



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:52 AM UTC

PDB ID : 8Z9H / pdb_00008z9h
EMDB ID : EMD-39862
Title : Cryo-EM structure of Thogoto virus polymerase in a transcription elongation-reception conformation
Authors : Xue, L.; Chang, T.; Li, Z.; Zhao, H.; Li, M.; He, J.; Chen, X.; Xiong, X.
Deposited on : 2024-04-23
Resolution : 2.70 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

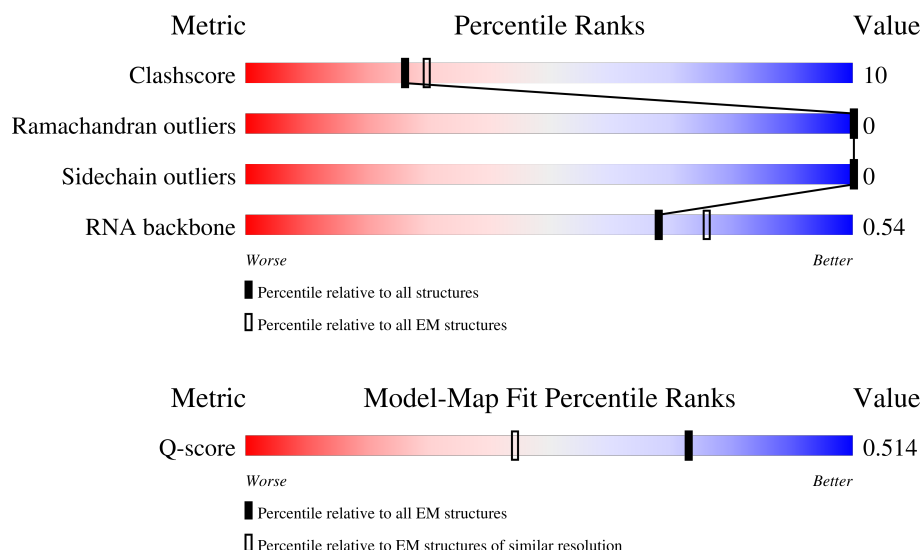
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	622	 79% 21%
1	H	622	 5% 51% 21% 28%
2	B	710	 71% 24% 5%

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Mol	Chain	Length	Quality of chain
2	I	710	13% 54% 27% 18%
3	C	827	5% 70% 20% 10%
3	J	827	6% 90%
4	D	18	22% 44% 33%
5	E	17	12% 18% 71%
5	F	17	24% 47% 6% 24%
6	G	9	56% 44%
6	K	9	22% 33% 44% 22%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 26469 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	621	Total	C	N	O	S	0	0
			5021	3172	874	947	28		
1	H	449	Total	C	N	O	S	0	0
			3616	2290	630	675	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	GLU	GLY	conflict	UNP P27194
H	471	GLU	GLY	conflict	UNP P27194

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	676	Total	C	N	O	S	0	0
			5422	3447	943	996	36		
2	I	580	Total	C	N	O	S	0	0
			4631	2954	790	854	33		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	LEU	ARG	conflict	UNP O41353
B	230	TRP	CYS	conflict	UNP O41353
I	7	LEU	ARG	conflict	UNP O41353
I	230	TRP	CYS	conflict	UNP O41353

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	748	Total	C	N	O	S	3	0
			6024	3812	1052	1125	35		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	79	Total	C	N	O	S	0	0
			649	422	109	116	2		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	770	LEU	-	expression tag	UNP Q9YNA4
C	771	GLU	-	expression tag	UNP Q9YNA4
C	772	VAL	-	expression tag	UNP Q9YNA4
C	773	LEU	-	expression tag	UNP Q9YNA4
C	774	PHE	-	expression tag	UNP Q9YNA4
C	775	GLN	-	expression tag	UNP Q9YNA4
C	776	GLY	-	expression tag	UNP Q9YNA4
C	777	PRO	-	expression tag	UNP Q9YNA4
C	778	GLY	-	expression tag	UNP Q9YNA4
C	779	HIS	-	expression tag	UNP Q9YNA4
C	780	HIS	-	expression tag	UNP Q9YNA4
C	781	HIS	-	expression tag	UNP Q9YNA4
C	782	HIS	-	expression tag	UNP Q9YNA4
C	783	HIS	-	expression tag	UNP Q9YNA4
C	784	HIS	-	expression tag	UNP Q9YNA4
C	785	HIS	-	expression tag	UNP Q9YNA4
C	786	HIS	-	expression tag	UNP Q9YNA4
C	787	SER	-	expression tag	UNP Q9YNA4
C	788	ALA	-	expression tag	UNP Q9YNA4
C	789	ASP	-	expression tag	UNP Q9YNA4
C	790	TYR	-	expression tag	UNP Q9YNA4
C	791	LYS	-	expression tag	UNP Q9YNA4
C	792	ASP	-	expression tag	UNP Q9YNA4
C	793	ASP	-	expression tag	UNP Q9YNA4
C	794	ASP	-	expression tag	UNP Q9YNA4
C	795	ASP	-	expression tag	UNP Q9YNA4
C	796	LYS	-	expression tag	UNP Q9YNA4
C	797	GLY	-	expression tag	UNP Q9YNA4
C	798	GLY	-	expression tag	UNP Q9YNA4
C	799	TRP	-	expression tag	UNP Q9YNA4
C	800	SER	-	expression tag	UNP Q9YNA4
C	801	HIS	-	expression tag	UNP Q9YNA4
C	802	PRO	-	expression tag	UNP Q9YNA4
C	803	GLN	-	expression tag	UNP Q9YNA4
C	804	PHE	-	expression tag	UNP Q9YNA4
C	805	GLU	-	expression tag	UNP Q9YNA4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	806	LYS	-	expression tag	UNP Q9YNA4
C	807	GLY	-	expression tag	UNP Q9YNA4
C	808	GLY	-	expression tag	UNP Q9YNA4
C	809	GLY	-	expression tag	UNP Q9YNA4
C	810	SER	-	expression tag	UNP Q9YNA4
C	811	GLY	-	expression tag	UNP Q9YNA4
C	812	GLY	-	expression tag	UNP Q9YNA4
C	813	GLY	-	expression tag	UNP Q9YNA4
C	814	GLY	-	expression tag	UNP Q9YNA4
C	815	SER	-	expression tag	UNP Q9YNA4
C	816	GLY	-	expression tag	UNP Q9YNA4
C	817	GLY	-	expression tag	UNP Q9YNA4
C	818	SER	-	expression tag	UNP Q9YNA4
C	819	ALA	-	expression tag	UNP Q9YNA4
C	820	TRP	-	expression tag	UNP Q9YNA4
C	821	SER	-	expression tag	UNP Q9YNA4
C	822	HIS	-	expression tag	UNP Q9YNA4
C	823	PRO	-	expression tag	UNP Q9YNA4
C	824	GLN	-	expression tag	UNP Q9YNA4
C	825	PHE	-	expression tag	UNP Q9YNA4
C	826	GLU	-	expression tag	UNP Q9YNA4
C	827	LYS	-	expression tag	UNP Q9YNA4
J	761	LEU	-	expression tag	UNP Q9YNA4
J	762	GLU	-	expression tag	UNP Q9YNA4
J	763	VAL	-	expression tag	UNP Q9YNA4
J	764	LEU	-	expression tag	UNP Q9YNA4
J	765	PHE	-	expression tag	UNP Q9YNA4
J	766	GLN	-	expression tag	UNP Q9YNA4
J	767	GLY	-	expression tag	UNP Q9YNA4
J	768	PRO	-	expression tag	UNP Q9YNA4
J	769	GLY	-	expression tag	UNP Q9YNA4
J	770	HIS	-	expression tag	UNP Q9YNA4
J	771	HIS	-	expression tag	UNP Q9YNA4
J	772	HIS	-	expression tag	UNP Q9YNA4
J	773	HIS	-	expression tag	UNP Q9YNA4
J	774	HIS	-	expression tag	UNP Q9YNA4
J	775	HIS	-	expression tag	UNP Q9YNA4
J	776	HIS	-	expression tag	UNP Q9YNA4
J	777	HIS	-	expression tag	UNP Q9YNA4
J	778	SER	-	expression tag	UNP Q9YNA4
J	779	ALA	-	expression tag	UNP Q9YNA4
J	780	ASP	-	expression tag	UNP Q9YNA4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	781	TYR	-	expression tag	UNP Q9YNA4
J	782	LYS	-	expression tag	UNP Q9YNA4
J	783	ASP	-	expression tag	UNP Q9YNA4
J	784	ASP	-	expression tag	UNP Q9YNA4
J	785	ASP	-	expression tag	UNP Q9YNA4
J	786	ASP	-	expression tag	UNP Q9YNA4
J	787	LYS	-	expression tag	UNP Q9YNA4
J	788	GLY	-	expression tag	UNP Q9YNA4
J	789	GLY	-	expression tag	UNP Q9YNA4
J	790	TRP	-	expression tag	UNP Q9YNA4
J	791	SER	-	expression tag	UNP Q9YNA4
J	792	HIS	-	expression tag	UNP Q9YNA4
J	793	PRO	-	expression tag	UNP Q9YNA4
J	794	GLN	-	expression tag	UNP Q9YNA4
J	795	PHE	-	expression tag	UNP Q9YNA4
J	796	GLU	-	expression tag	UNP Q9YNA4
J	797	LYS	-	expression tag	UNP Q9YNA4
J	798	GLY	-	expression tag	UNP Q9YNA4
J	799	GLY	-	expression tag	UNP Q9YNA4
J	800	GLY	-	expression tag	UNP Q9YNA4
J	801	SER	-	expression tag	UNP Q9YNA4
J	802	GLY	-	expression tag	UNP Q9YNA4
J	803	GLY	-	expression tag	UNP Q9YNA4
J	804	GLY	-	expression tag	UNP Q9YNA4
J	805	GLY	-	expression tag	UNP Q9YNA4
J	806	SER	-	expression tag	UNP Q9YNA4
J	807	GLY	-	expression tag	UNP Q9YNA4
J	808	GLY	-	expression tag	UNP Q9YNA4
J	809	SER	-	expression tag	UNP Q9YNA4
J	810	ALA	-	expression tag	UNP Q9YNA4
J	811	TRP	-	expression tag	UNP Q9YNA4
J	812	SER	-	expression tag	UNP Q9YNA4
J	813	HIS	-	expression tag	UNP Q9YNA4
J	814	PRO	-	expression tag	UNP Q9YNA4
J	815	GLN	-	expression tag	UNP Q9YNA4
J	816	PHE	-	expression tag	UNP Q9YNA4
J	817	GLU	-	expression tag	UNP Q9YNA4
J	818	LYS	-	expression tag	UNP Q9YNA4

- Molecule 4 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*AP*AP*AP*UP*CP*AP*AP*GP*GP*CP*AP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	12	Total	C	N	O	P	0	0
			260	118	55	76	11		

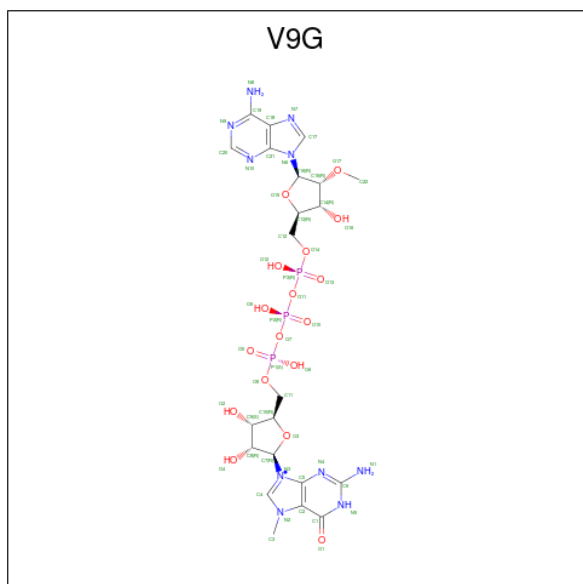
- Molecule 5 is a RNA chain called RNA (5'-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	5	Total	C	N	O	P	0	0
			103	46	14	38	5		
5	F	13	Total	C	N	O	P	0	0
			269	120	38	98	13		

- Molecule 6 is a RNA chain called RNA (5'-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	9	Total	C	N	O	P	0	0
			195	88	41	57	9		
6	K	9	Total	C	N	O	P	0	0
			195	88	41	57	9		

- Molecule 7 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-(2'-O-METHYL)-ADENOSINE (CCD ID: V9G) (formula: C₂₂H₃₂N₁₀O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

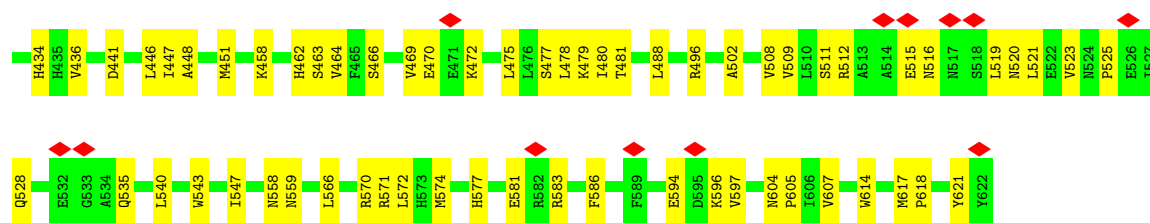


Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total	C	N	O	P	0
			52	22	10	17	3	

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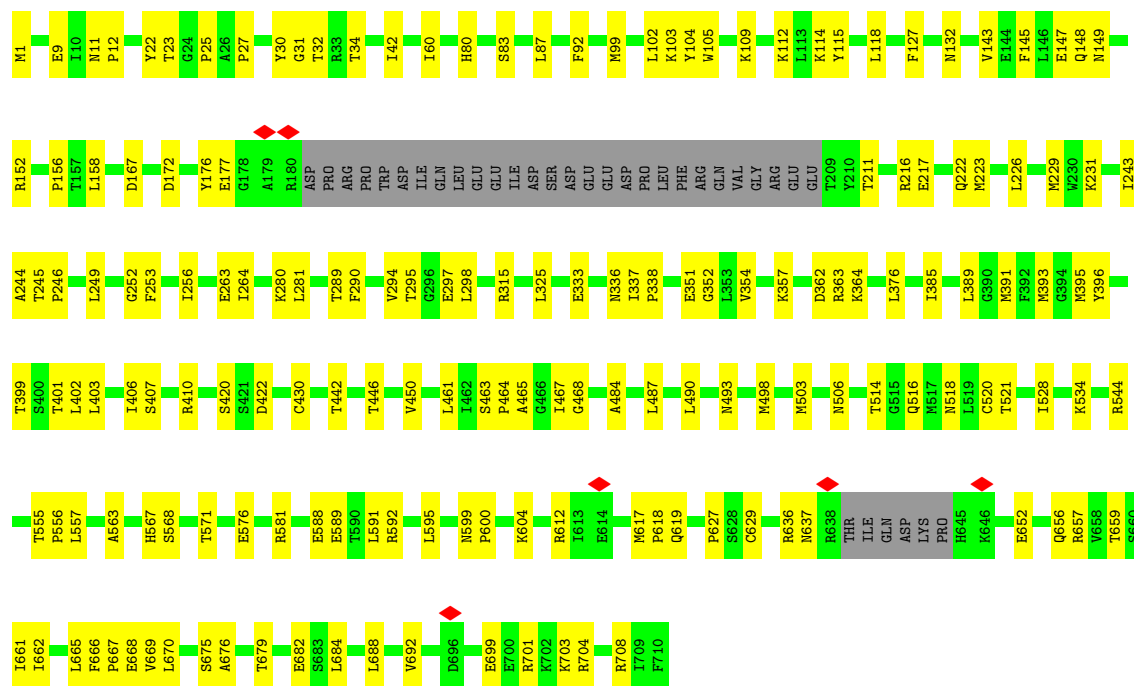
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	K	1	32	11	5	13	3	0



