



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:05 AM UTC

PDB ID : 8RQK / pdb_00008rqk
EMDB ID : EMD-19442
Title : Structure of the complete Vaccinia DNA-dependent RNA polymerase complex at 2.65Å resolution
Authors : Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on : 2024-01-18
Resolution : 2.65 Å(reported)
Based on initial model : 6rfl

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:

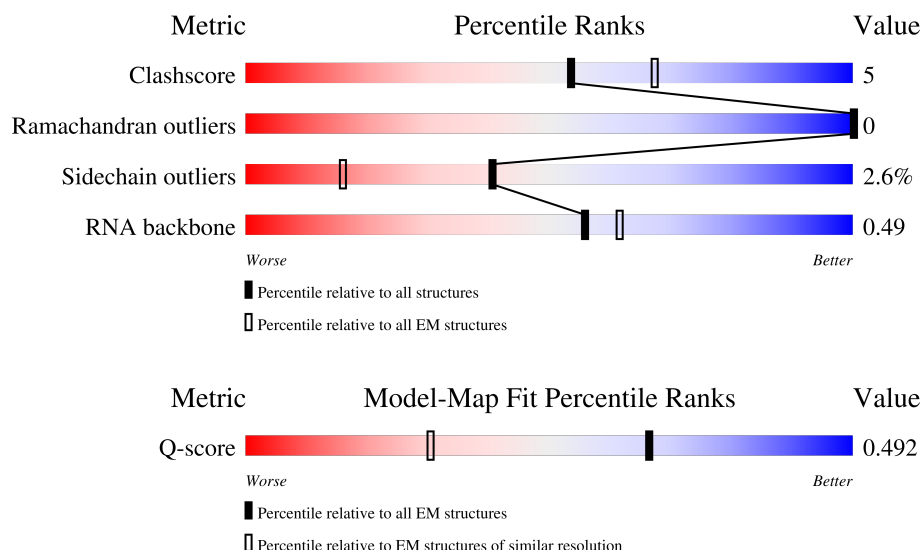
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 2.65 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	9050 (2.15 - 3.15)

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	1286	
2	B	1164	
3	C	305	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	185	
5	G	161	
6	I	795	
7	J	63	
8	K	710	
9	L	287	
10	O	844	
11	Q	129	
11	R	129	
12	S	259	
13	U	72	
14	Y	631	
15	F	164	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 104491 atoms, of which 51970 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1278	Total	C	H	N	O	S	0	0
			20643	6610	10368	1690	1929	46		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P20504
A	489	GLU	LYS	variant	UNP P20504
A	1015	LYS	ARG	variant	UNP P20504

- Molecule 2 is a protein called DNA-directed RNA polymerase 133 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1129	Total	C	H	N	O	S	0	0
			18210	5794	9119	1554	1695	48		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	variant	UNP P68694
B	343	PHE	TYR	variant	UNP P68694

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	304	Total	C	H	N	O	S	0	0
			4946	1608	2462	399	464	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ASN	ASP	variant	UNP P21087

- Molecule 4 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	184	Total	C	H	N	O	S	0	0
			3041	966	1546	248	276	5		

- Molecule 5 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	159	Total	C	H	N	O	S	0	0
			2460	782	1219	205	248	6		

- Molecule 6 is a protein called RNA polymerase-associated transcription-specificity factor RAP94.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	773	Total	C	H	N	O	S	0	0
			12934	4210	6488	1025	1190	21		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	61	Total	C	H	N	O	S	0	0
			1019	310	529	88	88	4		

- Molecule 8 is a protein called Early transcription factor 82 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	99	Total	C	H	N	O	S	0	0
			1618	523	796	145	144	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	133	ALA	VAL	variant	UNP P20635

- Molecule 9 is a protein called mRNA-capping enzyme regulatory subunit OPG124.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	284	Total	C	H	N	O	S	0	0
			4678	1492	2358	385	430	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	235	ASN	ASP	variant	UNP P20980

- Molecule 10 is a protein called mRNA-capping enzyme catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O	844	Total	C	H	N	O	S	0	0
			13715	4399	6884	1123	1290	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	8	PHE	SER	variant	UNP P20979
O	202	THR	LYS	variant	UNP P20979

- Molecule 11 is a protein called Core protein OPG073.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Q	124	Total	C	H	N	O	S	0	0
			2008	660	995	158	190	5		
11	R	129	Total	C	H	N	O	S	1	0
			2109	689	1053	165	197	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	S	189	Total	C	H	N	O	P S	0	0
			3004	950	1473	248	325	3 5		

- Molecule 13 is a RNA chain called URQ-UUG1-1 tRNA (72-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	U	72	Total	C	H	N	O	P	3	0
			2402	713	806	275	533	75		

- Molecule 14 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Y	605	Total	C	H	N	O	S	0	0
			9842	3140	4948	833	896	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	329	ASP	ASN	variant	UNP P20637

- Molecule 15 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	F	111	Total	C	H	N	O	S	0	0
			1845	588	926	158	170	3		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	U	3	Total	Mg	0
			3	3	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	I	1	Total	Zn	0
			1	1	

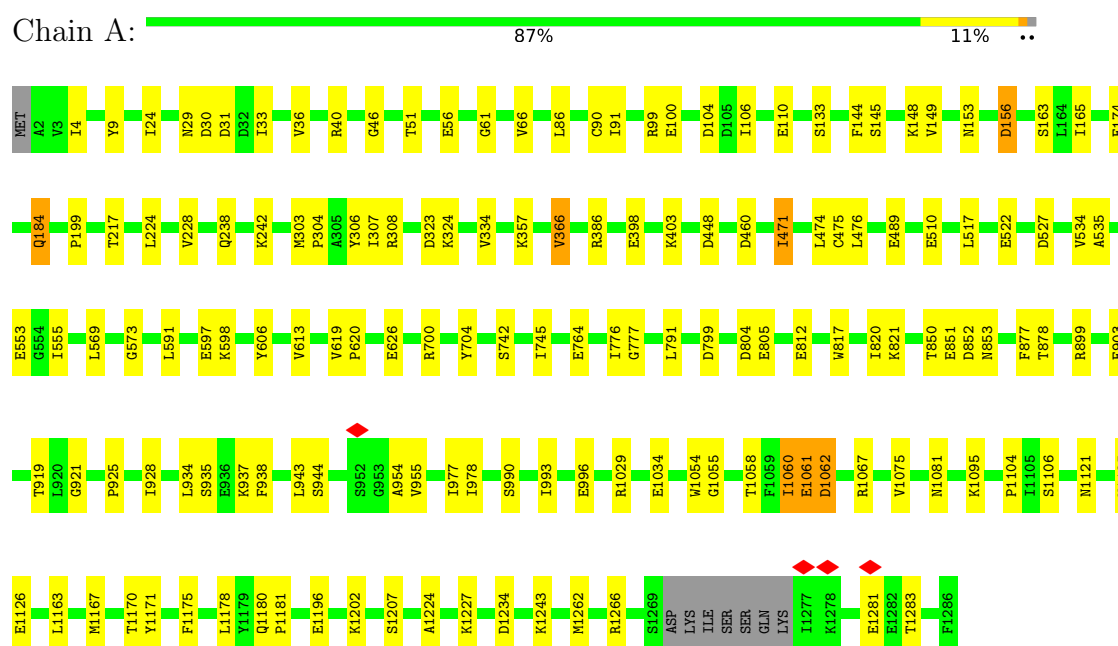
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	O	0
			2	2	
18	B	1	Total	O	0
			1	1	
18	I	1	Total	O	0
			1	1	
18	L	2	Total	O	0
			2	2	
18	S	2	Total	O	0
			2	2	
18	Y	1	Total	O	0
			1	1	

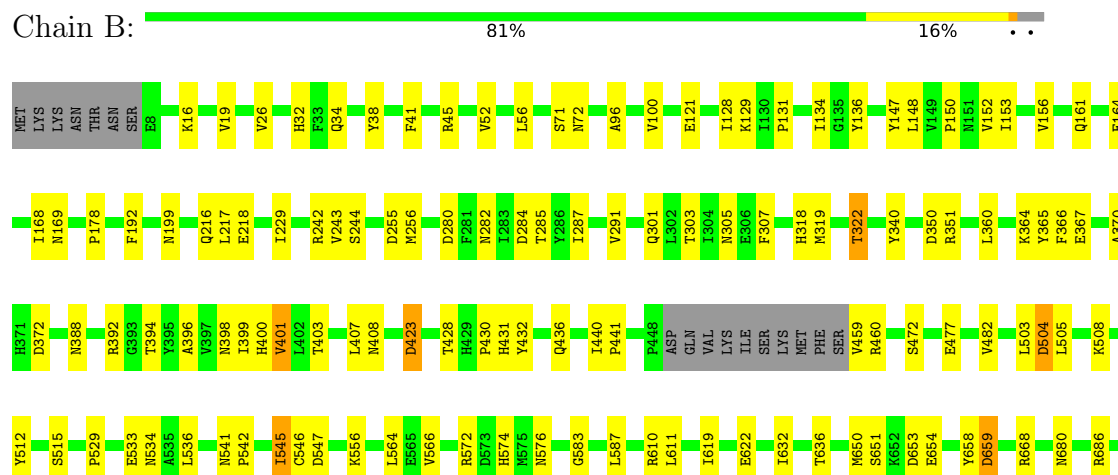
3 Residue-property plots

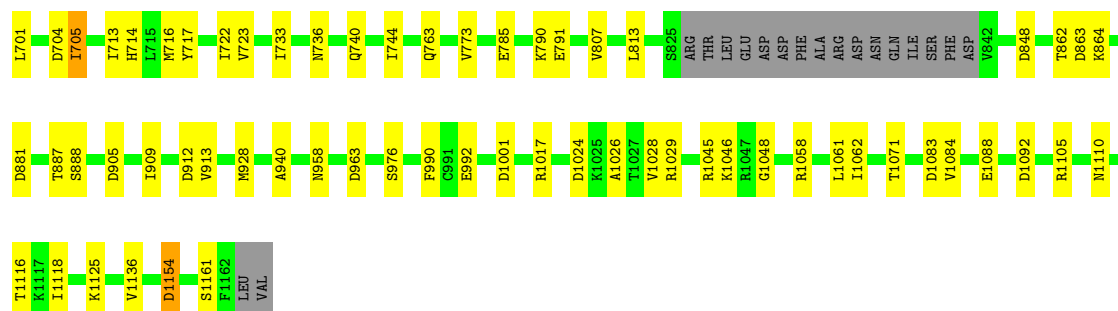
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 147 kDa polypeptide



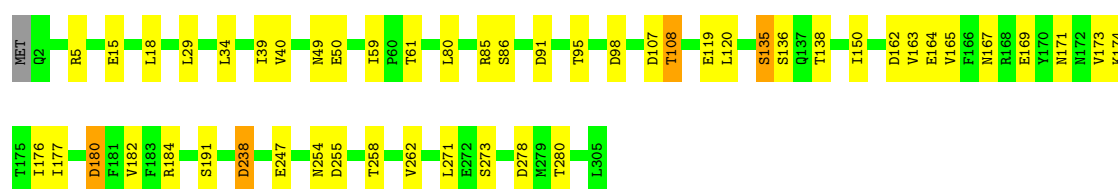
- Molecule 2: DNA-directed RNA polymerase 133 kDa polypeptide





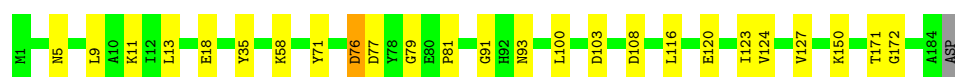
- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit

Chain C: 83% 15% .



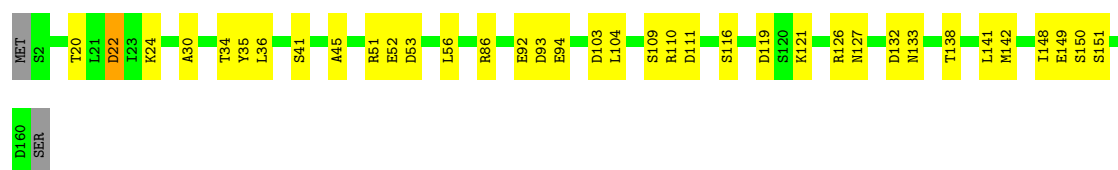
- Molecule 4: DNA-directed RNA polymerase 22 kDa subunit

Chain E: 86% 13% ..



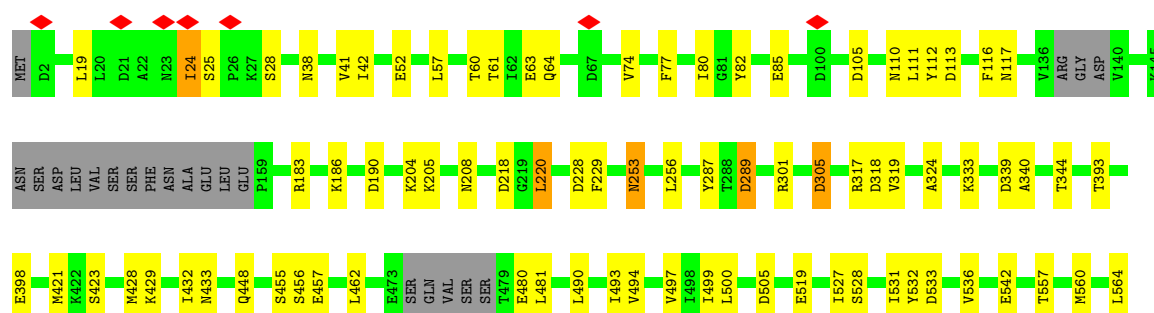
- Molecule 5: DNA-directed RNA polymerase 18 kDa subunit

Chain G: 76% 22% ..



- Molecule 6: RNA polymerase-associated transcription-specificity factor RAP94

Chain I: 82% 15% ..



