



Full wwPDB EM Validation Report ⓘ

Aug 2, 2026 – 06:18 PM EDT

PDB ID : 9Y3F / pdb_00009y3f
EMDB ID : EMD-72456
Title : Extended cryo-EM structure of human SRCAP-CFDP1-nucleosome complex
in the poised state
Authors : Louder, R.K.; Park, G.
Deposited on : 2025-09-02
Resolution : 4.50 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

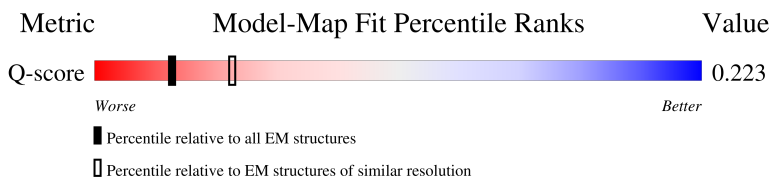
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



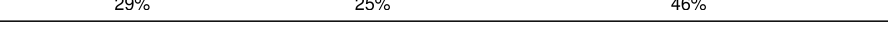
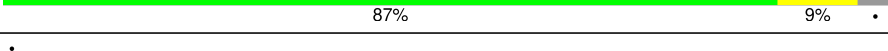
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	C	396	 89% 11%
2	F	463	 86% 9% 5%
2	H	463	 84% 9% 7%
2	J	463	 82% 9% 10%

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Mol	Chain	Length	Quality of chain
3	E	456	
3	G	456	
3	I	456	
4	N	467	
5	Q	128	
5	S	128	
6	R	125	
6	T	125	
7	U	135	
7	W	135	
8	V	102	
8	X	102	
9	Y	285	
10	Z	285	
11	A	3230	
12	B	364	
13	D	154	
14	K	429	
14	M	429	
15	L	375	
16	P	299	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 55482 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 Actin-related protein 6.

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

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

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

- Molecule 3 is a protein called RuvB-like 1.

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

- Molecule 4 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	41	Total	C	N	O	S	0	0
			360	237	68	53	2		

- Molecule 5 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	96	Total	C	N	O	0	0
			742	465	147	130		
5	S	104	Total	C	N	O	0	0
			800	504	156	140		

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
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 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
6	T	95	Total	C	N	O	S	0	0
			744	469	134	139	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 7 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	90	Total	C	N	O	S	0	0
			740	467	140	130	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	96	Total	C	N	O	S	0	0
			795	501	154	137	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 8 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	79	Total	C	N	O	S	0	0
			626	395	121	109	1		
8	X	81	Total	C	N	O	S	0	0
			645	407	126	111	1		

- Molecule 9 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	155	Total	C	N	O	P	0	0
			3168	1502	580	931	155		

- Molecule 10 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	155	Total	C	N	O	P	0	0
			3187	1508	595	929	155		

- Molecule 11 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	880	Total	C	N	O	S	0	0
			7255	4612	1329	1274	40		

- Molecule 12 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

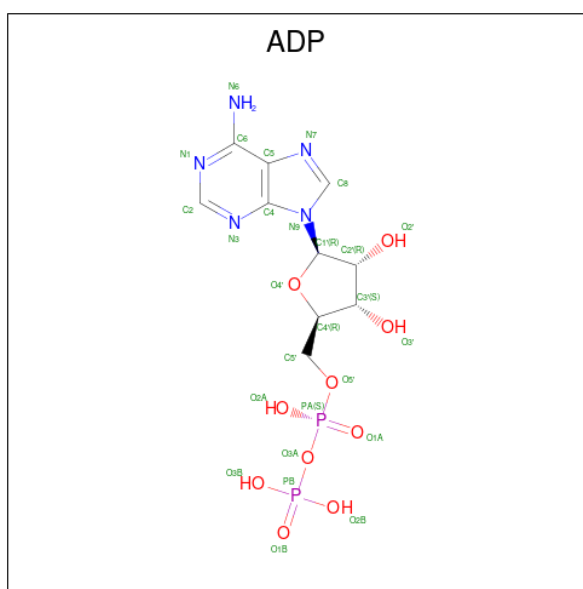
Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	166	Total	C	N	O	S	0	0
			1373	860	264	244	5		

Mol	Chain	Residues	Atoms					AltConf
17	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

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Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	E	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	
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 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

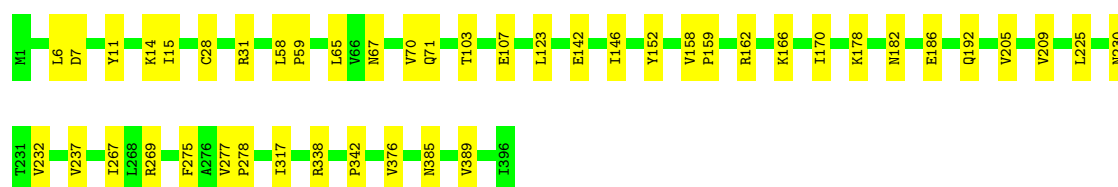
Mol	Chain	Residues	Atoms		AltConf
20	D	2	Total	Zn	0
			2	2	

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.

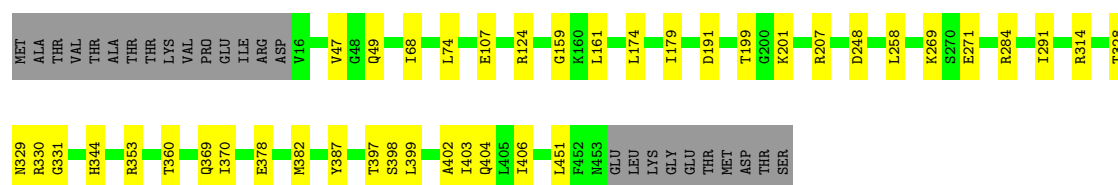
• Molecule 1: Actin-related protein 6

Chain C: 



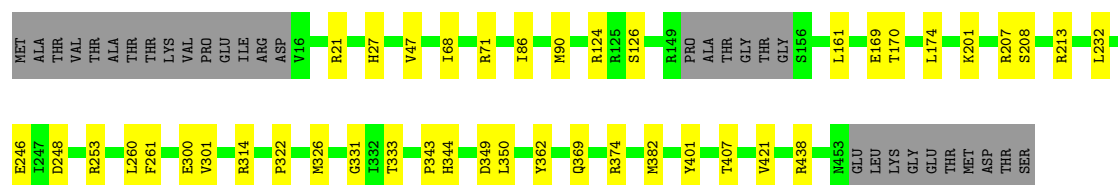
• Molecule 2: RuvB-like 2

Chain F: 



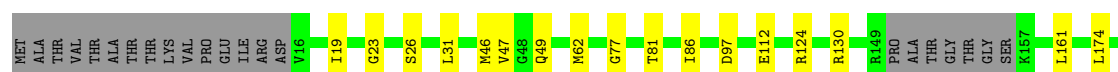
• Molecule 2: RuvB-like 2

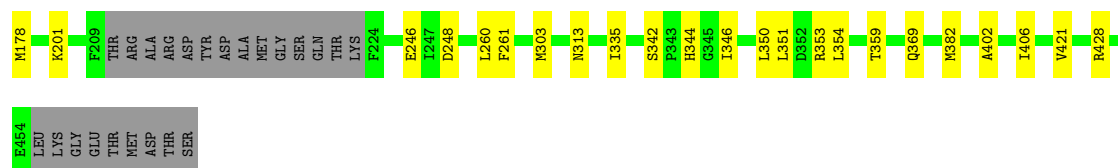
Chain H: 



• Molecule 2: RuvB-like 2

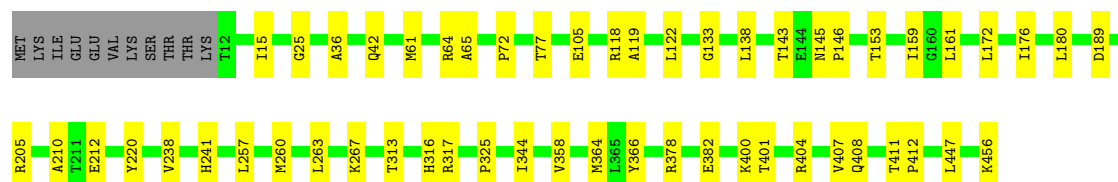
Chain J: 





- Molecule 3: RuvB-like 1

Chain G: 86% 12%



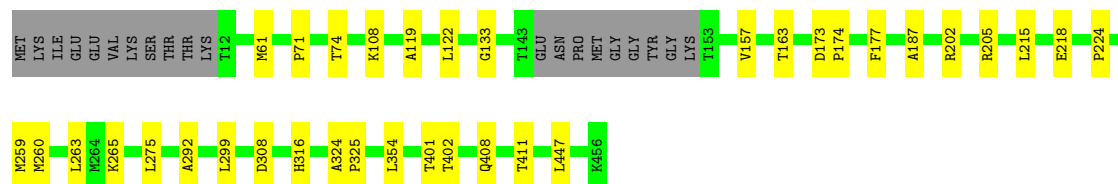
- Molecule 3: RuvB-like 1

Chain E: 82% 12% 5%



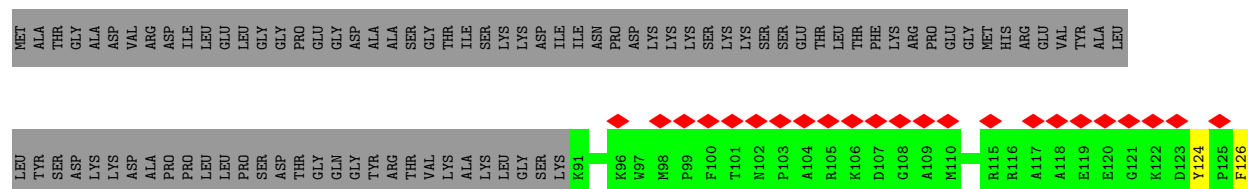
- Molecule 3: RuvB-like 1

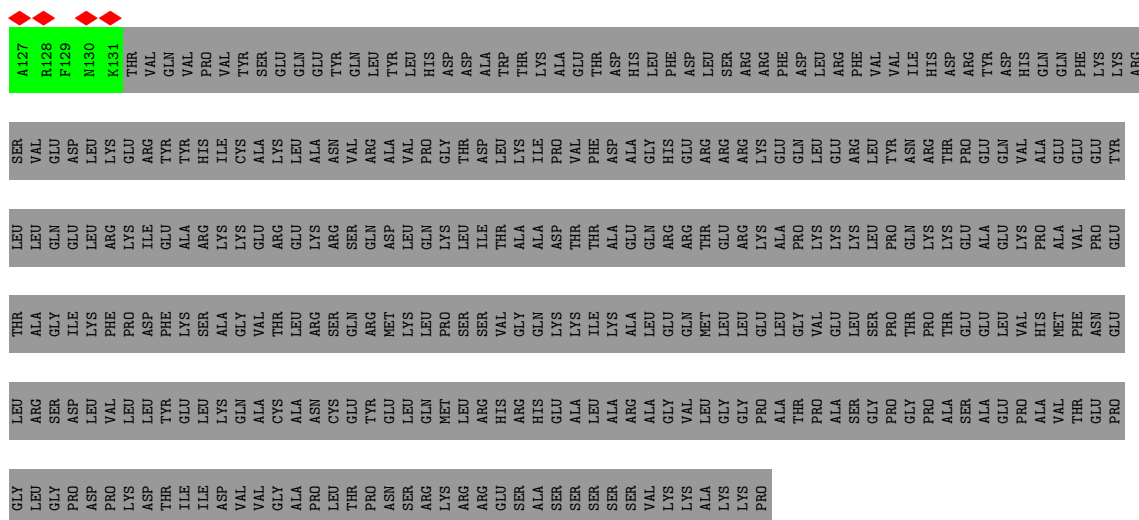
Chain I: 88% 8%



- Molecule 4: DNA methyltransferase 1-associated protein 1

Chain N: 6% 8% 91%





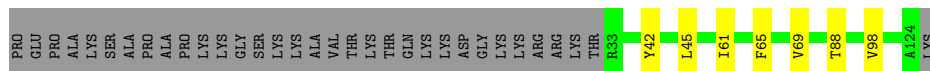
- Molecule 5: Histone H2A type 1



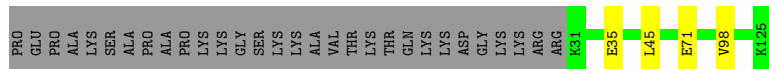
- Molecule 5: Histone H2A type 1



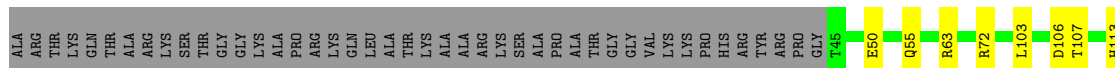
- Molecule 6: Histone H2B 1.1



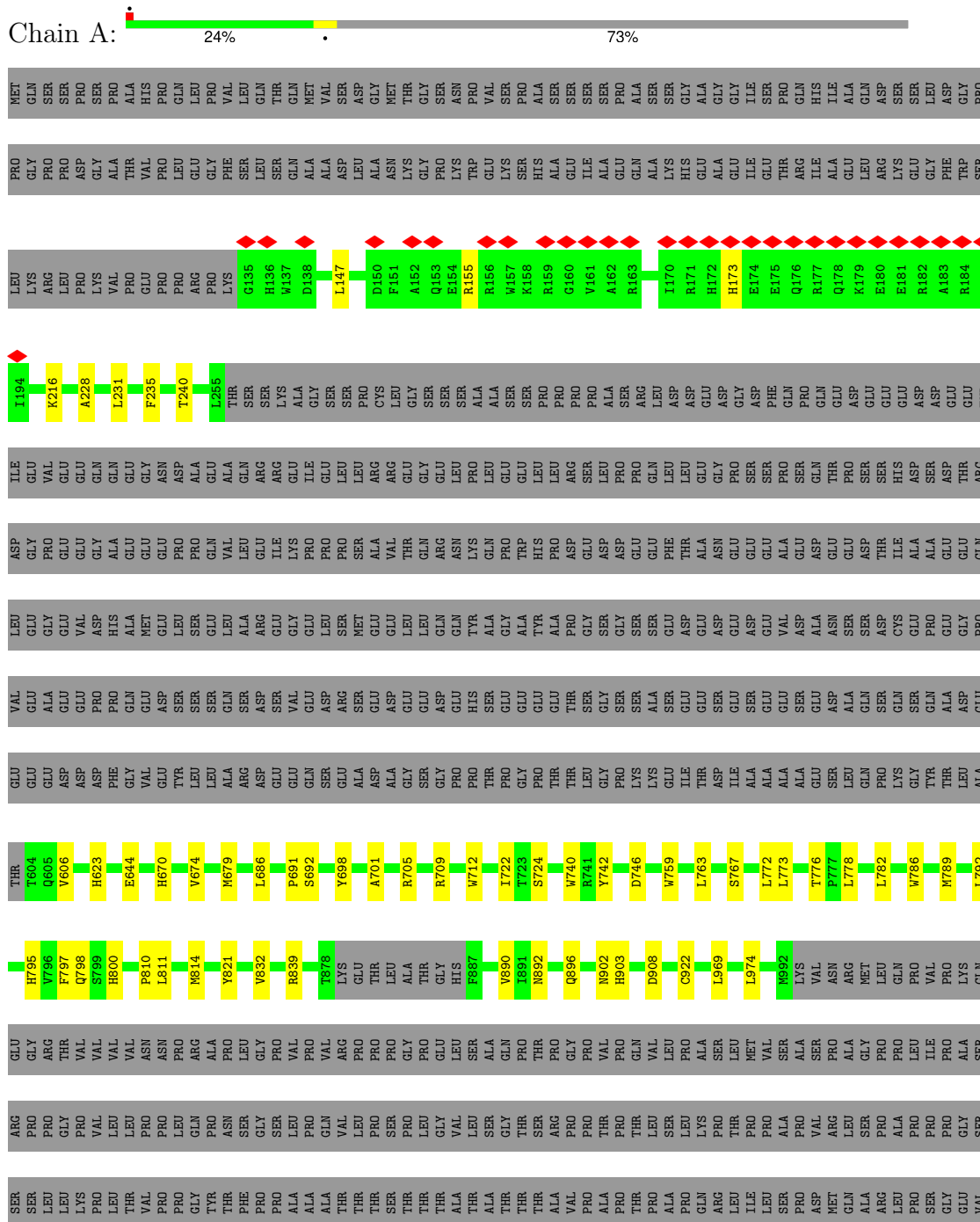
- Molecule 6: Histone H2B 1.1



- Molecule 7: Histone H3.2



- Molecule 11: Helicase SRCAP





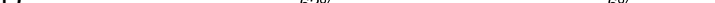
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	GLU	VAL	GLU	ASN	LEU	ALA	GLU	ALA	LEU	PRO	GLN	GLN	PRO	THR
	SER	SER	GLY	THR	SER	ASP	SER	ASP	SER	GLY	GLU	GLU	GLU	THR
	GLU	LEU	SER	THR	VAL	PRO	VAL	PRO	VAL	ARG	LEU	LEU	VAL	LEU
	ALA	THR	SER	THR	GLU	ARG	GLU	SER	SER	VAL	THR	THR	VAL	VAL
	GLU	PRO	SER	THR	GLY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

