



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:00 AM UTC

PDB ID : 9HVQ / pdb_00009hvq
EMDB ID : EMD-52443
Title : Structure of the transcribing Pol II-DSIF-PAF-SPT6-RECQL5 complex
Authors : Zhang, L.; Zhang, S.
Deposited on : 2024-12-31
Resolution : 2.00 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

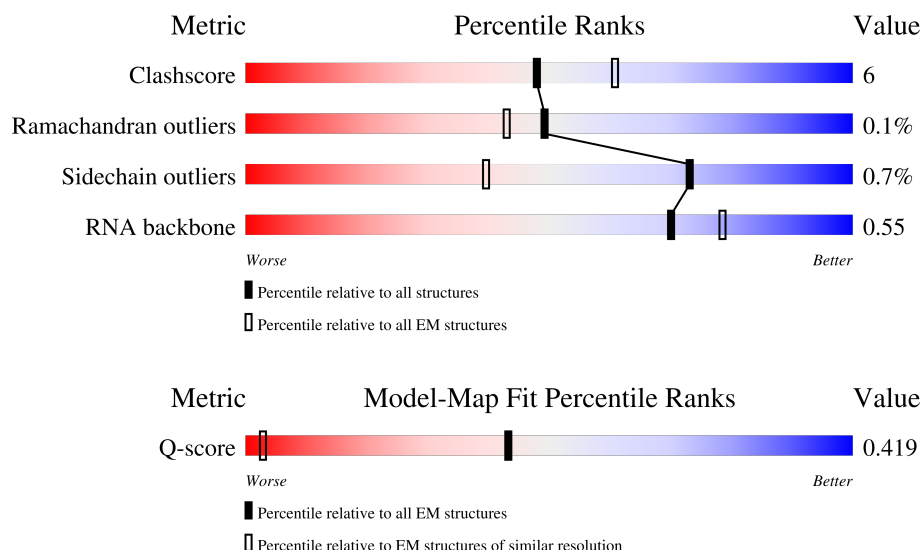
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.00 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.



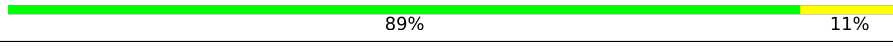
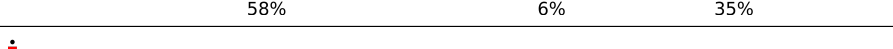
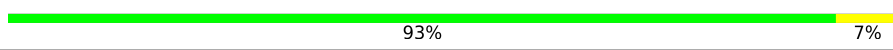
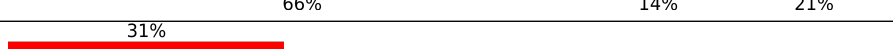
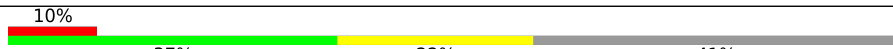
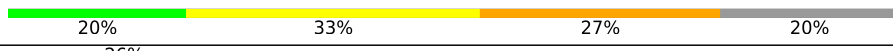
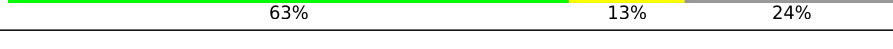
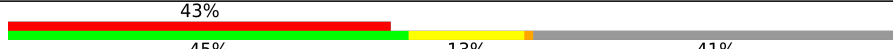
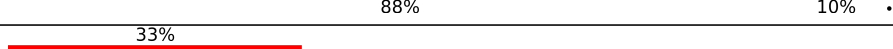
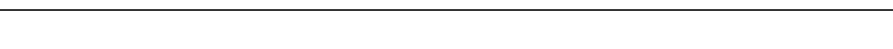
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1659 (1.50 - 2.50)

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	1726	
14	N	63	
15	O	991	
16	P	15	
17	Q	1173	
18	T	48	
19	U	666	
20	V	531	
21	W	305	
22	X	531	
23	Y	117	
24	Z	1087	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 63421 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11266	7084	2018	2093	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
			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 RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1030	642	175	209	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 polymerases I, II, and III subunit RPABC2.

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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	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	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 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, I and III 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	1120	Total	C	N	O	S	0	0
			9177	5819	1591	1725	42		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	37	Total	C	N	O	P	0	0
			769	361	149	222	37		

- Molecule 15 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	119	Total	C	N	O	S	0	0
			969	599	186	181	3		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	12	Total	C	N	O	P	0	0
			257	115	49	81	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			7222	4574	1264	1352	32		

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	37	Total	C	N	O	P	0	0
			749	355	128	229	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	154	Total	C	N	O	S	0	0
			1257	788	219	247	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	311	Total	C	N	O	S	0	0
			2569	1624	435	497	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	305	Total	C	N	O	S	0	0
			2373	1507	399	462	5		

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	229	Total	C	N	O	S	0	0
			1892	1213	342	332	5		

- Molecule 23 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	115	Total	C	N	O	S	0	0
			906	567	158	172	9		

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	515	Total	C	N	O	S	0	0
			4131	2626	731	756	18		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

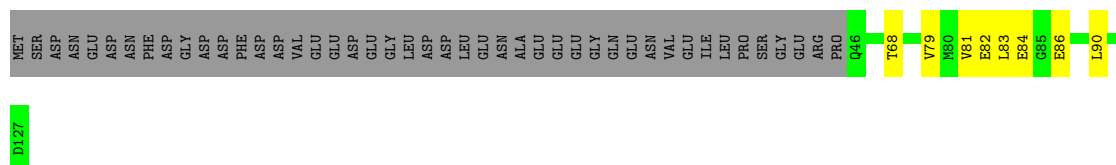
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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



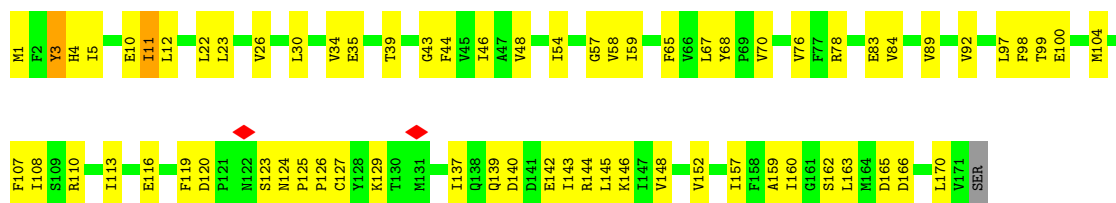
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 58% 6% 35%



- Molecule 7: DNA-directed RNA polymerase subunit

Chain G: 60% 38% ..



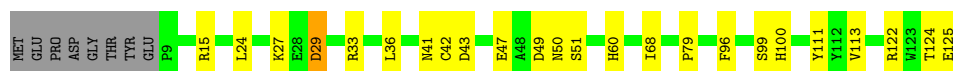
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 87% 11% .



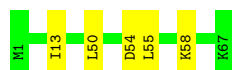
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 74% 18% 6%



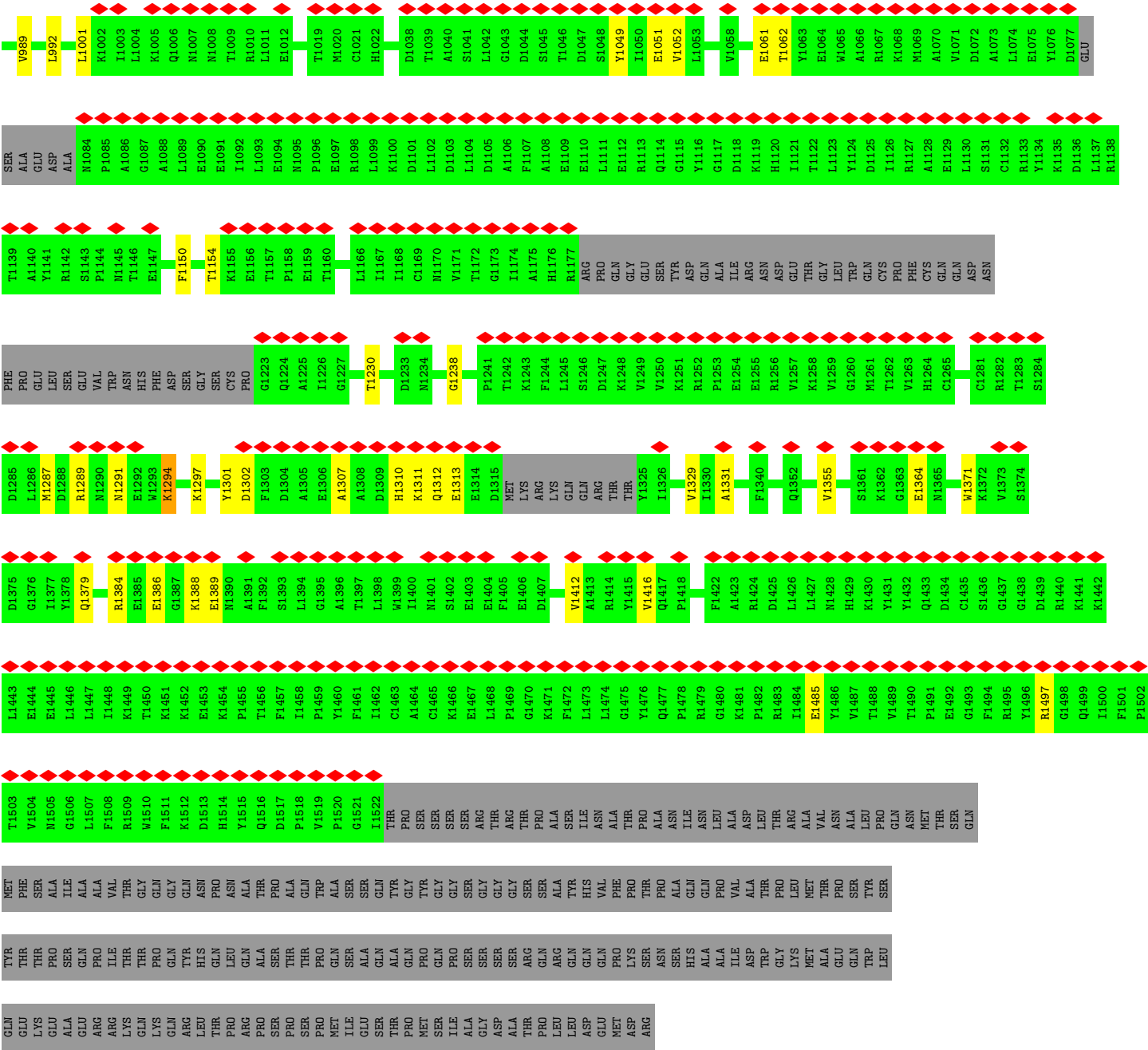
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 93% 7%