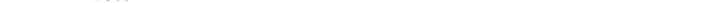


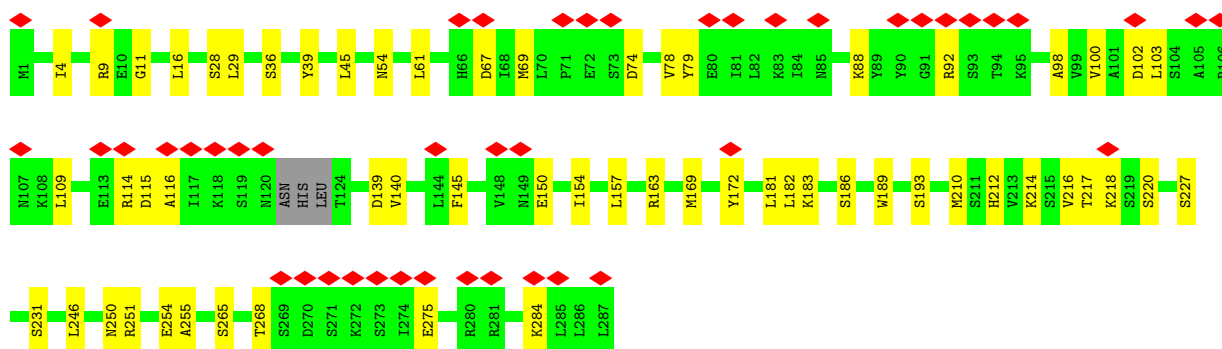
MET
V2
C7
D13
E17
R18
L21
V33
S34
V35
C39
C40
L44
Q47
T48
E49
N53
L60
D61
I62
ASN

- Molecule 8: Early transcription factor 82 kDa subunit

Tyr	Phe	Lys	Glu	Ala	Ile	Gly	Thr	Ile	Leu	Phe	Tyr	Met
Phe	Ser	Lys	Ile	Val	Ile	Val	Lys	Glu	Ala	Arg	Pro	Arg
Pro	Pro	Lys	Phe	Val	Phe	Thr	Val	Ala	Ser	Thr	Thr	Met
Lys	Leu	Lys	Val	Val	Thr	Thr	T365	Thr	Ser	Leu	Cys	Ile
Phe	Phe	Asn	Glu	Asn	Glu	Ser		Asn	Asp	Lys	Asp	Ser
Lys	Lys	Lys	Glu	Glu	Asp	Ser	N379	Asn	Gly	Leu	Phe	Lys
Tyr	Tyr	Phe	Asp	Asp	Asp	Lys		Ile	Asp	Thr	Leu	Gln
Val	Val	Pro	Lys	Lys	Met	MET	N386	Leu	Thr	Gly	Val	Pro
Ile	Ile	Pro	Asn	Asn	Ser	Ser	N387	Leu	Val	Leu	Ile	Val
Ser	Ser	Gln	Ile	Ile	Phe	PHE	L388	Ser	Met	Lys	Trp	Gly
Glu	Glu	Thr	Leu	Leu	Leu	Leu		Ser	Ile	Lys	Val	Leu
Ala	Ala	Ile	Ile	Ile	Pro	Pro	N392	Asp	Asn	Ile	Ala	Gln
Lys	Lys	Gln	Val	Val	Ile	Ile		Lys	Asn	Arg	Val	Val
Asp	Asp	Thr	Asn	Asn	Ile	Ile	E404	Lys	Val	Ile	Arg	Lys
Arg	Arg	Pro	Asp	Asp	Phe	PHE		Ile	Lys	Arg	Cys	Gly
Ile	Ile	Ile	Met	Met	Ala	Ala	T409	Ser	Leu	Val	Asp	Gln
Lys	Lys	Ser	Tyr	Phe	Phe	PHE	D411	Ile	Thr	Asp	Thr	Glu
Thr	Thr	Asp	Phe	Phe	Leu	Leu		Ile	Asp	Ile	Ile	Glu
Trp	Trp	Met	Met	Met	Asn	Asn	C418	Ala	Leu	Asp	Pro	Ile
Met	Met	Gly	Met	Met	Met	Met	N419	Lys	Val	Ile	Glu	Ala
Ile	Ile	Met	Asn	Asn	Gly	Gly	D420	Asn	Ser	Asn	Phe	Leu
Asn	Asn	Val	Ala	Ala	Met	Met		His	Asp	Tyr	Gly	Ser
Ile	Ile	Leu	Ser	Ser	Thr	Thr	C423	Ile	Ile	Lys	Ser	His
Met	Met	Thr	Asp	Asp	Ala	Ala		Ser	Asp	Leu	Tyr	Leu
Ile	Ile	Thr	Ile	Ile	Asn	Asn	N426	Ile	Thr	Ser	Glu	Leu
His	His	Asp	Gly	Gly	Met	Met	K427	Lys	Gln	Ser	Asn	Asn
Met	Met	Gly	Lys	Lys	Glu	Glu	V428	Val	Met	Ser	Val	Asp
Asn	Asn	Phe	Lys	Lys	Gln	Gln		Lys	Glu	Arg	Asp	Tyr
Val	Val	Tyr	Ile	Ile	Asp	Asp	N432	Asn	Arg	Tyr	Asn	Ile
Asp	Asp	Ile	His	His	Asn	Asn		His	Ile	Asn	Asp	Asp
Pro	Pro	Asp	Ile	Ile	Ile	Lys	L447	Ile	Ile	Glu	Ile	Tyr
Asn	Asn	Gly	Leu	Leu	Arg	Arg	H448	Pro	Gly	His	Ile	Lys
Lys	Lys	Lys	Ile	Ile	Leu	Leu	D449	Asn	Asp	Phe	Lys	Ser
Ile	Ile	Leu	Gln	Gln	Lys	Lys	Q450	Ile	Ile	Ile	Asn	Pro
Ile	Ile	Phe	Glu	Glu	Gly	Gly	S451	Glu	Thr	Asn	Thr	Ile
Pro	Pro	Asn	Ile	Ile	Thr	Thr		Lys	Tyr	Met	Met	Ile
Thr	Thr	Glu	Val	Val	His	Gly	T455	Phe	Val	Thr	Gly	Phe
Lys	Lys	Leu	Glu	Val	His	His	F456	Thr	His	Asn	Met	Arg
Tyr	Tyr	Ser	Met	Ile	Ile	Ile	S457	Phe	Leu	His	Glu	Arg
Thr	Thr	Lys	Met	Val	Val	Val		Leu	Ala	Val	Val	Val
Pro	Pro	Val	Val	Val	Arg	Arg	H461	Thr	Ala	Thr	Phe	His
Asn	Asn	Tyr	Lys	Lys	Cys	Cys	Q462	Ile	Pro	Leu	Thr	Leu
Ser	Ser	Thr	Lys	Lys	Cys	Cys	T463	Ile	Asn	Asp	Lys	Ile
Gly	Gly	Phe	Lys	Lys	Ala	Ala	ASP	Asn	Ser	Glu	Leu	Gln
Arg	Arg	Thr	Glu	Glu	Gly	Gly	VAL	Arg	Arg	Gln	Thr	Thr
Ala	Ala	Lys	Ser	Ser	Asp	Asp	Lys	Met	Ile	Glu	Leu	Pro
Gln	Gln	Asn	Ser	Ser	Asp	Asp	Lys	Phe	Lys	Asn	Glu	Pro
Ile	Ile	Val	Asp	Ile	Ile	Ile	Ile	Asn	Leu	Thr		

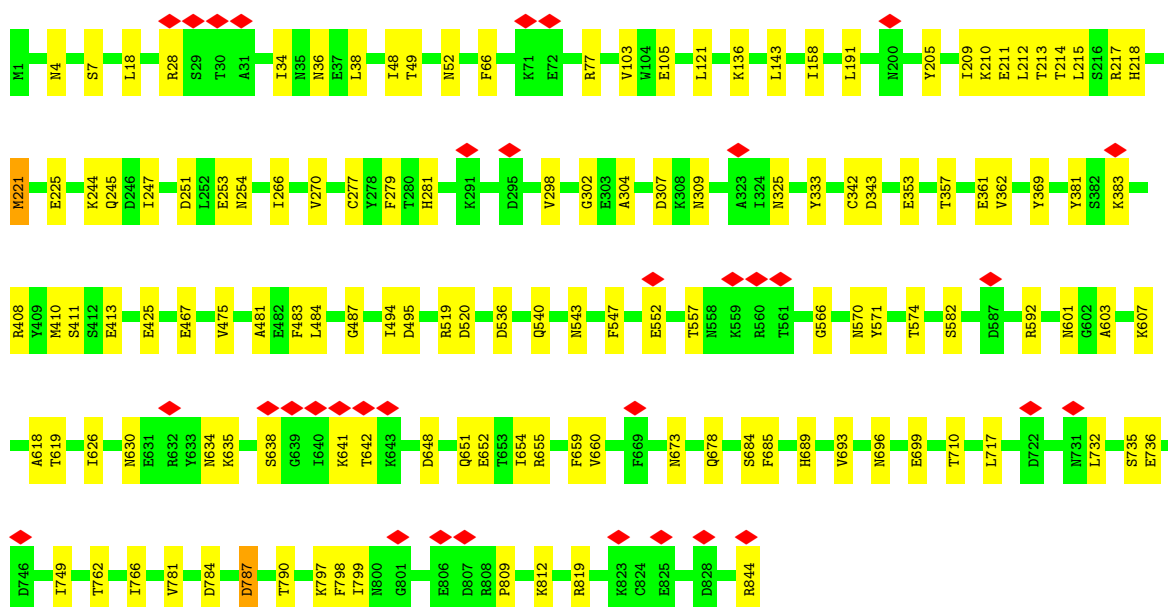
- Molecule 9: mRNA-capping enzyme regulatory subunit OPG124

Chain L:  16% 78% 21%



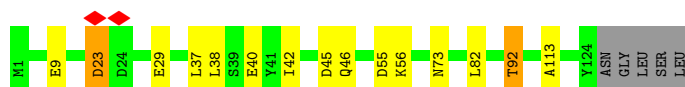
- Molecule 10: mRNA-capping enzyme catalytic subunit

Chain O: 84% 15%



- Molecule 11: Core protein OPG073

Chain Q: 84% 10%

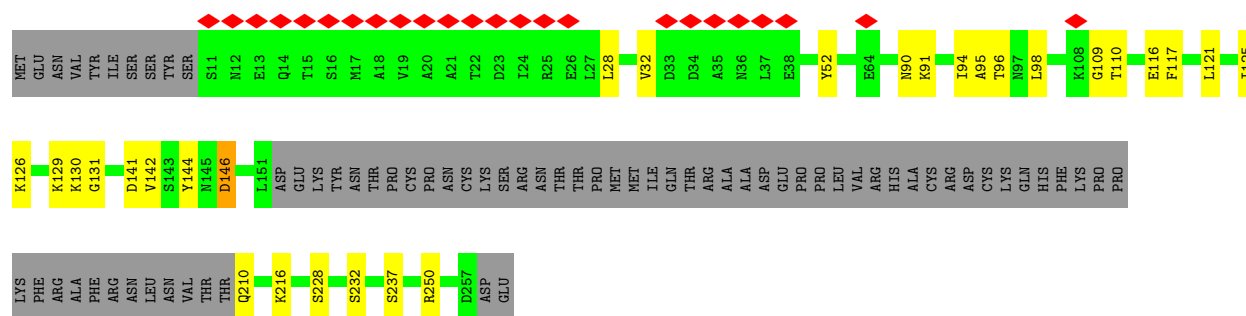


- Molecule 11: Core protein OPG073

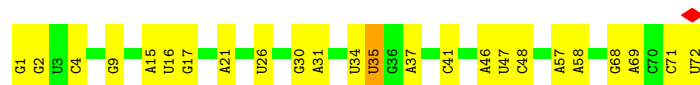
Chain R: 88% 11%



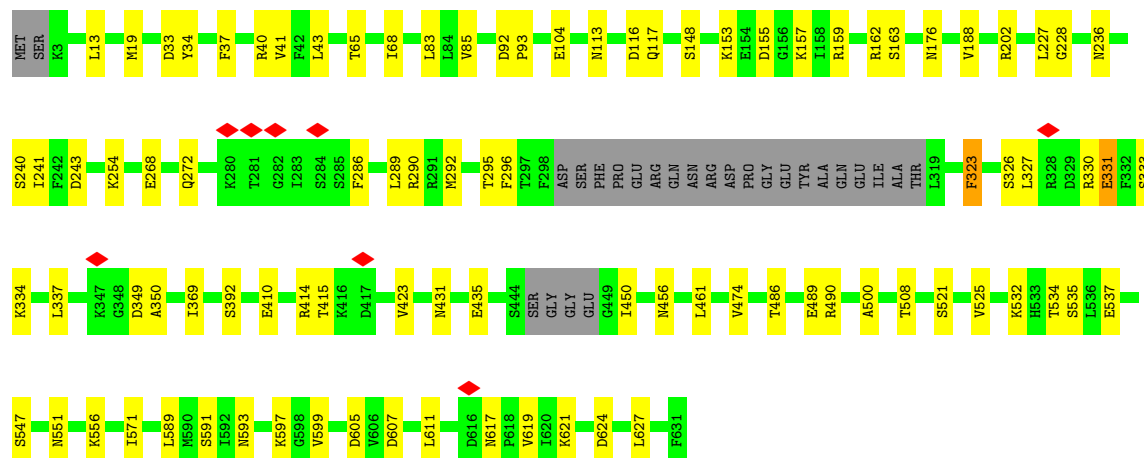
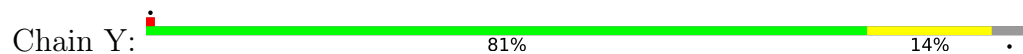
- Molecule 12: DNA-directed RNA polymerase 30 kDa polypeptide



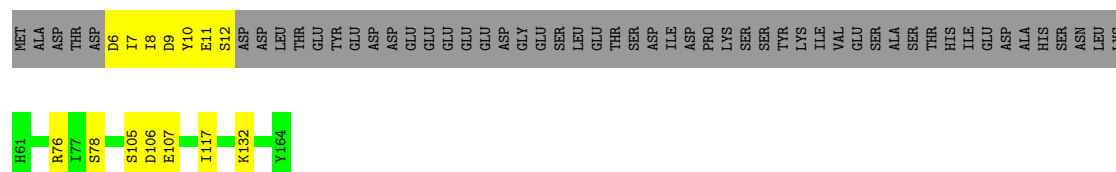
• Molecule 13: URQ-UUG1-1 tRNA (72-MER)



• Molecule 14: Nucleoside triphosphatase I



• Molecule 15: DNA-directed RNA polymerase 19 kDa subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	934606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	78	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.650	Depositor
Minimum map value	-0.338	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	382.86002, 382.86002, 382.86002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, 1MA, OMC, 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	0.27	0/10481	0.30	0/14166
2	B	0.27	0/9281	0.31	0/12537
3	C	0.26	0/2540	0.30	0/3440
4	E	0.25	0/1522	0.31	0/2069
5	G	0.24	0/1260	0.27	0/1709
6	I	0.23	0/6590	0.30	0/8918
7	J	0.27	0/494	0.32	0/663
8	K	0.17	0/843	0.28	0/1133
9	L	0.12	0/2365	0.26	0/3189
10	O	0.16	0/6973	0.27	0/9433
11	Q	0.18	0/1035	0.27	0/1402
11	R	0.20	0/1081	0.29	0/1463
12	S	0.17	0/1524	0.28	0/2050
13	U	0.20	0/1732	0.22	0/2695
14	Y	0.20	0/4989	0.29	0/6717
15	F	0.28	0/934	0.33	0/1252
All	All	0.23	0/53644	0.29	0/72836