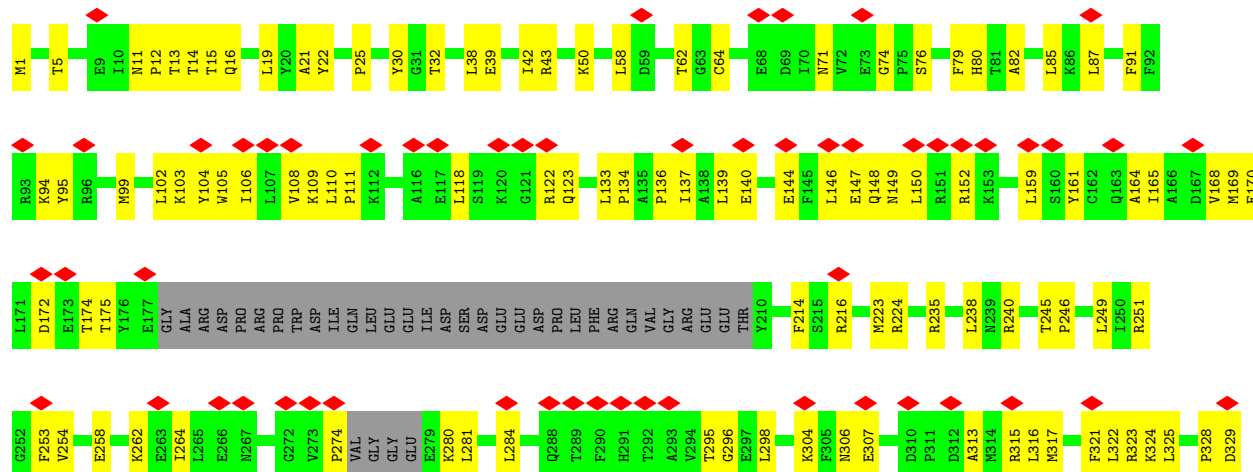
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

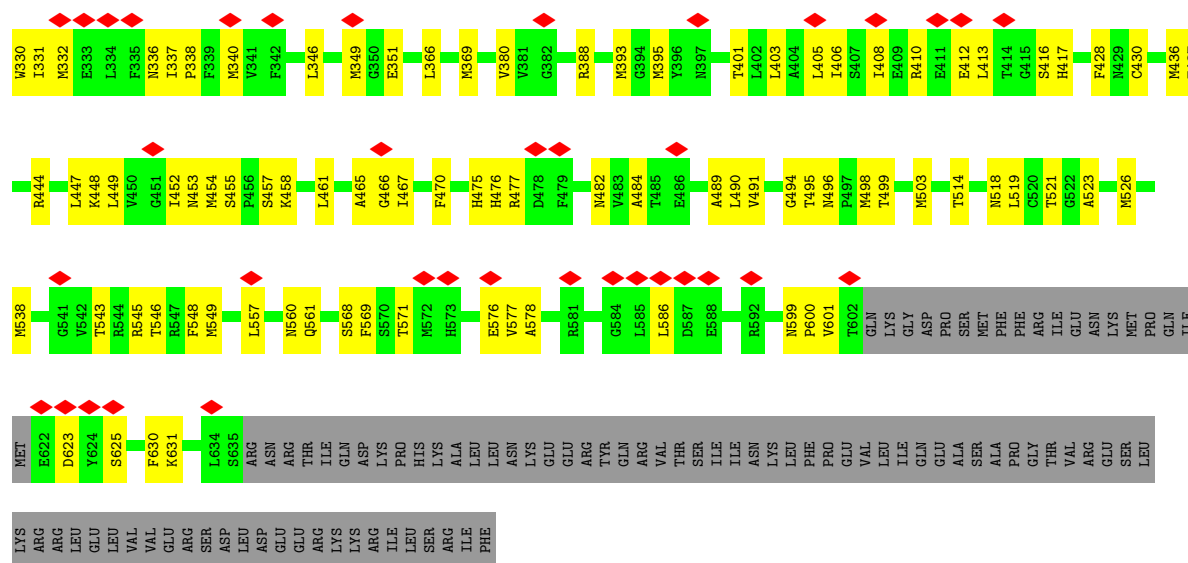
Chain B: 71% 24% 5%



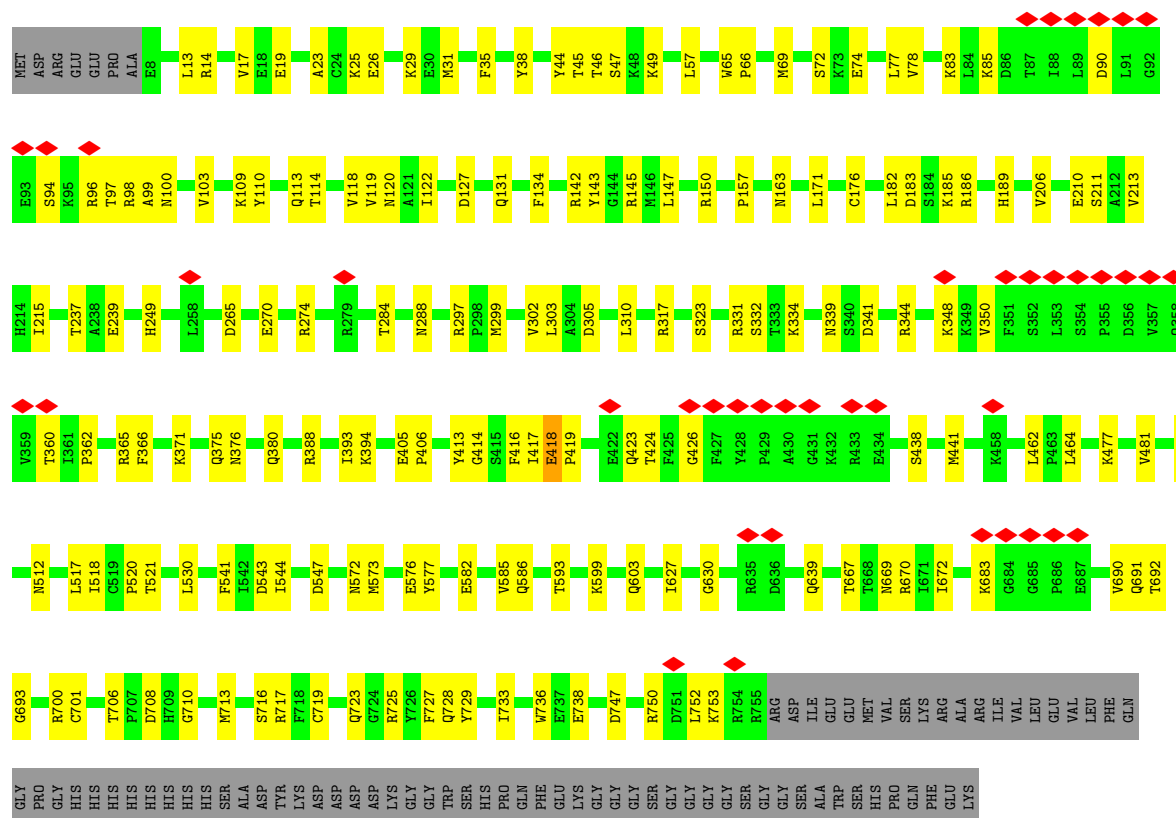
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain I: 13% 54% 27% 18%



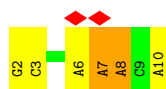


• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80060	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	262.80002, 262.80002, 262.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V9G