- Molecule 12: Vacuolar protein sorting-associated protein 72 homolog

Chain B:  41% 54%

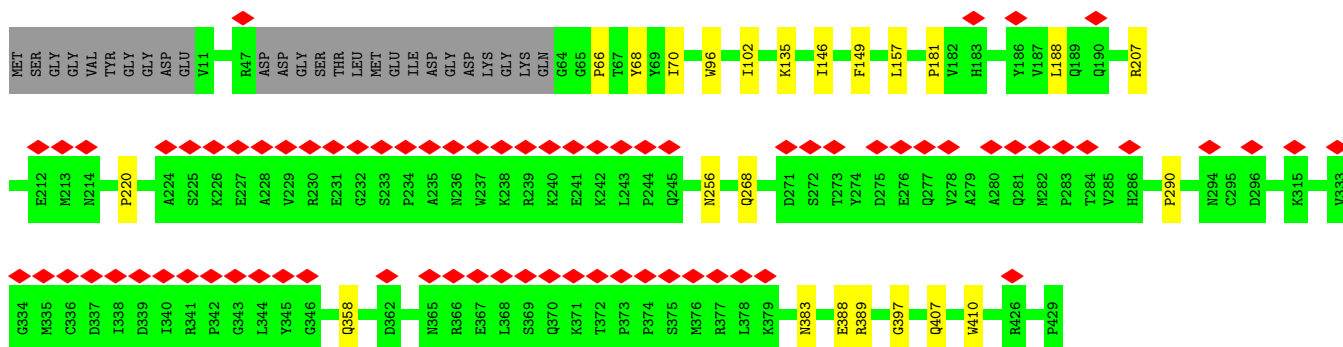
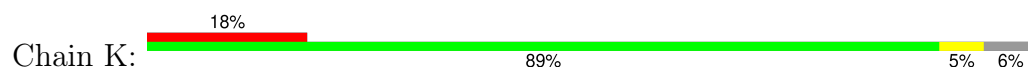
LYS	ILE	VAL	ILE	LYS	HIS	GLU	PHE	MET
ALA	GLY	ALA	GLY	ALA	GLN	LEU	ASP	SER
THR	THR	VAL	THR	THR	LEU	GLN	ILE	LEU
GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP	ALA
PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY
VAL	VAL	SER	ASP	SER	SER	SER	ASP	ARG
ASN	ASN	ASP	ASP	ASP	ASP	GLU	GLU	ALA
PRO	PRO	S129	PRO	PRO	S129	PRO	PRO	ARG
A269	A269	R134	R134	R134	R134	THR	THR	LYS
T266	T266	T144	T144	T144	T144	ALA	GLY	ALA
R289	R289	Q149	Q149	Q149	Q149	ALA	GLU	ASN
E290	E290	E150	E150	E150	E150	GLU	GLU	ARG
T295	T295	R151	R151	R151	R151	PRO	PRO	SER
H296	H296	Q152	Q152	Q152	Q152	ARG	ARG	GLY
R297	R297	G153	G153	G153	G153	LEU	LEU	LEU
R302	R302	Q154	Q154	Q154	Q154	ARG	ARG	GLU
D307	D307	S155	S155	S155	S155	ALA	ALA	GLU
Y310	Y310	R156	R156	R156	R156	VAL	VAL	GLU
A311	A311	R157	R157	R157	R157	VAL	VAL	GLU
T312	T312	R158	R158	R158	R158	THR	THR	ASP
A313	A313	K159	K159	K159	K159	LYS	LYS	GLY
R314	R314	A176	A176	A176	A176	ALA	ALA	GLY
G331	G331	N183	N183	N183	N183	LYS	LYS	THR
LEU	LEU	Y214	Y214	Y214	Y214	PRO	PRO	THR
PRO	PRO	L221	L221	L221	L221	LEU	LEU	TYR
THR	THR	VAL	VAL	VAL	VAL	SER	SER	GLY
ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY
SER	SER	PRO	PRO	PRO	PRO	ARG	ARG	PHE
ALA	ALA	GLU	GLU	GLU	GLU	PRO	PRO	THR
LEU	LEU	PRO	PRO	PRO	PRO	LYS	LYS	GLU
GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL	SER
PRO	PRO	PRO	PRO	PRO	PRO	ASN	ASN	GLY
PRO	PRO	GLU	GLU	GLU	GLU	THR	THR	ASP
PRO	PRO	ASN	ASN	ASN	ASN	PRO	PRO	ASP
PRO	PRO	VAL	VAL	VAL	VAL	ALA	ALA	GLU
GLU	GLU	ASP	ASP	ASP	ASP	GLY	GLY	TYR
LEU	LEU	ILE	ILE	ILE	ILE	SER	SER	GLN
PRO	PRO	GLU	GLU	GLU	GLU	SER	SER	GLY
PRO	PRO	GLY	GLY	GLY	GLY	GLN	GLN	ASN
PRO	PRO	LEU	LEU	LEU	LEU	LYS	LYS	GLN
GLY	GLY	LEU	LEU	LEU	LEU	ALA	ALA	SER
SER	SER	ASP	ASP	ASP	ASP	ARG	ARG	ASP
GLY	GLY	PRO	PRO	PRO	PRO	GLU	GLU	THR
PRO	PRO	ALA	ALA	ALA	ALA	GLU	GLU	THR
PRO	PRO	PRO	PRO	PRO	PRO	LYS	LYS	ASP
ARG	ARG	SER	SER	SER	SER	ALA	ALA	GLU
ALA	ALA	VAL	VAL	VAL	VAL	LEU	LEU	VAL
LEU	LEU	SER	SER	SER	SER	LEU	LEU	ASP
ARG	ARG	ALA	ALA	ALA	ALA	PRO	PRO	SER
GLN	GLN	LEU	LEU	LEU	LEU	ALA	ALA	ASP
		THR	THR	THR	THR	THR	THR	ASP

- Molecule 13: Zinc finger HIT domain-containing protein 1

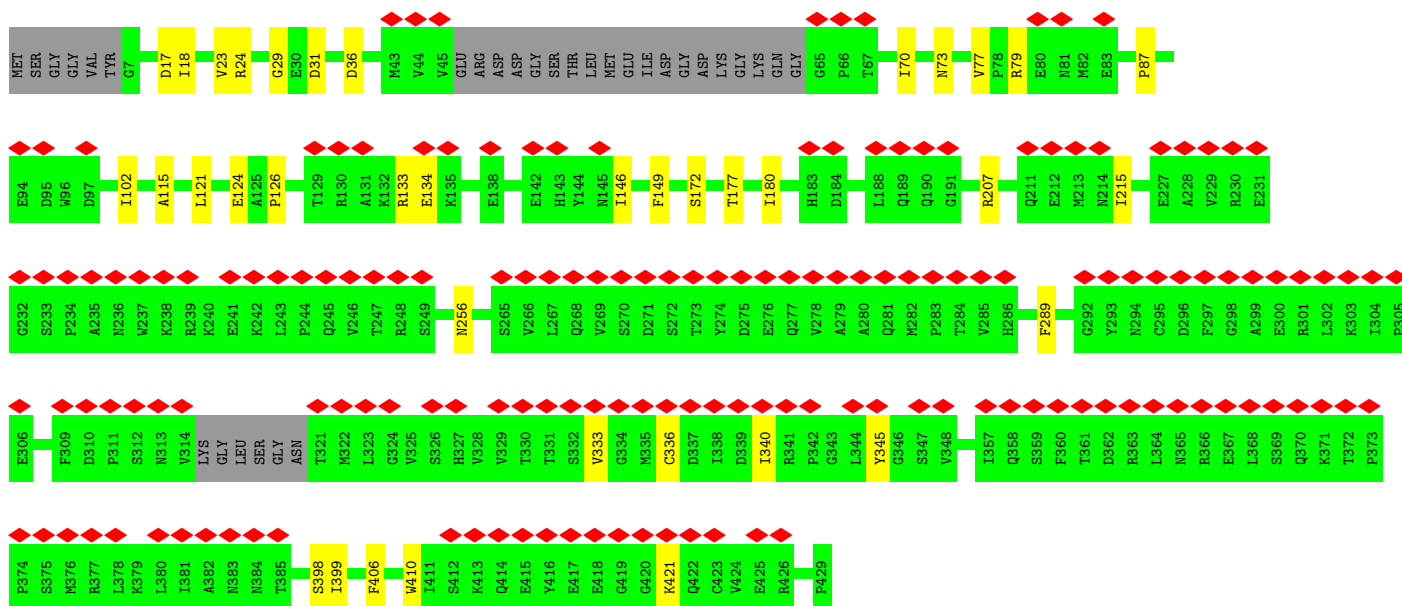
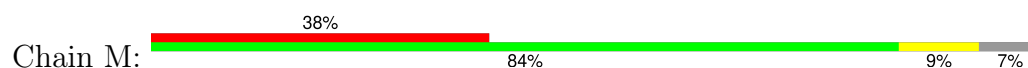
Chain D:  62% 6% 32%



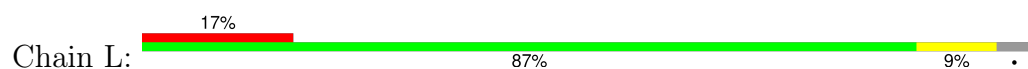
• Molecule 14: Actin-like protein 6A

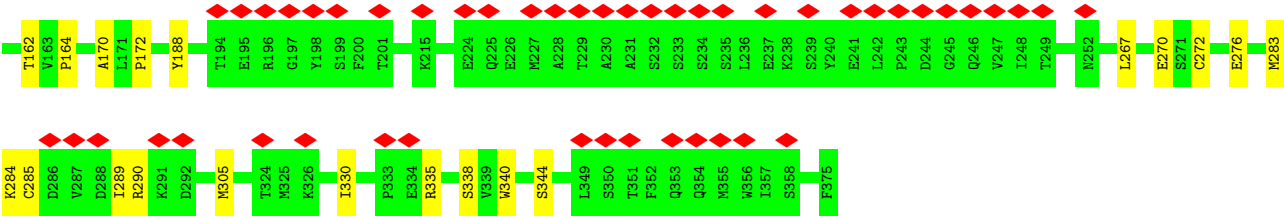


• Molecule 14: Actin-like protein 6A

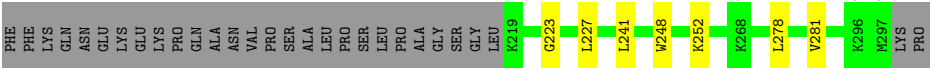
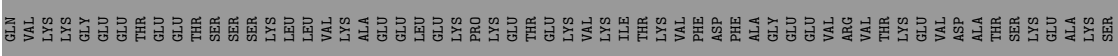
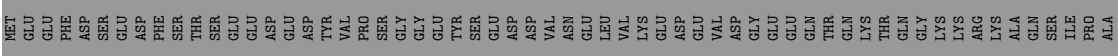


• Molecule 15: Actin, cytoplasmic 1





• Molecule 16: Craniofacial development protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22651	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	0.091	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	393.59998, 393.59998, 393.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: MG, ATP, ZN, ADP

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	C	0.08	0/3299	0.24	0/4467
2	F	0.07	0/3435	0.22	0/4625
2	H	0.08	0/3399	0.22	0/4573
2	J	0.07	0/3290	0.22	0/4426
3	E	0.10	0/3386	0.25	0/4561
3	G	0.08	0/3475	0.22	0/4683
3	I	0.08	0/3407	0.22	0/4591
4	N	0.10	0/376	0.32	0/505
5	Q	0.08	0/751	0.20	0/1013
5	S	0.08	0/810	0.20	0/1095
6	R	0.10	0/730	0.20	0/983
6	T	0.07	0/755	0.19	0/1015
7	U	0.09	0/748	0.22	0/1003
7	W	0.08	0/806	0.21	0/1081
8	V	0.09	0/633	0.20	0/848
8	X	0.11	0/652	0.24	0/873
9	Y	0.22	0/3551	0.54	0/5476
10	Z	0.22	0/3577	0.53	0/5521
11	A	0.11	0/7422	0.30	0/10020
12	B	0.10	0/1404	0.29	0/1892
13	D	0.07	0/848	0.25	0/1147
14	K	0.12	0/3214	0.36	0/4358
14	M	0.12	0/3175	0.35	0/4306
15	L	0.12	0/2883	0.37	0/3905
16	P	0.12	0/802	0.39	0/1058
All	All	0.12	0/56828	0.32	0/78025