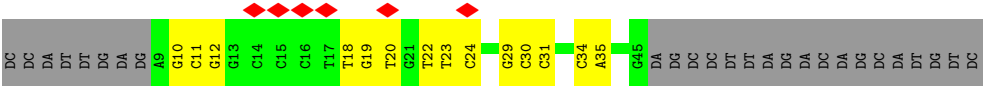


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 85% 14%



● Molecule 14: Non-template DNA

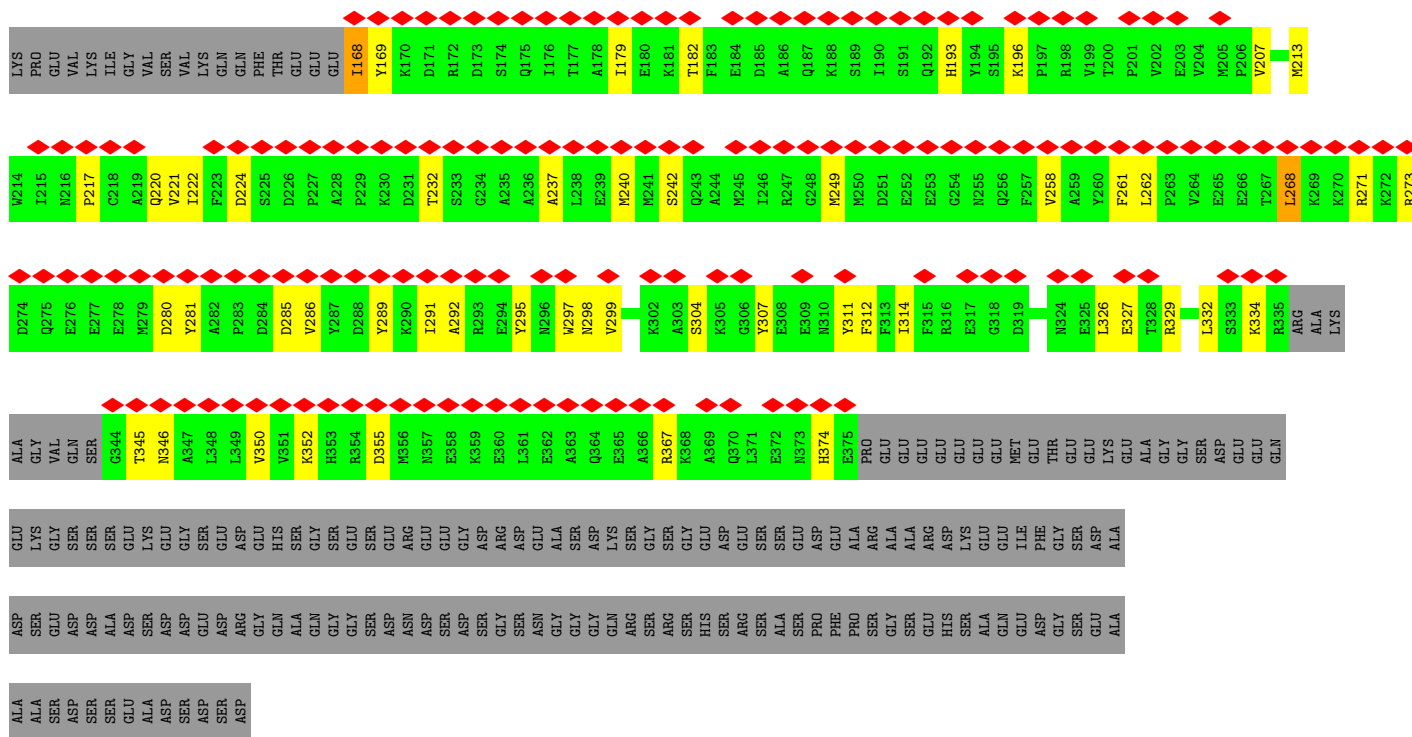


● Molecule 15: ATP-dependent DNA helicase Q5

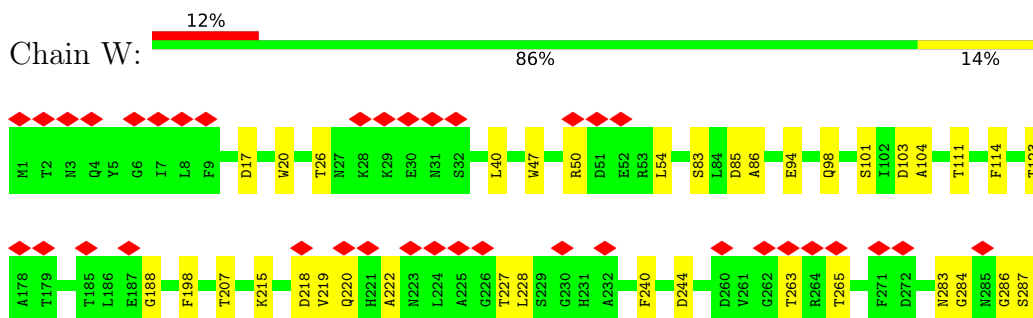




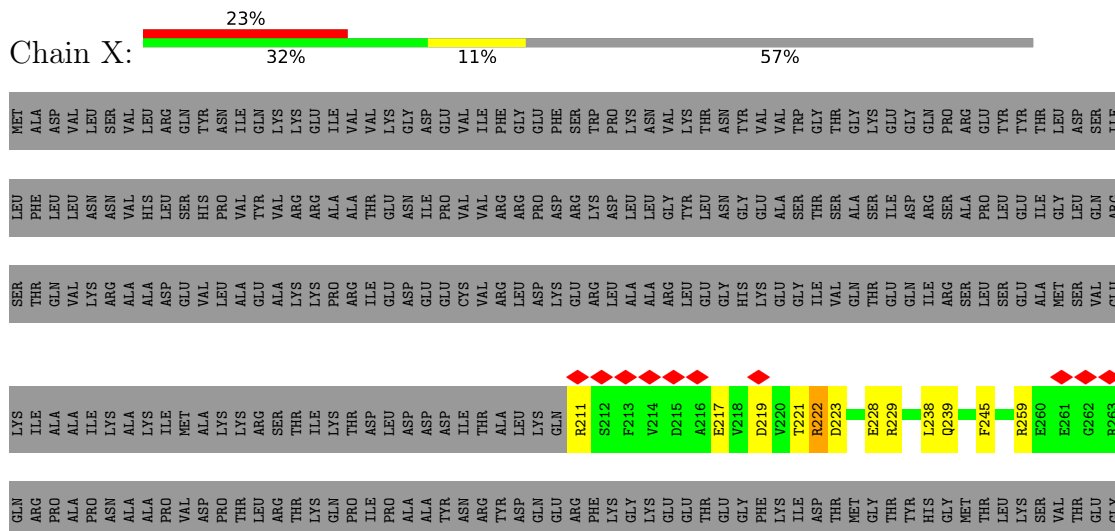


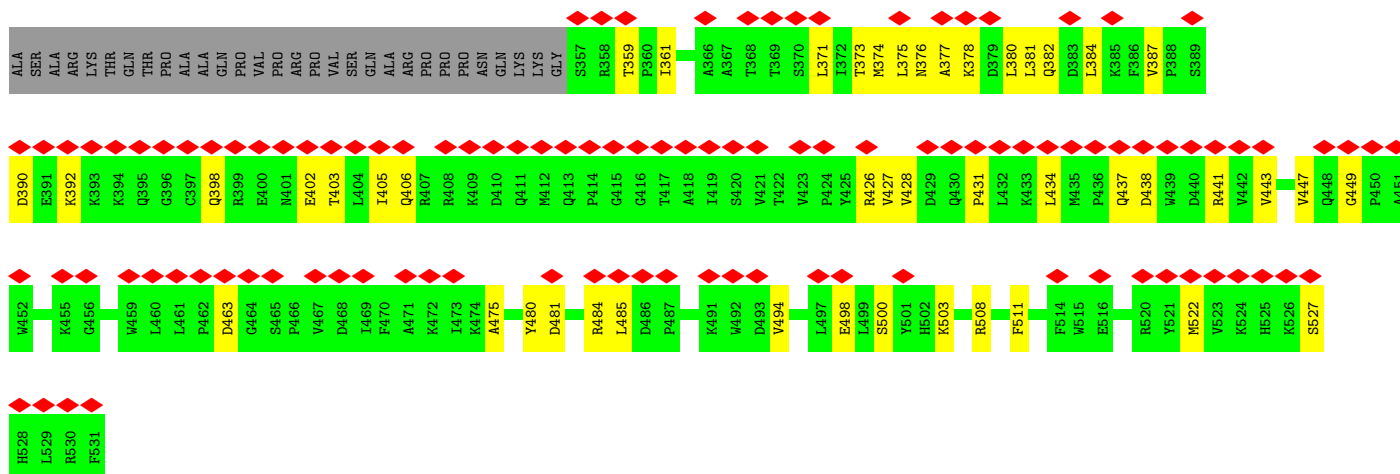


• Molecule 21: WD repeat-containing protein 61

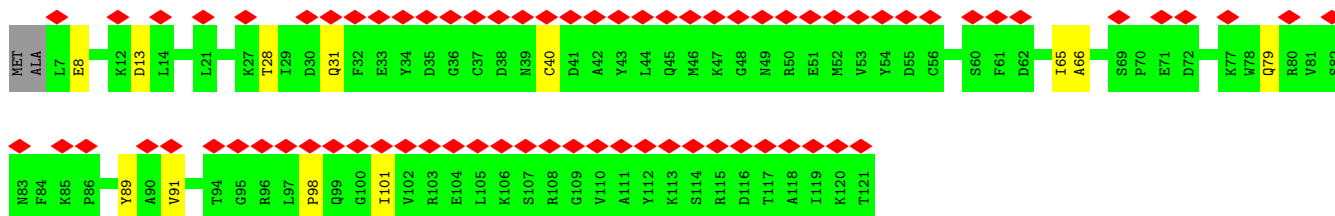
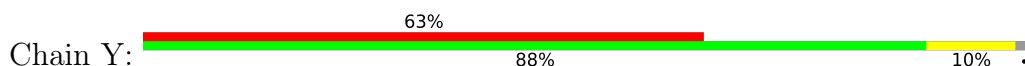


• Molecule 22: Parafibromin

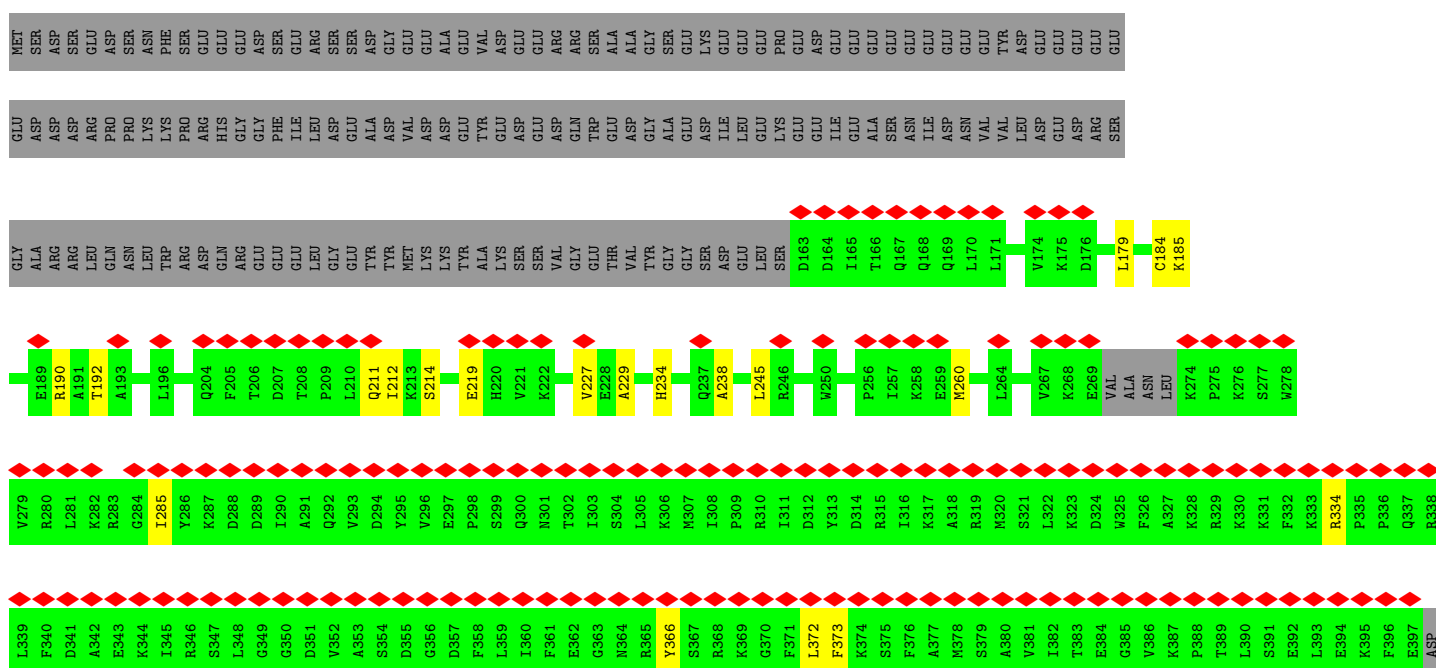
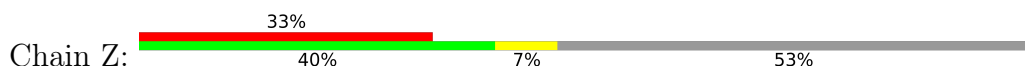


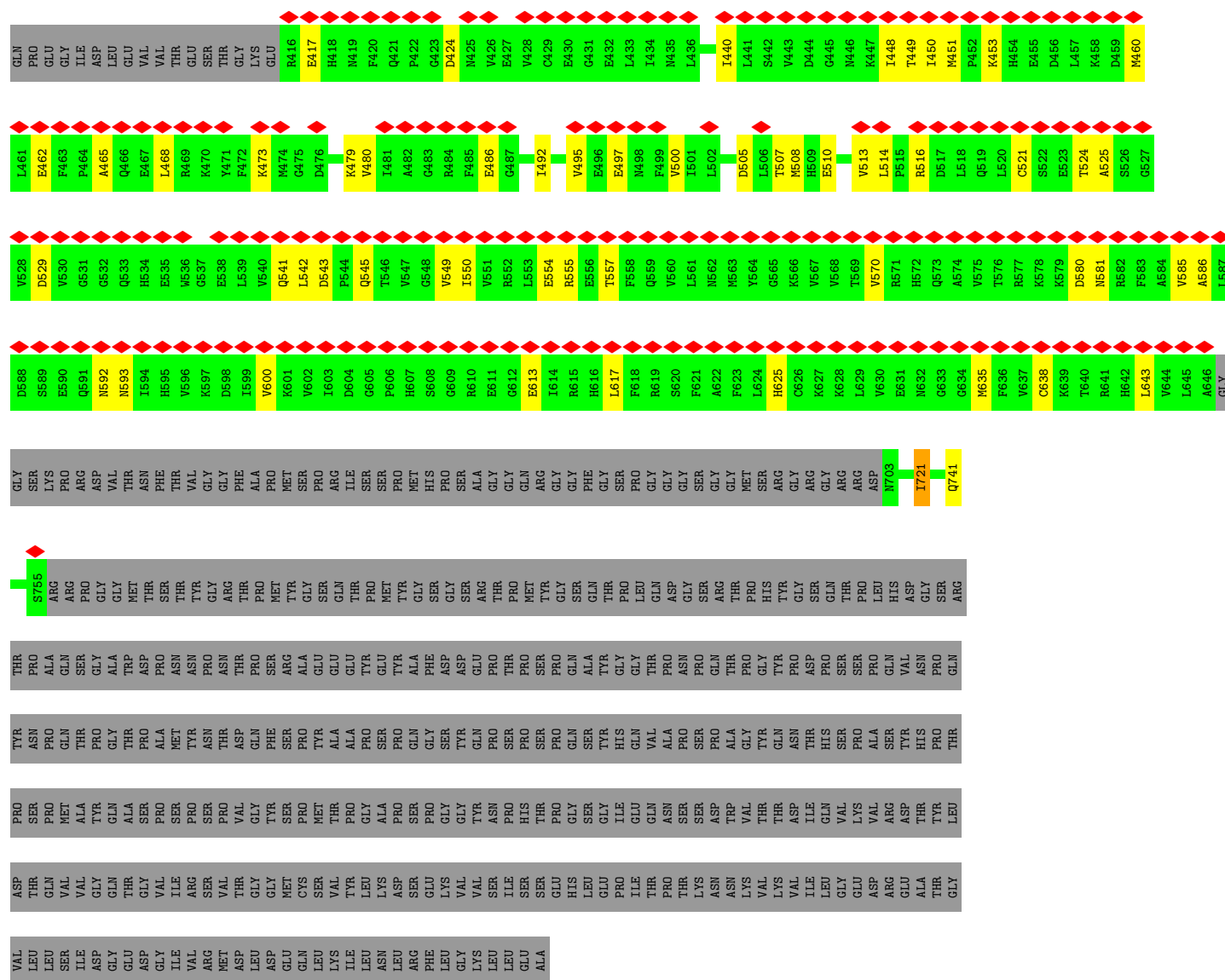


- Molecule 23: Transcription elongation factor SPT4



- Molecule 24: Transcription elongation factor SPT5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.002	Depositor
Map size ($\text{\AA}$)	391.48798, 391.48798, 391.48798	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8156, 0.8156, 0.8156	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	0.33	0/11471	0.41	0/15487
2	B	0.34	0/9233	0.40	0/12463
3	C	0.37	0/2132	0.41	0/2896
4	D	0.19	0/1043	0.63	0/1400
5	E	0.30	0/1751	0.33	0/2366
6	F	0.35	0/667	0.39	0/901
7	G	0.26	0/1382	0.59	0/1874
8	H	0.37	0/1207	0.36	0/1628
9	I	0.25	0/972	0.33	0/1316
10	J	0.37	0/542	0.45	0/730
11	K	0.38	0/939	0.40	0/1271
12	L	0.33	0/394	0.43	0/524
13	M	0.07	0/9369	0.21	1/12642 (0.0%)
14	N	0.21	0/864	0.43	0/1334
15	O	0.11	0/984	0.22	0/1319
16	P	0.37	0/287	0.37	0/445
17	Q	0.10	0/7360	0.27	0/9919
18	T	0.37	0/835	0.47	0/1285
19	U	0.14	0/1282	0.42	0/1730
20	V	0.11	0/2625	0.32	0/3543
21	W	0.09	0/2432	0.27	0/3311
22	X	0.12	0/1937	0.35	0/2621
23	Y	0.06	0/922	0.20	0/1243
24	Z	0.10	0/4205	0.23	0/5659
All	All	0.25	0/64835	0.35	1/87907 (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
20	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1052	VAL	CG1-CB-CG2	5.03	121.86	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	V	168	ILE	Peptide

5.2 Too-close contacts [i](#)

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	11266	0	11398	108	0
2	B	9052	0	9087	83	0
3	C	2089	0	2031	18	0
4	D	1030	0	1016	55	0
5	E	1720	0	1737	17	0
6	F	657	0	684	7	0
7	G	1351	0	1358	63	0
8	H	1186	0	1147	11	0
9	I	949	0	879	17	0
10	J	533	0	553	6	0
11	K	920	0	942	12	0
12	L	388	0	393	8	0
13	M	9177	0	9059	67	0
14	N	769	0	414	13	0
15	O	969	0	982	15	0
16	P	257	0	131	6	0
17	Q	7222	0	7170	113	0
18	T	749	0	417	2	0
19	U	1257	0	1206	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	V	2569	0	2488	59	0
21	W	2373	0	2290	26	0
22	X	1892	0	1929	47	0
23	Y	906	0	900	6	0
24	Z	4131	0	4206	53	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
26	A	1	0	0	0	0
All	All	63421	0	62417	742	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 6.

