



## Full wwPDB EM Validation Report ⓘ

May 26, 2024 – 08:01 PM EDT

PDB ID : 7SWL  
EMDB ID : EMD-25474  
Title : CryoEM structure of the N-terminal-deleted Rix7 AAA-ATPase  
Authors : Kocaman, S.; Stanley, R.E.; Lo, Y.H.; Krahn, J.; Dandey, V.P.; Sobhany, M.; Petrovich, M.; Williams, J.G.; Deterding, L.J.; Borgnia, M.J.; Etigunta, S.  
Deposited on : 2021-11-20  
Resolution : 2.88 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>.

---

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

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

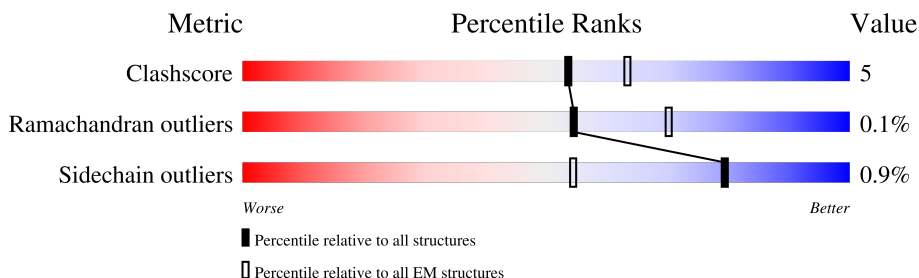
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.88 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	629	
1	B	629	
1	C	629	
1	D	629	
1	E	629	
1	F	629	
2	G	24	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23907 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 Rix7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	553	Total	C	N	O	S	0	0
			4238	2662	757	798	21		
1	B	551	Total	C	N	O	S	2	0
			4262	2674	766	801	21		
1	C	559	Total	C	N	O	S	2	0
			4320	2708	772	819	21		
1	D	555	Total	C	N	O	S	0	0
			4259	2672	761	805	21		
1	E	480	Total	C	N	O	S	0	0
			3652	2295	645	693	19		
1	F	348	Total	C	N	O	S	0	0
			2684	1689	477	506	12		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	MET	-	expression tag	UNP G0RZG1
A	186	ALA	-	expression tag	UNP G0RZG1
A	187	SER	-	expression tag	UNP G0RZG1
A	188	MET	-	expression tag	UNP G0RZG1
A	189	THR	-	expression tag	UNP G0RZG1
A	190	GLY	-	expression tag	UNP G0RZG1
A	191	GLY	-	expression tag	UNP G0RZG1
A	192	GLN	-	expression tag	UNP G0RZG1
A	193	GLN	-	expression tag	UNP G0RZG1
A	194	MET	-	expression tag	UNP G0RZG1
A	195	GLY	-	expression tag	UNP G0RZG1
A	196	ARG	-	expression tag	UNP G0RZG1
A	197	GLY	-	expression tag	UNP G0RZG1
A	198	SER	-	expression tag	UNP G0RZG1
A	199	MET	-	expression tag	UNP G0RZG1
A	303	GLN	GLU	conflict	UNP G0RZG1
A	602	GLN	GLU	conflict	UNP G0RZG1
A	803	ALA	-	expression tag	UNP G0RZG1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	804	ALA	-	expression tag	UNP G0RZG1
A	805	ALA	-	expression tag	UNP G0RZG1
A	806	LEU	-	expression tag	UNP G0RZG1
A	807	GLU	-	expression tag	UNP G0RZG1
A	808	HIS	-	expression tag	UNP G0RZG1
A	809	HIS	-	expression tag	UNP G0RZG1
A	810	HIS	-	expression tag	UNP G0RZG1
A	811	HIS	-	expression tag	UNP G0RZG1
A	812	HIS	-	expression tag	UNP G0RZG1
A	813	HIS	-	expression tag	UNP G0RZG1
B	185	MET	-	expression tag	UNP G0RZG1
B	186	ALA	-	expression tag	UNP G0RZG1
B	187	SER	-	expression tag	UNP G0RZG1
B	188	MET	-	expression tag	UNP G0RZG1
B	189	THR	-	expression tag	UNP G0RZG1
B	190	GLY	-	expression tag	UNP G0RZG1
B	191	GLY	-	expression tag	UNP G0RZG1
B	192	GLN	-	expression tag	UNP G0RZG1
B	193	GLN	-	expression tag	UNP G0RZG1
B	194	MET	-	expression tag	UNP G0RZG1
B	195	GLY	-	expression tag	UNP G0RZG1
B	196	ARG	-	expression tag	UNP G0RZG1
B	197	GLY	-	expression tag	UNP G0RZG1
B	198	SER	-	expression tag	UNP G0RZG1
B	199	MET	-	expression tag	UNP G0RZG1
B	303	GLN	GLU	conflict	UNP G0RZG1
B	602	GLN	GLU	conflict	UNP G0RZG1
B	803	ALA	-	expression tag	UNP G0RZG1
B	804	ALA	-	expression tag	UNP G0RZG1
B	805	ALA	-	expression tag	UNP G0RZG1
B	806	LEU	-	expression tag	UNP G0RZG1
B	807	GLU	-	expression tag	UNP G0RZG1
B	808	HIS	-	expression tag	UNP G0RZG1
B	809	HIS	-	expression tag	UNP G0RZG1
B	810	HIS	-	expression tag	UNP G0RZG1
B	811	HIS	-	expression tag	UNP G0RZG1
B	812	HIS	-	expression tag	UNP G0RZG1
B	813	HIS	-	expression tag	UNP G0RZG1
C	185	MET	-	expression tag	UNP G0RZG1
C	186	ALA	-	expression tag	UNP G0RZG1
C	187	SER	-	expression tag	UNP G0RZG1
C	188	MET	-	expression tag	UNP G0RZG1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	189	THR	-	expression tag	UNP G0RZG1
C	190	GLY	-	expression tag	UNP G0RZG1
C	191	GLY	-	expression tag	UNP G0RZG1
C	192	GLN	-	expression tag	UNP G0RZG1
C	193	GLN	-	expression tag	UNP G0RZG1
C	194	MET	-	expression tag	UNP G0RZG1
C	195	GLY	-	expression tag	UNP G0RZG1
C	196	ARG	-	expression tag	UNP G0RZG1
C	197	GLY	-	expression tag	UNP G0RZG1
C	198	SER	-	expression tag	UNP G0RZG1
C	199	MET	-	expression tag	UNP G0RZG1
C	303	GLN	GLU	conflict	UNP G0RZG1
C	602	GLN	GLU	conflict	UNP G0RZG1
C	803	ALA	-	expression tag	UNP G0RZG1
C	804	ALA	-	expression tag	UNP G0RZG1
C	805	ALA	-	expression tag	UNP G0RZG1
C	806	LEU	-	expression tag	UNP G0RZG1
C	807	GLU	-	expression tag	UNP G0RZG1
C	808	HIS	-	expression tag	UNP G0RZG1
C	809	HIS	-	expression tag	UNP G0RZG1
C	810	HIS	-	expression tag	UNP G0RZG1
C	811	HIS	-	expression tag	UNP G0RZG1
C	812	HIS	-	expression tag	UNP G0RZG1
C	813	HIS	-	expression tag	UNP G0RZG1
D	185	MET	-	expression tag	UNP G0RZG1
D	186	ALA	-	expression tag	UNP G0RZG1
D	187	SER	-	expression tag	UNP G0RZG1
D	188	MET	-	expression tag	UNP G0RZG1
D	189	THR	-	expression tag	UNP G0RZG1
D	190	GLY	-	expression tag	UNP G0RZG1
D	191	GLY	-	expression tag	UNP G0RZG1
D	192	GLN	-	expression tag	UNP G0RZG1
D	193	GLN	-	expression tag	UNP G0RZG1
D	194	MET	-	expression tag	UNP G0RZG1
D	195	GLY	-	expression tag	UNP G0RZG1
D	196	ARG	-	expression tag	UNP G0RZG1
D	197	GLY	-	expression tag	UNP G0RZG1
D	198	SER	-	expression tag	UNP G0RZG1
D	199	MET	-	expression tag	UNP G0RZG1
D	303	GLN	GLU	conflict	UNP G0RZG1
D	602	GLN	GLU	conflict	UNP G0RZG1
D	803	ALA	-	expression tag	UNP G0RZG1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	804	ALA	-	expression tag	UNP G0RZG1
D	805	ALA	-	expression tag	UNP G0RZG1
D	806	LEU	-	expression tag	UNP G0RZG1
D	807	GLU	-	expression tag	UNP G0RZG1
D	808	HIS	-	expression tag	UNP G0RZG1
D	809	HIS	-	expression tag	UNP G0RZG1
D	810	HIS	-	expression tag	UNP G0RZG1
D	811	HIS	-	expression tag	UNP G0RZG1
D	812	HIS	-	expression tag	UNP G0RZG1
D	813	HIS	-	expression tag	UNP G0RZG1
E	185	MET	-	expression tag	UNP G0RZG1
E	186	ALA	-	expression tag	UNP G0RZG1
E	187	SER	-	expression tag	UNP G0RZG1
E	188	MET	-	expression tag	UNP G0RZG1
E	189	THR	-	expression tag	UNP G0RZG1
E	190	GLY	-	expression tag	UNP G0RZG1
E	191	GLY	-	expression tag	UNP G0RZG1
E	192	GLN	-	expression tag	UNP G0RZG1
E	193	GLN	-	expression tag	UNP G0RZG1
E	194	MET	-	expression tag	UNP G0RZG1
E	195	GLY	-	expression tag	UNP G0RZG1
E	196	ARG	-	expression tag	UNP G0RZG1
E	197	GLY	-	expression tag	UNP G0RZG1
E	198	SER	-	expression tag	UNP G0RZG1
E	199	MET	-	expression tag	UNP G0RZG1
E	303	GLN	GLU	conflict	UNP G0RZG1
E	602	GLN	GLU	conflict	UNP G0RZG1
E	803	ALA	-	expression tag	UNP G0RZG1
E	804	ALA	-	expression tag	UNP G0RZG1
E	805	ALA	-	expression tag	UNP G0RZG1
E	806	LEU	-	expression tag	UNP G0RZG1
E	807	GLU	-	expression tag	UNP G0RZG1
E	808	HIS	-	expression tag	UNP G0RZG1
E	809	HIS	-	expression tag	UNP G0RZG1
E	810	HIS	-	expression tag	UNP G0RZG1
E	811	HIS	-	expression tag	UNP G0RZG1
E	812	HIS	-	expression tag	UNP G0RZG1
E	813	HIS	-	expression tag	UNP G0RZG1
F	185	MET	-	expression tag	UNP G0RZG1
F	186	ALA	-	expression tag	UNP G0RZG1
F	187	SER	-	expression tag	UNP G0RZG1
F	188	MET	-	expression tag	UNP G0RZG1

