



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:09 AM UTC

PDB ID : 8FCN / pdb_00008fcn
EMDB ID : EMD-28987
Title : Cryo-EM structure of p97:UBXD1 VIM-only state
Authors : Braxton, J.R.; Tucker, M.R.; Tse, E.; Southworth, D.R.
Deposited on : 2022-12-01
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

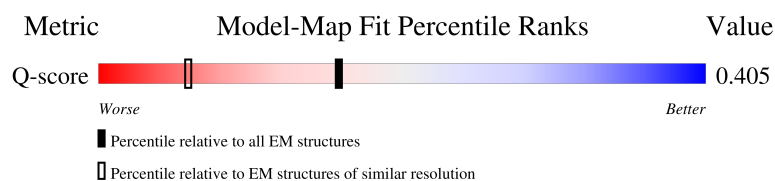
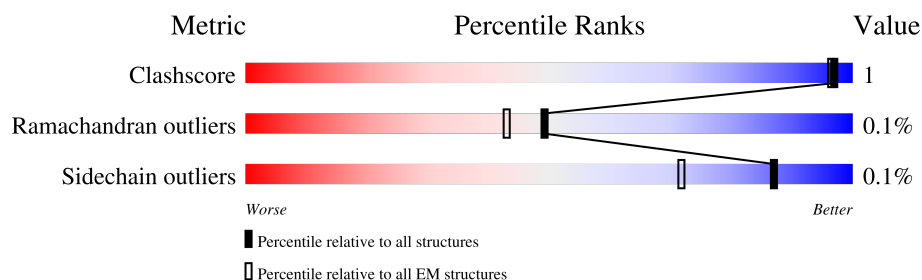
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

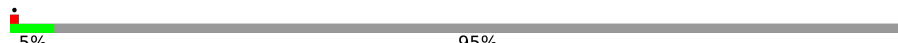
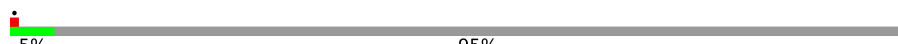
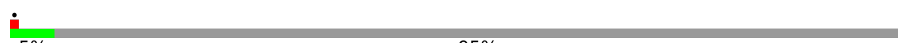
The reported resolution of this entry is 2.95 Å.

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



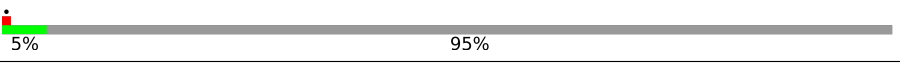
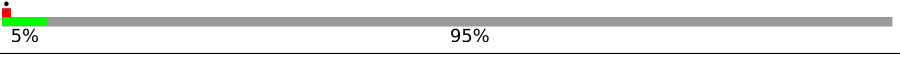
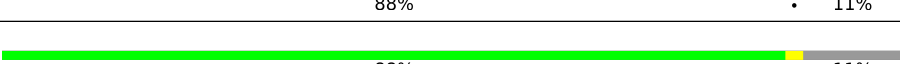
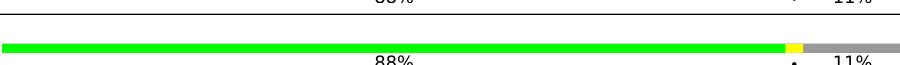
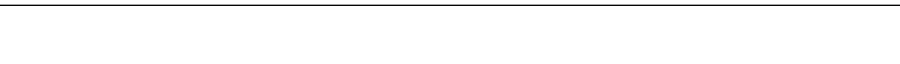
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13114 (2.45 - 3.45)

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

Mol	Chain	Length	Quality of chain
1	G	441	 5% 95%
1	H	441	 5% 95%
1	I	441	 5% 95%
1	J	441	 5% 95%

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Mol	Chain	Length	Quality of chain
1	K	441	 5% 95%
1	L	441	 5% 95%
2	A	806	 87% 11%
2	B	806	 87% 11%
2	C	806	 88% 11%
2	D	806	 88% 11%
2	E	806	 88% 11%
2	F	806	 88% 11%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35034 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 UBX domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	20	Total	C	N	O	S	0	0
			145	86	28	30	1		
1	K	20	Total	C	N	O	S	0	0
			145	86	28	30	1		
1	J	20	Total	C	N	O	S	0	0
			145	86	28	30	1		
1	I	20	Total	C	N	O	S	0	0
			145	86	28	30	1		
1	H	20	Total	C	N	O	S	0	0
			145	86	28	30	1		
1	G	20	Total	C	N	O	S	0	0
			145	86	28	30	1		

- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
2	E	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
2	D	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
2	C	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
2	B	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
2	A	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

[illegible]

- Molecule 1: UBX domain-containing protein 6



PRO	GLN	VAL	GLN	GLU	THR	TRP	MET
GLU	SER	GLU	SER	GLU	LEU	GLY	LYS
LEU	ASP	ARG	LEU	GLU	LYS	PRO	LYS
LEU	TRP	LEU	GLU	TYR	THR	THR	PHE
ALA	SER	SER	ARG	ARG	ASP	SER	PHE
ILE	PRO	VAL	HIS	LYS	GLN	GLN	GLN
	PHE	LEU	LYS	ILE	ARG	ASP	GLU
GLU	GLU	ARG	GLU	LYS	ASP	THR	PHE
LEU	LEU	THR	GLN	GLN	ILE	ARG	LYS
LEU	LEU	LYS	LEU	GLN	CYS	ARG	ALA
	ALA	ALA	LEU	ASN	ILE	ASN	ASP
SER	SER	MET	ALA	LYS	LYS	GLN	ILE
	GLY	ARG	ALA	VAL	GLU	VAL	LYS
	GLY	GLU	GLU	PHE	ALA	ARG	PHE
GLN	GLN	LYS	PRO	GLN	ILE	LYS	LYS
LYS	LYS	GLU	VAL	GLU	LEU	GLU	SER
LEU	LEU	GLU	ARG	ARG	LEU	LEU	ALA
	SER	GLN	ALA	ILE	HIS	GLN	GLY
	GLU	ARG	LYS	ASN	PHE	ALA	PRO
	ASP	GLY	LEU	CYS	SER	GLU	GLY
GLU	GLU	LEU	ASP	LEU	THR	ALA	GLN
ASN	ASN	ARG	ARG	GLU	ASP	THR	LYS
LEU	LEU	LYS	GLN	GLY	PRO	VAL	LEU
ALA	ALA	TYR	ARG	THR	VAL	SER	LYS
LEU	LEU	ASN	ARG	HIS	ALA	GLY	GLU
ASN	ASN	TYR	VAL	GLU	ALA	SER	SER
GLU	GLU	THR	PHE	PHE	SER	PRO	VAL
LYS	CYS	LEU	GLN	PHE	ILE	GLU	GLY
GLY	GLY	LEU	PRO	GLU	MET	ALA	GLU
LEU	LEU	ARG	SER	ALA	LYS	PRO	LYS
VAL	VAL	VAL	PRO	ILE	ILE	GLY	ALA
PRO	PRO	ARG	LEU	PHE	THR	THR	HIS
SER	SER	LEU	ALA	PHE	THR	ASN	LYS
ALA	ALA	PRO	SER	LYS	PHE	VAL	GLU
LEU	LEU	GLY	GLN	VAL	ASN	VAL	LYS
	GLY	ASP	PHE	VAL	LYS	SER	PRO
THR	THR	CYS	GLU	LEU	ASP	GLU	ASN
PHE	PHE	LEU	LEU	LEU	GLN	PRO	GLN
TRP	TRP	GLN	GLY	PRO	ASP	ARG	PRO
ASP	ASP	GLY	ASP	GLN	ARG	GLU	ALA
MET	MET	THR	PHE	ASP	LYS	GLY	ARG
ALA	ALA	PHE	PHE	GLN	LEU	SER	PRO
VAL	VAL	THR	ASN	GLU	ALA	ALA	PRO
LEU	LEU	ALA	ILE	TYR	LYS	HIS	ARG
GLY	GLY	VAL	ARG	VAL	THR	GLN	GLN
ASP	ASP	GLU	ALA	GLU	THR	ALA	GLY
ILE	ILE	ARG	GLU	GLU	ILE	VAL	PRO
LYS	LYS	LEU	GLU	PHE	ALA	PRO	T49
ALA	ALA	GLY	ILE	TYR	LYS	GLY	T49
ALA	ALA	VAL	ARG	VAL	TYR	VAL	A59
GLY	GLY	VAL	GLU	SER	LEU	PHE	L63
ALA	ALA	TYR	GLU	GLU	ASN	THR	E64
PRO	PRO	PHE	ARG	GLU	ILE	CYS	Q65
ASP	ASP	VAL	LEU	THR	HIS	PRO	K66
SER	SER	ARG	ARG	LEU	LEU	THR	Q67
ILE	ILE	GLU	SER	ALA	HIS	GLY	S68
LEU	LEU	ALA	GLU	GLN	PRO	ALA	ARG
LYS	LYS	LEU	ALA	PRO	GLU	GLY	ALA

- Molecule 1: UBX domain-containing protein 6



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

[illegible]

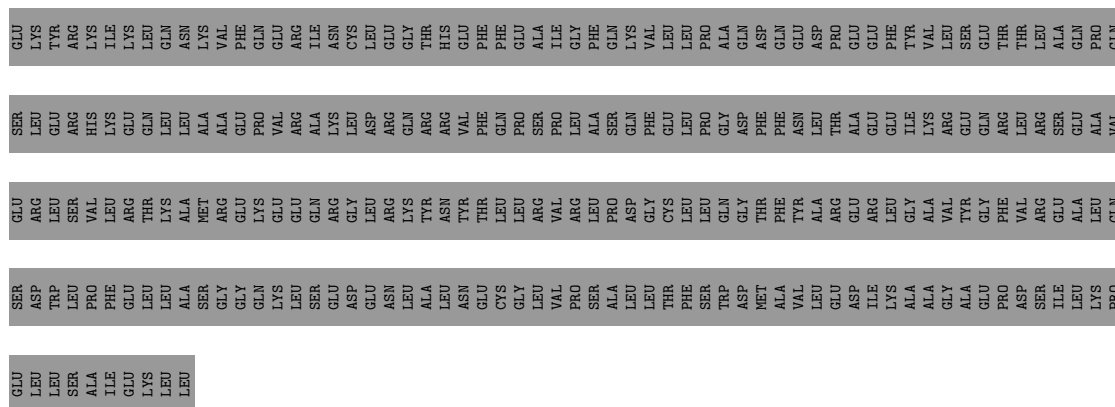
- Molecule 1: UBX domain-containing protein 6



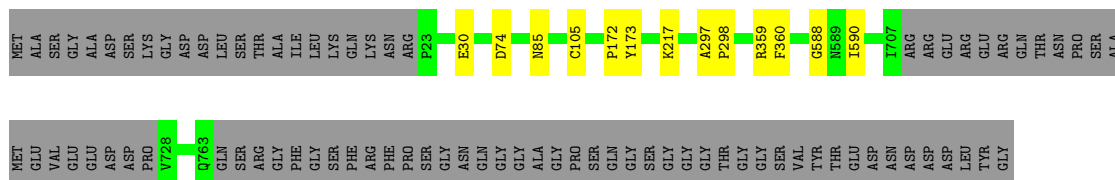
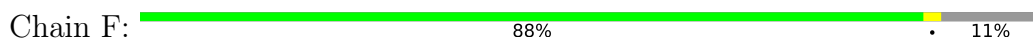
PRO	GLN	VAL	GLN	GLU	THR	TRP	MET
GLU	SER	GLU	SER	GLU	LEU	GLY	LYS
LEU	ASP	ARG	LEU	GLU	LYS	PRO	LYS
LEU	TRP	LEU	GLU	TYR	GLU	THR	PHE
SER	LEU	SER	ARG	ARG	ASP	SER	PHE
ALA	PRO	VAL	HIS	LYS	GLN	GLN	GLN
ILE	PHE	LEU	LYS	ILE	ARG	ASP	GLU
GLU	GLU	ARG	GLU	LYS	THR	THR	PHE
LEU	LEU	THR	GLN	LEU	ALA	ILE	LYS
LEU	LEU	LYS	LEU	GLN	CYS	ARG	ALA
LEU	ALA	ALA	LEU	ASN	ILE	ASN	ASP
SER	SER	MET	ALA	LYS	LYS	GLN	ILE
GLY	GLY	ARG	ALA	VAL	GLU	VAL	LYS
GLN	GLN	LYS	PRO	PHE	ALA	ARG	PHE
LYS	LYS	GLU	VAL	GLN	ILE	LYS	LYS
LEU	LYS	GLU	VAL	GLU	LEU	SER	SER
LEU	SER	GLN	ARG	ILE	HIS	GLN	ALA
ALA	GLU	ARG	LYS	ASN	PHE	ALA	PRO
LEU	GLU	GLY	LEU	CYS	SER	GLU	GLY
LEU	GLU	LEU	ASP	LEU	THR	THR	GLN
ALA	LEU	TYR	GLN	GLY	PRO	VAL	LYS
LEU	ALA	ASN	ARG	HIS	VAL	GLY	GLU
LYS	ASN	THR	VAL	GLU	ALA	SER	SER
GLU	GLU	THR	PHE	PHE	SER	PRO	VAL
LYS	CYS	LEU	GLN	ILE	GLN	GLU	GLY
LEU	GLY	LEU	PRO	ALA	MET	ALA	GLU
LEU	LEU	ARG	SER	ALA	LYS	PRO	LYS
VAL	VAL	VAL	PRO	ILE	ILE	GLY	ALA
PRO	PRO	ARG	LEU	GLY	TYR	THR	HIS
ALA	SER	LEU	ALA	PHE	THR	ASN	LYS
LEU	LEU	PRO	GLN	LYS	PHE	VAL	GLU
ASP	GLY	ASP	GLN	VAL	ASN	VAL	LYS
MET	THR	GLY	ASP	ASP	LYS	SER	PRO
ALA	ALA	PHE	PHE	GLN	LYS	GLY	ARG
VAL	VAL	TYR	ASN	GLU	LEU	SER	PRO
LEU	LEU	ALA	LEU	ASP	VAL	HIS	GLN
GLU	GLU	ARG	THR	PRO	ASP	LEU	ARG
ASP	ASP	GLU	ALA	GLU	THR	ALA	GLY
ILE	ILE	ARG	GLU	GLU	ILE	VAL	PRO
LYS	LYS	LEU	GLU	PHE	ALA	PRO	T49
ALA	ALA	GLY	ILE	TYR	LYS	GLY	T49
ALA	GLY	VAL	ARG	LEU	TYR	VAL	A59
ALA	TYR	GLY	GLU	SER	ASP	PHE	L63
GLU	GLU	GLY	GLN	GLU	ASN	THR	E54
PRO	PRO	PHE	ARG	GLU	ILE	CYS	Q65
ASP	ASP	VAL	LEU	THR	THR	PRO	Q65
SER	SER	ARG	ARG	LEU	HIS	LEU	K66
ILE	ILE	GLU	SER	ALA	HIS	THR	Q67
LEU	LEU	ALA	GLU	GLN	PRO	GLY	S68
LYS	LYS	LEU	ALA	PRO	GLU	ALA	ARG

