



Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 04:23 pm BST

PDB ID : 9G23 / pdb_00009g23
EMDB ID : EMD-50962
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site bound to nucleotide analog AMPCPP at A-site
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 3.40 Å(reported)
Based on initial model : 6hko

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

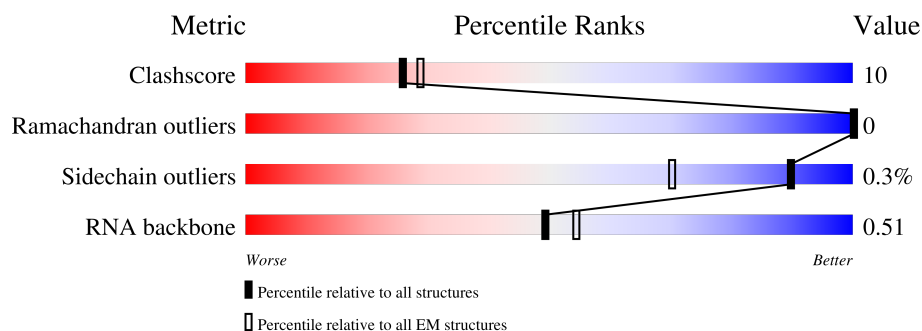
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1664	<div> <div>5%</div> <div>66%</div> <div>23%</div> <div>11%</div> </div>
2	B	1203	<div> <div>71%</div> <div>26%</div> <div>.</div> </div>
3	C	335	<div> <div>77%</div> <div>15%</div> <div>7%</div> </div>
4	D	137	<div> <div>31%</div> <div>34%</div> <div>9%</div> <div>57%</div> </div>
5	E	215	<div> <div>5%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
6	F	155	<div> <div>50%</div> <div>15%</div> <div>35%</div> </div>
7	G	326	<div> <div>23%</div> <div>34%</div> <div>15%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	12	
16	S	38	
17	T	38	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 34137 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1478	Total	C	N	O	S	0	0
			11664	7363	2034	2205	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1168	Total	C	N	O	S	0	0
			9274	5862	1629	1732	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	310	Total	C	N	O	S	0	0
			2461	1560	422	471	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	59	Total	C	N	O	0	0
			467	293	80	94		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1734	1102	306	315	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			827	524	145	155	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	162	Total	C	N	O	S	0	0
			1258	809	212	232	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	132	Total	C	N	O	S	0	0
			1060	670	177	209	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			479	300	79	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			766	481	124	156	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	103	Total	C	N	O	0	0
			816	518	137	161		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	116	Total	C	N	O	S	0	0
			921	597	152	168	4		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	11	Total	C	N	O	P	0	0
			239	107	47	74	11		

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	26	Total	C	N	O	P	0	0
			526	252	87	161	26		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	34	Total	C	N	O	P	0	0
			686	327	122	203	34		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

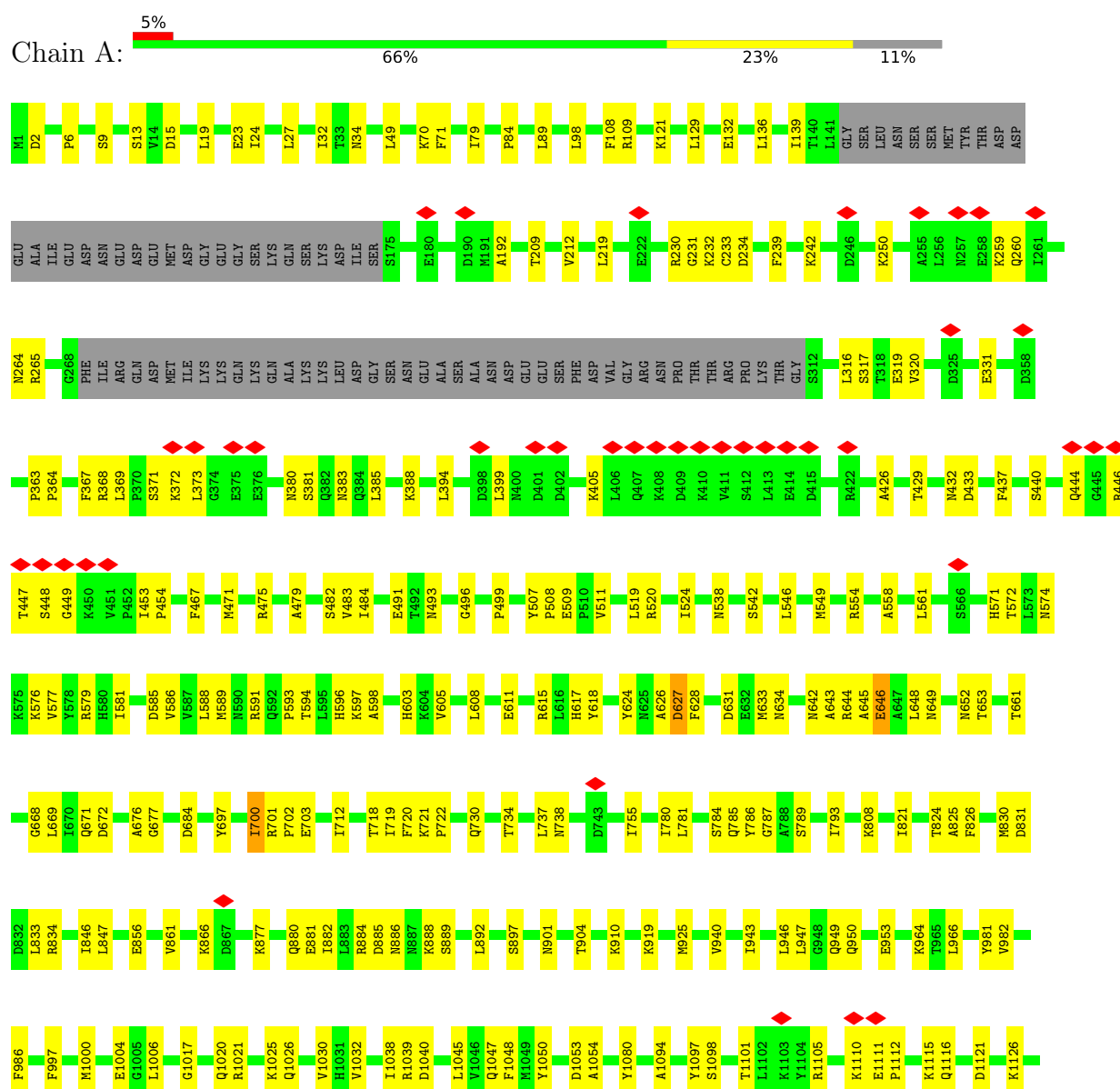
- Molecule 20 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

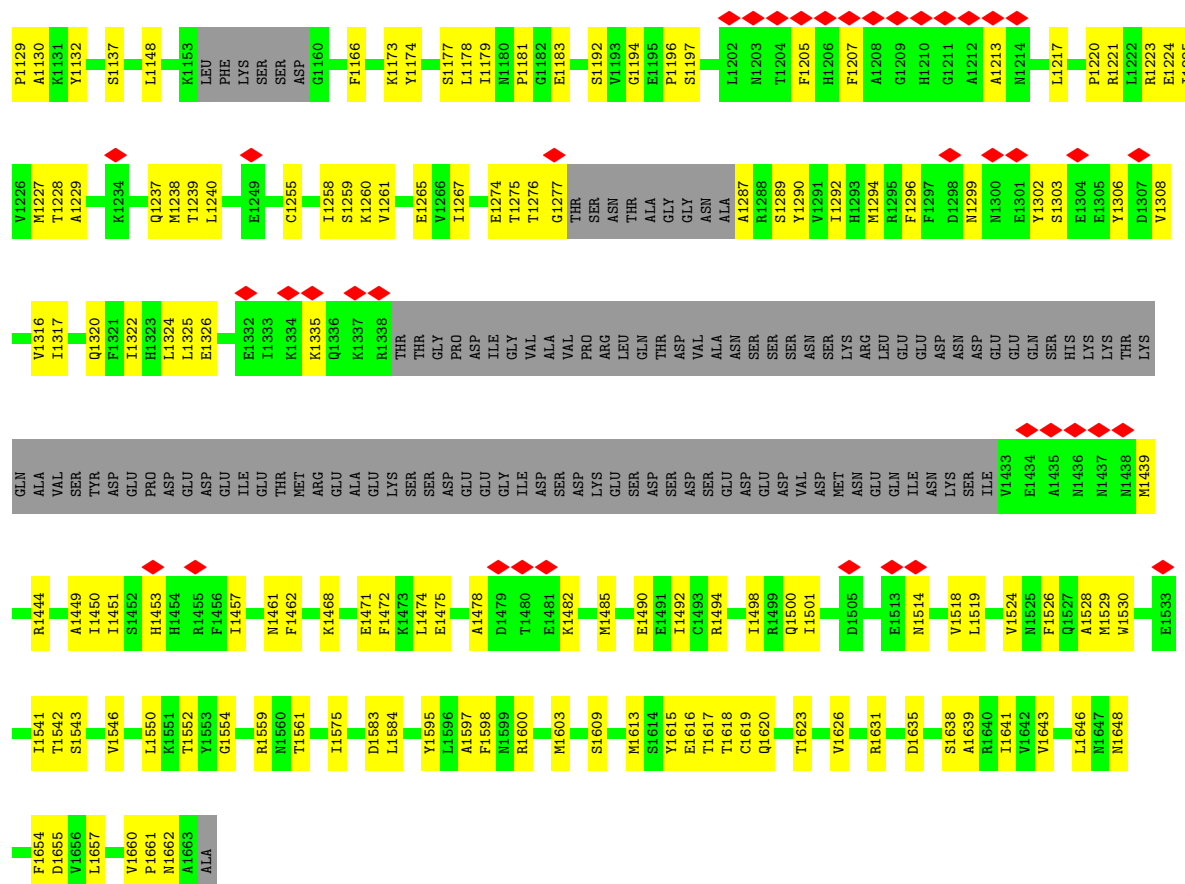


3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

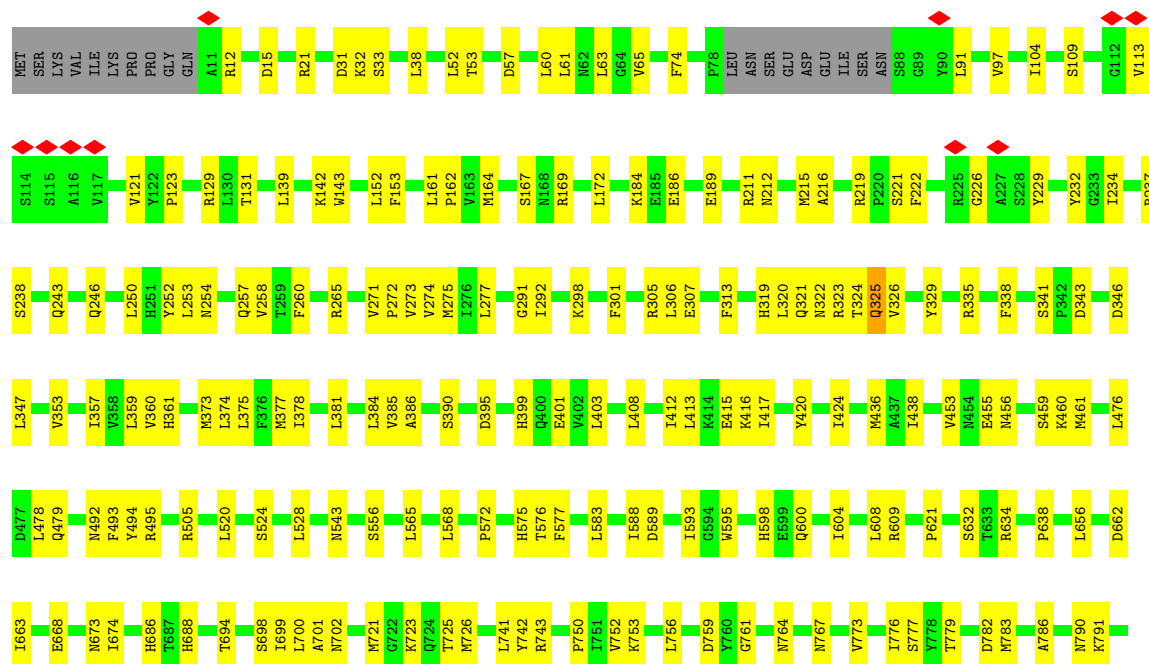
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

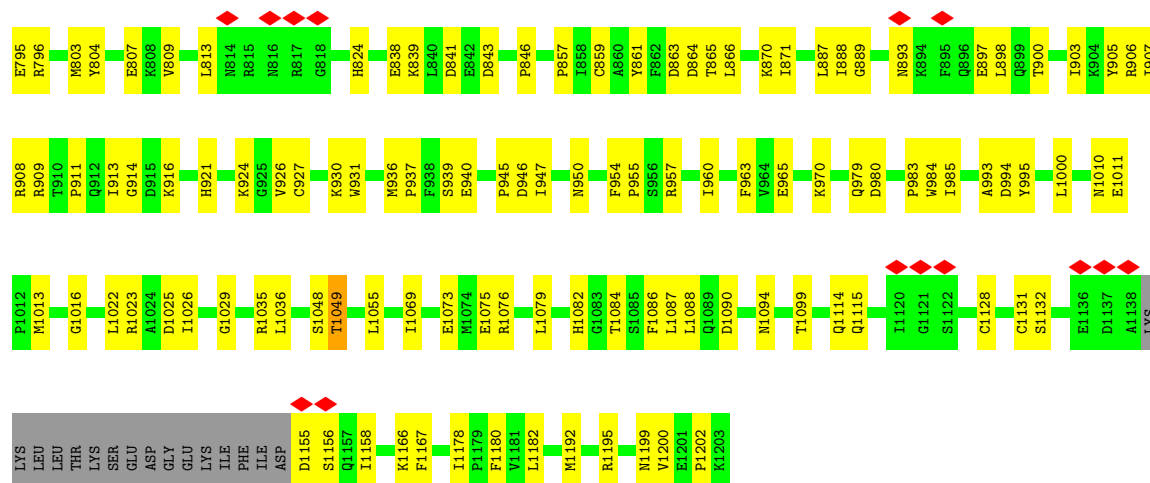




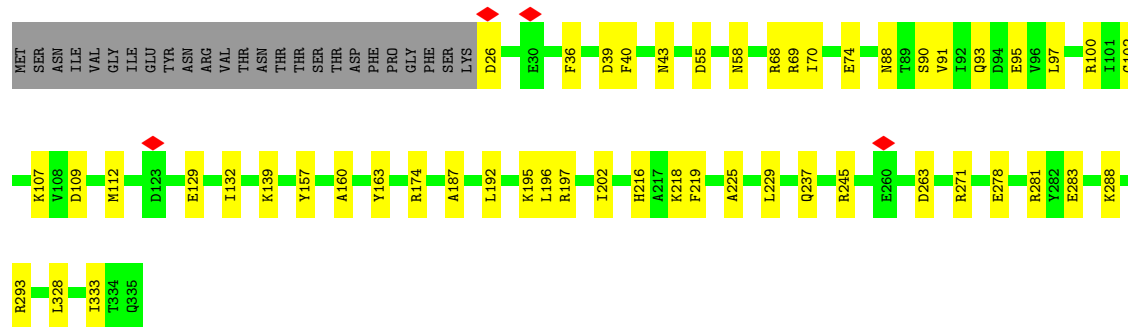
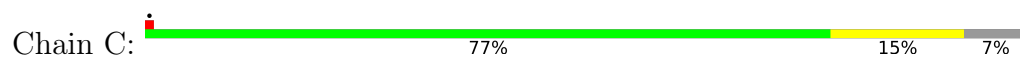
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B: 71% 26%

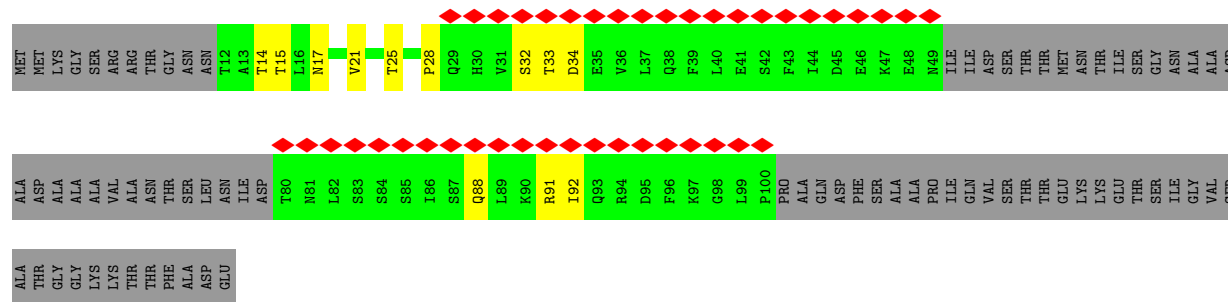
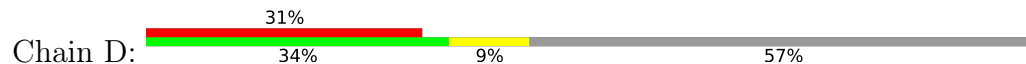




