



Full wwPDB EM Validation Report ⓘ

Oct 8, 2022 – 07:26 PM EDT

PDB ID : 7UD5
EMDB ID : EMD-26454
Title : Complex between MLL1-WRAD and an H2B-ubiquitinated nucleosome
Authors : Niklas, H.A.; Rahman, S.; Worden, E.J.; Wolberger, C.
Deposited on : 2022-03-18
Resolution : 4.25 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

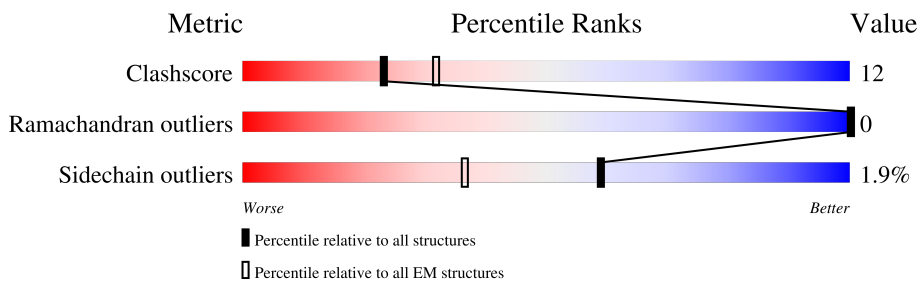
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	123	
4	H	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	146	73% 27%
6	J	146	58% 42%
7	K	226	14% 55% 22% 23%
8	L	335	9% 57% 34% 10%
9	M	534	25% 34% 26% 39%
10	N	538	7% 46% 21% 32%
11	O	81	67% 62% 31% 7%
12	P	104	38% 30% 20% 50%
12	Q	104	33% 33% 16% 51%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22713 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	97	802	508	155	138	1	0	0
1	E	95	785	497	151	136	1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	NLE	LYS	engineered mutation	UNP A0A310TTQ1
A	90	NLE	MET	engineered mutation	UNP A0A310TTQ1
A	120	NLE	MET	engineered mutation	UNP A0A310TTQ1
E	4	NLE	LYS	engineered mutation	UNP A0A310TTQ1
E	90	NLE	MET	engineered mutation	UNP A0A310TTQ1
E	120	NLE	MET	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	82	657	416	128	112	1	0	0
2	F	79	633	399	124	109	1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	106	820	517	160	143	0	0
3	G	105	809	510	158	141	0	0

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			754	472	139	140	3		
4	H	95	Total	C	N	O	S	0	0
			742	466	133	140	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	expression tag	UNP P02281
D	29	THR	SER	engineered mutation	UNP P02281
D	117	CYS	LYS	engineered mutation	UNP P02281
H	0	MET	-	expression tag	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281
H	117	CYS	LYS	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called 601 DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called 601 DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called cDNA FLJ56846, highly similar to Zinc finger protein HRX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	175	Total	C	N	O	S	0	0
			1398	887	253	244	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	3744	MET	-	initiating methionine	UNP B4DIJ7

- Molecule 8 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	303	2382	1523	394	454	11	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	GLY	-	expression tag	UNP P61964
L	1	SER	-	expression tag	UNP P61964

- Molecule 9 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	328	2625	1685	446	486	8	0	0

- Molecule 10 is a protein called Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	366	2879	1813	494	557	15	0	0

- Molecule 11 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	75	597	376	104	116	1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-4	GLN	-	expression tag	UNP J3QS39
O	-3	GLY	-	expression tag	UNP J3QS39
O	-2	SER	-	expression tag	UNP J3QS39
O	-1	HIS	-	expression tag	UNP J3QS39
O	0	MET	-	expression tag	UNP J3QS39
O	76	CYS	GLY	engineered mutation	UNP J3QS39

- Molecule 12 is a protein called Protein dpy-30 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	P	52	413	271	68	74	0	0

Continued on next page...

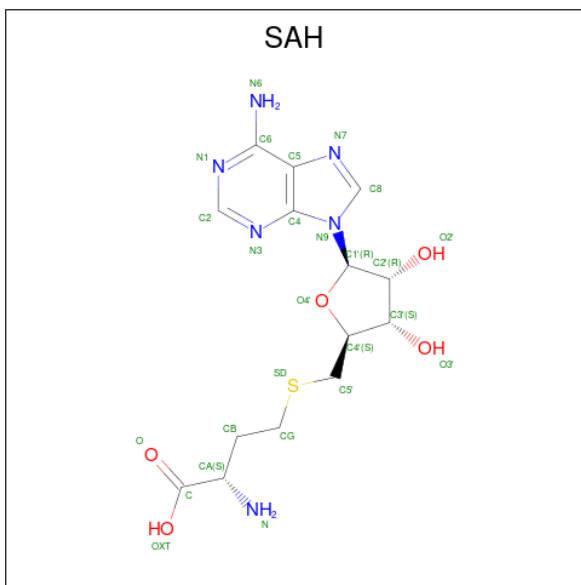
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Q	51	404	265	66	73	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	GLY	-	expression tag	UNP Q9C005
P	-3	ALA	-	expression tag	UNP Q9C005
P	-2	MET	-	expression tag	UNP Q9C005
P	-1	ASP	-	expression tag	UNP Q9C005
P	0	PRO	-	expression tag	UNP Q9C005
Q	-4	GLY	-	expression tag	UNP Q9C005
Q	-3	ALA	-	expression tag	UNP Q9C005
Q	-2	MET	-	expression tag	UNP Q9C005
Q	-1	ASP	-	expression tag	UNP Q9C005
Q	0	PRO	-	expression tag	UNP Q9C005

- Molecule 13 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
13	K	1	26	14	6	5	1	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

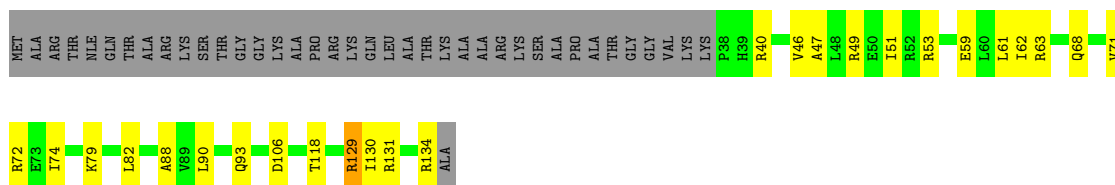
Mol	Chain	Residues	Atoms		AltConf
14	K	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

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.

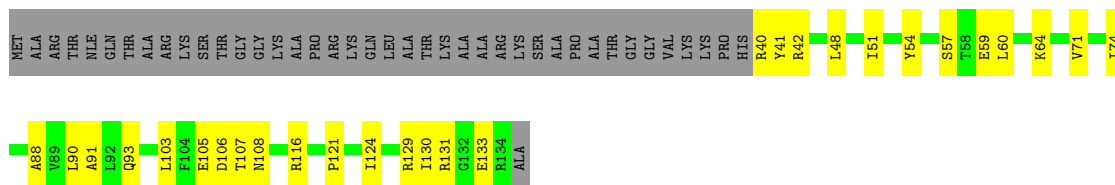
- Molecule 1: Histone H3

Chain A:  53% 18% 29%



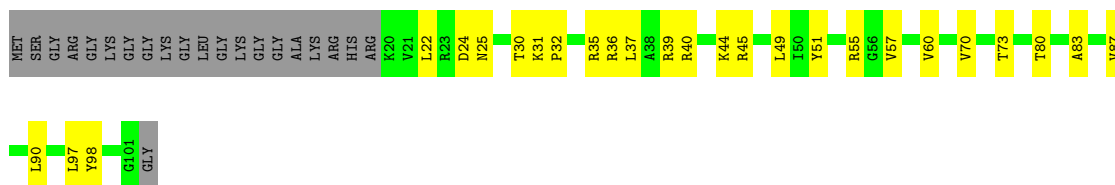
- Molecule 1: Histone H3

Chain E:  49% 21% 30%



- Molecule 2: Histone H4

Chain B:  54% 25% 20%



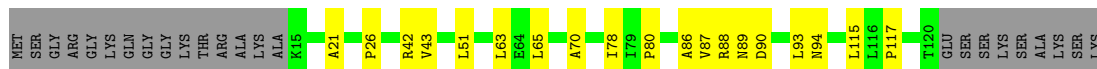
- Molecule 2: Histone H4

Chain F:  54% 22% 23%

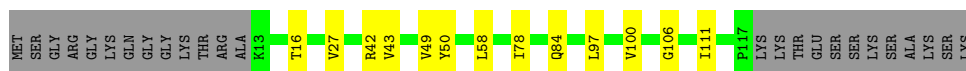




• Molecule 3: Histone H2A



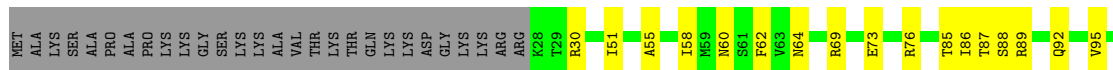
• Molecule 3: Histone H2A



• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1

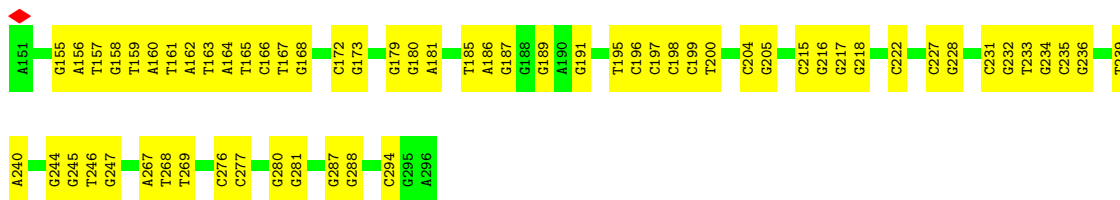


• Molecule 5: 601 DNA (146-MER)

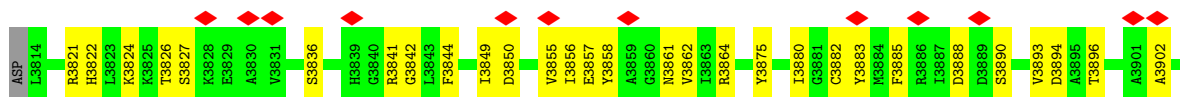
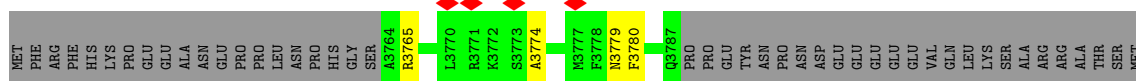


• Molecule 6: 601 DNA (146-MER)

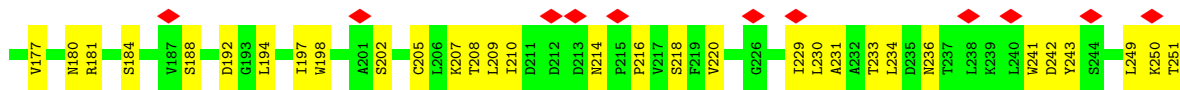
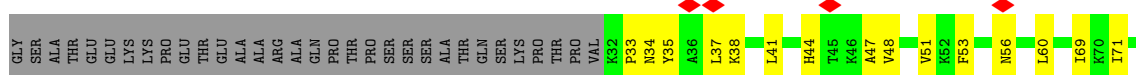




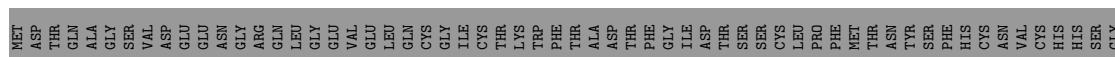
• Molecule 7: cDNA FLJ56846, highly similar to Zinc finger protein HRX

