



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:19 PM UTC

PDB ID : 7OPD / pdb_00007opd
EMDB ID : EMD-13016
Title : Pol II-CSB-CRL4CSA-UVSSA-SPT6-PAF (Structure 5)
Authors : Kokic, G.; Cramer, P.
Deposited on : 2021-05-31
Resolution : 3.00 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:

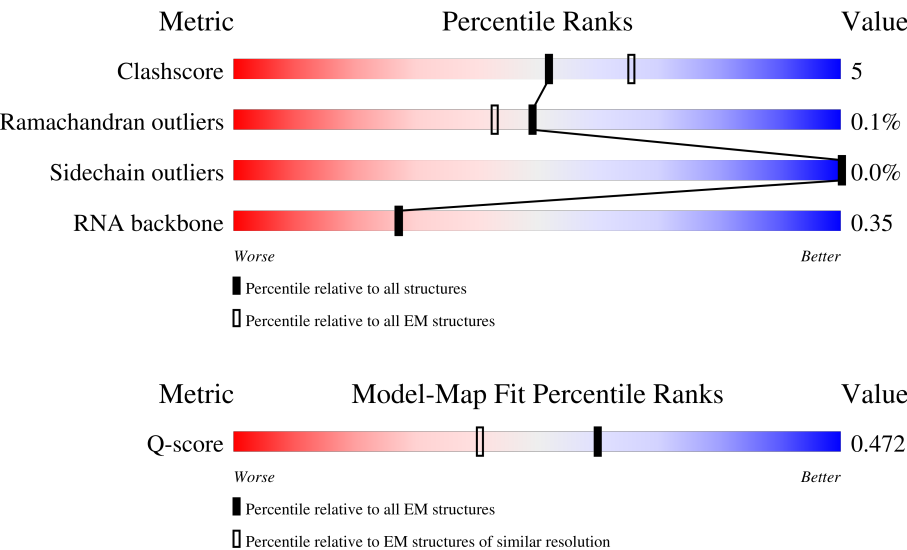
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.00 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	14081 (2.50 - 3.50)

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	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
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	M	1729	
14	N	47	
15	P	45	
16	R	40	
17	S	1179	
18	T	47	
19	U	666	
20	V	531	
21	Y	305	
22	Z	531	
23	a	396	
24	b	1496	
25	c	712	
26	d	1143	
27	e	762	
28	f	108	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 64227 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	1412	Total	C	N	O	S	0	0
			11179	7033	2002	2074	70		

- 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
			9052	5727	1592	1669	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	260	Total	C	N	O	S	0	0
			2089	1309	359	415	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1013	636	172	201	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
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	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
			1334	867	216	243	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	117	Total	C	N	O	S	0	0
			949	587	169	182	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	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

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	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	810	Total	C	N	O	S	0	0
			6648	4226	1155	1234	33		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 14 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			454	204	89	140	21		

- Molecule 16 is a protein called LEO1 helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	40	Total	C	N	O	0	0
			160	80	40	40		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S	890	Total	C	N	O	0	0
			3560	1780	890	890		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1174	GLU	-	expression tag	UNP Q6PD62
S	1175	ASN	-	expression tag	UNP Q6PD62
S	1176	LEU	-	expression tag	UNP Q6PD62
S	1177	TYR	-	expression tag	UNP Q6PD62
S	1178	PHE	-	expression tag	UNP Q6PD62
S	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	U	104	Total	C	N	O	0	0
			416	208	104	104		

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	217	Total	C	N	O	0	0
			868	434	217	217		

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	300	Total	C	N	O	0	0
			1200	600	300	300		

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Z	43	Total	C	N	O	0	0
			172	86	43	43		

- Molecule 23 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	365	Total	C	N	O	S	0	0
			2849	1775	507	548	19		

- Molecule 24 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	520	Total	C	N	O	S	0	0
			4261	2746	748	746	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q03468
b	-1	ASN	-	expression tag	UNP Q03468
b	0	ALA	-	expression tag	UNP Q03468
b	538	ARG	LYS	conflict	UNP Q03468

- Molecule 25 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	141	Total	C	N	O	0	0
			564	282	141	141		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	SER	-	expression tag	UNP Q2YD98
c	-1	ASN	-	expression tag	UNP Q2YD98
c	0	ALA	-	expression tag	UNP Q2YD98

- Molecule 26 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	1096	Total	C	N	O	S	0	0
			7443	4562	1354	1493	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 27 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	e	711	Total	C	N	O	0	0
			2845	1422	711	712		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-2	SER	-	expression tag	UNP Q13619
e	-1	ASN	-	expression tag	UNP Q13619
e	0	ALA	-	expression tag	UNP Q13619

- Molecule 28 is a protein called E3 ubiquitin-protein ligase RBX1.

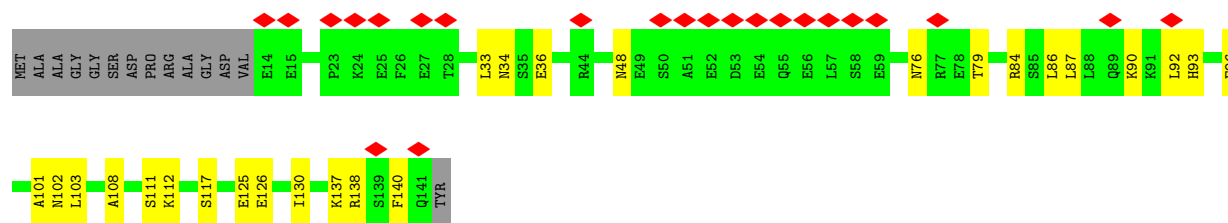
Mol	Chain	Residues	Atoms				AltConf	Trace
28	f	21	Total	C	N	O	0	0
			84	42	21	21		

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

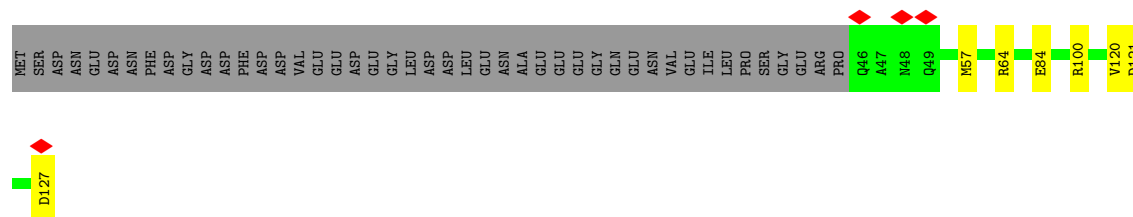
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	



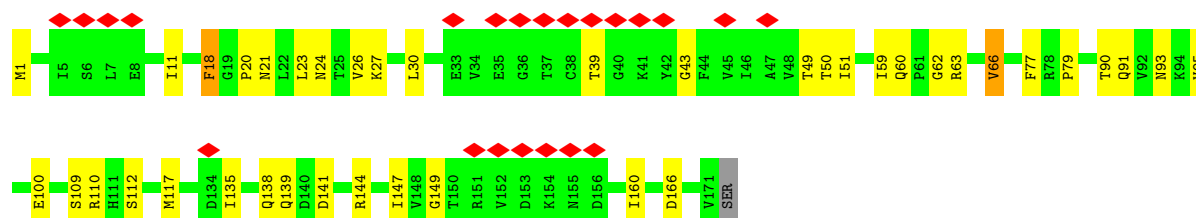
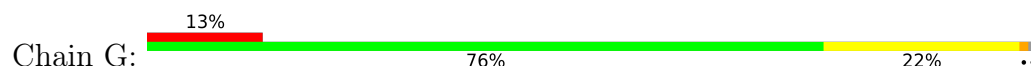
- Molecule 5: DNA-directed RNA polymerase II subunit E



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



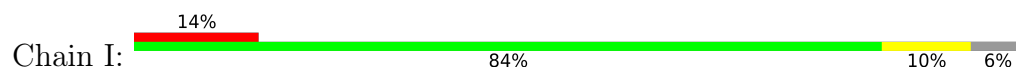
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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

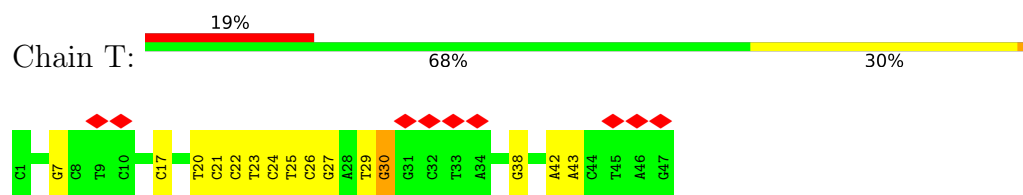


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

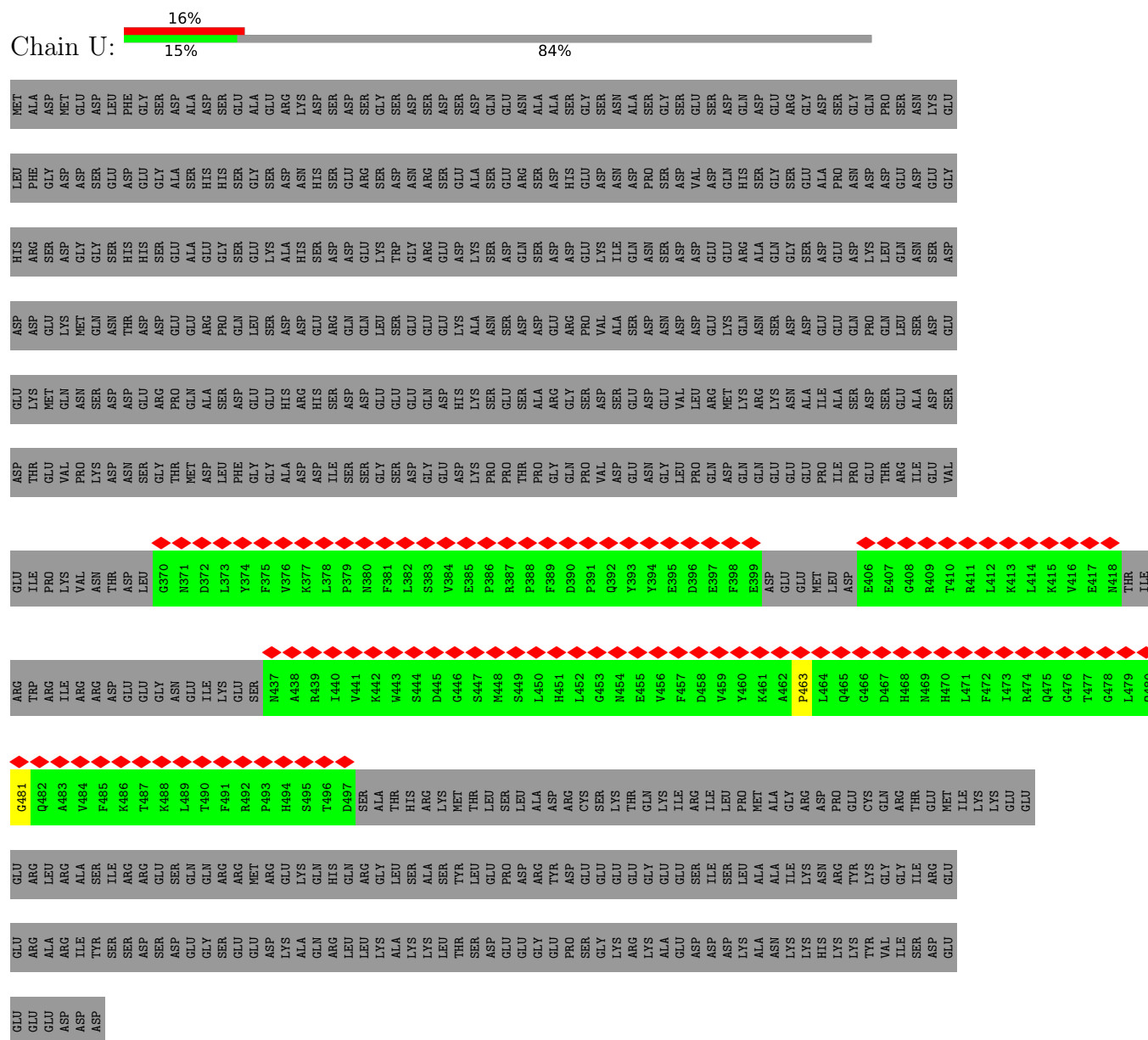




- Molecule 18: TS



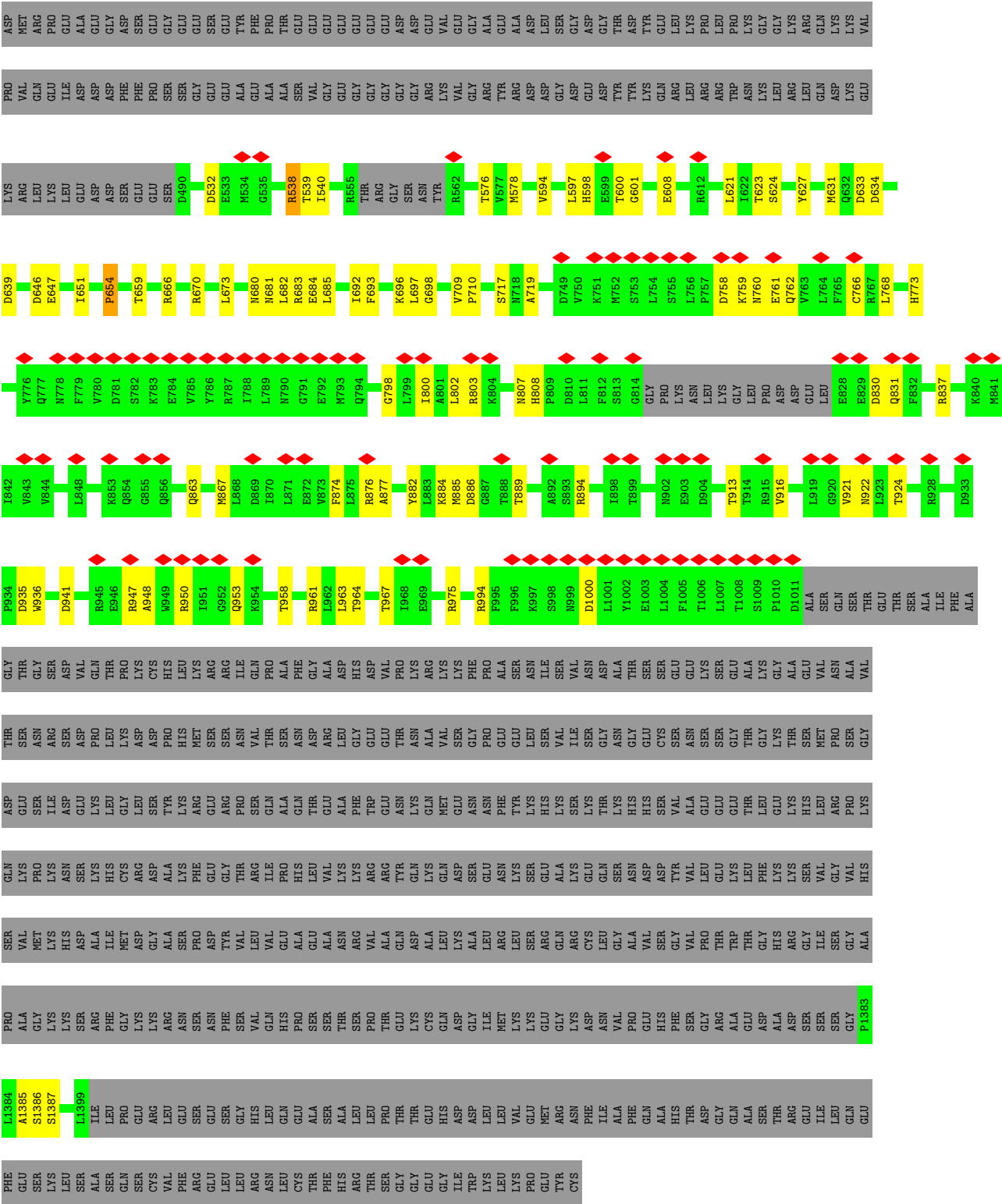
- Molecule 19: RNA polymerase-associated protein LEO1



