



Full wwPDB EM Validation Report ⓘ

Aug 2, 2026 – 06:14 PM EDT

PDB ID : 9Y3E / pdb_00009y3e
EMDB ID : EMD-72455
Title : Extended cryo-EM structure of human SRCAP-nucleosome complex in the pre-engaged state
Authors : Louder, R.K.; Park, G.
Deposited on : 2025-09-02
Resolution : 5.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

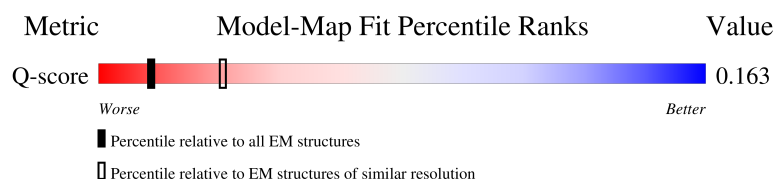
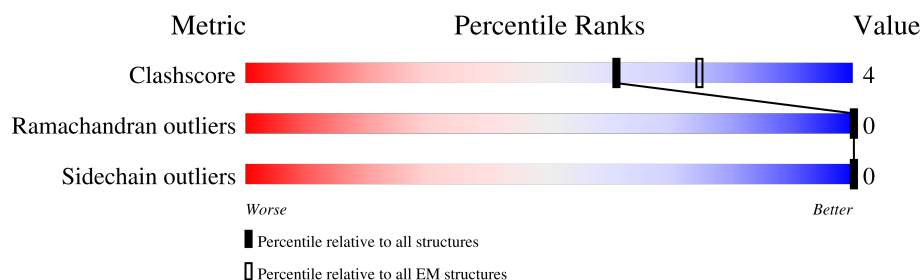
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 (4.50 - 5.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3230	 24% 73%
2	B	364	 17% 41% 5% 54%
3	C	396	 85% 15%
4	D	154	 62% 6% 32%

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Mol	Chain	Length	Quality of chain
5	E	456	
5	G	456	
5	I	456	
6	F	463	
6	H	463	
6	J	463	
7	K	429	
7	M	429	
8	L	375	
9	N	467	
10	Q	128	
10	S	128	
11	R	125	
11	T	125	
12	U	135	
12	W	135	
13	V	102	
13	X	102	
14	Y	285	
15	Z	285	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 56261 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 Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	859	Total	C	N	O	S	0	0
			7104	4525	1306	1236	37		

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	166	Total	C	N	O	S	0	0
			1373	860	264	244	5		

- Molecule 3 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3225	2064	528	615	18		

- Molecule 4 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	105	Total	C	N	O	S	0	0
			831	508	164	151	8		

- Molecule 5 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	433	Total	C	N	O	S	0	0
			3343	2107	574	645	17		
5	G	445	Total	C	N	O	S	0	0
			3429	2159	588	664	18		
5	I	436	Total	C	N	O	S	0	0
			3364	2119	577	651	17		

- Molecule 6 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	438	Total	C	N	O	S	0	0
			3395	2121	596	662	16		
6	H	432	Total	C	N	O	S	0	0
			3361	2101	590	654	16		
6	J	418	Total	C	N	O	S	0	0
			3254	2039	568	632	15		

- Molecule 7 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	403	Total	C	N	O	S	0	0
			3143	1987	538	594	24		
7	M	398	Total	C	N	O	S	0	0
			3105	1964	528	589	24		

- Molecule 8 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	361	Total	C	N	O	S	0	0
			2822	1791	473	538	20		

- Molecule 9 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	157	Total	C	N	O	S	0	0
			1348	864	251	230	3		

- Molecule 10 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Q	110	Total	C	N	O	0	0
			850	535	168	147		
10	S	110	Total	C	N	O	0	0
			850	535	168	147		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	99	ARG	GLY	conflict	UNP P06897
Q	123	SER	-	expression tag	UNP P06897
Q	124	LYS	-	expression tag	UNP P06897
Q	125	SER	-	expression tag	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	126	LYS	-	expression tag	UNP P06897
Q	127	SER	-	expression tag	UNP P06897
Q	128	LYS	-	expression tag	UNP P06897
S	99	ARG	GLY	conflict	UNP P06897
S	123	SER	-	expression tag	UNP P06897
S	124	LYS	-	expression tag	UNP P06897
S	125	SER	-	expression tag	UNP P06897
S	126	LYS	-	expression tag	UNP P06897
S	127	SER	-	expression tag	UNP P06897
S	128	LYS	-	expression tag	UNP P06897

- Molecule 11 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	98	Total	C	N	O	S	0	0
			775	487	144	142	2		
11	T	98	Total	C	N	O	S	0	0
			775	487	144	142	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	32	THR	SER	conflict	UNP P02281
T	32	THR	SER	conflict	UNP P02281

- Molecule 12 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	98	Total	C	N	O	S	0	0
			811	512	157	139	3		
12	W	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	102	ALA	GLY	variant	UNP P84233
W	102	ALA	GLY	variant	UNP P84233

- Molecule 13 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	81	Total 648	C 410	N 126	O 111	S 1	0	0
13	X	81	Total 648	C 410	N 126	O 111	S 1	0	0

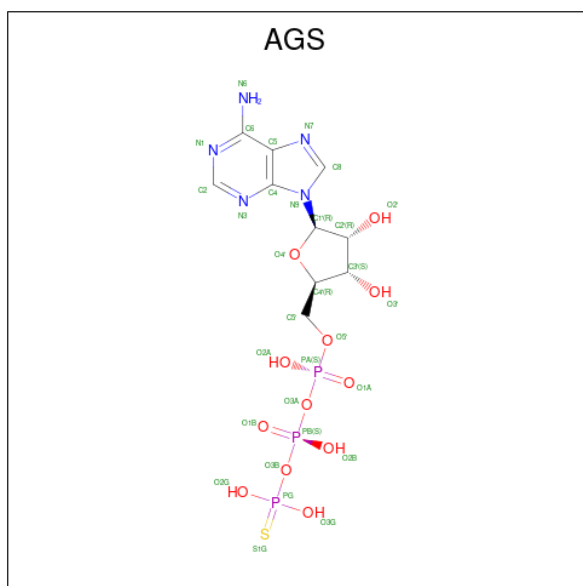
- Molecule 14 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	165	Total	C	N	O	P	0	0
			3365	1596	612	992	165		

- Molecule 15 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	165	Total	C	N	O	P	0	0
			3400	1607	640	988	165		

- Molecule 16 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$).



Mol	Chain	Residues	Atoms						AltConf
16	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
16	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

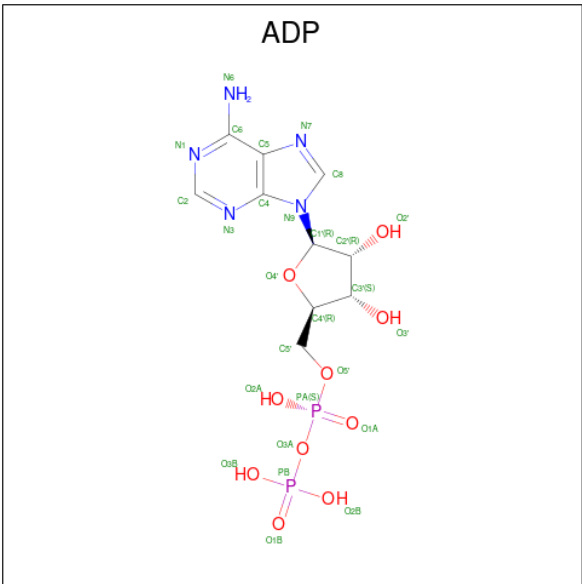
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	C	1	Total	Mg	0
			1	1	
17	F	1	Total	Mg	0
			1	1	
17	H	1	Total	Mg	0
			1	1	
17	J	1	Total	Mg	0
			1	1	
17	K	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
18	D	2	Total	Zn	0
			2	2	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



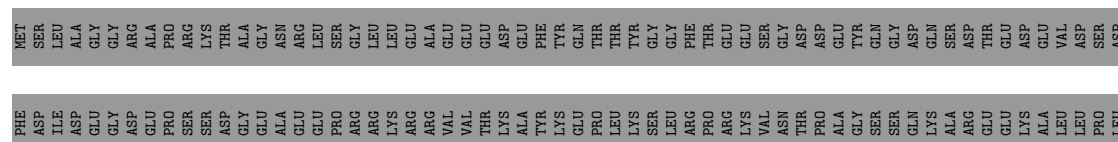
Mol	Chain	Residues	Atoms					AltConf
19	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

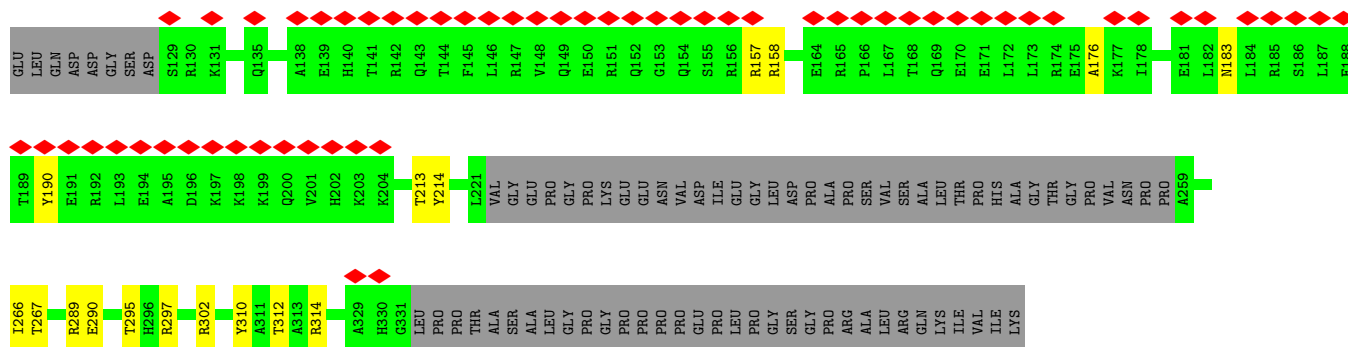
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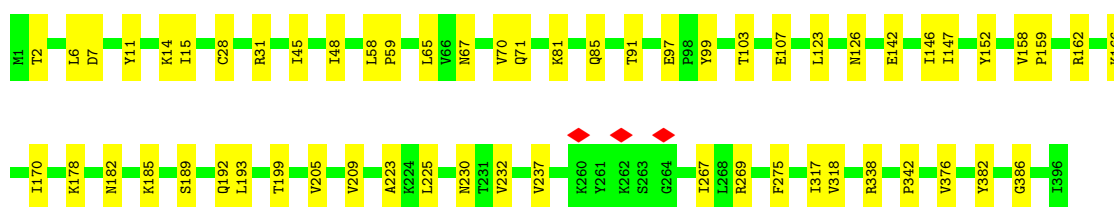
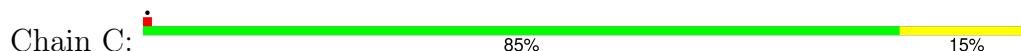
Mol	Chain	Residues	Atoms					AltConf
19	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	J	1	Total	C	N	O	P	0
			27	10	5	10	2	



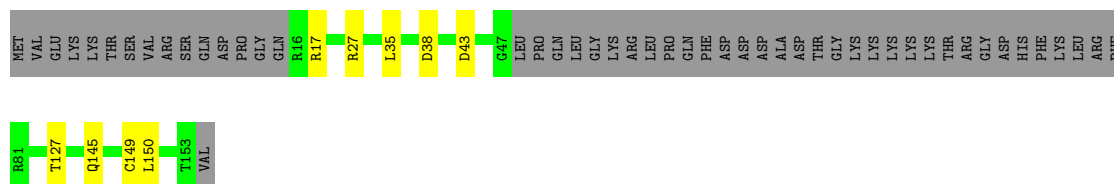




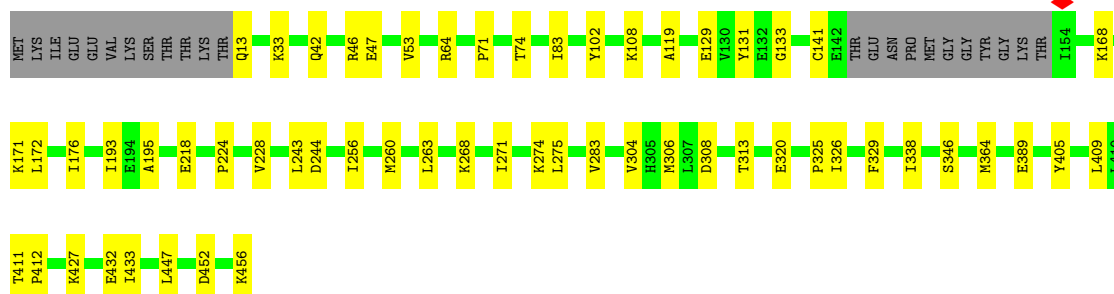
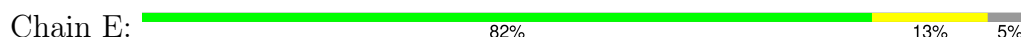
• Molecule 3: Actin-related protein 6



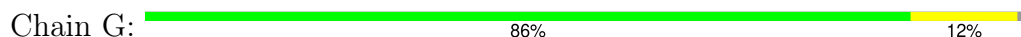
• Molecule 4: Zinc finger HIT domain-containing protein 1