*Continued on next page...*

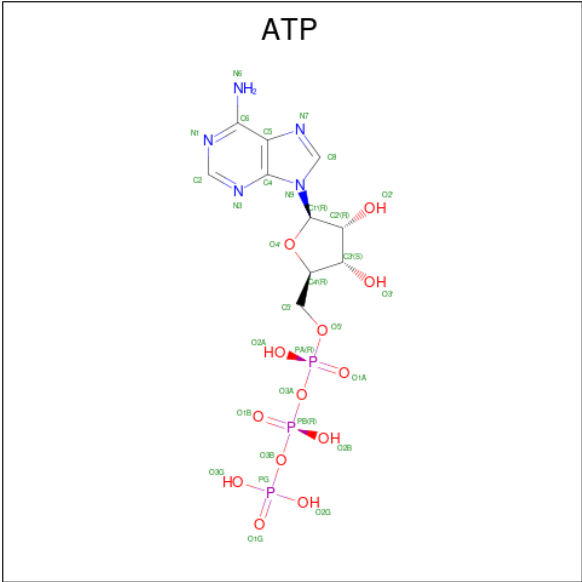
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	189	THR	-	expression tag	UNP G0RZG1
F	190	GLY	-	expression tag	UNP G0RZG1
F	191	GLY	-	expression tag	UNP G0RZG1
F	192	GLN	-	expression tag	UNP G0RZG1
F	193	GLN	-	expression tag	UNP G0RZG1
F	194	MET	-	expression tag	UNP G0RZG1
F	195	GLY	-	expression tag	UNP G0RZG1
F	196	ARG	-	expression tag	UNP G0RZG1
F	197	GLY	-	expression tag	UNP G0RZG1
F	198	SER	-	expression tag	UNP G0RZG1
F	199	MET	-	expression tag	UNP G0RZG1
F	303	GLN	GLU	conflict	UNP G0RZG1
F	602	GLN	GLU	conflict	UNP G0RZG1
F	803	ALA	-	expression tag	UNP G0RZG1
F	804	ALA	-	expression tag	UNP G0RZG1
F	805	ALA	-	expression tag	UNP G0RZG1
F	806	LEU	-	expression tag	UNP G0RZG1
F	807	GLU	-	expression tag	UNP G0RZG1
F	808	HIS	-	expression tag	UNP G0RZG1
F	809	HIS	-	expression tag	UNP G0RZG1
F	810	HIS	-	expression tag	UNP G0RZG1
F	811	HIS	-	expression tag	UNP G0RZG1
F	812	HIS	-	expression tag	UNP G0RZG1
F	813	HIS	-	expression tag	UNP G0RZG1

- Molecule 2 is a protein called polyleucine.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	24	Total	C	N	O	0	0
			177	129	24	24		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

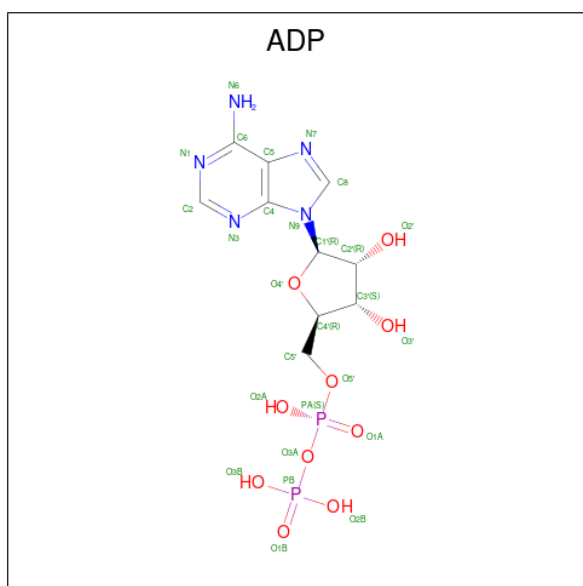
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total	Mg	0
			2	2	
4	D	2	Total	Mg	0
			2	2	
4	E	1	Total	Mg	0
			1	1	

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

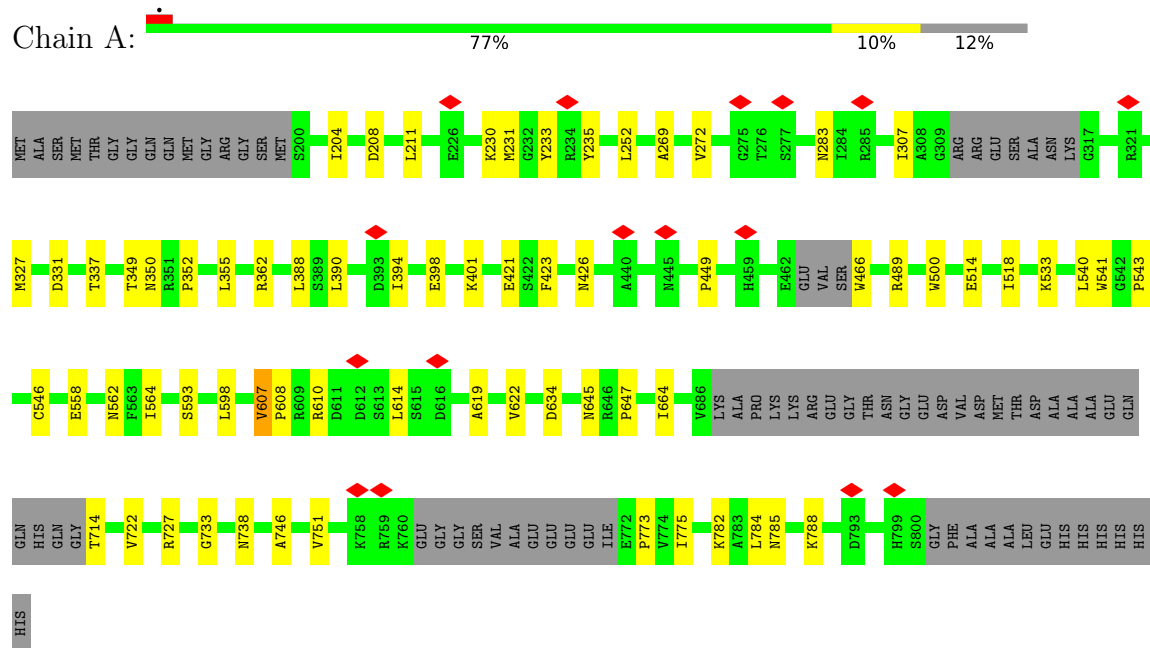


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

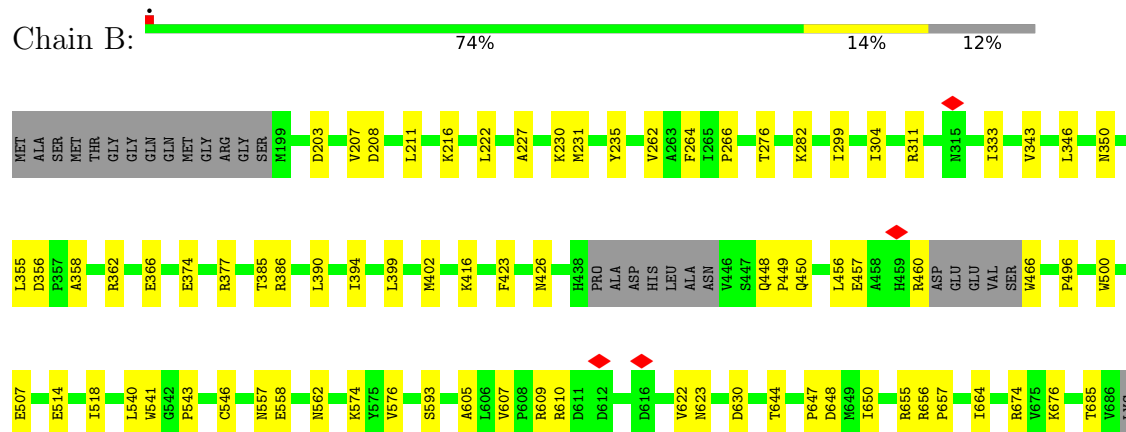
### 3 Residue-property plots [i](#)

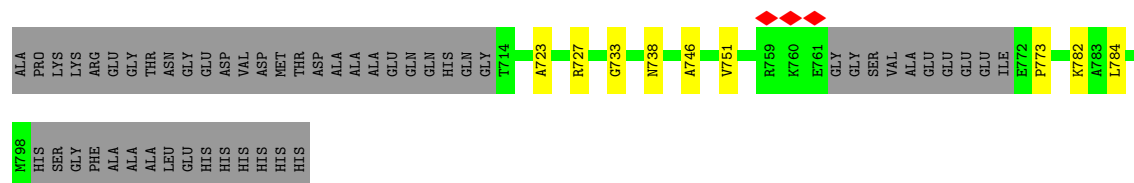
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Rix7



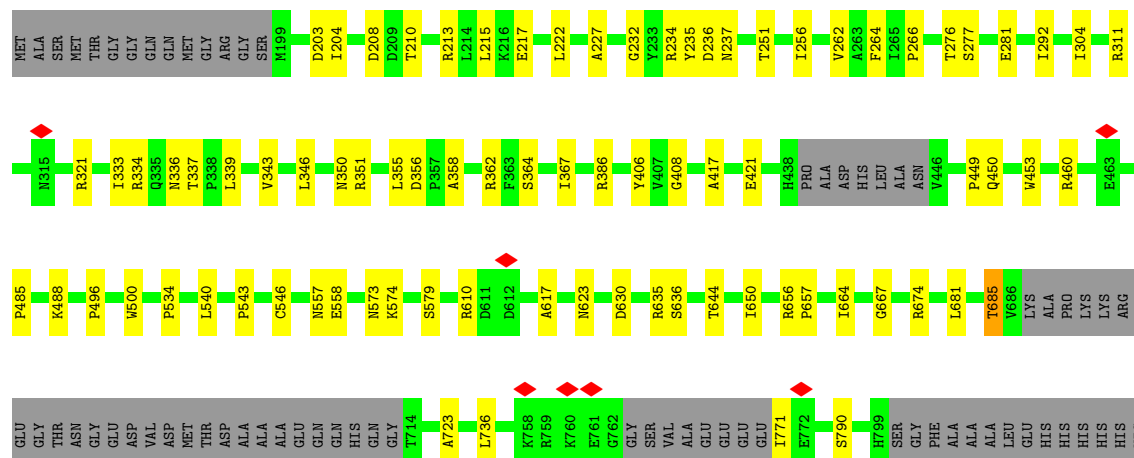
#### • Molecule 1: Rix7





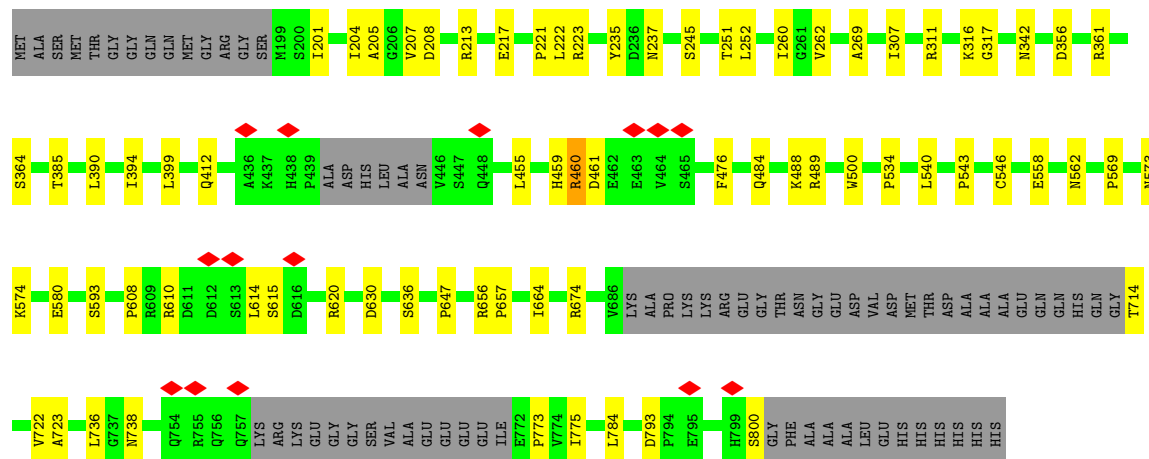
• Molecule 1: Rix7

Chain C: 76% 13% 11%



• Molecule 1: Rix7

Chain D: 77% 11% 12%



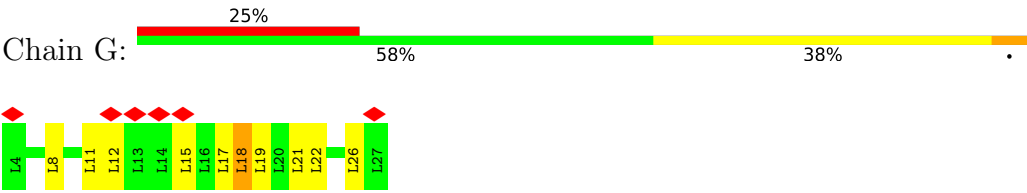
• Molecule 1: Rix7

Chain E: 6% 64% 13% 24%





● Molecule 2: polyleucine



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1200000	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.780	Depositor
Minimum map value	-3.134	Depositor
Average map value	0.049	Depositor
Map value standard deviation	0.336	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	132.867, 148.6845, 162.39299	wwPDB
Map dimensions	126, 141, 154	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0545, 1.0545, 1.0545	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0.24	0/4306	0.47	0/5820
1	B	0.25	0/4334	0.48	0/5850
1	C	0.25	0/4393	0.48	0/5932
1	D	0.25	0/4328	0.47	0/5851
1	E	0.24	0/3701	0.47	0/4995
1	F	0.23	0/2723	0.46	0/3675
2	G	0.21	0/176	0.48	0/241
All	All	0.24	0/23961	0.47	0/32364

