Full wwPDB EM Validation Report (i)

May 26, 2024 – 10:59 AM EDT

PDB ID	:	7S67
EMDB ID	:	EMD-24852
Title	:	Extended conformation of daytime state KaiC
Authors	:	Sandate, C.R.; Swan, J.A.; Partch, C.L.; Lander, G.C.
Deposited on	:	2021-09-13
Resolution	:	3.80 Å(reported)
Based on initial model	:	3K0C

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 (i) 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 (1)) were used in the production of this report:

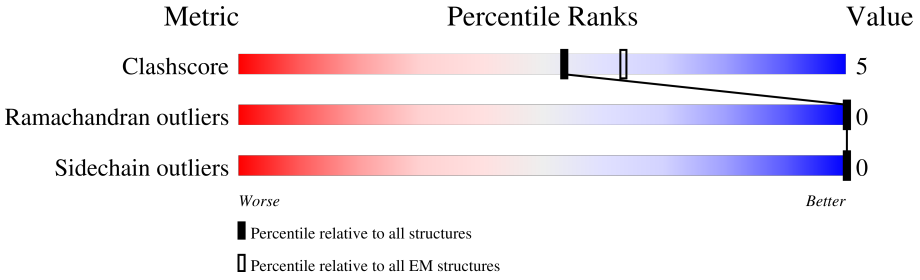
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	519	15% 87% 5% 7%
1	B	519	15% 87% 5% 7%
1	C	519	15% 88% 5% 7%
1	D	519	15% 88% 5% 7%
1	E	519	15% 88% 5% 7%
1	F	519	16% 87% 5% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	601	-	-	X	-
2	ATP	A	605	-	-	X	-
2	ATP	B	601	-	-	X	-
2	ATP	C	601	-	-	X	-
2	ATP	D	601	-	-	X	-
2	ATP	F	601	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23058 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.

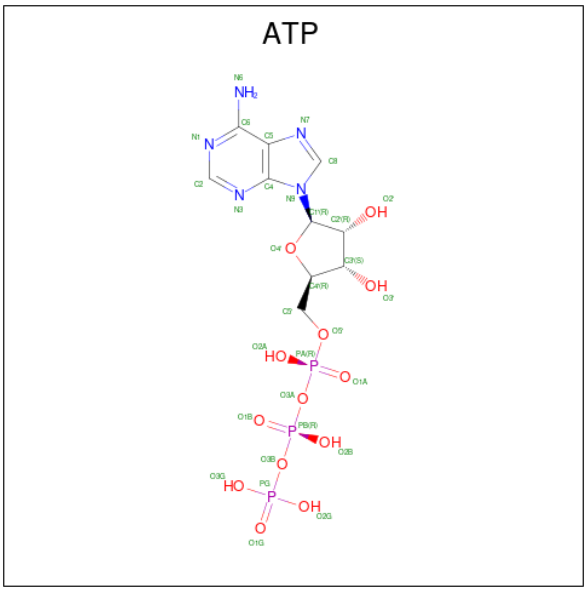
- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	482	3783	2385	666	717	15	0	0
1	B	482	3783	2385	666	717	15	0	0
1	C	482	3783	2385	666	717	15	0	0
1	D	482	3783	2385	666	717	15	0	0
1	E	482	3783	2385	666	717	15	0	0
1	F	482	3783	2385	666	717	15	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	engineered mutation	UNP Q79PF4
A	432	GLU	THR	engineered mutation	UNP Q79PF4
B	431	ALA	SER	engineered mutation	UNP Q79PF4
B	432	GLU	THR	engineered mutation	UNP Q79PF4
C	431	ALA	SER	engineered mutation	UNP Q79PF4
C	432	GLU	THR	engineered mutation	UNP Q79PF4
D	431	ALA	SER	engineered mutation	UNP Q79PF4
D	432	GLU	THR	engineered mutation	UNP Q79PF4
E	431	ALA	SER	engineered mutation	UNP Q79PF4
E	432	GLU	THR	engineered mutation	UNP Q79PF4
F	431	ALA	SER	engineered mutation	UNP Q79PF4
F	432	GLU	THR	engineered mutation	UNP Q79PF4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	Mg	0
			3	3	
3	B	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	D	2	Total	Mg	0
			2	2	
3	E	2	Total	Mg	0
			2	2	

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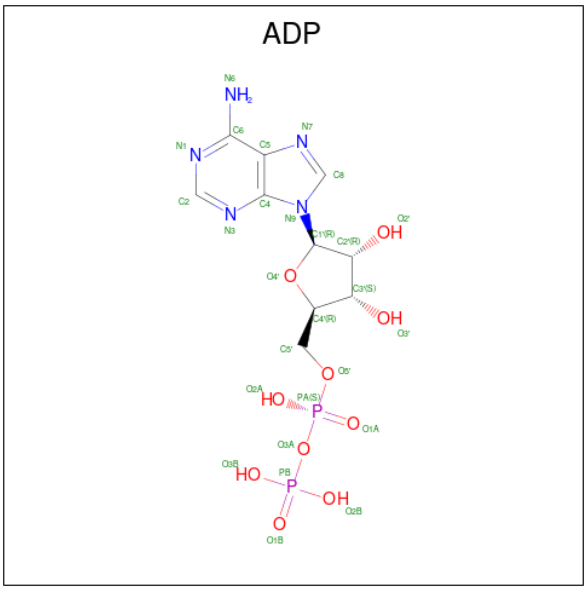
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	F	1	1	1	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



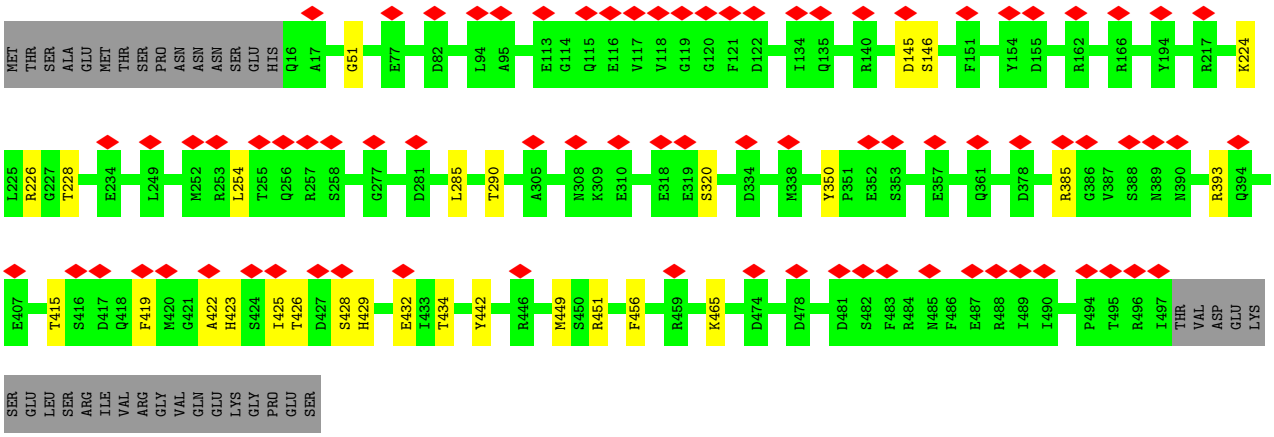
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	27	10	5	10	2	0
4	B	1	27	10	5	10	2	0
4	C	1	27	10	5	10	2	0
4	D	1	27	10	5	10	2	0
4	E	1	27	10	5	10	2	0
4	F	1	27	10	5	10	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

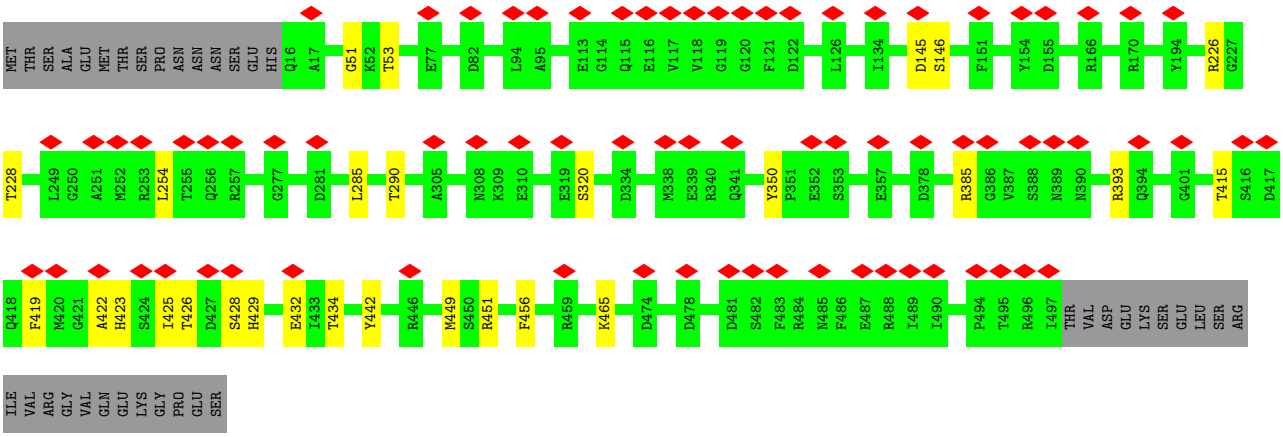
• Molecule 1: Circadian clock protein kinase KaiC

Chain A:



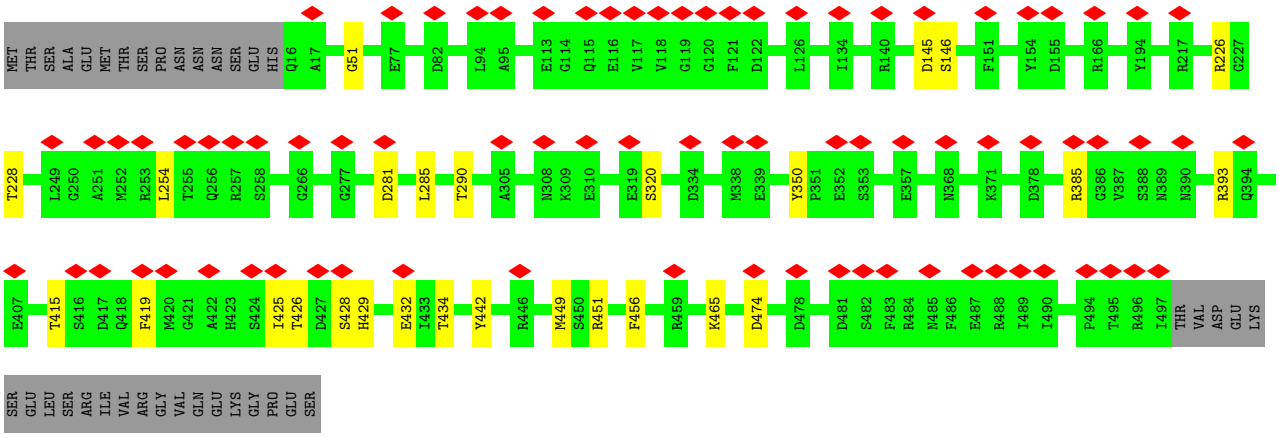
• Molecule 1: Circadian clock protein kinase KaiC

Chain B:



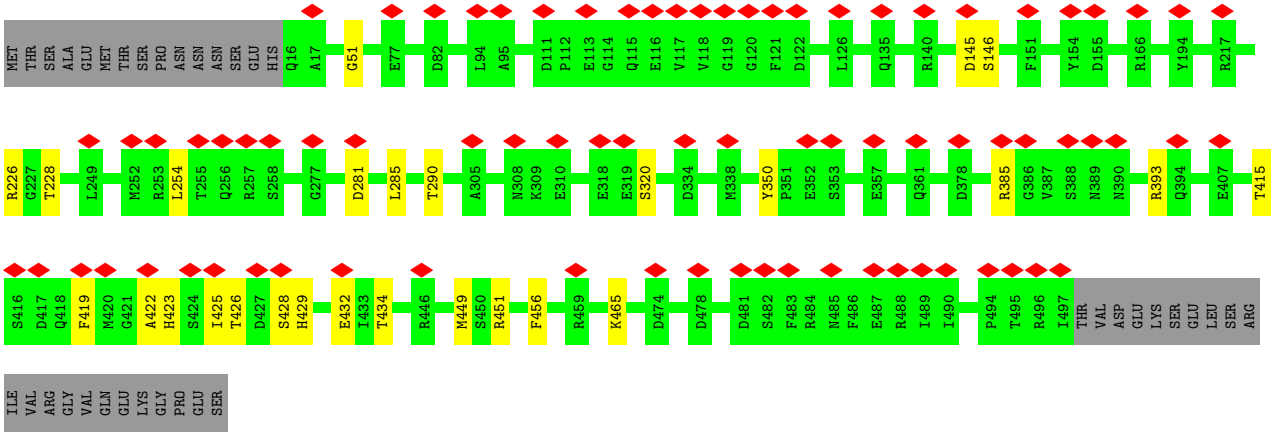
• Molecule 1: Circadian clock protein kinase KaiC

Chain C:



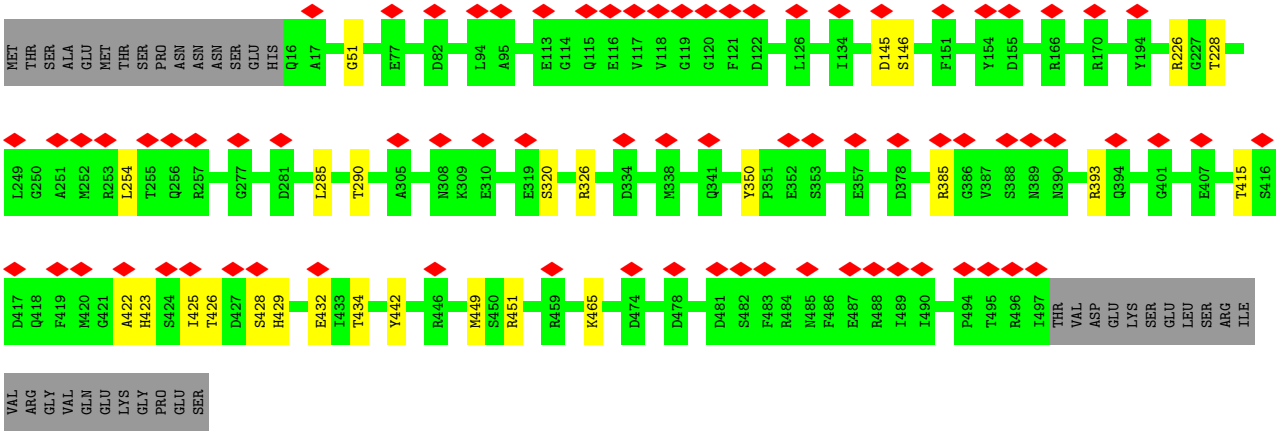
• Molecule 1: Circadian clock protein kinase KaiC

Chain D:



• Molecule 1: Circadian clock protein kinase KaiC

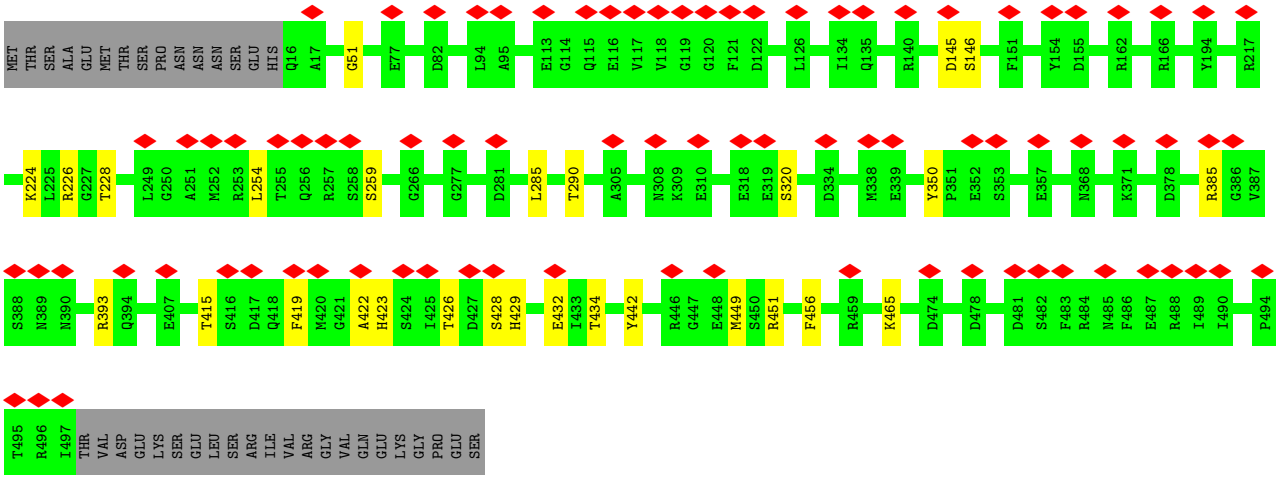
Chain E:



• Molecule 1: Circadian clock protein kinase KaiC

Chain F:

16%
87%
5%
7%


MET THR SER ALA GLU MET THR SER PRO ASN ASN ASN SER GLU HIS Q16 A17 G51 E77 D82 L94 A95 E113 G114 Q115 E116 V117 V118 G119 G120 F121 D122 L126 I134 Q135 R140 D145 S146 F151 Y154 D155 R162 R166 Y194 R217
K224 L225 R226 G227 T228 L249 G250 A251 M252 R253 L254 T255 Q256 R257 S258 S259 G266 G277 D281 L285 T290 A305 N308 K309 E310 E318 E319 S320 D334 M338 E339 Y350 P351 E352 S353 E357 N368 K371 D378 R385 G386 V387
S388 N389 N390 R393 Q394 E407 T415 S416 D417 Q418 F419 M420 G421 A422 H423 S424 I425 T426 D427 S428 H429 E432 I433 T434 Y442 R446 G447 E448 M449 S450 R451 F456 R459 K465 D474 D478 D481 S482 F483 R484 N485 F486 E487 R488 I489 I490 P494
T495 R496 I497 THR VAL ASP GLU LYS SER GLU LEU SER ARG ILE VAL ARG GLY VAL GLN GLU LYS GLY PRO GLU SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	89892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF Refinement performed in Relion	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40.3	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	43478	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	220.79999, 220.79999, 220.79999	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	A	0.77	0/3846	0.57	0/5183
1	B	0.77	0/3846	0.57	0/5183
1	C	0.77	0/3846	0.57	0/5183
1	D	0.77	0/3846	0.57	0/5183
1	E	0.77	0/3846	0.57	0/5183
1	F	0.77	0/3846	0.57	0/5183
All	All	0.77	0/23076	0.57	0/31098

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3783	0	3775	56	0
1	B	3783	0	3775	55	0
1	C	3783	0	3775	55	0
1	D	3783	0	3775	54	0
1	E	3783	0	3775	54	0
1	F	3783	0	3775	57	0
2	A	62	0	24	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	20	0
2	C	31	0	12	21	0
2	D	31	0	12	21	0
2	F	31	0	12	19	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
All	All	23058	0	22794	251	0

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

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ARG:CZ	2:F:601:ATP:O3G	1.85	1.25
1:A:226:ARG:NH2	2:A:605:ATP:O3G	1.74	1.20
1:F:226:ARG:NH2	2:F:601:ATP:O3G	1.74	1.20
2:D:601:ATP:O3G	1:E:226:ARG:NH2	1.76	1.18
2:C:601:ATP:O3G	1:D:226:ARG:CZ	1.92	1.18
2:D:601:ATP:O3G	1:E:226:ARG:CZ	1.91	1.18
2:B:601:ATP:O3G	1:C:226:ARG:CZ	1.91	1.17
2:C:601:ATP:O3G	1:D:226:ARG:NH2	1.76	1.17
2:B:601:ATP:O3G	1:C:226:ARG:NH2	1.77	1.15
2:A:601:ATP:O3G	1:B:226:ARG:NH2	1.81	1.13
1:F:226:ARG:NH1	2:F:601:ATP:PG	2.26	1.09
2:A:601:ATP:O3G	1:B:226:ARG:CZ	1.99	1.09
1:A:226:ARG:CZ	2:A:605:ATP:O3G	2.00	1.08
2:D:601:ATP:PG	1:E:226:ARG:HH12	1.77	1.07
2:C:601:ATP:PG	1:D:226:ARG:HH12	1.78	1.05
2:D:601:ATP:O2G	1:E:226:ARG:NH1	1.91	1.03
2:C:601:ATP:O2G	1:D:226:ARG:NH1	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:ATP:PG	1:B:226:ARG:HH12	1.83	1.00
2:B:601:ATP:PG	1:C:226:ARG:NH1	2.33	1.00
2:D:601:ATP:PG	1:E:226:ARG:NH1	2.34	1.00
2:C:601:ATP:PG	1:D:226:ARG:NH1	2.35	0.99
2:A:601:ATP:O2G	1:B:226:ARG:NH1	1.99	0.94
2:A:601:ATP:PG	1:B:226:ARG:NH1	2.43	0.91
1:A:226:ARG:NH1	2:A:605:ATP:PG	2.46	0.87
1:C:51:GLY:HA2	2:C:601:ATP:PA	2.15	0.87
1:D:51:GLY:HA2	2:D:601:ATP:PA	2.15	0.87
1:A:51:GLY:HA2	2:A:601:ATP:PA	2.15	0.86
1:A:226:ARG:HH22	2:A:605:ATP:PG	1.98	0.86
1:E:51:GLY:HA2	2:F:601:ATP:PA	2.15	0.86
1:B:51:GLY:HA2	2:B:601:ATP:PA	2.15	0.85
2:A:605:ATP:PA	1:F:51:GLY:HA2	2.15	0.85
1:A:226:ARG:NH2	2:A:605:ATP:PG	2.51	0.84
1:A:51:GLY:HA2	2:A:601:ATP:O3A	1.78	0.84
1:D:51:GLY:HA2	2:D:601:ATP:O3A	1.78	0.83
2:A:605:ATP:O3A	1:F:51:GLY:HA2	1.78	0.83
1:E:51:GLY:HA2	2:F:601:ATP:O3A	1.78	0.83
1:F:226:ARG:NH2	2:F:601:ATP:PG	2.50	0.83
1:F:226:ARG:HH22	2:F:601:ATP:PG	2.02	0.82
1:B:51:GLY:HA2	2:B:601:ATP:O3A	1.78	0.82
1:C:51:GLY:HA2	2:C:601:ATP:O3A	1.78	0.82
1:A:254:LEU:O	1:F:320:SER:HB2	1.79	0.80
1:F:226:ARG:NH1	2:F:601:ATP:O3G	2.11	0.80
2:C:601:ATP:O3G	1:D:226:ARG:NH1	2.15	0.80
2:B:601:ATP:PG	1:C:226:ARG:HH22	2.05	0.80
2:C:601:ATP:PG	1:D:226:ARG:HH22	2.05	0.80
1:C:429:HIS:O	1:C:429:HIS:CD2	2.35	0.79
1:D:429:HIS:CD2	1:D:429:HIS:O	2.36	0.79
2:D:601:ATP:PG	1:E:226:ARG:HH22	2.05	0.79
1:E:429:HIS:O	1:E:429:HIS:CD2	2.36	0.79
1:B:429:HIS:O	1:B:429:HIS:CD2	2.36	0.79
1:A:429:HIS:CD2	1:A:429:HIS:O	2.36	0.79
1:F:429:HIS:CD2	1:F:429:HIS:O	2.36	0.78
2:B:601:ATP:PG	1:C:226:ARG:NH2	2.55	0.78
2:D:601:ATP:O3G	1:E:226:ARG:NH1	2.15	0.78
1:A:320:SER:HB2	1:B:254:LEU:O	1.84	0.78
2:C:601:ATP:PG	1:D:226:ARG:NH2	2.56	0.77
2:D:601:ATP:PG	1:E:226:ARG:NH2	2.56	0.77
1:F:226:ARG:CZ	2:F:601:ATP:PG	2.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:ATP:O3G	1:B:226:ARG:NH1	2.18	0.77
1:D:320:SER:HB2	1:E:254:LEU:O	1.86	0.75
1:E:320:SER:HB2	1:F:254:LEU:O	1.87	0.75
2:B:601:ATP:O3G	1:C:226:ARG:NH1	2.15	0.74
1:C:320:SER:HB2	1:D:254:LEU:O	1.87	0.74
2:B:601:ATP:PG	1:C:226:ARG:CZ	2.74	0.73
1:B:320:SER:HB2	1:C:254:LEU:O	1.88	0.72
2:A:601:ATP:PG	1:B:226:ARG:HH22	2.12	0.72
1:E:449:MET:O	1:F:465:LYS:HD2	1.91	0.70
2:C:601:ATP:PG	1:D:226:ARG:CZ	2.76	0.70
2:D:601:ATP:PG	1:E:226:ARG:CZ	2.75	0.70
2:A:601:ATP:PG	1:B:226:ARG:NH2	2.65	0.70
1:A:226:ARG:CZ	2:A:605:ATP:PG	2.78	0.70
1:A:254:LEU:O	1:F:320:SER:CB	2.40	0.69
1:A:432:GLU:CD	1:F:415:THR:HG21	2.12	0.69
1:F:228:THR:O	2:F:601:ATP:C8	2.46	0.68
1:A:228:THR:O	2:A:605:ATP:C8	2.46	0.68
1:E:415:THR:HG21	1:F:432:GLU:CD	2.14	0.68
1:A:432:GLU:OE2	1:F:290:THR:HB	1.93	0.68
2:A:605:ATP:H5'2	1:F:51:GLY:HA2	1.76	0.67
1:D:51:GLY:HA2	2:D:601:ATP:H5'2	1.76	0.67
1:A:51:GLY:HA2	2:A:601:ATP:H5'2	1.76	0.67
1:C:51:GLY:HA2	2:C:601:ATP:H5'2	1.76	0.66
1:E:51:GLY:HA2	2:F:601:ATP:H5'2	1.76	0.66
1:D:449:MET:O	1:E:465:LYS:HD2	1.96	0.66
1:B:415:THR:HG21	1:C:432:GLU:CD	2.16	0.66
1:A:432:GLU:OE2	1:F:415:THR:HG21	1.94	0.66
1:B:51:GLY:HA2	2:B:601:ATP:H5'2	1.76	0.66
2:B:601:ATP:C8	1:C:228:THR:O	2.49	0.66
1:B:449:MET:O	1:C:465:LYS:HD2	1.97	0.65
1:B:415:THR:HG21	1:C:432:GLU:OE2	1.97	0.65
1:E:320:SER:CB	1:F:254:LEU:O	2.45	0.64
1:A:226:ARG:NH2	2:A:605:ATP:O2G	2.29	0.64
1:A:415:THR:HG21	1:B:432:GLU:OE2	1.97	0.64
1:C:449:MET:O	1:D:465:LYS:HD2	1.97	0.64
2:D:601:ATP:C8	1:E:228:THR:O	2.51	0.64
1:A:226:ARG:NH1	2:A:605:ATP:O3G	2.31	0.64
1:B:451:ARG:NH2	4:B:603:ADP:O2'	2.28	0.64
1:C:415:THR:HG21	1:D:432:GLU:CD	2.18	0.64
1:E:451:ARG:NH2	4:E:902:ADP:O2'	2.28	0.64
1:D:320:SER:CB	1:E:254:LEU:O	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HD2	1:F:449:MET:O	1.98	0.63
1:C:320:SER:CB	1:D:254:LEU:O	2.47	0.63
1:F:451:ARG:NH2	4:F:602:ADP:O2'	2.28	0.63
2:A:605:ATP:O3A	1:F:51:GLY:CA	2.46	0.63
1:A:226:ARG:HH12	2:A:605:ATP:PG	1.91	0.63
1:A:415:THR:HG21	1:B:432:GLU:CD	2.19	0.63
2:A:601:ATP:C8	1:B:228:THR:O	2.52	0.63
2:C:601:ATP:C8	1:D:228:THR:O	2.52	0.62
1:E:415:THR:HG21	1:F:432:GLU:OE2	1.98	0.62
1:A:290:THR:HB	1:B:432:GLU:OE2	1.99	0.62
1:A:449:MET:O	1:B:465:LYS:HD2	1.99	0.62
1:D:451:ARG:NH2	4:D:603:ADP:O2'	2.28	0.62
1:B:51:GLY:HA2	2:B:601:ATP:O2A	2.00	0.62
2:B:601:ATP:PG	1:C:226:ARG:HH12	1.77	0.62
1:D:415:THR:HG21	1:E:432:GLU:CD	2.19	0.62
1:E:51:GLY:CA	2:F:601:ATP:O3A	2.46	0.62
1:A:320:SER:CB	1:B:254:LEU:O	2.47	0.62
1:C:415:THR:HG21	1:D:432:GLU:OE2	2.00	0.62
1:C:51:GLY:CA	2:C:601:ATP:O3A	2.46	0.62
2:A:605:ATP:O2A	1:F:51:GLY:HA2	2.00	0.62
1:C:451:ARG:NH2	4:C:603:ADP:O2'	2.28	0.62
1:B:320:SER:CB	1:C:254:LEU:O	2.48	0.62
1:C:290:THR:HB	1:D:432:GLU:OE2	1.98	0.62
1:D:51:GLY:CA	2:D:601:ATP:O3A	2.46	0.62
1:A:51:GLY:CA	2:A:601:ATP:O3A	2.46	0.61
1:B:51:GLY:CA	2:B:601:ATP:O3A	2.46	0.61
1:B:290:THR:HB	1:C:432:GLU:OE2	1.99	0.61
1:D:290:THR:HB	1:E:432:GLU:OE2	1.99	0.61
1:E:51:GLY:HA2	2:F:601:ATP:O2A	2.00	0.61
1:A:51:GLY:HA2	2:A:601:ATP:O2A	2.00	0.61
1:C:51:GLY:HA2	2:C:601:ATP:O2A	2.00	0.61
1:D:51:GLY:HA2	2:D:601:ATP:O2A	2.00	0.61
1:D:415:THR:HG21	1:E:432:GLU:OE2	2.01	0.61
1:A:451:ARG:NH2	4:A:603:ADP:O2'	2.28	0.60
1:D:51:GLY:CA	2:D:601:ATP:H5'2	2.32	0.60
1:A:393:ARG:NH1	1:F:385:ARG:O	2.34	0.60
2:A:605:ATP:H5'2	1:F:51:GLY:CA	2.32	0.60
1:B:51:GLY:CA	2:B:601:ATP:H5'2	2.32	0.59
1:E:51:GLY:CA	2:F:601:ATP:H5'2	2.32	0.59
2:D:601:ATP:O2G	1:E:226:ARG:CZ	2.50	0.59
1:E:290:THR:HB	1:F:432:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLY:CA	2:C:601:ATP:H5'2	2.32	0.59
2:C:601:ATP:O2G	1:D:226:ARG:CZ	2.51	0.59
1:A:51:GLY:CA	2:A:601:ATP:H5'2	2.32	0.59
1:A:226:ARG:NH1	2:A:605:ATP:O1A	2.36	0.58
1:F:226:ARG:NH2	2:F:601:ATP:O2G	2.35	0.58
2:D:601:ATP:O2G	1:E:226:ARG:NH2	2.40	0.54
1:B:385:ARG:O	1:C:393:ARG:NH1	2.42	0.53
2:C:601:ATP:O2G	1:D:226:ARG:NH2	2.41	0.53
1:F:426:THR:HB	1:F:428:SER:OG	2.09	0.53
1:A:426:THR:HB	1:A:428:SER:OG	2.09	0.53
1:B:426:THR:HB	1:B:428:SER:OG	2.09	0.52
1:E:426:THR:HB	1:E:428:SER:OG	2.09	0.52
1:A:385:ARG:O	1:B:393:ARG:NH1	2.43	0.52
1:C:426:THR:HB	1:C:428:SER:OG	2.09	0.52
1:C:385:ARG:O	1:D:393:ARG:NH1	2.44	0.51
1:D:426:THR:HB	1:D:428:SER:OG	2.09	0.51
1:E:350:TYR:CZ	1:F:254:LEU:CD2	2.93	0.51
1:E:415:THR:HG21	1:F:432:GLU:OE1	2.11	0.51
1:E:350:TYR:CE1	1:F:254:LEU:HD21	2.46	0.50
1:D:385:ARG:O	1:E:393:ARG:NH1	2.45	0.50
2:B:601:ATP:O2G	1:C:226:ARG:NH2	2.39	0.50
1:B:350:TYR:CZ	1:C:254:LEU:CD2	2.95	0.50
1:D:350:TYR:CZ	1:E:254:LEU:CD2	2.95	0.50
1:E:385:ARG:O	1:F:393:ARG:NH1	2.45	0.49
2:A:601:ATP:O2G	1:B:226:ARG:CZ	2.60	0.49
1:C:350:TYR:CZ	1:D:254:LEU:CD2	2.95	0.49
1:D:429:HIS:O	1:D:429:HIS:HD2	1.95	0.49
1:A:419:PHE:CD1	1:B:425:ILE:HG22	2.48	0.49
1:A:145:ASP:OD1	1:A:146:SER:N	2.47	0.48
1:D:145:ASP:OD1	1:D:146:SER:N	2.47	0.48
1:B:145:ASP:OD1	1:B:146:SER:N	2.47	0.48
1:B:429:HIS:O	1:B:429:HIS:HD2	1.95	0.48
1:E:145:ASP:OD1	1:E:146:SER:N	2.47	0.48
1:F:145:ASP:OD1	1:F:146:SER:N	2.47	0.48
1:B:350:TYR:CE1	1:C:254:LEU:HD21	2.48	0.48
1:C:145:ASP:OD1	1:C:146:SER:N	2.47	0.47
1:D:350:TYR:CE1	1:E:254:LEU:HD21	2.49	0.47
1:A:432:GLU:OE1	1:F:415:THR:HG21	2.14	0.47
1:F:429:HIS:O	1:F:429:HIS:HD2	1.95	0.47
1:A:456:PHE:CZ	1:F:442:TYR:CE2	3.03	0.46
1:C:350:TYR:CE1	1:D:254:LEU:HD21	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:TYR:CE2	1:B:456:PHE:CZ	3.04	0.46
1:C:429:HIS:O	1:C:429:HIS:HD2	1.95	0.45
1:B:415:THR:HG21	1:C:432:GLU:OE1	2.16	0.45
1:D:429:HIS:O	1:D:429:HIS:CG	2.70	0.45
1:A:429:HIS:O	1:A:429:HIS:CG	2.70	0.45
1:A:425:ILE:HG22	1:F:419:PHE:CD1	2.52	0.44
2:A:605:ATP:PB	1:F:51:GLY:H	2.40	0.44
1:E:429:HIS:O	1:E:429:HIS:CG	2.70	0.44
1:A:51:GLY:H	2:A:601:ATP:PB	2.40	0.44
2:A:601:ATP:O2G	1:B:226:ARG:NH2	2.49	0.44
1:B:429:HIS:O	1:B:429:HIS:CG	2.70	0.44
1:C:51:GLY:H	2:C:601:ATP:PB	2.40	0.44
1:D:415:THR:HG21	1:E:432:GLU:OE1	2.18	0.44
1:A:425:ILE:HG22	1:F:419:PHE:HB2	1.99	0.44
1:B:51:GLY:H	2:B:601:ATP:PB	2.40	0.44
1:C:281:ASP:OD1	1:C:281:ASP:N	2.49	0.44
1:B:442:TYR:CE2	1:C:456:PHE:CZ	3.06	0.44
1:F:429:HIS:O	1:F:429:HIS:CG	2.70	0.44
1:D:51:GLY:H	2:D:601:ATP:PB	2.40	0.44
1:E:449:MET:O	1:F:465:LYS:HB2	2.18	0.44
1:E:51:GLY:H	2:F:601:ATP:PB	2.40	0.44
1:B:419:PHE:CD1	1:C:425:ILE:HG22	2.53	0.43
1:C:419:PHE:CD1	1:D:425:ILE:HG22	2.53	0.43
1:E:350:TYR:CZ	1:F:254:LEU:HD23	2.53	0.43
2:D:601:ATP:O1A	1:E:226:ARG:NH1	2.51	0.43
1:A:350:TYR:CZ	1:B:254:LEU:CD2	3.02	0.43
1:A:429:HIS:O	1:A:429:HIS:HD2	1.95	0.43
1:C:415:THR:HG21	1:D:432:GLU:OE1	2.18	0.43
1:F:226:ARG:NH1	2:F:601:ATP:O1A	2.52	0.43
1:C:429:HIS:O	1:C:429:HIS:CG	2.70	0.43
2:C:601:ATP:O1A	1:D:226:ARG:NH1	2.51	0.43
1:E:429:HIS:O	1:E:429:HIS:HD2	1.95	0.43
2:B:601:ATP:O1A	1:C:226:ARG:NH1	2.52	0.43
1:C:51:GLY:N	2:C:601:ATP:O2B	2.52	0.42
1:E:326:ARG:NH1	1:F:259:SER:O	2.45	0.42
1:A:254:LEU:CD2	1:F:350:TYR:CZ	3.02	0.42
1:F:224:LYS:HE3	2:F:601:ATP:O3G	2.19	0.42
2:A:605:ATP:O2B	1:F:51:GLY:N	2.52	0.42
1:A:51:GLY:N	2:A:601:ATP:O2B	2.52	0.42
1:A:465:LYS:HB2	1:F:449:MET:O	2.19	0.42
1:B:51:GLY:N	2:B:601:ATP:O2B	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:PHE:CD1	1:E:425:ILE:HG22	2.54	0.42
1:D:51:GLY:N	2:D:601:ATP:O2B	2.52	0.42
1:C:442:TYR:CE2	1:D:456:PHE:CZ	3.08	0.42
1:D:281:ASP:OD1	1:D:281:ASP:N	2.49	0.41
1:C:419:PHE:HB2	1:D:425:ILE:HG22	2.02	0.41
1:F:422:ALA:O	1:F:423:HIS:C	2.58	0.41
1:A:419:PHE:HB2	1:B:425:ILE:HG22	2.03	0.41
1:B:419:PHE:HB2	1:C:425:ILE:HG22	2.02	0.41
1:E:285:LEU:HB2	1:E:434:THR:HG21	2.02	0.41
1:F:285:LEU:HB2	1:F:434:THR:HG21	2.02	0.41
1:B:422:ALA:O	1:B:423:HIS:C	2.58	0.41
1:C:285:LEU:HB2	1:C:434:THR:HG21	2.02	0.41
1:E:422:ALA:O	1:E:423:HIS:C	2.58	0.41
1:A:415:THR:HG21	1:B:432:GLU:OE1	2.20	0.41
1:E:51:GLY:N	2:F:601:ATP:O2B	2.52	0.41
1:A:350:TYR:CE1	1:B:254:LEU:HD21	2.56	0.41
1:A:422:ALA:O	1:A:423:HIS:C	2.58	0.41
1:B:350:TYR:CZ	1:C:254:LEU:HD23	2.56	0.41
1:D:422:ALA:O	1:D:423:HIS:C	2.58	0.41
1:A:224:LYS:HE3	2:A:605:ATP:O3G	2.21	0.41
1:A:285:LEU:HB2	1:A:434:THR:HG21	2.02	0.41
1:B:285:LEU:HB2	1:B:434:THR:HG21	2.02	0.41
1:C:474:ASP:OD1	1:C:474:ASP:N	2.54	0.41
1:A:254:LEU:HD21	1:F:350:TYR:CE1	2.56	0.41
1:A:254:LEU:O	1:F:320:SER:HB3	2.20	0.40
1:B:53:THR:OG1	2:B:601:ATP:O1A	2.40	0.40
1:E:442:TYR:CE2	1:F:456:PHE:CZ	3.09	0.40
2:A:605:ATP:O3A	1:F:51:GLY:N	2.55	0.40
1:D:285:LEU:HB2	1:D:434:THR:HG21	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	A	480/519 (92%)	473 (98%)	7 (2%)	0	100	100
1	B	480/519 (92%)	473 (98%)	7 (2%)	0	100	100
1	C	480/519 (92%)	473 (98%)	7 (2%)	0	100	100
1	D	480/519 (92%)	473 (98%)	7 (2%)	0	100	100
1	E	480/519 (92%)	473 (98%)	7 (2%)	0	100	100
1	F	480/519 (92%)	473 (98%)	7 (2%)	0	100	100
All	All	2880/3114 (92%)	2838 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/443 (91%)	405 (100%)	0	100	100
1	B	405/443 (91%)	405 (100%)	0	100	100
1	C	405/443 (91%)	405 (100%)	0	100	100
1	D	405/443 (91%)	405 (100%)	0	100	100
1	E	405/443 (91%)	405 (100%)	0	100	100
1	F	405/443 (91%)	405 (100%)	0	100	100
All	All	2430/2658 (91%)	2430 (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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	B	429	HIS
1	C	429	HIS
1	D	429	HIS
1	E	429	HIS

