



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 01:50 pm GMT

PDB ID : 9QQR / pdb\_00009qqr  
EMDB ID : EMD-53312  
Title : S.aureus ClpC decameric resting state  
Authors : Engelhardt, L.; Carroni, M.  
Deposited on : 2025-04-02  
Resolution : 4.70 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

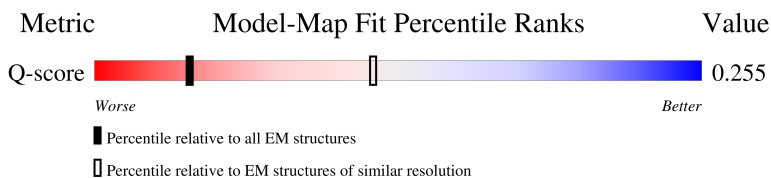
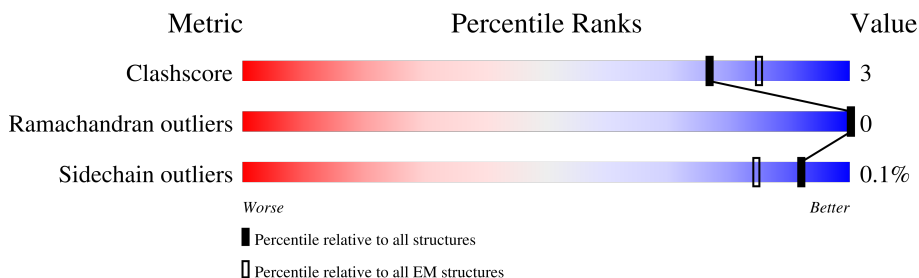
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.70 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	1989 ( 4.20 - 5.20 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	818	
1	B	818	
1	C	818	
1	D	818	

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Mol	Chain	Length	Quality of chain
1	E	818	
1	F	818	
1	G	818	
1	H	818	
1	I	818	
1	J	818	

## 2 Entry composition

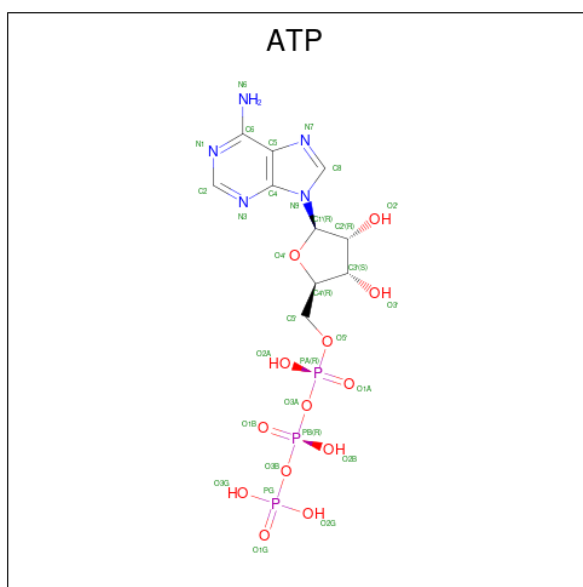
There are 3 unique types of molecules in this entry. The entry contains 53192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease ATP-binding subunit ClpC.

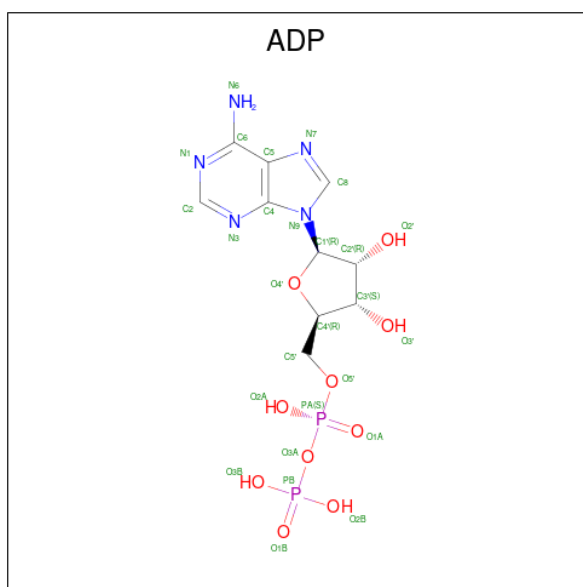
Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	618	Total	C	N	O	S	0	0
			4854	3032	851	958	13		
1	G	760	Total	C	N	O	S	0	0
			5963	3731	1055	1161	16		
1	H	760	Total	C	N	O	S	0	0
			5963	3731	1055	1161	16		
1	I	760	Total	C	N	O	S	0	0
			5963	3731	1055	1161	16		
1	J	618	Total	C	N	O	S	0	0
			4854	3032	851	958	13		
1	E	618	Total	C	N	O	S	0	0
			4854	3032	851	958	13		
1	D	760	Total	C	N	O	S	0	0
			5963	3731	1055	1161	16		
1	C	760	Total	C	N	O	S	0	0
			5963	3731	1055	1161	16		
1	B	760	Total	C	N	O	S	0	0
			5963	3731	1055	1161	16		
1	A	309	Total	C	N	O	S	0	0
			2411	1498	425	483	5		

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



Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total 31	C 10	N 5	O 13	P 3	0
2	G	1	Total 31	C 10	N 5	O 13	P 3	0
2	H	1	Total 31	C 10	N 5	O 13	P 3	0
2	I	1	Total 31	C 10	N 5	O 13	P 3	0
2	J	1	Total 31	C 10	N 5	O 13	P 3	0
2	E	1	Total 31	C 10	N 5	O 13	P 3	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0

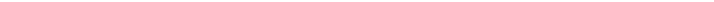
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total 27	C 10	N 5	O 10	P 2	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0



L471	P204	H1
1476	L234	H16
I511	V239	E19
R526	L242	M25
L531	V247	L36
P546	VAL	K39
K551	ALA	K40
V572	GLY	I45
L586	THR	V60
V594	LYS	V64
HIS	TVR	H70
ASP	ARG	L90
ASP	G255	E106
Q601	1278	R114
L602	D279	R122
L685	GLU	L129
A671	LEU	N130
G672	HIS	I131
F673	THR	A134
G674	THR	R135
F711	VAL	L142
H712	GLY	GLY
K713	GLY	ASN
E721	ALA	PRO
Q770	GLU	GLU
Q808	ILE	NET
THR	ASP	SER
GLU	ALA	ASN
THR	ALA	LYS
THR	K326	ASN
THR	I366	ALA
THR	A374	SER
PRO	D393	LYS
SER	E435	SER
GLN	D444	ASN
ALA	V461	N159
		L170
		T190
		T192

- Chain I:  87% 6% 7%

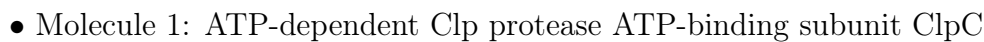
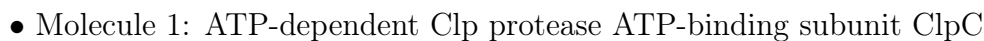
[illegible]

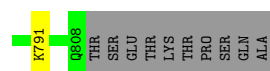
- Chain J:  69% 7% 24%

MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														
MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														
MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														
MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														
MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														
MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														
MET	ILE	ALA	TYR	H361	F670	F671	F672	F673	F674	F675	L719	L765	E774	T793	D804	Q808	THR	SER	SER	GLU	THR	LYS	THR	PRO	SER	SER	GLN	ALA	GLY	LEU	GLY	THR	ILE	MET
		ARG	ARG	G255																														

- 
- WORLDWIDE  
PDB  
PROTEIN DATA BANK

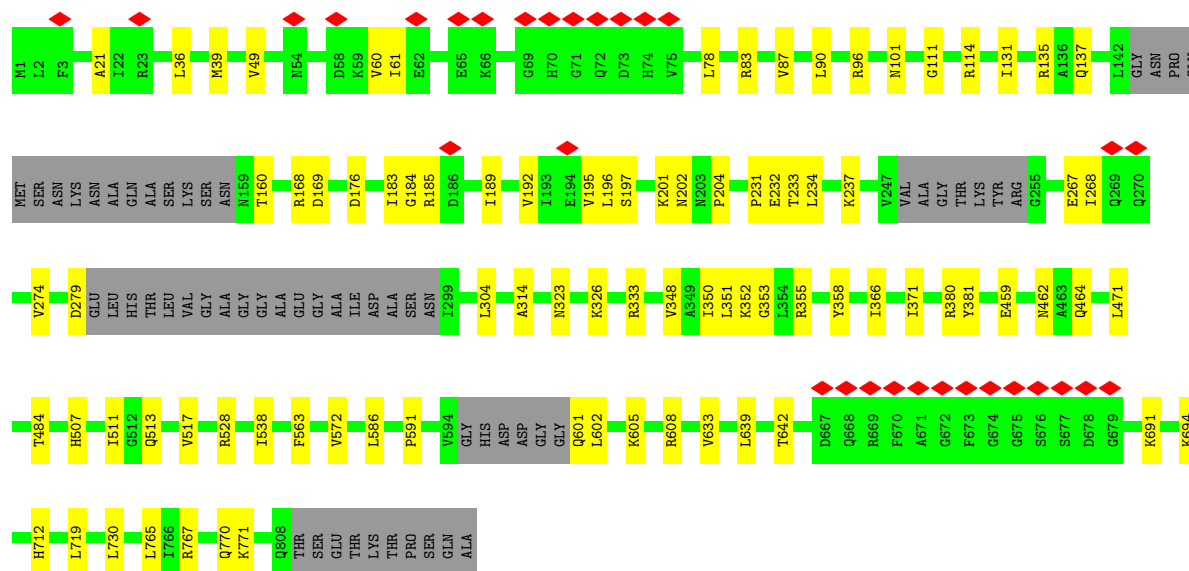






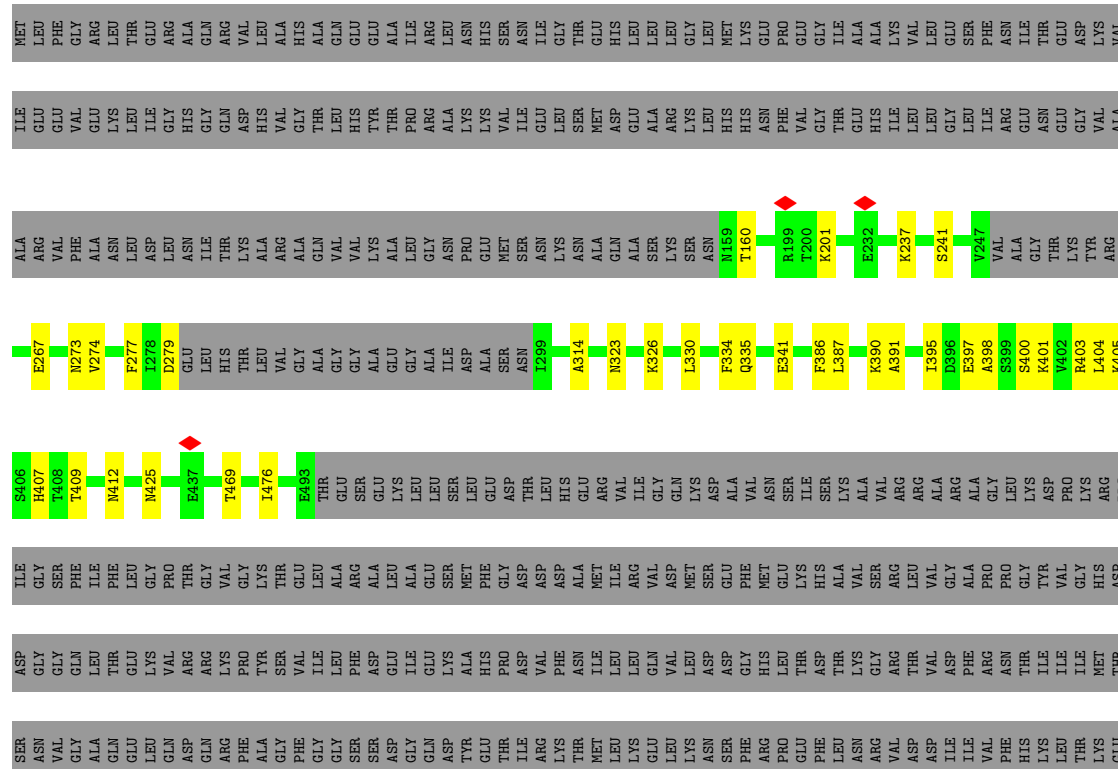
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain B: 82% 11% 7%



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

Chain A: 34% 62%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181306	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.430	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0593	Depositor
Map size (Å)	536.544, 536.544, 536.544	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.656, 1.656, 1.656	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.07	0/2436	0.19	0/3287
1	B	0.07	0/6036	0.20	0/8132
1	C	0.07	0/6036	0.21	0/8132
1	D	0.07	0/6036	0.22	0/8132
1	E	0.06	0/4913	0.19	0/6620
1	F	0.07	0/4913	0.20	0/6620
1	G	0.07	0/6036	0.21	0/8132
1	H	0.08	0/6036	0.22	0/8132
1	I	0.08	0/6036	0.22	0/8132
1	J	0.07	0/4913	0.19	0/6620
All	All	0.07	0/53391	0.21	0/71939

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2411	0	2432	25	0
1	B	5963	0	6039	54	0
1	C	5963	0	6039	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5963	0	6039	33	0
1	E	4854	0	4897	27	0
1	F	4854	0	4897	21	0
1	G	5963	0	6039	33	0
1	H	5963	0	6039	34	0
1	I	5963	0	6039	36	0
1	J	4854	0	4897	34	0
2	B	31	0	12	1	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	1	0
2	I	31	0	12	0	0
2	J	31	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	G	27	0	12	1	0
3	H	27	0	12	0	0
3	I	27	0	12	1	0
All	All	53192	0	53537	297	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 3.