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10275	10368	10388	105	0
2	B	9091	9119	9146	113	0
3	C	2484	2462	2470	30	0
4	E	1495	1546	1548	12	0
5	G	1241	1219	1222	22	0
6	I	6446	6488	6502	79	0
7	J	490	529	530	10	0
8	K	822	796	800	15	0
9	L	2320	2358	2363	40	0
10	O	6831	6884	6899	76	0
11	Q	1013	995	998	10	0
11	R	1056	1053	1056	10	0
12	S	1531	1473	1474	18	0
13	U	1596	806	806	8	0
14	Y	4894	4948	4963	53	0
15	F	919	926	930	9	0
16	A	1	0	0	0	0
16	U	3	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	I	1	0	0	0	0
18	A	2	0	0	0	0
18	B	1	0	0	1	0
18	I	1	0	0	0	0
18	L	2	0	0	0	0
18	S	2	0	0	1	0
18	Y	1	0	0	0	0
All	All	52521	51970	52095	548	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (548) 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:B:147:TYR:OH	6:I:594:SER:O	1.95	0.84
10:O:251:ASP:OD1	10:O:381:TYR:OH	1.95	0.84
10:O:28:ARG:NH1	10:O:36:ASN:O	2.10	0.83
8:K:423:GLY:O	8:K:426:ASN:ND2	2.12	0.82
2:B:477:GLU:N	2:B:477:GLU:OE1	2.12	0.82
2:B:1161:SER:OG	18:B:1301:HOH:O	1.96	0.82
6:I:398:GLU:O	14:Y:547:SER:OG	1.97	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:410:GLU:OE1	14:Y:414:ARG:NH2	2.14	0.80
13:U:31:A:OP2	14:Y:162:ARG:NH2	2.14	0.80
9:L:36:SER:OG	10:O:784:ASP:OD1	1.99	0.80
11:Q:73:ASN:OD1	14:Y:236:ASN:ND2	2.14	0.79
2:B:423:ASP:OD1	2:B:423:ASP:N	2.14	0.79
6:I:627:LYS:NZ	6:I:628:ILE:O	2.16	0.79
14:Y:532:LYS:O	14:Y:535:SER:OG	2.02	0.78
6:I:339:ASP:OD1	6:I:340:ALA:N	2.16	0.78
10:O:357:THR:N	10:O:361:GLU:OE2	2.16	0.78
14:Y:268:GLU:O	14:Y:272:GLN:NE2	2.16	0.78
10:O:582:SER:O	10:O:592:ARG:NH1	2.17	0.77
2:B:218:GLU:N	2:B:218:GLU:OE1	2.18	0.77
3:C:164:GLU:N	3:C:164:GLU:OE1	2.19	0.76
10:O:626:ILE:HD11	10:O:651:GLN:HB3	1.68	0.76
1:A:184:GLN:NE2	1:A:1224:ALA:O	2.20	0.75
1:A:553:GLU:N	1:A:553:GLU:OE1	2.20	0.74
2:B:1001:ASP:OD2	3:C:191:SER:OG	2.05	0.74
14:Y:456:ASN:OD1	14:Y:490:ARG:NH1	2.20	0.73
6:I:457:GLU:OE1	6:I:457:GLU:N	2.21	0.73
2:B:887:THR:O	2:B:888:SER:OG	2.06	0.73
1:A:996:GLU:O	1:A:1095:LYS:NZ	2.22	0.72
5:G:93:ASP:OD1	5:G:94:GLU:N	2.21	0.72
6:I:113:ASP:OD1	6:I:117:ASN:ND2	2.23	0.72
2:B:301:GLN:N	2:B:301:GLN:OE1	2.24	0.70
7:J:18:ARG:NH2	7:J:47:GLN:OE1	2.25	0.70
3:C:50:GLU:OE1	3:C:50:GLU:N	2.23	0.70
5:G:92:GLU:N	5:G:92:GLU:OE1	2.24	0.70
3:C:173:VAL:O	3:C:176:ILE:N	2.25	0.70
2:B:704:ASP:OD1	7:J:53:ASN:ND2	2.25	0.70
10:O:655:ARG:NH1	10:O:684:SER:OG	2.24	0.70
10:O:408:ARG:NH2	10:O:425:GLU:OE1	2.25	0.70
10:O:49:THR:HG21	10:O:191:LEU:HD22	1.74	0.69
1:A:510:GLU:OE1	1:A:510:GLU:N	2.26	0.69
2:B:242:ARG:O	6:I:738:ARG:NH2	2.26	0.69
14:Y:116:ASP:OD1	14:Y:117:GLN:N	2.25	0.69
2:B:651:SER:OG	2:B:653:ASP:OD1	2.09	0.69
2:B:763:GLN:OE1	2:B:763:GLN:N	2.24	0.68
9:L:54:ASN:OD1	9:L:114:ARG:NH2	2.26	0.68
11:R:55:ASP:OD1	11:R:55:ASP:N	2.26	0.68
2:B:121:GLU:N	2:B:121:GLU:OE1	2.27	0.68
2:B:164:GLU:OE1	2:B:431:HIS:NE2	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASP:OD1	2:B:351:ARG:N	2.27	0.67
1:A:100:GLU:N	1:A:100:GLU:OE1	2.28	0.67
4:E:18:GLU:OE1	4:E:35:TYR:OH	2.06	0.67
1:A:943:LEU:O	1:A:944:SER:OG	2.08	0.67
4:E:77:ASP:OD2	4:E:79:GLY:N	2.28	0.67
3:C:39:ILE:HG13	3:C:173:VAL:HG21	1.77	0.66
11:R:39:SER:O	11:R:109:LYS:NZ	2.28	0.66
1:A:1207:SER:OG	1:A:1234:ASP:OD2	2.13	0.66
2:B:848:ASP:OD1	2:B:1046:LYS:NZ	2.29	0.66
3:C:278:ASP:OD2	3:C:280:THR:OG1	2.13	0.66
10:O:342:CYS:SG	10:O:343:ASP:N	2.69	0.66
14:Y:117:GLN:N	14:Y:117:GLN:OE1	2.29	0.65
1:A:1266:ARG:NH2	5:G:22:ASP:OD1	2.29	0.65
1:A:1060:ILE:HD11	12:S:126:LYS:HB3	1.79	0.65
3:C:180:ASP:OD1	3:C:180:ASP:N	2.25	0.65
6:I:305:ASP:N	6:I:305:ASP:OD1	2.29	0.65
12:S:131:GLY:O	18:S:301:HOH:O	2.14	0.65
6:I:448:GLN:N	6:I:448:GLN:OE1	2.30	0.64
14:Y:327:LEU:O	14:Y:330:ARG:NH1	2.30	0.64
3:C:15:GLU:N	3:C:15:GLU:OE1	2.28	0.64
10:O:244:LYS:NZ	10:O:520:ASP:OD2	2.30	0.64
6:I:289:ASP:OD1	6:I:289:ASP:N	2.30	0.64
2:B:542:PRO:HA	2:B:545:ILE:HD13	1.79	0.64
10:O:630:ASN:O	10:O:634:ASN:ND2	2.31	0.64
2:B:242:ARG:NH2	2:B:284:ASP:OD2	2.31	0.64
5:G:110:ARG:NH2	14:Y:571:ILE:O	2.31	0.63
9:L:39:TYR:OH	9:L:163:ARG:NH2	2.31	0.63
1:A:323:ASP:OD1	1:A:324:LYS:N	2.31	0.63
2:B:807:VAL:HG21	2:B:813:LEU:HD21	1.79	0.63
2:B:1088:GLU:OE2	2:B:1116:THR:OG1	2.17	0.63
6:I:456:SER:OG	6:I:457:GLU:OE1	2.16	0.62
14:Y:521:SER:O	14:Y:525:VAL:HG23	2.00	0.62
1:A:1061:GLU:OE1	1:A:1067:ARG:NH1	2.33	0.62
1:A:764:GLU:OE2	2:B:1058:ARG:NH1	2.33	0.62
1:A:1196:GLU:OE2	1:A:1202:LYS:N	2.33	0.61
8:K:456:PHE:O	8:K:460:VAL:HG22	1.99	0.61
10:O:603:ALA:O	10:O:607:LYS:NZ	2.33	0.61
1:A:852:ASP:OD1	1:A:853:ASN:N	2.33	0.61
3:C:119:GLU:OE1	3:C:119:GLU:N	2.31	0.61
2:B:533:GLU:OE2	2:B:583:GLY:N	2.33	0.61
12:S:141:ASP:OD1	12:S:142:VAL:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:VAL:HG23	2:B:244:SER:H	1.65	0.61
1:A:1060:ILE:O	12:S:130:LYS:NZ	2.30	0.61
2:B:303:THR:OG1	2:B:305:ASN:O	2.15	0.61
6:I:82:TYR:OH	10:O:762:THR:OG1	2.13	0.61
1:A:149:VAL:HG21	1:A:242:LYS:HB2	1.83	0.61
6:I:753:ASN:O	6:I:753:ASN:ND2	2.35	0.60
8:K:420:ASP:OD2	8:K:423:GLY:N	2.33	0.60
14:Y:435:GLU:OE1	14:Y:435:GLU:N	2.34	0.60
15:F:9:ASP:OD1	15:F:10:TYR:N	2.34	0.60
1:A:522:GLU:N	1:A:522:GLU:OE1	2.35	0.60
4:E:11:LYS:NZ	4:E:103:ASP:OD2	2.35	0.60
9:L:74:ASP:O	9:L:78:VAL:HG23	2.02	0.60
2:B:881:ASP:OD2	2:B:1017:ARG:NH2	2.35	0.60
10:O:552:GLU:OE1	10:O:552:GLU:N	2.35	0.60
6:I:481:LEU:HD22	11:R:58:ILE:HG13	1.84	0.60
14:Y:13:LEU:O	14:Y:40:ARG:NH2	2.34	0.59
1:A:334:VAL:HG13	1:A:366:VAL:HG13	1.83	0.59
6:I:598:GLU:C	6:I:599:LEU:HD22	2.27	0.59
5:G:132:ASP:OD1	5:G:133:ASN:N	2.36	0.59
9:L:275:GLU:N	9:L:275:GLU:OE1	2.36	0.59
3:C:5:ARG:NH2	7:J:13:ASP:O	2.35	0.58
6:I:500:LEU:HD11	6:I:560:MET:HE1	1.84	0.58
1:A:306:TYR:OH	2:B:1026:ALA:HB1	2.04	0.58
1:A:817:TRP:O	1:A:821:LYS:N	2.36	0.58
6:I:519:GLU:N	6:I:519:GLU:OE1	2.36	0.58
10:O:225:GLU:OE1	10:O:225:GLU:N	2.34	0.58
1:A:156:ASP:OD1	1:A:156:ASP:N	2.33	0.58
1:A:163:SER:OG	6:I:183:ARG:NH2	2.37	0.58
1:A:174:GLU:N	1:A:174:GLU:OE1	2.34	0.58
2:B:650:MET:HE1	2:B:658:TYR:CE1	2.39	0.58
8:K:448:HIS:O	8:K:450:GLN:NE2	2.37	0.57
14:Y:537:GLU:OE1	14:Y:537:GLU:N	2.32	0.57
10:O:77:ARG:NH1	10:O:105:GLU:OE2	2.38	0.57
2:B:686:ARG:NH2	2:B:888:SER:O	2.37	0.57
2:B:717:TYR:O	2:B:740:GLN:NE2	2.37	0.57
3:C:107:ASP:OD1	3:C:108:THR:N	2.35	0.57
2:B:653:ASP:OD1	2:B:654:GLU:N	2.37	0.56
6:I:77:PHE:HA	6:I:80:ILE:HG22	1.87	0.56
1:A:153:ASN:ND2	1:A:156:ASP:OD1	2.37	0.56
1:A:1034:GLU:OE1	1:A:1034:GLU:N	2.35	0.56
12:S:109:GLY:O	12:S:110:THR:OG1	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:146:ASP:OD1	12:S:146:ASP:N	2.38	0.56
2:B:370:ALA:HA	2:B:407:LEU:HD21	1.87	0.56
10:O:689:HIS:O	10:O:693:VAL:HG12	2.05	0.56
2:B:388:ASN:ND2	2:B:396:ALA:O	2.36	0.56
10:O:557:THR:O	10:O:601:ASN:ND2	2.36	0.55
2:B:430:PRO:O	2:B:432:TYR:N	2.37	0.55
9:L:28:SER:N	9:L:231:SER:O	2.38	0.55
10:O:266:ILE:HD12	10:O:279:PHE:CE2	2.41	0.55
10:O:266:ILE:HD11	10:O:277:CYS:HB3	1.88	0.55
14:Y:333:SER:O	14:Y:337:LEU:HD13	2.06	0.55
1:A:903:GLU:OE1	1:A:903:GLU:N	2.36	0.55
12:S:90:ASN:OD1	12:S:91:LYS:N	2.38	0.55
1:A:851:GLU:OE1	1:A:899:ARG:NE	2.40	0.55
9:L:183:LYS:NZ	9:L:193:SER:O	2.39	0.55
1:A:133:SER:OG	6:I:218:ASP:OD1	2.14	0.55
6:I:190:ASP:OD1	6:I:190:ASP:N	2.40	0.55
1:A:919:THR:O	15:F:76:ARG:NH2	2.41	0.54
14:Y:104:GLU:OE1	14:Y:104:GLU:N	2.36	0.54
9:L:45:LEU:HD13	10:O:798:PHE:HD1	1.72	0.54
10:O:266:ILE:HG21	10:O:304:ALA:HB2	1.89	0.54
11:Q:45:ASP:OD1	11:Q:45:ASP:N	2.37	0.54
1:A:30:ASP:OD1	1:A:31:ASP:N	2.38	0.54
3:C:162:ASP:OD2	3:C:165:VAL:HG23	2.08	0.54
10:O:685:PHE:CD1	10:O:766:ILE:HG22	2.43	0.54
3:C:135:SER:O	3:C:135:SER:OG	2.26	0.54
8:K:449:ASP:OD1	8:K:450:GLN:N	2.41	0.54
10:O:266:ILE:HG22	10:O:302:GLY:O	2.08	0.54
2:B:399:ILE:HG22	2:B:400:HIS:H	1.73	0.53
6:I:735:ASN:ND2	6:I:747:VAL:O	2.36	0.53
1:A:877:PHE:O	1:A:878:THR:OG1	2.23	0.53
10:O:253:GLU:OE1	10:O:253:GLU:N	2.36	0.53
2:B:136:TYR:CD1	2:B:153:ILE:HG22	2.43	0.53
6:I:542:GLU:OE1	6:I:542:GLU:N	2.36	0.53
9:L:115:ASP:OD1	9:L:116:ALA:N	2.41	0.53
4:E:71:TYR:OH	4:E:77:ASP:OD2	2.22	0.53
12:S:117:PHE:CE2	12:S:121:LEU:HD11	2.43	0.53
10:O:566:GLY:O	10:O:570:ASN:ND2	2.40	0.53
10:O:799:ILE:HG22	10:O:819:ARG:HG2	1.91	0.53
1:A:489:GLU:OE1	1:A:489:GLU:N	2.40	0.53
1:A:1060:ILE:HD12	1:A:1060:ILE:H	1.74	0.53
7:J:39:CYS:SG	7:J:40:CYS:N	2.82	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ARG:NH2	2:B:636:THR:O	2.39	0.53
9:L:139:ASP:OD1	9:L:227:SER:OG	2.24	0.53
5:G:103:ASP:OD1	5:G:103:ASP:N	2.39	0.53
2:B:990:PHE:O	2:B:992:GLU:N	2.42	0.52
2:B:1110:ASN:ND2	6:I:110:ASN:OD1	2.37	0.52
2:B:504:ASP:OD2	2:B:508:LYS:NZ	2.42	0.52
7:J:17:GLU:OE1	7:J:17:GLU:N	2.41	0.52
1:A:386:ARG:NH2	1:A:448:ASP:OD1	2.43	0.52
10:O:4:ASN:O	10:O:7:SER:OG	2.22	0.52
10:O:660:VAL:HG11	10:O:699:GLU:OE1	2.09	0.52
3:C:258:THR:O	3:C:262:VAL:HG22	2.10	0.52
10:O:481:ALA:HB3	10:O:483:PHE:CE1	2.45	0.52
14:Y:202:ARG:NH2	14:Y:228:GLY:O	2.39	0.52
1:A:36:VAL:HG21	1:A:224:LEU:HB3	1.92	0.52
1:A:460:ASP:N	1:A:460:ASP:OD1	2.43	0.52
1:A:812:GLU:OE1	1:A:812:GLU:N	2.37	0.52
1:A:1262:MET:SD	5:G:56:LEU:HD22	2.50	0.52
1:A:29:ASN:ND2	1:A:33:ILE:O	2.39	0.52
2:B:430:PRO:O	2:B:436:GLN:NE2	2.33	0.52
9:L:79:TYR:OH	9:L:100:VAL:HG21	2.10	0.52
11:R:8:LEU:HB2	11:R:15:VAL:HG22	1.92	0.51
14:Y:333:SER:OG	14:Y:334:LYS:N	2.44	0.51
1:A:619:VAL:O	12:S:144:TYR:OH	2.25	0.51
7:J:35:VAL:HG21	7:J:44:LEU:HD12	1.92	0.51
8:K:456:PHE:CE1	8:K:460:VAL:HG21	2.46	0.51
9:L:45:LEU:HD13	10:O:798:PHE:CD1	2.45	0.51
2:B:460:ARG:NH2	2:B:482:VAL:O	2.44	0.51
14:Y:331:GLU:N	14:Y:331:GLU:OE1	2.43	0.51
5:G:51:ARG:NH2	5:G:53:ASP:OD2	2.44	0.51
6:I:19:LEU:HD21	6:I:63:GLU:HA	1.91	0.51
9:L:140:VAL:O	9:L:172:TYR:OH	2.29	0.51
14:Y:43:LEU:HD21	14:Y:68:ILE:HG23	1.92	0.51
2:B:887:THR:HG21	2:B:928:MET:HB2	1.91	0.51
8:K:449:ASP:OD1	8:K:451:SER:N	2.39	0.51
14:Y:500:ALA:O	14:Y:508:THR:OG1	2.29	0.51
6:I:584:SER:OG	7:J:62:ILE:N	2.44	0.51
4:E:120:GLU:O	4:E:124:VAL:HG23	2.10	0.51
3:C:173:VAL:O	3:C:177:ILE:N	2.44	0.51
5:G:34:THR:HG23	5:G:35:TYR:CD2	2.45	0.51
1:A:303:MET:O	1:A:308:ARG:NH1	2.44	0.50
1:A:1054:TRP:O	1:A:1054:TRP:CD2	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HD12	3:C:182:VAL:HG12	1.94	0.50
9:L:92:ARG:NH2	9:L:145:PHE:O	2.43	0.50
10:O:18:LEU:HD12	10:O:212:LEU:HD11	1.93	0.50
2:B:322:THR:O	6:I:728:GLN:NE2	2.43	0.50
9:L:74:ASP:N	9:L:74:ASP:OD1	2.43	0.50
10:O:411:SER:OG	10:O:413:GLU:O	2.29	0.50
1:A:217:THR:HG21	6:I:393:THR:HG23	1.93	0.50
2:B:785:GLU:OE1	2:B:785:GLU:N	2.42	0.50
6:I:710:ARG:NE	6:I:761:GLU:OE2	2.44	0.50
13:U:21:A:H61	13:U:46:A:H2'	1.76	0.50
13:U:35:U:N3	14:Y:163:SER:OG	2.45	0.50
1:A:776:ILE:HG23	1:A:777:GLY:H	1.77	0.50
1:A:1262:MET:O	5:G:24:LYS:NZ	2.38	0.50
14:Y:153:LYS:NZ	14:Y:157:LYS:O	2.45	0.50
10:O:536:ASP:OD2	10:O:540:GLN:NE2	2.45	0.50
1:A:475:CYS:SG	1:A:476:LEU:N	2.85	0.50
2:B:96:ALA:HB3	2:B:128:ILE:HB	1.94	0.50
2:B:16:LYS:O	2:B:19:VAL:HG22	2.12	0.49
2:B:199:ASN:CG	2:B:503:LEU:HD21	2.37	0.49
6:I:57:LEU:O	6:I:61:THR:HG23	2.12	0.49
2:B:34:GLN:NE2	2:B:169:ASN:OD1	2.45	0.49
9:L:251:ARG:O	9:L:254:GLU:HG2	2.12	0.49
10:O:52:ASN:ND2	10:O:221:MET:SD	2.85	0.49
1:A:66:VAL:HG21	1:A:228:VAL:HG22	1.94	0.49
2:B:705:ILE:HD12	2:B:714:HIS:CD2	2.47	0.49
2:B:659:ASP:OD1	2:B:659:ASP:N	2.44	0.49
3:C:163:VAL:O	3:C:167:ASN:ND2	2.42	0.49
6:I:723:ASP:OD1	6:I:723:ASP:N	2.46	0.49
1:A:238:GLN:N	1:A:238:GLN:OE1	2.41	0.49
10:O:205:TYR:O	10:O:209:ILE:HG22	2.12	0.49
10:O:210:LYS:O	10:O:213:THR:OG1	2.26	0.49
1:A:934:LEU:O	1:A:1171:TYR:OH	2.26	0.49
3:C:167:ASN:O	3:C:171:ASN:ND2	2.39	0.49
10:O:211:GLU:HA	10:O:214:THR:HG22	1.95	0.49
1:A:357:LYS:NZ	6:I:324:ALA:O	2.45	0.49
14:Y:92:ASP:HB3	14:Y:93:PRO:HD3	1.95	0.49
9:L:28:SER:O	9:L:231:SER:N	2.42	0.49
10:O:519:ARG:NH1	10:O:547:PHE:O	2.46	0.49
15:F:76:ARG:O	15:F:132:LYS:NZ	2.45	0.49
9:L:103:LEU:HD21	9:L:139:ASP:CB	2.42	0.48
2:B:545:ILE:HG22	2:B:546:CYS:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:66:PHE:CD2	10:O:143:LEU:HD22	2.47	0.48
1:A:1029:ARG:NH2	12:S:144:TYR:OH	2.45	0.48
6:I:557:THR:HA	6:I:560:MET:HE3	1.95	0.48
1:A:46:GLY:N	1:A:56:GLU:OE2	2.43	0.48
2:B:680:ASN:OD1	2:B:958:ASN:N	2.42	0.48
2:B:722:ILE:HD12	2:B:723:VAL:HG23	1.94	0.48
6:I:38:ASN:O	6:I:41:VAL:HG22	2.14	0.48
1:A:954:ALA:HB2	1:A:1104:PRO:HD2	1.96	0.48
9:L:100:VAL:HG22	9:L:154:ILE:HB	1.95	0.48
9:L:150:GLU:N	9:L:150:GLU:OE1	2.46	0.48
1:A:527:ASP:O	12:S:210:GLN:NE2	2.43	0.48
2:B:71:SER:OG	2:B:72:ASN:OD1	2.32	0.48
2:B:505:LEU:HD21	2:B:566:VAL:HG22	1.96	0.48
6:I:490:LEU:O	6:I:494:VAL:HG23	2.13	0.48
10:O:809:PRO:HA	10:O:812:LYS:HB3	1.95	0.48
1:A:1281:GLU:O	10:O:218:HIS:NE2	2.46	0.48
2:B:372:ASP:OD1	12:S:250:ARG:NE	2.41	0.48
1:A:1283:THR:O	10:O:217:ARG:NH1	2.47	0.48
2:B:940:ALA:O	2:B:976:SER:OG	2.31	0.48
4:E:58:LYS:NZ	4:E:76:ASP:OD2	2.44	0.48
1:A:471:ILE:HG21	1:A:474:LEU:HD11	1.95	0.47
2:B:360:LEU:HD22	2:B:364:LYS:HB3	1.96	0.47
2:B:1024:ASP:O	2:B:1045:ARG:NH1	2.47	0.47
1:A:1224:ALA:HB2	2:B:1136:VAL:HG13	1.96	0.47
9:L:250:ASN:OD1	9:L:251:ARG:N	2.47	0.47
2:B:129:LYS:N	2:B:408:ASN:OD1	2.44	0.47
2:B:255:ASP:O	2:B:574:HIS:ND1	2.46	0.47
9:L:169:MET:HA	9:L:169:MET:HE2	1.96	0.47
1:A:1180:GLN:HB2	1:A:1181:PRO:HD3	1.97	0.47
2:B:399:ILE:HG22	2:B:400:HIS:N	2.29	0.47
3:C:169:GLU:O	3:C:173:VAL:HG22	2.14	0.47