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	4238	0	4290	45	0
1	B	4262	0	4343	62	0
1	C	4320	0	4389	55	0
1	D	4259	0	4312	48	0
1	E	3652	0	3725	46	0
1	F	2684	0	2724	40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	177	0	218	8	0
3	A	62	0	24	2	0
3	B	62	0	24	2	0
3	C	62	0	24	2	0
3	D	62	0	24	3	0
3	E	31	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	E	27	0	12	1	0
All	All	23907	0	24121	262	0

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

All (262) 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:C:674:ARG:NH1	1:C:723:ALA:O	2.22	0.72
1:C:232:GLY:HA2	1:C:339:LEU:HD21	1.74	0.69
1:C:203:ASP:OD1	1:C:386:ARG:NH2	2.27	0.67
1:D:311:ARG:NH1	1:D:356:ASP:OD2	2.29	0.66
1:D:674:ARG:NH1	1:D:723:ALA:O	2.29	0.66
1:B:450:GLN:NE2	1:C:204:ILE:O	2.29	0.65
1:F:523:ASN:HB3	1:F:526:LEU:HB3	1.78	0.65
1:F:487:SER:HB2	1:F:492:PHE:HB3	1.79	0.64
1:D:390:LEU:HB3	1:D:394:ILE:HD12	1.79	0.64
3:B:902:ATP:O3'	1:C:334:ARG:NH2	2.32	0.63
1:E:644:THR:HG21	1:E:650:ILE:HD11	1.80	0.63
1:B:674:ARG:NH1	1:B:723:ALA:O	2.31	0.62
1:B:358:ALA:O	1:B:362:ARG:NH1	2.32	0.62
1:B:426:ASN:HB3	1:B:466:TRP:HD1	1.64	0.62
1:D:562:ASN:ND2	1:D:593:SER:O	2.33	0.62
1:B:423:PHE:HA	1:B:426:ASN:HD22	1.65	0.61
1:B:311:ARG:NH1	1:B:356:ASP:OD2	2.33	0.61
1:A:204:ILE:HG12	1:A:252:LEU:HD13	1.82	0.61
1:C:234:ARG:NH2	1:C:337:THR:O	2.28	0.61
1:A:489:ARG:NH1	1:B:366:GLU:OE2	2.33	0.61
1:C:610:ARG:NH1	1:C:623:ASN:OD1	2.34	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:GLN:HE21	1:F:488:LYS:HG3	1.66	0.61
1:E:656:ARG:NH1	1:E:657:PRO:O	2.33	0.60
1:E:550:LEU:HD22	5:E:901:ADP:H2'	1.82	0.60
1:D:630:ASP:OD2	1:D:656:ARG:NH2	2.32	0.60
1:D:213:ARG:NH2	1:D:217:GLU:OE2	2.34	0.60
1:D:656:ARG:NH1	1:D:657:PRO:O	2.33	0.60
1:B:203:ASP:OD1	1:B:386:ARG:NH2	2.33	0.60
1:D:459:HIS:O	1:D:461:ASP:N	2.35	0.59
1:A:390:LEU:HB3	1:A:394:ILE:HD12	1.84	0.59
1:C:256:ILE:HD11	1:C:346:LEU:HD11	1.84	0.59
1:F:647:PRO:O	1:F:655:ARG:NH1	2.35	0.59
1:C:311:ARG:NH1	1:C:356:ASP:OD2	2.34	0.59
3:A:902:ATP:O1G	1:B:362:ARG:NH2	2.36	0.58
1:E:213:ARG:NH2	1:E:217:GLU:OE2	2.36	0.58
1:A:398:GLU:HA	1:A:401:LYS:HE2	1.85	0.58
1:A:272:VAL:O	1:A:283:ASN:ND2	2.33	0.58
1:A:610:ARG:HA	1:A:614:LEU:HD22	1.85	0.58
1:A:349:THR:HG21	1:A:355:LEU:HD11	1.84	0.58
1:B:416:LYS:NZ	1:C:236:ASP:O	2.37	0.57
1:D:385:THR:HB	1:D:390:LEU:HD11	1.84	0.57
1:B:390:LEU:HB3	1:B:394:ILE:HD12	1.87	0.57
1:A:423:PHE:HA	1:A:426:ASN:HD22	1.69	0.57
1:A:211:LEU:HD21	1:A:252:LEU:HD11	1.87	0.57
1:C:656:ARG:NH1	1:C:657:PRO:O	2.37	0.57
1:D:773:PRO:HD2	1:E:529:ARG:HH11	1.71	0.56
1:A:533:LYS:HG2	1:A:634:ASP:HB3	1.86	0.56
1:C:358:ALA:O	1:C:362:ARG:NH1	2.37	0.56
1:A:449:PRO:HG2	1:B:208:ASP:HB3	1.87	0.56
1:D:460:ARG:NH2	1:E:258:GLY:O	2.38	0.56
1:F:385:THR:HG22	1:F:388:LEU:HD12	1.88	0.55
1:C:630:ASP:OD2	1:C:656:ARG:NH2	2.35	0.55
1:B:727:ARG:HE	1:B:784:LEU:HB3	1.71	0.55
1:F:472:THR:HG22	1:F:474:GLU:H	1.71	0.55
1:F:656:ARG:NH1	1:F:657:PRO:O	2.40	0.55
1:E:590:ALA:HB2	1:E:598:LEU:HD21	1.90	0.54
1:C:574:LYS:HE2	2:G:21:LEU:HD22	1.89	0.54
1:D:237:ASN:OD1	1:D:364:SER:OG	2.26	0.54
1:F:399:LEU:H	1:F:399:LEU:HD23	1.72	0.54
1:C:406:TYR:CE1	1:C:485:PRO:HG3	2.43	0.54
1:D:647:PRO:HG2	1:D:800:SER:HB3	1.90	0.54
1:B:751:VAL:HG21	1:B:773:PRO:HB3	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ALA:HB1	1:E:307:ILE:HG23	1.90	0.53
1:D:222:LEU:HD13	1:D:262:VAL:HG21	1.89	0.53
1:A:230:LYS:HD3	1:F:468:SER:HB3	1.89	0.53
1:F:377:ARG:NH2	1:F:400:ALA:O	2.34	0.53
1:D:580:GLU:OE2	1:D:620:ARG:NH1	2.39	0.53
1:E:573:ASN:OD1	1:E:574:LYS:N	2.42	0.52
1:D:738:ASN:HB2	1:E:657:PRO:HB3	1.90	0.52
1:B:304:ILE:HG23	1:B:355:LEU:HD21	1.92	0.52
1:E:537:GLY:HA3	1:E:640:VAL:O	2.10	0.52
1:C:222:LEU:HD13	1:C:262:VAL:HG21	1.91	0.51
1:E:610:ARG:HA	1:E:614:LEU:HD22	1.91	0.51
1:B:449:PRO:HG2	1:C:208:ASP:HB3	1.91	0.51
1:D:205:ALA:O	3:D:902:ATP:N6	2.36	0.51
1:D:610:ARG:HA	1:D:614:LEU:HD22	1.91	0.51
1:E:210:THR:HG23	1:E:367:ILE:HD13	1.92	0.51
1:C:292:ILE:HD13	1:C:336:ASN:HB2	1.92	0.51
1:D:500:TRP:CD1	1:D:558:GLU:HG3	2.46	0.51
1:B:496:PRO:O	1:B:557:ASN:ND2	2.43	0.51
1:B:350:ASN:OD1	1:C:311:ARG:NH2	2.41	0.51
1:F:722:VAL:HG21	1:F:780:TRP:HB3	1.93	0.51
1:F:374:GLU:HG2	1:F:377:ARG:HH22	1.77	0.50
1:C:281:GLU:OE2	1:C:321:ARG:NH1	2.44	0.50
1:F:630:ASP:OD1	1:F:659:ARG:NE	2.44	0.50
1:C:251:THR:HG21	3:C:902:ATP:H2'	1.94	0.50
1:C:304:ILE:HG23	1:C:355:LEU:HD21	1.92	0.50
1:E:566:ILE:HG22	1:E:568:GLY:H	1.77	0.50
1:B:609:ARG:HH21	1:B:655[B]:ARG:HH22	1.58	0.50
1:E:402:MET:HG3	1:E:403:THR:HG23	1.93	0.49
1:E:607:VAL:HG11	1:E:625:LEU:HD12	1.93	0.49
1:E:744:ALA:HB1	1:F:530:VAL:HB	1.94	0.49
2:G:17:LEU:H	2:G:17:LEU:HD12	1.76	0.49
1:A:388:LEU:HD22	1:B:231:MET:HE2	1.94	0.49
1:D:714:THR:OG1	1:D:775:ILE:O	2.29	0.49
1:B:644:THR:HG21	1:B:650:ILE:HD11	1.93	0.49
1:B:576:VAL:HG21	2:G:18:LEU:HD12	1.95	0.49
1:D:245:SER:OG	3:D:902:ATP:O1G	2.25	0.49
1:F:590:ALA:HB2	1:F:598:LEU:HD21	1.95	0.49
1:E:516:SER:HB3	1:E:538:ILE:HD11	1.94	0.48
1:E:530:VAL:HG23	1:E:532:ILE:HG13	1.95	0.48
1:E:514:GLU:HA	1:E:518:ILE:HB	1.94	0.48
1:B:399:LEU:HA	1:B:402:MET:HG2	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:ASP:N	1:D:793:ASP:OD1	2.46	0.48
1:B:222:LEU:HD13	1:B:262:VAL:HG21	1.94	0.48
1:A:614:LEU:HD23	1:A:619:ALA:HB2	1.95	0.48
1:C:350:ASN:OD1	1:D:311:ARG:NH2	2.47	0.48
1:A:785:ASN:O	1:A:788:LYS:NZ	2.45	0.48
1:C:450:GLN:NE2	1:D:204:ILE:O	2.47	0.48
1:B:605:ALA:HB2	1:C:623:ASN:HD22	1.79	0.48
1:C:237:ASN:OD1	1:C:364:SER:OG	2.30	0.48
1:B:733:GLY:HA3	3:B:901:ATP:C8	2.48	0.48
1:C:408:GLY:HA3	3:C:902:ATP:C8	2.49	0.48
1:E:207:VAL:HG23	1:E:211:LEU:HG	1.95	0.48
1:D:540:LEU:HD23	1:D:664:ILE:HB	1.95	0.47
1:A:350:ASN:OD1	1:B:311:ARG:NH2	2.45	0.47
1:B:574:LYS:HD2	2:G:19:LEU:HD23	1.96	0.47
1:A:466:TRP:CD2	1:B:227:ALA:HB2	2.50	0.47
1:B:207:VAL:HG23	1:B:211:LEU:HG	1.97	0.47
1:B:466:TRP:CD2	1:C:227:ALA:HB2	2.49	0.47
1:C:277:SER:HA	2:G:8:LEU:HG	1.96	0.47
1:D:455:LEU:O	1:D:459:HIS:ND1	2.43	0.47
1:D:722:VAL:HG13	1:D:784:LEU:HD21	1.97	0.47
1:E:240:LEU:HD11	1:E:349:THR:HG22	1.95	0.47
1:E:647:PRO:O	1:E:655:ARG:NH1	2.48	0.47
1:F:566:ILE:HG21	1:F:586:LEU:HD21	1.97	0.47
1:A:208:ASP:HB3	1:F:449:PRO:HG2	1.97	0.47
1:A:327:MET:O	1:A:362:ARG:NH1	2.48	0.47
1:A:727:ARG:HE	1:A:784:LEU:HB3	1.79	0.47
1:D:489:ARG:NH1	1:E:366:GLU:OE2	2.48	0.47
1:F:680:THR:HG23	1:F:683:ARG:HH22	1.80	0.47