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	0.11	0/5136	0.29	1/6967 (0.0%)
1	H	0.12	0/3697	0.32	0/5011
2	B	0.12	0/5532	0.31	0/7468
2	I	0.11	0/4730	0.30	0/6396
3	C	0.11	0/6161	0.34	1/8332 (0.0%)
3	J	0.12	0/666	0.37	0/905
4	D	0.10	0/293	0.32	0/456
5	E	0.08	0/113	0.14	0/173
5	F	0.10	0/297	0.23	0/459
6	G	0.10	0/219	0.14	0/339
6	K	0.12	0/219	0.35	0/339
All	All	0.11	0/27063	0.31	2/36845 (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
3	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	PRO	CA-N-CD	-5.67	104.06	112.00
3	C	94	SER	CB-CA-C	-5.59	110.12	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	418	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5021	0	4960	99	0
1	H	3616	0	3614	91	0
2	B	5422	0	5493	126	0
2	I	4631	0	4662	139	0
3	C	6024	0	6029	122	0
3	J	649	0	657	23	0
4	D	260	0	133	6	0
5	E	103	0	53	2	0
5	F	269	0	137	11	0
6	G	195	0	100	4	0
6	K	195	0	100	5	0
7	G	52	0	0	0	0
7	K	32	0	0	0	0
All	All	26469	0	25938	527	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 (527) 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)
2:I:253:PHE:HB3	2:I:338:PRO:HG3	1.57	0.86
1:A:396:THR:HG21	5:E:16:C:H41	1.40	0.85
1:A:538:MET:HE1	1:A:546:MET:HE2	1.62	0.79
2:B:656:GLN:NE2	3:C:44:TYR:O	2.17	0.77
2:I:102:LEU:HD23	2:I:264:ILE:HD13	1.68	0.75
2:I:538:MET:HB3	2:I:543:THR:HG21	1.68	0.74
3:C:150:ARG:O	3:C:489:GLN:NE2	2.20	0.73
1:H:436:VAL:HG23	1:H:441:ASP:HB2	1.71	0.73
2:B:253:PHE:HB3	2:B:338:PRO:HG3	1.68	0.73
2:I:304:LYS:HB3	2:I:307:GLU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:ASP:OD1	3:C:186:ARG:NH2	2.21	0.71
1:H:180:ARG:HG3	1:H:184:LYS:HE3	1.71	0.70
3:J:119:LEU:HD12	3:J:123:ARG:HH12	1.57	0.70
2:B:32:THR:HG22	2:B:34:THR:H	1.57	0.69
1:H:340:GLU:OE2	1:H:458:LYS:NZ	2.18	0.69
3:C:417:ILE:HG22	3:C:419:PRO:HD2	1.76	0.68
1:H:574:MET:HE3	2:I:467:ILE:HG22	1.74	0.67
2:I:599:ASN:ND2	2:I:601:VAL:O	2.27	0.67
2:B:396:TYR:HB3	2:B:399:THR:HB	1.75	0.67
2:I:306:ASN:ND2	2:I:393:MET:SD	2.68	0.67
3:C:317:ARG:NH1	3:C:323:SER:O	2.27	0.67
3:C:46:THR:HG22	3:C:47:SER:H	1.61	0.66
3:C:706:THR:OG1	3:C:708:ASP:O	2.13	0.66
3:C:99:ALA:HB1	3:C:103:VAL:HG21	1.77	0.66
3:C:331:ARG:HG3	3:C:332:SER:H	1.59	0.66
1:H:189:TRP:HB2	2:I:315:ARG:HH22	1.59	0.66
3:C:747:ASP:OD1	3:C:750:ARG:NH2	2.29	0.66
2:I:246:PRO:HD3	2:I:395:MET:HE1	1.78	0.66
2:I:467:ILE:HA	2:I:475:HIS:O	1.94	0.66
2:B:362:ASP:OD2	2:B:364:LYS:NZ	2.28	0.66
2:I:538:MET:HE3	3:J:52:VAL:HG12	1.77	0.65
1:H:618:PRO:HB2	1:H:621:TYR:HE1	1.60	0.65
3:C:157:PRO:HD3	3:C:237:THR:HG21	1.77	0.65
1:H:321:TRP:HB2	2:I:369:MET:HE1	1.79	0.65
2:I:251:ARG:HA	2:I:254:VAL:HG22	1.79	0.65
1:A:110:THR:HG22	1:A:111:SER:H	1.60	0.65
1:A:255:HIS:NE2	1:A:282:GLN:OE1	2.29	0.64
2:B:87:LEU:HD13	2:B:407:SER:HA	1.79	0.64
3:C:691:GLN:HE21	3:C:727:PHE:HB3	1.63	0.64
2:B:589:GLU:OE2	3:C:113:GLN:NE2	2.30	0.64
1:H:528:GLN:OE1	1:H:535:GLN:NE2	2.31	0.64
2:I:16:GLN:HA	2:I:19:LEU:HD23	1.80	0.64
2:B:148:GLN:NE2	2:B:176:TYR:O	2.30	0.64
2:B:627:PRO:HB3	3:C:122:ILE:HD13	1.78	0.64
3:C:237:THR:HG22	3:C:239:GLU:H	1.62	0.63
3:C:360:THR:HG22	3:C:362:PRO:HD3	1.79	0.63
1:H:469:VAL:O	1:H:472:LYS:HB2	1.97	0.63
3:C:547:ASP:OD2	1:H:248:GLN:NE2	2.22	0.63
3:C:576:GLU:OE2	3:C:599:LYS:NZ	2.27	0.62
2:B:104:TYR:HE1	2:B:109:LYS:HE3	1.64	0.62
3:C:77:LEU:HD23	3:C:78:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:MET:HE1	2:I:19:LEU:HD11	1.82	0.62
3:C:572:ASN:HA	3:C:577:TYR:HB2	1.81	0.62
1:A:190:ASP:O	2:B:315:ARG:NH2	2.33	0.61
1:A:232:LEU:HD13	1:A:390:LYS:HE3	1.83	0.61
3:J:61:THR:OG1	3:J:87:ARG:NH1	2.32	0.61
1:A:146:CYS:HB3	3:C:691:GLN:OE1	2.00	0.61
1:A:538:MET:HE3	1:A:542:GLN:HG3	1.83	0.61
2:B:351:GLU:HG2	2:B:363:ARG:HD3	1.81	0.61
3:C:691:GLN:NE2	3:C:693:GLY:O	2.30	0.60
2:I:106:ILE:HD13	2:I:110:LEU:HD13	1.83	0.60
1:A:229:ARG:NH2	4:D:4:G:OP2	2.35	0.60
1:A:517:ASN:ND2	3:C:143:TYR:O	2.32	0.60
2:B:290:PHE:O	3:C:394:LYS:NZ	2.35	0.60
2:I:148:GLN:NE2	2:I:149:ASN:OD1	2.35	0.60
3:C:270:GLU:OE1	3:C:274:ARG:NH1	2.35	0.60
1:A:110:THR:OG1	1:A:116:ASP:OD2	2.19	0.59
2:B:60:ILE:HD11	2:B:389:LEU:HD11	1.84	0.59
2:B:333:GLU:O	2:B:337:ILE:HG12	2.02	0.59
2:B:701:ARG:NH2	2:B:704:ARG:HH22	2.00	0.59
1:A:576:ARG:O	1:A:580:MET:HG3	2.02	0.59
3:J:118:ASP:O	3:J:121:VAL:N	2.35	0.59
3:C:284:THR:O	3:C:288:ASN:ND2	2.34	0.59
2:I:410:ARG:NH1	2:I:412:GLU:OE2	2.36	0.59
2:B:132:ASN:ND2	5:F:6:C:OP1	2.33	0.59
1:H:604:ASN:HB3	1:H:607:VAL:HB	1.84	0.59
2:B:376:LEU:HB3	2:B:385:ILE:HD11	1.84	0.59
2:B:514:THR:HG22	2:B:516:GLN:HE21	1.68	0.59
1:A:264:ARG:NH2	1:A:459:TYR:O	2.36	0.59
2:B:701:ARG:HH22	2:B:704:ARG:HH22	1.51	0.58
3:C:418:GLU:O	3:C:423:GLN:NE2	2.36	0.58
1:A:71:ILE:HG21	3:C:752:LEU:HD21	1.85	0.58
2:B:699:GLU:OE1	2:B:703:LYS:NZ	2.31	0.58
1:A:324:ALA:HB2	2:B:354:VAL:HG13	1.85	0.58
1:H:559:ASN:HD21	1:H:604:ASN:HD22	1.49	0.58
1:H:235:ALA:HB2	1:H:344:LEU:HD12	1.84	0.58
2:B:555:THR:HG23	2:B:557:LEU:HG	1.85	0.58
3:C:127:ASP:O	3:C:131:GLN:OE1	2.22	0.57
1:A:44:LEU:HD21	3:C:738:GLU:HG3	1.86	0.57
2:B:231:LYS:HE2	5:F:7:C:H41	1.68	0.57
1:A:430:LEU:HD12	1:A:446:LEU:HD23	1.86	0.57
1:H:203:ARG:NH1	1:H:204:ILE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:578:ALA:HB1	3:J:121:VAL:HG21	1.86	0.57
2:B:103:LYS:HE3	2:B:325:LEU:HD22	1.85	0.57
1:H:451:MET:HE1	1:H:464:VAL:HG22	1.85	0.57
1:H:368:ALA:HB2	2:I:519:LEU:HD12	1.87	0.57
1:A:56:GLN:OE1	1:A:134:ARG:NH2	2.37	0.57
1:A:344:LEU:O	1:A:384:VAL:HG23	2.04	0.57
3:C:69:MET:O	3:C:97:THR:OG1	2.20	0.57
1:H:273:VAL:HG23	1:H:478:LEU:HD13	1.87	0.57
2:I:38:LEU:HD21	2:I:366:LEU:HD22	1.87	0.57
3:C:365:ARG:HD2	3:C:388:ARG:HH22	1.70	0.56
3:C:72:SER:O	3:C:85:LYS:NZ	2.39	0.56
1:H:181:THR:O	1:H:185:ARG:HD3	2.05	0.56
2:B:652:GLU:OE2	3:C:46:THR:N	2.26	0.56
1:H:260:ILE:HG21	1:H:274:ILE:HG12	1.87	0.56
2:I:133:LEU:HB3	2:I:137:ILE:HD11	1.86	0.56
1:A:89:ASP:O	1:A:93:ALA:HA	2.05	0.56
2:I:91:PHE:HB3	2:I:321:PHE:HZ	1.71	0.56
3:C:670:ARG:HE	3:C:672:ILE:HD11	1.69	0.56
2:I:545:ARG:HG2	2:I:549:MET:HE1	1.86	0.56
2:I:22:TYR:OH	2:I:484:ALA:O	2.15	0.55
3:C:25:LYS:NZ	3:C:26:GLU:OE2	2.33	0.55
2:B:463:SER:OG	2:B:464:PRO:HD3	2.05	0.55
1:H:397:ARG:NH1	1:H:413:PRO:O	2.40	0.55
2:B:656:GLN:HE22	3:C:45:THR:HG22	1.72	0.55
3:C:670:ARG:NH2	1:H:470:GLU:OE1	2.40	0.55
2:B:692:VAL:HG22	3:C:13:LEU:HD22	1.87	0.55
3:J:61:THR:HA	3:J:87:ARG:HD2	1.88	0.55
2:I:295:THR:O	2:I:465:ALA:N	2.40	0.55
1:A:128:SER:O	1:A:132:VAL:HG23	2.06	0.54
1:H:417:ARG:NH1	1:H:423:CYS:SG	2.79	0.54
2:B:80:HIS:ND1	2:B:83:SER:OG	2.34	0.54
2:B:667:PRO:O	2:B:670:LEU:HB3	2.07	0.54
2:I:332:MET:O	2:I:336:ASN:ND2	2.39	0.54
2:B:289:THR:HG21	3:C:371:LYS:HD2	1.89	0.54
3:J:60:MET:N	3:J:88:THR:O	2.39	0.54
1:A:384:VAL:HG11	1:A:548:LEU:HG	1.88	0.54
1:H:180:ARG:O	1:H:184:LYS:HG3	2.08	0.54
1:A:71:ILE:HD13	3:C:752:LEU:HD21	1.90	0.54
1:H:434:HIS:ND1	1:H:434:HIS:O	2.41	0.54
1:A:356:GLU:OE1	2:B:534:LYS:NZ	2.40	0.54
2:B:102:LEU:HD22	2:B:264:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:ARG:NH1	2:B:637:ASN:OD1	2.41	0.54
1:H:430:LEU:HD12	1:H:446:LEU:HD23	1.89	0.54
2:B:668:GLU:HG3	3:C:723:GLN:HG2	1.90	0.54
1:H:519:LEU:HD21	1:H:521:LEU:HG	1.89	0.54
3:J:118:ASP:OD1	3:J:119:LEU:N	2.41	0.54
2:B:105:TRP:HH2	2:B:256:ILE:HG23	1.72	0.53
3:C:700:ARG:O	3:C:717:ARG:NH2	2.41	0.53
1:H:586:PHE:HB2	2:I:461:LEU:HB3	1.89	0.53
2:I:403:LEU:HD12	2:I:406:ILE:HD11	1.90	0.53
3:C:163:ASN:N	3:C:305:ASP:OD1	2.41	0.53
2:B:172:ASP:OD1	2:B:216:ARG:NH2	2.39	0.53
1:A:375:TYR:O	1:A:379:VAL:HG22	2.09	0.53
2:B:112:LYS:HD2	2:B:112:LYS:N	2.24	0.53
3:C:189:HIS:HD2	3:C:297:ARG:HH11	1.55	0.53
3:C:341:ASP:O	3:C:512:ASN:ND2	2.41	0.53
1:A:215:LEU:HG	1:A:579:MET:HE1	1.90	0.53
3:C:405:GLU:HG2	3:C:406:PRO:HD3	1.90	0.53
2:B:662:ILE:HG12	2:B:684:LEU:HD11	1.89	0.53
3:C:46:THR:O	3:C:47:SER:OG	2.23	0.53
3:C:211:SER:O	3:C:215:ILE:HD12	2.08	0.53
2:B:604:LYS:NZ	5:F:17:U:OP1	2.36	0.53
2:B:667:PRO:HB2	3:C:176:CYS:SG	2.49	0.53
2:I:111:PRO:HA	2:I:159:LEU:HD23	1.91	0.53
2:I:410:ARG:HB2	2:I:413:LEU:HD12	1.91	0.53
2:B:699:GLU:O	2:B:703:LYS:HG2	2.08	0.53
2:I:39:GLU:O	2:I:43:ARG:HG3	2.09	0.53
2:I:62:THR:HG22	2:I:64:CYS:H	1.74	0.53
1:H:192:ILE:HD12	2:I:332:MET:HB3	1.90	0.53
3:C:462:LEU:O	3:C:477:LYS:NZ	2.32	0.52
2:I:405:LEU:HD13	2:I:408:ILE:HD11	1.91	0.52
2:B:657:ARG:HD3	3:C:23:ALA:HA	1.91	0.52
1:H:353:ILE:HG21	1:H:376:ILE:HD12	1.91	0.52
1:A:41:ILE:HD11	1:A:145:LEU:HD21	1.91	0.52
2:I:102:LEU:HD11	2:I:325:LEU:HD22	1.90	0.52
2:B:152:ARG:NH2	2:B:167:ASP:OD2	2.43	0.52
2:B:229:MET:SD	2:B:243:ILE:HG13	2.49	0.52
2:I:557:LEU:HD12	2:I:586:LEU:HD23	1.91	0.52
1:A:482:SER:HB2	4:D:3:A:H1'	1.91	0.52
3:J:50:TYR:O	3:J:54:LYS:N	2.42	0.52
2:B:403:LEU:HG	2:B:450:VAL:HG11	1.91	0.52
2:B:229:MET:HE1	2:B:245:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:ARG:NH1	3:C:413:TYR:O	2.35	0.52
1:A:496:ARG:HG2	2:B:490:LEU:HD22	1.90	0.52
2:I:428:PHE:HB2	2:I:436:MET:HE2	1.92	0.52
2:I:545:ARG:HH12	2:I:561:GLN:HA	1.75	0.52
3:J:117:GLU:HA	3:J:120:LYS:NZ	2.25	0.52
1:A:89:ASP:O	1:A:93:ALA:N	2.43	0.52
1:H:558:ASN:HB3	2:I:25:PRO:HD2	1.92	0.52
1:A:610:LEU:HD22	2:B:1:MET:HE2	1.90	0.51
2:B:145:PHE:O	2:B:149:ASN:ND2	2.38	0.51
3:C:393:ILE:HB	3:C:481:VAL:HG22	1.91	0.51
2:I:223:MET:HE1	2:I:249:LEU:HB2	1.90	0.51
1:A:89:ASP:O	1:A:93:ALA:CA	2.58	0.51
2:B:391:MET:HE2	2:B:393:MET:O	2.10	0.51
2:I:12:PRO:HA	2:I:15:THR:HG22	1.91	0.51
2:I:455:SER:HB3	2:I:458:LYS:HB2	1.91	0.51
1:H:378:ILE:HG13	1:H:379:VAL:HG13	1.93	0.51
2:I:148:GLN:NE2	2:I:175:THR:O	2.34	0.51
1:A:344:LEU:HA	1:A:383:LYS:HB3	1.93	0.51
3:C:543:ASP:OD1	3:C:543:ASP:N	2.42	0.51
2:B:518:ASN:N	2:B:521:THR:OG1	2.44	0.51
1:H:334:PRO:HG2	1:H:605:PRO:HB3	1.92	0.51
1:H:515:GLU:OE1	1:H:516:ASN:ND2	2.42	0.51
2:I:568:SER:N	2:I:571:THR:OG1	2.39	0.51
3:C:599:LYS:O	3:C:603:GLN:HG2	2.11	0.51
1:H:218:LEU:HD23	1:H:614:TRP:CD1	2.45	0.51
1:H:232:LEU:HB2	1:H:391:TRP:CE2	2.46	0.51
1:H:263:ILE:HD11	1:H:466:SER:HB2	1.93	0.51
1:A:560:PRO:HD3	2:B:27:PRO:HB3	1.93	0.51
2:B:226:LEU:HD23	2:B:246:PRO:HB3	1.93	0.51
2:B:659:THR:HG23	3:C:38:TYR:HE1	1.75	0.51
2:I:21:ALA:O	2:I:235:ARG:NH2	2.44	0.51
2:B:567:HIS:HE1	2:B:576:GLU:HB2	1.76	0.51
1:H:216:PRO:HB3	1:H:594:GLU:HB3	1.93	0.51
2:I:296:GLY:HA3	2:I:436:MET:HE1	1.93	0.51
2:I:494:GLY:HA2	3:J:48:LEU:HD22	1.93	0.51
1:A:402:LEU:HB3	1:A:485:ARG:HD3	1.93	0.50
6:G:7:A:H2'	6:G:8:A:C8	2.45	0.50
2:I:105:TRP:CD1	2:I:110:LEU:HD12	2.46	0.50
3:C:299:MET:HA	3:C:302:VAL:HG12	1.94	0.50
2:I:74:GLY:O	2:I:448:LYS:NZ	2.44	0.50
1:A:46:SER:HB2	1:A:57:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:CYS:HB2	1:A:423:CYS:HB2	1.94	0.50
2:I:136:PRO:O	2:I:140:GLU:HG2	2.11	0.50
2:B:42:ILE:HB	2:B:376:LEU:HD11	1.94	0.50
3:C:171:LEU:HD23	3:C:213:VAL:HG13	1.93	0.50
2:B:675:SER:O	3:C:725:ARG:NH1	2.32	0.50
2:B:665:LEU:HD21	2:B:688:LEU:HD13	1.93	0.49
2:I:32:THR:HG22	2:I:351:GLU:HB2	1.94	0.49
2:B:295:THR:O	2:B:465:ALA:N	2.43	0.49
3:C:83:LYS:NZ	3:C:85:LYS:O	2.40	0.49
1:H:371:LEU:HD21	1:H:509:VAL:HG11	1.93	0.49
1:A:160:GLU:OE1	1:A:160:GLU:N	2.40	0.49
2:I:161:TYR:O	2:I:165:ILE:HG12	2.12	0.49
2:I:444:ARG:HA	2:I:454:MET:HE3	1.95	0.49
1:H:208:ARG:NH2	2:I:437:PHE:HB3	2.26	0.49
1:H:273:VAL:HG11	1:H:480:ILE:HD11	1.94	0.49
1:H:372:VAL:HG21	2:I:523:ALA:HB3	1.94	0.49
2:I:349:MET:HE1	2:I:380:VAL:HG22	1.95	0.49
2:B:143:VAL:O	2:B:147:GLU:HG2	2.12	0.49
1:H:183:LEU:HD23	2:I:340:MET:HG3	1.94	0.49
1:A:605:PRO:HG2	1:A:606:ILE:HD12	1.95	0.49
2:B:617:MET:HE3	2:B:619:GLN:HB2	1.95	0.49
2:I:546:THR:HA	2:I:549:MET:HE2	1.94	0.49
2:I:50:LYS:HE3	2:I:71:ASN:HA	1.93	0.49
2:I:146:LEU:HD12	2:I:164:ALA:HB1	1.95	0.49
2:B:493:ASN:O	3:C:57:LEU:HD22	2.13	0.48
1:H:373:ASP:O	1:H:376:ILE:N	2.46	0.48
2:B:490:LEU:O	2:B:490:LEU:HD23	2.12	0.48
2:B:556:PRO:HB2	2:B:563:ALA:HB2	1.95	0.48
2:B:666:PHE:O	2:B:669:VAL:HG12	2.13	0.48
3:C:708:ASP:C	3:C:710:GLY:H	2.19	0.48
2:B:595:LEU:HD12	3:C:119:VAL:HG13	1.95	0.48
1:H:194:THR:HG22	2:I:323:ARG:HH12	1.78	0.48
1:H:269:THR:O	1:H:463:SER:OG	2.31	0.48
2:I:238:LEU:O	2:I:240:ARG:NH1	2.46	0.48
2:I:245:THR:OG1	2:I:251:ARG:NH2	2.45	0.48
1:A:462:HIS:NE2	1:A:479:LYS:HD2	2.28	0.48
2:B:31:GLY:HA3	4:D:7:A:O3'	2.14	0.48
3:C:145:ARG:O	3:C:145:ARG:HD3	2.14	0.48
1:H:270:PRO:O	1:H:273:VAL:HG22	2.14	0.48
2:I:518:ASN:H	2:I:521:THR:HG1	1.61	0.48
3:C:265:ASP:OD2	3:C:310:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLN:O	1:A:311:GLN:HG3	2.13	0.48
2:I:103:LYS:HA	2:I:106:ILE:HG22	1.96	0.48
3:C:134:PHE:O	1:H:308:GLU:HG2	2.14	0.48