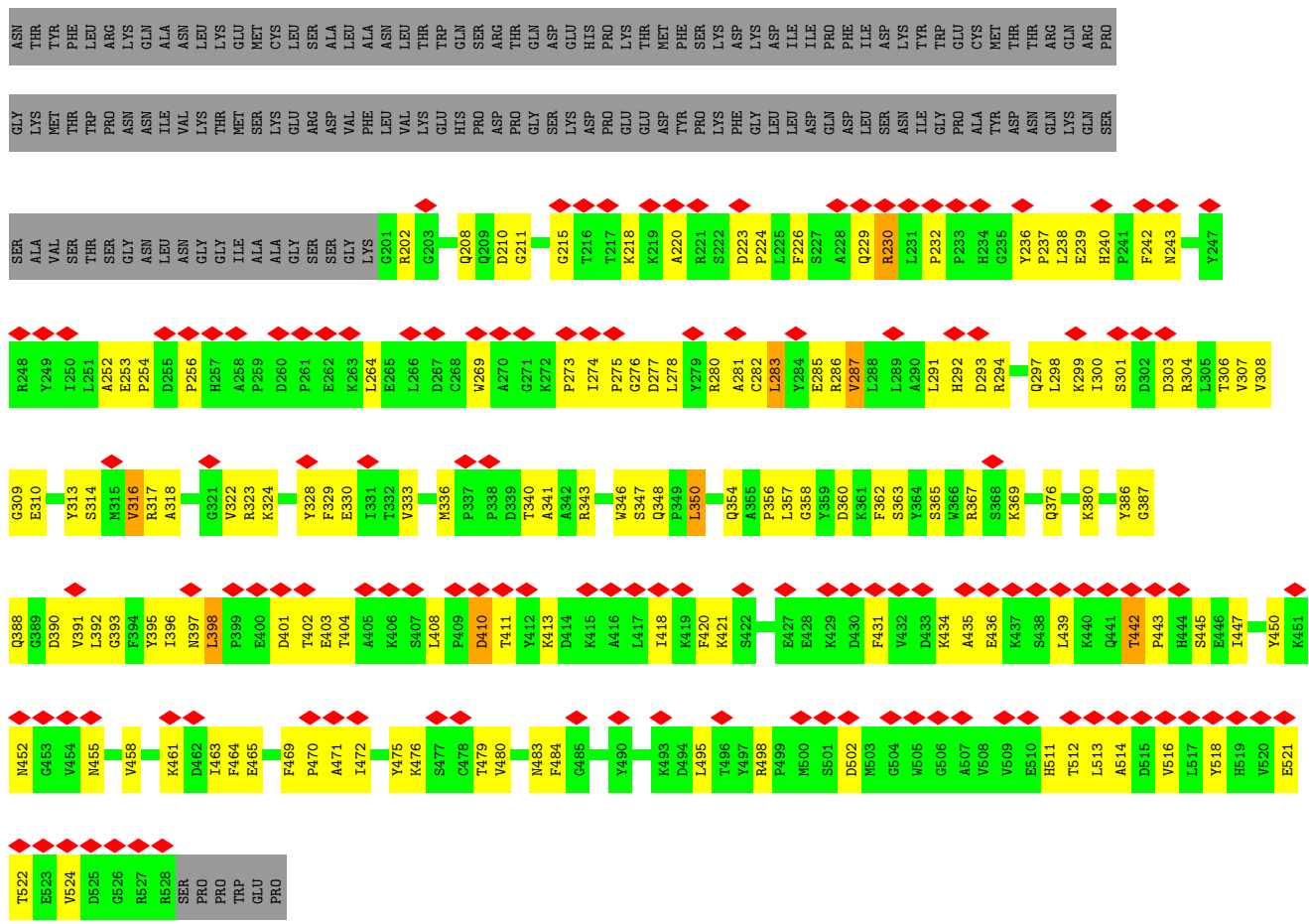


• Molecule 8: WD repeat-containing protein 5

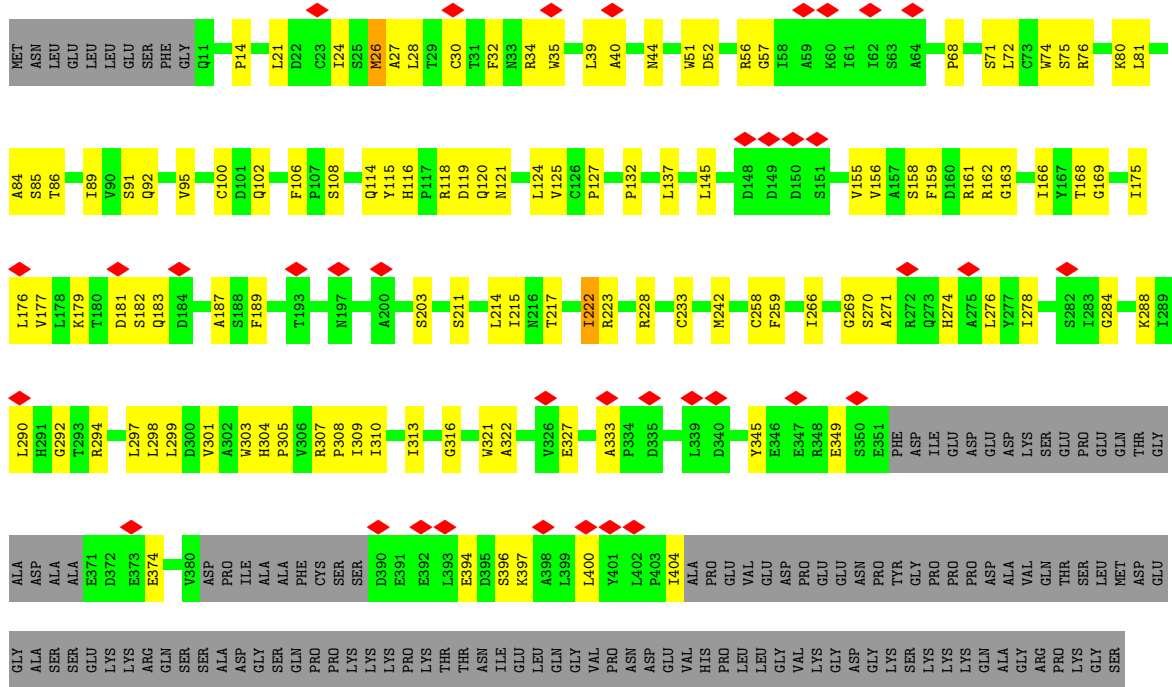


• Molecule 9: Set1/Ash2 histone methyltransferase complex subunit ASH2



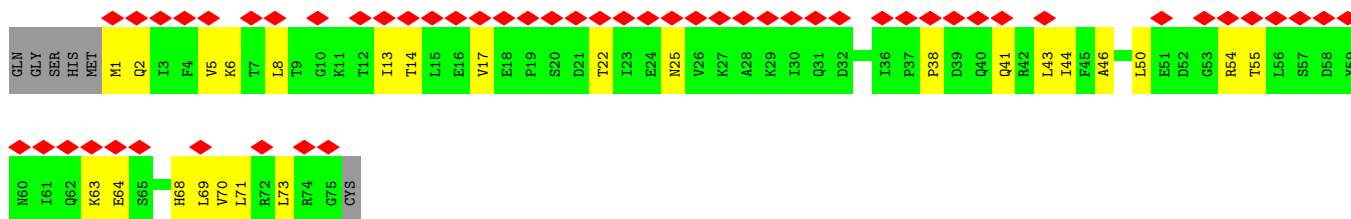


Molecule 10: Retinoblastoma-binding protein 5

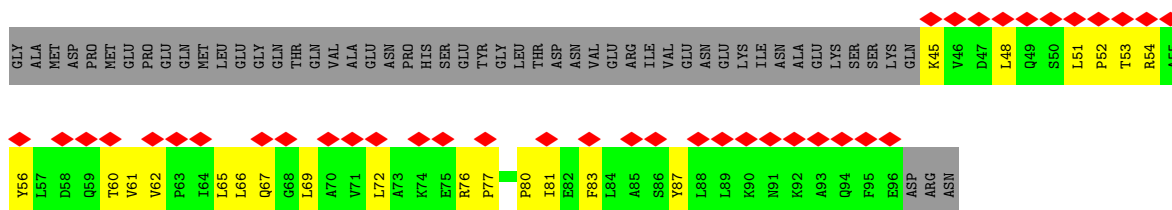
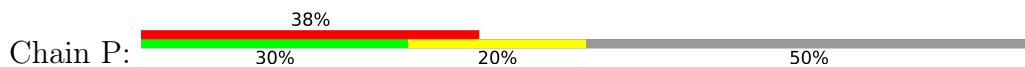


LYS
GLY
LYS
GLU
LYS
ASP
SER
PRO
PHE
LYS
PRO
LYS
LEU
TYR
LYS
GLY
ASP
ARG
GLY
LEU
PRO
GLU
GLY
SER
ALA
LYS
GLY
LYS
VAL
GLN
ALA
GLU
LEU
SER
GLN
PRO
LEU
THR

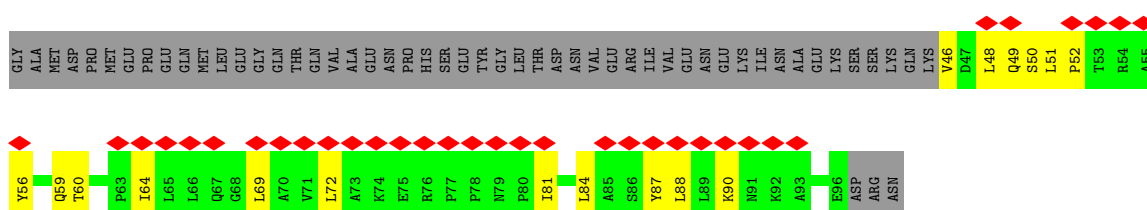
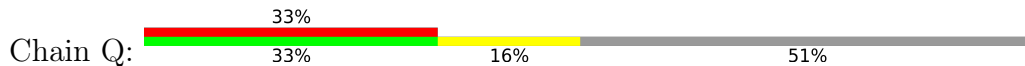
• Molecule 11: Polyubiquitin-B



• Molecule 12: Protein dpy-30 homolog



• Molecule 12: Protein dpy-30 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66449	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00732	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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: NLE, ZN, SAH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/796	0.54	0/1065
1	E	0.25	0/777	0.55	0/1039
2	B	0.24	0/664	0.56	0/889
2	F	0.24	0/640	0.57	0/857
3	C	0.24	0/830	0.53	0/1120
3	G	0.24	0/819	0.53	0/1106
4	D	0.24	0/765	0.49	0/1029
4	H	0.24	0/753	0.47	0/1012
5	I	0.49	0/3333	0.93	0/5137
6	J	0.46	0/3381	0.89	0/5221
7	K	0.24	0/1426	0.50	0/1907
8	L	0.23	0/2458	0.45	0/3332
9	M	0.28	0/2704	0.53	0/3662
10	N	0.23	0/2937	0.49	0/3988
11	O	0.23	0/603	0.50	0/811
12	P	0.25	0/421	0.51	0/573
12	Q	0.24	0/412	0.50	0/562
All	All	0.33	0/23719	0.66	0/33310

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	802	0	843	23	0
1	E	785	0	828	22	0
2	B	657	0	706	26	0
2	F	633	0	673	20	0
3	C	820	0	879	14	0
3	G	809	0	864	11	0
4	D	754	0	778	13	0
4	H	742	0	765	16	0
5	I	2975	0	1639	27	0
6	J	3011	0	1639	47	0
7	K	1398	0	1384	39	0
8	L	2382	0	2374	85	0
9	M	2625	0	2558	125	0
10	N	2879	0	2825	87	0
11	O	597	0	626	21	0
12	P	413	0	438	20	0
12	Q	404	0	425	16	0
13	K	26	0	19	3	0
14	K	1	0	0	0	0
All	All	22713	0	20263	524	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 12.