1:F:739:LEU:HA	1:F:787:VAL:HG21	1.96	0.47
1:A:327:MET:HB2	1:A:362:ARG:NE	2.30	0.47
1:A:733:GLY:HA3	3:A:901:ATP:C8	2.50	0.47
1:C:213:ARG:NH2	1:C:217:GLU:OE2	2.48	0.47
1:D:316:LYS:HG2	1:D:317:GLY:H	1.80	0.47
1:C:681:LEU:O	1:C:685:THR:OG1	2.30	0.47
1:D:251:THR:HG21	3:D:902:ATP:H2'	1.96	0.47
1:E:203:ASP:OD1	1:E:386:ARG:NH2	2.47	0.47
1:C:573:ASN:H	1:C:579:SER:HB3	1.80	0.46
1:B:385:THR:HB	1:B:390:LEU:HD11	1.98	0.46
1:C:674:ARG:HG2	1:C:736:LEU:HD11	1.96	0.46
1:A:540:LEU:HD23	1:A:664:ILE:HB	1.96	0.46
1:A:269:ALA:HB1	1:A:307:ILE:HG23	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:HA	1:A:518:ILE:HB	1.97	0.46
1:A:607:VAL:HA	1:A:622:VAL:HG22	1.97	0.46
1:E:748:LEU:HD11	1:F:530:VAL:HG21	1.97	0.46
1:F:509:VAL:HG13	1:F:664:ILE:HG21	1.96	0.46
1:B:514:GLU:HA	1:B:518:ILE:HB	1.97	0.46
1:D:543:PRO:HG2	1:D:546:CYS:SG	2.55	0.46
1:A:543:PRO:HG2	1:A:546:CYS:SG	2.55	0.46
1:A:746:ALA:HB1	1:A:782:LYS:HD2	1.98	0.46
1:D:221:PRO:O	1:D:342:ASN:ND2	2.41	0.46
1:A:231:MET:HE3	1:F:388:LEU:HD22	1.98	0.46
1:B:605:ALA:HB2	1:C:623:ASN:ND2	2.30	0.46
1:F:671:ALA:HB1	1:F:724:LEU:HD22	1.98	0.46
1:A:608:PRO:HG2	1:A:614:LEU:HD11	1.98	0.46
1:B:299:ILE:O	1:B:346:LEU:N	2.43	0.45
1:B:507:GLU:OE2	1:B:676:LYS:NZ	2.43	0.45
1:B:456:LEU:HD12	1:C:215:LEU:HD11	1.97	0.45
1:B:648:ASP:N	1:B:648:ASP:OD1	2.48	0.45
1:C:500:TRP:CD1	1:C:558:GLU:HG3	2.51	0.45
1:F:493:SER:OG	1:F:563:PHE:O	2.23	0.45
1:B:738:ASN:HB2	1:C:657:PRO:HB3	1.98	0.45
1:C:333:ILE:HG23	1:C:343:VAL:HB	1.99	0.45
1:C:449:PRO:HG2	1:D:208:ASP:HB3	1.99	0.45
1:E:610:ARG:HH11	1:E:623:ASN:HD21	1.63	0.45
1:F:739:LEU:HD11	1:F:784:LEU:HD23	1.99	0.45
1:C:350:ASN:OD1	1:C:351:ARG:NH1	2.50	0.45
1:C:534:PRO:HG2	1:C:636:SER:HB2	1.98	0.45
1:A:562:ASN:ND2	1:A:593:SER:HB3	2.31	0.45
1:E:263:ALA:HB1	1:E:294:LEU:HD23	1.99	0.45
1:C:540:LEU:HD23	1:C:664:ILE:HB	1.99	0.45
1:A:714:THR:OG1	1:A:775:ILE:O	2.35	0.45
1:F:599:PHE:CE2	1:F:601:ASP:HB3	2.51	0.45
1:A:541:TRP:HB2	1:A:647:PRO:HG3	1.97	0.45
1:C:496:PRO:O	1:C:557:ASN:ND2	2.50	0.44
1:A:564:ILE:HB	1:A:598:LEU:HD23	1.98	0.44
1:C:264:PHE:CE2	1:C:266:PRO:HG3	2.52	0.44
1:F:385:THR:HB	1:F:390:LEU:HD21	1.99	0.44
1:F:573:ASN:H	1:F:579:SER:HB2	1.83	0.44
1:A:500:TRP:CD1	1:A:558:GLU:HG3	2.52	0.44
1:B:333:ILE:HG23	1:B:343:VAL:HB	1.99	0.44
1:B:656:ARG:NH1	1:B:657:PRO:O	2.50	0.44
1:F:722:VAL:HG22	1:F:784:LEU:HD21	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:GLU:HG3	1:B:460:ARG:HH21	1.82	0.44
1:B:746:ALA:HB1	1:B:782:LYS:HD2	1.99	0.44
1:E:239:VAL:HB	1:E:346:LEU:HD23	2.00	0.44
1:C:543:PRO:HG2	1:C:546:CYS:SG	2.57	0.44
1:C:617:ALA:HB1	2:G:22:LEU:HD13	2.00	0.44
1:D:534:PRO:HG2	1:D:636:SER:HB2	1.99	0.44
1:F:414:VAL:HA	1:F:483:VAL:HG21	2.00	0.44
1:B:630:ASP:OD2	1:B:656:ARG:NH2	2.45	0.44
1:C:644:THR:HG21	1:C:650:ILE:HD11	1.99	0.44
1:F:399:LEU:HA	1:F:402:MET:HG2	2.00	0.44
1:A:233:TYR:OH	1:F:416:LYS:HG2	2.18	0.43
1:A:331:ASP:OD1	1:A:362:ARG:NH1	2.25	0.43
1:E:601:ASP:HA	1:E:643:ALA:HB3	2.00	0.43
1:A:466:TRP:O	1:B:230:LYS:NZ	2.46	0.43
1:B:540:LEU:HD23	1:B:664:ILE:HB	1.99	0.43
1:D:608:PRO:HB2	1:D:614:LEU:HD11	1.99	0.43
1:B:647:PRO:O	1:B:655[B]:ARG:NH1	2.51	0.43
1:E:310:ARG:NH2	1:E:353:GLU:O	2.51	0.43
1:F:517:ILE:HD12	1:F:639:TYR:HB3	2.01	0.43
1:B:610:ARG:HH11	1:B:623:ASN:HD21	1.66	0.43
1:E:297:CYS:SG	1:E:298:LEU:N	2.92	0.43
1:E:781:GLU:O	1:E:785:ASN:ND2	2.52	0.43
1:D:569:PRO:HG3	1:E:620:ARG:HB3	2.00	0.43
1:E:576:VAL:HA	2:G:26:LEU:HD21	1.99	0.43
1:D:269:ALA:HB1	1:D:307:ILE:HG23	1.99	0.43
1:E:540:LEU:HD23	1:E:664:ILE:HB	2.01	0.42
1:A:751:VAL:HG21	1:A:773:PRO:HB3	2.00	0.42
1:C:210:THR:HG23	1:C:367:ILE:HG21	2.01	0.42
1:F:604:ASP:OD1	1:F:604:ASP:N	2.52	0.42
1:D:573:ASN:OD1	1:D:574:LYS:N	2.52	0.42
1:E:659:ARG:O	1:E:661:GLY:N	2.51	0.42
1:C:790:SER:OG	1:D:657:PRO:HD3	2.19	0.42
1:D:399:LEU:HD21	1:D:476:PHE:HB3	2.01	0.42
1:A:722:VAL:HG13	1:A:784:LEU:HD21	1.99	0.42
1:C:573:ASN:OD1	1:C:574:LYS:N	2.53	0.42
1:B:500:TRP:CD1	1:B:558:GLU:HG3	2.55	0.42
1:C:488:LYS:HE3	1:C:488:LYS:HB3	1.82	0.42
1:D:614:LEU:O	1:D:615:SER:OG	2.35	0.42
1:E:232:GLY:HA2	1:E:339:LEU:HD13	2.01	0.42
1:E:316:LYS:HD3	1:E:319:GLU:HG3	2.02	0.42
1:B:282:LYS:HE2	1:B:282:LYS:HB3	1.92	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PRO:HG2	1:B:546:CYS:SG	2.59	0.42
1:F:514:GLU:HA	1:F:518:ILE:HB	2.01	0.42
1:F:632:VAL:HG23	1:F:638:ILE:HB	2.02	0.42
1:D:260:ILE:HG22	1:D:262:VAL:HG13	2.02	0.42
1:F:412:GLN:HG2	1:F:416:LYS:HE3	2.02	0.42
1:F:407:VAL:H	1:F:410:ASP:HB2	1.84	0.41
1:A:645:ASN:ND2	1:B:610:ARG:HH22	2.18	0.41
1:B:541:TRP:CE3	1:B:647:PRO:HG3	2.54	0.41
1:B:562:ASN:ND2	1:B:593:SER:HB3	2.35	0.41
1:C:417:ALA:O	1:C:421:GLU:HG2	2.20	0.41
1:D:204:ILE:HG12	1:D:252:LEU:HD13	2.01	0.41
1:B:264:PHE:CE2	1:B:266:PRO:HG3	2.55	0.41
1:B:607:VAL:HA	1:B:622:VAL:HG22	2.03	0.41
1:D:412:GLN:OE1	1:E:334:ARG:NH1	2.54	0.41
1:E:222:LEU:HD13	1:E:262:VAL:HG21	2.01	0.41
1:F:403:THR:HB	1:F:406:TYR:HB2	2.03	0.41
1:E:616:ASP:O	1:E:620:ARG:HG3	2.20	0.41
1:C:453:TRP:HB3	1:D:201:ILE:HG13	2.03	0.41
1:E:269:ALA:O	1:E:272:VAL:HG22	2.21	0.41
1:A:514:GLU:HG2	1:A:518:ILE:HD12	2.03	0.41
1:C:460:ARG:HD2	1:D:223:ARG:HH21	1.86	0.41
1:E:653:ALA:O	1:E:659:ARG:HD2	2.21	0.41
1:A:421:GLU:OE2	1:B:216:LYS:NZ	2.47	0.41
1:B:374:GLU:HG2	1:B:377:ARG:NH2	2.36	0.40
1:B:385:THR:HB	1:B:390:LEU:HD21	2.03	0.40
1:E:404:PRO:HB3	1:E:595:PRO:HD2	2.03	0.40
1:E:543:PRO:HG2	1:E:546:CYS:SG	2.61	0.40
1:D:674:ARG:HG2	1:D:736:LEU:HD11	2.03	0.40
1:F:496:PRO:O	1:F:557:ASN:ND2	2.49	0.40
1:A:738:ASN:HB2	1:B:657:PRO:HB3	2.02	0.40
1:B:448:GLN:HB3	1:B:449:PRO:HD3	2.03	0.40
1:B:562:ASN:ND2	1:B:593:SER:O	2.48	0.40
2:G:11:LEU:HG	2:G:12:LEU:H	1.86	0.40
1:A:352:PRO:HA	1:A:355:LEU:HD13	2.03	0.40
1:C:543:PRO:HD2	1:C:667:GLY:HA2	2.04	0.40
1:D:488:LYS:HE2	1:D:488:LYS:HB3	1.87	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	543/629 (86%)	523 (96%)	20 (4%)	0	100	100
1	B	543/629 (86%)	534 (98%)	9 (2%)	0	100	100
1	C	553/629 (88%)	542 (98%)	11 (2%)	0	100	100
1	D	547/629 (87%)	531 (97%)	15 (3%)	1 (0%)	47	76
1	E	466/629 (74%)	450 (97%)	16 (3%)	0	100	100
1	F	332/629 (53%)	314 (95%)	18 (5%)	0	100	100
2	G	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	2	8
All	All	3006/3798 (79%)	2914 (97%)	90 (3%)	2 (0%)	54	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	460	ARG
2	G	15	LEU