1:A:1167:MET:O	1:A:1170:THR:OG1	2.27	0.47
3:C:80:LEU:HD23	3:C:80:LEU:C	2.39	0.47
3:C:238:ASP:OD1	3:C:238:ASP:N	2.48	0.47
6:I:662:ASP:OD1	6:I:662:ASP:N	2.47	0.47
14:Y:431:ASN:O	14:Y:431:ASN:ND2	2.48	0.47
1:A:937:LYS:HG2	1:A:1178:LEU:HD11	1.97	0.47
6:I:220:LEU:N	6:I:220:LEU:HD23	2.30	0.47
14:Y:243:ASP:O	14:Y:254:LYS:NZ	2.40	0.47
8:K:409:ILE:HG23	8:K:409:ILE:O	2.14	0.47
11:Q:38:LEU:O	11:Q:42:ILE:N	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:295:THR:HG23	14:Y:296:PHE:CD2	2.50	0.46
3:C:59:ILE:O	3:C:61:THR:HG23	2.15	0.46
14:Y:19:MET:HE1	14:Y:43:LEU:HD12	1.97	0.46
10:O:38:LEU:HD11	10:O:121:LEU:HD11	1.98	0.46
11:Q:23:ASP:OD1	11:Q:23:ASP:N	2.47	0.46
10:O:732:LEU:HD23	10:O:736:GLU:O	2.16	0.46
14:Y:286:PHE:O	14:Y:290:ARG:NH2	2.42	0.46
4:E:81:PRO:O	4:E:93:ASN:ND2	2.43	0.46
1:A:1180:GLN:OE1	1:A:1180:GLN:N	2.43	0.46
2:B:744:ILE:HG22	2:B:913:VAL:HB	1.97	0.46
6:I:586:LEU:HD23	6:I:586:LEU:H	1.81	0.46
11:Q:9:GLU:O	11:Q:92:THR:OG1	2.30	0.46
2:B:388:ASN:O	2:B:392:ARG:N	2.49	0.46
2:B:1058:ARG:HH11	2:B:1062:ILE:HD12	1.81	0.46
14:Y:241:ILE:HD11	14:Y:474:VAL:HG21	1.97	0.46
3:C:254:ASN:HA	3:C:271:LEU:O	2.15	0.46
6:I:64:GLN:OE1	14:Y:621:LYS:N	2.39	0.46
6:I:613:ILE:HG22	6:I:614:VAL:H	1.81	0.46
1:A:1054:TRP:O	1:A:1054:TRP:CG	2.69	0.45
8:K:411:ASP:OD1	8:K:411:ASP:N	2.48	0.45
1:A:398:GLU:O	1:A:403:LYS:NZ	2.49	0.45
2:B:72:ASN:OD1	2:B:72:ASN:N	2.50	0.45
6:I:790:MET:O	6:I:795:ASN:N	2.38	0.45
10:O:495:ASP:OD1	10:O:495:ASP:N	2.50	0.45
1:A:925:PRO:HB2	1:A:928:ILE:HG22	1.98	0.45
2:B:1029:ARG:NH1	2:B:1048:GLY:O	2.50	0.45
9:L:54:ASN:O	9:L:114:ARG:NH2	2.39	0.45
10:O:484:LEU:O	10:O:487:GLY:N	2.49	0.45
1:A:24:ILE:HB	1:A:66:VAL:HG22	1.97	0.45
2:B:319:MET:HE1	2:B:536:LEU:H	1.82	0.45
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.98	0.45
10:O:787:ASP:OD1	10:O:787:ASP:N	2.49	0.45
14:Y:33:ASP:OD1	14:Y:34:TYR:N	2.46	0.45
6:I:699:TYR:OH	6:I:714:PRO:O	2.14	0.45
9:L:103:LEU:HD21	9:L:139:ASP:HB2	1.97	0.45
1:A:144:PHE:HB3	15:F:8:ILE:HB	1.98	0.45
1:A:820:ILE:HB	4:E:172:GLY:HA3	1.99	0.45
1:A:61:GLY:HA3	1:A:199:PRO:HB3	1.98	0.45
1:A:613:VAL:HG13	1:A:620:PRO:HG3	1.99	0.45
10:O:48:ILE:HD11	10:O:494:ILE:HD13	1.99	0.45
1:A:799:ASP:OD1	12:S:216:LYS:NZ	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:TYR:O	2:B:515:SER:OG	2.33	0.45
5:G:126:ARG:NH1	5:G:127:ASN:OD1	2.50	0.45
9:L:157:LEU:HD23	9:L:157:LEU:H	1.82	0.45
10:O:4:ASN:O	10:O:7:SER:N	2.45	0.45
10:O:353:GLU:OE2	10:O:369:TYR:OH	2.25	0.45
2:B:287:ILE:O	2:B:291:VAL:HG23	2.16	0.45
2:B:905:ASP:OD1	2:B:909:ILE:N	2.49	0.45
3:C:85:ARG:NH2	3:C:91:ASP:O	2.50	0.45
8:K:388:LEU:HD23	10:O:136:LYS:HB3	1.99	0.45
10:O:717:LEU:HD13	10:O:749:ILE:HD13	1.98	0.45
11:Q:113:ALA:HB2	11:R:107:ILE:HD11	1.98	0.45
11:R:25:VAL:HG21	11:R:29:GLU:HG2	1.97	0.45
1:A:517:LEU:HD12	1:A:517:LEU:H	1.81	0.44
2:B:147:TYR:CG	2:B:148:LEU:N	2.84	0.44
6:I:24:ILE:HD12	6:I:25:SER:H	1.83	0.44
6:I:695:ASN:O	6:I:698:LYS:NZ	2.50	0.44
1:A:104:ASP:N	1:A:104:ASP:OD1	2.50	0.44
7:J:2:VAL:HG12	7:J:2:VAL:O	2.16	0.44
6:I:715:MET:O	6:I:757:ARG:NH2	2.51	0.44
11:R:77:VAL:HG23	11:R:77:VAL:O	2.17	0.44
6:I:532:TYR:O	6:I:536:VAL:HG23	2.17	0.44
9:L:16:LEU:HD13	9:L:181:LEU:HD23	1.98	0.44
2:B:38:TYR:OH	2:B:131:PRO:O	2.26	0.44
2:B:45:ARG:NE	2:B:367:GLU:OE2	2.42	0.44
2:B:152:VAL:O	2:B:152:VAL:HG13	2.17	0.44
1:A:86:LEU:HD22	1:A:91:ILE:HD11	1.99	0.44
1:A:1175:PHE:HB3	1:A:1178:LEU:HD12	2.00	0.44
2:B:610:ARG:NH2	2:B:622:GLU:OE1	2.51	0.44
3:C:86:SER:CB	3:C:138:THR:HG22	2.48	0.44
6:I:674:HIS:HD2	6:I:685:ILE:HG23	1.82	0.44
14:Y:37:PHE:O	14:Y:41:VAL:HG23	2.18	0.44
12:S:95:ALA:HB1	12:S:98:LEU:HD21	2.00	0.44
1:A:304:PRO:HD2	1:A:307:ILE:HD12	1.99	0.44
2:B:152:VAL:O	2:B:153:ILE:C	2.61	0.44
11:R:27:ALA:O	11:R:28:SER:C	2.60	0.44
6:I:499:ILE:HD12	6:I:531:ILE:HG13	1.98	0.44
9:L:4:ILE:HD11	9:L:255:ALA:HA	2.00	0.44
10:O:221:MET:HE2	10:O:221:MET:HB2	1.92	0.44
13:U:30:G:OP2	14:Y:159:ARG:NH1	2.51	0.44
1:A:597:GLU:OE2	1:A:598:LYS:NZ	2.51	0.43
1:A:606:TYR:OH	1:A:626:GLU:OE2	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:ILE:O	2:B:736:ASN:O	2.36	0.43
5:G:119:ASP:O	5:G:121:LYS:NZ	2.47	0.43
8:K:418:CYS:SG	8:K:428:VAL:HG22	2.57	0.43
11:Q:55:ASP:OD1	11:Q:56:LYS:N	2.42	0.43
2:B:243:VAL:HG23	2:B:244:SER:N	2.31	0.43
8:K:379:ASN:OD1	8:K:379:ASN:N	2.51	0.43
8:K:460:VAL:HG23	8:K:461:HIS:ND1	2.33	0.43
11:Q:9:GLU:OE2	11:R:105:ARG:NH1	2.51	0.43
15:F:11:GLU:N	15:F:11:GLU:OE1	2.51	0.43
1:A:534:VAL:HG12	1:A:535:ALA:N	2.32	0.43
1:A:1075:VAL:O	1:A:1081:ASN:ND2	2.43	0.43
2:B:459:VAL:O	2:B:459:VAL:HG22	2.18	0.43
6:I:52:GLU:OE1	10:O:543:ASN:ND2	2.51	0.43
6:I:228:ASP:OD1	6:I:229:PHE:N	2.41	0.43
10:O:626:ILE:HD11	10:O:651:GLN:CB	2.45	0.43
2:B:256:MET:HE1	2:B:340:TYR:HB2	2.00	0.43
10:O:467:GLU:OE1	10:O:467:GLU:N	2.36	0.43
14:Y:227:LEU:O	14:Y:534:THR:HG22	2.19	0.43
14:Y:617:ASN:O	14:Y:619:VAL:N	2.52	0.43
2:B:1083:ASP:OD1	2:B:1083:ASP:N	2.50	0.43
10:O:307:ASP:C	10:O:309:ASN:H	2.26	0.43
13:U:68:G:H2'	13:U:69:A:H8	1.84	0.43
3:C:34:LEU:HD21	3:C:184:ARG:HD2	2.01	0.43
9:L:69:MET:HE1	9:L:109:LEU:HB2	1.99	0.43
14:Y:85:VAL:O	14:Y:113:ASN:HA	2.18	0.43
2:B:134:ILE:HD12	2:B:156:VAL:HG23	2.00	0.43
14:Y:349:ASP:OD1	14:Y:350:ALA:N	2.51	0.43
15:F:105:SER:O	15:F:107:GLU:N	2.52	0.43
1:A:938:PHE:CD1	1:A:938:PHE:C	2.97	0.43
1:A:1055:GLY:HA3	12:S:94:ILE:HB	2.01	0.43
2:B:587:LEU:HD12	2:B:632:ILE:HD12	2.00	0.43
5:G:36:LEU:O	5:G:45:ALA:O	2.37	0.43
6:I:220:LEU:HD23	6:I:220:LEU:H	1.84	0.43
13:U:1:G:H2'	13:U:2:G:C8	2.53	0.43
14:Y:617:ASN:O	14:Y:619:VAL:HG23	2.19	0.43
2:B:862:THR:O	6:I:505:ASP:HB3	2.18	0.43
3:C:150:ILE:HD12	3:C:150:ILE:N	2.33	0.43
5:G:150:SER:O	5:G:151:SER:OG	2.33	0.43
6:I:432:ILE:O	6:I:433:ASN:C	2.61	0.43
7:J:35:VAL:HG21	7:J:44:LEU:CD1	2.49	0.43
1:A:804:ASP:OD1	1:A:805:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:ASN:O	2:B:285:THR:N	2.52	0.43
2:B:1154:ASP:OD1	2:B:1154:ASP:N	2.49	0.43
6:I:653:ASP:OD1	6:I:653:ASP:N	2.52	0.43
11:Q:113:ALA:CB	11:R:105:ARG:HE	2.32	0.43
12:S:52:TYR:HD1	12:S:116:GLU:HG3	1.84	0.43
14:Y:423:VAL:HG11	14:Y:450:ILE:HG21	2.01	0.43
1:A:935:SER:HA	1:A:938:PHE:CE2	2.54	0.42
5:G:142:MET:HE2	5:G:142:MET:HA	2.01	0.42
1:A:978:ILE:N	1:A:978:ILE:HD12	2.35	0.42
1:A:1062:ASP:N	1:A:1062:ASP:OD1	2.51	0.42
9:L:212:HIS:O	9:L:216:VAL:HG23	2.19	0.42
10:O:571:TYR:O	10:O:574:THR:HG22	2.19	0.42
14:Y:589:LEU:HD13	14:Y:624:ASP:OD2	2.18	0.42
1:A:86:LEU:HD21	1:A:165:ILE:HG23	2.00	0.42
1:A:99:ARG:NH2	6:I:220:LEU:HD22	2.35	0.42
1:A:145:SER:HB3	1:A:148:LYS:O	2.20	0.42
2:B:863:ASP:OD1	2:B:864:LYS:N	2.50	0.42
5:G:41:SER:O	6:I:287:TYR:OH	2.36	0.42
13:U:26:U:O2	13:U:26:U:O4'	2.37	0.42
2:B:790:LYS:HG3	2:B:791:GLU:H	1.84	0.42
2:B:862:THR:O	6:I:505:ASP:CB	2.67	0.42
4:E:123:ILE:O	4:E:127:VAL:HG23	2.20	0.42
14:Y:597:LYS:O	14:Y:597:LYS:HG3	2.19	0.42
1:A:40:ARG:O	1:A:51:THR:OG1	2.38	0.42
2:B:178:PRO:HB3	2:B:192:PHE:HB3	2.01	0.42
10:O:266:ILE:HD12	10:O:279:PHE:CD2	2.55	0.42
11:Q:37:LEU:O	11:Q:40:GLU:HB3	2.19	0.42
1:A:955:VAL:HG11	1:A:977:ILE:HG21	2.02	0.42
1:A:1125:VAL:HG22	1:A:1126:GLU:N	2.34	0.42
2:B:716:MET:CG	2:B:773:VAL:HG23	2.49	0.42
3:C:40:VAL:HG21	3:C:49:ASN:HB3	2.02	0.42
3:C:95:THR:N	3:C:98:ASP:OD2	2.47	0.42
5:G:30:ALA:O	5:G:34:THR:HG22	2.19	0.42
5:G:86:ARG:NH1	5:G:138:THR:OG1	2.48	0.42
10:O:654:ILE:O	10:O:696:ASN:ND2	2.53	0.42
10:O:781:VAL:HG23	10:O:844:ARG:HD3	2.00	0.42
1:A:1106:SER:O	1:A:1121:ASN:HA	2.19	0.42
2:B:398:ASN:O	2:B:401:VAL:HG22	2.20	0.42
6:I:111:LEU:C	6:I:111:LEU:HD23	2.45	0.42
10:O:244:LYS:O	10:O:247:ILE:HG22	2.20	0.42
14:Y:593:ASN:N	14:Y:593:ASN:OD1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:TYR:OH	2:B:668:ARG:NH1	2.53	0.42
2:B:147:TYR:OH	6:I:593:GLU:HB3	2.20	0.42
6:I:428:MET:O	6:I:429:LYS:C	2.63	0.42
14:Y:83:LEU:N	14:Y:83:LEU:HD12	2.34	0.42
2:B:611:LEU:CD1	2:B:619:ILE:HD11	2.50	0.42
3:C:173:VAL:O	3:C:174:LYS:C	2.62	0.42
6:I:650:CYS:O	6:I:651:ASP:HB3	2.20	0.42
6:I:713:ASP:HB3	6:I:730:LYS:HG2	2.01	0.42
10:O:158:ILE:HG12	10:O:215:LEU:HD21	2.01	0.42
10:O:641:LYS:HD2	10:O:642:THR:HG23	2.01	0.42
10:O:678:GLN:HA	10:O:710:THR:OG1	2.19	0.42
12:S:28:LEU:HD22	12:S:125:ILE:HD11	2.01	0.42
6:I:748:PHE:O	6:I:748:PHE:CG	2.73	0.41
1:A:4:ILE:O	1:A:1243:LYS:NZ	2.41	0.41
1:A:569:LEU:O	1:A:573:GLY:N	2.52	0.41
2:B:529:PRO:HD2	2:B:576:ASN:O	2.20	0.41
6:I:208:ASN:OD1	6:I:208:ASN:C	2.63	0.41
12:S:125:ILE:O	12:S:129:LYS:HG2	2.20	0.41
2:B:168:ILE:O	2:B:365:TYR:OH	2.34	0.41
2:B:318:HIS:NE2	2:B:534:ASN:O	2.53	0.41
5:G:52:GLU:O	6:I:301:ARG:NH2	2.54	0.41
5:G:148:ILE:O	5:G:149:GLU:C	2.64	0.41
6:I:60:THR:O	6:I:63:GLU:HG3	2.20	0.41
6:I:493:ILE:O	6:I:497:VAL:HG23	2.20	0.41
8:K:432:ASN:HA	8:K:455:THR:HG21	2.02	0.41
9:L:67:ASP:OD1	9:L:67:ASP:N	2.53	0.41
9:L:254:GLU:OE1	10:O:797:LYS:NZ	2.52	0.41
10:O:254:ASN:O	10:O:381:TYR:HA	2.20	0.41
10:O:635:LYS:O	10:O:638:SER:OG	2.30	0.41
1:A:9:TYR:O	1:A:1227:LYS:HA	2.20	0.41
2:B:41:PHE:CZ	2:B:366:PHE:HB3	2.54	0.41
2:B:1084:VAL:HG11	2:B:1125:LYS:HE2	2.02	0.41
9:L:61:LEU:HD21	9:L:109:LEU:HD23	2.01	0.41
2:B:26:VAL:HG22	2:B:32:HIS:CE1	2.55	0.41
2:B:556:LYS:NZ	2:B:564:LEU:O	2.50	0.41
4:E:91:GLY:O	4:E:150:LYS:NZ	2.52	0.41
5:G:109:SER:OG	5:G:111:ASP:OD1	2.37	0.41
9:L:11:GLY:HA2	9:L:189:TRP:CZ2	2.55	0.41
9:L:210:MET:O	9:L:214:LYS:HG2	2.20	0.41
10:O:325:ASN:O	10:O:383:LYS:HB3	2.21	0.41
14:Y:461:LEU:N	14:Y:461:LEU:HD12	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:531:ILE:O	6:I:532:TYR:C	2.63	0.41
1:A:110:GLU:OE1	1:A:110:GLU:N	2.54	0.41
2:B:541:ASN:OD1	2:B:541:ASN:C	2.64	0.41
9:L:88:LYS:N	9:L:98:ALA:O	2.49	0.41
9:L:214:LYS:O	9:L:218:LYS:N	2.43	0.41
9:L:246:LEU:O	9:L:250:ASN:ND2	2.54	0.41
14:Y:489:GLU:OE1	14:Y:489:GLU:N	2.40	0.41
6:I:253:ASN:O	6:I:253:ASN:ND2	2.54	0.41
6:I:599:LEU:HD22	6:I:599:LEU:N	2.36	0.41
14:Y:605:ASP:HB2	14:Y:611:LEU:HD21	2.02	0.41
1:A:850:THR:O	1:A:852:ASP:N	2.54	0.41
4:E:9:LEU:O	4:E:13:LEU:HG	2.21	0.41
6:I:204:LYS:O	6:I:205:LYS:HB2	2.20	0.41
6:I:527:ILE:O	6:I:528:SER:C	2.63	0.41
8:K:388:LEU:HD12	8:K:392:MET:SD	2.61	0.41
9:L:102:ASP:O	9:L:103:LEU:HD23	2.21	0.41
9:L:214:LYS:NZ	9:L:220:SER:O	2.45	0.41
10:O:618:ALA:N	10:O:648:ASP:O	2.42	0.41
14:Y:176:ASN:OD1	14:Y:556:LYS:NZ	2.52	0.41
14:Y:155:ASP:OD1	14:Y:155:ASP:N	2.53	0.41
14:Y:289:LEU:HD23	14:Y:292:MET:HE3	2.03	0.41
1:A:306:TYR:CZ	2:B:1026:ALA:HB1	2.56	0.40
1:A:990:SER:O	1:A:993:ILE:HG22	2.20	0.40
9:L:9:ARG:NH2	9:L:284:LYS:O	2.47	0.40
10:O:245:GLN:C	10:O:245:GLN:OE1	2.64	0.40
1:A:145:SER:O	15:F:6:ASP:O	2.39	0.40
1:A:742:SER:HA	1:A:745:ILE:HG12	2.02	0.40
2:B:305:ASN:C	2:B:307:PHE:H	2.29	0.40
2:B:440:ILE:HB	2:B:441:PRO:HD3	2.02	0.40
6:I:74:VAL:HG13	10:O:735:SER:HB2	2.02	0.40
6:I:533:ASP:OD1	6:I:533:ASP:N	2.54	0.40
6:I:777:TRP:O	6:I:781:ASN:ND2	2.45	0.40
1:A:921:GLY:HA3	15:F:78:SER:CB	2.50	0.40
2:B:1092:ASP:OD2	2:B:1105:ARG:NE	2.46	0.40
6:I:112:TYR:O	6:I:116:PHE:HD1	2.04	0.40
7:J:2:VAL:HA	7:J:18:ARG:HD3	2.03	0.40
10:O:66:PHE:HD2	10:O:143:LEU:HD22	1.85	0.40
13:U:15:A:H2'	13:U:58:A:N6	2.37	0.40
14:Y:92:ASP:CB	14:Y:93:PRO:HD3	2.51	0.40
2:B:1084:VAL:HG21	2:B:1118:ILE:HG13	2.04	0.40
5:G:104:LEU:HD21	5:G:141:LEU:HD21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:564:LEU:N	6:I:564:LEU:HD12	2.37	0.40
10:O:652:GLU:HG2	10:O:659:PHE:HA	2.02	0.40
14:Y:323:PHE:O	14:Y:326:SER:OG	2.39	0.40
2:B:150:PRO:HG3	6:I:596:GLY:HA2	2.02	0.40
2:B:556:LYS:NZ	2:B:566:VAL:O	2.50	0.40
4:E:5:ASN:HB2	4:E:100:LEU:HB3	2.03	0.40
6:I:421:MET:O	6:I:423:SER:N	2.54	0.40
15:F:11:GLU:O	15:F:12:SER:OG	2.32	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	1274/1286 (99%)	1200 (94%)	74 (6%)	0	100	100
2	B	1123/1164 (96%)	1057 (94%)	66 (6%)	0	100	100
3	C	302/305 (99%)	281 (93%)	21 (7%)	0	100	100
4	E	182/185 (98%)	172 (94%)	10 (6%)	0	100	100
5	G	157/161 (98%)	150 (96%)	7 (4%)	0	100	100
6	I	765/795 (96%)	719 (94%)	46 (6%)	0	100	100
7	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
8	K	97/710 (14%)	93 (96%)	4 (4%)	0	100	100
9	L	280/287 (98%)	265 (95%)	15 (5%)	0	100	100
10	O	842/844 (100%)	815 (97%)	27 (3%)	0	100	100
11	Q	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
11	R	128/129 (99%)	119 (93%)	9 (7%)	0	100	100
12	S	182/259 (70%)	174 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	Y	599/631 (95%)	574 (96%)	25 (4%)	0	100	100
15	F	107/164 (65%)	105 (98%)	2 (2%)	0	100	100
All	All	6219/7112 (87%)	5899 (95%)	320 (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	1149/1157 (99%)	1135 (99%)	14 (1%)	63	79
2	B	1030/1064 (97%)	1002 (97%)	28 (3%)	39	61
3	C	286/287 (100%)	275 (96%)	11 (4%)	29	49
4	E	174/175 (99%)	170 (98%)	4 (2%)	44	66
5	G	142/144 (99%)	139 (98%)	3 (2%)	47	69
6	I	735/755 (97%)	709 (96%)	26 (4%)	32	52
7	J	60/62 (97%)	54 (90%)	6 (10%)	7	11
8	K	95/665 (14%)	90 (95%)	5 (5%)	20	35
9	L	269/272 (99%)	263 (98%)	6 (2%)	45	67
10	O	774/774 (100%)	760 (98%)	14 (2%)	51	72
11	Q	116/121 (96%)	111 (96%)	5 (4%)	26	44
11	R	122/121 (101%)	117 (96%)	5 (4%)	27	46
12	S	171/237 (72%)	168 (98%)	3 (2%)	51	72
14	Y	552/573 (96%)	537 (97%)	15 (3%)	39	61
15	F	102/151 (68%)	99 (97%)	3 (3%)	37	58
All	All	5777/6558 (88%)	5629 (97%)	148 (3%)	41	63