All (742) 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)
7:G:120:ASP:OD2	7:G:129:LYS:NZ	2.04	0.91
2:B:649:ASN:O	19:U:460:TYR:OH	1.87	0.90
2:B:756:LYS:NZ	20:V:134:THR:OG1	2.04	0.89
21:W:98:GLN:OE1	21:W:101:SER:OG	1.93	0.86
20:V:273:ARG:NH2	20:V:285:ASP:OD2	2.09	0.86
20:V:307:TYR:OH	20:V:326:LEU:O	1.92	0.85
3:C:158:GLU:OE2	3:C:160:ARG:NH1	2.10	0.85
5:E:4:GLU:N	5:E:4:GLU:OE1	2.10	0.85
17:Q:277:ASN:OD1	17:Q:311:GLN:NE2	2.12	0.82
2:B:230:ARG:NH2	2:B:346:GLU:OE1	2.13	0.82
3:C:225:LYS:NZ	3:C:227:GLU:OE2	2.14	0.81
8:H:67:ASP:OD1	8:H:69:THR:OG1	1.97	0.81
2:B:686:GLU:N	2:B:686:GLU:OE1	2.13	0.81
19:U:415:LYS:O	19:U:419:THR:OG1	1.99	0.80
17:Q:423:GLU:OE1	22:X:229:ARG:NH2	2.14	0.80
20:V:297:TRP:CE3	20:V:299:VAL:HG23	2.17	0.80
17:Q:121:ASP:OD2	17:Q:134:ARG:NH1	2.14	0.80
20:V:281:TYR:OH	20:V:355:ASP:OD1	2.00	0.80
9:I:68:ILE:O	9:I:122:ARG:NH1	2.16	0.79
22:X:374:MET:SD	22:X:403:THR:OG1	2.40	0.79
2:B:35:ASP:OD1	2:B:646:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:GLU:OE2	2:B:835:GLU:N	2.17	0.78
4:D:48:ASN:OD1	4:D:49:GLU:N	2.17	0.77
19:U:455:GLU:OE1	19:U:498:SER:OG	2.00	0.77
17:Q:94:VAL:HG13	17:Q:140:LEU:HD22	1.66	0.77
17:Q:35:LYS:NZ	17:Q:70:ASP:OD2	2.18	0.76
4:D:33:LEU:HD11	4:D:101:ALA:HB3	1.67	0.76
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.03	0.76
4:D:66:ASN:OD1	4:D:67:TYR:N	2.19	0.75
1:A:911:PRO:O	1:A:963:ARG:NH2	2.19	0.75
5:E:79:GLU:OE2	5:E:86:THR:HG21	1.86	0.75
24:Z:541:GLN:NE2	24:Z:543:ASP:O	2.20	0.75
1:A:48:GLU:OE2	1:A:53:LYS:NZ	2.17	0.75
15:O:541:ARG:NH2	15:O:591:ALA:O	2.20	0.74
13:M:441:ARG:O	13:M:471:TYR:OH	2.05	0.74
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.04	0.74
1:A:927:GLU:OE1	1:A:931:ARG:NH2	2.20	0.74
19:U:459:VAL:CG1	19:U:489:LEU:HD22	2.18	0.74
17:Q:498:THR:OG1	22:X:228:GLU:OE2	2.03	0.73
2:B:835:GLU:O	2:B:886:ARG:N	2.21	0.73
13:M:322:ARG:O	13:M:327:THR:OG1	2.05	0.73
22:X:437:GLN:N	22:X:437:GLN:OE1	2.21	0.73
24:Z:417:GLU:OE2	24:Z:516:ARG:NH1	2.21	0.73
21:W:188:GLY:O	21:W:215:LYS:NZ	2.19	0.72
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.06	0.72
3:C:44:ILE:HD12	3:C:238:SER:OG	1.90	0.72
17:Q:738:GLN:NE2	21:W:17:ASP:OD2	2.22	0.72
2:B:887:TYR:O	2:B:888:THR:HG22	1.90	0.72
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.71	0.72
7:G:107:PHE:CZ	7:G:160:ILE:HD12	2.25	0.71
15:O:565:ARG:O	15:O:569:ARG:N	2.22	0.71
8:H:36:LYS:NZ	17:Q:706:ASN:OD1	2.23	0.71
1:A:60:PRO:HA	1:A:65:ILE:HD11	1.73	0.71
4:D:103:LEU:HD23	4:D:114:LEU:HD13	1.73	0.71
1:A:154:CYS:SG	1:A:188:GLN:NE2	2.64	0.71
22:X:443:VAL:HG21	22:X:522:MET:HE3	1.73	0.70
17:Q:34:LEU:HD11	17:Q:47:LEU:HD12	1.71	0.70
17:Q:365:GLU:OE2	17:Q:385:TYR:OH	2.10	0.70
4:D:83:VAL:O	4:D:87:LEU:HD13	1.92	0.69
1:A:1279:MET:O	15:O:515:ARG:NH2	2.26	0.69
1:A:413:TYR:O	1:A:415:GLY:N	2.25	0.69
13:M:1294:LYS:HZ3	13:M:1294:LYS:HB2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:ALA:HB3	7:G:3:TYR:CE2	2.28	0.69
4:D:126:GLU:O	4:D:130:ILE:HD12	1.92	0.69
9:I:50:ASN:O	9:I:51:SER:OG	2.10	0.69
24:Z:486:GLU:OE2	24:Z:555:ARG:NH1	2.25	0.69
24:Z:554:GLU:OE1	24:Z:557:THR:OG1	2.10	0.69
7:G:97:LEU:HD23	7:G:98:PHE:N	2.08	0.68
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.26	0.68
19:U:482:GLN:O	20:V:242:SER:OG	2.11	0.68
13:M:695:ARG:NH2	13:M:697:GLU:OE2	2.26	0.68
1:A:1063:GLU:OE2	22:X:508:ARG:NE	2.27	0.68
1:A:1229:GLU:N	1:A:1229:GLU:OE1	2.26	0.68
13:M:802:GLU:O	13:M:981:TYR:OH	2.06	0.68
13:M:1311:LYS:HG3	13:M:1312:GLN:NE2	2.09	0.68
17:Q:665:GLU:OE2	22:X:259:ARG:NH1	2.27	0.68
13:M:586:GLU:OE1	13:M:589:ARG:NH2	2.27	0.67
1:A:211:GLU:N	1:A:211:GLU:OE1	2.27	0.67
1:A:1166:LEU:O	1:A:1170:THR:HG23	1.94	0.67
22:X:475:ALA:HB3	22:X:494:VAL:HG12	1.77	0.67
13:M:618:ILE:HD12	13:M:640:LEU:HD12	1.77	0.67
17:Q:191:ARG:NH1	20:V:104:ASP:OD1	2.28	0.67
7:G:89:VAL:HG13	7:G:97:LEU:HD21	1.76	0.67
24:Z:473:LYS:O	24:Z:492:ILE:HD11	1.95	0.67
17:Q:489:GLU:N	17:Q:489:GLU:OE1	2.28	0.67
22:X:373:THR:O	22:X:377:ALA:N	2.26	0.67
2:B:92:TYR:HA	19:U:506:LEU:HD12	1.75	0.66
1:A:111:CYS:SG	1:A:114:CYS:N	2.67	0.66
1:A:197:GLU:OE2	1:A:308:LYS:NZ	2.28	0.66
1:A:458:PHE:CE2	1:A:484:LEU:HD21	2.30	0.66
13:M:1307:ALA:HA	13:M:1310:HIS:CE1	2.29	0.66
17:Q:877:GLN:OE1	17:Q:880:GLN:NE2	2.29	0.66
3:C:44:ILE:HD11	3:C:239:LEU:HG	1.77	0.66
2:B:735:VAL:HG11	10:J:55:LEU:HD21	1.77	0.65
17:Q:609:ASN:ND2	20:V:37:ASN:O	2.30	0.65
1:A:1189:ASP:OD2	1:A:1258:ARG:NE	2.30	0.65
7:G:35:GLU:OE2	7:G:48:VAL:N	2.29	0.65
9:I:99:SER:O	9:I:100:HIS:ND1	2.30	0.65
24:Z:285:ILE:O	24:Z:334:ARG:NH2	2.30	0.65
13:M:421:GLN:NE2	13:M:443:LEU:O	2.30	0.65
9:I:50:ASN:OD1	9:I:51:SER:N	2.30	0.65
17:Q:191:ARG:HD2	20:V:100:LEU:HD21	1.79	0.65
17:Q:314:ARG:NH1	20:V:67:GLU:OE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:54:ILE:HD13	7:G:70:VAL:HG13	1.79	0.64
1:A:1202:PHE:CE2	1:A:1204:VAL:HG22	2.32	0.64
2:B:567:ILE:HD11	2:B:577:HIS:HB2	1.79	0.64
15:O:511:GLN:OE1	15:O:515:ARG:NH1	2.30	0.64
20:V:232:THR:O	20:V:237:ALA:HB2	1.98	0.64
1:A:187:TYR:N	1:A:206:ASN:OD1	2.31	0.63
8:H:72:ASP:OD1	8:H:74:GLU:N	2.28	0.63
10:J:58:LYS:HG2	20:V:137:ILE:HD11	1.81	0.63
13:M:894:MET:HE3	24:Z:545:GLN:NE2	2.14	0.63
17:Q:204:MET:HE3	17:Q:204:MET:HA	1.79	0.63
21:W:218:ASP:O	21:W:222:ALA:N	2.32	0.63
15:O:524:GLU:OE1	15:O:525:PHE:N	2.32	0.62
16:P:137:G:O2'	16:P:138:A:O5'	2.16	0.62
4:D:25:GLU:OE2	7:G:78:ARG:NH1	2.32	0.62
13:M:1049:TYR:OH	13:M:1051:GLU:OE2	2.16	0.62
1:A:1417:HIS:O	1:A:1421:ARG:HG2	2.00	0.62
2:B:1006:VAL:HG22	20:V:130:TRP:CG	2.34	0.62
17:Q:491:TYR:CE1	17:Q:495:ILE:HD11	2.34	0.62
19:U:436:SER:OG	20:V:207:VAL:O	2.17	0.61
13:M:1384:ARG:NH2	13:M:1386:GLU:OE2	2.33	0.61
17:Q:320:GLU:OE1	17:Q:320:GLU:N	2.33	0.61
9:I:41:ASN:OD1	9:I:42:CYS:N	2.33	0.61
2:B:1037:ILE:O	3:C:195:THR:HG22	1.99	0.61
19:U:405:ASP:O	19:U:408:GLY:N	2.33	0.61
5:E:79:GLU:N	5:E:79:GLU:OE1	2.34	0.61
1:A:109:CYS:SG	1:A:236:LEU:HD21	2.40	0.61
13:M:1355:VAL:HG22	13:M:1416:VAL:HG11	1.83	0.61
1:A:196:LEU:HD23	1:A:311:GLN:HG3	1.83	0.60
13:M:1289:ARG:HG2	13:M:1289:ARG:HH11	1.66	0.60
10:J:54:ASP:O	20:V:137:ILE:HD13	2.02	0.60
22:X:498:GLU:N	22:X:498:GLU:OE1	2.33	0.60
13:M:1355:VAL:CG2	13:M:1416:VAL:HG11	2.31	0.60
22:X:443:VAL:HG21	22:X:522:MET:CE	2.32	0.60
17:Q:91:ALA:CB	20:V:86:LEU:HD11	2.32	0.60
1:A:388:MET:HE1	1:A:503:LEU:HD22	1.82	0.60
4:D:33:LEU:HD11	4:D:101:ALA:CB	2.32	0.60
13:M:428:ILE:HG12	13:M:436:LEU:HD11	1.84	0.60
13:M:316:GLU:OE2	13:M:367:ARG:NH1	2.35	0.59
13:M:986:ILE:CD1	13:M:1001:LEU:HD21	2.32	0.59
17:Q:689:HIS:ND1	17:Q:704:TYR:OH	2.34	0.59
24:Z:179:LEU:HG	24:Z:260:MET:HE3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:497:GLU:OE1	24:Z:497:GLU:N	2.35	0.59
1:A:1282:ASP:OD2	1:A:1283:VAL:HG13	2.02	0.59
5:E:27:LEU:O	17:Q:877:GLN:NE2	2.35	0.59
17:Q:375:TYR:CE1	17:Q:404:VAL:HG13	2.37	0.59
22:X:217:GLU:OE1	22:X:221:THR:OG1	2.19	0.59
15:O:497:ASP:OD1	15:O:498:GLU:N	2.36	0.59
17:Q:243:LEU:HD23	17:Q:251:ILE:HD12	1.83	0.59
4:D:132:ASP:O	4:D:136:THR:HG23	2.01	0.59
13:M:1150:PHE:O	13:M:1154:THR:OG1	2.15	0.59
15:O:584:GLU:OE1	15:O:597:TYR:OH	2.20	0.59
2:B:994:GLY:HA2	10:J:50:LEU:HD11	1.85	0.59
8:H:8:ASP:OD2	8:H:32:SER:OG	2.13	0.59
13:M:1287:MET:HB3	13:M:1289:ARG:NH1	2.17	0.59
15:O:535:LYS:NZ	15:O:582:GLU:OE1	2.36	0.58
5:E:29:THR:OG1	5:E:31:ASP:OD1	2.15	0.58
17:Q:395:ASP:OD2	17:Q:396:ILE:N	2.36	0.58
1:A:937:ASP:OD1	1:A:937:ASP:N	2.37	0.58
17:Q:48:ALA:HB1	17:Q:60:PHE:CE2	2.38	0.58
20:V:291:ILE:HG21	20:V:345:THR:O	2.04	0.58
17:Q:591:ILE:O	17:Q:597:THR:OG1	2.20	0.58
13:M:1230:THR:O	13:M:1238:GLY:N	2.36	0.58
21:W:227:THR:C	21:W:228:LEU:HD23	2.29	0.57
17:Q:375:TYR:HE1	17:Q:404:VAL:HG13	1.69	0.57
10:J:58:LYS:NZ	20:V:138:SER:O	2.37	0.57
13:M:1291:ASN:HA	13:M:1294:LYS:NZ	2.20	0.57
20:V:312:PHE:HE1	20:V:314:ILE:HD11	1.68	0.57
4:D:17:ALA:O	4:D:20:LEU:HD22	2.05	0.57
13:M:639:TYR:HB3	13:M:1302:ASP:HB3	1.87	0.57
13:M:1364:GLU:O	13:M:1388:LYS:NZ	2.34	0.57
1:A:67:ARG:O	1:A:68:THR:OG1	2.13	0.57
4:D:123:GLU:OE2	4:D:126:GLU:N	2.37	0.57
5:E:118:LEU:HD22	5:E:127:LEU:HG	1.85	0.57
9:I:29:ASP:O	9:I:33:ARG:N	2.33	0.56
13:M:297:ARG:NE	13:M:372:GLU:OE2	2.34	0.56
4:D:29:ALA:HB3	7:G:3:TYR:CZ	2.41	0.56
22:X:380:LEU:HD22	22:X:511:PHE:CZ	2.41	0.56
17:Q:131:LEU:HD13	17:Q:154:PHE:HE2	1.70	0.56
17:Q:669:VAL:O	17:Q:673:VAL:HG23	2.06	0.56
1:A:693:ILE:HD13	1:A:828:LEU:CD2	2.36	0.56
5:E:104:ILE:HD11	5:E:127:LEU:HD12	1.87	0.56
22:X:500:SER:OG	22:X:503:LYS:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:212:ILE:HD13	24:Z:238:ALA:CB	2.36	0.56
21:W:20:TRP:CH2	21:W:40:LEU:HD13	2.41	0.56
1:A:1194:ASN:OD1	1:A:1195:VAL:N	2.38	0.56
4:D:60:VAL:HG11	7:G:44:PHE:CZ	2.41	0.56
21:W:83:SER:OG	21:W:85:ASP:OD1	2.12	0.56
2:B:20:ASP:N	2:B:20:ASP:OD1	2.39	0.55
24:Z:479:LYS:NZ	24:Z:521:CYS:O	2.36	0.55
17:Q:836:GLU:OE1	17:Q:837:GLU:N	2.39	0.55
24:Z:592:ASN:OD1	24:Z:593:ASN:N	2.39	0.55
20:V:220:GLN:HB2	20:V:326:LEU:HD13	1.89	0.55
21:W:287:SER:O	21:W:288:LYS:NZ	2.37	0.55
1:A:67:ARG:NH1	16:P:134:A:O4'	2.40	0.55
2:B:910:THR:HG22	12:L:42:ARG:O	2.07	0.55
21:W:198:PHE:HE1	21:W:219:VAL:HG11	1.71	0.55
1:A:693:ILE:HD13	1:A:828:LEU:HD21	1.88	0.55
21:W:244:ASP:OD1	21:W:244:ASP:O	2.24	0.55
4:D:31:THR:HG21	7:G:1:MET:HE2	1.87	0.55
1:A:706:ILE:HD11	1:A:787:VAL:CG1	2.38	0.54
2:B:861:SER:O	2:B:864:ASP:HB2	2.08	0.54
6:F:68:THR:HG21	7:G:59:ILE:HG21	1.90	0.54
24:Z:600:VAL:HG21	24:Z:643:LEU:HD22	1.89	0.54
24:Z:184:CYS:SG	24:Z:185:LYS:N	2.80	0.54
7:G:110:ARG:O	7:G:113:ILE:HG22	2.07	0.54
24:Z:500:VAL:HG22	24:Z:513:VAL:O	2.07	0.54
17:Q:556:GLU:OE2	22:X:211:ARG:NH1	2.35	0.54
1:A:1282:ASP:OD2	1:A:1283:VAL:N	2.40	0.54
3:C:26:THR:OG1	11:K:97:GLU:OE2	2.23	0.54
1:A:413:TYR:CD1	1:A:413:TYR:C	2.85	0.54
4:D:80:ILE:O	4:D:83:VAL:HG12	2.06	0.54
7:G:142:GLU:O	7:G:170:LEU:HD12	2.07	0.54
24:Z:453:LYS:HE3	24:Z:460:MET:HE1	1.89	0.54
7:G:22:LEU:HD23	7:G:23:LEU:HD22	1.90	0.54
13:M:1389:GLU:N	13:M:1389:GLU:OE1	2.41	0.54
17:Q:236:VAL:O	17:Q:240:VAL:HG23	2.08	0.54
24:Z:366:TYR:CE1	24:Z:372:LEU:HD13	2.42	0.54
7:G:146:LYS:O	7:G:162:SER:N	2.41	0.54
1:A:458:PHE:HE2	1:A:484:LEU:HD21	1.71	0.53
4:D:130:ILE:O	4:D:134:ILE:HG13	2.08	0.53
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.91	0.53
3:C:76:ASP:HA	3:C:239:LEU:HD23	1.91	0.53
8:H:148:LEU:HD12	8:H:148:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:522:ILE:HG23	15:O:522:ILE:O	2.07	0.53
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.74	0.53
17:Q:323:ASP:OD1	17:Q:324:GLN:N	2.42	0.53
17:Q:395:ASP:OD2	17:Q:396:ILE:HG13	2.09	0.53
7:G:30:LEU:O	7:G:34:VAL:HG22	2.08	0.53
17:Q:529:ASN:HA	17:Q:560:ILE:HG21	1.91	0.53
24:Z:492:ILE:HD12	24:Z:495:VAL:CG1	2.38	0.53
2:B:957:THR:HG22	2:B:1028:LEU:CD2	2.39	0.53
7:G:30:LEU:HD13	7:G:70:VAL:HG11	1.91	0.53
17:Q:277:ASN:ND2	17:Q:307:GLU:OE2	2.39	0.53
17:Q:665:GLU:OE1	17:Q:665:GLU:N	2.39	0.53
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.42	0.53
2:B:910:THR:HG21	12:L:43:ILE:HG12	1.91	0.53
7:G:3:TYR:N	7:G:76:VAL:O	2.40	0.53
8:H:55:LYS:HB3	8:H:148:LEU:HD11	1.91	0.53
4:D:25:GLU:OE2	7:G:78:ARG:NH2	2.41	0.52
6:F:82:GLU:OE1	13:M:1331:ALA:N	2.23	0.52
20:V:80:LEU:HD23	20:V:80:LEU:O	2.09	0.52
7:G:10:GLU:HA	7:G:68:TYR:O	2.09	0.52
20:V:134:THR:HG23	20:V:134:THR:O	2.10	0.52
1:A:513:ALA:HB2	6:F:90:LEU:HD21	1.92	0.52
17:Q:860:GLN:OE1	17:Q:864:ARG:NH1	2.41	0.52
20:V:127:VAL:HG23	20:V:128:VAL:N	2.25	0.52
1:A:123:ASN:OD1	1:A:125:LYS:N	2.40	0.52
2:B:837:CYS:SG	2:B:891:ASP:N	2.83	0.52
20:V:249:MET:HE3	20:V:261:PHE:HZ	1.74	0.52
9:I:49:ASP:OD1	9:I:49:ASP:N	2.42	0.52
17:Q:60:PHE:CE2	17:Q:64:LEU:HD22	2.45	0.52
1:A:139:LYS:O	1:A:142:THR:OG1	2.24	0.52
7:G:146:LYS:N	7:G:162:SER:O	2.29	0.52
19:U:373:LEU:HD11	20:V:312:PHE:CD1	2.44	0.52
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.36	0.52
1:A:1279:MET:HG2	15:O:511:GLN:NE2	2.25	0.51
2:B:15:ASP:OD1	2:B:15:ASP:N	2.43	0.51
2:B:971:ALA:O	2:B:975:ARG:HG3	2.09	0.51
4:D:114:LEU:HD22	7:G:84:VAL:HG11	1.91	0.51
19:U:400:ASP:O	19:U:401:GLU:C	2.54	0.51
1:A:931:ARG:NE	1:A:936:GLU:OE1	2.43	0.51
4:D:31:THR:CG2	7:G:1:MET:HE2	2.40	0.51
13:M:1289:ARG:HG2	13:M:1289:ARG:NH1	2.25	0.51
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:428:ILE:CG1	13:M:436:LEU:HD11	2.39	0.51
7:G:124:ASN:HB3	7:G:125:PRO:CD	2.40	0.51
13:M:1307:ALA:HA	13:M:1310:HIS:NE2	2.25	0.51
2:B:792:ASP:O	2:B:943:GLY:HA3	2.11	0.51
7:G:124:ASN:O	7:G:126:PRO:HD3	2.11	0.51
13:M:1289:ARG:NE	13:M:1289:ARG:HA	2.26	0.51
13:M:1311:LYS:HG3	13:M:1312:GLN:HE22	1.74	0.51
17:Q:304:MET:HE1	17:Q:308:SER:OG	2.11	0.51
22:X:221:THR:HG22	22:X:222:ARG:NH2	2.26	0.51
5:E:114:ALA:O	5:E:117:SER:OG	2.25	0.51
13:M:814:PHE:O	13:M:829:LYS:NZ	2.40	0.51
21:W:220:GLN:HA	21:W:220:GLN:OE1	2.10	0.51
17:Q:273:ASN:ND2	17:Q:304:MET:SD	2.84	0.51
19:U:459:VAL:HG12	19:U:489:LEU:HD22	1.91	0.51
1:A:394:VAL:O	1:A:442:THR:O	2.29	0.51
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.92	0.51
13:M:412:ASN:OD1	13:M:415:ARG:NH2	2.41	0.51
24:Z:450:ILE:HD12	24:Z:468:LEU:HD13	1.93	0.51
7:G:140:ASP:OD1	7:G:140:ASP:C	2.54	0.50
17:Q:359:ASN:OD1	17:Q:362:GLN:NE2	2.44	0.50
24:Z:600:VAL:CG2	24:Z:643:LEU:HD22	2.40	0.50
17:Q:279:PHE:HB3	17:Q:288:VAL:HG22	1.93	0.50
21:W:283:ASN:OD1	21:W:286:GLY:N	2.44	0.50
2:B:484:ARG:HE	2:B:525:ASN:HD21	1.58	0.50
17:Q:524:LEU:HD22	17:Q:534:TYR:CE2	2.47	0.50
15:O:541:ARG:NH2	15:O:588:PHE:O	2.45	0.50
22:X:381:LEU:HB2	22:X:405:ILE:HD13	1.93	0.50
1:A:327:ARG:HB2	1:A:329:MET:HE2	1.94	0.50
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.94	0.50
13:M:338:TYR:OH	13:M:961:GLU:OE2	2.28	0.50
17:Q:304:MET:C	17:Q:304:MET:HE3	2.36	0.50
2:B:35:ASP:OD2	20:V:142:ASN:ND2	2.44	0.50
4:D:48:ASN:OD1	4:D:48:ASN:C	2.55	0.50
5:E:84:ILE:HD11	5:E:113:SER:HB2	1.94	0.50
21:W:263:THR:OG1	21:W:265:THR:OG1	2.26	0.50
24:Z:581:ASN:ND2	24:Z:617:LEU:O	2.45	0.50
24:Z:638:CYS:SG	24:Z:643:LEU:HD21	2.52	0.50
2:B:957:THR:O	2:B:959:GLU:O	2.30	0.50
1:A:384:ILE:HG23	1:A:388:MET:HE2	1.94	0.50
17:Q:145:MET:SD	17:Q:172:ILE:HG23	2.52	0.50
21:W:288:LYS:NZ	21:W:302:ASP:OD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:THR:CG2	2:B:732:ALA:O	2.60	0.49
5:E:47:LYS:N	5:E:52:ARG:O	2.38	0.49
22:X:387:VAL:HG21	22:X:392:LYS:HE3	1.92	0.49
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.47	0.49
4:D:17:ALA:N	7:G:83:GLU:OE2	2.44	0.49
5:E:79:GLU:H	5:E:79:GLU:CD	2.20	0.49
17:Q:884:LYS:O	17:Q:887:ASN:N	2.45	0.49
1:A:58:MET:HE1	1:A:271:ARG:HD2	1.94	0.49
17:Q:280:PHE:HA	17:Q:288:VAL:HG21	1.93	0.49
19:U:378:LEU:HD11	20:V:311:TYR:CD2	2.47	0.49
22:X:223:ASP:C	22:X:223:ASP:OD1	2.55	0.49
1:A:1261:ILE:HD11	15:O:512:MET:HE1	1.94	0.49
17:Q:836:GLU:OE1	17:Q:836:GLU:C	2.55	0.49
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.94	0.49
9:I:99:SER:O	9:I:100:HIS:CG	2.66	0.49
17:Q:253:ASN:OD1	17:Q:254:GLY:N	2.45	0.49
20:V:179:ILE:O	20:V:182:THR:OG1	2.29	0.49
4:D:99:CYS:O	4:D:102:ASN:OD1	2.31	0.49
13:M:635:TYR:CE1	13:M:1297:LYS:HE3	2.48	0.49
21:W:94:GLU:HA	21:W:94:GLU:OE1	2.12	0.49
24:Z:613:GLU:O	24:Z:625:HIS:N	2.45	0.49
13:M:1061:GLU:HG3	13:M:1062:THR:HG23	1.94	0.49
17:Q:531:VAL:HG13	17:Q:557:ALA:HB1	1.94	0.49
1:A:119:VAL:CG2	1:A:126:ILE:HD11	2.43	0.49
1:A:1350:LYS:O	1:A:1351:ASP:HB2	2.13	0.49
17:Q:491:TYR:O	17:Q:495:ILE:HG12	2.13	0.49
1:A:478:PRO:O	11:K:2:ASN:HB3	2.13	0.49
2:B:102:ASP:OD1	2:B:103:GLY:N	2.46	0.49
7:G:54:ILE:CD1	7:G:70:VAL:HG13	2.42	0.49
2:B:687:VAL:HG23	2:B:687:VAL:O	2.13	0.49
2:B:715:ASP:OD1	2:B:715:ASP:N	2.46	0.49
17:Q:495:ILE:HG23	20:V:49:ILE:HD13	1.95	0.49
24:Z:211:GLN:OE1	24:Z:234:HIS:NE2	2.46	0.49
1:A:357:LYS:NZ	2:B:1107:LEU:O	2.37	0.48
7:G:39:THR:O	7:G:43:GLY:N	2.45	0.48
17:Q:187:LYS:O	17:Q:191:ARG:HG2	2.13	0.48
17:Q:448:ASP:OD1	17:Q:448:ASP:N	2.46	0.48
7:G:44:PHE:HD2	7:G:46:ILE:HD13	1.78	0.48
17:Q:715:GLN:N	17:Q:715:GLN:OE1	2.46	0.48
22:X:387:VAL:O	22:X:387:VAL:HG23	2.12	0.48
1:A:657:TYR:O	1:A:660:MET:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:297:ARG:NH2	13:M:989:VAL:O	2.46	0.48
1:A:186:ARG:NH2	1:A:210:GLN:OE1	2.46	0.48
4:D:99:CYS:HB3	4:D:115:ILE:HD11	1.95	0.48
5:E:110:MET:HG2	5:E:114:ALA:HB3	1.95	0.48
7:G:143:ILE:HG22	7:G:144:ARG:N	2.29	0.48
18:T:33:DC:H2''	18:T:34:DT:OP1	2.13	0.48
20:V:193:HIS:HB3	20:V:196:LYS:O	2.13	0.48
1:A:155:GLU:O	1:A:183:GLY:N	2.40	0.48
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.13	0.48
22:X:371:LEU:HD11	22:X:480:TYR:CE2	2.49	0.48
22:X:434:LEU:HD23	22:X:438:ASP:HB3	1.94	0.48
5:E:38:GLU:OE1	5:E:38:GLU:N	2.44	0.48
7:G:3:TYR:HD2	7:G:5:ILE:HD11	1.79	0.48
17:Q:6:ILE:HD13	17:Q:47:LEU:HD22	1.96	0.48
21:W:198:PHE:CE1	21:W:219:VAL:HG11	2.49	0.48
2:B:489:ILE:CD1	2:B:498:PRO:HB2	2.44	0.48
17:Q:151:GLN:O	17:Q:155:VAL:HG23	2.13	0.48
17:Q:471:LYS:HB2	17:Q:506:LEU:HD21	1.96	0.48
19:U:474:ARG:HB3	20:V:217:PRO:HG2	1.96	0.48
12:L:26:ASN:HD21	12:L:44:MET:HE1	1.79	0.47
19:U:358:ILE:HG23	19:U:358:ILE:O	2.12	0.47
1:A:83:GLY:HA3	1:A:257:PRO:HB2	1.96	0.47
1:A:713:VAL:HG11	1:A:817:PRO:HD3	1.96	0.47
2:B:492:ASP:OD1	2:B:492:ASP:N	2.38	0.47
7:G:92:VAL:HG11	7:G:127:CYS:HA	1.96	0.47
13:M:1311:LYS:HD2	13:M:1311:LYS:O	2.13	0.47
15:O:597:TYR:O	15:O:601:VAL:HG23	2.14	0.47
1:A:695:ASP:N	1:A:695:ASP:OD1	2.47	0.47
17:Q:156:LEU:HD23	17:Q:156:LEU:C	2.40	0.47
17:Q:791:ARG:NH2	21:W:103:ASP:OD2	2.46	0.47
7:G:11:ILE:HG13	7:G:11:ILE:O	2.13	0.47
2:B:650:ASN:C	19:U:460:TYR:OH	2.58	0.47
14:N:10:DG:H1'	14:N:11:DC:C5	2.49	0.47