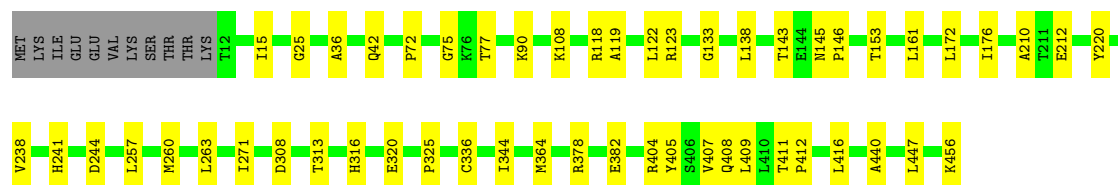


• Molecule 5: RuvB-like 1



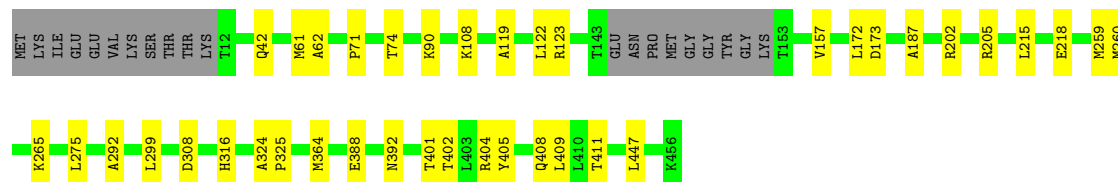
• Molecule 5: RuvB-like 1





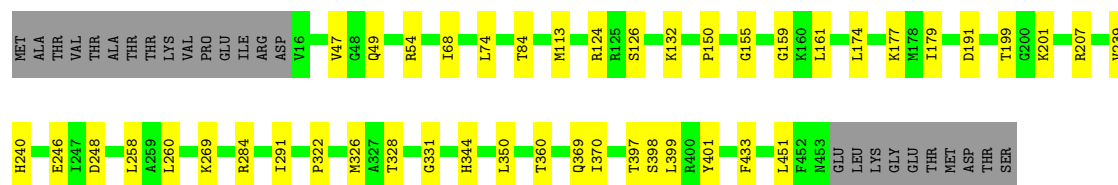
• Molecule 5: RuvB-like 1

Chain I: 87% 9%



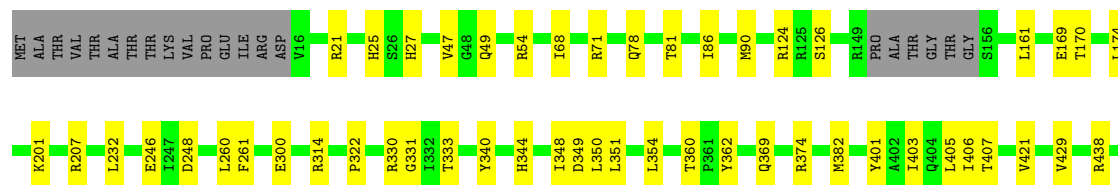
• Molecule 6: RuvB-like 2

Chain F: 85% 10% 5%



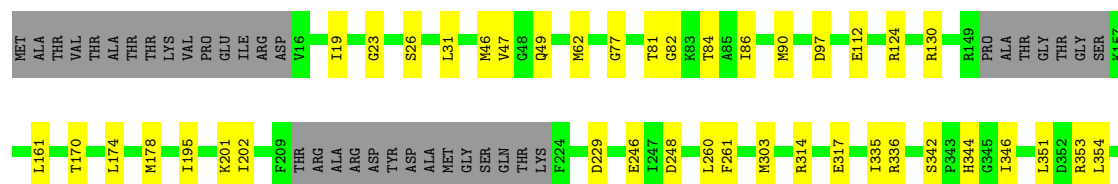
• Molecule 6: RuvB-like 2

Chain H: 82% 11% 7%



• Molecule 6: RuvB-like 2

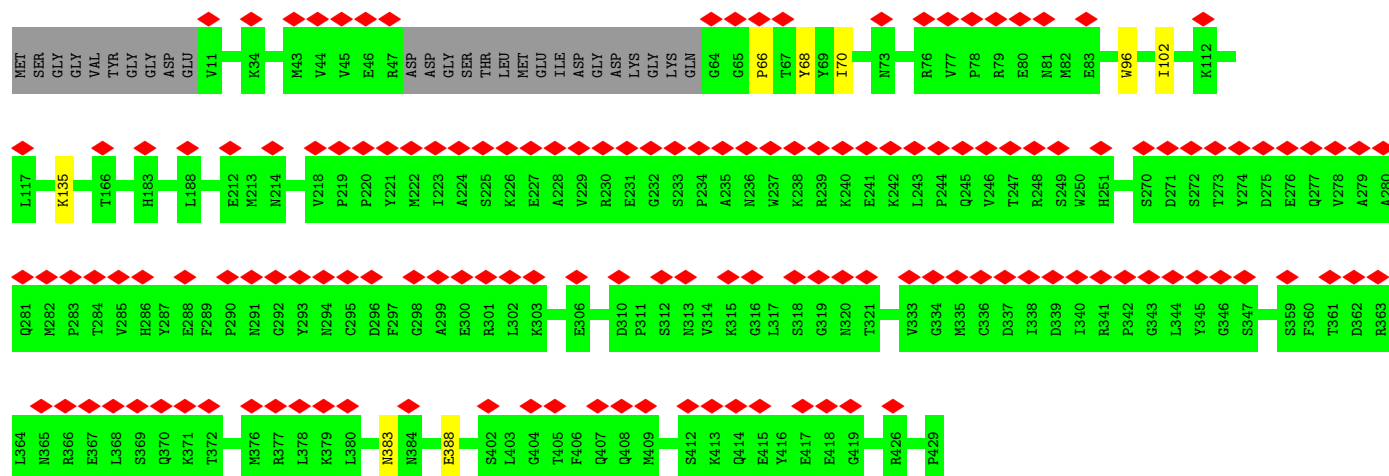
Chain J: 80% 10% 10%





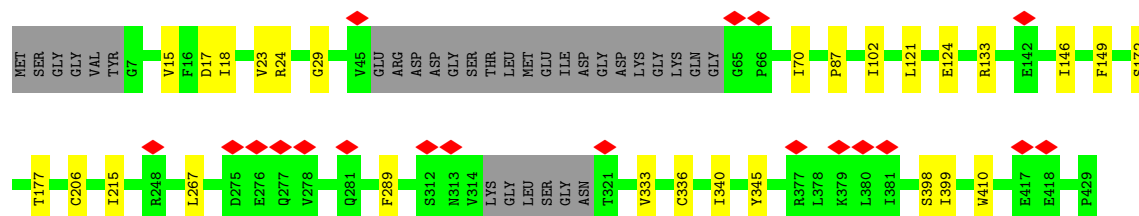
- Molecule 7: Actin-like protein 6A

Chain K: 34% 92% 6%



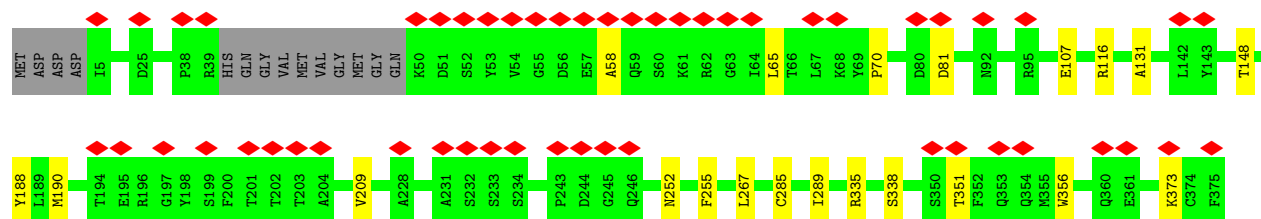
- Molecule 7: Actin-like protein 6A

Chain M: 86% 6% 7%



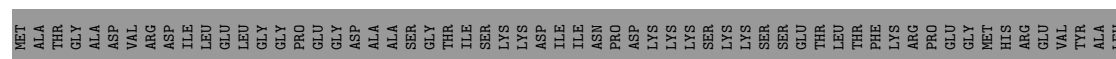
- Molecule 8: Actin, cytoplasmic 1

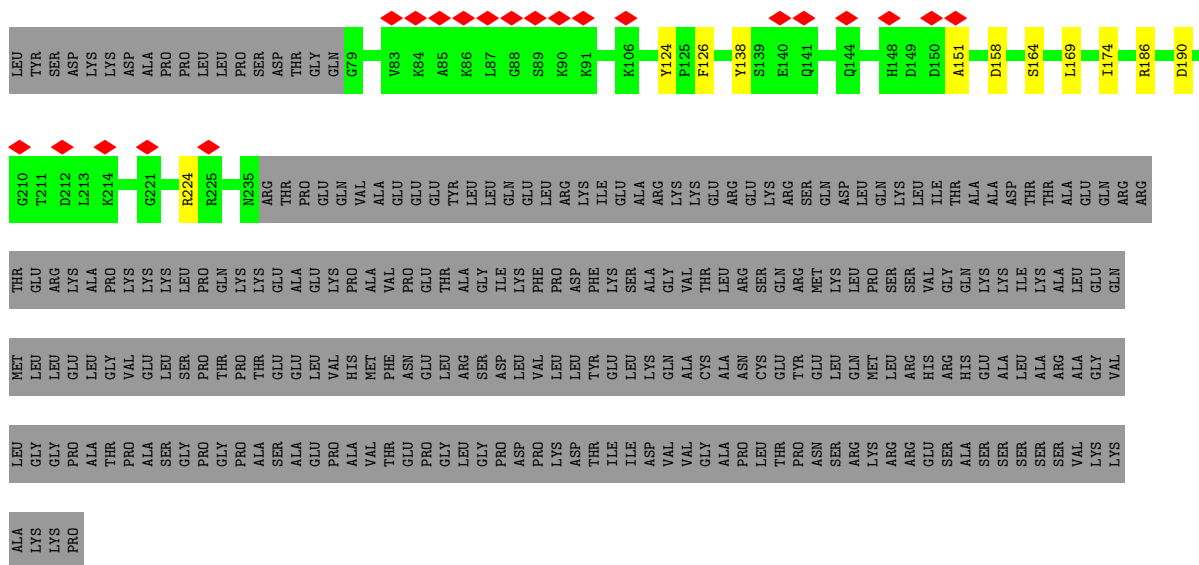
Chain L: 14% 91% 6%



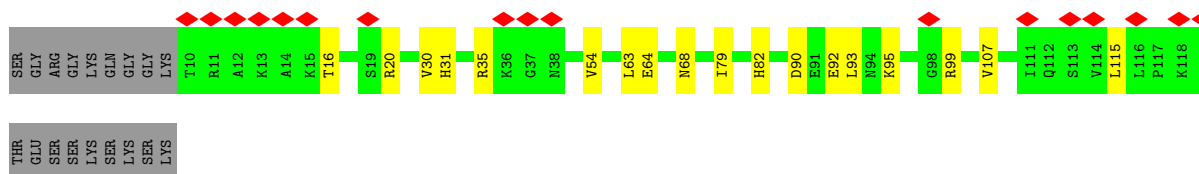
- Molecule 9: DNA methyltransferase 1-associated protein 1

Chain N: 31% 66% 3%

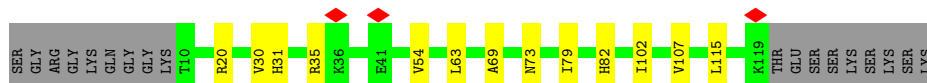




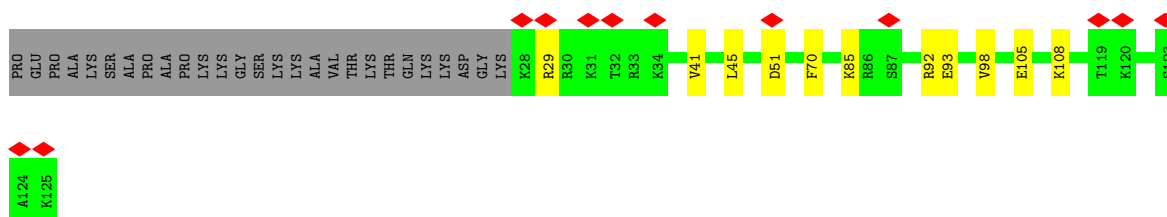
- Molecule 10: Histone H2A type 1



- Molecule 10: Histone H2A type 1



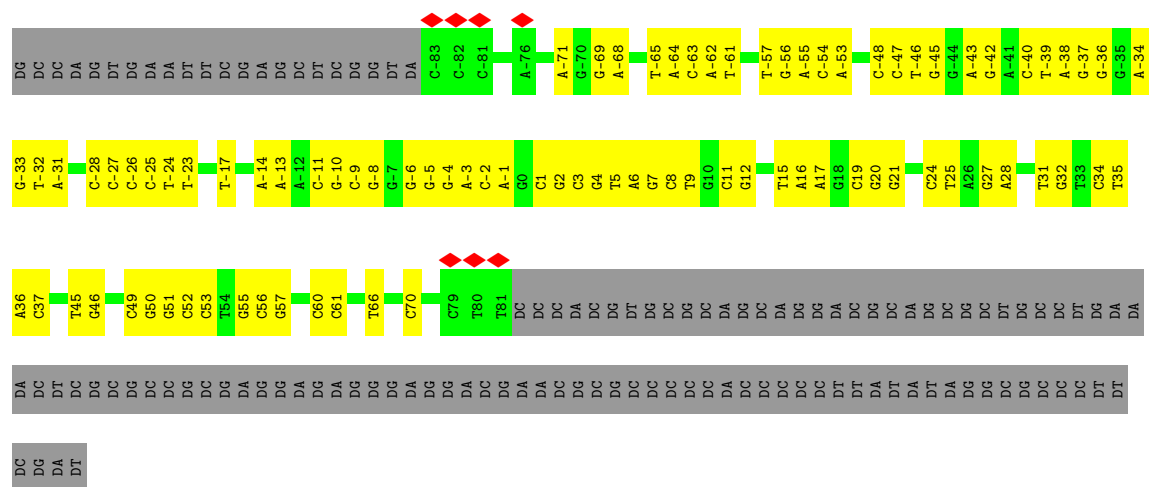
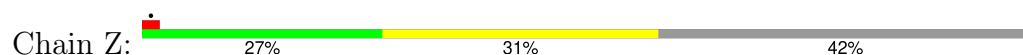
- Molecule 11: Histone H2B 1.1



- Molecule 11: Histone H2B 1.1



- Molecule 15: DNA (285-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	393.59998, 393.59998, 393.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.025, 1.025, 1.025	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AGS, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/7272	0.33	0/9821
2	B	0.13	0/1404	0.37	0/1892
3	C	0.07	0/3299	0.23	0/4467
4	D	0.07	0/848	0.23	0/1147
5	E	0.09	0/3386	0.22	0/4561
5	G	0.08	0/3475	0.22	0/4683
5	I	0.08	0/3407	0.21	0/4591
6	F	0.07	0/3435	0.21	0/4625
6	H	0.07	0/3399	0.21	0/4573
6	J	0.08	0/3290	0.23	0/4426
7	K	0.12	0/3214	0.38	0/4358
7	M	0.12	0/3175	0.37	0/4306
8	L	0.13	0/2883	0.39	0/3905
9	N	0.10	0/1388	0.33	0/1869
10	Q	0.08	0/860	0.21	0/1159
10	S	0.12	0/860	0.22	0/1159
11	R	0.07	0/786	0.20	0/1054
11	T	0.08	0/786	0.22	0/1054
12	U	0.07	0/823	0.18	0/1104
12	W	0.08	0/823	0.20	0/1104
13	V	0.09	0/655	0.20	0/878
13	X	0.09	0/655	0.20	0/878
14	Y	0.19	0/3770	0.46	0/5812
15	Z	0.19	0/3818	0.44	0/5895
All	All	0.12	0/57711	0.31	0/79321

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

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	7104	0	7206	51	0
2	B	1373	0	1394	14	0
3	C	3225	0	3147	36	0
4	D	831	0	798	9	0
5	E	3343	0	3449	42	0
5	G	3429	0	3530	42	0
5	I	3364	0	3470	29	0
6	F	3395	0	3467	29	0
6	H	3361	0	3435	41	0
6	J	3254	0	3329	37	0
7	K	3143	0	3092	4	0
7	M	3105	0	3044	16	0
8	L	2822	0	2798	12	0
9	N	1348	0	1320	6	0
10	Q	850	0	915	15	0
10	S	850	0	915	12	0
11	R	775	0	812	11	0
11	T	775	0	812	13	0
12	U	811	0	853	13	0
12	W	811	0	853	12	0
13	V	648	0	693	5	0
13	X	648	0	693	10	0
14	Y	3365	0	1851	63	0
15	Z	3400	0	1849	67	0
16	C	31	0	12	0	0
16	K	31	0	12	0	0
17	C	1	0	0	0	0
17	F	1	0	0	0	0
17	H	1	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
18	D	2	0	0	0	0
19	E	27	0	12	0	0
19	F	27	0	12	0	0
19	G	27	0	12	2	0
19	H	27	0	12	2	0
19	I	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	27	0	12	1	0
All	All	56261	0	53821	484	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 4.