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	CYS
1	A	106	ILE
1	A	156	ASP
1	A	184	GLN
1	A	366	VAL
1	A	471	ILE
1	A	555	ILE
1	A	591	LEU
1	A	791	LEU
1	A	1058	THR
1	A	1060	ILE
1	A	1061	GLU
1	A	1062	ASP
1	A	1163	LEU
2	B	52	VAL
2	B	56	LEU
2	B	100	VAL
2	B	161	GLN
2	B	216	GLN
2	B	217	LEU
2	B	229	ILE
2	B	280	ASP
2	B	322	THR
2	B	394	THR
2	B	401	VAL
2	B	403	THR
2	B	423	ASP
2	B	428	THR
2	B	472	SER
2	B	504	ASP
2	B	545	ILE
2	B	547	ASP
2	B	572	ARG
2	B	659	ASP
2	B	705	ILE
2	B	713	ILE
2	B	912	ASP
2	B	963	ASP
2	B	1028	VAL
2	B	1061	LEU
2	B	1071	THR
2	B	1154	ASP
3	C	18	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	29	LEU
3	C	108	THR
3	C	120	LEU
3	C	135	SER
3	C	136	SER
3	C	180	ASP
3	C	238	ASP
3	C	247	GLU
3	C	255	ASP
3	C	273	SER
4	E	76	ASP
4	E	108	ASP
4	E	116	LEU
4	E	171	THR
5	G	20	THR
5	G	22	ASP
5	G	116	SER
6	I	24	ILE
6	I	28	SER
6	I	42	ILE
6	I	85	GLU
6	I	105	ASP
6	I	186	LYS
6	I	220	LEU
6	I	253	ASN
6	I	256	LEU
6	I	289	ASP
6	I	305	ASP
6	I	317	ARG
6	I	318	ASP
6	I	319	VAL
6	I	333	LYS
6	I	344	THR
6	I	455	SER
6	I	462	LEU
6	I	480	GLU
6	I	589	ASN
6	I	614	VAL
6	I	652	GLU
6	I	662	ASP
6	I	744	ASP
6	I	747	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	I	749	VAL
7	J	7	CYS
7	J	13	ASP
7	J	21	LEU
7	J	33	VAL
7	J	49	GLU
7	J	60	LEU
8	K	379	ASN
8	K	386	ASN
8	K	388	LEU
8	K	447	LEU
8	K	457	SER
9	L	29	LEU
9	L	182	LEU
9	L	186	SER
9	L	217	THR
9	L	265	SER
9	L	268	THR
10	O	34	ILE
10	O	103	VAL
10	O	221	MET
10	O	270	VAL
10	O	281	HIS
10	O	298	VAL
10	O	333	TYR
10	O	362	VAL
10	O	410	MET
10	O	475	VAL
10	O	619	THR
10	O	673	ASN
10	O	787	ASP
10	O	790	THR
11	Q	23	ASP
11	Q	29	GLU
11	Q	46	GLN
11	Q	82	LEU
11	Q	92	THR
11	R	15	VAL
11	R	55	ASP
11	R	57	ASP
11	R	71	VAL
11	R	89	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	S	32	VAL
12	S	96	THR
12	S	146	ASP
14	Y	65	THR
14	Y	148	SER
14	Y	188	VAL
14	Y	240	SER
14	Y	323	PHE
14	Y	331	GLU
14	Y	369	ILE
14	Y	392	SER
14	Y	415	THR
14	Y	486	THR
14	Y	551	ASN
14	Y	591	SER
14	Y	599	VAL
14	Y	607	ASP
14	Y	627	LEU
15	F	7	ILE
15	F	106	ASP
15	F	117	ILE