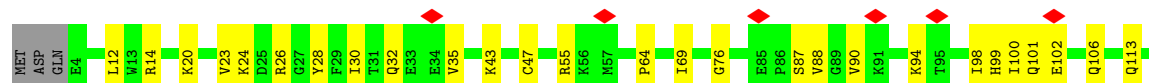
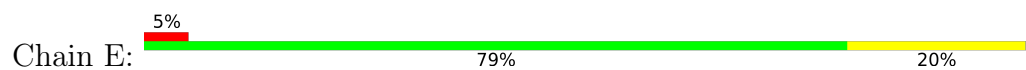
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

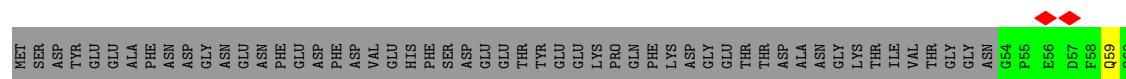


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

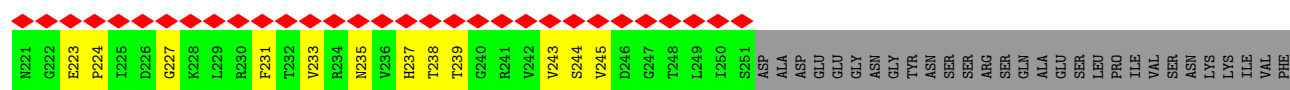
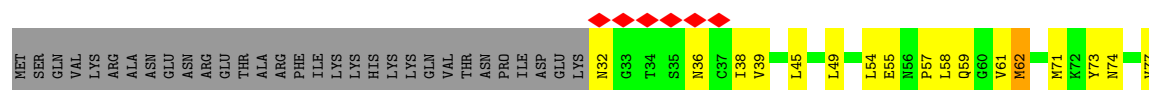
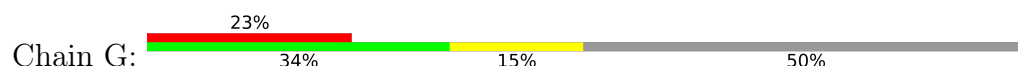




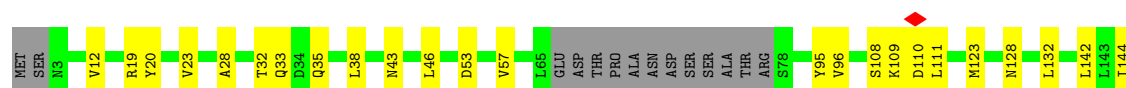
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



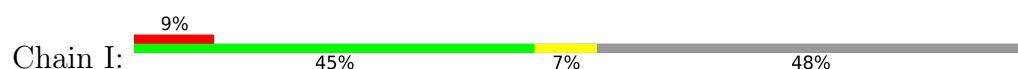
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

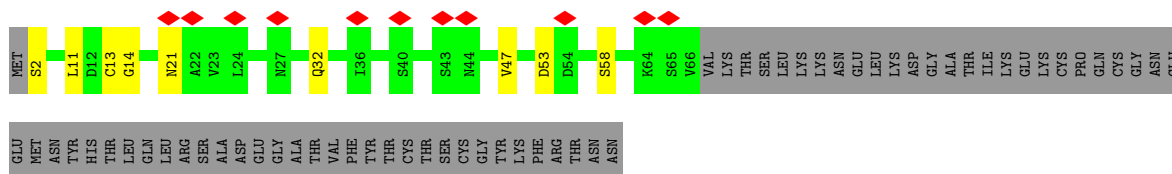


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase I subunit RPA12





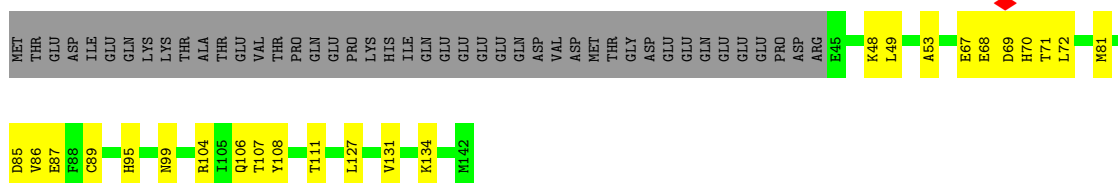
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 63% 36% .



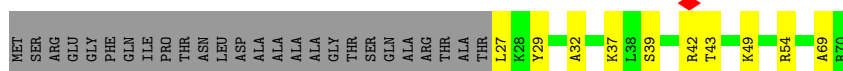
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 52% 17% 31%



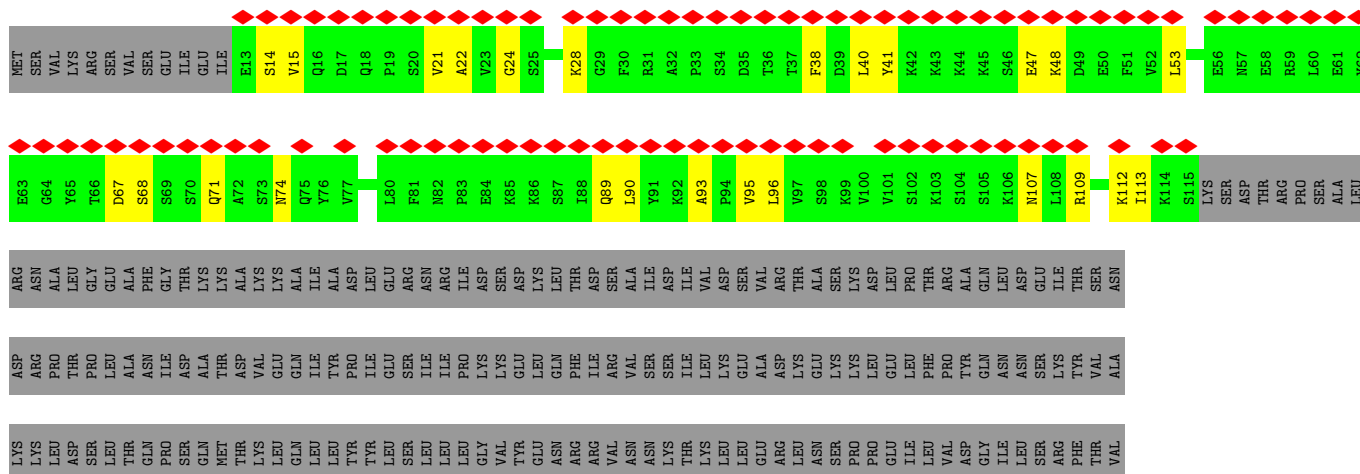
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 49% 14% 37%



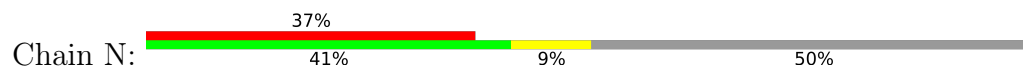
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M: 19% 22% 6% 75%



ILE	LYS	PRO	GLY	GLN	PHE	GLY	ARG	LYS	ASP	ASP	ARG	SER	THR	ALA	GLN	PHE	ASP	ALA	ASP	PRO	GLN	ASN	LYS	ASP	GLU	LEU	ILE	LEU	CYS	TYR	ILE	LEU	ALA	ILE	ILE	MET	HIS	LYS	VAL	PRO	ASN	PHE	LYS	LEU	VAL	ILE	GLU	THR	PRO	LEU	ALA	HIS	GLY	GLY	PRO	SER	LYS	VAL	VAL	SER	LEU	PHE
ARG	VAL	LEU	GLY	ALA	ILE	VAL	LYS	GLY	ALA	THR	VAL	ASP	ALA	GLN	ALA	ASP	GLU	ALA	PHE	GLY	ILE	ASN	PRO	LYS	SER	GLU	PHE	ALA	ALA	SER	TYR	ILE	LYS	ALA	THR	MET	LYS	VAL	PRO	PHE	LYS	LEU	PRO	GLU	MET	THR	ARG	ARG	GLY	GLY	PRO	ARG	ARG									

• Molecule 14: DNA-directed RNA polymerase I subunit RPA34



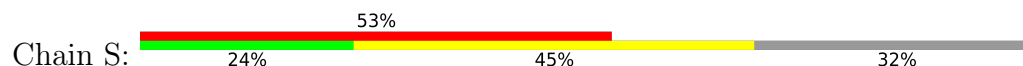
VAL	LYS	GLU	ASN	LYS	GLU	PRO	LYS	LYS	ARG	SER	HIS	HIS	ASP	GLU	GLU	GLU	SER	SER	LYS	LYS	LYS	LYS	GLU	ARG	GLU	LYS	ARG	GLU	LYS	ASP	LYS	LYS	LYS	LYS	HIS	ARG	ASP																						
I121	A122	S123	T124	A125	LYS	ASP	ASN	ALA	P130	L131	Q132	F133	D134	K135	V136	F137	S138	V139	S140	E141	T142	A143	K144	I145	P146	D149	Y150	S151	K152	V153	R154	V155	P156	R157	K158	D159	K162	V163	K167	L168	E169	H170	F171	A172	Y175	ASP	ALA	GLU	ASP	PHE	HIS	VAL	ALA	GLU	GLU				
M61	V62	D63	I64	S65	K66	L67	LYS	SER	LEU	PRO	VAL	ASP	PHE	GLU	GLU	SER	T78	T79	M80	T81	I82	D83	K84	H85	D86	Y87	K88	I89	M90	ASP	THR	ASP	ILE	GLU	SER	SER	LEU	THR	GLN	ASP	ASN	LEU	S105	N106	M107	T108	L109	L110	V111	P112	S113	E114	S115	K116	E117	S118	L119		
MET	SER	LYS	LEU	SER	LYS	ASP	TYR	VAL	LYS	ASP	SER	SER	ASP	GLU	VAL	ILE	SER	ASN	ASN	GLU	PHE	S24	I25	P26	D27	G28	F29	K30	K31	C32	K33	H34	L35	K36	N37	F38	P39	L40	M41	G42	ASP	ASN	LYS	LYS	LYS	ALA	LYS	LYS	GLN	Q51	Q52	V53	W54	L55	I56	K57	F58	P59	S60

• Molecule 15: RNA



A	U2	A3	A4	A5	U6	C7	G8	G12
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• Molecule 16: Non-template DNA



DG	DA	DT	DT	T5	C6	A7	T8	C10	G11	C12	C13	DA	DT	DT	DC	DC	DT	DC	T22	C23	T24	C25	T26	G27	C28	T29	T30	A31	T32	C33	G34	G35	T36	A37	G38
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• Molecule 17: Template DNA



C1	T2	A3	C4	C5	G6	A7	T8	A9	A10	G11	C12	M17	C20	G27	C28	G29	T30	A31	T32	G33	A34	DA	DA	DT	DC
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	207080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.155	Depositor
Minimum map value	-2.798	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.43	Depositor
Map size (\AA)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, 3DR, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.12	0/11879	0.29	0/16045
2	B	0.12	0/9480	0.27	0/12816
3	C	0.10	0/2513	0.24	0/3407
4	D	0.12	0/473	0.42	0/641
5	E	0.11	0/1770	0.27	0/2383
6	F	0.14	0/842	0.31	0/1135
7	G	0.10	0/1288	0.27	0/1755
8	H	0.09	0/1078	0.24	0/1460
9	I	0.08	0/485	0.30	0/657
10	J	0.10	0/578	0.22	0/775
11	K	0.11	0/776	0.28	0/1047
12	L	0.09	0/354	0.21	0/468
13	M	0.06	0/832	0.20	0/1116
14	N	0.08	0/938	0.21	0/1258
15	R	0.11	0/268	0.18	0/416
16	S	0.16	0/585	0.40	0/897
17	T	0.20	0/755	0.38	0/1160
All	All	0.11	0/34894	0.28	0/47436