- Molecule 1: UBX domain-containing protein 6

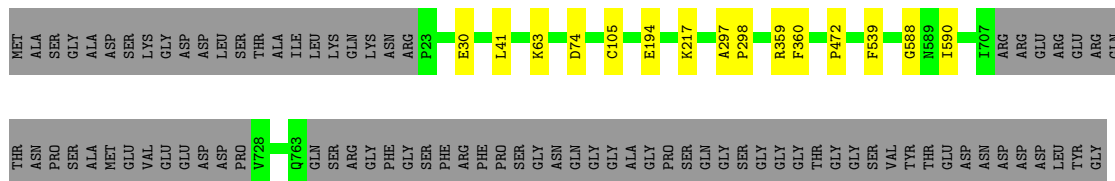
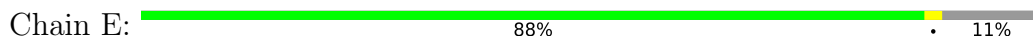
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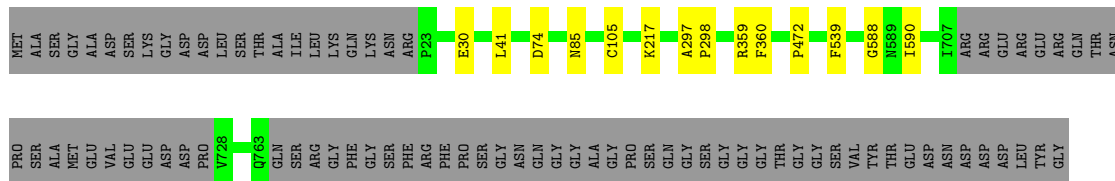
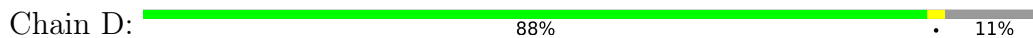
- Molecule 2: Transitional endoplasmic reticulum ATPase



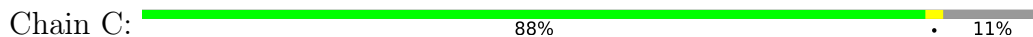
- Molecule 2: Transitional endoplasmic reticulum ATPase



- Molecule 2: Transitional endoplasmic reticulum ATPase

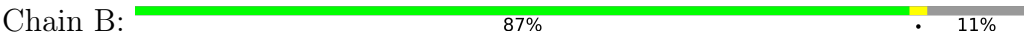


- Molecule 2: Transitional endoplasmic reticulum ATPase

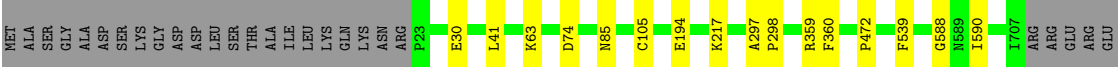
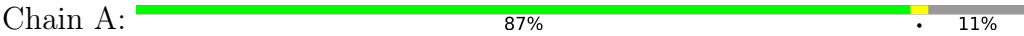




● Molecule 2: Transitional endoplasmic reticulum ATPase



● Molecule 2: Transitional endoplasmic reticulum ATPase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	59952	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.998	Depositor
Minimum map value	-0.374	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	333.6, 333.6, 333.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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	G	0.69	0/144	0.99	0/192
1	H	0.69	0/144	0.99	0/192
1	I	0.69	0/144	0.99	0/192
1	J	0.68	0/144	0.99	0/192
1	K	0.69	0/144	0.99	0/192
1	L	0.69	0/144	1.00	0/192
2	A	0.58	0/5732	0.48	1/7741 (0.0%)
2	B	0.58	0/5732	0.48	1/7741 (0.0%)
2	C	0.57	0/5732	0.49	1/7741 (0.0%)
2	D	0.58	0/5732	0.48	1/7741 (0.0%)
2	E	0.58	0/5732	0.48	1/7741 (0.0%)
2	F	0.57	0/5732	0.49	1/7741 (0.0%)
All	All	0.58	0/35256	0.50	6/47598 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	590	ILE	N-CA-C	-5.70	106.66	111.56
2	E	590	ILE	N-CA-C	-5.68	106.68	111.56
2	B	590	ILE	N-CA-C	-5.67	106.69	111.56
2	D	590	ILE	N-CA-C	-5.65	106.70	111.56
2	A	590	ILE	N-CA-C	-5.64	106.71	111.56
2	F	590	ILE	N-CA-C	-5.63	106.72	111.56

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	G	145	0	145	0	0
1	H	145	0	145	0	0
1	I	145	0	145	0	0
1	J	145	0	145	0	0
1	K	145	0	145	0	0
1	L	145	0	145	0	0
2	A	5640	0	5713	8	0
2	B	5640	0	5713	11	0
2	C	5640	0	5713	8	0
2	D	5640	0	5713	7	0
2	E	5640	0	5713	7	0
2	F	5640	0	5713	7	0
3	A	54	0	24	0	0
3	B	54	0	24	0	0
3	C	54	0	24	0	0
3	D	54	0	24	0	0
3	E	54	0	24	0	0
3	F	54	0	24	0	0
All	All	35034	0	35292	48	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 1.

All (48) 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)
2:C:30:GLU:OE2	2:C:217:LYS:NZ	2.40	0.52
2:B:30:GLU:OE2	2:B:217:LYS:NZ	2.41	0.51
2:E:30:GLU:OE2	2:E:217:LYS:NZ	2.44	0.51
2:A:30:GLU:OE2	2:A:217:LYS:NZ	2.44	0.50
2:D:30:GLU:OE2	2:D:217:LYS:NZ	2.43	0.49
2:F:30:GLU:OE2	2:F:217:LYS:NZ	2.45	0.48
2:D:359:ARG:O	2:D:360:PHE:C	2.56	0.48
2:E:359:ARG:O	2:E:360:PHE:C	2.57	0.48
2:A:359:ARG:O	2:A:360:PHE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:ARG:O	2:C:360:PHE:C	2.57	0.48
2:F:359:ARG:O	2:F:360:PHE:C	2.57	0.47
2:B:359:ARG:O	2:B:360:PHE:C	2.57	0.47
2:D:74:ASP:OD1	2:D:74:ASP:C	2.59	0.46
2:A:74:ASP:OD1	2:A:74:ASP:C	2.59	0.46
2:F:74:ASP:OD1	2:F:74:ASP:C	2.58	0.46
2:C:74:ASP:OD1	2:C:74:ASP:C	2.59	0.46
2:E:74:ASP:OD1	2:E:74:ASP:C	2.59	0.46
2:D:105:CYS:SG	2:D:105:CYS:O	2.75	0.45
2:B:105:CYS:SG	2:B:105:CYS:O	2.75	0.45
2:B:123:VAL:O	2:B:123:VAL:HG13	2.16	0.45
2:A:105:CYS:SG	2:A:105:CYS:O	2.75	0.44
2:B:297:ALA:HA	2:B:298:PRO:C	2.42	0.44
2:C:297:ALA:HA	2:C:298:PRO:C	2.42	0.44
2:C:105:CYS:O	2:C:105:CYS:SG	2.75	0.44
2:B:74:ASP:C	2:B:74:ASP:OD1	2.60	0.44
2:D:297:ALA:HA	2:D:298:PRO:C	2.42	0.44
2:F:105:CYS:SG	2:F:105:CYS:O	2.76	0.44
2:E:105:CYS:SG	2:E:105:CYS:O	2.76	0.43
2:A:63:LYS:NZ	2:A:194:GLU:OE1	2.51	0.43
2:C:172:PRO:HG2	2:C:173:TYR:CD2	2.53	0.43
2:B:172:PRO:HG2	2:B:173:TYR:CD2	2.53	0.43
2:A:297:ALA:HA	2:A:298:PRO:C	2.42	0.43
2:F:297:ALA:HA	2:F:298:PRO:C	2.43	0.42
2:E:297:ALA:HA	2:E:298:PRO:C	2.43	0.42
2:B:119:ILE:O	2:B:122:THR:HG22	2.19	0.42
2:D:472:PRO:HD3	2:D:539:PHE:HB2	2.02	0.42
2:B:472:PRO:HD3	2:B:539:PHE:HB2	2.02	0.42
2:C:472:PRO:HD3	2:C:539:PHE:HB2	2.02	0.41
2:E:63:LYS:NZ	2:E:194:GLU:OE1	2.54	0.41
2:D:85:ASN:OD1	2:D:85:ASN:C	2.64	0.41
2:A:472:PRO:HD3	2:A:539:PHE:HB2	2.02	0.41
2:A:85:ASN:OD1	2:A:85:ASN:C	2.65	0.40
2:F:85:ASN:OD1	2:F:85:ASN:C	2.64	0.40
2:F:172:PRO:HG2	2:F:173:TYR:CD2	2.56	0.40
2:E:472:PRO:HD3	2:E:539:PHE:HB2	2.02	0.40
2:B:85:ASN:OD1	2:B:85:ASN:C	2.64	0.40
2:C:172:PRO:HG2	2:C:173:TYR:HD2	1.85	0.40
2:B:63:LYS:NZ	2:B:194:GLU:OE1	2.55	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	G	18/441 (4%)	18 (100%)	0	0	100	100
1	H	18/441 (4%)	18 (100%)	0	0	100	100
1	I	18/441 (4%)	18 (100%)	0	0	100	100
1	J	18/441 (4%)	18 (100%)	0	0	100	100
1	K	18/441 (4%)	18 (100%)	0	0	100	100
1	L	18/441 (4%)	18 (100%)	0	0	100	100
2	A	717/806 (89%)	707 (99%)	9 (1%)	1 (0%)	48	72
2	B	717/806 (89%)	707 (99%)	9 (1%)	1 (0%)	48	72
2	C	717/806 (89%)	707 (99%)	9 (1%)	1 (0%)	48	72
2	D	717/806 (89%)	707 (99%)	9 (1%)	1 (0%)	48	72
2	E	717/806 (89%)	708 (99%)	8 (1%)	1 (0%)	48	72
2	F	717/806 (89%)	707 (99%)	9 (1%)	1 (0%)	48	72
All	All	4410/7482 (59%)	4351 (99%)	53 (1%)	6 (0%)	49	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	588	GLY
2	E	588	GLY
2	D	588	GLY
2	C	588	GLY
2	B	588	GLY
2	A	588	GLY

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	G	13/374 (4%)	13 (100%)	0	100	100
1	H	13/374 (4%)	13 (100%)	0	100	100
1	I	13/374 (4%)	13 (100%)	0	100	100
1	J	13/374 (4%)	13 (100%)	0	100	100
1	K	13/374 (4%)	13 (100%)	0	100	100
1	L	13/374 (4%)	13 (100%)	0	100	100
2	A	613/678 (90%)	612 (100%)	1 (0%)	87	94
2	B	613/678 (90%)	613 (100%)	0	100	100
2	C	613/678 (90%)	612 (100%)	1 (0%)	87	94
2	D	613/678 (90%)	612 (100%)	1 (0%)	87	94
2	E	613/678 (90%)	612 (100%)	1 (0%)	87	94
2	F	613/678 (90%)	613 (100%)	0	100	100
All	All	3756/6312 (60%)	3752 (100%)	4 (0%)	87	95

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

Mol	Chain	Res	Type
2	E	41	LEU
2	D	41	LEU
2	C	41	LEU
2	A	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	103	GLN
2	F	215	GLN
2	F	340	HIS
2	F	458	GLN
2	F	603	GLN
2	F	616	ASN
2	F	680	ASN
2	E	103	GLN

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Mol	Chain	Res	Type
2	E	215	GLN
2	E	340	HIS
2	E	603	GLN
2	E	680	ASN
2	D	215	GLN
2	D	340	HIS
2	D	458	GLN
2	C	215	GLN
2	C	340	HIS
2	C	458	GLN
2	C	603	GLN
2	C	680	ASN
2	B	215	GLN
2	B	340	HIS
2	B	406	HIS
2	B	458	GLN
2	A	215	GLN
2	A	458	GLN
2	A	603	GLN

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](#)