- Molecule 20: RNA polymerase II-associated factor 1 homolog

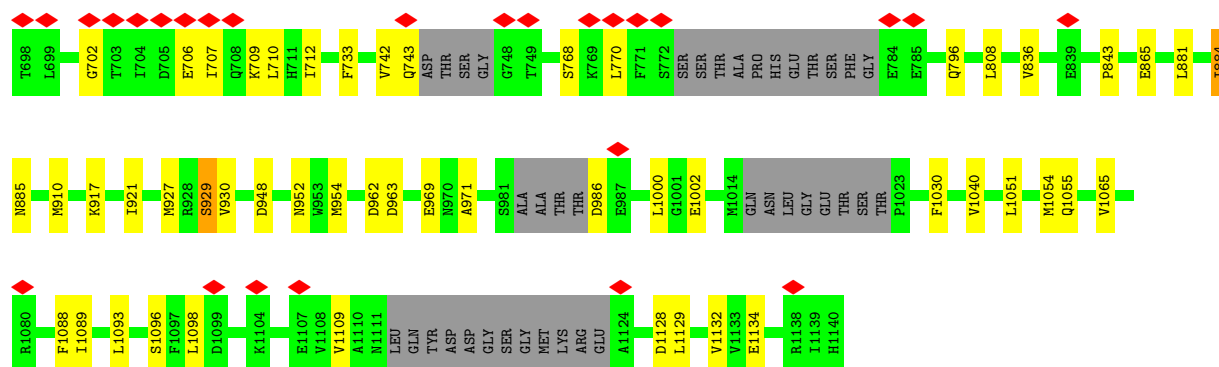




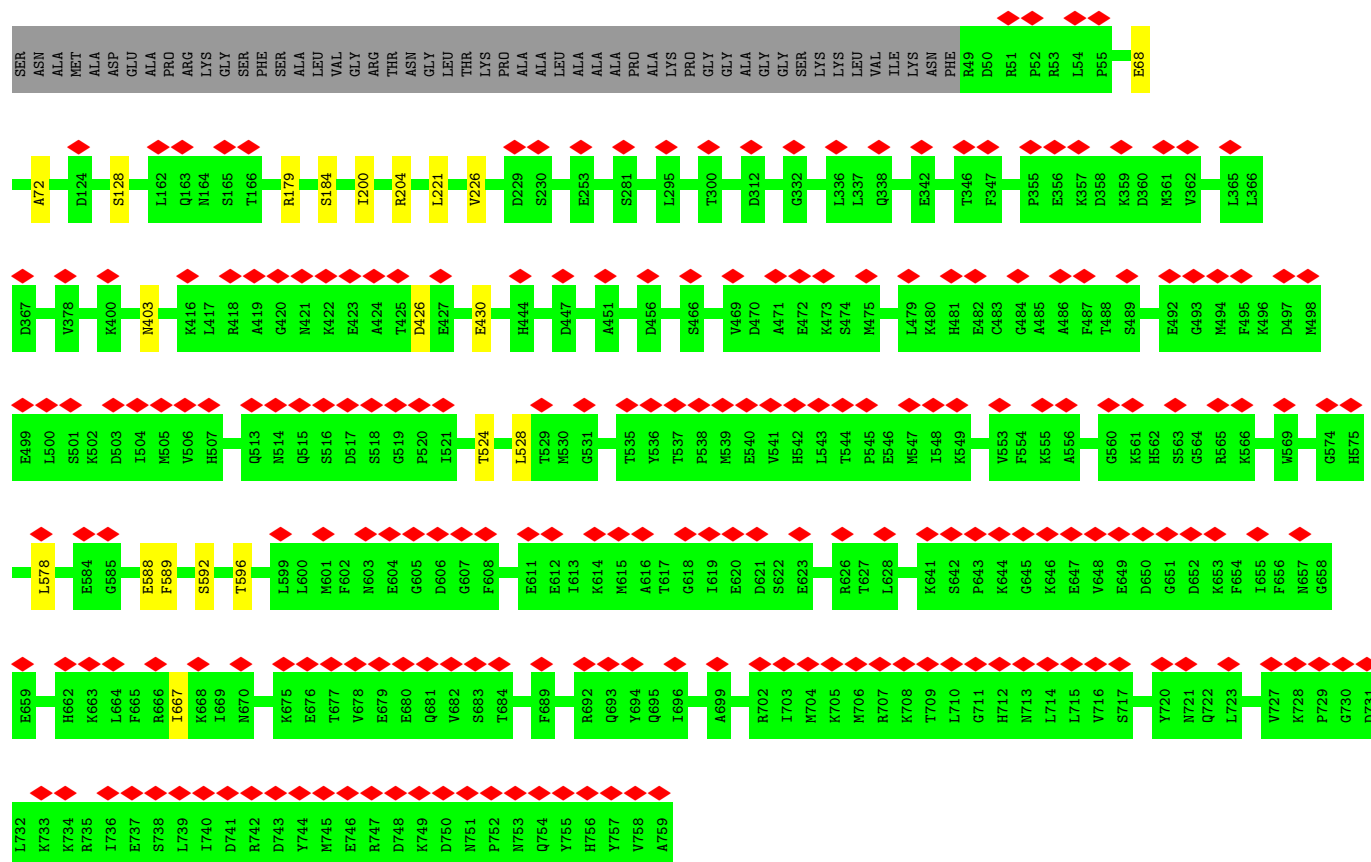


● Molecule 25: UV-stimulated scaffold protein A

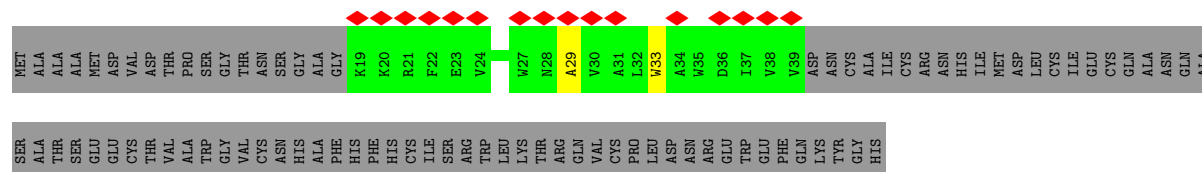




• Molecule 27: Cullin-4A



• Molecule 28: E3 ubiquitin-protein ligase RBX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	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 ($e^-/\text{\AA}^2$)	40.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	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	0.24	0/11382	0.41	0/15368
2	B	0.24	0/9233	0.39	0/12463
3	C	0.27	0/2132	0.42	0/2896
4	D	0.93	0/1027	0.81	0/1384
5	E	0.21	0/1751	0.35	0/2366
6	F	0.23	0/667	0.36	0/901
7	G	1.22	2/1365 (0.1%)	0.85	1/1853 (0.1%)
8	H	0.23	0/1207	0.37	0/1628
9	I	0.20	0/972	0.40	0/1316
10	J	0.24	0/542	0.37	0/730
11	K	0.23	0/939	0.34	0/1271
12	L	0.26	0/394	0.42	0/524
13	M	1.76	34/6770 (0.5%)	1.05	6/9119 (0.1%)
14	N	1.05	0/817	0.57	0/1258
15	P	2.14	18/510 (3.5%)	0.82	1/793 (0.1%)
17	S	0.32	0/3559	0.76	2/4447 (0.0%)
18	T	1.90	13/1056 (1.2%)	0.79	2/1624 (0.1%)
19	U	0.33	0/413	0.66	0/511
20	V	0.34	0/864	0.80	2/1073 (0.2%)
21	Y	0.33	0/1199	0.76	0/1497
22	Z	0.36	0/171	0.86	0/212
23	a	1.93	16/2908 (0.6%)	0.95	1/3939 (0.0%)
24	b	1.13	2/4364 (0.0%)	0.73	0/5893
25	c	0.11	0/563	0.27	0/702
26	d	0.30	0/7551	0.45	1/10076 (0.0%)
27	e	0.34	0/2844	0.85	1/3552 (0.0%)
28	f	0.22	0/83	0.81	0/102
All	All	0.88	85/65283 (0.1%)	0.65	17/87498 (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	1
13	M	0	1
16	R	0	1
23	a	0	1
26	d	0	2
27	e	0	1
All	All	0	7

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	19	ARG	CB-CG	-8.38	1.27	1.52
23	a	215	ASP	CA-CB	-8.07	1.42	1.53
23	a	312	TYR	CA-CB	-8.02	1.28	1.53
13	M	912	GLN	CB-CG	-7.90	1.28	1.52
15	P	50	A	P-OP1	-7.42	1.34	1.49
13	M	1014	ARG	CD-NE	-7.10	1.36	1.46
7	G	59	ILE	CG1-CD1	-6.85	1.25	1.51
15	P	49	G	P-OP1	-6.80	1.35	1.49
13	M	946	GLN	CB-CG	-6.78	1.32	1.52
15	P	31	U	C1'-N1	6.72	1.57	1.47
23	a	279	ASN	CB-CG	-6.52	1.35	1.52
15	P	35	U	C1'-N1	6.40	1.57	1.47
23	a	105	VAL	CB-CG2	-6.27	1.31	1.52
18	T	23	DT	P-OP1	-6.26	1.35	1.48
15	P	48	G	C5-C4	-6.25	1.25	1.38
23	a	251	LEU	CG-CD2	-6.24	1.31	1.52
15	P	49	G	P-OP2	-6.18	1.36	1.49
15	P	46	G	C2-N3	-6.11	1.20	1.32
15	P	37	C	C1'-N1	6.08	1.57	1.48
13	M	603	ARG	CG-CD	-5.99	1.34	1.52
13	M	1030	ASN	CB-CG	-5.99	1.37	1.52
13	M	1014	ARG	CZ-NH1	-5.91	1.24	1.32
23	a	9	GLN	CB-CG	-5.91	1.34	1.52
13	M	987	GLN	CB-CG	-5.85	1.34	1.52
13	M	397	TRP	CG-CD2	-5.79	1.33	1.43
13	M	600	PRO	CB-CG	-5.78	1.20	1.49
15	P	48	G	O3'-P	-5.71	1.52	1.61
18	T	25	DT	N1-C2	-5.71	1.26	1.38
23	a	268	ARG	CA-CB	-5.71	1.43	1.54
15	P	46	G	N1-C2	-5.69	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	25	DT	C5-C6	-5.68	1.22	1.34
18	T	22	DC	N3-C4	-5.68	1.22	1.33
13	M	653	PHE	CB-CG	-5.66	1.37	1.50
13	M	404	THR	CA-CB	-5.66	1.44	1.53
23	a	228	GLN	CB-CG	-5.65	1.35	1.52
15	P	50	A	P-OP2	-5.64	1.37	1.49
13	M	755	VAL	CB-CG2	-5.58	1.34	1.52
15	P	46	G	N9-C4	-5.55	1.26	1.38
13	M	720	PHE	CB-CG	-5.55	1.37	1.50
15	P	49	G	N1-C2	-5.55	1.26	1.37
23	a	289	ASN	CB-CG	-5.54	1.38	1.52
13	M	301	ARG	CG-CD	-5.54	1.35	1.52
13	M	549	ASN	CB-CG	-5.53	1.38	1.52
13	M	893	TYR	CB-CG	-5.51	1.39	1.51
13	M	316	GLU	CB-CG	-5.49	1.35	1.52
23	a	147	HIS	CA-CB	-5.48	1.45	1.53
18	T	25	DT	C4-C5	-5.48	1.33	1.44
23	a	196	PRO	CB-CG	-5.47	1.22	1.49
23	a	189	ILE	CG1-CD1	-5.44	1.30	1.51
15	P	50	A	P-O5'	-5.41	1.51	1.59
24	b	670	ARG	CG-CD	-5.40	1.36	1.52
18	T	27	DG	C5-C6	-5.39	1.31	1.42
13	M	887	ASN	C-N	-5.38	1.23	1.33
13	M	1034	PHE	CD2-CE2	-5.38	1.22	1.38
15	P	46	G	N9-C8	-5.35	1.27	1.37
13	M	924	LEU	CG-CD2	-5.35	1.34	1.52
7	G	66	VAL	CB-CG1	-5.35	1.34	1.52
23	a	107	TRP	CB-CG	-5.32	1.33	1.50
15	P	46	G	C5-C4	-5.31	1.27	1.38
13	M	379	TYR	CA-CB	-5.25	1.42	1.53
13	M	566	PRO	CB-CG	-5.25	1.23	1.49
13	M	946	GLN	CG-CD	-5.24	1.39	1.52
13	M	379	TYR	CB-CG	-5.22	1.40	1.51
13	M	319	TRP	CD2-CE2	-5.22	1.32	1.41
13	M	693	TYR	CB-CG	-5.21	1.40	1.51
13	M	948	HIS	C-N	-5.18	1.24	1.33
13	M	397	TRP	CB-CG	-5.18	1.34	1.50
13	M	578	PHE	C-N	-5.17	1.21	1.33
18	T	26	DC	O5'-C5'	-5.17	1.27	1.42
15	P	30	A	C1'-N9	-5.17	1.40	1.48
18	T	24	DC	N1-C2	-5.16	1.30	1.40
23	a	49	LEU	CA-CB	-5.12	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	654	PRO	CB-CG	-5.11	1.24	1.49
18	T	25	DT	P-OP2	-5.11	1.38	1.48
23	a	249	ASN	CB-CG	-5.11	1.39	1.52
18	T	23	DT	C1'-N1	-5.10	1.34	1.49
18	T	25	DT	C2-N3	-5.09	1.27	1.37
13	M	401	GLU	CB-CG	-5.09	1.37	1.52
13	M	741	VAL	CB-CG2	-5.06	1.35	1.52
13	M	1034	PHE	CG-CD2	-5.06	1.28	1.38
15	P	45	A	C5-C6	-5.05	1.30	1.41
18	T	22	DC	P-OP1	-5.05	1.38	1.48
18	T	24	DC	C2-O2	-5.01	1.14	1.24
13	M	400	ASP	CB-CG	-5.01	1.39	1.52
13	M	595	GLN	CG-CD	-5.01	1.39	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1014	ARG	NE-CZ-NH1	-7.79	113.71	121.50
27	e	128	SER	N-CA-C	-7.67	103.27	114.39
13	M	1014	ARG	NE-CZ-NH2	7.07	125.57	119.20
13	M	724	GLN	N-CA-CB	6.31	120.06	110.28
17	S	772	GLU	CA-C-N	5.91	132.33	121.70
17	S	772	GLU	C-N-CA	5.91	132.33	121.70
26	d	929	SER	N-CA-C	5.70	122.94	110.80
13	M	450	ARG	NE-CZ-NH2	5.62	124.25	119.20
15	P	50	A	O5'-P-OP1	-5.54	91.38	108.00
7	G	18	PHE	N-CA-C	-5.48	102.90	110.35
23	a	174	LYS	N-CA-C	-5.43	103.32	110.43
20	V	71	TYR	CA-C-N	5.34	131.32	121.70
20	V	71	TYR	C-N-CA	5.34	131.32	121.70
13	M	1056	SER	CA-CB-OG	-5.29	100.52	111.10
13	M	316	GLU	N-CA-CB	5.13	117.62	109.82
18	T	30	DG	N9-C1'-C2'	5.02	121.03	113.50
18	T	30	DG	O4'-C1'-C2'	-5.01	98.89	106.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
13	M	575	CYS	Peptide
16	R	11	UNK	Peptide

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Mol	Chain	Res	Type	Group
23	a	174	LYS	Peptide
26	d	35	LYS	Peptide
26	d	884	ILE	Peptide
27	e	403	ASN	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	11179	0	11313	105	0
2	B	9052	0	9087	60	0
3	C	2089	0	2031	14	0
4	D	1013	0	972	21	0
5	E	1720	0	1737	14	0
6	F	657	0	684	5	0
7	G	1334	0	1333	26	0
8	H	1186	0	1147	7	0
9	I	949	0	879	9	0
10	J	533	0	553	5	0
11	K	920	0	942	7	0
12	L	388	0	393	2	0
13	M	6648	0	6644	142	0
14	N	727	0	393	1	0
15	P	454	0	210	12	0
16	R	160	0	2	3	0
17	S	3560	0	940	8	0
18	T	947	0	519	14	0
19	U	416	0	111	0	0
20	V	868	0	212	3	0
21	Y	1200	0	341	15	0
22	Z	172	0	44	2	0
23	a	2849	0	2778	44	0
24	b	4261	0	4302	71	0
25	c	564	0	143	1	0
26	d	7443	0	6536	95	0
27	e	2845	0	753	10	0
28	f	84	0	20	2	0
29	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
30	A	1	0	0	0	0
All	All	64227	0	55019	634	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 5.