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	628	PHE	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	11664	0	11740	282	0
2	B	9274	0	9160	216	0
3	C	2461	0	2439	43	0
4	D	467	0	468	8	0
5	E	1734	0	1764	30	0
6	F	827	0	843	19	0
7	G	1258	0	1255	42	0
8	H	1060	0	1032	19	0
9	I	479	0	480	7	0
10	J	569	0	585	18	0
11	K	766	0	765	22	0
12	L	352	0	374	8	0
13	M	816	0	816	21	0
14	N	921	0	956	16	0
15	R	239	0	120	8	0
16	S	526	0	297	16	0
17	T	686	0	381	10	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
20	B	31	0	14	1	0
All	All	34137	0	33489	675	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (675) 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)
1:A:631:ASP:OD1	15:R:12:G:O3'	1.73	1.03
1:A:89:LEU:HD11	2:B:1192:MET:HG2	1.62	0.81
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.65	0.78
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.67	0.76
2:B:694:THR:OG1	2:B:702:ASN:ND2	2.18	0.76
1:A:363:PRO:O	1:A:368:ARG:NH1	2.19	0.76
2:B:273:VAL:HG11	2:B:378:ILE:HD11	1.67	0.76
1:A:49:LEU:O	1:A:368:ARG:NH2	2.19	0.75
5:E:124:VAL:HG23	5:E:125:PRO:HD3	1.69	0.74
1:A:1662:ASN:HD21	7:G:103:LYS:HD2	1.52	0.74
2:B:741:LEU:HB2	2:B:804:TYR:HB2	1.70	0.73
1:A:1439:MET:HE2	1:A:1461:ASN:HD22	1.53	0.72
5:E:20:LYS:HB3	5:E:35:VAL:HG22	1.72	0.72
3:C:109:ASP:HB3	3:C:112:MET:HG3	1.72	0.72
5:E:101:GLN:N	5:E:101:GLN:OE1	2.22	0.72
7:G:111:THR:HG22	7:G:113:PHE:H	1.55	0.71
3:C:237:GLN:HB2	3:C:288:LYS:HG3	1.73	0.70
2:B:1156:SER:H	7:G:238:THR:HG23	1.57	0.70
5:E:180:ARG:HD2	5:E:192:ARG:HG3	1.72	0.70
2:B:492:ASN:ND2	2:B:767:ASN:OD1	2.24	0.70
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.23	0.69
3:C:43:ASN:HB3	3:C:55:ASP:HB2	1.74	0.69
1:A:1662:ASN:HB3	7:G:57:PRO:HG2	1.74	0.69
4:D:88:GLN:HA	4:D:91:ARG:HE	1.58	0.69
1:A:1662:ASN:HB2	7:G:58:LEU:HD23	1.74	0.68
16:S:37:DA:H61	17:T:2:DT:H3	1.42	0.68
2:B:494:TYR:HB3	2:B:700:LEU:HD21	1.76	0.68
1:A:634:ASN:HD22	2:B:1069:ILE:HD12	1.59	0.68
1:A:1635:ASP:O	1:A:1648:ASN:ND2	2.25	0.68
1:A:2:ASP:OD1	1:A:576:LYS:NZ	2.26	0.67
1:A:919:LYS:HD2	8:H:19:ARG:HH21	1.59	0.67
2:B:911:PRO:O	2:B:930:LYS:NZ	2.23	0.67
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.77	0.67
2:B:415:GLU:HG3	2:B:476:LEU:HD21	1.75	0.67
2:B:424:ILE:HG22	2:B:453:VAL:HG11	1.75	0.67
14:N:53:VAL:HG23	14:N:133:PHE:HA	1.75	0.67
2:B:413:LEU:HD13	2:B:461:MET:HE2	1.76	0.66
7:G:238:THR:HB	7:G:243:VAL:HG23	1.77	0.66
1:A:265:ARG:O	1:A:265:ARG:NH1	2.28	0.66
13:M:112:LYS:HG2	13:M:113:ILE:HG13	1.76	0.66
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.78	0.66
3:C:129:GLU:OE2	3:C:129:GLU:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14:SER:HB3	13:M:89:GLN:HE22	1.62	0.65
1:A:671:GLN:NE2	2:B:783:MET:O	2.30	0.65
1:A:846:ILE:HD11	1:A:910:LYS:HD3	1.78	0.65
2:B:970:LYS:HG2	2:B:1000:LEU:HD21	1.79	0.64
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.14	0.64
11:K:127:LEU:O	11:K:131:VAL:HG23	1.98	0.64
1:A:1238:MET:HA	1:A:1543:SER:HA	1.80	0.64
1:A:448:SER:HB3	16:S:13:DC:H2''	1.80	0.64
1:A:484:ILE:HD13	1:A:633:MET:HE3	1.79	0.64
2:B:186:GLU:HB2	2:B:189:GLU:HB2	1.78	0.63
2:B:274:VAL:HG11	2:B:313:PHE:HB2	1.80	0.63
1:A:721:LYS:HG3	1:A:722:PRO:HA	1.81	0.63
1:A:524:ILE:O	1:A:554:ARG:NH1	2.32	0.63
2:B:97:VAL:HG11	2:B:424:ILE:HD11	1.81	0.62
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	1.82	0.62
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.82	0.61
1:A:1616:GLU:HG3	1:A:1617:THR:HG23	1.82	0.61
12:L:42:ARG:HG3	12:L:43:THR:HG23	1.82	0.61
1:A:108:PHE:N	1:A:331:GLU:OE2	2.30	0.61
1:A:446:ARG:HE	1:A:449:GLY:HA3	1.65	0.61
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.83	0.61
11:K:81:MET:HE3	11:K:89:CYS:HB3	1.83	0.61
16:S:25:DC:H2'	16:S:26:DT:C6	2.35	0.61
1:A:369:LEU:O	1:A:380:ASN:ND2	2.34	0.61
16:S:34:DG:H2'	16:S:35:DG:C8	2.36	0.61
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.83	0.61
2:B:53:THR:OG1	2:B:169:ARG:NH1	2.34	0.60
1:A:1223:ARG:HA	1:A:1227:MET:HG2	1.83	0.60
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.29	0.60
7:G:235:ASN:OD1	7:G:237:HIS:NE2	2.34	0.60
2:B:74:PHE:HB3	2:B:91:LEU:HB3	1.84	0.60
17:T:28:DC:H2''	17:T:29:DG:H2'	1.82	0.60
14:N:59:PRO:HD3	14:N:139:VAL:HB	1.83	0.60
3:C:100:ARG:NH2	3:C:192:LEU:O	2.33	0.60
2:B:321:GLN:O	9:I:32:GLN:NE2	2.33	0.60
1:A:1194:GLY:O	1:A:1197:SER:OG	2.19	0.60
1:A:109:ARG:HE	1:A:231:GLY:HA2	1.67	0.60
1:A:1101:THR:O	1:A:1105:ARG:HG3	2.02	0.60
2:B:662:ASP:OD1	2:B:663:ILE:N	2.35	0.60
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.29	0.60
2:B:32:LYS:NZ	2:B:33:SER:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.83	0.59
1:A:1609:SER:O	1:A:1613:MET:HG3	2.03	0.59
2:B:21:ARG:NH2	10:J:53:HIS:O	2.36	0.59
11:K:67:GLU:HA	11:K:99:ASN:HB2	1.83	0.59
2:B:721:MET:HE1	2:B:924:LYS:HE3	1.84	0.59
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.85	0.59
1:A:1275:THR:HG22	1:A:1277:GLY:H	1.67	0.58
2:B:803:MET:HB3	2:B:907:ILE:HB	1.85	0.58
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.85	0.58
1:A:364:PRO:HD2	1:A:367:PHE:HD2	1.69	0.58
1:A:1482:LYS:HD3	2:B:307:GLU:HG2	1.84	0.58
2:B:752:VAL:HG11	2:B:965:GLU:HG3	1.84	0.58
8:H:12:VAL:HG22	8:H:53:ASP:H	1.68	0.58
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.86	0.58
1:A:1317:ILE:HD12	1:A:1462:PHE:HE2	1.69	0.58
2:B:889:GLY:HA3	12:L:54:ARG:HB3	1.86	0.58
2:B:1132:SER:HB2	2:B:1167:PHE:HB3	1.86	0.58
1:A:721:LYS:HB3	8:H:96:VAL:HG12	1.86	0.58
6:F:99:LEU:HD13	7:G:112:PRO:HD3	1.86	0.58
1:A:264:ASN:OD1	1:A:265:ARG:N	2.37	0.57
1:A:1296:PHE:HZ	1:A:1317:ILE:HD11	1.68	0.57
2:B:359:LEU:HD11	2:B:373:MET:HG2	1.86	0.57
2:B:1016:GLY:O	3:C:69:ARG:NH1	2.36	0.57
1:A:897:SER:O	1:A:901:ASN:ND2	2.38	0.57
2:B:568:LEU:HD13	2:B:604:ILE:HG23	1.86	0.57
13:M:21:VAL:HG23	13:M:93:ALA:HB2	1.86	0.57
2:B:600:GLN:O	2:B:604:ILE:HG13	2.04	0.57
2:B:756:LEU:HA	2:B:759:ASP:HB2	1.87	0.57
3:C:88:ASN:ND2	3:C:90:SER:OG	2.37	0.57
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.85	0.57
2:B:123:PRO:HG2	2:B:172:LEU:HD11	1.86	0.57
14:N:159:ASP:OD1	14:N:159:ASP:N	2.38	0.57
2:B:906:ARG:NE	3:C:95:GLU:OE2	2.35	0.57
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.85	0.57
2:B:222:PHE:O	2:B:226:GLY:HA3	2.03	0.57
2:B:824:HIS:ND1	2:B:897:GLU:OE1	2.37	0.57
1:A:661:THR:HA	1:A:1192:SER:HB2	1.87	0.57
1:A:1260:LYS:HD2	1:A:1500:GLN:HG3	1.86	0.57
2:B:104:ILE:HD12	2:B:161:LEU:HD23	1.86	0.57
2:B:215:MET:HE1	2:B:399:HIS:HB3	1.84	0.57
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:85:ASP:OD2	11:K:111:THR:OG1	2.20	0.57
1:A:718:THR:HG23	1:A:719:ILE:HG13	1.87	0.57
1:A:546:LEU:HA	1:A:549:MET:HG3	1.87	0.56
1:A:1258:ILE:HG12	1:A:1529:MET:HE1	1.87	0.56
2:B:985:ILE:O	14:N:157:ARG:NH1	2.38	0.56
7:G:49:LEU:HD13	7:G:61:VAL:HG23	1.86	0.56
11:K:104:ARG:NH1	11:K:106:GLN:OE1	2.38	0.56
9:I:13:CYS:SG	9:I:14:GLY:N	2.79	0.56
16:S:34:DG:H2'	16:S:35:DG:H8	1.69	0.56
1:A:591:ARG:HB2	1:A:633:MET:HE2	1.87	0.56
13:M:38:PHE:HB2	14:N:119:LEU:HB2	1.85	0.56
1:A:1296:PHE:O	1:A:1468:LYS:NZ	2.33	0.56
2:B:995:TYR:O	14:N:162:LYS:NZ	2.38	0.56
16:S:37:DA:N6	17:T:2:DT:H3	2.02	0.56
13:M:68:SER:HA	13:M:71:GLN:HG2	1.87	0.56
16:S:36:DT:H2''	16:S:37:DA:C8	2.41	0.56
1:A:388:LYS:HG3	1:A:433:ASP:OD2	2.06	0.56
1:A:1449:ALA:O	1:A:1453:HIS:ND1	2.38	0.56
2:B:970:LYS:NZ	2:B:1011:GLU:OE1	2.37	0.56
4:D:25:THR:OG1	6:F:59:GLN:NE2	2.38	0.56
1:A:475:ARG:NH1	17:T:20:DC:OP1	2.38	0.56
1:A:1559:ARG:NH1	1:A:1583:ASP:OD1	2.39	0.56
2:B:479:GLN:N	2:B:479:GLN:OE1	2.39	0.56
3:C:229:LEU:O	3:C:293:ARG:NH1	2.40	0.55
13:M:14:SER:O	13:M:89:GLN:NE2	2.40	0.55
2:B:888:ILE:HB	2:B:900:THR:HG23	1.87	0.55
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.88	0.55
13:M:22:ALA:HB1	13:M:96:LEU:HD11	1.88	0.55
1:A:668:GLY:HA3	1:A:787:GLY:HA2	1.88	0.55
1:A:1111:GLU:HB3	1:A:1116:GLN:HG3	1.89	0.55
1:A:1265:GLU:HA	9:I:58:SER:HB3	1.87	0.55
2:B:292:ILE:HD13	2:B:378:ILE:HG21	1.88	0.55
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.89	0.55
1:A:697:TYR:OH	1:A:703:GLU:OE2	2.24	0.55
1:A:1322:ILE:O	1:A:1326:GLU:HG2	2.06	0.55
2:B:104:ILE:HG23	2:B:169:ARG:HG3	1.89	0.55
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.88	0.55
7:G:71:MET:HE3	7:G:71:MET:HA	1.88	0.55
2:B:565:LEU:HD21	2:B:608:LEU:HD11	1.90	0.54
1:A:1137:SER:OG	1:A:1174:TYR:OH	2.25	0.54
2:B:857:PRO:HB3	2:B:871:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLN:O	1:A:734:THR:HG22	2.07	0.54
1:A:230:ARG:NH2	1:A:234:ASP:OD1	2.40	0.54
1:A:1000:MET:O	1:A:1004:GLU:HG2	2.06	0.54
2:B:916:LYS:HE2	2:B:1036:LEU:HD12	1.89	0.54
1:A:1290:TYR:HB2	1:A:1474:LEU:HB3	1.89	0.54
3:C:283:GLU:N	3:C:283:GLU:OE2	2.41	0.54
13:M:15:VAL:HA	13:M:90:LEU:HB3	1.90	0.54
1:A:15:ASP:N	1:A:15:ASP:OD1	2.40	0.54
2:B:1079:LEU:O	2:B:1084:THR:OG1	2.25	0.54
1:A:593:PRO:HG3	20:B:3002:APC:H2	1.90	0.54
7:G:233:VAL:HG12	7:G:245:VAL:HG11	1.89	0.54
11:K:68:GLU:N	11:K:68:GLU:OE1	2.41	0.54
14:N:144:LYS:HE2	14:N:146:PRO:HG3	1.90	0.54
1:A:1000:MET:HG2	2:B:520:LEU:HD22	1.90	0.54
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.40	0.54
3:C:333:ILE:HD11	11:K:49:LEU:HB2	1.88	0.54
1:A:1274:GLU:HB3	9:I:47:VAL:HG22	1.90	0.53
2:B:390:SER:OG	2:B:634:ARG:O	2.26	0.53
11:K:81:MET:HE2	11:K:81:MET:HA	1.89	0.53
2:B:743:ARG:HH21	3:C:93:GLN:NE2	2.06	0.53
1:A:617:HIS:CD2	1:A:618:TYR:H	2.27	0.53
1:A:831:ASP:N	1:A:831:ASP:OD1	2.41	0.53
1:A:1039:ARG:HB3	1:A:1045:LEU:HD12	1.91	0.53
1:A:1112:PRO:HG2	1:A:1115:LYS:HD2	1.90	0.53
7:G:237:HIS:N	7:G:244:SER:O	2.37	0.53
1:A:722:PRO:HD2	8:H:46:LEU:HD23	1.91	0.53
1:A:877:LYS:O	1:A:881:GLU:HG3	2.08	0.53
1:A:885:ASP:OD1	1:A:886:ASN:N	2.42	0.53
7:G:74:ASN:HB3	7:G:77:VAL:HG12	1.91	0.53
1:A:645:ALA:O	1:A:649:ASN:ND2	2.41	0.53
1:A:1289:SER:HA	1:A:1475:GLU:HA	1.90	0.53
1:A:109:ARG:HG2	1:A:233:CYS:HB2	1.90	0.52
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.34	0.52
2:B:216:ALA:HB1	2:B:384:LEU:HD13	1.90	0.52
11:K:69:ASP:OD1	11:K:69:ASP:N	2.41	0.52
1:A:1439:MET:HB3	1:A:1444:ARG:HH21	1.74	0.52
6:F:133:VAL:HG22	6:F:147:SER:HB2	1.91	0.52
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.90	0.52
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.82	0.52
2:B:320:LEU:HD13	2:B:326:VAL:HG23	1.91	0.52
3:C:70:ILE:HG23	3:C:74:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:128:ASN:H	8:H:132:LEU:HD13	1.74	0.52
1:A:1177:SER:O	1:A:1177:SER:OG	2.23	0.52
6:F:82:THR:HG22	6:F:84:TYR:H	1.74	0.52
8:H:53:ASP:OD2	8:H:146:ARG:NH2	2.42	0.52
1:A:1239:THR:N	1:A:1542:THR:O	2.40	0.52
2:B:319:HIS:O	2:B:321:GLN:NE2	2.43	0.52
7:G:149:ILE:HD12	7:G:153:PHE:HD2	1.75	0.52
2:B:234:ILE:HG13	2:B:381:LEU:HB2	1.92	0.52
2:B:320:LEU:HD11	2:B:329:TYR:HD2	1.75	0.52
17:T:29:DG:H4'	17:T:30:DT:OP1	2.10	0.52
1:A:34:ASN:OD1	1:A:34:ASN:N	2.43	0.51
1:A:1129:PRO:HB2	1:A:1178:LEU:HD11	1.93	0.51
2:B:936:MET:HG3	2:B:937:PRO:HD2	1.93	0.51
16:S:5:DT:OP1	16:S:6:DC:N4	2.44	0.51
1:A:1038:ILE:HG12	1:A:1047:GLN:HB2	1.92	0.51
2:B:57:ASP:HB3	2:B:63:LEU:HD21	1.92	0.51
2:B:420:TYR:O	2:B:424:ILE:HG23	2.10	0.51
2:B:865:THR:OG1	2:B:866:LEU:HD22	2.10	0.51
1:A:381:SER:HB3	1:A:453:ILE:HG23	1.93	0.51
3:C:102:GLY:HA3	12:L:69:ALA:HB1	1.93	0.51
7:G:62:MET:HE2	7:G:84:TYR:HE2	1.76	0.51
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.75	0.51
2:B:1128:CYS:HB3	2:B:1131:CYS:HB2	1.92	0.51
2:B:773:VAL:HG23	2:B:947:ILE:HG22	1.93	0.51
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.93	0.51
1:A:1600:ARG:HA	1:A:1603:MET:HB3	1.92	0.51
2:B:750:PRO:HG2	2:B:753:LYS:HB3	1.93	0.51
2:B:807:GLU:OE2	2:B:905:TYR:OH	2.28	0.51
11:K:53:ALA:O	11:K:104:ARG:NH2	2.43	0.51
14:N:149:ASP:HB3	14:N:152:LYS:HG2	1.93	0.51
1:A:588:LEU:HD11	2:B:1087:LEU:HD22	1.93	0.51
2:B:211:ARG:HH12	2:B:243:GLN:HE22	1.58	0.51
7:G:85:GLU:HG2	7:G:123:TYR:HE2	1.76	0.51
7:G:237:HIS:O	7:G:244:SER:N	2.33	0.51
1:A:1020:GLN:HG3	1:A:1194:GLY:HA3	1.94	0.50
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.93	0.50
1:A:1641:ILE:HD11	2:B:1088:LEU:HD21	1.92	0.50
2:B:1114:GLN:NE2	2:B:1115:GLN:O	2.40	0.50
5:E:12:LEU:HD21	5:E:55:ARG:HH21	1.76	0.50
1:A:1213:ALA:HB1	1:A:1237:GLN:HE22	1.77	0.50
7:G:148:LEU:HB3	7:G:151:ASP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.92	0.50
1:A:949:GLN:NE2	1:A:950:GLN:O	2.44	0.50
2:B:142:LYS:HG3	2:B:153:PHE:HE1	1.77	0.50
2:B:164:MET:O	2:B:167:SER:OG	2.29	0.50
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.92	0.50
17:T:6:DG:H2"	17:T:7:DA:C8	2.47	0.50
1:A:519:LEU:HD13	1:A:577:VAL:HB	1.94	0.50
1:A:925:MET:HG3	1:A:940:VAL:HG22	1.93	0.50
13:M:107:ASN:OD1	13:M:109:ARG:NH2	2.43	0.50
1:A:479:ALA:HB1	2:B:1069:ILE:HD11	1.93	0.50
2:B:576:THR:HG21	2:B:595:TRP:CD1	2.46	0.50
10:J:7:CYS:HA	10:J:49:MET:HE2	1.92	0.50
1:A:642:ASN:O	1:A:646:GLU:HB3	2.11	0.50
1:A:1306:TYR:HB2	1:A:1308:VAL:HG12	1.93	0.50
7:G:223:GLU:HG2	7:G:224:PRO:HD2	1.93	0.50
1:A:1255:CYS:O	1:A:1259:SER:OG	2.24	0.50
2:B:61:LEU:O	2:B:65:VAL:HG22	2.12	0.50
1:A:861:VAL:HG11	1:A:892:LEU:HB2	1.94	0.50
1:A:943:ILE:HD13	2:B:960:ILE:HD11	1.93	0.50
7:G:137:ILE:HG12	7:G:227:GLY:HA2	1.94	0.50
1:A:1094:ALA:O	1:A:1098:SER:OG	2.27	0.49
3:C:163:TYR:OH	10:J:19:GLU:OE1	2.25	0.49
1:A:949:GLN:HA	1:A:981:TYR:HA	1.93	0.49
1:A:1240:LEU:HB2	1:A:1519:LEU:HB3	1.94	0.49
2:B:234:ILE:HG22	2:B:377:MET:HE3	1.94	0.49
2:B:725:THR:OG1	2:B:767:ASN:ND2	2.45	0.49
3:C:174:ARG:HG3	3:C:174:ARG:HH11	1.77	0.49
1:A:901:ASN:HA	1:A:904:THR:HG22	1.95	0.49
2:B:238:SER:OG	2:B:361:HIS:ND1	2.35	0.49
1:A:380:ASN:HB3	1:A:383:ASN:HB2	1.93	0.49
1:A:755:ILE:HD13	1:A:780:ILE:HD11	1.95	0.49
1:A:882:ILE:HG12	1:A:888:LYS:HB3	1.94	0.49
5:E:99:HIS:HA	5:E:102:GLU:HB2	1.93	0.49
8:H:23:VAL:HA	8:H:43:ASN:HA	1.94	0.49
1:A:209:THR:H	1:A:212:VAL:HG22	1.78	0.49
1:A:1038:ILE:HD11	1:A:1584:LEU:HD13	1.95	0.49
1:A:1238:MET:HE3	1:A:1524:VAL:HA	1.94	0.49
2:B:219:ARG:HG2	2:B:221:SER:H	1.77	0.49
6:F:140:ASP:OD1	6:F:141:GLY:N	2.45	0.49
11:K:71:THR:OG1	11:K:72:LEU:N	2.45	0.49
1:A:594:THR:HG21	2:B:1075:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:PRO:HB3	1:A:1575:ILE:HG21	1.94	0.49
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.93	0.49
1:A:260:GLN:N	1:A:260:GLN:OE1	2.46	0.49
1:A:684:ASP:HB2	8:H:20:TYR:HD1	1.78	0.49
1:A:830:MET:HE2	2:B:993:ALA:HB2	1.94	0.49
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.94	0.49
2:B:212:ASN:ND2	2:B:589:ASP:OD1	2.45	0.48
1:A:781:LEU:HD22	1:A:785:GLN:HG3	1.95	0.48
1:A:1111:GLU:O	1:A:1116:GLN:NE2	2.46	0.48
8:H:108:SER:OG	8:H:109:LYS:N	2.45	0.48
2:B:572:PRO:HG3	13:M:74:ASN:HD21	1.78	0.48
4:D:14:THR:OG1	4:D:15:THR:N	2.46	0.48
1:A:129:LEU:HB3	1:A:132:GLU:HB2	1.95	0.48
1:A:880:GLN:HE22	2:B:632:SER:HB2	1.79	0.48
1:A:1121:ASP:OD1	1:A:1121:ASP:N	2.46	0.48
2:B:495:ARG:HD2	2:B:723:LYS:HB3	1.95	0.48
5:E:177:ARG:HD2	5:E:215:MET:HB3	1.95	0.48
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.95	0.48
14:N:24:SER:O	14:N:24:SER:OG	2.31	0.48
1:A:1299:ASN:HA	1:A:1302:TYR:CD2	2.48	0.48
2:B:699:ILE:O	2:B:700:LEU:HB2	2.14	0.48
10:J:32:GLU:OE1	10:J:32:GLU:N	2.31	0.48
2:B:861:TYR:CZ	2:B:870:LYS:HB2	2.48	0.48
13:M:40:LEU:HB2	14:N:119:LEU:HD21	1.95	0.48
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.94	0.48
14:N:115:SER:O	14:N:116:LYS:HG2	2.13	0.48
1:A:672:ASP:OD2	2:B:950:ASN:ND2	2.34	0.48
6:F:149:GLU:OE2	6:F:149:GLU:N	2.46	0.48
8:H:35:GLN:N	8:H:35:GLN:OE1	2.46	0.48
1:A:482:SER:OG	1:A:483:VAL:N	2.46	0.48
1:A:597:LYS:HD2	2:B:1082:HIS:ND1	2.29	0.48
1:A:1490:GLU:OE1	1:A:1494:ARG:NH2	2.46	0.48
1:A:1641:ILE:HD13	2:B:1076:ARG:HD2	1.96	0.48
1:A:833:LEU:HD22	1:A:943:ILE:HG21	1.95	0.47
1:A:833:LEU:HD11	2:B:963:PHE:HD2	1.79	0.47
1:A:1526:PHE:CD1	1:A:1552:THR:HG21	2.48	0.47
2:B:598:HIS:HE1	2:B:638:PRO:HB2	1.79	0.47
2:B:796:ARG:NH1	10:J:8:PHE:O	2.44	0.47
1:A:121:LYS:HD3	1:A:219:LEU:HD11	1.95	0.47
1:A:373:LEU:HD12	15:R:3:A:N7	2.29	0.47
1:A:1623:THR:HA	1:A:1626:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1158:ILE:HD11	2:B:1166:LYS:HB3	1.95	0.47
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.47	0.47
1:A:1287:ALA:HB3	1:A:1478:ALA:HB2	1.96	0.47
2:B:939:SER:OG	2:B:940:GLU:N	2.46	0.47
1:A:1026:GLN:HB2	1:A:1598:PHE:HD1	1.79	0.47
2:B:1099:THR:HG21	2:B:1180:PHE:HD2	1.78	0.47
9:I:2:SER:HB3	9:I:11:LEU:HG	1.95	0.47
1:A:947:LEU:HB3	1:A:982:VAL:HG23	1.97	0.47
2:B:258:VAL:HG23	2:B:273:VAL:HB	1.97	0.47
6:F:135:ARG:NH2	7:G:92:ALA:O	2.39	0.47
1:A:1017:GLY:HA3	17:T:17:3DR:H1'1	1.96	0.47
17:T:8:DT:H2''	17:T:9:DA:C8	2.49	0.47
17:T:32:DT:H2''	17:T:33:DG:N7	2.30	0.47
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.80	0.47
1:A:701:ARG:HG2	1:A:703:GLU:OE1	2.14	0.47
1:A:1045:LEU:HD22	5:E:170:LEU:HD11	1.96	0.47
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.96	0.47
2:B:887:LEU:HD11	12:L:29:TYR:CE1	2.50	0.47
2:B:1155:ASP:HA	7:G:239:THR:HG22	1.96	0.47
5:E:90:VAL:HG12	5:E:94:LYS:HE3	1.97	0.47
1:A:1613:MET:HB3	1:A:1618:THR:HG23	1.96	0.47
2:B:184:LYS:NZ	12:L:32:ALA:O	2.45	0.47
3:C:69:ARG:HE	11:K:71:THR:HG22	1.79	0.47
6:F:118:LEU:O	6:F:122:MET:HG3	2.15	0.47
1:A:1320:GLN:HE21	1:A:1324:LEU:HD11	1.80	0.47
1:A:1299:ASN:O	1:A:1303:SER:OG	2.28	0.47
2:B:139:LEU:HD21	2:B:417:ILE:HG12	1.97	0.47
2:B:292:ILE:HD12	2:B:306:LEU:HD11	1.97	0.47
15:R:6:U:H2'	15:R:7:C:C6	2.50	0.47
6:F:135:ARG:HH22	7:G:92:ALA:C	2.23	0.46
16:S:32:DT:H2''	16:S:33:DC:C5	2.50	0.46
1:A:6:PRO:HB3	7:G:111:THR:HG21	1.96	0.46
1:A:720:PHE:HB2	8:H:96:VAL:HG13	1.97	0.46
1:A:1130:ALA:HB1	6:F:82:THR:HG23	1.97	0.46
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.43	0.46
7:G:45:LEU:H	7:G:45:LEU:HD23	1.81	0.46
1:A:997:PHE:HD1	1:A:1000:MET:HE3	1.81	0.46
6:F:140:ASP:OD1	6:F:142:SER:OG	2.34	0.46
2:B:161:LEU:HD12	2:B:162:PRO:HD2	1.98	0.46
2:B:246:GLN:HB3	2:B:360:VAL:HG21	1.97	0.46
1:A:1181:PRO:HD2	6:F:86:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:OE1	2:B:1086:PHE:HB2	2.16	0.46
1:A:1030:VAL:HA	1:A:1040:ASP:HA	1.98	0.46
3:C:40:PHE:CZ	11:K:131:VAL:HG13	2.51	0.46
2:B:250:LEU:HD22	2:B:377:MET:HB3	1.97	0.46
2:B:773:VAL:N	2:B:1029:GLY:O	2.47	0.46
2:B:838:GLU:HG3	2:B:839:LYS:HG2	1.97	0.46
2:B:846:PRO:HG3	2:B:903:ILE:HD13	1.97	0.46
2:B:945:PRO:HD3	2:B:1013:MET:HE1	1.97	0.46
1:A:1316:VAL:HG11	1:A:1498:ILE:HG12	1.98	0.46
2:B:253:LEU:HD13	2:B:257:GLN:HE21	1.80	0.46
11:K:86:VAL:HA	11:K:107:THR:HA	1.96	0.46
13:M:15:VAL:HG12	13:M:90:LEU:HD13	1.98	0.46
1:A:372:LYS:HG3	1:A:373:LEU:O	2.15	0.46
1:A:467:PHE:HA	1:A:471:MET:CE	2.46	0.46
1:A:538:ASN:HB2	1:A:542:SER:HB2	1.98	0.46
1:A:1179:ILE:HD11	1:A:1183:GLU:HG2	1.99	0.46
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.47	0.46
2:B:575:HIS:CD2	13:M:95:VAL:HG11	2.50	0.45
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.85	0.45
1:A:1205:PHE:HE1	1:A:1217:LEU:HD12	1.81	0.45
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.51	0.45
2:B:913:ILE:HG22	2:B:927:CYS:SG	2.56	0.45
1:A:467:PHE:HA	1:A:471:MET:HE3	1.98	0.45
1:A:1220:PRO:O	1:A:1224:GLU:HG3	2.16	0.45
1:A:1530:TRP:O	5:E:14:ARG:NH2	2.48	0.45
2:B:113:VAL:HG13	2:B:893:ASN:HB2	1.98	0.45
2:B:1079:LEU:HD12	2:B:1079:LEU:HA	1.82	0.45
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.44	0.45
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.99	0.45
1:A:259:LYS:HD2	1:A:259:LYS:HA	1.78	0.45
1:A:1221:ARG:HG3	1:A:1225:ILE:HD12	1.98	0.45
2:B:416:LYS:HA	2:B:416:LYS:HD3	1.78	0.45
2:B:556:SER:HB3	2:B:621:PRO:HG3	1.98	0.45
3:C:55:ASP:OD1	3:C:271:ARG:NH1	2.49	0.45
1:A:23:GLU:O	1:A:27:LEU:N	2.44	0.45
1:A:1550:LEU:HD13	1:A:1595:TYR:HB2	1.99	0.45
16:S:27:DG:H2'	16:S:28:DC:C6	2.52	0.45
4:D:17:ASN:OD1	4:D:17:ASN:N	2.50	0.45
16:S:35:DG:H2'	16:S:36:DT:C6	2.51	0.45
1:A:493:ASN:HA	1:A:653:THR:HG21	1.99	0.45
1:A:856:GLU:O	1:A:866:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1657:LEU:HD13	7:G:106:LYS:HA	1.99	0.45
3:C:197:ARG:HD3	3:C:197:ARG:HA	1.65	0.45
3:C:245:ARG:NH1	3:C:263:ASP:OD1	2.49	0.45
1:A:405:LYS:HA	1:A:405:LYS:HD3	1.77	0.45
1:A:644:ARG:HE	1:A:644:ARG:HB3	1.50	0.45
1:A:1048:PHE:CZ	5:E:211:TYR:HB2	2.52	0.45
1:A:1261:VAL:HG11	1:A:1306:TYR:HB3	1.98	0.45
2:B:232:TYR:CG	2:B:385:VAL:HG12	2.51	0.45
2:B:543:ASN:OD1	2:B:543:ASN:N	2.46	0.45
3:C:328:LEU:HD23	3:C:328:LEU:HA	1.86	0.45
5:E:76:GLY:N	5:E:106:GLN:OE1	2.49	0.45
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.98	0.45
1:A:388:LYS:HA	1:A:388:LYS:HE2	1.99	0.45
1:A:571:HIS:CE1	1:A:572:THR:HG23	2.52	0.45
1:A:1635:ASP:OD1	1:A:1635:ASP:N	2.44	0.45
1:A:1655:ASP:OD2	7:G:106:LYS:NZ	2.36	0.45
2:B:260:PHE:N	2:B:271:VAL:O	2.50	0.45
3:C:97:LEU:HD21	3:C:202:ILE:HD13	1.99	0.45
5:E:166:LYS:HE3	5:E:166:LYS:HB3	1.70	0.45
11:K:68:GLU:HG2	11:K:72:LEU:HD23	1.98	0.45
13:M:24:GLY:N	14:N:108:THR:O	2.49	0.45
16:S:26:DT:H2'	16:S:27:DG:C8	2.52	0.45
1:A:631:ASP:CG	15:R:12:G:O3'	2.53	0.45
1:A:700:ILE:HG21	1:A:738:ASN:HB3	1.99	0.45
2:B:265:ARG:HD3	2:B:265:ARG:HA	1.74	0.45
2:B:395:ASP:HA	2:B:505:ARG:HH21	1.82	0.45
16:S:10:DC:H5'	16:S:10:DC:C6	2.52	0.45
1:A:491:GLU:O	1:A:493:ASN:N	2.51	0.44
1:A:784:SER:O	1:A:789:SER:OG	2.33	0.44
1:A:964:LYS:HB3	1:A:964:LYS:HE3	1.81	0.44
1:A:1080:TYR:OH	1:A:1173:LYS:NZ	2.32	0.44
7:G:77:VAL:HG22	7:G:124:VAL:HG11	1.99	0.44
15:R:4:A:H2'	15:R:5:A:C8	2.51	0.44
1:A:611:GLU:HG3	2:B:913:ILE:HD13	1.99	0.44
1:A:109:ARG:NE	1:A:231:GLY:HA2	2.31	0.44
1:A:618:TYR:CZ	2:B:783:MET:HG2	2.51	0.44
1:A:953:GLU:OE2	1:A:953:GLU:N	2.50	0.44
2:B:323:ARG:HA	2:B:326:VAL:HG12	1.99	0.44
2:B:324:THR:HG21	13:M:109:ARG:HG2	1.99	0.44
3:C:192:LEU:HG	10:J:2:ILE:HD11	2.00	0.44
1:A:643:ALA:HB1	2:B:1087:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:LYS:NZ	1:A:1638:SER:OG	2.50	0.44
1:A:1229:ALA:HB2	1:A:1597:ALA:HB2	1.98	0.44
1:A:1451:ILE:HA	1:A:1457:ILE:HG23	2.00	0.44
2:B:15:ASP:OD1	2:B:15:ASP:N	2.50	0.44
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.38	0.44
7:G:32:ASN:HD22	7:G:134:GLU:HB2	1.82	0.44
1:A:1276:THR:HB	9:I:21:ASN:HD21	1.82	0.44
2:B:274:VAL:HA	2:B:277:LEU:HB2	1.99	0.44
2:B:577:PHE:CE2	13:M:28:LYS:HB2	2.53	0.44
2:B:791:LYS:O	2:B:795:GLU:HG3	2.17	0.44
1:A:232:LYS:HD3	1:A:239:PHE:CE1	2.53	0.44
1:A:808:LYS:HB2	1:A:808:LYS:HE2	1.69	0.44
1:A:1290:TYR:CD1	1:A:1485:MET:HG2	2.53	0.44
15:R:7:C:H2'	15:R:8:G:H8	1.83	0.44
1:A:426:ALA:HA	1:A:429:THR:HG22	2.00	0.44
1:A:591:ARG:HD2	1:A:626:ALA:HB2	2.00	0.44
2:B:321:GLN:H	2:B:325:GLN:NE2	2.16	0.44
2:B:761:GLY:O	2:B:764:ASN:ND2	2.50	0.44
2:B:779:THR:HG22	2:B:931:TRP:CE2	2.53	0.44
2:B:782:ASP:HA	2:B:786:ALA:HB3	2.00	0.44
1:A:507:TYR:CD1	1:A:509:GLU:HG2	2.52	0.43
1:A:588:LEU:HD21	2:B:1087:LEU:HD13	2.00	0.43
1:A:608:LEU:HD22	11:K:95:HIS:CE1	2.53	0.43
1:A:824:THR:HB	2:B:1023:ARG:HB2	2.00	0.43
15:R:6:U:H2'	15:R:7:C:H6	1.83	0.43
1:A:1267:ILE:HG12	1:A:1296:PHE:CE1	2.53	0.43
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.99	0.43
2:B:909:ARG:HD3	2:B:909:ARG:HA	1.74	0.43
3:C:39:ASP:O	3:C:58:ASN:ND2	2.45	0.43
3:C:107:LYS:HG3	3:C:187:ALA:HA	1.99	0.43
1:A:136:LEU:O	1:A:139:ILE:HG13	2.18	0.43
1:A:1032:VAL:HG12	1:A:1181:PRO:HA	2.00	0.43
1:A:1335:LYS:HA	1:A:1335:LYS:HD2	1.85	0.43
2:B:12:ARG:HA	14:N:163:VAL:HG22	1.99	0.43
3:C:26:ASP:OD1	3:C:26:ASP:N	2.51	0.43
7:G:88:LYS:NZ	7:G:88:LYS:HB3	2.34	0.43
8:H:108:SER:HB3	8:H:111:LEU:HD12	1.99	0.43
1:A:603:HIS:NE2	1:A:624:TYR:OH	2.36	0.43
2:B:776:ILE:HG13	2:B:1026:ILE:HD12	1.99	0.43
8:H:110:ASP:HB3	8:H:128:ASN:ND2	2.33	0.43
1:A:491:GLU:C	1:A:493:ASN:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:ALA:HB3	2:B:1022:LEU:HD13	1.99	0.43
7:G:130:GLY:H	7:G:233:VAL:HG23	1.84	0.43
2:B:420:TYR:CE1	2:B:455:GLU:HG2	2.53	0.43
2:B:1055:LEU:HD23	2:B:1055:LEU:H	1.83	0.43
3:C:100:ARG:NH1	10:J:3:VAL:O	2.41	0.43
5:E:64:PRO:HB2	5:E:69:ILE:HG12	1.99	0.43
12:L:27:LEU:HD12	12:L:37:LYS:HB3	2.00	0.43
1:A:209:THR:H	1:A:212:VAL:CG2	2.31	0.43
1:A:596:HIS:HD2	1:A:598:ALA:H	1.67	0.43
1:A:1148:LEU:HD21	1:A:1166:PHE:HD2	1.83	0.43
1:A:1239:THR:HG23	1:A:1518:VAL:HG13	2.00	0.43
1:A:1514:ASN:OD1	1:A:1514:ASN:N	2.51	0.43
3:C:132:ILE:HD13	3:C:132:ILE:HA	1.86	0.43
1:A:13:SER:OG	2:B:1199:ASN:ND2	2.43	0.43
1:A:132:GLU:HG2	1:A:192:ALA:HB1	2.00	0.43
1:A:242:LYS:HD2	1:A:242:LYS:HA	1.70	0.43
1:A:586:VAL:HG11	1:A:648:LEU:HG	2.01	0.43
1:A:1546:VAL:HG22	1:A:1561:THR:HG23	1.99	0.43
1:A:1554:GLY:HA2	5:E:183:PRO:HD2	2.01	0.43
2:B:374:LEU:HD23	2:B:374:LEU:HA	1.83	0.43
2:B:983:PRO:HB2	2:B:984:TRP:CE3	2.53	0.43
5:E:185:ALA:HA	5:E:190:LEU:HD12	2.00	0.43
1:A:432:ASN:HD21	1:A:444:GLN:H	1.66	0.43
2:B:673:ASN:HB3	2:B:686:HIS:HD2	1.84	0.43
2:B:809:VAL:HG11	2:B:859:CYS:SG	2.59	0.43
2:B:908:ARG:HD2	3:C:95:GLU:HG2	2.00	0.43
1:A:496:GLY:HA3	1:A:615:ARG:HB2	2.00	0.43
1:A:511:VAL:O	1:A:574:ASN:ND2	2.51	0.43
1:A:1255:CYS:SG	1:A:1519:LEU:HD11	2.59	0.43
1:A:1325:LEU:HA	1:A:1492:ILE:HD13	2.00	0.43
2:B:229:TYR:O	2:B:254:ASN:ND2	2.52	0.43
4:D:32:SER:O	4:D:33:THR:HG22	2.18	0.43
12:L:39:SER:O	12:L:49:LYS:NZ	2.48	0.43
1:A:1501:ILE:HD13	1:A:1528:ALA:HB1	2.00	0.42
6:F:72:LYS:HA	6:F:72:LYS:HD3	1.78	0.42
16:S:8:DT:H2"	16:S:9:DA:N7	2.34	0.42
2:B:31:ASP:OD1	2:B:31:ASP:N	2.52	0.42
1:A:1661:PRO:HD2	7:G:55:GLU:HA	2.02	0.42
2:B:298:LYS:HD3	2:B:298:LYS:HA	1.75	0.42
2:B:656:LEU:HD23	2:B:656:LEU:HA	1.77	0.42
8:H:57:VAL:HG22	8:H:144:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:HB3	2:B:1200:VAL:HG13	2.01	0.42
1:A:440:SER:HB2	1:A:454:PRO:HA	2.01	0.42
1:A:669:LEU:H	1:A:669:LEU:HG	1.66	0.42
1:A:946:LEU:HD12	1:A:947:LEU:H	1.83	0.42
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	2.01	0.42
2:B:335:ARG:NH2	2:B:346:ASP:OD1	2.44	0.42
3:C:69:ARG:NH2	11:K:70:HIS:HB2	2.34	0.42
16:S:37:DA:H2''	16:S:38:DG:O5'	2.20	0.42
1:A:371:SER:HB3	15:R:3:A:N3	2.35	0.42
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.89	0.42
1:A:634:ASN:HB3	2:B:1069:ILE:HD12	2.00	0.42
2:B:813:LEU:HD12	2:B:813:LEU:HA	1.86	0.42
11:K:87:GLU:HB2	11:K:108:TYR:CE1	2.54	0.42
17:T:29:DG:C8	17:T:30:DT:H72	2.54	0.42
1:A:511:VAL:HG11	1:A:561:LEU:HG	2.02	0.42
1:A:1646:LEU:HD22	7:G:109:PRO:HB3	2.02	0.42
2:B:341:SER:C	2:B:343:ASP:H	2.28	0.42
2:B:753:LYS:O	2:B:980:ASP:HA	2.19	0.42
13:M:47:GLU:HB3	13:M:48:LYS:HE2	2.00	0.42
13:M:67:ASP:OD1	13:M:67:ASP:N	2.51	0.42
1:A:317:SER:HA	1:A:320:VAL:HG22	2.02	0.42
2:B:416:LYS:HD2	2:B:460:LYS:HD2	2.01	0.42
2:B:954:PHE:N	2:B:955:PRO:HD2	2.34	0.42
3:C:40:PHE:O	11:K:134:LYS:NZ	2.51	0.42
1:A:447:THR:HB	16:S:13:DC:C6	2.54	0.42
1:A:520:ARG:HG3	1:A:558:ALA:HB1	2.00	0.42
1:A:1207:PHE:HE2	1:A:1217:LEU:HD22	1.84	0.42
2:B:698:SER:OG	2:B:699:ILE:N	2.53	0.42
5:E:55:ARG:NH1	5:E:113:GLN:OE1	2.47	0.42
5:E:87:SER:OG	5:E:88:VAL:N	2.53	0.42
8:H:32:THR:OG1	8:H:33:GLN:N	2.52	0.42
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.55	0.42
2:B:272:PRO:O	2:B:275:MET:HB3	2.20	0.42
2:B:957:ARG:H	2:B:957:ARG:HG2	1.72	0.42
6:F:61:HIS:N	6:F:61:HIS:CD2	2.87	0.42
8:H:12:VAL:HA	8:H:28:ALA:HA	2.00	0.42
1:A:19:LEU:HD22	1:A:24:ILE:HG23	2.00	0.42
1:A:953:GLU:O	1:A:953:GLU:HG2	2.20	0.42
2:B:237:ARG:NH2	2:B:401:GLU:OE2	2.53	0.42
2:B:277:LEU:HD23	2:B:277:LEU:HA	1.92	0.42
5:E:20:LYS:HA	5:E:20:LYS:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ILE:HD13	5:E:100:ILE:HA	1.91	0.42
7:G:36:ASN:ND2	7:G:38:ILE:O	2.52	0.42
10:J:10:CYS:SG	10:J:11:GLY:N	2.93	0.42
2:B:322:ASN:OD1	2:B:323:ARG:N	2.53	0.41
2:B:436:MET:HB2	2:B:438:ILE:HG23	2.01	0.41
2:B:863:ASP:OD2	2:B:866:LEU:HD23	2.20	0.41
8:H:123:MET:HE1	8:H:142:LEU:HD13	2.02	0.41
14:N:26:PRO:HB2	14:N:29:PHE:CD1	2.55	0.41
1:A:499:PRO:HD3	1:A:608:LEU:O	2.19	0.41
2:B:109:SER:HB2	2:B:121:VAL:HG22	2.02	0.41
2:B:129:ARG:HB3	2:B:131:THR:HG23	2.01	0.41
2:B:324:THR:HG23	2:B:347:LEU:HD13	2.02	0.41
10:J:5:VAL:HA	10:J:15:GLY:HA3	2.03	0.41
13:M:112:LYS:HE2	13:M:112:LYS:HB2	1.82	0.41
1:A:627:ASP:O	1:A:631:ASP:HB2	2.20	0.41
2:B:841:ASP:HB3	2:B:843:ASP:OD1	2.20	0.41
4:D:28:PRO:HB2	7:G:39:VAL:HG11	2.01	0.41
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.55	0.41
1:A:884:ARG:HD3	1:A:884:ARG:HA	1.84	0.41
2:B:52:LEU:HA	2:B:60:LEU:HB2	2.02	0.41
2:B:301:PHE:CE2	2:B:386:ALA:HB2	2.55	0.41
3:C:36:PHE:CE2	11:K:127:LEU:HG	2.55	0.41
1:A:579:ARG:NH1	1:A:585:ASP:OD2	2.53	0.41
1:A:1110:LYS:H	1:A:1110:LYS:HG2	1.66	0.41
1:A:1292:ILE:O	1:A:1471:GLU:HA	2.21	0.41
2:B:864:ASP:OD1	2:B:864:ASP:N	2.53	0.41
1:A:826:PHE:HB3	2:B:777:SER:HB3	2.02	0.41
2:B:408:LEU:O	2:B:412:ILE:HG13	2.20	0.41
7:G:59:GLN:HA	7:G:62:MET:SD	2.61	0.41
11:K:48:LYS:HB2	11:K:48:LYS:HE3	1.78	0.41
1:A:15:ASP:HB3	1:A:1631:ARG:HB2	2.02	0.41
1:A:32:ILE:HB	1:A:79:ILE:HG22	2.01	0.41
1:A:589:MET:HB2	1:A:603:HIS:CD2	2.56	0.41
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.89	0.41
2:B:338:PHE:CZ	2:B:353:VAL:HG23	2.56	0.41
3:C:196:LEU:O	3:C:197:ARG:NH1	2.47	0.41
5:E:43:LYS:O	5:E:47:CYS:HB2	2.21	0.41
5:E:98:ILE:HG13	5:E:99:HIS:N	2.35	0.41
7:G:54:LEU:HD23	7:G:54:LEU:HA	1.86	0.41
2:B:909:ARG:O	2:B:1035:ARG:NH1	2.47	0.41
2:B:1048:SER:OG	2:B:1049:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:ARG:HG3	3:C:225:ALA:O	2.21	0.41
3:C:174:ARG:HG3	3:C:174:ARG:NH1	2.35	0.41
5:E:20:LYS:HD2	5:E:30:ILE:HG21	2.03	0.41
5:E:155:ARG:HD3	5:E:190:LEU:HD23	2.03	0.41
6:F:147:SER:HB3	6:F:150:GLU:OE2	2.20	0.41
7:G:133:LEU:HD13	7:G:233:VAL:HG11	2.03	0.41
1:A:433:ASP:OD1	1:A:433:ASP:C	2.63	0.41
1:A:507:TYR:HA	1:A:508:PRO:HD3	1.91	0.41
1:A:648:LEU:O	1:A:652:ASN:ND2	2.54	0.41
1:A:882:ILE:O	1:A:889:SER:OG	2.37	0.41
1:A:1006:LEU:HD23	1:A:1006:LEU:HA	1.92	0.41
1:A:1097:TYR:CZ	1:A:1126:LYS:HD2	2.56	0.41
1:A:1223:ARG:HB3	1:A:1223:ARG:CZ	2.50	0.41
1:A:1639:ALA:O	1:A:1643:VAL:HG23	2.20	0.41
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.55	0.41
2:B:357:ILE:HD13	2:B:357:ILE:HA	1.92	0.41
2:B:403:LEU:HD12	2:B:403:LEU:HA	1.96	0.41
2:B:699:ILE:C	2:B:701:ALA:H	2.28	0.41
2:B:752:VAL:HA	2:B:979:GLN:O	2.19	0.41
5:E:28:TYR:HA	5:E:64:PRO:HA	2.03	0.41
10:J:1:MET:HB3	10:J:2:ILE:H	1.56	0.41
11:K:134:LYS:HB2	11:K:134:LYS:HE3	1.64	0.41
1:A:24:ILE:H	1:A:24:ILE:HG12	1.69	0.41
1:A:70:LYS:HG3	1:A:71:PHE:CD1	2.56	0.41
1:A:1450:ILE:HD12	1:A:1450:ILE:HA	1.88	0.41
2:B:129:ARG:NH2	2:B:889:GLY:O	2.42	0.41
2:B:1178:ILE:HB	2:B:1182:LEU:HD23	2.03	0.41
3:C:218:LYS:HE3	3:C:219:PHE:CE2	2.56	0.41
14:N:30:LYS:HB2	14:N:30:LYS:HE3	1.88	0.41
1:A:250:LYS:HB2	1:A:250:LYS:HE2	1.74	0.40
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.57	0.40
2:B:795:GLU:OE1	3:C:216:HIS:HA	2.21	0.40
3:C:139:LYS:HB3	3:C:139:LYS:HE3	1.65	0.40
10:J:24:LEU:HD21	10:J:38:ARG:HD2	2.03	0.40
1:A:84:PRO:O	1:A:317:SER:OG	2.34	0.40
1:A:1021:ARG:NH1	2:B:1073:GLU:OE1	2.55	0.40
2:B:38:LEU:HD11	2:B:493:PHE:HZ	1.86	0.40
2:B:887:LEU:HB3	2:B:898:LEU:HD13	2.03	0.40
2:B:914:GLY:HA2	2:B:926:VAL:HB	2.03	0.40
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.28	0.40
7:G:55:GLU:N	7:G:55:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:149:ILE:HD11	7:G:231:PHE:HZ	1.86	0.40
10:J:56:LEU:HD23	10:J:56:LEU:HA	1.90	0.40
1:A:1294:MET:HE2	1:A:1472:PHE:HE1	1.86	0.40
2:B:97:VAL:HG21	2:B:424:ILE:HD11	2.03	0.40
2:B:588:ILE:HG13	2:B:593:ILE:HG13	2.03	0.40
5:E:23:VAL:HG13	5:E:28:TYR:HD2	1.86	0.40
7:G:73:TYR:CE1	7:G:79:GLY:HA2	2.56	0.40
1:A:316:LEU:O	1:A:319:GLU:HG2	2.20	0.40
1:A:947:LEU:HB3	1:A:982:VAL:CG2	2.52	0.40
1:A:947:LEU:HD11	1:A:986:PHE:CZ	2.56	0.40
2:B:381:LEU:O	2:B:385:VAL:HG13	2.22	0.40
2:B:456:ASN:HB3	2:B:459:SER:HB3	2.03	0.40
2:B:476:LEU:O	2:B:478:LEU:HD13	2.20	0.40
2:B:1202:PRO:O	4:D:21:VAL:HG21	2.21	0.40
4:D:32:SER:C	4:D:34:ASP:H	2.30	0.40
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.20	0.40
1:A:847:LEU:HD21	1:A:946:LEU:HD22	2.02	0.40
2:B:583:LEU:HD13	2:B:583:LEU:HA	1.97	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	1466/1664 (88%)	1398 (95%)	68 (5%)	0	100	100
2	B	1162/1203 (97%)	1110 (96%)	52 (4%)	0	100	100
3	C	308/335 (92%)	298 (97%)	10 (3%)	0	100	100
4	D	55/137 (40%)	51 (93%)	4 (7%)	0	100	100
5	E	210/215 (98%)	199 (95%)	11 (5%)	0	100	100
6	F	99/155 (64%)	97 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	158/326 (48%)	154 (98%)	4 (2%)	0	100	100
8	H	128/146 (88%)	127 (99%)	1 (1%)	0	100	100
9	I	63/125 (50%)	60 (95%)	3 (5%)	0	100	100
10	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
11	K	96/142 (68%)	90 (94%)	6 (6%)	0	100	100
12	L	42/70 (60%)	41 (98%)	1 (2%)	0	100	100
13	M	101/415 (24%)	98 (97%)	3 (3%)	0	100	100
14	N	106/233 (46%)	104 (98%)	2 (2%)	0	100	100
All	All	4061/5236 (78%)	3891 (96%)	170 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1301/1465 (89%)	1295 (100%)	6 (0%)	86	91
2	B	1020/1053 (97%)	1018 (100%)	2 (0%)	92	96
3	C	273/296 (92%)	273 (100%)	0	100	100
4	D	56/116 (48%)	55 (98%)	1 (2%)	54	73
5	E	194/197 (98%)	193 (100%)	1 (0%)	86	91
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	141/291 (48%)	140 (99%)	1 (1%)	81	88
8	H	116/128 (91%)	116 (100%)	0	100	100
9	I	57/110 (52%)	56 (98%)	1 (2%)	54	73
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	88/130 (68%)	88 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
13	M	93/371 (25%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	107/220 (49%)	107 (100%)	0	100	100
All	All	3639/4636 (78%)	3627 (100%)	12 (0%)	90	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	LEU
1	A	627	ASP
1	A	646	GLU
1	A	700	ILE
1	A	737	LEU
1	A	1228	THR
2	B	325	GLN
2	B	1049	THR
4	D	92	ILE
5	E	124	VAL
7	G	62	MET
9	I	53	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	221	HIS
1	A	336	GLN
1	A	384	GLN
1	A	521	GLN
1	A	525	ASN
1	A	617	HIS
1	A	636	HIS
1	A	748	ASN
1	A	767	ASN
1	A	840	ASN
1	A	863	ASN
1	A	901	ASN
1	A	939	ASN
1	A	942	GLN
1	A	1108	HIS
1	A	1116	GLN
1	A	1237	GLN
1	A	1320	GLN