All (297) 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:D:9:ARG:HH22	1:C:435:GLU:HG3	1.60	0.67
1:B:201:LYS:HB2	1:A:400:SER:HB3	1.77	0.67
1:I:586:LEU:HA	1:I:601:GLN:HB3	1.76	0.66
1:J:586:LEU:HA	1:J:601:GLN:HB3	1.78	0.66
1:I:198:ARG:HG2	1:J:396:ASP:HA	1.77	0.65
1:B:201:LYS:HB3	1:A:397:GLU:HA	1.79	0.65
1:A:387:LEU:HD22	1:A:391:ALA:HB2	1.78	0.65
1:B:511:ILE:H	2:B:901:ATP:HN62	1.45	0.64
1:I:196:LEU:HD11	1:I:310:GLN:HB3	1.80	0.64
1:J:511:ILE:HB	2:J:901:ATP:HN62	1.62	0.63
1:D:785:ASN:HB3	1:D:788:GLU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:GLU:HA	1:C:331:GLU:HB2	1.80	0.62
1:F:366:ILE:HG12	1:F:471:LEU:HD12	1.80	0.62
1:B:196:LEU:HD12	1:B:202:ASN:HB2	1.81	0.62
1:B:87:VAL:HG13	1:B:111:GLY:HA3	1.82	0.62
1:B:184:GLY:HA3	1:B:350:ILE:HG12	1.82	0.62
1:I:526:ARG:HG3	1:I:531:LEU:HD12	1.82	0.61
1:H:39:MET:HG3	1:H:60:VAL:HG21	1.81	0.61
1:J:620:GLU:HG2	1:J:621:LYS:HG3	1.82	0.61
1:E:586:LEU:HA	1:E:601:GLN:HB3	1.81	0.61
1:G:785:ASN:HB3	1:G:788:GLU:HB2	1.83	0.59
1:H:131:ILE:HD11	1:H:135:ARG:HH21	1.66	0.59
1:E:698:ARG:HB2	1:E:701:PHE:HB2	1.83	0.59
1:G:90:LEU:HD13	1:G:114:ARG:HB3	1.84	0.59
1:B:719:LEU:HD22	1:B:765:LEU:HD11	1.83	0.59
1:I:511:ILE:HD13	1:I:721:GLU:HB3	1.85	0.59
1:C:25:ASN:HB2	1:C:70:HIS:HE1	1.67	0.59
1:H:90:LEU:HD13	1:H:114:ARG:HB3	1.85	0.58
1:G:546:PRO:HG3	1:G:713:LYS:HD2	1.84	0.58
1:H:374:ALA:HA	1:H:476:ILE:HG21	1.85	0.58
1:D:83:ARG:HH12	1:D:465:ASN:HA	1.69	0.58
1:A:404:LEU:HA	1:A:407:HIS:HD2	1.69	0.58
1:I:90:LEU:HD13	1:I:114:ARG:HB3	1.85	0.58
1:I:198:ARG:HE	1:I:199:ARG:H	1.52	0.58
1:B:49:VAL:HG13	1:B:137:GLN:HG2	1.84	0.57
1:D:160:THR:HG22	1:D:267:GLU:HB3	1.86	0.57
1:C:719:LEU:HD23	1:C:722:ILE:HD12	1.86	0.57
1:B:39:MET:HG3	1:B:60:VAL:HG21	1.85	0.57
1:C:742:ILE:HD12	1:C:791:LYS:HE3	1.85	0.56
1:A:341:GLU:HB2	1:A:387:LEU:HB2	1.85	0.56
1:D:374:ALA:HB2	1:D:476:ILE:HD13	1.86	0.56
1:F:785:ASN:HB3	1:F:788:GLU:HB2	1.86	0.56
1:H:511:ILE:HD13	1:H:721:GLU:HB3	1.88	0.56
1:D:729:LYS:HE3	1:D:733:ARG:HH21	1.71	0.55
1:F:719:LEU:HD22	1:F:765:LEU:HD11	1.87	0.55
1:C:131:ILE:HD11	1:C:135:ARG:HH21	1.71	0.55
1:G:374:ALA:HA	1:G:476:ILE:HG21	1.87	0.55
1:H:45:ILE:HB	1:H:106:GLU:HB3	1.88	0.55
1:F:698:ARG:HB2	1:F:701:PHE:HB2	1.89	0.55
1:A:160:THR:HG22	1:A:267:GLU:HB3	1.89	0.55
1:H:16:HIS:HD2	1:H:40:LYS:HE3	1.73	0.54
1:I:374:ALA:HA	1:I:476:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ALA:HB3	1:B:78:LEU:HD13	1.89	0.54
1:I:591:PRO:HD3	1:I:642:THR:HB	1.88	0.54
1:C:115:GLU:HG3	1:C:117:GLU:H	1.72	0.54
1:B:380:ARG:HH22	1:B:563:PHE:HA	1.72	0.54
1:F:374:ALA:HA	1:F:476:ILE:HG21	1.88	0.54
1:B:232:GLU:HB2	1:A:409:THR:HG23	1.89	0.54
1:C:16:HIS:HD2	1:C:40:LYS:HE3	1.72	0.54
1:I:201:LYS:HG2	1:I:335:GLN:HB2	1.90	0.54
1:A:279:ASP:HA	1:A:314:ALA:HB3	1.89	0.54
1:C:5:ARG:HH21	1:C:176:ASP:HA	1.73	0.54
1:H:546:PRO:HG3	1:H:713:LYS:HD2	1.89	0.54
1:G:45:ILE:HB	1:G:106:GLU:HB3	1.90	0.54
1:G:590:PRO:HA	1:G:642:THR:HG21	1.90	0.54
1:C:785:ASN:HB3	1:C:788:GLU:HB2	1.90	0.54
1:B:234:LEU:HA	1:B:237:LYS:HD2	1.89	0.53
1:H:511:ILE:H	2:H:901:ATP:HN62	1.56	0.53
1:B:183:ILE:HG21	1:B:353:GLY:HA3	1.90	0.53
1:J:543:PHE:HB3	1:J:551:LYS:HD3	1.90	0.53
1:G:9:ARG:HH22	1:H:435:GLU:HG3	1.74	0.53
1:I:279:ASP:HA	1:I:314:ALA:HB3	1.90	0.53
1:H:299:ILE:HG22	1:H:300:LEU:HG	1.92	0.52
1:C:300:LEU:HB3	1:C:303:ALA:HB3	1.91	0.52
1:B:591:PRO:HD3	1:B:642:THR:HB	1.91	0.52
1:E:268:ILE:HG23	1:E:274:VAL:HB	1.91	0.52
1:H:90:LEU:HD22	1:H:114:ARG:HD3	1.92	0.52
1:I:213:GLY:HA3	3:I:902:ADP:H8	1.75	0.52
1:C:201:LYS:HA	1:C:333:ARG:HA	1.91	0.52
1:B:83:ARG:HH12	1:B:464:GLN:HG2	1.75	0.52
1:E:785:ASN:HB3	1:E:788:GLU:HB2	1.92	0.51
1:H:36:LEU:HD21	1:H:64:VAL:HG11	1.91	0.51
1:D:90:LEU:HD13	1:D:114:ARG:HB3	1.93	0.51
1:I:131:ILE:HD11	1:I:135:ARG:HH21	1.74	0.51
1:J:719:LEU:HD22	1:J:765:LEU:HD11	1.90	0.51
1:G:201:LYS:HE2	1:G:332:ARG:HA	1.93	0.51
1:J:241:SER:HA	1:J:277:PHE:HB3	1.93	0.51
1:B:195:VAL:HA	1:A:401:LYS:HE2	1.91	0.51
1:J:323:ASN:HA	1:J:326:LYS:HE3	1.93	0.51
1:D:719:LEU:HD23	1:D:722:ILE:HD12	1.92	0.50
1:H:170:LEU:HD13	1:H:239:VAL:HG12	1.94	0.50
1:J:160:THR:HG22	1:J:267:GLU:HB3	1.93	0.50
1:C:261:LEU:HD13	1:C:300:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:730:LEU:HD12	1:E:733:ARG:HD2	1.93	0.50
1:B:513:GLN:HG2	1:B:712:HIS:HB2	1.94	0.50
1:H:122:ARG:HD3	1:H:461:LYS:HE2	1.93	0.50
1:E:768:ALA:HA	1:E:771:LYS:HE3	1.93	0.50
1:B:192:VAL:HG13	1:B:204:PRO:HG3	1.93	0.50
1:A:403:ARG:HA	1:A:469:THR:HG21	1.93	0.50
1:G:39:MET:HB3	1:G:57:GLU:HG3	1.93	0.50
1:G:787:ILE:HA	1:G:790:LYS:HD2	1.94	0.50
1:H:204:PRO:HG2	1:H:312:ILE:HG12	1.93	0.50
1:I:168:ARG:HH11	1:I:169:ASP:H	1.60	0.49
1:J:443:ARG:HH21	1:E:436:PHE:HB2	1.76	0.49
1:I:129:LEU:HD11	1:I:134:ALA:HB2	1.94	0.49
1:C:546:PRO:HG3	1:C:713:LYS:HD2	1.93	0.49
1:J:279:ASP:HA	1:J:314:ALA:HB3	1.95	0.49
1:G:366:ILE:HG12	1:G:471:LEU:HD12	1.94	0.49
1:I:90:LEU:HD22	1:I:114:ARG:HD3	1.94	0.49
1:J:374:ALA:HA	1:J:476:ILE:HG21	1.93	0.49
1:A:201:LYS:HB3	1:A:335:GLN:HB2	1.94	0.49
1:I:546:PRO:HG3	1:I:713:LYS:HD2	1.93	0.49
1:E:719:LEU:HD22	1:E:765:LEU:HD11	1.93	0.49
1:B:168:ARG:HH11	1:B:169:ASP:H	1.58	0.49
1:B:381:TYR:HB3	1:B:484:THR:HG21	1.95	0.49
1:G:719:LEU:HD22	1:G:765:LEU:HD11	1.95	0.49
1:F:522:LYS:HA	1:F:525:ARG:HH11	1.77	0.48
1:A:409:THR:HB	1:A:412:ASN:HB2	1.95	0.48
1:I:330:LEU:HD22	1:I:334:PHE:HE1	1.77	0.48
1:C:531:LEU:HD22	1:B:730:LEU:HD11	1.95	0.48
1:D:546:PRO:HG3	1:D:713:LYS:HD2	1.95	0.48
1:D:623:HIS:HB3	1:D:626:VAL:HG23	1.95	0.48
1:B:279:ASP:HA	1:B:314:ALA:HB3	1.95	0.48
1:H:572:VAL:HG21	1:H:602:LEU:HD13	1.96	0.48
1:G:90:LEU:HD22	1:G:114:ARG:HD3	1.95	0.48
1:F:768:ALA:HA	1:F:771:LYS:HE3	1.95	0.48
1:D:46:ALA:HB2	1:D:106:GLU:HA	1.94	0.48
1:C:572:VAL:HG21	1:C:602:LEU:HD13	1.96	0.48
1:A:323:ASN:HA	1:A:326:LYS:HE3	1.96	0.48
1:F:729:LYS:HE3	1:F:733:ARG:HH21	1.78	0.48
1:G:94:GLU:HG3	1:G:110:LEU:HB3	1.95	0.48
1:J:793:THR:HB	1:J:804:ASP:HB3	1.95	0.48
1:B:304:LEU:HB3	1:B:333:ARG:HG3	1.95	0.47
1:G:330:LEU:HD22	1:G:334:PHE:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:527:ALA:HB3	1:J:538:ILE:HG23	1.96	0.47
1:C:39:MET:HG3	1:C:60:VAL:HG21	1.96	0.47
1:I:199:ARG:HD3	1:J:361:HIS:CG	2.49	0.47
1:I:242:LEU:HB2	1:I:276:LEU:HD11	1.97	0.47
1:B:197:SER:HB3	1:A:405:LYS:HB2	1.96	0.47
1:A:160:THR:HG21	1:A:274:VAL:HG21	1.97	0.47
1:J:330:LEU:HD22	1:J:334:PHE:HE1	1.78	0.47
1:B:351:LEU:HD12	1:B:371:ILE:HG23	1.95	0.47
1:G:25:ASN:HB2	1:G:70:HIS:HE1	1.79	0.47
1:J:348:VAL:HG22	1:J:375:VAL:HG11	1.96	0.47
1:E:590:PRO:HA	1:E:642:THR:HG21	1.95	0.47
1:A:404:LEU:HA	1:A:407:HIS:CD2	2.49	0.47
1:E:751:ILE:HD11	1:E:768:ALA:HB1	1.96	0.47
1:C:45:ILE:HB	1:C:106:GLU:HB3	1.97	0.47
1:E:181:PRO:HB3	1:E:223:GLN:HE22	1.79	0.47
1:H:366:ILE:HG12	1:H:471:LEU:HD12	1.96	0.47
1:E:550:GLY:HA3	2:E:901:ATP:H8	1.80	0.47
1:G:6:LEU:HD23	1:G:103:VAL:HB	1.97	0.46
1:I:299:ILE:HG22	1:I:300:LEU:HG	1.97	0.46
1:D:751:ILE:HD11	1:D:768:ALA:HB1	1.96	0.46
1:I:49:VAL:HG13	1:I:137:GLN:HG2	1.97	0.46
1:H:586:LEU:HA	1:H:601:GLN:HB3	1.97	0.46
1:D:603:THR:HB	1:D:647:VAL:HG11	1.98	0.46
1:B:201:LYS:HE2	1:A:395:ILE:HG23	1.98	0.46
1:A:330:LEU:HD22	1:A:334:PHE:HE1	1.80	0.46
1:G:323:ASN:HA	1:G:326:LYS:HE3	1.97	0.46
1:I:231:PRO:HB2	1:J:407:HIS:HD2	1.80	0.46
1:B:183:ILE:HG13	1:B:353:GLY:HA3	1.98	0.46
1:D:234:LEU:HD13	1:D:237:LYS:HD2	1.97	0.46
1:D:435:GLU:HB3	1:D:438:ASN:HD22	1.80	0.46
1:B:352:LYS:HG2	1:B:355:ARG:HH21	1.81	0.46
1:B:767:ARG:HH12	1:B:771:LYS:HB3	1.81	0.46
1:J:196:LEU:HD11	1:J:312:ILE:HD11	1.97	0.46
1:E:261:LEU:HD13	1:E:300:LEU:HD21	1.98	0.46
1:B:268:ILE:HG23	1:B:274:VAL:HB	1.98	0.45
1:H:531:LEU:HD23	1:I:734:LEU:HD21	1.98	0.45
1:E:347:THR:HG21	1:E:387:LEU:HD22	1.97	0.45
1:D:430:ALA:HB1	1:D:435:GLU:HB2	1.98	0.45
1:C:590:PRO:HA	1:C:642:THR:HG21	1.99	0.45
1:A:398:ALA:HB1	1:A:476:ILE:HA	1.99	0.45
1:H:551:LYS:HG2	1:H:711:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:HE2	1:C:335:GLN:HA	1.99	0.45
1:C:526:ARG:NH1	1:B:770:GLN:HB3	2.31	0.45
1:B:459:GLU:HA	1:B:462:ASN:HD22	1.81	0.45
1:B:323:ASN:HA	1:B:326:LYS:HE3	1.98	0.45
1:B:691:LYS:HD2	1:B:694:LYS:HZ3	1.81	0.45
1:D:330:LEU:HD22	1:D:334:PHE:HE1	1.81	0.45
1:F:402:VAL:HG11	1:F:471:LEU:HD21	1.99	0.45
1:G:399:SER:HB3	1:G:471:LEU:HD11	1.99	0.45
1:G:603:THR:HB	1:G:647:VAL:HG11	1.99	0.45
1:F:625:ASP:HA	1:F:628:ASN:HD22	1.81	0.45
1:E:323:ASN:HA	1:E:326:LYS:HE3	1.98	0.45
1:F:526:ARG:NH1	1:G:770:GLN:HB3	2.32	0.44
1:H:526:ARG:NH1	1:I:770:GLN:HB3	2.32	0.44
1:J:320:TYR:HA	1:J:324:ILE:HD13	1.98	0.44
1:G:698:ARG:HB2	1:G:701:PHE:HB2	1.99	0.44
1:D:698:ARG:HH21	1:C:573:ASP:HB2	1.83	0.44
1:G:213:GLY:HA2	3:G:902:ADP:H5'1	1.99	0.44
1:D:531:LEU:HD22	1:C:730:LEU:HD11	1.98	0.44
1:C:234:LEU:HD13	1:C:237:LYS:HD2	2.00	0.44
1:B:233:THR:HG21	1:A:404:LEU:HD11	1.99	0.44
1:F:577:PHE:HD1	1:F:582:ALA:HB1	1.82	0.44
1:H:25:ASN:HB2	1:H:70:HIS:HE1	1.83	0.44
1:I:572:VAL:HG21	1:I:602:LEU:HD13	2.00	0.44
1:B:101:ASN:HB3	1:A:425:ASN:HB3	2.00	0.44
1:D:364:ILE:HD11	1:D:403:ARG:HB2	2.00	0.44
1:D:526:ARG:NH1	1:C:770:GLN:HB3	2.33	0.44
1:B:36:LEU:HD22	1:B:61:ILE:HG12	2.00	0.44
1:A:241:SER:HA	1:A:277:PHE:HB3	2.00	0.44
1:J:184:GLY:HA3	1:J:350:ILE:HD11	2.00	0.44
1:J:480:ILE:HG23	1:J:491:ILE:HD13	2.00	0.44
1:E:366:ILE:HG12	1:E:471:LEU:HD12	2.00	0.44
1:J:443:ARG:NH2	1:E:436:PHE:HB2	2.33	0.43
1:H:242:LEU:HB3	1:H:278:ILE:HG22	2.01	0.43
1:E:743:VAL:HG22	1:E:794:VAL:HB	2.01	0.43
1:H:129:LEU:HD11	1:H:134:ALA:HB2	2.01	0.43
1:D:355:ARG:HG3	1:D:371:ILE:HD11	2.00	0.43
1:F:620:GLU:HG2	1:F:621:LYS:HG3	1.99	0.43
1:D:526:ARG:HH12	1:C:770:GLN:HB3	1.83	0.43
1:G:526:ARG:NH1	1:H:770:GLN:HB3	2.33	0.43
1:H:374:ALA:HB2	1:H:476:ILE:HG12	2.00	0.43
1:D:6:LEU:HD23	1:D:103:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ARG:HH21	1:B:538:ILE:HD13	1.84	0.43
1:G:316:THR:HG23	1:G:319:GLU:H	1.84	0.43
1:J:364:ILE:HD11	1:J:403:ARG:HD2	2.01	0.43
1:J:604:GLU:HG3	1:J:608:ARG:HH12	1.83	0.43
1:C:565:ASP:HB3	1:C:568:ALA:HB2	2.00	0.43
1:G:46:ALA:HB2	1:G:106:GLU:HA	2.01	0.43
1:I:242:LEU:HD12	1:I:276:LEU:HD21	2.01	0.43
1:E:526:ARG:HH12	1:D:770:GLN:HB3	1.84	0.43
1:B:131:ILE:HD11	1:B:135:ARG:HH21	1.84	0.43
1:B:366:ILE:HG12	1:B:471:LEU:HD12	2.00	0.43
1:F:416:ILE:HG21	1:F:453:TYR:HB2	2.00	0.42
1:G:237:LYS:HZ3	1:G:273:ASN:HA	1.84	0.42
1:H:546:PRO:HD3	1:H:665:LEU:HD23	2.01	0.42
1:J:552:THR:HG23	1:J:571:ARG:HH22	1.84	0.42
1:H:16:HIS:HA	1:H:19:GLU:HG2	2.00	0.42
1:C:199:ARG:HD3	1:B:358:TYR:HE1	1.85	0.42
1:B:96:ARG:HD3	1:B:176:ASP:HB3	2.01	0.42
1:G:265:MET:HB2	1:G:309:LEU:HD21	2.00	0.42
1:J:377:LEU:HD12	1:J:476:ILE:HG22	2.01	0.42
1:I:198:ARG:NE	1:I:199:ARG:H	2.17	0.42
1:B:231:PRO:HD2	1:B:234:LEU:HB2	2.01	0.42
1:A:237:LYS:HA	1:A:273:ASN:HB2	2.01	0.42
1:F:546:PRO:HG3	1:F:713:LYS:HD2	2.02	0.42
1:G:122:ARG:HD3	1:G:461:LYS:NZ	2.35	0.42
1:H:190:THR:HA	1:H:193:ILE:HG12	2.00	0.42
1:J:419:GLU:HA	1:J:422:LYS:HG2	2.02	0.42
1:E:526:ARG:NH1	1:D:770:GLN:HB3	2.34	0.42
1:D:299:ILE:HG22	1:D:300:LEU:HG	2.01	0.42
1:C:8:GLU:HB3	1:C:12:ARG:HH12	1.84	0.42
1:C:303:ALA:HA	1:C:308:GLU:HB2	2.02	0.42
1:B:160:THR:HG22	1:B:267:GLU:HB3	2.00	0.42
1:F:348:VAL:HG22	1:F:375:VAL:HG11	2.01	0.42
1:I:526:ARG:HD2	1:J:774:GLU:OE1	2.20	0.42
1:J:341:GLU:HB2	1:J:387:LEU:HB2	2.01	0.42
1:E:363:ARG:HH11	1:E:403:ARG:HH12	1.67	0.42
1:C:323:ASN:HA	1:C:326:LYS:HE3	2.02	0.42
1:I:198:ARG:HH12	1:J:364:ILE:HG13	1.85	0.42
1:A:386:PHE:N	1:A:390:LYS:HD3	2.35	0.42
1:H:531:LEU:HD22	1:I:730:LEU:HD11	2.01	0.41
1:D:122:ARG:HD3	1:D:461:LYS:NZ	2.35	0.41
1:D:142:LEU:HD11	1:C:432:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:VAL:HG21	1:B:602:LEU:HD13	2.02	0.41
1:H:39:MET:HE3	1:H:60:VAL:HG11	2.01	0.41
1:I:456:ALA:HA	1:I:459:GLU:HG2	2.02	0.41
1:C:586:LEU:HA	1:C:601:GLN:HB3	2.01	0.41
1:I:232:GLU:HB3	1:J:407:HIS:NE2	2.36	0.41
1:D:664:GLU:HB3	1:D:689:MET:HE1	2.03	0.41
1:B:90:LEU:HD13	1:B:114:ARG:HD3	2.03	0.41
1:J:342:PRO:HB2	1:J:346:ASP:HB3	2.02	0.41
1:G:198:ARG:NH2	1:H:393:ASP:HB2	2.36	0.41
1:I:168:ARG:HA	1:I:168:ARG:HD2	1.93	0.41
1:C:546:PRO:HD3	1:C:665:LEU:HD23	2.03	0.41
1:B:586:LEU:HA	1:B:601:GLN:HB3	2.02	0.41
1:F:419:GLU:HA	1:F:422:LYS:HG2	2.02	0.41
1:J:206:LEU:HD22	1:J:339:VAL:HG21	2.02	0.41
1:E:546:PRO:HD3	1:E:665:LEU:HD23	2.02	0.41
1:C:90:LEU:HD13	1:C:114:ARG:HB3	2.03	0.41
1:C:122:ARG:HD3	1:C:461:LYS:HE2	2.03	0.41
1:F:563:PHE:CD1	1:F:611:TYR:HB3	2.56	0.41
1:I:5:ARG:HH22	1:I:176:ASP:C	2.29	0.41
1:E:409:THR:HB	1:E:414:LYS:HZ3	1.86	0.41
1:E:546:PRO:HG3	1:E:713:LYS:HD2	2.03	0.41
1:E:623:HIS:HB3	1:E:626:VAL:HG23	2.01	0.41
1:B:197:SER:HA	1:A:404:LEU:HB3	2.03	0.41
1:B:605:LYS:HG2	1:B:608:ARG:HH22	1.86	0.41
1:F:430:ALA:HB1	1:F:435:GLU:HB2	2.02	0.41
1:I:45:ILE:HB	1:I:106:GLU:HB3	2.03	0.41
1:D:363:ARG:HD2	1:D:403:ARG:HH12	1.85	0.41
1:D:409:THR:HB	1:D:414:LYS:NZ	2.36	0.41
1:B:348:VAL:HG12	1:B:352:LYS:HE3	2.03	0.41
1:B:185:ARG:HB3	1:B:189:ILE:HG12	2.03	0.40
1:E:241:SER:HA	1:E:277:PHE:HB3	2.04	0.40
1:G:419:GLU:HA	1:G:422:LYS:HG2	2.02	0.40
1:B:633:VAL:HG22	1:B:639:LEU:HD11	2.03	0.40
1:F:190:THR:HA	1:F:193:ILE:HG12	2.04	0.40
1:G:546:PRO:HD3	1:G:665:LEU:HD23	2.03	0.40
1:C:623:HIS:HB3	1:C:626:VAL:HG23	2.03	0.40
1:B:507:HIS:CD2	1:B:517:VAL:HG11	2.57	0.40
1:F:526:ARG:HH12	1:G:770:GLN:HB3	1.87	0.40
1:H:323:ASN:HA	1:H:326:LYS:HE3	2.03	0.40
1:E:231:PRO:HB2	1:D:407:HIS:HD2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	303/818 (37%)	292 (96%)	11 (4%)	0	100	100
1	B	750/818 (92%)	741 (99%)	9 (1%)	0	100	100
1	C	750/818 (92%)	744 (99%)	6 (1%)	0	100	100
1	D	750/818 (92%)	743 (99%)	7 (1%)	0	100	100
1	E	610/818 (75%)	605 (99%)	5 (1%)	0	100	100
1	F	610/818 (75%)	602 (99%)	8 (1%)	0	100	100
1	G	750/818 (92%)	742 (99%)	8 (1%)	0	100	100
1	H	750/818 (92%)	741 (99%)	9 (1%)	0	100	100
1	I	750/818 (92%)	745 (99%)	5 (1%)	0	100	100
1	J	610/818 (75%)	603 (99%)	7 (1%)	0	100	100
All	All	6633/8180 (81%)	6558 (99%)	75 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/695 (38%)	262 (100%)	0	100	100
1	B	646/695 (93%)	646 (100%)	0	100	100
1	C	646/695 (93%)	645 (100%)	1 (0%)	92	94
1	D	646/695 (93%)	646 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	530/695 (76%)	530 (100%)	0	100	100
1	F	530/695 (76%)	530 (100%)	0	100	100
1	G	646/695 (93%)	645 (100%)	1 (0%)	92	94
1	H	646/695 (93%)	644 (100%)	2 (0%)	91	92
1	I	646/695 (93%)	646 (100%)	0	100	100
1	J	530/695 (76%)	530 (100%)	0	100	100
All	All	5728/6950 (82%)	5724 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	706	ASP
1	H	234	LEU
1	H	444	ASP
1	C	711	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	362	HIS
1	F	412	ASN
1	F	628	ASN
1	F	737	GLN
1	F	738	ASN
1	G	70	HIS
1	G	507	HIS
1	G	601	GLN
1	G	703	ASN
1	G	738	ASN
1	H	16	HIS
1	H	70	HIS
1	H	464	GLN
1	H	776	ASN
1	H	796	HIS
1	H	808	GLN
1	I	26	HIS
1	I	28	ASN
1	I	33	HIS
1	I	70	HIS