All (634) 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)
26:d:392:ASN:OD1	26:d:710:LEU:CD2	1.82	1.28
1:A:114:CYS:SG	1:A:184:CYS:HB3	1.83	1.18
26:d:392:ASN:OD1	26:d:710:LEU:HD23	1.41	1.13
24:b:975:ARG:NH2	24:b:1000:ASP:OD1	1.92	1.02
26:d:392:ASN:OD1	26:d:710:LEU:HD21	1.58	1.00
24:b:532:ASP:O	24:b:538:ARG:NH1	1.97	0.97
13:M:926:GLU:OE1	13:M:981:TYR:OH	1.90	0.88
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.88
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.57	0.87
13:M:1014:ARG:NH1	13:M:1032:ALA:O	2.08	0.87
2:B:565:THR:OG1	2:B:610:ARG:O	1.95	0.85
13:M:886:ASP:OD1	13:M:887:ASN:N	2.12	0.83
23:a:1:MET:O	23:a:4:PHE:N	2.11	0.83
26:d:917:LYS:NZ	26:d:962:ASP:OD1	2.11	0.83
13:M:1167:ILE:HD12	13:M:1232:LEU:HD11	1.60	0.81
1:A:266:MET:HE3	1:A:270:ALA:HB3	1.63	0.80
1:A:114:CYS:SG	1:A:184:CYS:CB	2.68	0.79
9:I:68:ILE:O	9:I:122:ARG:NH1	2.16	0.79
13:M:561:GLN:NE2	13:M:697:GLU:OE2	2.15	0.79
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.16	0.78
24:b:885:MET:HE2	24:b:894:ARG:HG3	1.66	0.78
13:M:825:GLU:O	13:M:828:LYS:N	2.15	0.78
23:a:33:ASN:OD1	23:a:35:ASP:N	2.16	0.78
13:M:893:TYR:O	13:M:896:SER:OG	2.01	0.77
4:D:93:HIS:HB3	4:D:96:GLU:OE1	1.85	0.76
23:a:37:ASP:OD2	23:a:81:TYR:OH	2.04	0.76
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.58	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:LYS:HE2	4:D:130:ILE:HD12	1.66	0.75
26:d:102:THR:OG1	26:d:1065:VAL:O	2.05	0.75
24:b:538:ARG:HG2	24:b:538:ARG:HH21	1.51	0.74
26:d:130:MET:HE1	26:d:195:VAL:HG11	1.68	0.74
24:b:717:SER:O	24:b:994:ARG:NH2	2.20	0.74
24:b:863:GLN:NE2	24:b:941:ASP:OD1	2.20	0.74
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.21	0.74
13:M:445:THR:O	13:M:448:MET:N	2.20	0.74
2:B:352:GLY:O	2:B:361:LYS:NZ	2.20	0.74
1:A:374:SER:OG	1:A:376:ASP:OD1	2.06	0.73
2:B:430:ASN:ND2	16:R:20:UNK:O	2.22	0.72
1:A:70:ARG:NH2	1:A:75:ALA:O	2.21	0.72
1:A:576:GLN:O	1:A:590:GLN:NE2	2.23	0.72
1:A:538:VAL:HG12	1:A:539:GLN:H	1.53	0.72
13:M:445:THR:O	13:M:449:GLU:N	2.21	0.71
3:C:180:ALA:O	10:J:42:ARG:NH2	2.23	0.71
26:d:226:PHE:O	26:d:241:ASN:ND2	2.23	0.71
1:A:413:TYR:OH	1:A:450:MET:O	2.08	0.71
24:b:831:GLN:N	24:b:831:GLN:OE1	2.24	0.71
1:A:549:THR:O	1:A:589:LYS:NZ	2.24	0.71
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.64	0.70
1:A:67:ARG:NH2	15:P:38:A:OP1	2.24	0.70
2:B:198:GLU:OE2	2:B:388:TYR:OH	2.09	0.70
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.24	0.70
13:M:692:PHE:O	13:M:694:TYR:N	2.25	0.70
24:b:639:ASP:OD2	24:b:666:ARG:NH1	2.25	0.69
2:B:957:THR:OG1	2:B:959:GLU:O	2.11	0.69
24:b:935:ASP:OD1	24:b:936:TRP:N	2.25	0.69
1:A:321:GLU:OE1	1:A:341:GLN:NE2	2.26	0.69
13:M:1145:ASN:O	13:M:1148:GLU:N	2.26	0.69
26:d:134:ARG:NH1	26:d:164:VAL:O	2.26	0.69
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.74	0.68
13:M:1148:GLU:N	13:M:1148:GLU:OE1	2.26	0.68
26:d:1093:LEU:O	26:d:1096:SER:OG	2.10	0.68
13:M:580:THR:O	13:M:582:GLU:N	2.26	0.68
1:A:266:MET:SD	18:T:30:DG:N3	2.67	0.68
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.76	0.68
26:d:130:MET:HE2	26:d:169:PHE:HZ	1.59	0.68
26:d:19:VAL:HG22	26:d:64:MET:HE3	1.75	0.67
1:A:431:PHE:HE2	15:P:38:A:H61	1.42	0.67
2:B:551:GLU:OE2	2:B:578:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:608:GLU:N	24:b:608:GLU:OE2	2.27	0.67
2:B:591:ARG:HE	2:B:603:MET:HE2	1.60	0.67
26:d:1054:MET:SD	26:d:1129:LEU:HD22	2.35	0.67
7:G:100:GLU:N	7:G:100:GLU:OE1	2.29	0.66
24:b:921:VAL:O	24:b:947:ARG:NH1	2.29	0.66
26:d:47:GLU:OE1	26:d:47:GLU:N	2.29	0.66
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.29	0.66
26:d:248:ILE:HD12	26:d:250:PRO:HG3	1.78	0.66
26:d:282:MET:HE2	26:d:305:LEU:HD11	1.78	0.66
13:M:1145:ASN:OD1	13:M:1146:THR:N	2.28	0.66
2:B:329:GLY:O	2:B:335:ARG:NE	2.29	0.65
23:a:170:LEU:HD12	23:a:180:HIS:CD2	2.31	0.65
1:A:1198:GLU:OE1	1:A:1198:GLU:N	2.29	0.65
7:G:91:GLN:NE2	7:G:93:ASN:OD1	2.28	0.65
24:b:762:GLN:OE1	24:b:958:THR:OG1	2.14	0.65
24:b:922:ASN:OD1	24:b:950:ARG:NE	2.29	0.65
26:d:706:GLU:O	26:d:706:GLU:HG2	1.96	0.65
26:d:929:SER:O	26:d:930:VAL:HG13	1.97	0.65
13:M:529:SER:OG	13:M:530:ALA:N	2.30	0.65
26:d:1051:LEU:HD23	26:d:1054:MET:CE	2.27	0.65
26:d:768:SER:HB3	26:d:808:LEU:HD11	1.79	0.65
23:a:26:ARG:NH1	26:d:927:MET:SD	2.70	0.65
13:M:582:GLU:N	13:M:582:GLU:OE1	2.30	0.64
24:b:633:ASP:OD1	24:b:634:ASP:N	2.29	0.64
24:b:766:CYS:N	24:b:963:LEU:O	2.29	0.64
1:A:373:LEU:O	1:A:485:ASN:ND2	2.30	0.64
1:A:413:TYR:O	1:A:415:GLY:N	2.30	0.64
13:M:979:HIS:O	13:M:981:TYR:N	2.30	0.64
23:a:119:SER:OG	23:a:120:PHE:N	2.29	0.64
2:B:1104:ARG:NH1	2:B:1109:GLU:OE2	2.31	0.63
23:a:192:VAL:HG12	23:a:204:THR:HG22	1.80	0.63
24:b:924:THR:O	24:b:953:GLN:NE2	2.32	0.63
13:M:934:ASP:OD1	13:M:935:GLU:N	2.32	0.63
13:M:1031:CYS:SG	13:M:1032:ALA:N	2.72	0.62
24:b:538:ARG:HH21	24:b:538:ARG:CG	2.12	0.62
3:C:190:ASN:O	3:C:193:ARG:NH1	2.33	0.62
7:G:149:GLY:O	7:G:160:ILE:N	2.33	0.62
23:a:33:ASN:HB2	23:a:362:VAL:HG22	1.81	0.62
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.35	0.62
2:B:347:MET:HE1	2:B:365:LEU:HD22	1.82	0.62
2:B:841:ARG:NH2	15:P:40:A:N7	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:d:684:SER:N	26:d:687:TYR:O	2.33	0.62
1:A:507:GLN:N	2:B:1105:GLU:OE2	2.33	0.62
13:M:551:ARG:NH1	13:M:552:ASP:OD1	2.32	0.62
13:M:1123:LEU:O	13:M:1126:ILE:N	2.33	0.62
1:A:1311:LEU:HD12	1:A:1332:GLN:HG3	1.82	0.61
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.18	0.61
24:b:964:THR:OG1	24:b:967:THR:OG1	2.17	0.61
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.82	0.61
26:d:381:ALA:O	26:d:385:GLY:N	2.33	0.61
2:B:210:LYS:NZ	2:B:212:ASP:O	2.33	0.61
9:I:50:ASN:O	9:I:51:SER:OG	2.16	0.61
13:M:474:ASP:OD1	13:M:474:ASP:N	2.22	0.61
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.14	0.61
1:A:808:PRO:HG2	2:B:675:LEU:HD12	1.83	0.61
2:B:927:ARG:NH1	2:B:1057:ASP:OD1	2.33	0.61
4:D:33:LEU:HD22	4:D:101:ALA:HB3	1.81	0.61
1:A:41:ILE:HD12	1:A:255:VAL:HG11	1.82	0.61
13:M:444:ASP:OD1	13:M:444:ASP:N	2.33	0.61
7:G:95:VAL:O	7:G:110:ARG:N	2.34	0.60
16:R:11:UNK:O	16:R:15:UNK:N	2.34	0.60
13:M:369:GLN:O	13:M:1026:LYS:NZ	2.30	0.60
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.34	0.60
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.19	0.60
5:E:93:ARG:CZ	17:S:891:PHE:CA	2.79	0.60
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.83	0.60
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.34	0.60
13:M:853:GLU:OE1	13:M:854:ASN:ND2	2.35	0.60
20:V:243:VAL:O	20:V:248:PRO:N	2.35	0.60
24:b:680:ASN:N	24:b:684:GLU:OE1	2.34	0.60
24:b:761:GLU:OE2	24:b:961:ARG:NH1	2.34	0.59
13:M:1108:ALA:HA	13:M:1111:LEU:HD12	1.84	0.59
7:G:49:THR:OG1	7:G:50:THR:N	2.31	0.59
13:M:572:ASP:OD1	13:M:572:ASP:N	2.33	0.59
1:A:521:VAL:HG13	1:A:535:MET:HE1	1.84	0.59
26:d:367:LEU:HD11	26:d:796:GLN:O	2.02	0.58
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.36	0.58
26:d:1109:VAL:HG12	26:d:1109:VAL:O	2.03	0.58
13:M:800:ASN:OD1	13:M:801:GLY:N	2.36	0.58
24:b:539:THR:HG23	24:b:540:ILE:HD12	1.85	0.58
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.86	0.58
13:M:699:SER:OG	13:M:701:GLN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:167:LYS:NZ	23:a:183:GLN:OE1	2.36	0.58
1:A:266:MET:CE	18:T:30:DG:H2'	2.34	0.58
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.21	0.58
21:Y:212:GLY:O	21:Y:230:GLY:N	2.37	0.58
13:M:870:GLU:OE1	13:M:870:GLU:N	2.36	0.58
13:M:1062:THR:HG21	13:M:1126:ILE:HD11	1.86	0.58
2:B:501:LEU:HD12	2:B:505:LEU:CD1	2.32	0.58
21:Y:48:LYS:N	21:Y:55:ASP:O	2.37	0.58
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.86	0.58
24:b:538:ARG:HD3	24:b:673:LEU:HB3	1.86	0.58
26:d:119:GLY:O	26:d:134:ARG:NH2	2.36	0.57
23:a:168:VAL:HG22	23:a:189:ILE:HD13	1.86	0.57
26:d:884:ILE:HG22	26:d:885:ASN:H	1.70	0.57
26:d:35:LYS:O	26:d:38:ARG:N	2.38	0.57
27:e:426:ASP:O	27:e:430:GLU:N	2.35	0.57
1:A:296:ASN:OD1	24:b:683:ARG:NH2	2.34	0.57
25:c:137:PHE:O	25:c:141:ASN:N	2.37	0.57
24:b:682:LEU:O	24:b:685:LEU:N	2.38	0.57
7:G:109:SER:O	7:G:112:SER:OG	2.22	0.57
7:G:117:MET:HE2	7:G:135:ILE:HG13	1.86	0.56
2:B:413:LYS:O	2:B:417:ILE:HD12	2.03	0.56
24:b:646:ASP:OD1	24:b:647:GLU:N	2.38	0.56
27:e:578:LEU:O	27:e:589:PHE:N	2.34	0.56
4:D:36:GLU:OE2	4:D:84:ARG:NH1	2.39	0.56
13:M:787:SER:HG	13:M:792:HIS:CE1	2.21	0.56
26:d:881:LEU:HD21	26:d:921:ILE:HG21	1.86	0.56
1:A:421:ARG:NH1	1:A:444:TYR:OH	2.39	0.56
1:A:904:GLN:NE2	1:A:981:CYS:O	2.37	0.56
21:Y:172:ILE:O	21:Y:186:LEU:N	2.38	0.56
24:b:800:ILE:HD13	24:b:803:ARG:NH2	2.21	0.56
26:d:308:THR:O	26:d:383:LYS:NZ	2.35	0.56
13:M:297:ARG:NE	13:M:372:GLU:OE2	2.39	0.56
26:d:707:ILE:HG22	26:d:707:ILE:O	2.04	0.56
1:A:1180:ASN:ND2	1:A:1183:SER:OG	2.38	0.56
13:M:473:ARG:NE	13:M:473:ARG:HA	2.19	0.56
13:M:565:GLU:N	13:M:565:GLU:OE1	2.39	0.56
13:M:1002:LYS:O	13:M:1005:LYS:N	2.38	0.56
5:E:120:ASP:OD1	5:E:121:MET:N	2.38	0.56
13:M:650:ASP:OD1	13:M:651:ASP:N	2.37	0.56
23:a:179:SER:OG	24:b:696:LYS:O	2.19	0.56
24:b:538:ARG:CZ	24:b:538:ARG:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:627:TYR:HD1	24:b:631:MET:HE1	1.71	0.56
24:b:808:HIS:HB3	24:b:867:MET:HE1	1.86	0.55
24:b:800:ILE:HD13	24:b:803:ARG:HH21	1.71	0.55
27:e:68:GLU:O	27:e:72:ALA:N	2.37	0.55
4:D:33:LEU:O	4:D:36:GLU:N	2.39	0.55
13:M:1151:ASN:ND2	13:M:1156:GLU:O	2.38	0.55
13:M:807:ASP:OD1	13:M:807:ASP:N	2.37	0.55
13:M:965:ARG:NH1	13:M:968:GLU:OE2	2.40	0.55
24:b:882:TYR:HE2	24:b:884:LYS:HB2	1.69	0.55
1:A:54:LEU:O	1:A:61:ARG:NH2	2.40	0.55
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.39	0.55
24:b:760:ASN:OD1	24:b:761:GLU:N	2.40	0.55
26:d:1055:GLN:HG3	26:d:1093:LEU:HD23	1.89	0.55
13:M:610:PHE:O	13:M:614:ALA:HB2	2.07	0.55
26:d:397:HIS:O	26:d:702:GLY:HA3	2.07	0.55
13:M:316:GLU:O	13:M:319:TRP:N	2.39	0.55
3:C:59:LEU:HD13	3:C:63:PHE:CD1	2.42	0.55
23:a:93:ASP:OD1	23:a:93:ASP:N	2.32	0.55
2:B:602:SER:OG	2:B:620:ARG:NH1	2.41	0.54
23:a:153:SER:HA	23:a:199:ASP:OD1	2.07	0.54
7:G:138:GLN:N	7:G:141:ASP:OD2	2.36	0.54
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.41	0.54
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.90	0.54
13:M:951:LYS:O	13:M:955:LEU:HD23	2.07	0.54
23:a:338:ASP:OD1	23:a:354:ARG:NH1	2.40	0.54
5:E:78:GLU:OE1	5:E:78:GLU:N	2.41	0.54
6:F:84:GLU:OE2	6:F:84:GLU:N	2.40	0.54
13:M:306:LYS:O	13:M:367:ARG:NH2	2.41	0.54
1:A:108:ARG:NH2	1:A:191:ILE:O	2.41	0.54
26:d:1051:LEU:HB2	26:d:1089:ILE:HD13	1.88	0.54
13:M:301:ARG:NH2	13:M:305:VAL:HG22	2.23	0.54
23:a:111:ASP:OD2	24:b:1386:SER:OG	2.21	0.54
24:b:876:ARG:HH21	24:b:876:ARG:HG2	1.73	0.53
1:A:499:ASP:OD1	15:P:50:A:H4'	2.09	0.53
2:B:959:GLU:O	2:B:961:ILE:N	2.40	0.53
4:D:103:LEU:O	7:G:144:ARG:NH2	2.41	0.53
13:M:552:ASP:OD2	13:M:556:ARG:NE	2.41	0.53
13:M:1031:CYS:O	13:M:1033:GLY:N	2.42	0.53
1:A:413:TYR:O	1:A:449:HIS:ND1	2.41	0.53
17:S:279:PHE:O	17:S:284:ASP:N	2.40	0.53
27:e:588:GLU:O	27:e:667:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:e:592:SER:O	27:e:596:THR:N	2.39	0.53
23:a:17:ARG:NH1	26:d:117:GLU:O	2.42	0.53
26:d:213:GLU:OE2	26:d:236:SER:N	2.42	0.53
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.22	0.52
13:M:613:ARG:O	13:M:613:ARG:HG3	2.09	0.52
23:a:208:ASP:OD1	23:a:208:ASP:N	2.40	0.52
24:b:693:PHE:CD1	24:b:696:LYS:HB2	2.45	0.52
27:e:528:LEU:O	28:f:33:TRP:N	2.41	0.52
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.42	0.52
13:M:287:ASN:O	13:M:290:ARG:HG2	2.10	0.52
1:A:862:ARG:NH1	2:B:1088:GLU:OE2	2.42	0.52
13:M:288:GLU:O	13:M:292:THR:N	2.41	0.52
26:d:31:LEU:HD21	26:d:33:ILE:HD11	1.90	0.52
1:A:889:LEU:O	1:A:890:ARG:NH1	2.42	0.52
13:M:802:GLU:N	13:M:802:GLU:OE2	2.42	0.52
3:C:7:PRO:O	11:K:104:ARG:NH1	2.43	0.52
3:C:86:ARG:HD3	11:K:11:LEU:HD11	1.92	0.52
13:M:622:LYS:HA	13:M:625:ARG:HE	1.75	0.52
24:b:540:ILE:HD12	24:b:540:ILE:H	1.74	0.52
26:d:310:ILE:O	26:d:326:SER:OG	2.12	0.52
26:d:356:LEU:HD11	26:d:712:ILE:HD13	1.91	0.52
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	1.91	0.51
13:M:1056:SER:OG	13:M:1058:VAL:HG22	2.09	0.51
24:b:876:ARG:HA	24:b:876:ARG:NE	2.25	0.51
26:d:707:ILE:HD12	26:d:709:LYS:HE3	1.93	0.51
7:G:39:THR:O	7:G:43:GLY:N	2.40	0.51
26:d:130:MET:HE2	26:d:169:PHE:CZ	2.44	0.51
21:Y:86:ALA:O	21:Y:104:ALA:N	2.43	0.51
13:M:1051:GLU:OE1	13:M:1051:GLU:N	2.44	0.51
13:M:329:THR:HG22	13:M:329:THR:O	2.11	0.51
13:M:551:ARG:HD3	13:M:601:LEU:HD11	1.92	0.51
13:M:1113:ARG:HA	13:M:1116:TYR:HE1	1.76	0.51
23:a:209:SER:OG	23:a:246:GLY:O	2.18	0.51
26:d:742:VAL:HG13	26:d:743:GLN:N	2.25	0.51
1:A:951:GLU:OE2	1:A:954:ARG:NH2	2.44	0.51
4:D:90:LYS:CE	4:D:130:ILE:HD12	2.36	0.51
13:M:532:LEU:HD11	13:M:584:VAL:HG23	1.93	0.51
13:M:574:VAL:O	13:M:574:VAL:HG13	2.10	0.50
24:b:538:ARG:CG	24:b:538:ARG:NH2	2.73	0.50
7:G:90:THR:O	7:G:139:GLN:NE2	2.43	0.50
13:M:1165:LYS:HE3	13:M:1167:ILE:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:d:232:ILE:HD13	26:d:237:ILE:HG23	1.93	0.50
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.43	0.50
26:d:1128:ASP:O	26:d:1132:VAL:HG23	2.11	0.50
13:M:316:GLU:HG2	13:M:403:TRP:CE2	2.46	0.50
24:b:1385:ALA:O	24:b:1387:SER:N	2.45	0.50
23:a:65:ASP:OD2	23:a:67:VAL:HG22	2.12	0.50
24:b:886:ASP:O	24:b:889:THR:OG1	2.28	0.50
5:E:114:ALA:O	5:E:117:SER:OG	2.26	0.50
24:b:975:ARG:HA	24:b:975:ARG:NE	2.26	0.50
13:M:288:GLU:O	13:M:291:ALA:N	2.44	0.50
26:d:289:GLU:OE1	26:d:289:GLU:N	2.44	0.50
3:C:175:LYS:NZ	12:L:57:ALA:O	2.44	0.50
5:E:141:GLU:N	5:E:141:GLU:OE1	2.45	0.50
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.94	0.50
13:M:963:ILE:O	13:M:967:ASN:ND2	2.45	0.50
23:a:153:SER:O	23:a:153:SER:OG	2.28	0.49
24:b:719:ALA:O	24:b:994:ARG:NH2	2.45	0.49
26:d:1051:LEU:HD23	26:d:1054:MET:HE3	1.94	0.49
4:D:90:LYS:HD2	4:D:92:LEU:HD12	1.93	0.49
13:M:1156:GLU:OE1	13:M:1156:GLU:N	2.46	0.49
2:B:312:GLN:NE2	9:I:22:ASN:OD1	2.46	0.49
9:I:109:ARG:HE	9:I:124:THR:HG21	1.78	0.49
23:a:351:SER:O	23:a:351:SER:OG	2.31	0.49
24:b:538:ARG:HB3	24:b:538:ARG:NH2	2.28	0.49
13:M:606:LEU:HD23	13:M:721:LEU:HD22	1.93	0.49
13:M:999:HIS:O	13:M:1003:ILE:HD12	2.12	0.49
1:A:481:THR:O	1:A:483:ARG:NE	2.46	0.49
13:M:550:LEU:HD22	13:M:689:ILE:CD1	2.43	0.49
13:M:575:CYS:SG	13:M:576:SER:N	2.85	0.49
13:M:1109:GLU:OE2	13:M:1113:ARG:NH1	2.46	0.49
21:Y:35:VAL:N	21:Y:47:TRP:O	2.44	0.49
21:Y:176:ASP:O	21:Y:180:GLY:N	2.38	0.49
1:A:1477:ALA:HB1	7:G:23:LEU:HD21	1.95	0.49
7:G:21:ASN:OD1	7:G:24:ASN:HB2	2.13	0.49
9:I:72:VAL:HG22	9:I:78:LEU:HD11	1.95	0.49
2:B:812:ARG:NH2	2:B:900:GLU:OE2	2.45	0.48
5:E:209:VAL:O	5:E:210:GLN:NE2	2.44	0.48
3:C:70:LEU:O	10:J:6:ARG:NE	2.40	0.48
13:M:522:ASP:C	13:M:523:MET:HG3	2.38	0.48
21:Y:130:VAL:O	21:Y:144:LEU:N	2.43	0.48
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:HG	1:A:184:CYS:CB	2.20	0.48
1:A:728:THR:H	1:A:736:THR:HG21	1.79	0.48
2:B:777:ASN:O	10:J:47:ARG:NH1	2.40	0.48
13:M:450:ARG:HH21	13:M:450:ARG:HG3	1.77	0.48
13:M:1062:THR:O	13:M:1062:THR:HG22	2.14	0.48
13:M:394:TRP:O	13:M:398:GLN:HG3	2.12	0.48
1:A:523:ARG:NH1	6:F:127:ASP:OD2	2.47	0.48
26:d:390:ILE:HD12	26:d:390:ILE:N	2.29	0.48
7:G:100:GLU:O	7:G:100:GLU:HG2	2.13	0.48
9:I:50:ASN:ND2	9:I:52:CYS:O	2.46	0.48
1:A:455:ILE:HG23	1:A:520:MET:HE1	1.96	0.48