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	C	3225	0	3147	26	0
2	F	3395	0	3467	28	0
2	H	3361	0	3434	30	0
2	J	3254	0	3329	30	0
3	E	3343	0	3449	44	0
3	G	3429	0	3530	42	0
3	I	3364	0	3470	29	0
4	N	360	0	345	1	0
5	Q	742	0	784	11	0
5	S	800	0	851	9	0
6	R	719	0	740	6	0
6	T	744	0	773	4	0
7	U	740	0	781	10	0
7	W	795	0	833	10	0
8	V	626	0	663	5	0
8	X	645	0	687	10	0
9	Y	3168	0	1739	51	0
10	Z	3187	0	1738	56	0
11	A	7255	0	7330	66	0
12	B	1373	0	1394	13	0
13	D	831	0	798	10	0
14	K	3143	0	3092	13	0
14	M	3105	0	3044	24	0
15	L	2822	0	2798	21	0
16	P	793	0	804	6	0
17	A	31	0	12	0	0
17	C	31	0	12	0	0
17	K	31	0	12	0	0
18	A	1	0	0	0	0
18	C	1	0	0	0	0
18	F	1	0	0	0	0
18	H	1	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	E	27	0	12	1	0
19	F	27	0	12	0	0
19	G	27	0	12	2	0
19	H	27	0	12	1	0
19	I	27	0	12	0	0
19	J	27	0	12	0	0
20	D	2	0	0	0	0
All	All	55482	0	53128	454	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 (454) 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)
9:Y:39:DA:H2'	9:Y:40:DG:C8	2.19	0.77
9:Y:27:DG:H2'	9:Y:28:DG:C8	2.19	0.76
2:F:68:ILE:HG13	3:E:411:THR:HG21	1.68	0.75
3:E:125:LYS:HE2	16:P:278:LEU:HD23	1.68	0.74
3:G:411:THR:HG21	2:H:68:ILE:HG13	1.72	0.70
10:Z:49:DC:H2'	10:Z:50:DG:C8	2.27	0.70
14:M:17:ASP:OD2	14:M:24:ARG:NH1	2.26	0.68
2:F:124:ARG:NE	2:F:248:ASP:OD2	2.27	0.66
9:Y:-22:DA:H2''	9:Y:-21:DC:H5''	1.78	0.66
9:Y:-70:DG:H2''	9:Y:-69:DA:C8	2.31	0.66
9:Y:15:DT:H2''	9:Y:16:DA:C8	2.31	0.65
15:L:188:TYR:HB2	15:L:267:LEU:HD21	1.76	0.65
11:A:709:ARG:O	11:A:712:TRP:HD1	1.80	0.65
3:G:263:LEU:O	2:H:253:ARG:NH2	2.30	0.64
10:Z:35:DT:H2''	10:Z:36:DA:C8	2.33	0.64
3:G:447:LEU:HD22	2:H:331:GLY:HA2	1.79	0.64
9:Y:-62:DC:H2'	9:Y:-61:DG:C8	2.33	0.64
9:Y:26:DG:H2'	9:Y:27:DG:C8	2.33	0.64
11:A:890:VAL:HG23	16:P:241:LEU:HD22	1.79	0.64
3:I:108:LYS:NZ	3:I:308:ASP:OD2	2.30	0.63
9:Y:-66:DA:H2''	9:Y:-65:DT:H5''	1.80	0.63
1:C:65:LEU:HD11	1:C:71:GLN:HG2	1.81	0.63
9:Y:-44:DA:H2'	9:Y:-43:DT:H71	1.79	0.63
9:Y:15:DT:H2''	9:Y:16:DA:N7	2.13	0.63
2:H:124:ARG:NE	2:H:248:ASP:OD2	2.31	0.63
14:M:336:CYS:HB3	14:M:340:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:285:CYS:HB3	15:L:289:ILE:HD11	1.81	0.63
2:F:159:GLY:HA3	2:F:179:ILE:HD11	1.81	0.62
9:Y:-26:DT:H2''	9:Y:-25:DA:C8	2.34	0.62
10:Z:66:DT:H2'	10:Z:67:DT:H71	1.80	0.62
3:E:125:LYS:HD2	16:P:281:VAL:HG11	1.80	0.62
8:X:30:THR:HG22	8:X:32:PRO:HD2	1.82	0.62
10:Z:50:DG:H2''	10:Z:51:DG:H8	1.65	0.62
2:J:124:ARG:NE	2:J:248:ASP:OD2	2.32	0.61
10:Z:15:DT:H2''	10:Z:16:DA:C8	2.35	0.61
3:E:404:ARG:NH2	19:E:501:ADP:O1A	2.32	0.61
11:A:692:SER:HB2	12:B:176:ALA:HB1	1.81	0.61
3:E:275:LEU:HD13	2:J:261:PHE:HB3	1.83	0.61
2:H:207:ARG:NH1	3:I:173:ASP:OD1	2.34	0.61
14:M:121:LEU:HB2	14:M:410:TRP:HH2	1.66	0.60
2:F:451:LEU:HD21	3:G:72:PRO:HG3	1.84	0.60
10:Z:39:DA:H2''	10:Z:40:DC:H5''	1.82	0.60
15:L:107:GLU:OE2	15:L:116:ARG:NH2	2.28	0.60
3:G:408:GLN:O	2:H:71:ARG:NH2	2.34	0.59
11:A:1973:ILE:HG23	11:A:1977:ILE:HD12	1.84	0.59
2:F:331:GLY:HA2	3:E:447:LEU:HD22	1.85	0.59
10:Z:50:DG:H2''	10:Z:51:DG:C8	2.38	0.59
10:Z:37:DC:H2''	10:Z:38:DG:C8	2.37	0.59
1:C:182:ASN:ND2	13:D:35:LEU:O	2.36	0.59
11:A:778:LEU:HD23	11:A:2187:GLY:HA2	1.85	0.59
11:A:922:CYS:SG	2:J:201:LYS:NZ	2.74	0.59
11:A:1924:ASP:OD2	2:H:201:LYS:NZ	2.34	0.58
3:E:47:GLU:OE1	2:J:428:ARG:NH2	2.33	0.58
1:C:142:GLU:O	1:C:162:ARG:NH2	2.36	0.58
9:Y:39:DA:H2'	9:Y:40:DG:H8	1.65	0.58
11:A:644:GLU:OE2	11:A:839:ARG:NH2	2.34	0.58
14:K:70:ILE:HD13	14:K:102:ILE:HA	1.86	0.58
2:F:269:LYS:HE2	3:E:268:LYS:HG2	1.85	0.58
9:Y:45:DC:H2''	9:Y:46:DA:C8	2.38	0.58
3:I:401:THR:OG1	3:I:402:THR:N	2.33	0.58
11:A:147:LEU:HD23	14:M:399:ILE:HG23	1.85	0.57
9:Y:-47:DT:H2''	9:Y:-46:DC:C5	2.40	0.57
9:Y:8:DC:H2''	9:Y:9:DG:C8	2.39	0.57
11:A:240:THR:HG21	11:A:832:VAL:HA	1.87	0.57
2:F:191:ASP:OD1	2:F:207:ARG:NH1	2.37	0.57
3:G:172:LEU:HB3	3:G:176:ILE:HD12	1.87	0.57
9:Y:-20:DC:H2'	9:Y:-19:DG:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:691:PRO:O	12:B:183:ASN:ND2	2.30	0.57
2:J:49:GLN:NE2	2:J:81:THR:O	2.30	0.57
3:E:283:VAL:HB	2:J:19:ILE:HD11	1.86	0.57
9:Y:-57:DC:H2"	9:Y:-56:DG:C8	2.40	0.57
11:A:173:HIS:NE2	15:L:143:TYR:O	2.34	0.57
2:F:107:GLU:OE2	3:G:317:ARG:NH1	2.38	0.56
7:U:50:GLU:OE1	8:V:39:ARG:NH1	2.38	0.56
11:A:155:ARG:NH2	14:M:31:ASP:O	2.33	0.56
5:Q:64:GLU:OE2	5:Q:68:ASN:ND2	2.37	0.56
2:F:284:ARG:NH2	3:E:13:GLN:OE1	2.39	0.56
9:Y:-27:DC:H2"	9:Y:-26:DT:H71	1.87	0.56
11:A:903:HIS:HB2	11:A:2071:MET:HE1	1.87	0.56
3:G:212:GLU:OE2	12:B:289:ARG:NH2	2.37	0.56
1:C:103:THR:O	1:C:107:GLU:HG3	2.05	0.56
1:C:123:LEU:HB2	1:C:376:VAL:HG12	1.87	0.56
2:F:161:LEU:HB2	2:F:174:LEU:HD11	1.88	0.56
3:I:447:LEU:HD11	2:J:344:HIS:CE1	2.41	0.56
9:Y:-12:DC:H2"	9:Y:-11:DG:C8	2.41	0.55
3:G:15:ILE:HD13	3:G:382:GLU:HA	1.87	0.55
9:Y:-63:DC:H2"	9:Y:-62:DC:C5	2.42	0.55
6:T:71:GLU:OE1	8:X:91:LYS:NZ	2.39	0.55
2:H:401:TYR:OH	2:H:438:ARG:NH2	2.39	0.55
3:I:187:ALA:O	3:I:205:ARG:NH1	2.38	0.55
5:Q:77:ARG:NH1	10:Z:-56:DG:O3'	2.35	0.55
3:I:119:ALA:HB3	3:I:325:PRO:HG3	1.88	0.55
14:M:18:ILE:HG23	14:M:23:VAL:HG22	1.87	0.55
7:W:51:ILE:HG13	8:X:39:ARG:HD2	1.89	0.55
9:Y:33:DC:H2'	9:Y:34:DT:C6	2.42	0.55
5:S:63:LEU:HD13	6:T:45:LEU:HB2	1.89	0.54
3:E:129:GLU:HB2	3:E:195:ALA:HB3	1.87	0.54
14:M:121:LEU:HB2	14:M:410:TRP:CH2	2.42	0.54
5:S:54:VAL:HG21	6:T:98:VAL:HG21	1.90	0.54
2:F:199:THR:HG23	2:F:201:LYS:H	1.71	0.54
3:G:263:LEU:HD22	3:I:260:MET:HE2	1.90	0.54
7:W:119:ILE:HD11	8:X:46:ILE:HG23	1.90	0.54
9:Y:32:DA:H2"	9:Y:33:DC:H6	1.72	0.54
9:Y:49:DC:H2"	9:Y:50:DA:C8	2.43	0.54
2:J:335:ILE:HD11	2:J:342:SER:HB2	1.90	0.54
2:F:49:GLN:NE2	2:F:360:THR:O	2.41	0.54
3:G:119:ALA:HB3	3:G:325:PRO:HG3	1.90	0.54
3:E:304:VAL:HG21	3:E:329:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:100:LEU:HD11	8:X:58:LEU:HD22	1.89	0.53
11:A:892:ASN:O	11:A:896:GLN:HG2	2.07	0.53
1:C:159:PRO:HG2	1:C:166:LYS:HB2	1.90	0.53
1:C:338:ARG:NH2	1:C:342:PRO:O	2.41	0.53
7:U:72:ARG:NH1	9:Y:-23:DC:OP1	2.39	0.53
5:Q:54:VAL:HG21	6:R:98:VAL:HG21	1.90	0.53
2:J:351:LEU:HD23	2:J:354:LEU:HD12	1.90	0.53
14:K:383:ASN:HD22	14:K:388:GLU:HB3	1.72	0.53
3:G:77:THR:OG1	2:H:314:ARG:NH1	2.41	0.53
2:H:27:HIS:HD2	2:H:374:ARG:HH11	1.56	0.53
10:Z:0:DG:OP1	13:D:26:ARG:NH2	2.37	0.53
3:I:119:ALA:HB2	3:I:299:LEU:HB2	1.91	0.53
9:Y:32:DA:H2''	9:Y:33:DC:C6	2.43	0.53
3:I:408:GLN:HE22	2:J:353:ARG:HA	1.74	0.53
1:C:186:GLU:OE2	13:D:148:ARG:NH2	2.36	0.52
3:G:344:ILE:HG13	3:E:456:LYS:HE3	1.92	0.52
9:Y:-28:DT:H2''	9:Y:-27:DC:C6	2.44	0.52
2:F:370:ILE:HG21	2:F:399:LEU:HD21	1.92	0.51
11:A:772:LEU:HG	11:A:792:LEU:HD21	1.92	0.51
3:E:411:THR:OG1	3:E:412:PRO:HD3	2.10	0.51
2:H:349:ASP:OD1	2:H:350:LEU:N	2.43	0.51
2:J:313:ASN:HD21	2:J:350:LEU:HB2	1.74	0.51
15:L:270:GLU:HB3	14:M:79:ARG:HH21	1.76	0.51
10:Z:-37:DG:H2''	10:Z:-36:DG:N7	2.26	0.51
10:Z:-17:DT:H2''	10:Z:-16:DT:C5	2.46	0.51
10:Z:22:DT:H4'	10:Z:23:DG:OP1	2.09	0.51
2:J:46:MET:HE1	2:J:86:ILE:HA	1.91	0.51
2:J:31:LEU:HD23	2:J:46:MET:HE3	1.92	0.51
10:Z:-19:DG:H5''	11:A:2120:SER:HB3	1.92	0.51
2:J:382:MET:HE2	2:J:421:VAL:HG11	1.92	0.51
11:A:686:LEU:HD12	11:A:722:ILE:HD11	1.91	0.51
11:A:2305:LEU:HD12	16:P:227:LEU:HD22	1.92	0.51
3:E:260:MET:HE1	3:I:260:MET:HE3	1.92	0.51
16:P:248:TRP:CD1	16:P:252:LYS:HE3	2.46	0.51
9:Y:40:DG:C8	9:Y:41:DT:H72	2.45	0.50
11:A:782:LEU:HD11	11:A:811:LEU:HD12	1.93	0.50
2:F:271:GLU:OE2	3:E:118:ARG:NH1	2.41	0.50
14:M:172:SER:HA	14:M:177:THR:HA	1.92	0.50
8:V:24:ASP:OD1	8:V:24:ASP:N	2.43	0.50
11:A:606:VAL:HG11	11:A:623:HIS:ND1	2.26	0.50
2:H:27:HIS:CD2	2:H:374:ARG:HH11	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:181:PRO:HG2	14:K:188:LEU:HB2	1.94	0.50
9:Y:29:DA:C8	9:Y:30:DT:H72	2.46	0.50
11:A:231:LEU:HD13	11:A:2343:ARG:HB2	1.93	0.50
1:C:11:TYR:HB2	1:C:152:TYR:CG	2.47	0.50
2:H:161:LEU:HB3	2:H:174:LEU:HD21	1.93	0.50
3:G:105:GLU:HG2	3:G:267:LYS:HZ2	1.77	0.50
9:Y:-55:DC:H2''	9:Y:-54:DA:N7	2.26	0.50
14:K:207:ARG:NH2	14:K:256:ASN:OD1	2.36	0.50
1:C:192:GLN:NE2	1:C:269:ARG:O	2.44	0.50
8:X:52:GLU:OE2	8:X:55:ARG:NH1	2.42	0.50
7:U:107:THR:HG21	7:U:124:ILE:HG12	1.93	0.50
2:J:402:ALA:O	2:J:406:ILE:HG13	2.12	0.49
1:C:7:ASP:HB3	1:C:14:LYS:HB2	1.92	0.49
4:N:124:TYR:CE2	4:N:126:PHE:HB2	2.46	0.49
10:Z:-49:DG:H2''	10:Z:-48:DC:C6	2.48	0.49
10:Z:31:DT:H2''	10:Z:32:DG:C8	2.47	0.49
10:Z:74:DC:H2''	10:Z:75:DA:C8	2.46	0.49
11:A:789:MET:HB3	11:A:797:PHE:CE1	2.47	0.49
3:E:133:GLY:HA2	3:E:224:PRO:HG2	1.94	0.49
3:G:404:ARG:NH2	19:G:501:ADP:O3A	2.45	0.49
10:Z:19:DC:H2''	10:Z:20:DG:H8	1.78	0.49
11:A:235:PHE:HB2	11:A:2346:LEU:HB3	1.93	0.49
11:A:2167:ILE:HG13	11:A:2177:LEU:HD22	1.95	0.49
7:U:117:VAL:HG13	8:V:44:LYS:HE3	1.94	0.49
9:Y:-7:DC:H2''	9:Y:-6:DT:C6	2.48	0.49
14:M:134:GLU:HB3	14:M:421:LYS:HD2	1.95	0.49
11:A:216:LYS:NZ	11:A:2321:GLU:OE2	2.32	0.49
2:J:342:SER:OG	2:J:346:ILE:O	2.28	0.49
1:C:225:LEU:O	1:C:230:ASN:ND2	2.40	0.49
3:G:143:THR:HG22	3:G:145:ASN:H	1.76	0.49
5:Q:102:ILE:HG23	6:R:61:ILE:HD12	1.94	0.49
9:Y:-10:DC:H1'	9:Y:-9:DA:H5'	1.95	0.49
9:Y:25:DG:O3'	9:Y:26:DG:H8	1.96	0.49
12:B:295:THR:HG23	12:B:297:ARG:H	1.78	0.49
3:G:447:LEU:HD11	2:H:344:HIS:CE1	2.48	0.48
11:A:155:ARG:CZ	14:M:31:ASP:HB2	2.43	0.48
15:L:70:PRO:HB3	15:L:81:ASP:HB2	1.94	0.48
15:L:284:LYS:NZ	14:M:36:ASP:O	2.46	0.48
10:Z:-7:DG:H2''	10:Z:-6:DG:C8	2.48	0.48
15:L:153:MET:HG2	15:L:162:THR:HG22	1.95	0.48
3:G:133:GLY:HA3	3:G:161:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:103:LEU:O	7:U:107:THR:HG23	2.12	0.48
2:H:86:ILE:HG22	2:H:90:MET:HE2	1.95	0.48
3:E:119:ALA:HB3	3:E:325:PRO:HG3	1.95	0.48
2:H:382:MET:HG2	2:H:421:VAL:HB	1.95	0.48
1:C:59:PRO:HB3	1:C:70:VAL:HG13	1.96	0.48
9:Y:-18:DC:H2''	9:Y:-17:DT:H5'	1.95	0.48
10:Z:5:DT:H2''	10:Z:6:DA:C8	2.49	0.48
3:E:172:LEU:HD13	3:E:176:ILE:HG21	1.96	0.48
9:Y:-54:DA:H2''	9:Y:-53:DG:C8	2.49	0.48
2:F:258:LEU:HD12	3:G:257:LEU:HD13	1.94	0.48
10:Z:65:DA:OP1	12:B:159:LYS:NZ	2.47	0.48
9:Y:14:DT:H5'	9:Y:14:DT:C6	2.49	0.48
10:Z:-23:DT:H2''	10:Z:-22:DG:C8	2.49	0.48
5:Q:63:LEU:HD13	6:R:45:LEU:HB2	1.94	0.47
7:W:74:ILE:HG12	8:X:59:LYS:HE3	1.96	0.47
10:Z:25:DT:H2''	10:Z:26:DA:N7	2.28	0.47
5:Q:42:ARG:NH1	6:R:88:THR:OG1	2.39	0.47
5:S:72:ASP:OD1	12:B:144:THR:HG23	2.14	0.47
7:W:46:VAL:HG21	9:Y:9:DG:H3'	1.95	0.47
9:Y:-2:DC:H2''	9:Y:-1:DG:C8	2.49	0.47
15:L:151:ILE:HA	15:L:164:PRO:HA	1.97	0.47
5:S:71:ARG:HD2	12:B:144:THR:HG22	1.96	0.47
11:A:1983:VAL:HG11	3:E:243:LEU:HD23	1.96	0.47
3:G:260:MET:HE3	3:E:263:LEU:HB2	1.96	0.47
3:G:366:TYR:OH	19:G:501:ADP:N7	2.36	0.47
5:S:61:GLU:OE1	12:B:134:ARG:NH2	2.44	0.47
7:U:114:ALA:HA	7:W:114:ALA:HB2	1.96	0.47
15:L:335:ARG:HA	15:L:338:SER:OG	2.14	0.47
11:A:786:TRP:CH2	11:A:800:HIS:HB3	2.50	0.47
3:G:146:PRO:HA	3:G:153:THR:HG22	1.96	0.47
6:R:65:PHE:O	6:R:69:VAL:HG12	2.15	0.47
11:A:2094:ARG:NE	11:A:2096:GLU:OE2	2.33	0.47
2:J:47:VAL:HG11	2:J:369:GLN:HB3	1.97	0.47
1:C:59:PRO:HA	1:C:67:ASN:HB3	1.96	0.47
10:Z:2:DG:H2''	10:Z:3:DC:H5''	1.96	0.47
11:A:2009:GLN:HB3	3:I:259:MET:HE1	1.96	0.47
14:M:70:ILE:HD13	14:M:102:ILE:HA	1.96	0.47
1:C:182:ASN:HD22	13:D:35:LEU:C	2.23	0.47
2:F:74:LEU:HD11	2:F:328:THR:HG22	1.97	0.47
1:C:205:VAL:O	1:C:209:VAL:HG22	2.15	0.47
13:D:145:GLN:HA	13:D:149:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:105:LEU:HD11	15:L:123:MET:HE3	1.97	0.47
3:G:42:GLN:NE2	3:G:364:MET:O	2.48	0.47
3:G:411:THR:OG1	3:G:412:PRO:HD3	2.14	0.47
10:Z:8:DC:H2'	10:Z:9:DT:H71	1.97	0.47
11:A:709:ARG:O	11:A:712:TRP:CD1	2.66	0.47
1:C:237:VAL:HG22	1:C:267:ILE:HG12	1.96	0.46
10:Z:21:DG:H2'	10:Z:22:DT:H71	1.97	0.46
2:H:170:THR:HG22	2:H:232:LEU:HD13	1.96	0.46
15:L:24:ASP:HB2	15:L:340:TRP:HH2	1.80	0.46
14:M:29:GLY:N	14:M:398:SER:OG	2.48	0.46
3:G:400:LYS:HG3	3:G:401:THR:HG23	1.97	0.46
10:Z:53:DC:H2''	10:Z:54:DT:C6	2.50	0.46
2:J:97:ASP:HB3	2:J:130:ARG:NH2	2.29	0.46