3:C:667:THR:OG1	3:C:669:ASN:OD1	2.24	0.48
3:C:701:CYS:HB2	3:C:719:CYS:SG	2.53	0.48
3:C:299:MET:HE3	3:C:303:LEU:HG	1.96	0.47
2:I:80:HIS:CE1	2:I:82:ALA:HB3	2.49	0.47
3:J:56:TRP:HB3	3:J:89:ARG:HB3	1.96	0.47
2:B:568:SER:H	2:B:571:THR:HG1	1.57	0.47
3:C:593:THR:HB	3:C:639:GLN:HA	1.96	0.47
2:I:106:ILE:HD11	2:I:331:ILE:HD12	1.96	0.47
2:I:548:PHE:HE2	3:J:96:ASP:HB3	1.78	0.47
2:B:127:PHE:HB2	2:B:222:GLN:HB3	1.96	0.47
3:C:332:SER:OG	3:C:376:ASN:ND2	2.47	0.47
1:H:528:GLN:HB3	1:H:535:GLN:HE21	1.79	0.47
2:I:447:LEU:HD12	2:I:452:ILE:HG21	1.95	0.47
1:A:326:TYR:CZ	4:D:7:A:H8	2.33	0.47
1:H:418:ASP:HB3	1:H:424:GLN:NE2	2.30	0.47
2:I:105:TRP:CZ3	2:I:109:LYS:HE2	2.50	0.47
2:I:494:GLY:HA2	3:J:48:LEU:HD13	1.96	0.47
1:A:499:ILE:HD11	2:B:528:ILE:HD12	1.96	0.47
2:B:294:VAL:HB	2:B:430:CYS:O	2.14	0.47
3:C:573:MET:HE1	3:C:630:GLY:HA3	1.97	0.47
5:F:8:U:H2'	5:F:9:G:H8	1.79	0.47
3:C:118:VAL:HG13	3:C:206:VAL:HG11	1.97	0.47
1:H:226:SER:HA	1:H:331:MET:HE2	1.96	0.47
2:I:13:THR:HG21	2:I:476:HIS:HB2	1.97	0.47
2:B:401:THR:OG1	2:B:420:SER:O	2.24	0.46
1:H:211:GLN:NE2	1:H:212:MET:O	2.47	0.46
3:C:90:ASP:O	3:C:96:ARG:HG2	2.15	0.46
1:A:365:ASP:O	1:A:369:GLU:HG2	2.16	0.46
2:B:410:ARG:HH11	2:B:446:THR:HG22	1.79	0.46
2:I:623:ASP:OD2	2:I:625:SER:OG	2.31	0.46
1:A:538:MET:CE	1:A:546:MET:HE2	2.40	0.46
2:B:32:THR:HG21	2:B:352:GLY:O	2.16	0.46
1:H:342:VAL:HG12	1:H:345:ARG:HH22	1.81	0.46
1:H:375:TYR:CE2	1:H:502:ALA:HB2	2.50	0.46
1:H:543:TRP:O	1:H:547:ILE:HG12	2.15	0.46
3:C:365:ARG:HD2	3:C:388:ARG:NH2	2.31	0.46
1:H:525:PRO:HD2	1:H:540:LEU:HD22	1.97	0.46
2:I:475:HIS:NE2	2:I:477:ARG:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LEU:O	2:B:406:ILE:HG23	2.15	0.46
1:A:568:ASN:OD1	1:A:571:ARG:NH2	2.43	0.46
2:B:422:ASP:OD1	2:B:422:ASP:N	2.49	0.46
1:H:265:GLU:OE1	1:H:271:ALA:HB2	2.16	0.46
2:I:317:MET:HG3	2:I:406:ILE:HD13	1.98	0.46
3:C:438:SER:HA	3:C:441:MET:HG2	1.97	0.46
3:C:585:VAL:HG13	3:C:627:ILE:HG23	1.97	0.46
2:I:274:PRO:HA	2:I:280:LYS:HE3	1.98	0.46
2:I:601:VAL:HG13	3:J:60:MET:SD	2.54	0.46
3:C:517:LEU:HG	3:C:518:ILE:HG13	1.98	0.46
2:I:523:ALA:HA	2:I:526:MET:HG2	1.97	0.46
1:A:126:GLU:O	1:A:130:ALA:N	2.46	0.45
1:A:557:TYR:CG	1:A:606:ILE:HD13	2.51	0.45
2:B:600:PRO:HG2	3:C:74:GLU:HB2	1.98	0.45
2:I:172:ASP:H	2:I:216:ARG:HH21	1.64	0.45
1:A:483:PHE:HD2	1:A:488:LEU:HG	1.80	0.45
1:A:614:TRP:HB2	2:B:1:MET:HG3	1.99	0.45
2:I:322:LEU:HD23	2:I:325:LEU:HD21	1.98	0.45
1:A:512:ARG:NH1	2:B:9:GLU:OE2	2.50	0.45
2:B:612:ARG:HB2	2:B:618:PRO:HA	1.98	0.45
3:C:348:LYS:NZ	3:C:360:THR:HG21	2.30	0.45
3:C:669:ASN:OD1	3:C:670:ARG:N	2.50	0.45
2:I:489:ALA:HB1	2:I:491:VAL:HG12	1.98	0.45
2:I:576:GLU:HG2	2:I:577:VAL:N	2.31	0.45
2:B:393:MET:HE2	2:B:395:MET:HG2	1.98	0.45
3:C:530:LEU:HD11	3:C:544:ILE:HG22	1.97	0.45
2:B:391:MET:HE3	2:B:396:TYR:HD1	1.81	0.45
3:C:334:LYS:HE2	3:C:375:GLN:HE21	1.82	0.45
3:C:683:LYS:HE3	3:C:713:MET:HA	1.98	0.45
2:I:11:ASN:OD1	2:I:14:THR:HG23	2.17	0.45
2:I:122:ARG:HG2	2:I:123:GLN:H	1.82	0.45
1:A:450:ILE:HA	1:A:475:LEU:O	2.17	0.45
2:B:298:LEU:HB2	2:B:461:LEU:HD13	1.98	0.45
1:H:583:ARG:HH12	2:I:466:GLY:HA3	1.81	0.45
1:A:185:ARG:NH1	2:B:217:GLU:OE2	2.43	0.45
1:A:191:VAL:O	2:B:336:ASN:ND2	2.50	0.45
1:A:353:ILE:HD12	1:A:380:GLY:HA2	1.98	0.45
2:B:105:TRP:HB2	2:B:263:GLU:HG2	1.99	0.45
3:C:189:HIS:CD2	3:C:297:ARG:HH11	2.34	0.45
6:G:3:C:H2'	6:G:4:A:C8	2.52	0.45
2:I:85:LEU:HD21	2:I:316:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD1	1:A:83:ASP:N	2.50	0.44
1:H:508:VAL:O	1:H:511:SER:HB3	2.18	0.44
2:B:281:LEU:HB3	3:C:150:ARG:NH1	2.31	0.44
3:C:414:GLY:HA3	3:C:416:PHE:CZ	2.52	0.44
2:I:58:LEU:O	2:I:388:ARG:NH1	2.49	0.44
2:I:165:ILE:HA	2:I:168:VAL:HG12	2.00	0.44
2:I:499:THR:O	2:I:503:MET:HG2	2.16	0.44
1:A:232:LEU:HB2	1:A:391:TRP:CE2	2.53	0.44
3:C:185:LYS:HZ3	3:C:708:ASP:CG	2.25	0.44
3:C:464:LEU:HD22	3:C:481:VAL:HG11	1.99	0.44
1:H:374:LYS:O	1:H:378:ILE:HG12	2.17	0.44
2:B:357:LYS:HB2	2:B:357:LYS:HE3	1.81	0.44
3:C:582:GLU:O	3:C:586:GLN:HG3	2.17	0.44
3:C:690:VAL:HG23	3:C:692:THR:OG1	2.18	0.44
1:H:614:TRP:HB2	2:I:1:MET:HG2	1.98	0.44
2:I:99:MET:HA	2:I:102:LEU:HG	1.98	0.44
3:C:424:THR:HG22	3:C:426:GLY:H	1.82	0.44
3:C:520:PRO:O	3:C:521:THR:OG1	2.33	0.44
2:I:495:THR:OG1	2:I:496:ASN:N	2.49	0.44
3:J:56:TRP:HH2	3:J:74:LYS:HB3	1.81	0.44
1:A:103:ASP:OD2	1:A:105:SER:OG	2.27	0.44
5:F:15:G:H2'	5:F:16:C:C6	2.52	0.44
1:H:581:GLU:OE2	1:H:583:ARG:HD2	2.18	0.44
2:I:94:LYS:HG2	2:I:95:TYR:H	1.81	0.44
2:I:545:ARG:HH22	2:I:561:GLN:HA	1.82	0.44
1:A:3:ASP:OD1	1:A:3:ASP:N	2.48	0.44
1:A:418:ASP:OD1	1:A:422:ASN:N	2.51	0.44
1:A:3:ASP:HB3	2:B:104:TYR:HE2	1.83	0.44
2:B:592:ARG:NE	3:C:114:THR:O	2.50	0.44
1:H:496:ARG:HG2	2:I:490:LEU:HD12	1.99	0.44
1:A:577:HIS:ND1	2:B:12:PRO:HD2	2.32	0.44
3:C:142:ARG:O	3:C:249:HIS:HA	2.16	0.44
2:I:324:LYS:HB3	2:I:324:LYS:HE3	1.78	0.44
1:A:139:GLN:OE1	3:C:733:ILE:HG12	2.18	0.43
1:A:577:HIS:CE1	2:B:11:ASN:HB2	2.53	0.43
2:B:177:GLU:O	2:B:177:GLU:HG3	2.18	0.43
3:C:49:LYS:NZ	6:G:4:A:OP1	2.49	0.43
1:H:520:ASN:HB3	1:H:523:VAL:HG13	2.00	0.43
2:I:150:LEU:HG	2:I:152:ARG:HG2	2.00	0.43
1:A:543:TRP:CE2	1:A:547:ILE:HD11	2.53	0.43
2:B:544:ARG:NH1	5:E:14:U:OP1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:LYS:C	3:C:31:MET:H	2.27	0.43
2:I:174:THR:O	2:I:214:PHE:N	2.50	0.43
1:A:442:ASN:HB3	1:A:482:SER:HB3	2.00	0.43
3:C:274:ARG:HB3	3:C:541:PHE:CE1	2.54	0.43
1:H:566:LEU:O	1:H:570:ARG:HG3	2.18	0.43
2:I:39:GLU:HA	2:I:42:ILE:HG22	2.01	0.43
2:I:79:PHE:HA	2:I:449:LEU:O	2.18	0.43
2:B:22:TYR:O	2:B:23:THR:OG1	2.24	0.43
1:A:343:LEU:C	1:A:345:ARG:H	2.26	0.43
2:B:581:ARG:NH2	3:C:120:ASN:OD1	2.46	0.43
6:G:3:C:H2'	6:G:4:A:H8	1.83	0.43
1:A:228:TRP:NE1	1:A:232:LEU:O	2.45	0.43
2:B:246:PRO:HD3	2:B:393:MET:HE1	2.00	0.43
2:I:258:GLU:O	2:I:262:LYS:HG3	2.19	0.43
1:A:465:PHE:CE1	1:A:478:LEU:HD23	2.54	0.43
1:A:582:ARG:HH22	1:A:621:TYR:HB3	1.83	0.43
1:H:179:PHE:HZ	2:I:337:ILE:HD13	1.83	0.43
1:H:451:MET:HE3	1:H:475:LEU:HB3	2.00	0.43
2:I:76:SER:H	2:I:453:ASN:CG	2.27	0.43
2:I:284:LEU:HD11	2:I:416:SER:HB3	2.01	0.43
1:A:344:LEU:HG	1:A:384:VAL:HG22	2.00	0.43
1:A:487:LYS:HG2	2:B:25:PRO:HB3	2.00	0.43
3:C:182:LEU:HD13	3:C:729:TYR:CE1	2.54	0.43
1:H:180:ARG:HH22	1:H:190:ASP:HB2	1.84	0.43
2:I:146:LEU:HD11	2:I:165:ILE:HD13	2.00	0.43
2:B:280:LYS:HB3	2:B:280:LYS:HE2	1.83	0.43
2:B:498:MET:H	2:B:498:MET:HG2	1.69	0.43
2:I:144:GLU:O	2:I:147:GLU:HG3	2.19	0.43
2:I:430:CYS:SG	2:I:436:MET:HG3	2.59	0.43
2:I:600:PRO:HB2	3:J:60:MET:SD	2.58	0.43
1:A:65:ARG:HH12	1:A:81:GLU:HA	1.83	0.42
1:A:454:ASP:CG	1:A:464:VAL:HG21	2.44	0.42
2:B:506:ASN:ND2	5:F:14:U:O5'	2.52	0.42
3:C:210:GLU:OE2	5:F:17:U:H5''	2.19	0.42
3:C:339:ASN:HD21	3:C:371:LYS:HE2	1.84	0.42
1:A:375:TYR:HA	1:A:378:ILE:HG12	2.00	0.42
1:A:440:THR:OG1	5:F:5:G:O6	2.30	0.42
1:A:468:LYS:HE3	1:A:471:GLU:HA	2.01	0.42
2:B:588:GLU:HA	2:B:591:LEU:HB2	2.00	0.42
3:C:66:PRO:HD2	3:C:100:ASN:HA	2.01	0.42
2:I:122:ARG:HG2	2:I:123:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:617:MET:HE1	2:I:5:THR:HG21	2.02	0.42
2:I:118:LEU:HD22	2:I:139:LEU:HD13	2.01	0.42
2:I:298:LEU:HD13	2:I:461:LEU:HB2	2.01	0.42
3:J:63:SER:O	3:J:76:LYS:NZ	2.52	0.42
3:C:690:VAL:HG23	3:C:692:THR:HG1	1.84	0.42
1:H:571:ARG:CZ	2:I:458:LYS:HG2	2.49	0.42
2:I:328:PRO:HB2	2:I:330:TRP:CD1	2.54	0.42
3:C:65:TRP:HB3	3:C:98:ARG:HB3	2.01	0.42
2:I:104:TYR:CE1	2:I:108:VAL:HG21	2.55	0.42
1:A:35:GLU:HB3	1:A:62:TRP:HZ2	1.84	0.42
1:A:451:MET:HB2	1:A:475:LEU:HB2	2.02	0.42
3:C:728:GLN:HG3	3:C:728:GLN:O	2.19	0.42
1:H:383:LYS:O	1:H:387:VAL:HG23	2.20	0.42
2:I:224:ARG:O	2:I:346:LEU:N	2.45	0.42
2:I:408:ILE:HD12	2:I:417:HIS:HB3	2.00	0.42
1:A:239:TYR:HA	1:A:425:PHE:O	2.18	0.42
2:B:118:LEU:HD21	2:B:252:GLY:HA2	2.02	0.42
2:I:32:THR:H	6:K:7:A:H5'	1.84	0.42
2:I:281:LEU:HD12	2:I:470:PHE:HB3	2.02	0.42
2:I:498:MET:HE1	2:I:630:PHE:HB2	2.02	0.42
2:B:30:TYR:HB3	4:D:8:U:H1'	2.01	0.42
1:H:231:LEU:HG	1:H:232:LEU:HD22	2.02	0.42
1:H:334:PRO:HA	1:H:335:PRO:HD3	1.96	0.42
2:I:87:LEU:HD12	2:I:406:ILE:O	2.20	0.42
5:F:8:U:H2'	5:F:9:G:C8	2.54	0.42
1:A:4:ARG:HG3	1:A:13:TRP:CG	2.54	0.41
3:C:365:ARG:NH2	3:C:366:PHE:O	2.50	0.41
3:C:417:ILE:CG2	3:C:419:PRO:HD2	2.49	0.41
1:H:402:LEU:HD11	1:H:488:LEU:HD12	2.02	0.41
1:H:429:VAL:HG23	1:H:447:ILE:HG12	2.02	0.41
1:H:583:ARG:NH1	2:I:467:ILE:HG13	2.35	0.41
3:J:58:ILE:O	3:J:90:ALA:N	2.43	0.41
1:A:506:SER:HB3	2:B:520:CYS:HB3	2.02	0.41
1:A:577:HIS:CD2	2:B:467:ILE:HD13	2.55	0.41
2:B:115:TYR:HA	2:B:158:LEU:HD13	2.03	0.41
1:H:572:LEU:HD11	1:H:597:VAL:HG21	2.02	0.41
1:H:596:LYS:HD3	2:I:457:SER:HB2	2.02	0.41
2:I:329:ASP:O	2:I:332:MET:HB2	2.20	0.41
2:I:560:ASN:OD1	2:I:560:ASN:N	2.52	0.41
1:A:58:ASP:OD1	1:A:88:TYR:HB3	2.20	0.41
1:A:538:MET:CE	1:A:542:GLN:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:60:MET:O	3:J:87:ARG:HB3	2.20	0.41
1:A:583:ARG:HA	2:B:464:PRO:HG2	2.01	0.41
3:C:350:VAL:HA	3:C:360:THR:HG23	2.03	0.41
1:H:481:THR:HA	6:K:2:G:O2'	2.21	0.41
2:I:79:PHE:CG	2:I:313:ALA:HB2	2.55	0.41
2:I:482:ASN:HD22	2:I:514:THR:HB	1.86	0.41
2:I:496:ASN:OD1	2:I:499:THR:HB	2.20	0.41
2:B:484:ALA:HA	2:B:487:LEU:HG	2.03	0.41
2:B:661:ILE:HD13	3:C:19:GLU:HB3	2.03	0.41
3:C:109:LYS:HG2	3:C:110:TYR:H	1.86	0.41
3:C:716:SER:O	3:C:717:ARG:HG3	2.21	0.41
1:H:236:ASP:O	1:H:451:MET:HA	2.20	0.41
2:I:134:PRO:HD2	2:I:137:ILE:HD11	2.01	0.41
2:I:401:THR:O	2:I:405:LEU:HD23	2.20	0.41
1:H:208:ARG:HE	1:H:209:TRP:N	2.19	0.41
1:H:508:VAL:O	1:H:512:ARG:HG2	2.21	0.41
6:K:3:C:H42	6:K:8:A:H61	1.68	0.41
2:B:92:PHE:CD2	2:B:99:MET:HG3	2.55	0.41
3:C:147:LEU:HB3	3:C:380:GLN:NE2	2.36	0.41
1:H:462:HIS:NE2	1:H:479:LYS:HD2	2.36	0.41
2:B:223:MET:HG3	2:B:249:LEU:HB2	2.03	0.41
1:A:48:MET:HG3	3:C:736:TRP:CE2	2.55	0.41
1:A:64:ASP:OD2	3:C:753:LYS:NZ	2.52	0.41
1:A:71:ILE:O	1:A:75:LYS:NZ	2.52	0.41
1:A:468:LYS:HD3	1:A:473:GLN:NE2	2.36	0.41
1:A:586:PHE:HE2	2:B:463:SER:HB3	1.86	0.41
2:B:114:LYS:HD2	2:B:156:PRO:HB2	2.03	0.41
2:B:244:ALA:O	5:F:7:C:H1'	2.21	0.41
2:B:708:ARG:NE	3:C:14:ARG:HH12	2.19	0.41
2:I:30:TYR:HB2	6:K:7:A:H2	1.85	0.41
2:I:50:LYS:HE2	2:I:50:LYS:HB3	1.92	0.41
2:I:498:MET:HE2	2:I:631:LYS:HG2	2.01	0.41
3:C:210:GLU:HG2	3:C:211:SER:N	2.36	0.41
1:H:175:VAL:HG23	1:H:179:PHE:HD2	1.86	0.41
2:I:519:LEU:HD13	2:I:569:PHE:CE2	2.56	0.41
3:J:60:MET:HE3	3:J:94:VAL:HG11	2.03	0.41
1:A:374:LYS:HE3	1:A:374:LYS:HB3	1.90	0.40
1:A:520:ASN:HB3	1:A:523:VAL:HG13	2.02	0.40
2:B:297:GLU:OE2	2:B:468:GLY:HA3	2.20	0.40
3:C:691:GLN:HE21	3:C:727:PHE:CB	2.32	0.40
5:F:7:C:H2'	5:F:8:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:ARG:HH22	2:I:437:PHE:HB3	1.86	0.40
1:H:309:LYS:HE2	6:K:10:A:N1	2.36	0.40
1:H:375:TYR:HA	1:H:378:ILE:HG12	2.03	0.40
1:H:389:GLU:O	1:H:393:ILE:HG12	2.21	0.40
3:J:91:ASN:OD1	3:J:92:ILE:N	2.51	0.40
1:A:390:LYS:HD2	1:A:426:TRP:CE3	2.56	0.40
1:A:546:MET:HA	1:A:549:CYS:SG	2.62	0.40
2:B:708:ARG:HG3	3:C:17:VAL:HG11	2.03	0.40
1:H:232:LEU:HB2	1:H:391:TRP:NE1	2.37	0.40
1:H:242:CYS:HB2	1:H:423:CYS:HB2	2.02	0.40
1:H:448:ALA:HA	1:H:477:SER:O	2.22	0.40
2:I:467:ILE:HG12	2:I:476:HIS:HD2	1.86	0.40
1:A:269:THR:HG21	1:A:478:LEU:O	2.20	0.40
1:A:430:LEU:HB2	1:A:446:LEU:HB3	2.03	0.40
1:A:449:GLU:HG2	1:A:477:SER:HB2	2.03	0.40
1:A:560:PRO:HD2	4:D:5:A:OP1	2.21	0.40
2:B:679:THR:HG23	2:B:682:GLU:H	1.86	0.40
2:B:177:GLU:OE1	2:B:211:THR:OG1	2.33	0.40
2:B:442:THR:O	2:B:446:THR:HG23	2.20	0.40
2:B:493:ASN:ND2	2:B:503:MET:SD	2.94	0.40
2:B:599:ASN:HD22	2:B:629:CYS:HB3	1.86	0.40
2:B:676:ALA:HB3	3:C:35:PHE:CD2	2.56	0.40
1:H:577:HIS:ND1	2:I:12:PRO:HD2	2.36	0.40
2:I:169:MET:SD	2:I:170:GLU:HG2	2.61	0.40
3:J:119:LEU:HA	3:J:122:GLN:NE2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	619/622 (100%)	598 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	447/622 (72%)	426 (95%)	21 (5%)	0	100	100
2	B	670/710 (94%)	643 (96%)	27 (4%)	0	100	100
2	I	572/710 (81%)	547 (96%)	25 (4%)	0	100	100
3	C	748/827 (90%)	696 (93%)	52 (7%)	0	100	100
3	J	75/827 (9%)	75 (100%)	0	0	100	100
All	All	3131/4318 (72%)	2985 (95%)	146 (5%)	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	560/561 (100%)	560 (100%)	0	100	100
1	H	403/561 (72%)	403 (100%)	0	100	100
2	B	600/633 (95%)	600 (100%)	0	100	100
2	I	513/633 (81%)	513 (100%)	0	100	100
3	C	676/736 (92%)	676 (100%)	0	100	100
3	J	73/736 (10%)	73 (100%)	0	100	100
All	All	2825/3860 (73%)	2825 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	351	ASN
1	A	486	ASN
1	A	500	GLN
1	A	577	HIS