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.29	0.48
13:M:865:LYS:O	13:M:869:HIS:ND1	2.41	0.48
1:A:1229:GLU:OE1	1:A:1229:GLU:N	2.45	0.48
13:M:780:ARG:O	13:M:846:HIS:N	2.47	0.48
13:M:1002:LYS:O	13:M:1003:ILE:C	2.57	0.48
21:Y:14:ALA:N	21:Y:296:GLN:O	2.47	0.48
23:a:1:MET:SD	26:d:910:MET:HE1	2.54	0.48
24:b:807:ASN:CG	24:b:867:MET:HE3	2.39	0.48
13:M:311:ASP:N	13:M:311:ASP:OD1	2.38	0.48
13:M:795:PHE:CD2	13:M:910:LEU:HG	2.49	0.48
23:a:355:ASP:N	23:a:355:ASP:OD1	2.36	0.47
27:e:179:ARG:O	27:e:184:SER:N	2.40	0.47
24:b:964:THR:HG1	24:b:967:THR:HG1	1.51	0.47
1:A:98:GLY:HA3	1:A:1440:MET:HE3	1.97	0.47
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.47	0.47
4:D:96:GLU:OE2	4:D:117:SER:HB3	2.14	0.47
18:T:20:DT:H2'	18:T:21:DC:O4'	2.13	0.47
21:Y:33:GLU:O	21:Y:49:TRP:N	2.48	0.47
26:d:6:VAL:HG22	26:d:1040:VAL:HG22	1.96	0.47
4:D:34:ASN:OD1	4:D:102:ASN:ND2	2.48	0.47
7:G:20:PRO:O	7:G:21:ASN:HB3	2.14	0.47
26:d:1055:GLN:CG	26:d:1093:LEU:HD23	2.44	0.47
21:Y:90:LEU:O	21:Y:99:ILE:N	2.41	0.47
24:b:681:ASN:N	24:b:681:ASN:OD1	2.45	0.47
2:B:105:PRO:HG2	16:R:9:UNK:C	2.44	0.47
3:C:144:GLU:OE1	3:C:144:GLU:N	2.48	0.47
13:M:808:PHE:HB2	13:M:910:LEU:HD21	1.96	0.47
17:S:205:GLY:O	17:S:209:VAL:N	2.48	0.47
23:a:251:LEU:HD23	23:a:262:THR:HG22	1.96	0.47
26:d:275:ASP:OD2	26:d:279:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:206:SER:OG	23:a:207:ALA:N	2.48	0.47
4:D:125:GLU:OE2	4:D:125:GLU:N	2.42	0.47
13:M:1111:LEU:O	13:M:1116:TYR:N	2.45	0.47
1:A:1297:THR:HG23	1:A:1297:THR:O	2.15	0.46
1:A:1357:THR:O	5:E:142:HIS:NE2	2.45	0.46
24:b:651:ILE:HG22	24:b:651:ILE:O	2.15	0.46
26:d:31:LEU:CD2	26:d:33:ILE:HD11	2.45	0.46
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.46	0.46
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.13	0.46
2:B:905:ASP:N	2:B:922:ARG:O	2.47	0.46
4:D:140:PHE:CZ	13:M:523:MET:HE1	2.50	0.46
24:b:768:LEU:HD12	24:b:773:HIS:HA	1.98	0.46
26:d:284:LEU:HD22	26:d:301:ARG:NH1	2.31	0.46
26:d:929:SER:O	26:d:930:VAL:CG1	2.63	0.46
26:d:929:SER:HB2	26:d:952:ASN:HB2	1.98	0.46
9:I:109:ARG:NE	9:I:124:THR:HG21	2.30	0.46
23:a:76:SER:O	23:a:76:SER:OG	2.34	0.46
24:b:654:PRO:HA	24:b:659:THR:HG21	1.96	0.46
26:d:1000:LEU:HD23	26:d:1002:GLU:HB2	1.97	0.46
1:A:1478:GLU:N	1:A:1478:GLU:OE1	2.49	0.46
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.48	0.46
23:a:266:ASP:OD1	23:a:266:ASP:N	2.44	0.46
26:d:45:THR:HG22	26:d:46:ALA:N	2.31	0.46
24:b:913:THR:CG2	24:b:916:VAL:HG22	2.46	0.46
3:C:189:ASP:O	3:C:191:ALA:N	2.48	0.46
2:B:438:ARG:NH2	2:B:442:ASP:OD1	2.48	0.46
13:M:311:ASP:OD1	13:M:312:GLU:N	2.49	0.46
26:d:165:ILE:HG21	26:d:217:SER:HA	1.97	0.46
1:A:78:MET:O	2:B:1072:ARG:NH2	2.49	0.46
4:D:84:ARG:O	4:D:87:LEU:N	2.48	0.46
4:D:108:ALA:HB1	4:D:112:LYS:HZ3	1.81	0.46
8:H:136:GLU:O	8:H:139:SER:OG	2.27	0.46
24:b:808:HIS:CB	24:b:867:MET:HE1	2.45	0.46
26:d:986:ASP:OD1	26:d:986:ASP:N	2.49	0.46
26:d:1051:LEU:CB	26:d:1089:ILE:HD13	2.46	0.46
1:A:67:ARG:NH2	15:P:38:A:H5'	2.31	0.45
1:A:321:GLU:OE1	1:A:321:GLU:N	2.50	0.45
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.80	0.45
1:A:844:ARG:NH2	2:B:501:LEU:HD13	2.31	0.45
7:G:117:MET:CE	7:G:135:ILE:HG13	2.46	0.45
26:d:38:ARG:NE	26:d:54:GLU:OE2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:754:ARG:HD2	13:M:754:ARG:O	2.16	0.45
13:M:755:VAL:HG23	13:M:923:PRO:HG2	1.98	0.45
13:M:1150:PHE:CZ	13:M:1161:PHE:CE2	3.04	0.45
13:M:296:GLU:HB2	13:M:996:LYS:HD2	1.98	0.45
13:M:296:GLU:OE2	13:M:300:LEU:HD21	2.16	0.45
13:M:542:THR:O	13:M:542:THR:HG23	2.15	0.45
13:M:915:SER:O	13:M:918:ARG:N	2.50	0.45
24:b:874:PHE:O	24:b:877:ALA:N	2.49	0.45
26:d:196:SER:O	26:d:200:LYS:N	2.49	0.45
7:G:27:LYS:HE3	7:G:51:ILE:HD11	1.97	0.45
1:A:332:SER:HB3	18:T:29:DT:H5''	1.97	0.45
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.52	0.45
13:M:379:TYR:O	13:M:380:ARG:NH1	2.46	0.45
13:M:590:TYR:CZ	13:M:594:LEU:HD21	2.52	0.45
21:Y:35:VAL:O	21:Y:47:TRP:N	2.40	0.45
24:b:758:ASP:OD1	24:b:759:LYS:N	2.49	0.45
1:A:695:ASP:OD1	1:A:698:THR:OG1	2.30	0.45
5:E:112:PRO:HB3	18:T:7:DG:H5'	1.98	0.45
7:G:62:GLY:O	7:G:63:ARG:HG2	2.17	0.45
13:M:783:GLY:O	13:M:796:CYS:HA	2.17	0.45
13:M:1126:ILE:O	13:M:1130:LEU:HD23	2.16	0.45
24:b:597:LEU:HB2	24:b:621:LEU:HD11	1.97	0.45
26:d:72:GLU:OE1	26:d:103:ARG:NH2	2.47	0.45
26:d:308:THR:HG22	26:d:347:VAL:HG11	1.98	0.45
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.98	0.45
13:M:554:TYR:O	13:M:556:ARG:N	2.49	0.45
20:V:292:ALA:C	20:V:294:GLU:H	2.25	0.45
8:H:88:PHE:CD1	8:H:144:LEU:HD12	2.52	0.45
26:d:61:ILE:HG23	26:d:79:ILE:HG23	1.99	0.45
24:b:600:THR:OG1	24:b:601:GLY:N	2.49	0.45
24:b:948:ALA:O	24:b:950:ARG:N	2.49	0.45
4:D:76:ASN:O	4:D:79:THR:OG1	2.24	0.44
13:M:413:LEU:HD12	13:M:460:LEU:HD11	1.99	0.44
13:M:753:LEU:HD13	13:M:924:LEU:HD13	1.98	0.44
13:M:1113:ARG:HA	13:M:1116:TYR:CE1	2.51	0.44
18:T:29:DT:O3'	18:T:30:DG:O4'	2.35	0.44
22:Z:247:LYS:O	22:Z:251:ALA:N	2.44	0.44
1:A:332:SER:HB3	18:T:29:DT:C5'	2.47	0.44
2:B:294:ASP:OD1	2:B:379:ARG:NH2	2.48	0.44
13:M:849:THR:HB	13:M:885:VAL:HG21	1.99	0.44
1:A:896:LEU:O	1:A:1396:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ASP:OD1	2:B:15:ASP:N	2.47	0.44
13:M:613:ARG:HG3	13:M:671:ILE:HG23	1.99	0.44
24:b:830:ASP:O	24:b:837:ARG:NH2	2.48	0.44
26:d:6:VAL:HG23	26:d:1088:PHE:HD1	1.81	0.44
26:d:884:ILE:HD12	26:d:884:ILE:H	1.81	0.44
18:T:29:DT:C4	18:T:30:DG:C2	3.05	0.44
21:Y:88:ILE:N	21:Y:102:ILE:O	2.39	0.44
23:a:164:ARG:HG2	23:a:164:ARG:O	2.17	0.44
26:d:929:SER:HA	26:d:954:MET:HG2	2.00	0.44
1:A:883:ILE:HD11	1:A:1424:THR:HA	1.99	0.44
3:C:5:ASN:OD1	11:K:52:LYS:NZ	2.51	0.44
21:Y:214:ILE:O	21:Y:228:LEU:N	2.40	0.44
26:d:43:VAL:HG23	26:d:52:VAL:HG11	1.99	0.44
4:D:108:ALA:O	4:D:111:SER:OG	2.20	0.44
13:M:1023:MET:HE3	13:M:1027:VAL:HG23	1.99	0.44
4:D:138:ARG:HH12	13:M:523:MET:HG2	1.83	0.44
13:M:355:THR:HG23	13:M:356:ILE:N	2.33	0.44
23:a:79:GLN:OE1	23:a:79:GLN:N	2.51	0.44
26:d:677:ASN:N	26:d:694:ALA:O	2.48	0.44
1:A:272:ASN:ND2	18:T:30:DG:H2''	2.32	0.44
1:A:1189:ASP:OD2	1:A:1258:ARG:NE	2.51	0.44
8:H:71:ASP:OD1	8:H:72:ASP:N	2.51	0.44
13:M:756:ALA:N	13:M:1139:THR:O	2.48	0.44
17:S:413:GLU:O	17:S:416:ILE:N	2.51	0.44
23:a:290:ASN:N	23:a:290:ASN:OD1	2.51	0.44
1:A:266:MET:CE	1:A:270:ALA:HB3	2.40	0.43
4:D:48:ASN:C	4:D:48:ASN:HD22	2.25	0.43
18:T:38:DG:OP1	24:b:913:THR:HG21	2.18	0.43
23:a:2:LEU:HD11	26:d:843:PRO:HG2	2.00	0.43
27:e:221:LEU:O	27:e:226:VAL:N	2.45	0.43
2:B:84:TYR:HE2	2:B:132:VAL:HG22	1.83	0.43
23:a:289:ASN:N	23:a:289:ASN:OD1	2.50	0.43
26:d:275:ASP:OD1	26:d:279:ARG:N	2.52	0.43
26:d:310:ILE:HG21	26:d:328:LEU:HD12	2.00	0.43
26:d:963:ASP:OD1	26:d:963:ASP:N	2.51	0.43
1:A:467:MET:SD	1:A:524:MET:HB3	2.58	0.43
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.33	0.43
13:M:699:SER:OG	13:M:702:VAL:N	2.51	0.43
15:P:45:A:H2'	15:P:46:G:O4'	2.17	0.43
2:B:256:ILE:HD11	2:B:373:LEU:HD21	2.00	0.43
2:B:887:TYR:O	2:B:888:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:ARG:NH2	17:S:891:PHE:CA	2.81	0.43
13:M:608:GLN:O	13:M:612:GLU:OE1	2.36	0.43
13:M:1123:LEU:O	13:M:1124:TYR:C	2.61	0.43
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	2.01	0.43
1:A:937:ASP:OD1	1:A:938:LEU:N	2.51	0.43
13:M:1119:LYS:O	13:M:1123:LEU:HD23	2.18	0.43
21:Y:287:SER:O	21:Y:303:CYS:N	2.46	0.43
2:B:628:VAL:HG12	2:B:629:GLU:O	2.18	0.43
3:C:123:ASN:OD1	3:C:124:SER:N	2.51	0.43
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.54	0.43
13:M:330:ILE:HG13	13:M:332:LEU:HD23	2.01	0.43
13:M:608:GLN:O	13:M:609:THR:C	2.60	0.43
13:M:966:VAL:O	13:M:970:GLY:N	2.46	0.43
20:V:206:LYS:O	20:V:208:ARG:N	2.49	0.43
24:b:576:THR:HG23	24:b:894:ARG:HG2	2.01	0.43
13:M:1145:ASN:HB3	13:M:1148:GLU:OE1	2.19	0.43
26:d:273:LEU:HD11	26:d:283:LEU:HB2	2.00	0.43
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.47	0.43
13:M:473:ARG:NH2	13:M:520:ARG:HE	2.16	0.43
23:a:174:LYS:O	23:a:175:SER:C	2.61	0.43
1:A:1475:LEU:HB2	7:G:66:VAL:HG21	2.00	0.43
13:M:542:THR:HG22	13:M:545:GLN:CD	2.42	0.43
13:M:755:VAL:HG23	13:M:755:VAL:O	2.17	0.43
2:B:850:ASP:OD1	2:B:850:ASP:N	2.52	0.43
27:e:524:THR:O	28:f:29:ALA:N	2.51	0.43
22:Z:246:SER:O	22:Z:250:PHE:N	2.42	0.42
23:a:2:LEU:HD12	26:d:836:VAL:CG2	2.48	0.42
23:a:320:THR:OG1	23:a:327:ILE:HD11	2.19	0.42
24:b:623:THR:OG1	24:b:624:SER:N	2.49	0.42
13:M:303:ILE:HG21	13:M:404:THR:HG21	2.01	0.42
13:M:1018:VAL:HG12	13:M:1023:MET:O	2.19	0.42
23:a:1:MET:C	23:a:3:GLY:N	2.76	0.42
24:b:692:ILE:HG13	24:b:693:PHE:N	2.34	0.42
1:A:255:VAL:HG23	1:A:280:LEU:HD22	2.01	0.42
7:G:27:LYS:O	7:G:30:LEU:N	2.51	0.42
1:A:381:PRO:HG2	1:A:384:ILE:HD12	2.01	0.42
1:A:413:TYR:HB3	1:A:414:PRO:HD3	2.01	0.42
13:M:671:ILE:HG22	13:M:671:ILE:O	2.18	0.42
17:S:535:LEU:O	17:S:539:ALA:N	2.47	0.42
1:A:94:VAL:HG21	1:A:311:GLN:HA	2.01	0.42
26:d:18:CYS:SG	26:d:315:THR:HG23	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:ARG:NH2	6:F:121:ASP:O	2.52	0.42
7:G:1:MET:O	7:G:77:PHE:HA	2.19	0.42
13:M:559:THR:HG22	13:M:560:GLU:N	2.35	0.42
26:d:207:TRP:CB	26:d:242:GLY:HA2	2.50	0.42
26:d:930:VAL:HG22	26:d:948:ASP:HB3	2.00	0.42
26:d:1000:LEU:HD21	26:d:1030:PHE:CE1	2.54	0.42
2:B:1091:ARG:NH2	2:B:1092:ASP:OD1	2.53	0.42
13:M:864:VAL:O	13:M:868:VAL:HG13	2.20	0.42
13:M:866:ARG:O	13:M:870:GLU:OE1	2.38	0.42
15:P:41:A:H2'	15:P:42:U:C6	2.54	0.42
1:A:410:ASN:OD1	1:A:449:HIS:NE2	2.46	0.42
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.52	0.42
24:b:578:MET:HE1	24:b:598:HIS:CG	2.55	0.42
24:b:709:VAL:HB	24:b:710:PRO:HD3	2.01	0.42
1:A:266:MET:SD	18:T:30:DG:H2'	2.60	0.42
1:A:595:ILE:HD11	1:A:675:VAL:HG11	2.02	0.42
1:A:695:ASP:OD1	1:A:695:ASP:N	2.52	0.42
2:B:761:THR:H	2:B:764:MET:HE3	1.85	0.42
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.18	0.42
17:S:649:ALA:O	17:S:652:GLY:N	2.53	0.42
23:a:37:ASP:HB2	23:a:83:THR:HG22	2.01	0.42
23:a:309:PHE:CD2	23:a:318:VAL:HG22	2.55	0.42
1:A:431:PHE:HE2	15:P:38:A:N6	2.12	0.42
2:B:629:GLU:N	2:B:632:LYS:O	2.41	0.42
13:M:702:VAL:HG23	13:M:703:GLN:OE1	2.20	0.42
4:D:86:LEU:HB2	4:D:137:LYS:HZ3	1.85	0.41
7:G:79:PRO:HB3	7:G:147:ILE:HD13	2.02	0.41
13:M:381:LYS:O	13:M:384:VAL:N	2.46	0.41
13:M:855:ARG:NE	13:M:1275:PHE:HD2	2.18	0.41
13:M:889:LEU:HG	13:M:930:VAL:HG11	2.00	0.41
13:M:1057:ARG:NH1	13:M:1134:TYR:CE1	2.88	0.41
26:d:285:LEU:HB3	26:d:297:LEU:HD13	2.01	0.41
26:d:1109:VAL:HG22	26:d:1129:LEU:HD12	2.02	0.41
5:E:110:MET:HG2	5:E:114:ALA:HB3	2.03	0.41
13:M:382:GLU:HB3	13:M:1121:ILE:HG22	2.01	0.41
13:M:672:ASP:OD1	13:M:672:ASP:N	2.52	0.41
23:a:22:GLU:O	23:a:26:ARG:HG3	2.20	0.41
24:b:594:VAL:O	24:b:594:VAL:HG23	2.19	0.41
24:b:627:TYR:CD1	24:b:631:MET:HE1	2.54	0.41
1:A:86:GLY:C	1:A:255:VAL:HG12	2.46	0.41
5:E:84:ILE:HG22	14:N:45:DG:P	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:MET:HE1	6:F:120:VAL:HG13	2.02	0.41
13:M:621:THR:O	13:M:622:LYS:C	2.64	0.41
13:M:937:ILE:HG23	13:M:938:LEU:N	2.36	0.41
23:a:273:ASN:O	23:a:277:GLY:N	2.54	0.41
26:d:969:GLU:HG2	26:d:971:ALA:H	1.85	0.41
1:A:431:PHE:CE2	15:P:38:A:N6	2.84	0.41
1:A:883:ILE:O	1:A:883:ILE:HG22	2.20	0.41
26:d:284:LEU:HD22	26:d:301:ARG:HH12	1.84	0.41
5:E:127:LEU:HD23	5:E:127:LEU:H	1.86	0.41
23:a:111:ASP:OD1	23:a:112:THR:N	2.53	0.41
26:d:81:THR:HG22	26:d:83:LYS:H	1.85	0.41
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.02	0.41
2:B:733:MET:HE1	2:B:1054:MET:HE2	2.02	0.41
7:G:60:GLN:O	7:G:62:GLY:O	2.39	0.41
13:M:758:TYR:CD1	13:M:759:ARG:N	2.89	0.41
23:a:1:MET:HE2	23:a:1:MET:HB3	1.92	0.41
24:b:697:LEU:O	24:b:698:GLY:O	2.39	0.41
26:d:6:VAL:HG23	26:d:1088:PHE:CD1	2.56	0.41
26:d:72:GLU:OE1	26:d:103:ARG:NH1	2.51	0.41
4:D:126:GLU:O	4:D:130:ILE:HG12	2.21	0.41
9:I:49:ASP:OD1	9:I:49:ASP:N	2.49	0.41
12:L:25:GLU:O	12:L:25:GLU:HG2	2.20	0.41
13:M:610:PHE:O	13:M:611:GLN:C	2.62	0.41
24:b:886:ASP:HA	24:b:913:THR:HG22	2.03	0.41
1:A:1433:GLU:OE1	18:T:17:DC:H4'	2.20	0.41
13:M:332:LEU:HD11	13:M:740:TYR:HB2	2.02	0.41
13:M:832:ASP:O	13:M:835:THR:HG22	2.21	0.41
13:M:894:MET:SD	13:M:912:GLN:HG3	2.61	0.41
24:b:798:GLY:O	24:b:802:LEU:HD13	2.20	0.41
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.35	0.41
2:B:899:SER:OG	11:K:1:MET:HE2	2.21	0.41
4:D:48:ASN:C	4:D:48:ASN:ND2	2.78	0.41
7:G:18:PHE:N	7:G:18:PHE:CD1	2.87	0.41
7:G:166:ASP:HB3	13:M:516:LYS:HB2	2.03	0.41
13:M:917:ALA:O	13:M:921:GLN:HG3	2.21	0.41
15:P:32:A:O2'	15:P:33:U:OP1	2.26	0.41
26:d:770:LEU:HD13	26:d:865:GLU:HB2	2.03	0.41
26:d:1098:LEU:HD21	26:d:1134:GLU:OE2	2.21	0.41
27:e:200:ILE:O	27:e:204:ARG:N	2.53	0.41
1:A:848:ILE:HG21	2:B:496:ALA:HB1	2.03	0.41
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:VAL:HG21	10:J:55:LEU:HD13	2.02	0.41
13:M:541:LEU:HD23	13:M:541:LEU:O	2.21	0.41
26:d:413:LEU:O	26:d:424:THR:N	2.54	0.41
2:B:292:PHE:HD1	2:B:298:MET:HE1	1.85	0.40
2:B:962:THR:O	10:J:9:THR:HG23	2.21	0.40
13:M:1150:PHE:HD1	13:M:1275:PHE:CE1	2.38	0.40
13:M:301:ARG:HD2	13:M:401:GLU:HG2	2.03	0.40
13:M:1107:PHE:HA	13:M:1110:GLU:HG2	2.02	0.40
23:a:316:ILE:CD1	23:a:337:VAL:HG11	2.52	0.40
24:b:532:ASP:C	24:b:538:ARG:HH12	2.11	0.40
26:d:311:ALA:HB2	26:d:324:VAL:HG13	2.02	0.40
26:d:742:VAL:HG13	26:d:743:GLN:H	1.86	0.40
1:A:67:ARG:HH21	15:P:38:A:H5'	1.86	0.40
1:A:457:ILE:HD11	1:A:515:ILE:HG23	2.03	0.40
8:H:49:PRO:O	8:H:147:LYS:NZ	2.50	0.40
13:M:1111:LEU:HD13	13:M:1119:LYS:HB2	2.02	0.40
15:P:41:A:H2'	15:P:42:U:H6	1.87	0.40
21:Y:214:ILE:N	21:Y:228:LEU:O	2.38	0.40
26:d:170:LEU:HD21	26:d:179:CYS:CB	2.51	0.40
1:A:266:MET:SD	18:T:30:DG:C4	3.15	0.40
1:A:630:VAL:HG21	1:A:652:LEU:HD21	2.04	0.40
1:A:811:ILE:HD12	9:I:79:PRO:HB3	2.03	0.40
2:B:864:ASP:OD1	2:B:865:VAL:N	2.51	0.40
13:M:1156:GLU:HG2	13:M:1161:PHE:CE2	2.56	0.40
23:a:2:LEU:HD12	26:d:836:VAL:HG22	2.03	0.40
26:d:390:ILE:HG22	26:d:710:LEU:HD22	2.03	0.40
1:A:286:ILE:HD12	1:A:309:LEU:HD23	2.04	0.40
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.03	0.40
3:C:210:GLU:O	3:C:210:GLU:HG2	2.22	0.40
17:S:507:TYR:O	17:S:512:GLU:N	2.45	0.40
18:T:42:DA:H4'	18:T:43:DA:OP1	2.21	0.40
24:b:947:ARG:NE	24:b:947:ARG:HA	2.37	0.40
26:d:365:VAL:HG11	26:d:733:PHE:HE1	1.87	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	1402/1970 (71%)	1366 (97%)	36 (3%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	126/142 (89%)	118 (94%)	8 (6%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	M	788/1729 (46%)	710 (90%)	76 (10%)	2 (0%)	36	70
17	S	888/1179 (75%)	842 (95%)	46 (5%)	0	100	100
19	U	98/666 (15%)	82 (84%)	14 (14%)	2 (2%)	6	28
20	V	209/531 (39%)	174 (83%)	31 (15%)	4 (2%)	6	30
21	Y	298/305 (98%)	278 (93%)	20 (7%)	0	100	100
22	Z	41/531 (8%)	40 (98%)	1 (2%)	0	100	100
23	a	363/396 (92%)	336 (93%)	27 (7%)	0	100	100
24	b	512/1496 (34%)	470 (92%)	42 (8%)	0	100	100
25	c	139/712 (20%)	136 (98%)	3 (2%)	0	100	100
26	d	1082/1143 (95%)	1004 (93%)	78 (7%)	0	100	100
27	e	709/762 (93%)	652 (92%)	57 (8%)	0	100	100
28	f	19/108 (18%)	18 (95%)	1 (5%)	0	100	100
All	All	8992/14145 (64%)	8457 (94%)	527 (6%)	8 (0%)	49	80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	V	248	PRO
19	U	481	GLY
19	U	463	PRO
20	V	238	GLU
20	V	259	ASP
20	V	301	ASN
13	M	946	GLN
13	M	581	PRO