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Mol	Chain	Res	Type
1	A	1454	HIS
1	A	1461	ASN
1	A	1544	ASN
1	A	1567	ASN
1	A	1601	GLN
2	B	27	ASN
2	B	101	GLN
2	B	248	ASN
2	B	254	ASN
2	B	257	GLN
2	B	321	GLN
2	B	325	GLN
2	B	422	GLN
2	B	462	GLN
2	B	492	ASN
2	B	600	GLN
2	B	673	ASN
2	B	702	ASN
2	B	735	HIS
2	B	764	ASN
2	B	767	ASN
2	B	923	GLN
2	B	944	GLN
2	B	975	HIS
2	B	1008	HIS
2	B	1165	ASN
2	B	1199	ASN
3	C	88	ASN
3	C	158	ASN
3	C	207	HIS
3	C	335	GLN
4	D	23	HIS
4	D	26	GLN
4	D	81	ASN
5	E	61	GLN
5	E	99	HIS
6	F	59	GLN
7	G	36	ASN
7	G	140	GLN
8	H	64	ASN
9	I	21	ASN
9	I	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	64	GLN
11	K	95	HIS
11	K	102	ASN
13	M	16	GLN
13	M	89	GLN
14	N	132	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	10/12 (83%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	3	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	3DR	T	17	17	8,11,12	1.54	1 (12%)	9,14,17	1.67	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3DR	T	17	17	-	1/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	17	3DR	C2'-C1'	2.48	1.58	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	17	3DR	O4'-C4'-C3'	3.55	108.96	103.73
17	T	17	3DR	C2'-C3'-C4'	3.20	109.39	102.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	T	17	3DR	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	17	3DR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	APC	B	3002	-	27,33,33	4.51	8 (29%)	31,52,52	1.33	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	APC	B	3002	-	-	5/15/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	3002	APC	O4'-C1'	14.36	1.61	1.41
20	B	3002	APC	C2'-C1'	-12.40	1.34	1.53
20	B	3002	APC	PB-O3B	8.38	1.67	1.58
20	B	3002	APC	O4'-C4'	-6.45	1.30	1.45
20	B	3002	APC	PA-O5'	5.93	1.66	1.57
20	B	3002	APC	O2'-C2'	3.18	1.50	1.43
20	B	3002	APC	C6-N6	3.03	1.45	1.34
20	B	3002	APC	O3'-C3'	-2.58	1.36	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	3002	APC	N3-C2-N1	-4.51	121.63	128.68
20	B	3002	APC	C3'-C2'-C1'	2.85	105.26	100.98
20	B	3002	APC	PB-O3B-PG	-2.55	123.63	132.62
20	B	3002	APC	C4-C5-N7	-2.16	107.15	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