16:P:137:G:O2'	16:P:138:A:P	2.73	0.47
17:Q:84:THR:O	17:Q:88:THR:OG1	2.29	0.47
20:V:297:TRP:HE3	20:V:299:VAL:HG23	1.73	0.47
6:F:83:LEU:O	6:F:84:GLU:C	2.56	0.47
17:Q:225:LEU:HD11	17:Q:235:LEU:CD2	2.45	0.47
20:V:224:ASP:OD2	20:V:334:LYS:N	2.39	0.47
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.55	0.47
4:D:118:LEU:O	4:D:118:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:LEU:HD21	4:D:127:LEU:HD13	1.97	0.47
7:G:12:LEU:HB3	7:G:65:PHE:HD2	1.79	0.47
11:K:64:PRO:HG3	11:K:72:ILE:HD12	1.95	0.47
17:Q:200:VAL:HG12	20:V:82:VAL:HG21	1.97	0.47
20:V:262:LEU:HD12	20:V:292:ALA:HB2	1.96	0.47
20:V:327:GLU:OE1	20:V:367:ARG:NH2	2.41	0.47
22:X:380:LEU:HD22	22:X:511:PHE:HZ	1.80	0.47
24:Z:507:THR:C	24:Z:508:MET:HE2	2.39	0.47
12:L:22:CYS:SG	12:L:24:THR:OG1	2.62	0.47
13:M:1329:VAL:HG13	13:M:1329:VAL:O	2.15	0.47
17:Q:605:LEU:HD12	22:X:238:LEU:HD13	1.97	0.47
20:V:295:TYR:HB2	20:V:332:LEU:HD22	1.97	0.47
24:Z:505:ASP:OD1	24:Z:505:ASP:N	2.48	0.47
1:A:190:ARG:NH2	14:N:34:DC:OP1	2.48	0.47
2:B:329:GLY:O	2:B:335:ARG:NE	2.48	0.47
17:Q:624:LYS:HA	17:Q:627:ARG:HG2	1.96	0.47
19:U:479:LEU:HD12	19:U:479:LEU:N	2.30	0.47
1:A:1262:MET:SD	15:O:544:ARG:NH1	2.85	0.47
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.96	0.47
17:Q:91:ALA:HB3	20:V:86:LEU:HD11	1.96	0.47
24:Z:212:ILE:HD12	24:Z:227:VAL:HG13	1.96	0.47
24:Z:424:ASP:HB2	24:Z:440:ILE:HD12	1.96	0.47
24:Z:448:ILE:HG12	24:Z:465:ALA:HB2	1.97	0.47
1:A:882:SER:OG	1:A:1428:MET:HE1	2.15	0.46
3:C:44:ILE:HD11	3:C:239:LEU:CG	2.44	0.46
13:M:639:TYR:O	13:M:1301:TYR:HA	2.15	0.46
2:B:19:PRO:O	2:B:22:TRP:N	2.48	0.46
7:G:165:ASP:OD2	7:G:166:ASP:N	2.47	0.46
20:V:95:ASP:OD1	20:V:95:ASP:N	2.45	0.46
21:W:26:THR:HG21	21:W:284:GLY:HA3	1.97	0.46
2:B:473:LEU:HD11	2:B:1052:LYS:HD2	1.97	0.46
3:C:11:ILE:HG12	11:K:108:ALA:HB1	1.97	0.46
3:C:44:ILE:HD11	3:C:239:LEU:CD1	2.45	0.46
19:U:405:ASP:CG	19:U:506:LEU:HD22	2.41	0.46
23:Y:79:GLN:NE2	23:Y:91:VAL:O	2.46	0.46
1:A:970:PHE:O	1:A:972:THR:O	2.33	0.46
2:B:255:ARG:NH1	2:B:307:GLU:OE2	2.47	0.46
6:F:68:THR:CG2	7:G:59:ILE:HG21	2.45	0.46
13:M:1287:MET:HE3	13:M:1289:ARG:HH11	1.81	0.46
5:E:56:THR:N	5:E:78:GLU:OE2	2.49	0.46
23:Y:8:GLU:O	23:Y:31:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:372:LEU:HD12	24:Z:373:PHE:N	2.31	0.46
1:A:299:ALA:O	1:A:302:VAL:HG22	2.15	0.46
1:A:381:PRO:HB3	1:A:479:TRP:O	2.15	0.46
2:B:474:THR:HG21	2:B:732:ALA:O	2.15	0.46
7:G:108:ILE:HD11	7:G:145:LEU:HD13	1.97	0.46
17:Q:592:LEU:HD21	17:Q:603:SER:HB2	1.97	0.46
1:A:981:CYS:HB3	1:A:986:MET:HE1	1.97	0.46
4:D:86:LEU:HG	4:D:87:LEU:HD12	1.96	0.46
17:Q:524:LEU:HD22	17:Q:534:TYR:CZ	2.51	0.46
20:V:258:VAL:HG21	20:V:297:TRP:HB3	1.98	0.46
24:Z:542:LEU:CD2	24:Z:570:VAL:HG11	2.46	0.46
1:A:205:VAL:HG13	1:A:207:GLU:O	2.16	0.46
2:B:735:VAL:HG11	10:J:55:LEU:CD2	2.44	0.46
2:B:908:MET:SD	2:B:910:THR:HG23	2.56	0.46
13:M:475:ILE:N	13:M:476:PRO:HD2	2.31	0.46
17:Q:877:GLN:HG3	17:Q:881:TYR:CE2	2.51	0.46
24:Z:480:VAL:O	24:Z:480:VAL:HG13	2.16	0.46
24:Z:492:ILE:HD12	24:Z:495:VAL:HG13	1.97	0.46
4:D:17:ALA:O	4:D:20:LEU:CD2	2.64	0.46
4:D:19:GLN:HB3	4:D:21:ILE:HG12	1.98	0.46
4:D:60:VAL:HG11	7:G:44:PHE:CE2	2.51	0.46
16:P:135:G:C4'	16:P:136:G:O5'	2.64	0.46
24:Z:510:GLU:N	24:Z:510:GLU:OE1	2.48	0.46
1:A:1158:LEU:C	1:A:1158:LEU:HD23	2.41	0.45
13:M:807:ASP:OD1	13:M:808:PHE:N	2.48	0.45
20:V:295:TYR:CB	20:V:332:LEU:HD22	2.45	0.45
4:D:57:LEU:HG	4:D:61:PHE:HB2	1.96	0.45
8:H:91:VAL:HG22	8:H:144:LEU:HD13	1.98	0.45
1:A:896:LEU:CD1	1:A:980:PRO:HG3	2.47	0.45
4:D:87:LEU:HB3	4:D:97:LEU:HD22	1.98	0.45
13:M:340:ASP:OD1	13:M:340:ASP:N	2.49	0.45
17:Q:438:THR:HG23	17:Q:449:VAL:CG2	2.46	0.45
20:V:240:MET:HG3	20:V:268:LEU:HD11	1.98	0.45
24:Z:542:LEU:HD23	24:Z:570:VAL:HG11	1.99	0.45
1:A:1257:LEU:HD11	1:A:1259:ILE:HD11	1.98	0.45
21:W:146:THR:HG22	21:W:175:PHE:CZ	2.52	0.45
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.97	0.45
7:G:152:VAL:HA	7:G:157:ILE:HA	1.99	0.45
8:H:131:ASN:HD21	17:Q:702:GLN:HE22	1.65	0.45
13:M:1289:ARG:HA	13:M:1289:ARG:CZ	2.47	0.45
22:X:382:GLN:OE1	22:X:406:GLN:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:384:LEU:HD12	22:X:508:ARG:HE	1.81	0.45
24:Z:549:VAL:HG21	24:Z:635:MET:HE1	1.98	0.45
1:A:294:GLU:OE1	1:A:303:ILE:HD12	2.17	0.45
1:A:431:PHE:O	1:A:432:HIS:C	2.60	0.45
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.97	0.45
17:Q:643:ASP:OD2	22:X:239:GLN:NE2	2.41	0.45
22:X:378:LYS:HB2	22:X:403:THR:HG21	1.99	0.45
9:I:15:ARG:HB3	9:I:24:LEU:HD12	1.99	0.45
17:Q:272:LEU:HD11	17:Q:291:LEU:HD22	1.98	0.45
17:Q:436:THR:O	17:Q:440:ILE:HG13	2.17	0.45
23:Y:66:ALA:O	24:Z:214:SER:OG	2.26	0.45
24:Z:212:ILE:HG22	24:Z:229:ALA:HB2	1.98	0.45
1:A:1189:ASP:O	1:A:1193:VAL:HG23	2.16	0.45
22:X:375:LEU:HD12	22:X:376:ASN:N	2.32	0.45
13:M:1291:ASN:HA	13:M:1294:LYS:HZ2	1.81	0.45
14:N:19:DG:H3'	14:N:20:DT:H5'	1.99	0.45
22:X:398:GLN:C	22:X:398:GLN:OE1	2.60	0.45
4:D:66:ASN:OD1	4:D:66:ASN:C	2.60	0.45
7:G:97:LEU:HD22	7:G:99:THR:CG2	2.47	0.45
17:Q:358:GLU:O	17:Q:361:SER:OG	2.24	0.45
17:Q:775:ASN:OD1	17:Q:775:ASN:N	2.48	0.45
19:U:472:PHE:CD2	20:V:221:VAL:HG21	2.52	0.45
11:K:37:LYS:N	11:K:69:HIS:O	2.48	0.44
14:N:34:DC:H2''	14:N:35:DA:C8	2.52	0.44
17:Q:166:LEU:HD23	17:Q:189:ALA:CA	2.47	0.44
17:Q:400:HIS:O	17:Q:404:VAL:HG23	2.17	0.44
20:V:286:VAL:CG1	20:V:350:VAL:HG13	2.47	0.44
1:A:83:GLY:HA3	1:A:257:PRO:CB	2.46	0.44
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.99	0.44
1:A:384:ILE:CG2	1:A:388:MET:HE2	2.48	0.44
2:B:607:ILE:O	2:B:609:GLU:O	2.35	0.44
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.98	0.44
20:V:127:VAL:HG23	20:V:128:VAL:H	1.81	0.44
20:V:168:ILE:HG22	20:V:169:TYR:CD1	2.52	0.44
2:B:728:MET:SD	2:B:942:LYS:HD3	2.58	0.44
7:G:148:VAL:HG13	7:G:160:ILE:HG23	1.99	0.44
9:I:47:GLU:OE1	9:I:47:GLU:N	2.50	0.44
16:P:139:A:H2'	16:P:140:C:O4'	2.17	0.44
1:A:412:GLN:O	1:A:413:TYR:C	2.59	0.44
2:B:547:GLU:HG3	20:V:298:ASN:ND2	2.33	0.44
13:M:1355:VAL:HG21	13:M:1412:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:667:ARG:HB2	17:Q:690:ILE:HG21	1.98	0.44
1:A:467:MET:HG2	1:A:534:VAL:HG21	2.00	0.44
2:B:910:THR:CG2	12:L:43:ILE:HG12	2.47	0.44
3:C:33:SER:OG	11:K:45:ILE:HG23	2.17	0.44
17:Q:886:LYS:O	17:Q:890:MET:N	2.43	0.44
1:A:140:ARG:NH1	1:A:234:PHE:O	2.50	0.44
1:A:208:ASP:OD2	1:A:209:SER:N	2.51	0.44
1:A:503:LEU:C	1:A:503:LEU:HD23	2.43	0.44
1:A:1227:THR:N	1:A:1230:GLN:OE1	2.45	0.44
2:B:473:LEU:HD11	2:B:1052:LYS:CD	2.48	0.44
4:D:23:PRO:HB2	4:D:25:GLU:HG2	2.00	0.44
4:D:29:ALA:HB2	7:G:5:ILE:HG23	2.00	0.44
4:D:116:PRO:HA	4:D:119:GLU:OE2	2.16	0.44
13:M:1291:ASN:OD1	13:M:1294:LYS:NZ	2.32	0.44
24:Z:495:VAL:HG23	24:Z:495:VAL:O	2.17	0.44
1:A:54:LEU:O	1:A:59:ASP:OD1	2.36	0.44
1:A:621:ILE:HG23	1:A:621:ILE:O	2.17	0.44
1:A:693:ILE:HG22	1:A:694:ALA:N	2.32	0.44
1:A:693:ILE:CD1	1:A:828:LEU:HD21	2.48	0.44
7:G:137:ILE:HD13	7:G:143:ILE:HD12	1.98	0.44
13:M:1294:LYS:HB2	13:M:1294:LYS:NZ	2.30	0.44
22:X:481:ASP:OD1	22:X:481:ASP:N	2.50	0.44
22:X:361:ILE:HD11	22:X:426:ARG:NH2	2.33	0.44
2:B:18:THR:O	2:B:22:TRP:N	2.51	0.44
2:B:624:PRO:HA	2:B:663:GLU:O	2.16	0.44
4:D:26:PHE:HE2	7:G:78:ARG:NH1	2.16	0.44
4:D:112:LYS:NZ	4:D:124:ASP:OD2	2.48	0.44
7:G:139:GLN:O	7:G:140:ASP:CG	2.61	0.44
8:H:80:ASP:OD1	8:H:80:ASP:N	2.50	0.44
13:M:676:VAL:HG12	13:M:676:VAL:O	2.17	0.44
22:X:402:GLU:OE2	22:X:428:VAL:HG12	2.18	0.44
4:D:24:LYS:HD3	4:D:24:LYS:H	1.82	0.43
7:G:89:VAL:HG22	7:G:97:LEU:HD21	2.00	0.43
9:I:42:CYS:SG	9:I:43:ASP:N	2.90	0.43
17:Q:48:ALA:HB1	17:Q:60:PHE:CD2	2.52	0.43
1:A:1193:VAL:O	1:A:1197:TYR:N	2.51	0.43
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.53	0.43
9:I:113:VAL:HG22	9:I:122:ARG:HG3	2.00	0.43
4:D:104:CYS:SG	4:D:138:ARG:NH2	2.85	0.43
20:V:222:ILE:HD11	20:V:329:ARG:HE	1.84	0.43
24:Z:513:VAL:HG12	24:Z:514:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:VAL:HG13	2:B:767:LEU:HD22	2.00	0.43
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.51	0.43
17:Q:374:ASN:HB3	17:Q:377:THR:HG22	2.00	0.43
17:Q:438:THR:HG23	17:Q:449:VAL:HG22	2.00	0.43
17:Q:619:THR:HG22	17:Q:621:ASP:H	1.83	0.43
1:A:1147:SER:HA	1:A:1153:ARG:HB2	1.99	0.43
4:D:57:LEU:HD22	4:D:62:MET:SD	2.59	0.43
4:D:98:ALA:O	4:D:102:ASN:CG	2.62	0.43
13:M:989:VAL:HB	13:M:992:LEU:HD12	1.99	0.43
13:M:1485:GLU:OE2	13:M:1497:ARG:NH2	2.49	0.43
21:W:169:ASP:OD1	21:W:169:ASP:N	2.43	0.43
22:X:382:GLN:NE2	22:X:406:GLN:O	2.51	0.43
19:U:376:VAL:HG13	19:U:491:PHE:HE2	1.84	0.43
22:X:359:THR:HG23	22:X:359:THR:O	2.19	0.43
24:Z:524:THR:HG22	24:Z:525:ALA:N	2.34	0.43
1:A:565:MET:HE1	11:K:74:ARG:HB2	2.01	0.43
1:A:858:GLY:HA2	1:A:861:GLN:HE21	1.83	0.43
2:B:503:ASN:H	2:B:503:ASN:HD22	1.66	0.43
4:D:98:ALA:O	4:D:102:ASN:ND2	2.52	0.43
5:E:9:ARG:O	5:E:13:ILE:HG12	2.17	0.43
17:Q:48:ALA:HB2	17:Q:63:LEU:HD11	2.01	0.43
17:Q:166:LEU:HD23	17:Q:189:ALA:N	2.33	0.43
1:A:91:ALA:HB3	1:A:290:LEU:HD23	2.01	0.43
1:A:1302:GLU:O	1:A:1303:GLN:HB2	2.18	0.43
2:B:327:LYS:HE3	14:N:20:DT:H72	2.00	0.43
4:D:99:CYS:HA	4:D:102:ASN:OD1	2.19	0.43
6:F:79:VAL:HG12	6:F:81:VAL:H	1.84	0.43
17:Q:166:LEU:HD23	17:Q:189:ALA:HA	2.01	0.43
2:B:190:SER:OG	2:B:192:LYS:HE2	2.19	0.43
7:G:116:GLU:OE1	7:G:116:GLU:N	2.50	0.43
17:Q:393:LYS:HA	17:Q:396:ILE:HD12	2.01	0.43
23:Y:13:ASP:OD1	23:Y:28:THR:HG21	2.19	0.43
23:Y:65:ILE:O	23:Y:89:TYR:N	2.42	0.43
14:N:29:DG:H2'	14:N:30:DC:C5	2.53	0.43
1:A:154:CYS:O	1:A:155:GLU:HB3	2.18	0.42
12:L:53:VAL:HG23	12:L:53:VAL:O	2.19	0.42
13:M:541:LEU:HD12	13:M:693:TYR:HD1	1.83	0.42
17:Q:94:VAL:HG11	17:Q:137:PHE:HA	2.01	0.42
20:V:271:ARG:NH2	20:V:289:TYR:OH	2.51	0.42
24:Z:448:ILE:O	24:Z:449:THR:OG1	2.32	0.42
13:M:464:TYR:CE1	13:M:468:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:398:PHE:O	19:U:398:PHE:CG	2.73	0.42
22:X:374:MET:HE1	22:X:427:VAL:HG12	2.01	0.42
1:A:549:THR:O	1:A:589:LYS:NZ	2.52	0.42
2:B:778:SER:O	2:B:1045:PRO:HA	2.20	0.42
7:G:123:SER:OG	13:M:409:ARG:NH2	2.52	0.42
22:X:447:VAL:HG22	22:X:449:GLY:H	1.84	0.42
24:Z:192:THR:HG21	24:Z:245:LEU:HD21	2.00	0.42
1:A:413:TYR:O	1:A:449:HIS:ND1	2.25	0.42
1:A:910:LYS:N	1:A:911:PRO:HD2	2.34	0.42
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.55	0.42
12:L:52:LEU:HD21	24:Z:721:ILE:HD13	2.02	0.42
4:D:33:LEU:HD21	4:D:98:ALA:HA	2.01	0.42
13:M:779:ILE:O	13:M:921:GLN:NE2	2.53	0.42
13:M:824:GLU:OE1	13:M:824:GLU:N	2.43	0.42
13:M:895:ASN:OD1	24:Z:545:GLN:NE2	2.52	0.42
17:Q:79:GLU:OE1	17:Q:79:GLU:N	2.41	0.42
22:X:219:ASP:OD1	22:X:219:ASP:C	2.63	0.42
2:B:489:ILE:HD13	2:B:498:PRO:HB2	2.01	0.42
4:D:23:PRO:HB2	4:D:25:GLU:CG	2.49	0.42
9:I:27:LYS:O	9:I:36:LEU:N	2.37	0.42
17:Q:486:GLU:OE2	17:Q:486:GLU:N	2.41	0.42
22:X:431:PRO:HA	22:X:434:LEU:HD13	2.01	0.42
23:Y:98:PRO:HG2	23:Y:101:ILE:HD12	2.02	0.42
13:M:413:LEU:HD22	13:M:460:LEU:HD11	2.02	0.42
13:M:897:LYS:NZ	13:M:900:GLU:OE2	2.44	0.42
15:O:568:THR:HG22	15:O:568:THR:O	2.20	0.42
19:U:368:ASP:HB3	20:V:213:MET:HE3	2.01	0.42
1:A:957:GLU:OE2	1:A:960:ARG:NH1	2.53	0.42
2:B:225:LEU:O	2:B:226:GLU:C	2.61	0.42
2:B:473:LEU:C	2:B:473:LEU:HD23	2.45	0.42
2:B:651:TYR:N	19:U:460:TYR:OH	2.52	0.42
7:G:22:LEU:O	7:G:26:VAL:HG23	2.20	0.42
7:G:83:GLU:N	7:G:83:GLU:OE1	2.53	0.42
7:G:163:LEU:O	7:G:163:LEU:HD12	2.20	0.42
14:N:10:DG:H2"	14:N:11:DC:C5	2.54	0.42
1:A:760:LEU:HD11	1:A:781:ILE:HG21	2.02	0.42
9:I:60:HIS:O	9:I:60:HIS:CG	2.71	0.42
3:C:27:ASP:OD1	11:K:52:LYS:HD2	2.20	0.41
5:E:82:VAL:HG21	5:E:106:VAL:HG12	2.02	0.41
17:Q:304:MET:HE3	17:Q:305:GLN:N	2.34	0.41
20:V:79:ASP:OD1	20:V:79:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:LEU:CD1	1:A:1259:ILE:HD11	2.50	0.41
2:B:626:LEU:HD23	2:B:662:VAL:HG22	2.00	0.41
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.39	0.41
7:G:57:GLY:HA2	7:G:67:LEU:O	2.20	0.41
7:G:113:ILE:HD12	7:G:163:LEU:HD11	2.02	0.41
18:T:4:DC:O2	18:T:4:DC:O4'	2.36	0.41
21:W:128:GLY:O	21:W:146:THR:OG1	2.28	0.41
2:B:756:LYS:NZ	20:V:134:THR:HG1	2.13	0.41
3:C:44:ILE:HD13	3:C:44:ILE:HA	1.84	0.41
3:C:79:VAL:HG22	3:C:167:LYS:HD2	2.01	0.41
4:D:93:HIS:HB3	4:D:96:GLU:OE1	2.20	0.41
7:G:119:PHE:N	7:G:119:PHE:CD1	2.88	0.41
21:W:295:ASP:OD1	21:W:295:ASP:N	2.45	0.41
22:X:484:ARG:HD2	22:X:485:LEU:O	2.20	0.41
2:B:728:MET:SD	2:B:942:LYS:HB3	2.59	0.41
22:X:438:ASP:OD1	22:X:441:ARG:NH2	2.53	0.41
24:Z:550:ILE:O	24:Z:550:ILE:HG23	2.20	0.41
2:B:380:ARG:NH1	2:B:609:GLU:HG2	2.35	0.41
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.20	0.41
13:M:942:PHE:N	13:M:946:GLN:OE1	2.50	0.41
14:N:34:DC:C2'	14:N:35:DA:C8	3.04	0.41
17:Q:317:HIS:CE1	17:Q:350:MET:SD	3.14	0.41
20:V:48:PHE:O	22:X:229:ARG:N	2.53	0.41
22:X:371:LEU:N	22:X:371:LEU:HD22	2.35	0.41
2:B:791:GLU:O	2:B:792:ASP:HB2	2.20	0.41
2:B:818:GLU:O	2:B:916:TYR:HB3	2.20	0.41
4:D:61:PHE:O	4:D:64:THR:HG22	2.20	0.41
13:M:586:GLU:OE2	13:M:715:ARG:NH2	2.54	0.41
14:N:22:DT:H4'	14:N:23:DT:OP1	2.19	0.41
22:X:221:THR:CG2	22:X:222:ARG:NH2	2.83	0.41
24:Z:529:ASP:OD1	24:Z:529:ASP:N	2.51	0.41
2:B:629:GLU:HB2	2:B:634:LEU:HD21	2.02	0.41
14:N:23:DT:H2''	14:N:24:DC:OP1	2.21	0.41
14:N:30:DC:H2''	14:N:31:DC:C6	2.56	0.41
17:Q:350:MET:HA	17:Q:350:MET:HE3	2.03	0.41
17:Q:425:THR:O	17:Q:425:THR:HG22	2.21	0.41
17:Q:836:GLU:CD	17:Q:837:GLU:N	2.79	0.41
19:U:366:ASN:ND2	20:V:280:ASP:OD1	2.54	0.41
21:W:47:TRP:HB3	21:W:54:LEU:HG	2.02	0.41
22:X:428:VAL:O	22:X:428:VAL:HG23	2.21	0.41
1:A:613:GLU:OE1	1:A:622:SER:OG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:794:VAL:HG12	2:B:967:ILE:HG22	2.03	0.41
6:F:83:LEU:O	6:F:86:GLU:N	2.52	0.41
14:N:11:DC:H2''	14:N:12:DG:C8	2.56	0.41
14:N:18:DT:O2	14:N:18:DT:O4'	2.39	0.41
1:A:111:CYS:SG	1:A:115:SER:N	2.93	0.41
1:A:1185:VAL:HG12	1:A:1185:VAL:O	2.20	0.41
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.51	0.41
2:B:910:THR:HG22	12:L:43:ILE:HA	2.02	0.41
4:D:29:ALA:HB1	7:G:4:HIS:O	2.19	0.41
7:G:104:MET:SD	7:G:159:ALA:HB3	2.61	0.41
9:I:96:PHE:HA	9:I:111:TYR:O	2.21	0.41
17:Q:138:CYS:SG	17:Q:148:ALA:HB2	2.61	0.41
17:Q:186:TYR:CG	17:Q:204:MET:SD	3.14	0.41
17:Q:200:VAL:HG23	17:Q:201:ARG:N	2.36	0.41
17:Q:318:VAL:HG13	17:Q:319:GLN:OE1	2.21	0.41
17:Q:879:ALA:O	17:Q:882:VAL:HG12	2.19	0.41
24:Z:190:ARG:NH2	24:Z:219:GLU:OE1	2.54	0.41
24:Z:450:ILE:HG22	24:Z:451:MET:N	2.35	0.41
24:Z:451:MET:HE1	24:Z:462:GLU:HG3	2.03	0.41
1:A:562:ASN:O	1:A:565:MET:CB	2.69	0.41
2:B:451:GLY:CA	2:B:466:VAL:O	2.69	0.41
8:H:33:GLU:HG3	17:Q:674:ARG:HH22	1.86	0.41
16:P:143:A:O2'	16:P:144:C:H5'	2.21	0.41
17:Q:48:ALA:CB	17:Q:63:LEU:HD11	2.51	0.41
21:W:111:THR:O	21:W:123:THR:HA	2.21	0.41
2:B:157:ARG:HG3	2:B:182:GLY:HA3	2.02	0.40
2:B:623:ARG:HH22	2:B:697:GLU:CD	2.28	0.40
2:B:1143:LYS:O	2:B:1143:LYS:HG3	2.21	0.40
4:D:21:ILE:HG13	4:D:21:ILE:O	2.19	0.40
13:M:1371:TRP:NE1	13:M:1379:GLN:OE1	2.49	0.40
17:Q:522:ASN:OD1	17:Q:525:ARG:NH1	2.48	0.40
20:V:291:ILE:O	20:V:291:ILE:HG23	2.21	0.40
21:W:86:ALA:O	21:W:104:ALA:HB3	2.21	0.40
1:A:527:THR:HB	1:A:534:VAL:CG1	2.51	0.40
1:A:1165:THR:HG21	1:A:1294:THR:O	2.20	0.40
4:D:32:LEU:HD11	7:G:4:HIS:HB2	2.03	0.40
7:G:30:LEU:HD13	7:G:70:VAL:CG1	2.51	0.40
17:Q:163:ILE:N	17:Q:164:PRO:CD	2.84	0.40
19:U:405:ASP:O	19:U:406:GLU:C	2.64	0.40
22:X:405:ILE:HD11	22:X:427:VAL:HG21	2.03	0.40
2:B:747:LEU:HD21	2:B:812:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.54	0.40
4:D:32:LEU:CD1	7:G:4:HIS:HB2	2.51	0.40
4:D:118:LEU:HD23	4:D:118:LEU:C	2.45	0.40
17:Q:193:ASN:ND2	20:V:93:ARG:O	2.54	0.40
20:V:69:GLN:O	20:V:69:GLN:OE1	2.39	0.40
24:Z:585:VAL:HG22	24:Z:586:ALA:N	2.37	0.40
2:B:754:PRO:HB2	2:B:773:PRO:HG2	2.03	0.40
4:D:39:MET:O	4:D:42:GLU:HG2	2.22	0.40
13:M:894:MET:HG2	24:Z:545:GLN:HE21	1.86	0.40
17:Q:225:LEU:HD11	17:Q:235:LEU:HD21	2.03	0.40
17:Q:419:ALA:HB2	17:Q:433:ALA:HB3	2.04	0.40
20:V:224:ASP:OD1	20:V:224:ASP:N	2.54	0.40
21:W:50:ARG:HB3	21:W:50:ARG:NH1	2.36	0.40
24:Z:212:ILE:HD13	24:Z:238:ALA:HB1	2.03	0.40
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.21	0.40
2:B:473:LEU:HD13	2:B:731:GLN:HA	2.02	0.40
2:B:635:LEU:HD21	2:B:640:ILE:HD11	2.04	0.40
4:D:24:LYS:HD3	4:D:24:LYS:N	2.37	0.40
9:I:124:THR:HG22	9:I:125:GLU:N	2.36	0.40
13:M:689:ILE:HD11	13:M:717:LEU:HD11	2.04	0.40
17:Q:39:THR:OG1	17:Q:43:ILE:HD13	2.22	0.40
17:Q:815:ARG:O	17:Q:818:SER:OG	2.32	0.40
19:U:361:GLU:HA	20:V:352:LYS:O	2.22	0.40
22:X:463:ASP:OD1	22:X:463:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1414/1970 (72%)	1370 (97%)	44 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1123/1174 (96%)	1072 (96%)	51 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	124/142 (87%)	123 (99%)	1 (1%)	0	100	100
5	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	80/127 (63%)	76 (95%)	4 (5%)	0	100	100
7	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	115/125 (92%)	109 (95%)	6 (5%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
13	M	1106/1726 (64%)	1093 (99%)	13 (1%)	0	100	100
15	O	117/991 (12%)	113 (97%)	4 (3%)	0	100	100
17	Q	888/1173 (76%)	880 (99%)	8 (1%)	0	100	100
19	U	150/666 (22%)	140 (93%)	7 (5%)	3 (2%)	6	2
20	V	303/531 (57%)	292 (96%)	9 (3%)	2 (1%)	18	14
21	W	303/305 (99%)	289 (95%)	14 (5%)	0	100	100
22	X	225/531 (42%)	217 (96%)	8 (4%)	0	100	100
23	Y	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
24	Z	507/1087 (47%)	502 (99%)	5 (1%)	0	100	100
All	All	7568/11714 (65%)	7356 (97%)	207 (3%)	5 (0%)	49	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	U	400	ASP
19	U	406	GLU
20	V	374	HIS
20	V	346	ASN
19	U	401	GLU