5.3.2 Protein sidechains [i](#)

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	1242/1749 (71%)	1242 (100%)	0	100	100
2	B	992/1027 (97%)	992 (100%)	0	100	100
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	108/126 (86%)	108 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	722/1524 (47%)	721 (100%)	1 (0%)	88	93
23	a	320/348 (92%)	320 (100%)	0	100	100
24	b	466/1299 (36%)	465 (100%)	1 (0%)	87	92
26	d	690/1001 (69%)	690 (100%)	0	100	100
All	All	5623/8242 (68%)	5621 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
13	M	572	ASP
24	b	538	ARG

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	HIS
1	A	295	GLN
1	A	735	GLN
1	A	792	ASN
1	A	1077	ASN
1	A	1078	GLN
2	B	227	ASN
2	B	319	ASN
2	B	1160	GLN
4	D	19	GLN
4	D	66	ASN
4	D	93	HIS
7	G	4	HIS
8	H	29	HIS
11	K	36	ASN
13	M	921	GLN
13	M	948	HIS
13	M	979	HIS
13	M	1007	ASN
23	a	110	HIS
24	b	511	GLN
24	b	524	GLN
24	b	649	HIS
26	d	163	HIS
26	d	261	HIS
26	d	991	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/45 (44%)	9 (45%)	1 (5%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	31	U
15	P	32	A
15	P	33	U
15	P	34	A
15	P	35	U
15	P	38	A
15	P	39	A
15	P	40	A
15	P	41	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	32	A

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

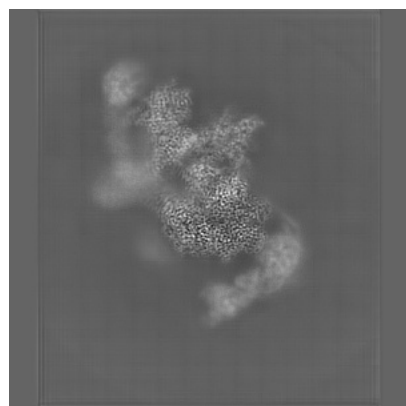
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13016. These allow visual inspection of the internal detail of the map and identification of artifacts.