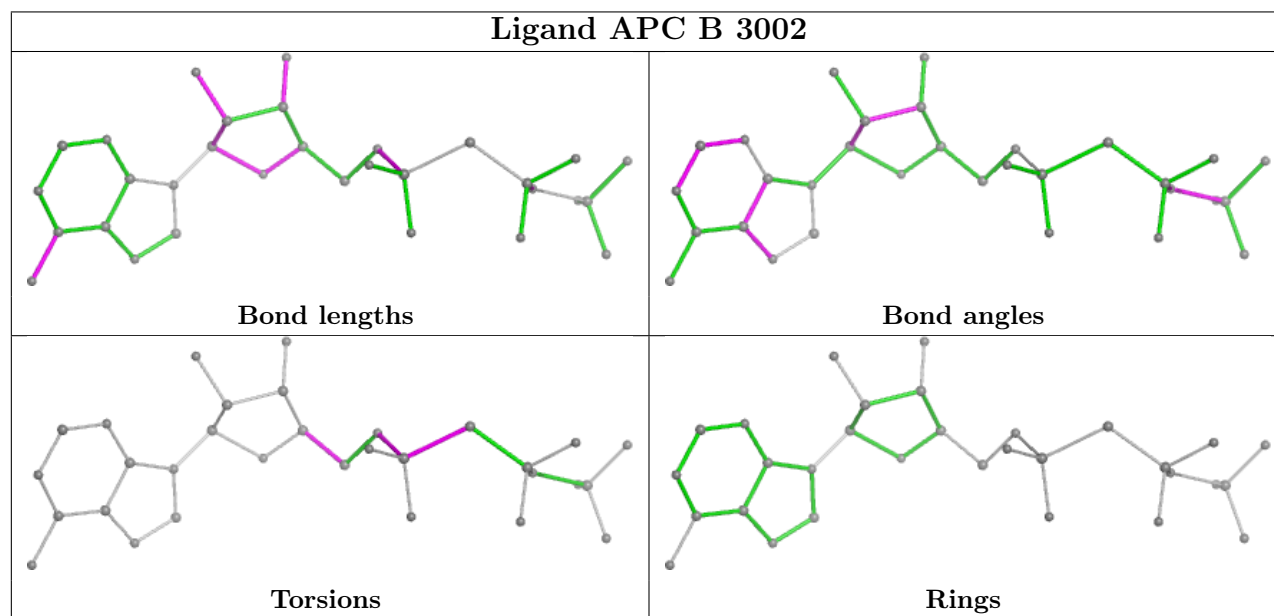
Mol	Chain	Res	Type	Atoms
20	B	3002	APC	PB-C3A-PA-O1A
20	B	3002	APC	PB-C3A-PA-O5'
20	B	3002	APC	C5'-O5'-PA-O1A
20	B	3002	APC	O4'-C4'-C5'-O5'
20	B	3002	APC	PB-C3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	3002	APC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