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Mol	Chain	Res	Type
1	I	116	ASN
1	I	203	ASN
1	I	310	GLN
1	I	507	HIS
1	I	737	GLN
1	J	412	ASN
1	J	432	HIS
1	J	507	HIS
1	J	638	HIS
1	J	703	ASN
1	J	737	GLN
1	J	738	ASN
1	J	776	ASN
1	J	786	GLN
1	E	159	ASN
1	E	412	ASN
1	E	432	HIS
1	E	507	HIS
1	E	518	ASN
1	E	659	ASN
1	E	738	ASN
1	E	786	GLN
1	D	33	HIS
1	D	159	ASN
1	D	412	ASN
1	D	434	GLN
1	D	438	ASN
1	D	703	ASN
1	D	738	ASN
1	D	776	ASN
1	D	786	GLN
1	C	16	HIS
1	C	70	HIS
1	C	432	HIS
1	C	808	GLN
1	B	107	HIS
1	B	203	ASN
1	B	228	ASN
1	B	323	ASN
1	B	518	ASN
1	B	601	GLN
1	B	703	ASN

*Continued on next page...*



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Mol	Chain	Res	Type
1	B	776	ASN
1	B	786	GLN
1	A	425	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 [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADP	B	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
2	ATP	C	901	-	26,33,33	0.58	0	31,52,52	0.82	2 (6%)
2	ATP	H	901	-	26,33,33	0.59	0	31,52,52	0.84	3 (9%)
3	ADP	H	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
3	ADP	G	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
2	ATP	J	901	-	26,33,33	0.59	0	31,52,52	0.83	3 (9%)
2	ATP	F	901	-	26,33,33	0.59	0	31,52,52	0.83	3 (9%)
2	ATP	B	901	-	26,33,33	0.58	0	31,52,52	0.84	3 (9%)
3	ADP	D	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	I	901	-	26,33,33	0.60	0	31,52,52	0.83	3 (9%)
3	ADP	I	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
2	ATP	E	901	-	26,33,33	0.58	0	31,52,52	0.83	3 (9%)
2	ATP	D	901	-	26,33,33	0.60	0	31,52,52	0.82	2 (6%)
3	ADP	C	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
2	ATP	G	901	-	26,33,33	0.58	0	31,52,52	0.83	3 (9%)

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
3	ADP	B	902	-	-	0/12/32/32	0/3/3/3
2	ATP	C	901	-	-	1/18/38/38	0/3/3/3
2	ATP	H	901	-	-	2/18/38/38	0/3/3/3
3	ADP	H	902	-	-	1/12/32/32	0/3/3/3
3	ADP	G	902	-	-	3/12/32/32	0/3/3/3
2	ATP	J	901	-	-	1/18/38/38	0/3/3/3
2	ATP	F	901	-	-	2/18/38/38	0/3/3/3
2	ATP	B	901	-	-	2/18/38/38	0/3/3/3
3	ADP	D	902	-	-	1/12/32/32	0/3/3/3
2	ATP	I	901	-	-	2/18/38/38	0/3/3/3
3	ADP	I	902	-	-	1/12/32/32	0/3/3/3
2	ATP	E	901	-	-	1/18/38/38	0/3/3/3
2	ATP	D	901	-	-	3/18/38/38	0/3/3/3
3	ADP	C	902	-	-	2/12/32/32	0/3/3/3
2	ATP	G	901	-	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	902	ADP	C5-C4	2.52	1.47	1.40
3	I	902	ADP	C5-C4	2.48	1.47	1.40
3	B	902	ADP	C5-C4	2.47	1.47	1.40
3	H	902	ADP	C5-C4	2.45	1.47	1.40
3	D	902	ADP	C5-C4	2.45	1.47	1.40
3	C	902	ADP	C5-C4	2.44	1.47	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	902	ADP	PA-O3A-PB	-4.04	118.98	132.83
3	C	902	ADP	PA-O3A-PB	-3.96	119.23	132.83
3	D	902	ADP	PA-O3A-PB	-3.91	119.41	132.83
3	B	902	ADP	PA-O3A-PB	-3.80	119.79	132.83
3	G	902	ADP	PA-O3A-PB	-3.72	120.04	132.83
3	I	902	ADP	PA-O3A-PB	-3.63	120.38	132.83
3	G	902	ADP	C3'-C2'-C1'	3.38	106.06	100.98
3	I	902	ADP	C3'-C2'-C1'	3.33	105.98	100.98
3	B	902	ADP	C3'-C2'-C1'	3.21	105.81	100.98
3	C	902	ADP	N3-C2-N1	-3.19	123.69	128.68
3	H	902	ADP	N3-C2-N1	-3.19	123.69	128.68
3	G	902	ADP	N3-C2-N1	-3.18	123.70	128.68
3	D	902	ADP	N3-C2-N1	-3.18	123.71	128.68
3	B	902	ADP	N3-C2-N1	-3.17	123.72	128.68
3	I	902	ADP	N3-C2-N1	-3.15	123.76	128.68
3	H	902	ADP	C3'-C2'-C1'	3.11	105.66	100.98
3	D	902	ADP	C3'-C2'-C1'	3.11	105.66	100.98
3	C	902	ADP	C3'-C2'-C1'	3.03	105.54	100.98
3	I	902	ADP	C4-C5-N7	-2.72	106.56	109.40
3	D	902	ADP	C4-C5-N7	-2.71	106.58	109.40
3	G	902	ADP	C4-C5-N7	-2.68	106.60	109.40
3	H	902	ADP	C4-C5-N7	-2.67	106.61	109.40
3	B	902	ADP	C4-C5-N7	-2.66	106.63	109.40
3	C	902	ADP	C4-C5-N7	-2.65	106.64	109.40
2	D	901	ATP	C5-C6-N6	2.31	123.86	120.35
2	C	901	ATP	C5-C6-N6	2.30	123.85	120.35
2	F	901	ATP	C5-C6-N6	2.28	123.82	120.35
2	E	901	ATP	C5-C6-N6	2.28	123.81	120.35
2	G	901	ATP	C5-C6-N6	2.27	123.81	120.35
2	H	901	ATP	C5-C6-N6	2.27	123.80	120.35
2	B	901	ATP	C5-C6-N6	2.26	123.79	120.35
2	J	901	ATP	C5-C6-N6	2.25	123.78	120.35
2	I	901	ATP	C5-C6-N6	2.25	123.76	120.35
2	H	901	ATP	C3'-C2'-C1'	2.22	104.32	100.98
2	B	901	ATP	C3'-C2'-C1'	2.15	104.22	100.98
2	J	901	ATP	C3'-C2'-C1'	2.15	104.22	100.98
2	I	901	ATP	C3'-C2'-C1'	2.14	104.20	100.98
2	F	901	ATP	C3'-C2'-C1'	2.11	104.15	100.98
2	G	901	ATP	C3'-C2'-C1'	2.09	104.13	100.98
2	E	901	ATP	C3'-C2'-C1'	2.07	104.10	100.98
2	B	901	ATP	PB-O3B-PG	2.06	139.91	132.83
2	G	901	ATP	PB-O3B-PG	2.06	139.90	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	ATP	PB-O3B-PG	2.06	139.89	132.83
2	F	901	ATP	PB-O3B-PG	2.05	139.87	132.83
2	J	901	ATP	PB-O3B-PG	2.05	139.87	132.83
2	E	901	ATP	PB-O3B-PG	2.05	139.86	132.83
2	C	901	ATP	PB-O3B-PG	2.05	139.85	132.83
2	I	901	ATP	PB-O3B-PG	2.04	139.84	132.83
2	D	901	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

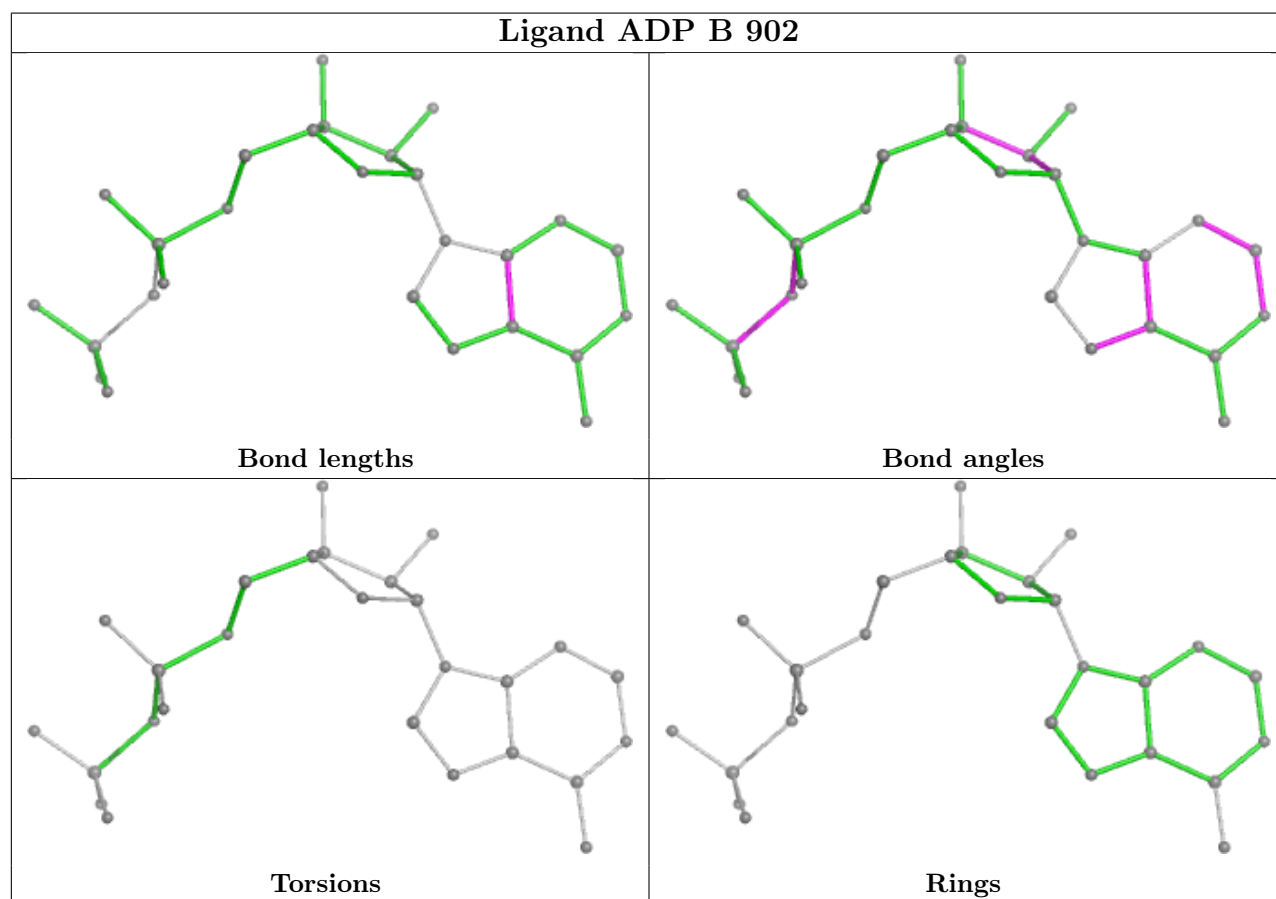
Mol	Chain	Res	Type	Atoms
3	G	902	ADP	C5'-O5'-PA-O1A
3	G	902	ADP	C5'-O5'-PA-O3A
3	H	902	ADP	C5'-O5'-PA-O1A
3	D	902	ADP	C5'-O5'-PA-O1A
3	C	902	ADP	C5'-O5'-PA-O1A
3	C	902	ADP	C5'-O5'-PA-O3A
2	G	901	ATP	O4'-C4'-C5'-O5'
2	I	901	ATP	O4'-C4'-C5'-O5'
2	D	901	ATP	C3'-C4'-C5'-O5'
2	D	901	ATP	O4'-C4'-C5'-O5'
2	C	901	ATP	PB-O3A-PA-O5'
3	G	902	ADP	O4'-C4'-C5'-O5'
2	D	901	ATP	C4'-C5'-O5'-PA
2	J	901	ATP	O4'-C4'-C5'-O5'
2	G	901	ATP	C4'-C5'-O5'-PA
2	H	901	ATP	O4'-C4'-C5'-O5'
2	H	901	ATP	C4'-C5'-O5'-PA
2	E	901	ATP	O4'-C4'-C5'-O5'
2	F	901	ATP	C4'-C5'-O5'-PA
2	I	901	ATP	C4'-C5'-O5'-PA
2	B	901	ATP	C4'-C5'-O5'-PA
3	I	902	ADP	C5'-O5'-PA-O1A
2	F	901	ATP	O4'-C4'-C5'-O5'
2	B	901	ATP	O4'-C4'-C5'-O5'