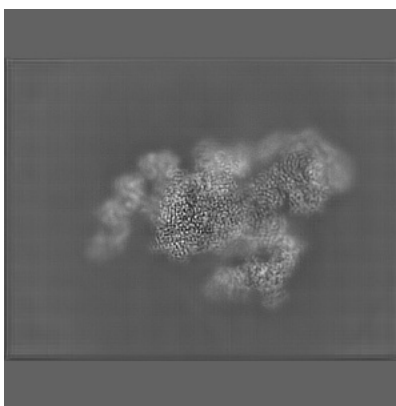
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

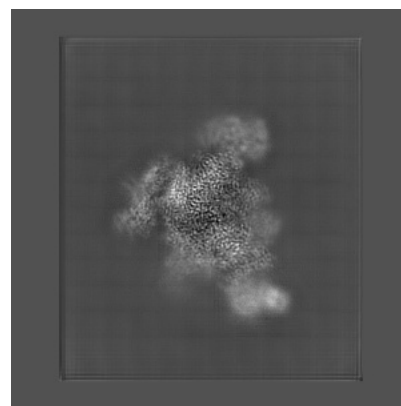
6.1.1 Primary map



X

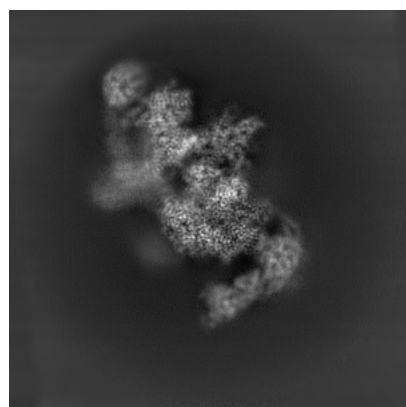


Y

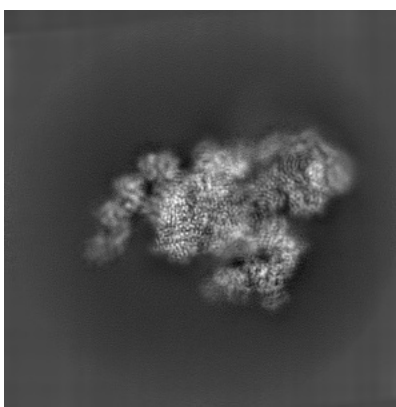


Z

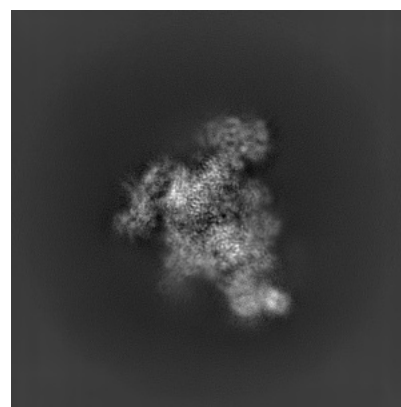
6.1.2 Raw map



X



Y

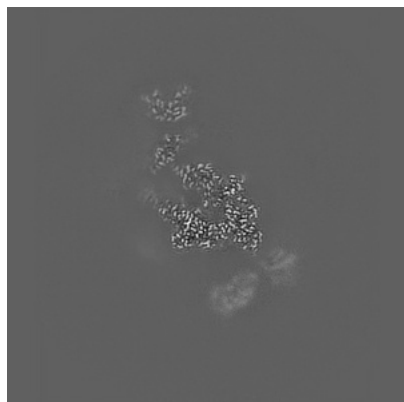


Z

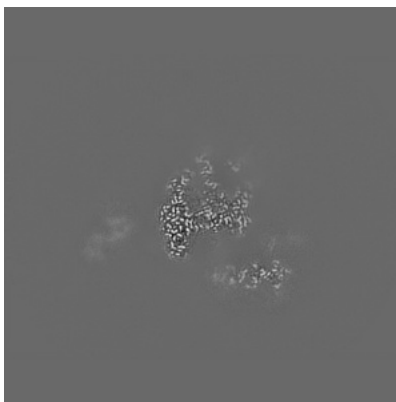
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

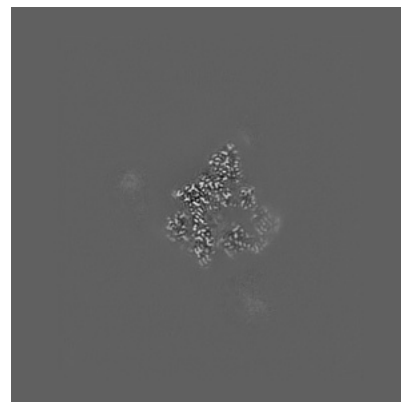
6.2.1 Primary map



X Index: 210

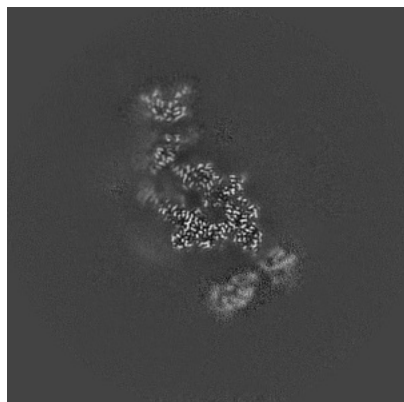


Y Index: 210

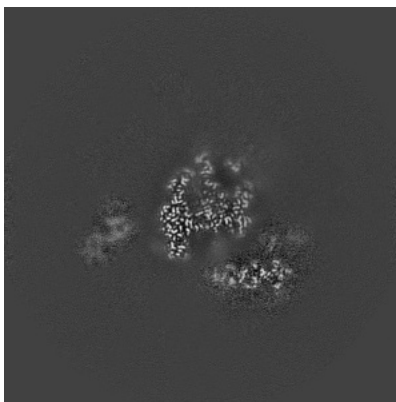


Z Index: 210

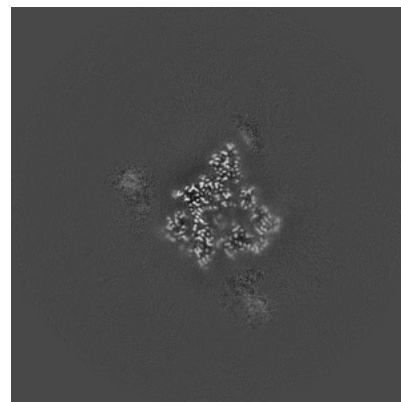
6.2.2 Raw map



X Index: 210



Y Index: 210

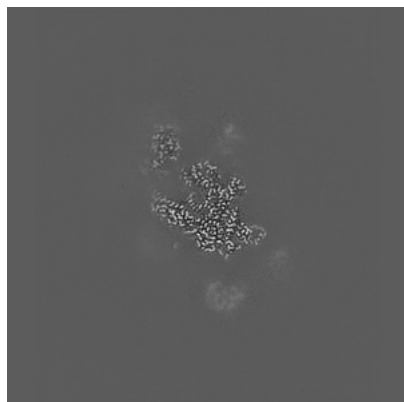


Z Index: 210

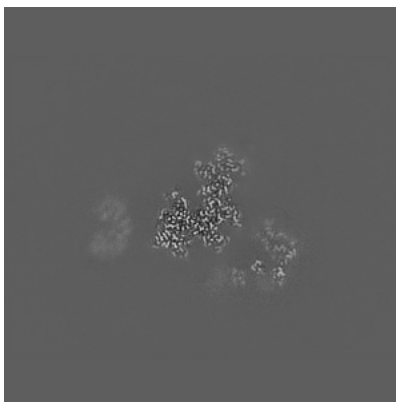
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

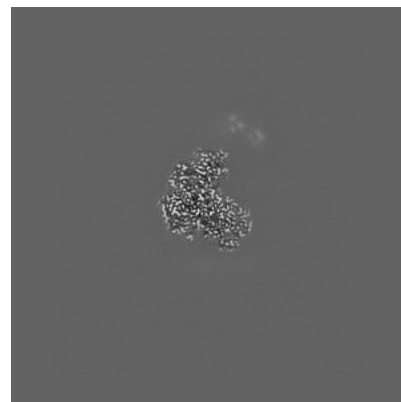
6.3.1 Primary map



X Index: 197

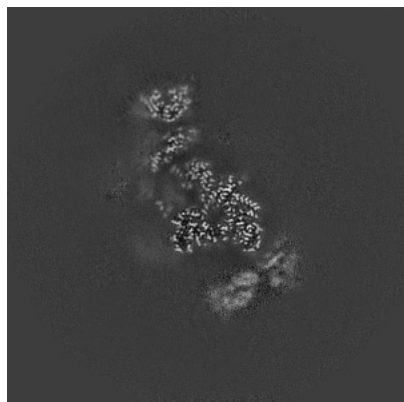


Y Index: 222

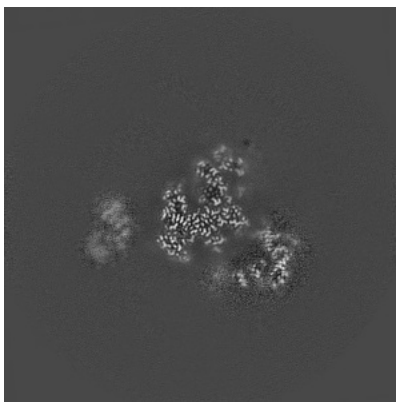


Z Index: 183

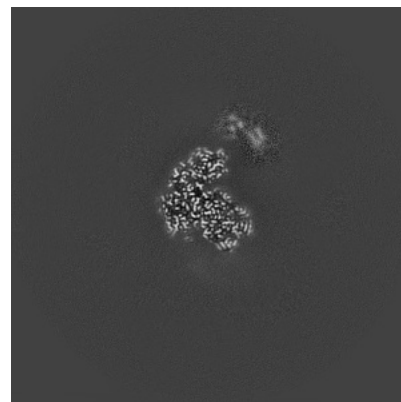
6.3.2 Raw map



X Index: 213



Y Index: 218

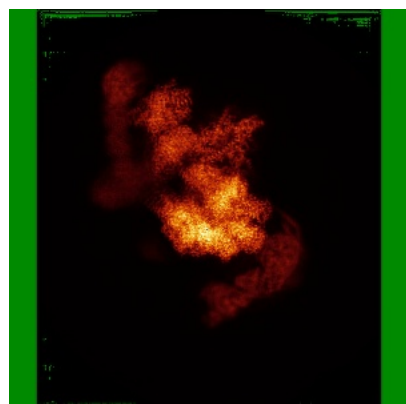


Z Index: 181

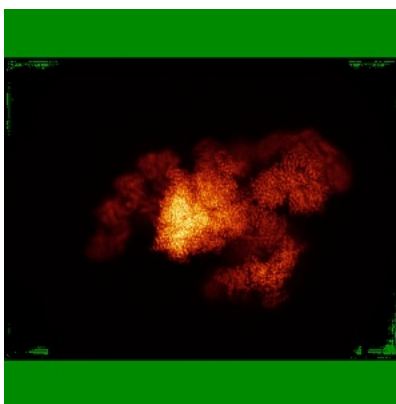
The images above show the largest variance slices of the map in three orthogonal directions.

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

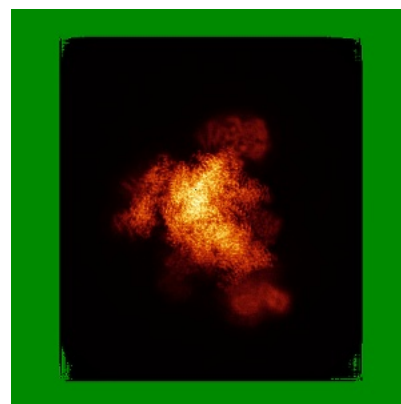
6.4.1 Primary map



X

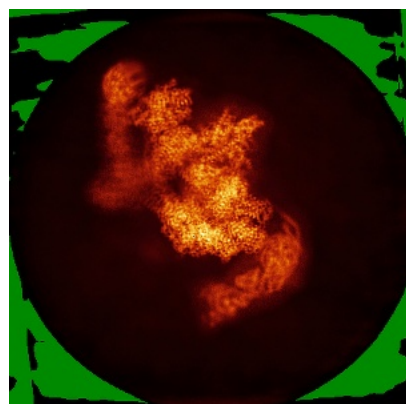


Y

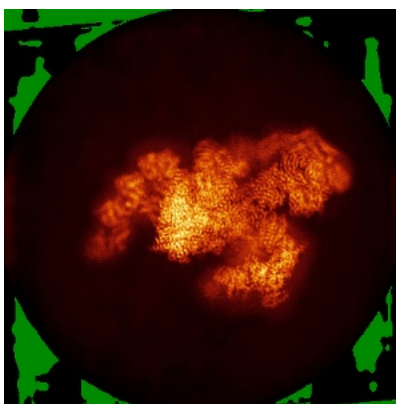


Z

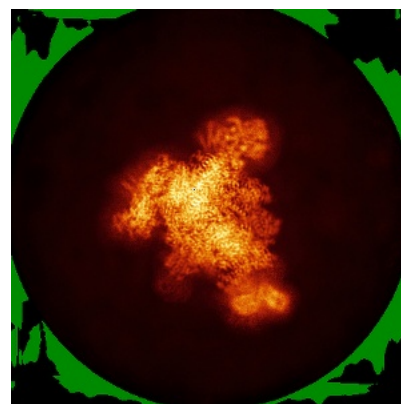
6.4.2 Raw map



X



Y

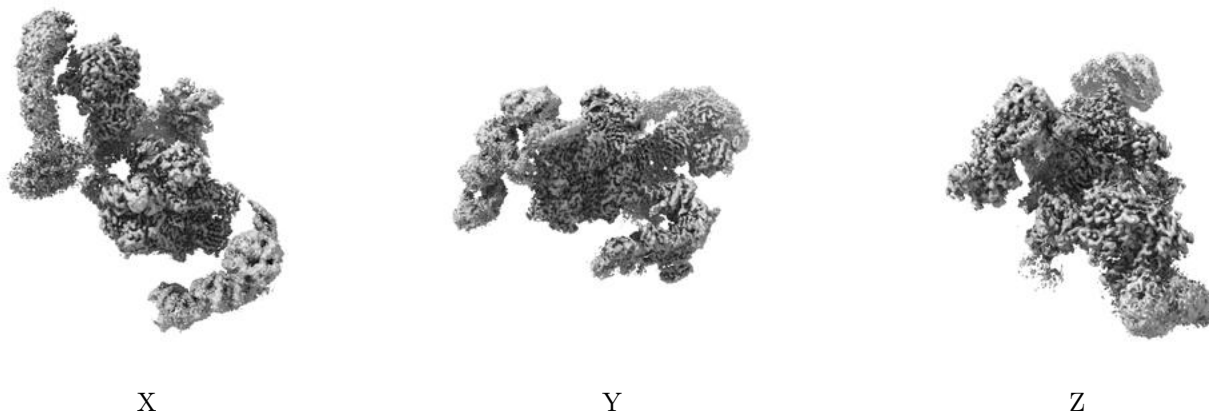


Z

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.

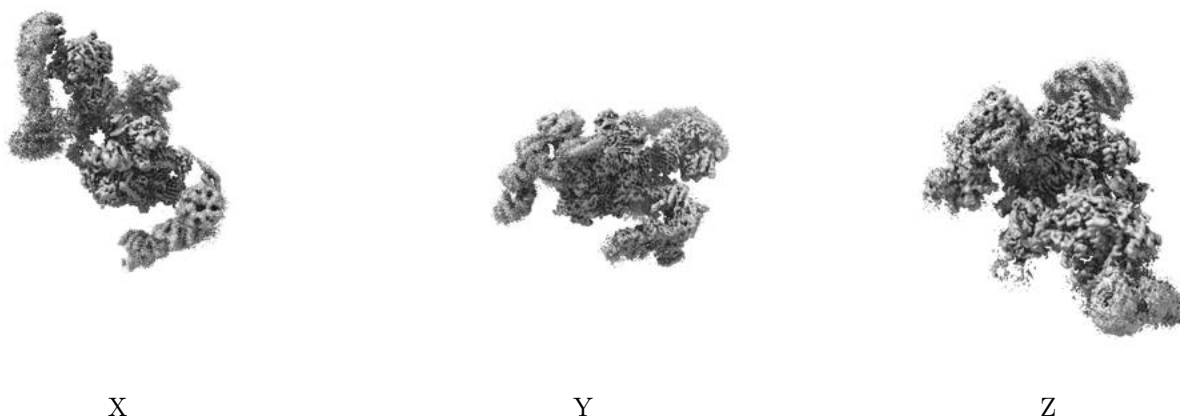
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

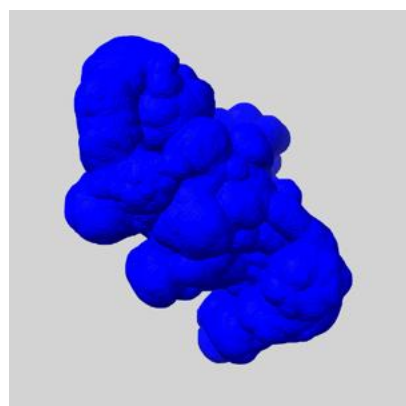
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

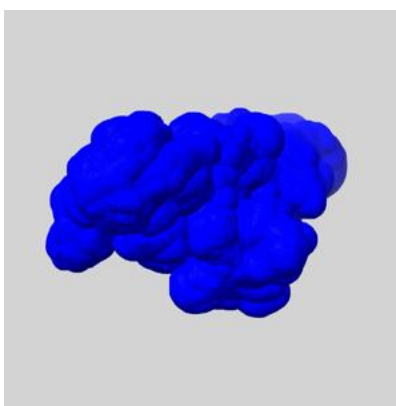
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