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	1253/1749 (72%)	1249 (100%)	4 (0%)	86	91
2	B	992/1027 (97%)	985 (99%)	7 (1%)	76	82
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	116/126 (92%)	112 (97%)	4 (3%)	32	33
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	148 (97%)	4 (3%)	40	44
8	H	129/131 (98%)	128 (99%)	1 (1%)	73	80
9	I	105/112 (94%)	104 (99%)	1 (1%)	68	75
10	J	56/56 (100%)	55 (98%)	1 (2%)	51	58
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	993/1522 (65%)	991 (100%)	2 (0%)	87	92
15	O	104/820 (13%)	104 (100%)	0	100	100
17	Q	761/1005 (76%)	754 (99%)	7 (1%)	70	78
19	U	139/590 (24%)	135 (97%)	4 (3%)	37	40
20	V	283/462 (61%)	279 (99%)	4 (1%)	59	66
21	W	260/260 (100%)	257 (99%)	3 (1%)	63	70
22	X	209/467 (45%)	205 (98%)	4 (2%)	50	56
23	Y	102/103 (99%)	101 (99%)	1 (1%)	68	75
24	Z	455/940 (48%)	452 (99%)	3 (1%)	76	82
All	All	6755/10239 (66%)	6705 (99%)	50 (1%)	73	82

