ85
S	-1	ASN	-	expression tag	UNP Q7KZ85
S	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	C	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	

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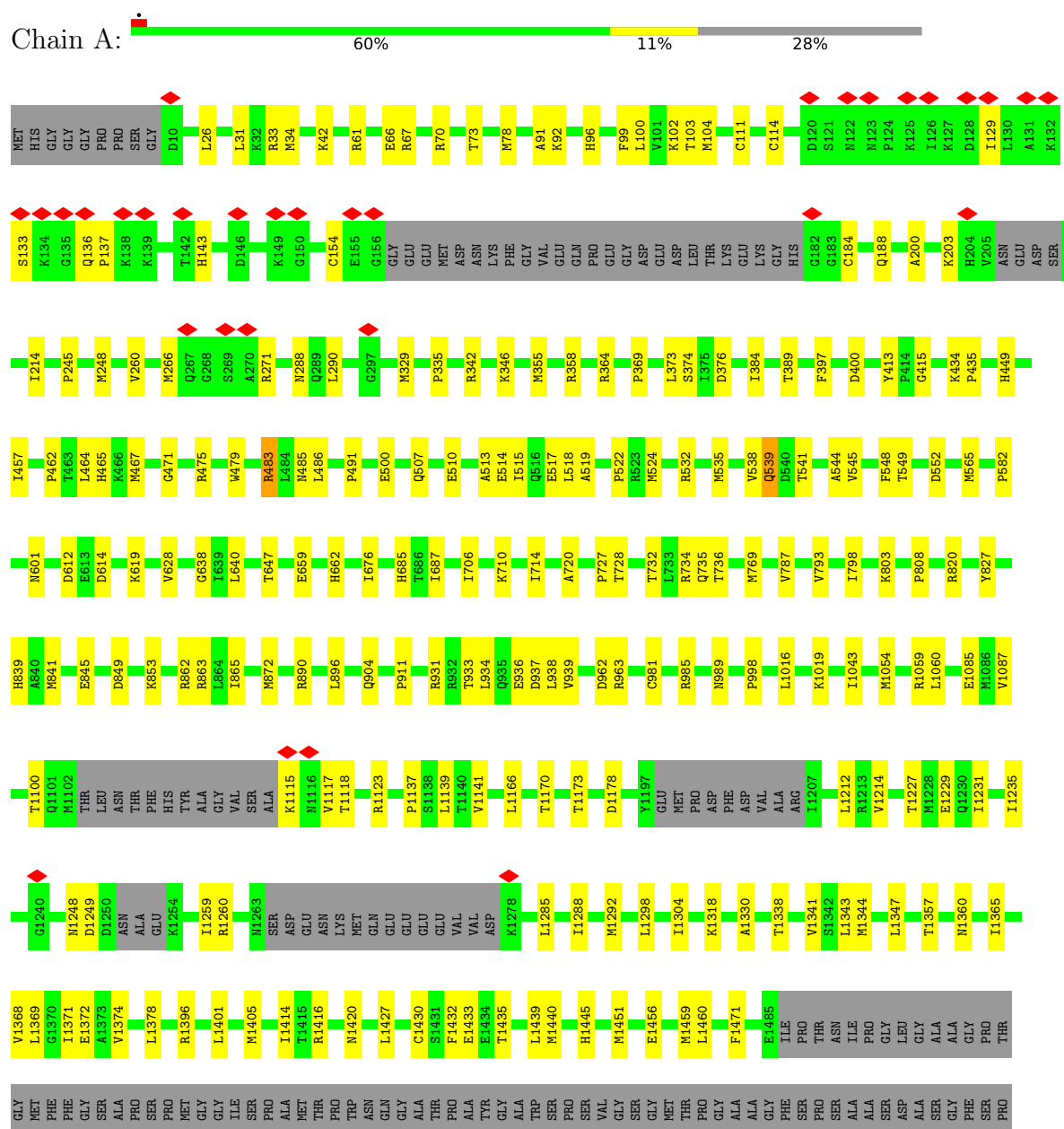
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	L	1	1	1	0

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 II subunit RPB1



[illegible]

- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B: 74% 16% 10%

1944	1948	1951	1954	1958	1963	1964	1971	1980	1982	1985	1990	1993	1997	1998	1999	2000	2001	2010	2015	2016	2019	2032	2044	2060	2105	2112	2113	2117	2130	2135	2138															
S803	A804	M805	G806	K807	Q808	A809	M810	I814	T815	V819	R820	M821	A825	H826	P831	Y843	L844	P850	V871	V878	R884	Y888	K897	F900	D901	Q902	E903	E904	E912	T913	C914	Q915	G916	M917	R918	H919	K924	R936	H937	S938	G939	D940	D941			
I644	E658	L664	Q670	M671	I674	M680	I681	R685	E686	R687	E688	I689	R690	C699	L702	L703	E706	L711	E722	Y725	V739	D743	T744	L745	E748	L752	A753	D758	K762	E763	V764	A765	C767	R768	R769	R775	M779									
L454	D461	H464	L470	G474	L476	M484	L489	V492	K504	A511	L521	M530	K534	K535	A536	H537	Q538	T551	S554	L562	N563	R568	D569	G570	K571	Q577	L578	L582	E590	L603	A604	L605	M606	I618	M627											
G320	GLY	GLN	GLY	ALA	LYS	LYS	SER	A328	Q331	R332	T336	R351	V356	S357	D358	L362	I366	M374	M375	V378	E384	A385	F386	V387	I388	Q389	E390	V393	A394	I398	K404	V407	E410	Q421	H427	V428	G429	D432	K438	V446						
L163	Q167	I168	Y169	L170	S171	R172	P173	E177	R178	D179	L195	P200	L281	Y202	T208	V209	I210	K211	E212	G213	E214	L217	I231	R234	L248	N252	E253	C254	I142	L271	D289	S300	C301	R304	R307	P308	T309	W313	V314	S315	M316	L317	A318	R319		
VAL	CYS	CYS	VAL	SER	LEU	ARG	GLY	PRO	GLY	SER	CYS	ALA	ASN	MET	LEU	ASP	ALA	ASP	GLU	ASP	GLN	TYR	ASP	GLU	ASP	ASP	D92	S108	F127	A139	P140	P141	I142	D143	A146	GLU	ALA	GLN	HIS	SER	PRO	ARG	TRP	LEU	LEU	ALA



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

Chain C: 75% 19% 6%



- Molecule 4: RNA polymerase II subunit D

Chain D: 46% 18% 36%



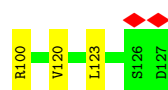
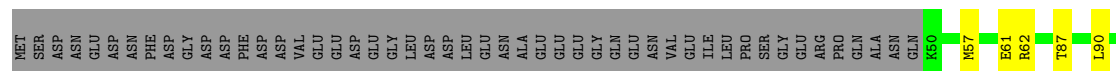
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 82% 17%



- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 55% 6% 39%



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

Chain G:  75% 24% ..



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

Chain H:  86% 13% .



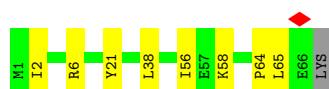
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  80% 13% 7%



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

Chain J:  87% 12% .



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

Chain K:  87% 11% .

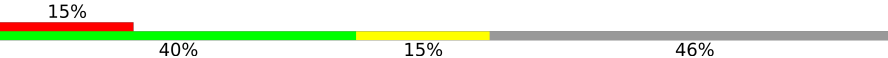


- Molecule 12: RNA polymerase II subunit K

Chain L:  67% 9% 24%



- Molecule 13: Non-template DNA

Chain N:  15% 40% 15% 46%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174029	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 ($e^-/\text{\AA}^2$)	40.09	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	59.731	Depositor
Minimum map value	-28.119	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.105	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/11360	0.50	2/15328 (0.0%)
2	B	0.29	0/9227	0.52	2/12454 (0.0%)
3	C	0.27	0/2115	0.42	0/2873
4	D	0.32	0/979	0.71	0/1312
5	E	0.27	0/1752	0.52	0/2366
6	F	0.26	0/636	0.49	0/859
7	G	0.38	0/1378	0.71	0/1870
8	H	0.24	0/1207	0.44	0/1628
9	I	0.22	0/954	0.56	0/1293
10	J	0.28	0/533	0.47	0/719
11	K	0.27	0/939	0.45	0/1271
12	L	0.27	0/372	0.53	0/493
13	N	0.18	0/619	0.29	0/954
14	P	0.17	0/313	0.22	0/486
15	T	0.24	0/857	0.39	0/1319
16	S	0.31	1/6826 (0.0%)	0.65	7/9194 (0.1%)
All	All	0.28	1/40067 (0.0%)	0.54	11/54419 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
7	G	0	1
16	S	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	S	860	LEU	C-O	6.20	1.32	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	867	ILE	N-CA-C	-7.41	103.06	110.62
1	A	483	ARG	CG-CD-NE	7.32	128.09	112.00
16	S	863	ASP	CA-C-N	-6.48	110.01	120.64
16	S	863	ASP	C-N-CA	-6.48	110.01	120.64
16	S	869	HIS	N-CA-C	-6.43	103.52	111.75
16	S	860	LEU	N-CA-C	-6.08	105.12	112.54
1	A	539	GLN	N-CA-C	5.66	122.85	110.80
16	S	863	ASP	CB-CA-C	-5.63	102.28	110.96
2	B	141	PRO	CA-N-CD	-5.51	104.28	112.00
16	S	866	ARG	N-CA-C	-5.30	106.66	113.23
2	B	900	PHE	N-CA-C	-5.15	106.95	113.18