All (524) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:TYR:HB3	2:F:40:ARG:HH12	1.27	0.95
9:M:285:GLU:HG2	9:M:495:LEU:HB2	1.53	0.89
9:M:223:ASP:H	9:M:243:ASN:HD21	1.21	0.88
3:C:21:ALA:HB2	4:D:118:TYR:HB2	1.64	0.79
1:A:79:LYS:HE3	1:A:82:LEU:HD21	1.66	0.78
9:M:410:ASP:N	9:M:410:ASP:OD1	2.17	0.77
9:M:299:LYS:HB2	9:M:308:VAL:HB	1.66	0.77
1:E:42:ARG:HG3	6:J:294:DC:H5"	1.68	0.75
9:M:330:GLU:OE2	9:M:483:ASN:ND2	2.20	0.74
8:L:216:PRO:HG2	8:L:234:LEU:HB2	1.71	0.72
9:M:439:LEU:HA	9:M:464:PHE:HE1	1.55	0.72
10:N:71:SER:HB3	10:N:84:ALA:HB3	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:76:ARG:HB3	10:N:120:GLN:HB3	1.70	0.72
9:M:293:ASP:OD2	9:M:317:ARG:NE	2.23	0.71
9:M:253:GLU:HG3	9:M:514:ALA:HB1	1.73	0.70
9:M:318:ALA:H	9:M:469:PHE:HB3	1.57	0.69
8:L:194:LEU:HD22	8:L:210:ILE:HG13	1.74	0.69
9:M:340:THR:HG22	9:M:476:LYS:HB2	1.74	0.69
9:M:346:TRP:HE3	9:M:447:ILE:HG23	1.56	0.69
8:L:177:VAL:HG12	8:L:188:SER:HA	1.75	0.68
8:L:111:LEU:HD21	8:L:132:VAL:HG11	1.76	0.68
9:M:211:GLY:HA2	9:M:218:LYS:H	1.59	0.68
9:M:253:GLU:HB3	9:M:518:TYR:HB2	1.76	0.68
10:N:155:VAL:HA	10:N:169:GLY:O	1.93	0.67
7:K:3909:CYS:HB2	7:K:3964:CYS:HA	1.76	0.67
7:K:3948:ILE:HG12	7:K:3969:ASN:HB2	1.76	0.67
10:N:214:LEU:HB3	10:N:222:ILE:HD11	1.76	0.66
8:L:41:LEU:HB2	8:L:327:ILE:HB	1.78	0.66
8:L:250:LYS:HB3	8:L:291:LYS:HD3	1.77	0.66
9:M:297:GLN:NE2	9:M:354:GLN:OE1	2.29	0.65
9:M:396:ILE:HG13	9:M:398:LEU:HD22	1.78	0.65
9:M:397:ASN:OD1	9:M:450:TYR:OH	2.14	0.65
9:M:223:ASP:N	9:M:243:ASN:HD21	1.94	0.65
8:L:51:VAL:HG22	8:L:319:ALA:HB2	1.79	0.64
9:M:357:LEU:HD12	9:M:363:SER:HB3	1.79	0.64
1:A:62:ILE:HD11	2:B:37:LEU:HD11	1.78	0.64
10:N:307:ARG:HH11	10:N:308:PRO:HD2	1.62	0.64
9:M:348:GLN:HG3	9:M:464:PHE:HB3	1.80	0.64
1:A:63:ARG:HH12	2:B:36:ARG:HH12	1.45	0.64
10:N:217:THR:HG21	10:N:223:ARG:HH21	1.63	0.64
10:N:278:ILE:HD11	10:N:288:LYS:HB3	1.80	0.64
8:L:262:ILE:HD11	8:L:279:GLU:HG3	1.80	0.63
9:M:329:PHE:HB2	9:M:484:PHE:HA	1.79	0.63
10:N:159:PHE:HB3	10:N:163:GLY:HA2	1.81	0.63
9:M:297:GLN:HB2	9:M:310:GLU:HB2	1.82	0.62
3:G:78:ILE:HB	4:H:51:ILE:HG22	1.80	0.62
8:L:102:LEU:HD23	8:L:114:TRP:HB2	1.82	0.62
9:M:521:GLU:HA	9:M:524:VAL:HG22	1.81	0.62
8:L:283:VAL:HB	8:L:297:LEU:HB2	1.81	0.62
7:K:3911:PRO:HG3	7:K:3943:ASP:HB2	1.82	0.61
5:I:100:DG:N2	6:J:199:DC:O2	2.33	0.61
9:M:323:ARG:NH1	9:M:402:THR:O	2.31	0.61
8:L:275:VAL:HG13	8:L:285:ILE:HG12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:3875:TYR:OH	7:K:3894:ASP:OD1	2.18	0.61
9:M:393:GLY:H	9:M:452:ASN:H	1.46	0.61
10:N:292:GLY:O	10:N:294:ARG:NH1	2.33	0.61
8:L:279:GLU:HA	8:L:303:VAL:HG13	1.83	0.61
10:N:35:TRP:O	10:N:304:HIS:NE2	2.34	0.61
12:P:61:VAL:HG23	12:P:65:LEU:HD23	1.82	0.61
4:H:89:ARG:HA	4:H:92:GLN:HG2	1.83	0.61
12:P:52:PRO:O	12:P:56:TYR:N	2.32	0.61
9:M:341:ALA:H	9:M:475:TYR:HB3	1.65	0.61
9:M:274:ILE:O	12:P:54:ARG:NH2	2.34	0.60
7:K:3780:PHE:HB3	7:K:3841:ARG:HE	1.66	0.60
8:L:81:LYS:NZ	8:L:118:SER:O	2.32	0.60
3:G:84:GLN:NE2	3:G:106:GLY:O	2.35	0.60
8:L:102:LEU:H	8:L:113:ILE:HG23	1.67	0.60
8:L:233:THR:O	8:L:257:ASN:ND2	2.35	0.60
7:K:3765:ARG:HD3	8:L:91:SER:HA	1.83	0.60
8:L:197:ILE:HD11	8:L:229:ILE:HD13	1.84	0.60
9:M:269:TRP:HE1	9:M:274:ILE:HG12	1.67	0.60
5:I:75:DT:H2'	5:I:76:DG:C8	2.37	0.59
10:N:258:CYS:SG	10:N:259:PHE:N	2.75	0.59
7:K:3875:TYR:HA	7:K:3880:ILE:HB	1.84	0.59
9:M:410:ASP:OD2	9:M:434:LYS:HB3	2.01	0.59
10:N:156:VAL:HG21	10:N:203:SER:HA	1.84	0.59
1:E:51:ILE:HD11	2:F:42:GLY:HA2	1.84	0.59
7:K:3864:ARG:NH2	9:M:313:TYR:O	2.36	0.59
7:K:3890:SER:HB2	9:M:243:ASN:CG	2.23	0.59
9:M:224:PRO:HB2	9:M:297:GLN:HB3	1.85	0.59
10:N:91:SER:HG	10:N:100:CYS:HG	1.45	0.59
1:A:90:NLE:O	1:A:93:GLN:HG2	2.02	0.59
8:L:136:ASN:ND2	8:L:177:VAL:O	2.27	0.59
8:L:111:LEU:HB2	8:L:125:LEU:HB2	1.83	0.58
10:N:81:LEU:HG	10:N:95:VAL:HG22	1.84	0.58
8:L:34:ASN:OD1	8:L:332:SER:OG	2.20	0.58
7:K:3883:TYR:OH	13:K:4001:SAH:N	2.36	0.58
8:L:139:PRO:HG2	8:L:181:ARG:HA	1.84	0.58
10:N:91:SER:OG	10:N:100:CYS:SG	2.59	0.58
7:K:3779:ASN:ND2	8:L:169:ALA:O	2.37	0.58
4:H:73:GLU:OE1	4:H:76:ARG:NH2	2.36	0.57
1:A:106:ASP:OD2	1:A:131:ARG:NH2	2.36	0.57
10:N:228:ARG:HD2	11:O:6:LYS:HD2	1.86	0.57
8:L:56:ASN:ND2	8:L:99:SER:OG	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:2:GLN:HE21	11:O:14:THR:HB	1.70	0.57
8:L:51:VAL:HB	8:L:60:LEU:HD11	1.87	0.57
9:M:350:LEU:HG	9:M:435:ALA:HB1	1.85	0.56
10:N:177:VAL:HB	10:N:187:ALA:HB3	1.87	0.56
2:B:35:ARG:HH21	2:B:39:ARG:HH21	1.54	0.56
8:L:218:SER:HB2	8:L:261:CYS:HA	1.87	0.56
12:P:60:THR:HG23	12:P:61:VAL:HG13	1.87	0.56
3:G:42:ARG:HB2	4:H:85:THR:HG22	1.88	0.56
8:L:218:SER:HB3	8:L:234:LEU:HD21	1.87	0.56
9:M:442:THR:HB	9:M:465:GLU:HB2	1.88	0.56
9:M:215:GLY:HA2	9:M:413:LYS:NZ	2.21	0.56
9:M:220:ALA:HB1	9:M:240:HIS:CE1	2.40	0.56
4:D:27:ARG:HB2	5:I:104:DT:H4'	1.88	0.56
2:F:70:VAL:HA	2:F:73:THR:HG22	1.87	0.56
6:J:185:DT:H2''	6:J:186:DA:C8	2.41	0.56
11:O:44:ILE:O	11:O:68:HIS:N	2.36	0.56
8:L:69:ILE:HG21	8:L:102:LEU:HD21	1.87	0.56
9:M:323:ARG:NH1	9:M:401:ASP:HB2	2.20	0.56
9:M:277:ASP:OD1	9:M:277:ASP:N	2.40	0.55
9:M:439:LEU:HA	9:M:464:PHE:CE1	2.40	0.55
9:M:512:THR:HG21	12:P:53:THR:HG22	1.89	0.55
9:M:404:THR:H	12:Q:49:GLN:HB3	1.71	0.55
1:E:57:SER:OG	1:E:59:GLU:OE1	2.24	0.55
3:C:70:ALA:HB2	3:C:78:ILE:HG12	1.89	0.55
9:M:256:PRO:HB3	9:M:273:PRO:HG3	1.87	0.55
2:B:22:LEU:HG	2:B:24:ASP:H	1.72	0.55
7:K:3882:CYS:O	13:K:4001:SAH:O3'	2.25	0.55
12:P:62:VAL:HA	12:P:65:LEU:HG	1.89	0.55
8:L:198:TRP:HA	8:L:205:CYS:HA	1.89	0.55
5:I:110:DC:O2	6:J:189:DG:N2	2.40	0.55
8:L:35:TYR:H	8:L:295:GLN:HE22	1.53	0.55
8:L:265:ASN:HD22	8:L:308:ALA:HA	1.71	0.55
9:M:362:PHE:CE2	9:M:436:GLU:HG2	2.41	0.55
2:F:73:THR:OG1	2:F:80:THR:O	2.24	0.54
1:E:88:ALA:O	1:E:91:ALA:HB3	2.08	0.54
10:N:127:PRO:HD2	10:N:132:PRO:HA	1.89	0.54
8:L:301:THR:OG1	8:L:323:ASN:O	2.25	0.54
10:N:269:GLY:HA2	10:N:276:LEU:HD13	1.89	0.54
10:N:132:PRO:HG2	10:N:145:LEU:HB2	1.88	0.54
1:A:47:ALA:O	1:A:51:ILE:HG12	2.08	0.54
1:A:61:LEU:HD12	2:B:37:LEU:HD23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:75:SER:HA	10:N:115:TYR:CG	2.43	0.54
2:B:87:VAL:HG23	2:B:97:LEU:HB2	1.90	0.54
3:C:63:LEU:HD12	4:D:42:LEU:HD13	1.90	0.54
7:K:3779:ASN:HD21	8:L:170:HIS:HA	1.73	0.53
7:K:3836:SER:HB2	7:K:3842:GLY:HA3	1.89	0.53
10:N:181:ASP:O	10:N:183:GLN:NE2	2.41	0.53
1:A:129:ARG:HG3	1:A:134:ARG:HH11	1.73	0.53
8:L:83:ILE:HG21	8:L:114:TRP:HB3	1.88	0.53
11:O:1:MET:HG2	11:O:63:LYS:HD2	1.90	0.53
8:L:216:PRO:HB2	8:L:234:LEU:HD12	1.91	0.53
9:M:280:ARG:NH1	9:M:282:CYS:HB3	2.23	0.53
10:N:309:ILE:HG13	10:N:322:ALA:HA	1.90	0.53
10:N:233:CYS:HA	11:O:46:ALA:HB1	1.91	0.53
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.41	0.53
8:L:207:LYS:HG2	8:L:243:TYR:HB2	1.91	0.53
1:A:61:LEU:O	2:B:36:ARG:NH2	2.41	0.53
4:D:92:GLN:HA	4:D:95:VAL:HG22	1.89	0.53
9:M:218:LYS:HZ1	9:M:418:ILE:HD13	1.72	0.53
9:M:283:LEU:HD12	9:M:304:ARG:HH21	1.74	0.53
4:H:30:ARG:HH12	6:J:179:DG:H5'	1.74	0.53
9:M:294:ARG:NH1	9:M:300:ILE:HG13	2.25	0.53
9:M:358:GLY:O	9:M:376:GLN:N	2.34	0.53
7:K:3821:ARG:HA	7:K:3824:LYS:HZ3	1.72	0.52
10:N:34:ARG:HG3	10:N:35:TRP:HD1	1.72	0.52
10:N:116:HIS:NE2	10:N:162:ARG:O	2.40	0.52
8:L:260:TYR:N	8:L:279:GLU:OE2	2.40	0.52
9:M:282:CYS:SG	9:M:283:LEU:N	2.81	0.52
10:N:28:LEU:HD12	10:N:299:LEU:HD13	1.91	0.52
10:N:40:ALA:HB2	10:N:74:TRP:HE1	1.74	0.52
11:O:44:ILE:HB	11:O:68:HIS:HB2	1.91	0.52
8:L:155:ILE:HG13	8:L:164:LEU:HB2	1.91	0.52
10:N:394:GLU:OE2	10:N:397:LYS:NZ	2.43	0.52
12:P:69:LEU:HD23	12:P:72:LEU:HD21	1.91	0.52
2:F:68:ASP:OD2	2:F:92:ARG:NH2	2.34	0.52
6:J:233:DT:H2''	6:J:234:DG:H5'	1.91	0.52
9:M:333:VAL:HA	9:M:480:VAL:HG23	1.91	0.52
10:N:299:LEU:HB2	10:N:313:ILE:HG23	1.91	0.52
12:Q:69:LEU:HD23	12:Q:72:LEU:HD21	1.90	0.52
10:N:284:GLY:H	11:O:73:LEU:HD13	1.73	0.52
1:A:61:LEU:HD11	2:B:40:ARG:HE	1.75	0.52
10:N:270:SER:OG	10:N:271:ALA:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:3961:ALA:HB3	7:K:3964:CYS:HB2	1.92	0.52
10:N:32:PHE:HD2	10:N:305:PRO:HD3	1.74	0.52
1:A:106:ASP:HB3	1:E:130:ILE:HD11	1.92	0.51
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.92	0.51
9:M:445:SER:OG	9:M:463:ILE:N	2.44	0.51
9:M:387:GLY:N	9:M:390:ASP:OD2	2.43	0.51
10:N:21:LEU:HD12	10:N:56:ARG:HH11	1.74	0.51
2:F:40:ARG:HA	2:F:40:ARG:NE	2.26	0.51
6:J:179:DG:H2''	6:J:180:DG:C8	2.46	0.51
6:J:172:DC:H2''	6:J:173:DG:C8	2.45	0.51
8:L:180:ASN:OD1	8:L:184:SER:N	2.42	0.51
8:L:276:SER:HB2	8:L:286:TRP:HZ3	1.73	0.51
9:M:232:PRO:O	9:M:238:LEU:HD11	2.11	0.51
10:N:75:SER:HB3	10:N:80:LYS:HB2	1.93	0.51
10:N:304:HIS:HB3	10:N:307:ARG:O	2.10	0.51
5:I:119:DC:O2	6:J:180:DG:N2	2.43	0.51
1:A:130:ILE:HD11	1:E:106:ASP:HB3	1.93	0.51
7:K:3890:SER:HB3	9:M:243:ASN:CB	2.40	0.51
8:L:229:ILE:HG13	8:L:241:TRP:HB2	1.92	0.51
9:M:346:TRP:HB2	9:M:447:ILE:HG12	1.93	0.51
7:K:3862:VAL:HG12	7:K:3893:VAL:HG22	1.93	0.50
9:M:298:LEU:HG	9:M:316:VAL:HG13	1.93	0.50
9:M:316:VAL:O	9:M:471:ALA:HA	2.10	0.50
9:M:323:ARG:HB2	12:Q:50:SER:HB2	1.92	0.50
10:N:26:MET:SD	10:N:26:MET:N	2.78	0.50
5:I:93:DC:H2'	5:I:94:DG:C8	2.46	0.50
6:J:165:DT:H4'	6:J:166:DC:OP1	2.10	0.50
10:N:116:HIS:CD2	10:N:118:ARG:H	2.29	0.50
2:F:44:LYS:HG3	2:F:45:ARG:HG2	1.92	0.50
3:C:89:ASN:OD1	3:C:90:ASP:N	2.45	0.50
12:P:76:ARG:HD3	12:Q:48:LEU:HA	1.93	0.50
2:B:31:LYS:HG3	2:B:32:PRO:HD3	1.94	0.50
1:E:105:GLU:O	1:E:108:ASN:HB3	2.12	0.50
7:K:3850:ASP:HA	7:K:3933:LYS:HA	1.94	0.50
8:L:242:ASP:HB2	8:L:249:LEU:HD11	1.94	0.50
10:N:102:GLN:NE2	10:N:137:LEU:O	2.42	0.50
10:N:114:GLN:H	10:N:124:LEU:HB3	1.75	0.50
6:J:164:DA:H2''	6:J:165:DT:H5'	1.93	0.50
7:K:3885:PHE:HB3	7:K:3893:VAL:HB	1.93	0.50
9:M:286:ARG:HH12	12:Q:60:THR:HA	1.76	0.50
1:E:54:TYR:HB3	2:F:40:ARG:NH1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:3861:ASN:HD21	10:N:345:TYR:HB2	1.76	0.49
9:M:313:TYR:CZ	9:M:356:PRO:HA	2.46	0.49
9:M:401:ASP:OD1	9:M:401:ASP:N	2.44	0.49
10:N:24:ILE:HG22	10:N:51:TRP:HZ2	1.77	0.49
2:B:57:VAL:HA	2:B:60:VAL:HG22	1.95	0.49
3:C:87:VAL:HA	3:C:93:LEU:HD23	1.94	0.49
9:M:300:ILE:HG22	9:M:304:ARG:HA	1.93	0.49
10:N:304:HIS:HD2	10:N:305:PRO:HD2	1.77	0.49
5:I:33:DG:H2''	5:I:34:DG:H5''	1.94	0.49
6:J:167:DT:H2''	6:J:168:DG:C8	2.48	0.49
10:N:242:MET:HG3	11:O:71:LEU:H	1.78	0.49
12:P:72:LEU:HA	12:P:77:PRO:HD2	1.93	0.49
5:I:108:DT:O2	6:J:191:DG:N2	2.46	0.49
9:M:367:ARG:NH1	10:N:349:GLU:O	2.43	0.49
3:G:43:VAL:HG22	4:H:86:ILE:HD11	1.95	0.49
9:M:215:GLY:HA2	9:M:413:LYS:HZ3	1.78	0.49
9:M:516:VAL:HG11	12:P:65:LEU:HD22	1.95	0.49
3:C:78:ILE:HB	4:D:51:ILE:HD12	1.95	0.49
6:J:246:DT:H2''	6:J:247:DG:C8	2.48	0.49
2:F:24:ASP:OD1	2:F:24:ASP:N	2.46	0.49
11:O:22:THR:HA	11:O:55:THR:HG23	1.95	0.49
7:K:3888:ASP:OD2	7:K:3890:SER:OG	2.29	0.48
9:M:220:ALA:HB1	9:M:240:HIS:NE2	2.27	0.48
9:M:328:TYR:HD1	9:M:395:TYR:HB2	1.77	0.48
1:A:51:ILE:HG21	3:G:111:ILE:HD11	1.95	0.48
8:L:236:ASN:N	8:L:257:ASN:O	2.34	0.48
9:M:276:GLY:O	9:M:511:HIS:ND1	2.46	0.48
3:G:27:VAL:HG11	3:G:49:VAL:HG22	1.96	0.48
8:L:159:LYS:NZ	10:N:404:ILE:O	2.36	0.48
10:N:310:ILE:CG1	10:N:321:TRP:HB3	2.43	0.48
12:P:77:PRO:HG2	12:P:80:PRO:HB3	1.95	0.48
5:I:31:DT:H2''	5:I:32:DT:H5'	1.95	0.48
6:J:180:DG:H2''	6:J:181:DA:C8	2.48	0.48
6:J:267:DA:H2''	6:J:268:DT:C5	2.48	0.48
4:H:95:VAL:HG13	4:H:99:LEU:HD12	1.95	0.48
2:B:35:ARG:O	2:B:39:ARG:HG2	2.14	0.48
8:L:75:TYR:O	8:L:331:LYS:NZ	2.46	0.48
9:M:237:PRO:HB3	9:M:252:ALA:HB2	1.96	0.48
1:E:90:NLE:O	1:E:93:GLN:HB3	2.14	0.48
2:F:37:LEU:O	2:F:40:ARG:HB2	2.13	0.48
9:M:336:MET:O	9:M:388:GLN:NE2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:121:ASN:OD1	10:N:137:LEU:N	2.47	0.48
9:M:367:ARG:HG3	9:M:369:LYS:H	1.79	0.48
12:P:69:LEU:HA	12:P:72:LEU:HG	1.96	0.48
2:B:90:LEU:HD13	2:B:97:LEU:HD23	1.96	0.47
5:I:140:DC:H2''	5:I:141:DA:C8	2.48	0.47
6:J:267:DA:H2''	6:J:268:DT:C6	2.49	0.47
8:L:35:TYR:HA	8:L:332:SER:HB2	1.95	0.47
8:L:265:ASN:ND2	8:L:307:THR:O	2.44	0.47
12:Q:52:PRO:O	12:Q:56:TYR:N	2.38	0.47
10:N:14:PRO:HB2	10:N:321:TRP:HD1	1.79	0.47
10:N:44:ASN:HA	10:N:68:PRO:HB3	1.96	0.47
5:I:3:DC:H2''	5:I:4:DG:C8	2.50	0.47
9:M:275:PRO:HD3	12:P:52:PRO:HB3	1.97	0.47
9:M:298:LEU:HD13	9:M:309:GLY:HA2	1.96	0.47
9:M:367:ARG:HH12	10:N:349:GLU:HB3	1.80	0.47
9:M:502:ASP:N	9:M:502:ASP:OD1	2.48	0.47
6:J:215:DC:H2''	6:J:216:DG:C8	2.50	0.47
9:M:224:PRO:CB	9:M:297:GLN:HB3	2.45	0.47
9:M:357:LEU:HB3	9:M:365:SER:HB3	1.96	0.47
10:N:274:HIS:CD2	10:N:294:ARG:HA	2.50	0.47
11:O:63:LYS:O	11:O:64:GLU:HG3	2.15	0.47
8:L:78:LYS:NZ	8:L:80:GLU:OE2	2.40	0.47
10:N:85:SER:OG	10:N:89:ILE:N	2.45	0.47
11:O:5:VAL:HG23	11:O:13:ILE:HB	1.97	0.47
12:Q:46:VAL:HB	12:Q:51:LEU:HD22	1.96	0.47
5:I:82:DC:H2''	5:I:83:DG:C8	2.50	0.47
6:J:163:DT:H2''	6:J:164:DA:C8	2.50	0.47
7:K:3822:HIS:ND1	7:K:3826:THR:OG1	2.46	0.47
8:L:53:PHE:H	8:L:308:ALA:HB1	1.80	0.47
1:A:71:VAL:HA	1:A:74:ILE:HG22	1.96	0.46
4:D:55:ALA:HA	4:D:58:ILE:HG22	1.97	0.46
6:J:227:DC:H2''	6:J:228:DG:C8	2.50	0.46
8:L:95:TRP:HB3	8:L:99:SER:HA	1.96	0.46
1:A:88:ALA:HA	2:B:83:ALA:HB2	1.97	0.46
8:L:33:PRO:O	8:L:295:GLN:NE2	2.48	0.46
9:M:420:PHE:HD2	9:M:421:LYS:HG2	1.81	0.46
4:H:87:THR:OG1	4:H:88:SER:N	2.48	0.46
5:I:72:DC:H2''	5:I:73:DG:C8	2.51	0.46
6:J:204:DC:H2''	6:J:205:DG:C8	2.50	0.46
10:N:27:ALA:H	10:N:316:GLY:HA2	1.79	0.46
4:D:69:ARG:HG2	4:D:98:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:195:DT:H2''	6:J:196:DC:C6	2.51	0.46
9:M:291:LEU:HD11	9:M:304:ARG:HD3	1.97	0.46
8:L:47:ALA:HA	8:L:325:LYS:HG2	1.98	0.46
8:L:37:LEU:HD13	8:L:328:LYS:HB3	1.98	0.46
9:M:329:PHE:HB2	9:M:483:ASN:O	2.16	0.46
10:N:116:HIS:CD2	10:N:163:GLY:HA3	2.51	0.46
6:J:287:DG:H2''	6:J:288:DG:C8	2.51	0.46
9:M:285:GLU:OE2	9:M:498:ARG:NE	2.33	0.46
12:P:51:LEU:HD23	12:P:56:TYR:HD1	1.81	0.46
12:P:67:GLN:HB3	12:P:83:PHE:HE2	1.81	0.46
3:C:43:VAL:HG12	4:D:86:ILE:HB	1.98	0.45
1:E:103:LEU:HA	1:E:131:ARG:HH22	1.80	0.45
9:M:318:ALA:HB3	9:M:470:PRO:HD2	1.97	0.45
10:N:95:VAL:HG12	10:N:400:LEU:HB2	1.98	0.45
6:J:161:DT:H2''	6:J:162:DA:C8	2.51	0.45
8:L:44:HIS:HB2	8:L:48:VAL:HG22	1.98	0.45
8:L:320:ALA:HB3	8:L:324:ASP:HB3	1.98	0.45
2:B:49:LEU:H	2:B:49:LEU:HD23	1.81	0.45
9:M:218:LYS:HZ2	9:M:418:ILE:HG21	1.80	0.45
1:A:59:GLU:OE1	2:B:40:ARG:NH2	2.46	0.45
1:E:40:ARG:HH11	1:E:41:TYR:HD2	1.65	0.45
3:G:97:LEU:HB3	3:G:100:VAL:HG11	1.99	0.45
8:L:35:TYR:HB3	8:L:330:TRP:HB3	1.98	0.45
2:B:98:TYR:HE2	4:H:62:PHE:HA	1.80	0.45
7:K:3858:TYR:HD1	7:K:3902:ALA:HB3	1.81	0.45
8:L:71:ILE:HB	8:L:80:GLU:HB2	1.97	0.45
9:M:230:ARG:HH21	9:M:240:HIS:HD2	1.64	0.45
10:N:124:LEU:HD21	10:N:158:SER:HA	1.98	0.45
3:G:16:THR:HA	6:J:181:DA:H5''	1.98	0.45
4:H:69:ARG:HG2	4:H:98:LEU:HD11	1.98	0.45
7:K:3855:VAL:HG22	7:K:3928:ILE:O	2.17	0.45
9:M:236:TYR:HB3	9:M:278:LEU:HD11	1.98	0.45
10:N:242:MET:HG3	11:O:71:LEU:N	2.31	0.45
4:D:89:ARG:O	4:D:92:GLN:HG2	2.16	0.45
7:K:3857:GLU:OE1	7:K:3925:HIS:HB3	2.17	0.45
8:L:95:TRP:CE3	8:L:99:SER:HB2	2.51	0.45
9:M:210:ASP:OD1	9:M:211:GLY:N	2.50	0.45
10:N:276:LEU:HB2	10:N:290:LEU:HB3	1.99	0.45
10:N:298:LEU:HD21	10:N:301:VAL:HG13	1.98	0.45
2:F:85:ASP:OD1	2:F:85:ASP:N	2.49	0.45
8:L:111:LEU:HB2	8:L:125:LEU:HD22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:OG1	2:F:31:LYS:N	2.50	0.45
7:K:3890:SER:CB	9:M:243:ASN:ND2	2.80	0.45
7:K:3890:SER:CB	9:M:243:ASN:CG	2.86	0.45
8:L:265:ASN:ND2	8:L:308:ALA:HA	2.32	0.45
10:N:124:LEU:HB2	10:N:159:PHE:CE2	2.52	0.45
10:N:242:MET:HG2	11:O:8:LEU:HD22	1.99	0.45
6:J:244:DG:H2'	6:J:245:DG:C8	2.52	0.45
9:M:410:ASP:CG	9:M:434:LYS:HB3	2.37	0.45
8:L:38:LYS:HG3	8:L:331:LYS:HD2	1.99	0.44
7:K:3822:HIS:O	7:K:3827:SER:OG	2.23	0.44
9:M:323:ARG:HG2	9:M:402:THR:H	1.82	0.44
10:N:175:ILE:HD13	10:N:189:PHE:HD2	1.81	0.44
11:O:22:THR:HG23	11:O:25:ASN:H	1.82	0.44
3:C:117:PRO:HD2	1:E:48:LEU:HD11	1.99	0.44
1:E:121:PRO:HB3	2:F:53:GLU:OE2	2.18	0.44
8:L:130:ASN:HB3	8:L:149:PHE:HB2	2.00	0.44
11:O:43:LEU:O	11:O:50:LEU:HB2	2.17	0.44
8:L:192:ASP:OD1	8:L:192:ASP:N	2.49	0.44
9:M:218:LYS:NZ	9:M:418:ILE:HD13	2.33	0.44
2:F:60:VAL:O	2:F:63:GLU:HG3	2.18	0.44
9:M:301:SER:HB3	9:M:306:THR:HG22	1.99	0.44
9:M:322:VAL:HG21	9:M:396:ILE:HG21	1.99	0.44
2:B:98:TYR:HB3	4:H:58:ILE:HG13	1.98	0.44
1:E:107:THR:HG21	1:E:124:ILE:HG12	2.00	0.44
3:G:50:TYR:CZ	4:H:111:GLY:HA3	2.53	0.44
7:K:3906:ASN:ND2	7:K:3939:GLU:OE2	2.51	0.44
8:L:285:ILE:HD12	8:L:295:GLN:HB3	2.00	0.44
9:M:341:ALA:N	9:M:475:TYR:HB3	2.32	0.44
3:C:26:PRO:HD3	4:D:37:TYR:CD1	2.53	0.44
1:E:116:ARG:NH1	6:J:222:DC:OP2	2.51	0.44
10:N:116:HIS:HB3	10:N:119:ASP:O	2.18	0.44
12:P:65:LEU:HD12	12:P:66:LEU:N	2.33	0.44
1:E:41:TYR:HE1	6:J:294:DC:H4'	1.83	0.43
7:K:3917:VAL:HG22	7:K:3924:LYS:HE3	2.00	0.43
9:M:450:TYR:CD1	9:M:455:ASN:HB2	2.53	0.43
9:M:461:LYS:HE2	9:M:461:LYS:HB2	1.90	0.43
10:N:161:ARG:HD2	10:N:211:SER:H	1.83	0.43
9:M:347:SER:OG	9:M:348:GLN:N	2.51	0.43
11:O:41:GLN:HB2	11:O:69:LEU:HD12	2.00	0.43
11:O:54:ARG:HG3	11:O:55:THR:H	1.84	0.43
10:N:214:LEU:HD11	10:N:266:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:87:TYR:O	12:Q:90:LYS:HG2	2.18	0.43
1:A:68:GLN:HA	1:A:71:VAL:HG22	2.01	0.43
9:M:282:CYS:SG	9:M:292:HIS:NE2	2.84	0.43
9:M:403:GLU:HA	12:Q:49:GLN:HB2	2.00	0.43
10:N:168:THR:OG1	10:N:176:LEU:HB2	2.18	0.43
11:O:1:MET:N	11:O:17:VAL:O	2.41	0.43
6:J:186:DA:H2''	6:J:187:DG:C8	2.53	0.43
6:J:231:DC:H2''	6:J:232:DG:N7	2.34	0.43
7:K:3955:LEU:HD21	13:K:4001:SAH:H1'	2.00	0.43
10:N:34:ARG:HG3	10:N:35:TRP:CD1	2.51	0.43
10:N:179:LYS:HD2	10:N:182:SER:HB2	2.00	0.43
2:B:45:ARG:HE	6:J:231:DC:H4'	1.82	0.43
8:L:251:THR:HG22	8:L:253:THR:HG23	1.99	0.43
11:O:38:PRO:HA	11:O:41:GLN:HG2	1.99	0.43
2:B:51:TYR:O	2:B:55:ARG:HG3	2.19	0.43
3:C:42:ARG:HE	4:D:85:THR:HG22	1.82	0.43
3:G:58:LEU:HD21	4:H:103:LEU:HD21	2.01	0.43
6:J:244:DG:H2''	6:J:245:DG:O5'	2.18	0.43
9:M:450:TYR:HD1	9:M:455:ASN:HB2	1.84	0.43
3:C:115:LEU:HD21	2:F:44:LYS:HG2	2.01	0.43
10:N:52:ASP:HB2	10:N:57:GLY:H	1.82	0.43
1:E:64:LYS:HD2	1:E:90:NLE:HE1	2.01	0.43
2:F:78:ARG:NH2	5:I:102:DG:H8	2.17	0.43
10:N:30:CYS:SG	10:N:313:ILE:HD12	2.59	0.43
4:D:58:ILE:HG13	2:F:98:TYR:HB3	2.01	0.42
9:M:226:PHE:CE1	9:M:229:GLN:HB2	2.54	0.42
10:N:108:SER:HB3	10:N:127:PRO:HB3	2.01	0.42
1:A:46:VAL:HG23	1:A:49:ARG:HD3	1.99	0.42
6:J:217:DG:H2''	6:J:218:DG:C8	2.54	0.42
6:J:276:DC:H2''	6:J:277:DC:O5'	2.19	0.42
9:M:386:TYR:CD2	9:M:392:LEU:HD21	2.55	0.42
1:A:72:ARG:NH2	5:I:51:DC:OP2	2.52	0.42
5:I:7:DA:H2''	5:I:8:DA:C8	2.54	0.42
6:J:197:DC:H2''	6:J:198:DC:C5	2.55	0.42
6:J:239:DT:H2''	6:J:240:DA:C8	2.54	0.42
8:L:234:LEU:HB3	8:L:258:GLU:O	2.19	0.42
9:M:285:GLU:O	9:M:286:ARG:NH1	2.51	0.42
9:M:380:LYS:HE2	9:M:380:LYS:HB2	1.92	0.42
9:M:393:GLY:H	9:M:452:ASN:N	2.14	0.42
10:N:106:PHE:HE2	10:N:125:VAL:HG21	1.84	0.42
5:I:5:DA:H3'	9:M:202:ARG:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:280:DG:H2''	6:J:281:DG:N7	2.35	0.42
11:O:38:PRO:HA	11:O:41:GLN:HE21	1.85	0.42
2:B:30:THR:HG21	5:I:61:DA:H5''	2.00	0.42
5:I:60:DA:H2''	5:I:61:DA:C8	2.55	0.42
10:N:124:LEU:HB2	10:N:159:PHE:HE2	1.84	0.42
2:B:98:TYR:CE1	3:G:100:VAL:HG23	2.54	0.42
10:N:303:TRP:NE1	10:N:310:ILE:HG22	2.33	0.42
12:Q:64:ILE:HG21	12:Q:88:LEU:HD23	2.00	0.42
2:B:39:ARG:NH1	2:B:44:LYS:HA	2.33	0.42
2:F:97:LEU:HD21	2:F:100:PHE:HD2	1.85	0.42
4:H:30:ARG:NH1	6:J:179:DG:H5'	2.34	0.42
6:J:157:DT:H2''	6:J:158:DG:C8	2.55	0.42
7:K:3855:VAL:HG23	7:K:3856:ILE:H	1.84	0.42
8:L:152:SER:HA	8:L:169:ALA:H	1.85	0.42
9:M:286:ARG:HA	9:M:286:ARG:HD3	1.65	0.42
9:M:313:TYR:HA	9:M:475:TYR:HA	2.01	0.42
10:N:92:GLN:HB2	10:N:102:GLN:H	1.85	0.42
2:B:73:THR:OG1	2:B:80:THR:O	2.37	0.42
8:L:208:THR:H	10:N:333:ALA:HB2	1.84	0.42
12:P:45:LYS:HE2	12:P:48:LEU:HB3	2.01	0.42
12:P:81:ILE:HG12	12:Q:84:LEU:HD13	2.02	0.42
12:Q:46:VAL:HA	12:Q:51:LEU:HD13	2.01	0.42
6:J:159:DT:H2''	6:J:160:DA:C8	2.55	0.42
8:L:220:VAL:HG12	8:L:231:ALA:HA	2.02	0.42
8:L:273:TRP:HB3	8:L:285:ILE:HG21	2.02	0.42
8:L:297:LEU:HD13	8:L:330:TRP:CD1	2.55	0.42
9:M:254:PRO:HG3	12:P:54:ARG:NH1	2.34	0.42
9:M:316:VAL:HG23	9:M:472:ILE:HB	2.01	0.42
9:M:362:PHE:HE2	9:M:436:GLU:HG2	1.84	0.42
6:J:199:DC:H2''	6:J:200:DT:C5	2.55	0.41
7:K:3849:ILE:HD13	7:K:3855:VAL:HG12	2.01	0.41
12:P:81:ILE:HG21	12:Q:88:LEU:HD11	2.02	0.41
1:A:40:ARG:HA	6:J:234:DG:H5''	2.01	0.41
8:L:255:HIS:HB3	8:L:286:TRP:CZ2	2.55	0.41
8:L:287:ASN:ND2	8:L:290:THR:OG1	2.52	0.41
9:M:323:ARG:CZ	12:Q:48:LEU:HB2	2.50	0.41
9:M:343:ARG:HG2	9:M:367:ARG:HA	2.02	0.41
10:N:114:GLN:HB2	10:N:124:LEU:HD23	2.02	0.41
10:N:215:ILE:O	10:N:222:ILE:HD12	2.19	0.41
8:L:272:LYS:HE3	10:N:374:GLU:HB2	2.02	0.41
9:M:220:ALA:HA	9:M:242:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:287:VAL:HG22	12:Q:59:GLN:NE2	2.35	0.41
1:E:48:LEU:HA	1:E:51:ILE:HG22	2.03	0.41
2:F:30:THR:HG23	2:F:32:PRO:HD2	2.02	0.41
10:N:34:ARG:NH1	10:N:396:SER:OG	2.53	0.41
10:N:68:PRO:O	10:N:86:THR:OG1	2.27	0.41
5:I:87:DT:H1'	5:I:88:DT:H5'	2.03	0.41
5:I:98:DA:H2''	5:I:99:DG:N7	2.35	0.41
9:M:298:LEU:HD21	9:M:314:SER:HB3	2.03	0.41
10:N:274:HIS:HB2	10:N:294:ARG:HD3	2.02	0.41
6:J:217:DG:H2''	6:J:218:DG:N7	2.35	0.41
7:K:3917:VAL:HB	7:K:3926:ILE:HG22	2.01	0.41
9:M:223:ASP:OD1	9:M:224:PRO:HD3	2.21	0.41
9:M:442:THR:HG23	9:M:443:PRO:O	2.21	0.41
1:E:131:ARG:HD2	1:E:133:GLU:HG2	2.02	0.41
6:J:268:DT:H2''	6:J:269:DT:H5'	2.02	0.41
8:L:209:LEU:HD23	8:L:241:TRP:HB3	2.02	0.41
8:L:253:THR:O	8:L:286:TRP:NE1	2.54	0.41
5:I:15:DT:H2''	5:I:16:DG:C8	2.56	0.41
5:I:23:DC:H2''	5:I:24:DC:H5'	2.01	0.41
6:J:235:DC:H2''	6:J:236:DG:C8	2.55	0.41
8:L:302:ASP:CG	8:L:321:LEU:HB2	2.41	0.41
9:M:223:ASP:H	9:M:243:ASN:ND2	2.01	0.41
9:M:447:ILE:HG13	9:M:463:ILE:HG21	2.03	0.41
10:N:40:ALA:HB1	10:N:72:LEU:HD13	2.02	0.41
1:A:118:THR:HA	2:B:45:ARG:HB3	2.02	0.41
1:A:118:THR:HG22	2:B:45:ARG:HG2	2.03	0.41
3:C:80:PRO:HG2	4:D:54:LYS:HD2	2.03	0.41
5:I:119:DC:H2''	5:I:120:DA:C8	2.55	0.41
8:L:314:ASN:O	8:L:332:SER:N	2.54	0.41
9:M:208:GLN:O	9:M:218:LYS:HD2	2.21	0.41
9:M:239:GLU:OE2	9:M:281:ALA:HB1	2.21	0.41
9:M:328:TYR:HA	9:M:395:TYR:HB2	2.02	0.41
10:N:242:MET:HG3	11:O:70:VAL:HG13	2.03	0.41
4:H:60:ASN:OD1	4:H:64:ASN:ND2	2.54	0.41
8:L:202:SER:OG	10:N:327:GLU:OE2	2.38	0.41
8:L:258:GLU:H	8:L:279:GLU:CD	2.23	0.41
9:M:307:VAL:O	9:M:479:THR:HA	2.21	0.41
1:E:71:VAL:HA	1:E:74:ILE:HG22	2.02	0.40
4:H:55:ALA:HA	4:H:58:ILE:HG22	2.02	0.40
5:I:21:DG:H2''	5:I:22:DG:C8	2.56	0.40
9:M:360:ASP:OD1	9:M:360:ASP:N	2.48	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:204:DC:H2''	6:J:205:DG:H8	1.86	0.40
7:K:3774:ALA:H	8:L:214:ASN:HD21	1.70	0.40
7:K:3849:ILE:H	7:K:3934:ILE:HB	1.86	0.40
8:L:125:LEU:HD21	8:L:144:ILE:HD13	2.04	0.40
8:L:315:ILE:HG12	8:L:331:LYS:HG2	2.03	0.40
12:Q:81:ILE:HD12	12:Q:84:LEU:HD11	2.03	0.40
3:C:88:ARG:HA	3:C:94:ASN:OD1	2.22	0.40
8:L:310:HIS:CG	8:L:311:PRO:HD2	2.57	0.40
1:A:59:GLU:OE1	1:A:59:GLU:N	2.55	0.40
2:B:70:VAL:HA	2:B:73:THR:HG22	2.04	0.40
2:F:40:ARG:HA	2:F:40:ARG:CZ	2.51	0.40
8:L:220:VAL:HA	8:L:230:LEU:O	2.22	0.40
9:M:346:TRP:HA	9:M:470:PRO:HA	2.03	0.40
5:I:32:DT:H6	5:I:32:DT:H2'	1.69	0.40
5:I:86:DT:H2'	5:I:87:DT:C6	2.56	0.40
6:J:155:DG:H2''	6:J:156:DA:C8	2.57	0.40
7:K:3836:SER:HA	7:K:3844:PHE:HE1	1.87	0.40
7:K:3880:ILE:HD13	7:K:3896:THR:OG1	2.22	0.40
8:L:125:LEU:HD21	8:L:144:ILE:CD1	2.51	0.40
10:N:39:LEU:HB2	10:N:51:TRP:HB2	2.03	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	93/136 (68%)	89 (96%)	4 (4%)	0	100	100
1	E	91/136 (67%)	84 (92%)	7 (8%)	0	100	100
2	B	80/103 (78%)	75 (94%)	5 (6%)	0	100	100
2	F	77/103 (75%)	75 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	104/130 (80%)	101 (97%)	3 (3%)	0	100	100
3	G	103/130 (79%)	102 (99%)	1 (1%)	0	100	100
4	D	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
4	H	93/123 (76%)	87 (94%)	6 (6%)	0	100	100
7	K	169/226 (75%)	154 (91%)	15 (9%)	0	100	100
8	L	307/335 (92%)	274 (89%)	33 (11%)	0	100	100
9	M	326/534 (61%)	291 (89%)	35 (11%)	0	100	100
10	N	360/538 (67%)	328 (91%)	32 (9%)	0	100	100
11	O	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
12	P	50/104 (48%)	46 (92%)	4 (8%)	0	100	100
12	Q	49/104 (47%)	43 (88%)	6 (12%)	0	100	100
All	All	2069/2906 (71%)	1911 (92%)	158 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/108 (77%)	81 (98%)	2 (2%)	49	69
1	E	81/108 (75%)	79 (98%)	2 (2%)	47	68
2	B	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	F	65/79 (82%)	64 (98%)	1 (2%)	65	80
3	C	85/102 (83%)	84 (99%)	1 (1%)	71	84
3	G	83/102 (81%)	83 (100%)	0	100	100
4	D	82/103 (80%)	79 (96%)	3 (4%)	34	59
4	H	81/103 (79%)	80 (99%)	1 (1%)	71	84
7	K	147/198 (74%)	147 (100%)	0	100	100
8	L	271/291 (93%)	271 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	M	278/460 (60%)	260 (94%)	18 (6%)	17	44
10	N	322/462 (70%)	318 (99%)	4 (1%)	71	84
11	O	68/73 (93%)	68 (100%)	0	100	100
12	P	46/92 (50%)	45 (98%)	1 (2%)	52	71
12	Q	45/92 (49%)	45 (100%)	0	100	100
All	All	1805/2452 (74%)	1771 (98%)	34 (2%)	59	75