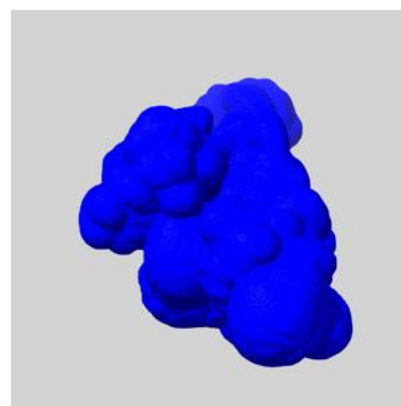
6.6.1 emd_13016_msk_1.map [i](#)



X

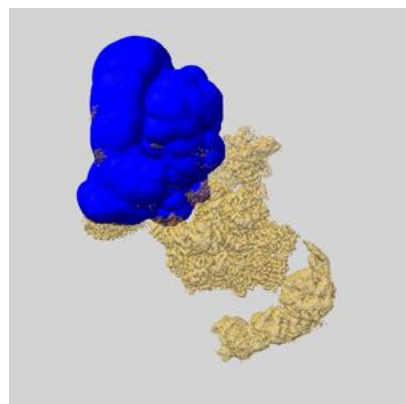


Y

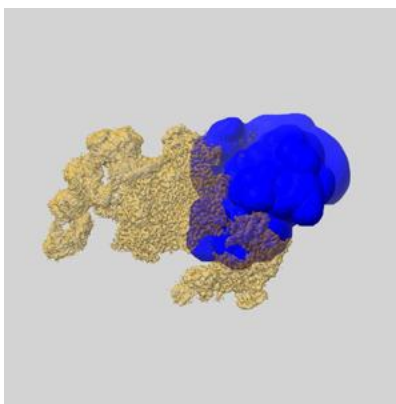


Z

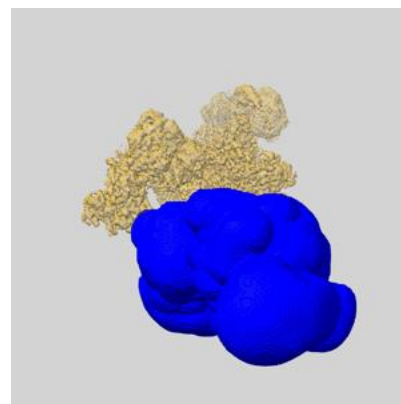
6.6.2 emd_13016_msk_2.map [i](#)



X

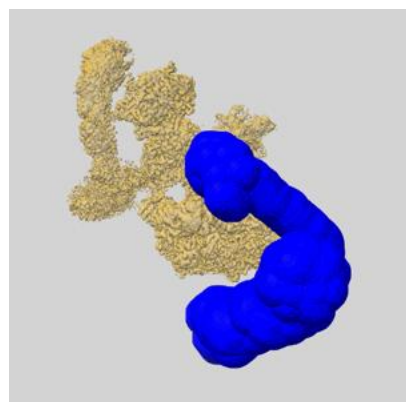


Y

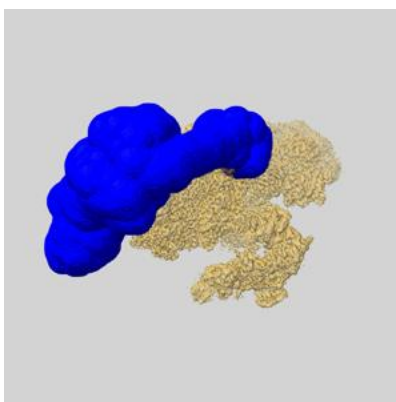


Z

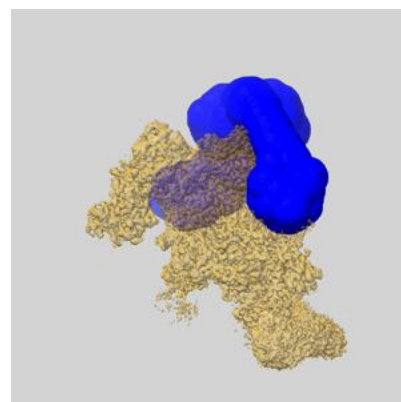
6.6.3 emd_13016_msk_3.map [i](#)



X

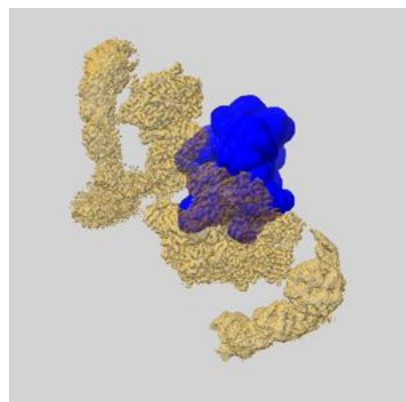


Y

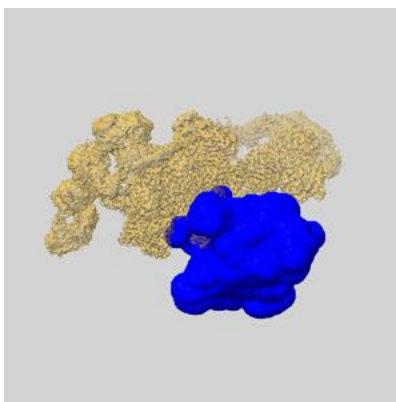


Z

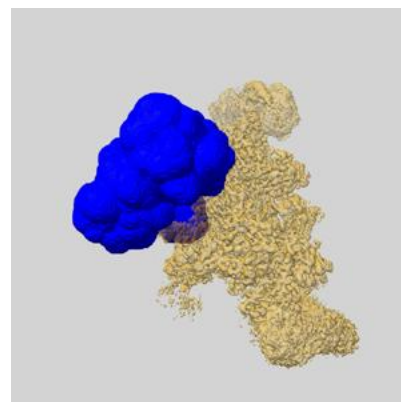
6.6.4 emd_13016_msk_4.map [i](#)



X

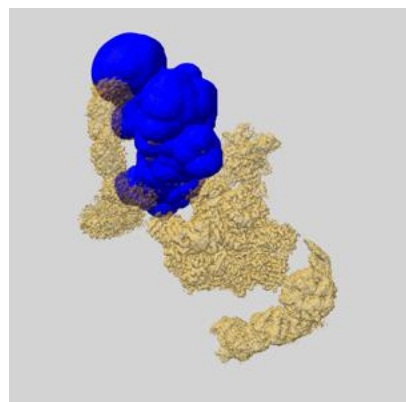


Y

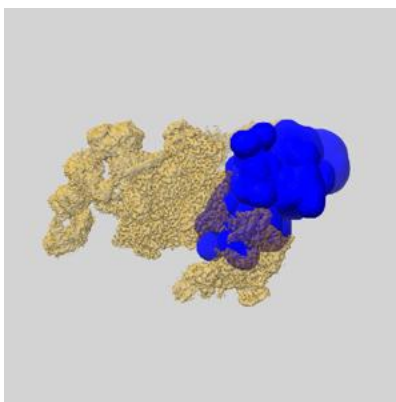


Z

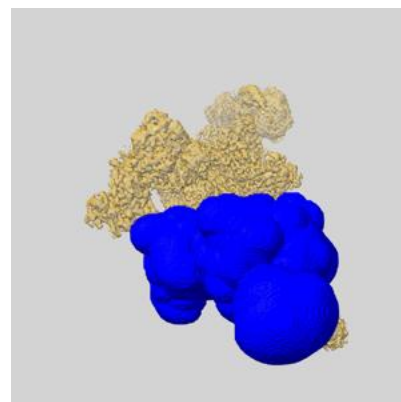
6.6.5 emd_13016_msk_5.map [i](#)



X

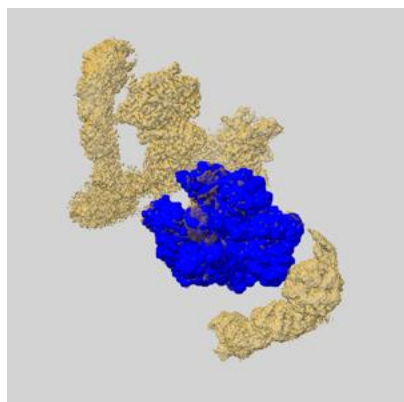


Y

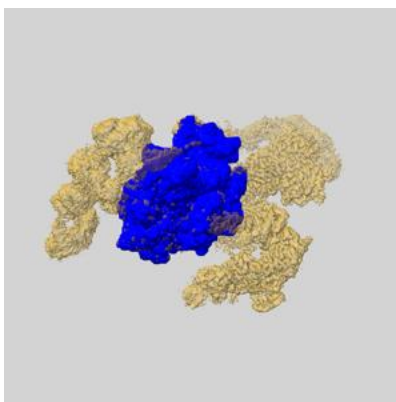


Z

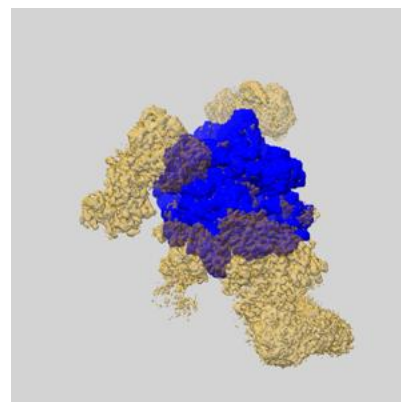
6.6.6 emd_13016_msk_6.map [i](#)



X



Y

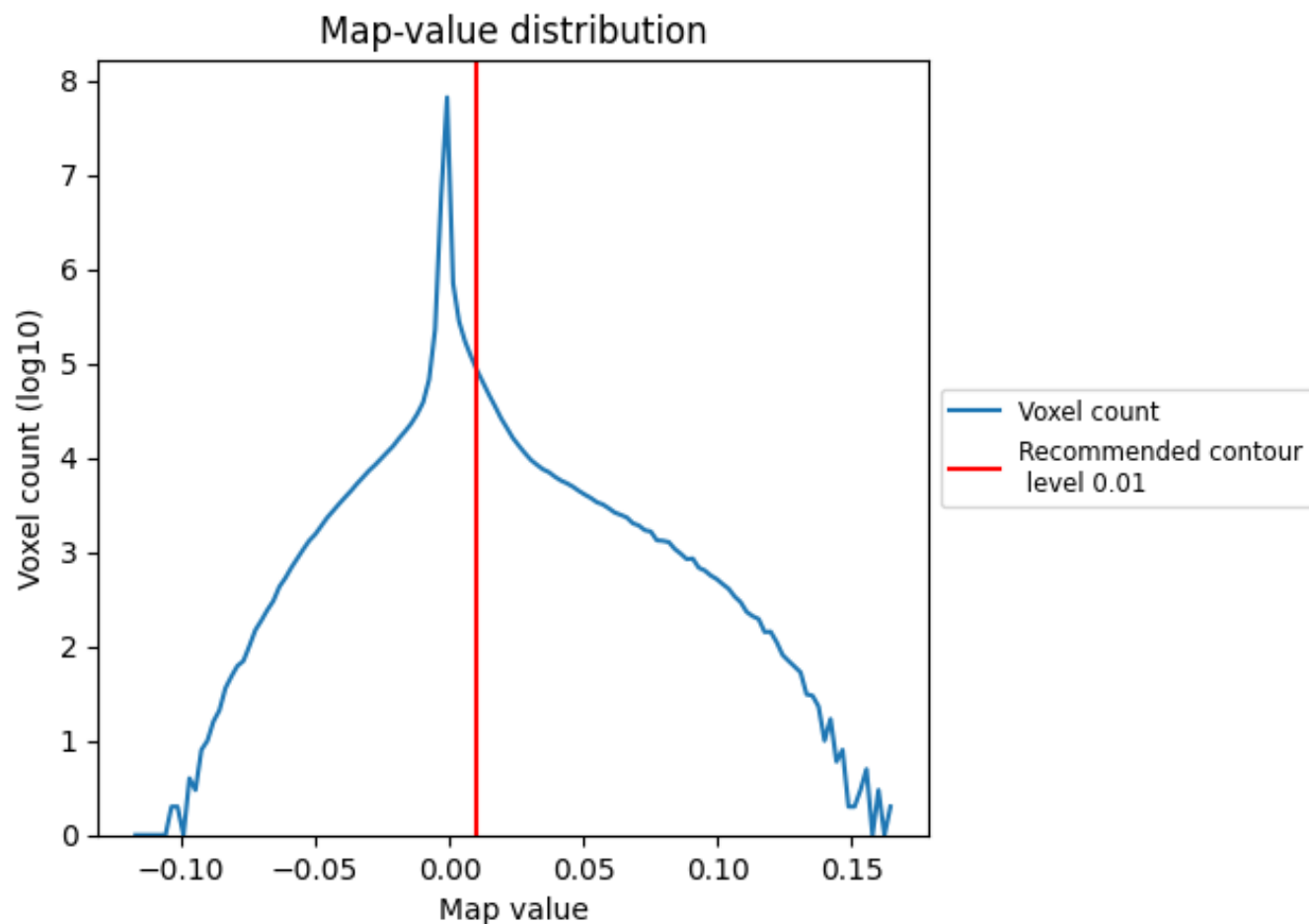


Z

7 Map analysis [i](#)

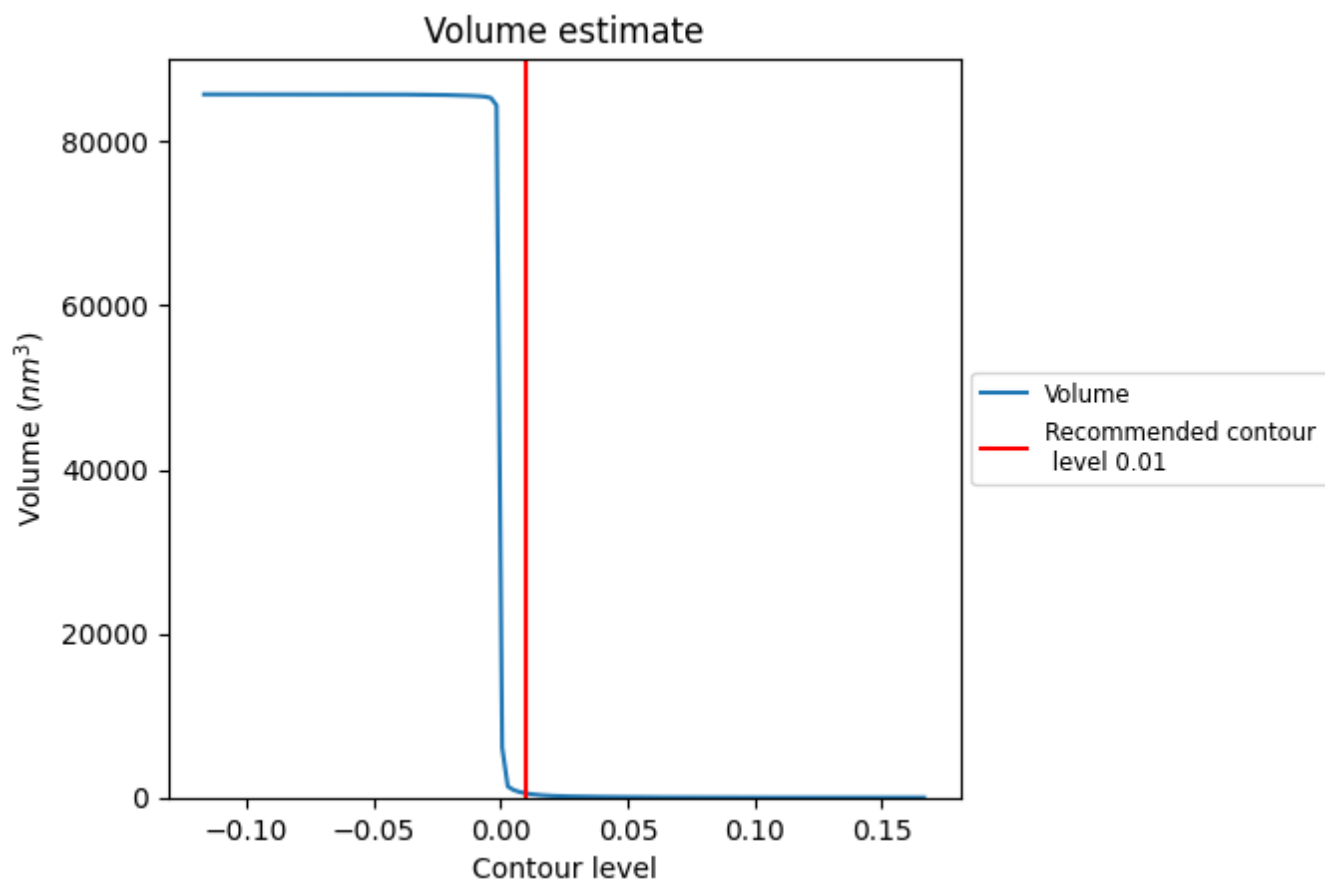
This section contains the results of statistical analysis of the map.

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.