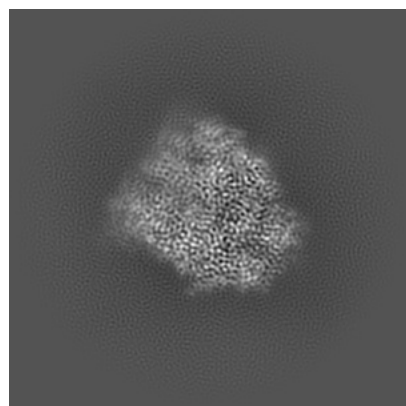
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50962. These allow visual inspection of the internal detail of the map and identification of artifacts.

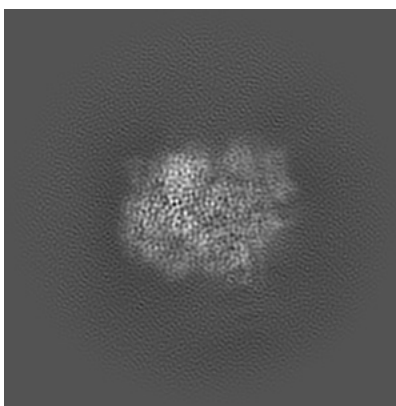
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

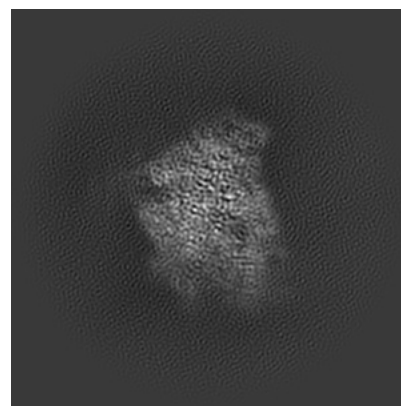
6.1.1 Primary map



X

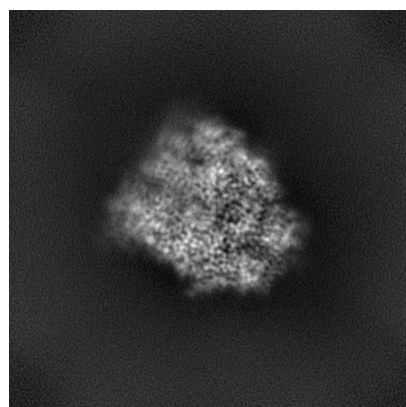


Y

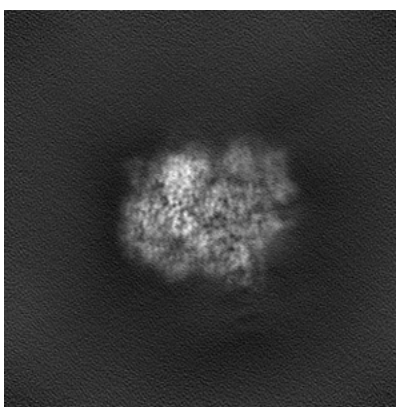


Z

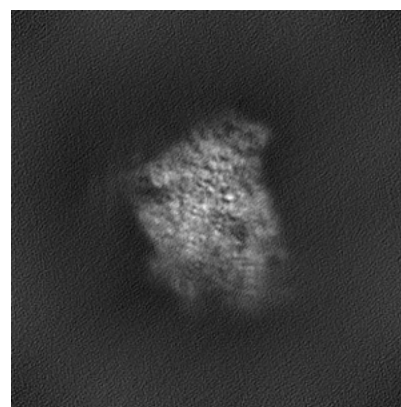
6.1.2 Raw map



X



Y

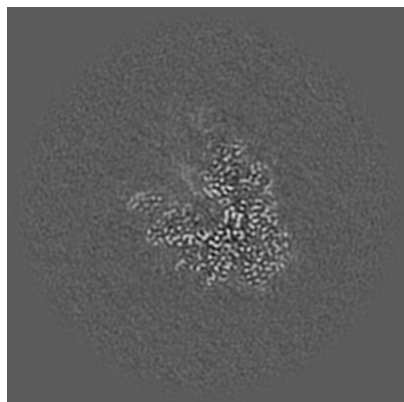


Z

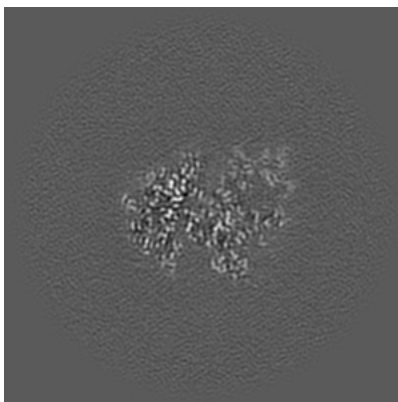
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

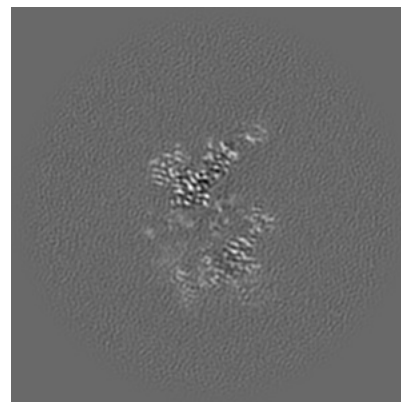
6.2.1 Primary map



X Index: 144

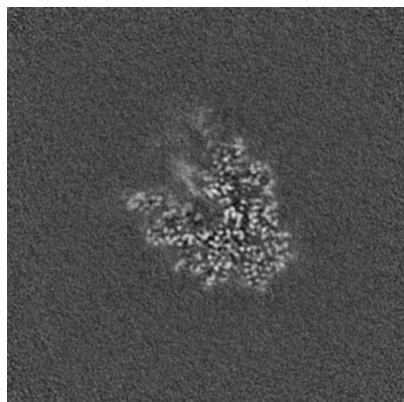


Y Index: 144

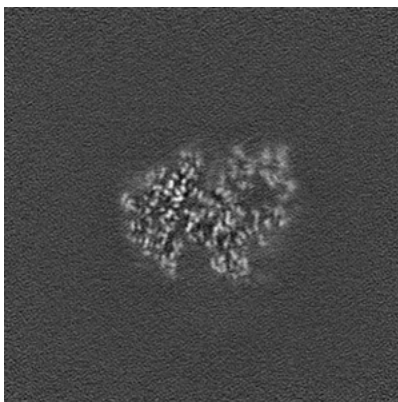


Z Index: 144

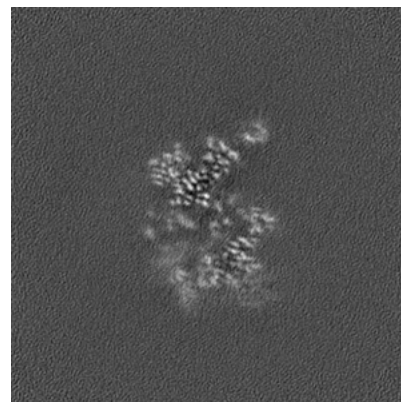
6.2.2 Raw map



X Index: 144



Y Index: 144

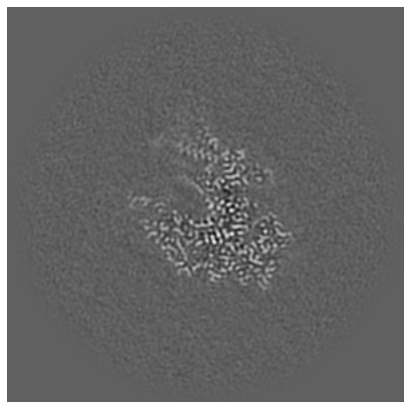


Z Index: 144

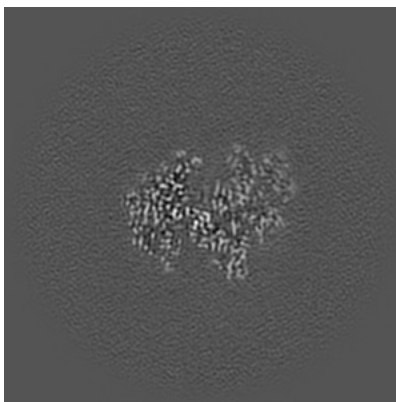
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

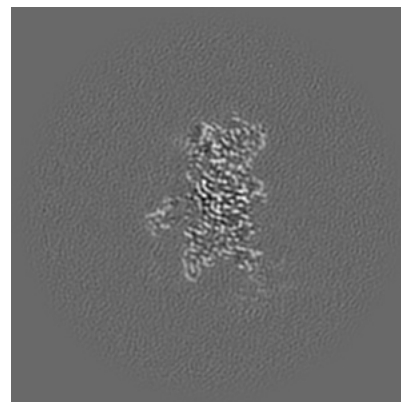
6.3.1 Primary map



X Index: 139

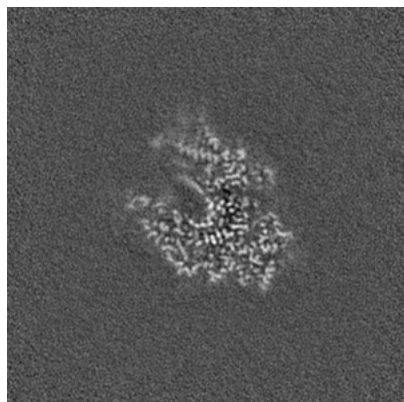


Y Index: 147

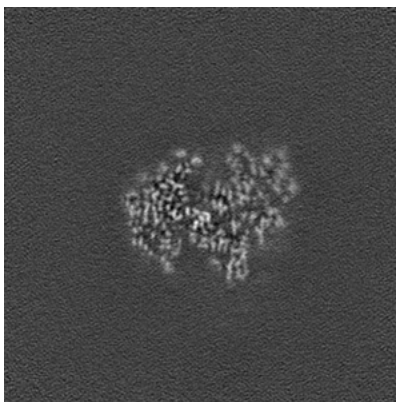


Z Index: 124

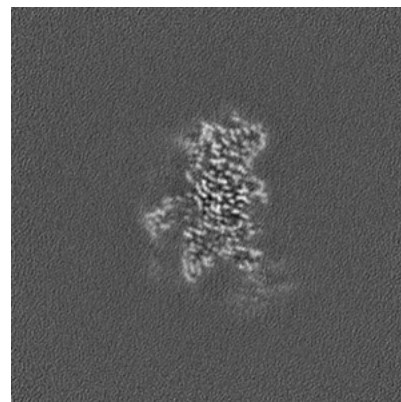
6.3.2 Raw map



X Index: 139



Y Index: 147

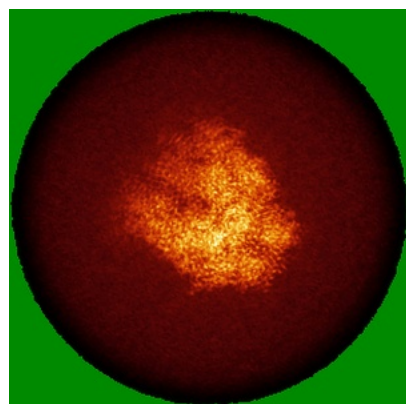


Z Index: 124

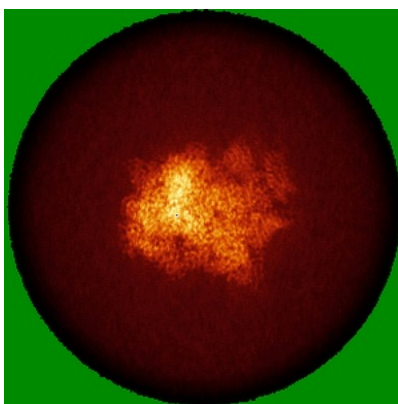
The images above show the largest variance slices of the map in three orthogonal directions.