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	129	ARG
2	B	25	ASN
3	C	51	LEU
4	D	27	ARG
4	D	87	THR
4	D	98	LEU
1	E	60	LEU
1	E	129	ARG
2	F	49	LEU
4	H	98	LEU
9	M	230	ARG
9	M	264	LEU
9	M	283	LEU
9	M	287	VAL
9	M	303	ASP
9	M	316	VAL
9	M	324	LYS
9	M	350	LEU
9	M	391	VAL
9	M	398	LEU
9	M	408	LEU
9	M	410	ASP
9	M	411	THR
9	M	431	PHE
9	M	442	THR
9	M	458	VAL
9	M	513	LEU
9	M	522	THR
10	N	26	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	N	166	ILE
10	N	222	ILE
10	N	297	LEU
12	P	87	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
3	C	112	GLN
1	E	68	GLN
3	G	31	HIS
3	G	112	GLN
7	K	3779	ASN
7	K	3906	ASN
8	L	204	GLN
8	L	295	GLN
9	M	243	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	NLE	E	120	1	6,7,8	0.49	0	2,7,9	0.44	0
1	NLE	E	90	1	6,7,8	0.49	0	2,7,9	0.42	0
1	NLE	A	120	1	6,7,8	0.48	0	2,7,9	0.40	0
1	NLE	A	90	1	6,7,8	0.51	0	2,7,9	0.42	0