12 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	-	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
3	ADP	A	902	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
3	ADP	F	902	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	8 (18%)
3	ADP	C	901	-	28,29,29	0.53	0	43,45,45	0.43	0
3	ADP	F	901	-	28,29,29	0.52	0	43,45,45	0.43	0
3	ADP	B	901	-	28,29,29	0.53	0	43,45,45	0.43	0
3	ADP	E	902	-	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
3	ADP	A	901	-	28,29,29	0.53	0	43,45,45	0.43	0
3	ADP	D	902	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	9 (20%)
3	ADP	C	902	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
3	ADP	D	901	-	28,29,29	0.52	0	43,45,45	0.43	0
3	ADP	E	901	-	28,29,29	0.53	0	43,45,45	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	902	-	-	0/16/32/32	0/3/3/3
3	ADP	A	902	-	-	0/16/32/32	0/3/3/3
3	ADP	F	902	-	-	0/16/32/32	0/3/3/3
3	ADP	C	901	-	-	1/16/32/32	0/3/3/3
3	ADP	F	901	-	-	0/16/32/32	0/3/3/3
3	ADP	B	901	-	-	1/16/32/32	0/3/3/3
3	ADP	E	902	-	-	0/16/32/32	0/3/3/3
3	ADP	A	901	-	-	1/16/32/32	0/3/3/3
3	ADP	D	902	-	-	0/16/32/32	0/3/3/3
3	ADP	C	902	-	-	0/16/32/32	0/3/3/3
3	ADP	D	901	-	-	0/16/32/32	0/3/3/3
3	ADP	E	901	-	-	0/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	ADP	C5-C4	4.68	1.47	1.39
3	F	902	ADP	C5-C4	4.66	1.47	1.39
3	C	902	ADP	C5-C4	4.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	ADP	C5-C4	4.62	1.47	1.39
3	B	902	ADP	C5-C4	4.61	1.47	1.39
3	E	902	ADP	C5-C4	4.60	1.47	1.39
3	F	902	ADP	C5-C6	2.59	1.48	1.41
3	E	902	ADP	C5-C6	2.59	1.48	1.41
3	C	902	ADP	C5-C6	2.58	1.48	1.41
3	B	902	ADP	C5-C6	2.58	1.48	1.41
3	A	902	ADP	C5-C6	2.57	1.48	1.41
3	D	902	ADP	C5-C6	2.54	1.48	1.41
3	E	902	ADP	C5-N7	-2.43	1.34	1.39
3	F	902	ADP	C5-N7	-2.43	1.34	1.39
3	C	902	ADP	C5-N7	-2.42	1.34	1.39
3	B	902	ADP	C5-N7	-2.41	1.34	1.39
3	A	902	ADP	C5-N7	-2.40	1.34	1.39
3	D	902	ADP	C5-N7	-2.40	1.34	1.39
3	B	902	ADP	C8-N7	2.29	1.36	1.31
3	F	902	ADP	C8-N7	2.27	1.36	1.31
3	E	902	ADP	C8-N7	2.25	1.36	1.31
3	A	902	ADP	C8-N7	2.24	1.36	1.31
3	C	902	ADP	C8-N7	2.22	1.35	1.31
3	D	902	ADP	C8-N7	2.20	1.35	1.31

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	ADP	C5-C4-N3	-6.00	118.46	126.72
3	F	902	ADP	C5-C4-N3	-6.00	118.46	126.72
3	B	902	ADP	C5-C4-N3	-5.97	118.50	126.72
3	C	902	ADP	C5-C4-N3	-5.96	118.51	126.72
3	A	902	ADP	C5-C4-N3	-5.94	118.53	126.72
3	E	902	ADP	C5-C4-N3	-5.94	118.54	126.72
3	F	902	ADP	N3-C4-N9	4.85	135.41	127.17
3	E	902	ADP	N3-C4-N9	4.84	135.39	127.17
3	D	902	ADP	N3-C4-N9	4.83	135.38	127.17
3	C	902	ADP	N3-C4-N9	4.82	135.37	127.17
3	B	902	ADP	N3-C4-N9	4.82	135.36	127.17
3	A	902	ADP	N3-C4-N9	4.79	135.31	127.17
3	D	902	ADP	C2-N3-C4	3.81	121.13	111.83
3	F	902	ADP	C2-N3-C4	3.81	121.13	111.83
3	C	902	ADP	C2-N3-C4	3.80	121.11	111.83
3	B	902	ADP	C2-N3-C4	3.79	121.08	111.83
3	A	902	ADP	C2-N3-C4	3.78	121.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	902	ADP	C2-N3-C4	3.78	121.05	111.83
3	D	902	ADP	C4-C5-N7	-3.41	106.69	110.58
3	C	902	ADP	C4-C5-N7	-3.38	106.72	110.58
3	A	902	ADP	C4-C5-N7	-3.37	106.73	110.58
3	F	902	ADP	C4-C5-N7	-3.37	106.73	110.58
3	B	902	ADP	C4-C5-N7	-3.33	106.77	110.58
3	E	902	ADP	C4-C5-N7	-3.30	106.81	110.58
3	C	902	ADP	N3-C2-N1	-3.28	123.62	128.58
3	A	902	ADP	N3-C2-N1	-3.27	123.62	128.58
3	D	902	ADP	N3-C2-N1	-3.27	123.63	128.58
3	B	902	ADP	N3-C2-N1	-3.27	123.63	128.58
3	F	902	ADP	N3-C2-N1	-3.25	123.66	128.58
3	E	902	ADP	N3-C2-N1	-3.22	123.70	128.58
3	E	902	ADP	C4-N9-C8	2.68	108.55	105.74
3	F	902	ADP	C4-N9-C8	2.66	108.53	105.74
3	C	902	ADP	C4-N9-C8	2.64	108.51	105.74
3	B	902	ADP	C4-N9-C8	2.64	108.50	105.74
3	D	902	ADP	C3'-C2'-C1'	2.63	106.44	101.46
3	C	902	ADP	C3'-C2'-C1'	2.63	106.44	101.46
3	F	902	ADP	C3'-C2'-C1'	2.62	106.42	101.46
3	B	902	ADP	C3'-C2'-C1'	2.62	106.41	101.46
3	A	902	ADP	C4-N9-C8	2.61	108.48	105.74
3	A	902	ADP	C3'-C2'-C1'	2.60	106.39	101.46
3	D	902	ADP	C4-N9-C8	2.60	108.47	105.74
3	E	902	ADP	C3'-C2'-C1'	2.59	106.37	101.46
3	D	902	ADP	C5-N7-C8	2.52	107.41	103.45
3	C	902	ADP	C5-N7-C8	2.52	107.40	103.45
3	F	902	ADP	C5-N7-C8	2.49	107.36	103.45
3	E	902	ADP	C5-N7-C8	2.47	107.34	103.45
3	B	902	ADP	C5-N7-C8	2.47	107.34	103.45
3	A	902	ADP	C5-N7-C8	2.47	107.33	103.45
3	D	902	ADP	C6-C5-N7	2.02	135.97	132.09

There are no chirality outliers.

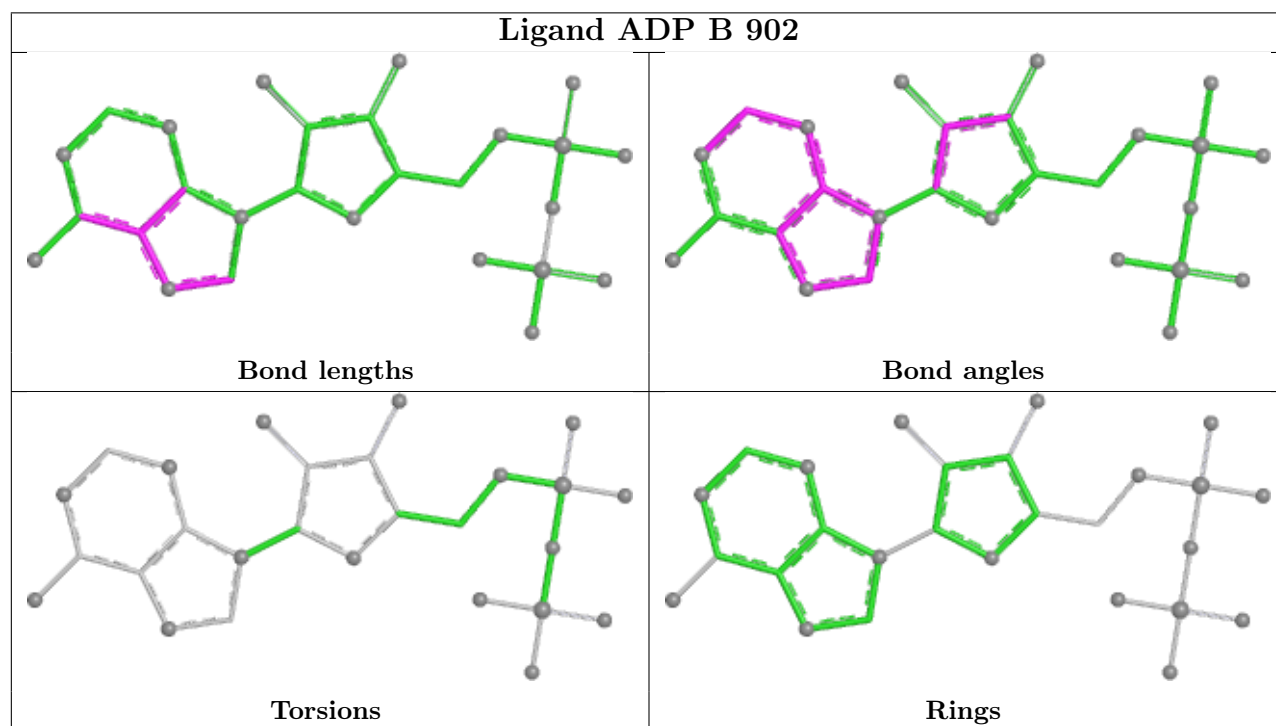
All (3) torsion outliers are listed below:

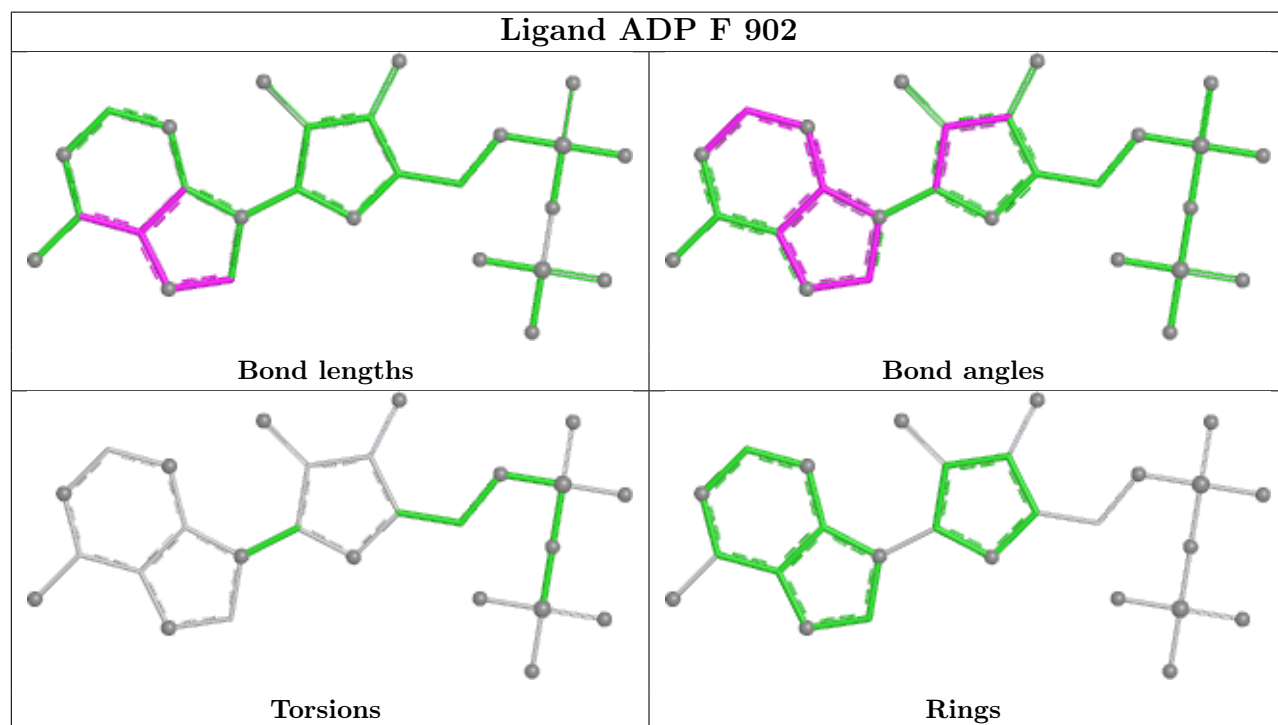
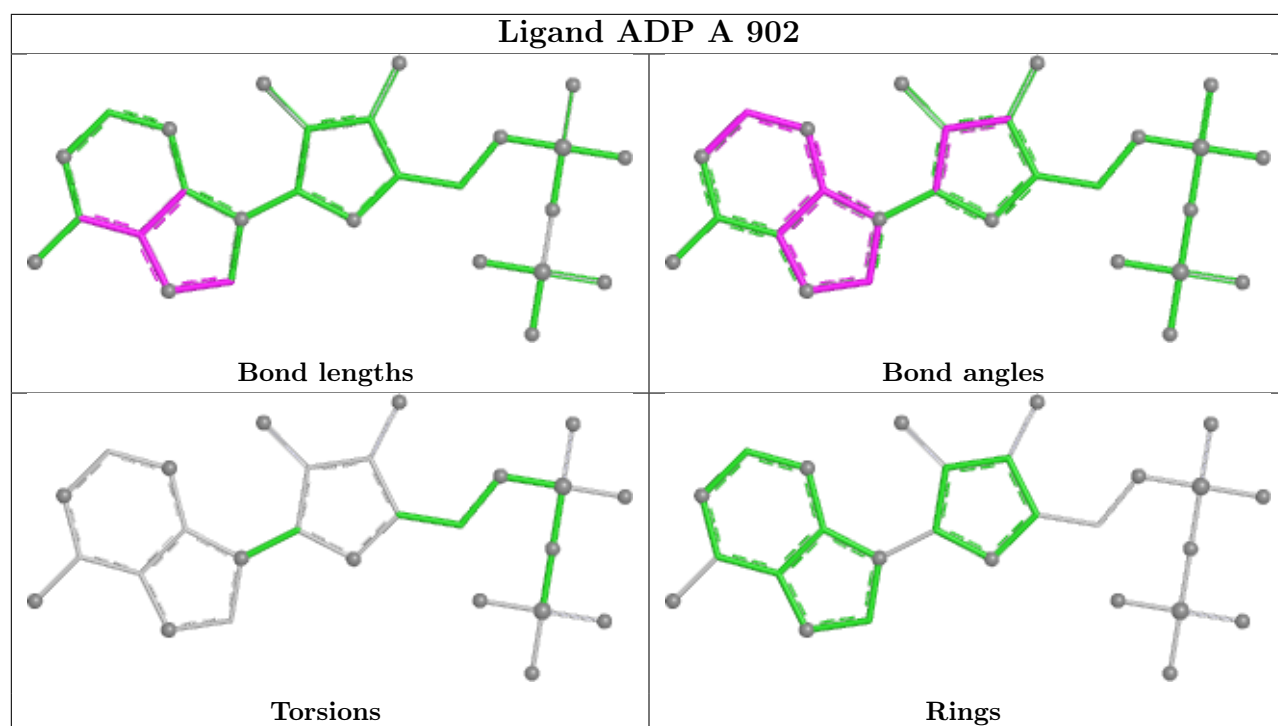
Mol	Chain	Res	Type	Atoms
3	C	901	ADP	PB-O3A-PA-O2A
3	B	901	ADP	PB-O3A-PA-O2A
3	A	901	ADP	PB-O3A-PA-O2A