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	385	HIS
1	A	648	HIS
1	A	686	GLN
1	A	830	GLN
2	B	357	HIS
2	B	371	HIS
2	B	543	ASN
2	B	714	HIS
2	B	1023	GLN
3	C	8	ASN
3	C	137	GLN
6	I	99	ASN
6	I	178	ASN
6	I	252	HIS
6	I	253	ASN
6	I	664	ASN
7	J	16	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	O	512	ASN
10	O	539	HIS
10	O	550	ASN
10	O	558	ASN
10	O	689	HIS
12	S	36	ASN
12	S	55	ASN
12	S	62	ASN
12	S	72	ASN
12	S	213	HIS
14	Y	483	HIS
14	Y	587	ASN
15	F	150	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	U	68/72 (94%)	12 (17%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	U	4	C
13	U	9	G
13	U	16	U
13	U	17	G
13	U	34	U
13	U	35	U
13	U	37	A
13	U	41	C
13	U	47	U
13	U	48	C
13	U	71	C
13	U	72	U

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
12	SEP	S	228	12	8,9,10	1.55	1 (12%)	7,12,14	1.30	1 (14%)
13	OMC	U	32	13	19,22,23	0.59	0	25,31,34	0.59	0
12	SEP	S	232	12	8,9,10	1.59	1 (12%)	7,12,14	1.14	1 (14%)
13	1MA	U	57	13	21,25,26	0.50	0	30,37,40	0.77	1 (3%)
12	SEP	S	237	12	8,9,10	1.57	1 (12%)	7,12,14	1.29	1 (14%)

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
12	SEP	S	228	12	-	2/6/8/10	-
13	OMC	U	32	13	-	0/9/27/28	0/2/2/2
12	SEP	S	232	12	-	0/6/8/10	-
13	1MA	U	57	13	-	0/7/25/26	0/3/3/3
12	SEP	S	237	12	-	3/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	232	SEP	P-O1P	3.46	1.61	1.50
12	S	237	SEP	P-O1P	3.43	1.61	1.50
12	S	228	SEP	P-O1P	3.40	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	228	SEP	OG-CB-CA	2.81	110.88	108.14
12	S	237	SEP	OG-CB-CA	2.66	110.73	108.14
12	S	232	SEP	OG-CB-CA	2.37	110.45	108.14
13	U	57	1MA	N1-C6-N6	2.26	125.39	119.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	S	237	SEP	CB-OG-P-O2P
12	S	237	SEP	CB-OG-P-O3P
12	S	237	SEP	CB-OG-P-O1P
12	S	228	SEP	CB-OG-P-O1P
12	S	228	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

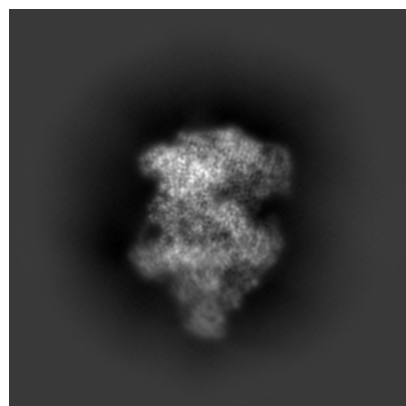
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19442. These allow visual inspection of the internal detail of the map and identification of artifacts.

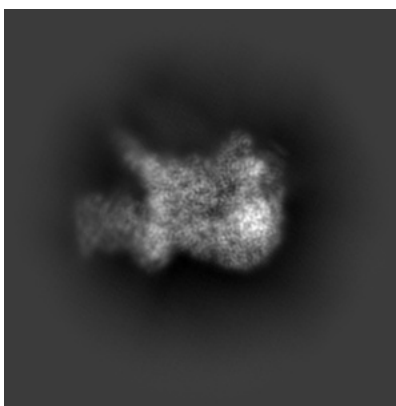
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

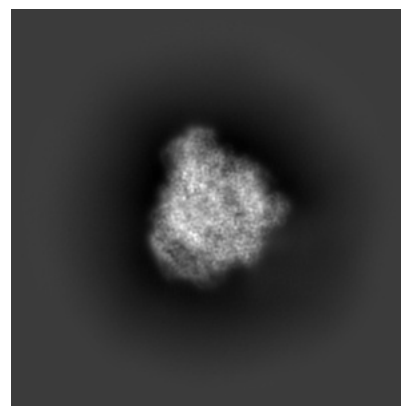
6.1.1 Primary map



X

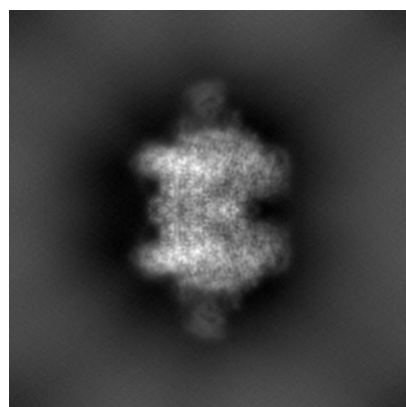


Y

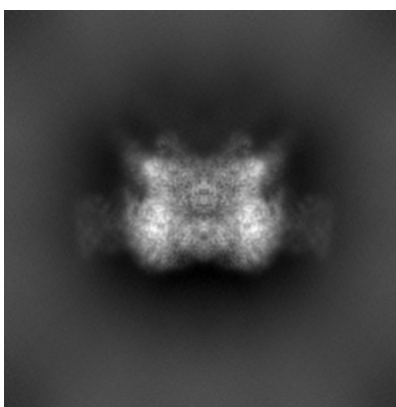


Z

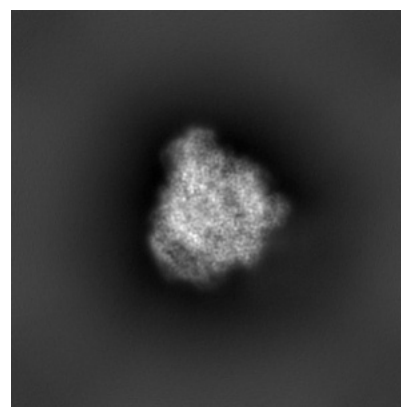
6.1.2 Raw map



X



Y

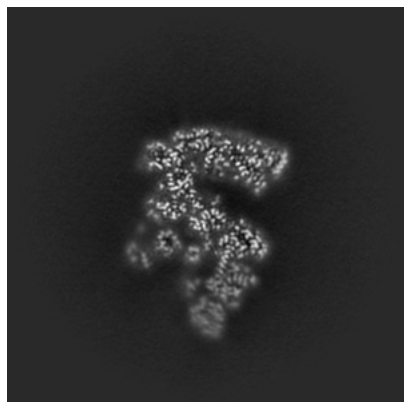


Z

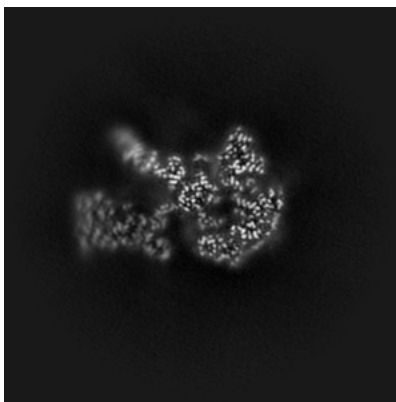
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

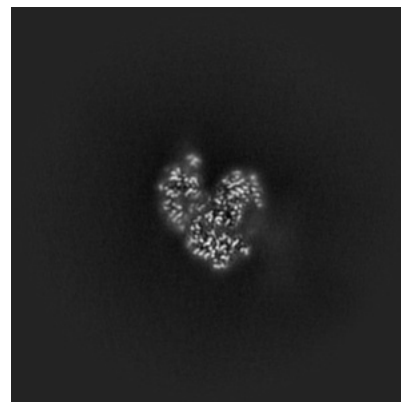
6.2.1 Primary map



X Index: 180

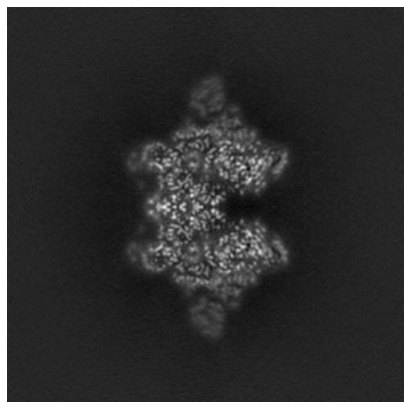


Y Index: 180

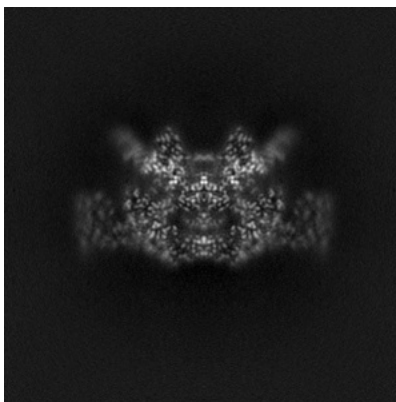


Z Index: 180

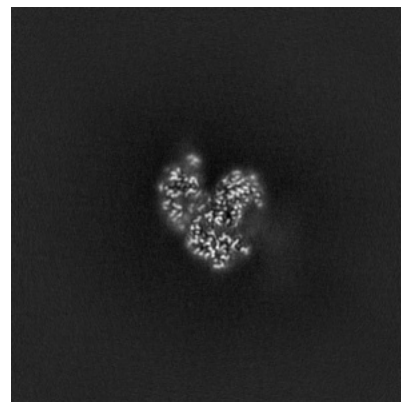
6.2.2 Raw map



X Index: 180



Y Index: 180

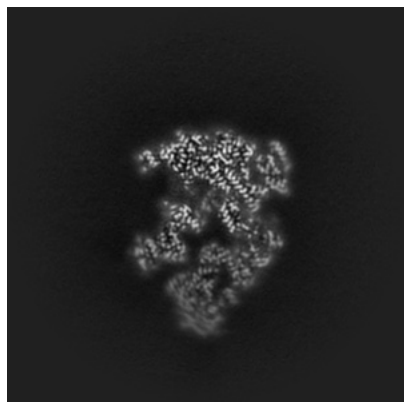


Z Index: 180

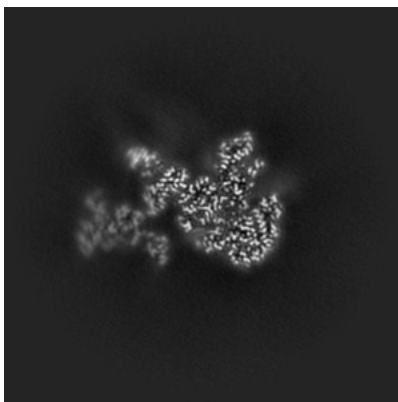
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