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
1	NLE	E	120	1	-	0/5/6/8	-
1	NLE	E	90	1	-	0/5/6/8	-
1	NLE	A	120	1	-	0/5/6/8	-
1	NLE	A	90	1	-	0/5/6/8	-

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	90	NLE	2	0
1	A	90	NLE	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	SAH	K	4001	7	24,28,28	1.21	3 (12%)	25,40,40	1.75	5 (20%)

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
13	SAH	K	4001	7	-	5/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	4001	SAH	C2-N3	4.01	1.38	1.32
13	K	4001	SAH	C2-N1	2.43	1.38	1.33
13	K	4001	SAH	OXT-C	-2.17	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	4001	SAH	N3-C2-N1	-5.40	120.24	128.68
13	K	4001	SAH	C5'-SD-CG	-4.09	90.00	102.27
13	K	4001	SAH	C3'-C2'-C1'	3.03	105.54	100.98
13	K	4001	SAH	OXT-C-O	-2.60	118.18	124.09
13	K	4001	SAH	OXT-C-CA	2.19	120.84	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	K	4001	SAH	N-CA-CB-CG
13	K	4001	SAH	C-CA-CB-CG
13	K	4001	SAH	CA-CB-CG-SD
13	K	4001	SAH	O-C-CA-CB
13	K	4001	SAH	OXT-C-CA-CB