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Mol	Chain	Res	Type
1	F	429	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	ADP	D	603	3	24,29,29	1.18	2 (8%)	29,45,45	1.60	7 (24%)
2	ATP	F	601	3	26,33,33	1.15	3 (11%)	31,52,52	1.76	7 (22%)
4	ADP	F	602	3	24,29,29	1.18	2 (8%)	29,45,45	1.60	7 (24%)
4	ADP	A	603	3	24,29,29	1.18	2 (8%)	29,45,45	1.60	8 (27%)
4	ADP	C	603	3	24,29,29	1.18	2 (8%)	29,45,45	1.60	7 (24%)
2	ATP	C	601	3	26,33,33	1.15	3 (11%)	31,52,52	1.76	7 (22%)
4	ADP	B	603	3	24,29,29	1.18	2 (8%)	29,45,45	1.60	8 (27%)
2	ATP	B	601	3	26,33,33	1.15	3 (11%)	31,52,52	1.76	7 (22%)
2	ATP	D	601	3	26,33,33	1.14	3 (11%)	31,52,52	1.76	7 (22%)
4	ADP	E	902	3	24,29,29	1.18	2 (8%)	29,45,45	1.60	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	A	601	3	26,33,33	1.15	3 (11%)	31,52,52	1.76	7 (22%)
2	ATP	A	605	3	26,33,33	1.15	2 (7%)	31,52,52	1.76	7 (22%)

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
4	ADP	D	603	3	-	3/12/32/32	0/3/3/3
2	ATP	F	601	3	-	2/18/38/38	0/3/3/3
4	ADP	F	602	3	-	3/12/32/32	0/3/3/3
4	ADP	A	603	3	-	3/12/32/32	0/3/3/3
4	ADP	C	603	3	-	3/12/32/32	0/3/3/3
2	ATP	C	601	3	-	2/18/38/38	0/3/3/3
4	ADP	B	603	3	-	3/12/32/32	0/3/3/3
2	ATP	B	601	3	-	2/18/38/38	0/3/3/3
2	ATP	D	601	3	-	2/18/38/38	0/3/3/3
4	ADP	E	902	3	-	3/12/32/32	0/3/3/3
2	ATP	A	601	3	-	2/18/38/38	0/3/3/3
2	ATP	A	605	3	-	2/18/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	ADP	O4'-C1'	2.53	1.44	1.41
4	B	603	ADP	O4'-C1'	2.50	1.44	1.41
4	F	602	ADP	O4'-C1'	2.49	1.44	1.41
4	A	603	ADP	O4'-C1'	2.49	1.44	1.41
4	E	902	ADP	O4'-C1'	2.46	1.44	1.41
4	C	603	ADP	O4'-C1'	2.43	1.44	1.41
2	B	601	ATP	PG-O3G	-2.34	1.45	1.54
2	A	605	ATP	PG-O3G	-2.33	1.45	1.54
2	A	601	ATP	PG-O3G	-2.32	1.45	1.54
2	C	601	ATP	PG-O3G	-2.32	1.45	1.54
2	F	601	ATP	PG-O3G	-2.32	1.45	1.54
2	D	601	ATP	PG-O3G	-2.32	1.45	1.54
2	F	601	ATP	O4'-C1'	2.23	1.44	1.41
2	B	601	ATP	O4'-C1'	2.22	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ATP	O4'-C1'	2.22	1.44	1.41
2	A	605	ATP	O4'-C1'	2.20	1.44	1.41
2	D	601	ATP	O4'-C1'	2.20	1.44	1.41
2	C	601	ATP	O4'-C1'	2.19	1.44	1.41
4	F	602	ADP	C5-C4	-2.18	1.35	1.40
4	E	902	ADP	C5-C4	-2.17	1.35	1.40
4	D	603	ADP	C5-C4	-2.17	1.35	1.40
4	C	603	ADP	C5-C4	-2.17	1.35	1.40
4	A	603	ADP	C5-C4	-2.16	1.35	1.40
4	B	603	ADP	C5-C4	-2.15	1.35	1.40
2	F	601	ATP	PG-O2G	-2.03	1.47	1.54
2	C	601	ATP	PG-O2G	-2.02	1.47	1.54
2	D	601	ATP	PG-O2G	-2.01	1.47	1.54
2	B	601	ATP	PG-O2G	-2.01	1.47	1.54
2	A	601	ATP	PG-O2G	-2.00	1.47	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	ATP	PA-O3A-PB	-4.87	116.10	132.83
2	B	601	ATP	PA-O3A-PB	-4.87	116.11	132.83
2	A	601	ATP	PA-O3A-PB	-4.87	116.11	132.83
2	C	601	ATP	PA-O3A-PB	-4.87	116.12	132.83
2	D	601	ATP	PA-O3A-PB	-4.87	116.13	132.83
2	A	605	ATP	PA-O3A-PB	-4.86	116.14	132.83
4	C	603	ADP	C4-C5-N7	4.40	113.98	109.40
4	A	603	ADP	C4-C5-N7	4.36	113.94	109.40
4	B	603	ADP	C4-C5-N7	4.35	113.93	109.40
4	E	902	ADP	C4-C5-N7	4.35	113.93	109.40
4	D	603	ADP	C4-C5-N7	4.34	113.92	109.40
4	F	602	ADP	C4-C5-N7	4.34	113.92	109.40
2	A	605	ATP	C4-C5-N7	4.27	113.85	109.40
2	B	601	ATP	C4-C5-N7	4.24	113.82	109.40
2	C	601	ATP	C4-C5-N7	4.23	113.81	109.40
2	F	601	ATP	C4-C5-N7	4.22	113.79	109.40
2	A	601	ATP	C4-C5-N7	4.20	113.78	109.40
2	D	601	ATP	C4-C5-N7	4.18	113.75	109.40
2	C	601	ATP	PB-O3B-PG	-3.42	121.11	132.83
2	B	601	ATP	PB-O3B-PG	-3.41	121.11	132.83
2	D	601	ATP	PB-O3B-PG	-3.41	121.12	132.83
2	A	601	ATP	PB-O3B-PG	-3.41	121.13	132.83
2	F	601	ATP	PB-O3B-PG	-3.41	121.13	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	605	ATP	PB-O3B-PG	-3.40	121.15	132.83
4	E	902	ADP	PA-O3A-PB	-3.26	121.63	132.83
4	D	603	ADP	PA-O3A-PB	-3.26	121.64	132.83
4	C	603	ADP	PA-O3A-PB	-3.26	121.64	132.83
4	B	603	ADP	PA-O3A-PB	-3.25	121.67	132.83
4	A	603	ADP	PA-O3A-PB	-3.25	121.67	132.83
4	F	602	ADP	PA-O3A-PB	-3.25	121.67	132.83
4	F	602	ADP	O3B-PB-O1B	-3.08	98.62	110.68
4	C	603	ADP	O3B-PB-O1B	-3.08	98.62	110.68
4	A	603	ADP	O3B-PB-O1B	-3.08	98.63	110.68
4	D	603	ADP	O3B-PB-O1B	-3.08	98.63	110.68
4	B	603	ADP	O3B-PB-O1B	-3.08	98.63	110.68
4	E	902	ADP	O3B-PB-O1B	-3.07	98.64	110.68
2	A	601	ATP	O4'-C4'-C3'	-2.48	100.20	105.11
2	F	601	ATP	O4'-C4'-C3'	-2.48	100.20	105.11
2	C	601	ATP	O4'-C4'-C3'	-2.48	100.21	105.11
2	A	605	ATP	O4'-C4'-C3'	-2.48	100.21	105.11
2	D	601	ATP	O4'-C4'-C3'	-2.47	100.22	105.11
2	B	601	ATP	O4'-C4'-C3'	-2.47	100.22	105.11
2	C	601	ATP	O2G-PG-O3B	2.45	112.86	104.64
2	F	601	ATP	O2G-PG-O3B	2.45	112.86	104.64
2	A	605	ATP	O2G-PG-O3B	2.45	112.85	104.64
2	D	601	ATP	O2G-PG-O3B	2.45	112.84	104.64
2	A	601	ATP	O2G-PG-O3B	2.44	112.83	104.64
2	B	601	ATP	O2G-PG-O3B	2.42	112.77	104.64
4	E	902	ADP	N6-C6-N1	-2.41	113.57	118.57
4	B	603	ADP	N6-C6-N1	-2.41	113.58	118.57
4	D	603	ADP	N6-C6-N1	-2.39	113.61	118.57
4	A	603	ADP	N6-C6-N1	-2.39	113.61	118.57
4	C	603	ADP	N6-C6-N1	-2.39	113.61	118.57
4	F	602	ADP	N6-C6-N1	-2.38	113.63	118.57
2	D	601	ATP	N6-C6-N1	-2.21	113.98	118.57
2	C	601	ATP	N6-C6-N1	-2.21	114.00	118.57
2	A	601	ATP	N6-C6-N1	-2.20	114.01	118.57
2	F	601	ATP	N6-C6-N1	-2.19	114.03	118.57
2	A	605	ATP	N6-C6-N1	-2.19	114.03	118.57
2	B	601	ATP	N6-C6-N1	-2.19	114.03	118.57
4	E	902	ADP	O3B-PB-O3A	2.17	111.93	104.64
4	A	603	ADP	O3B-PB-O3A	2.17	111.93	104.64
4	F	602	ADP	O3B-PB-O3A	2.17	111.92	104.64
2	F	601	ATP	C5-C6-N6	2.17	123.65	120.35
4	C	603	ADP	O3B-PB-O3A	2.17	111.90	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	603	ADP	O3B-PB-O3A	2.17	111.90	104.64
2	A	605	ATP	C5-C6-N6	2.17	123.64	120.35
2	C	601	ATP	C5-C6-N6	2.17	123.64	120.35
4	B	603	ADP	O3B-PB-O3A	2.17	111.90	104.64
2	A	601	ATP	C5-C6-N6	2.16	123.63	120.35
2	D	601	ATP	C5-C6-N6	2.15	123.62	120.35
2	B	601	ATP	C5-C6-N6	2.14	123.61	120.35
4	E	902	ADP	C5-C6-N6	2.10	123.55	120.35
4	A	603	ADP	C5-C6-N6	2.07	123.50	120.35
4	B	603	ADP	C5-C6-N6	2.07	123.49	120.35
4	F	602	ADP	C5-C6-N6	2.07	123.49	120.35
4	D	603	ADP	C2-N1-C6	-2.07	115.22	118.75
4	B	603	ADP	C2-N1-C6	-2.06	115.23	118.75
4	C	603	ADP	C5-C6-N6	2.06	123.48	120.35
4	D	603	ADP	C5-C6-N6	2.05	123.46	120.35
4	A	603	ADP	C2-N1-C6	-2.04	115.27	118.75
4	C	603	ADP	C2-N1-C6	-2.04	115.27	118.75
4	E	902	ADP	C2-N1-C6	-2.03	115.28	118.75
4	F	602	ADP	C2-N1-C6	-2.02	115.30	118.75
4	B	603	ADP	O2B-PB-O3A	2.00	111.35	104.64
4	A	603	ADP	O2B-PB-O3A	2.00	111.35	104.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	O4'-C4'-C5'-O5'
2	A	605	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	O4'-C4'-C5'-O5'
2	C	601	ATP	O4'-C4'-C5'-O5'
2	D	601	ATP	O4'-C4'-C5'-O5'
2	F	601	ATP	O4'-C4'-C5'-O5'
2	A	601	ATP	C3'-C4'-C5'-O5'
2	A	605	ATP	C3'-C4'-C5'-O5'
2	B	601	ATP	C3'-C4'-C5'-O5'
2	C	601	ATP	C3'-C4'-C5'-O5'
2	D	601	ATP	C3'-C4'-C5'-O5'
2	F	601	ATP	C3'-C4'-C5'-O5'
4	A	603	ADP	PA-O3A-PB-O1B
4	B	603	ADP	PA-O3A-PB-O1B
4	C	603	ADP	PA-O3A-PB-O1B
4	D	603	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	E	902	ADP	PA-O3A-PB-O1B
4	F	602	ADP	PA-O3A-PB-O1B
4	A	603	ADP	PA-O3A-PB-O2B
4	A	603	ADP	PA-O3A-PB-O3B
4	B	603	ADP	PA-O3A-PB-O2B
4	B	603	ADP	PA-O3A-PB-O3B
4	C	603	ADP	PA-O3A-PB-O2B
4	C	603	ADP	PA-O3A-PB-O3B
4	D	603	ADP	PA-O3A-PB-O2B
4	D	603	ADP	PA-O3A-PB-O3B
4	E	902	ADP	PA-O3A-PB-O2B
4	E	902	ADP	PA-O3A-PB-O3B
4	F	602	ADP	PA-O3A-PB-O2B
4	F	602	ADP	PA-O3A-PB-O3B