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Mol	Chain	Res	Type
2	B	55	GLN
2	B	129	HIS
2	B	433	HIS
2	B	598	ASN
2	B	619	GLN
2	B	656	GLN
3	C	100	ASN
3	C	209	GLN
3	C	249	HIS
3	C	288	ASN
3	C	375	GLN
3	C	376	ASN
3	C	380	GLN
3	C	423	GLN
3	C	469	ASN
3	C	509	GLN
3	C	562	HIS
3	C	639	GLN
1	H	435	HIS
1	H	528	GLN
1	H	535	GLN
1	H	577	HIS
2	I	46	GLN
2	I	163	GLN
2	I	476	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	11/18 (61%)	2 (18%)	1 (9%)
5	E	4/17 (23%)	1 (25%)	0
5	F	12/17 (70%)	1 (8%)	0
6	G	8/9 (88%)	0	0
6	K	8/9 (88%)	3 (37%)	1 (12%)
All	All	43/70 (61%)	7 (16%)	2 (4%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	6	A
4	D	12	G

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Mol	Chain	Res	Type
5	E	17	U
5	F	17	U
6	K	6	A
6	K	7	A
6	K	8	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	11	A
6	K	7	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
7	V9G	G	1	6	55,57,57	3.81	28 (50%)	78,89,89	2.41	20 (25%)
7	V9G	K	1	6	33,34,57	3.87	13 (39%)	48,53,89	2.31	12 (25%)

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
7	V9G	G	1	6	-	10/32/94/94	0/6/6/6
7	V9G	K	1	6	-	9/24/40/94	0/3/3/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	V9G	C14-C15	-11.79	1.27	1.53
7	K	1	V9G	C14-C15	-11.71	1.27	1.53
7	K	1	V9G	P2-O11	7.72	1.67	1.59
7	G	1	V9G	C9-C8	-7.72	1.32	1.53
7	G	1	V9G	P2-O11	7.57	1.67	1.59
7	G	1	V9G	C5-N4	7.52	1.48	1.33
7	K	1	V9G	O15-C13	-7.19	1.29	1.45
7	G	1	V9G	O15-C13	-7.14	1.29	1.45
7	G	1	V9G	C19-N8	6.34	1.50	1.34
7	K	1	V9G	O15-C16	6.32	1.56	1.42
7	K	1	V9G	C19-N8	6.31	1.50	1.34
7	G	1	V9G	O15-C16	6.29	1.56	1.42
7	G	1	V9G	O3-C10	-6.16	1.31	1.45
7	G	1	V9G	C14-C13	6.05	1.68	1.53
7	K	1	V9G	C14-C13	5.98	1.68	1.53
7	G	1	V9G	P3-O11	5.69	1.65	1.59
7	K	1	V9G	P3-O11	5.67	1.65	1.59
7	G	1	V9G	C6-N4	5.63	1.46	1.33
7	K	1	V9G	C16-N6	-5.14	1.32	1.46
7	G	1	V9G	C16-N6	-5.04	1.32	1.46
7	G	1	V9G	P1-O7	4.44	1.64	1.59
7	G	1	V9G	C6-N1	4.37	1.44	1.34
7	G	1	V9G	C9-C10	4.16	1.63	1.53
7	G	1	V9G	C2-C1	4.16	1.53	1.43
7	G	1	V9G	O17-C15	3.86	1.52	1.42
7	K	1	V9G	O17-C15	3.84	1.52	1.42
7	G	1	V9G	C4-N3	3.60	1.36	1.33
7	K	1	V9G	P2-O7	3.26	1.63	1.59
7	K	1	V9G	P1-O8	3.22	1.66	1.54
7	G	1	V9G	P2-O7	3.22	1.63	1.59
7	G	1	V9G	C6-N5	2.98	1.44	1.37
7	G	1	V9G	O4-C8	2.82	1.49	1.43
7	G	1	V9G	O1-C1	-2.47	1.18	1.23
7	K	1	V9G	C18-C21	-2.43	1.34	1.39
7	G	1	V9G	C18-C21	-2.33	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	V9G	C18-N7	-2.20	1.35	1.39
7	G	1	V9G	C1-N5	2.20	1.43	1.38
7	G	1	V9G	C2-N2	-2.19	1.34	1.38
7	G	1	V9G	C5-N3	-2.18	1.33	1.37
7	K	1	V9G	C18-N7	-2.16	1.35	1.39
7	G	1	V9G	C3-N2	2.11	1.50	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	1	V9G	N8-C19-N9	-7.89	100.80	118.38
7	G	1	V9G	N8-C19-N9	-7.87	100.85	118.38
7	G	1	V9G	C6-N4-C5	7.86	120.12	112.71
7	K	1	V9G	C18-C19-N8	6.43	139.21	123.29
7	G	1	V9G	C18-C19-N8	6.41	139.17	123.29
7	K	1	V9G	N10-C20-N9	-5.65	120.02	128.58
7	G	1	V9G	N10-C20-N9	-5.58	120.13	128.58
7	G	1	V9G	N4-C5-N3	5.38	132.04	125.61
7	G	1	V9G	C2-C1-N5	5.10	119.91	110.94
7	G	1	V9G	C18-C21-N10	-4.84	120.05	126.72
7	K	1	V9G	C18-C21-N10	-4.82	120.08	126.72
7	K	1	V9G	N6-C17-N7	-4.36	107.75	113.94
7	G	1	V9G	N6-C17-N7	-4.16	108.03	113.94
7	G	1	V9G	C7-N3-C4	-4.06	119.40	127.00
7	G	1	V9G	C2-C5-N4	-3.59	120.17	126.90
7	K	1	V9G	C20-N10-C21	3.36	120.03	111.83
7	G	1	V9G	C20-N10-C21	3.34	119.98	111.83
7	G	1	V9G	C3-N2-C4	-3.19	120.06	125.33
7	G	1	V9G	O1-C1-C2	-2.99	120.28	127.62
7	G	1	V9G	N10-C21-N6	2.98	132.24	127.17
7	K	1	V9G	C18-N7-C17	2.96	108.10	103.45
7	K	1	V9G	N10-C21-N6	2.94	132.16	127.17
7	G	1	V9G	C6-N5-C1	-2.91	119.84	125.11
7	G	1	V9G	C18-N7-C17	2.86	107.95	103.45
7	G	1	V9G	C10-O3-C7	-2.75	106.94	109.74
7	K	1	V9G	C21-N6-C17	2.56	108.42	105.74
7	G	1	V9G	C9-C8-C7	2.48	104.42	100.84
7	G	1	V9G	C21-N6-C17	2.33	108.19	105.74
7	K	1	V9G	C21-C18-N7	-2.29	107.96	110.58
7	K	1	V9G	C15-C16-N6	-2.23	110.08	113.75
7	K	1	V9G	C21-N6-C16	-2.22	121.44	126.63
7	G	1	V9G	C21-C18-N7	-2.15	108.12	110.58

There are no chirality outliers.