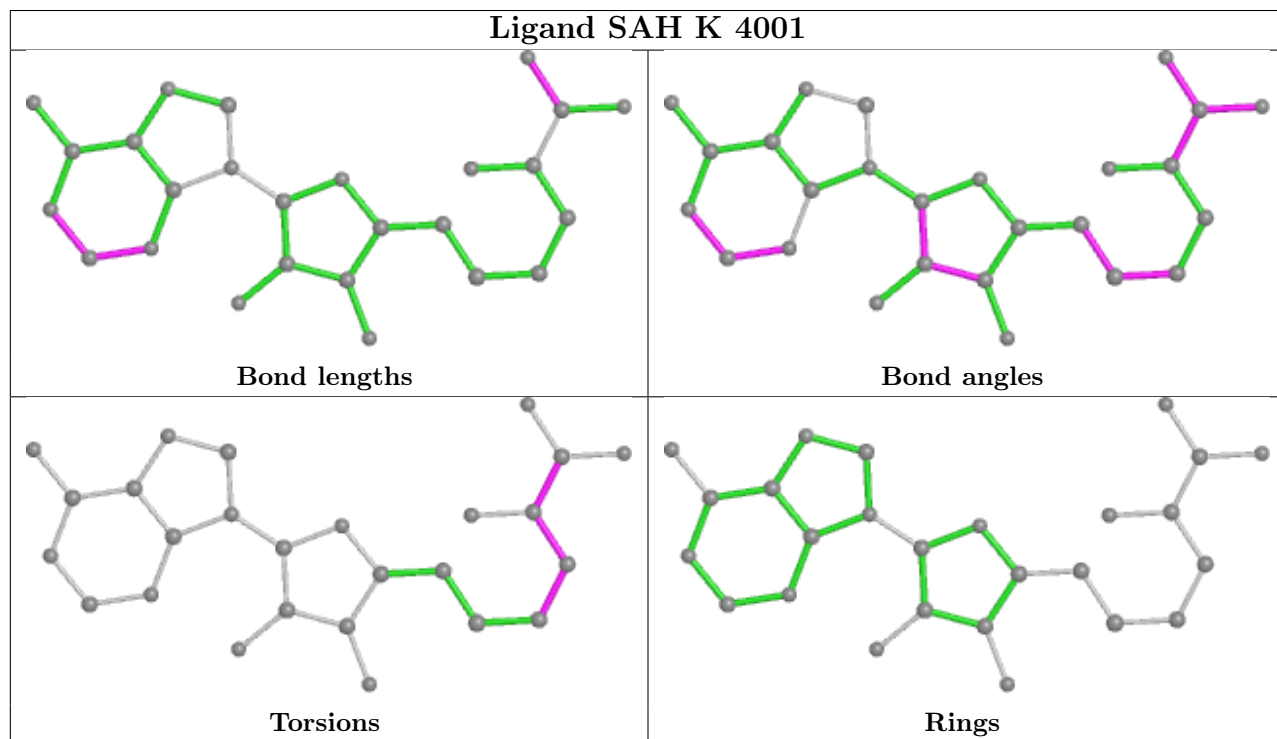
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	K	4001	SAH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

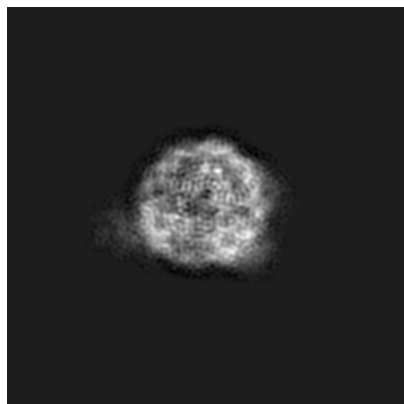
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26454. These allow visual inspection of the internal detail of the map and identification of artifacts.

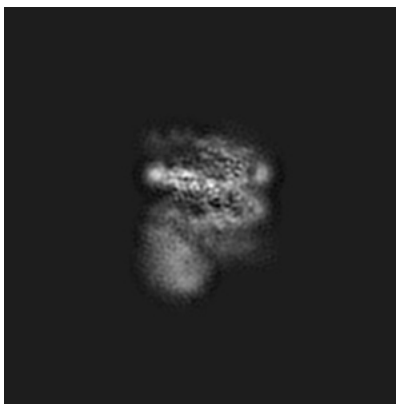
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

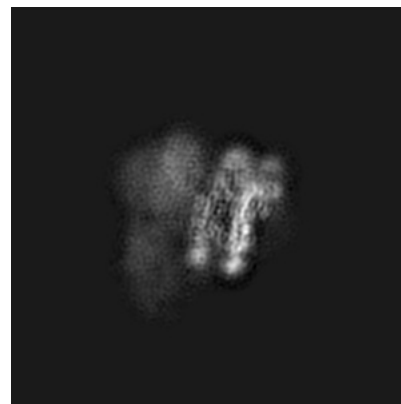
6.1.1 Primary map



X

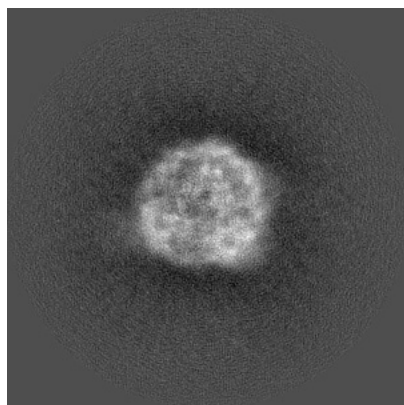


Y

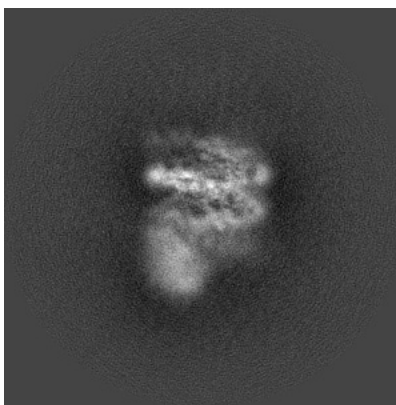


Z

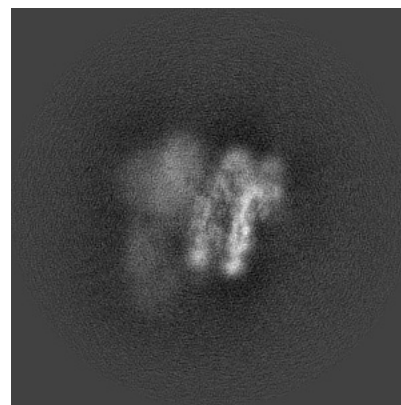
6.1.2 Raw map



X



Y

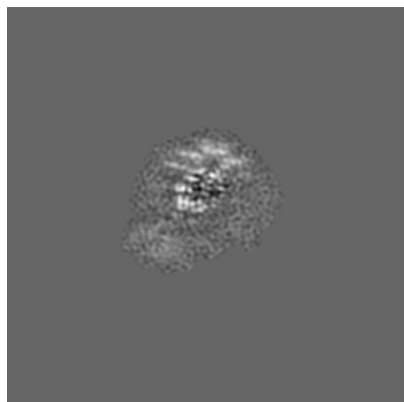


Z

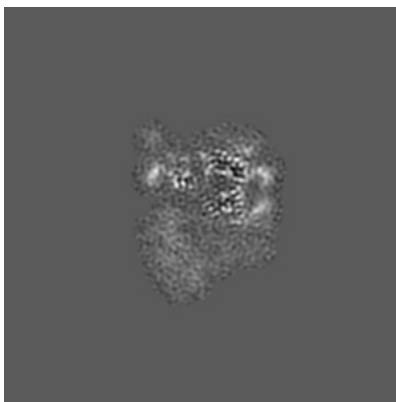
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

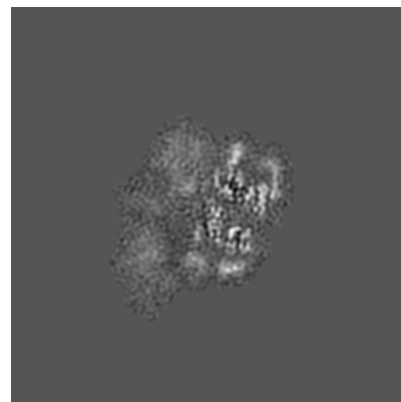
6.2.1 Primary map



X Index: 150

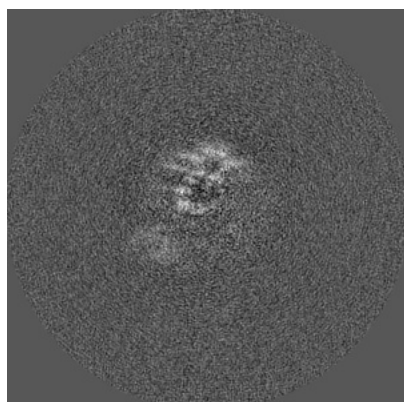


Y Index: 150

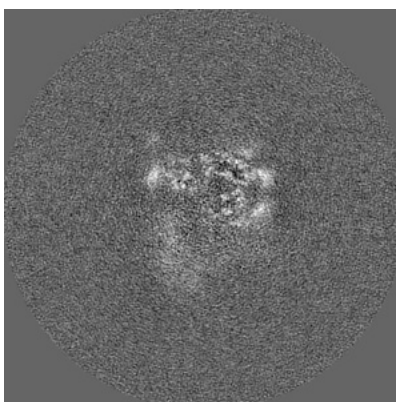


Z Index: 150

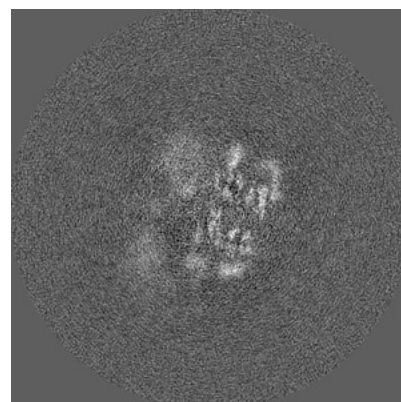
6.2.2 Raw map



X Index: 150



Y Index: 150

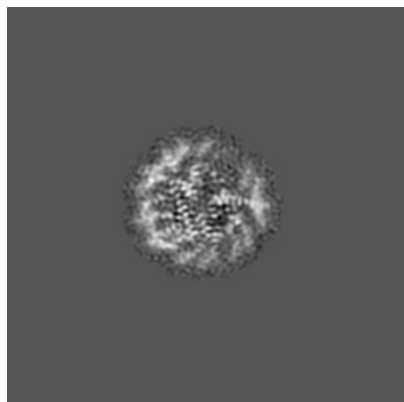


Z Index: 150

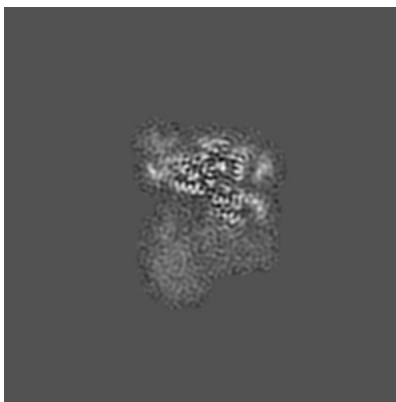
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

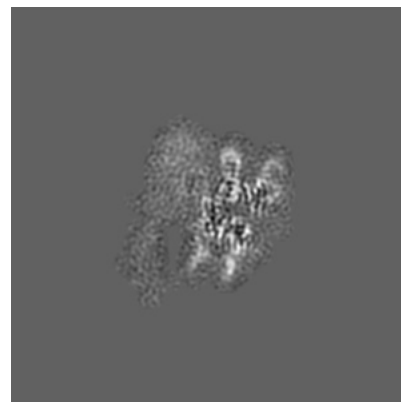
6.3.1 Primary map



X Index: 168

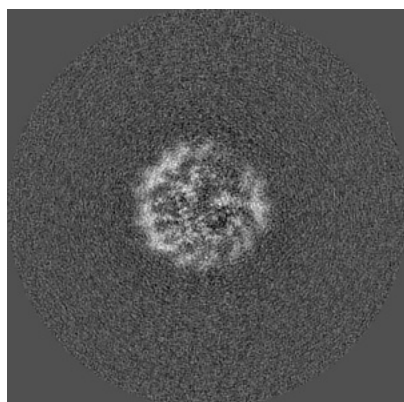


Y Index: 158

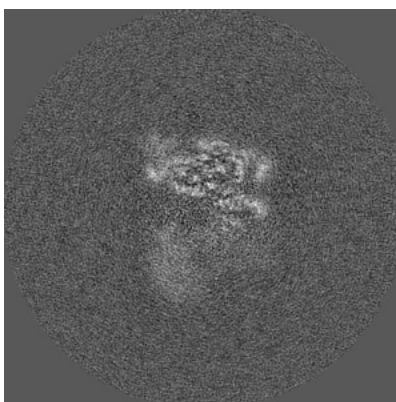


Z Index: 156

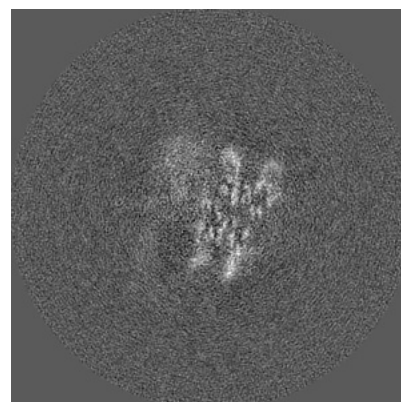
6.3.2 Raw map



X Index: 168



Y Index: 159

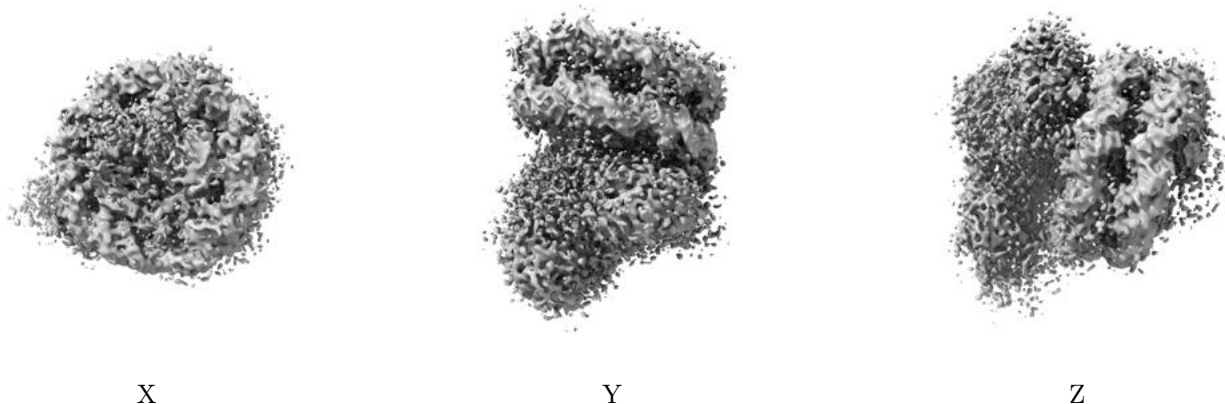


Z Index: 155

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

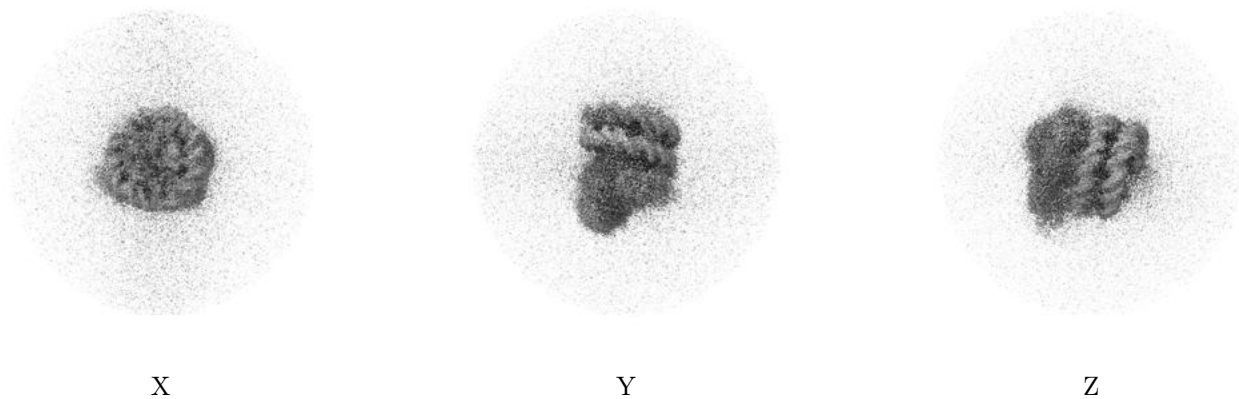
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00732. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