There are no ring outliers.

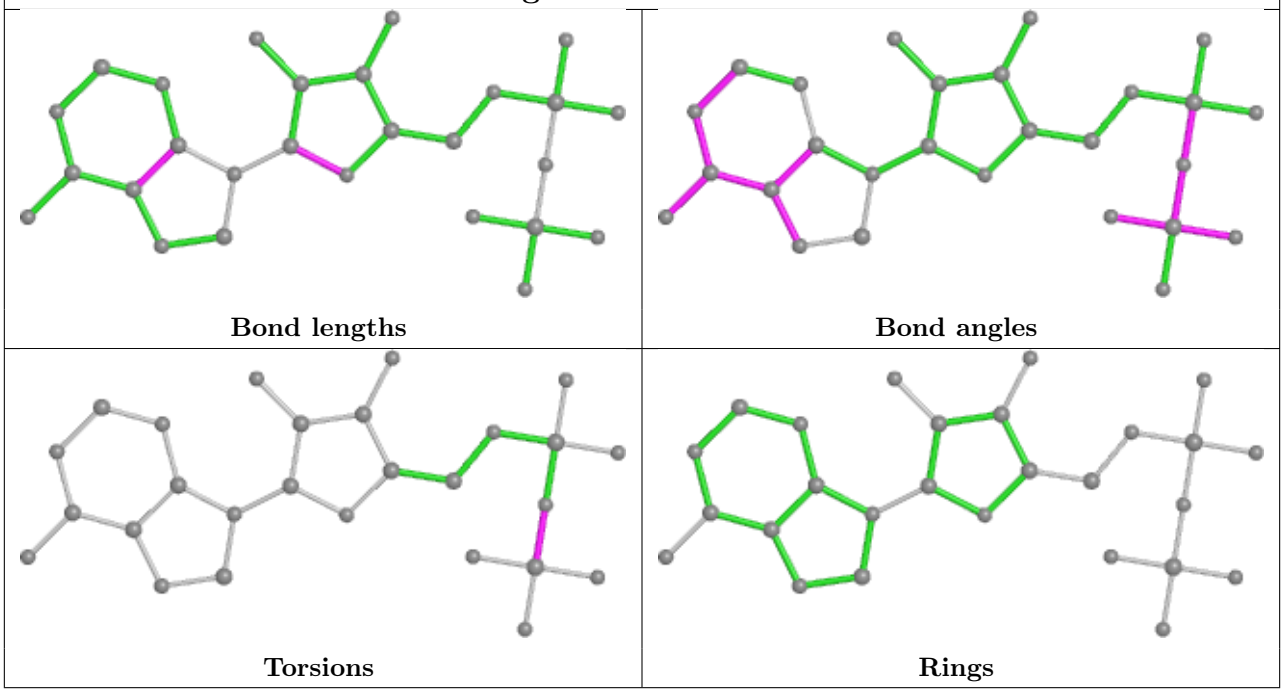
12 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	ADP	1	0
2	F	601	ATP	19	0
4	F	602	ADP	1	0
4	A	603	ADP	1	0
4	C	603	ADP	1	0
2	C	601	ATP	21	0
4	B	603	ADP	1	0
2	B	601	ATP	20	0
2	D	601	ATP	21	0
4	E	902	ADP	1	0
2	A	601	ATP	19	0
2	A	605	ATP	21	0

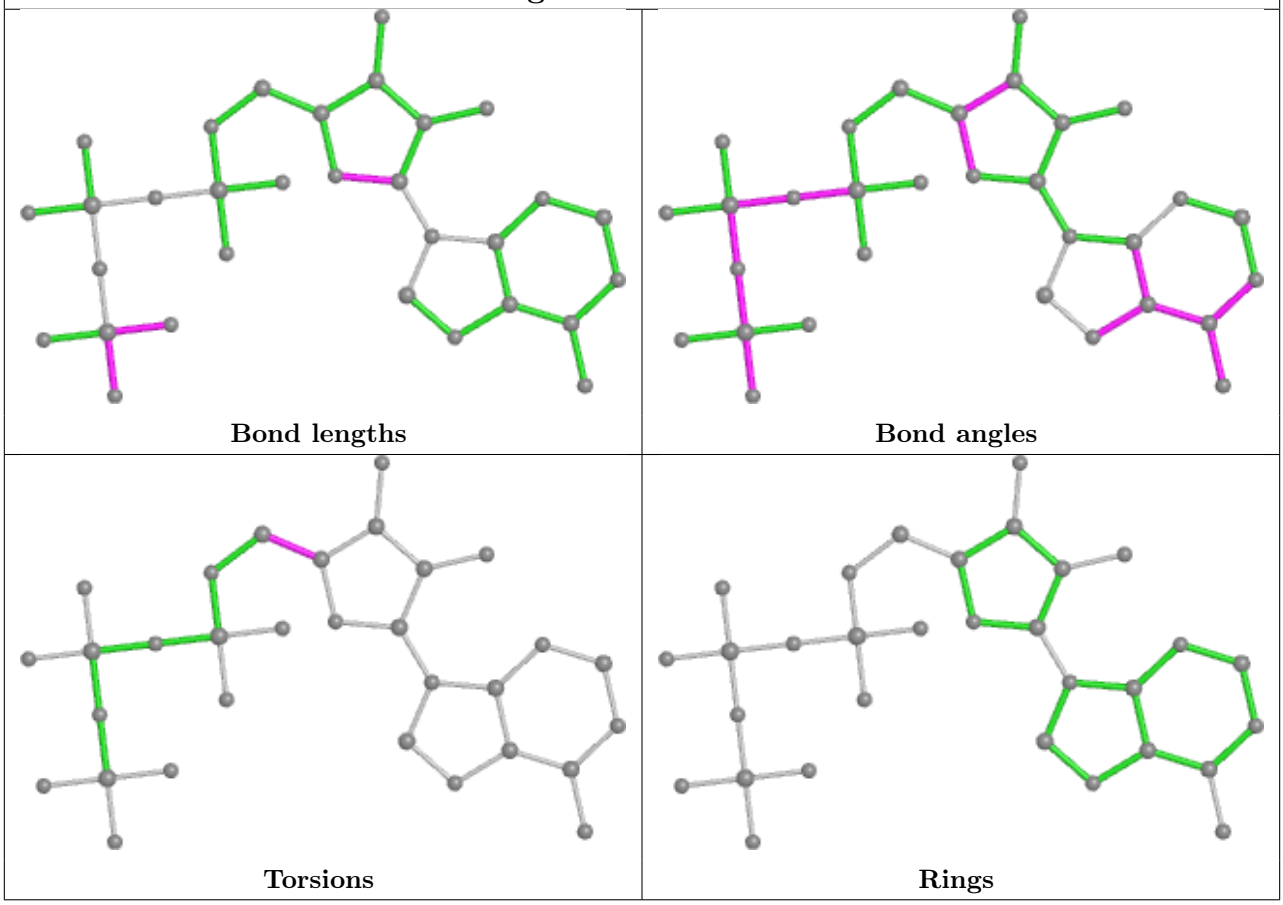
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