16:P:223:GLY:O	16:P:227:LEU:HG	2.16	0.46
11:A:2011:ALA:HB1	11:A:2015:TRP:HD1	1.80	0.46
12:B:290:GLU:OE2	12:B:302:ARG:NH1	2.37	0.46
11:A:795:HIS:O	11:A:798:GLN:NE2	2.49	0.46
1:C:28:CYS:HB3	1:C:58:LEU:HD13	1.97	0.46
3:I:71:PRO:HD2	3:I:74:THR:HG21	1.97	0.46
9:Y:-40:DG:H2'	9:Y:-39:DT:C6	2.51	0.46
3:I:265:LYS:NZ	2:J:112:GLU:OE2	2.48	0.46
8:V:31:LYS:HG3	8:V:51:TYR:CE1	2.51	0.46
3:I:122:LEU:HD11	3:I:292:ALA:HB1	1.96	0.46
2:H:362:TYR:OH	19:H:501:ADP:N7	2.43	0.46
14:M:207:ARG:NH2	14:M:256:ASN:OD1	2.43	0.46
1:C:178:LYS:NZ	13:D:38:ASP:OD1	2.40	0.45
3:I:202:ARG:NH2	3:I:218:GLU:OE2	2.37	0.45
14:K:181:PRO:HB2	14:K:188:LEU:HD12	1.98	0.45
3:G:313:THR:HA	3:G:316:HIS:CD2	2.51	0.45
9:Y:49:DC:H2''	9:Y:50:DA:N7	2.30	0.45
14:M:333:VAL:HG11	14:M:345:TYR:CE2	2.51	0.45
2:F:403:ILE:HA	2:F:406:ILE:HD12	1.98	0.45
7:W:73:GLU:O	7:W:76:GLN:HG2	2.16	0.45
9:Y:37:DC:H5''	9:Y:37:DC:H6	1.81	0.45
2:J:161:LEU:HB2	2:J:174:LEU:HD11	1.98	0.45
3:G:263:LEU:HD22	3:I:260:MET:HB3	1.97	0.45
10:Z:-20:DC:H5'	11:A:2069:THR:HG23	1.98	0.45
11:A:228:ALA:HB2	11:A:2339:VAL:HG22	1.99	0.45
15:L:23:GLY:N	15:L:344:SER:OG	2.49	0.45
6:R:42:TYR:OH	10:Z:-55:DA:H3'	2.16	0.45
10:Z:54:DT:H2''	10:Z:55:DG:N7	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:404:GLN:HA	3:G:64:ARG:HH12	1.82	0.45
9:Y:13:DT:H2''	9:Y:14:DT:H72	1.99	0.45
10:Z:-7:DG:H2''	10:Z:-6:DG:N7	2.31	0.45
7:U:63:ARG:HD3	10:Z:17:DA:H4'	1.99	0.45
9:Y:-63:DC:H2''	9:Y:-62:DC:C6	2.52	0.45
9:Y:36:DC:H2''	9:Y:37:DC:C5	2.52	0.45
14:M:146:ILE:HD11	14:M:149:PHE:HB2	1.98	0.45
5:Q:88:ARG:HA	5:Q:88:ARG:HD3	1.85	0.45
11:A:759:TRP:CH2	11:A:763:LEU:HD22	2.52	0.45
15:L:283:MET:O	15:L:290:ARG:NH2	2.50	0.45
1:C:232:VAL:HG11	1:C:275:PHE:HE2	1.82	0.44
2:F:344:HIS:CE1	3:E:447:LEU:HD11	2.52	0.44
10:Z:20:DG:H2''	10:Z:21:DG:H5''	1.98	0.44
12:B:310:TYR:OH	2:H:169:GLU:O	2.27	0.44
3:E:71:PRO:HD2	3:E:74:THR:HG21	1.98	0.44
3:E:168:LYS:HB3	3:E:228:VAL:HG11	2.00	0.44
2:H:47:VAL:HG11	2:H:369:GLN:HB3	1.99	0.44
14:K:157:LEU:HD22	14:K:397:GLY:HA2	1.99	0.44
14:M:73:ASN:O	14:M:77:VAL:HG23	2.18	0.44
11:A:2073:ASP:OD1	11:A:2088:ARG:NH1	2.43	0.44
3:E:274:LYS:NZ	2:J:246:GLU:OE2	2.45	0.44
2:H:407:THR:HG21	3:I:61:MET:HG3	2.00	0.44
2:F:382:MET:HB3	2:F:387:TYR:CE2	2.52	0.44
3:G:118:ARG:HE	3:G:241:HIS:CE1	2.35	0.44
2:H:126:SER:HB2	2:H:322:PRO:HG3	2.00	0.44
9:Y:-51:DC:H1'	9:Y:-50:DC:H5'	1.99	0.44
10:Z:5:DT:H2''	10:Z:6:DA:N7	2.32	0.44
12:B:302:ARG:NE	12:B:307:ASP:OD1	2.46	0.44
2:H:21:ARG:NH2	3:I:324:ALA:O	2.50	0.44
2:H:300:GLU:OE2	3:I:316:HIS:ND1	2.36	0.44
7:W:65:LEU:HB3	7:W:66:PRO:HD3	2.00	0.44
10:Z:-19:DG:H2''	10:Z:-18:DG:C8	2.53	0.44
10:Z:-6:DG:H2''	10:Z:-5:DG:C8	2.53	0.44
14:M:115:ALA:HB1	14:M:146:ILE:HG22	2.00	0.44
3:G:404:ARG:HA	3:G:407:VAL:HG22	1.99	0.43
10:Z:1:DC:H2''	10:Z:2:DG:C8	2.53	0.43
1:C:158:VAL:HG22	1:C:170:ILE:HG23	1.99	0.43
3:G:25:GLY:HA3	3:G:36:ALA:HB3	1.99	0.43
5:Q:29:ARG:HG3	5:Q:32:ARG:HH21	1.83	0.43
7:W:62:ILE:HD11	8:X:37:LEU:HD11	2.00	0.43
2:H:246:GLU:HA	2:H:260:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:679:MET:HG3	11:A:722:ILE:HG22	2.00	0.43
11:A:746:ASP:HA	11:A:773:LEU:HB2	1.99	0.43
11:A:2042:CYS:SG	11:A:2044:LYS:HB2	2.58	0.43
14:K:268:GLN:HG3	14:K:358:GLN:HB3	2.00	0.43
3:G:122:LEU:N	3:G:238:VAL:O	2.40	0.43
10:Z:-5:DG:H2''	10:Z:-4:DG:C8	2.54	0.43
10:Z:0:DG:H2'	10:Z:1:DC:C6	2.54	0.43
3:G:378:ARG:HD2	3:G:378:ARG:HA	1.87	0.43
1:C:6:LEU:HD13	1:C:15:ILE:HB	2.00	0.43
2:F:269:LYS:HD3	3:E:268:LYS:HE2	2.00	0.43
2:H:208:SER:O	2:H:213:ARG:NH1	2.49	0.43
9:Y:-14:DA:H2''	9:Y:-13:DA:C8	2.54	0.43
7:U:113:HIS:CG	7:W:126:LEU:HD22	2.54	0.43
10:Z:-17:DT:H2''	10:Z:-16:DT:C7	2.49	0.43
11:A:810:PRO:O	11:A:814:MET:HG3	2.19	0.43
3:E:264:MET:HE1	3:I:263:LEU:HB3	2.00	0.43
3:I:215:LEU:HG	2:J:178:MET:HE3	2.00	0.43
14:K:66:PRO:HG2	14:K:68:TYR:CZ	2.53	0.43
3:I:316:HIS:HD2	3:I:354:LEU:HD13	1.84	0.42
11:A:776:THR:HG21	11:A:2143:THR:HG23	2.01	0.42
11:A:2116:LEU:HD12	11:A:2117:SER:H	1.83	0.42
11:A:2157:GLN:NE2	11:A:2159:ARG:O	2.50	0.42
2:H:261:PHE:HD2	3:I:275:LEU:HD13	1.84	0.42
2:J:77:GLY:HA3	2:J:359:THR:OG1	2.19	0.42
2:F:47:VAL:HG11	2:F:369:GLN:HB3	2.01	0.42
11:A:2010:LEU:HG	11:A:2014:LEU:HD12	2.01	0.42
11:A:2011:ALA:HB1	11:A:2015:TRP:CD1	2.54	0.42
11:A:2137:ASP:OD1	11:A:2137:ASP:N	2.51	0.42
10:Z:51:DG:C5	10:Z:52:DC:C4	3.08	0.42
3:E:338:ILE:HD11	3:E:346:SER:OG	2.19	0.42
2:H:301:VAL:HG21	2:H:326:MET:HB3	2.02	0.42
3:G:189:ASP:OD1	3:G:205:ARG:NH1	2.52	0.42
11:A:814:MET:SD	11:A:821:TYR:HA	2.59	0.42
1:C:146:ILE:HG23	1:C:317:ILE:HA	2.01	0.42
5:S:79:ILE:HG12	5:S:82:HIS:CE1	2.54	0.42
10:Z:19:DC:C2	10:Z:20:DG:N7	2.88	0.42
14:K:146:ILE:HD11	14:K:149:PHE:HB2	2.01	0.42
15:L:107:GLU:CD	15:L:116:ARG:HE	2.28	0.42
2:F:314:ARG:NH1	2:F:353:ARG:HH22	2.17	0.42
2:F:402:ALA:O	2:F:406:ILE:HG13	2.20	0.42
3:G:138:LEU:HD12	3:G:138:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:107:VAL:HG23	7:U:55:GLN:OE1	2.20	0.42
9:Y:38:DT:H2''	9:Y:39:DA:N7	2.35	0.42
11:A:173:HIS:CD2	15:L:146:GLY:HA2	2.55	0.42
14:M:124:GLU:CD	14:M:133:ARG:HE	2.27	0.42
9:Y:6:DC:H2''	9:Y:7:DC:C5	2.54	0.42
10:Z:-38:DA:H2''	10:Z:-37:DG:C8	2.55	0.42
10:Z:24:DC:H2''	10:Z:25:DT:C6	2.55	0.42
11:A:2069:THR:O	11:A:2072:LEU:HB2	2.20	0.42
3:E:323:ILE:HG12	2:J:19:ILE:HG22	2.01	0.42
2:J:246:GLU:HA	2:J:260:LEU:HD21	2.02	0.42
14:K:96:TRP:CE2	14:K:135:LYS:HD3	2.54	0.42
14:K:407:GLN:HA	14:K:410:TRP:CD1	2.55	0.42
9:Y:47:DG:O3'	9:Y:48:DG:C8	2.73	0.42
10:Z:-56:DG:H2''	10:Z:-55:DA:C8	2.54	0.42
3:I:316:HIS:NE2	3:I:354:LEU:HB2	2.35	0.42
2:F:284:ARG:HD3	2:F:291:ILE:HD12	2.02	0.42
5:S:76:THR:N	10:Z:58:DC:OP1	2.53	0.42
15:L:58:ALA:HA	15:L:65:LEU:HD12	2.02	0.42
15:L:147:ARG:NH2	15:L:330:ILE:HG12	2.35	0.42
14:M:87:PRO:HG3	14:M:102:ILE:HD12	2.01	0.42
5:Q:65:LEU:HB3	5:Q:86:ALA:HB1	2.02	0.41
10:Z:-60:DA:H2'	10:Z:-59:DT:H72	2.01	0.41
10:Z:75:DA:C6	10:Z:76:DG:C6	3.08	0.41
11:A:908:ASP:OD1	11:A:908:ASP:N	2.52	0.41
3:E:119:ALA:O	3:E:297:GLY:HA3	2.19	0.41
3:E:256:ILE:O	3:E:260:MET:HG2	2.20	0.41
3:E:405:TYR:O	3:E:409:LEU:HG	2.20	0.41
2:J:382:MET:HG2	2:J:421:VAL:HB	2.02	0.41
2:F:397:THR:OG1	2:F:398:SER:N	2.53	0.41
8:X:38:ALA:HB1	8:X:43:VAL:HB	2.01	0.41
10:Z:-53:DA:C6	10:Z:-52:DG:C6	3.08	0.41
10:Z:-19:DG:H4'	11:A:2119:ARG:O	2.20	0.41
11:A:1885:TYR:CE2	11:A:1890:GLU:HG3	2.56	0.41
5:Q:32:ARG:HD3	10:Z:-45:DG:OP2	2.20	0.41
11:A:969:LEU:HD13	11:A:974:LEU:HD13	2.02	0.41
7:U:106:ASP:OD2	7:U:131:ARG:NH2	2.35	0.41
3:E:110:GLU:HG2	3:E:270:GLU:HA	2.02	0.41
3:I:163:THR:HG22	3:I:224:PRO:HB2	2.01	0.41
5:S:88:ARG:HB2	5:S:108:LEU:HD21	2.03	0.41
10:Z:70:DC:H2''	10:Z:71:DC:C5	2.56	0.41
10:Z:80:DT:H2'	10:Z:81:DT:H71	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:698:TYR:CE2	11:A:705:ARG:HD2	2.54	0.41
11:A:789:MET:HB3	11:A:797:PHE:CD1	2.55	0.41
13:D:135:TYR:CE2	13:D:141:LEU:HD13	2.55	0.41
3:E:452:ASP:OD1	3:E:452:ASP:N	2.54	0.41
3:I:157:VAL:HG21	3:I:177:PHE:HB2	2.02	0.41
3:I:411:THR:HG21	2:J:62:MET:HE3	2.02	0.41
14:M:126:PRO:HG2	14:M:180:ILE:HD13	2.02	0.41
9:Y:-56:DG:H2''	9:Y:-55:DC:C5	2.56	0.41
13:D:20:ASP:N	13:D:20:ASP:OD1	2.53	0.41
15:L:305:MET:HA	15:L:335:ARG:NH2	2.36	0.41
11:A:674:VAL:O	11:A:724:SER:HA	2.21	0.41
11:A:740:TRP:O	11:A:767:SER:HA	2.21	0.41
13:D:145:GLN:HA	13:D:149:CYS:CB	2.51	0.41
1:C:31:ARG:NH1	13:D:43:ASP:OD2	2.53	0.41
2:F:329:ASN:OD1	2:F:330:ARG:NH1	2.52	0.41
11:A:670:HIS:ND1	11:A:742:TYR:HB2	2.35	0.41
12:B:312:THR:HG22	12:B:314:ARG:H	1.85	0.41
2:J:23:GLY:H	2:J:26:SER:HG	1.68	0.41
3:G:159:ILE:HD11	3:G:180:LEU:HD11	2.03	0.41
11:A:902:ASN:HB3	11:A:2071:MET:HE3	2.02	0.41
3:E:107:LYS:HG3	3:E:110:GLU:H	1.85	0.41
3:E:313:THR:HG21	2:J:303:MET:HG3	2.02	0.41
3:E:316:HIS:HD2	3:E:354:LEU:HD13	1.86	0.41
2:J:351:LEU:HA	2:J:354:LEU:HG	2.01	0.41
14:K:383:ASN:O	14:K:389:ARG:NE	2.46	0.41
3:G:65:ALA:HB3	3:G:358:VAL:HG12	2.03	0.41
10:Z:45:DT:H2''	10:Z:46:DG:C8	2.56	0.41
1:C:385:ASN:O	1:C:389:VAL:HG22	2.21	0.40
2:F:378:GLU:HG2	3:G:61:MET:HE1	2.03	0.40
8:V:45:ARG:HA	10:Z:8:DC:OP1	2.20	0.40
11:A:2073:ASP:HB3	3:E:225:LYS:HG3	2.03	0.40
3:E:64:ARG:HB2	3:E:326:ILE:HD12	2.03	0.40
14:K:220:PRO:HG3	14:K:290:PRO:HB3	2.03	0.40
1:C:277:VAL:HB	1:C:278:PRO:HD3	2.03	0.40
3:G:210:ALA:HB2	3:G:220:TYR:CD1	2.56	0.40
3:G:447:LEU:HD13	2:H:343:PRO:O	2.20	0.40
10:Z:-15:DA:H2''	10:Z:-14:DA:C8	2.56	0.40
12:B:214:TYR:HA	12:B:266:ILE:HD13	2.04	0.40
3:I:173:ASP:OD1	3:I:174:PRO:HD2	2.21	0.40
3:G:456:LYS:HB3	2:H:333:THR:HG21	2.02	0.40
5:S:29:ARG:NH2	6:T:35:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:705:ARG:O	11:A:709:ARG:HG3	2.21	0.40
3:E:423:ASP:OD1	3:E:423:ASP:N	2.55	0.40
3:G:64:ARG:HE	3:G:64:ARG:HB3	1.61	0.40
9:Y:30:DT:H2'	9:Y:31:DT:H72	2.03	0.40
11:A:235:PHE:CG	11:A:2346:LEU:HD22	2.56	0.40
11:A:701:ALA:O	11:A:705:ARG:HG3	2.22	0.40
3:E:42:GLN:NE2	3:E:364:MET:O	2.47	0.40
15:L:170:ALA:O	15:L:172:PRO:HD3	2.21	0.40
14:M:215:ILE:HG21	14:M:289:PHE:CZ	2.57	0.40
14:M:406:PHE:HE2	14:M:410:TRP:CZ2	2.39	0.40
8:X:69:ALA:O	8:X:73:THR:HG23	2.21	0.40
9:Y:-52:DG:H2''	9:Y:-51:DC:C6	2.57	0.40
11:A:2072:LEU:O	11:A:2076:GLU:HG3	2.22	0.40
3:E:16:ALA:N	3:E:19:SER:OG	2.49	0.40
3:E:53:VAL:HG22	3:E:83:ILE:HG23	2.04	0.40
3:E:389:GLU:HG2	3:E:427:LYS:HD3	2.04	0.40
3:I:133:GLY:HA2	3:I:224:PRO:HG2	2.02	0.40
15:L:272:CYS:HB3	15:L:276:GLU:HB2	2.02	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	C	394/396 (100%)	379 (96%)	15 (4%)	0	100	100
2	F	436/463 (94%)	429 (98%)	7 (2%)	0	100	100
2	H	428/463 (92%)	419 (98%)	9 (2%)	0	100	100
2	J	412/463 (89%)	404 (98%)	8 (2%)	0	100	100
3	E	429/456 (94%)	424 (99%)	5 (1%)	0	100	100
3	G	443/456 (97%)	440 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	432/456 (95%)	424 (98%)	8 (2%)	0	100	100
4	N	39/467 (8%)	38 (97%)	1 (3%)	0	100	100
5	Q	94/128 (73%)	91 (97%)	3 (3%)	0	100	100
5	S	102/128 (80%)	101 (99%)	1 (1%)	0	100	100
6	R	90/125 (72%)	88 (98%)	2 (2%)	0	100	100
6	T	93/125 (74%)	91 (98%)	2 (2%)	0	100	100
7	U	88/135 (65%)	88 (100%)	0	0	100	100
7	W	94/135 (70%)	91 (97%)	3 (3%)	0	100	100
8	V	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
8	X	79/102 (78%)	78 (99%)	1 (1%)	0	100	100
11	A	870/3230 (27%)	857 (98%)	13 (2%)	0	100	100
12	B	162/364 (44%)	160 (99%)	2 (1%)	0	100	100
13	D	101/154 (66%)	99 (98%)	2 (2%)	0	100	100
14	K	399/429 (93%)	391 (98%)	8 (2%)	0	100	100
14	M	392/429 (91%)	389 (99%)	3 (1%)	0	100	100
15	L	357/375 (95%)	352 (99%)	5 (1%)	0	100	100
16	P	93/299 (31%)	90 (97%)	3 (3%)	0	100	100
All	All	6104/9880 (62%)	5999 (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	C	361/361 (100%)	361 (100%)	0	100	100
2	F	368/390 (94%)	368 (100%)	0	100	100
2	H	365/390 (94%)	365 (100%)	0	100	100
2	J	354/390 (91%)	354 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	367/387 (95%)	367 (100%)	0	100	100
3	G	376/387 (97%)	376 (100%)	0	100	100
3	I	370/387 (96%)	370 (100%)	0	100	100
4	N	34/400 (8%)	34 (100%)	0	100	100
5	Q	75/101 (74%)	75 (100%)	0	100	100
5	S	82/101 (81%)	82 (100%)	0	100	100
6	R	78/105 (74%)	78 (100%)	0	100	100
6	T	81/105 (77%)	81 (100%)	0	100	100
7	U	79/110 (72%)	79 (100%)	0	100	100
7	W	84/110 (76%)	84 (100%)	0	100	100
8	V	64/78 (82%)	64 (100%)	0	100	100
8	X	66/78 (85%)	66 (100%)	0	100	100
11	A	790/2721 (29%)	790 (100%)	0	100	100
12	B	150/312 (48%)	150 (100%)	0	100	100
13	D	89/133 (67%)	89 (100%)	0	100	100
14	K	345/364 (95%)	345 (100%)	0	100	100
14	M	341/364 (94%)	341 (100%)	0	100	100
15	L	307/318 (96%)	307 (100%)	0	100	100
16	P	84/261 (32%)	84 (100%)	0	100	100
All	All	5310/8353 (64%)	5310 (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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	203	ASN
2	F	275	GLN
3	G	115	ASN
3	G	316	HIS
3	G	380	GLN
4	N	113	HIS
6	R	84	ASN
5	S	38	ASN
7	U	68	GLN