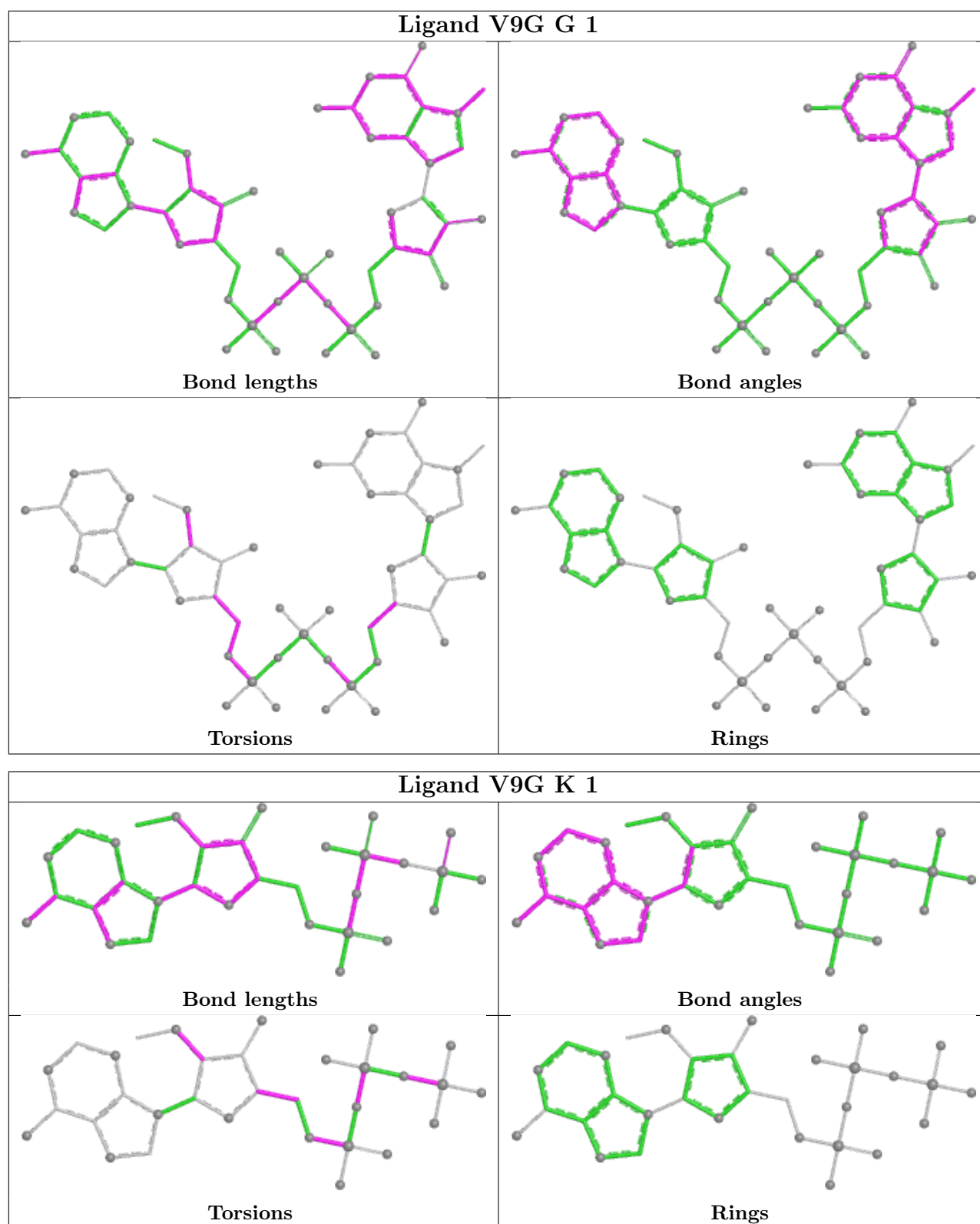
All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1	V9G	O14-C12-C13-O15
7	G	1	V9G	C16-C15-O17-C22
7	G	1	V9G	C12-O14-P3-O13
7	G	1	V9G	C12-O14-P3-O12
7	G	1	V9G	C12-O14-P3-O11
7	K	1	V9G	C16-C15-O17-C22
7	K	1	V9G	C12-O14-P3-O13
7	K	1	V9G	C12-O14-P3-O12
7	K	1	V9G	C12-O14-P3-O11
7	K	1	V9G	P2-O7-P1-O6
7	K	1	V9G	O14-C12-C13-O15
7	G	1	V9G	C9-C10-C11-O8
7	G	1	V9G	O3-C10-C11-O8
7	G	1	V9G	O14-C12-C13-C14
7	K	1	V9G	O14-C12-C13-C14
7	G	1	V9G	P2-O7-P1-O8
7	K	1	V9G	P2-O7-P1-O5
7	K	1	V9G	P3-O11-P2-O10
7	G	1	V9G	C13-C12-O14-P3

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no chain breaks in this entry.

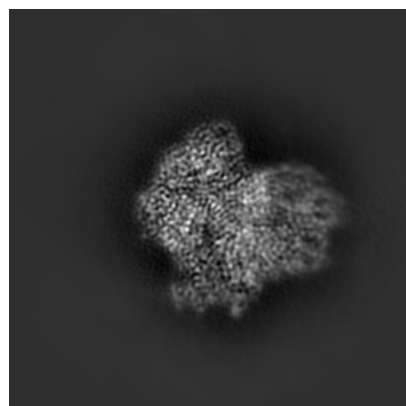
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39862. These allow visual inspection of the internal detail of the map and identification of artifacts.

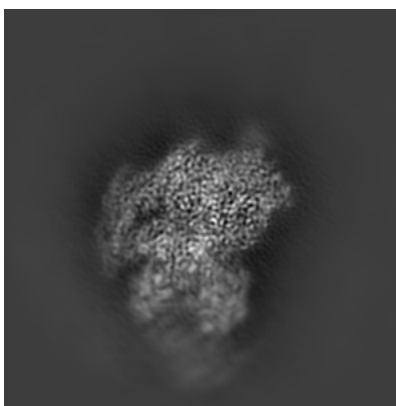
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

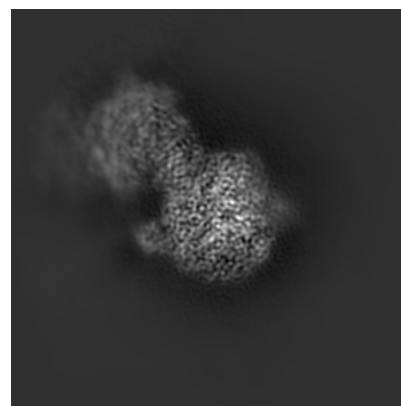
6.1.1 Primary map



X

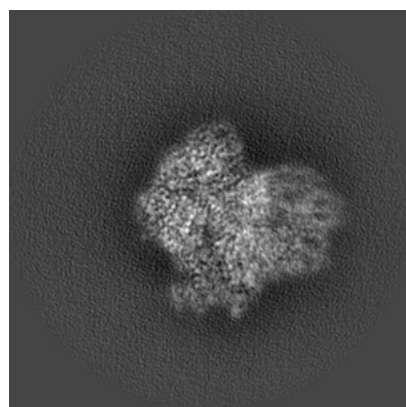


Y

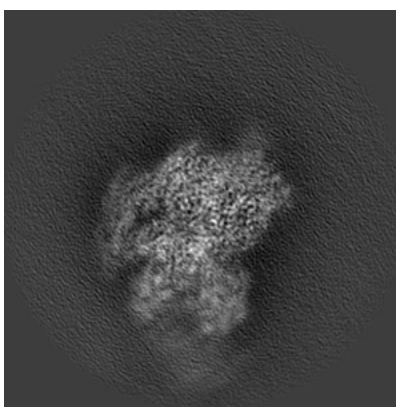


Z

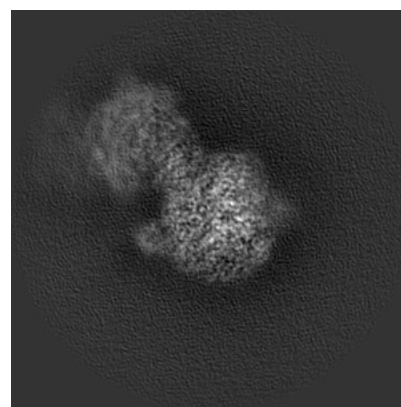
6.1.2 Raw map



X



Y

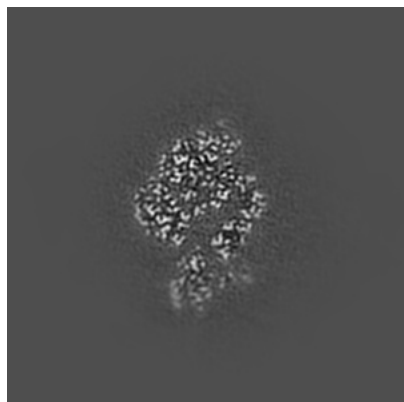


Z

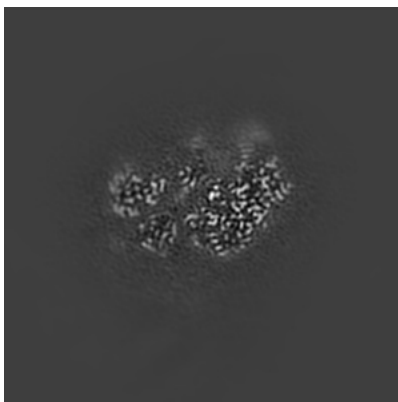
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

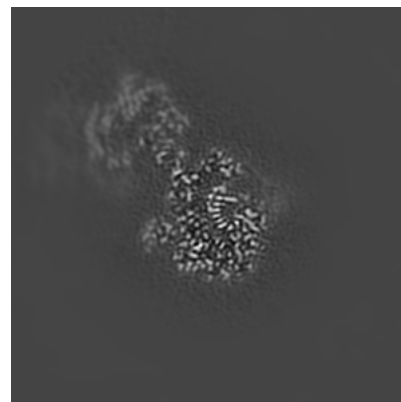
6.2.1 Primary map



X Index: 120

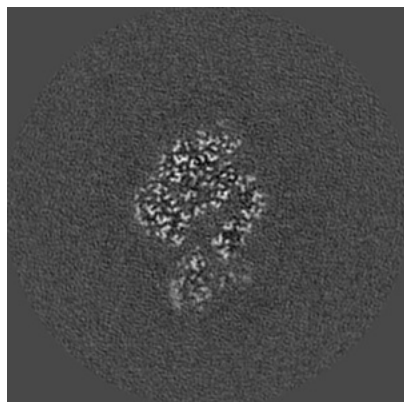


Y Index: 120

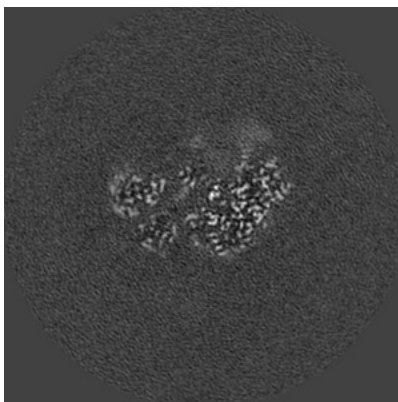


Z Index: 120

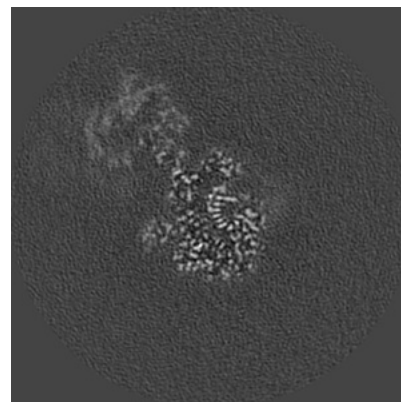
6.2.2 Raw map



X Index: 120



Y Index: 120

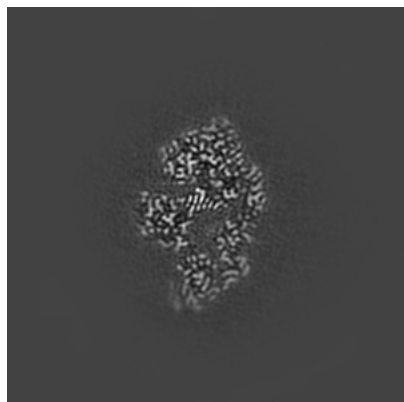


Z Index: 120

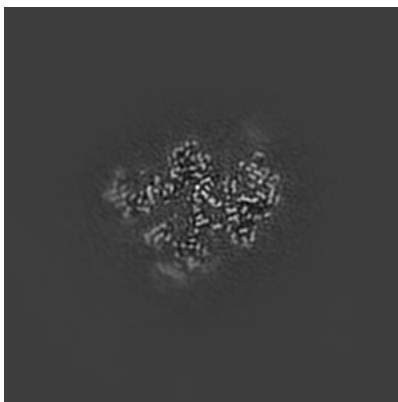
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

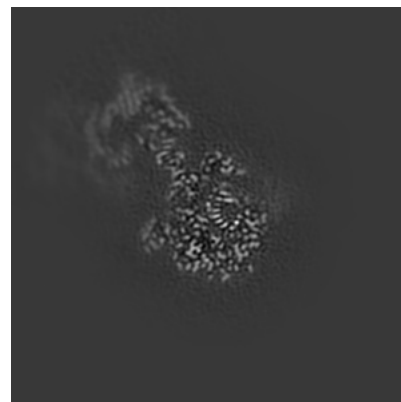
6.3.1 Primary map



X Index: 124

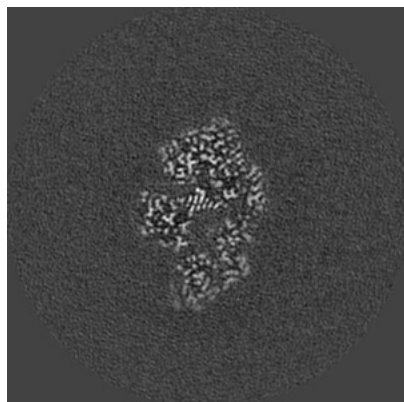


Y Index: 109

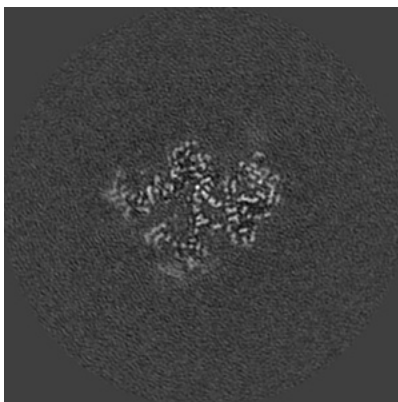


Z Index: 119

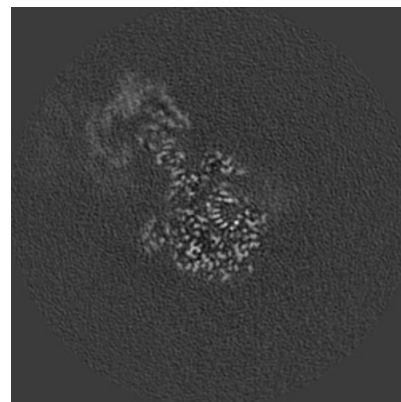
6.3.2 Raw map



X Index: 124



Y Index: 109

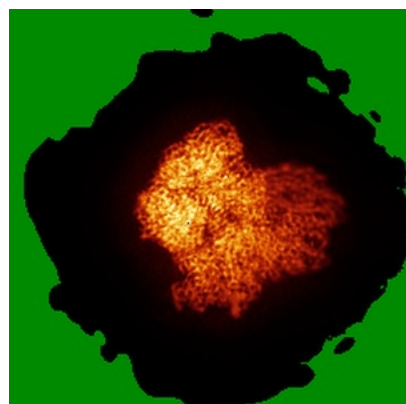


Z Index: 119

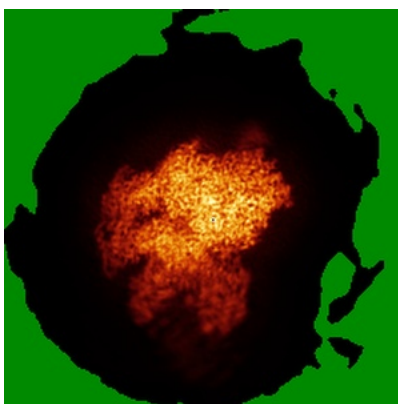
The images above show the largest variance slices of the map in three orthogonal directions.