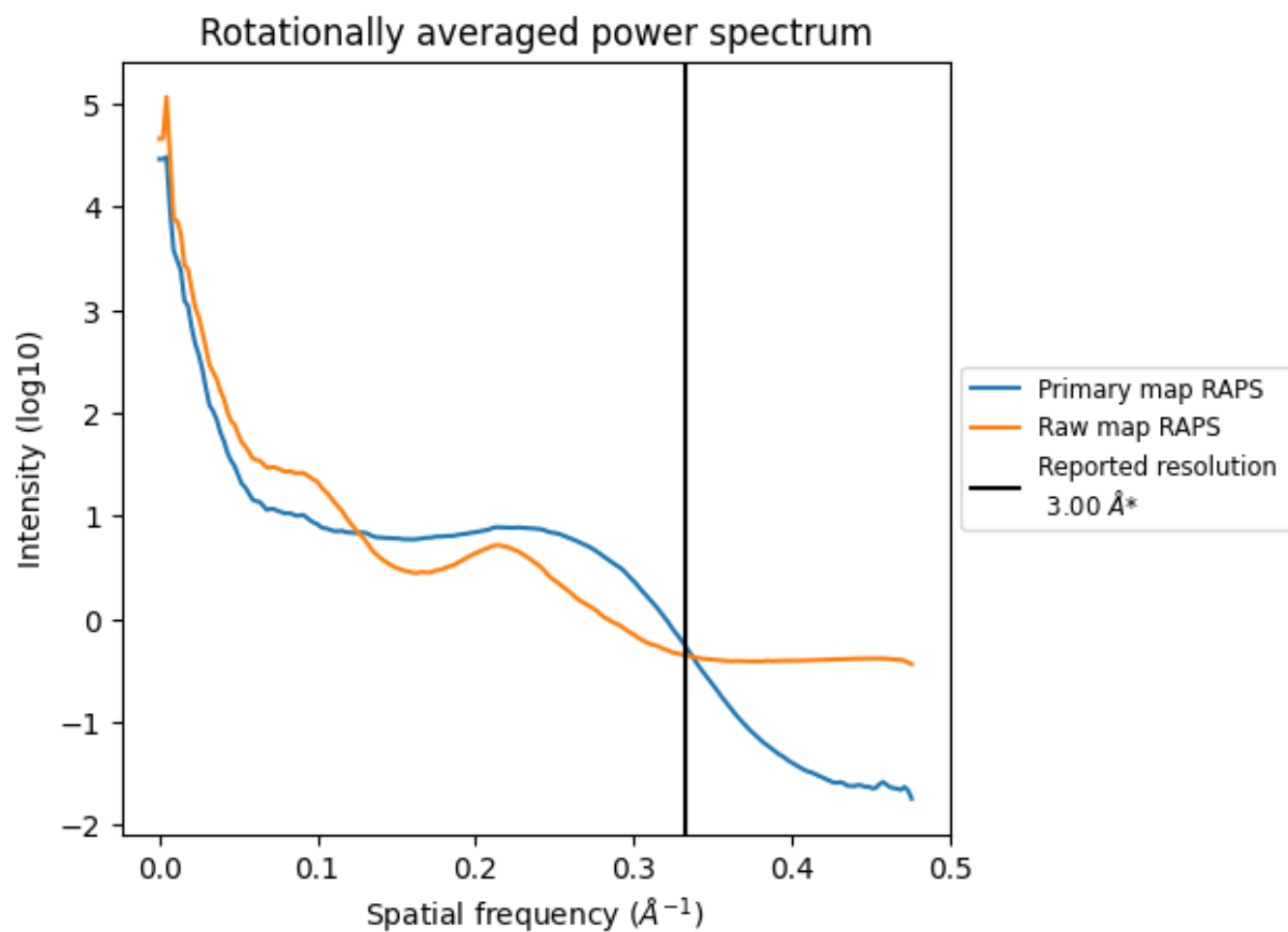
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 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 ⓘ

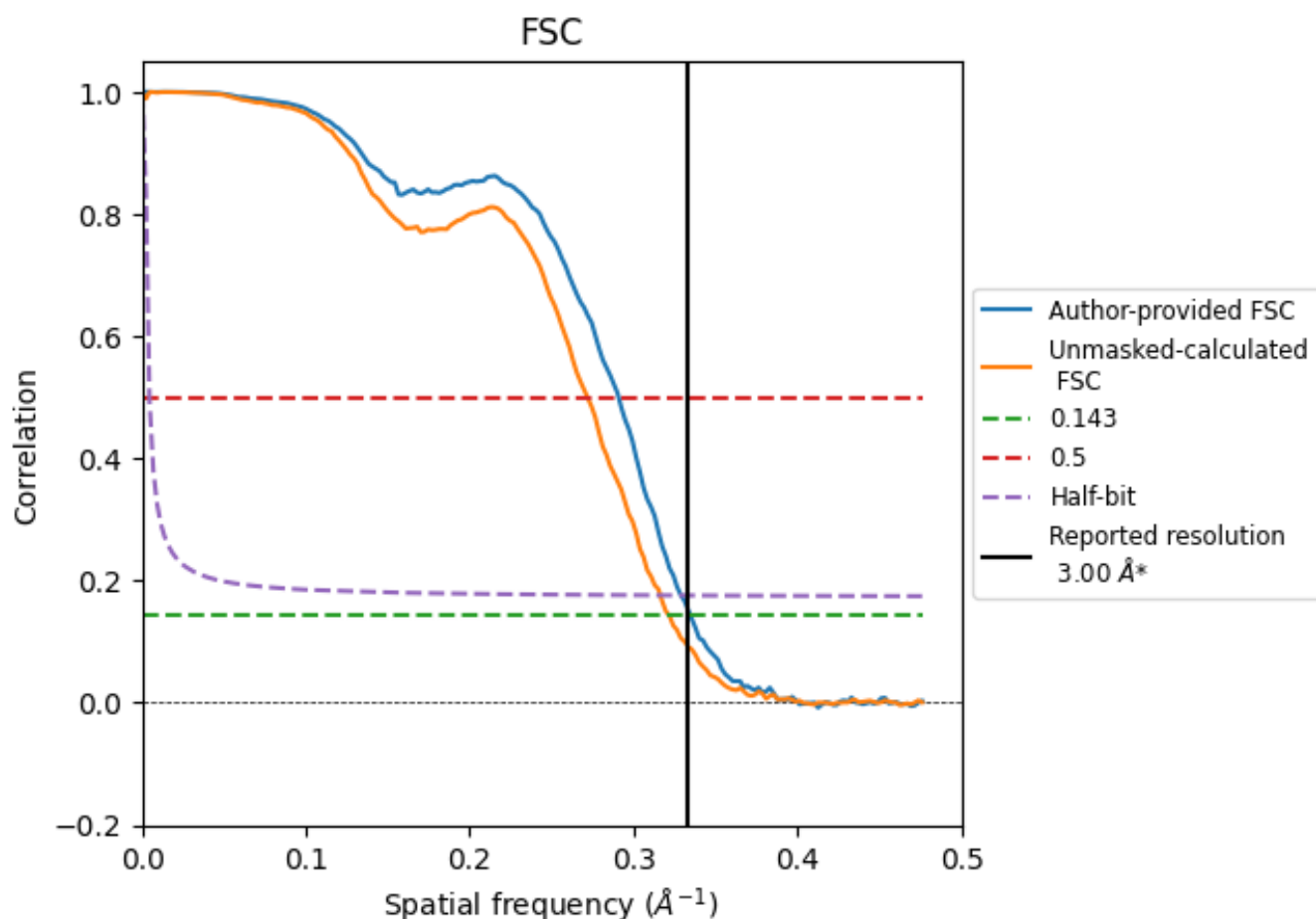


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

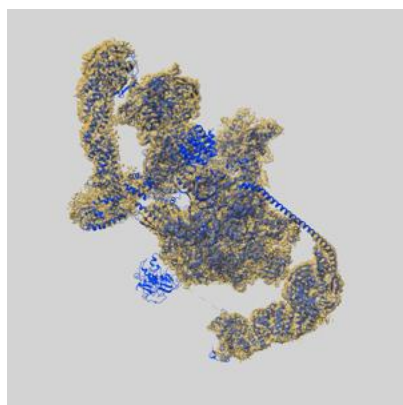
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.44	3.04
Unmasked-calculated*	3.11	3.68	3.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

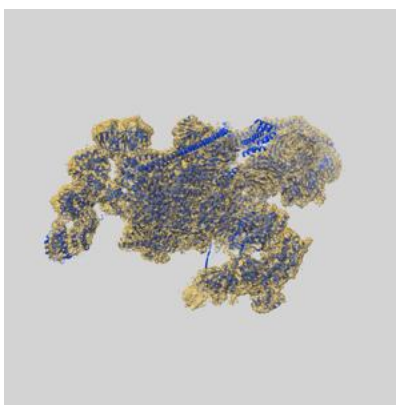
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13016 and PDB model 7OPD. Per-residue inclusion information can be found in section [3](#) on page [10](#).

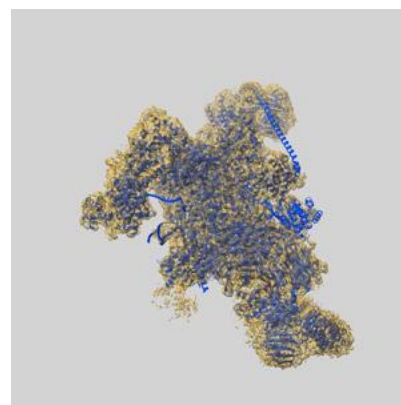
9.1 Map-model overlay [i](#)



X



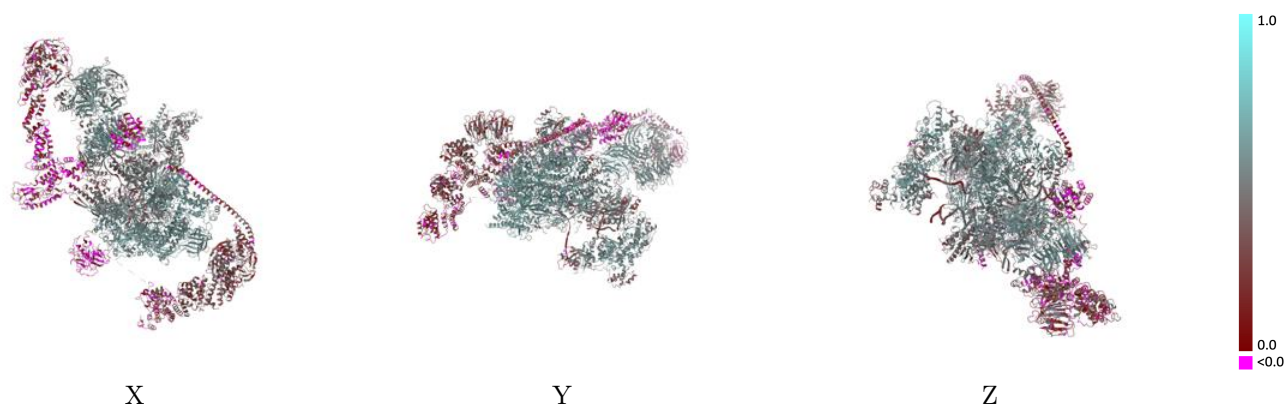
Y



Z

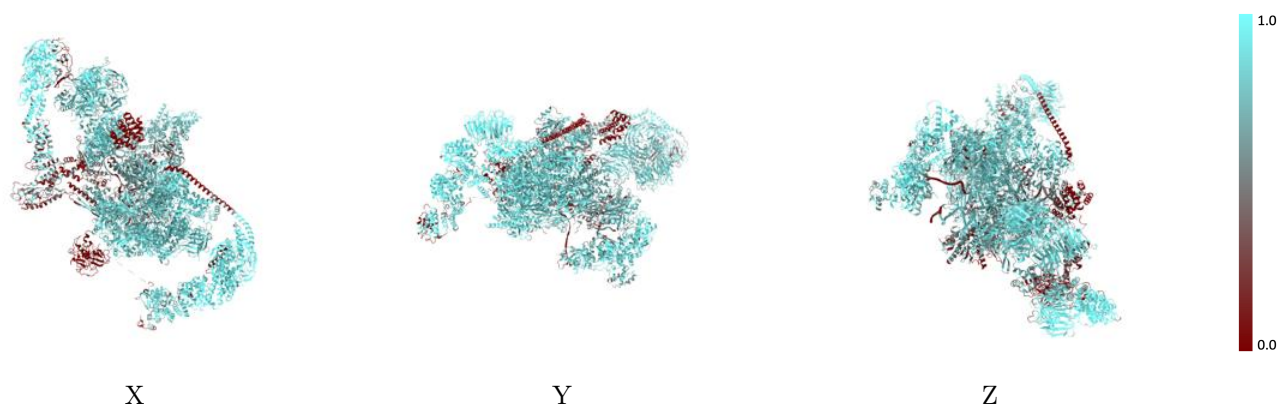
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



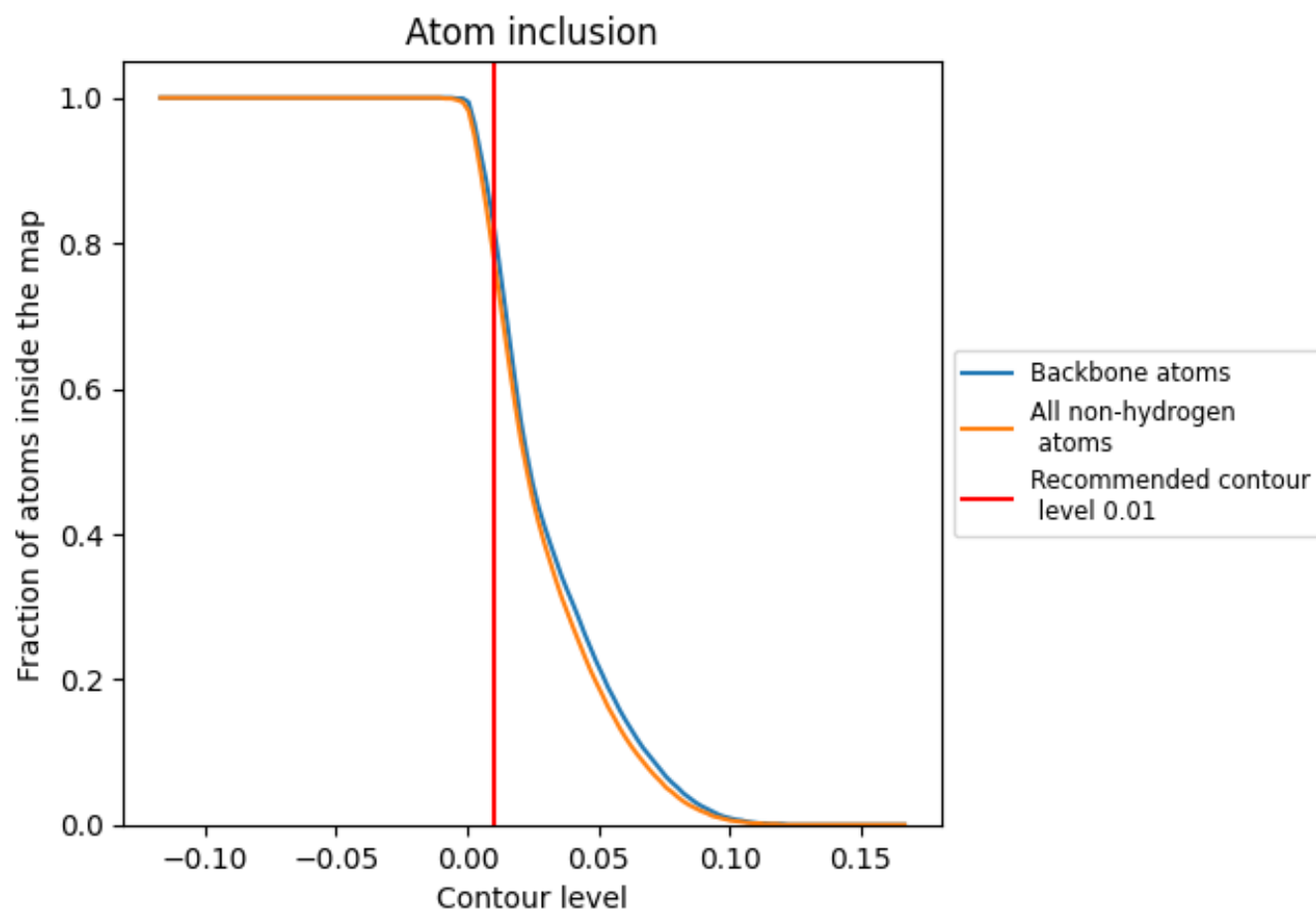
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.4720
A	 0.8420	 0.5530
B	 0.8510	 0.5600
C	 0.9120	 0.5890
D	 0.6760	 0.4030
E	 0.8620	 0.5410
F	 0.8720	 0.5720
G	 0.7160	 0.4960
H	 0.8900	 0.5830
I	 0.7500	 0.4910
J	 0.9330	 0.6180
K	 0.9200	 0.5950
L	 0.8090	 0.5080
M	 0.8370	 0.5000
N	 0.6600	 0.4260
P	 0.5020	 0.3840
R	 0.2000	 0.3300
S	 0.7810	 0.2280
T	 0.6830	 0.4590
U	 0.0000	 0.0120
V	 0.2500	 0.0820
Y	 0.9600	 0.3240
Z	 0.8550	 0.3060
a	 0.9070	 0.5870
b	 0.6660	 0.4790
c	 0.0050	 0.0250
d	 0.8000	 0.4670
e	 0.5960	 0.1270
f	 0.2380	 0.1570