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Mol	Chain	Res	Type
8	V	93	GLN
8	X	27	GLN
11	A	232	HIS
11	A	768	GLN
11	A	1906	GLN
12	B	296	HIS
2	H	25	HIS
2	H	27	HIS
2	H	146	GLN
2	H	245	HIS
2	H	453	ASN
3	I	34	GLN
3	I	115	ASN
3	I	169	GLN
3	I	241	HIS
3	I	262	GLN
3	I	393	HIS
3	I	408	GLN
2	J	78	GLN
2	J	245	HIS
14	K	251	HIS
14	K	365	ASN
14	K	383	ASN
15	L	12	ASN
15	L	263	GLN
14	M	73	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](#)

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

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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
19	ADP	I	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.77	8 (18%)
19	ADP	J	501	18	28,29,29	1.41	4 (14%)	43,45,45	1.77	9 (20%)
19	ADP	E	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.76	8 (18%)
19	ADP	H	501	18	28,29,29	1.41	4 (14%)	43,45,45	1.79	9 (20%)
17	ATP	K	501	18	32,33,33	0.38	0	48,52,52	0.45	0
19	ADP	G	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.76	8 (18%)
17	ATP	C	401	18	32,33,33	0.27	0	48,52,52	0.44	0
19	ADP	F	501	18	28,29,29	1.40	4 (14%)	43,45,45	1.76	7 (16%)
17	ATP	A	3301	18	32,33,33	0.29	0	48,52,52	0.44	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
19	ADP	I	501	-	-	3/16/32/32	0/3/3/3
19	ADP	J	501	18	-	7/16/32/32	0/3/3/3
19	ADP	E	501	-	-	3/16/32/32	0/3/3/3
19	ADP	H	501	18	-	0/16/32/32	0/3/3/3
17	ATP	K	501	18	-	1/22/38/38	0/3/3/3
19	ADP	G	501	-	-	5/16/32/32	0/3/3/3
17	ATP	C	401	18	-	0/22/38/38	0/3/3/3
19	ADP	F	501	18	-	4/16/32/32	0/3/3/3
17	ATP	A	3301	18	-	2/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	E	501	ADP	C5-C4	4.73	1.47	1.39
19	I	501	ADP	C5-C4	4.71	1.47	1.39
19	J	501	ADP	C5-C4	4.68	1.47	1.39
19	G	501	ADP	C5-C4	4.67	1.47	1.39
19	F	501	ADP	C5-C4	4.67	1.47	1.39
19	H	501	ADP	C5-C4	4.64	1.47	1.39
19	J	501	ADP	C5-C6	2.73	1.48	1.41
19	H	501	ADP	C5-C6	2.72	1.48	1.41
19	E	501	ADP	C5-C6	2.71	1.48	1.41
19	I	501	ADP	C5-C6	2.71	1.48	1.41
19	G	501	ADP	C5-C6	2.68	1.48	1.41
19	F	501	ADP	C5-C6	2.68	1.48	1.41
19	H	501	ADP	C8-N7	2.33	1.36	1.31
19	J	501	ADP	C8-N7	2.33	1.36	1.31
19	E	501	ADP	C8-N7	2.33	1.36	1.31
19	I	501	ADP	C8-N7	2.32	1.36	1.31
19	F	501	ADP	C5-N7	-2.31	1.34	1.39
19	G	501	ADP	C5-N7	-2.31	1.34	1.39
19	I	501	ADP	C5-N7	-2.29	1.34	1.39
19	J	501	ADP	C5-N7	-2.29	1.34	1.39
19	F	501	ADP	C8-N7	2.29	1.36	1.31
19	E	501	ADP	C5-N7	-2.29	1.34	1.39
19	G	501	ADP	C8-N7	2.29	1.36	1.31
19	H	501	ADP	C5-N7	-2.29	1.34	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	501	ADP	C5-C4-N3	-5.91	118.58	126.72
19	I	501	ADP	C5-C4-N3	-5.87	118.63	126.72
19	E	501	ADP	C5-C4-N3	-5.87	118.63	126.72
19	G	501	ADP	C5-C4-N3	-5.82	118.70	126.72
19	J	501	ADP	C5-C4-N3	-5.81	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	135.09	127.17
19	H	501	ADP	N3-C4-N9	4.65	135.07	127.17
19	I	501	ADP	N3-C4-N9	4.64	135.06	127.17
19	G	501	ADP	N3-C4-N9	4.62	135.03	127.17
19	F	501	ADP	N3-C4-N9	4.61	135.00	127.17
19	J	501	ADP	N3-C4-N9	4.59	134.97	127.17
19	H	501	ADP	C2-N3-C4	3.73	120.94	111.83
19	I	501	ADP	C2-N3-C4	3.68	120.83	111.83
19	E	501	ADP	C2-N3-C4	3.68	120.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	501	ADP	C2-N3-C4	3.63	120.71	111.83
19	F	501	ADP	C2-N3-C4	3.61	120.65	111.83
19	J	501	ADP	C2-N3-C4	3.61	120.65	111.83
19	J	501	ADP	C4-C5-N7	-3.54	106.54	110.58
19	H	501	ADP	C4-C5-N7	-3.52	106.56	110.58
19	G	501	ADP	C4-C5-N7	-3.46	106.63	110.58
19	E	501	ADP	C4-C5-N7	-3.46	106.63	110.58
19	I	501	ADP	C4-C5-N7	-3.45	106.64	110.58
19	F	501	ADP	C4-C5-N7	-3.43	106.66	110.58
19	H	501	ADP	N3-C2-N1	-3.21	123.73	128.58
19	E	501	ADP	N3-C2-N1	-3.16	123.80	128.58
19	I	501	ADP	N3-C2-N1	-3.16	123.81	128.58
19	G	501	ADP	N3-C2-N1	-3.12	123.86	128.58
19	F	501	ADP	N3-C2-N1	-3.07	123.93	128.58
19	J	501	ADP	N3-C2-N1	-3.03	124.00	128.58
19	J	501	ADP	C4-N9-C8	2.70	108.57	105.74
19	F	501	ADP	C4-N9-C8	2.65	108.52	105.74
19	G	501	ADP	C4-N9-C8	2.64	108.51	105.74
19	H	501	ADP	C4-N9-C8	2.63	108.50	105.74
19	J	501	ADP	C5-N7-C8	2.61	107.55	103.45
19	H	501	ADP	C5-N7-C8	2.59	107.53	103.45
19	E	501	ADP	C4-N9-C8	2.59	108.46	105.74
19	G	501	ADP	C5-N7-C8	2.53	107.43	103.45
19	I	501	ADP	C4-N9-C8	2.52	108.39	105.74
19	E	501	ADP	C5-N7-C8	2.52	107.41	103.45
19	F	501	ADP	C5-N7-C8	2.52	107.41	103.45
19	I	501	ADP	C5-N7-C8	2.51	107.40	103.45
19	H	501	ADP	C6-C5-N7	2.06	136.06	132.09
19	J	501	ADP	N9-C8-N7	-2.05	111.02	113.94
19	J	501	ADP	C6-C5-N7	2.05	136.04	132.09
19	E	501	ADP	C6-C5-N7	2.04	136.01	132.09
19	I	501	ADP	C6-C5-N7	2.02	135.99	132.09
19	G	501	ADP	C6-C5-N7	2.02	135.99	132.09
19	H	501	ADP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	3301	ATP	O4'-C4'-C5'-O5'
19	F	501	ADP	PA-O3A-PB-O2B
19	G	501	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
19	G	501	ADP	C5'-O5'-PA-O3A
19	G	501	ADP	O4'-C4'-C5'-O5'
19	J	501	ADP	C5'-O5'-PA-O1A
19	J	501	ADP	C3'-C4'-C5'-O5'
19	G	501	ADP	C3'-C4'-C5'-O5'
19	J	501	ADP	O4'-C4'-C5'-O5'
17	A	3301	ATP	C3'-C4'-C5'-O5'
19	E	501	ADP	PA-O3A-PB-O1B
19	I	501	ADP	PA-O3A-PB-O1B
19	F	501	ADP	PA-O3A-PB-O3B
19	J	501	ADP	PA-O3A-PB-O2B
19	J	501	ADP	PA-O3A-PB-O3B
19	G	501	ADP	C5'-O5'-PA-O2A
19	J	501	ADP	C5'-O5'-PA-O2A
19	J	501	ADP	C5'-O5'-PA-O3A
19	F	501	ADP	PA-O3A-PB-O1B
19	E	501	ADP	PA-O3A-PB-O2B
19	E	501	ADP	PA-O3A-PB-O3B
19	I	501	ADP	PA-O3A-PB-O2B
19	I	501	ADP	PA-O3A-PB-O3B
19	F	501	ADP	C4'-C5'-O5'-PA
17	K	501	ATP	PG-O3B-PB-O2B

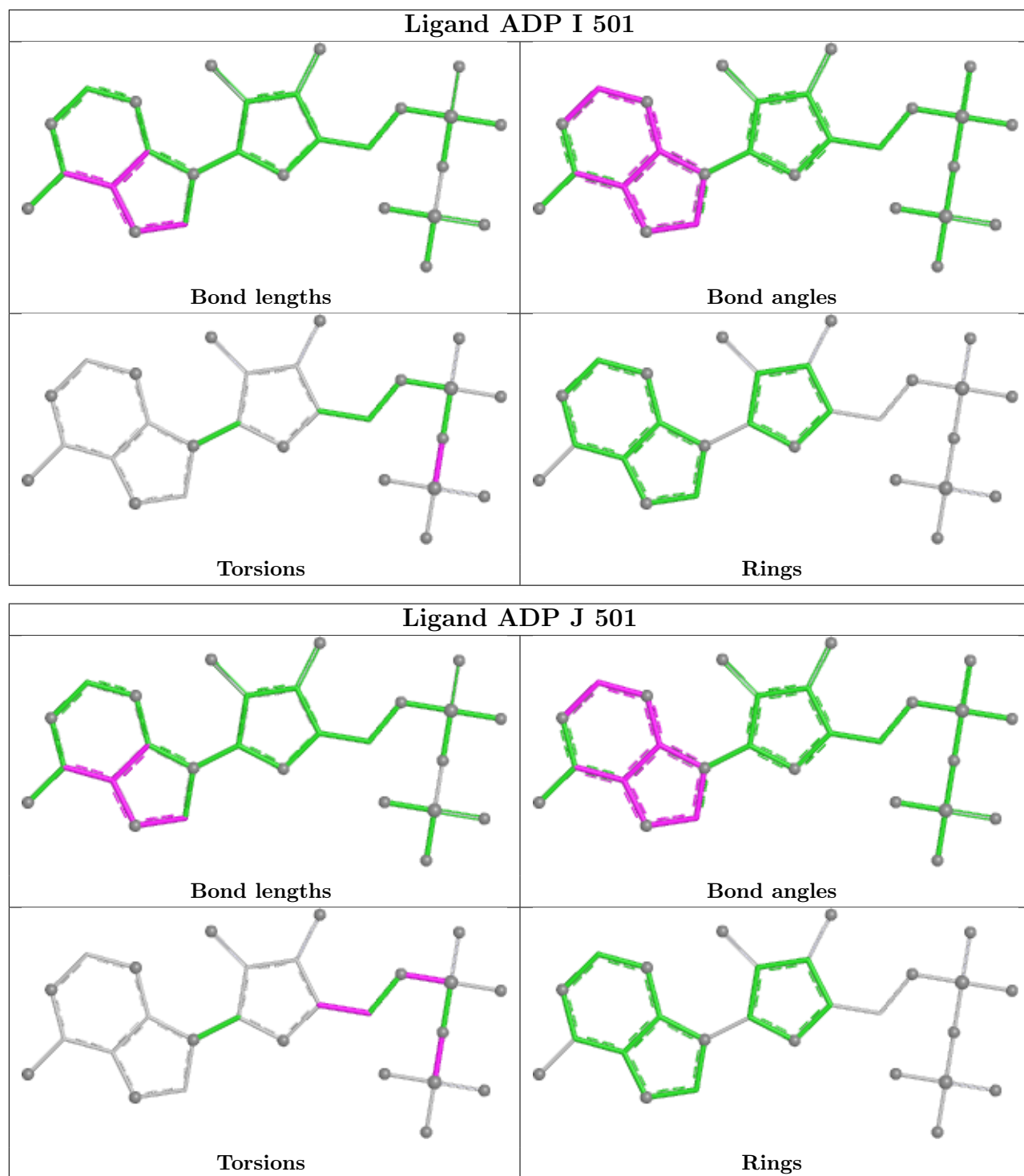
There are no ring outliers.

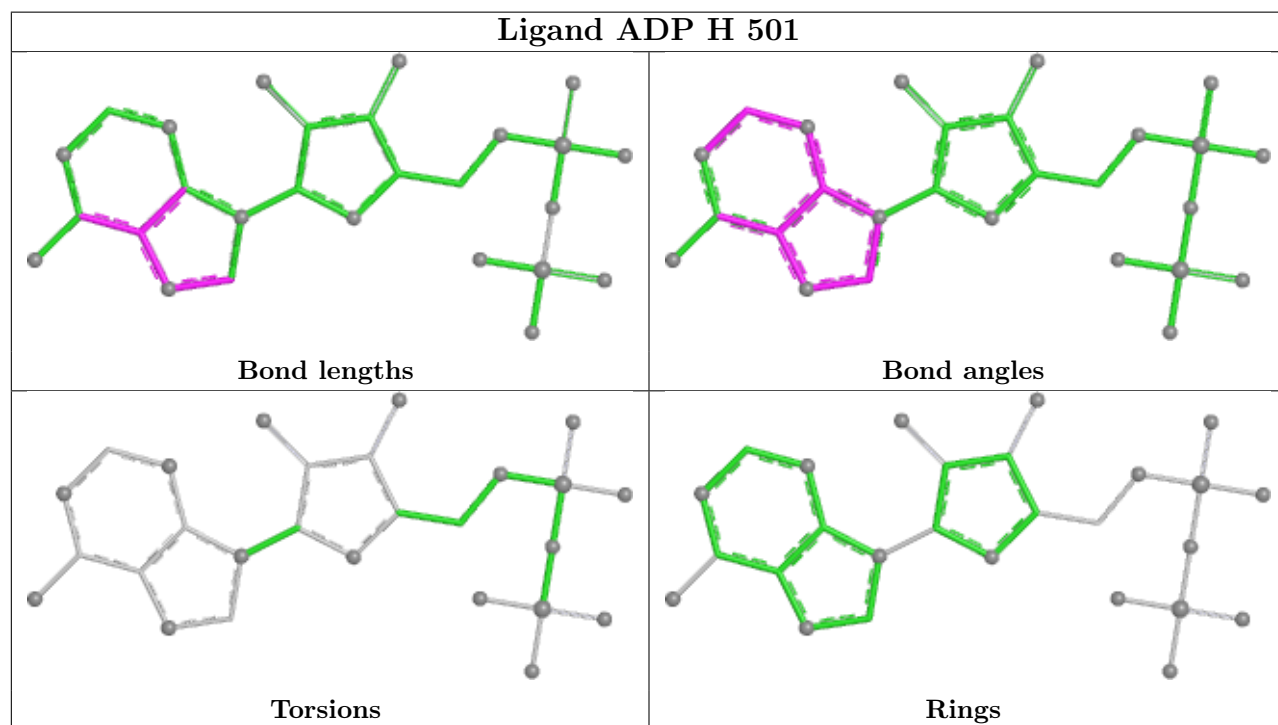
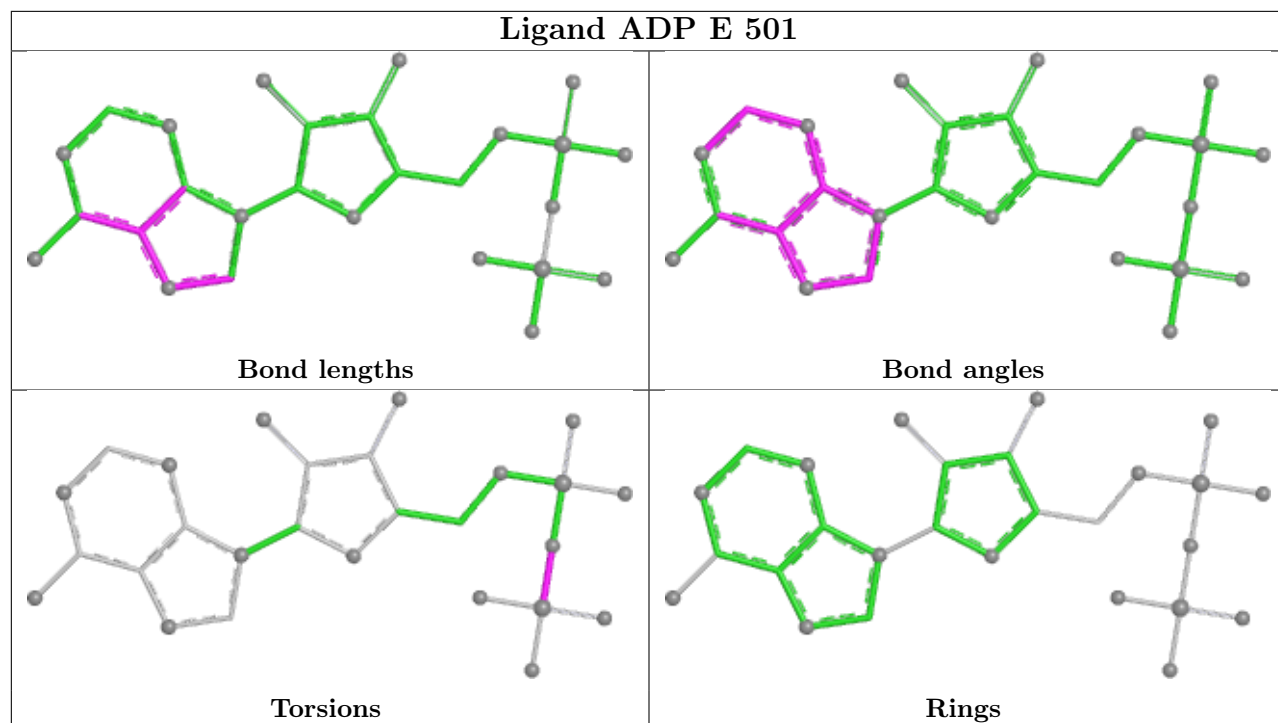
3 monomers are involved in 4 short contacts:

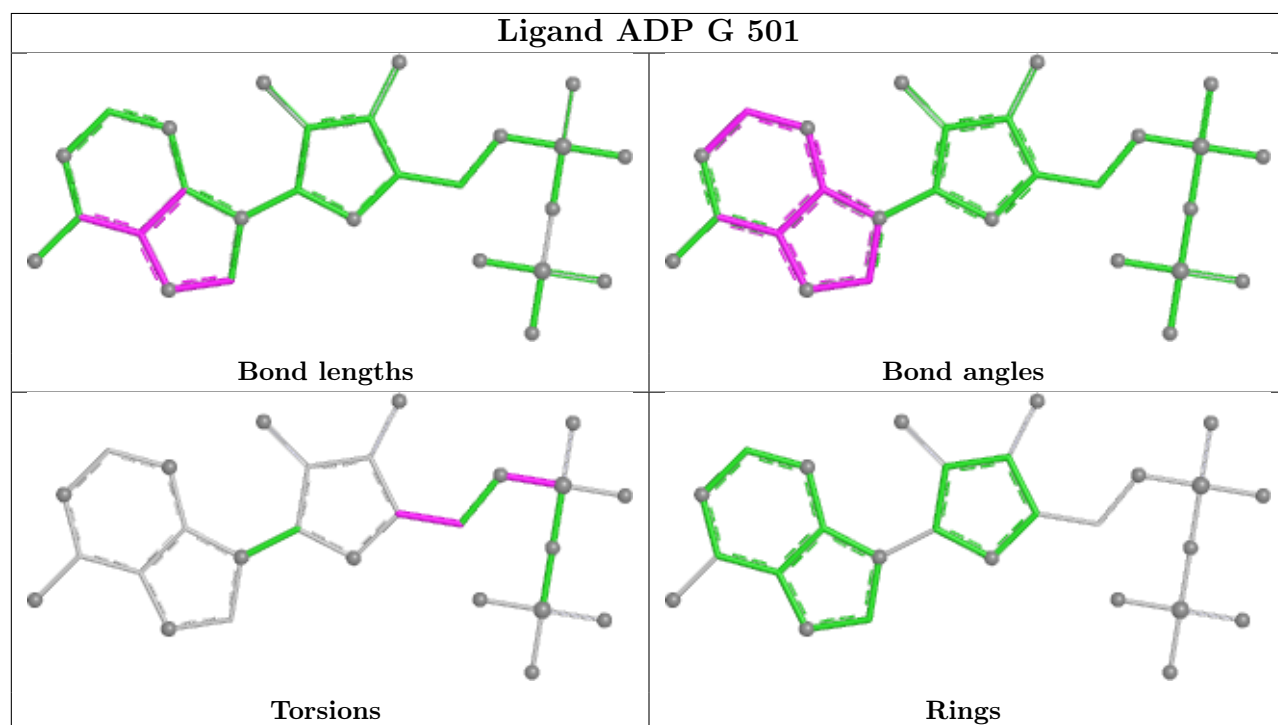
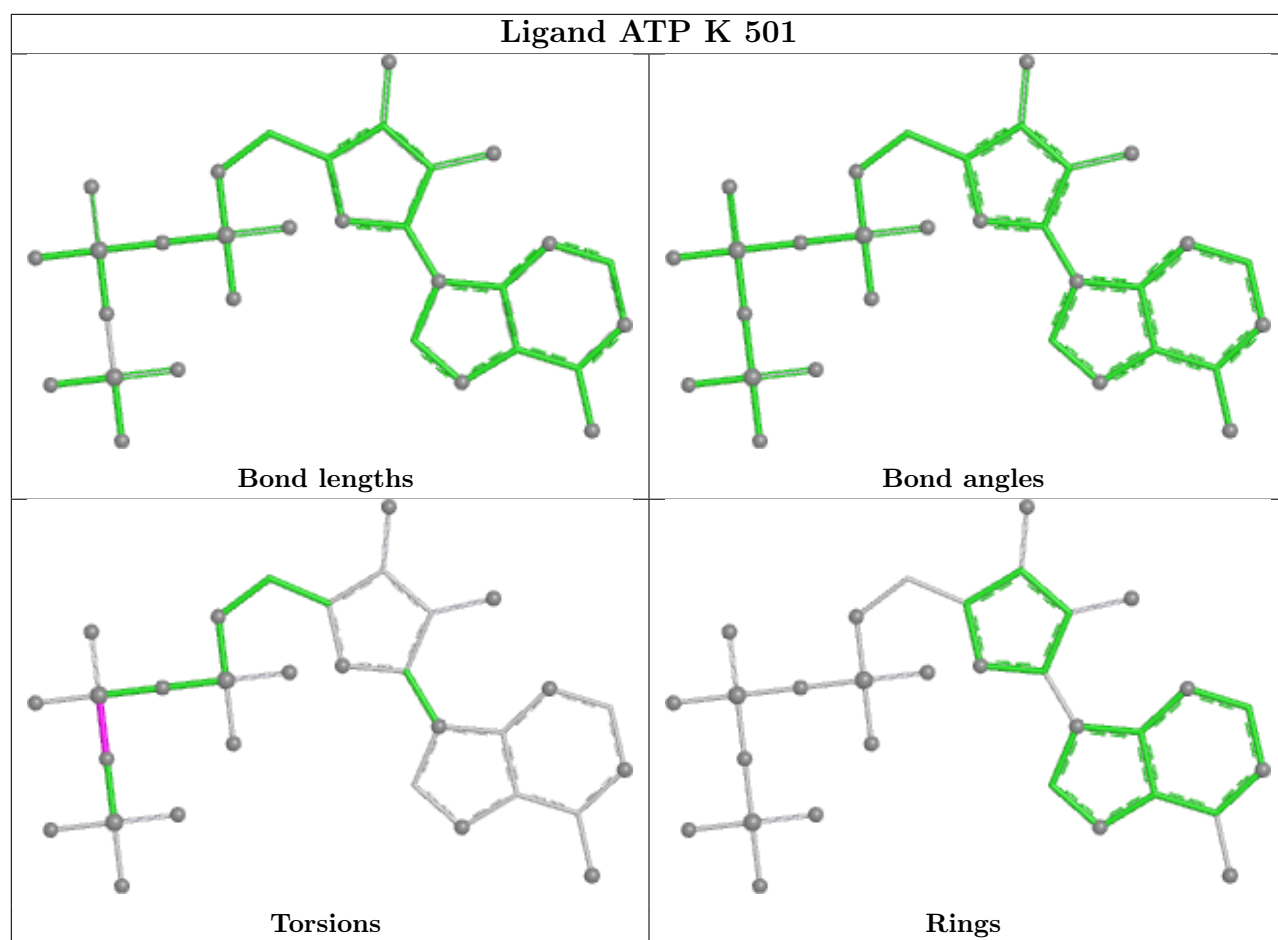
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	E	501	ADP	1	0
19	H	501	ADP	1	0
19	G	501	ADP	2	0

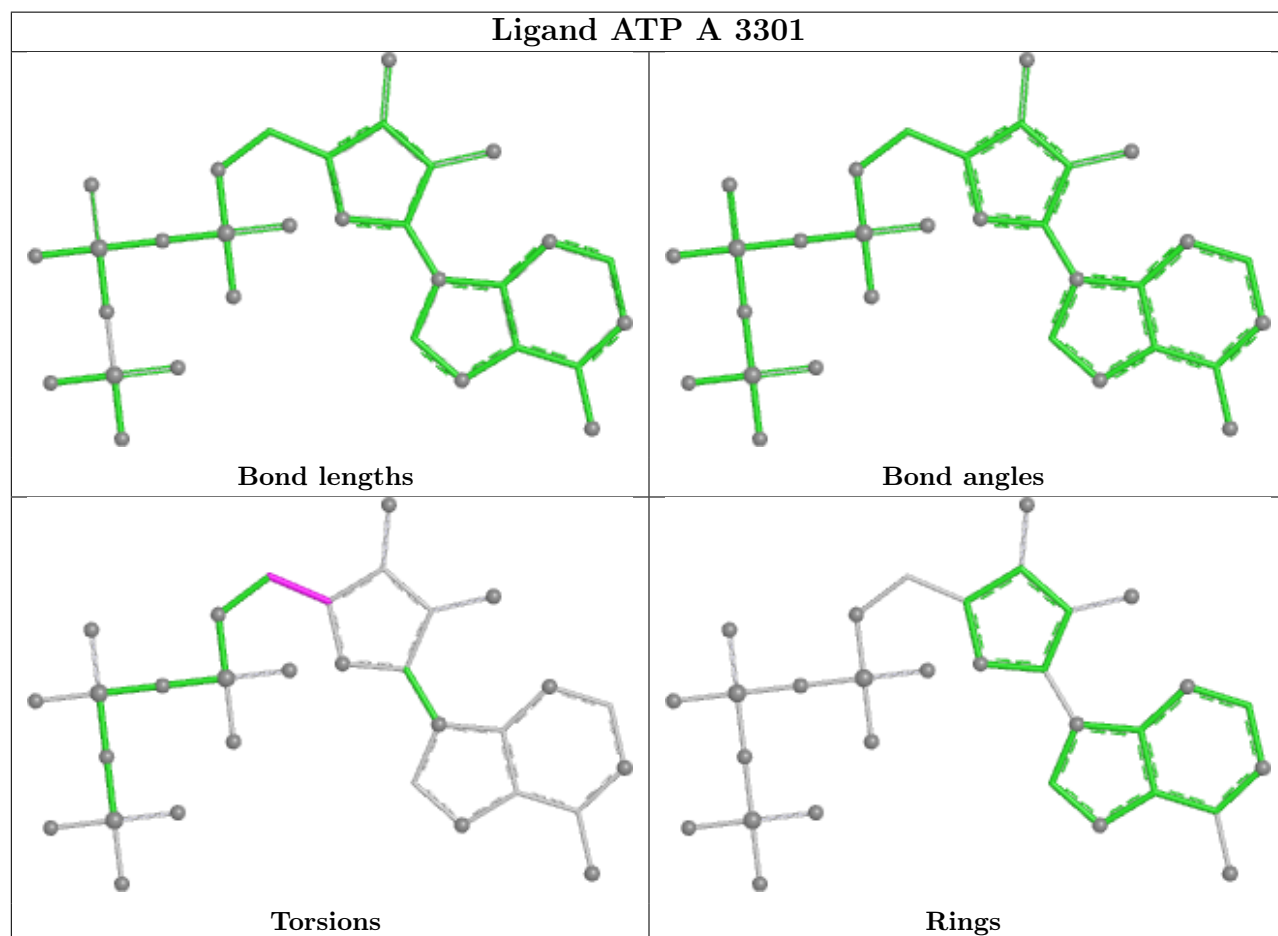
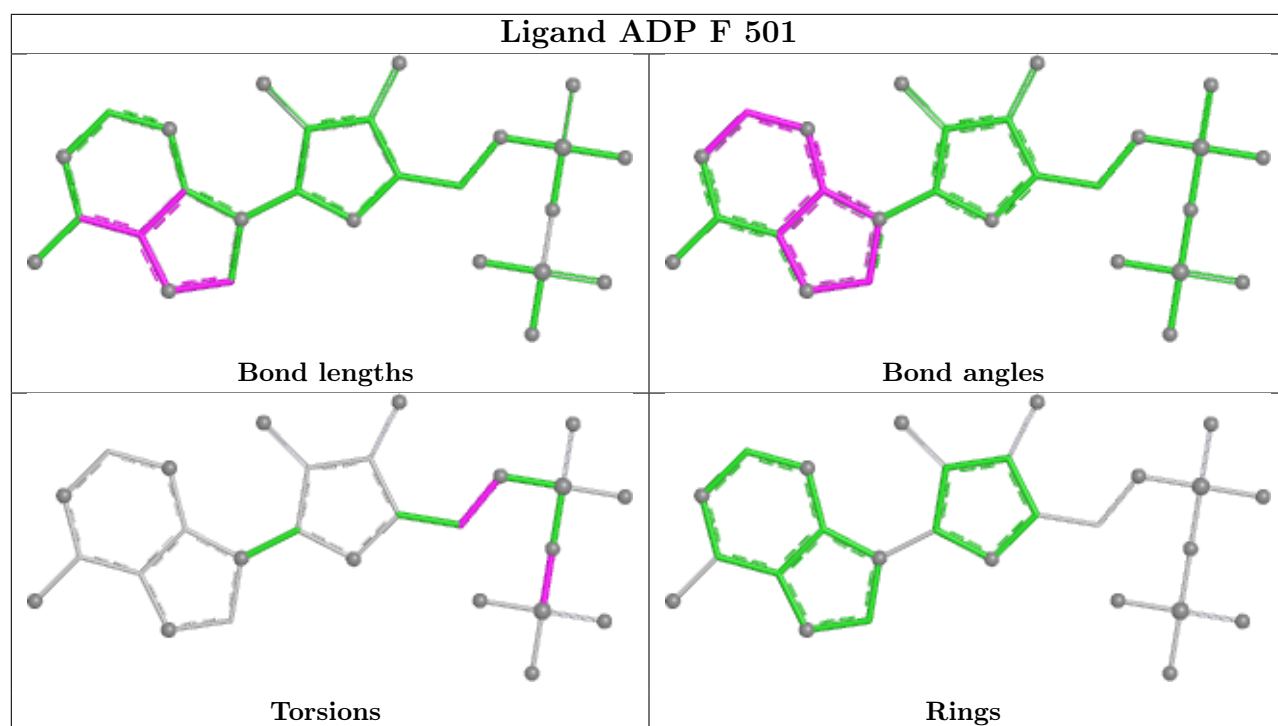
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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.

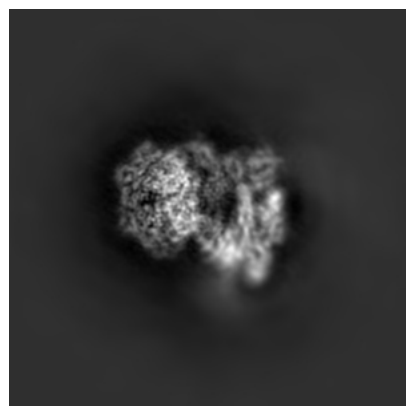
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72456. These allow visual inspection of the internal detail of the map and identification of artifacts.

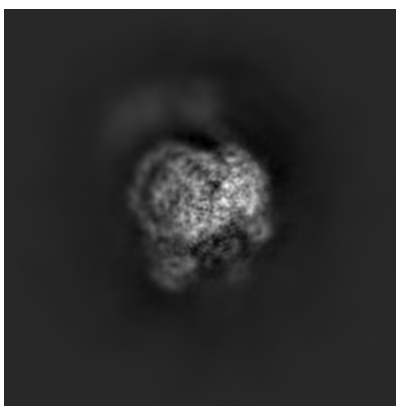
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

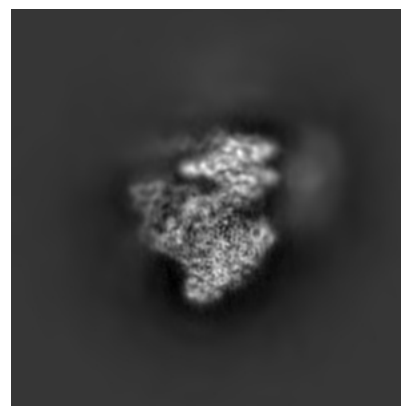
6.1.1 Primary map



X

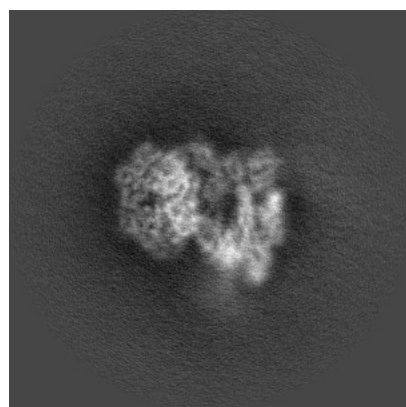


Y

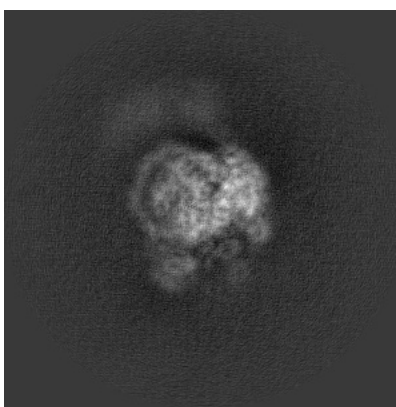


Z

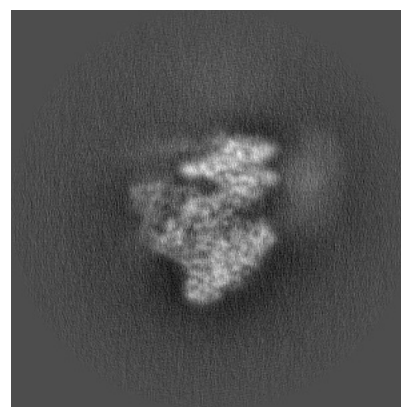
6.1.2 Raw map



X



Y

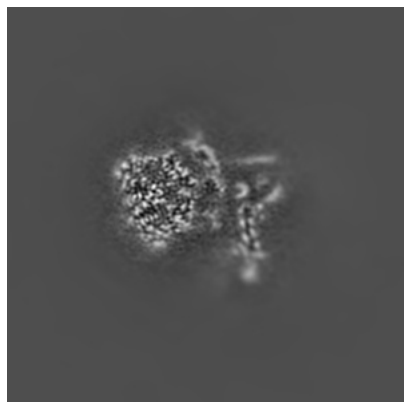


Z

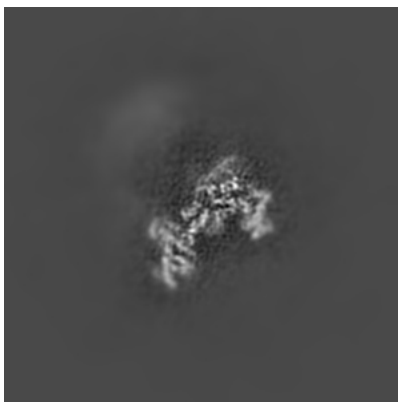
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