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
1	A	539	GLN	Peptide
7	G	124	ASN	Peptide
16	S	1156	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11159	0	11304	148	0
2	B	9047	0	9080	131	0
3	C	2072	0	2019	36	0
4	D	967	0	973	22	0
5	E	1721	0	1737	25	0
6	F	626	0	657	6	0
7	G	1347	0	1347	29	0
8	H	1186	0	1147	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	932	0	856	14	0
10	J	524	0	540	7	0
11	K	920	0	942	9	0
12	L	367	0	367	5	0
13	N	549	0	289	5	0
14	P	280	0	142	2	0
15	T	769	0	429	10	0
16	S	6703	0	6683	126	0
17	A	1	0	0	0	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	39178	0	38512	524	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (524) 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)
16:S:836:LEU:HD12	16:S:867:ILE:CD1	1.85	1.05
16:S:836:LEU:CD1	16:S:867:ILE:CD1	2.52	0.87
5:E:115:LYS:NZ	5:E:129:GLN:OE1	2.07	0.86
16:S:836:LEU:HD12	16:S:867:ILE:HD13	1.56	0.85
16:S:836:LEU:CD1	16:S:867:ILE:HD13	2.11	0.78
2:B:208:THR:HA	2:B:217:LEU:O	1.85	0.76
16:S:925:ILE:HA	16:S:985:LEU:HD21	1.69	0.74
3:C:106:ARG:HG2	3:C:158:GLU:HG3	1.69	0.73
1:A:514:GLU:O	1:A:518:LEU:HB2	1.88	0.73
2:B:1219:ASN:HD21	2:B:1222:GLN:HB2	1.54	0.72
4:D:82:LEU:HD11	7:G:75:ILE:HD11	1.72	0.72
1:A:565:MET:HE1	11:K:74:ARG:HB3	1.71	0.71
1:A:1416:ARG:O	1:A:1420:ASN:HB2	1.91	0.70
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.75	0.69
16:S:864:VAL:HA	16:S:867:ILE:HD12	1.75	0.68
1:A:734:ARG:NH1	9:I:108:MET:SD	2.67	0.68
16:S:836:LEU:HD12	16:S:867:ILE:HD11	1.74	0.68
16:S:1016:GLN:HA	16:S:1020:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:PRO:HB2	2:B:850:PRO:HG2	1.77	0.67
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.77	0.66
1:A:129:ILE:HD13	1:A:143:HIS:HB3	1.76	0.66
6:F:100:ARG:NH1	6:F:123:LEU:O	2.29	0.66
1:A:1166:LEU:HG	1:A:1298:LEU:HD21	1.78	0.66
2:B:160:ARG:HB3	2:B:210:ILE:HB	1.78	0.65
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.62	0.64
2:B:627:MET:HG3	2:B:644:ILE:HD12	1.78	0.64
2:B:1153:GLU:HB2	2:B:1157:ARG:HH21	1.63	0.64
2:B:936:ARG:HE	2:B:980:ILE:HD11	1.63	0.64
2:B:578:LEU:HD12	2:B:582:LEU:HD12	1.81	0.63
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.79	0.63
16:S:755:VAL:HG23	16:S:923:PRO:HG2	1.80	0.63
2:B:301:CYS:HB2	2:B:309:THR:HG22	1.81	0.63
16:S:410:LYS:HD3	16:S:454:VAL:HB	1.80	0.62
16:S:1018:VAL:HG13	16:S:1019:THR:HG23	1.80	0.62
9:I:15:ARG:HE	9:I:37:TYR:HE2	1.48	0.62
16:S:1167:ILE:HD12	16:S:1232:LEU:HD11	1.79	0.61
7:G:52:ASP:HB2	7:G:71:LYS:HG3	1.82	0.61
1:A:517:GLU:OE1	6:F:62:ARG:NH1	2.32	0.61
2:B:317:LEU:O	2:B:331:GLN:NE2	2.34	0.61
16:S:322:ARG:NH2	16:S:455:GLN:OE1	2.33	0.61
16:S:604:GLN:O	16:S:608:GLN:NE2	2.33	0.61
16:S:866:ARG:HA	16:S:869:HIS:HB2	1.83	0.60
4:D:166:ASP:HA	4:D:169:LEU:HD12	1.82	0.60
2:B:300:SER:OG	2:B:427:HIS:ND1	2.31	0.59
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.83	0.59
7:G:82:GLY:N	7:G:147:ILE:O	2.33	0.59
2:B:387:VAL:HG13	2:B:388:ILE:HD12	1.85	0.59
16:S:644:PRO:HG2	16:S:647:GLU:HB2	1.85	0.59
1:A:1344:MET:HE2	5:E:134:GLU:HA	1.85	0.59
2:B:211:LYS:HB2	2:B:214:GLU:HB3	1.85	0.59
16:S:297:ARG:NH2	16:S:989:VAL:O	2.36	0.58
16:S:963:ILE:O	16:S:967:ASN:ND2	2.34	0.58
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	1.84	0.58
16:S:858:GLN:O	16:S:861:ILE:HG12	2.04	0.58
2:B:388:ILE:HG23	2:B:393:VAL:HG13	1.85	0.58
2:B:1186:GLU:HA	2:B:1190:PRO:HG3	1.86	0.58
4:D:76:ASN:OD1	4:D:144:ASN:ND2	2.37	0.58
2:B:1112:ARG:NH1	2:B:1113:LYS:O	2.37	0.58
16:S:523:MET:HA	16:S:526:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ASN:O	3:C:193:ARG:NH1	2.36	0.58
2:B:1197:ASN:HB2	2:B:1222:GLN:HB3	1.84	0.58
2:B:702:LEU:HD13	2:B:752:LEU:HD21	1.85	0.58
2:B:1192:GLN:HB3	2:B:1225:LEU:HD11	1.85	0.57
4:D:105:LYS:HE3	7:G:103:PRO:HA	1.86	0.57
1:A:798:ILE:O	1:A:820:ARG:NH1	2.37	0.57
2:B:252:ASN:HB3	2:B:819:VAL:HG21	1.86	0.57
3:C:59:LEU:HD13	3:C:63:PHE:HE2	1.69	0.57
13:N:31:DC:H42	15:T:18:DG:H1	1.52	0.57
16:S:836:LEU:HB2	16:S:867:ILE:HD13	1.87	0.57
2:B:1015:ARG:NH2	2:B:1060:GLU:OE2	2.36	0.57
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.87	0.57
16:S:369:GLN:O	16:S:1026:LYS:NZ	2.26	0.57
2:B:142:ILE:HB	2:B:163:LEU:HB2	1.87	0.57
2:B:307:ARG:HH11	2:B:308:PRO:HD2	1.70	0.57
3:C:81:LYS:HZ1	3:C:126:ARG:HH22	1.50	0.57
16:S:915:SER:O	16:S:919:ARG:N	2.36	0.57
16:S:1136:ASP:OD2	16:S:1138:ARG:NH2	2.36	0.57
7:G:130:THR:HG1	7:G:134:ASP:H	1.50	0.57
9:I:73:SER:HB2	9:I:115:THR:HA	1.87	0.57
15:T:41:DC:H2''	15:T:42:DT:H5''	1.86	0.57
2:B:982:ASP:OD1	2:B:1001:ARG:NH1	2.38	0.57
2:B:127:PHE:HB2	2:B:474:GLY:HA2	1.87	0.56
1:A:1365:ILE:HG23	1:A:1369:LEU:HD12	1.87	0.56
16:S:752:TRP:HZ3	16:S:940:LEU:HD23	1.71	0.56
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.76	0.56
2:B:703:LEU:HG	2:B:775:ILE:HG12	1.87	0.56
2:B:815:THR:HG21	10:J:58:LYS:HG3	1.87	0.56
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.39	0.56
7:G:97:LEU:HD21	7:G:137:ILE:HD12	1.87	0.56
16:S:884:LEU:HD23	16:S:1149:ILE:HG12	1.86	0.56
3:C:13:GLU:HB3	3:C:20:LYS:HB2	1.86	0.56
9:I:14:ILE:HG23	9:I:23:MET:HG3	1.87	0.56
2:B:351:ARG:NH1	2:B:388:ILE:O	2.39	0.56
2:B:606:MET:HE1	2:B:775:ILE:HD12	1.88	0.56
4:D:129:LEU:HB3	4:D:139:LEU:HG	1.88	0.56
1:A:346:LYS:NZ	15:T:24:DG:OP1	2.36	0.56
16:S:857:ALA:O	16:S:861:ILE:HG23	2.04	0.56
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.39	0.56
16:S:1111:LEU:HD13	16:S:1119:LYS:HB2	1.87	0.56
2:B:484:MET:HE1	2:B:521:LEU:HG	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:172:ARG:NH1	5:E:210:GLN:OE1	2.38	0.55
1:A:687:ILE:HB	1:A:769:MET:HE1	1.88	0.55
2:B:658:GLU:OE1	9:I:74:GLN:NE2	2.40	0.55
1:A:1173:THR:HG22	1:A:1214:VAL:HG13	1.88	0.55
1:A:373:LEU:O	1:A:485:ASN:ND2	2.40	0.55
1:A:479:TRP:H	1:A:483:ARG:HH22	1.54	0.55
3:C:211:LEU:HD23	3:C:215:GLU:HB3	1.87	0.55
16:S:1014:ARG:HH11	16:S:1060:PRO:HD3	1.72	0.55
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.88	0.55
1:A:1401:LEU:HG	1:A:1405:MET:HE2	1.88	0.55
1:A:33:ARG:HB3	2:B:1216:GLY:HA2	1.88	0.54
1:A:78:MET:O	2:B:1149:ARG:NH2	2.39	0.54
4:D:150:ALA:N	4:D:170:GLN:OE1	2.39	0.54
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.89	0.54
2:B:421:GLN:NE2	2:B:432:ASP:OD1	2.40	0.54
13:N:32:DA:H61	15:T:17:DT:H3	1.54	0.54
16:S:552:ASP:OD2	16:S:556:ARG:NE	2.39	0.54
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.89	0.54
1:A:845:GLU:OE1	2:B:577:GLN:NE2	2.40	0.54
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.89	0.54
16:S:1156:GLU:OE1	16:S:1160:THR:OG1	2.19	0.54
11:K:40:HIS:O	11:K:44:ASN:HB2	2.07	0.54
16:S:1014:ARG:NH1	16:S:1058:VAL:O	2.39	0.54
16:S:589:ARG:NH1	16:S:708:GLN:OE1	2.40	0.54