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	PHE
1	A	413	TYR
1	A	1050	CYS
1	A	1192	TRP
2	B	474	THR

Continued on next page...

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Mol	Chain	Res	Type
2	B	492	ASP
2	B	528	LEU
2	B	675	LEU
2	B	710	ILE
2	B	901	THR
2	B	924	ARG
4	D	36	GLU
4	D	64	THR
4	D	88	LEU
4	D	123	GLU
7	G	3	TYR
7	G	11	ILE
7	G	58	VAL
7	G	100	GLU
8	H	45	ILE
9	I	29	ASP
10	J	13	ILE
13	M	1294	LYS
13	M	1313	GLU
17	Q	98	ARG
17	Q	134	ARG
17	Q	186	TYR
17	Q	241	LEU
17	Q	352	ILE
17	Q	836	GLU
17	Q	839	ARG
19	U	356	THR
19	U	464	LEU
19	U	506	LEU
19	U	515	THR
20	V	64	THR
20	V	137	ILE
20	V	268	LEU
20	V	304	SER
21	W	114	PHE
21	W	207	THR
21	W	240	PHE
22	X	222	ARG
22	X	245	PHE
22	X	390	ASP
22	X	527	SER
23	Y	40	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Z	580	ASP
24	Z	721	ILE
24	Z	741	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	222	HIS
1	A	278	HIS
1	A	459	ASN
1	A	531	ASN
1	A	576	GLN
1	A	673	GLN
1	A	711	GLN
1	A	731	ASN
1	A	742	ASN
1	A	757	GLN
1	A	792	ASN
1	A	1182	GLN
1	A	1244	ASN
1	A	1422	GLN
2	B	144	HIS
2	B	461	GLN
2	B	503	ASN
2	B	525	ASN
2	B	631	GLN
2	B	654	GLN
2	B	930	GLN
2	B	1025	ASN
2	B	1094	GLN
3	C	108	ASN
3	C	217	GLN
5	E	116	GLN
7	G	4	HIS
7	G	28	GLN
7	G	111	HIS
9	I	22	ASN
9	I	118	HIS
11	K	29	ASN
11	K	49	GLN
11	K	89	ASN

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Continued from previous page...

Mol	Chain	Res	Type
13	M	323	ASN
13	M	595	GLN
13	M	632	HIS
13	M	731	ASN
13	M	1151	ASN
13	M	1170	ASN
13	M	1390	ASN
15	O	500	HIS
15	O	585	HIS
15	O	595	ASN
17	Q	40	GLN
17	Q	206	HIS
17	Q	331	GLN
17	Q	362	GLN
17	Q	400	HIS
17	Q	559	GLN
17	Q	702	GLN
17	Q	745	HIS
19	U	468	HIS
19	U	469	ASN
19	U	470	HIS
19	U	475	GLN
20	V	373	ASN
21	W	95	ASN
21	W	268	HIS
21	W	285	ASN
24	Z	252	GLN
24	Z	435	ASN
24	Z	545	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	11/15 (73%)	2 (18%)	2 (18%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	136	G
16	P	138	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	135	G
16	P	137	G

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.

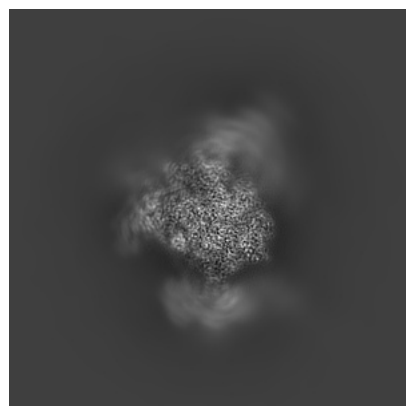
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52443. These allow visual inspection of the internal detail of the map and identification of artifacts.

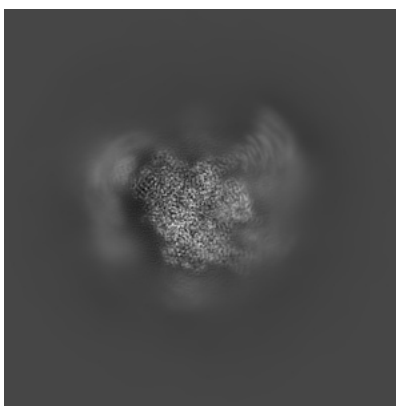
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

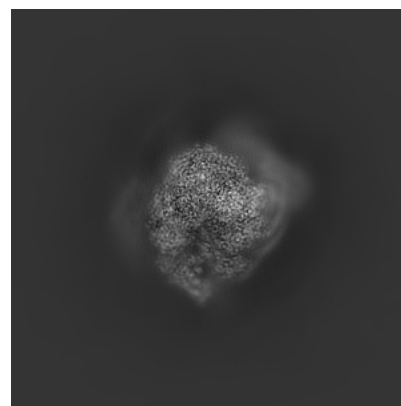
6.1.1 Primary map



X

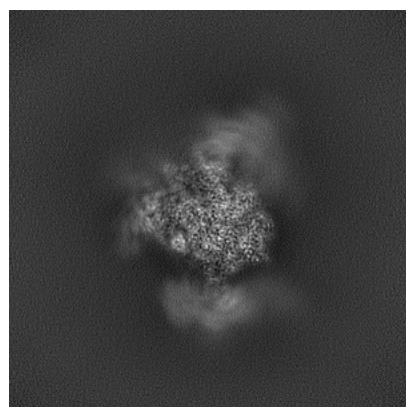


Y

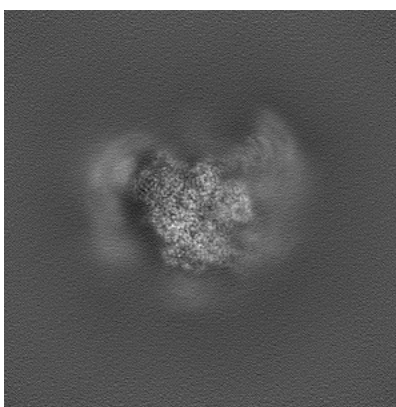


Z

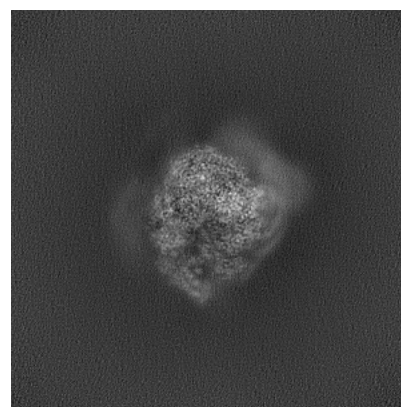
6.1.2 Raw map



X



Y

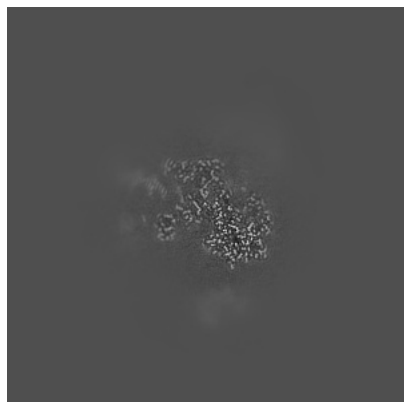


Z

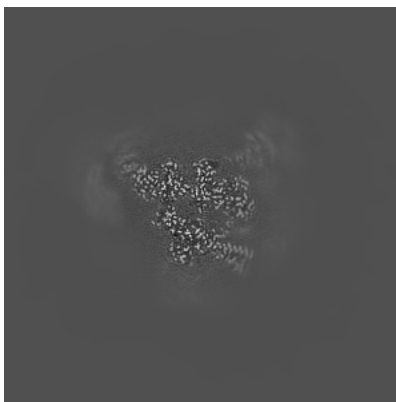
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

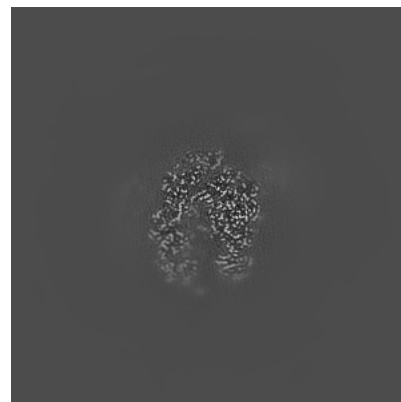
6.2.1 Primary map



X Index: 240

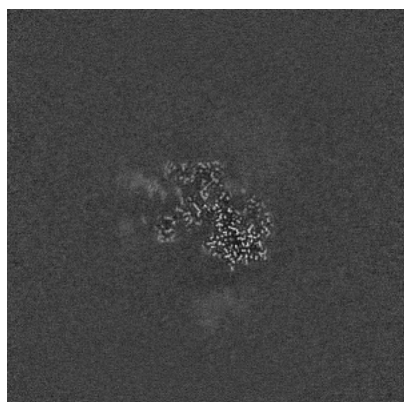


Y Index: 240

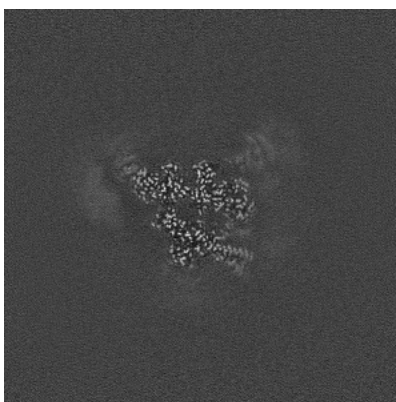


Z Index: 240

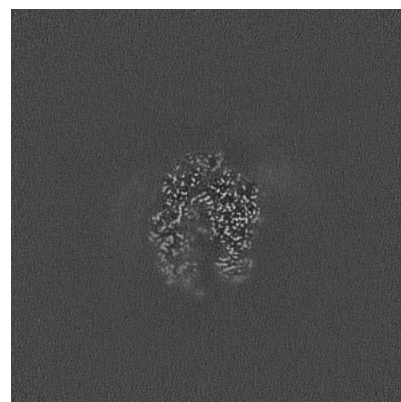
6.2.2 Raw map



X Index: 240



Y Index: 240

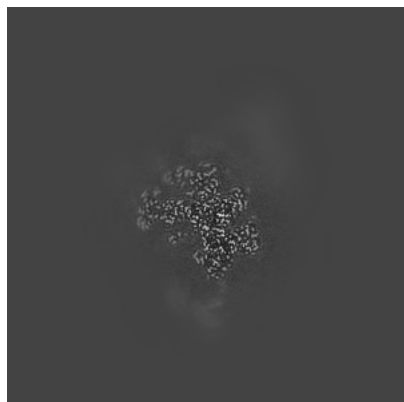


Z Index: 240

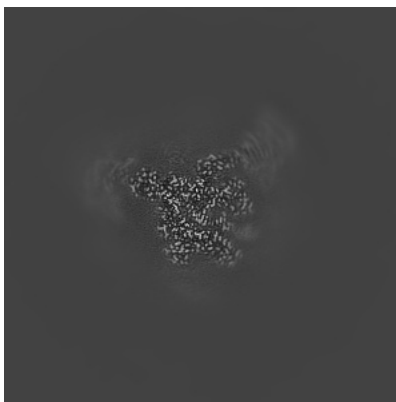
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