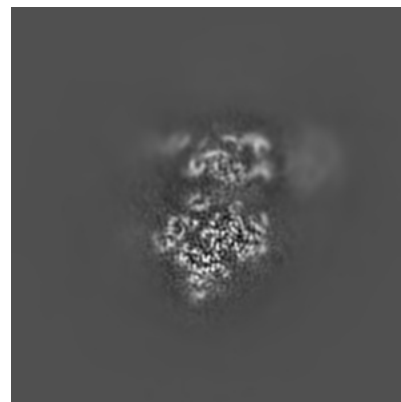
6.2.1 Primary map



X Index: 192

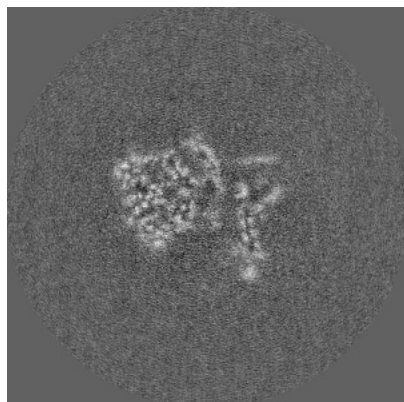


Y Index: 192

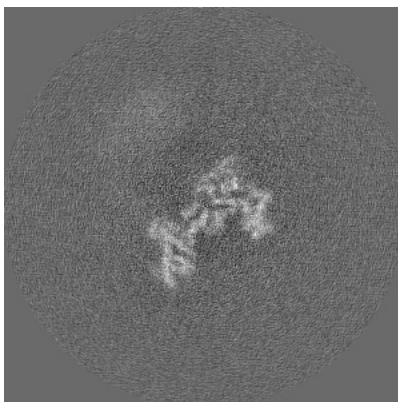


Z Index: 192

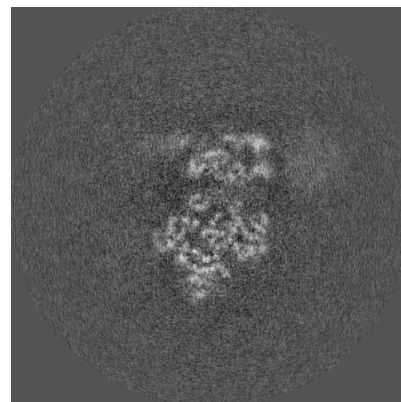
6.2.2 Raw map



X Index: 192



Y Index: 192

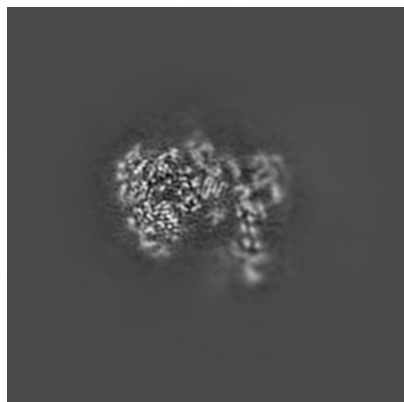


Z Index: 192

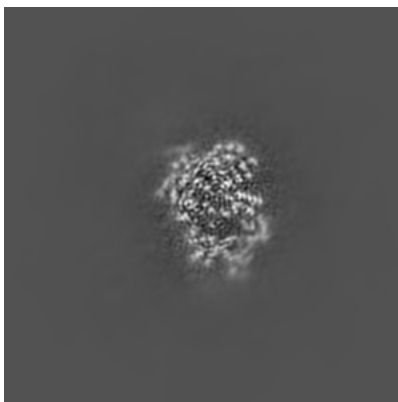
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

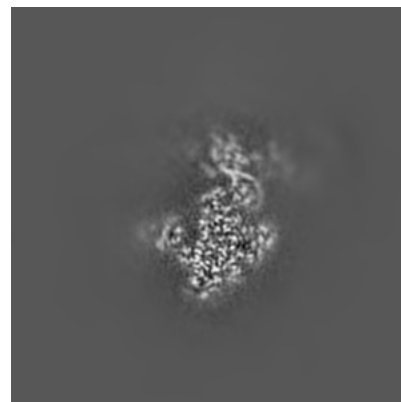
6.3.1 Primary map



X Index: 197

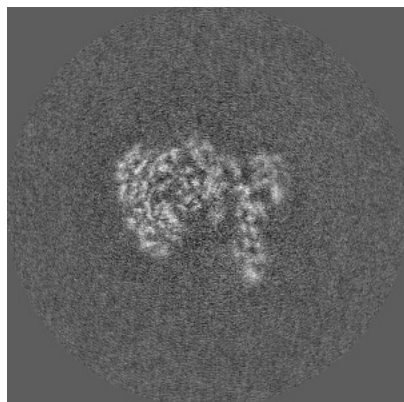


Y Index: 161

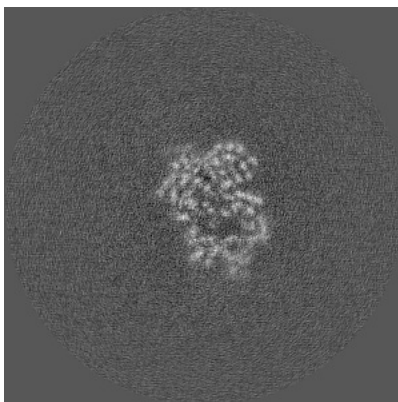


Z Index: 214

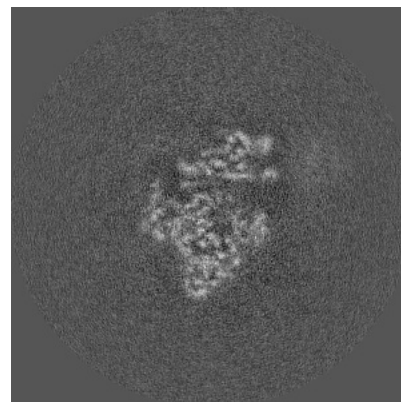
6.3.2 Raw map



X Index: 197



Y Index: 161

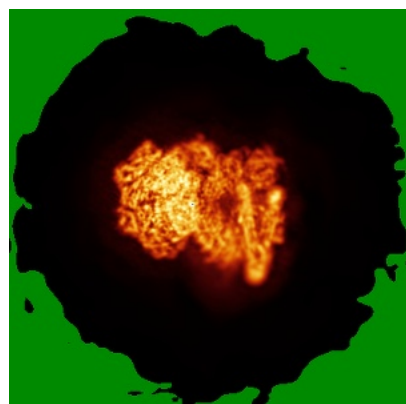


Z Index: 181

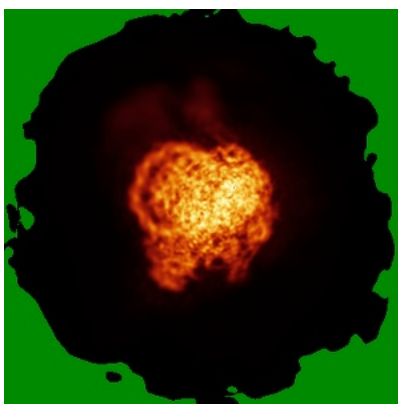
The images above show the largest variance slices of the map in three orthogonal directions.

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

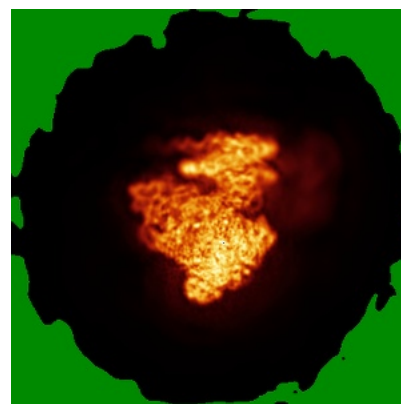
6.4.1 Primary map



X

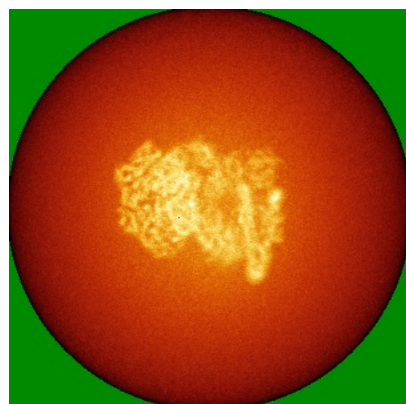


Y

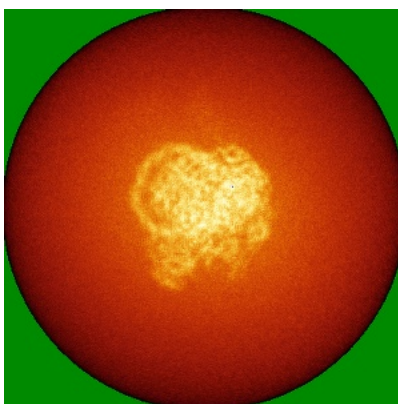


Z

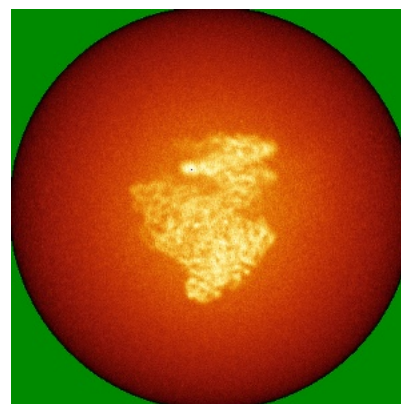
6.4.2 Raw map



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.

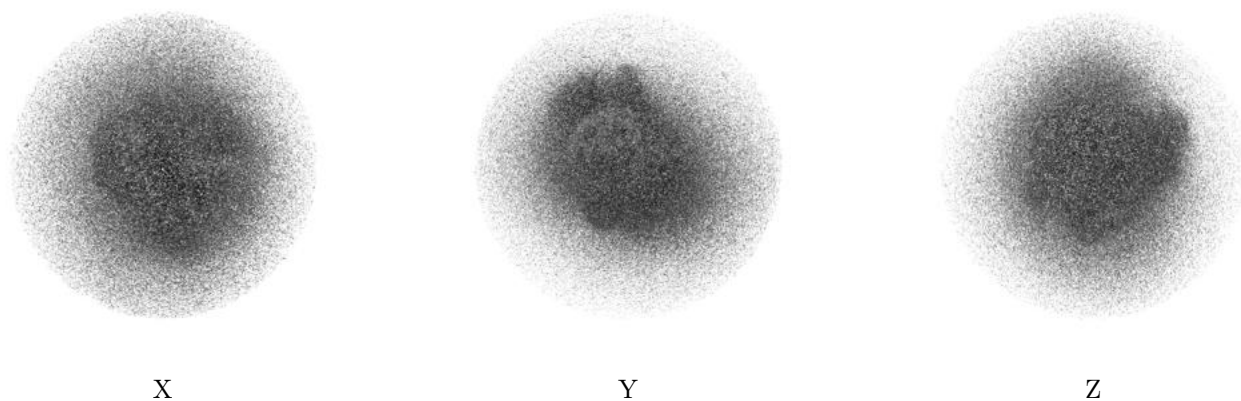
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

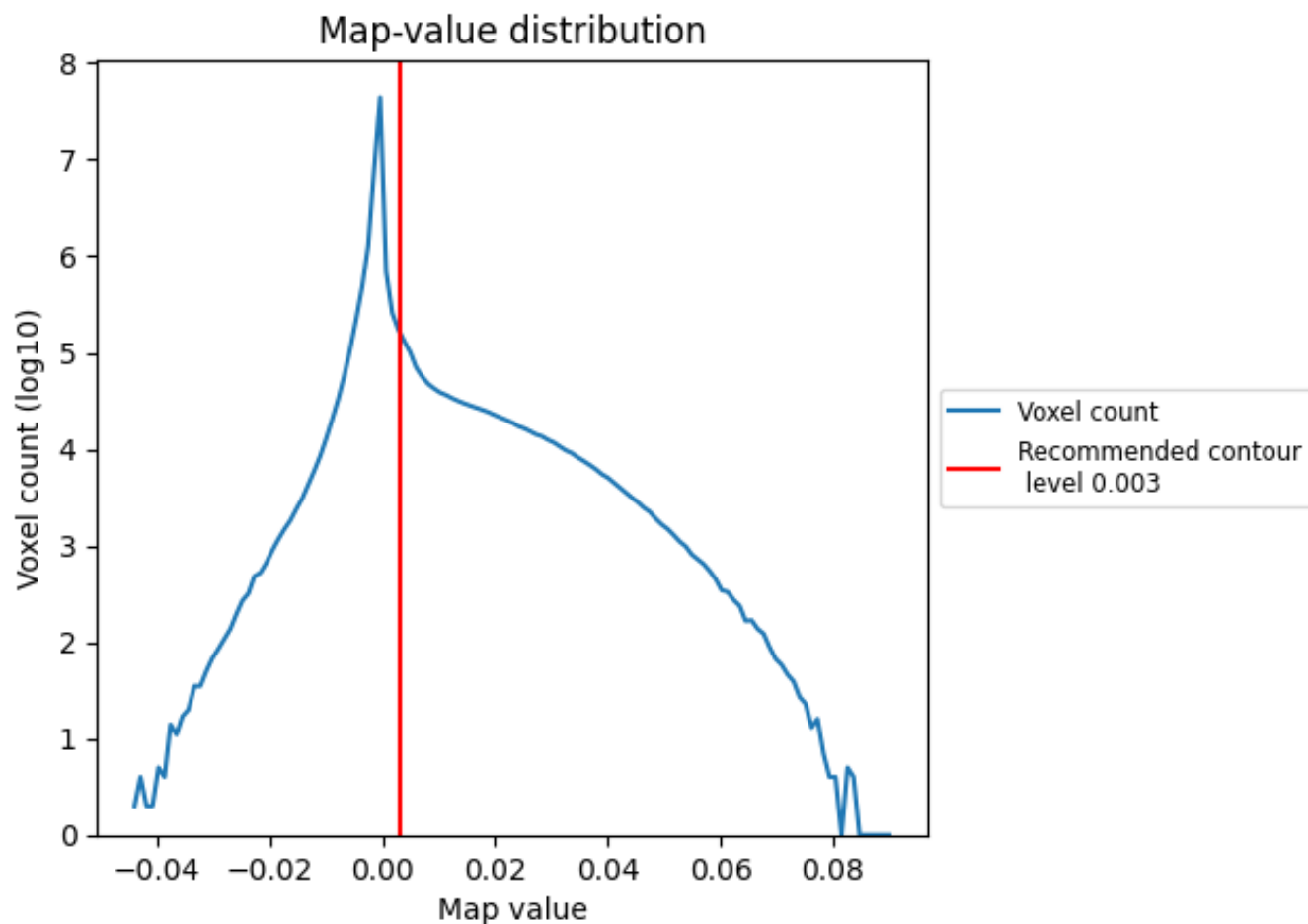
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

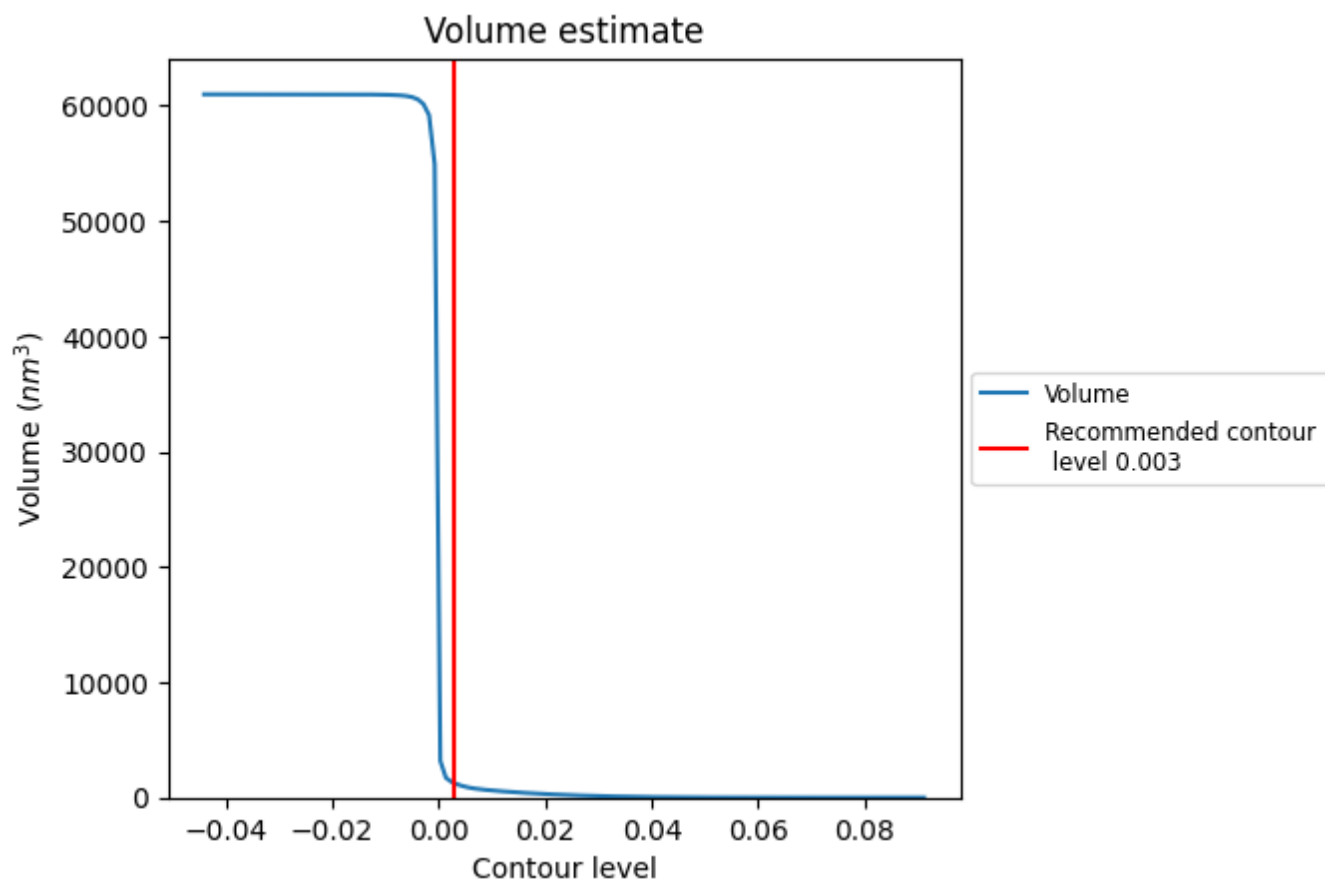
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