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

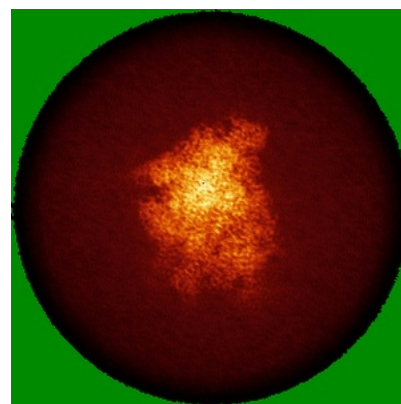
6.4.1 Primary map



X

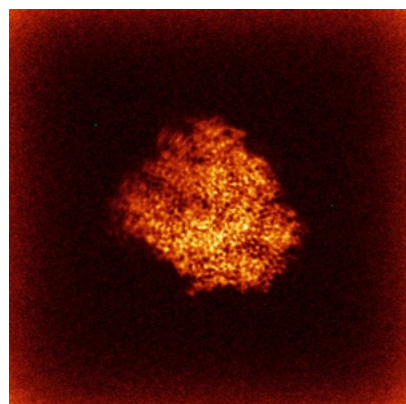


Y

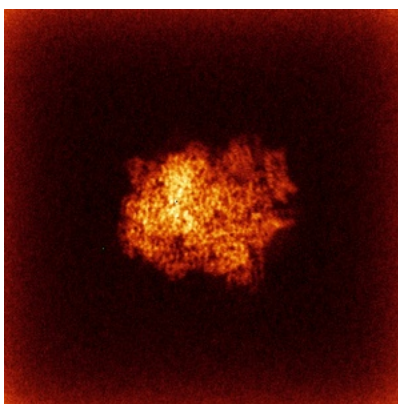


Z

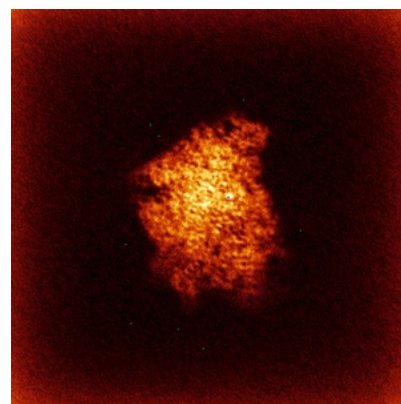
6.4.2 Raw map



X



Y

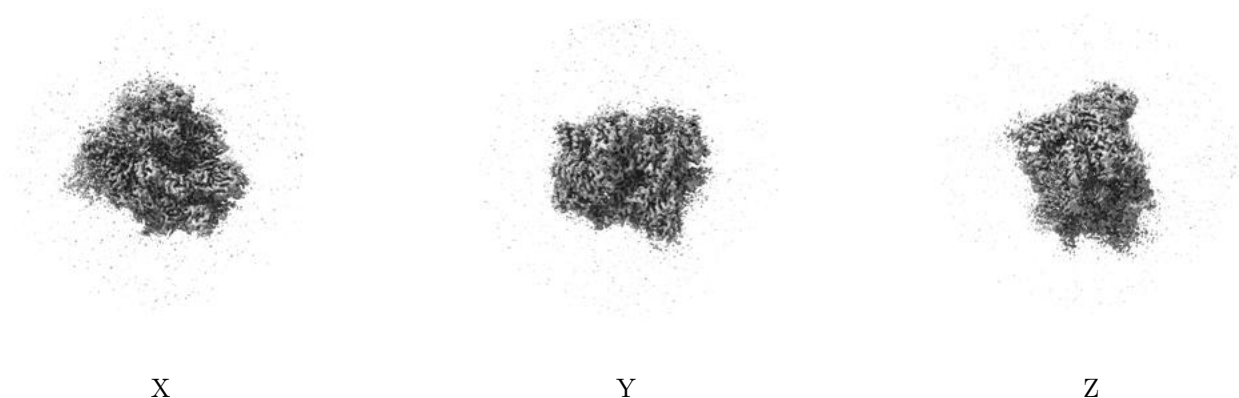


Z

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.

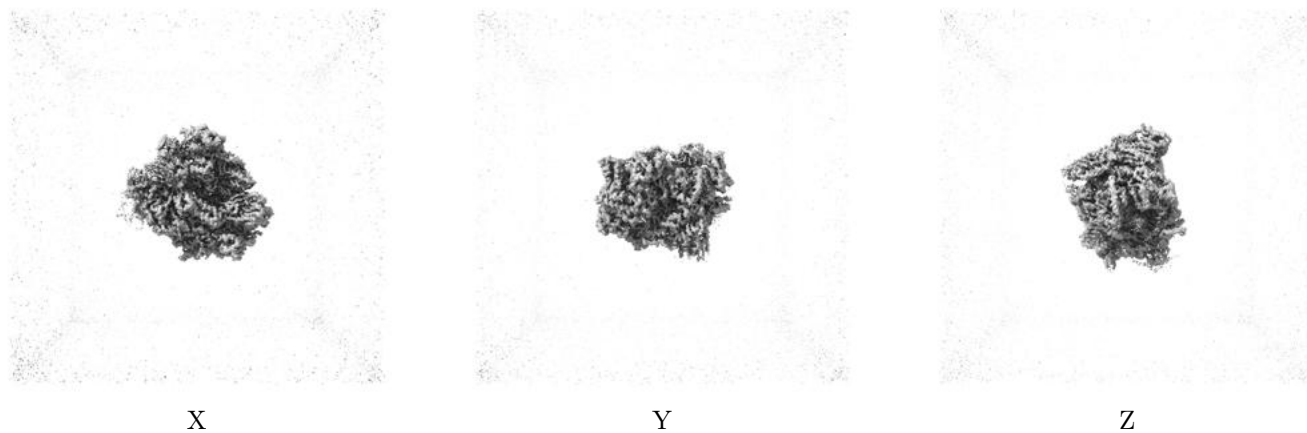
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. 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.

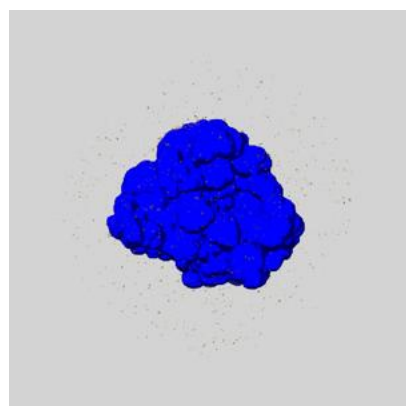
6.6 Mask visualisation [i](#)

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

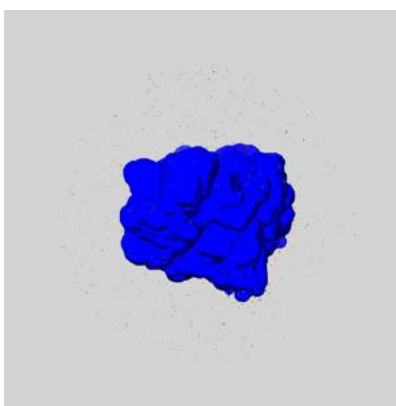
A mask typically either:

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

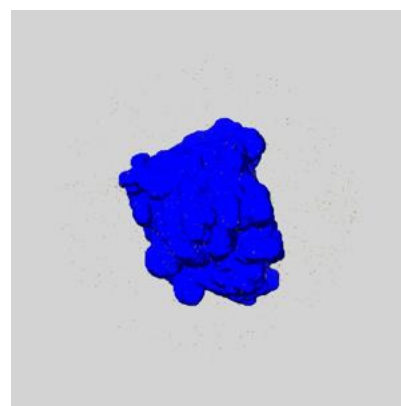
6.6.1 emd_50962_msk_1.map [i](#)



X

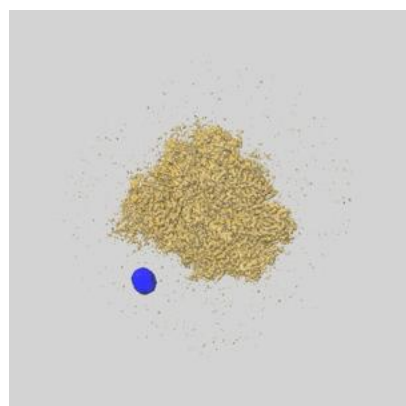


Y

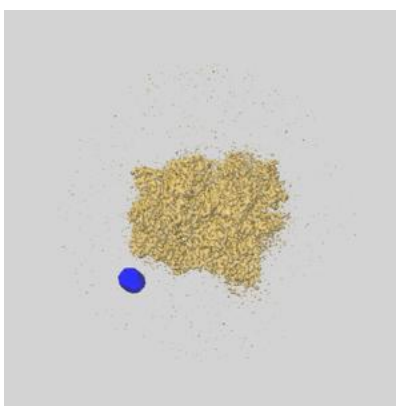


Z

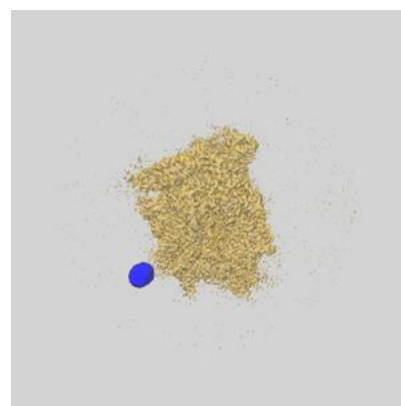
6.6.2 emd_50962_msk_2.map [i](#)



X



Y

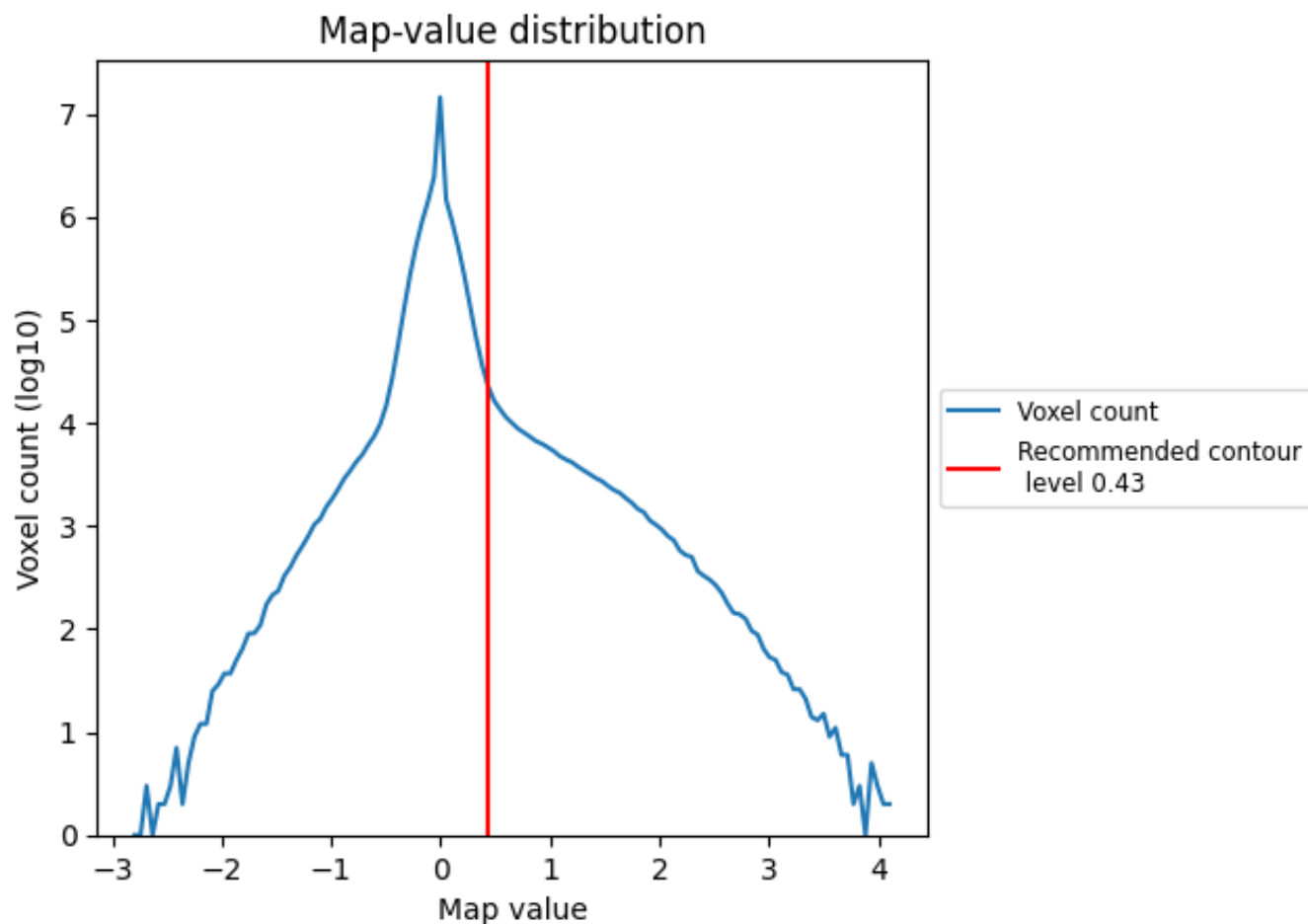


Z

7 Map analysis [i](#)

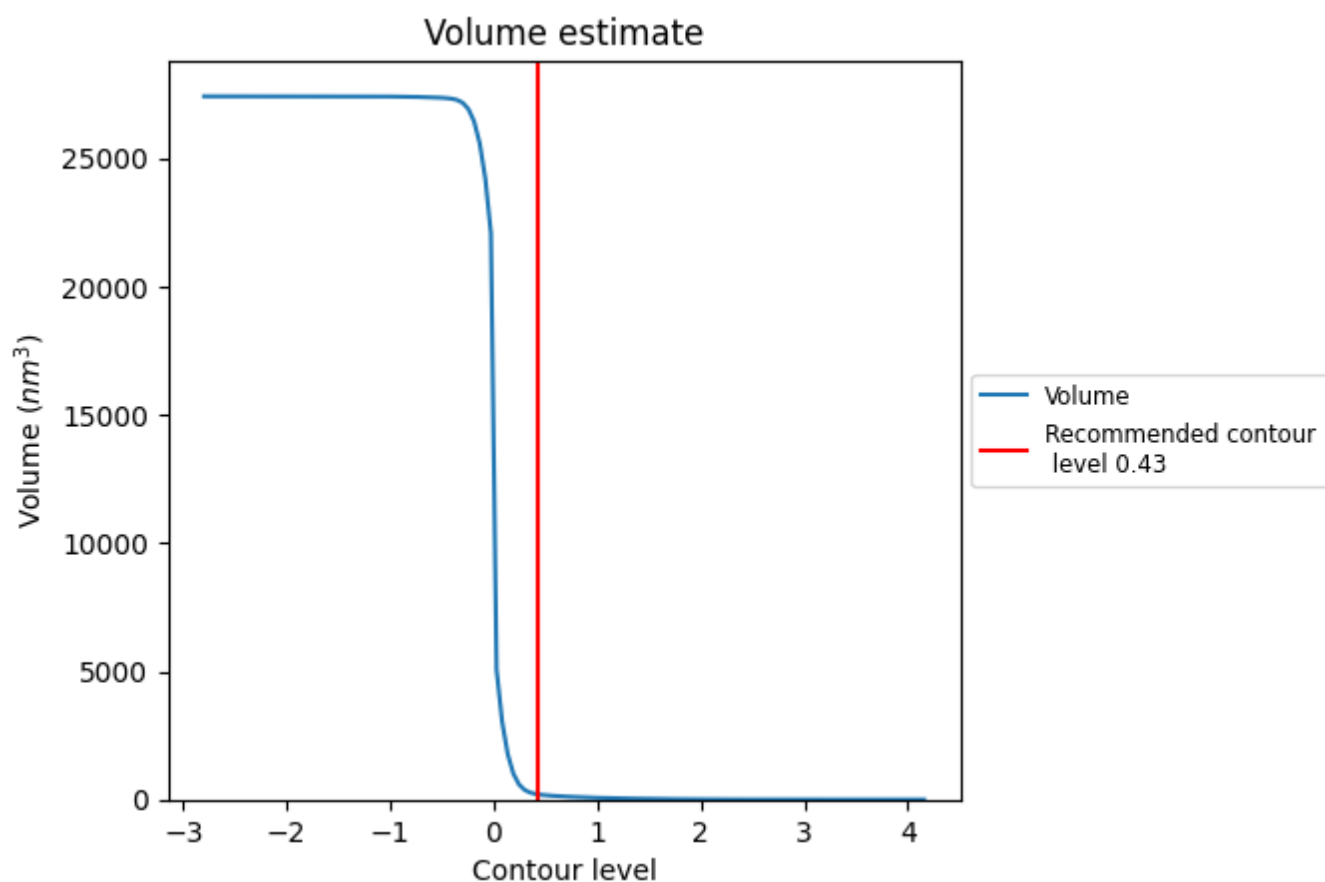
This section contains the results of statistical analysis of the map.

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.