All (484) 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)
5:E:411:THR:HG21	6:F:68:ILE:HG13	1.62	0.82
3:C:65:LEU:HD11	3:C:71:GLN:HG2	1.69	0.73
1:A:611:PRO:HG3	1:A:659:HIS:HB2	1.74	0.70
5:G:411:THR:HG21	6:H:68:ILE:HG13	1.74	0.70
6:H:207:ARG:NH1	5:I:173:ASP:OD1	2.24	0.69
6:J:124:ARG:NE	6:J:248:ASP:OD2	2.28	0.67
1:A:644:GLU:OE2	1:A:839:ARG:NH2	2.29	0.65
13:V:22:LEU:HB3	13:V:25:ASN:HD21	1.61	0.65
7:M:336:CYS:HB3	7:M:340:ILE:HD11	1.79	0.65
6:F:191:ASP:OD1	6:F:207:ARG:NH1	2.30	0.64
6:F:451:LEU:HD21	5:G:72:PRO:HG3	1.79	0.64
6:F:49:GLN:NE2	6:F:360:THR:O	2.31	0.64
1:A:692:SER:HB2	2:B:176:ALA:HB1	1.79	0.64
10:S:20:ARG:NH2	14:Y:-42:DT:OP1	2.30	0.64
1:A:240:THR:HG21	1:A:832:VAL:HA	1.79	0.63
15:Z:15:DT:H2''	15:Z:16:DA:C8	2.34	0.62
7:M:17:ASP:OD2	7:M:24:ARG:NH1	2.31	0.62
14:Y:61:DA:H2''	14:Y:62:DT:H5'	1.80	0.62
14:Y:35:DC:H2''	14:Y:36:DC:C5	2.34	0.62
3:C:182:ASN:ND2	4:D:35:LEU:O	2.32	0.62
5:E:275:LEU:HD13	6:J:261:PHE:HB3	1.82	0.62
6:H:401:TYR:OH	6:H:438:ARG:NH2	2.33	0.62
6:H:124:ARG:NE	6:H:248:ASP:OD2	2.34	0.61
15:Z:-62:DA:H2'	15:Z:-61:DT:H71	1.83	0.61
8:L:285:CYS:HB3	8:L:289:ILE:HD11	1.82	0.60
15:Z:-47:DC:H2''	15:Z:-46:DT:C5	2.36	0.60
1:A:1924:ASP:OD2	6:H:201:LYS:NZ	2.33	0.60
3:C:159:PRO:HG2	3:C:166:LYS:HB2	1.82	0.60
5:G:447:LEU:HD22	6:H:331:GLY:HA2	1.84	0.60
6:F:124:ARG:NE	6:F:248:ASP:OD2	2.34	0.59
5:I:408:GLN:HE22	6:J:353:ARG:HA	1.67	0.59
5:I:447:LEU:HD11	6:J:344:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:51:DG:H2''	14:Y:52:DC:H5''	1.85	0.59
6:J:49:GLN:NE2	6:J:81:THR:O	2.31	0.59
14:Y:55:DT:H2''	14:Y:56:DC:C5	2.38	0.59
5:G:172:LEU:HB3	5:G:176:ILE:HD12	1.85	0.59
5:E:447:LEU:HD22	6:F:331:GLY:HA2	1.85	0.59
15:Z:-54:DC:H2''	15:Z:-53:DA:C8	2.37	0.59
5:G:108:LYS:NZ	5:G:308:ASP:OD2	2.33	0.59
10:S:63:LEU:HD13	11:T:45:LEU:HB2	1.84	0.58
5:G:404:ARG:NH2	19:G:501:ADP:O3A	2.37	0.58
6:H:27:HIS:HD2	6:H:374:ARG:HH11	1.52	0.58
10:Q:63:LEU:HD13	11:R:45:LEU:HB2	1.85	0.58
6:F:159:GLY:HA3	6:F:179:ILE:HD11	1.84	0.58
14:Y:-47:DT:H2''	14:Y:-46:DC:C5	2.39	0.58
10:Q:16:THR:HA	15:Z:-43:DA:H5''	1.86	0.58
4:D:27:ARG:NH2	4:D:150:LEU:O	2.29	0.57
5:I:90:LYS:HB2	5:I:123:ARG:HH22	1.68	0.57
1:A:730:GLN:HE21	15:Z:-17:DT:H5''	1.69	0.57
1:A:1971:GLU:OE1	6:F:240:HIS:NE2	2.29	0.57
12:W:60:LEU:HD12	12:W:64:LYS:HE2	1.86	0.57
2:B:290:GLU:OE2	2:B:302:ARG:NH1	2.33	0.57
12:U:73:GLU:OE1	13:V:25:ASN:ND2	2.36	0.57
5:I:202:ARG:NH2	5:I:218:GLU:OE2	2.35	0.57
14:Y:66:DC:H2''	14:Y:67:DA:C8	2.40	0.57
3:C:123:LEU:HB2	3:C:376:VAL:HG12	1.87	0.56
5:E:304:VAL:HG21	5:E:329:PHE:HB3	1.87	0.56
1:A:922:CYS:SG	6:J:201:LYS:NZ	2.78	0.56
13:X:22:LEU:HB3	13:X:25:ASN:HD21	1.70	0.56
8:L:107:GLU:OE2	8:L:116:ARG:NH2	2.31	0.56
13:X:35:ARG:NH1	14:Y:8:DC:OP2	2.37	0.56
14:Y:-57:DC:H2''	14:Y:-56:DG:N7	2.20	0.56
3:C:142:GLU:O	3:C:162:ARG:NH2	2.39	0.56
14:Y:-71:DG:H2''	14:Y:-70:DG:C8	2.41	0.56
5:E:13:GLN:OE1	6:F:284:ARG:NH2	2.39	0.56
5:G:77:THR:OG1	6:H:314:ARG:NH1	2.39	0.56
2:B:289:ARG:NH2	5:G:212:GLU:OE2	2.39	0.56
6:F:199:THR:HG23	6:F:201:LYS:H	1.69	0.56
14:Y:49:DC:H2''	14:Y:50:DA:C8	2.41	0.55
1:A:772:LEU:HG	1:A:792:LEU:HD21	1.87	0.55
5:E:411:THR:OG1	5:E:412:PRO:HD3	2.07	0.55
4:D:127:THR:H	6:J:170:THR:HG23	1.71	0.55
6:J:246:GLU:HA	6:J:260:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:VAL:HG22	3:C:170:ILE:HG23	1.88	0.55
15:Z:-46:DT:H2''	15:Z:-45:DG:C8	2.42	0.55
15:Z:8:DC:H2'	15:Z:9:DT:H71	1.89	0.55
12:U:37:LYS:HD2	12:U:38:PRO:HD2	1.89	0.55
5:I:402:THR:HG22	5:I:404:ARG:H	1.70	0.54
15:Z:-65:DT:H2''	15:Z:-64:DA:C8	2.42	0.54
15:Z:49:DC:H2''	15:Z:50:DG:C8	2.42	0.54
5:E:33:LYS:O	5:E:46:ARG:NH2	2.41	0.54
8:L:188:TYR:HB2	8:L:267:LEU:HD21	1.89	0.54
5:E:263:LEU:HB2	5:G:260:MET:HE3	1.88	0.54
6:H:382:MET:HG2	6:H:421:VAL:HB	1.90	0.54
1:A:1973:ILE:HG23	1:A:1977:ILE:HD12	1.88	0.54
1:A:2094:ARG:NE	1:A:2096:GLU:OE2	2.31	0.54
14:Y:-32:DC:H2''	14:Y:-31:DA:C8	2.43	0.54
15:Z:3:DC:H2''	15:Z:4:DG:C8	2.42	0.54
10:Q:64:GLU:OE2	10:Q:68:ASN:ND2	2.37	0.54
11:R:29:ARG:HH12	15:Z:31:DT:H5''	1.72	0.54
3:C:178:LYS:NZ	4:D:38:ASP:OD1	2.38	0.53
5:G:119:ALA:HB3	5:G:325:PRO:HG3	1.91	0.53
7:K:383:ASN:HD22	7:K:388:GLU:HB3	1.72	0.53
15:Z:60:DC:H2''	15:Z:61:DC:C6	2.43	0.53
5:E:268:LYS:HG2	6:F:269:LYS:HE2	1.89	0.53
5:G:408:GLN:O	6:H:71:ARG:NH2	2.41	0.53
5:I:119:ALA:HB3	5:I:325:PRO:HG3	1.90	0.53
7:K:70:ILE:HD13	7:K:102:ILE:HA	1.89	0.53
15:Z:35:DT:H2''	15:Z:36:DA:C8	2.43	0.53
12:U:116:ARG:HD3	14:Y:-3:DG:H3'	1.89	0.53
15:Z:-24:DT:H2'	15:Z:-23:DT:H71	1.91	0.53
6:H:362:TYR:OH	19:H:501:ADP:N7	2.36	0.53
14:Y:-14:DA:H2''	14:Y:-13:DA:C8	2.44	0.53
10:Q:90:ASP:HB3	10:Q:93:LEU:HB2	1.90	0.53
5:I:108:LYS:NZ	5:I:308:ASP:OD2	2.37	0.53
10:S:30:VAL:HG13	11:T:70:PHE:HE2	1.73	0.53
14:Y:-57:DC:H2''	14:Y:-56:DG:C8	2.44	0.53
14:Y:-48:DC:H2''	14:Y:-47:DT:H72	1.91	0.53
15:Z:-57:DT:H2''	15:Z:-56:DG:C8	2.44	0.53
1:A:751:ILE:HG22	1:A:759:TRP:HD1	1.74	0.52
15:Z:16:DA:H2''	15:Z:17:DA:C8	2.44	0.52
5:E:47:GLU:OE1	6:J:428:ARG:NH2	2.37	0.52
5:E:283:VAL:HB	6:J:19:ILE:HD11	1.90	0.52
14:Y:30:DT:H2'	14:Y:31:DT:H71	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:263:LEU:HD22	5:I:260:MET:HB3	1.90	0.52
1:A:2134:VAL:HG22	1:A:2164:TYR:HB2	1.92	0.52
14:Y:-70:DG:H2''	14:Y:-69:DA:C8	2.45	0.52
1:A:2009:GLN:HB3	5:I:259:MET:HE1	1.91	0.52
14:Y:-72:DT:H2''	14:Y:-71:DG:C8	2.45	0.52
3:C:382:TYR:HA	3:C:386:GLY:HA3	1.92	0.52
5:E:42:GLN:NE2	5:E:364:MET:O	2.42	0.52
14:Y:45:DC:H2''	14:Y:46:DA:N7	2.25	0.52
3:C:192:GLN:NE2	3:C:269:ARG:O	2.42	0.51
6:H:246:GLU:HA	6:H:260:LEU:HD21	1.91	0.51
6:H:300:GLU:OE2	5:I:316:HIS:ND1	2.36	0.51
14:Y:-73:DC:H2'	14:Y:-72:DT:H72	1.91	0.51
1:A:700:GLY:O	1:A:705:ARG:NH1	2.40	0.51
14:Y:73:DT:H1'	14:Y:74:DG:C8	2.45	0.51
9:N:124:TYR:CE2	9:N:126:PHE:HB2	2.46	0.51
15:Z:-9:DC:H2''	15:Z:-8:DG:C8	2.45	0.51
14:Y:-41:DG:H2''	14:Y:-40:DG:H5''	1.91	0.51
14:Y:8:DC:H2''	14:Y:9:DG:C8	2.45	0.51
15:Z:55:DG:H2''	15:Z:56:DC:C5	2.45	0.51
11:T:33:ARG:HG3	15:Z:49:DC:H4'	1.91	0.51
12:U:126:LEU:HD22	12:W:113:HIS:CG	2.46	0.51
10:Q:31:HIS:CD2	10:Q:35:ARG:HE	2.28	0.51
5:E:172:LEU:HD13	5:E:176:ILE:HG21	1.93	0.51
7:M:18:ILE:HG23	7:M:23:VAL:HG22	1.93	0.51
14:Y:6:DC:H2''	14:Y:7:DC:C5	2.45	0.51
1:A:686:LEU:HD13	1:A:695:ILE:HD12	1.92	0.50
6:F:161:LEU:HB2	6:F:174:LEU:HD11	1.92	0.50
6:H:78:GLN:O	6:H:81:THR:OG1	2.25	0.50
1:A:680:LEU:HD21	2:B:190:TYR:OH	2.11	0.50
1:A:892:ASN:O	1:A:896:GLN:HG2	2.11	0.50
5:G:15:ILE:HD13	5:G:382:GLU:HA	1.93	0.50
5:G:336:CYS:SG	6:H:340:TYR:OH	2.55	0.50
6:H:49:GLN:NE2	6:H:360:THR:O	2.43	0.50
12:U:119:ILE:HD11	13:V:46:ILE:HG23	1.92	0.50
3:C:225:LEU:O	3:C:230:ASN:ND2	2.42	0.50
6:J:46:MET:HE1	6:J:86:ILE:HA	1.93	0.50
5:I:187:ALA:O	5:I:205:ARG:NH1	2.44	0.50
5:E:456:LYS:HE3	5:G:344:ILE:HG13	1.92	0.50
3:C:31:ARG:NH1	4:D:43:ASP:OD2	2.45	0.50
3:C:232:VAL:HG11	3:C:275:PHE:HE2	1.75	0.50
5:G:143:THR:HG22	5:G:145:ASN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:388:GLU:O	5:I:392:ASN:ND2	2.38	0.50
13:V:22:LEU:HB3	13:V:25:ASN:ND2	2.26	0.50
1:A:686:LEU:HD12	1:A:722:ILE:HD11	1.94	0.50
5:G:118:ARG:HE	5:G:241:HIS:CE1	2.30	0.50
10:Q:30:VAL:HG13	11:R:70:PHE:HE2	1.76	0.50
1:A:2011:ALA:HB1	1:A:2015:TRP:HD1	1.77	0.49
8:L:131:ALA:HB1	8:L:356:TRP:HB3	1.94	0.49
10:Q:63:LEU:HD11	11:R:41:VAL:HG13	1.94	0.49
11:R:93:GLU:HG3	13:X:75:HIS:CE1	2.47	0.49
15:Z:20:DG:H4'	15:Z:21:DG:OP1	2.12	0.49
7:M:121:LEU:HB2	7:M:410:TRP:CH2	2.48	0.49
10:S:31:HIS:CD2	10:S:35:ARG:HE	2.30	0.49
12:U:113:HIS:HE1	12:W:122:LYS:HG3	1.78	0.49
3:C:11:TYR:HB2	3:C:152:TYR:CG	2.48	0.49
6:J:31:LEU:HD23	6:J:46:MET:HE3	1.94	0.49
11:R:92:ARG:NH1	13:X:75:HIS:O	2.28	0.49
15:Z:-37:DG:H2''	15:Z:-36:DG:C8	2.47	0.49
6:F:401:TYR:OH	6:F:433:PHE:O	2.26	0.49
6:J:382:MET:HE2	6:J:421:VAL:HG11	1.95	0.49
7:M:121:LEU:HB2	7:M:410:TRP:HH2	1.76	0.49
1:A:742:TYR:CD1	1:A:769:ARG:HB2	2.48	0.49
8:L:70:PRO:HB3	8:L:81:ASP:HB2	1.95	0.49
10:Q:79:ILE:HG12	10:Q:82:HIS:CE1	2.47	0.49
10:Q:92:GLU:OE2	11:R:105:GLU:N	2.42	0.49
10:S:79:ILE:HG12	10:S:82:HIS:CE1	2.47	0.49
4:D:145:GLN:HA	4:D:149:CYS:HB2	1.94	0.49
12:U:113:HIS:CG	12:W:126:LEU:HD22	2.47	0.49
5:G:133:GLY:HA3	5:G:161:LEU:HB3	1.94	0.49
5:G:263:LEU:HD22	5:I:260:MET:HE2	1.94	0.49
14:Y:-6:DT:H2''	14:Y:-5:DA:N7	2.27	0.49
1:A:2044:LYS:NZ	1:A:2173:GLU:OE2	2.34	0.48
2:B:295:THR:HG23	2:B:297:ARG:H	1.78	0.48
14:Y:4:DC:H2''	14:Y:5:DC:C5	2.48	0.48
15:Z:-34:DA:H2''	15:Z:-33:DG:C8	2.48	0.48
5:I:122:LEU:HD11	5:I:292:ALA:HB1	1.96	0.48
5:I:215:LEU:HG	6:J:178:MET:HE3	1.95	0.48
9:N:164:SER:HA	9:N:174:ILE:HD11	1.95	0.48
1:A:2067:GLN:OE1	1:A:2118:THR:OG1	2.28	0.48
15:Z:-38:DA:H5'	15:Z:-38:DA:C8	2.48	0.48
15:Z:11:DC:H2''	15:Z:12:DG:C8	2.48	0.48
14:Y:67:DA:C8	14:Y:67:DA:H5'	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:351:LEU:HD23	6:H:354:LEU:HD11	1.96	0.48
6:J:351:LEU:HD23	6:J:354:LEU:HD12	1.96	0.48
5:E:129:GLU:HB2	5:E:195:ALA:HB3	1.96	0.48
6:H:27:HIS:CD2	6:H:374:ARG:HH11	2.30	0.48
6:J:335:ILE:HD11	6:J:342:SER:HB2	1.96	0.48
15:Z:-6:DG:H2"	15:Z:-5:DG:C8	2.49	0.48
15:Z:5:DT:H2"	15:Z:6:DA:C8	2.49	0.48
6:J:195:ILE:HG12	6:J:202:ILE:HG12	1.95	0.48
14:Y:15:DT:H2"	14:Y:16:DA:C8	2.49	0.48
6:F:258:LEU:HD12	5:G:257:LEU:HD13	1.94	0.48
5:G:90:LYS:HE3	5:G:123:ARG:HD2	1.96	0.48
6:J:402:ALA:O	6:J:406:ILE:HG13	2.14	0.48
14:Y:-55:DC:H2"	14:Y:-54:DA:N7	2.29	0.48
3:C:81:LYS:HD3	3:C:85:GLN:HG2	1.96	0.47
5:E:218:GLU:OE2	6:F:177:LYS:NZ	2.27	0.47
5:I:265:LYS:NZ	6:J:112:GLU:OE2	2.47	0.47
13:X:38:ALA:HB1	13:X:43:VAL:HB	1.96	0.47
6:F:284:ARG:HD3	6:F:291:ILE:HD12	1.96	0.47
6:H:261:PHE:HD2	5:I:275:LEU:HD13	1.79	0.47
14:Y:-46:DC:H2"	14:Y:-45:DA:N7	2.29	0.47
6:H:86:ILE:HG22	6:H:90:MET:HE2	1.96	0.47
14:Y:3:DT:H2"	14:Y:4:DC:C6	2.49	0.47
3:C:237:VAL:HG22	3:C:267:ILE:HG12	1.95	0.47
11:T:105:GLU:HA	11:T:108:LYS:HG2	1.95	0.47
5:G:447:LEU:HD11	6:H:344:HIS:CE1	2.49	0.47
1:A:147:LEU:HD23	7:M:399:ILE:HG23	1.96	0.47
5:G:146:PRO:HA	5:G:153:THR:HG22	1.97	0.47
14:Y:-12:DC:H2"	14:Y:-11:DG:C8	2.49	0.47
2:B:158:ARG:NH2	14:Y:-61:DG:OP2	2.41	0.47
10:Q:95:LYS:HE3	10:Q:95:LYS:HB2	1.74	0.47
14:Y:53:DT:H2"	14:Y:54:DG:C8	2.49	0.47
15:Z:-48:DC:H2"	15:Z:-47:DC:C5	2.49	0.47
5:E:168:LYS:HB3	5:E:228:VAL:HG11	1.97	0.47
6:H:25:HIS:NE2	19:H:501:ADP:O1A	2.38	0.47
6:J:23:GLY:H	6:J:26:SER:HG	1.59	0.47
11:T:55:SER:HA	14:Y:-54:DA:H5"	1.96	0.47
15:Z:45:DT:H2"	15:Z:46:DG:N7	2.30	0.47
5:E:432:GLU:OE2	6:F:54:ARG:NH1	2.35	0.47
14:Y:15:DT:H2"	14:Y:16:DA:N7	2.30	0.47
1:A:2157:GLN:NE2	1:A:2159:ARG:O	2.47	0.47
5:G:313:THR:HA	5:G:316:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:54:VAL:HG21	11:R:98:VAL:HG21	1.97	0.47
15:Z:34:DC:H2"	15:Z:35:DT:C5	2.50	0.47
5:E:141:CYS:SG	5:E:171:LYS:NZ	2.80	0.46
6:J:97:ASP:HB3	6:J:130:ARG:NH2	2.30	0.46
15:Z:6:DA:H2"	15:Z:7:DG:C8	2.50	0.46
15:Z:24:DC:H2"	15:Z:25:DT:C6	2.50	0.46
3:C:99:TYR:CZ	3:C:158:VAL:HG21	2.51	0.46
5:E:260:MET:HE1	5:I:260:MET:HE3	1.96	0.46
6:J:314:ARG:NH1	6:J:317:GLU:OE2	2.47	0.46
15:Z:-32:DT:H2"	15:Z:-31:DA:H8	1.80	0.46
15:Z:27:DG:H2"	15:Z:28:DA:C8	2.50	0.46
15:Z:45:DT:H2"	15:Z:46:DG:C8	2.50	0.46
14:Y:-16:DT:H2"	14:Y:-15:DA:N7	2.30	0.46
15:Z:-26:DC:H2"	15:Z:-25:DC:C6	2.50	0.46
3:C:205:VAL:O	3:C:209:VAL:HG22	2.15	0.46
5:G:411:THR:OG1	5:G:412:PRO:HD3	2.14	0.46
12:W:61:LEU:HD12	13:X:37:LEU:HD23	1.96	0.46
15:Z:-28:DC:H2"	15:Z:-27:DC:C6	2.50	0.46
11:T:90:THR:OG1	11:T:93:GLU:OE1	2.25	0.46
7:M:87:PRO:HG3	7:M:102:ILE:HD12	1.97	0.46
1:A:216:LYS:NZ	1:A:2321:GLU:OE2	2.37	0.46
1:A:714:LYS:HG3	1:A:715:PRO:HD2	1.97	0.46
14:Y:-2:DC:H2"	14:Y:-1:DG:C8	2.51	0.46
5:E:119:ALA:HB3	5:E:325:PRO:HG3	1.97	0.46
5:I:71:PRO:HD2	5:I:74:THR:HG21	1.96	0.46
14:Y:64:DT:H2"	14:Y:65:DA:C8	2.51	0.46
15:Z:-4:DG:H2"	15:Z:-3:DA:C8	2.51	0.46
1:A:1918:TYR:CZ	6:H:260:LEU:HD13	2.51	0.46
3:C:182:ASN:HD22	4:D:35:LEU:C	2.22	0.46
6:H:170:THR:HG22	6:H:232:LEU:HD13	1.98	0.46
5:G:416:LEU:HD11	6:H:54:ARG:NH2	2.31	0.45
6:J:342:SER:OG	6:J:346:ILE:O	2.29	0.45
15:Z:20:DG:H2"	15:Z:21:DG:O5'	2.16	0.45