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

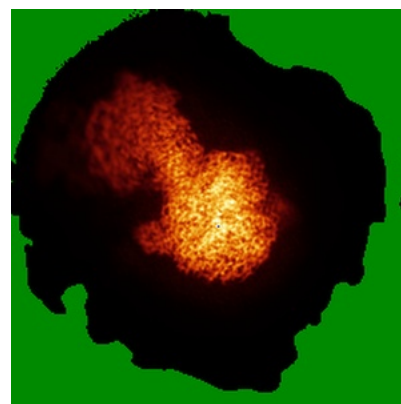
6.4.1 Primary map



X

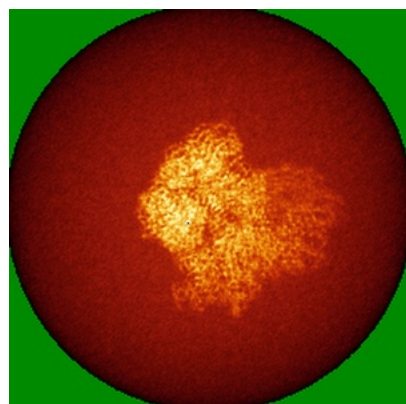


Y

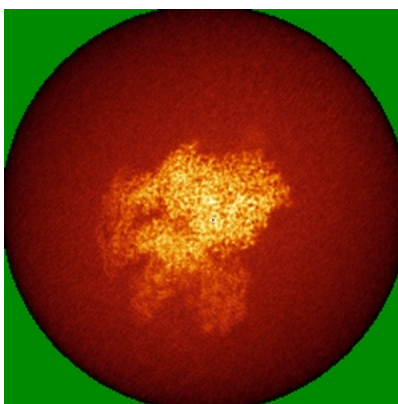


Z

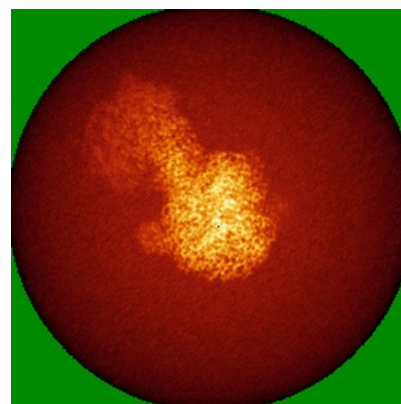
6.4.2 Raw map



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.

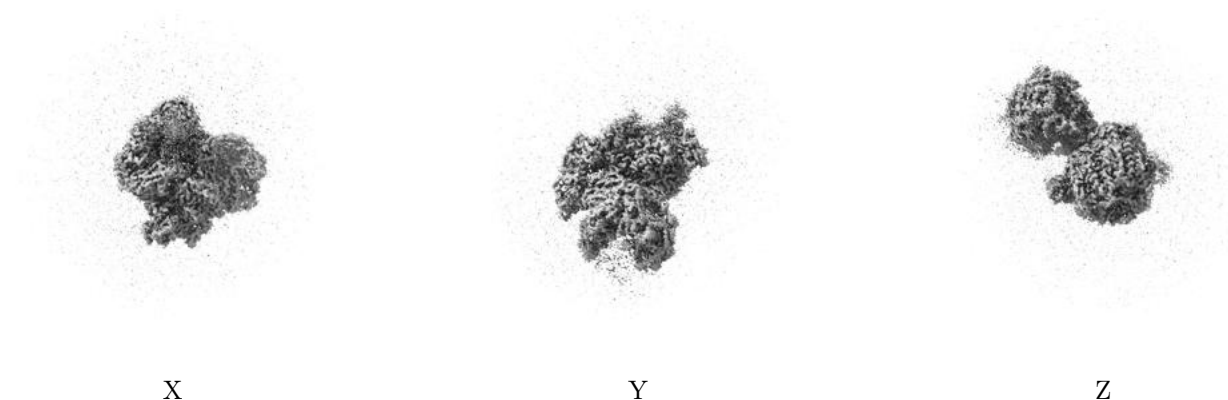
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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.

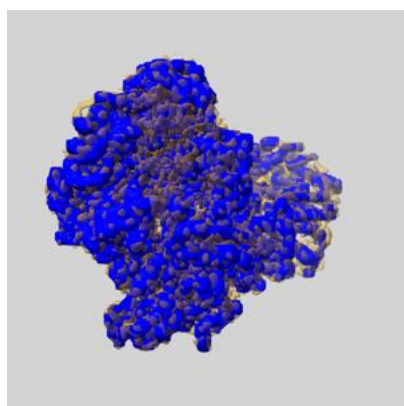
6.6 Mask visualisation [i](#)

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

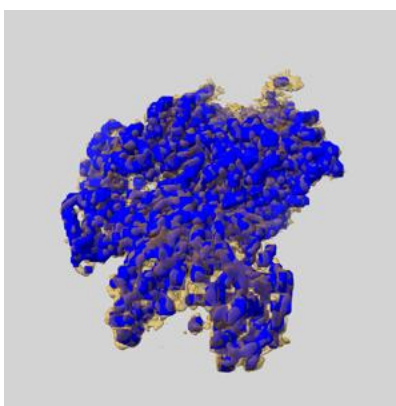
A mask typically either:

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

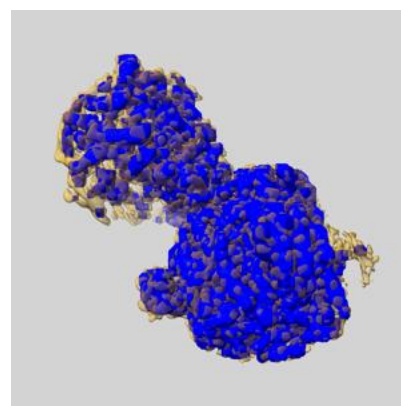
6.6.1 emd_39862_msk_1.map [i](#)



X



Y

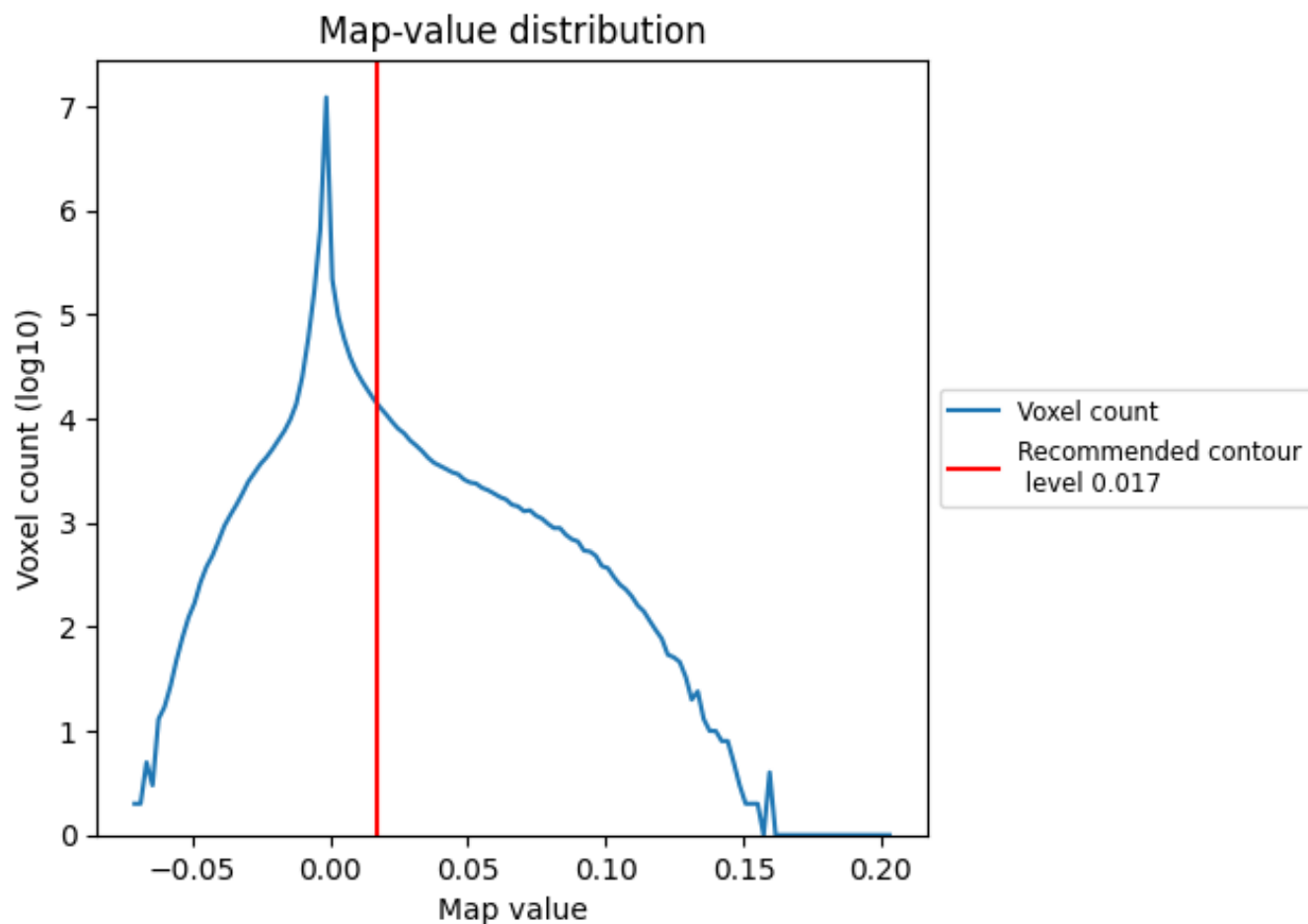


Z

7 Map analysis [i](#)

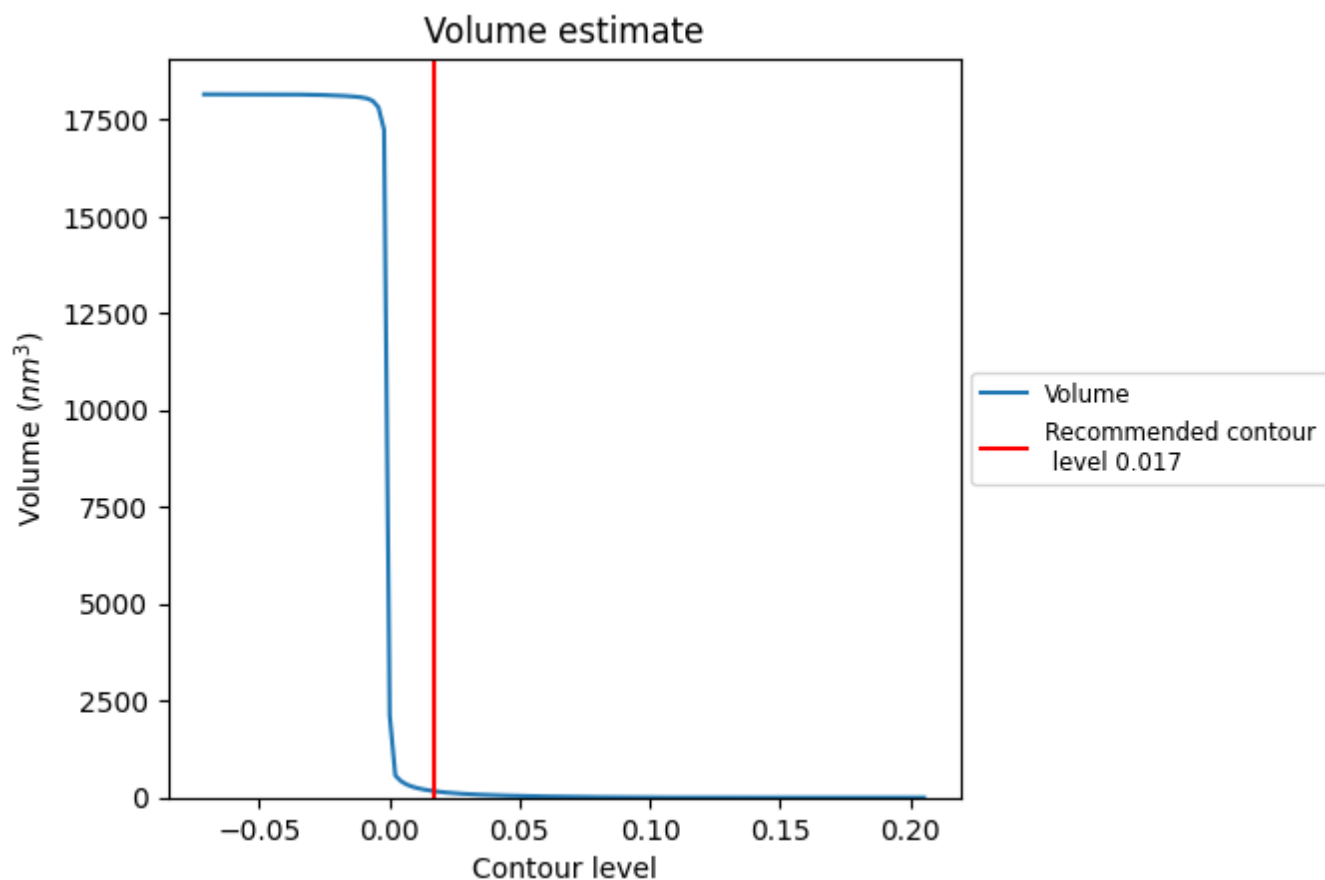
This section contains the results of statistical analysis of the map.

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.