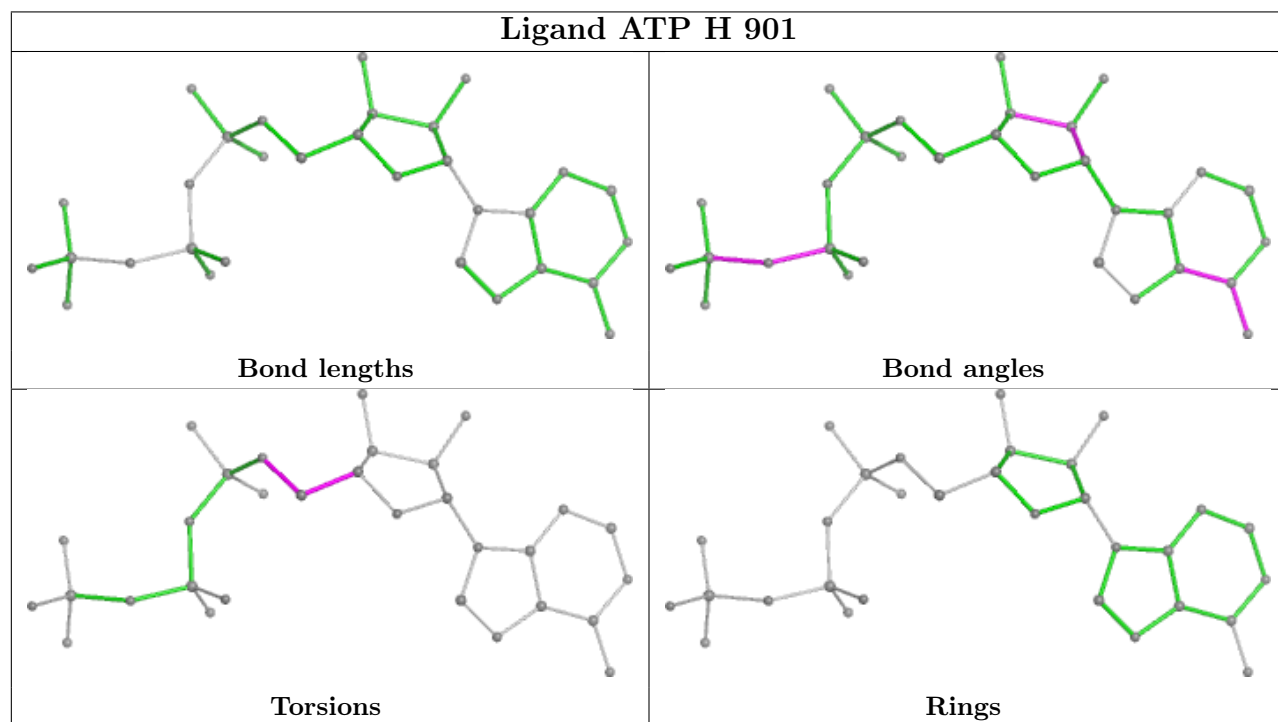
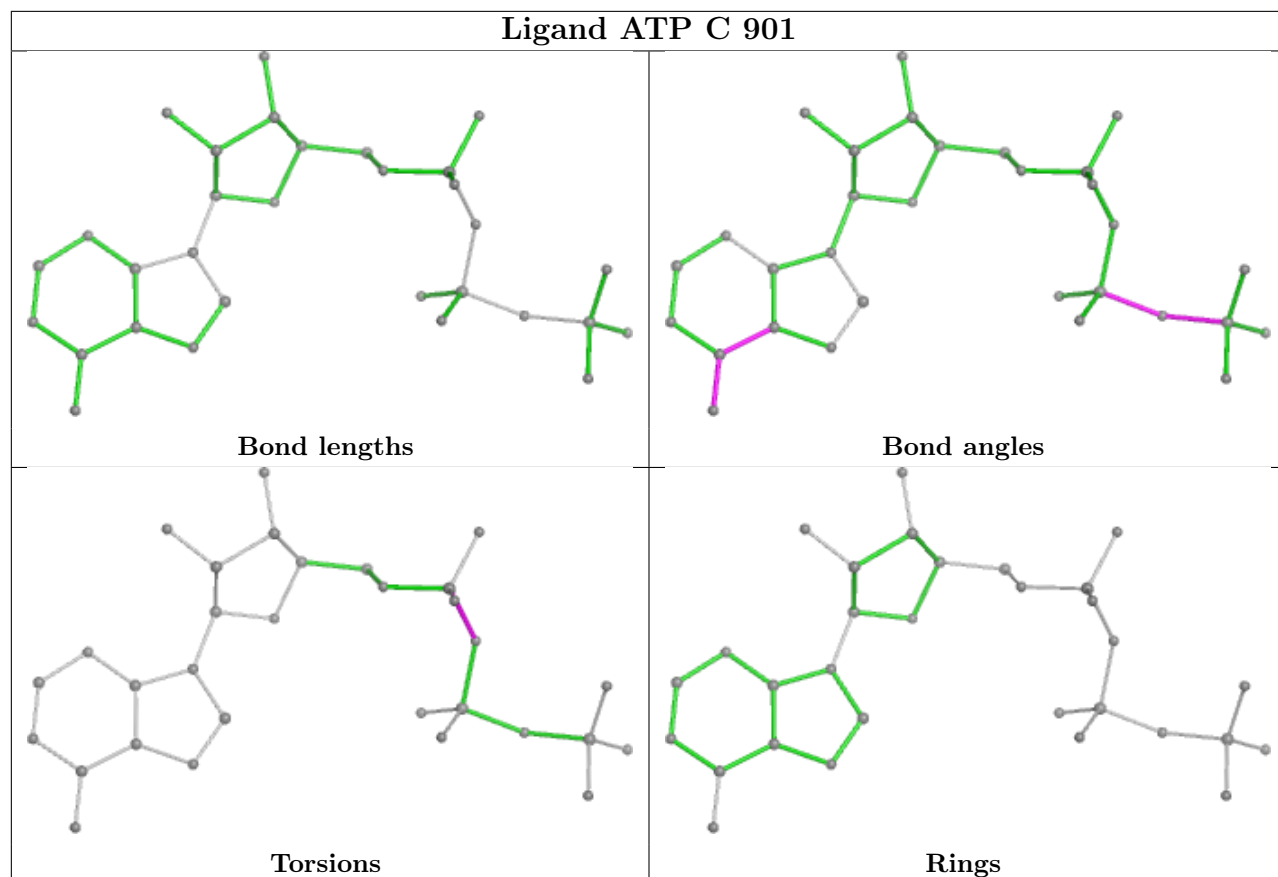
There are no ring outliers.

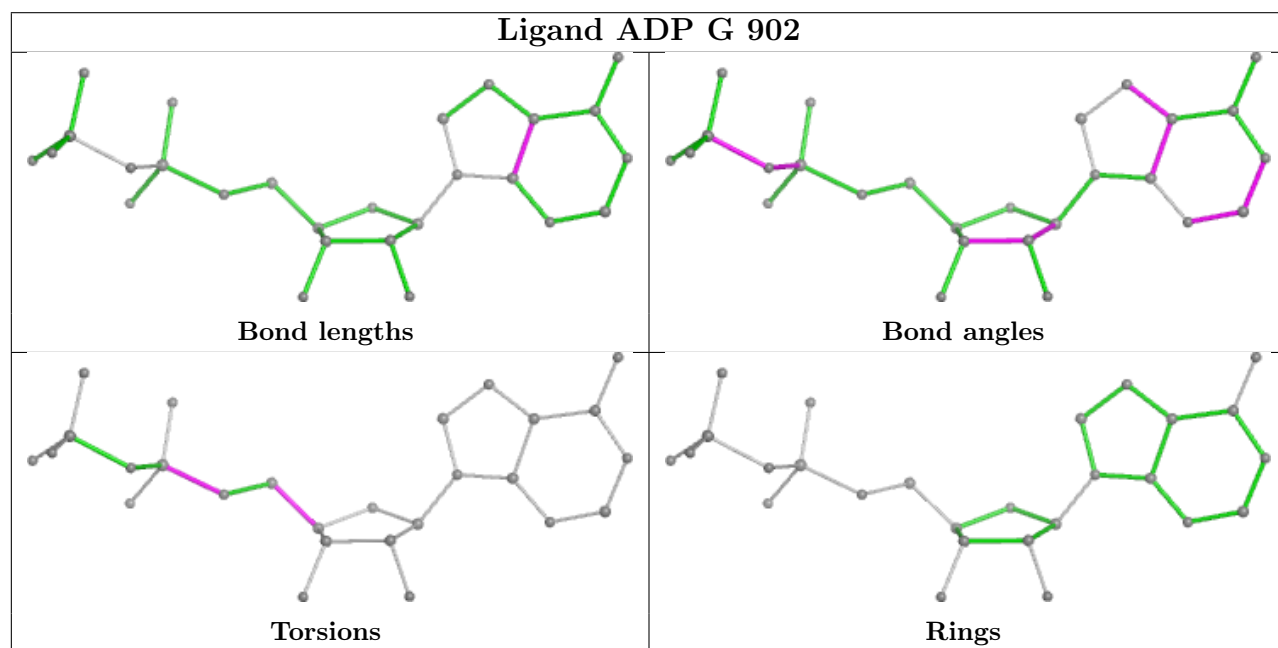
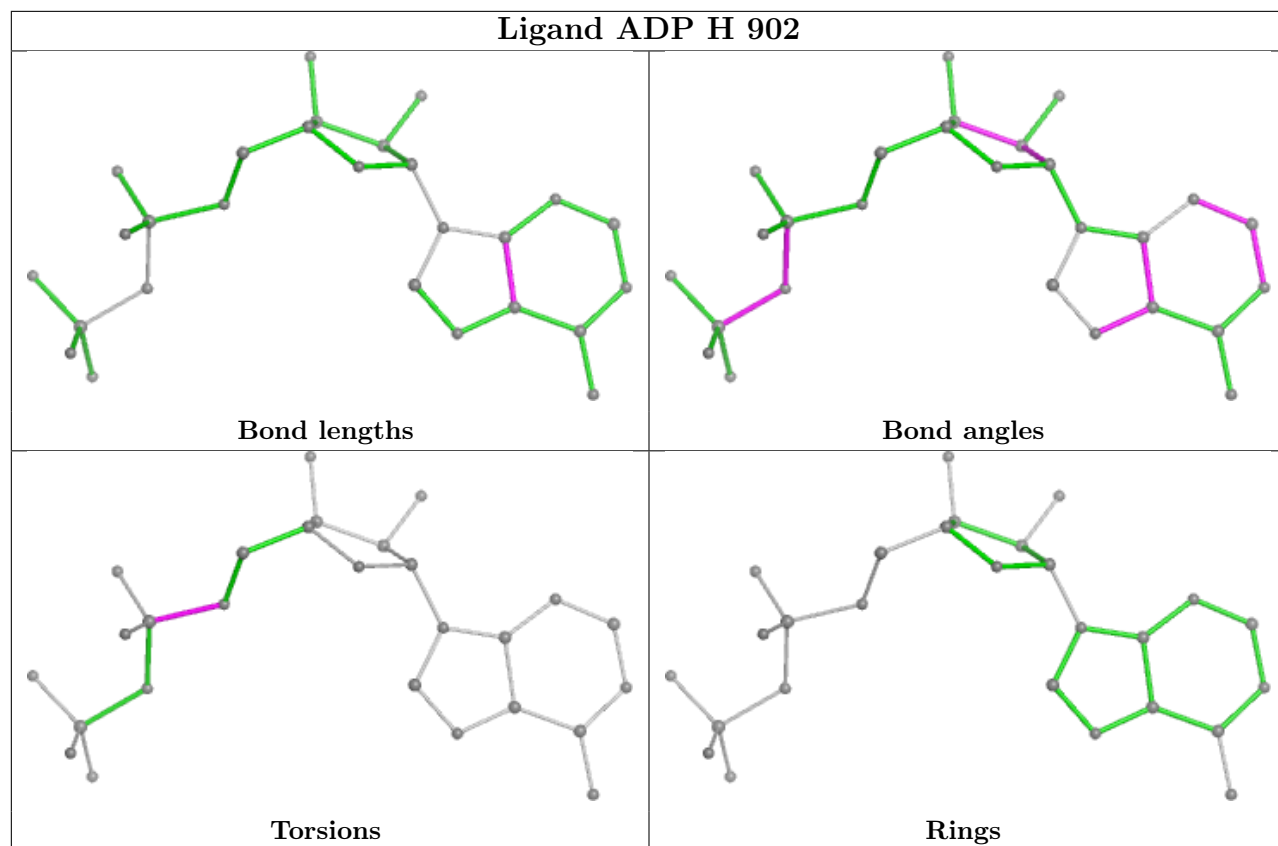
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	901	ATP	1	0
3	G	902	ADP	1	0
2	J	901	ATP	1	0
2	B	901	ATP	1	0
3	I	902	ADP	1	0
2	E	901	ATP	1	0

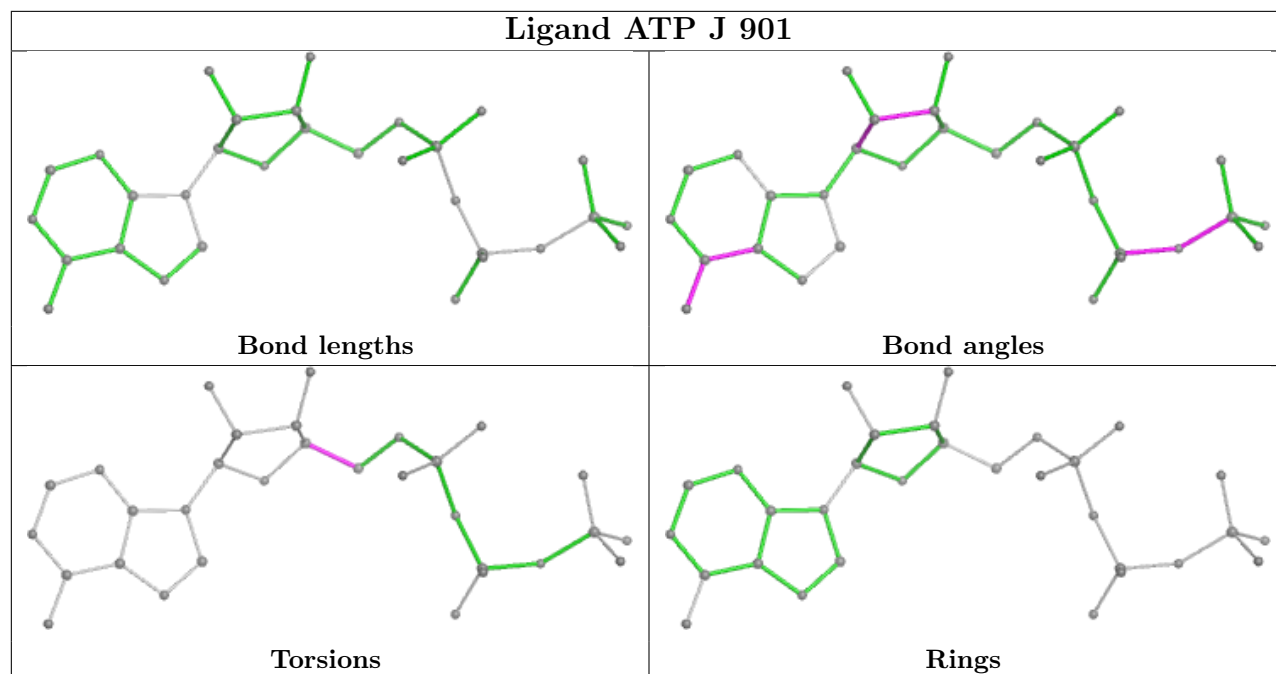
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