5:I:401:THR:O	5:I:402:THR:OG1	2.33	0.45
7:M:172:SER:HA	7:M:177:THR:HA	1.99	0.45
13:V:38:ALA:HB1	13:V:43:VAL:HB	1.98	0.45
15:Z:1:DC:H2"	15:Z:2:DG:C8	2.50	0.45
1:A:163:ARG:O	1:A:166:VAL:HG12	2.16	0.45
1:A:674:VAL:O	1:A:724:SER:HA	2.16	0.45
6:H:126:SER:HB2	6:H:322:PRO:HG3	1.98	0.45
15:Z:-69:DG:H2"	15:Z:-68:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:79:LYS:HD3	12:U:82:LEU:HD21	1.98	0.45
12:U:113:HIS:CE1	12:W:122:LYS:HG3	2.51	0.45
12:W:79:LYS:HD3	12:W:82:LEU:HD21	1.98	0.45
14:Y:-6:DT:H2''	14:Y:-5:DA:C8	2.52	0.45
15:Z:-40:DC:H2'	15:Z:-39:DT:H72	1.99	0.45
1:A:759:TRP:CH2	1:A:763:LEU:HD22	2.51	0.45
1:A:903:HIS:HB2	1:A:2071:MET:HE1	1.97	0.45
13:X:22:LEU:HB3	13:X:25:ASN:ND2	2.31	0.45
1:A:1983:VAL:HG11	5:E:243:LEU:HD23	1.98	0.45
3:C:59:PRO:HA	3:C:67:ASN:HB3	1.99	0.45
6:J:77:GLY:HA3	6:J:359:THR:OG1	2.16	0.45
14:Y:5:DC:H2''	14:Y:6:DC:C5	2.51	0.45
1:A:906:LEU:O	1:A:2070:ARG:NH1	2.50	0.45
2:B:158:ARG:HE	14:Y:-61:DG:P	2.40	0.45
5:E:64:ARG:HB2	5:E:326:ILE:HD12	1.99	0.45
6:J:86:ILE:HG22	6:J:90:MET:HE2	1.99	0.45
6:F:74:LEU:HD11	6:F:328:THR:HG22	1.99	0.45
14:Y:42:DC:H2'	14:Y:43:DT:H71	1.98	0.45
1:A:854:GLU:HA	1:A:2163:ILE:HB	1.98	0.45
2:B:213:THR:HB	2:B:267:THR:HB	1.98	0.45
12:W:70:LEU:HD22	13:X:29:ILE:HD11	1.99	0.45
15:Z:-2:DC:H2''	15:Z:-1:DA:C8	2.52	0.45
3:C:28:CYS:HB3	3:C:58:LEU:HD13	1.98	0.44
5:E:102:TYR:OH	5:E:306:MET:O	2.31	0.44
9:N:190:ASP:OD1	9:N:224:ARG:NH2	2.49	0.44
14:Y:24:DA:H2''	14:Y:25:DG:C8	2.52	0.44
5:E:108:LYS:NZ	5:E:308:ASP:OD2	2.35	0.44
9:N:138:TYR:OH	9:N:158:ASP:OD1	2.34	0.44
12:W:46:VAL:HB	14:Y:9:DG:P	2.58	0.44
15:Z:19:DC:H2''	15:Z:20:DG:H8	1.82	0.44
6:F:326:MET:HE1	6:F:350:LEU:HD21	1.99	0.44
6:J:303:MET:O	6:J:336:ARG:NH1	2.44	0.44
7:M:206:CYS:SG	7:M:267:LEU:HD11	2.57	0.44
6:J:49:GLN:NE2	6:J:359:THR:HB	2.33	0.44
10:Q:20:ARG:NH2	15:Z:-42:DG:OP1	2.50	0.44
2:B:312:THR:HG22	2:B:314:ARG:H	1.82	0.44
3:C:147:ILE:HD13	3:C:318:VAL:HB	2.00	0.44
5:G:378:ARG:HD2	5:G:378:ARG:HA	1.82	0.44
6:H:161:LEU:HB3	6:H:174:LEU:HD21	1.99	0.44
7:M:333:VAL:HG11	7:M:345:TYR:CE2	2.52	0.44
15:Z:56:DC:H2''	15:Z:57:DG:N7	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HD11	8:L:148:THR:CG2	2.47	0.44
2:B:302:ARG:N	6:H:170:THR:OG1	2.43	0.44
5:E:53:VAL:HG22	5:E:83:ILE:HG23	2.00	0.44
5:E:338:ILE:HD11	5:E:346:SER:OG	2.17	0.44
9:N:151:ALA:O	9:N:186:ARG:NH2	2.49	0.44
7:M:15:VAL:HG21	7:M:398:SER:HA	2.00	0.44
11:R:105:GLU:HA	11:R:108:LYS:HG2	2.00	0.44
14:Y:45:DC:H2''	14:Y:46:DA:C8	2.52	0.44
2:B:310:TYR:OH	6:H:169:GLU:O	2.27	0.44
5:G:405:TYR:O	5:G:409:LEU:HG	2.18	0.44
14:Y:69:DC:H2''	14:Y:70:DC:C6	2.53	0.44
5:E:71:PRO:HD2	5:E:74:THR:HG21	1.99	0.44
19:J:501:ADP:H5'1	19:J:501:ADP:H8	1.82	0.44
14:Y:11:DG:H2'	14:Y:12:DT:H71	1.99	0.44
15:Z:-32:DT:H2''	15:Z:-31:DA:C8	2.53	0.44
5:G:42:GLN:HE22	5:G:364:MET:N	2.16	0.43
5:G:244:ASP:HB3	5:G:271:ILE:HD13	2.00	0.43
5:I:411:THR:HG21	6:J:62:MET:HE3	2.00	0.43
11:R:85:LYS:HE3	11:R:85:LYS:HB2	1.72	0.43
12:W:37:LYS:HB2	12:W:38:PRO:HD3	2.00	0.43
8:L:335:ARG:HA	8:L:338:SER:OG	2.17	0.43
5:E:405:TYR:O	5:E:409:LEU:HG	2.18	0.43
6:F:47:VAL:HG11	6:F:369:GLN:HB3	2.00	0.43
6:F:132:LYS:HG3	6:F:239:VAL:HG22	2.01	0.43
5:G:440:ALA:HB1	6:H:348:ILE:HD11	2.00	0.43
6:H:47:VAL:HG11	6:H:369:GLN:HB3	2.00	0.43
11:T:46:LYS:HD3	11:T:46:LYS:HA	1.76	0.43
14:Y:75:DA:C8	14:Y:76:DT:H72	2.53	0.43
1:A:168:MET:HE3	8:L:351:THR:HG21	2.01	0.43
3:C:81:LYS:HA	3:C:85:GLN:HG2	2.00	0.43
3:C:223:ALA:O	3:C:230:ASN:ND2	2.51	0.43
5:G:122:LEU:N	5:G:238:VAL:O	2.35	0.43
5:G:404:ARG:HA	5:G:407:VAL:HG22	2.00	0.43
9:N:164:SER:HB3	9:N:169:LEU:HD23	1.99	0.43
3:C:158:VAL:HG13	3:C:170:ILE:HG12	2.01	0.43
3:C:185:LYS:HE2	3:C:199:THR:HA	2.00	0.43
4:D:17:ARG:HH21	4:D:150:LEU:HD13	1.83	0.43
6:J:314:ARG:HA	6:J:314:ARG:HD3	1.79	0.43
8:L:190:MET:HG2	8:L:209:VAL:HG21	2.00	0.43
8:L:252:ASN:HA	8:L:255:PHE:CE2	2.53	0.43
1:A:691:PRO:O	2:B:183:ASN:ND2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:ASP:HB3	3:C:14:LYS:HB2	2.00	0.43
3:C:382:TYR:HA	3:C:386:GLY:CA	2.48	0.43
5:E:244:ASP:HB3	5:E:271:ILE:HD13	2.01	0.43
5:G:447:LEU:HD11	6:H:344:HIS:NE2	2.33	0.43
5:E:405:TYR:CE2	5:E:409:LEU:HD11	2.53	0.43
12:W:42:ARG:HD3	15:Z:70:DC:P	2.59	0.43
15:Z:-26:DC:H2''	15:Z:-25:DC:C5	2.54	0.43
8:L:356:TRP:O	8:L:373:LYS:NZ	2.47	0.43
14:Y:-56:DG:H2''	14:Y:-55:DC:C5	2.53	0.43
15:Z:4:DG:H2''	15:Z:5:DT:C5	2.54	0.43
4:D:145:GLN:HA	4:D:149:CYS:CB	2.48	0.42
6:F:150:PRO:HG3	6:F:155:GLY:HA3	2.01	0.42
5:G:456:LYS:HE3	6:H:330:ARG:HE	1.84	0.42
13:X:31:LYS:HG3	13:X:51:TYR:CZ	2.54	0.42
15:Z:16:DA:H2''	15:Z:17:DA:N7	2.33	0.42
15:Z:35:DT:H2''	15:Z:36:DA:N7	2.33	0.42
15:Z:-71:DA:H5'	15:Z:-71:DA:C8	2.54	0.42
1:A:151:PHE:HZ	7:M:29:GLY:HA2	1.84	0.42
5:G:210:ALA:HB2	5:G:220:TYR:CD1	2.54	0.42
5:I:119:ALA:HB2	5:I:299:LEU:HB2	2.01	0.42
10:S:63:LEU:HD11	11:T:41:VAL:HG13	2.01	0.42
10:S:102:ILE:HG23	11:T:61:ILE:HD13	2.01	0.42
10:S:115:LEU:HD13	13:X:44:LYS:HB2	2.02	0.42
14:Y:-20:DC:H2''	14:Y:-19:DG:H8	1.84	0.42
5:E:320:GLU:OE1	6:J:84:THR:HG21	2.19	0.42
6:H:349:ASP:OD1	6:H:350:LEU:N	2.52	0.42
6:J:161:LEU:HB2	6:J:174:LEU:HD11	2.00	0.42
12:U:101:VAL:O	12:U:105:GLU:HG3	2.19	0.42
15:Z:-2:DC:H2''	15:Z:-1:DA:H8	1.83	0.42
3:C:2:THR:HG23	3:C:91:THR:HG23	2.01	0.42
5:G:25:GLY:HA3	5:G:36:ALA:HB3	2.01	0.42
6:H:407:THR:HG21	5:I:61:MET:HG3	2.02	0.42
7:M:70:ILE:HD13	7:M:102:ILE:HA	2.02	0.42
10:S:69:ALA:O	10:S:73:ASN:ND2	2.42	0.42
15:Z:-40:DC:H2'	15:Z:-39:DT:C7	2.49	0.42
15:Z:50:DG:H2''	15:Z:51:DG:H8	1.85	0.42
3:C:45:ILE:O	3:C:48:ILE:HG22	2.20	0.42
6:F:113:MET:HE2	6:F:113:MET:HB3	1.96	0.42
5:G:75:GLY:N	19:G:501:ADP:O1A	2.44	0.42
6:J:47:VAL:HG11	6:J:369:GLN:HB3	2.02	0.42
11:R:51:ASP:OD1	11:R:51:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:102:LEU:HB2	11:T:107:ALA:HB2	2.00	0.42
5:E:42:GLN:HE22	5:E:364:MET:H	1.68	0.42
15:Z:36:DA:H2"	15:Z:37:DC:C5	2.54	0.42
1:A:2065:PHE:HB3	1:A:2118:THR:HG23	2.01	0.42
6:F:370:ILE:HG21	6:F:399:LEU:HD21	2.02	0.42
14:Y:38:DT:H2"	14:Y:39:DA:C8	2.55	0.42
1:A:608:THR:O	1:A:623:HIS:HE1	2.03	0.41
1:A:679:MET:HG3	1:A:722:ILE:HG22	2.02	0.41
3:C:103:THR:O	3:C:107:GLU:HG3	2.20	0.41
5:E:131:TYR:HB2	5:E:193:ILE:HB	2.02	0.41
6:J:229:ASP:OD1	6:J:229:ASP:N	2.43	0.41
14:Y:-32:DC:H2"	14:Y:-31:DA:H8	1.84	0.41
14:Y:-5:DA:H2"	14:Y:-4:DC:C5	2.55	0.41
14:Y:10:DC:H2"	14:Y:11:DG:C8	2.55	0.41
15:Z:-14:DA:H2"	15:Z:-13:DA:H8	1.85	0.41
3:C:59:PRO:HB3	3:C:70:VAL:HG13	2.02	0.41
3:C:338:ARG:NH2	3:C:342:PRO:O	2.52	0.41
1:A:698:TYR:OH	1:A:709:ARG:NH1	2.54	0.41
3:C:6:LEU:HD13	3:C:15:ILE:HB	2.02	0.41
5:E:409:LEU:HD22	5:E:433:ILE:HG22	2.02	0.41
5:I:42:GLN:NE2	5:I:364:MET:O	2.53	0.41
14:Y:-20:DC:H2"	14:Y:-19:DG:C8	2.55	0.41
1:A:786:TRP:CH2	1:A:800:HIS:HB3	2.55	0.41
3:C:97:GLU:O	3:C:126:ASN:ND2	2.49	0.41
5:E:313:THR:HG21	6:J:303:MET:HG3	2.02	0.41
6:F:126:SER:HB2	6:F:322:PRO:HG3	2.03	0.41
10:S:20:ARG:NH1	11:T:125:LYS:HD2	2.35	0.41
5:E:274:LYS:NZ	6:J:246:GLU:OE2	2.43	0.41
6:J:382:MET:HG2	6:J:421:VAL:HB	2.03	0.41
8:L:58:ALA:HA	8:L:65:LEU:HD12	2.03	0.41
7:M:215:ILE:HG21	7:M:289:PHE:CZ	2.56	0.41
14:Y:-14:DA:H2"	14:Y:-13:DA:H8	1.84	0.41
6:F:84:THR:HG21	5:G:320:GLU:OE1	2.21	0.41
6:F:246:GLU:HA	6:F:260:LEU:HD21	2.03	0.41
6:H:21:ARG:NH2	5:I:324:ALA:O	2.54	0.41
5:I:157:VAL:HB	5:I:172:LEU:HB2	2.02	0.41
15:Z:31:DT:H2"	15:Z:32:DG:C8	2.54	0.41
1:A:737:ARG:CZ	14:Y:-60:DG:H21	2.34	0.41
1:A:2069:THR:HA	1:A:2072:LEU:HD12	2.02	0.41
5:I:405:TYR:O	5:I:409:LEU:HG	2.19	0.41
6:J:82:GLY:O	6:J:86:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:66:PRO:HG2	7:K:68:TYR:CZ	2.56	0.41
10:Q:99:ARG:HD3	10:Q:99:ARG:H	1.86	0.41
10:S:54:VAL:HG21	11:T:98:VAL:HG21	2.02	0.41
11:T:106:LEU:HD23	11:T:106:LEU:HA	1.94	0.41
14:Y:-44:DA:C2'	14:Y:-43:DT:H71	2.51	0.41
15:Z:-14:DA:H2''	15:Z:-13:DA:C8	2.56	0.41
15:Z:-11:DC:H2''	15:Z:-10:DG:H8	1.86	0.41
3:C:146:ILE:HG23	3:C:317:ILE:HA	2.02	0.41
14:Y:-53:DG:H2''	14:Y:-52:DG:C8	2.56	0.41
1:A:724:SER:O	1:A:728:VAL:HG23	2.21	0.40
1:A:2011:ALA:HB1	1:A:2015:TRP:CD1	2.55	0.40
1:A:2139:ASP:OD1	1:A:2140:TRP:N	2.54	0.40
5:G:138:LEU:HD12	5:G:138:LEU:HA	1.90	0.40
10:Q:115:LEU:HD11	12:U:108:ASN:HD21	1.86	0.40
15:Z:-63:DC:H2''	15:Z:-62:DA:C8	2.57	0.40
15:Z:52:DC:H2''	15:Z:53:DC:O5'	2.21	0.40
2:B:157:ARG:NH2	15:Z:66:DT:OP1	2.51	0.40
5:E:389:GLU:HG2	5:E:427:LYS:HD3	2.03	0.40
5:E:447:LEU:HD11	6:F:344:HIS:CE1	2.56	0.40
6:F:397:THR:OG1	6:F:398:SER:N	2.54	0.40
7:M:146:ILE:HD11	7:M:149:PHE:HB2	2.02	0.40
15:Z:-47:DC:H2''	15:Z:-46:DT:C6	2.56	0.40
7:K:96:TRP:CE2	7:K:135:LYS:HD3	2.56	0.40
10:Q:107:VAL:HG11	12:U:101:VAL:HG11	2.04	0.40
12:U:42:ARG:HD3	14:Y:70:DC:P	2.61	0.40
1:A:908:ASP:OD1	1:A:908:ASP:N	2.54	0.40
2:B:214:TYR:HA	2:B:266:ILE:HD13	2.03	0.40
5:G:456:LYS:HB3	6:H:333:THR:HG21	2.02	0.40
6:H:405:LEU:HD22	6:H:429:VAL:HG23	2.03	0.40
7:M:124:GLU:CD	7:M:133:ARG:HE	2.28	0.40
10:S:107:VAL:HG11	12:W:101:VAL:HG11	2.03	0.40
15:Z:-56:DG:H2''	15:Z:-55:DA:C8	2.57	0.40
1:A:2137:ASP:OD1	1:A:2137:ASP:N	2.55	0.40
3:C:189:SER:HA	3:C:193:LEU:O	2.21	0.40
5:E:133:GLY:HA2	5:E:224:PRO:HG2	2.03	0.40
5:E:256:ILE:O	5:E:260:MET:HG2	2.20	0.40
5:E:452:ASP:OD1	5:E:452:ASP:N	2.53	0.40
5:G:456:LYS:HE3	6:H:330:ARG:NE	2.37	0.40
6:H:21:ARG:HB2	5:I:62:ALA:HB2	2.04	0.40
6:H:403:ILE:HA	6:H:406:ILE:HD12	2.03	0.40
14:Y:-29:DC:C6	14:Y:-28:DT:H72	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Z:-27:DC:H2"	15:Z:-26:DC:C5	2.57	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	847/3230 (26%)	833 (98%)	14 (2%)	0	100	100
2	B	162/364 (44%)	156 (96%)	6 (4%)	0	100	100
3	C	394/396 (100%)	379 (96%)	15 (4%)	0	100	100
4	D	101/154 (66%)	98 (97%)	3 (3%)	0	100	100
5	E	429/456 (94%)	425 (99%)	4 (1%)	0	100	100
5	G	443/456 (97%)	441 (100%)	2 (0%)	0	100	100
5	I	432/456 (95%)	424 (98%)	8 (2%)	0	100	100
6	F	436/463 (94%)	429 (98%)	7 (2%)	0	100	100
6	H	428/463 (92%)	417 (97%)	11 (3%)	0	100	100
6	J	412/463 (89%)	404 (98%)	8 (2%)	0	100	100
7	K	399/429 (93%)	395 (99%)	4 (1%)	0	100	100
7	M	392/429 (91%)	388 (99%)	4 (1%)	0	100	100
8	L	357/375 (95%)	352 (99%)	5 (1%)	0	100	100
9	N	155/467 (33%)	152 (98%)	3 (2%)	0	100	100
10	Q	108/128 (84%)	106 (98%)	2 (2%)	0	100	100
10	S	108/128 (84%)	108 (100%)	0	0	100	100
11	R	96/125 (77%)	95 (99%)	1 (1%)	0	100	100
11	T	96/125 (77%)	93 (97%)	3 (3%)	0	100	100
12	U	96/135 (71%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	W	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
13	V	79/102 (78%)	78 (99%)	1 (1%)	0	100	100
13	X	79/102 (78%)	79 (100%)	0	0	100	100
All	All	6145/9581 (64%)	6040 (98%)	105 (2%)	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	776/2721 (28%)	776 (100%)	0	100	100
2	B	150/312 (48%)	150 (100%)	0	100	100
3	C	361/361 (100%)	361 (100%)	0	100	100
4	D	89/133 (67%)	89 (100%)	0	100	100
5	E	367/387 (95%)	367 (100%)	0	100	100
5	G	376/387 (97%)	376 (100%)	0	100	100
5	I	370/387 (96%)	370 (100%)	0	100	100
6	F	368/390 (94%)	368 (100%)	0	100	100
6	H	365/390 (94%)	365 (100%)	0	100	100
6	J	354/390 (91%)	354 (100%)	0	100	100
7	K	345/364 (95%)	345 (100%)	0	100	100
7	M	341/364 (94%)	341 (100%)	0	100	100
8	L	307/318 (96%)	307 (100%)	0	100	100
9	N	139/400 (35%)	139 (100%)	0	100	100
10	Q	87/101 (86%)	87 (100%)	0	100	100
10	S	87/101 (86%)	87 (100%)	0	100	100
11	R	84/105 (80%)	84 (100%)	0	100	100
11	T	84/105 (80%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	U	86/110 (78%)	86 (100%)	0	100	100
12	W	86/110 (78%)	86 (100%)	0	100	100
13	V	67/78 (86%)	67 (100%)	0	100	100
13	X	67/78 (86%)	67 (100%)	0	100	100
All	All	5356/8092 (66%)	5356 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	232	HIS
1	A	239	GLN
1	A	623	HIS
1	A	659	HIS
1	A	730	GLN
1	A	779	GLN
1	A	2077	GLN
2	B	202	HIS
2	B	296	HIS
5	E	34	GLN
5	E	85	GLN
5	E	373	GLN
6	F	25	HIS
6	F	275	GLN
6	F	447	GLN
5	G	42	GLN
5	G	289	GLN
5	G	380	GLN
5	G	450	GLN
6	H	146	GLN
6	H	245	HIS
6	H	453	ASN
5	I	34	GLN
5	I	115	ASN
5	I	169	GLN
5	I	408	GLN
6	J	78	GLN
6	J	245	HIS