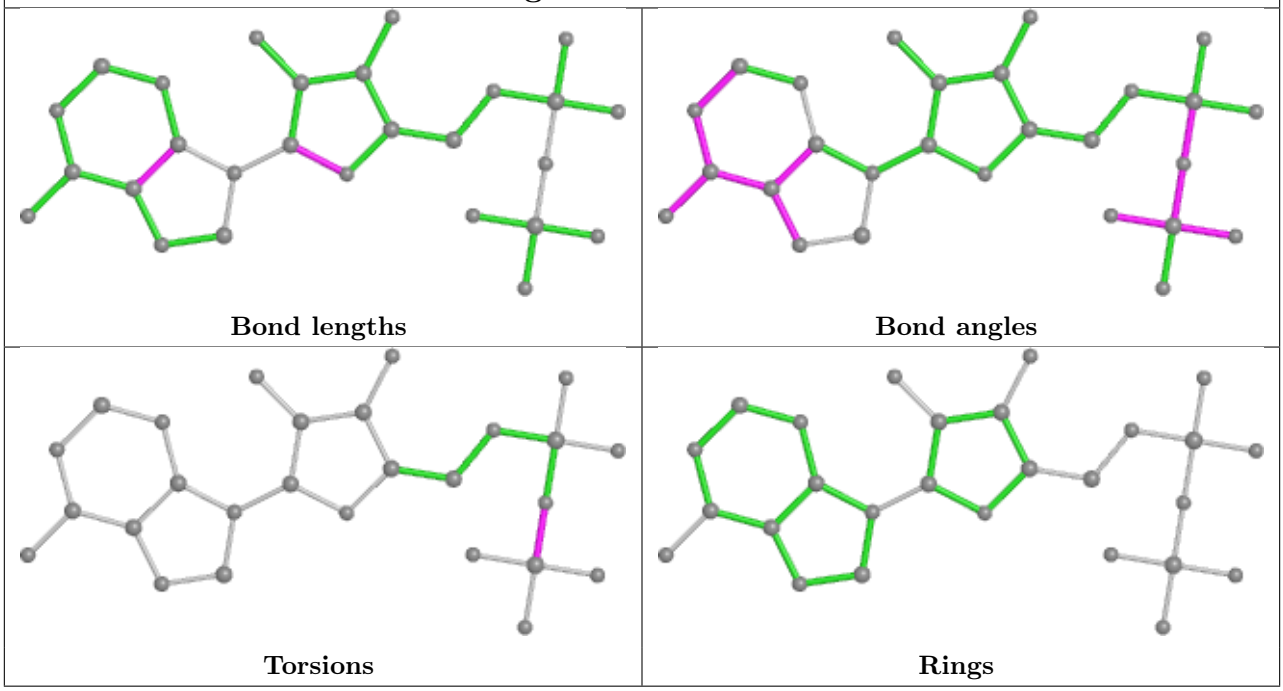
Ligand ADP D 603



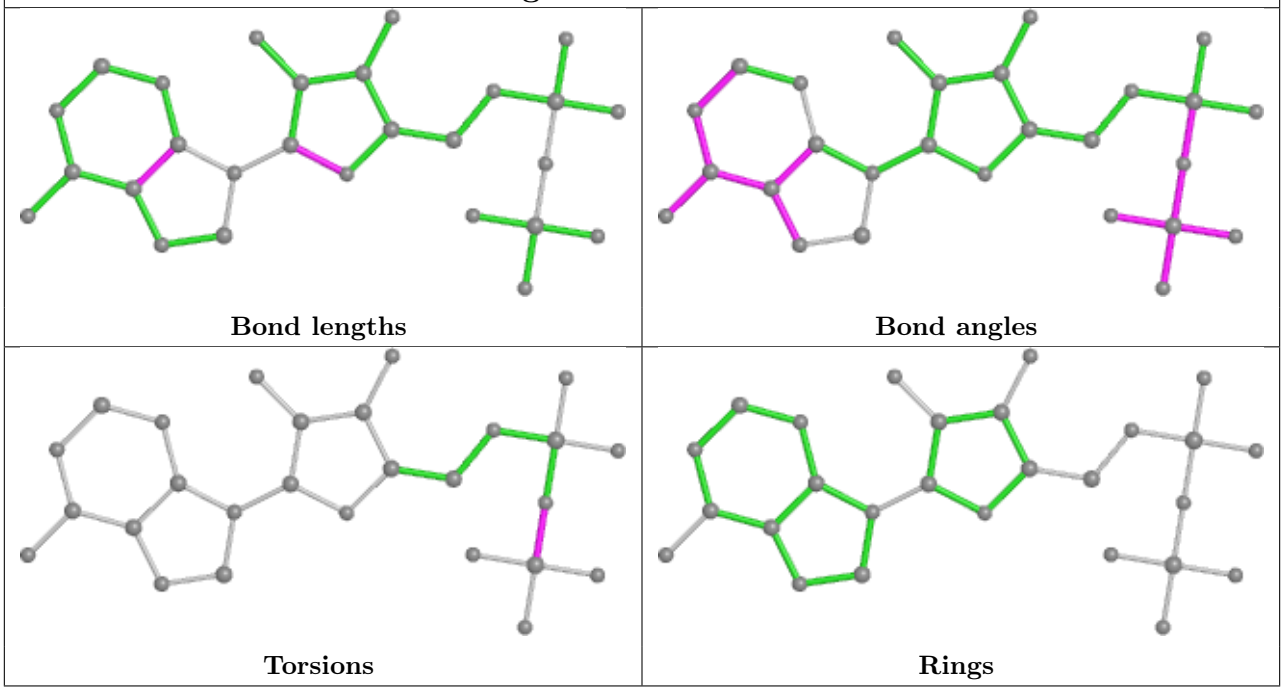
Ligand ATP F 601



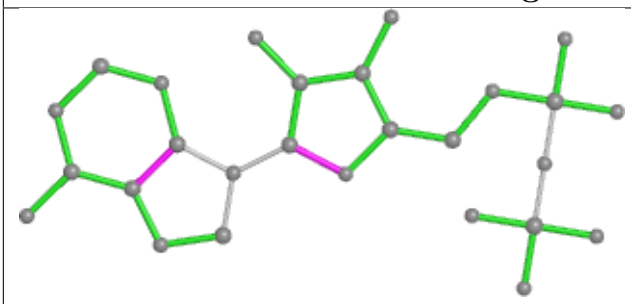
Ligand ADP F 602



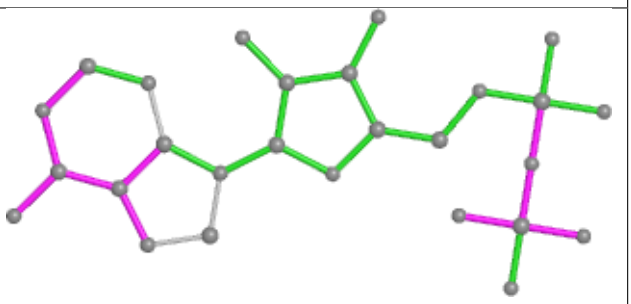
Ligand ADP A 603



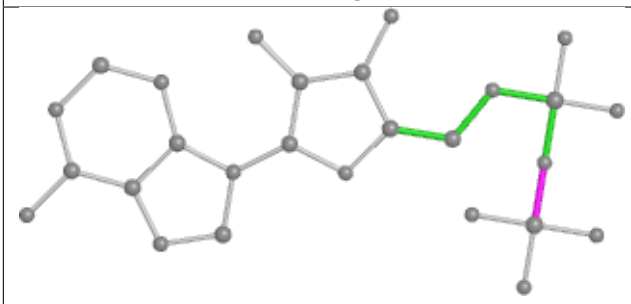
Ligand ADP C 603



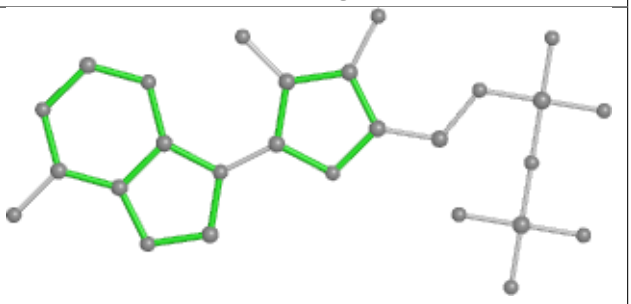
Bond lengths



Bond angles

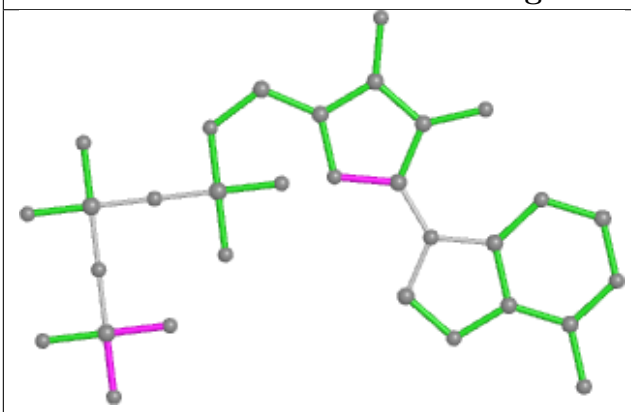


Torsions

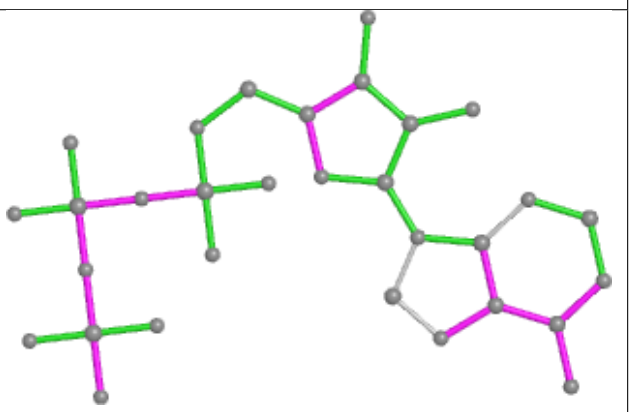


Rings

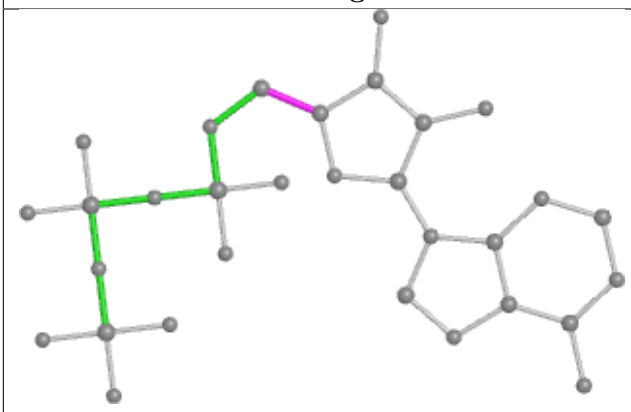
Ligand ATP C 601



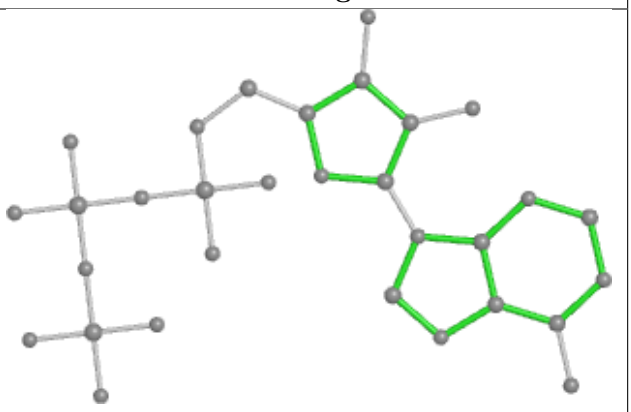
Bond lengths



Bond angles

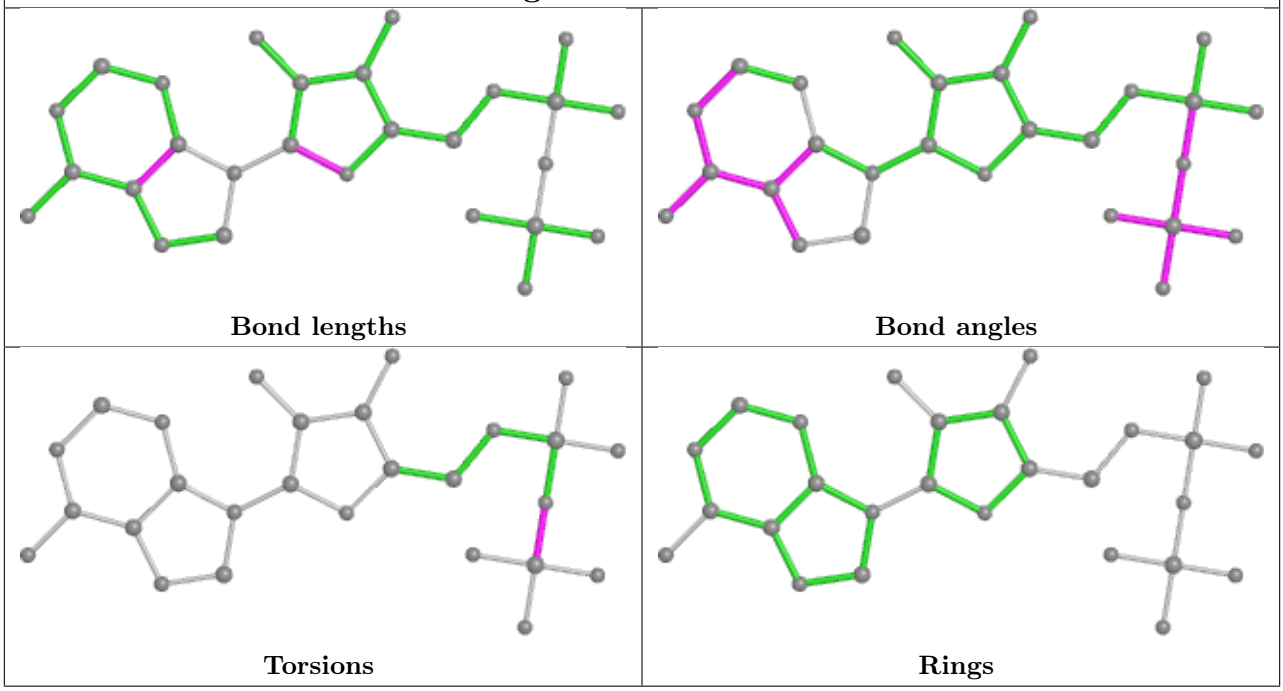


Torsions



Rings

Ligand ADP B 603



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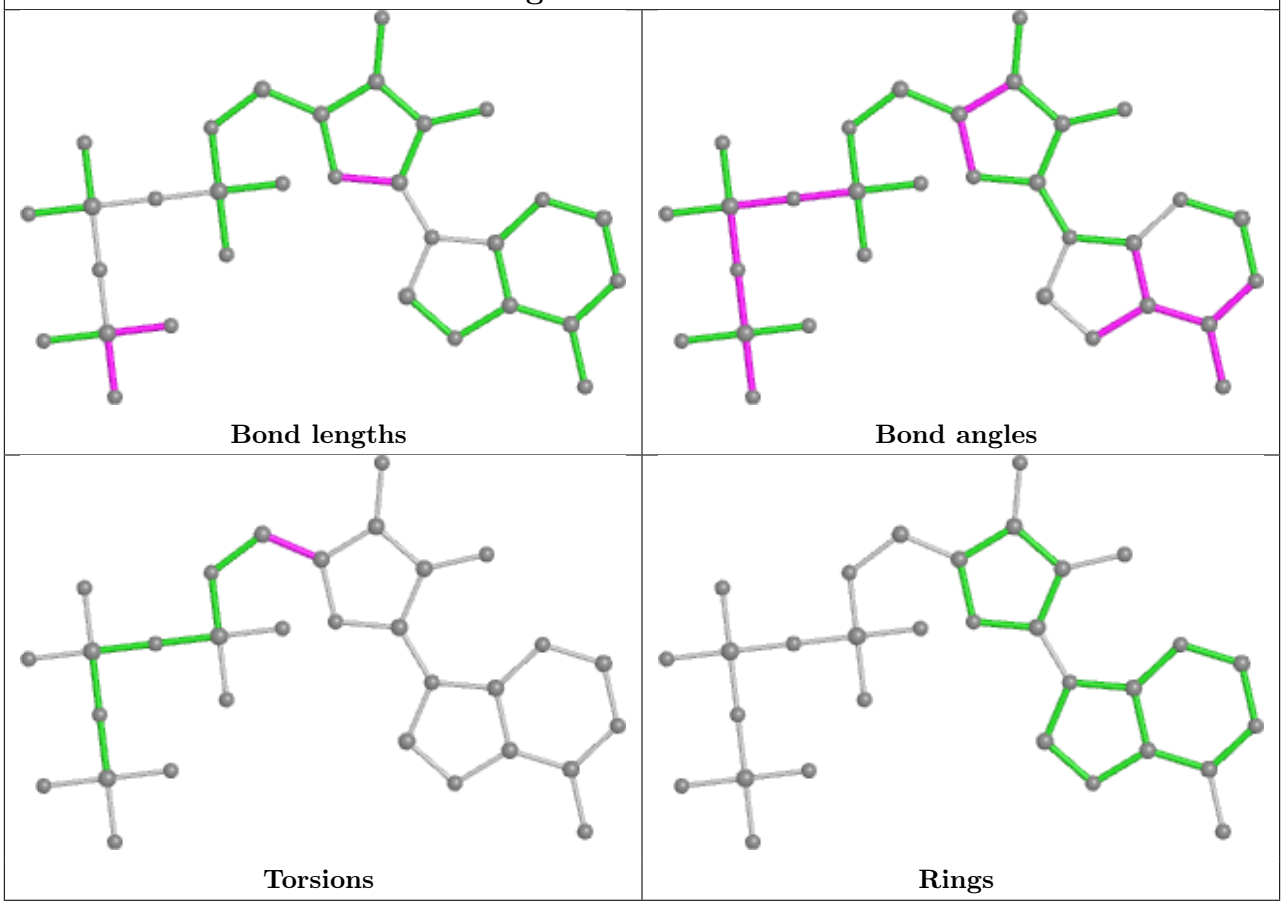
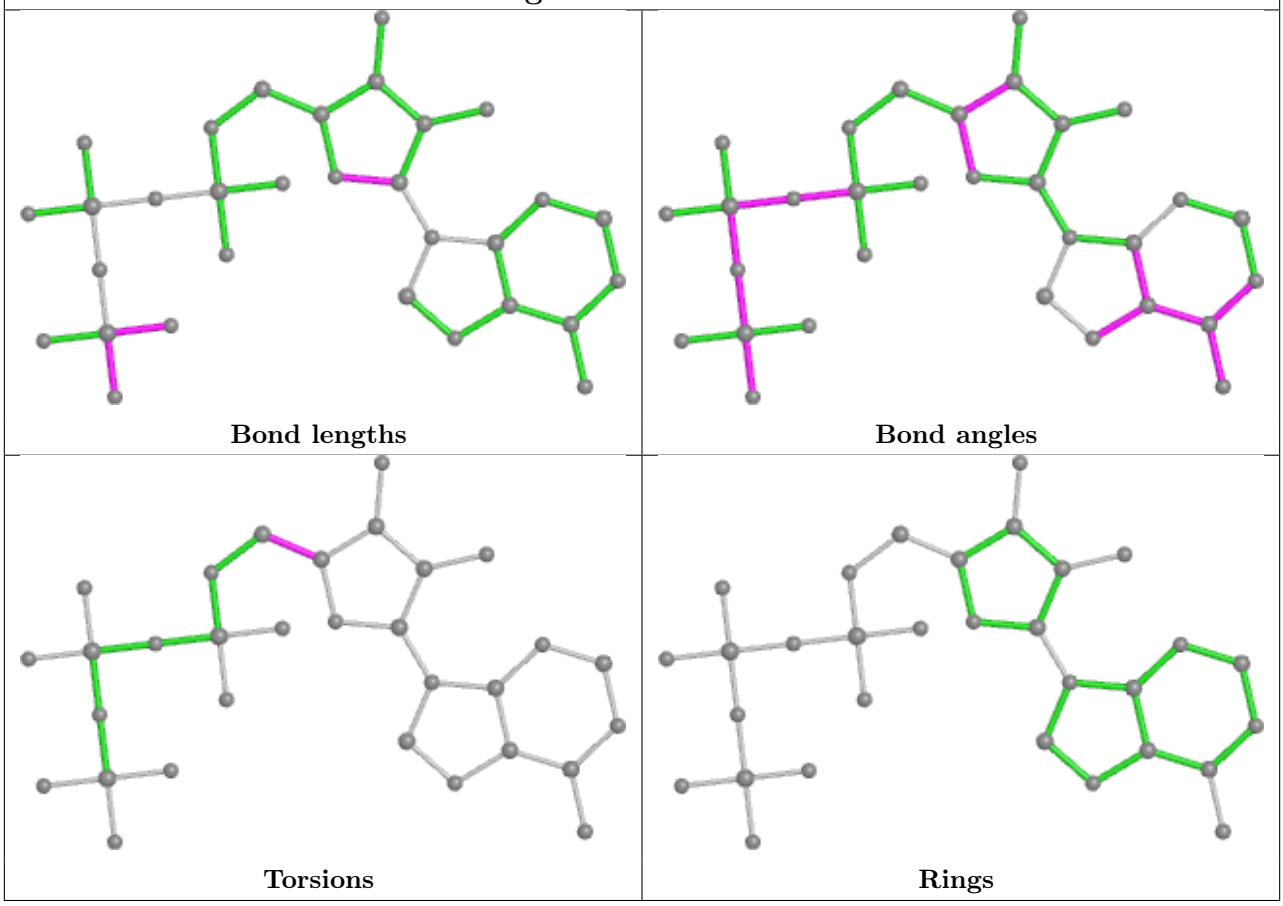
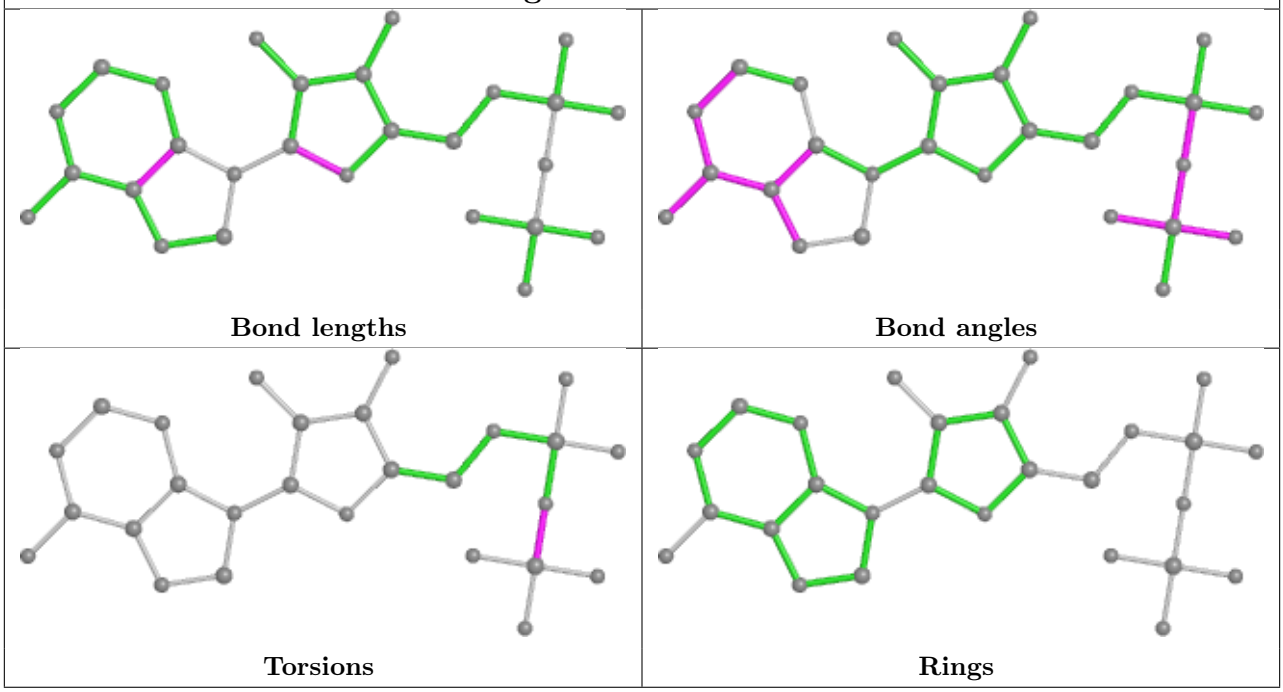