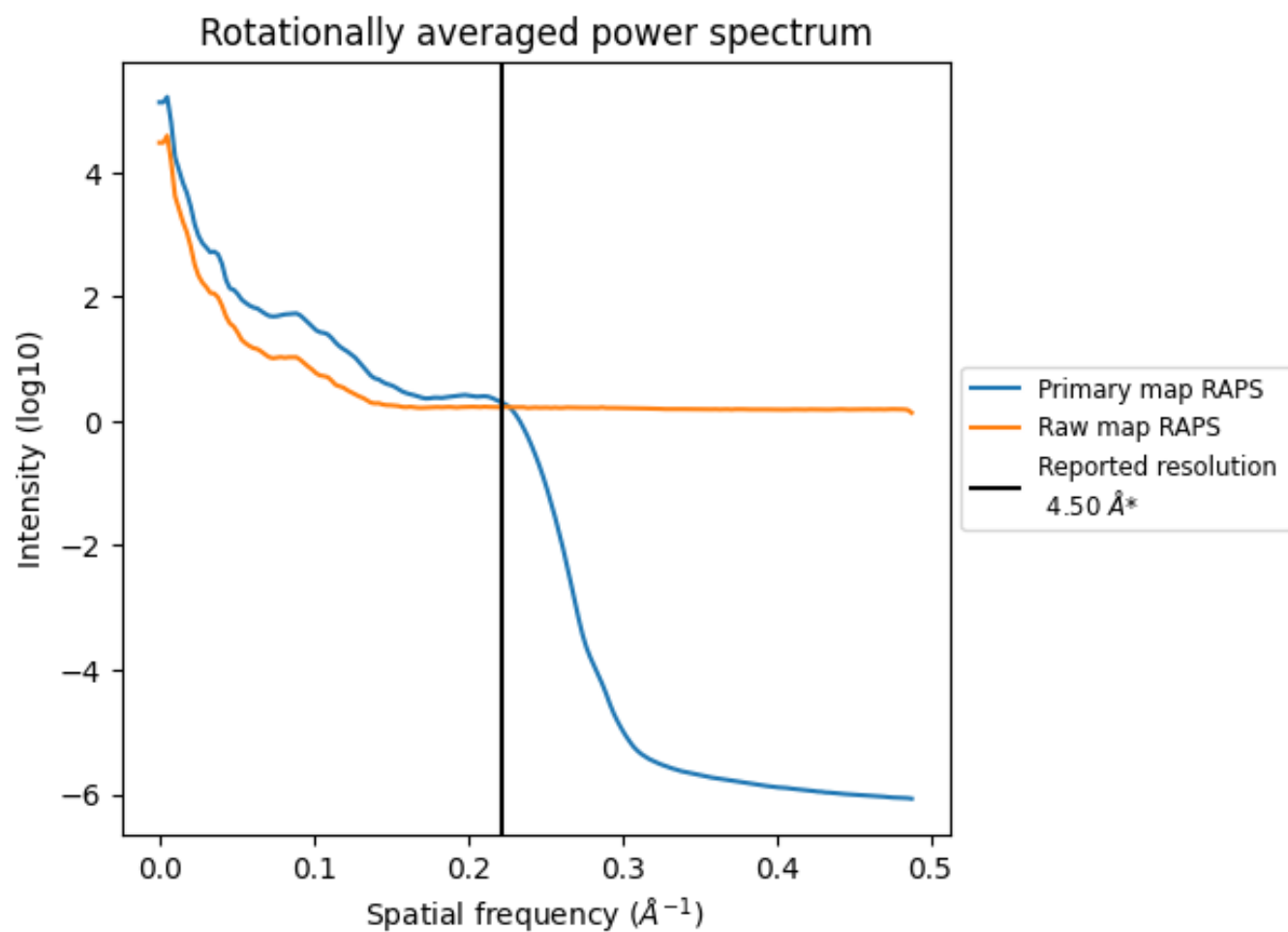
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1245 nm^3 ; this corresponds to an approximate mass of 1124 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 ⓘ

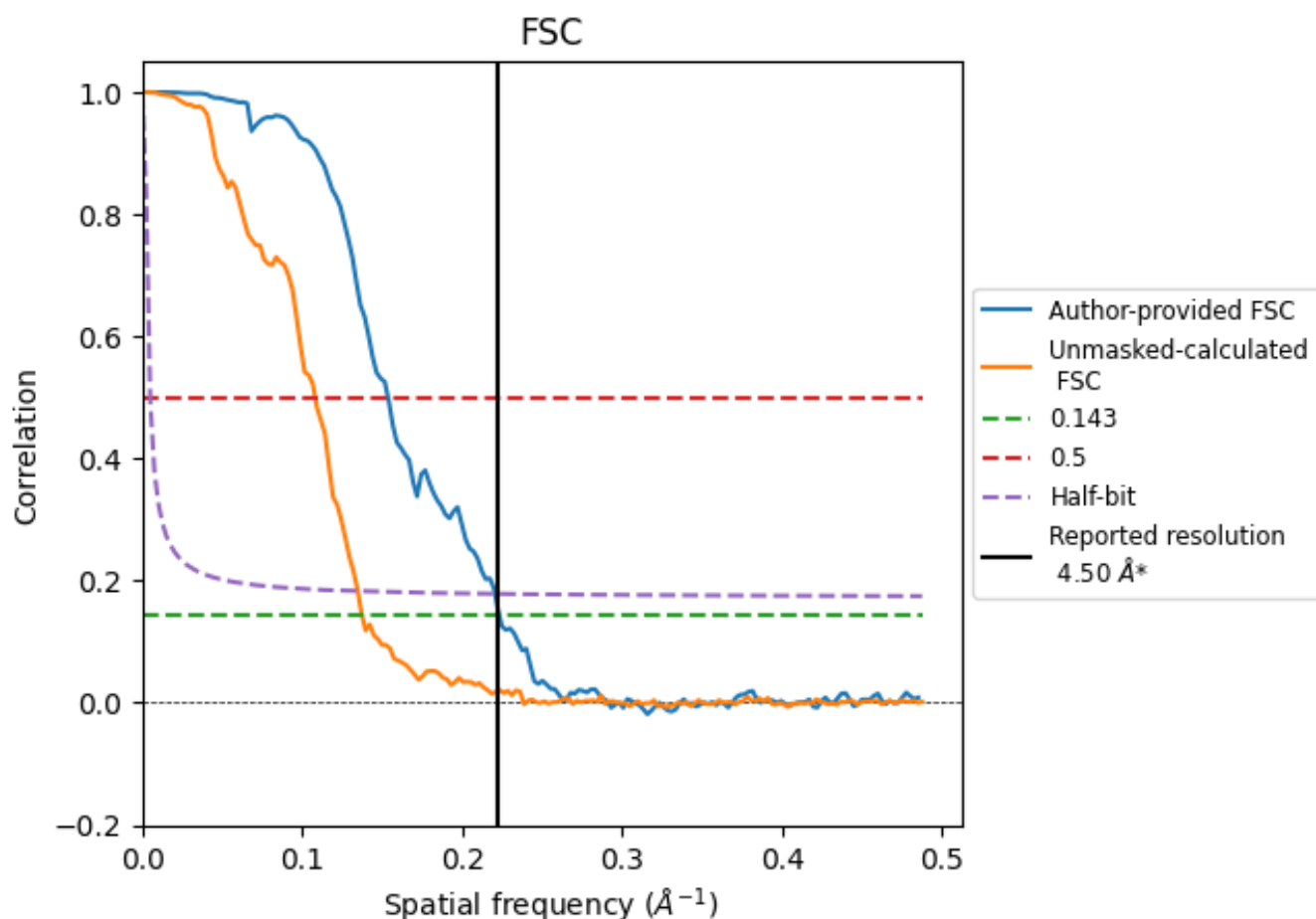


*Reported resolution corresponds to spatial frequency of 0.222 $\text{\AA}^{-1}$

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

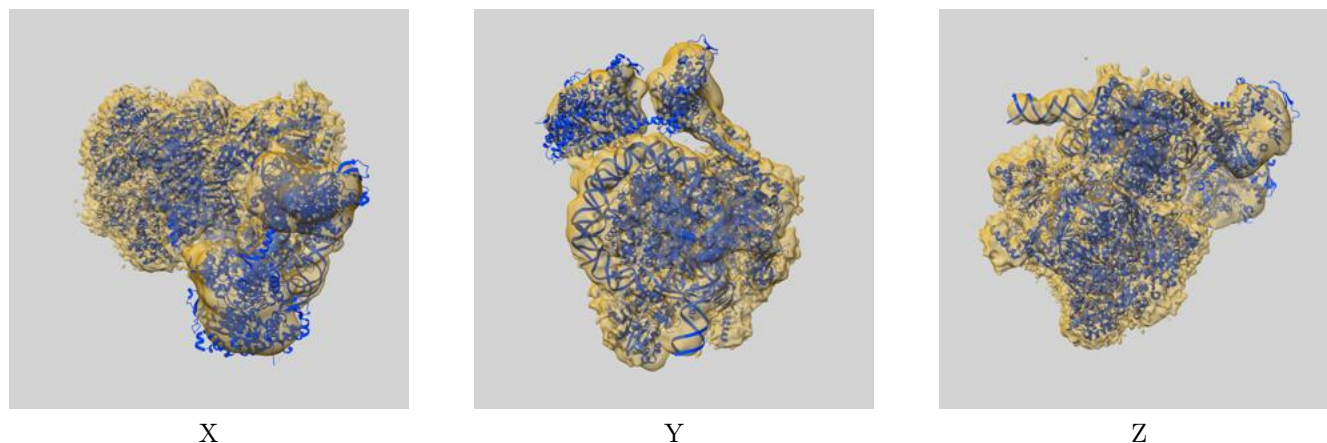
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.48	6.50	4.53
Unmasked-calculated*	7.28	9.24	7.42

*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 7.28 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

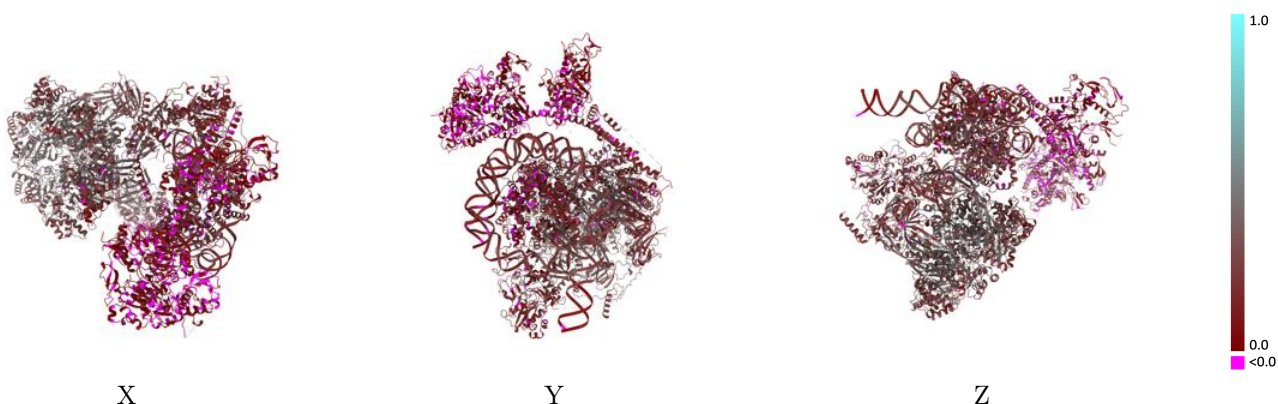
This section contains information regarding the fit between EMDB map EMD-72456 and PDB model 9Y3F. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



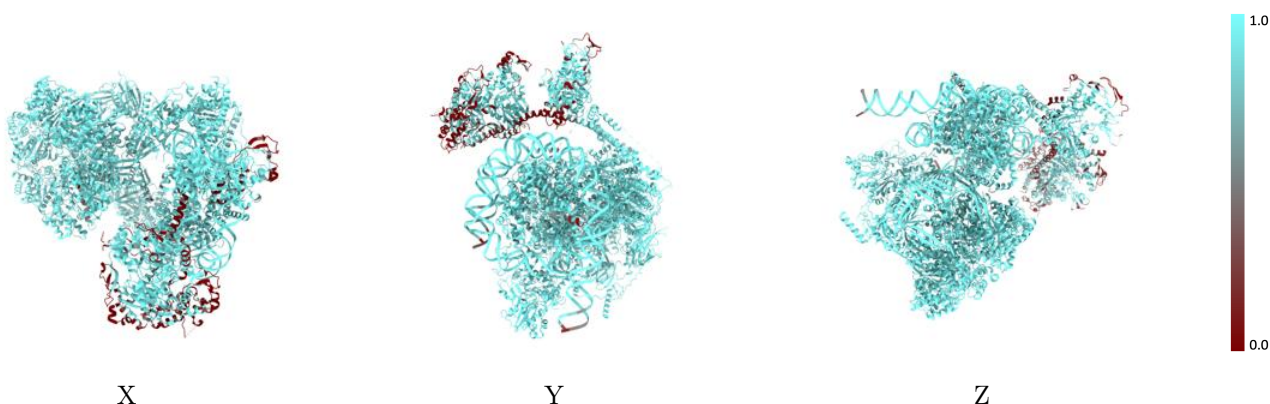
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



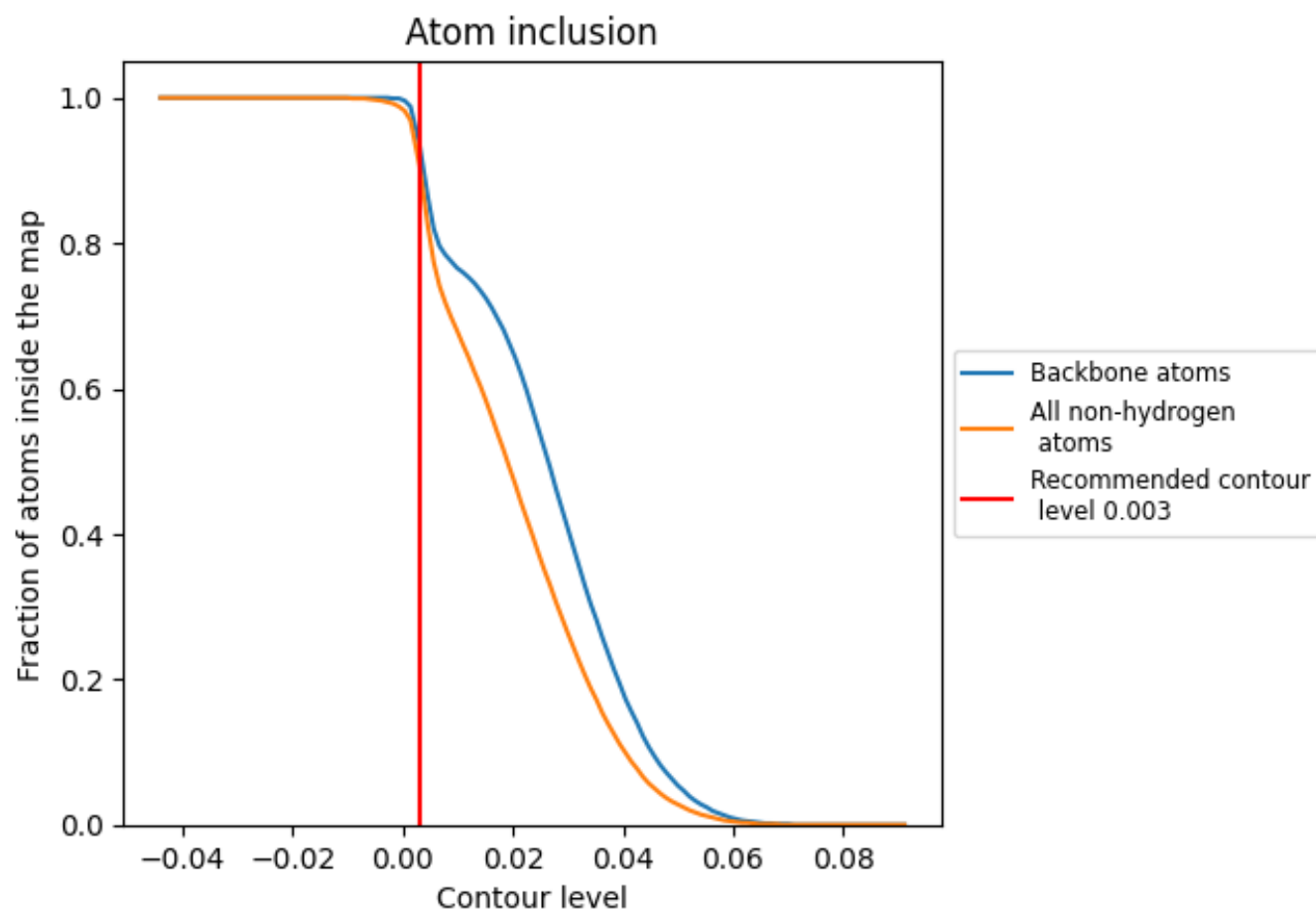
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.2230
A	 0.9150	 0.2390
B	 0.9030	 0.1860
C	 0.9740	 0.1940
D	 0.9510	 0.2410
E	 0.9560	 0.3210
F	 0.9680	 0.3290
G	 0.9720	 0.3210
H	 0.9710	 0.3370
I	 0.9660	 0.3330
J	 0.9620	 0.3170
K	 0.7910	 0.0670
L	 0.7960	 0.0510
M	 0.5640	 0.0300
N	 0.4050	 0.0310
P	 0.8490	 0.1160
Q	 0.9360	 0.1540
R	 0.9430	 0.1510
S	 0.9600	 0.1990
T	 0.9420	 0.1760
U	 0.9480	 0.1480
V	 0.9520	 0.1610
W	 0.9170	 0.2150
X	 0.9320	 0.2150
Y	 0.9480	 0.2000
Z	 0.9550	 0.2140