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Mol	Chain	Res	Type
7	K	143	HIS
7	K	365	ASN
7	K	383	ASN
8	L	12	ASN
8	L	263	GLN
7	M	105	HIS
7	M	408	GLN
10	Q	24	GLN
10	Q	31	HIS
10	Q	110	ASN
11	R	84	ASN
11	R	95	GLN
10	S	31	HIS
12	U	85	GLN
12	U	108	ASN
13	V	75	HIS
13	V	93	GLN
13	X	75	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\# Z > 2$
16	AGS	K	501	17	32,33,33	0.48	1 (3%)	45,52,52	0.80	1 (2%)
19	ADP	I	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
19	ADP	J	501	17	28,29,29	1.42	4 (14%)	43,45,45	1.81	8 (18%)
16	AGS	C	401	17	32,33,33	0.49	1 (3%)	45,52,52	0.68	1 (2%)
19	ADP	G	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	8 (18%)
19	ADP	F	501	17	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
19	ADP	H	501	17	28,29,29	1.42	5 (17%)	43,45,45	1.85	9 (20%)
19	ADP	E	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.81	8 (18%)

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
16	AGS	K	501	17	-	0/21/38/38	0/3/3/3
19	ADP	I	501	-	-	3/16/32/32	0/3/3/3
19	ADP	J	501	17	-	5/16/32/32	0/3/3/3
16	AGS	C	401	17	-	4/21/38/38	0/3/3/3
19	ADP	G	501	-	-	5/16/32/32	0/3/3/3
19	ADP	F	501	17	-	3/16/32/32	0/3/3/3
19	ADP	H	501	17	-	4/16/32/32	0/3/3/3
19	ADP	E	501	-	-	3/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	E	501	ADP	C5-C4	4.75	1.47	1.39
19	J	501	ADP	C5-C4	4.73	1.47	1.39
19	F	501	ADP	C5-C4	4.69	1.47	1.39
19	I	501	ADP	C5-C4	4.69	1.47	1.39
19	G	501	ADP	C5-C4	4.68	1.47	1.39
19	H	501	ADP	C5-C4	4.65	1.47	1.39
19	J	501	ADP	C5-C6	2.72	1.48	1.41
19	E	501	ADP	C5-C6	2.72	1.48	1.41
19	I	501	ADP	C5-C6	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	501	ADP	C5-C6	2.71	1.48	1.41
19	G	501	ADP	C5-C6	2.71	1.48	1.41
19	F	501	ADP	C5-C6	2.71	1.48	1.41
19	G	501	ADP	C8-N7	2.36	1.36	1.31
19	J	501	ADP	C8-N7	2.35	1.36	1.31
19	H	501	ADP	C8-N7	2.35	1.36	1.31
19	F	501	ADP	C8-N7	2.34	1.36	1.31
19	I	501	ADP	C8-N7	2.32	1.36	1.31
19	E	501	ADP	C8-N7	2.31	1.36	1.31
19	H	501	ADP	C5-N7	-2.30	1.34	1.39
19	F	501	ADP	C5-N7	-2.28	1.34	1.39
19	I	501	ADP	C5-N7	-2.27	1.34	1.39
19	J	501	ADP	C5-N7	-2.27	1.34	1.39
19	E	501	ADP	C5-N7	-2.27	1.34	1.39
19	G	501	ADP	C5-N7	-2.26	1.35	1.39
16	C	401	AGS	PG-S1G	2.14	1.95	1.90
16	K	501	AGS	PG-S1G	2.11	1.95	1.90
19	H	501	ADP	PA-O3A	2.03	1.61	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	501	ADP	C5-C4-N3	-5.86	118.65	126.72
19	E	501	ADP	C5-C4-N3	-5.86	118.65	126.72
19	H	501	ADP	C5-C4-N3	-5.85	118.66	126.72
19	I	501	ADP	C5-C4-N3	-5.82	118.70	126.72
19	G	501	ADP	C5-C4-N3	-5.82	118.71	126.72
19	F	501	ADP	C5-C4-N3	-5.80	118.73	126.72
19	E	501	ADP	N3-C4-N9	4.66	135.10	127.17
19	I	501	ADP	N3-C4-N9	4.63	135.04	127.17
19	J	501	ADP	N3-C4-N9	4.62	135.02	127.17
19	G	501	ADP	N3-C4-N9	4.61	135.01	127.17
19	H	501	ADP	N3-C4-N9	4.61	135.00	127.17
19	F	501	ADP	N3-C4-N9	4.60	134.98	127.17
19	H	501	ADP	C2-N3-C4	3.71	120.88	111.83
19	G	501	ADP	C2-N3-C4	3.68	120.83	111.83
19	E	501	ADP	C2-N3-C4	3.68	120.82	111.83
19	I	501	ADP	C2-N3-C4	3.67	120.80	111.83
19	J	501	ADP	C2-N3-C4	3.65	120.75	111.83
19	F	501	ADP	C2-N3-C4	3.65	120.74	111.83
16	K	501	AGS	PB-O3B-PG	-3.58	120.06	133.17
19	H	501	ADP	C4-C5-N7	-3.51	106.57	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	401	AGS	PB-O3B-PG	-3.49	120.39	133.17
19	F	501	ADP	C4-C5-N7	-3.46	106.62	110.58
19	J	501	ADP	C4-C5-N7	-3.46	106.63	110.58
19	G	501	ADP	C4-C5-N7	-3.45	106.64	110.58
19	I	501	ADP	C4-C5-N7	-3.44	106.64	110.58
19	E	501	ADP	C4-C5-N7	-3.43	106.66	110.58
19	H	501	ADP	N3-C2-N1	-3.24	123.68	128.58
19	G	501	ADP	N3-C2-N1	-3.21	123.72	128.58
19	I	501	ADP	N3-C2-N1	-3.18	123.76	128.58
19	E	501	ADP	N3-C2-N1	-3.17	123.79	128.58
19	F	501	ADP	N3-C2-N1	-3.15	123.82	128.58
19	J	501	ADP	N3-C2-N1	-3.10	123.88	128.58
19	I	501	ADP	C4-N9-C8	2.68	108.55	105.74
19	G	501	ADP	C4-N9-C8	2.66	108.53	105.74
19	F	501	ADP	C4-N9-C8	2.65	108.52	105.74
19	H	501	ADP	C4-N9-C8	2.63	108.50	105.74
19	E	501	ADP	C4-N9-C8	2.61	108.48	105.74
19	H	501	ADP	C5-N7-C8	2.59	107.52	103.45
19	F	501	ADP	C5-N7-C8	2.55	107.46	103.45
19	J	501	ADP	C4-N9-C8	2.55	108.41	105.74
19	G	501	ADP	C5-N7-C8	2.54	107.44	103.45
19	I	501	ADP	C5-N7-C8	2.53	107.43	103.45
19	J	501	ADP	C5-N7-C8	2.52	107.41	103.45
19	E	501	ADP	C5-N7-C8	2.49	107.36	103.45
19	H	501	ADP	C6-C5-N7	2.07	136.09	132.09
19	G	501	ADP	C6-C5-N7	2.05	136.05	132.09
19	I	501	ADP	C6-C5-N7	2.04	136.03	132.09
19	I	501	ADP	C3'-C2'-C1'	2.04	105.32	101.46
19	F	501	ADP	C6-C5-N7	2.03	136.01	132.09
19	E	501	ADP	C6-C5-N7	2.02	135.98	132.09
19	H	501	ADP	N9-C8-N7	-2.02	111.08	113.94
19	J	501	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	C	401	AGS	C5'-O5'-PA-O1A
19	E	501	ADP	PA-O3A-PB-O2B
19	F	501	ADP	C5'-O5'-PA-O2A
19	F	501	ADP	C5'-O5'-PA-O3A
19	G	501	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
19	G	501	ADP	C5'-O5'-PA-O2A
19	G	501	ADP	C5'-O5'-PA-O3A
19	H	501	ADP	PA-O3A-PB-O3B
19	I	501	ADP	C5'-O5'-PA-O1A
19	I	501	ADP	C5'-O5'-PA-O2A
19	I	501	ADP	C5'-O5'-PA-O3A
19	J	501	ADP	C5'-O5'-PA-O1A
19	J	501	ADP	C5'-O5'-PA-O2A
19	J	501	ADP	C5'-O5'-PA-O3A
19	G	501	ADP	O4'-C4'-C5'-O5'
19	J	501	ADP	O4'-C4'-C5'-O5'
19	G	501	ADP	C3'-C4'-C5'-O5'
19	J	501	ADP	C3'-C4'-C5'-O5'
16	C	401	AGS	C5'-O5'-PA-O2A
16	C	401	AGS	C5'-O5'-PA-O3A
19	F	501	ADP	C5'-O5'-PA-O1A
16	C	401	AGS	PG-O3B-PB-O2B
19	E	501	ADP	C3'-C4'-C5'-O5'
19	H	501	ADP	PA-O3A-PB-O1B
19	H	501	ADP	PA-O3A-PB-O2B
19	E	501	ADP	O4'-C4'-C5'-O5'
19	H	501	ADP	C4'-C5'-O5'-PA

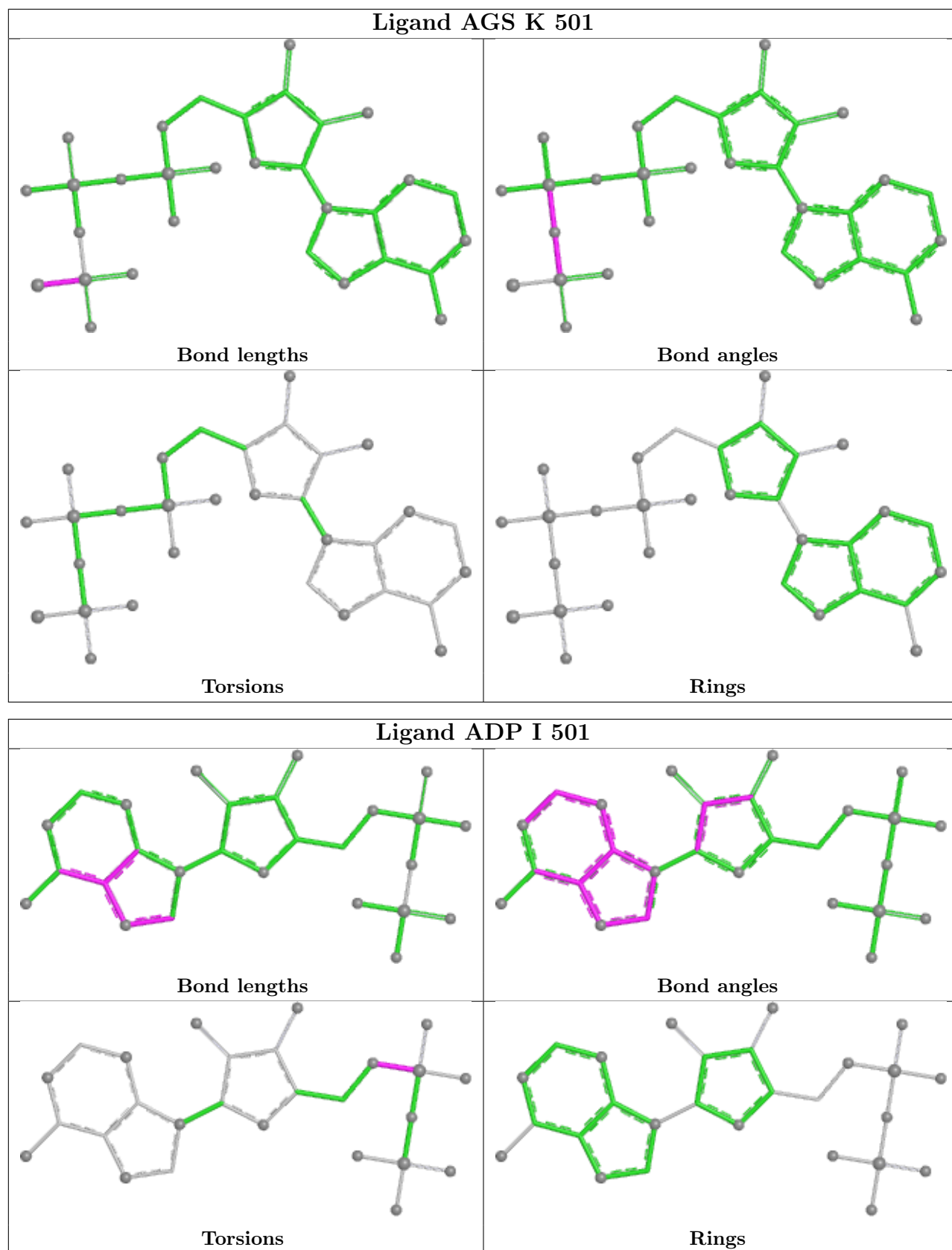
There are no ring outliers.

3 monomers are involved in 5 short contacts:

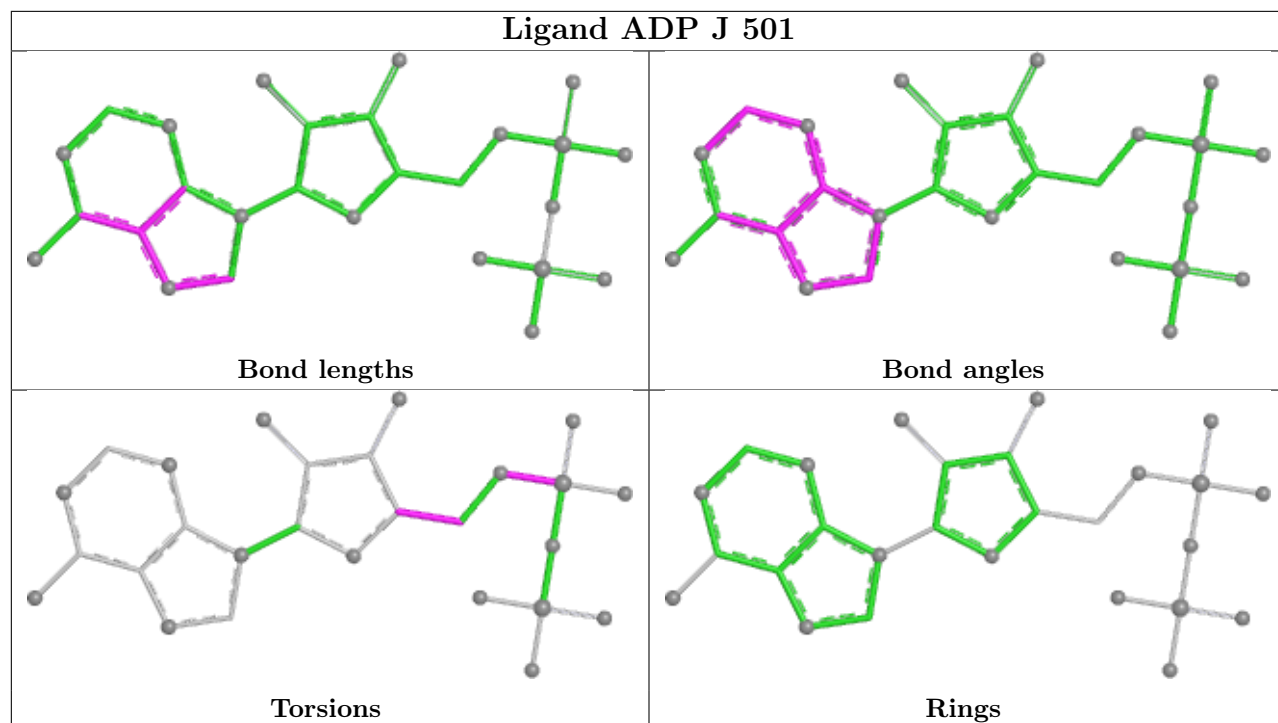
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	J	501	ADP	1	0
19	G	501	ADP	2	0
19	H	501	ADP	2	0