1:A:1285:LEU:HA	1:A:1288:ILE:HG12	1.88	0.54
2:B:108:SER:HG	2:B:843:TYR:HH	1.54	0.54
2:B:924:LYS:HA	12:L:51:ARG:HH22	1.72	0.54
1:A:544:ALA:O	1:A:548:PHE:HB2	2.08	0.54
2:B:429:GLY:O	2:B:438:LYS:NZ	2.39	0.54
2:B:878:VAL:O	2:B:884:ARG:NH2	2.35	0.54
2:B:606:MET:HE2	2:B:779:MET:HG3	1.90	0.54
9:I:29:ASP:O	9:I:33:ARG:N	2.41	0.54
16:S:329:THR:OG1	16:S:331:SER:O	2.24	0.54
16:S:373:VAL:HG13	16:S:393:LEU:HB3	1.90	0.54
16:S:378:PHE:O	16:S:381:LYS:NZ	2.35	0.53
5:E:110:MET:HE3	5:E:129:GLN:HG3	1.90	0.53
16:S:312:GLU:OE1	16:S:367:ARG:NH1	2.41	0.53
16:S:751:ASN:OD1	16:S:754:ARG:NH2	2.41	0.53
16:S:980:PRO:HA	16:S:983:GLN:HG3	1.90	0.53
2:B:810:MET:HG2	2:B:826:HIS:HB3	1.90	0.53
1:A:342:ARG:NH1	2:B:1238:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:PRO:O	1:A:1059:ARG:NH1	2.42	0.53
9:I:29:ASP:O	9:I:33:ARG:HA	2.09	0.53
5:E:104:ILE:HD11	5:E:127:LEU:HD23	1.90	0.53
16:S:836:LEU:HD13	16:S:864:VAL:HG13	1.89	0.53
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.44	0.52
5:E:17:ILE:HG21	5:E:74:VAL:HG11	1.92	0.52
16:S:365:PHE:HB3	16:S:371:PHE:HB2	1.91	0.52
7:G:124:ASN:OD1	7:G:125:PRO:HD3	2.09	0.52
16:S:687:GLU:HA	16:S:690:LYS:HD2	1.91	0.52
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	1.92	0.52
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.41	0.52
16:S:885:VAL:HB	16:S:916:LEU:HD23	1.91	0.52
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.90	0.52
5:E:192:LYS:HE3	5:E:194:ILE:HD11	1.92	0.52
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.91	0.52
1:A:26:LEU:HG	2:B:1245:ALA:HB2	1.92	0.52
2:B:904:GLU:HG2	2:B:948:VAL:HB	1.92	0.52
16:S:748:LYS:HD2	16:S:942:PHE:HA	1.91	0.52
1:A:1416:ARG:NH2	15:T:21:DT:O2	2.43	0.52
2:B:470:LEU:HD22	2:B:562:LEU:HD22	1.92	0.52
3:C:70:LEU:HD22	10:J:6:ARG:HG3	1.91	0.52
5:E:18:MET:HE1	5:E:60:VAL:HG11	1.92	0.52
1:A:358:ARG:NH1	15:T:27:DT:OP1	2.43	0.51
1:A:565:MET:HG3	11:K:62:LYS:HD2	1.93	0.51
4:D:146:CYS:HB3	4:D:177:GLN:HE22	1.75	0.51
16:S:1241:PRO:HG2	16:S:1244:PHE:HB2	1.92	0.51
16:S:420:MET:HE1	16:S:474:ASP:HB2	1.93	0.51
2:B:944:ILE:HB	2:B:971:THR:HB	1.92	0.51
1:A:931:ARG:NE	1:A:936:GLU:OE2	2.43	0.51
1:A:720:ALA:HB1	9:I:108:MET:HG3	1.92	0.51
2:B:688:GLU:OE1	2:B:690:ARG:NH1	2.44	0.51
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.92	0.51
2:B:554:SER:HA	2:B:807:LYS:HG2	1.93	0.51
6:F:57:MET:HE1	6:F:120:VAL:HG13	1.91	0.51
9:I:68:ILE:HB	9:I:122:ARG:HD3	1.92	0.51
2:B:551:THR:OG1	2:B:809:ALA:O	2.24	0.51
2:B:825:ALA:HB3	2:B:888:TYR:HB2	1.91	0.51
16:S:316:GLU:OE2	16:S:367:ARG:NH1	2.43	0.51
1:A:1139:LEU:HD21	1:A:1343:LEU:HA	1.91	0.51
16:S:1054:ASP:OD1	16:S:1063:TYR:OH	2.22	0.51
2:B:605:LEU:HD21	2:B:844:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:2:ALA:O	8:H:84:ARG:NH2	2.42	0.51
1:A:467:MET:HG3	1:A:524:MET:HB3	1.93	0.50
1:A:491:PRO:HG3	1:A:535:MET:HE2	1.93	0.50
1:A:1368:VAL:HG12	1:A:1369:LEU:HG	1.92	0.50
3:C:19:VAL:HG12	3:C:241:PRO:HB2	1.92	0.50
1:A:114:CYS:HB3	1:A:184:CYS:SG	2.51	0.50
2:B:685:ARG:NH1	2:B:686:GLU:OE2	2.39	0.50
4:D:112:ARG:NH2	7:G:142:GLU:OE2	2.32	0.50
2:B:139:ALA:HB1	2:B:489:LEU:HD11	1.92	0.50
2:B:1032:PRO:HB2	2:B:1105:LEU:HD23	1.93	0.50
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.44	0.50
1:A:1433:GLU:HG2	15:T:22:DC:H5"	1.94	0.50
16:S:1236:VAL:HG12	16:S:1275:PHE:HD2	1.76	0.50
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.93	0.50
2:B:167:GLN:NE2	2:B:168:ILE:O	2.40	0.50
2:B:871:VAL:HG12	2:B:1044:ILE:HG22	1.94	0.50
2:B:897:LYS:HG3	2:B:993:TYR:HE1	1.77	0.50
16:S:903:PHE:HB3	16:S:906:TYR:HB2	1.93	0.50
2:B:664:LEU:HB3	2:B:680:MET:SD	2.51	0.50
2:B:703:LEU:HD23	2:B:739:VAL:HG12	1.93	0.50
1:A:541:THR:HG23	1:A:676:ILE:HB	1.94	0.50
1:A:911:PRO:O	1:A:963:ARG:NH2	2.39	0.50
9:I:29:ASP:O	9:I:33:ARG:CA	2.59	0.50
2:B:234:ARG:NH2	2:B:254:CYS:O	2.45	0.50
2:B:351:ARG:NH2	2:B:358:ASP:OD1	2.45	0.50
16:S:992:LEU:HD23	16:S:997:GLY:HA2	1.93	0.50
1:A:329:MET:HA	1:A:335:PRO:HA	1.94	0.49
2:B:706:GLU:HB2	2:B:711:LEU:HD21	1.94	0.49
16:S:379:TYR:OH	16:S:1033:GLY:O	2.26	0.49
1:A:200:ALA:HB3	1:A:214:ILE:HG22	1.94	0.49
2:B:673:ILE:HD12	2:B:673:ILE:H	1.77	0.49
16:S:412:ASN:OD1	16:S:415:ARG:NH2	2.44	0.49
16:S:787:SER:HB2	16:S:792:HIS:CD2	2.48	0.49
16:S:1059:HIS:HB3	16:S:1062:THR:HG22	1.95	0.49
1:A:510:GLU:HG3	7:G:62:GLY:HA2	1.93	0.49
1:A:614:ASP:HA	1:A:619:LYS:HG3	1.93	0.49
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.95	0.49
2:B:1171:GLN:HB2	2:B:1180:LEU:HD13	1.93	0.49
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.94	0.49
16:S:862:GLU:OE1	16:S:865:LYS:HD3	2.13	0.49
2:B:390:GLU:HG2	2:B:393:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:ASN:O	4:D:110:THR:OG1	2.30	0.49
7:G:122:ASN:O	16:S:405:GLN:NE2	2.45	0.49
16:S:618:ILE:HG21	16:S:665:LEU:HD13	1.95	0.49
1:A:465:HIS:CD2	1:A:467:MET:HE2	2.45	0.49
2:B:924:LYS:HG2	12:L:51:ARG:HH12	1.78	0.49
5:E:106:VAL:HG23	5:E:131:LEU:HD13	1.94	0.49
16:S:597:ALA:HA	16:S:721:LEU:HD21	1.95	0.49
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.95	0.49
1:A:728:THR:H	1:A:736:THR:HG21	1.76	0.49
2:B:177:GLU:HG2	2:B:179:ASP:H	1.77	0.49
3:C:20:LYS:NZ	3:C:207:GLU:OE2	2.45	0.49
2:B:362:LEU:HD11	2:B:378:VAL:HG11	1.95	0.48
11:K:42:LEU:HD23	11:K:45:ILE:HD11	1.94	0.48
16:S:800:ASN:O	16:S:921:GLN:NE2	2.45	0.48
5:E:56:THR:N	5:E:78:GLU:OE2	2.41	0.48
16:S:421:GLN:NE2	16:S:443:LEU:O	2.42	0.48
1:A:66:GLU:OE2	1:A:271:ARG:NH1	2.47	0.48
16:S:1111:LEU:HD12	16:S:1123:LEU:HD11	1.96	0.48
1:A:1430:CYS:O	1:A:1435:THR:OG1	2.27	0.48
16:S:319:TRP:NE1	16:S:455:GLN:O	2.47	0.48
16:S:800:ASN:N	16:S:804:GLU:O	2.43	0.48
1:A:827:TYR:OH	1:A:839:HIS:NE2	2.40	0.48
4:D:86:ARG:NH2	7:G:35:GLU:OE2	2.47	0.48
1:A:706:ILE:HD11	1:A:787:VAL:HG21	1.95	0.48
1:A:1451:MET:HE1	1:A:1460:LEU:HD13	1.95	0.48
7:G:39:THR:O	7:G:43:GLY:N	2.47	0.48
1:A:96:HIS:HB3	1:A:99:PHE:HB2	1.96	0.48
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.96	0.47
4:D:71:ALA:HB1	7:G:5:ILE:HG22	1.95	0.47
7:G:93:ASN:OD1	7:G:94:LYS:N	2.47	0.47
1:A:374:SER:OG	1:A:376:ASP:OD1	2.26	0.47
7:G:34:VAL:O	7:G:37:THR:OG1	2.29	0.47
5:E:66:ASP:OD1	5:E:66:ASP:N	2.46	0.47
1:A:727:PRO:HA	1:A:736:THR:HG21	1.95	0.47
16:S:1265:CYS:SG	16:S:1279:LEU:HD23	2.55	0.47
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.96	0.47
1:A:1372:GLU:HG3	5:E:193:ILE:HG12	1.97	0.47
2:B:1130:HIS:HB3	2:B:1135:LYS:HE3	1.96	0.47
16:S:454:VAL:HG11	16:S:460:LEU:HD13	1.95	0.47
2:B:162:LEU:HB3	2:B:208:THR:OG1	2.15	0.47
2:B:315:SER:OG	2:B:316:MET:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:PHE:O	2:B:389:GLN:NE2	2.45	0.47
2:B:765:ALA:C	2:B:767:CYS:H	2.22	0.47
3:C:108:ASN:O	3:C:155:LYS:NZ	2.42	0.47