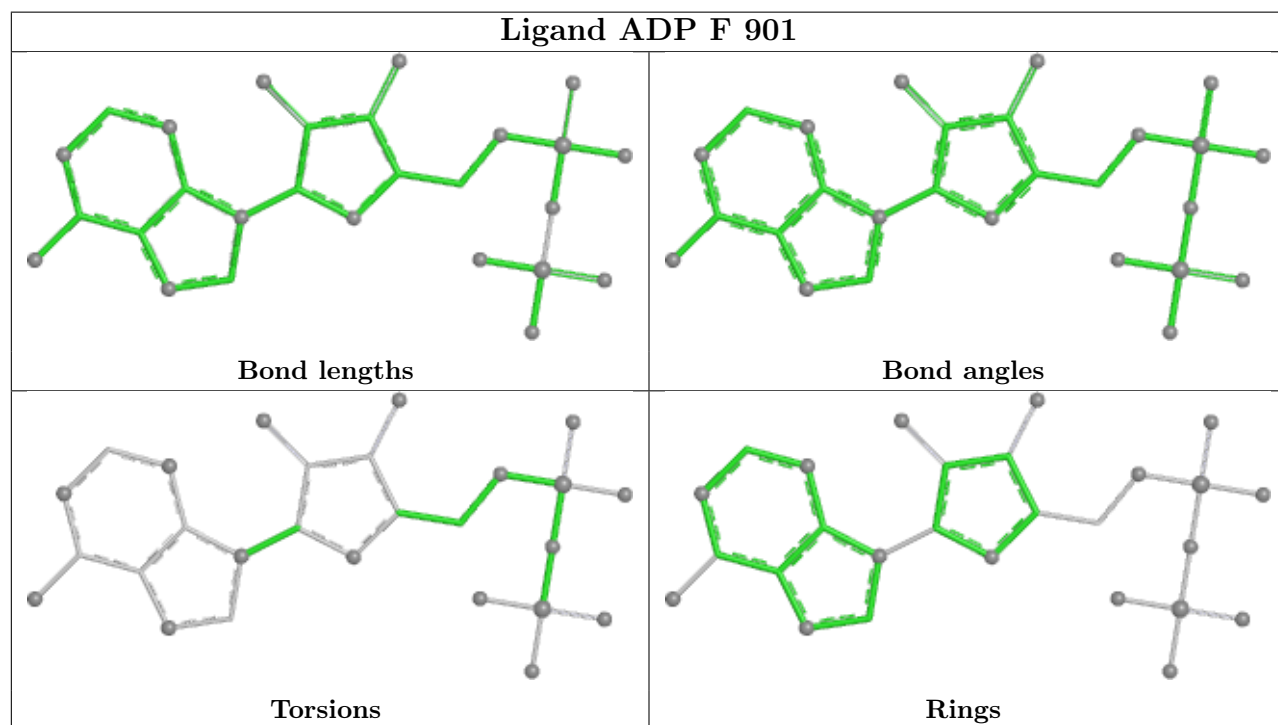
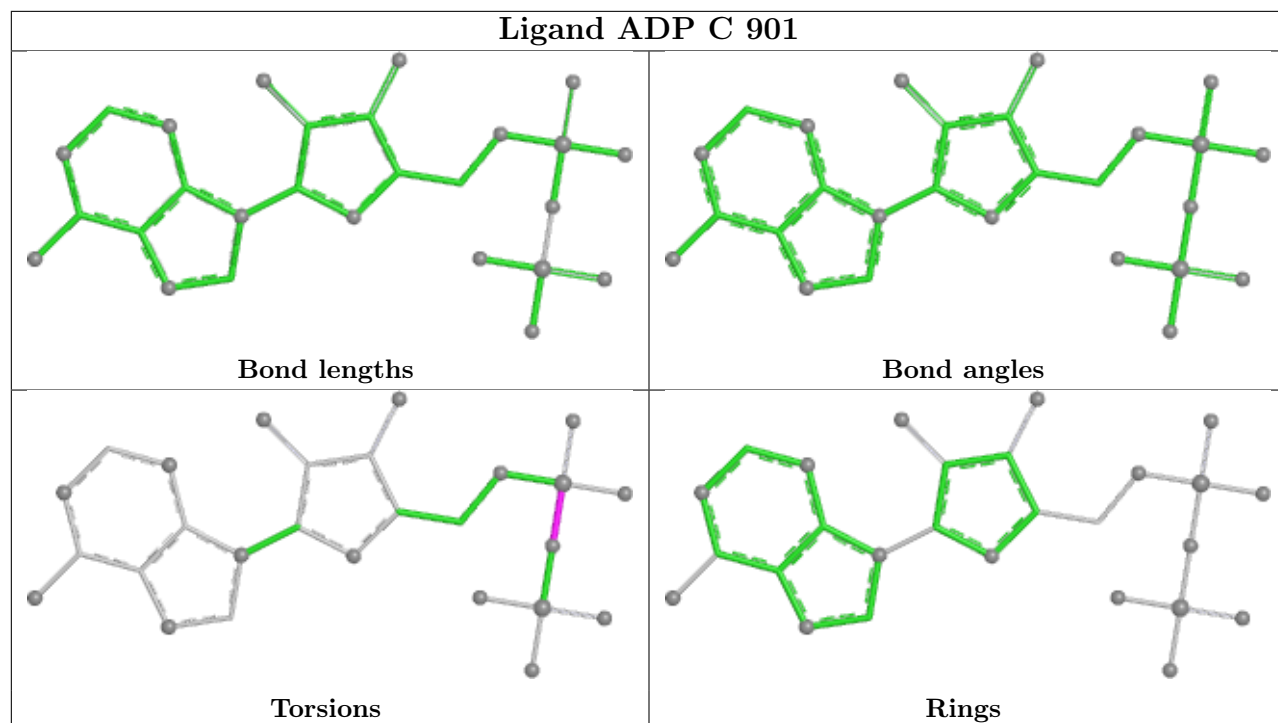
There are no ring outliers.

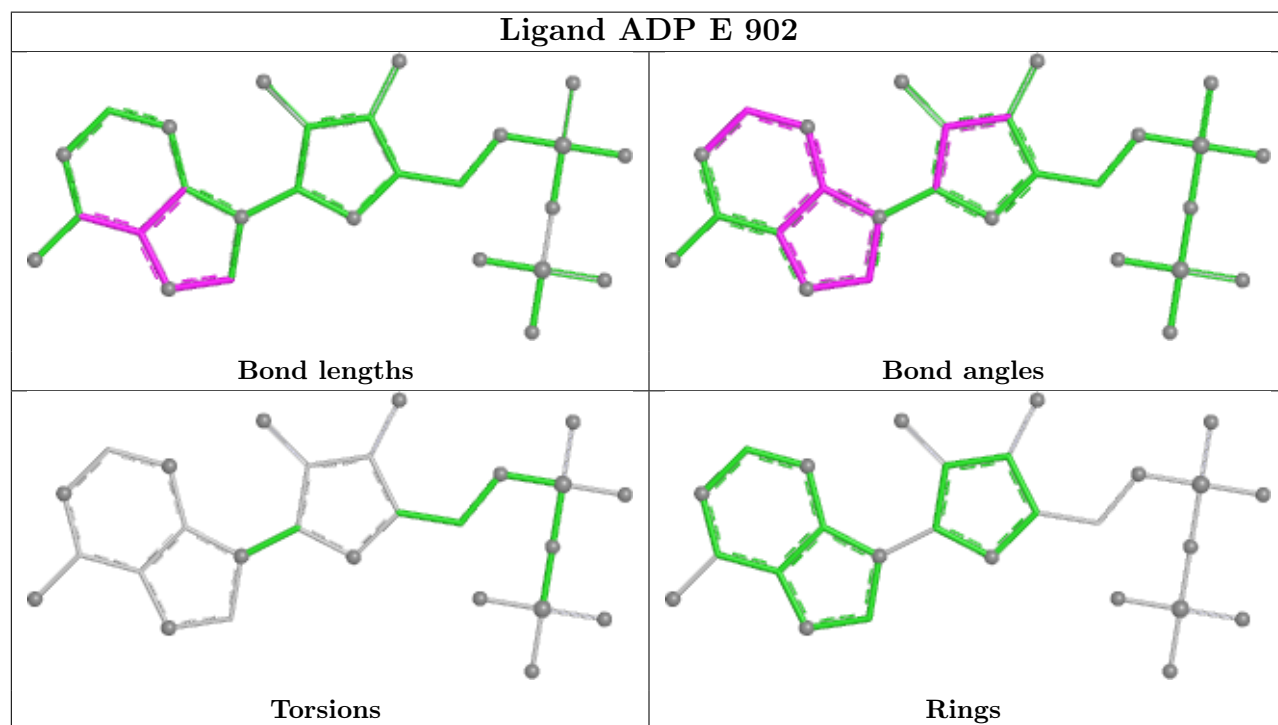
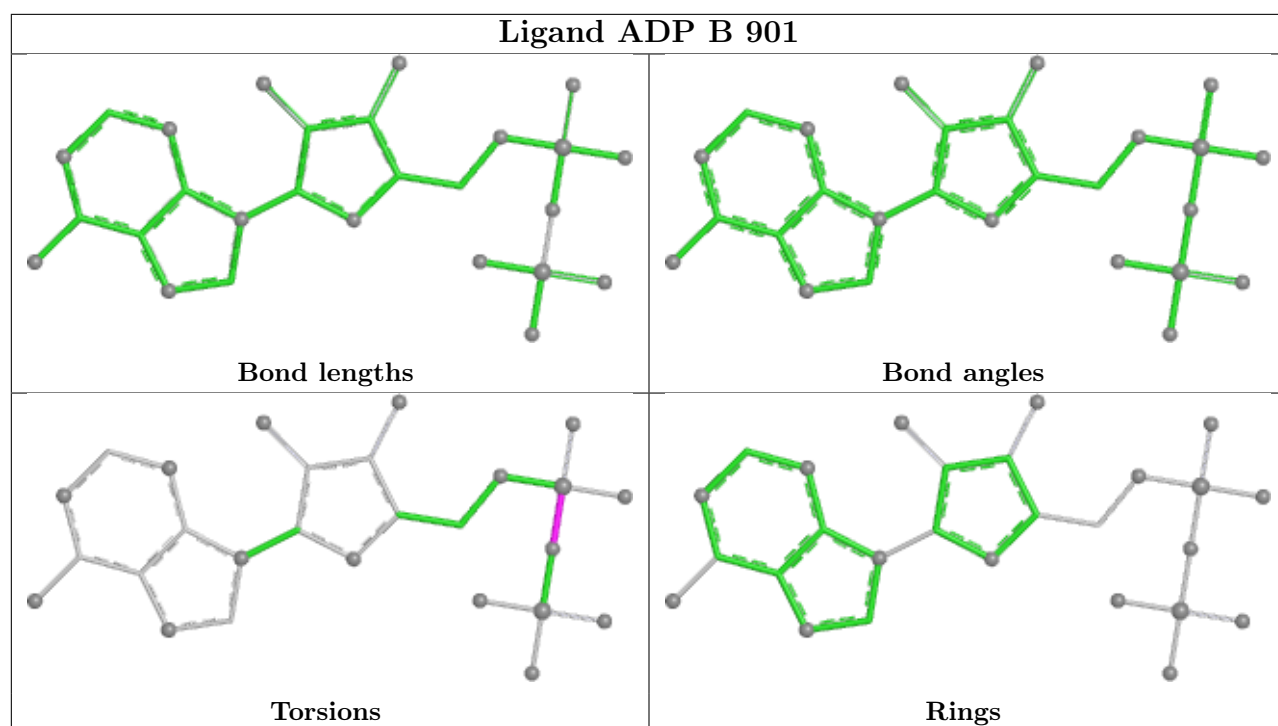
No monomer is involved in short contacts.