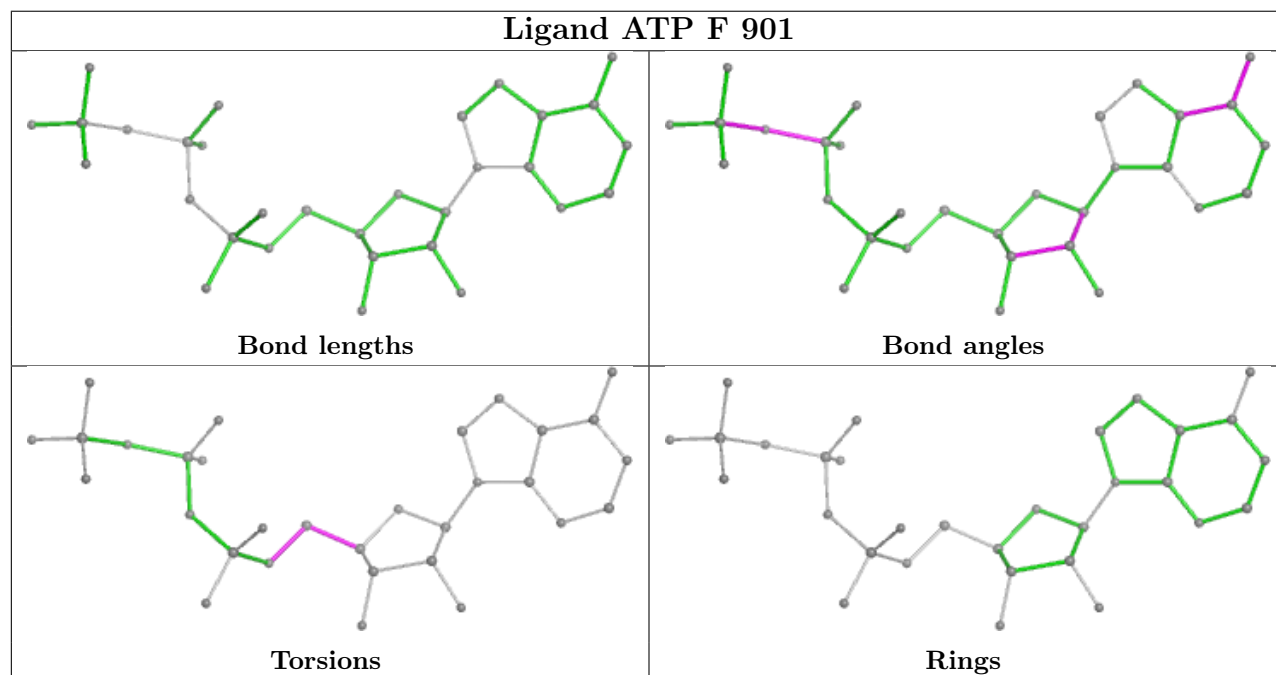




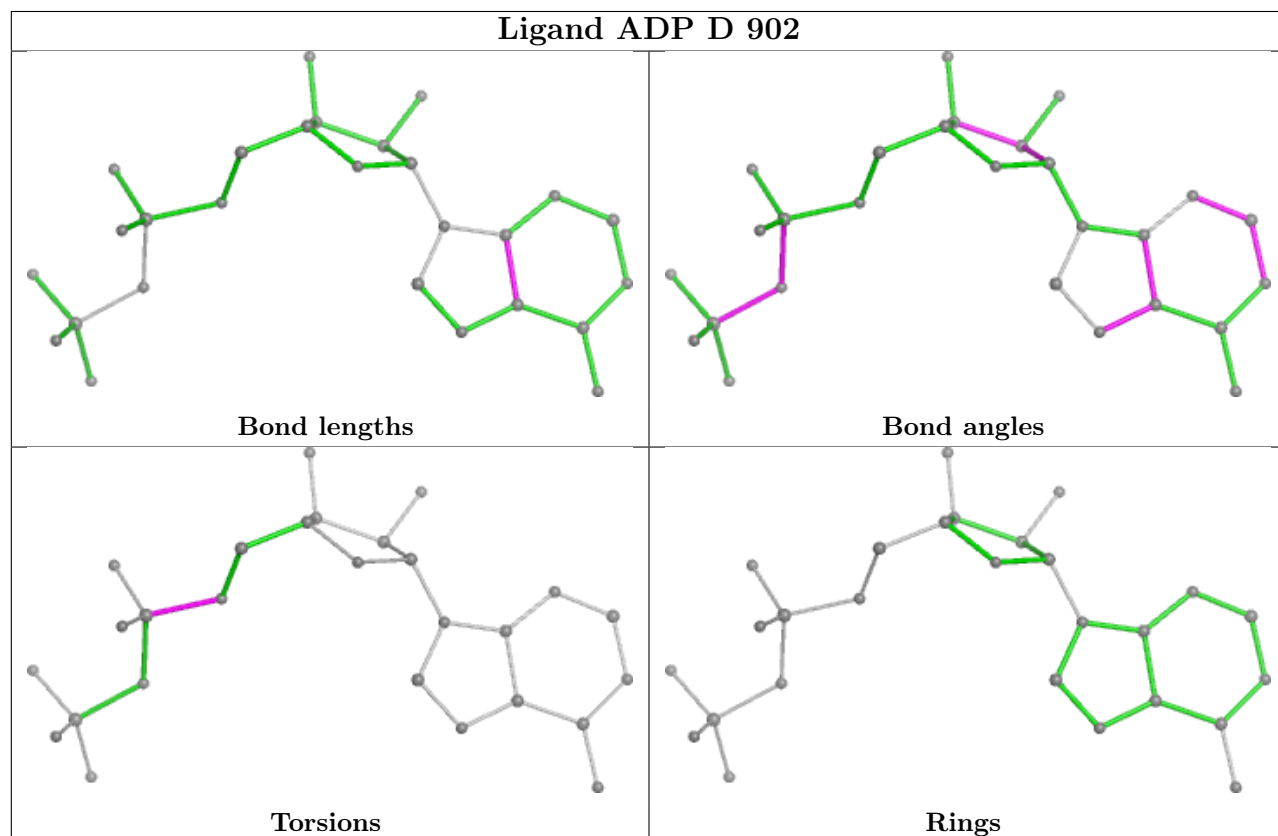
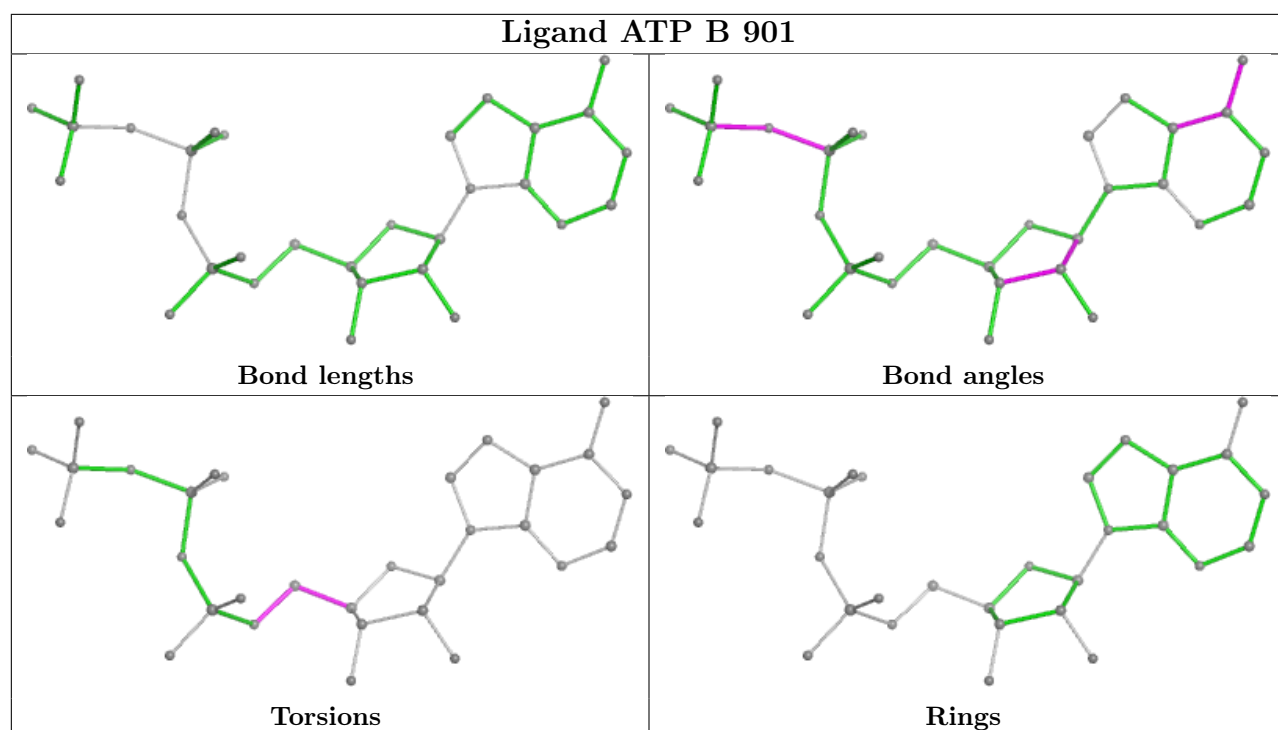
## Ligand ATP J 901