7:G:13:LEU:HD21	7:G:17:TYR:HB2	1.97	0.47
16:S:853:GLU:OE2	16:S:887:ASN:ND2	2.47	0.47
2:B:699:CYS:HA	2:B:743:ASP:HA	1.97	0.47
2:B:753:ALA:HB1	2:B:758:ASP:HB2	1.97	0.47
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.96	0.47
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.95	0.47
16:S:836:LEU:CB	16:S:867:ILE:HD13	2.45	0.47
16:S:915:SER:HA	16:S:918:ARG:HB2	1.97	0.47
1:A:364:ARG:NE	1:A:500:GLU:OE1	2.38	0.47
16:S:742:ILE:HG23	16:S:954:LEU:HD12	1.97	0.47
16:S:890:ALA:HB1	16:S:912:GLN:HG3	1.97	0.47
1:A:808:PRO:HG2	2:B:752:LEU:HD12	1.97	0.47
1:A:91:ALA:HB3	1:A:290:LEU:HD22	1.97	0.47
1:A:732:THR:HG23	1:A:735:GLN:H	1.80	0.47
1:A:1235:ILE:HG12	1:A:1292:MET:HE3	1.97	0.47
1:A:1115:LYS:HE3	1:A:1117:VAL:HB	1.96	0.46
12:L:18:ILE:HD11	12:L:47:LYS:HD3	1.96	0.46
1:A:397:PHE:HB3	6:F:87:THR:HG23	1.96	0.46
1:A:896:LEU:O	1:A:1396:ARG:NH1	2.49	0.46
1:A:1318:LYS:HD2	1:A:1330:ALA:HB1	1.97	0.46
2:B:940:ASP:OD2	14:P:34:G:N2	2.47	0.46
3:C:7:PRO:HB3	3:C:26:THR:HB	1.97	0.46
16:S:836:LEU:CD1	16:S:867:ILE:HD12	2.43	0.46
1:A:389:THR:O	1:A:507:GLN:NE2	2.47	0.46
2:B:386:PHE:CZ	9:I:40:ARG:HG3	2.50	0.46
2:B:461:ASP:HB3	2:B:464:HIS:HB2	1.97	0.46
3:C:214:ASP:OD1	3:C:214:ASP:N	2.47	0.46
7:G:14:HIS:ND1	7:G:16:ARG:HG3	2.30	0.46
1:A:266:MET:HE1	14:P:37:G:H1'	1.96	0.46
1:A:471:GLY:N	1:A:519:ALA:O	2.40	0.46
1:A:260:VAL:O	1:A:342:ARG:NH2	2.44	0.46
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.97	0.46
2:B:1168:ARG:HG2	2:B:1180:LEU:HD11	1.97	0.46
1:A:475:ARG:NH2	11:K:68:GLU:OE2	2.42	0.46
1:A:552:ASP:O	8:H:24:ARG:NH1	2.48	0.46
1:A:1304:ILE:HG23	1:A:1338:THR:HB	1.97	0.46
2:B:142:ILE:O	2:B:162:LEU:HA	2.16	0.46
2:B:313:TRP:HB2	2:B:336:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:LEU:HD21	4:D:156:LEU:HD13	1.97	0.46
16:S:1036:LYS:HG2	16:S:1134:TYR:CZ	2.50	0.46
1:A:104:MET:HE2	1:A:104:MET:HB3	1.80	0.46
1:A:931:ARG:HG3	1:A:939:VAL:HG11	1.97	0.46
2:B:670:GLN:NE2	2:B:672:ASP:OD2	2.36	0.46
5:E:5:GLU:OE1	5:E:9:ARG:NH2	2.49	0.46
3:C:130:VAL:HG11	3:C:237:GLY:HA3	1.97	0.46
1:A:154:CYS:SG	1:A:184:CYS:HB2	2.56	0.46
1:A:904:GLN:NE2	1:A:981:CYS:O	2.49	0.46
15:T:34:DT:H3'	15:T:35:DG:H3'	1.98	0.46
2:B:618:ILE:HG12	2:B:674:ILE:HG13	1.99	0.45
2:B:1182:GLU:HG3	2:B:1186:GLU:HG2	1.97	0.45
3:C:7:PRO:HB2	11:K:101:LEU:HD13	1.98	0.45
8:H:136:GLU:O	8:H:139:SER:OG	2.32	0.45
1:A:102:LYS:HZ2	1:A:1445:HIS:CE1	2.35	0.45
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.43	0.45
8:H:40:ILE:O	8:H:123:MET:HA	2.17	0.45
1:A:100:LEU:O	1:A:103:THR:OG1	2.32	0.45
1:A:413:TYR:O	1:A:449:HIS:ND1	2.33	0.45
2:B:209:VAL:HB	2:B:217:LEU:HB3	1.97	0.45
2:B:454:LEU:O	9:I:103:ARG:NH1	2.49	0.45
1:A:1248:ASN:OD1	1:A:1249:ASP:N	2.50	0.45
16:S:836:LEU:HD13	16:S:867:ILE:CD1	2.40	0.45
2:B:351:ARG:HD3	2:B:356:VAL:HA	1.98	0.45
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.81	0.45
9:I:61:GLU:OE2	9:I:61:GLU:N	2.50	0.45
4:D:61:GLN:HA	4:D:159:SER:HB3	1.99	0.45
16:S:1025:PRO:HA	16:S:1028:PHE:HB3	1.98	0.45
7:G:51:ILE:HD12	7:G:54:ILE:HD11	1.98	0.45
16:S:1107:PHE:O	16:S:1111:LEU:N	2.45	0.45
2:B:332:ARG:HD2	2:B:384:GLU:HG3	1.99	0.45
16:S:303:ILE:HG21	16:S:404:THR:HG21	1.99	0.45
16:S:889:LEU:HD12	16:S:930:VAL:HG11	1.98	0.45
1:A:513:ALA:HB2	6:F:90:LEU:HD11	1.99	0.45
1:A:1439:LEU:HD13	2:B:1239:LEU:HD21	1.99	0.45
16:S:374:PRO:HG2	16:S:990:CYS:HB3	1.99	0.45
16:S:658:LEU:HD12	16:S:658:LEU:HA	1.81	0.45
1:A:1378:LEU:HD21	1:A:1405:MET:HE3	1.98	0.45
2:B:314:VAL:HG11	2:B:446:VAL:HG22	1.99	0.44
4:D:135:HIS:HB3	4:D:138:GLU:HG2	1.99	0.44
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:174:ASP:O	4:D:178:THR:OG1	2.31	0.44
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.98	0.44
1:A:849:ASP:O	1:A:853:LYS:HB3	2.16	0.44
2:B:985:MET:HE3	2:B:997:LYS:HB2	1.99	0.44
5:E:15:LYS:NZ	5:E:33:LEU:O	2.48	0.44
1:A:582:PRO:HD2	8:H:47:ILE:HD12	2.00	0.44
1:A:1427:LEU:HD22	1:A:1459:MET:HE1	1.99	0.44
2:B:590:GLU:HG3	2:B:803:SER:HB3	1.99	0.44
7:G:59:ILE:HG13	7:G:66:VAL:HG22	1.99	0.44
2:B:1139:ARG:NH1	2:B:1158:ASP:O	2.50	0.44
1:A:545:VAL:O	1:A:549:THR:OG1	2.29	0.44
2:B:171:SER:HB3	2:B:200:PRO:HG2	1.99	0.44
16:S:413:LEU:HD12	16:S:413:LEU:HA	1.85	0.44
1:A:793:VAL:HG21	1:A:841:MET:HE2	2.00	0.44
2:B:897:LYS:HG3	2:B:993:TYR:CE1	2.53	0.44
3:C:61:ASP:OD2	12:L:48:ARG:NH2	2.38	0.44
4:D:118:ASN:O	4:D:121:THR:OG1	2.34	0.44
16:S:474:ASP:O	16:S:477:LYS:NZ	2.33	0.44
16:S:668:ASP:OD1	16:S:668:ASP:N	2.51	0.44
16:S:859:MET:C	16:S:861:ILE:N	2.75	0.44
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.99	0.43
2:B:606:MET:HG3	2:B:779:MET:HG3	2.00	0.43
16:S:938:LEU:HD11	16:S:955:LEU:HD21	1.98	0.43
16:S:989:VAL:HB	16:S:992:LEU:HD13	1.99	0.43
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.82	0.43
2:B:563:ASN:OD1	2:B:568:ARG:NH2	2.46	0.43
2:B:1016:HIS:NE2	2:B:1060:GLU:OE1	2.40	0.43
3:C:225:LYS:CG	3:C:226:PRO:HD2	2.48	0.43
5:E:60:VAL:HB	5:E:74:VAL:HB	2.00	0.43
11:K:12:LEU:HD11	11:K:18:LYS:HD3	2.00	0.43
13:N:34:DC:H2'	13:N:35:DA:C8	2.53	0.43
1:A:102:LYS:HD3	1:A:102:LYS:HA	1.88	0.43
1:A:355:MET:HB3	2:B:1165:GLU:HG2	1.99	0.43
5:E:9:ARG:O	5:E:13:ILE:HG12	2.18	0.43
7:G:89:VAL:HG21	7:G:97:LEU:HD23	1.99	0.43
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.53	0.43
16:S:1147:GLU:O	16:S:1151:ASN:ND2	2.51	0.43
1:A:865:ILE:HG21	2:B:1169:ASP:CG	2.43	0.43
13:N:37:DG:H2''	13:N:38:DG:H5'	2.00	0.43
1:A:1085:GLU:HB3	1:A:1087:VAL:HG13	2.00	0.43
7:G:38:CYS:SG	7:G:157:ILE:HG13	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:756:ALA:HB3	16:S:1140:ALA:HA	2.01	0.43
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.54	0.43
2:B:375:MET:HA	2:B:378:VAL:HG12	2.00	0.43
2:B:897:LYS:HG2	2:B:903:GLU:HG2	2.00	0.43
1:A:61:ARG:O	1:A:73:THR:OG1	2.35	0.43
4:D:142:LEU:HD21	4:D:157:ILE:HG13	2.00	0.43
2:B:169:TYR:N	2:B:202:TYR:O	2.44	0.43
7:G:12:LEU:HD23	7:G:12:LEU:HA	1.89	0.43
8:H:88:PHE:CG	8:H:144:LEU:HB3	2.54	0.43
10:J:2:ILE:HD12	10:J:56:ILE:HD13	2.00	0.43
16:S:574:VAL:HG11	16:S:581:PRO:HG3	1.99	0.43
16:S:695:ARG:HB2	16:S:706:ASN:HD21	1.83	0.43
16:S:1167:ILE:HD13	16:S:1267:ILE:HD11	2.00	0.43
1:A:70:ARG:HH12	2:B:1208:ARG:HH22	1.65	0.43
8:H:6:PHE:HE1	8:H:37:MET:HE3	1.83	0.43
16:S:686:PHE:HE1	16:S:713:ILE:HG23	1.84	0.43
16:S:754:ARG:HE	16:S:754:ARG:HB3	1.51	0.43
1:A:26:LEU:HD11	2:B:1240:MET:HG2	2.01	0.42
1:A:129:ILE:O	1:A:133:SER:N	2.46	0.42
1:A:464:LEU:HD13	1:A:1100:THR:HG21	2.01	0.42
1:A:1123:ARG:NH2	1:A:1360:ASN:O	2.48	0.42
16:S:370:HIS:HB2	16:S:1026:LYS:HE2	2.00	0.42
16:S:1065:TRP:CD1	16:S:1111:LEU:HD21	2.54	0.42
1:A:434:LYS:HG2	1:A:435:PRO:HD2	2.00	0.42
1:A:532:ARG:HD2	1:A:647:THR:O	2.18	0.42