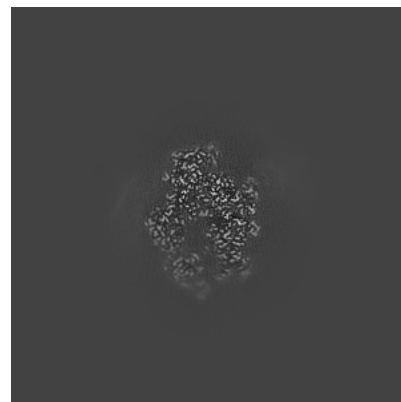
6.3.1 Primary map



X Index: 261

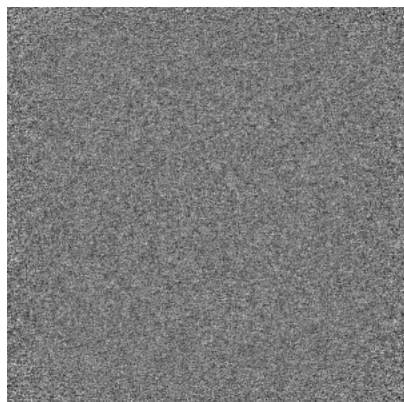


Y Index: 252

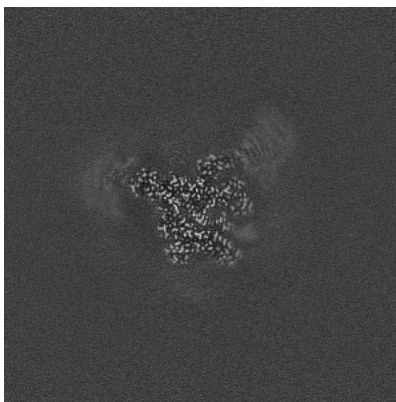


Z Index: 232

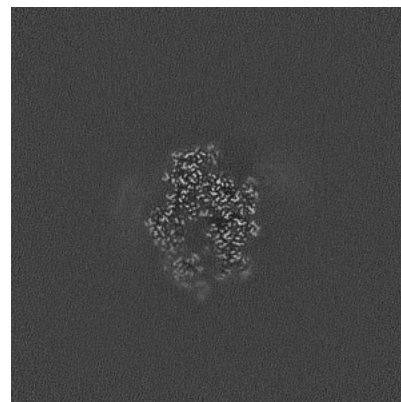
6.3.2 Raw map



X Index: 0



Y Index: 252

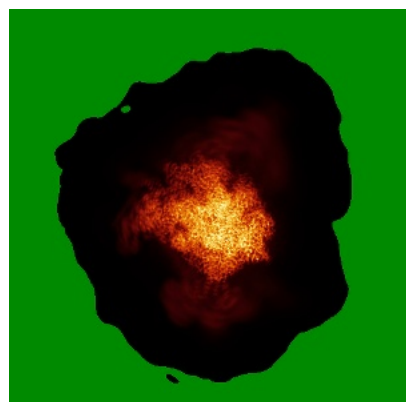


Z Index: 232

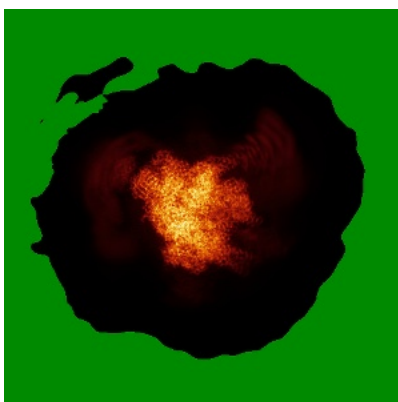
The images above show the largest variance slices of the map in three orthogonal directions.

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

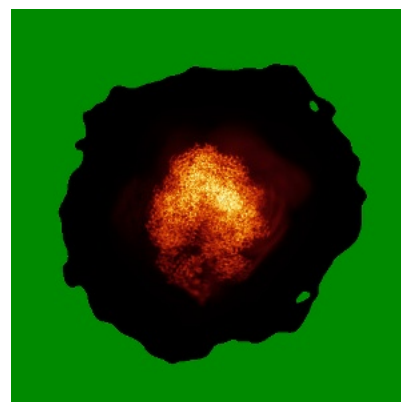
6.4.1 Primary map



X

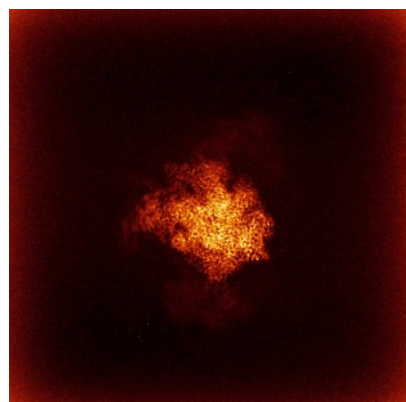


Y

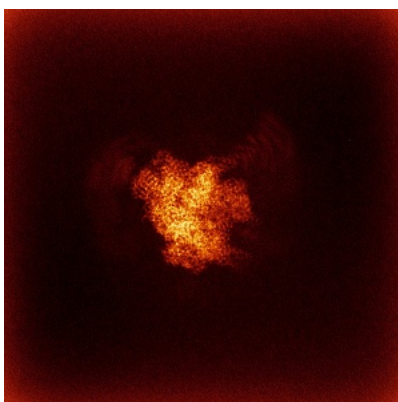


Z

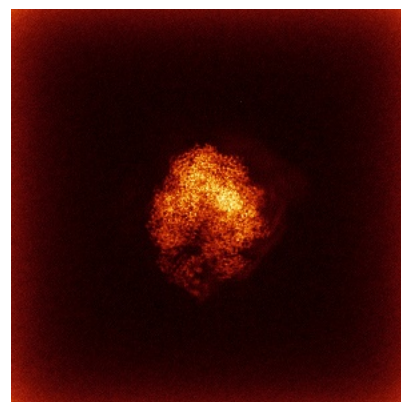
6.4.2 Raw map



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.

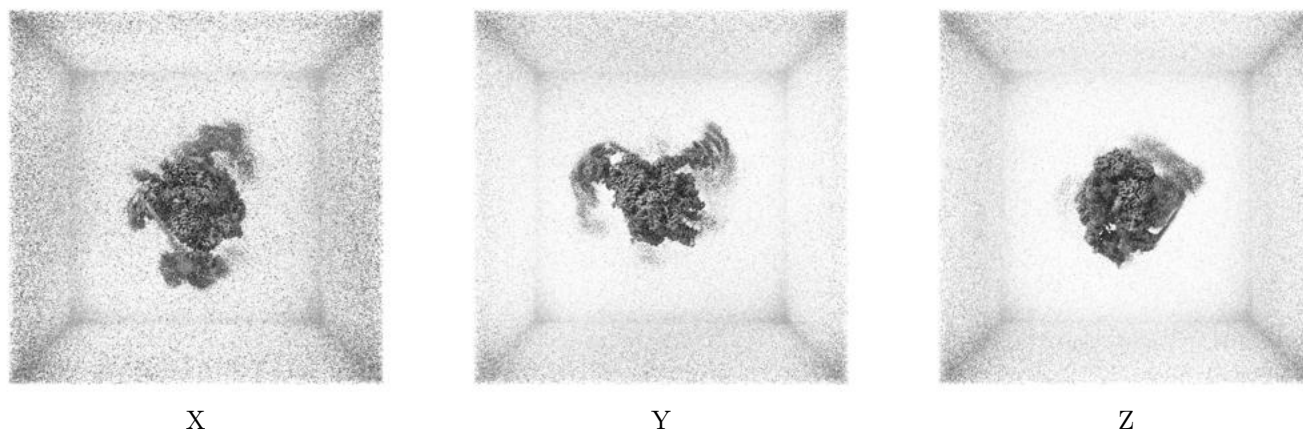
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.002. 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.

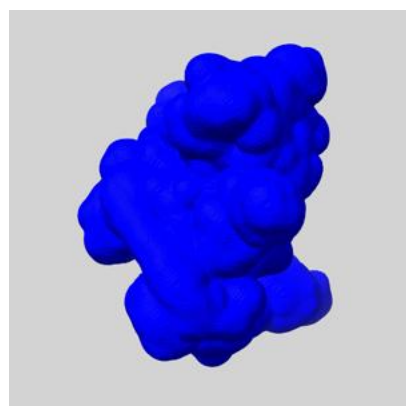
6.6 Mask visualisation [i](#)

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

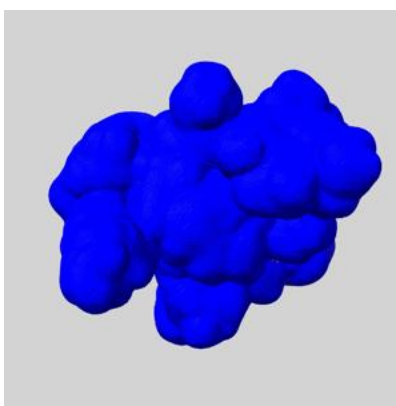
A mask typically either:

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

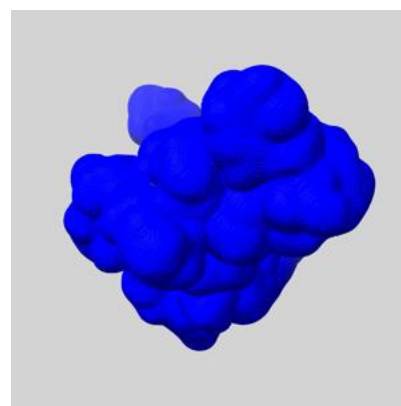
6.6.1 emd_52443_msk_1.map [i](#)



X



Y

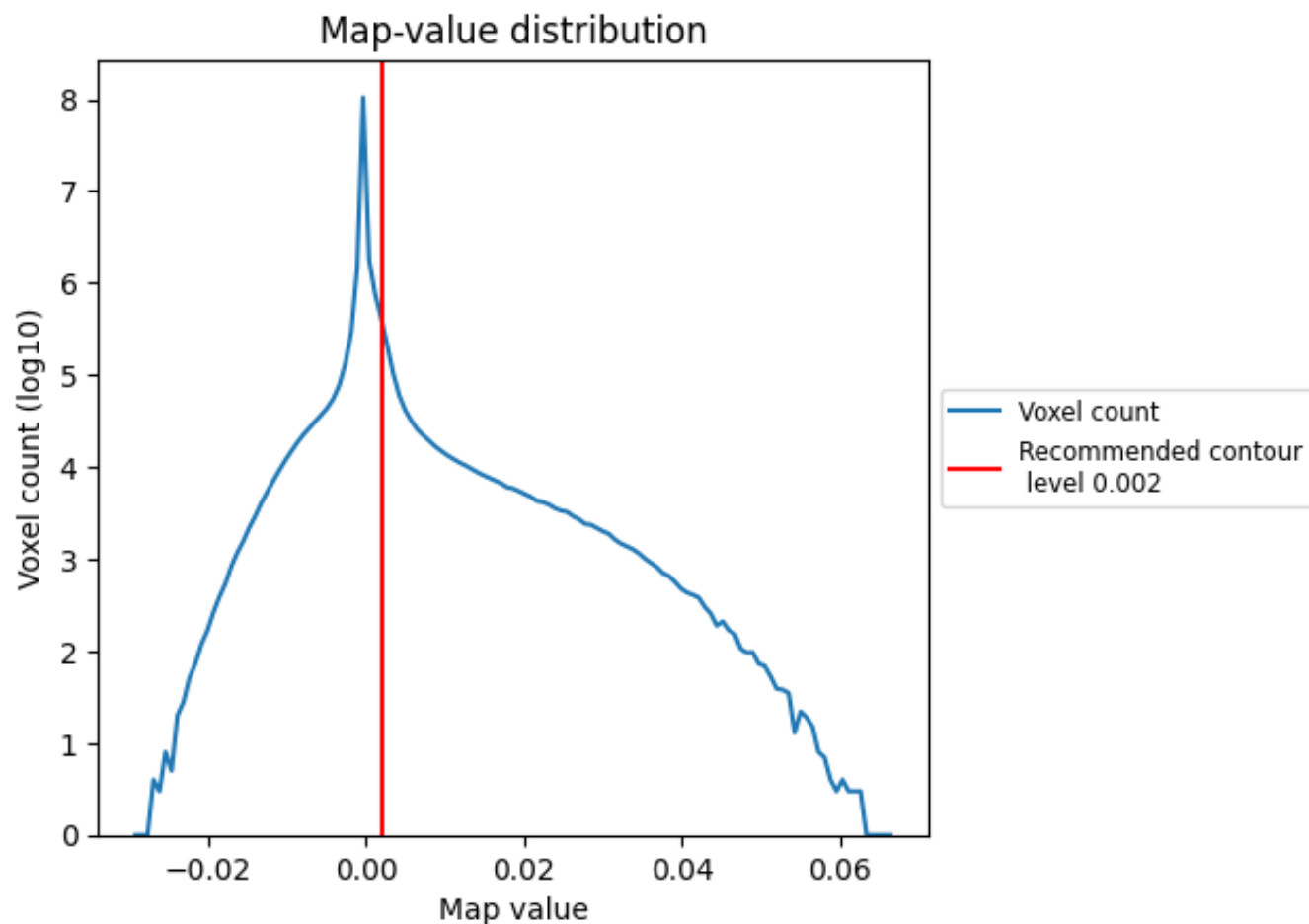


Z

7 Map analysis [i](#)

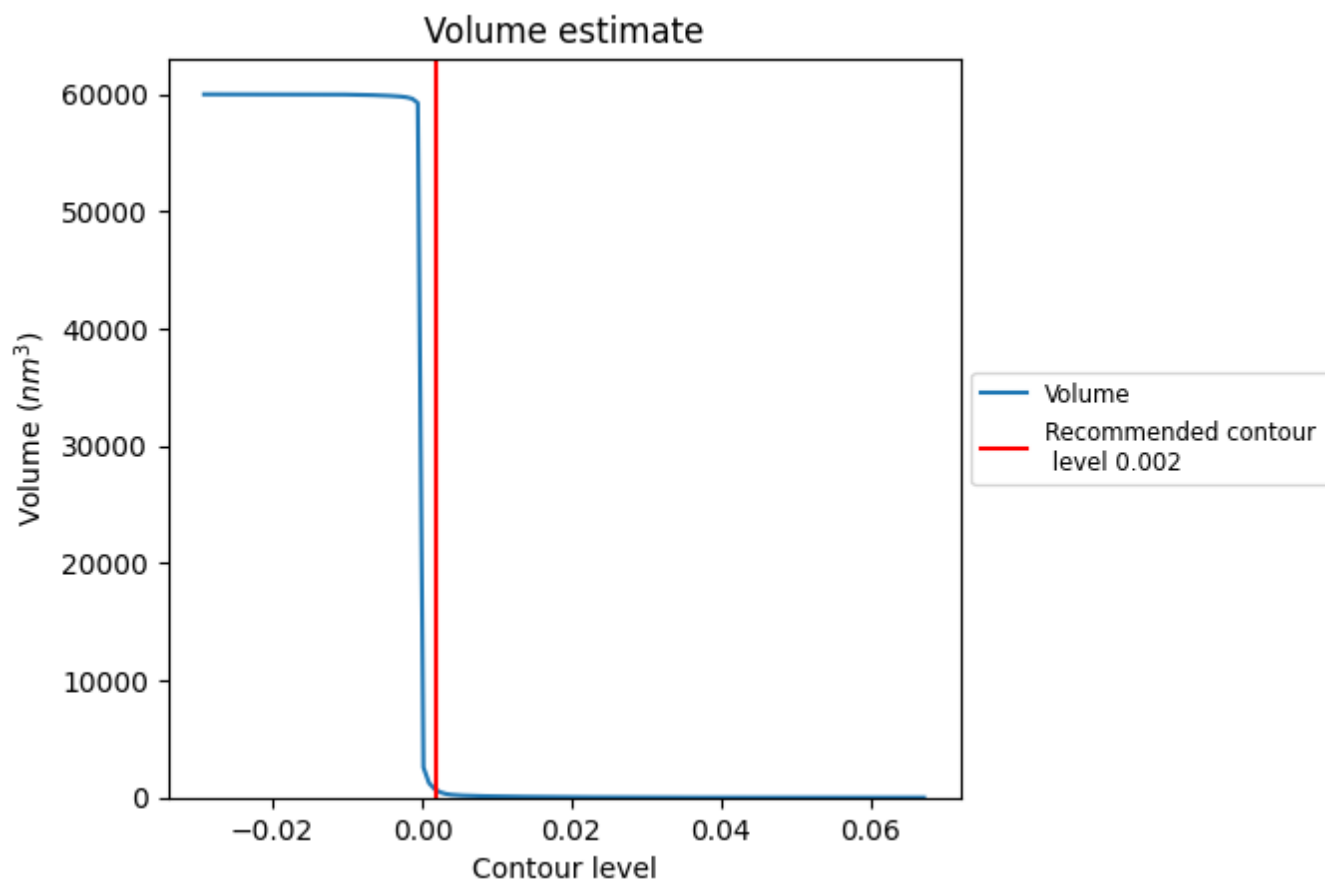
This section contains the results of statistical analysis of the map.

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.