### 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	453/516 (88%)	450 (99%)	3 (1%)	84	94
1	B	459/516 (89%)	456 (99%)	3 (1%)	84	94
1	C	466/516 (90%)	461 (99%)	5 (1%)	73	90
1	D	458/516 (89%)	454 (99%)	4 (1%)	78	92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	392/516 (76%)	390 (100%)	2 (0%)	88	96
1	F	289/516 (56%)	284 (98%)	5 (2%)	60	84
2	G	19/24 (79%)	18 (95%)	1 (5%)	22	52
All	All	2536/3120 (81%)	2513 (99%)	23 (1%)	79	92

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	TYR
1	A	337	THR
1	A	607	VAL
1	B	235	TYR
1	B	276	THR
1	B	685	THR
1	C	235	TYR
1	C	276	THR
1	C	635	ARG
1	C	685	THR
1	C	771	ILE
1	D	207	VAL
1	D	235	TYR
1	D	361	ARG
1	D	484	GLN
1	E	235	TYR
1	E	472	THR
1	F	371	MET
1	F	399	LEU
1	F	476	PHE
1	F	566	ILE
1	F	586	LEU
2	G	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	GLN
1	B	424	GLN
1	B	426	ASN
1	B	623	ASN
1	C	379	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	562	ASN
1	D	335	GLN
1	D	433	GLN
1	D	484	GLN
1	E	602	GLN
1	E	623	ASN
1	E	745	GLN
1	E	785	ASN
1	F	433	GLN
1	F	450	GLN
1	F	484	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	C	902	4	26,33,33	0.76	0	31,52,52	0.81	1 (3%)
5	ADP	E	901	-	24,29,29	0.94	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
3	ATP	C	901	4	26,33,33	0.76	0	31,52,52	0.79	1 (3%)
3	ATP	B	901	4	26,33,33	0.75	0	31,52,52	0.78	1 (3%)
3	ATP	B	902	4	26,33,33	0.74	0	31,52,52	0.83	1 (3%)
3	ATP	D	902	4	26,33,33	0.74	0	31,52,52	0.81	1 (3%)
3	ATP	D	901	4	26,33,33	0.75	0	31,52,52	0.77	1 (3%)
3	ATP	E	902	4	26,33,33	0.72	0	31,52,52	0.76	1 (3%)
3	ATP	A	902	4	26,33,33	0.73	0	31,52,52	0.79	1 (3%)
3	ATP	A	901	4	26,33,33	0.75	0	31,52,52	0.80	1 (3%)

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	ATP	C	902	4	-	4/18/38/38	0/3/3/3
5	ADP	E	901	-	-	3/12/32/32	0/3/3/3
3	ATP	C	901	4	-	3/18/38/38	0/3/3/3
3	ATP	B	901	4	-	3/18/38/38	0/3/3/3
3	ATP	B	902	4	-	3/18/38/38	0/3/3/3
3	ATP	D	902	4	-	3/18/38/38	0/3/3/3
3	ATP	D	901	4	-	4/18/38/38	0/3/3/3
3	ATP	E	902	4	-	1/18/38/38	0/3/3/3
3	ATP	A	902	4	-	1/18/38/38	0/3/3/3
3	ATP	A	901	4	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	901	ADP	C5-C4	2.48	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	901	ADP	C3'-C2'-C1'	3.69	106.53	100.98
5	E	901	ADP	PA-O3A-PB	-3.34	121.37	132.83
5	E	901	ADP	N3-C2-N1	-3.20	123.67	128.68
5	E	901	ADP	C4-C5-N7	-2.58	106.71	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	ATP	C5-C6-N6	2.24	123.76	120.35
3	D	901	ATP	C5-C6-N6	2.24	123.76	120.35
3	A	901	ATP	C5-C6-N6	2.22	123.72	120.35
3	B	901	ATP	C5-C6-N6	2.22	123.72	120.35
3	B	902	ATP	C5-C6-N6	2.21	123.71	120.35
3	E	902	ATP	C5-C6-N6	2.19	123.67	120.35
3	C	902	ATP	C5-C6-N6	2.18	123.67	120.35
3	A	902	ATP	C5-C6-N6	2.17	123.66	120.35
3	D	902	ATP	C5-C6-N6	2.17	123.64	120.35

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O2A
3	B	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O3G
3	C	902	ATP	PB-O3B-PG-O2G
3	D	901	ATP	PB-O3B-PG-O2G
3	B	902	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	PB-O3B-PG-O3G
3	B	902	ATP	PA-O3A-PB-O1B
3	A	901	ATP	PA-O3A-PB-O1B
3	C	902	ATP	O4'-C4'-C5'-O5'
3	D	902	ATP	O4'-C4'-C5'-O5'
5	E	901	ADP	PB-O3A-PA-O1A
3	D	901	ATP	PB-O3B-PG-O1G
3	D	902	ATP	PB-O3B-PG-O1G
3	B	901	ATP	PB-O3B-PG-O3G
3	C	902	ATP	PB-O3B-PG-O3G
3	A	901	ATP	C5'-O5'-PA-O3A
3	A	902	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PA-O3A-PB-O2B
3	B	902	ATP	PA-O3A-PB-O2B
3	D	902	ATP	PG-O3B-PB-O2B
5	E	901	ADP	PB-O3A-PA-O2A
3	C	901	ATP	O4'-C4'-C5'-O5'
3	E	902	ATP	O4'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

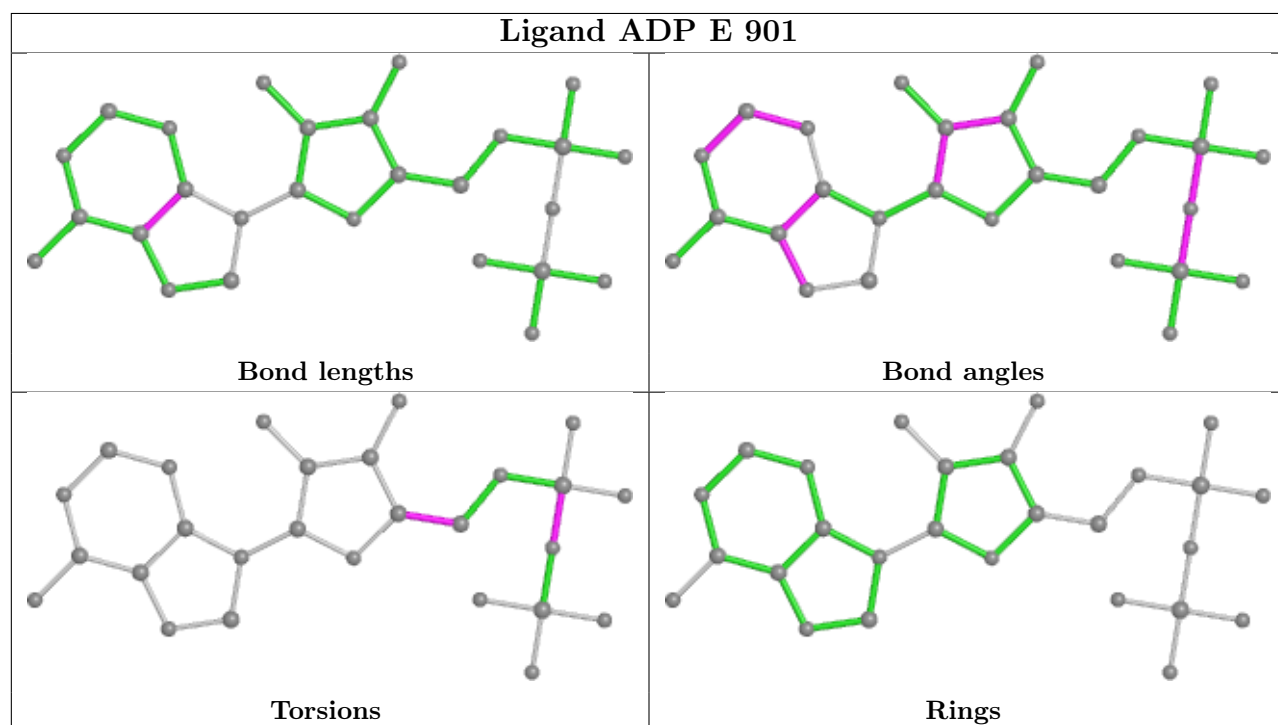
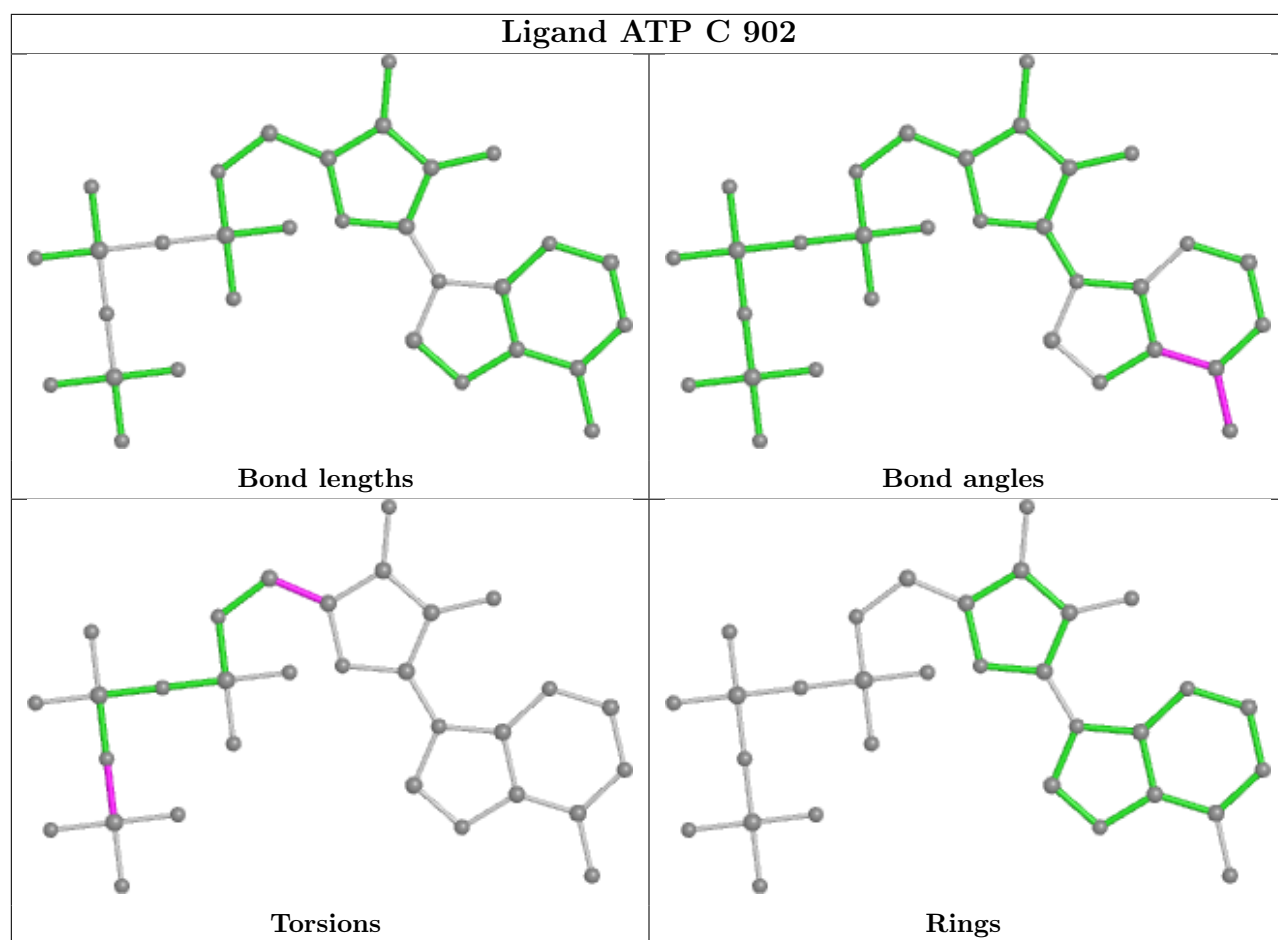
Mol	Chain	Res	Type	Atoms
5	E	901	ADP	O4'-C4'-C5'-O5'
3	C	902	ATP	PB-O3B-PG-O1G