1:A:1170:THR:HG21	1:A:1173:THR:HG23	2.01	0.42
2:B:234:ARG:HH21	2:B:248:LEU:HD13	1.83	0.42
16:S:303:ILE:HD11	16:S:405:GLN:HG3	2.02	0.42
16:S:1070:ALA:HB1	16:S:1088:ALA:HB1	2.01	0.42
2:B:394:ALA:O	2:B:398:ILE:HG12	2.20	0.42
7:G:84:VAL:HA	7:G:145:LEU:O	2.19	0.42
16:S:382:GLU:HG3	16:S:1121:ILE:HG12	2.00	0.42
16:S:863:ASP:O	16:S:867:ILE:HG13	2.19	0.42
1:A:203:LYS:HD3	1:A:203:LYS:HA	1.87	0.42
2:B:1143:PRO:HB2	2:B:1152:MET:HG3	2.01	0.42
3:C:49:TRP:O	3:C:163:ALA:HA	2.19	0.42
4:D:65:PRO:HG2	4:D:68:PHE:CD2	2.55	0.42
16:S:366:MET:HE1	16:S:396:VAL:HG12	2.01	0.42
1:A:384:ILE:HG12	2:B:1138:SER:HB3	2.01	0.42
1:A:1231:ILE:O	1:A:1235:ILE:HD12	2.20	0.42
16:S:445:THR:O	16:S:449:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:O	1:A:288:ASN:ND2	2.32	0.42
1:A:685:HIS:NE2	1:A:769:MET:HE2	2.35	0.42
2:B:1113:LYS:HB2	3:C:194:HIS:HB3	2.02	0.42
16:S:379:TYR:HE2	16:S:1033:GLY:HA3	1.85	0.42
16:S:1036:LYS:HG2	16:S:1134:TYR:CE2	2.55	0.42
1:A:937:ASP:OD1	1:A:938:LEU:N	2.53	0.42
1:A:1372:GLU:OE1	5:E:195:ARG:NH1	2.50	0.42
2:B:173:PRO:HG3	2:B:231:ILE:HG13	2.01	0.42
2:B:722:GLU:HB3	2:B:725:TYR:HB2	2.00	0.42
4:D:129:LEU:HD13	4:D:132:LYS:HE2	2.01	0.42
16:S:793:PRO:HB3	16:S:812:PRO:HB3	2.01	0.42
3:C:154:ARG:HH11	10:J:64:PRO:HD3	1.85	0.42
7:G:104:MET:HB2	7:G:104:MET:HE3	1.79	0.42
16:S:516:LYS:HE2	16:S:516:LYS:HB3	1.84	0.42
16:S:796:CYS:SG	16:S:809:LEU:HB3	2.60	0.42
1:A:136:GLN:HA	1:A:137:PRO:HD3	1.90	0.41
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.01	0.41
2:B:938:SER:N	2:B:941:ASP:OD2	2.52	0.41
5:E:81:LYS:HE2	5:E:81:LYS:HB3	1.85	0.41
2:B:535:LYS:HB3	2:B:538:GLN:HE21	1.85	0.41
2:B:562:LEU:HD11	2:B:603:LEU:HD23	2.02	0.41
3:C:189:ASP:HB3	3:C:218:ALA:HB2	2.02	0.41
4:D:177:GLN:OE1	4:D:180:ARG:NH1	2.51	0.41
1:A:612:ASP:OD1	1:A:612:ASP:N	2.48	0.41
1:A:1118:THR:HG23	1:A:1123:ARG:HD3	2.01	0.41
1:A:1440:MET:HE2	2:B:1242:MET:HE2	2.02	0.41
3:C:103:LEU:HB3	3:C:161:LEU:HG	2.01	0.41
13:N:30:DC:H42	15:T:19:DG:H1	1.68	0.41
16:S:686:PHE:CZ	16:S:714:GLU:HB3	2.55	0.41
7:G:83:GLU:O	7:G:146:LYS:HA	2.20	0.41
8:H:20:LYS:HE2	8:H:22:PHE:O	2.20	0.41
9:I:118:HIS:O	9:I:118:HIS:ND1	2.46	0.41
16:S:606:LEU:O	16:S:609:THR:OG1	2.32	0.41
16:S:861:ILE:HG13	16:S:862:GLU:N	2.36	0.41
1:A:803:LYS:HG3	2:B:748:GLU:OE2	2.20	0.41
4:D:127:SER:O	4:D:131:GLN:OE1	2.39	0.41
7:G:14:HIS:CE1	7:G:16:ARG:HG3	2.56	0.41
7:G:122:ASN:HD22	16:S:302:SER:HB2	1.85	0.41
16:S:754:ARG:O	16:S:1139:THR:OG1	2.38	0.41
16:S:836:LEU:HD13	16:S:867:ILE:HD12	2.01	0.41
1:A:710:LYS:O	1:A:714:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:LEU:HA	1:A:1019:LYS:HG2	2.03	0.41
2:B:476:LEU:HB3	2:B:530:TRP:CZ2	2.56	0.41
5:E:194:ILE:HG13	5:E:204:ILE:HG12	2.02	0.41
16:S:792:HIS:HA	16:S:793:PRO:HD3	1.91	0.41
1:A:245:PRO:HA	1:A:248:MET:HE1	2.01	0.41
1:A:413:TYR:O	1:A:415:GLY:N	2.51	0.41
1:A:462:PRO:HG3	15:T:24:DG:H21	1.86	0.41
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.45	0.41
1:A:890:ARG:HA	1:A:890:ARG:HD3	1.86	0.41
2:B:982:ASP:OD2	2:B:999:ARG:NH2	2.44	0.41
7:G:30:LEU:O	7:G:34:VAL:HG12	2.21	0.41
16:S:917:ALA:O	16:S:921:GLN:HB2	2.21	0.41
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.73	0.41
1:A:872:MET:HE3	1:A:872:MET:HB2	1.89	0.41
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.88	0.41
4:D:129:LEU:HD22	4:D:132:LYS:HZ1	1.86	0.41
16:S:695:ARG:O	16:S:706:ASN:ND2	2.54	0.41
16:S:1059:HIS:CD2	16:S:1060:PRO:HD2	2.55	0.41
2:B:366:ILE:HG12	2:B:374:MET:SD	2.61	0.41
2:B:492:VAL:HG13	2:B:511:ALA:HB1	2.03	0.41
2:B:605:LEU:HD23	2:B:605:LEU:HA	1.81	0.41
2:B:743:ASP:OD1	2:B:743:ASP:N	2.53	0.41
2:B:805:MET:SD	2:B:1019:LYS:HE3	2.60	0.41
3:C:7:PRO:HD2	11:K:100:LEU:HD23	2.03	0.41
16:S:332:LEU:O	16:S:333:GLN:NE2	2.54	0.41
16:S:992:LEU:HD12	16:S:1031:CYS:SG	2.60	0.41
16:S:1057:ARG:H	16:S:1129:GLU:CD	2.28	0.41
2:B:814:ILE:HD12	2:B:814:ILE:HA	1.94	0.41
16:S:1004:LEU:O	16:S:1008:ASN:N	2.51	0.41
1:A:92:LYS:HG2	1:A:290:LEU:HD21	2.01	0.40
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	2.02	0.40
5:E:153:LYS:HE3	5:E:153:LYS:HB2	1.91	0.40
7:G:145:LEU:HD12	7:G:161:GLY:HA3	2.02	0.40
16:S:308:ALA:HB3	16:S:313:LEU:HD12	2.02	0.40
16:S:1099:LEU:HD12	16:S:1127:ARG:HD3	2.02	0.40
1:A:933:THR:HG22	1:A:934:LEU:HG	2.03	0.40
2:B:195:LEU:HA	2:B:990:GLN:HE21	1.85	0.40
2:B:821:MET:HE1	2:B:985:MET:HB2	2.02	0.40
16:S:1268:MET:HB2	16:S:1268:MET:HE3	1.83	0.40
1:A:31:LEU:HD23	1:A:34:MET:HE2	2.02	0.40
1:A:369:PRO:HB3	1:A:486:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:THR:HG23	1:A:1229:GLU:HG3	2.04	0.40
2:B:681:ILE:HD13	2:B:745:LEU:HD23	2.03	0.40
2:B:1117:GLN:HE21	3:C:195:THR:HG1	1.62	0.40
3:C:56:SER:HB2	3:C:158:GLU:H	1.86	0.40
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.56	0.40
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.96	0.40
10:J:65:LEU:HD21	12:L:45:TYR:CG	2.57	0.40
11:K:61:TYR:HA	11:K:72:ILE:O	2.21	0.40
16:S:550:LEU:HB3	16:S:605:VAL:HG11	2.04	0.40
16:S:1026:LYS:HA	16:S:1026:LYS:HD2	1.88	0.40
1:A:400:ASP:OD1	1:A:400:ASP:N	2.54	0.40
3:C:246:LEU:HD23	3:C:246:LEU:HA	1.89	0.40
5:E:105:VAL:HA	5:E:130:PHE:O	2.22	0.40
16:S:473:ARG:NH1	16:S:520:ARG:HG2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1395/1970 (71%)	1362 (98%)	33 (2%)	0	100	100
2	B	1123/1251 (90%)	1090 (97%)	33 (3%)	0	100	100
3	C	254/275 (92%)	252 (99%)	2 (1%)	0	100	100
4	D	114/184 (62%)	109 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	148 (88%)	21 (12%)	0	100	100
8	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
9	I	114/125 (91%)	111 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
16	S	795/1729 (46%)	756 (95%)	39 (5%)	0	100	100
All	All	4612/6435 (72%)	4463 (97%)	149 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1239/1749 (71%)	1239 (100%)	0	100	100
2	B	991/1084 (91%)	989 (100%)	2 (0%)	87	90
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	151 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	40/55 (73%)	40 (100%)	0	100	100
16	S	726/1524 (48%)	724 (100%)	2 (0%)	86	88
All	All	4140/5685 (73%)	4136 (100%)	4 (0%)	87	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	762	LYS
2	B	764	VAL
16	S	864	VAL
16	S	869	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	377	GLN
1	A	439	HIS
1	A	504	HIS
1	A	685	HIS
1	A	746	ASN
1	A	792	ASN
1	A	949	GLN
1	A	1042	ASN
1	A	1422	GLN
1	A	1445	HIS
2	B	222	GLN
2	B	241	ASN
2	B	265	ASN
2	B	342	GLN
2	B	487	ASN
2	B	538	GLN
2	B	614	GLN
2	B	659	GLN
2	B	731	GLN
2	B	874	ASN
2	B	990	GLN
2	B	1107	ASN
2	B	1237	GLN
5	E	35	GLN
5	E	92	GLN
7	G	24	ASN
7	G	60	GLN
8	H	29	HIS
9	I	32	ASN
11	K	69	HIS
11	K	89	ASN
12	L	26	ASN
16	S	389	HIS
16	S	517	GLN