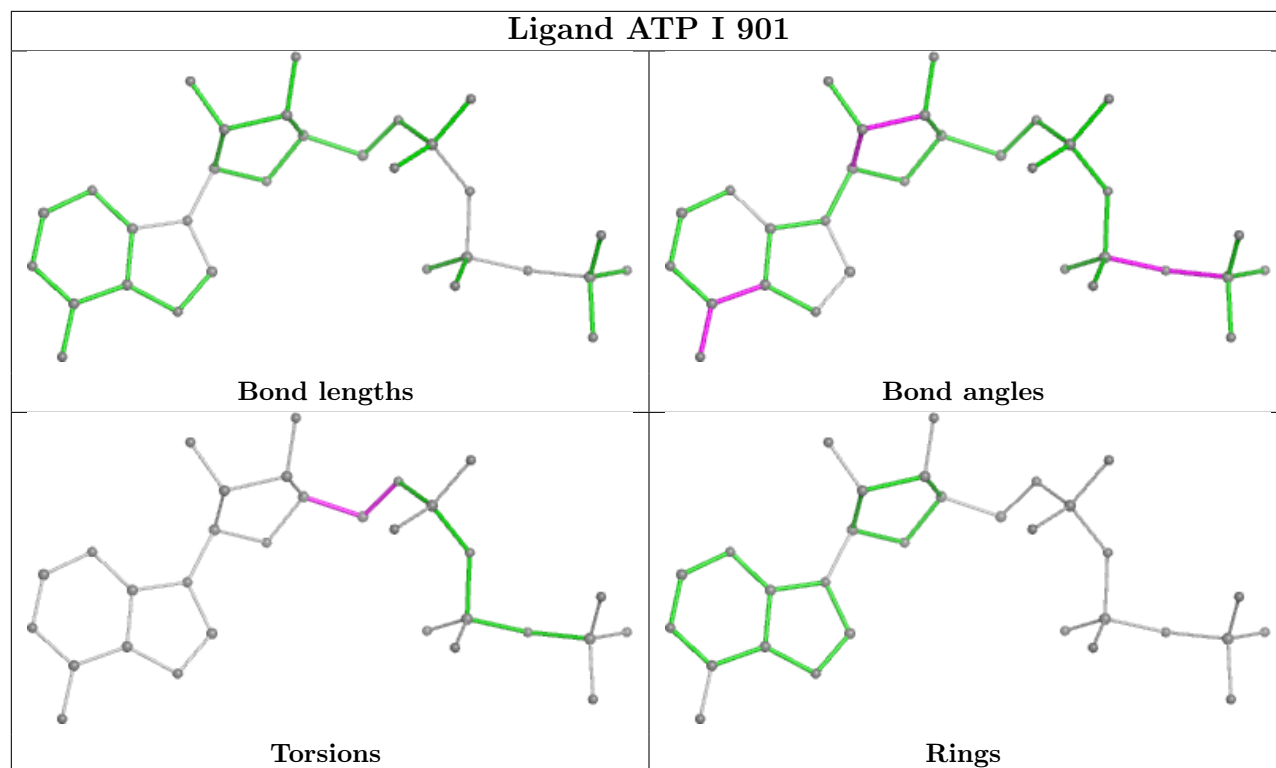
## Ligand ATP F 901



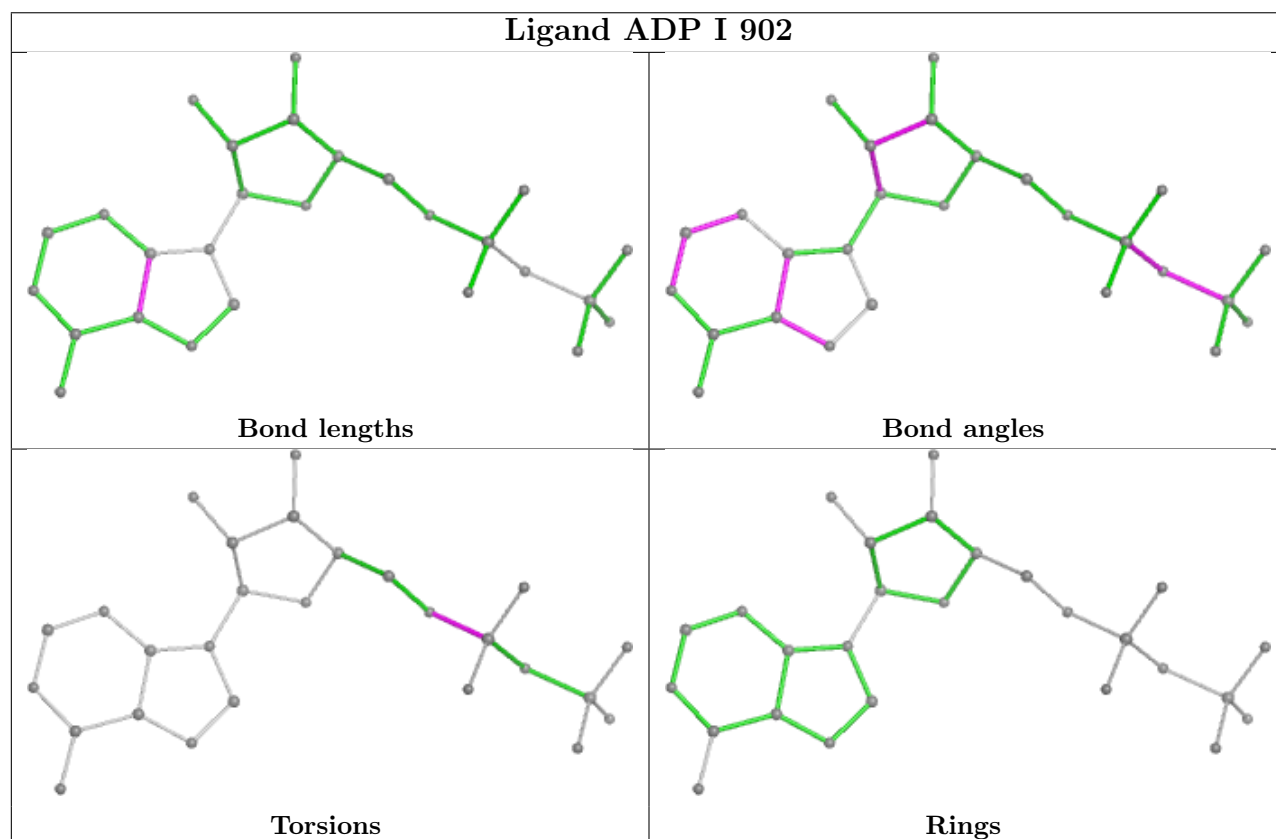




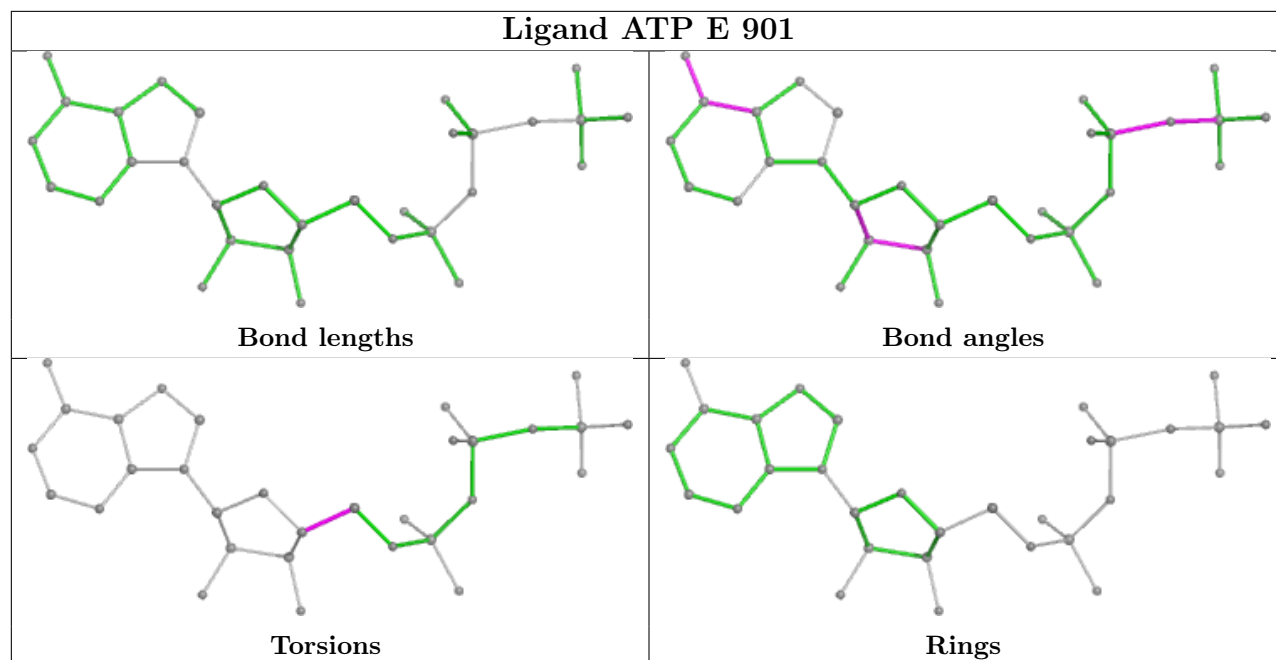
## Ligand ATP I 901



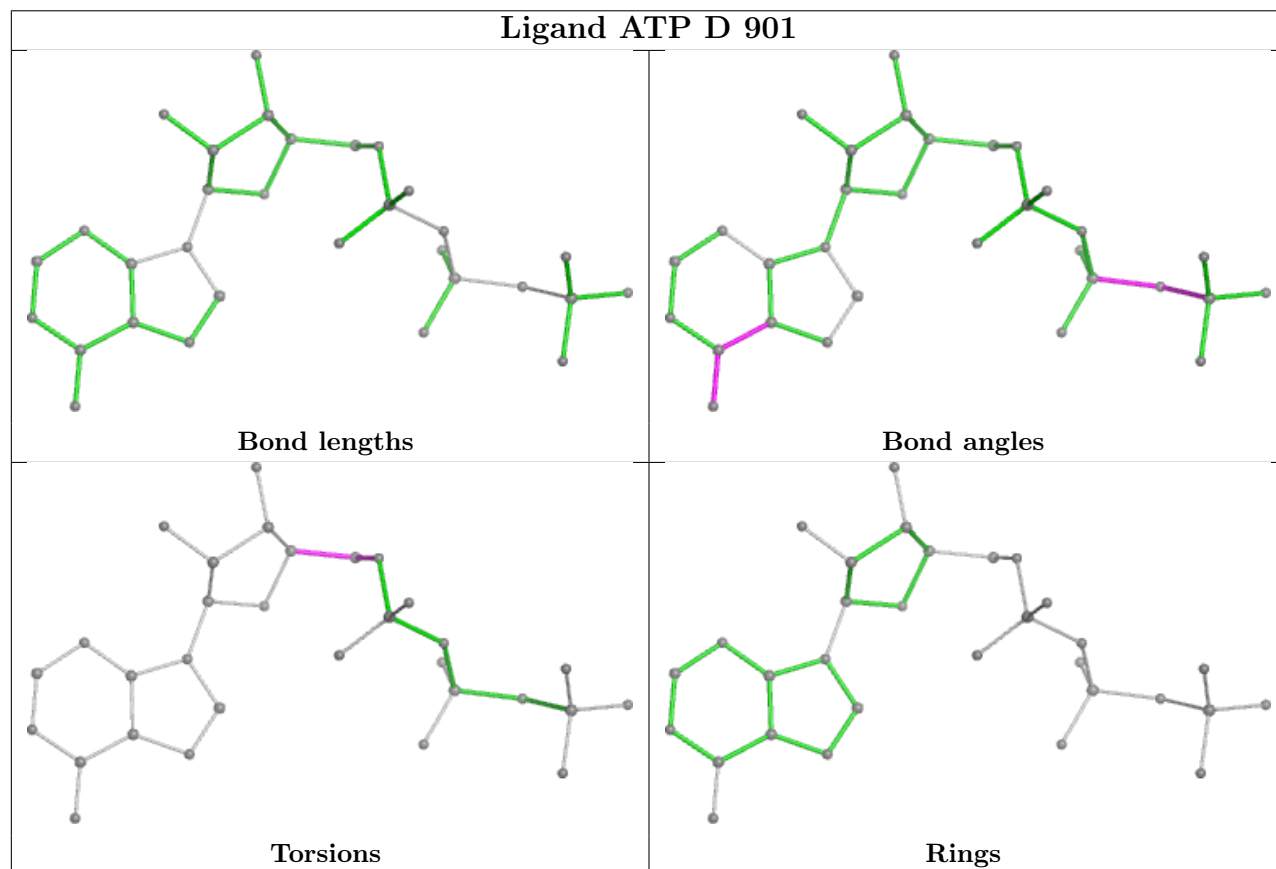
## Ligand ADP I 902

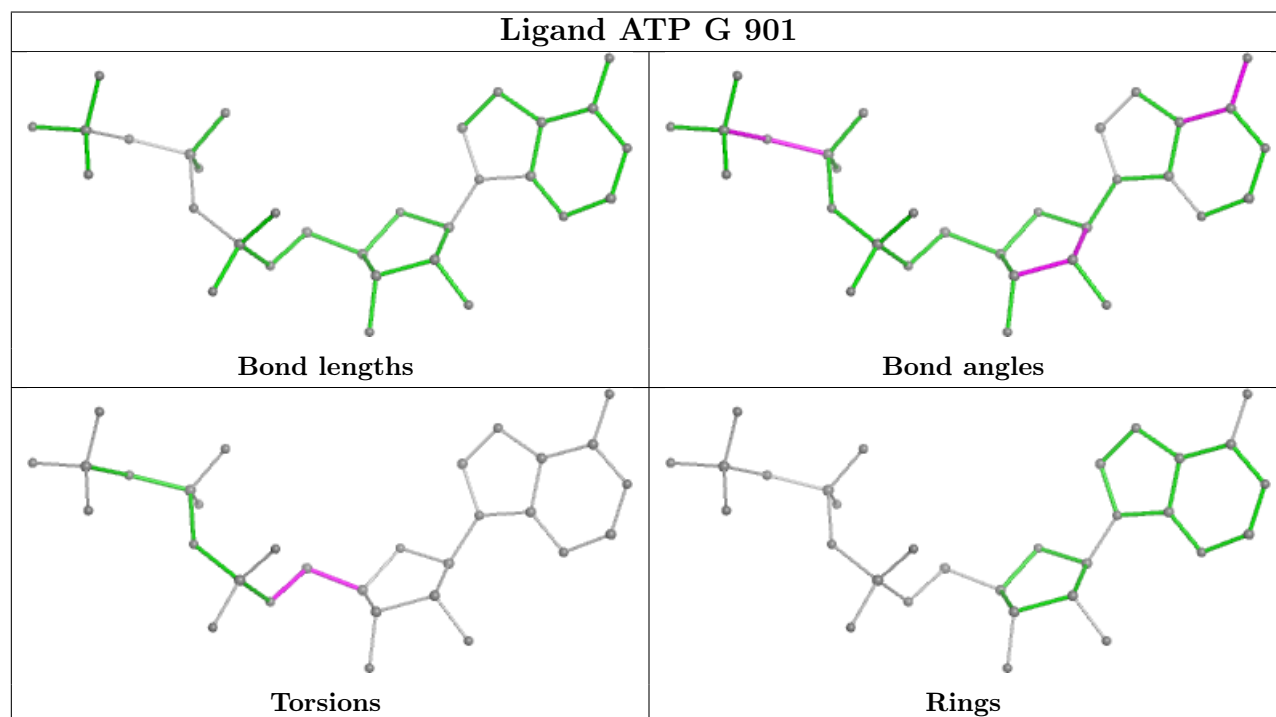
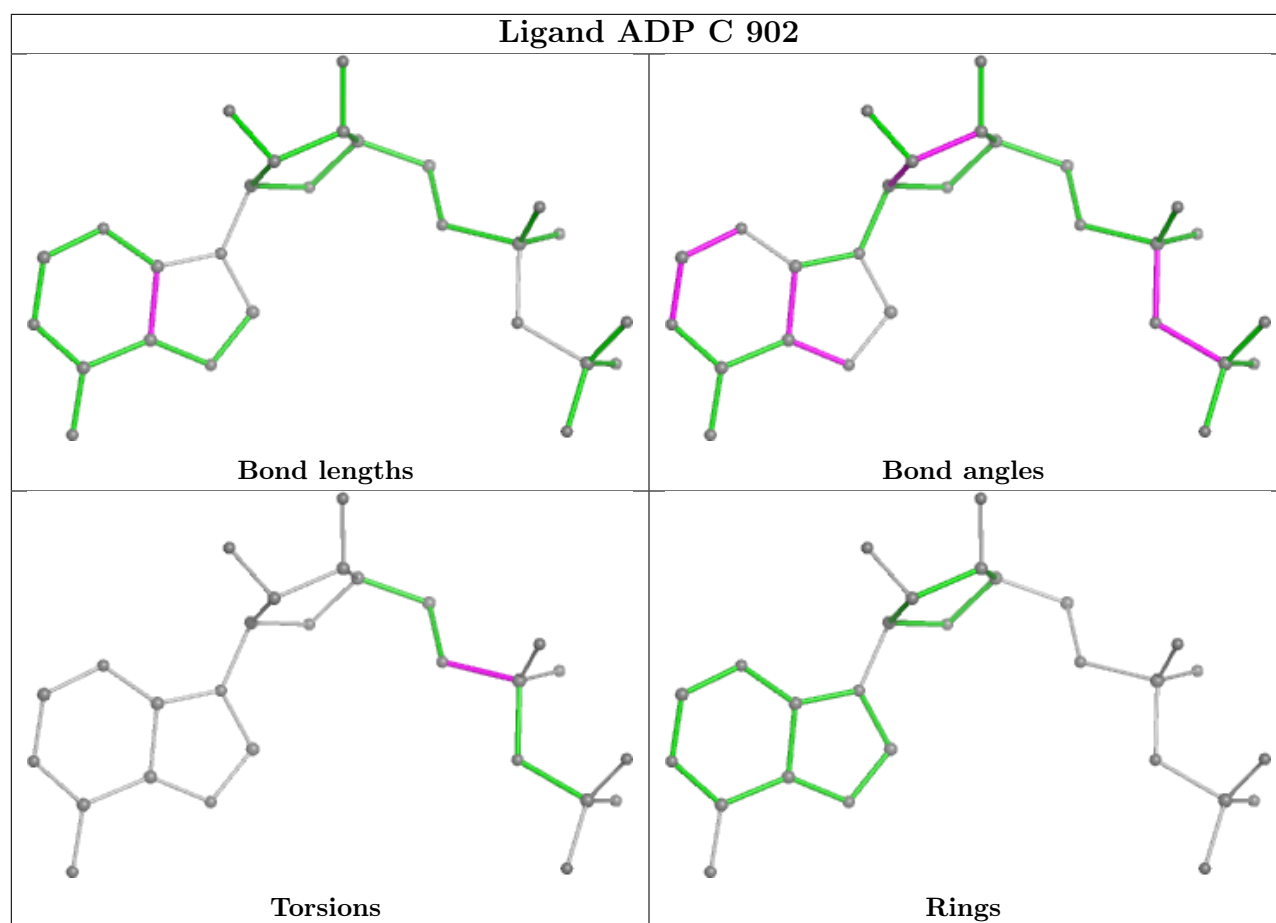


## Ligand ATP E 901



## Ligand ATP D 901





## 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.

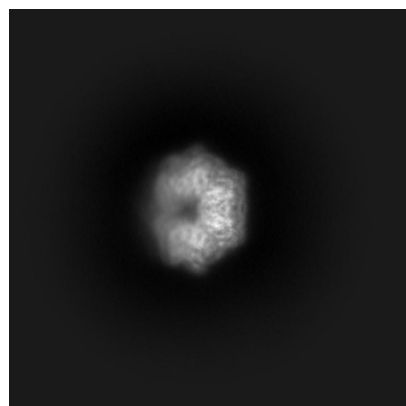
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53312. These allow visual inspection of the internal detail of the map and identification of artifacts.

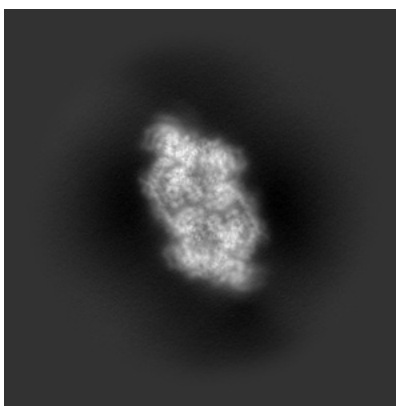
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

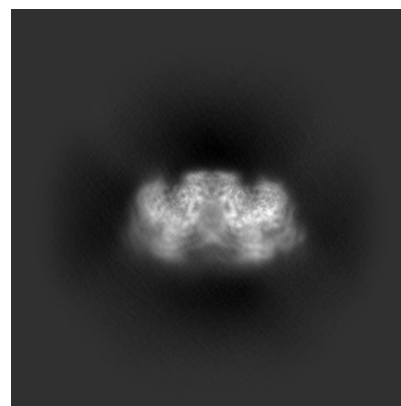
#### 6.1.1 Primary map



X

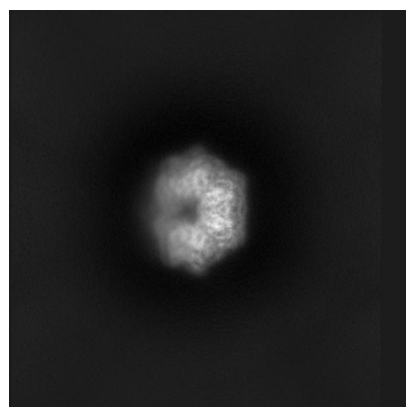


Y

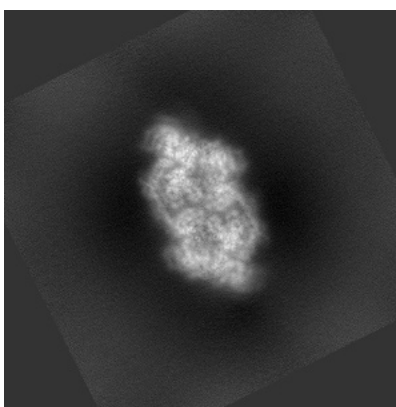


Z

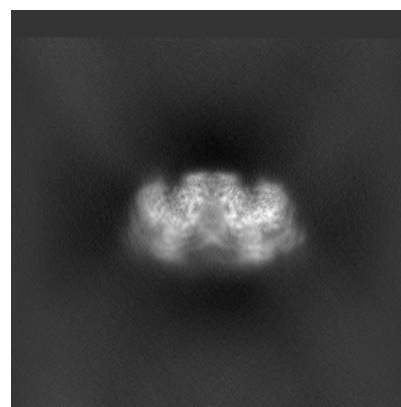
#### 6.1.2 Raw map



X



Y

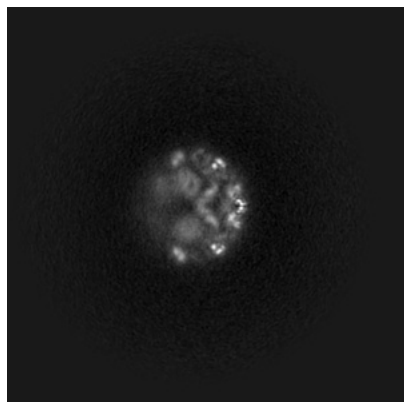


Z

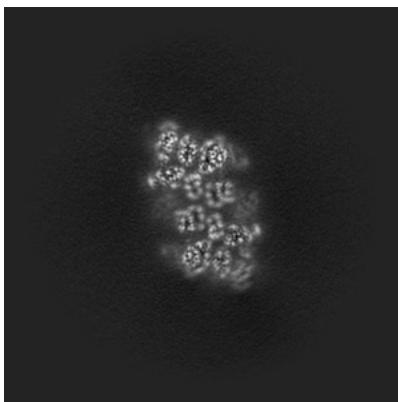
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