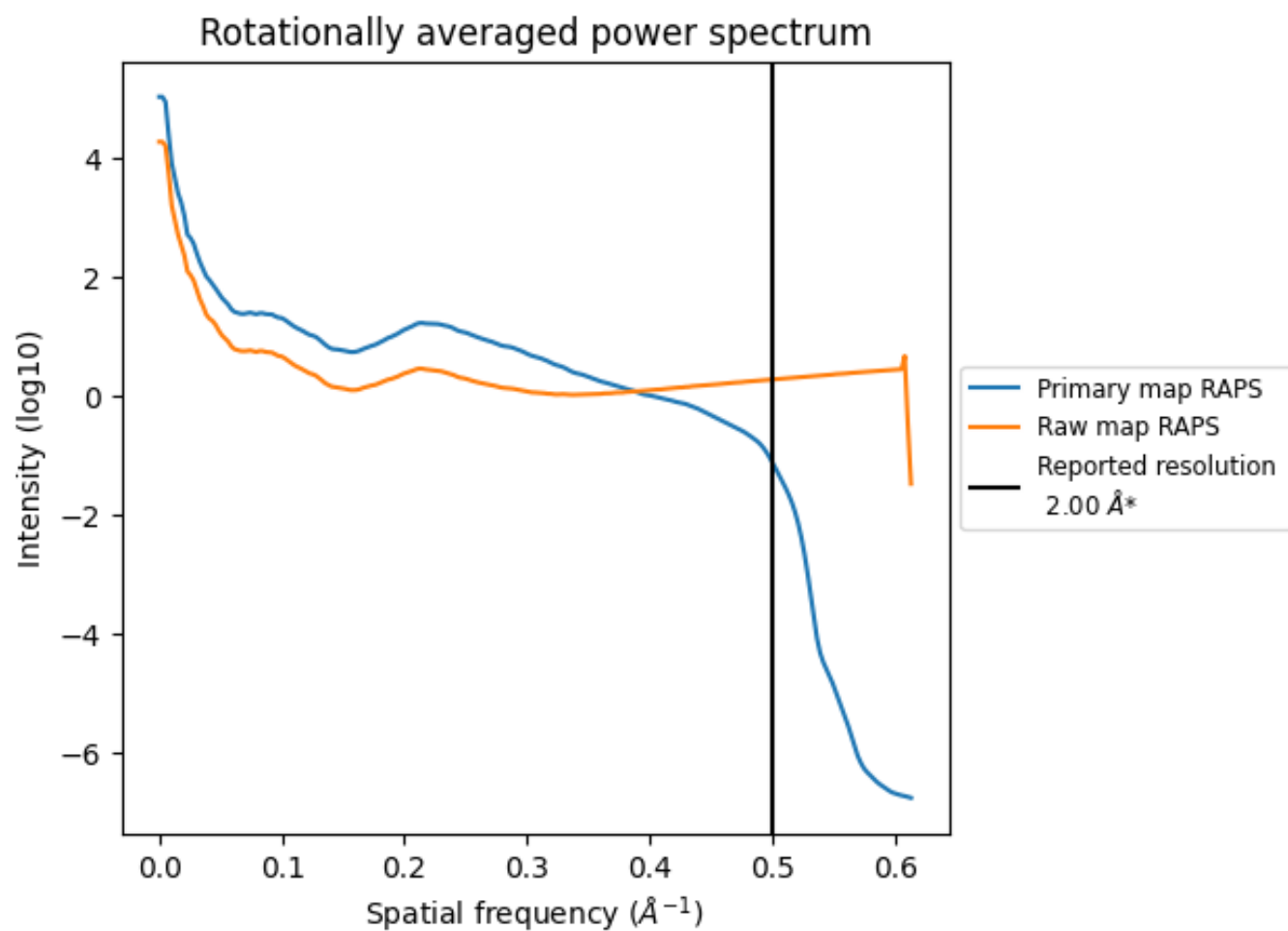
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 614 nm^3 ; this corresponds to an approximate mass of 554 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 ⓘ

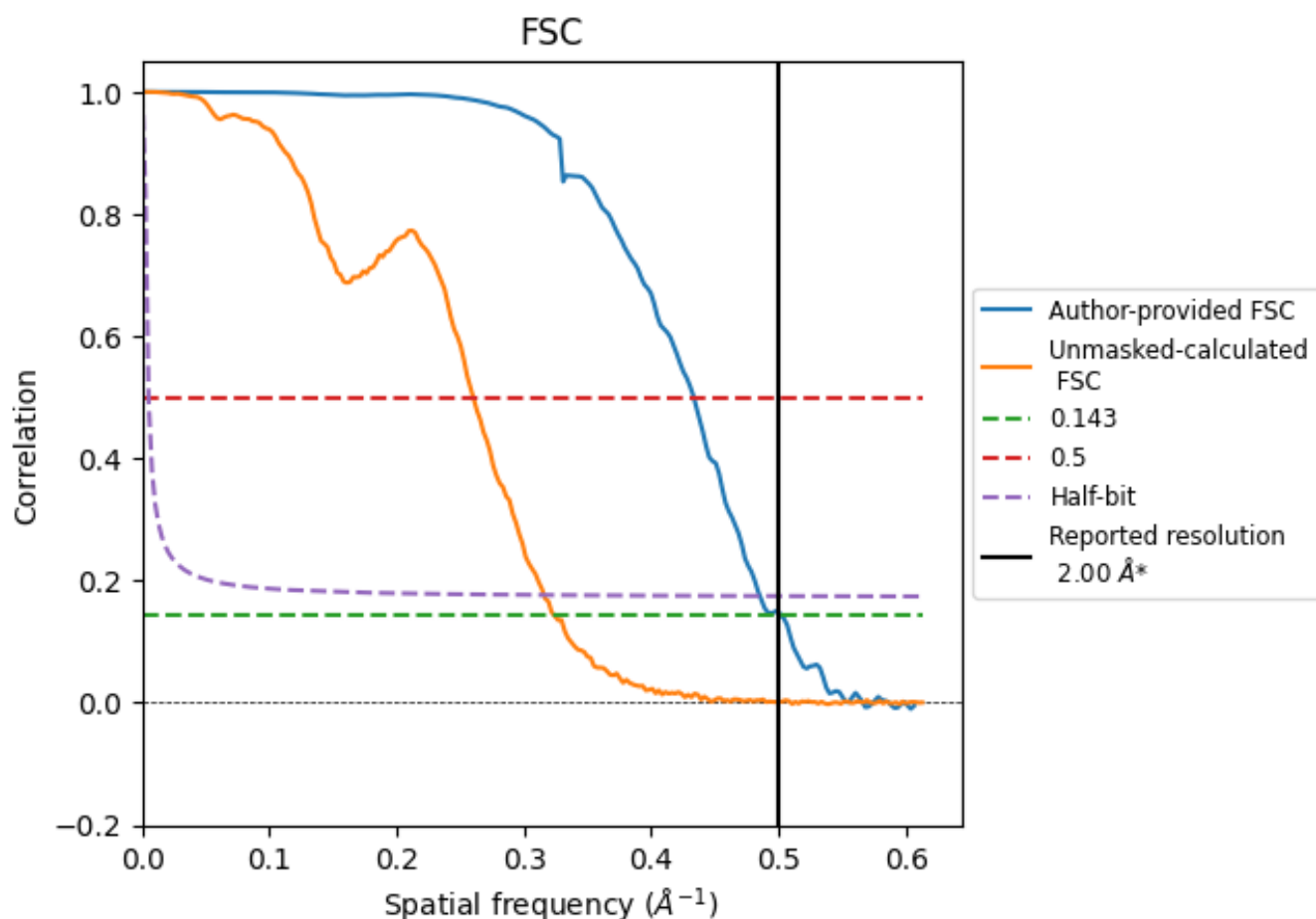


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

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 0.500 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

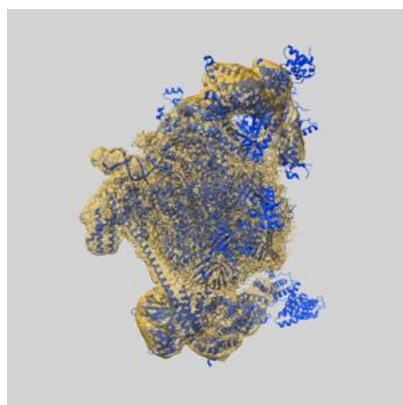
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	1.99	2.31	2.06
Unmasked-calculated*	3.09	3.84	3.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.0 by more than 10 %

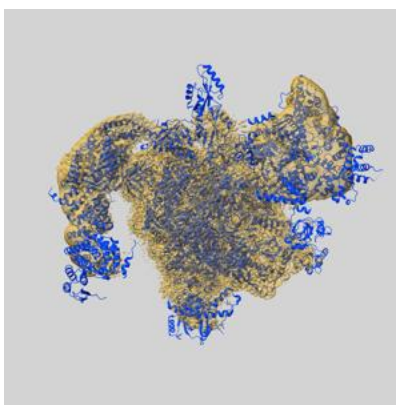
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52443 and PDB model 9HVQ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

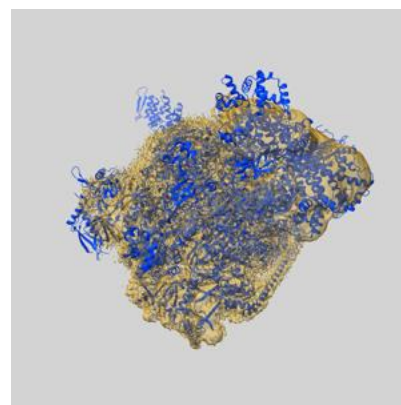
9.1 Map-model overlay [i](#)



X



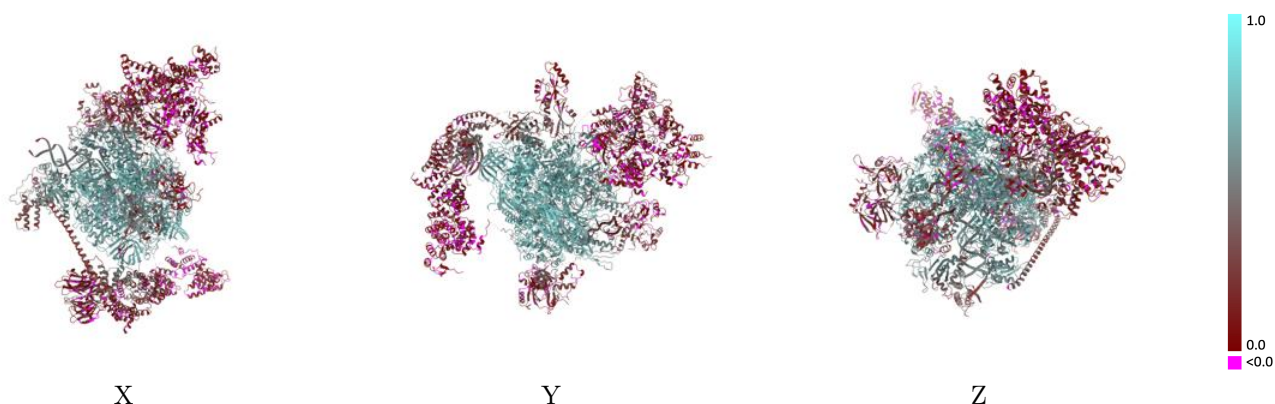
Y



Z

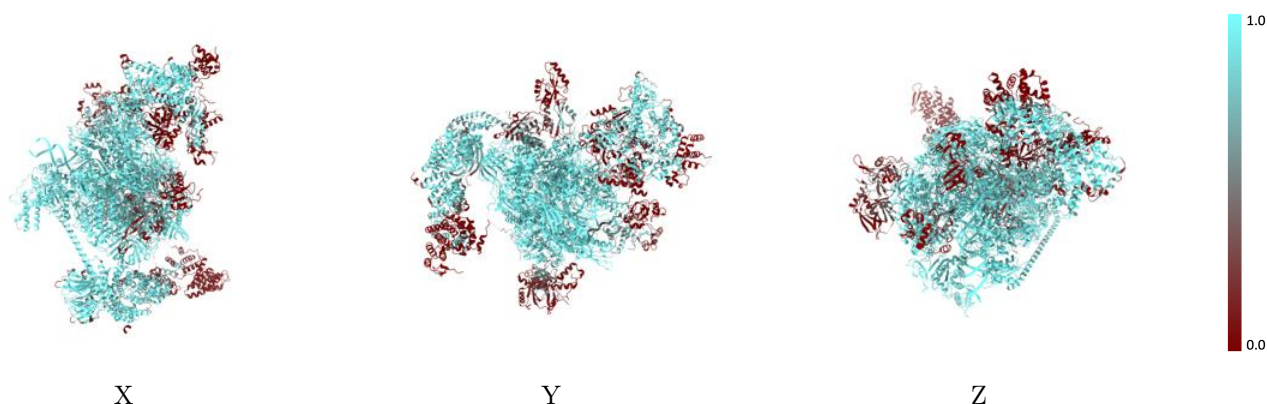
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



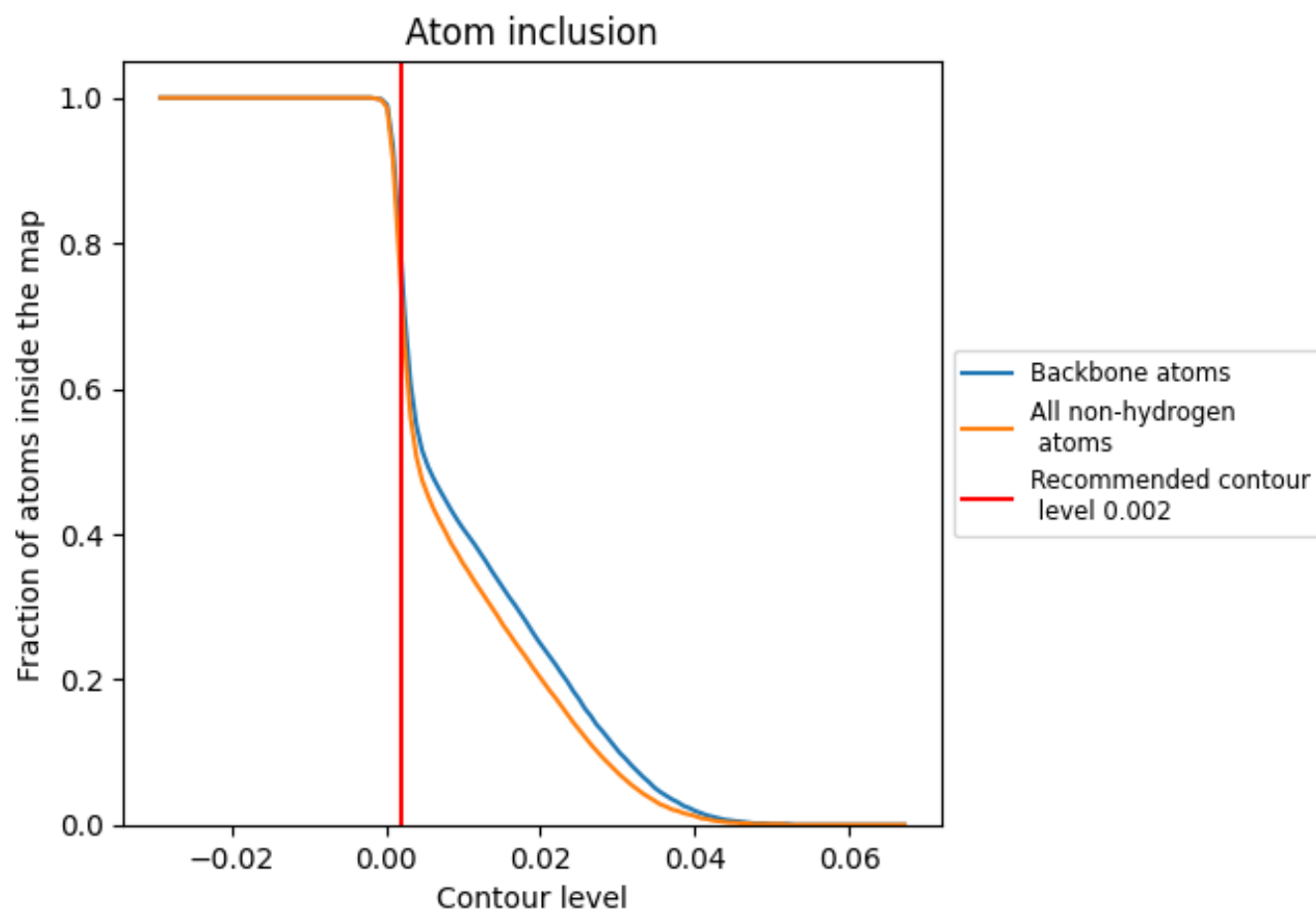
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.002).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.4190
A	 0.9810	 0.6760
B	 0.9830	 0.6850
C	 0.9920	 0.7190
D	 0.8410	 0.2310
E	 0.9860	 0.6380
F	 0.9730	 0.6840
G	 0.8960	 0.3820
H	 0.9850	 0.6880
I	 0.9650	 0.5700
J	 0.9900	 0.7350
K	 0.9880	 0.7180
L	 0.9950	 0.6510
M	 0.4900	 0.1180
N	 0.7960	 0.3560
O	 0.9110	 0.3460
P	 0.9460	 0.6020
Q	 0.5980	 0.1720
T	 0.9650	 0.5560
U	 0.2710	 0.2310
V	 0.2470	 0.1670
W	 0.8150	 0.1500
X	 0.4260	 0.3240
Y	 0.3170	 0.1950
Z	 0.2610	 0.2160