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Mol	Chain	Res	Type
16	S	577	GLN
16	S	608	GLN
16	S	842	ASN
16	S	854	ASN
16	S	887	ASN
16	S	912	GLN
16	S	929	GLN
16	S	1006	GLN
16	S	1234	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/46 (26%)	2 (16%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	36	G
14	P	37	G

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

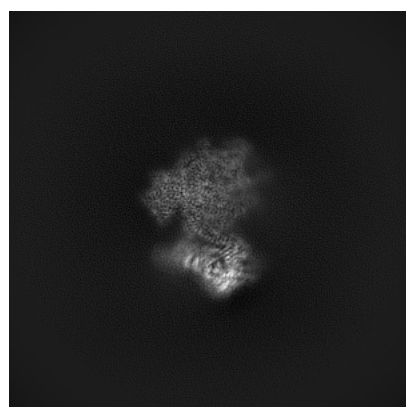
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16835. These allow visual inspection of the internal detail of the map and identification of artifacts.

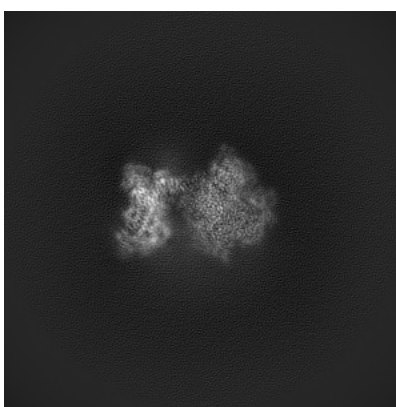
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

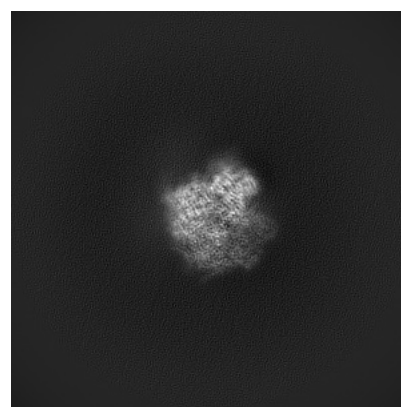
6.1.1 Primary map



X



Y

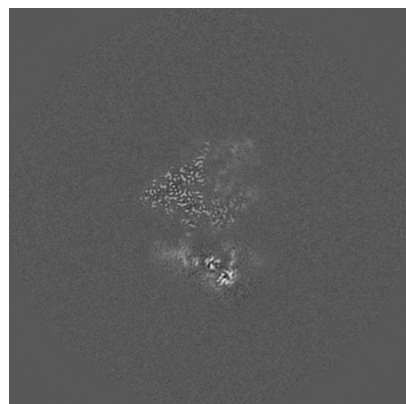


Z

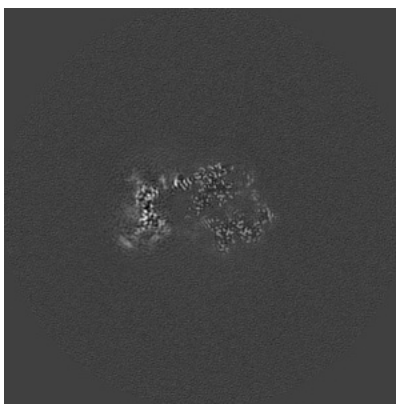
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

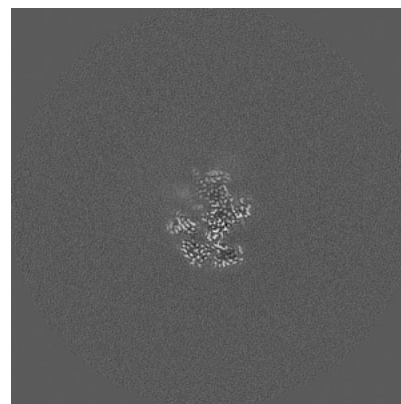
6.2.1 Primary map



X Index: 220



Y Index: 220

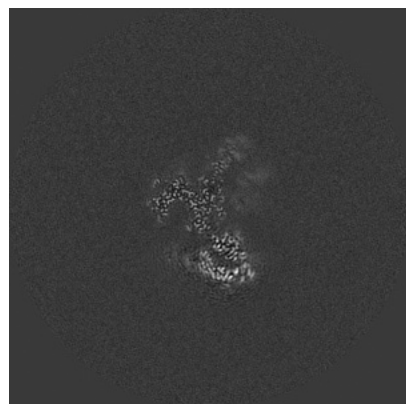


Z Index: 220

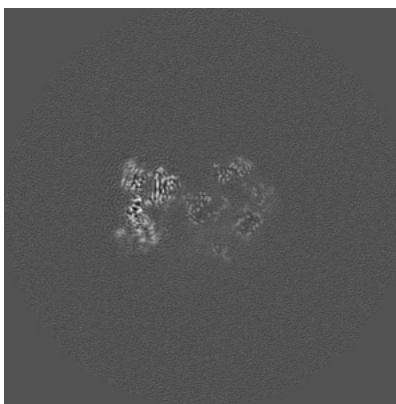
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

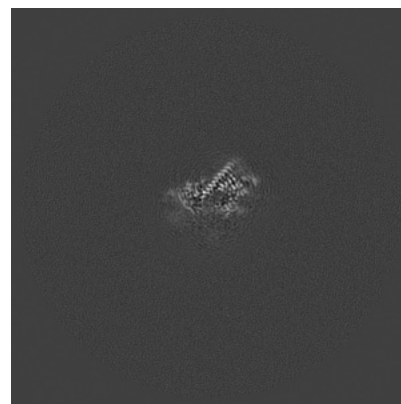
6.3.1 Primary map



X Index: 240



Y Index: 241

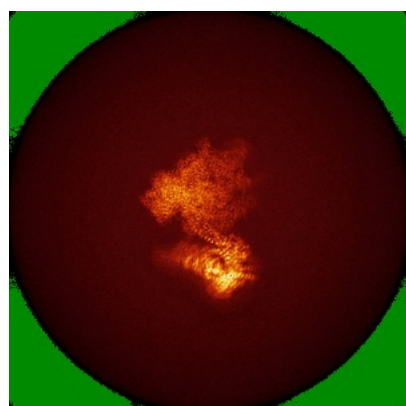


Z Index: 148

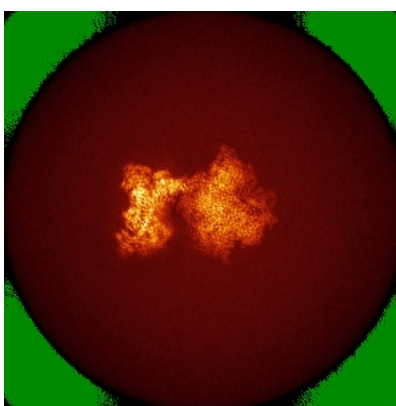
The images above show the largest variance slices of the map in three orthogonal directions.

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

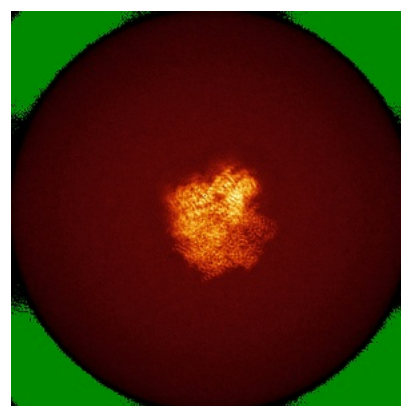
6.4.1 Primary map



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

This section was not generated.