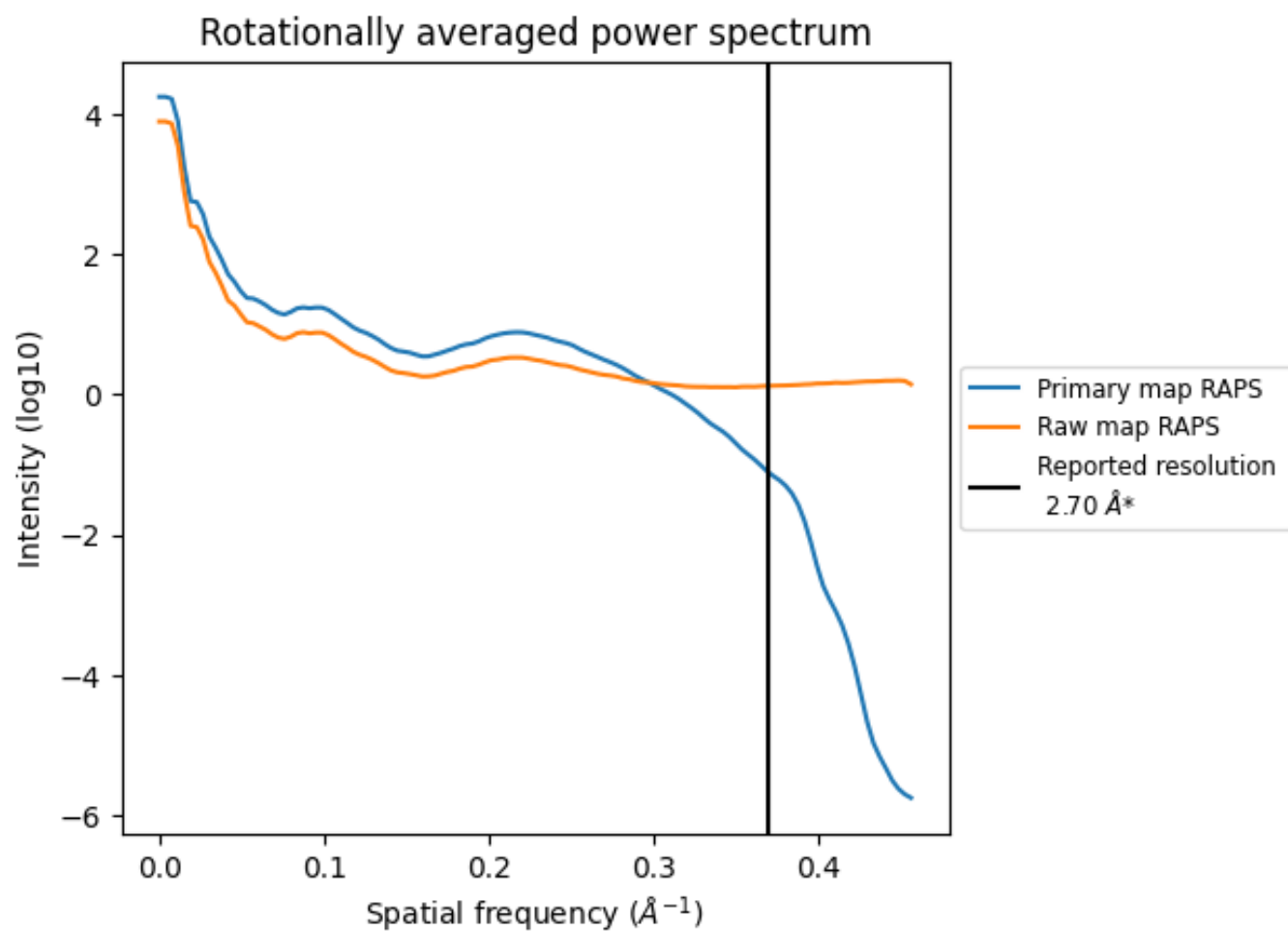
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm^3 ; this corresponds to an approximate mass of 151 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 ⓘ

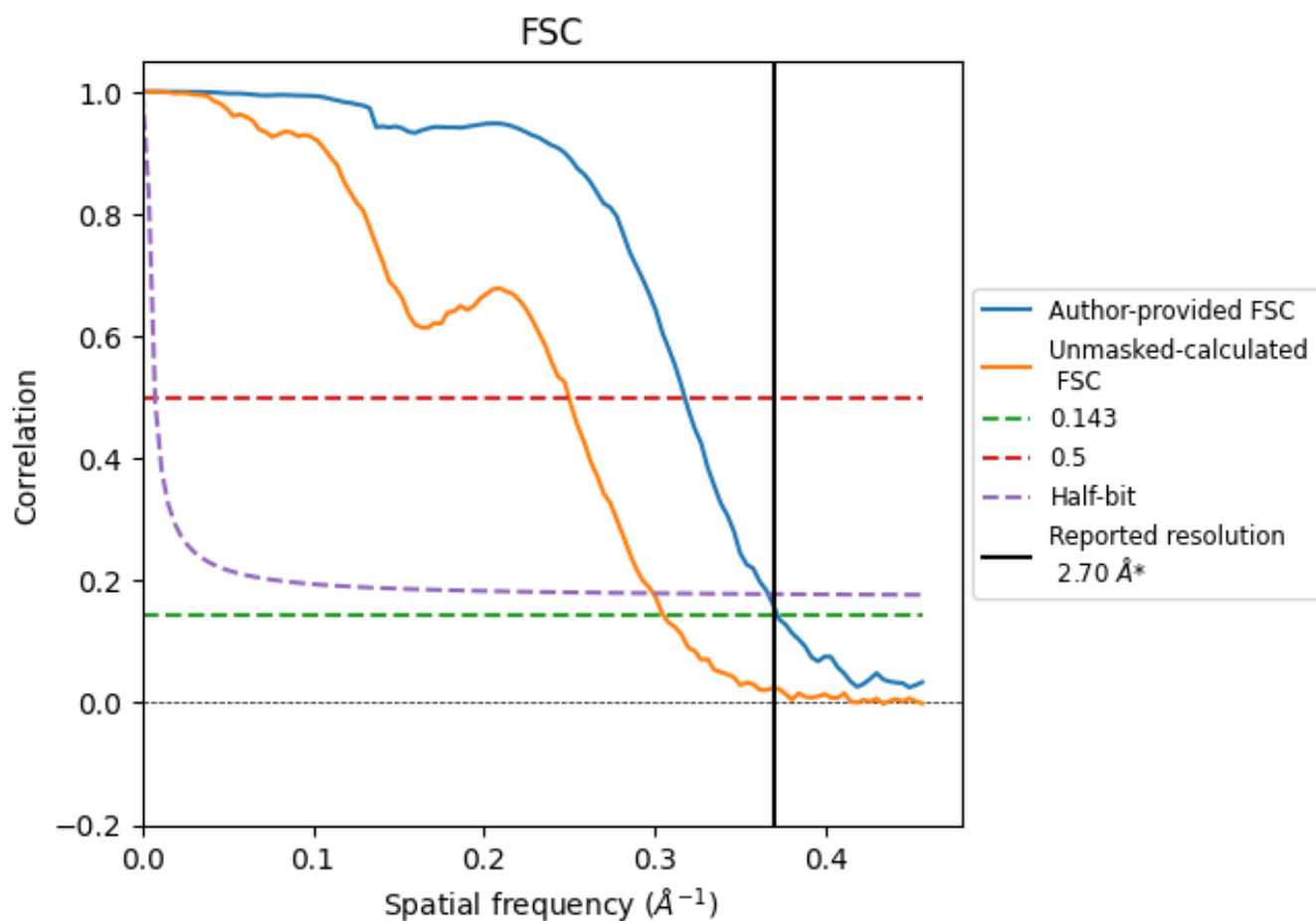


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

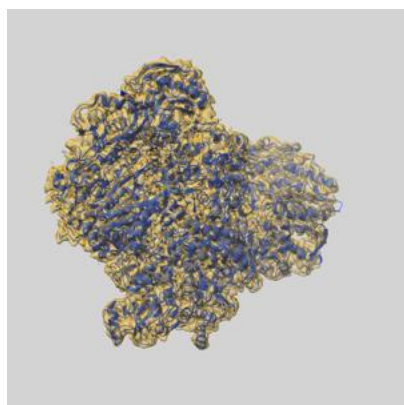
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.15	2.73
Unmasked-calculated*	3.28	4.00	3.34

*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 3.28 differs from the reported value 2.7 by more than 10 %

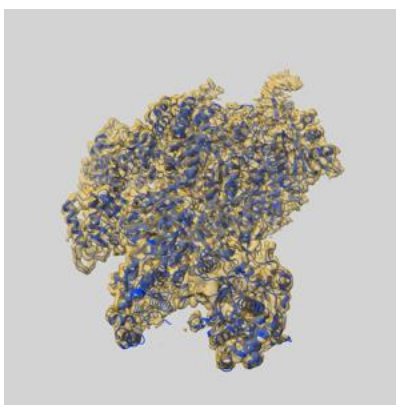
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39862 and PDB model 8Z9H. Per-residue inclusion information can be found in section [3](#) on page [10](#).

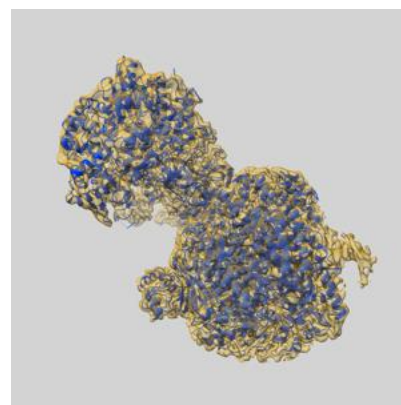
9.1 Map-model overlay [i](#)



X



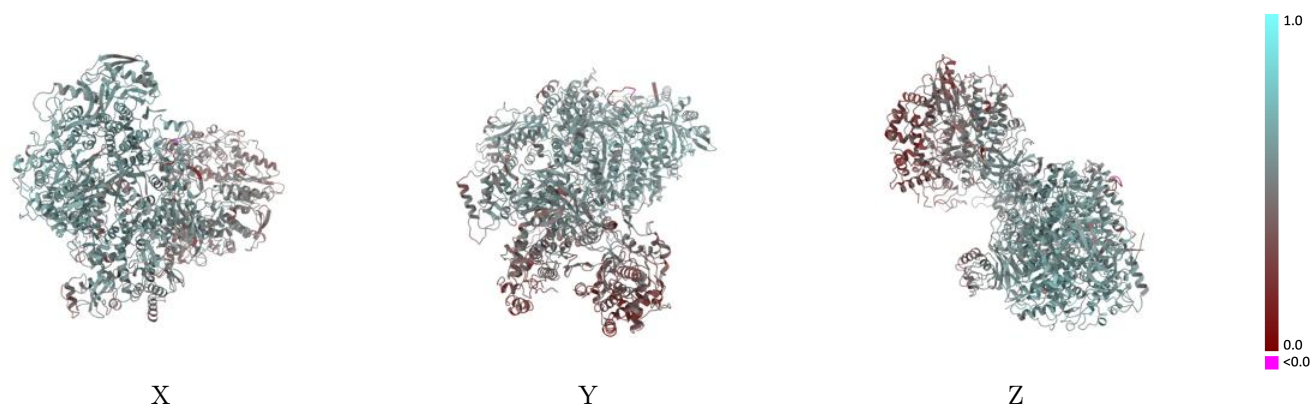
Y



Z

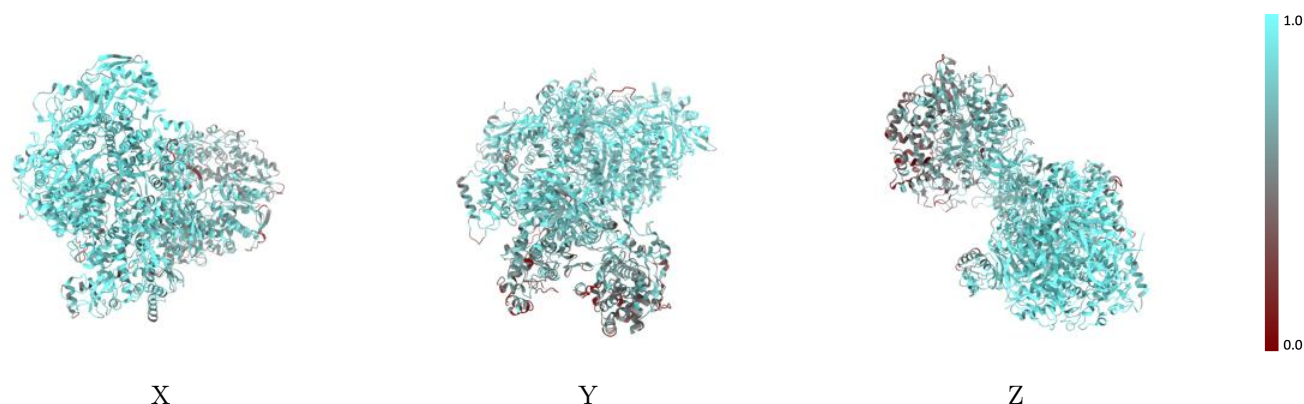
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



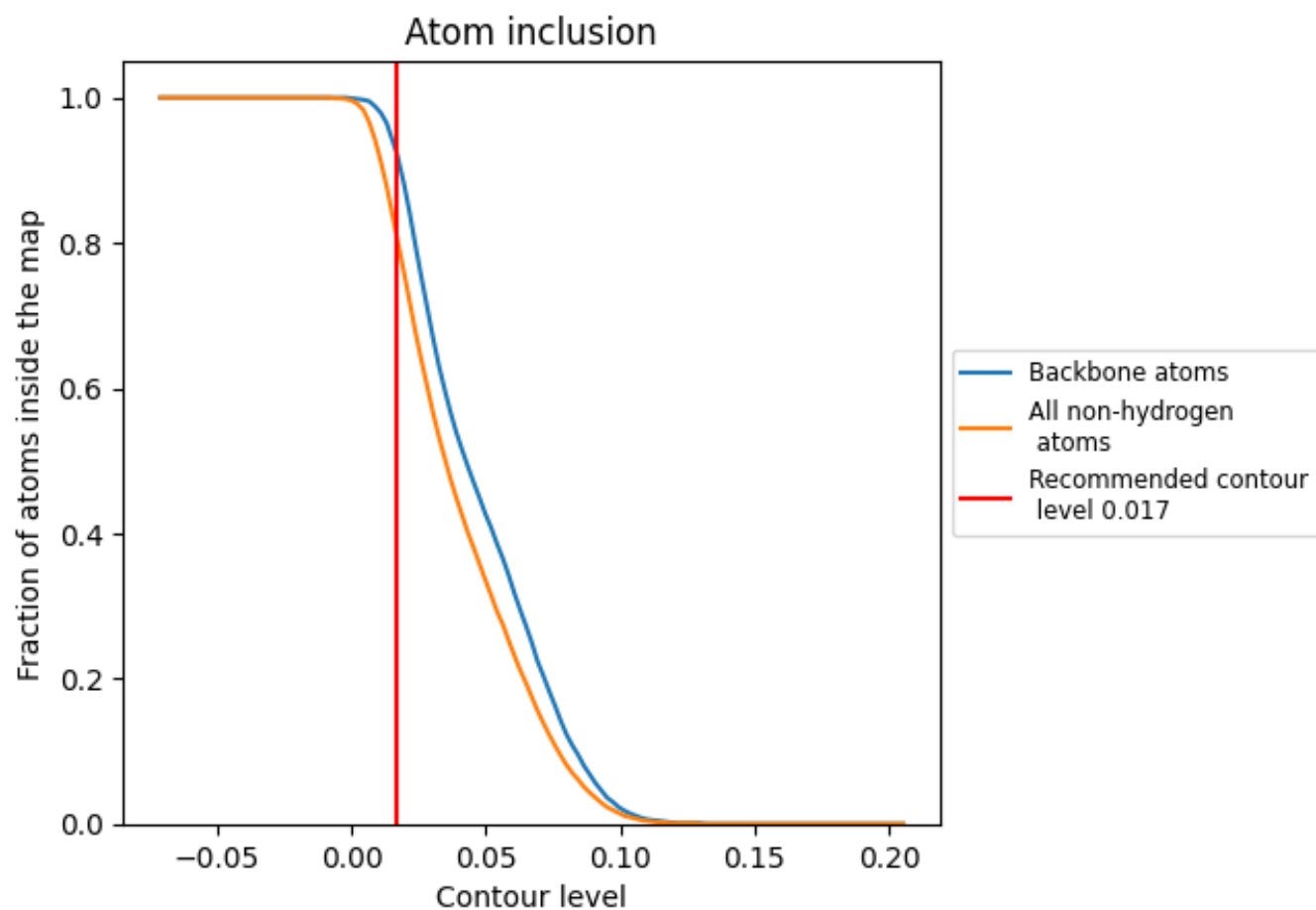
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 81% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5140
A	0.9040	0.5750
B	0.9250	0.5900
C	0.8170	0.5210
D	0.9500	0.5480
E	0.9810	0.5880
F	0.9440	0.5730
G	0.9310	0.5730
H	0.7630	0.4900
I	0.6050	0.3820
J	0.4920	0.3430
K	0.8060	0.4780

1.0

0.0

<0.0