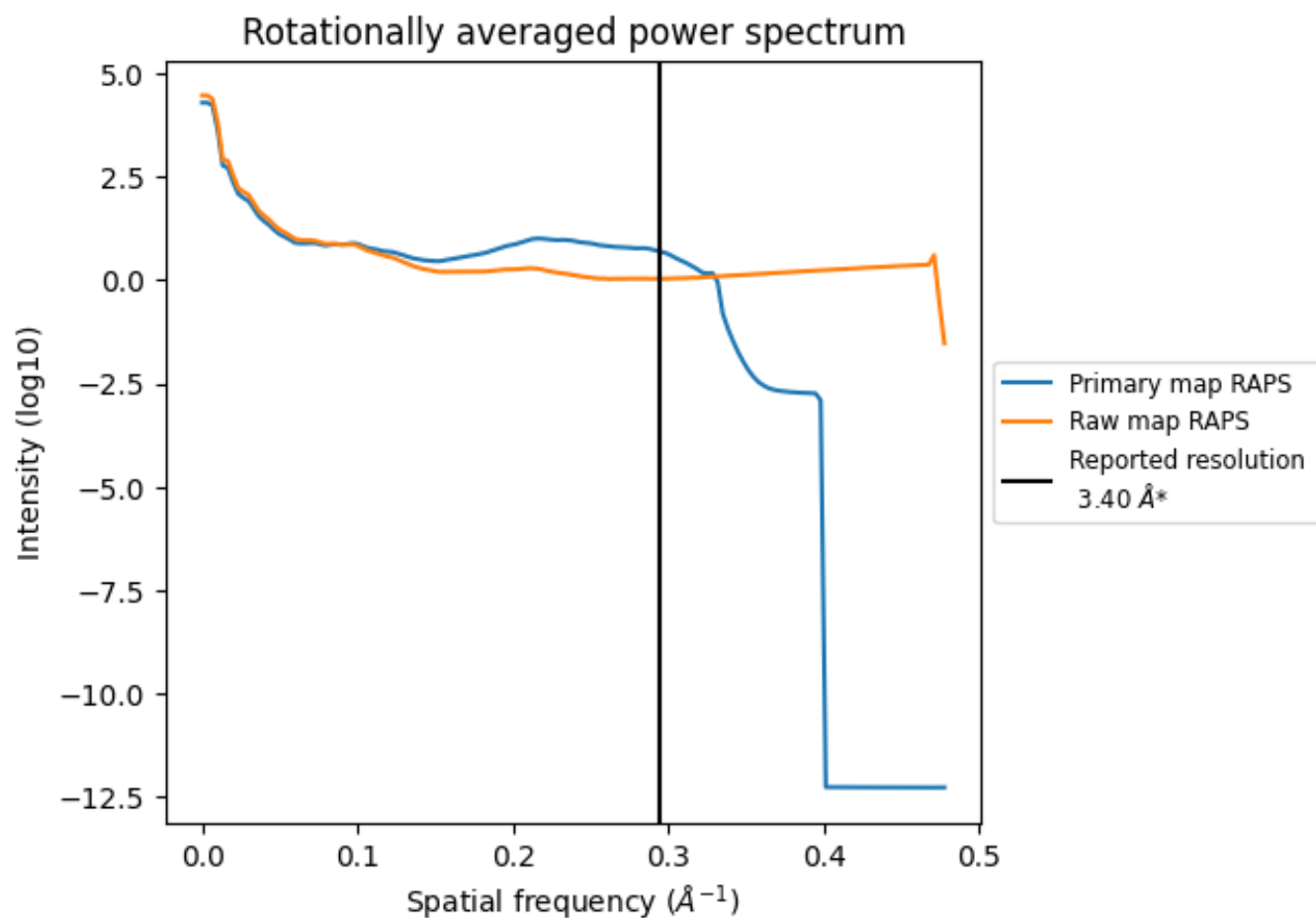
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 ⓘ

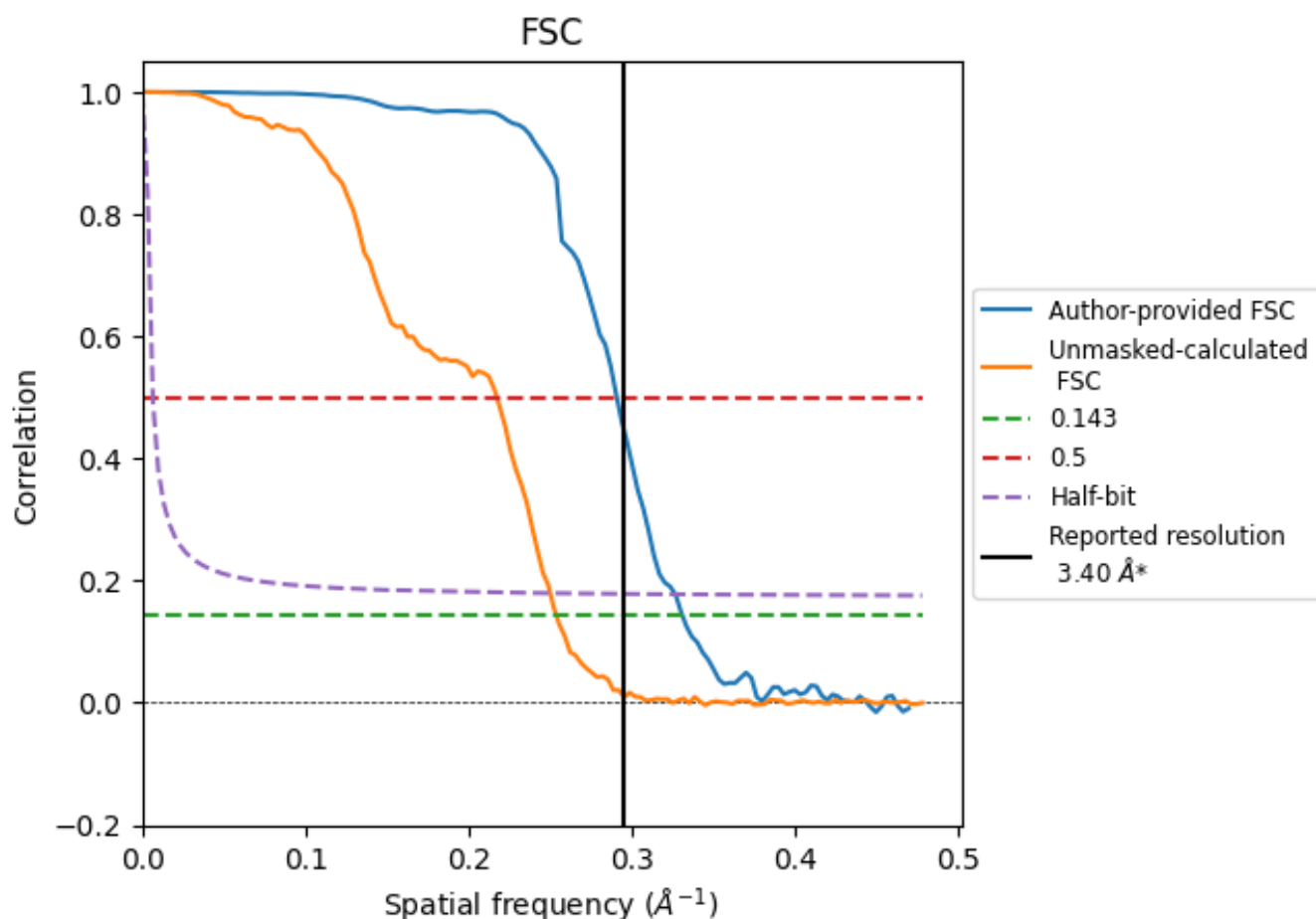


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.02	3.44	3.06
Unmasked-calculated*	3.94	4.61	4.00

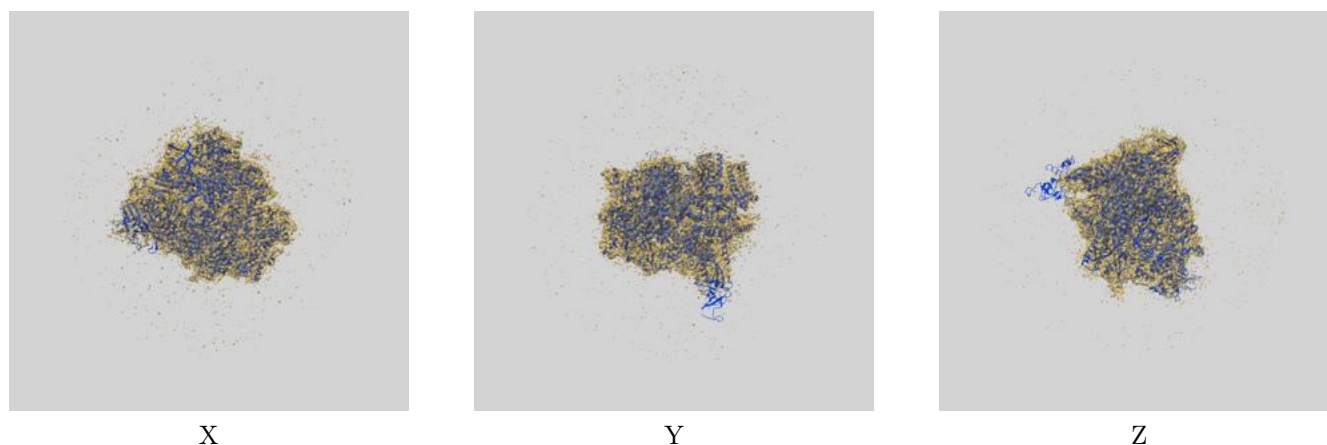
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 3.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

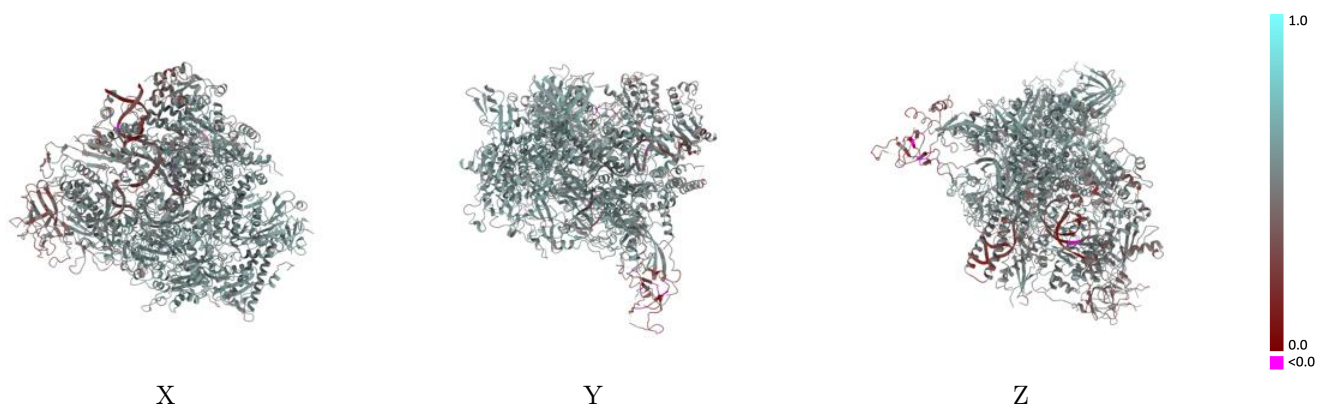
This section contains information regarding the fit between EMDB map EMD-50962 and PDB model 9G23. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



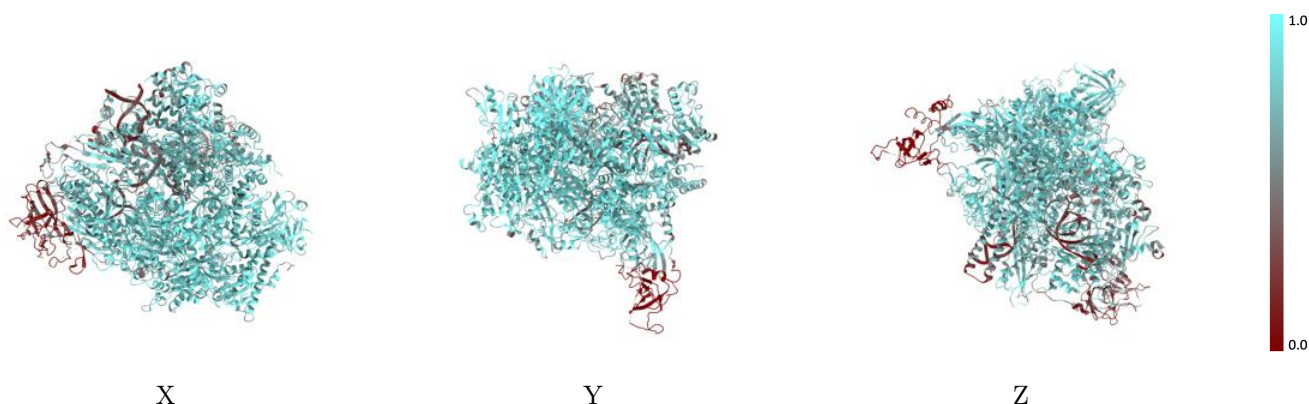
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



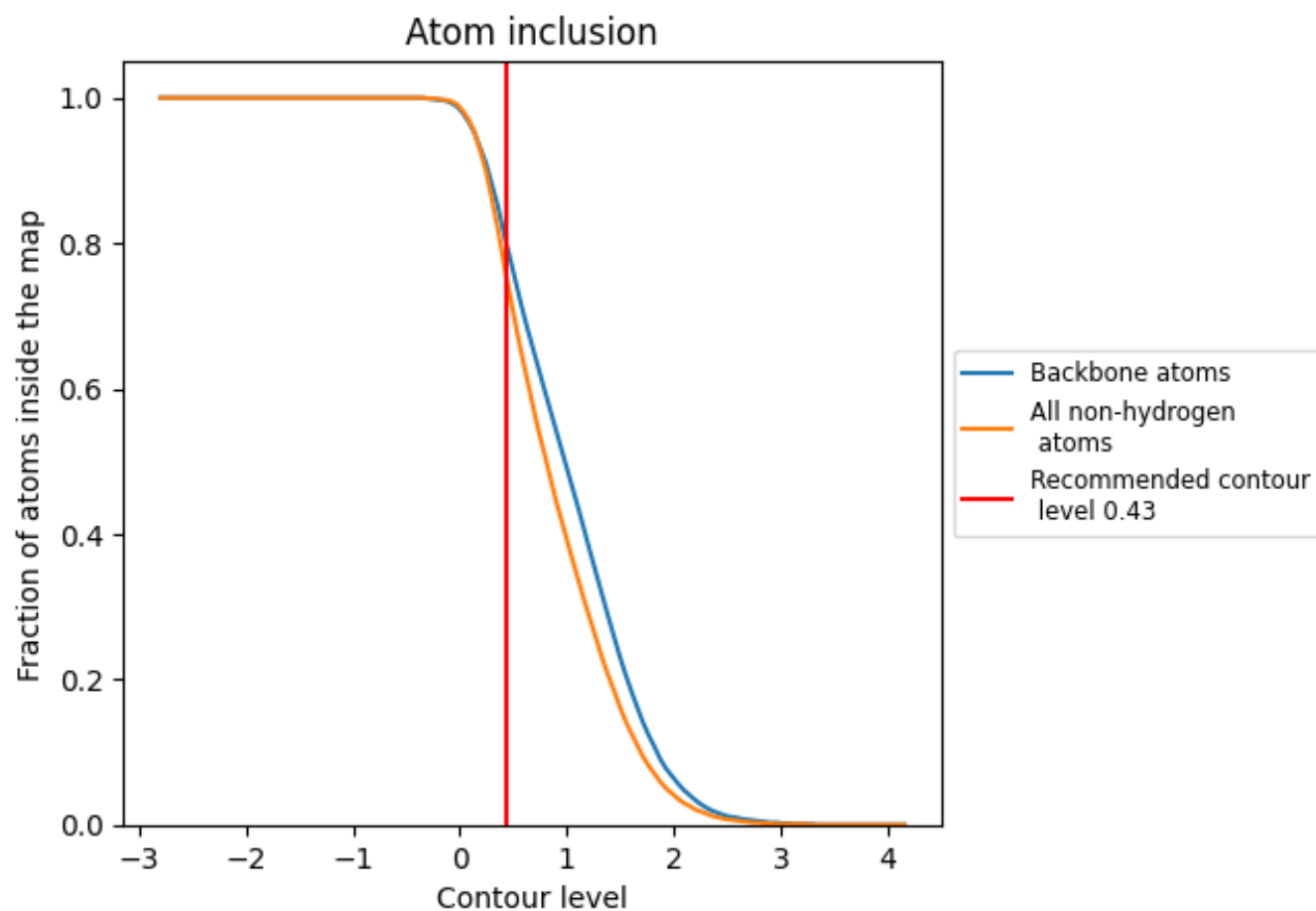
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7570	<div></div> 0.5150
A	<div></div> 0.7980	<div></div> 0.5260
B	<div></div> 0.8520	<div></div> 0.5480
C	<div></div> 0.8580	<div></div> 0.5560
D	<div></div> 0.2790	<div></div> 0.3720
E	<div></div> 0.7830	<div></div> 0.5070
F	<div></div> 0.8560	<div></div> 0.5570
G	<div></div> 0.4460	<div></div> 0.4090
H	<div></div> 0.8540	<div></div> 0.5570
I	<div></div> 0.6120	<div></div> 0.4800
J	<div></div> 0.9130	<div></div> 0.5830
K	<div></div> 0.8770	<div></div> 0.5650
L	<div></div> 0.8760	<div></div> 0.5570
M	<div></div> 0.2010	<div></div> 0.3820
N	<div></div> 0.2540	<div></div> 0.4330
R	<div></div> 0.7990	<div></div> 0.4890
S	<div></div> 0.2760	<div></div> 0.2390
T	<div></div> 0.4690	<div></div> 0.3130

1.0

0.0

<0.0