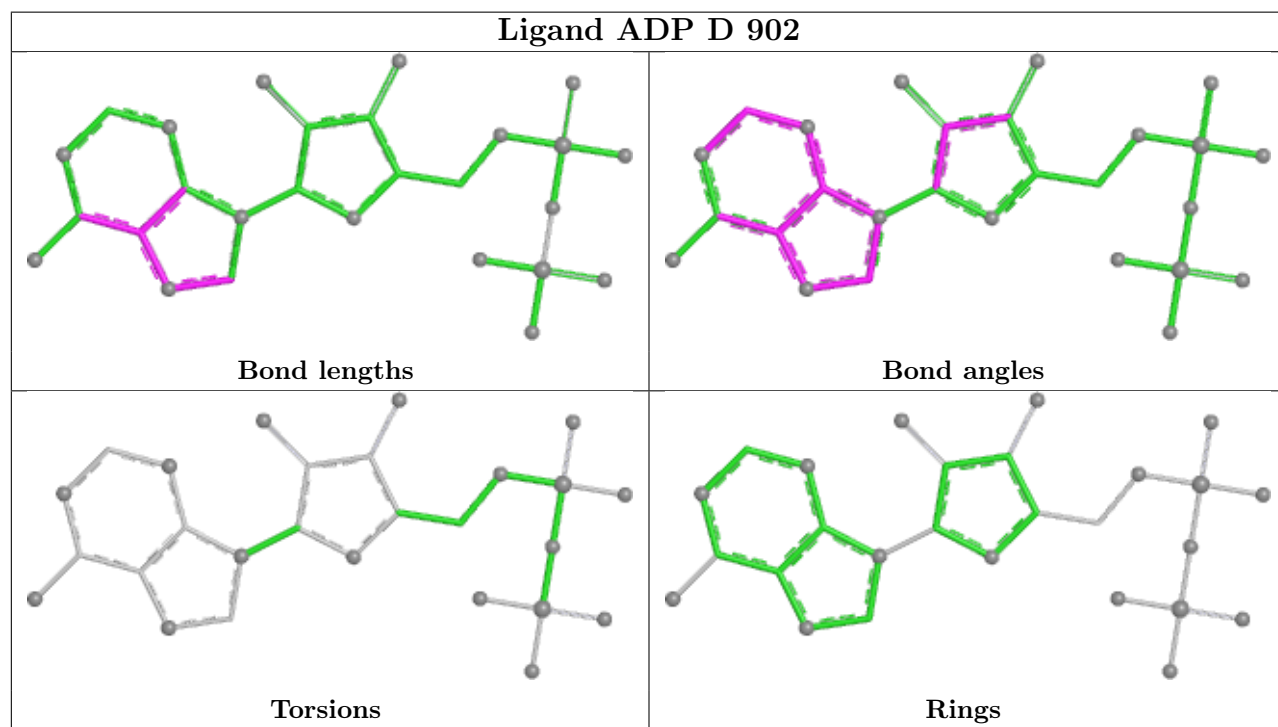
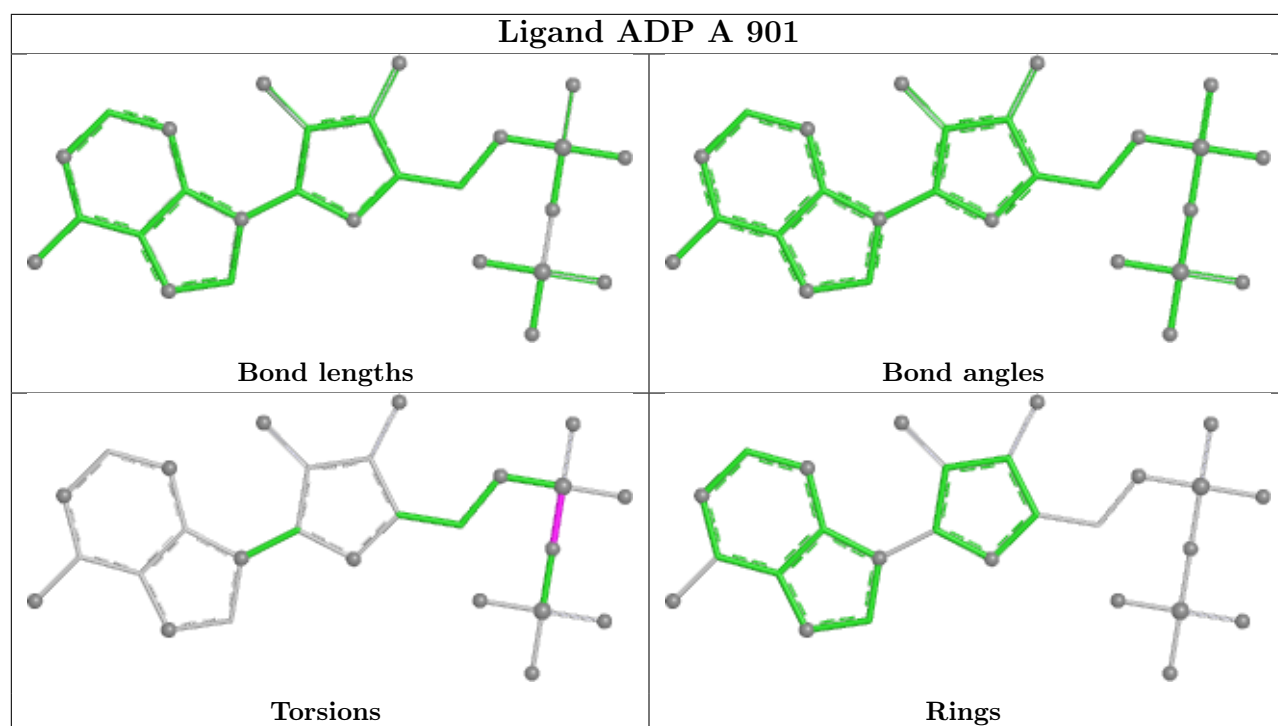
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

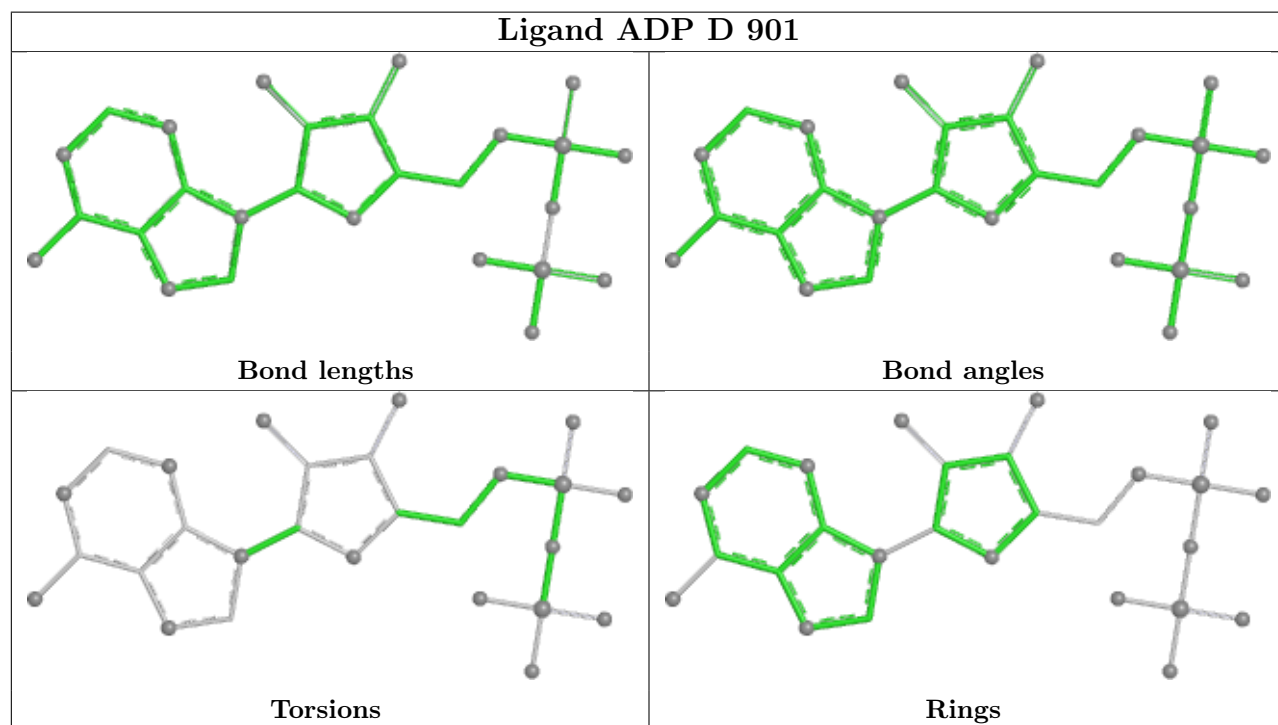
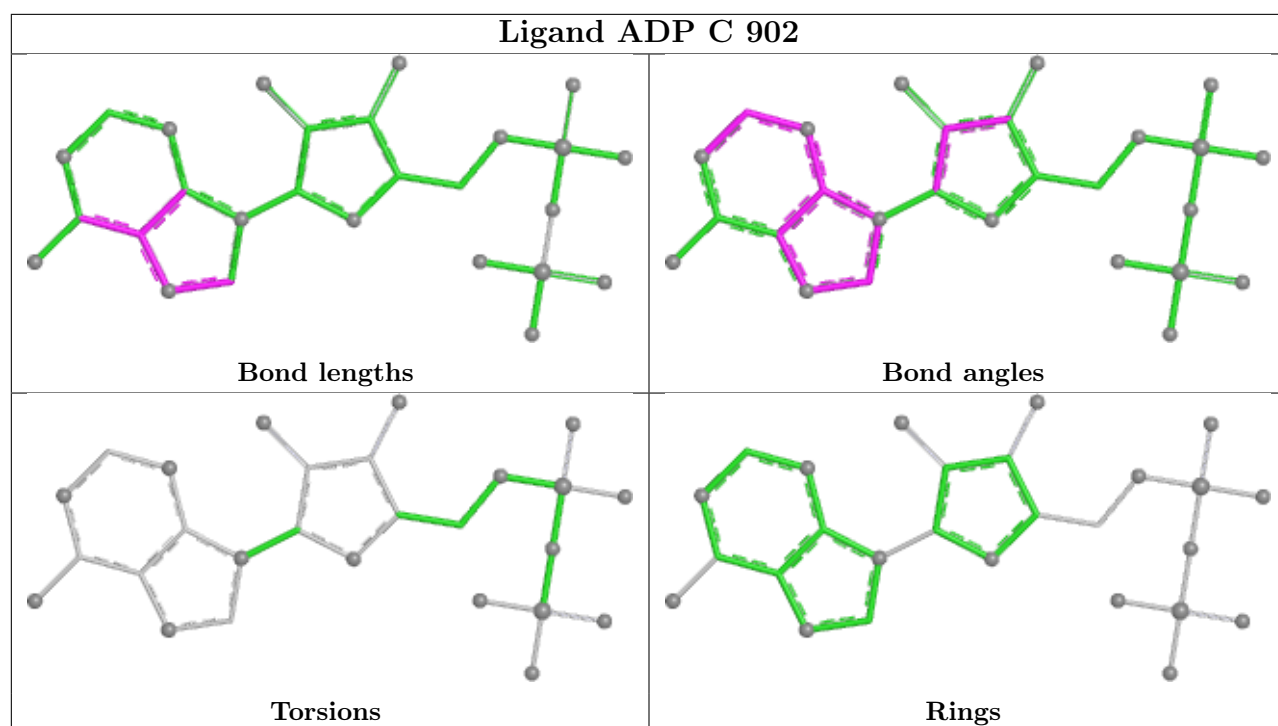


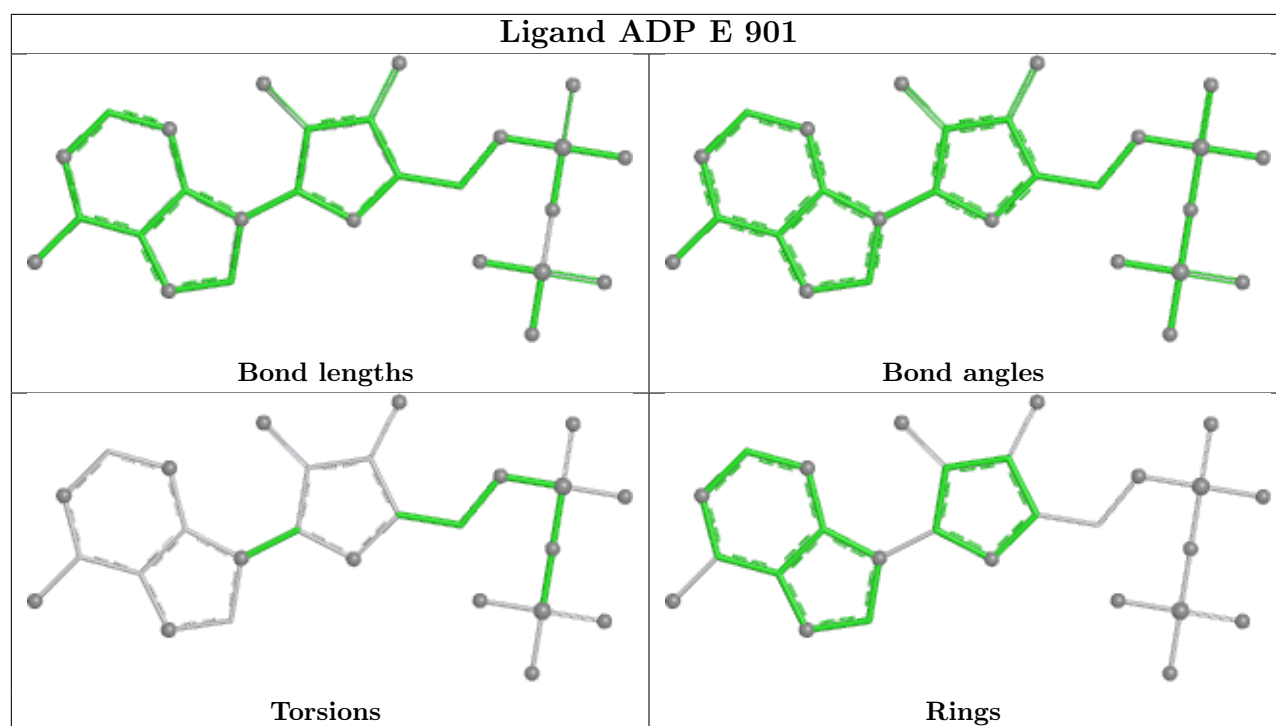












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

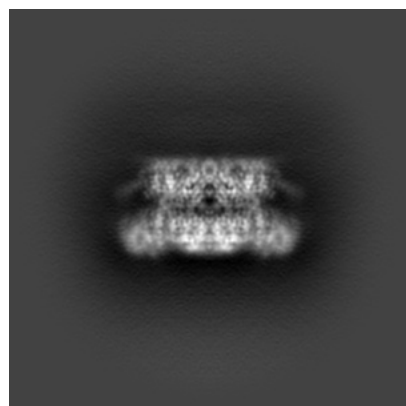
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28987. These allow visual inspection of the internal detail of the map and identification of artifacts.