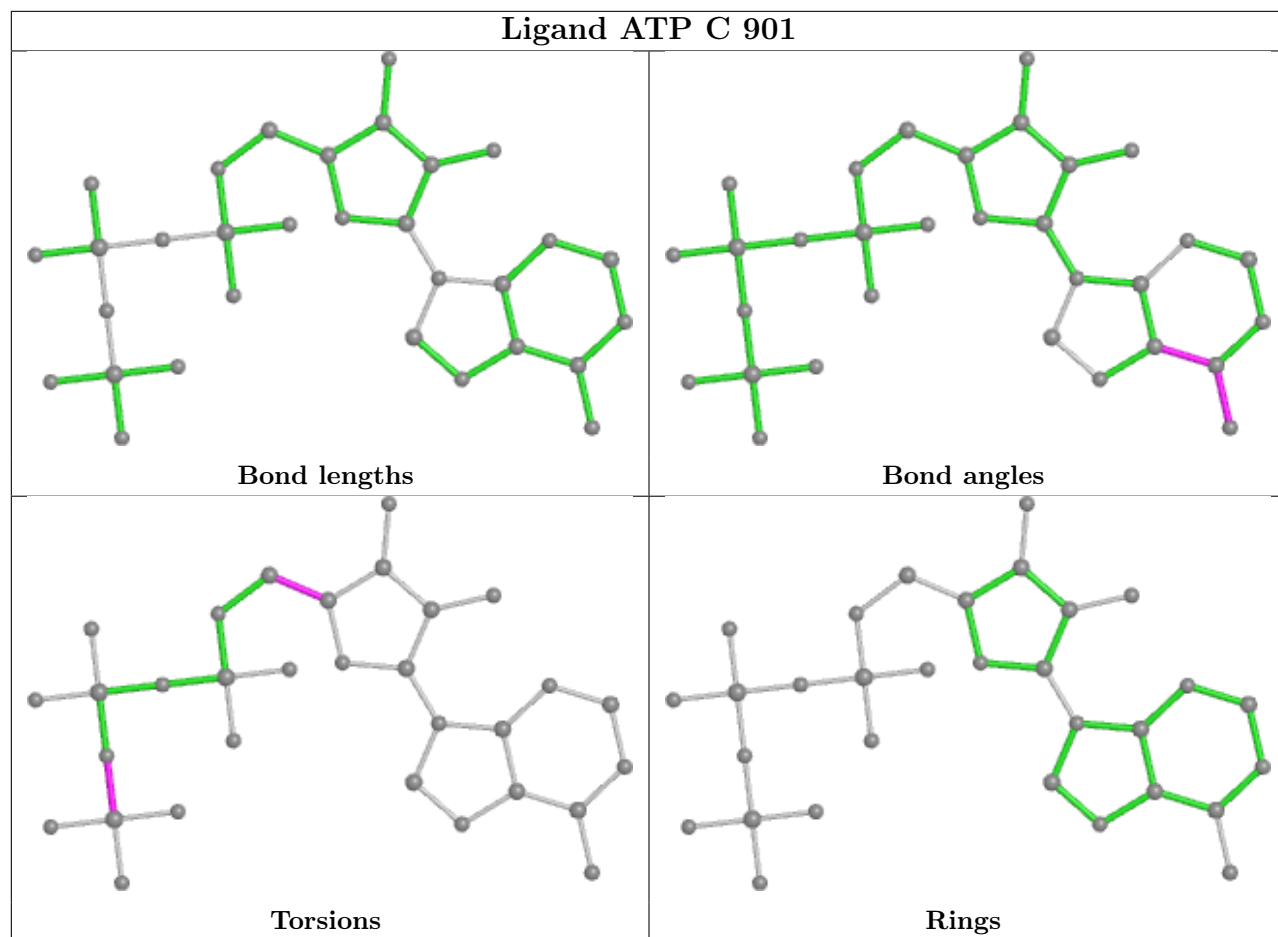
There are no ring outliers.

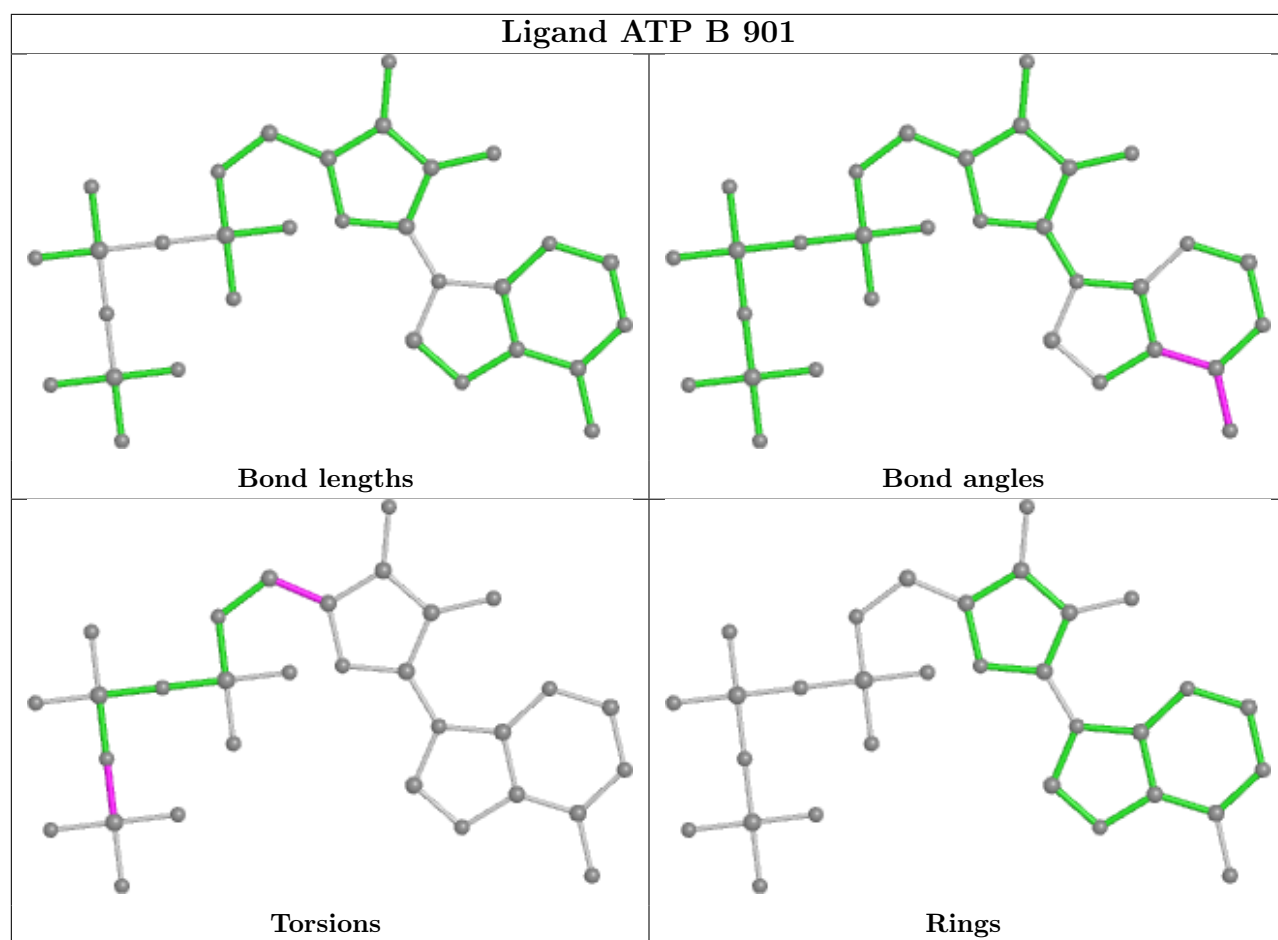
7 monomers are involved in 10 short contacts:

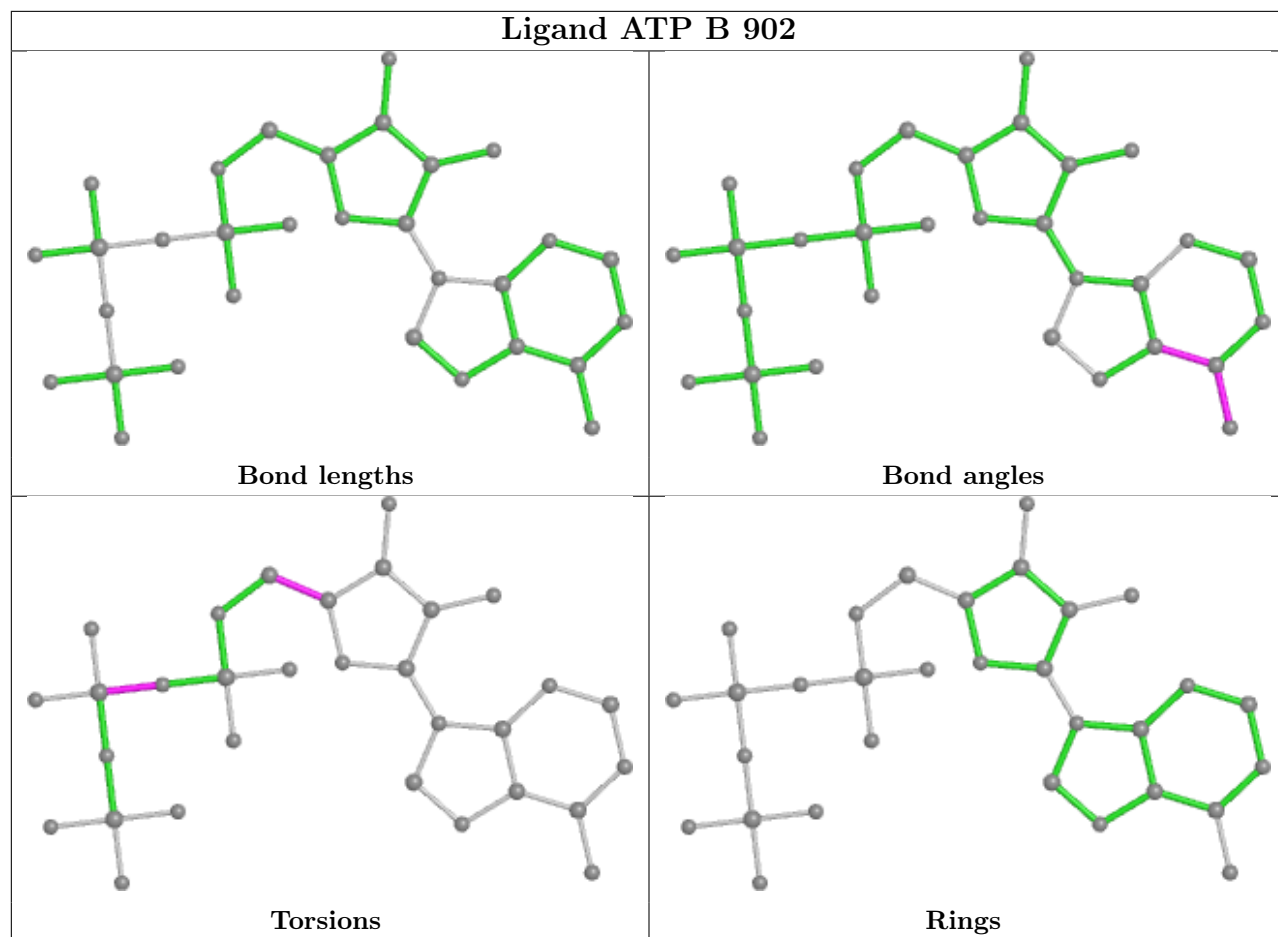
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	902	ATP	2	0
5	E	901	ADP	1	0
3	B	901	ATP	1	0
3	B	902	ATP	1	0
3	D	902	ATP	3	0
3	A	902	ATP	1	0
3	A	901	ATP	1	0

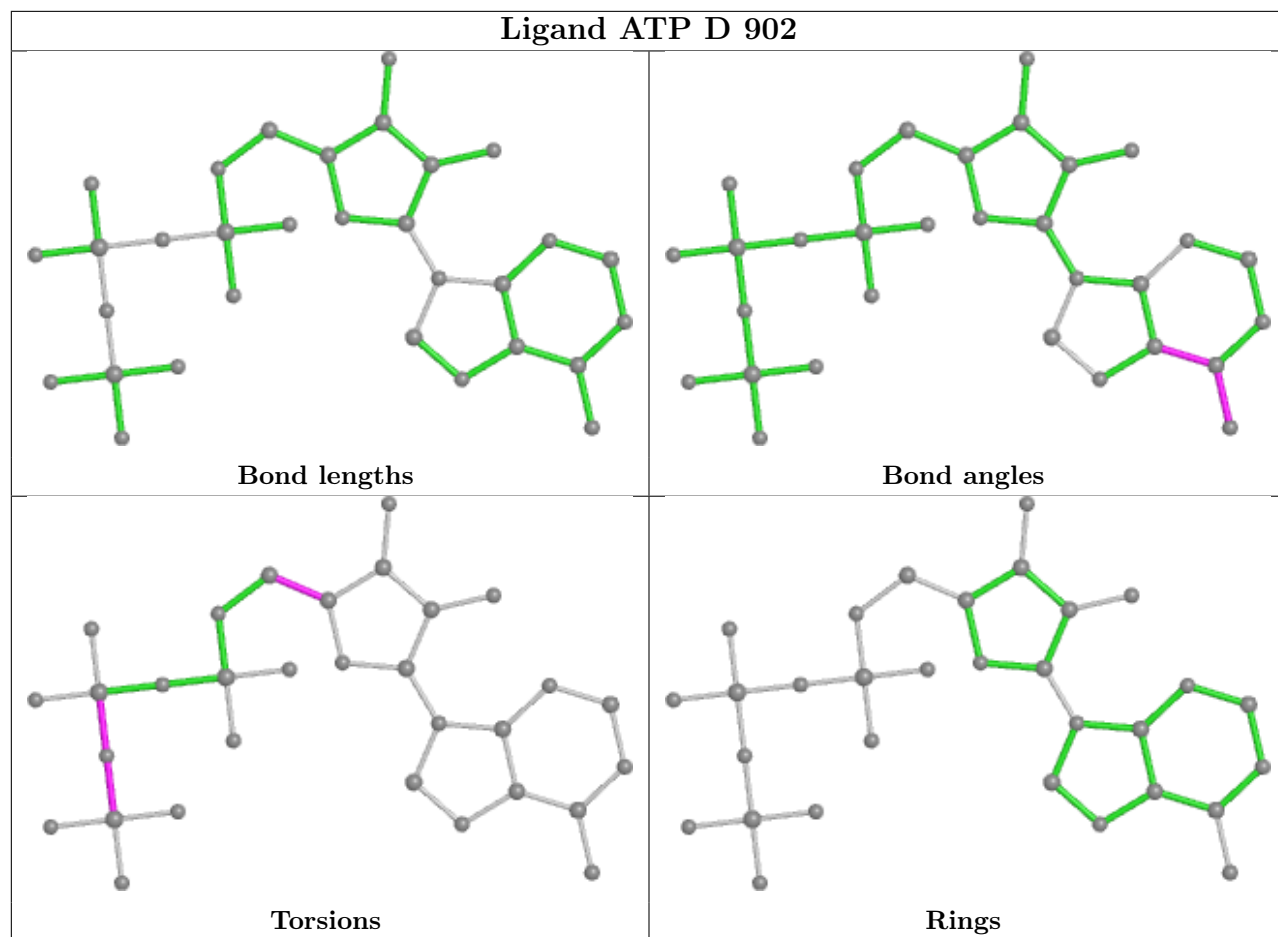
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