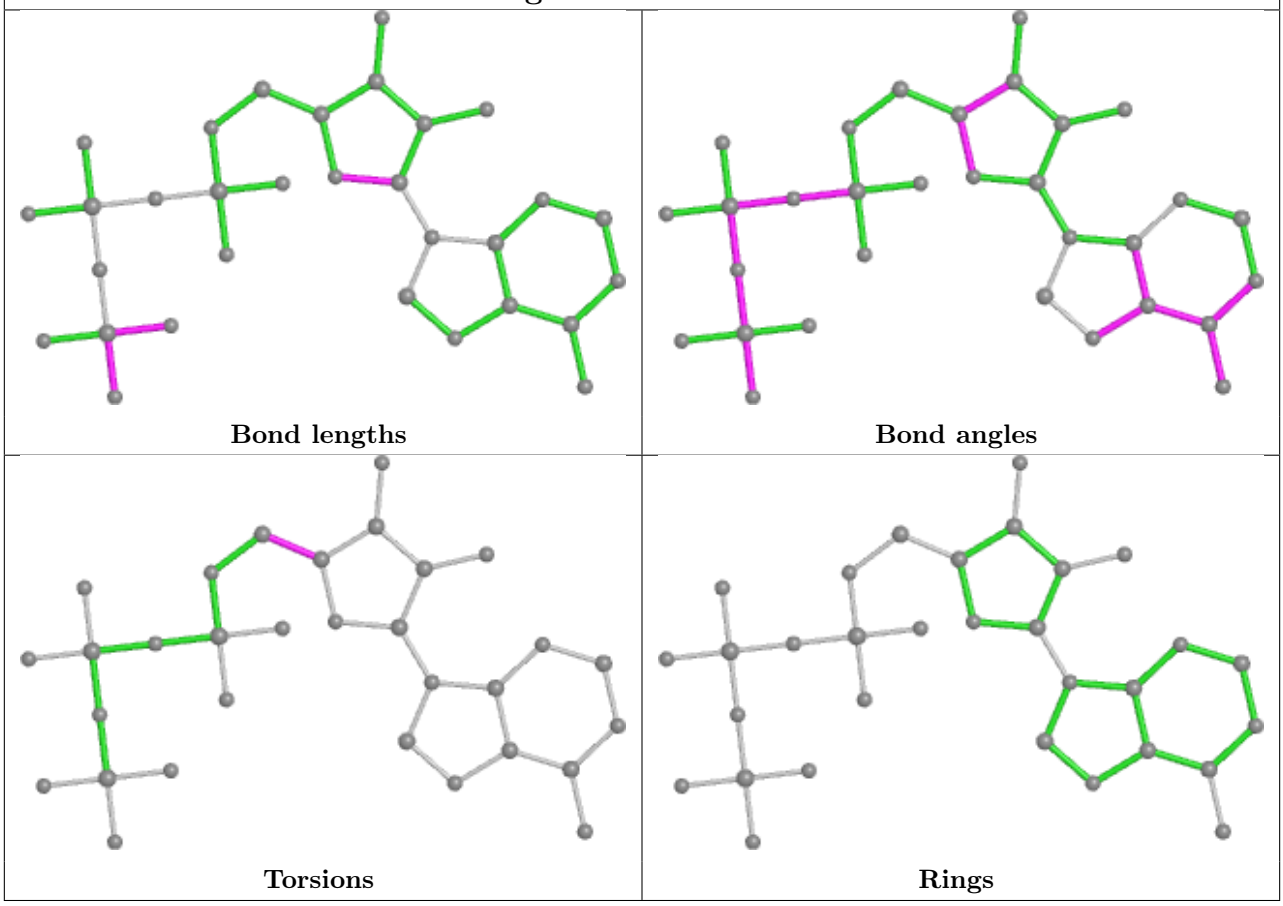
Ligand ATP D 601

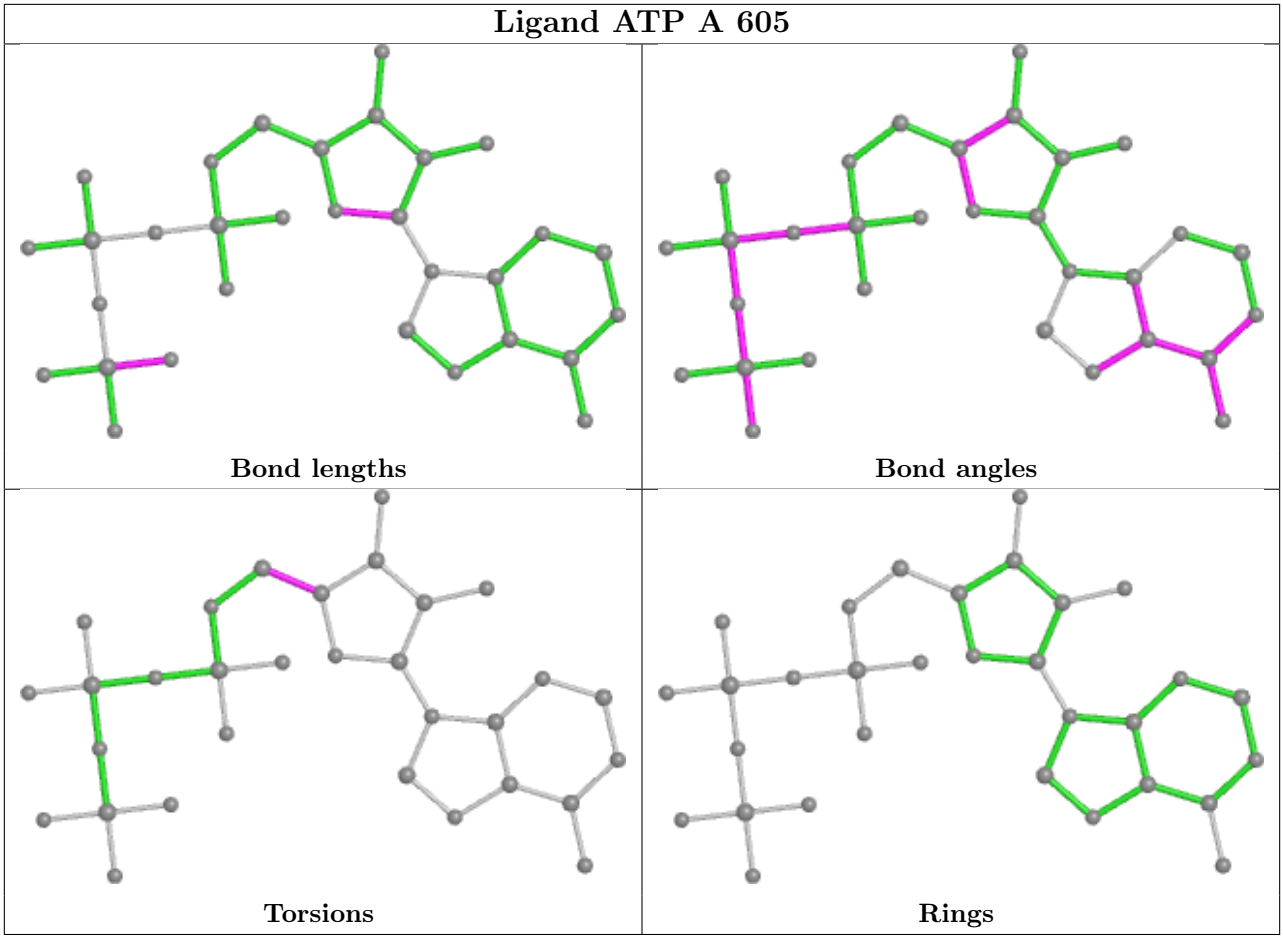


Ligand ADP E 902



Ligand ATP A 601





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.

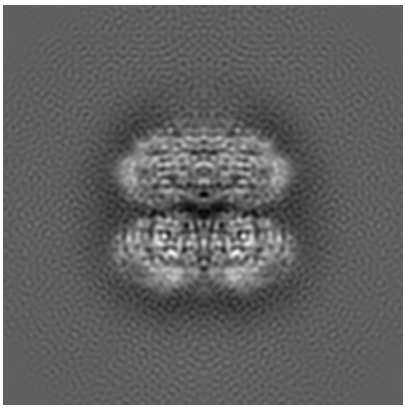
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24852. 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



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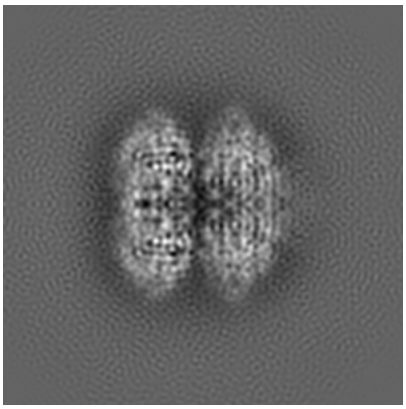

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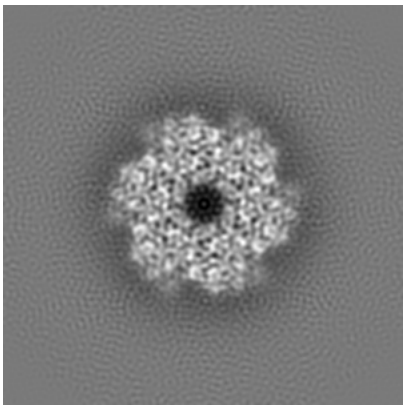
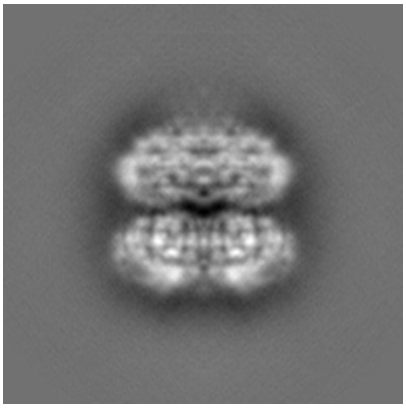


Z

6.1.2 Raw map



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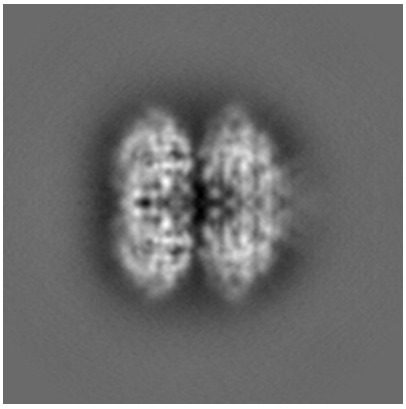
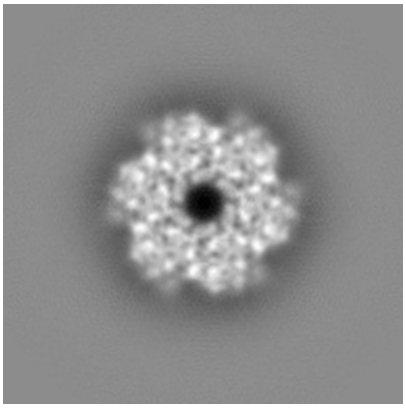


Y

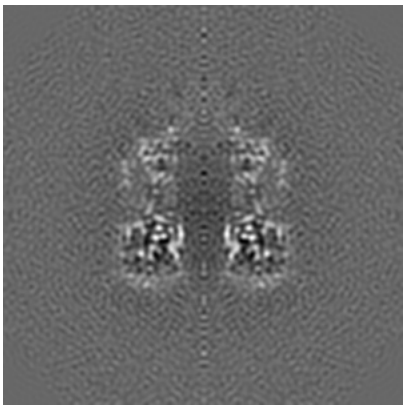


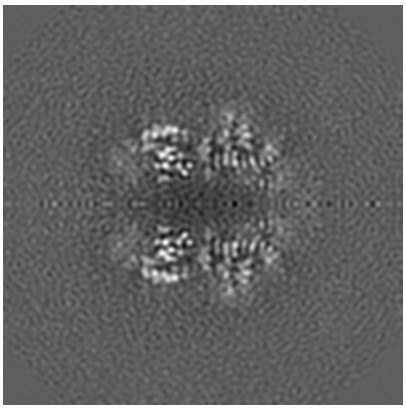
Z

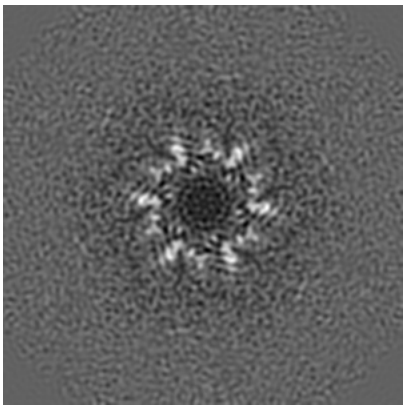
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