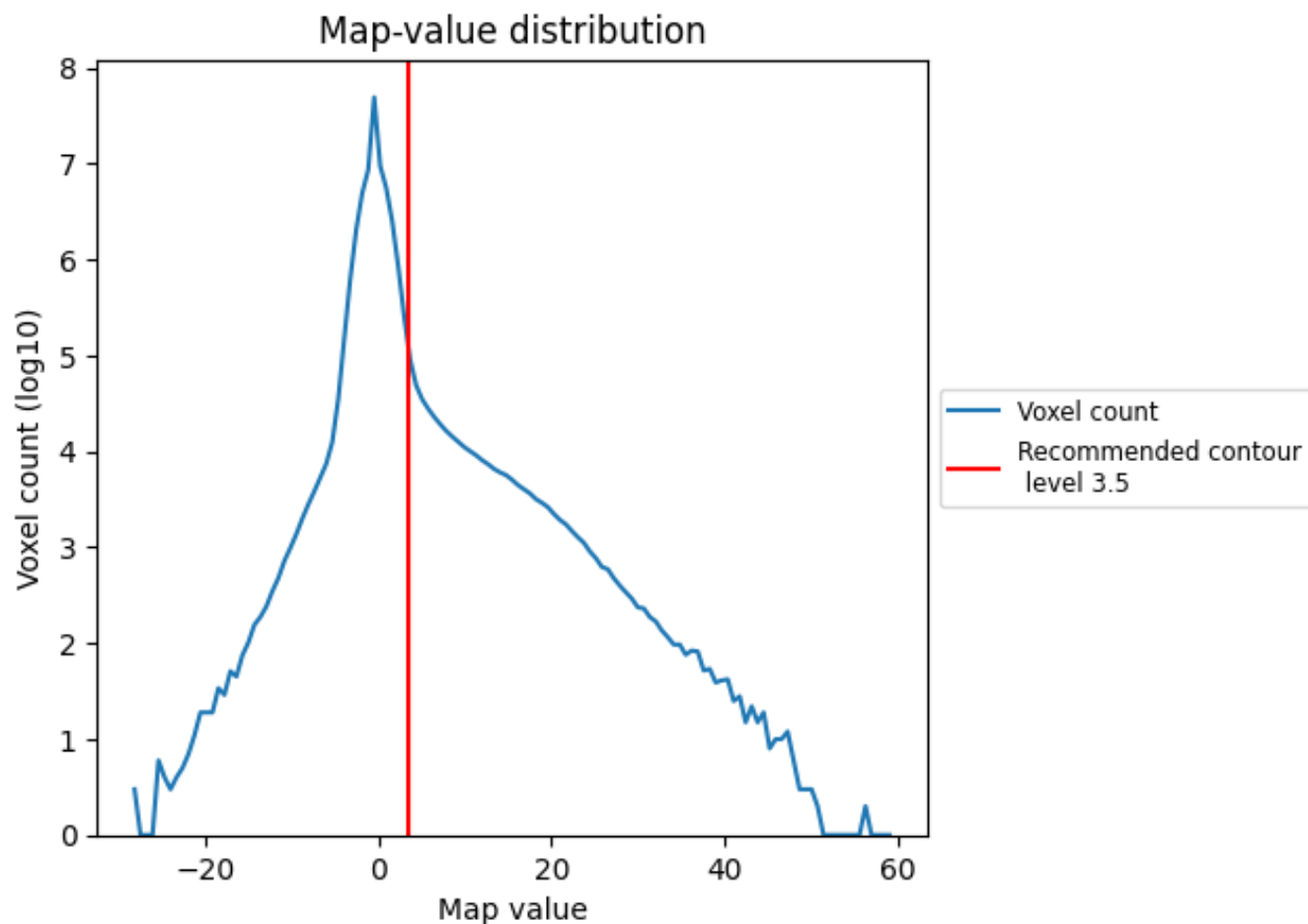
6.6 Mask visualisation

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

7 Map analysis [i](#)

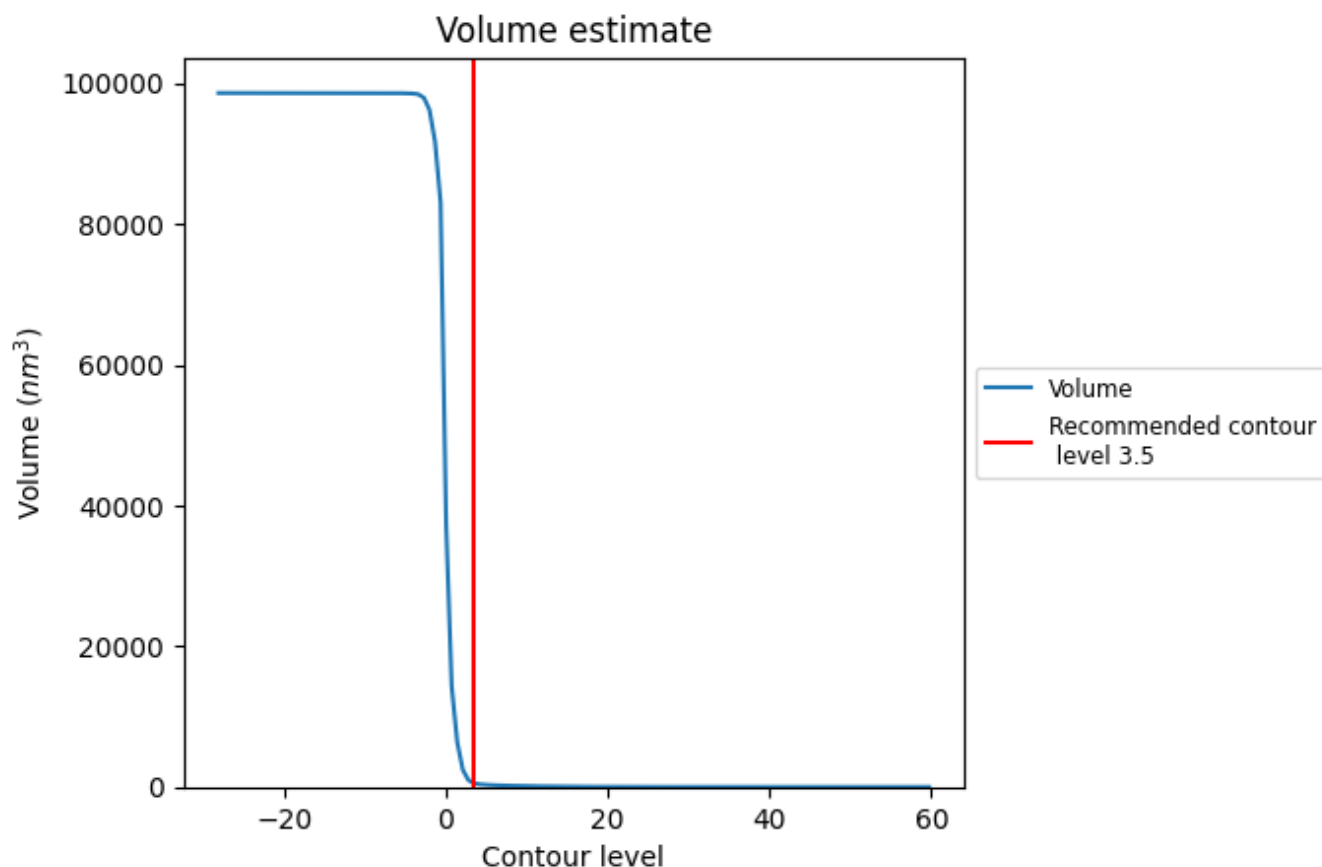
This section contains the results of statistical analysis of the map.

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.

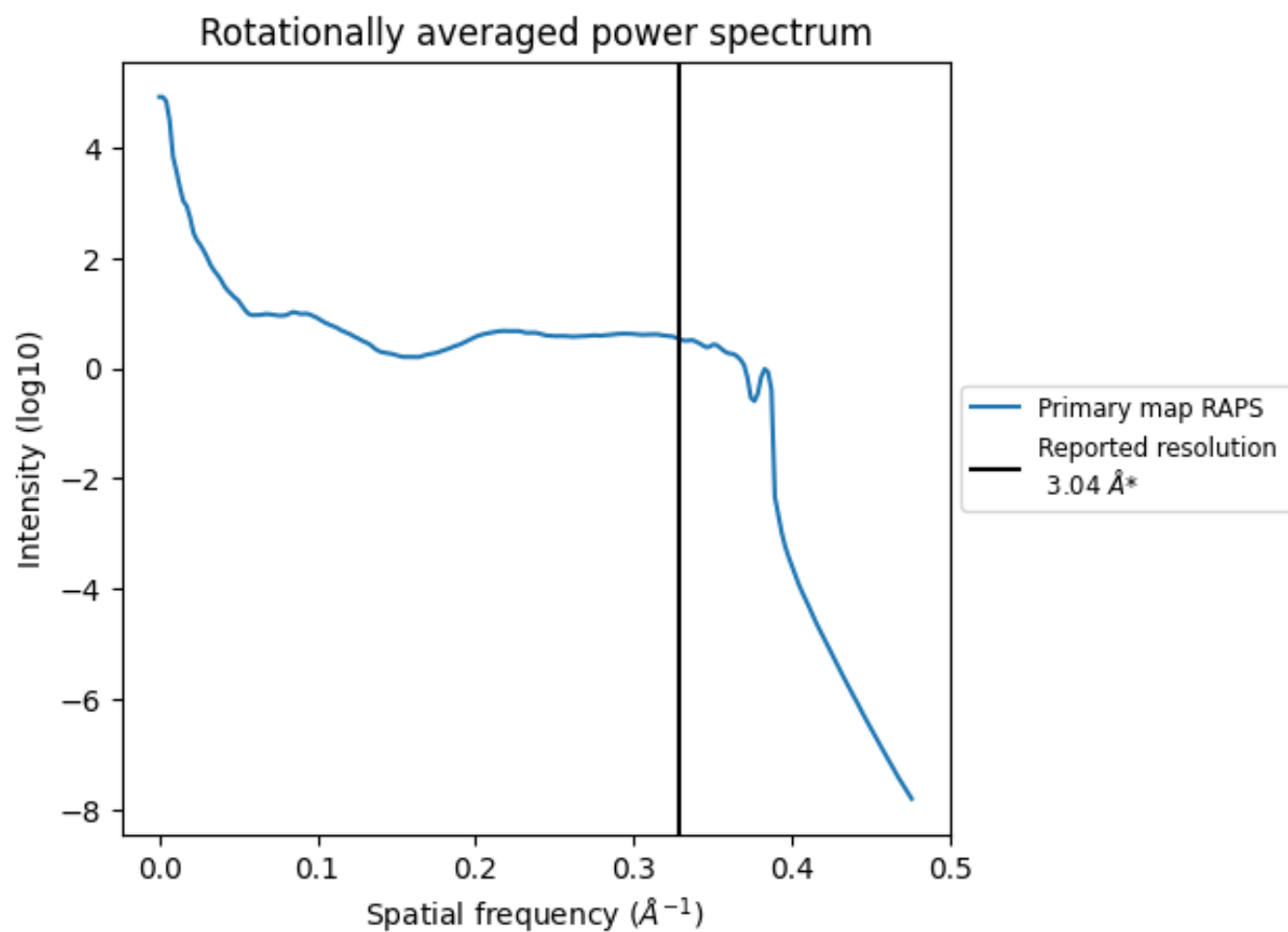
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm^3 ; this corresponds to an approximate mass of 466 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 0.329 Å⁻¹