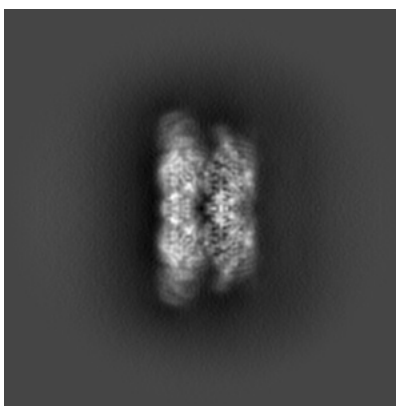
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

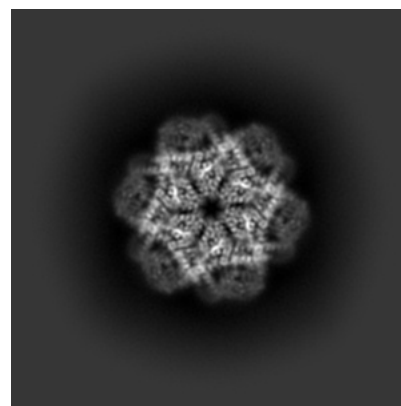
6.1.1 Primary map



X

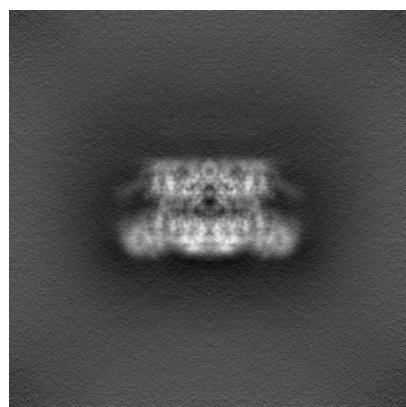


Y

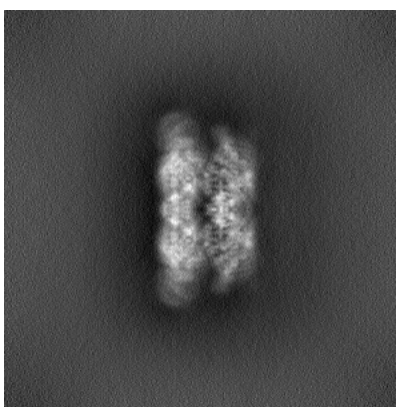


Z

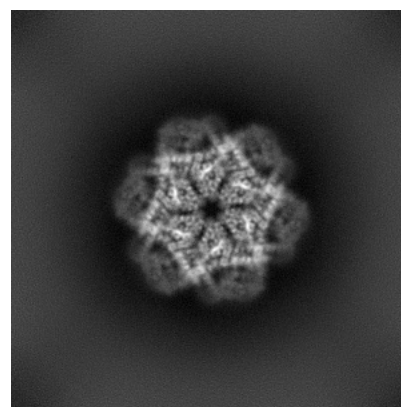
6.1.2 Raw map



X



Y

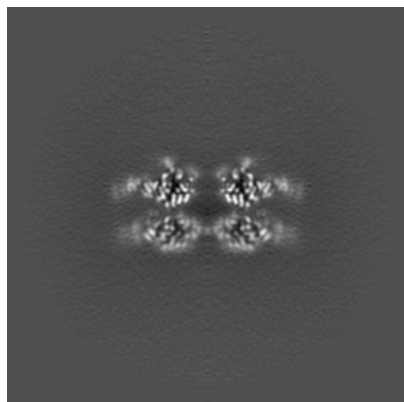


Z

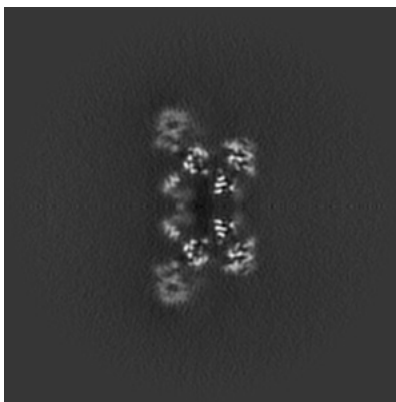
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

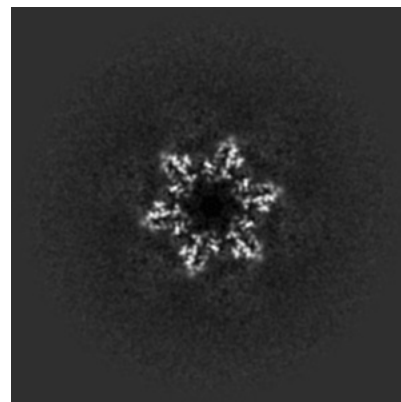
6.2.1 Primary map



X Index: 200

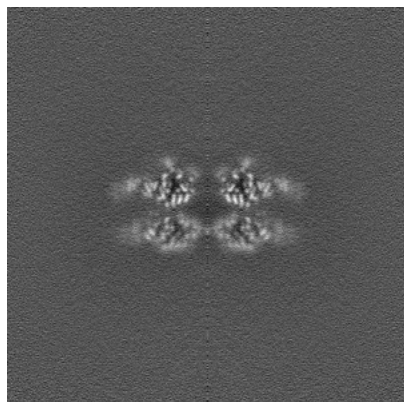


Y Index: 200

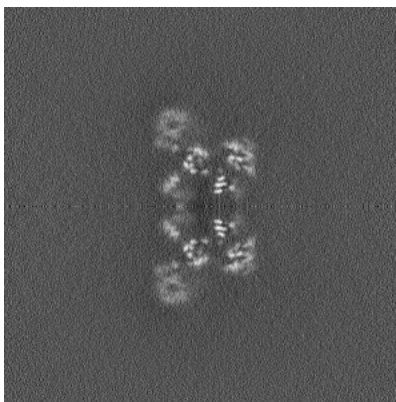


Z Index: 200

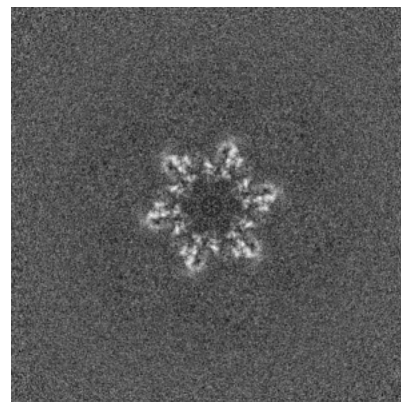
6.2.2 Raw map



X Index: 200



Y Index: 200

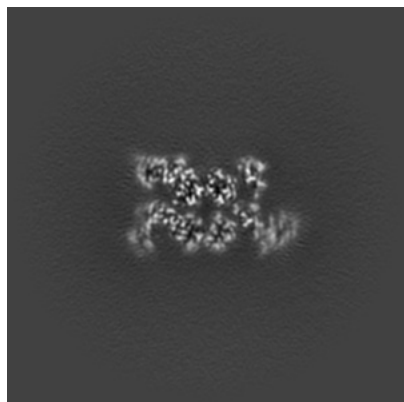


Z Index: 200

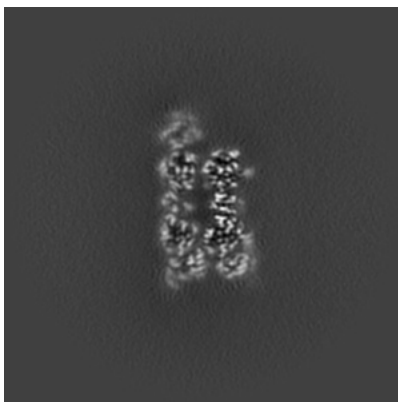
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

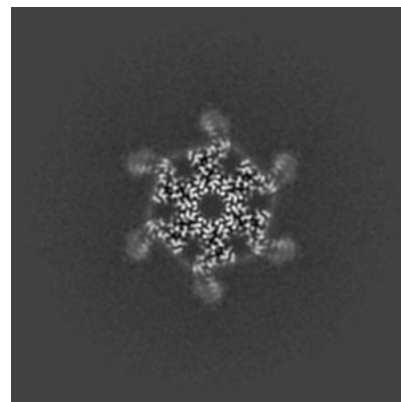
6.3.1 Primary map



X Index: 176

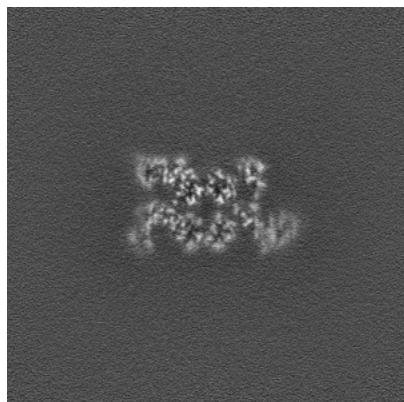


Y Index: 181

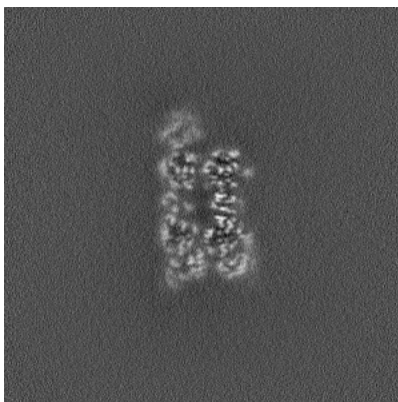


Z Index: 217

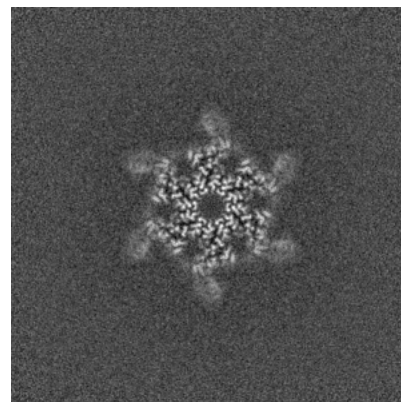
6.3.2 Raw map



X Index: 176



Y Index: 181

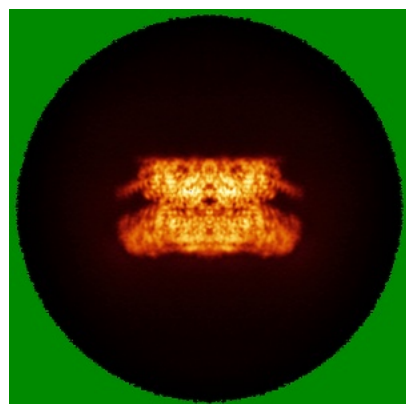


Z Index: 217

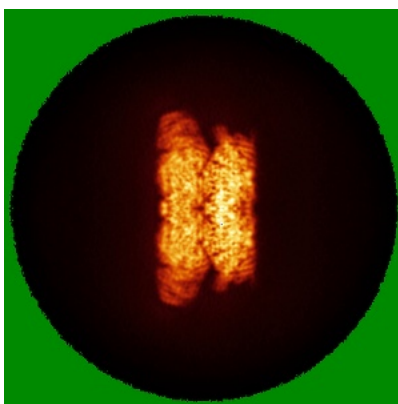
The images above show the largest variance slices of the map in three orthogonal directions.