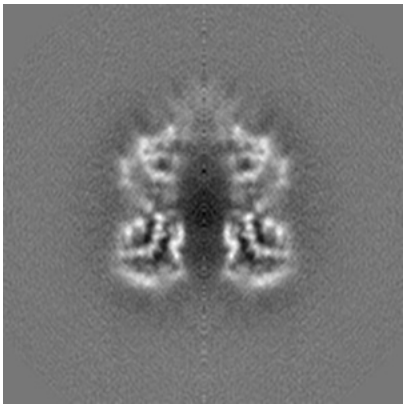
6.2.1 Primary map

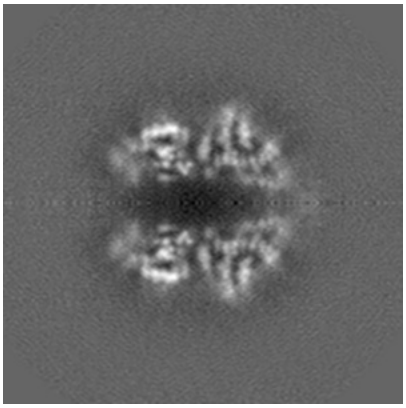

X Index: 96

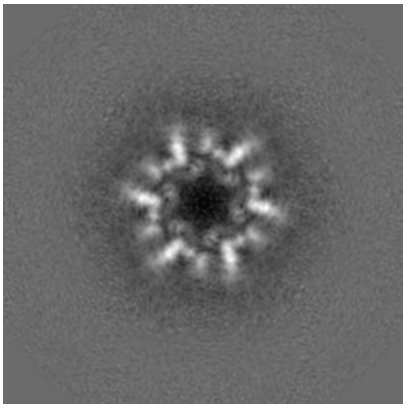

Y Index: 96


Z Index: 96

6.2.2 Raw map


X Index: 96

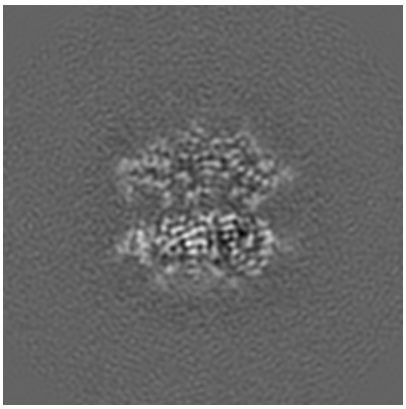

Y Index: 96

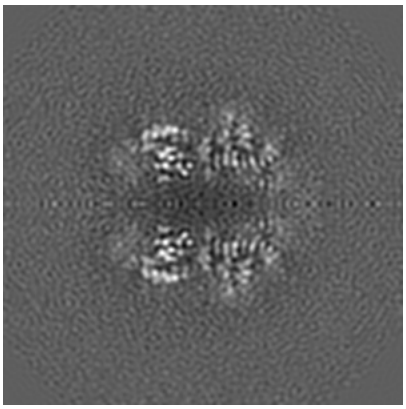

Z Index: 96

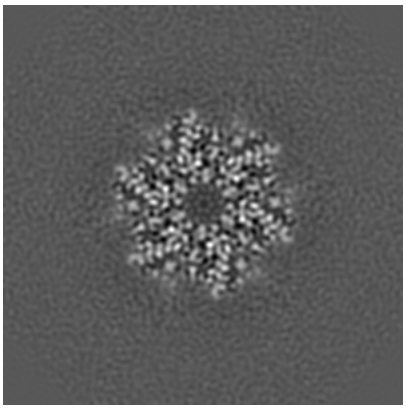
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

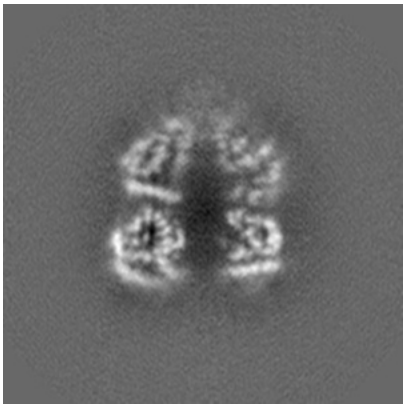
6.3.1 Primary map

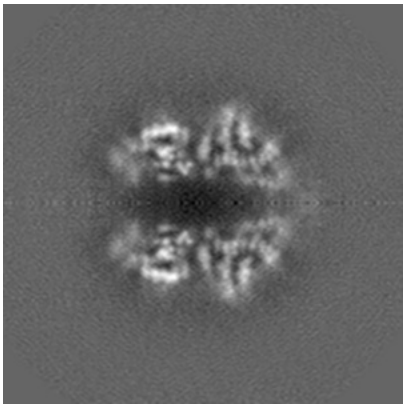

X Index: 114

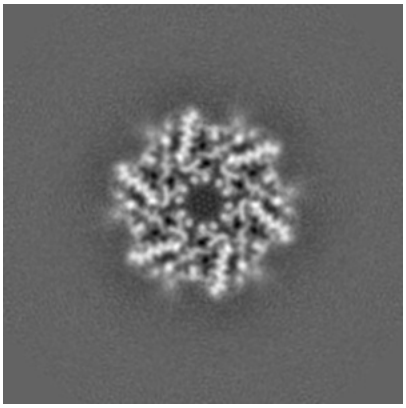

Y Index: 96


Z Index: 77

6.3.2 Raw map


X Index: 101

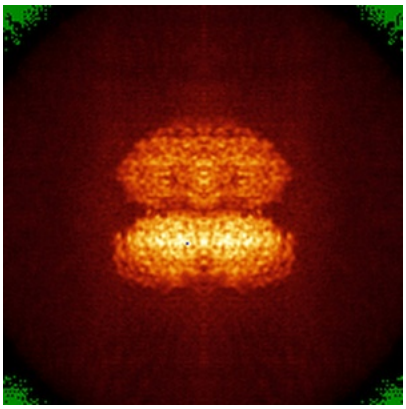

Y Index: 96

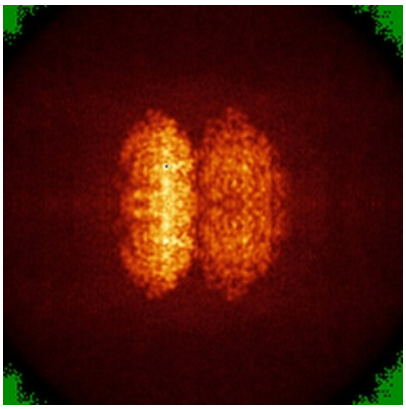

Z Index: 78

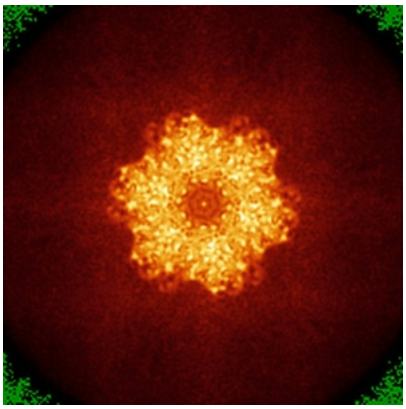
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

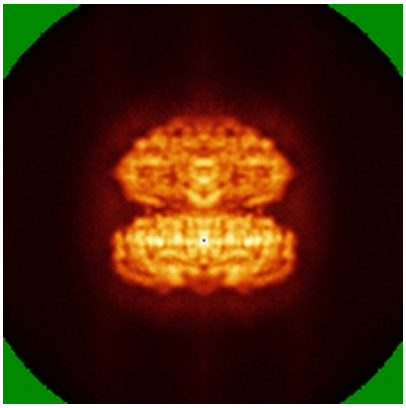
6.4.1 Primary map

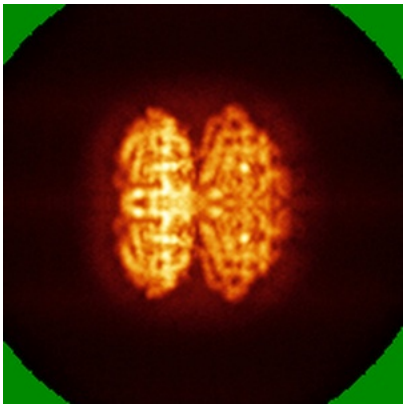

X

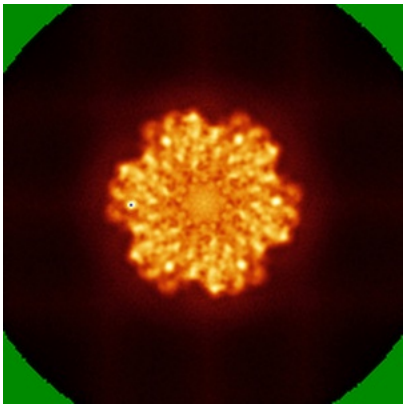

Y


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.

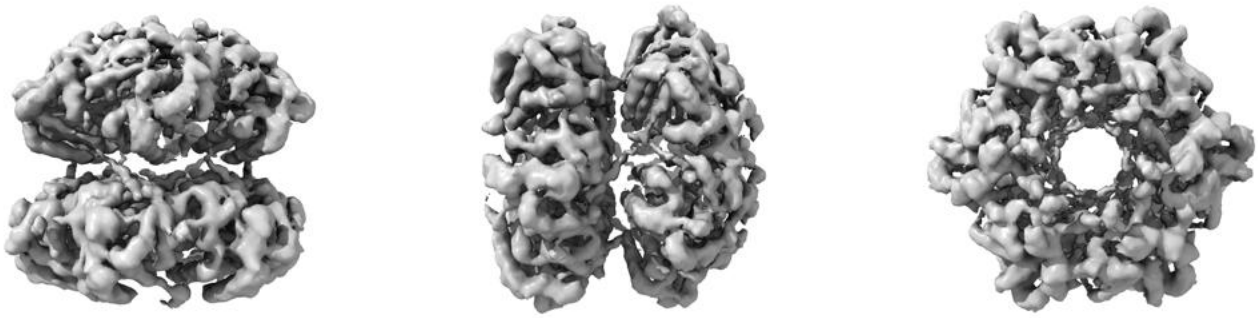
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



X Y Z

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.

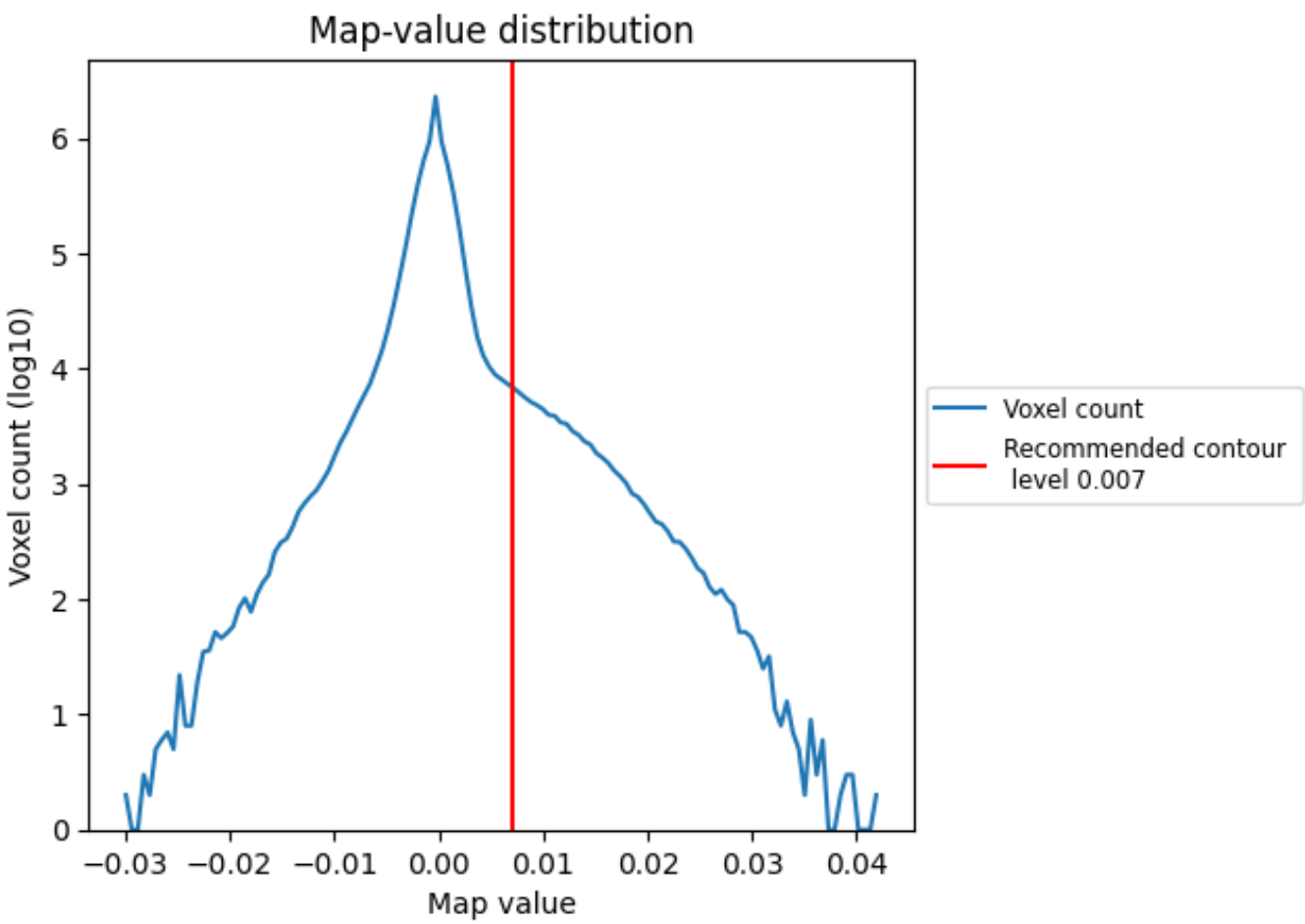
6.6 Mask visualisation (i)

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

7 Map analysis (i)

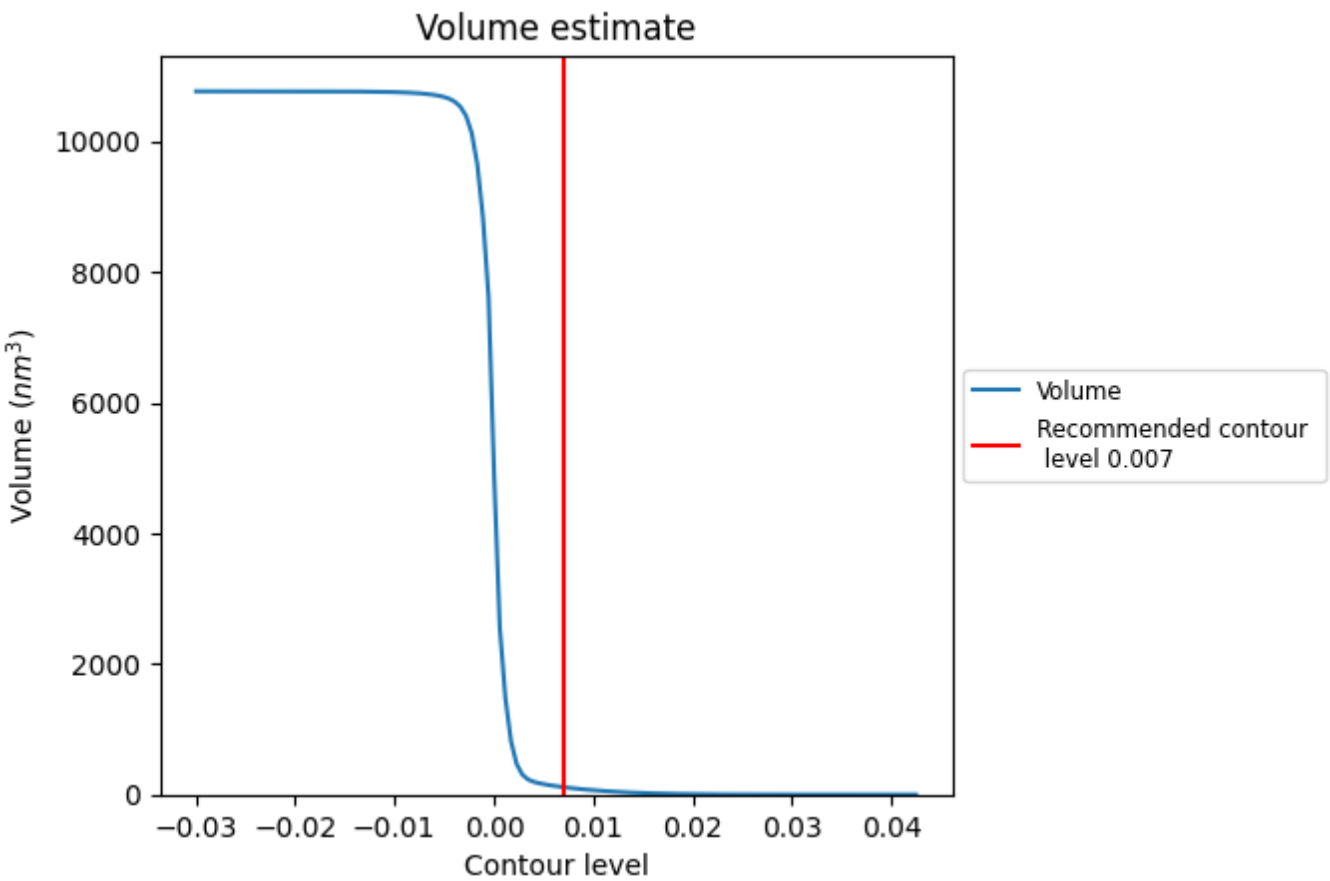
This section contains the results of statistical analysis of the map.

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.