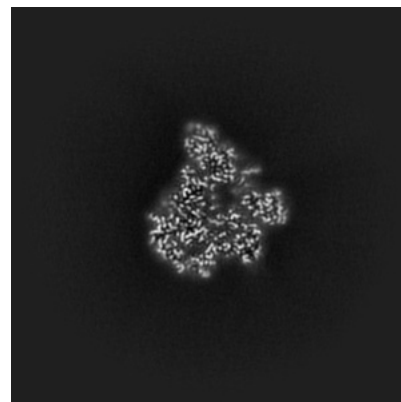
6.3.1 Primary map



X Index: 162

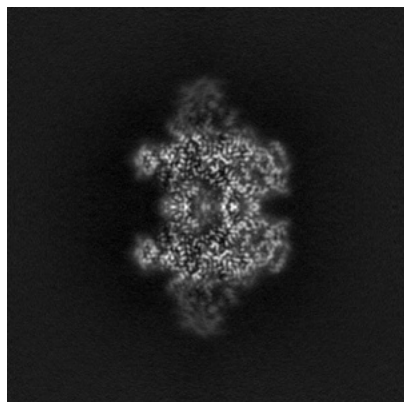


Y Index: 167

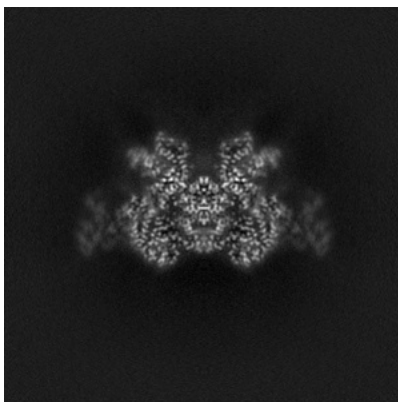


Z Index: 217

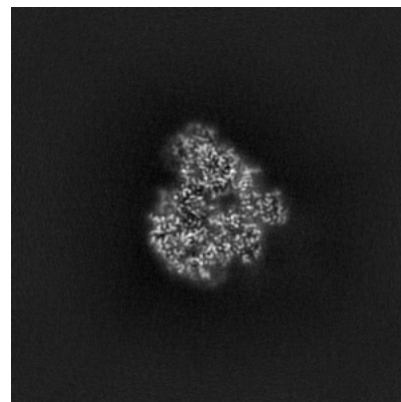
6.3.2 Raw map



X Index: 162



Y Index: 167

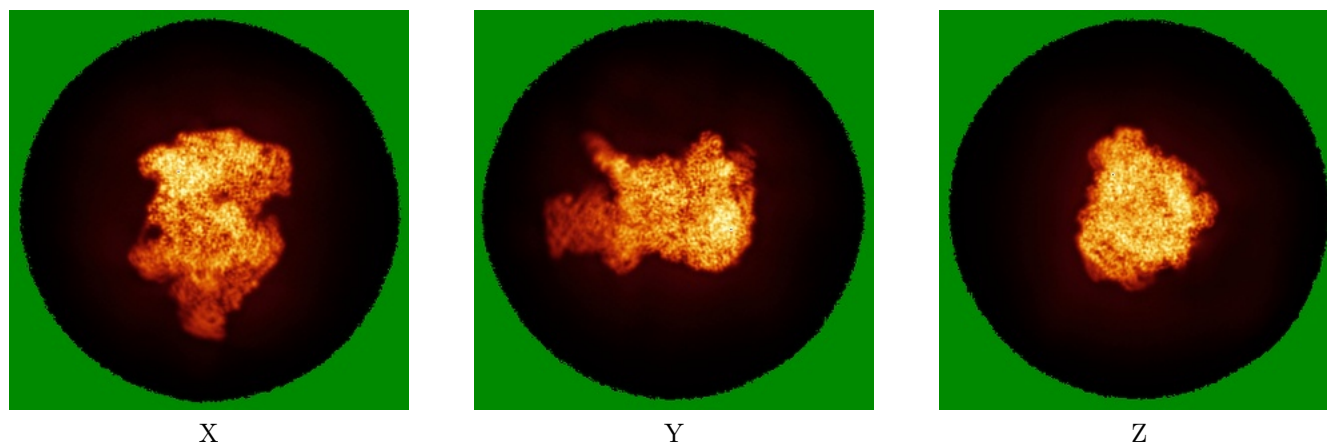


Z Index: 142

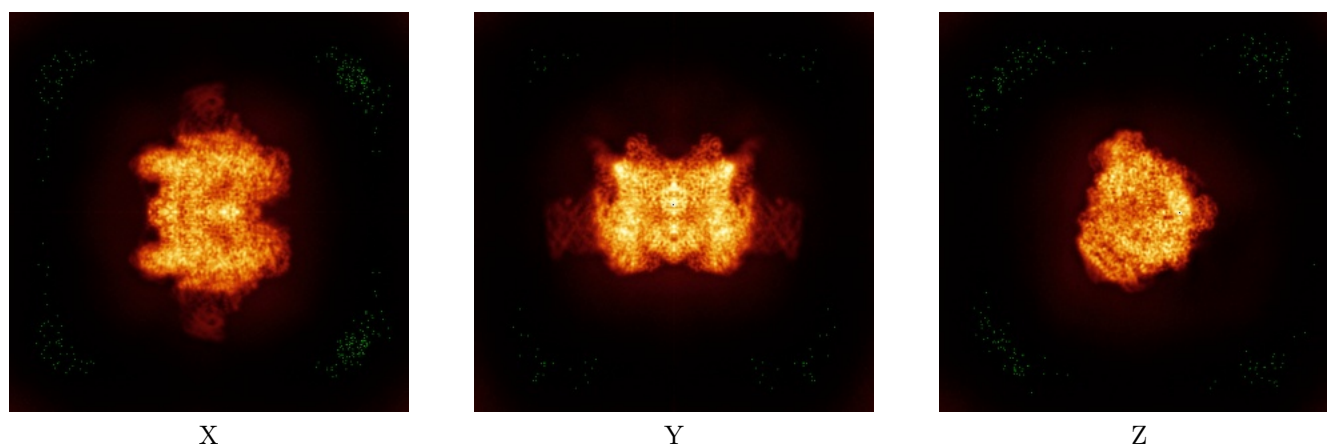
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

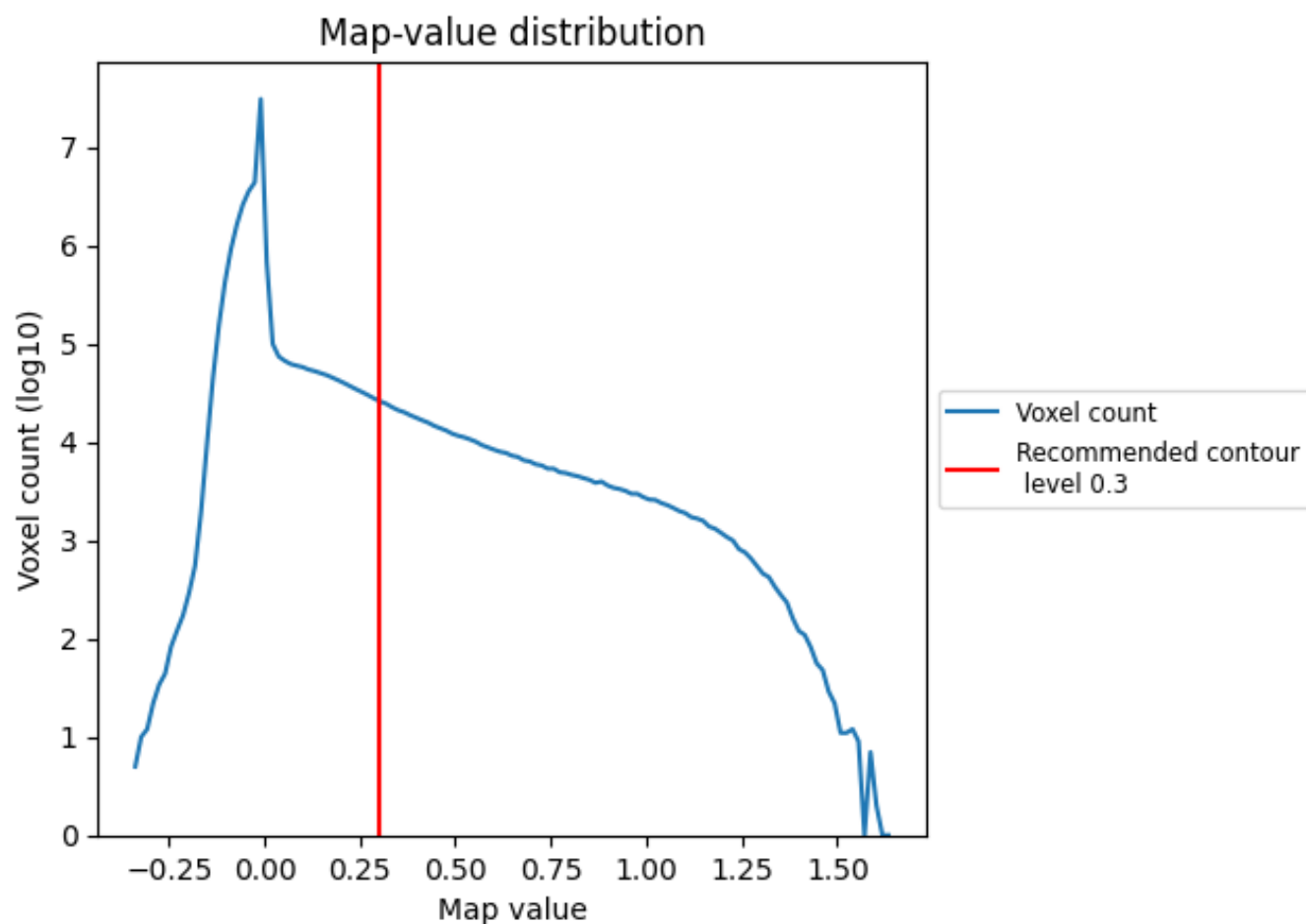
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

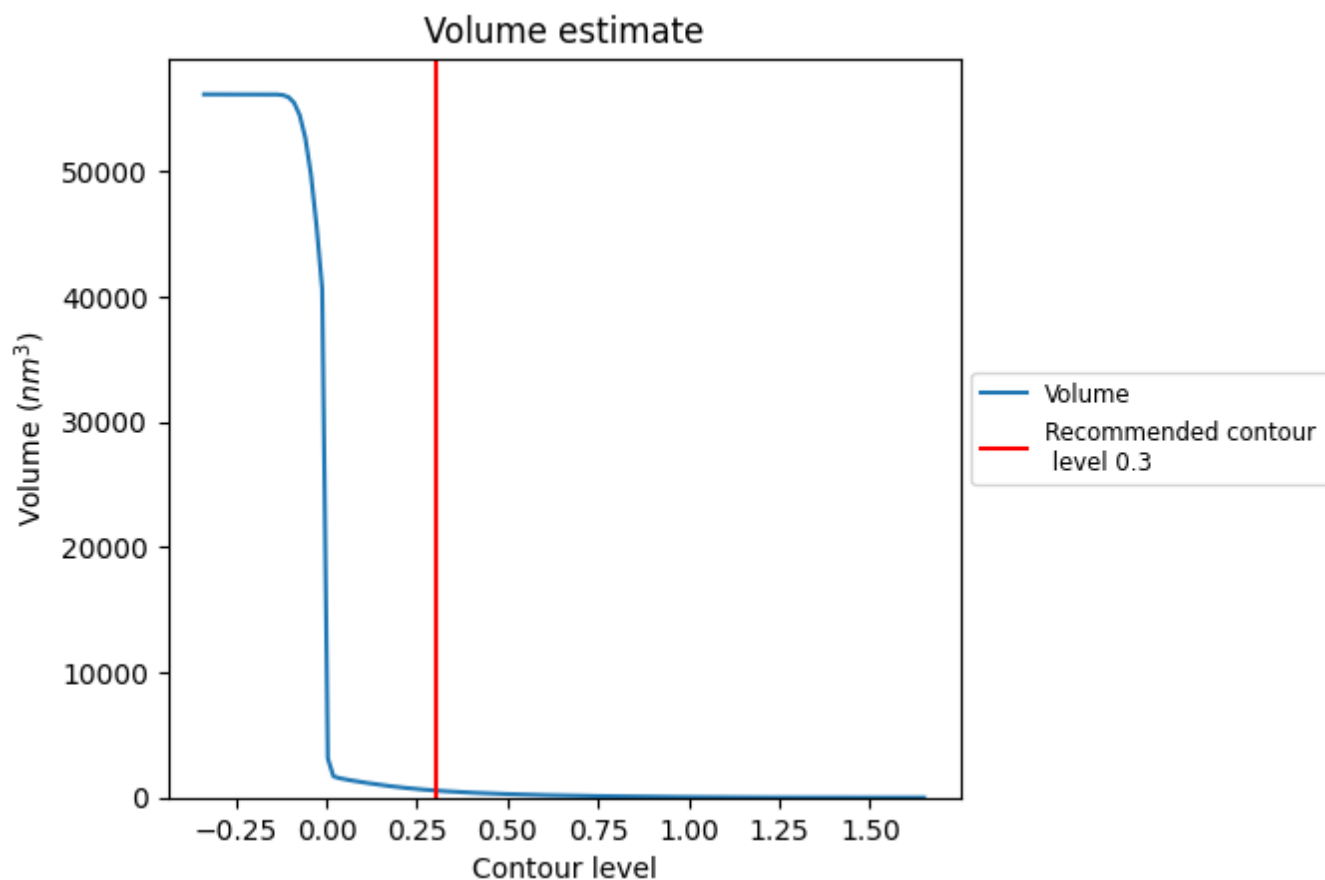
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