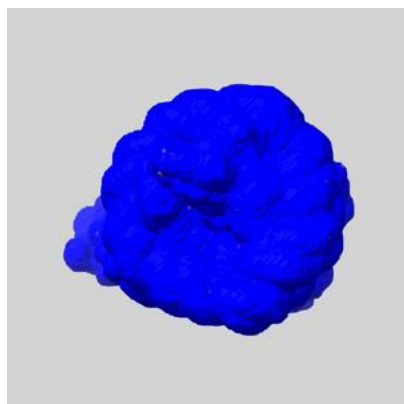
6.5 Mask visualisation [i](#)

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

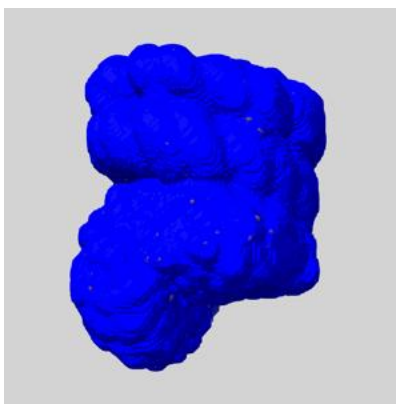
A mask typically either:

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

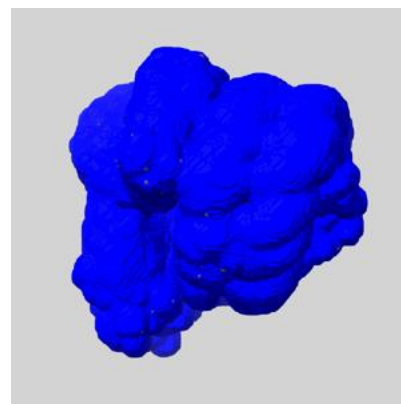
6.5.1 emd_26454_msk_1.map [i](#)



X



Y

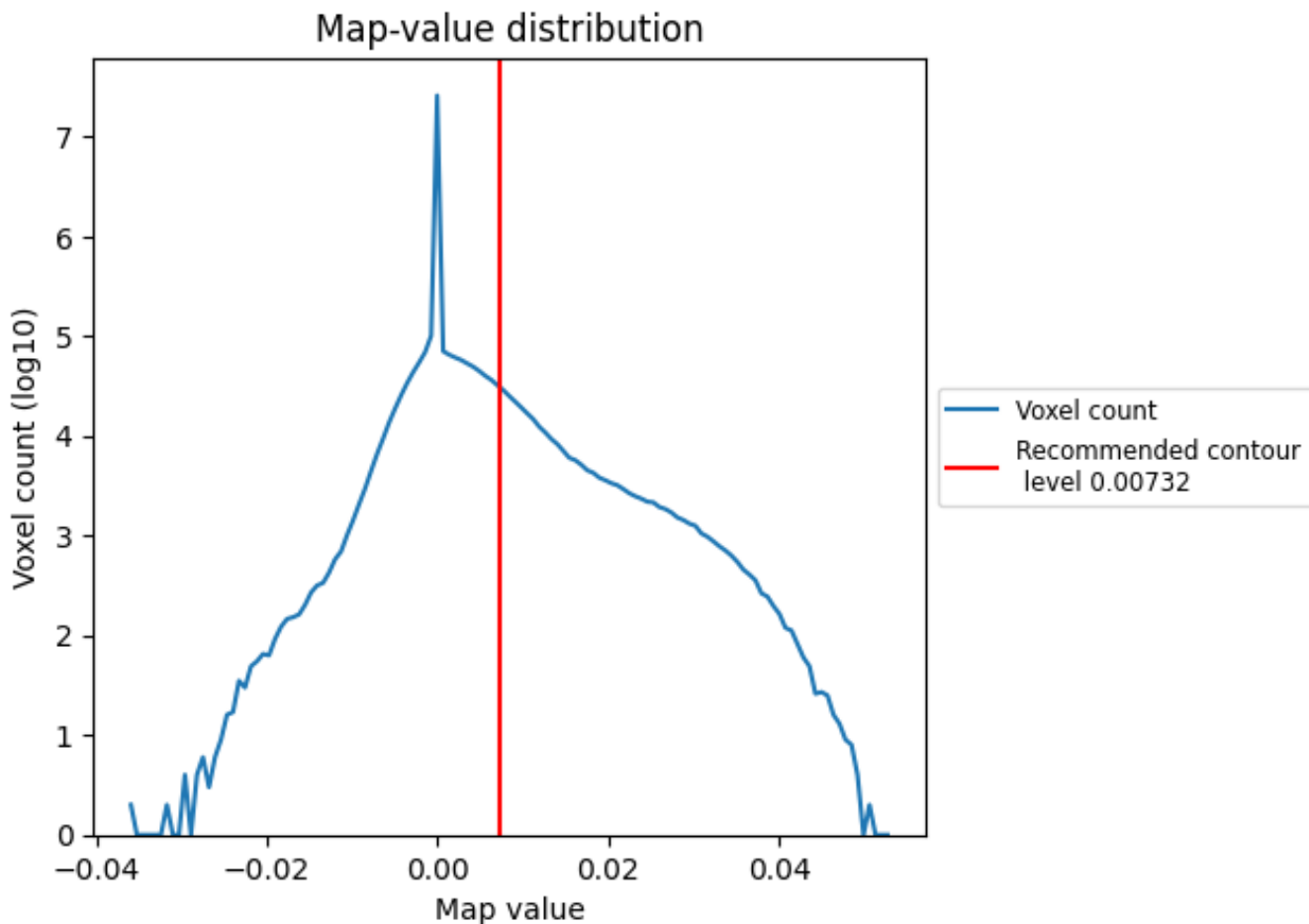


Z

7 Map analysis [i](#)

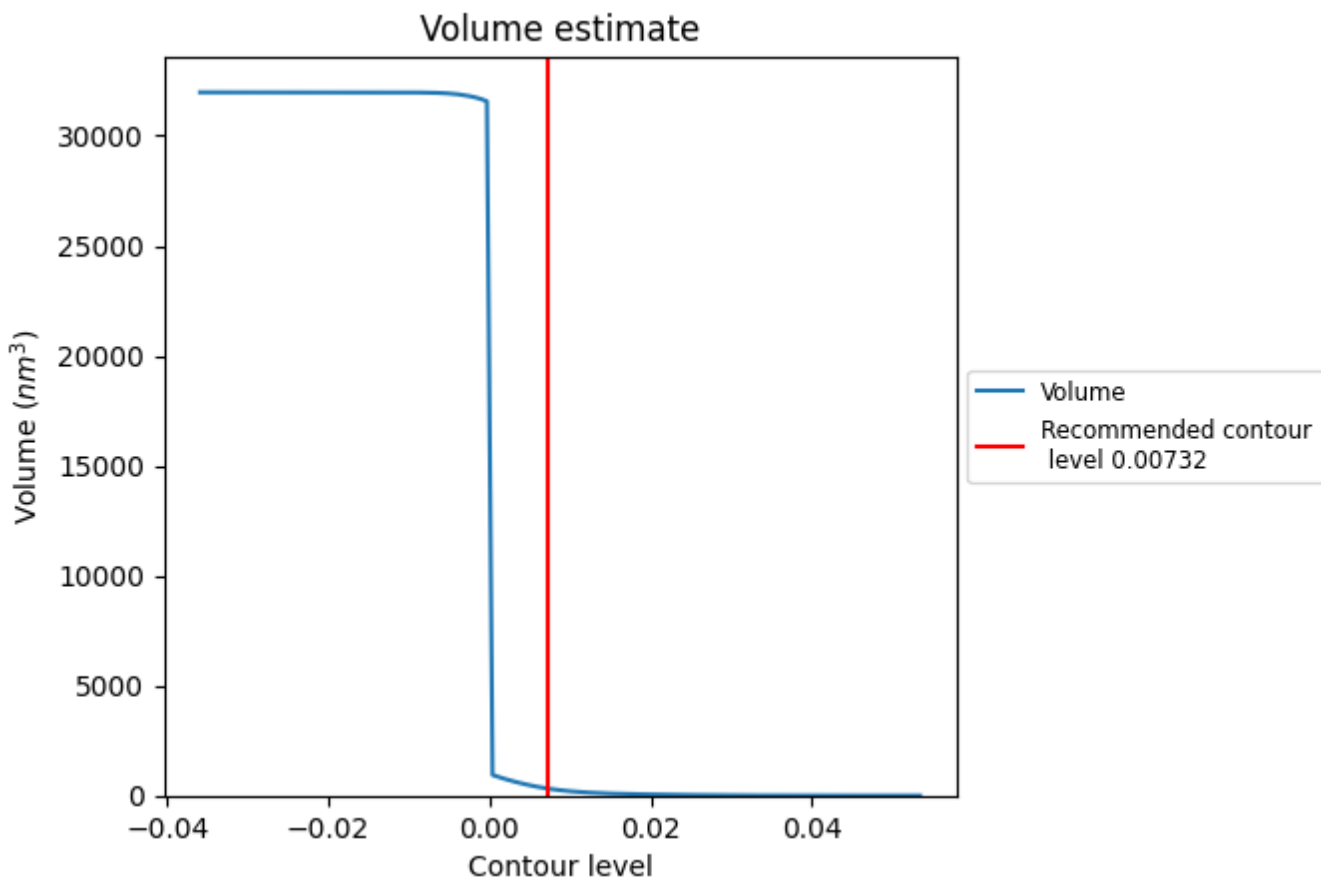
This section contains the results of statistical analysis of the map.

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.

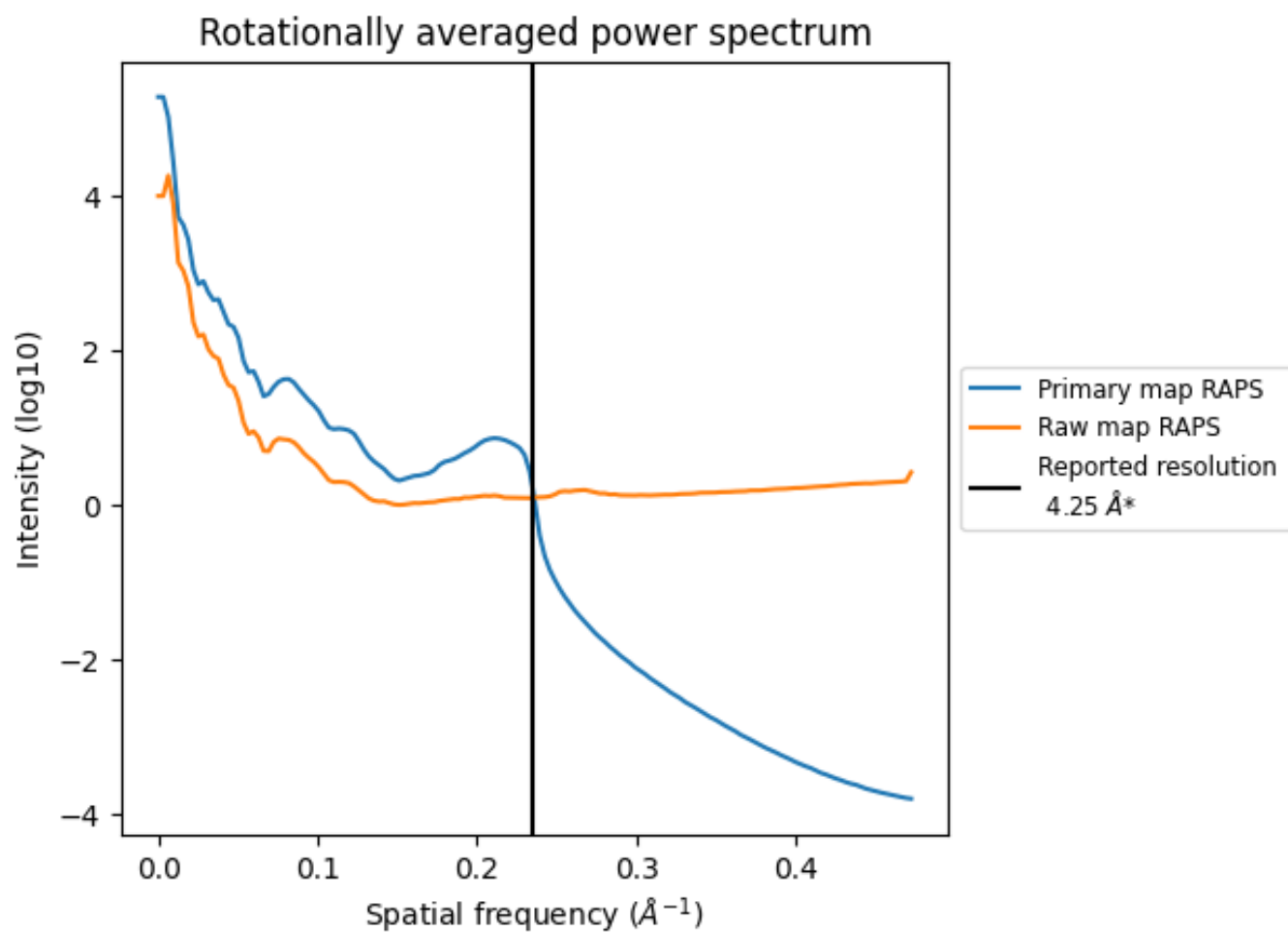
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; this corresponds to an approximate mass of 284 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 [i](#)