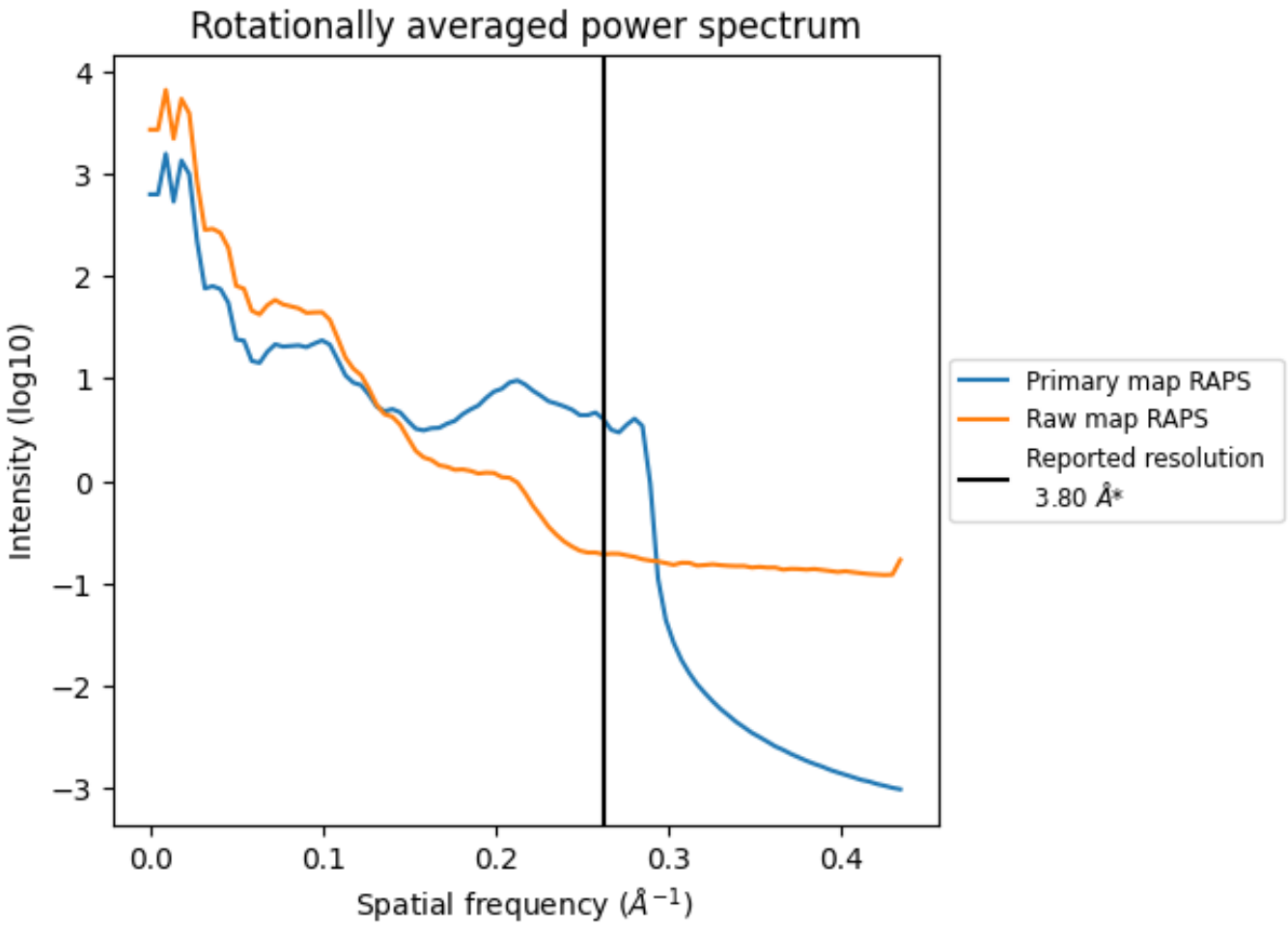
7.2 Volume estimate (i)



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

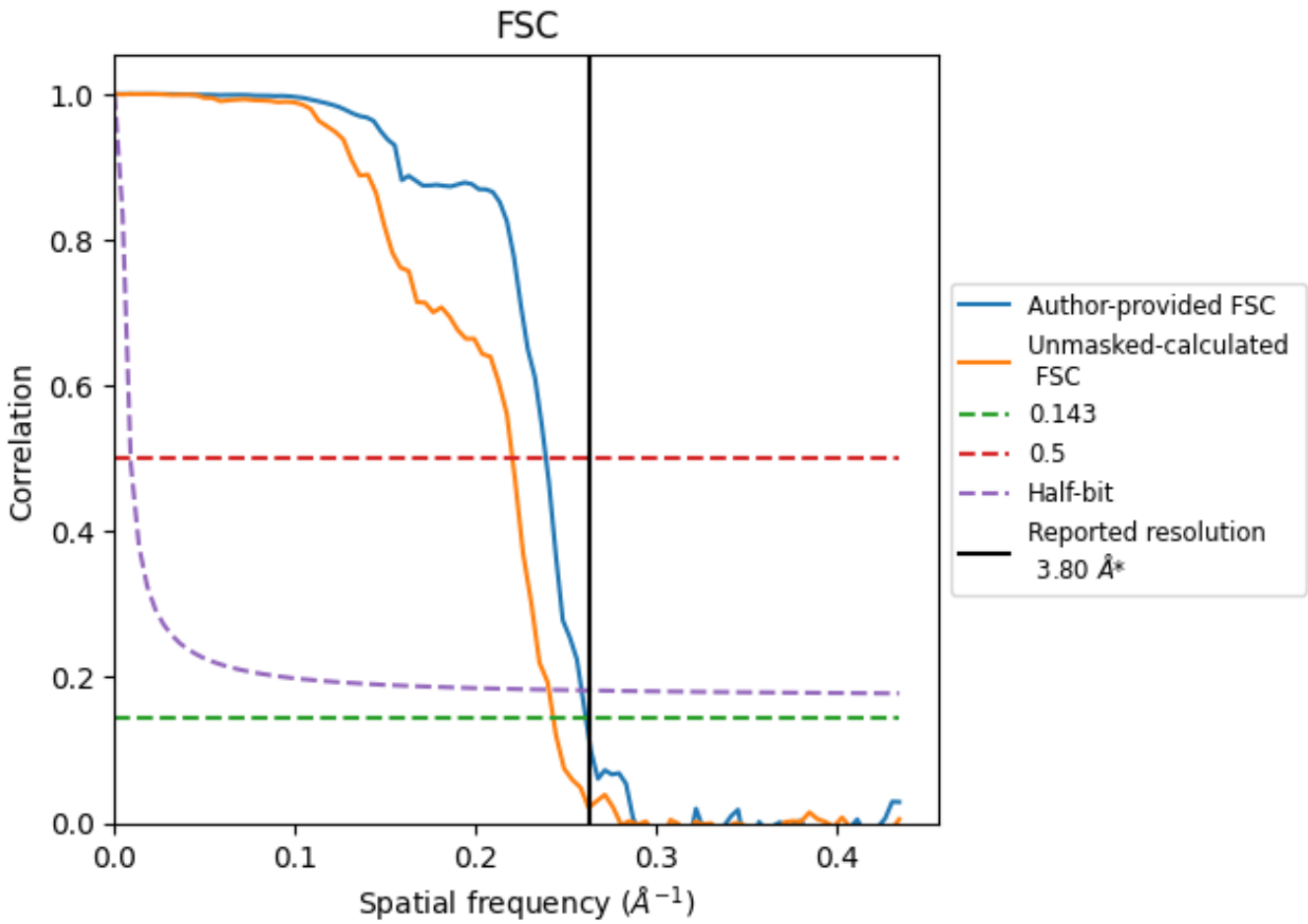


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

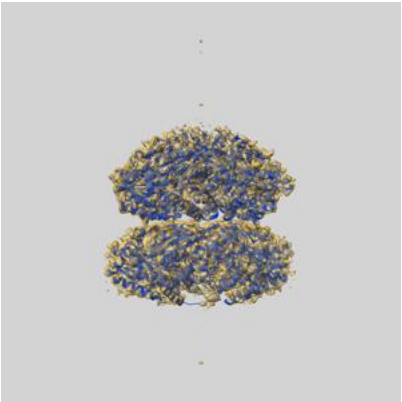
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.18	3.86
Unmasked-calculated*	4.11	4.54	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

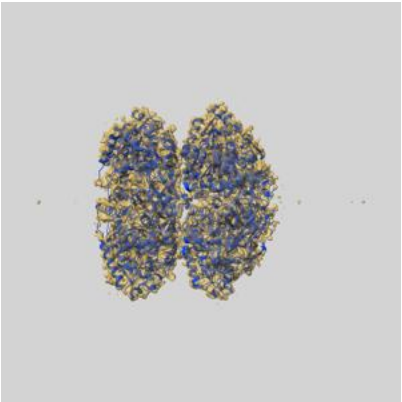
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24852 and PDB model 7S67. Per-residue inclusion information can be found in section 3 on page 7.

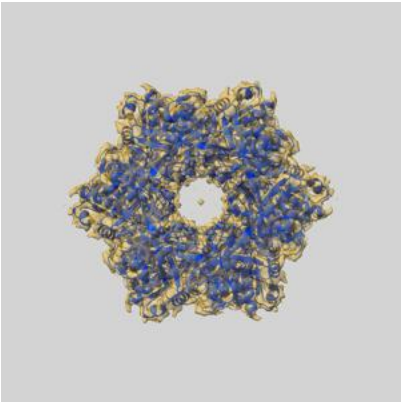
9.1 Map-model overlay (i)



X



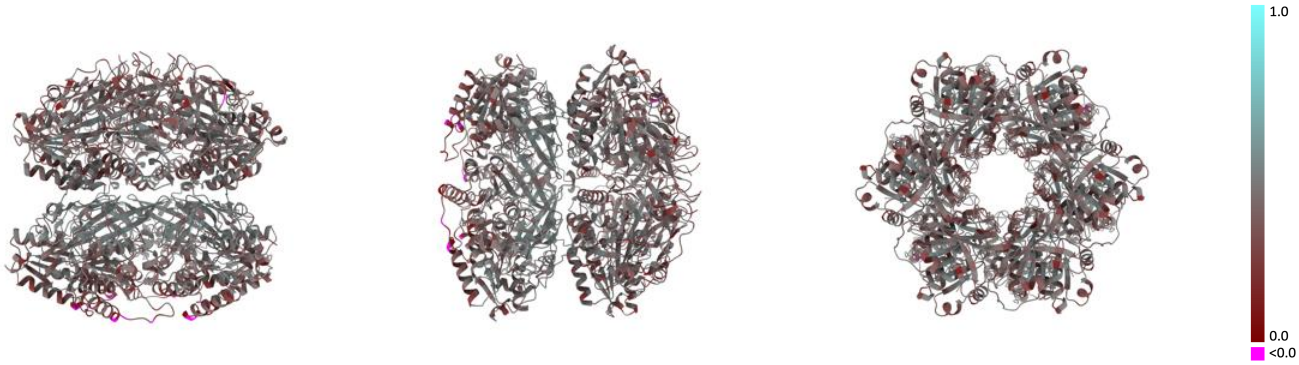
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

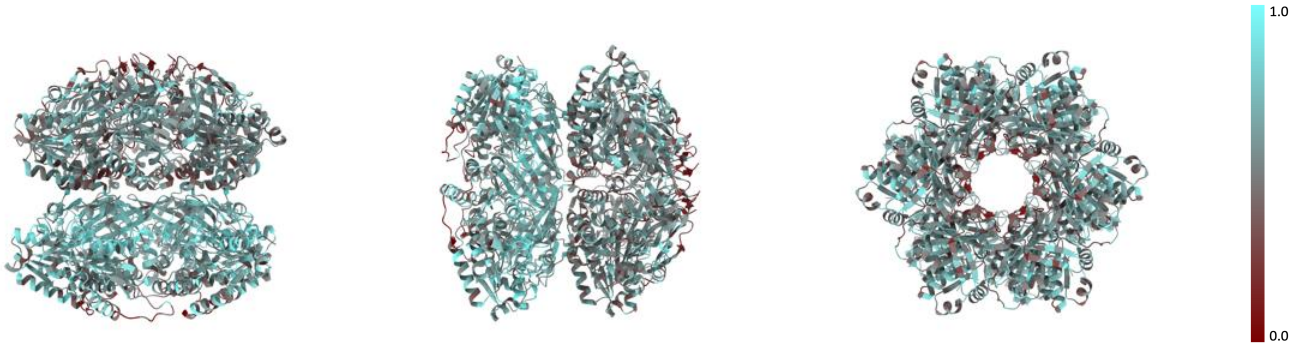
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

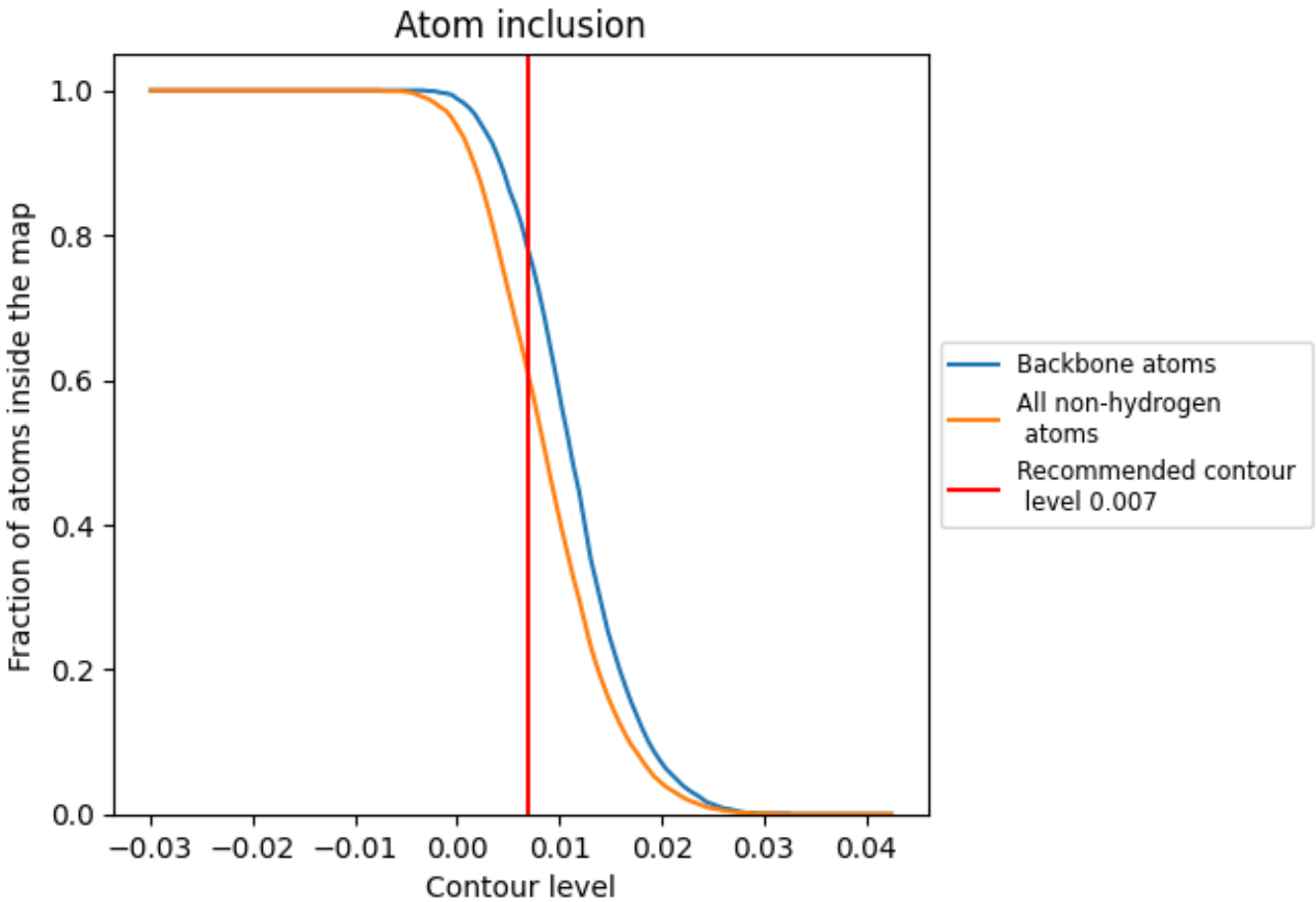
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6040	0.4080
A	0.6050	0.4110
B	0.6070	0.4080
C	0.6060	0.4080
D	0.5990	0.4080
E	0.6030	0.4070
F	0.6040	0.4090