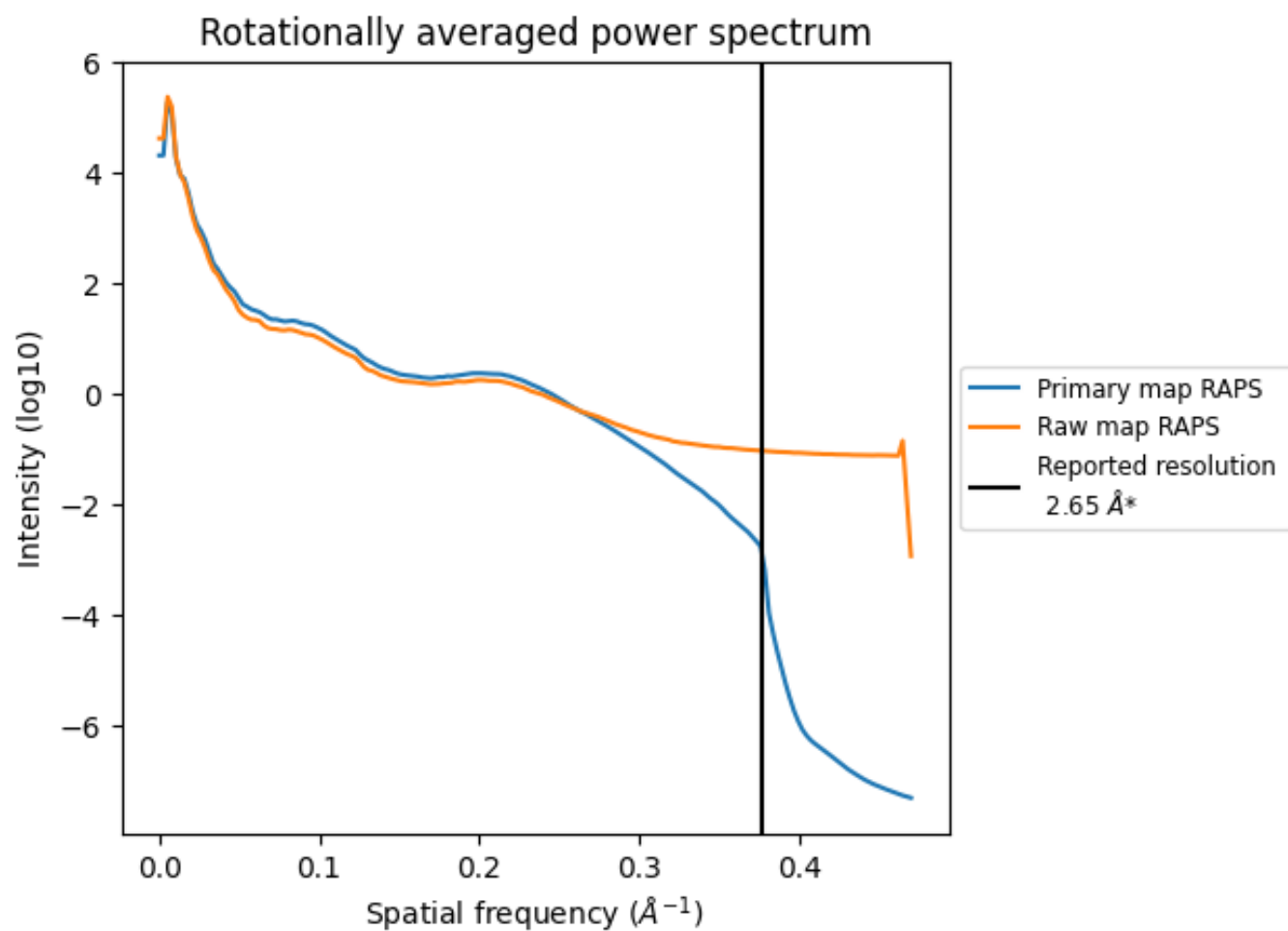
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 563 nm³; this corresponds to an approximate mass of 509 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 ⓘ

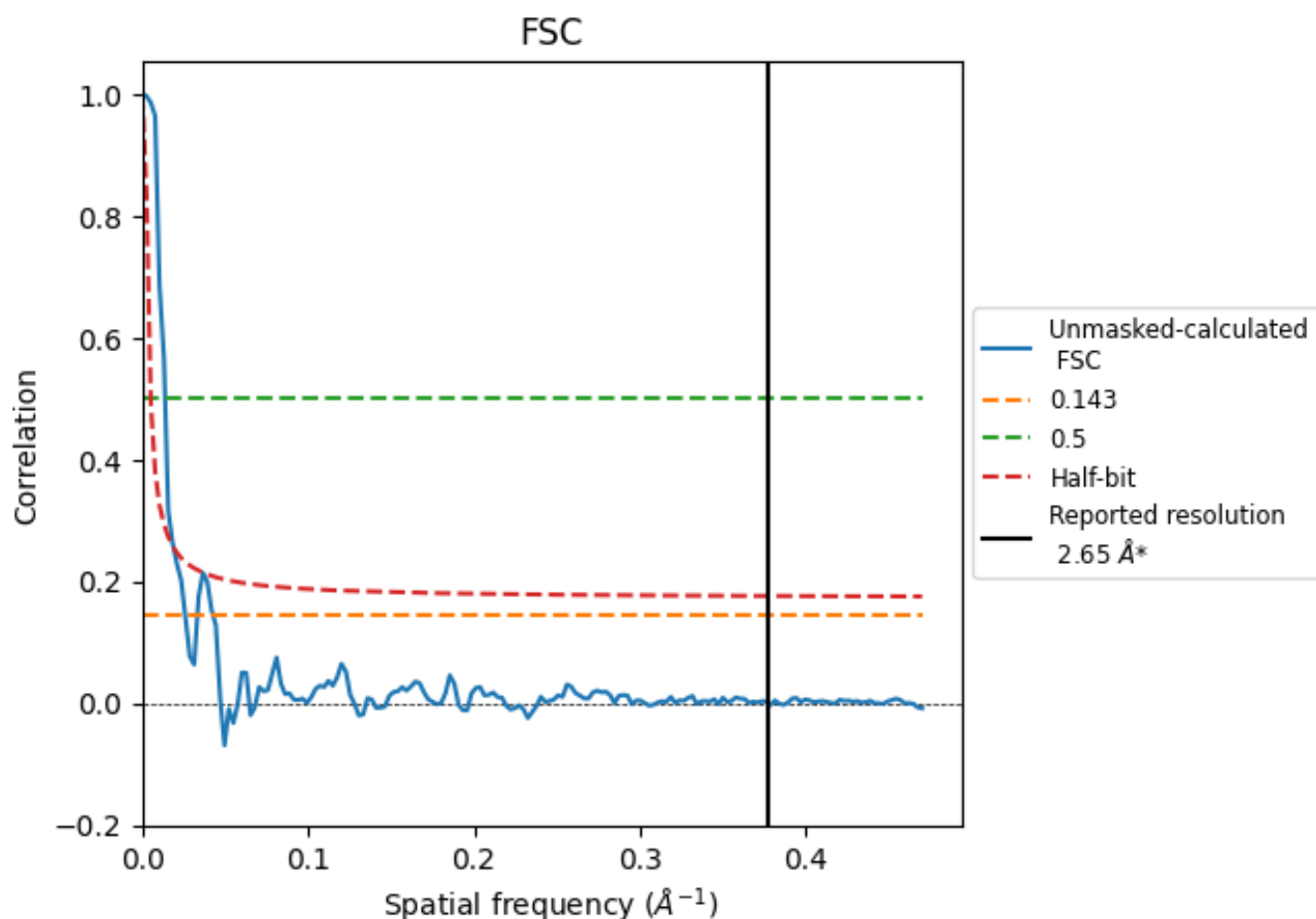


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

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 $0.377 \text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

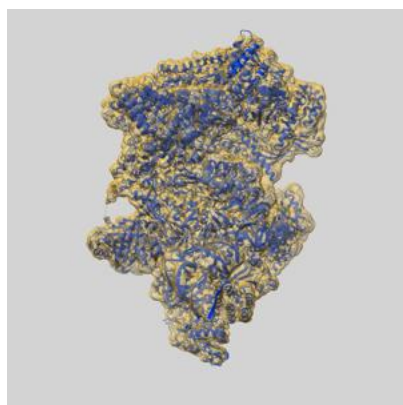
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	38.61	72.99	53.19

*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 38.61 differs from the reported value 2.65 by more than 10 %

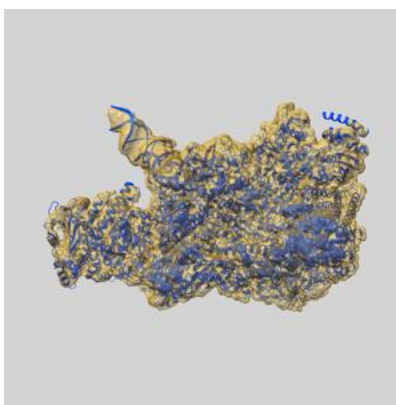
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19442 and PDB model 8RQK. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

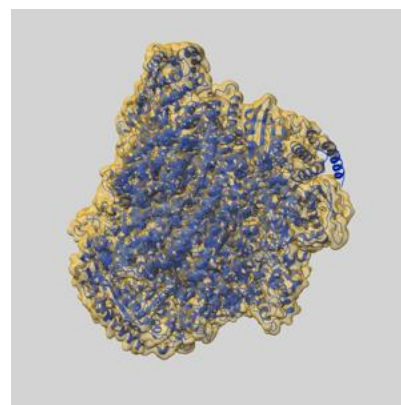
9.1 Map-model overlay [i](#)



X



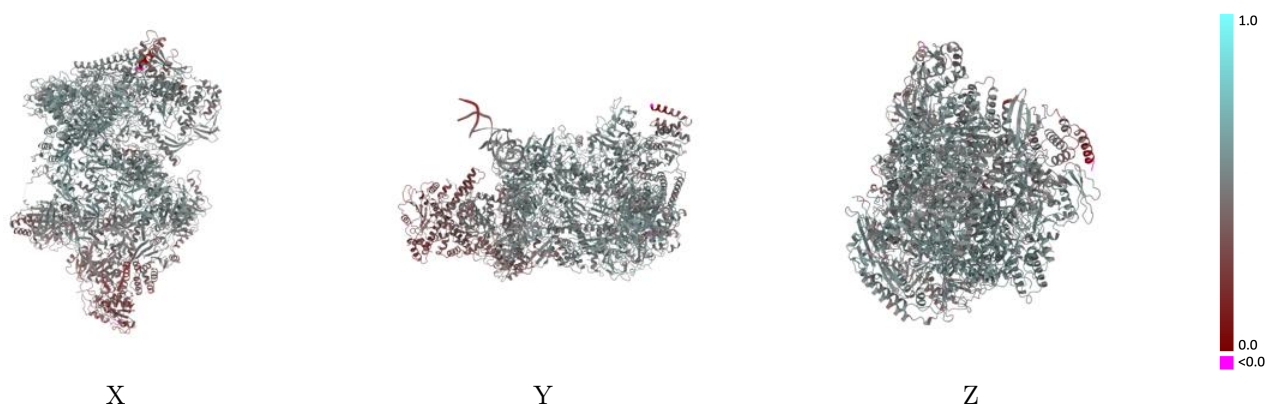
Y



Z

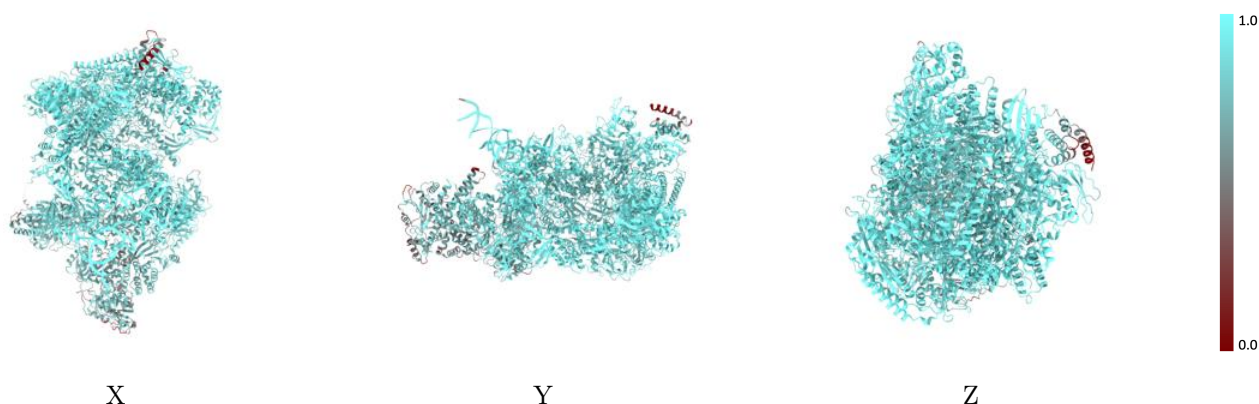
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



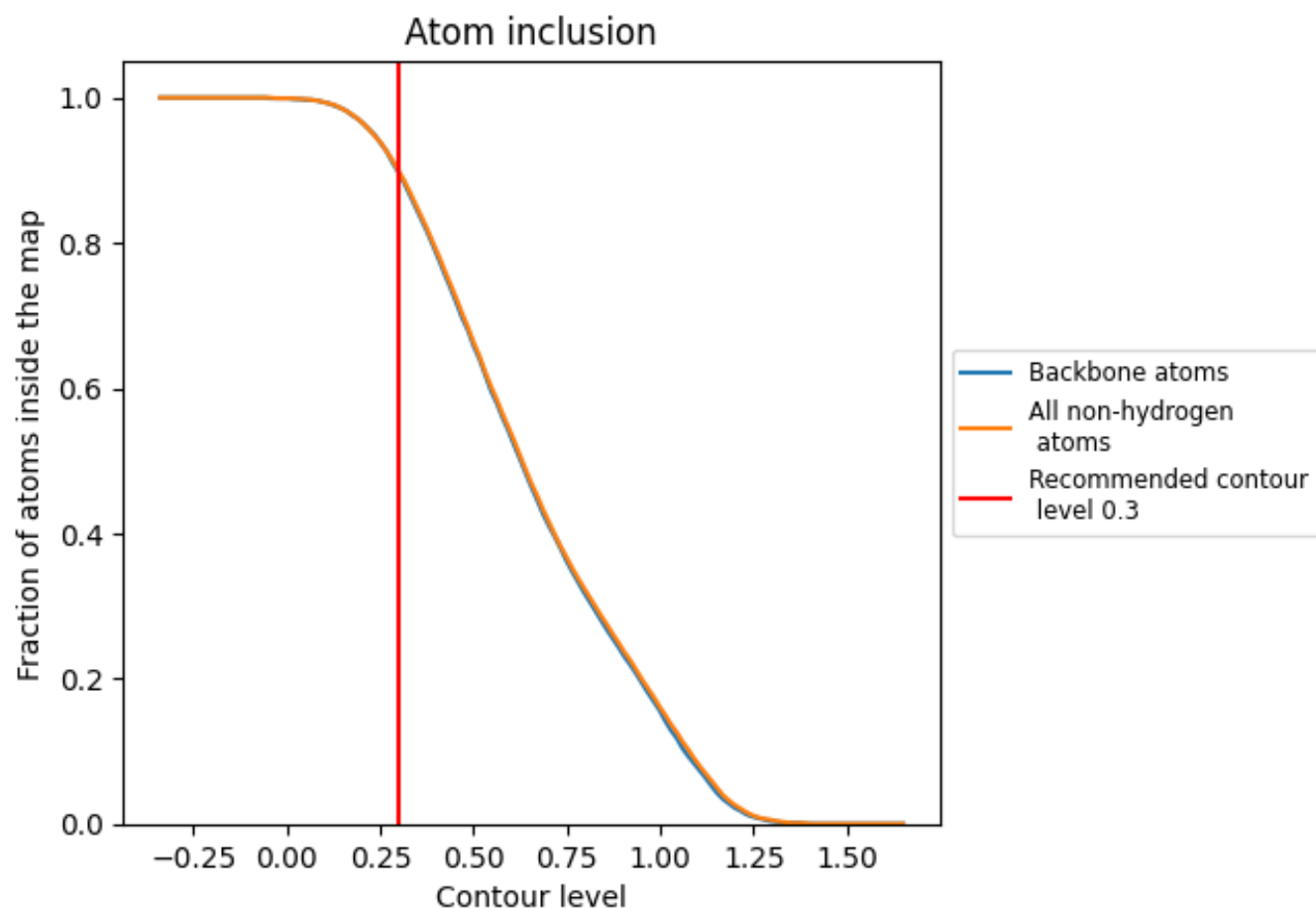
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8990	 0.4920
A	 0.9600	 0.5390
B	 0.9710	 0.5440
C	 0.9710	 0.5310
E	 0.9720	 0.5360
F	 0.9690	 0.5440
G	 0.9620	 0.5310
I	 0.9120	 0.4900
J	 0.9810	 0.5450
K	 0.8830	 0.4820
L	 0.6520	 0.3110
O	 0.7860	 0.4230
Q	 0.8920	 0.4520
R	 0.9290	 0.4750
S	 0.7450	 0.4340
U	 0.9770	 0.4490
Y	 0.8620	 0.4690