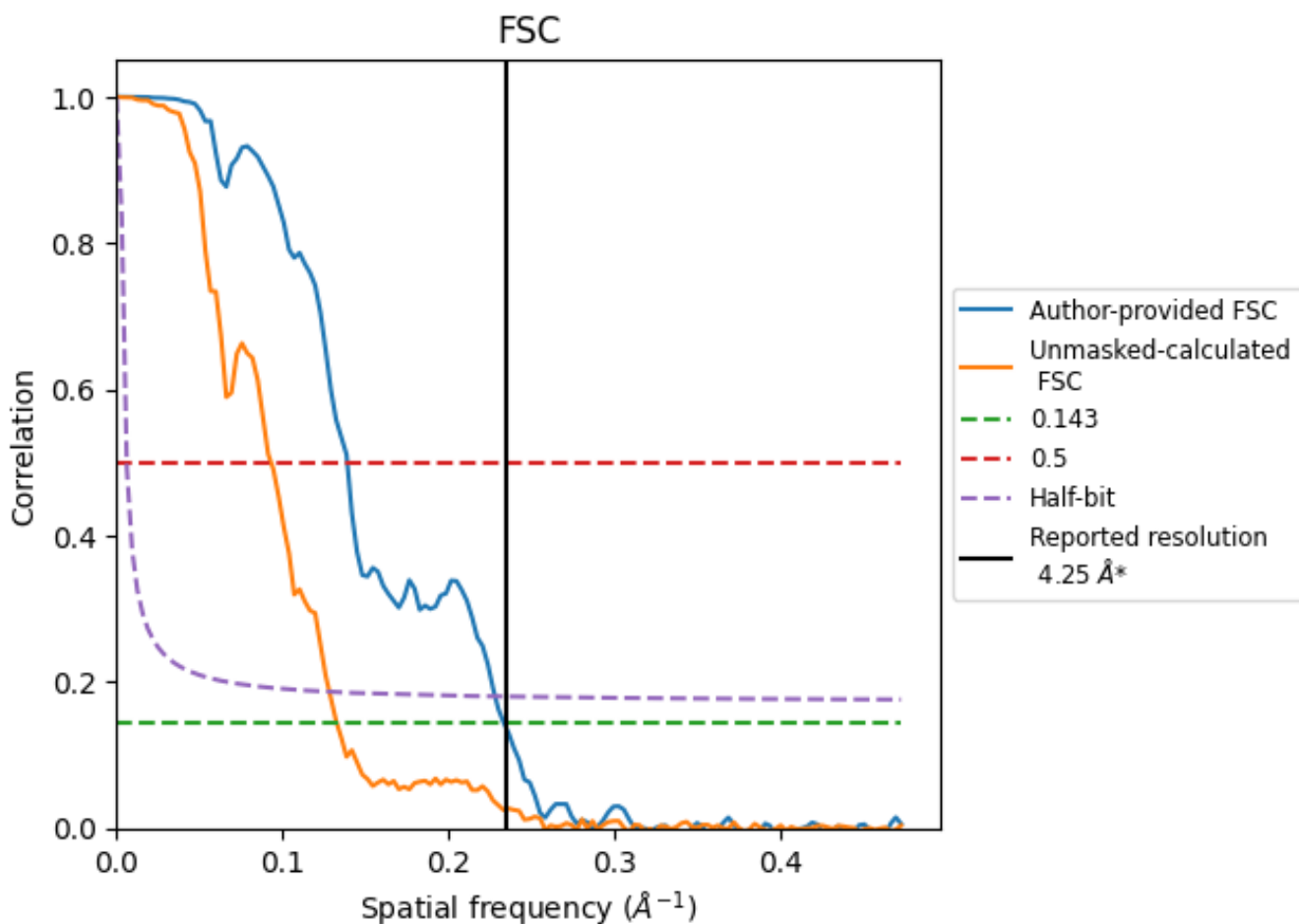


*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

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 0.235 Å⁻¹

8.2 Resolution estimates [i](#)

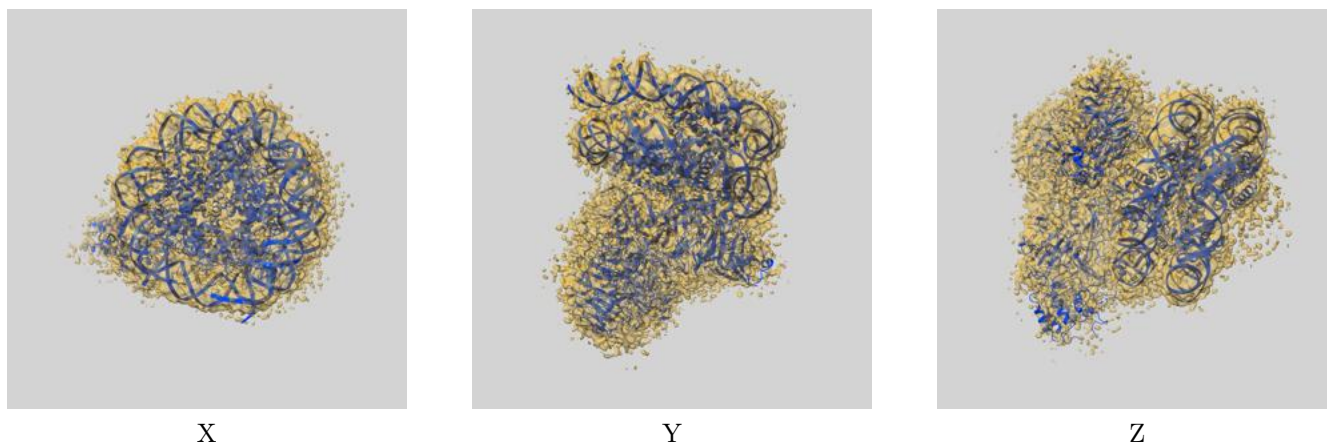
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.28	7.19	4.38
Unmasked-calculated*	7.53	10.74	7.80

*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 7.53 differs from the reported value 4.25 by more than 10 %

9 Map-model fit [i](#)

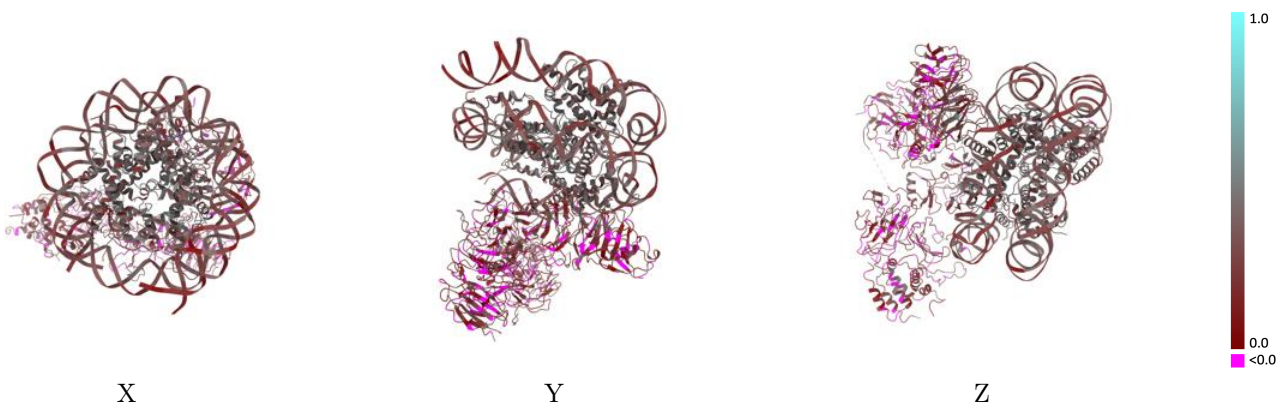
This section contains information regarding the fit between EMDB map EMD-26454 and PDB model 7UD5. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



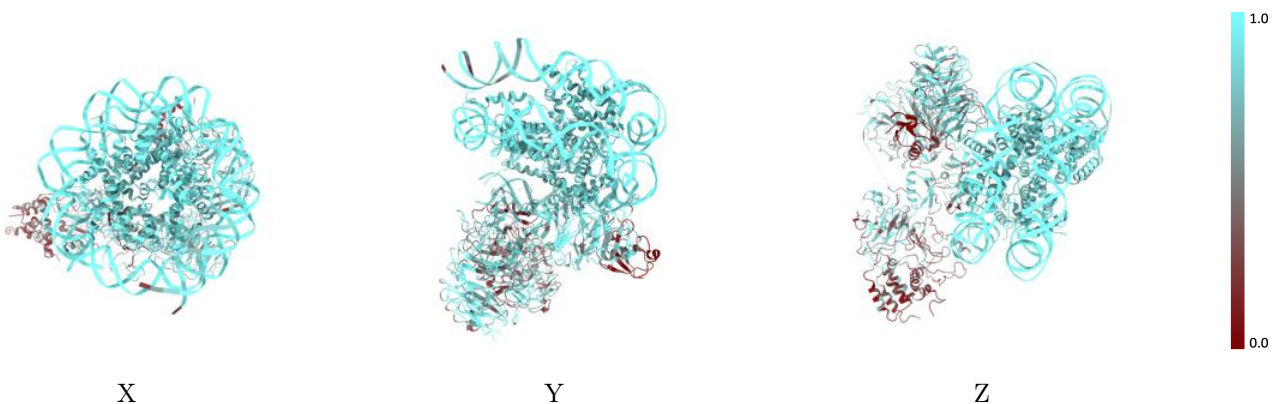
The images above show the 3D surface view of the map at the recommended contour level 0.00732 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



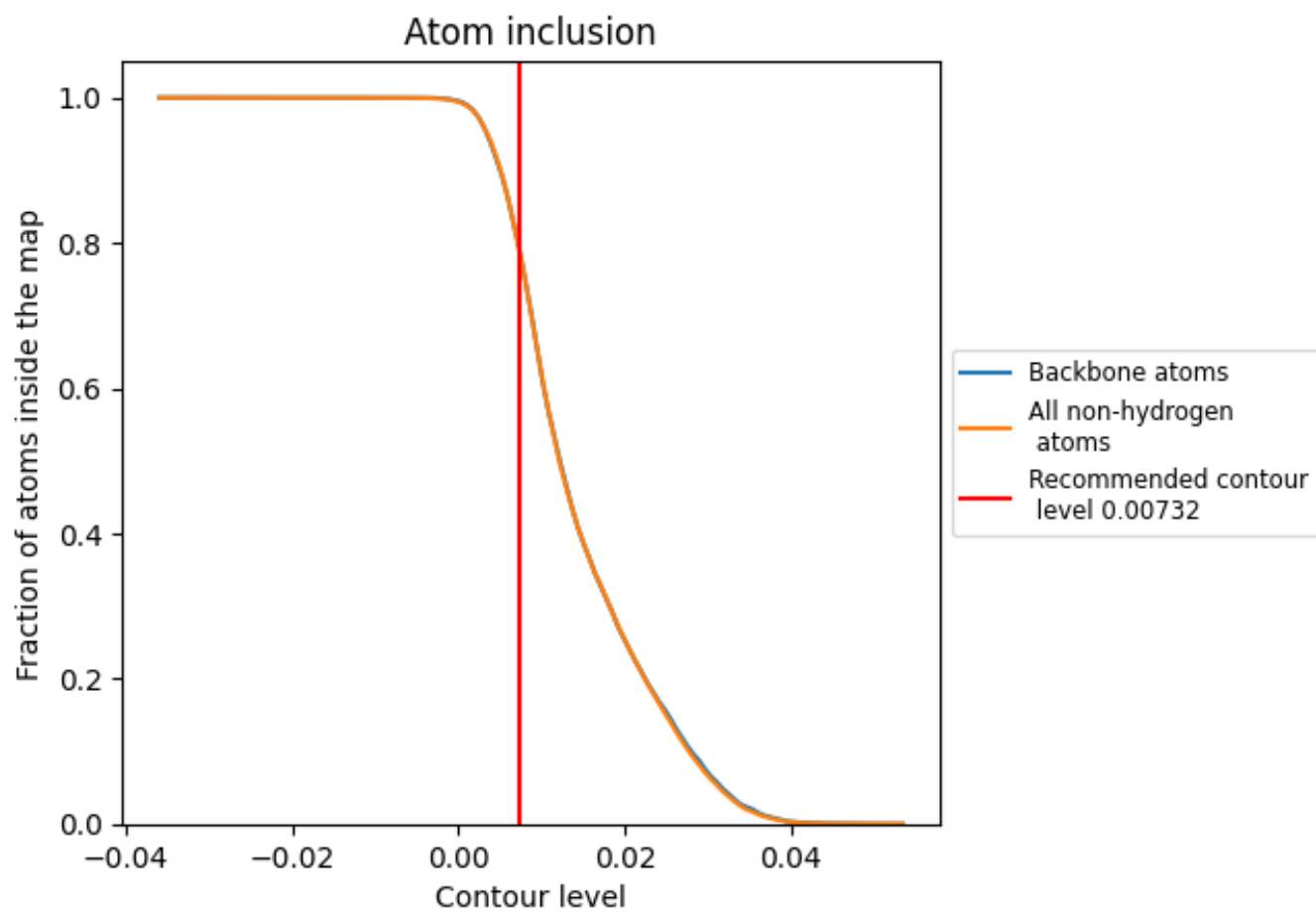
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00732).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.00732) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7919	 0.2630
A	 0.9416	 0.3900
B	 0.9097	 0.3950
C	 0.9069	 0.3860
D	 0.9236	 0.3910
E	 0.9350	 0.3960
F	 0.9308	 0.3950
G	 0.9464	 0.4060
H	 0.9393	 0.3860
I	 0.9694	 0.2990
J	 0.9645	 0.2960
K	 0.6748	 0.1890
L	 0.7475	 0.1460
M	 0.5199	 0.1350
N	 0.7384	 0.2230
O	 0.2568	 0.1470
P	 0.2432	 0.1850
Q	 0.3065	 0.1240