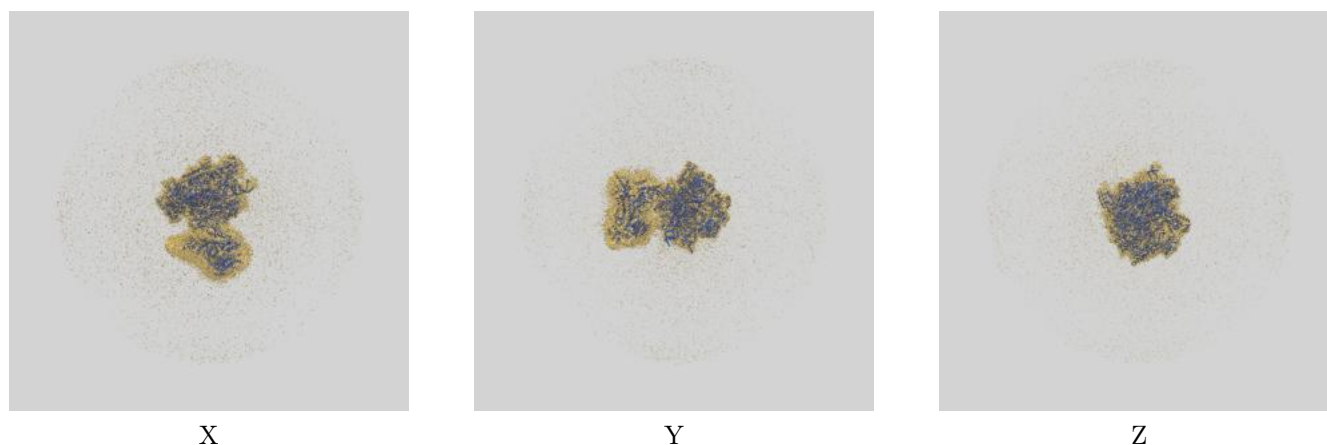
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

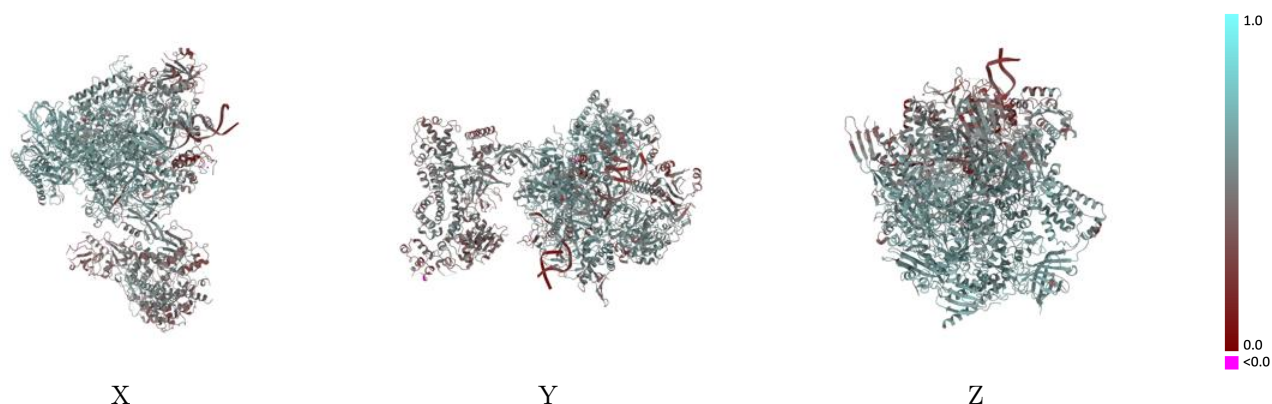
This section contains information regarding the fit between EMDB map EMD-16835 and PDB model 8OEU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



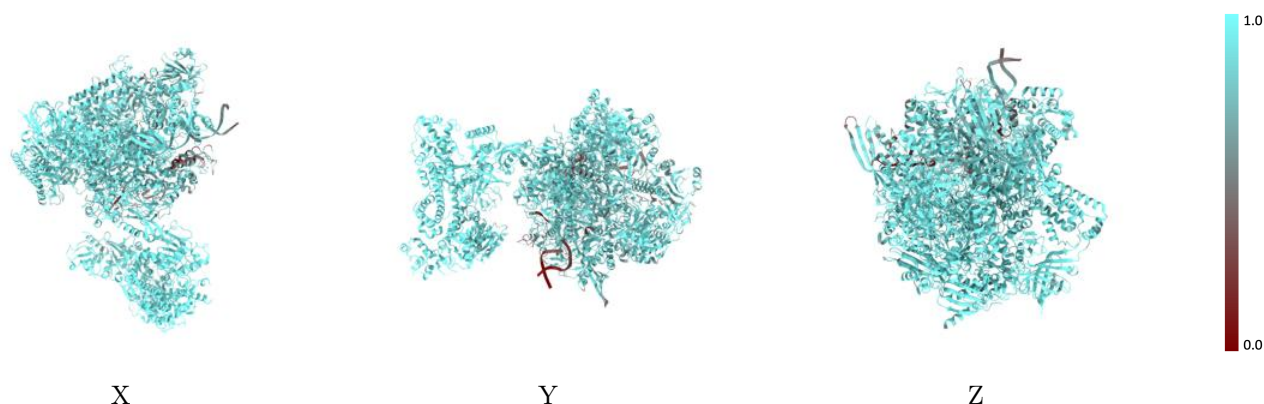
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



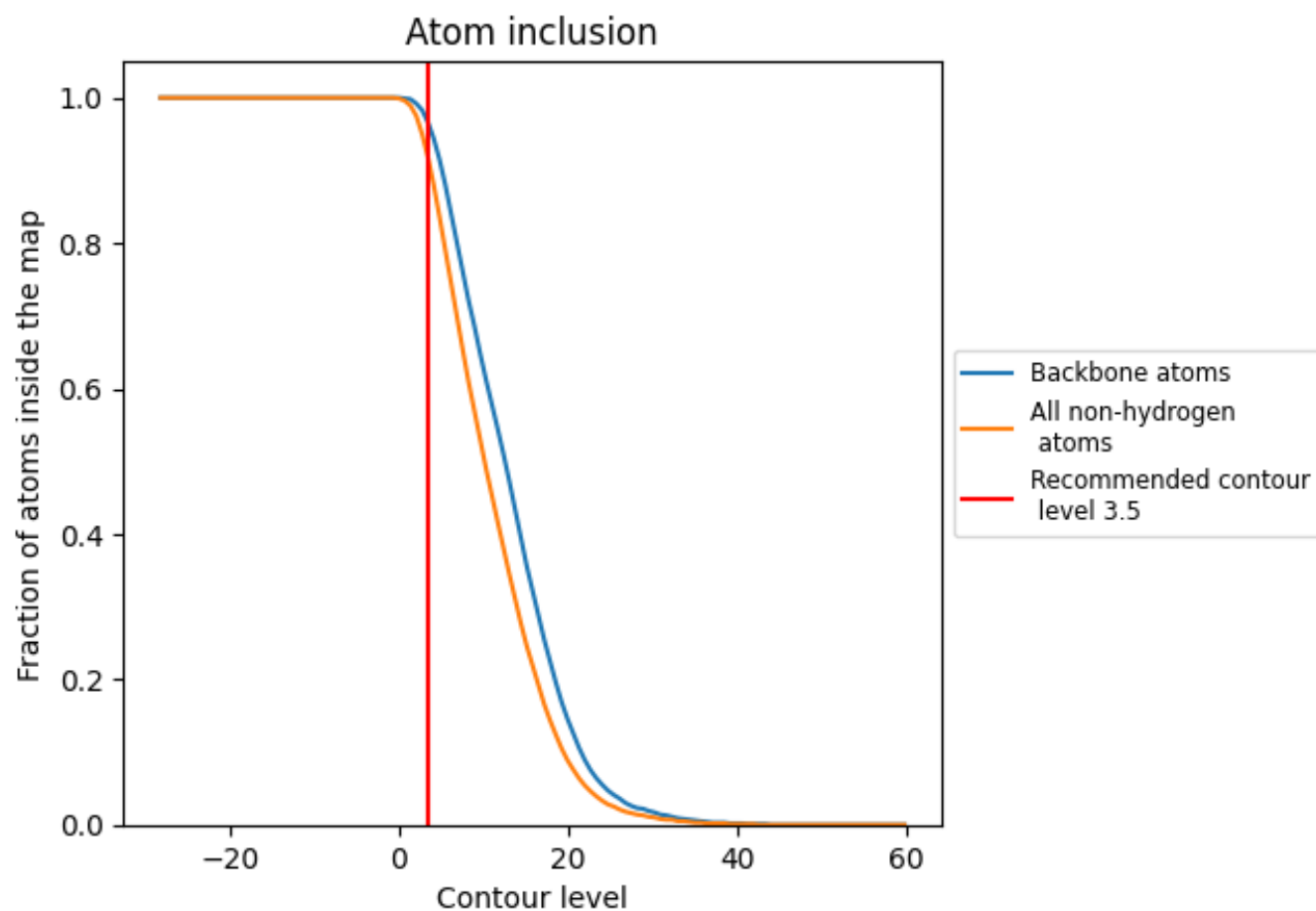
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.5260
A	 0.8980	 0.5530
B	 0.9080	 0.5640
C	 0.9510	 0.6010
D	 0.9620	 0.4280
E	 0.9120	 0.5260
F	 0.9390	 0.5780
G	 0.9610	 0.4980
H	 0.9430	 0.5860
I	 0.8530	 0.4750
J	 0.9570	 0.6030
K	 0.9550	 0.6010
L	 0.8890	 0.5220
N	 0.6140	 0.2890
P	 0.7890	 0.5060
S	 0.9800	 0.4350
T	 0.7060	 0.4170