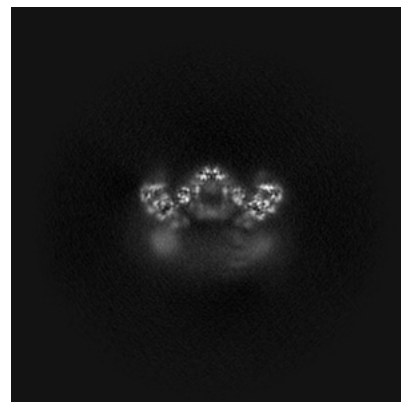
### 6.2.1 Primary map



X Index: 162

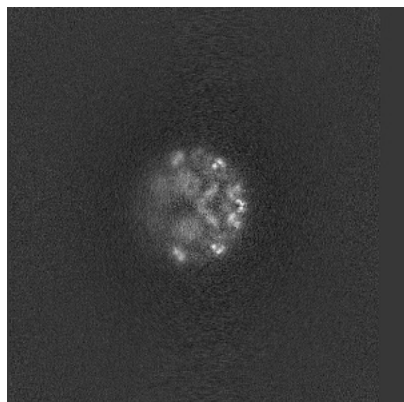


Y Index: 162

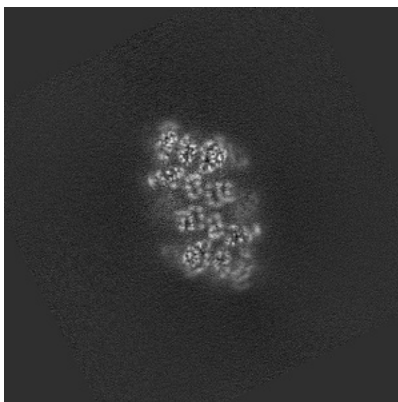


Z Index: 162

### 6.2.2 Raw map



X Index: 162



Y Index: 162

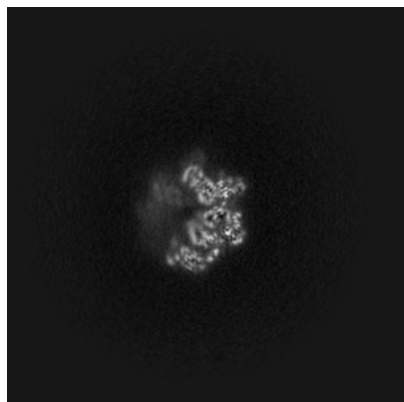


Z Index: 162

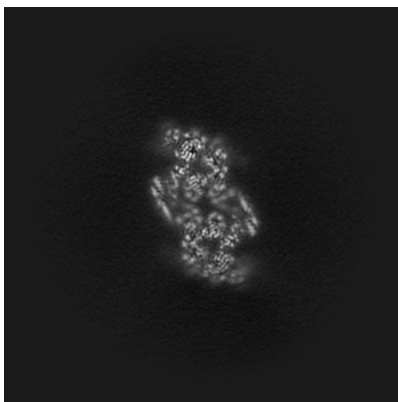
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

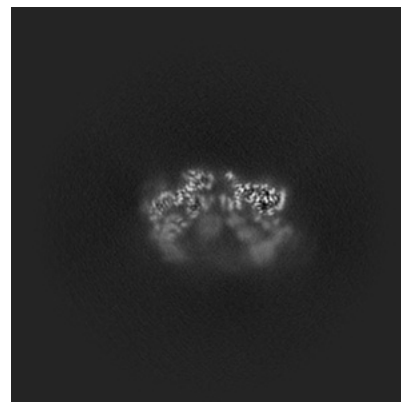
### 6.3.1 Primary map



X Index: 179

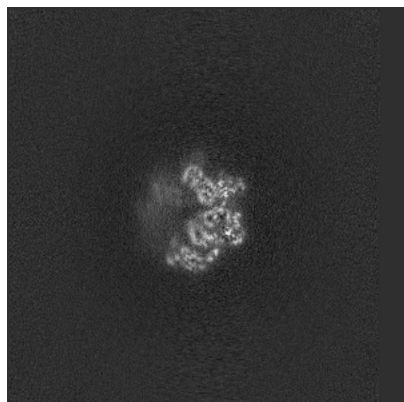


Y Index: 168

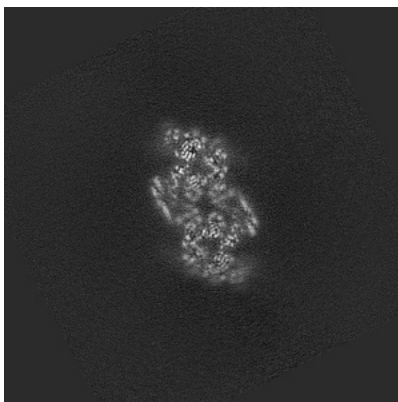


Z Index: 148

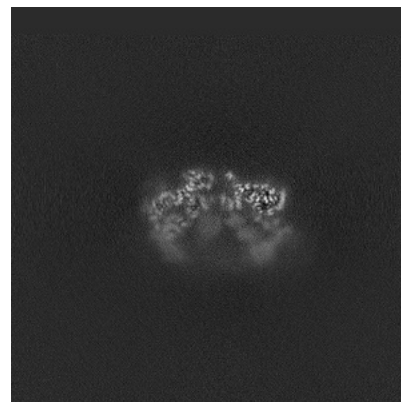
### 6.3.2 Raw map



X Index: 179



Y Index: 168



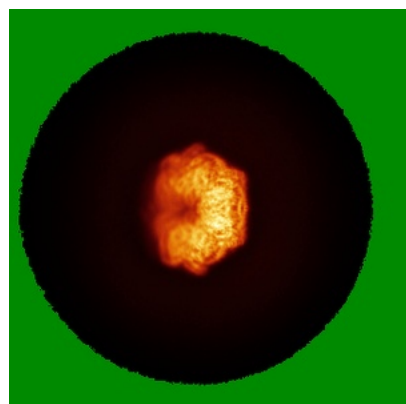
Z Index: 148

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

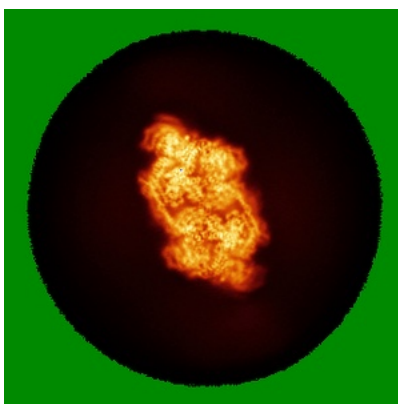


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

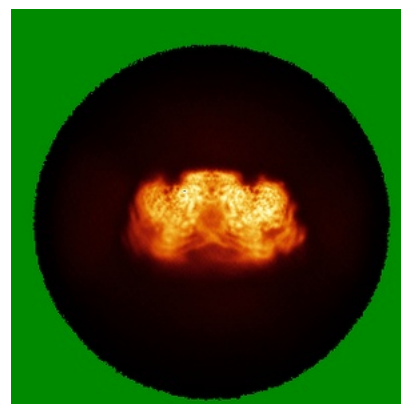
### 6.4.1 Primary map



X

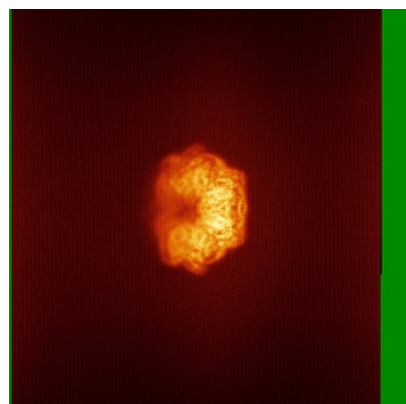


Y

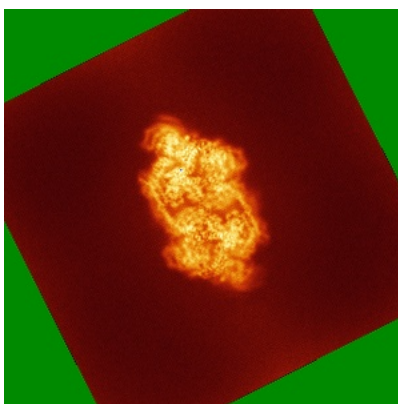


Z

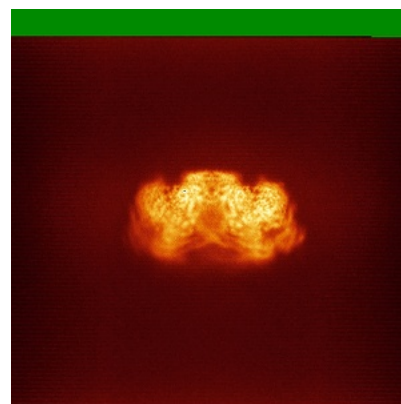
### 6.4.2 Raw map



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.

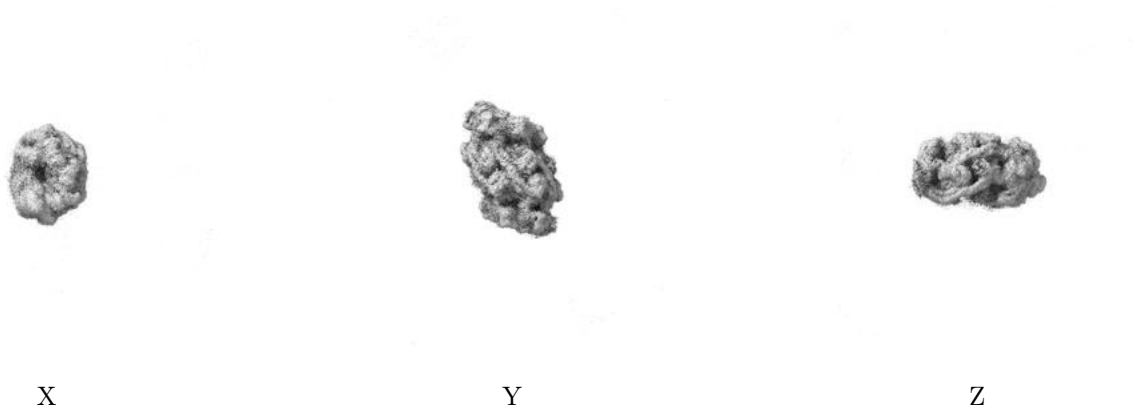
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0593. 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.

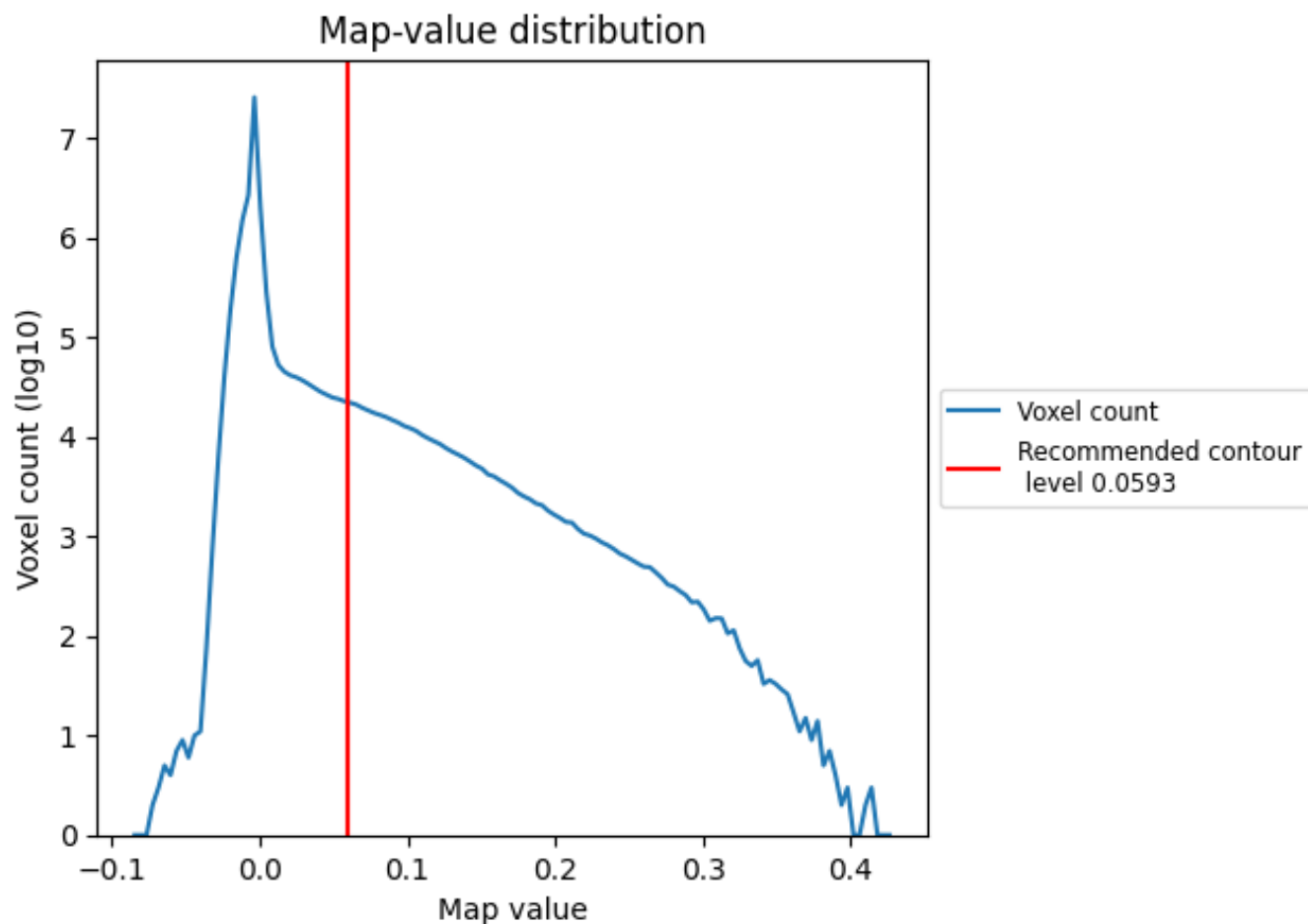
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

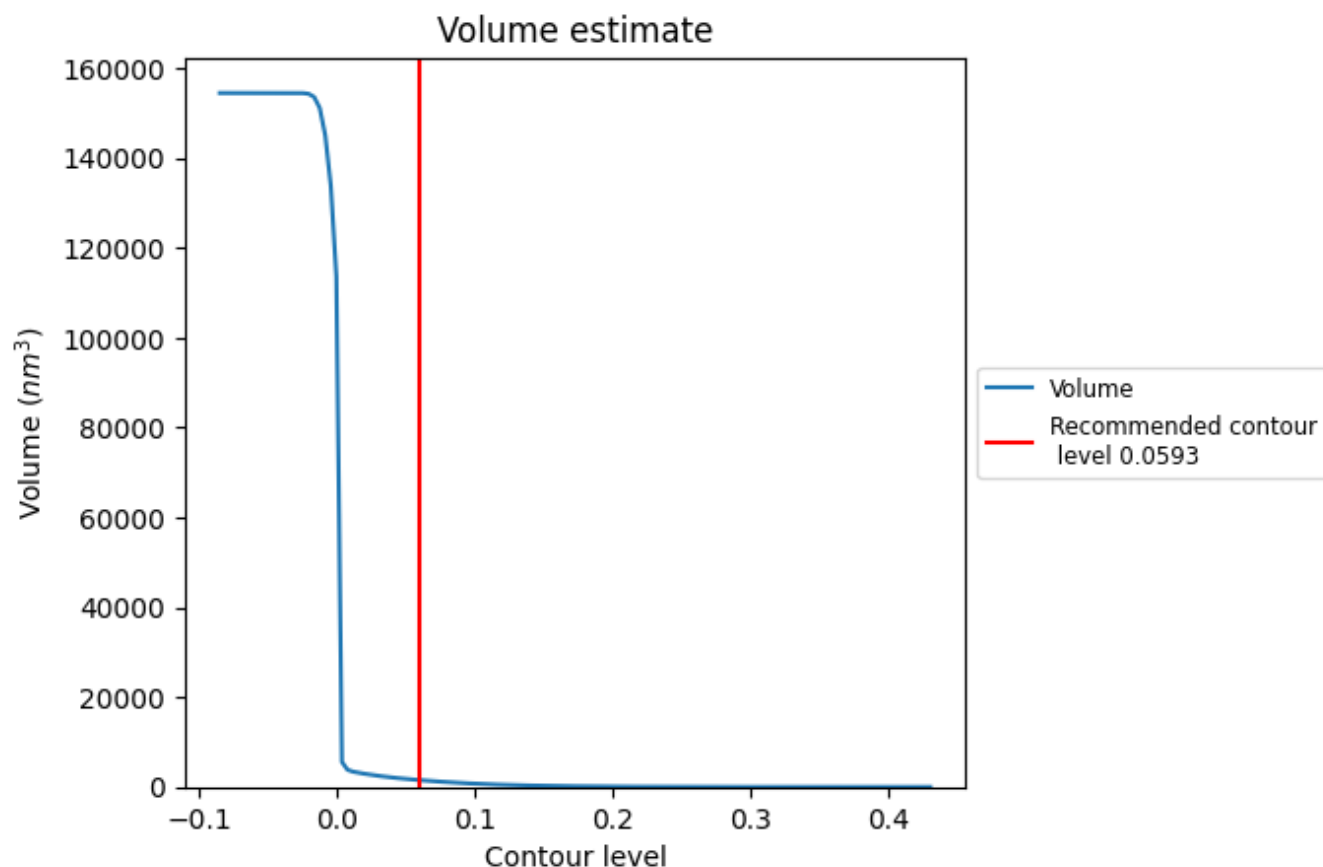
This section contains the results of statistical analysis of the map.