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

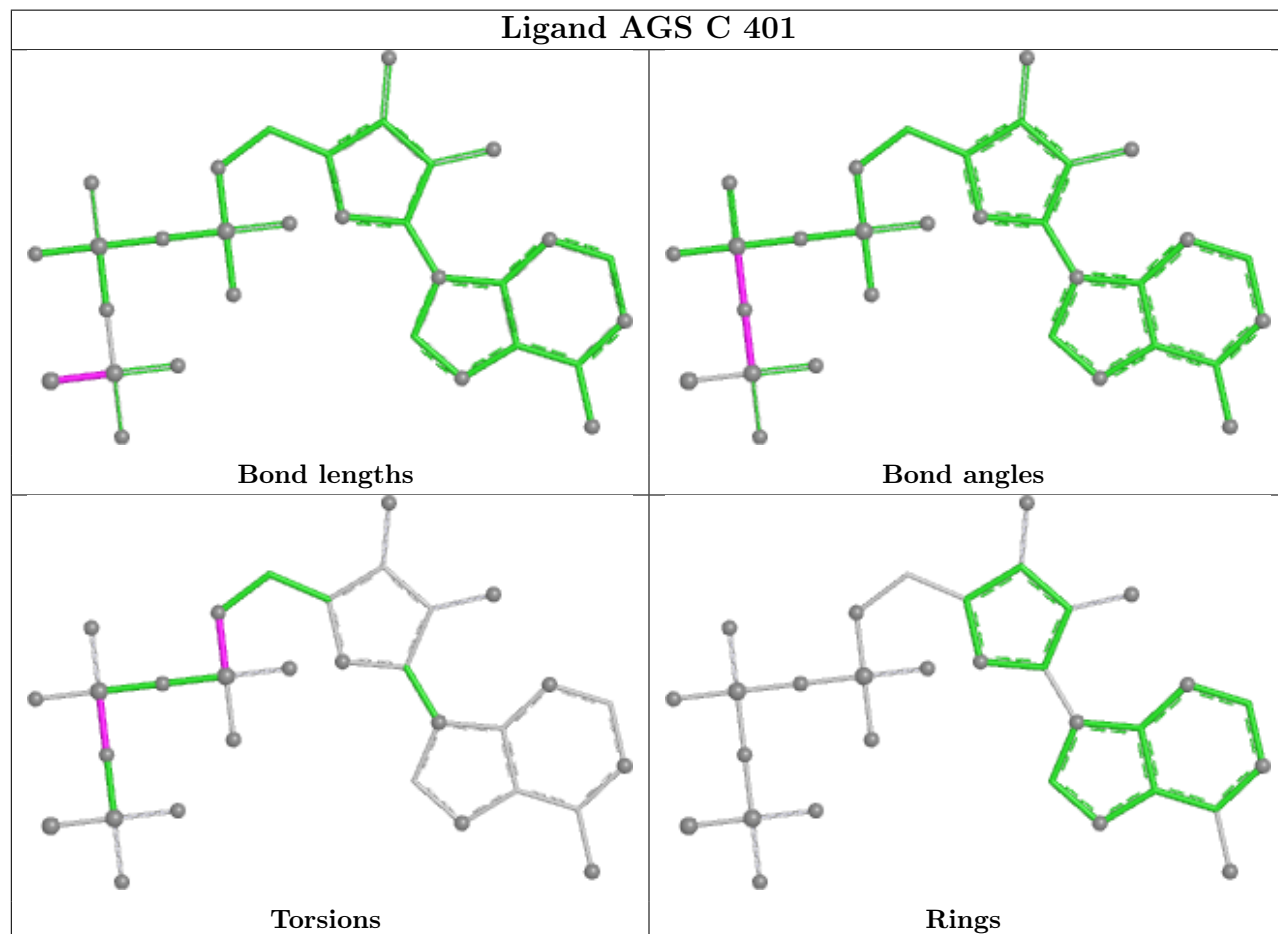
equivalents in the CSD to analyse the geometry.

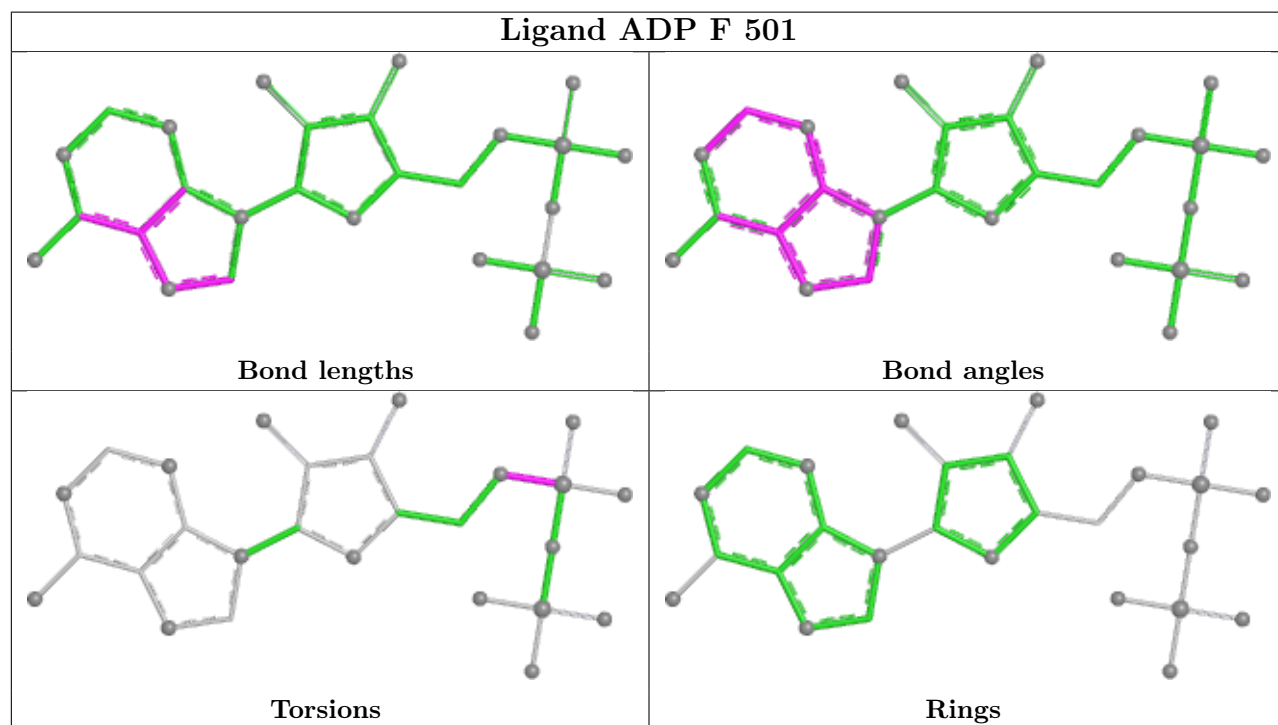
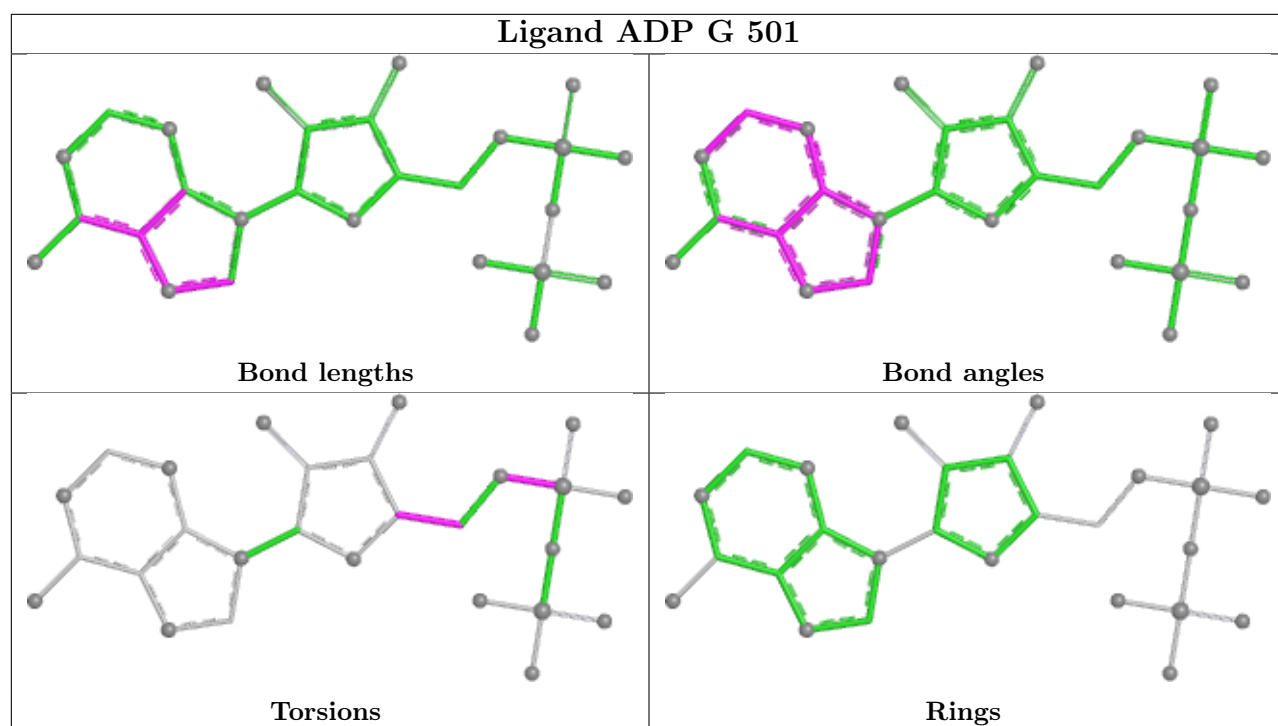


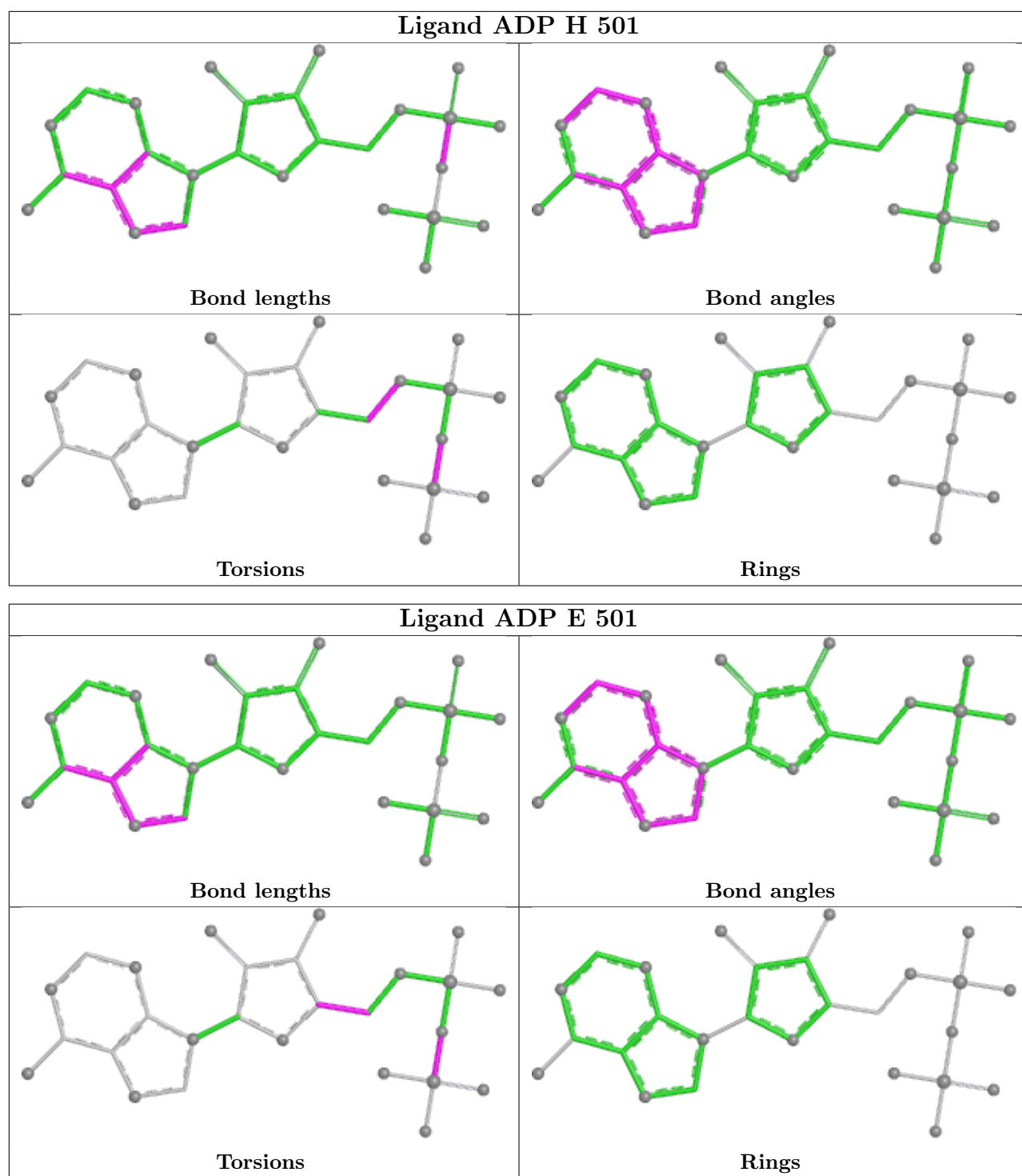
Ligand ADP J 501



Ligand AGS C 401







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

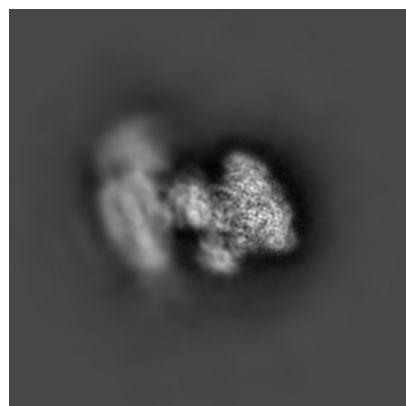
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72455. These allow visual inspection of the internal detail of the map and identification of artifacts.

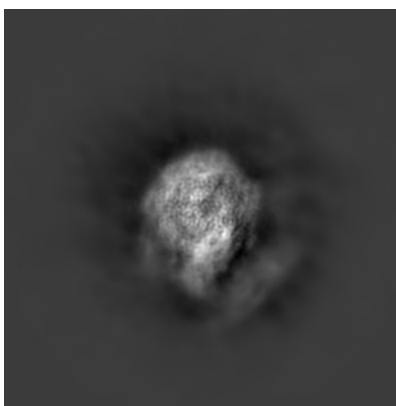
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

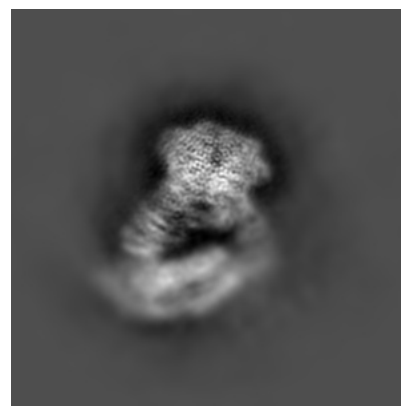
6.1.1 Primary map



X

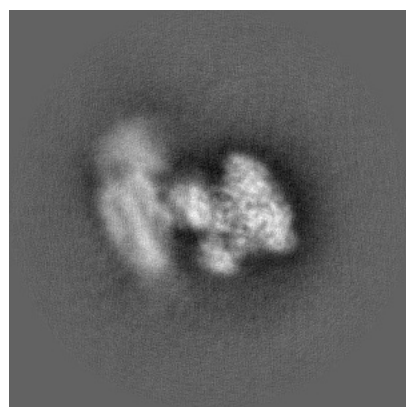


Y

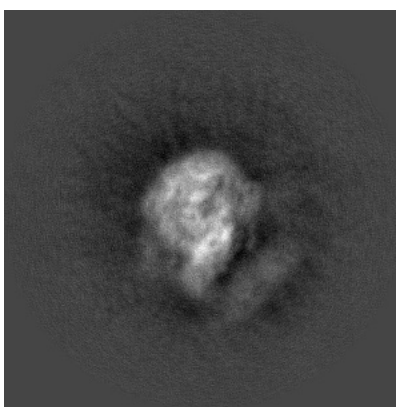


Z

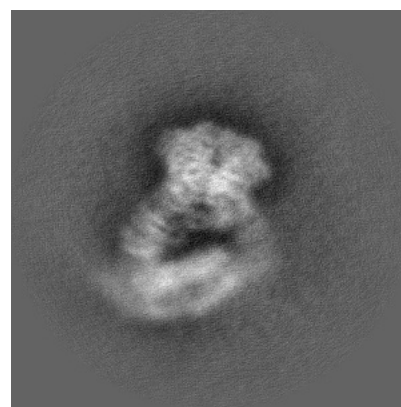
6.1.2 Raw map



X



Y

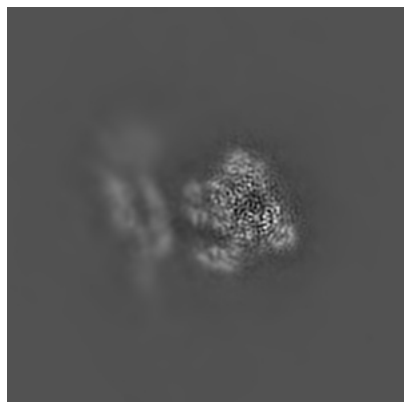


Z

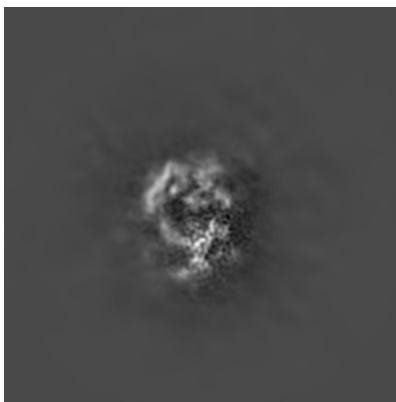
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