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

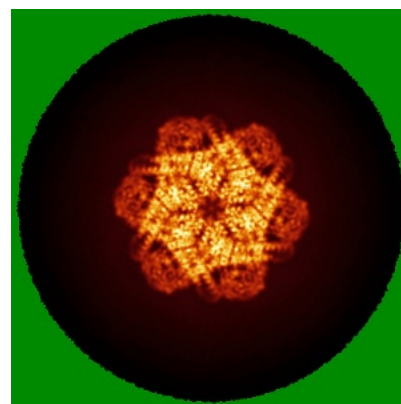
6.4.1 Primary map



X

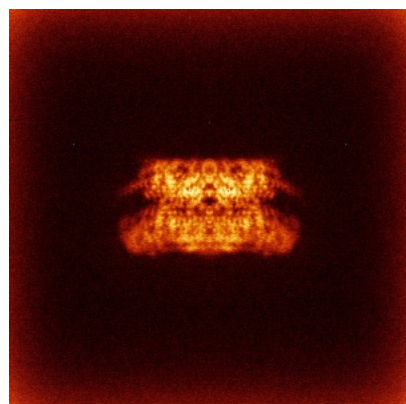


Y

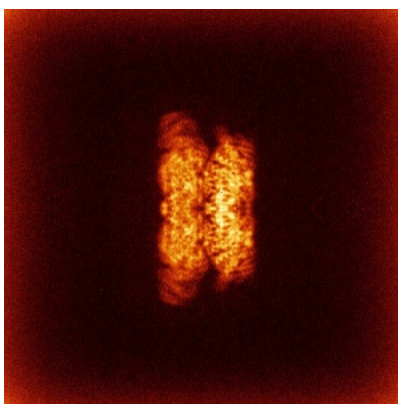


Z

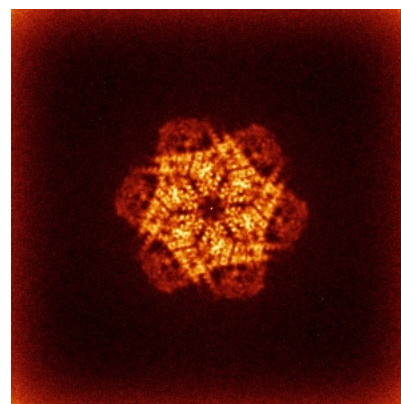
6.4.2 Raw map



X



Y

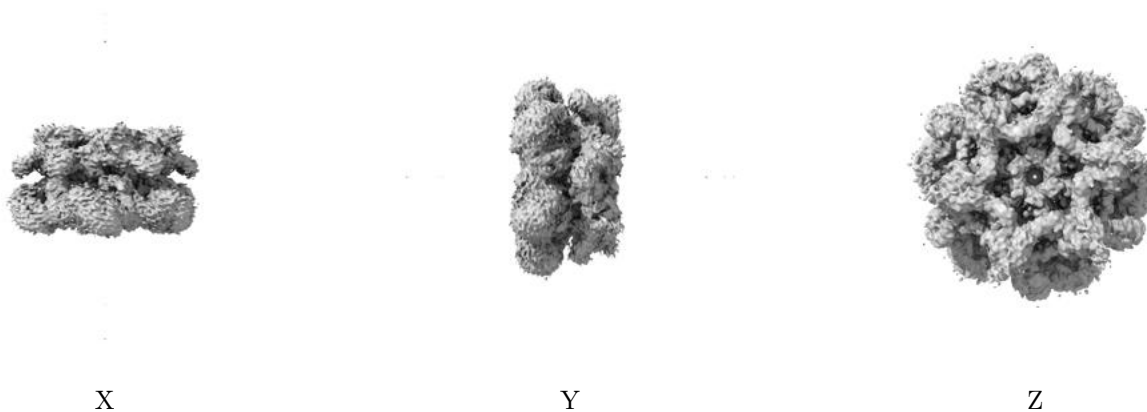


Z

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.

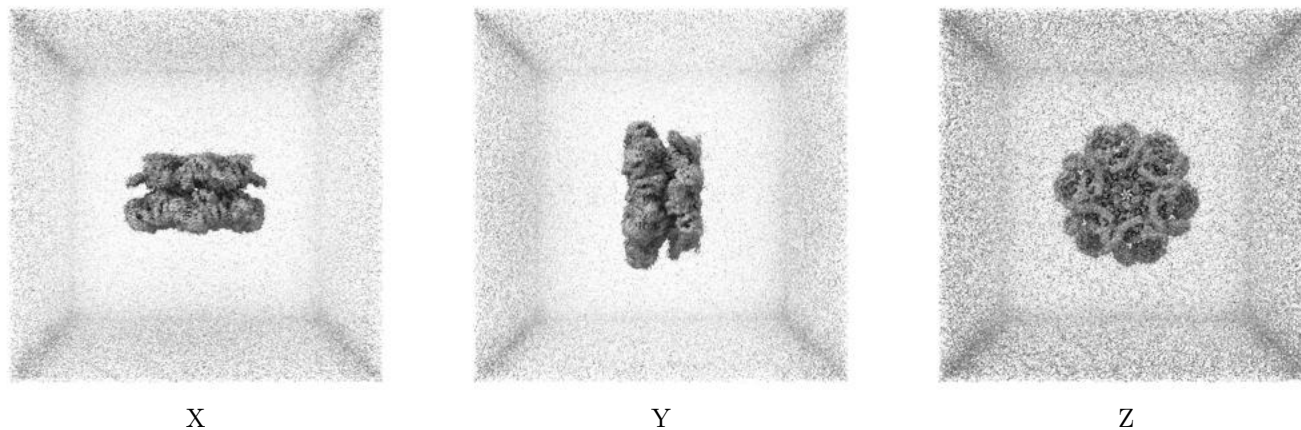
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

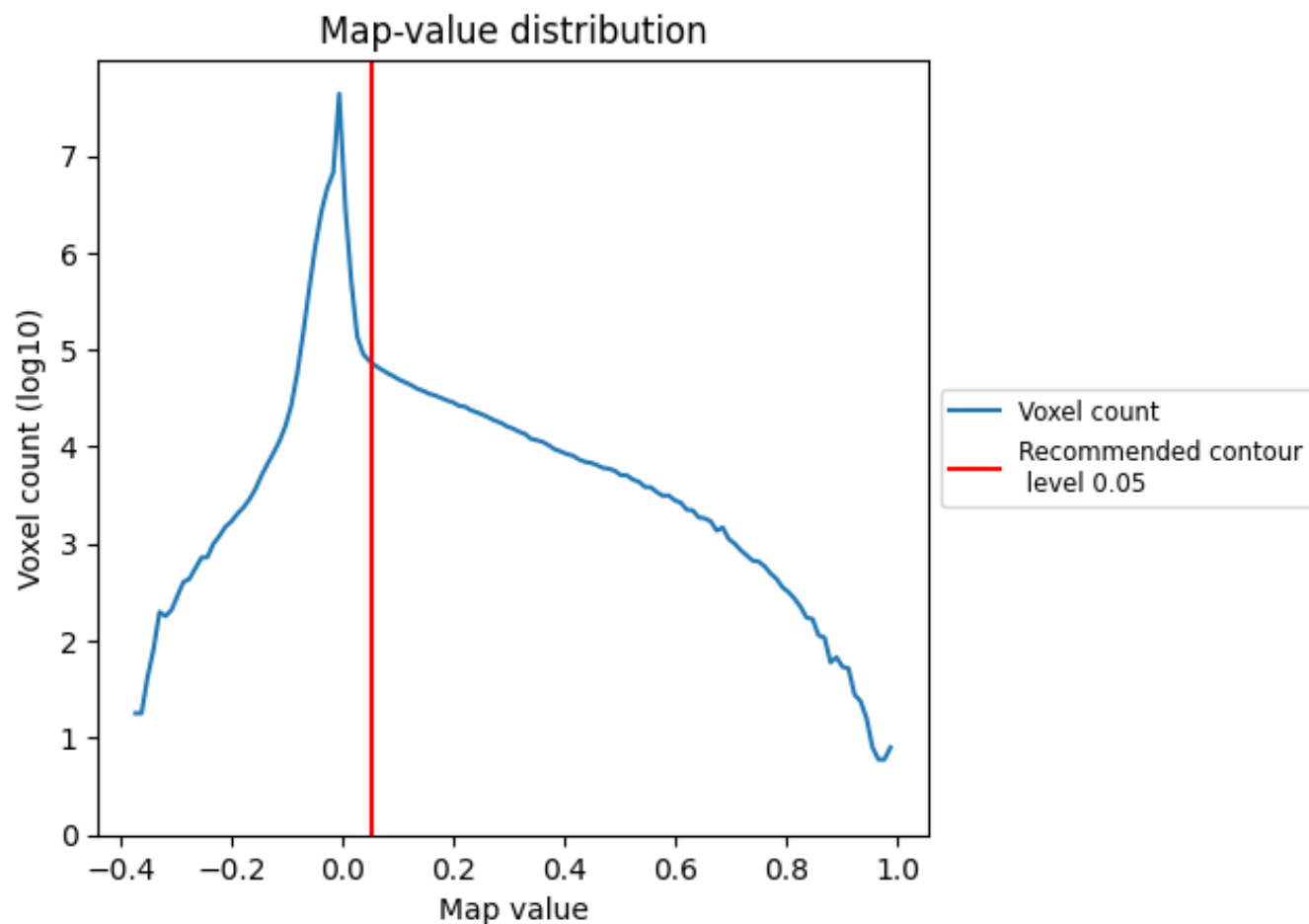
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

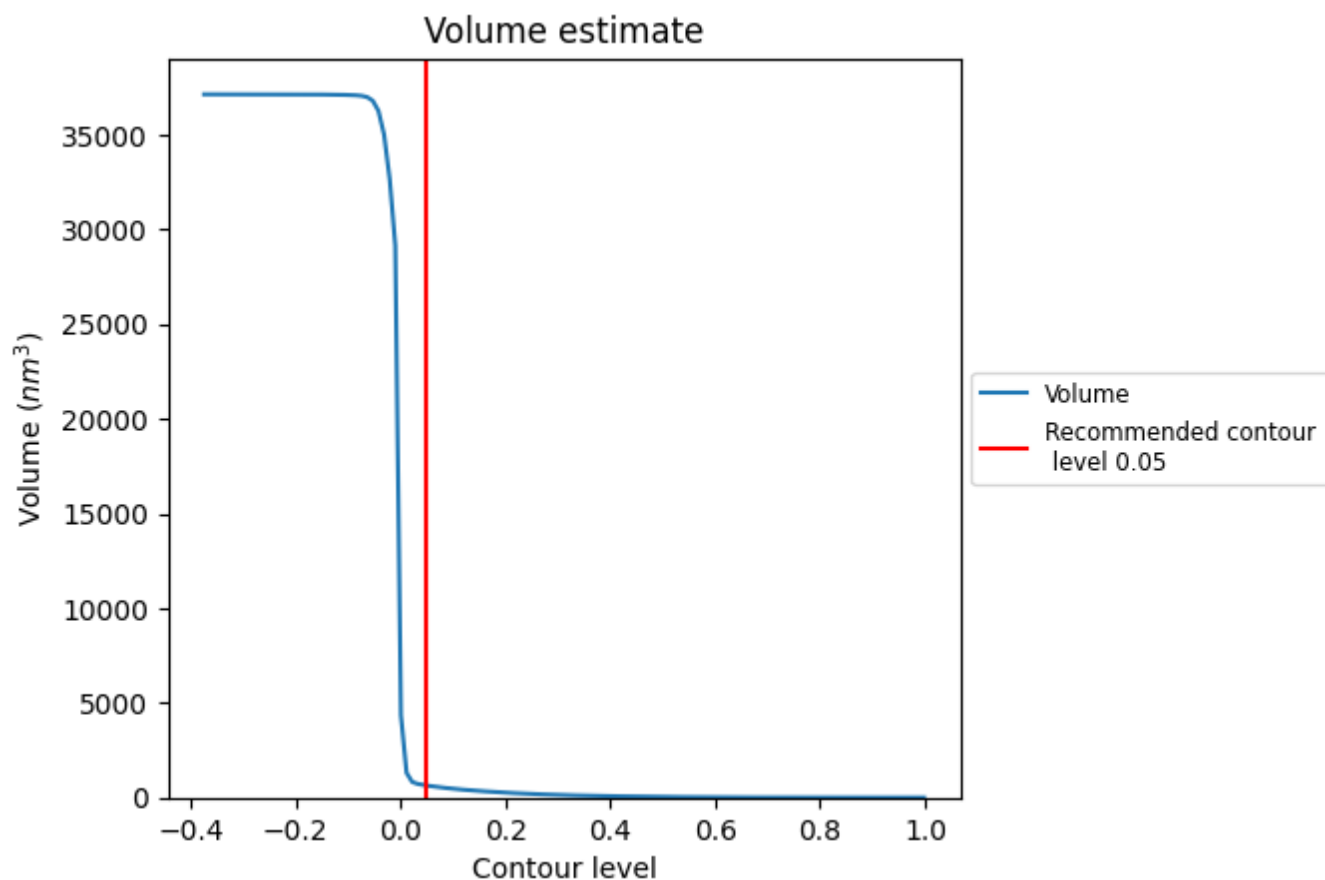
This section contains the results of statistical analysis of the map.

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.