### 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.

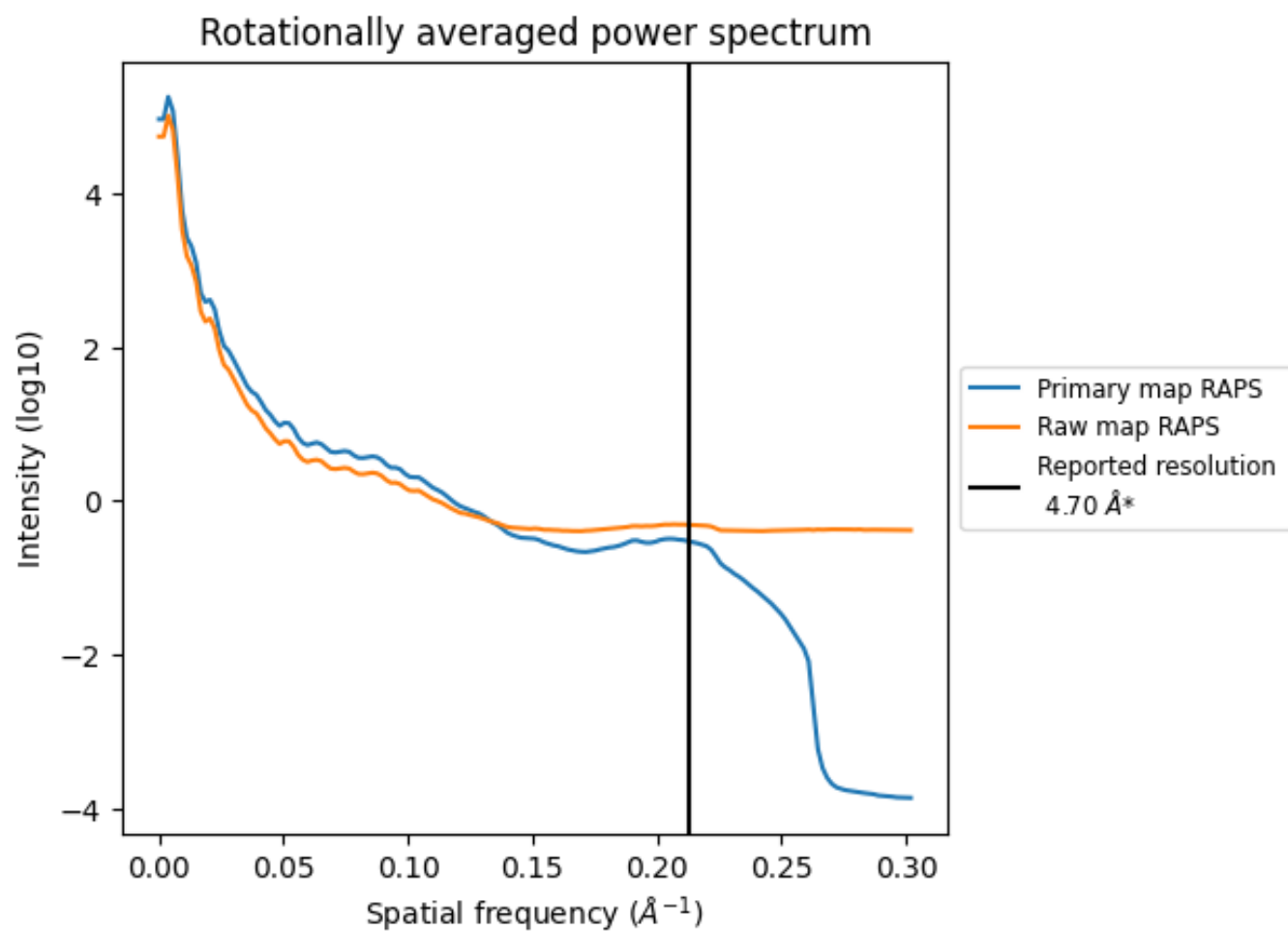
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1544 nm<sup>3</sup>; this corresponds to an approximate mass of 1395 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 ⓘ

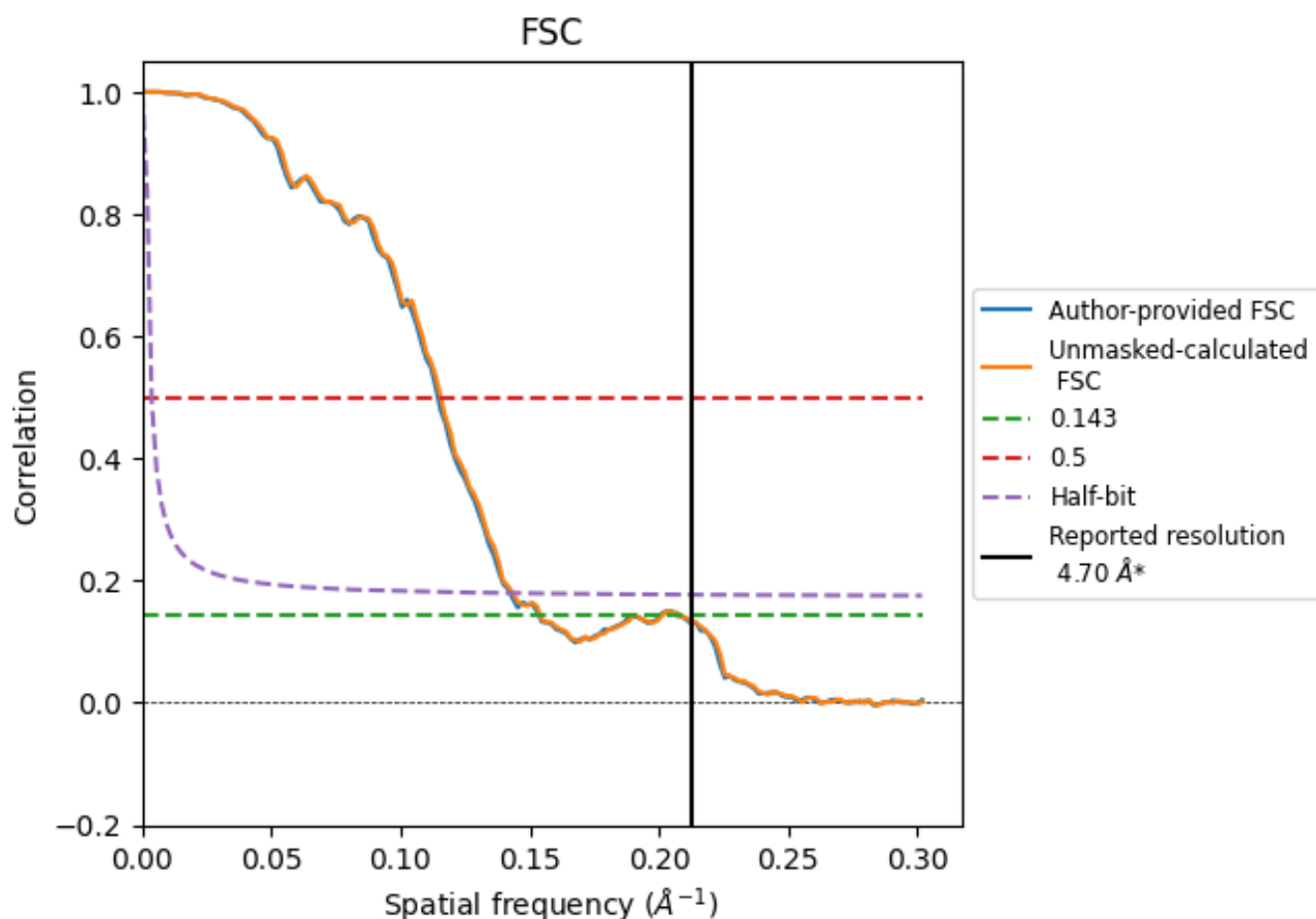


\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

## 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 0.213 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	6.51	8.74	7.02
Unmasked-calculated*	6.49	8.67	6.97

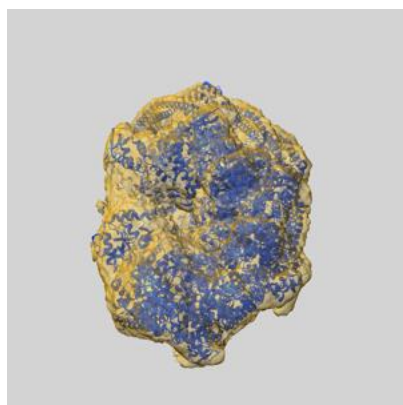
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.51 differs from the reported value 4.7 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.49 differs from the reported value 4.7 by more than 10 %

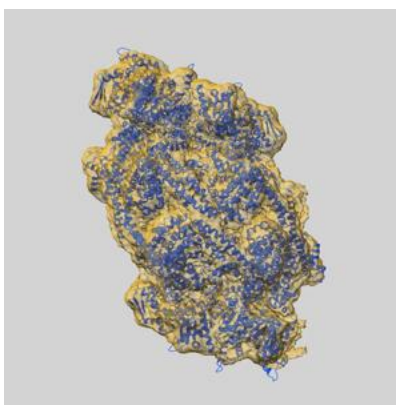
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53312 and PDB model 9QQR. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

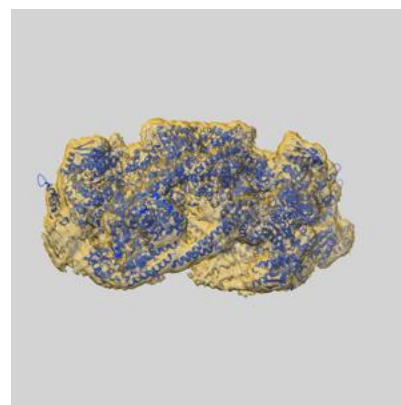
### 9.1 Map-model overlay [i](#)



X



Y

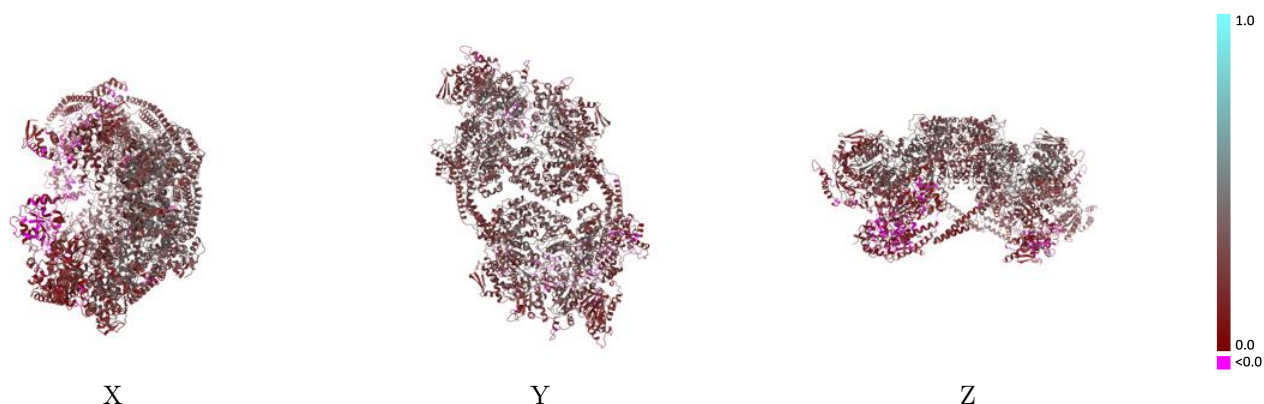


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0593 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

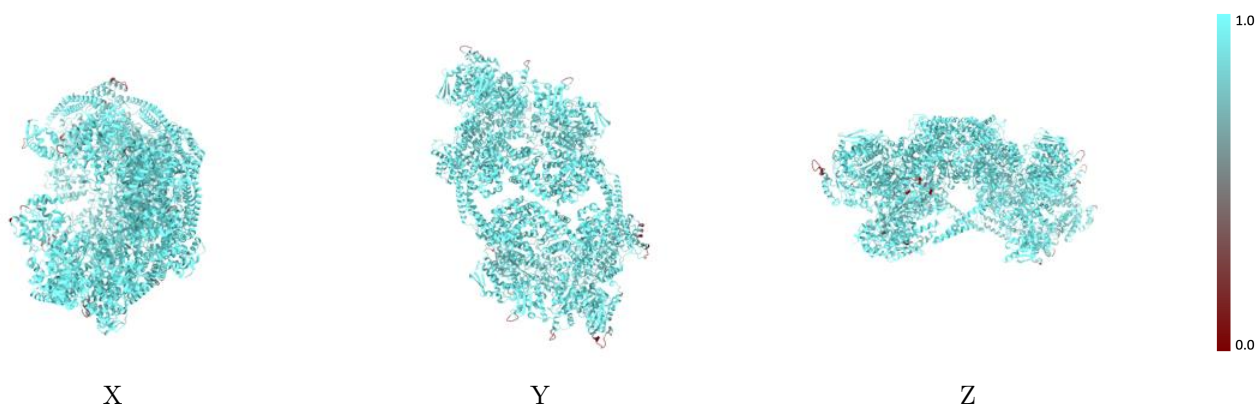


## 9.2 Q-score mapped to coordinate model [i](#)



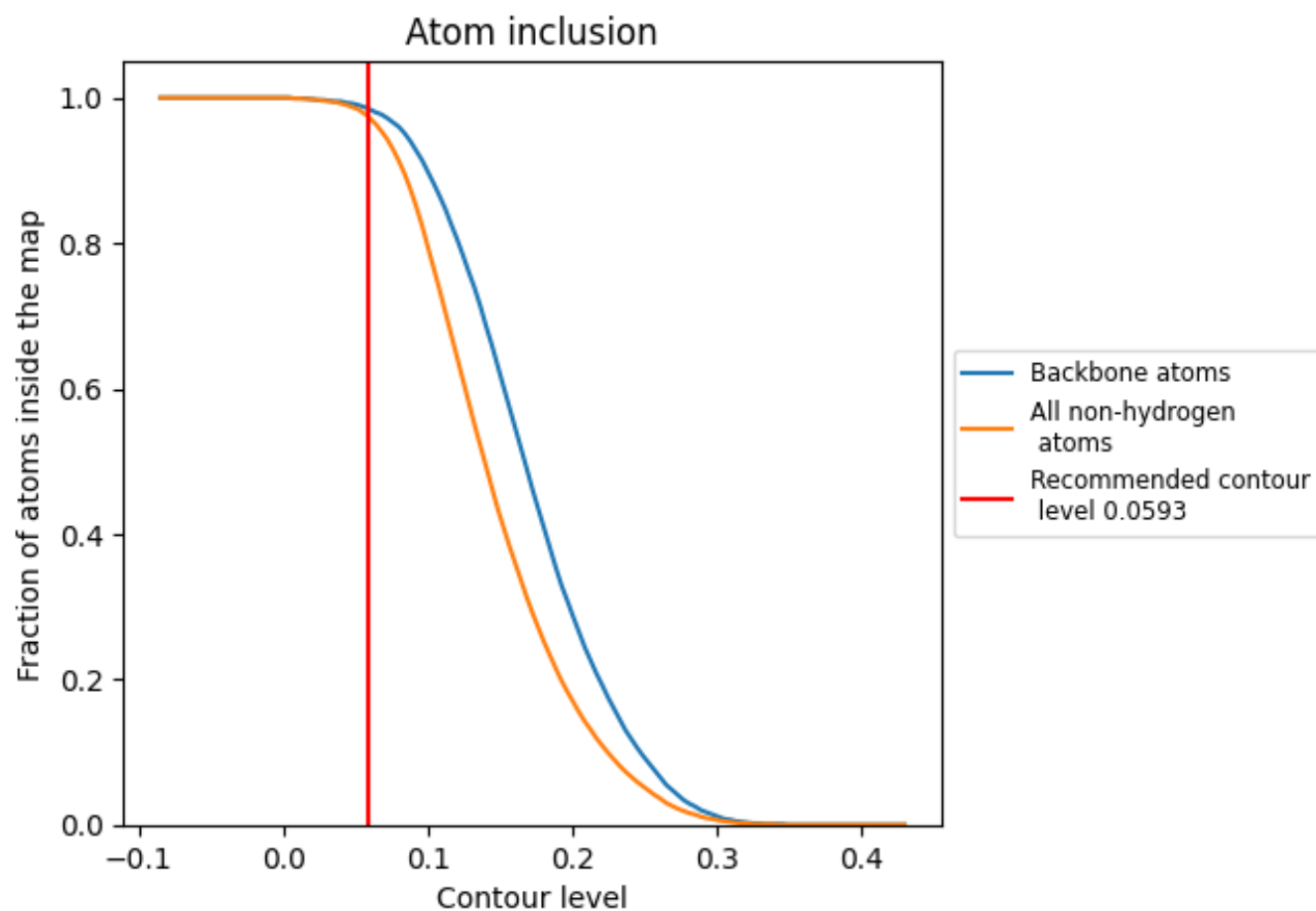
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0593).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.0593) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9740</div>	<div><div></div>0.2550</div>
A	<div><div></div>0.9650</div>	<div><div></div>0.0920</div>
B	<div><div></div>0.9260</div>	<div><div></div>0.1630</div>
C	<div><div></div>0.9830</div>	<div><div></div>0.3160</div>
D	<div><div></div>0.9850</div>	<div><div></div>0.3130</div>
E	<div><div></div>0.9540</div>	<div><div></div>0.2060</div>
F	<div><div></div>0.9810</div>	<div><div></div>0.2210</div>
G	<div><div></div>0.9890</div>	<div><div></div>0.3180</div>
H	<div><div></div>0.9890</div>	<div><div></div>0.3530</div>
I	<div><div></div>0.9860</div>	<div><div></div>0.2880</div>
J	<div><div></div>0.9720</div>	<div><div></div>0.1500</div>

1.0

0.0

<0.0