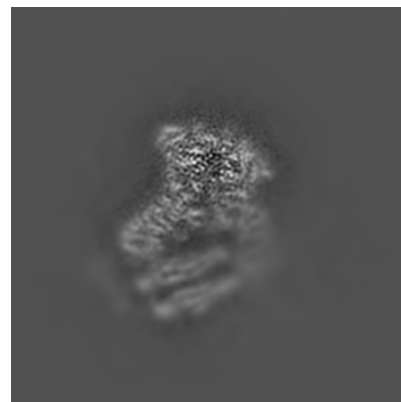
6.2.1 Primary map



X Index: 192

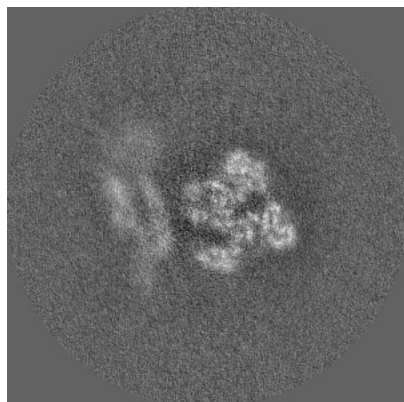


Y Index: 192

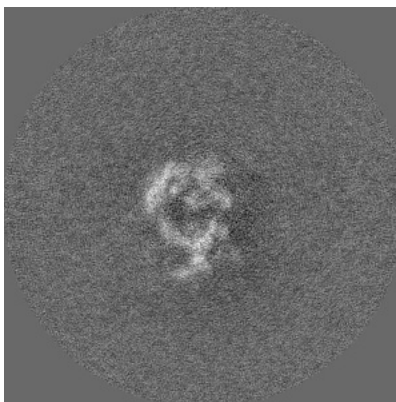


Z Index: 192

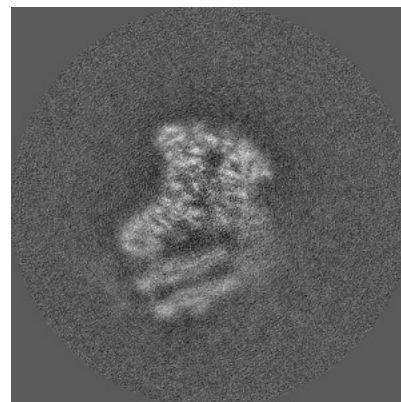
6.2.2 Raw map



X Index: 192



Y Index: 192

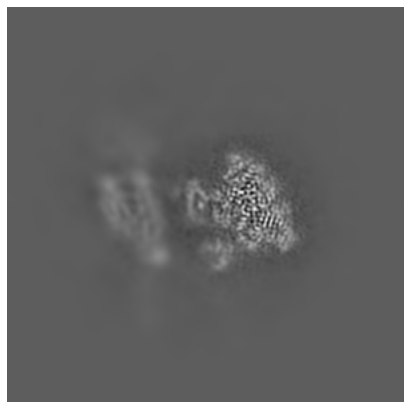


Z Index: 192

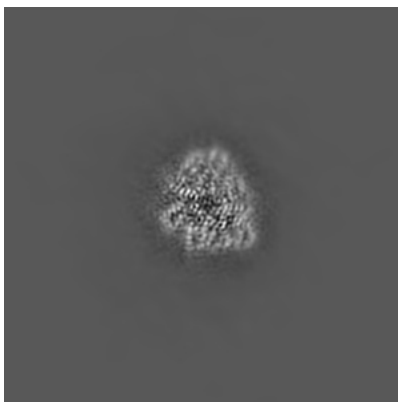
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

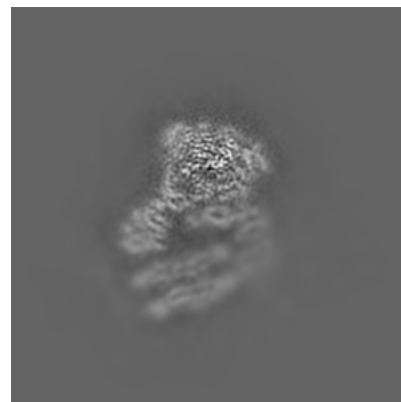
6.3.1 Primary map



X Index: 178

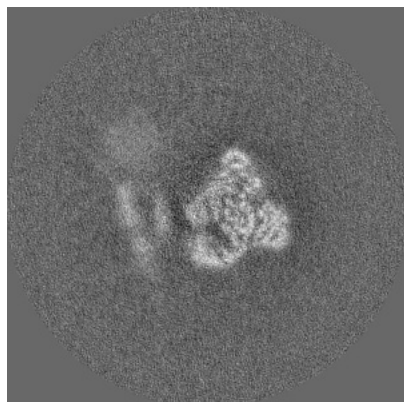


Y Index: 233

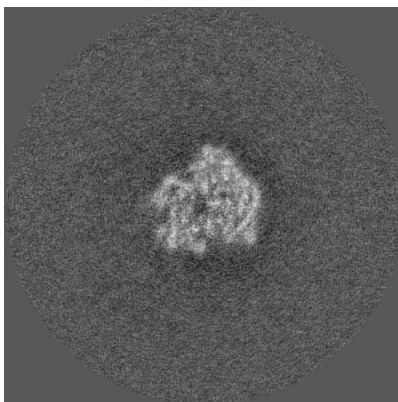


Z Index: 184

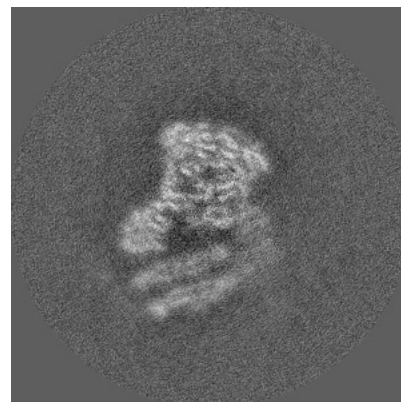
6.3.2 Raw map



X Index: 204



Y Index: 223

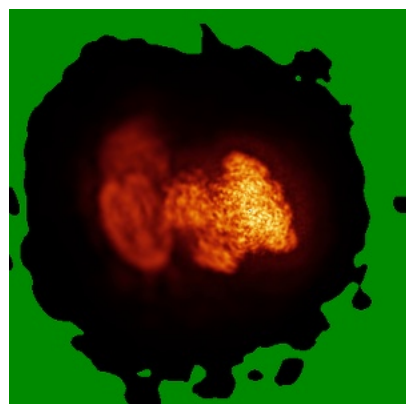


Z Index: 185

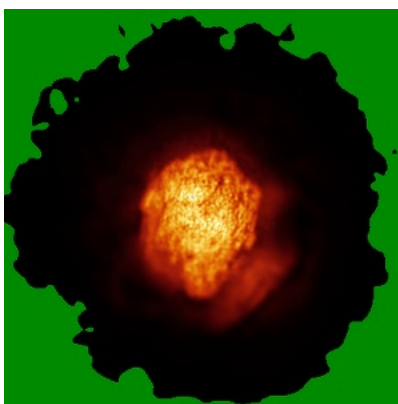
The images above show the largest variance slices of the map in three orthogonal directions.

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

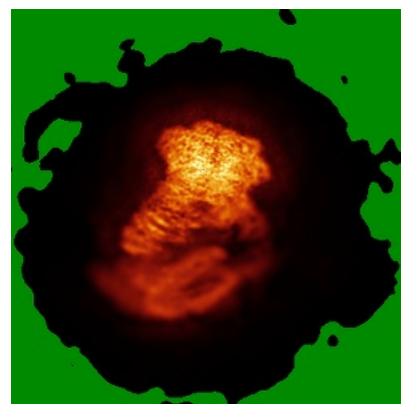
6.4.1 Primary map



X

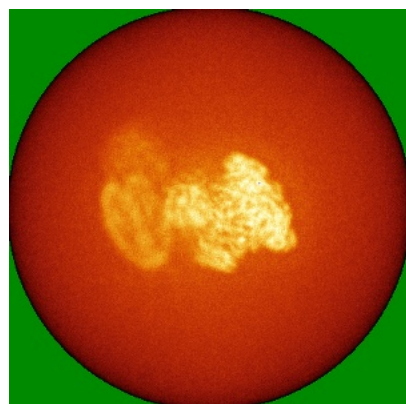


Y

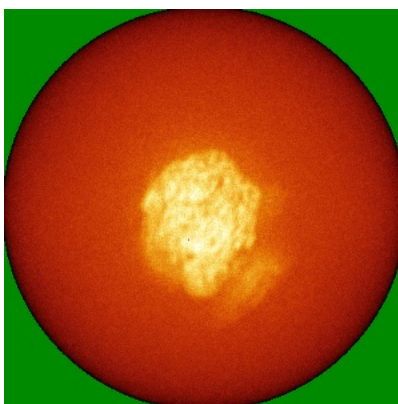


Z

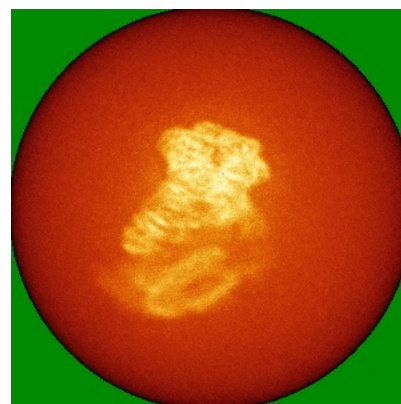
6.4.2 Raw map



X



Y

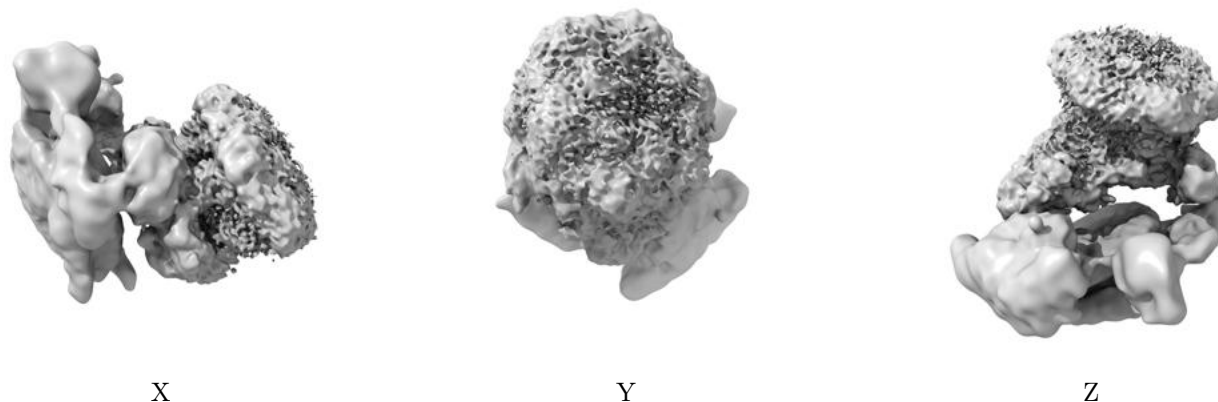


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

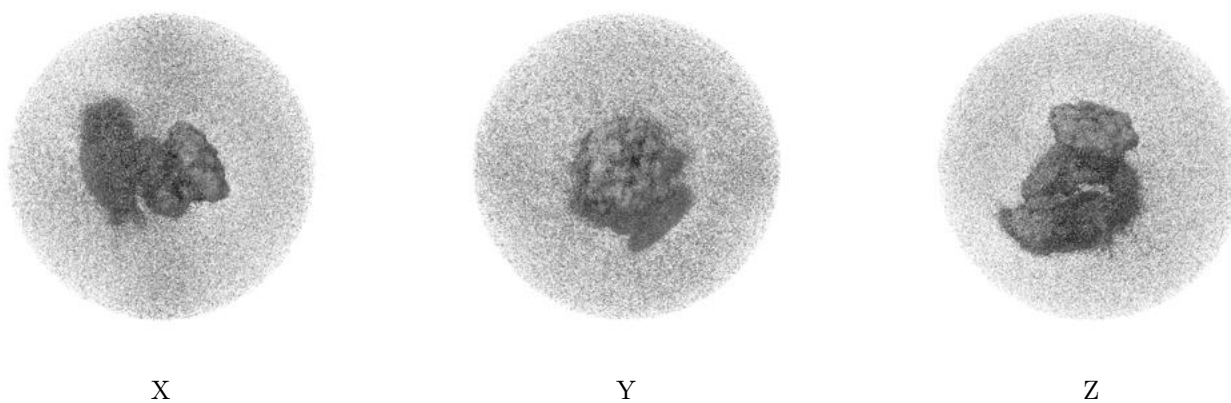
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

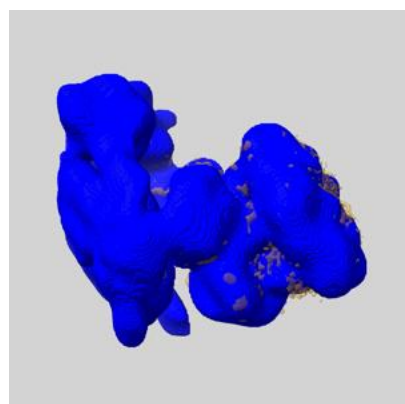
6.6 Mask visualisation [i](#)

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

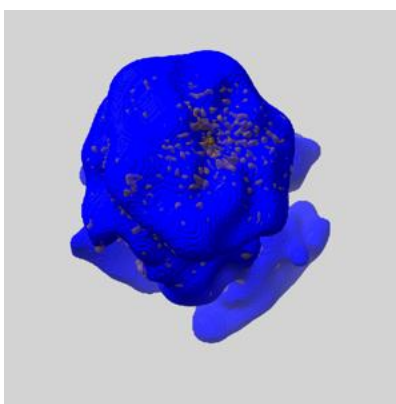
A mask typically either:

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

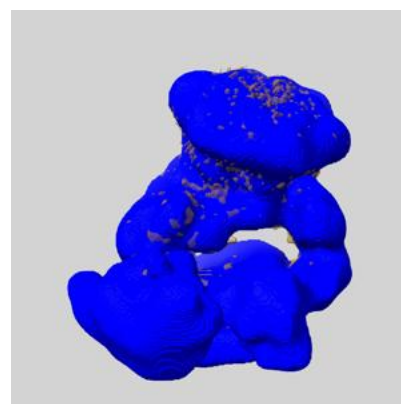
6.6.1 emd_72455_msk_1.map [i](#)



X



Y

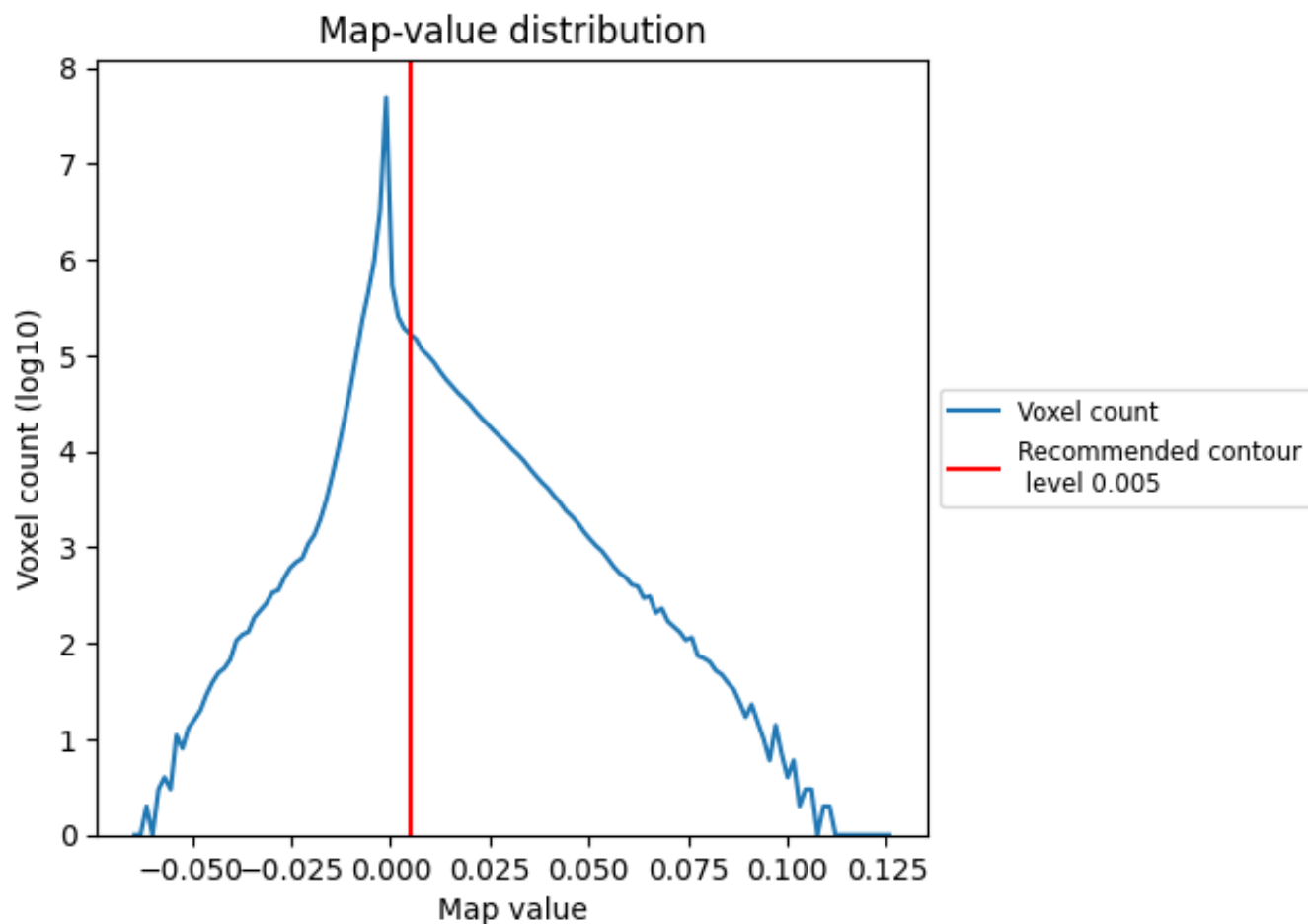


Z

7 Map analysis [i](#)

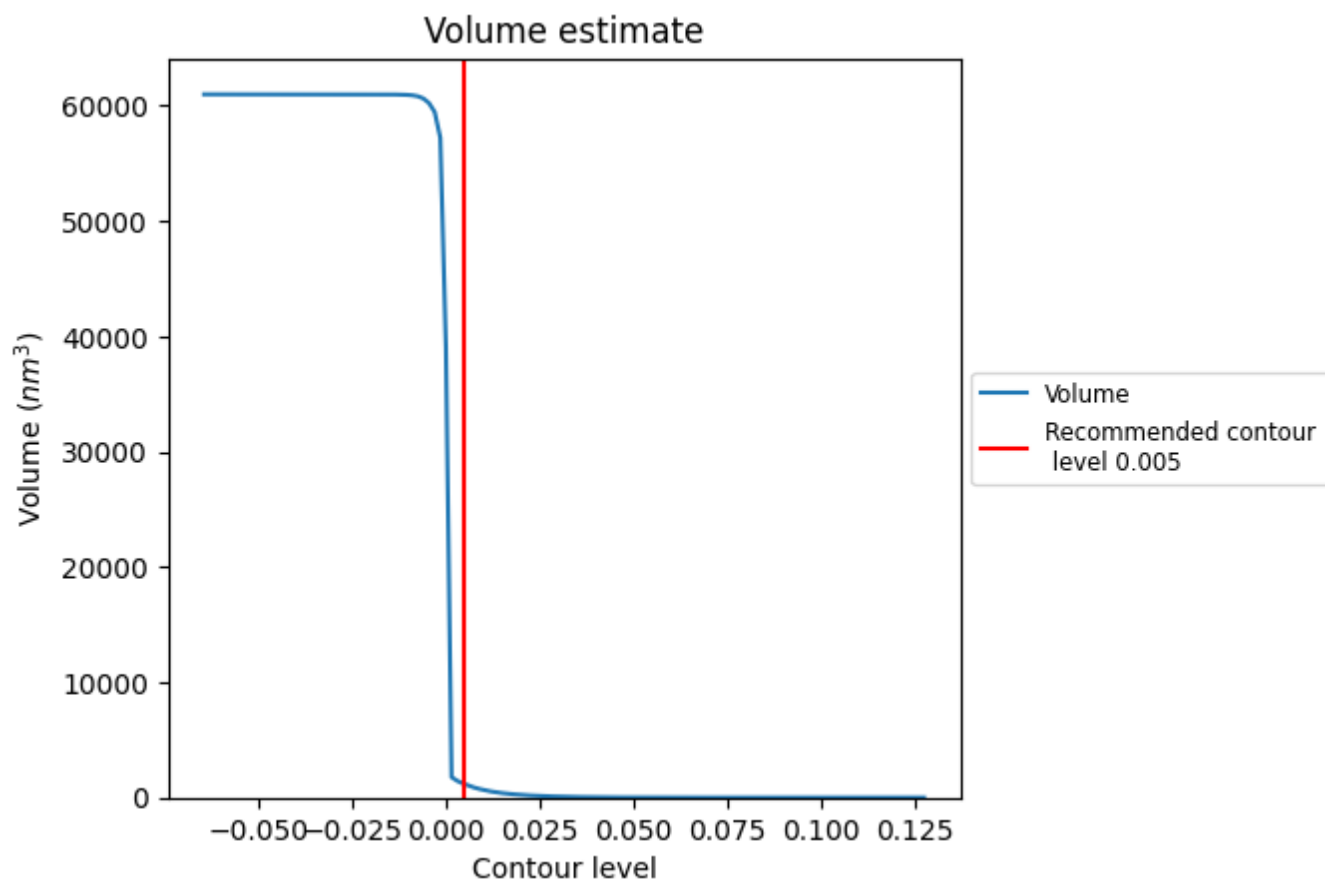
This section contains the results of statistical analysis of the map.