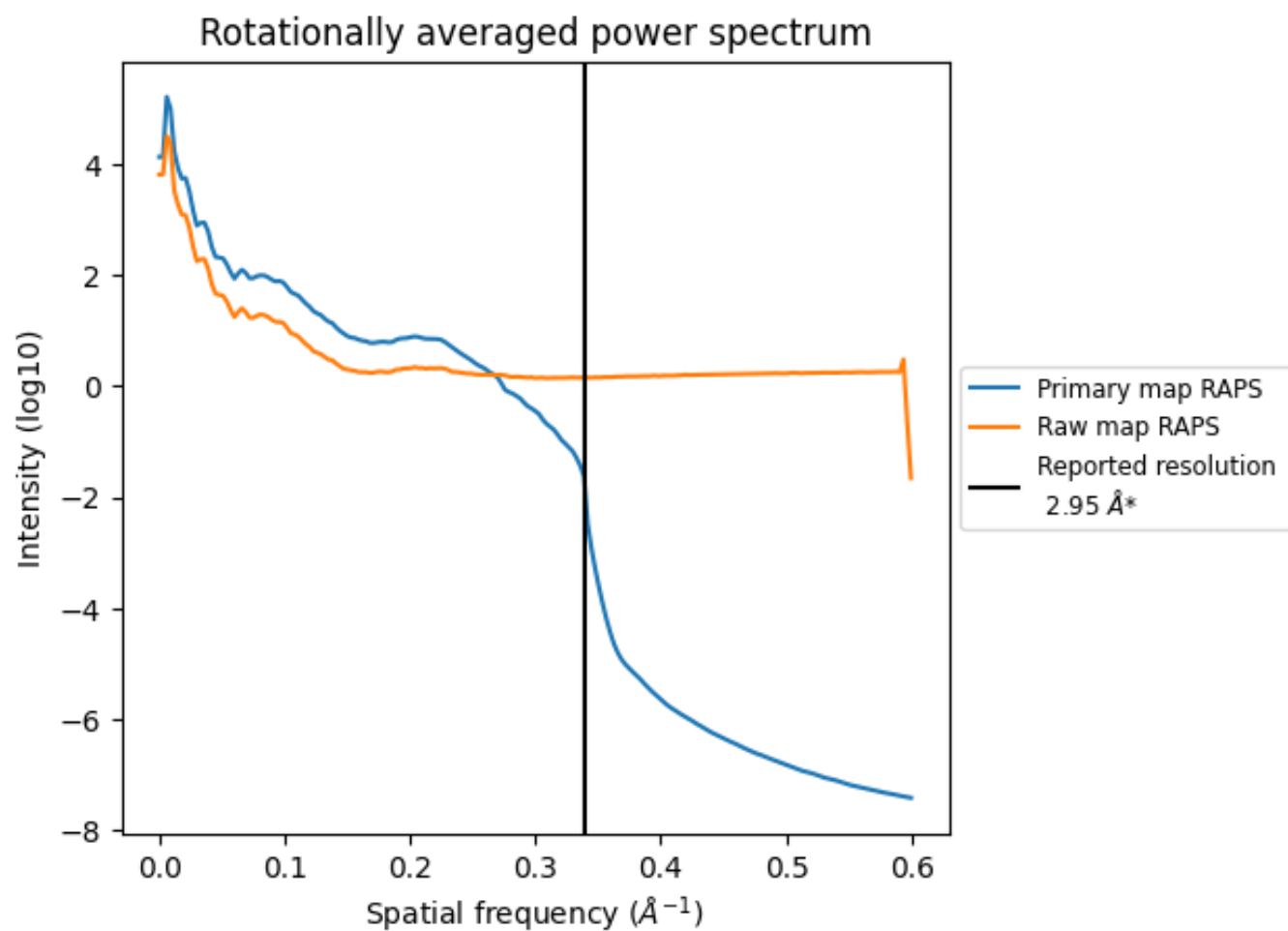
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm^3 ; this corresponds to an approximate mass of 576 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 ⓘ

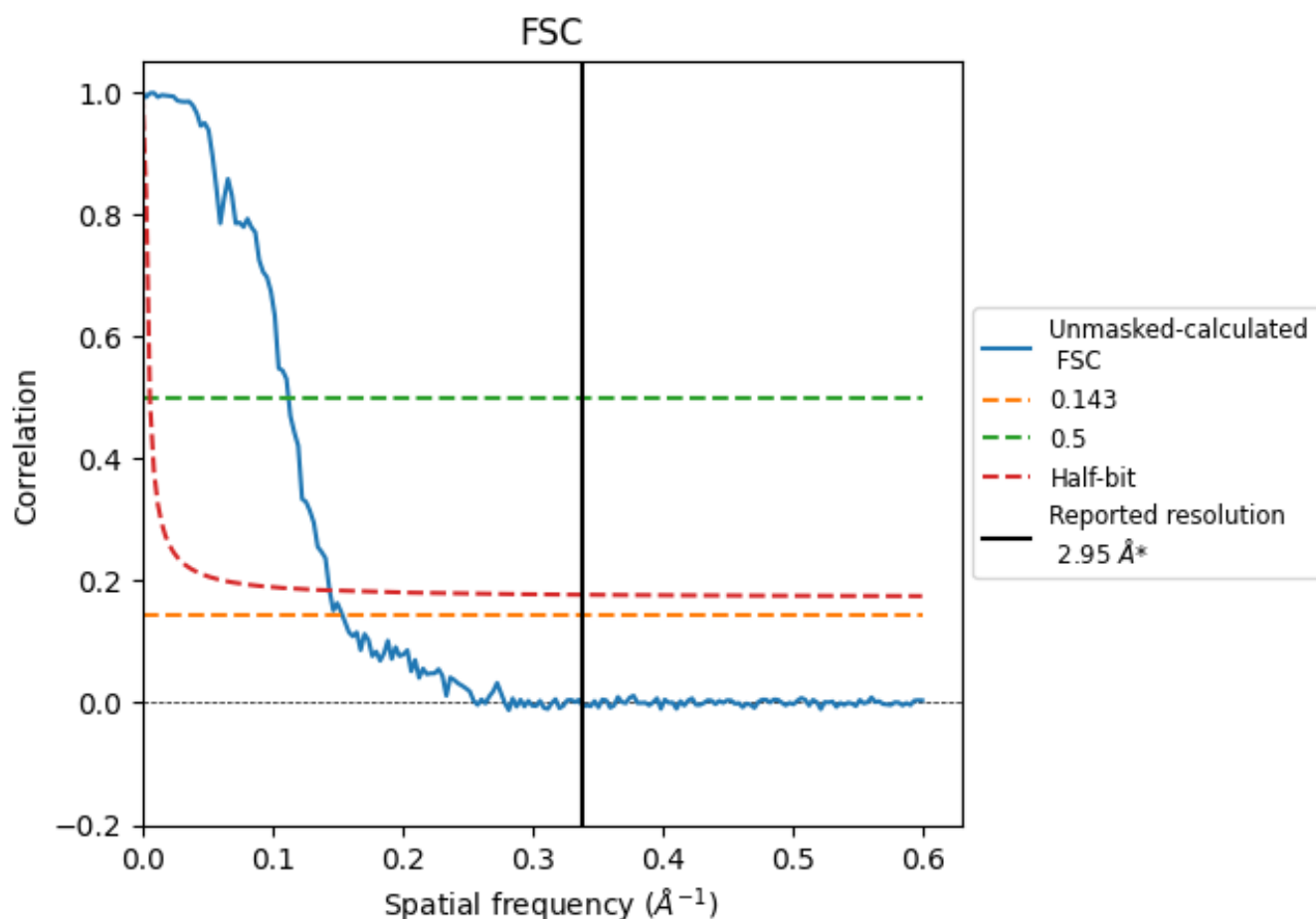


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

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 0.339 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.50	8.90	6.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.50 differs from the reported value 2.95 by more than 10 %

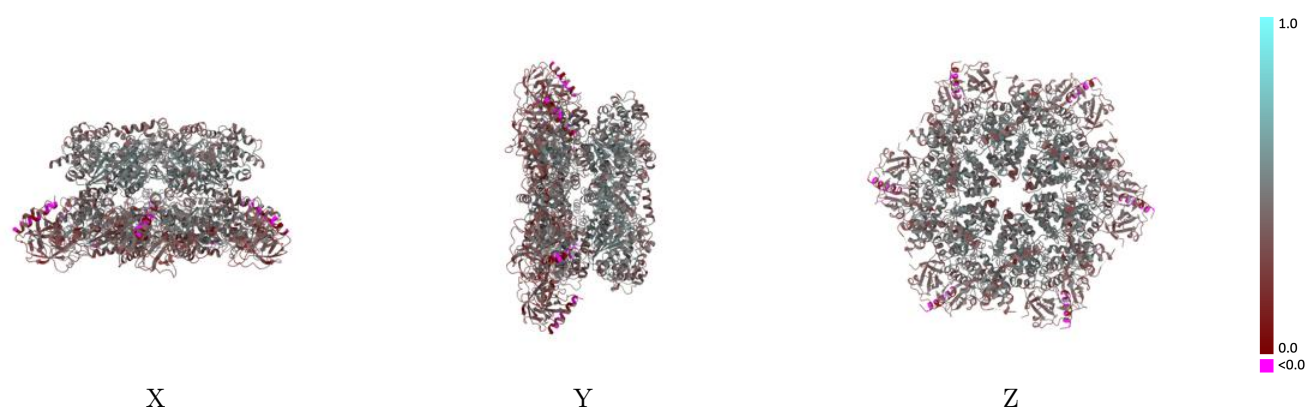
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28987 and PDB model 8FCN. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

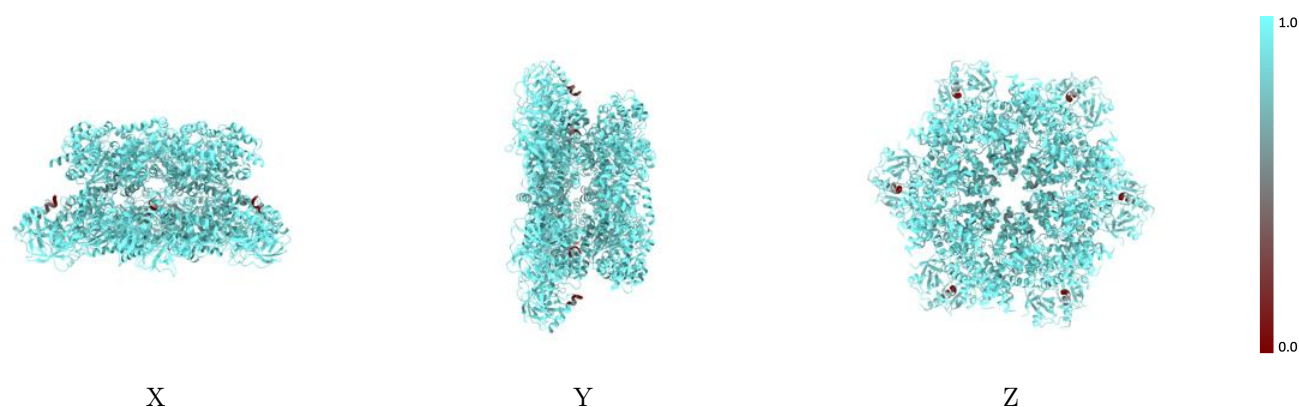
This section was not generated.

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



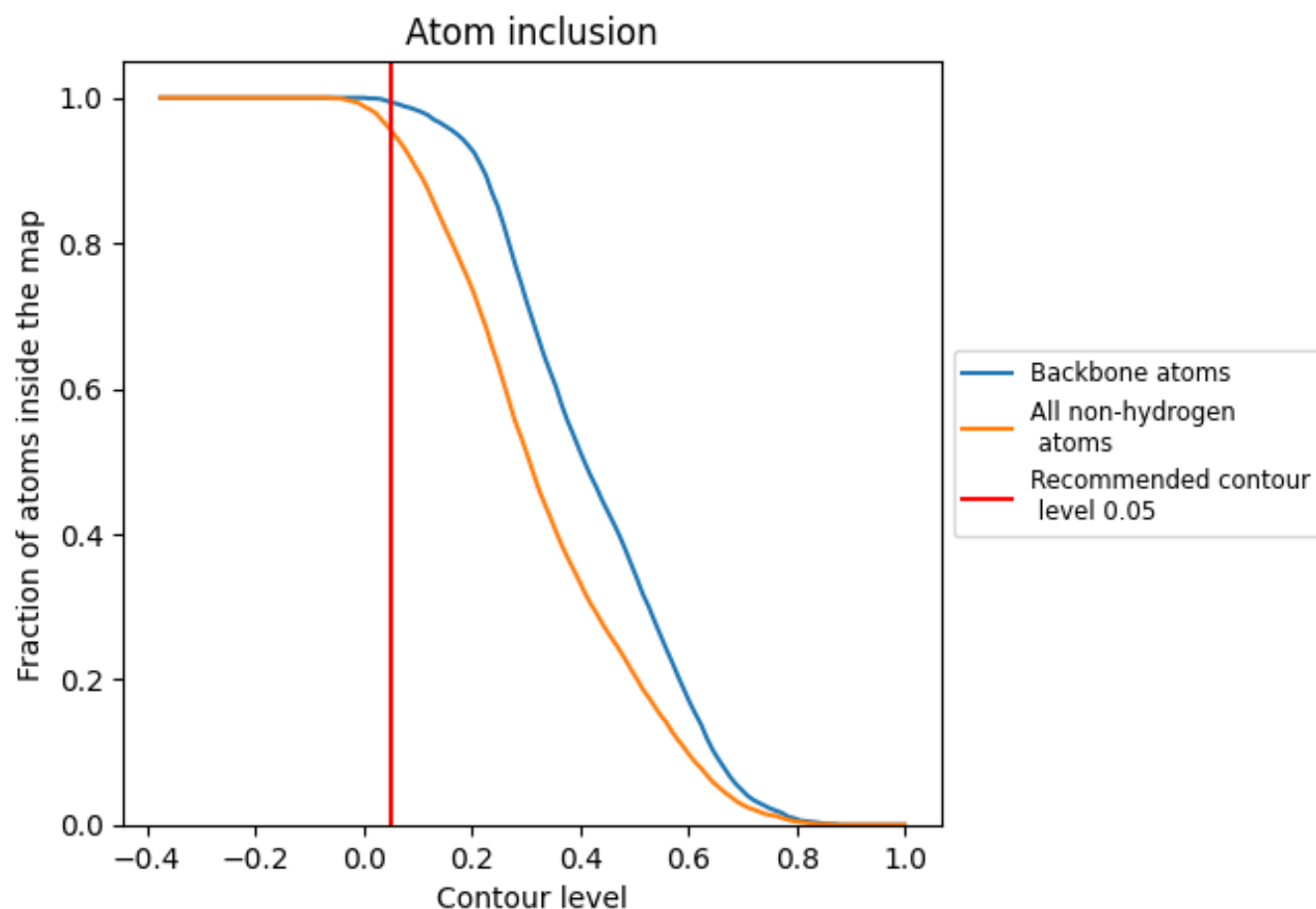
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.4050
A	0.9630	0.4130
B	0.9660	0.4130
C	0.9650	0.4130
D	0.9660	0.4120
E	0.9640	0.4120
F	0.9640	0.4120
G	0.6290	0.1180
H	0.6220	0.1130
I	0.6290	0.1150
J	0.6290	0.1200
K	0.6360	0.1180
L	0.6290	0.1290

1.0

0.0

<0.0