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.

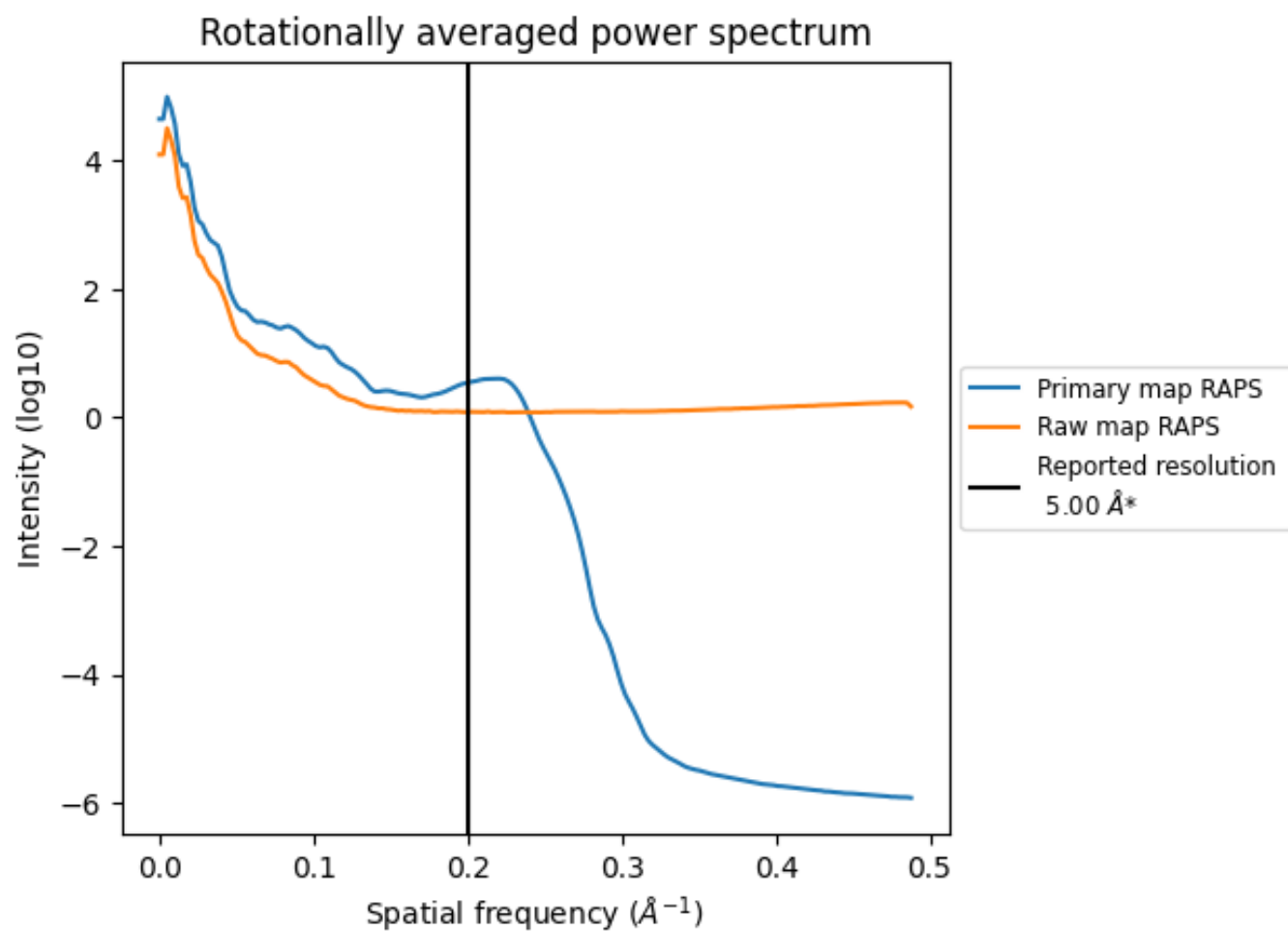
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1165 nm^3 ; this corresponds to an approximate mass of 1052 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 ⓘ

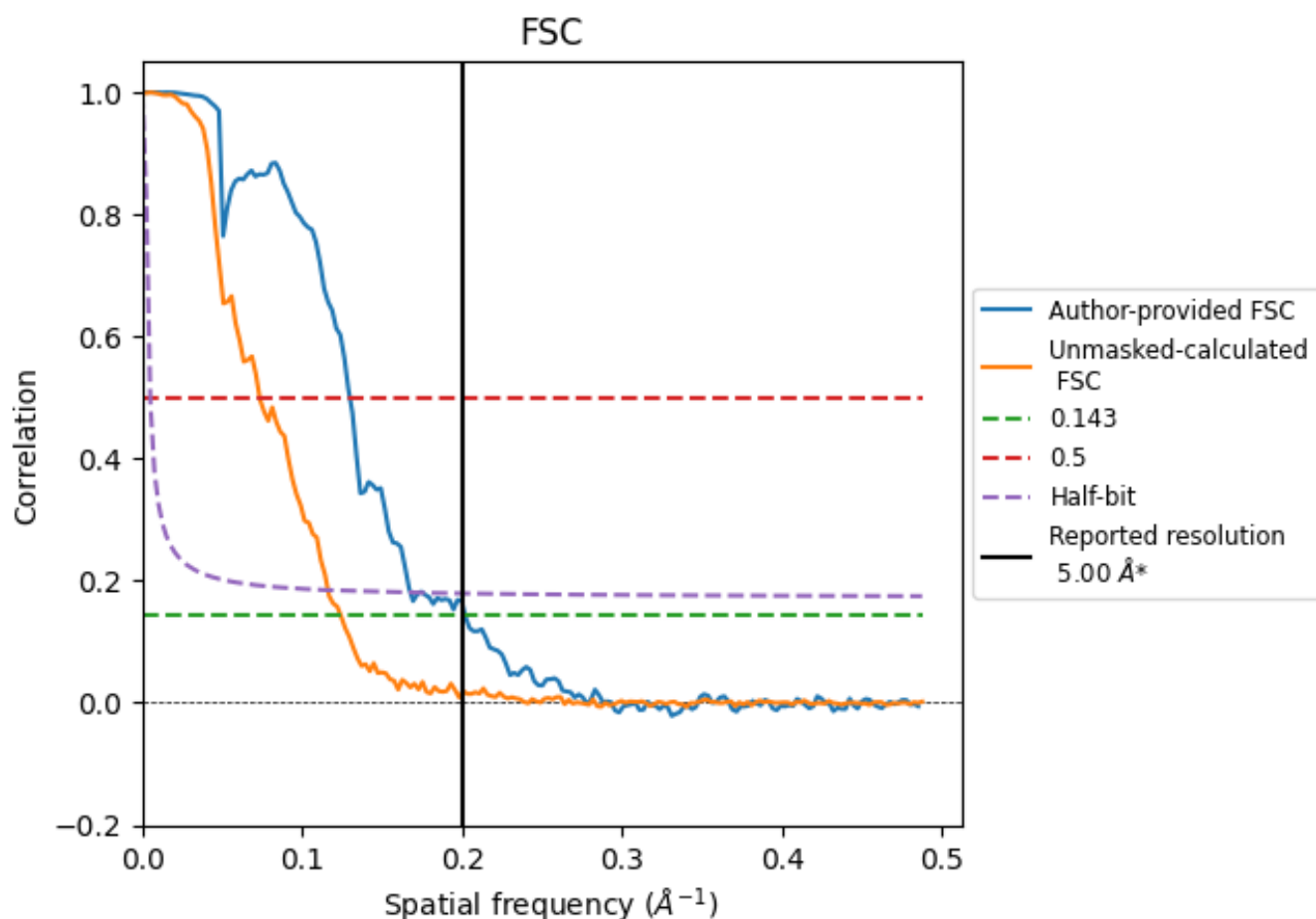


*Reported resolution corresponds to spatial frequency of 0.200 $\text{\AA}^{-1}$

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 0.200 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

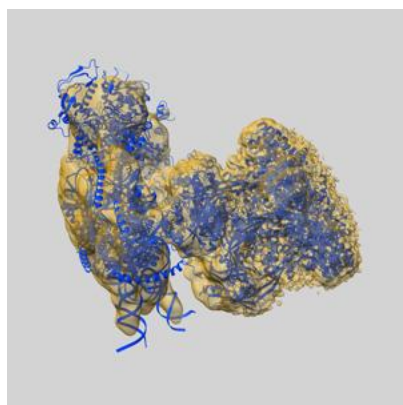
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.95	7.70	5.96
Unmasked-calculated*	8.06	13.61	8.61

*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 8.06 differs from the reported value 5.0 by more than 10 %

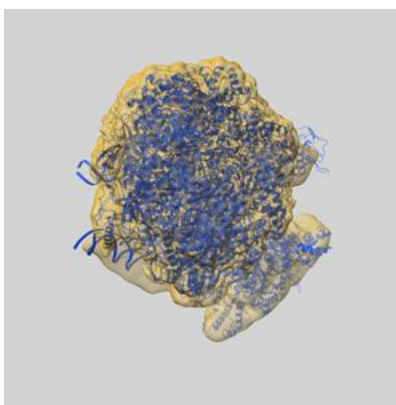
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72455 and PDB model 9Y3E. Per-residue inclusion information can be found in section [3](#) on page [10](#).

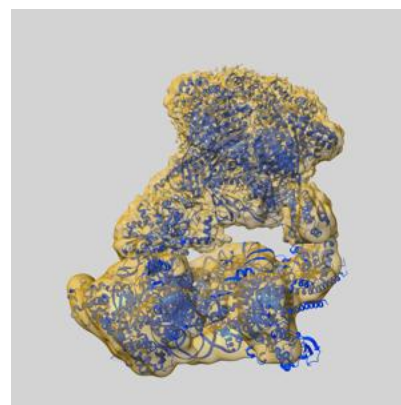
9.1 Map-model overlay [i](#)



X



Y



Z

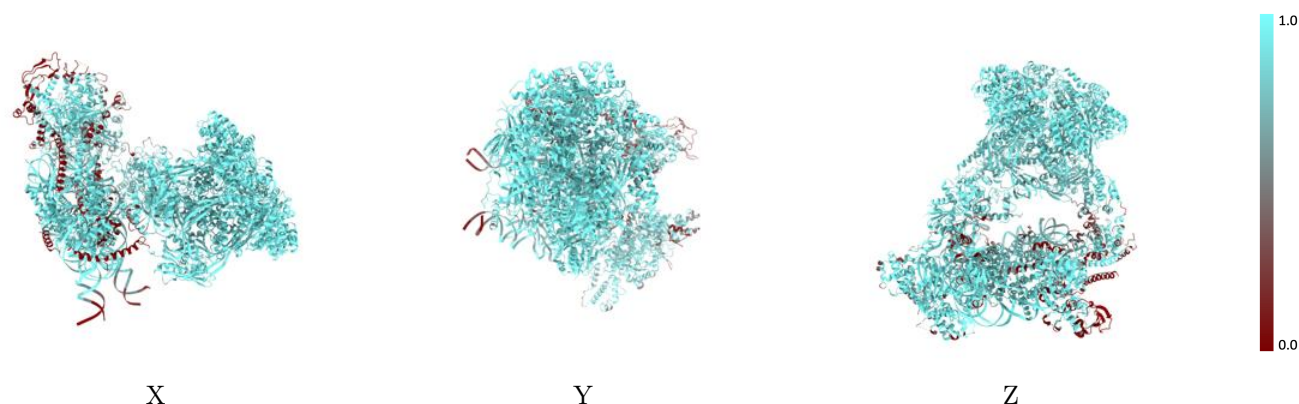
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



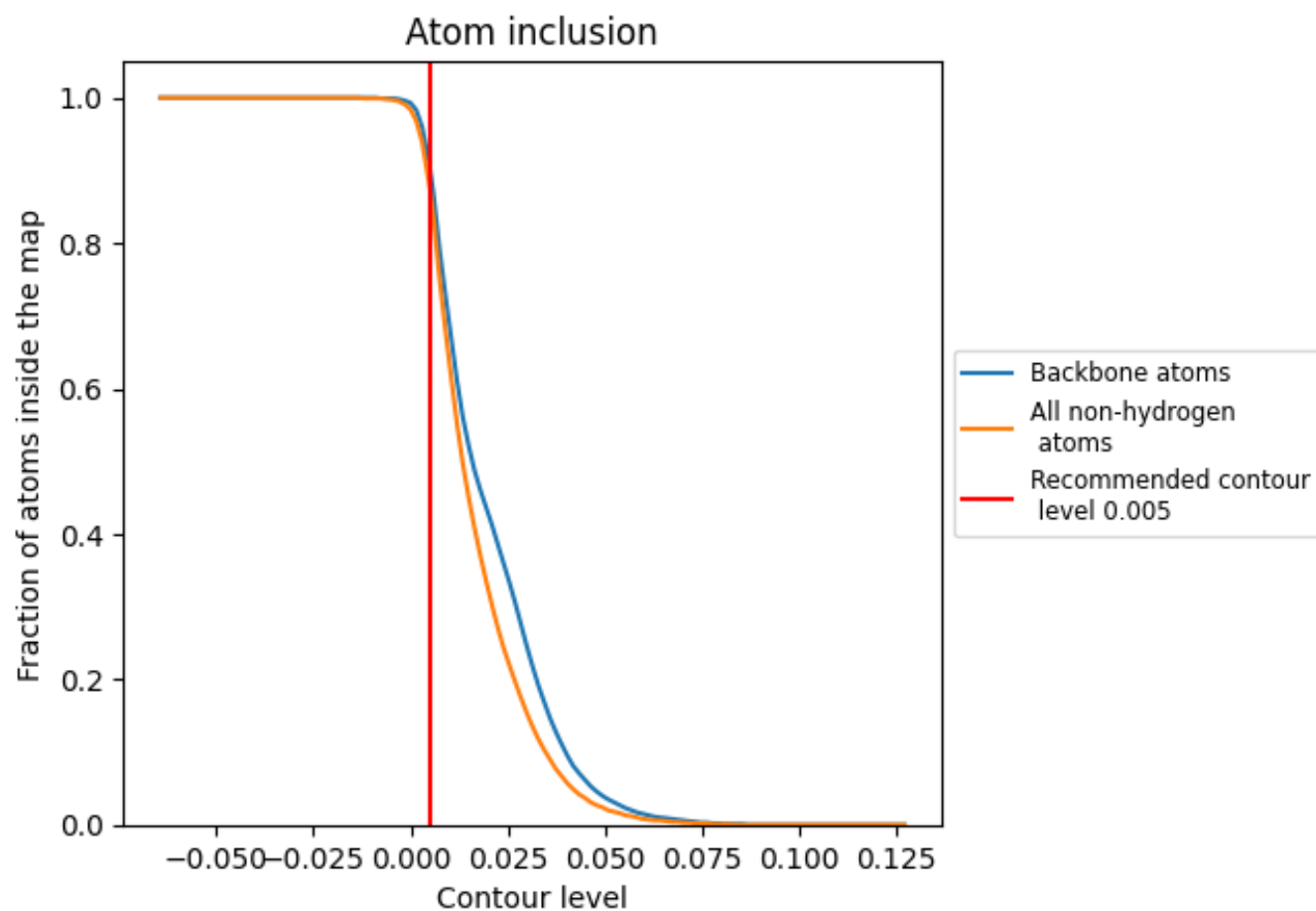
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.1630
A	 0.7930	 0.1300
B	 0.5990	 0.0990
C	 0.9580	 0.1860
D	 0.9020	 0.2110
E	 0.9540	 0.2480
F	 0.9700	 0.2600
G	 0.9560	 0.2690
H	 0.9630	 0.2710
I	 0.9570	 0.2800
J	 0.9450	 0.2670
K	 0.6070	 0.0470
L	 0.8220	 0.0570
M	 0.9170	 0.0690
N	 0.8460	 0.0810
Q	 0.7820	 0.0940
R	 0.7940	 0.1000
S	 0.9360	 0.0920
T	 0.8750	 0.0980
U	 0.9400	 0.0830
V	 0.8950	 0.0880
W	 0.8400	 0.0820
X	 0.8380	 0.0930
Y	 0.8690	 0.1060
Z	 0.8630	 0.1140