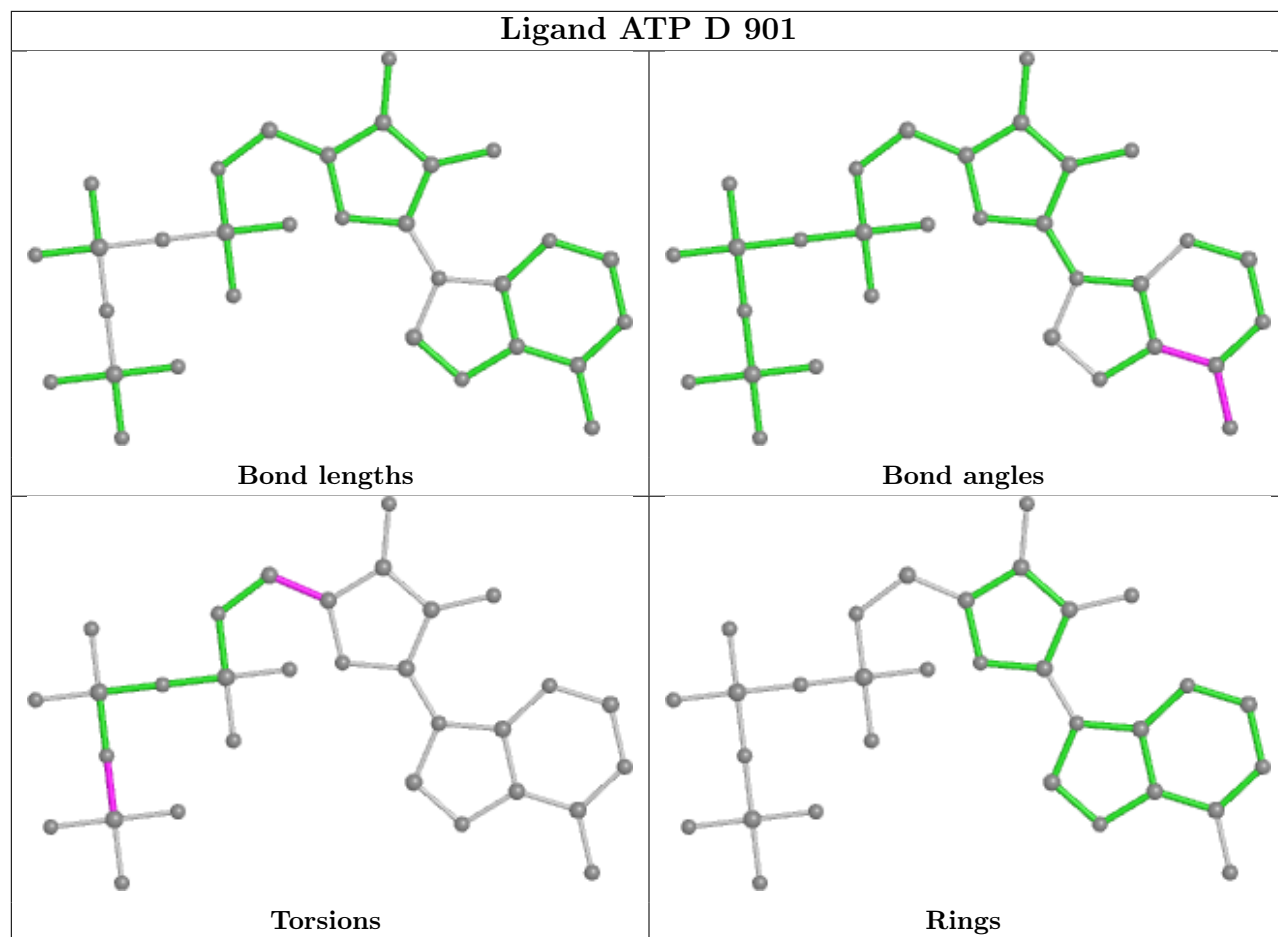


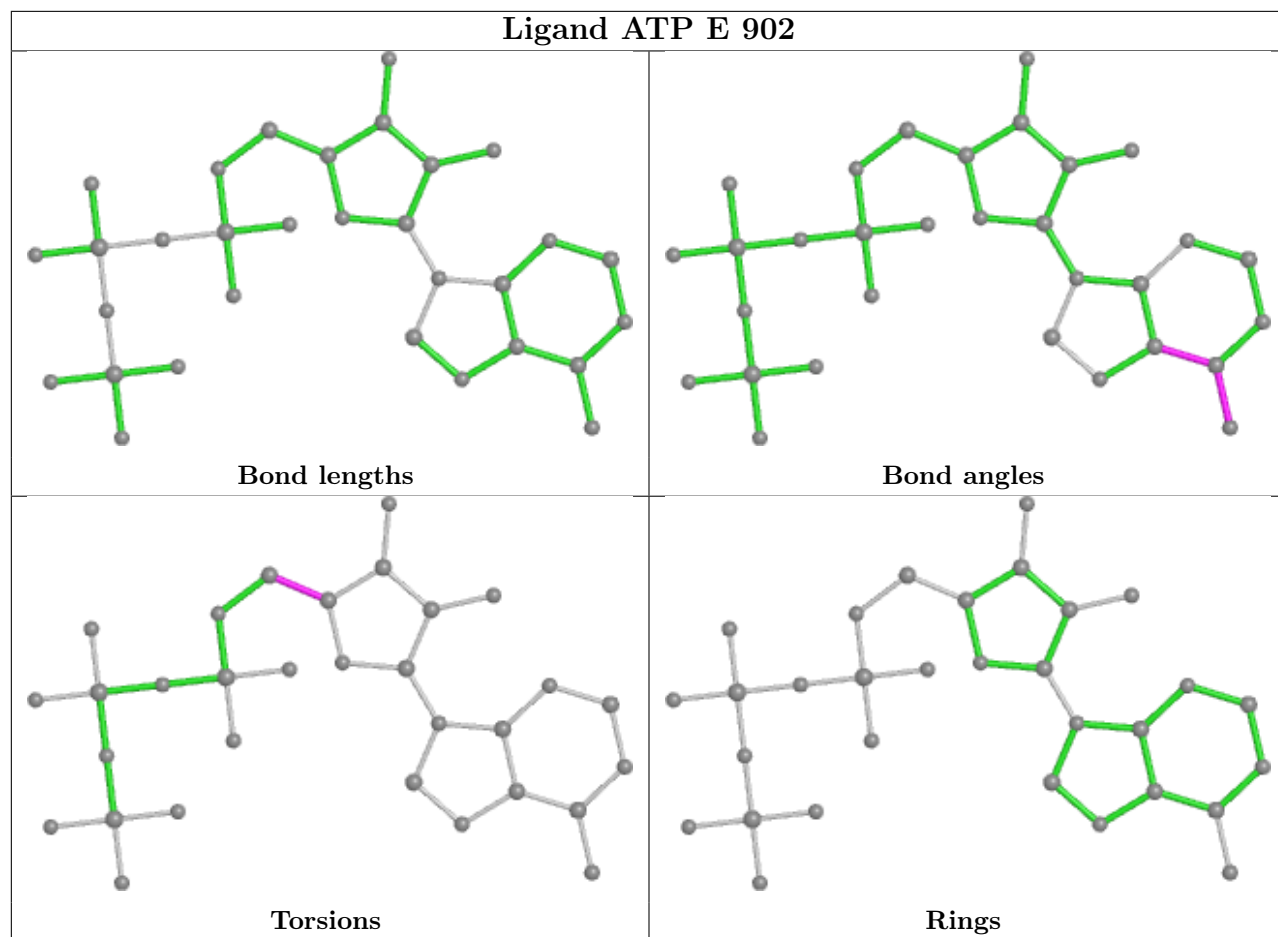


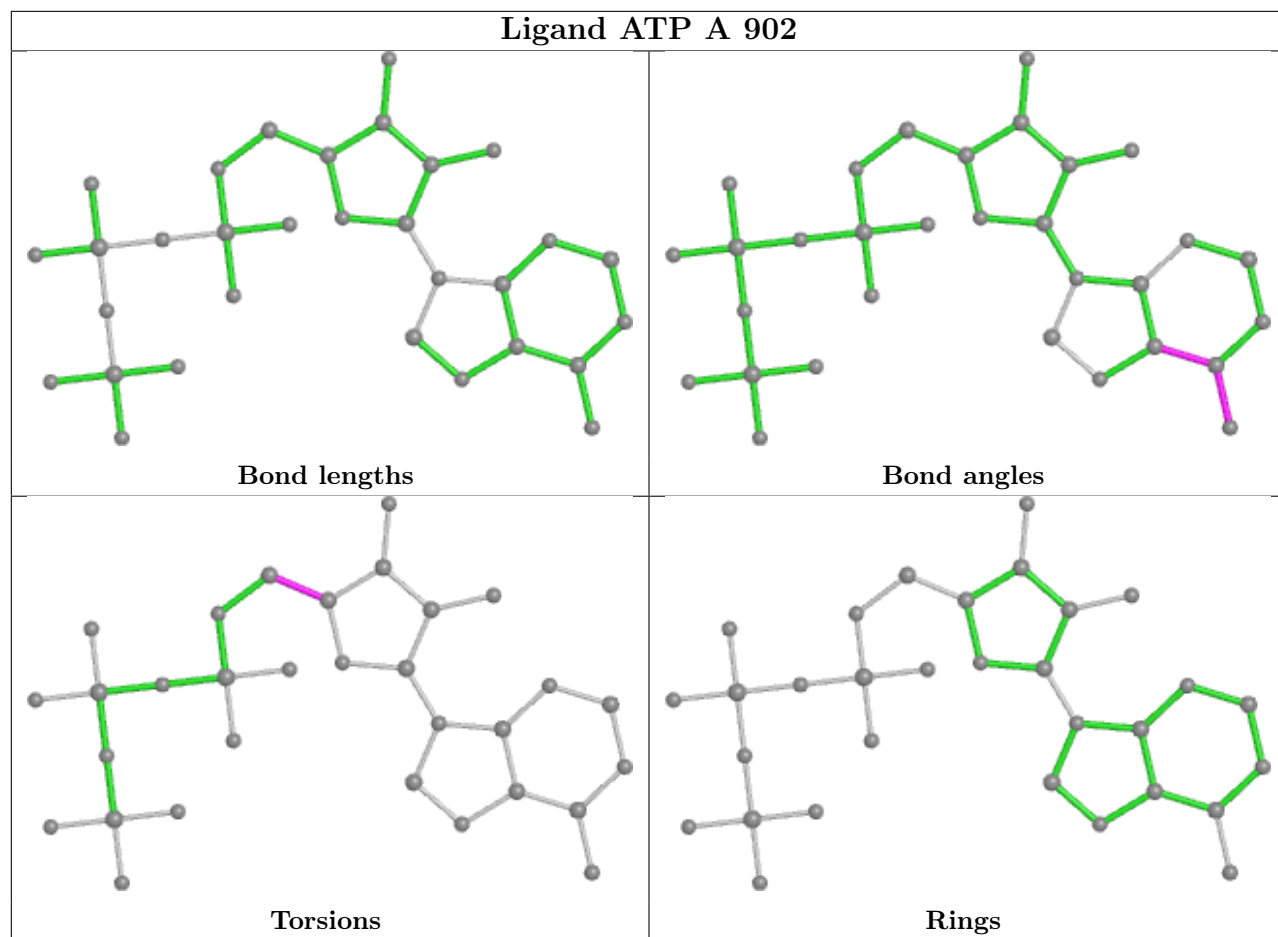


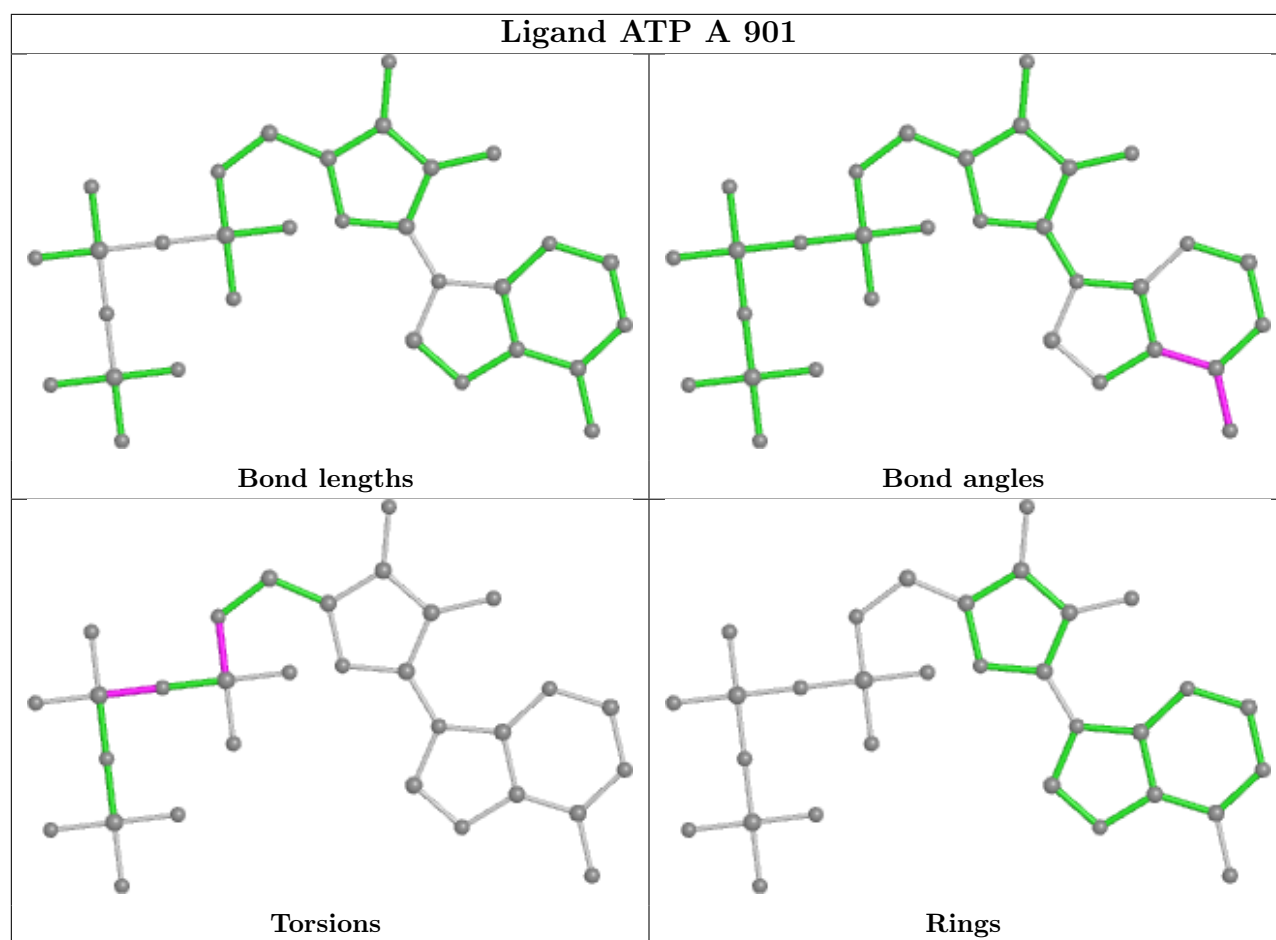












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

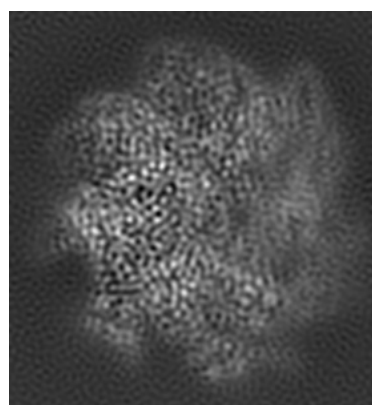
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25474. These allow visual inspection of the internal detail of the map and identification of artifacts.

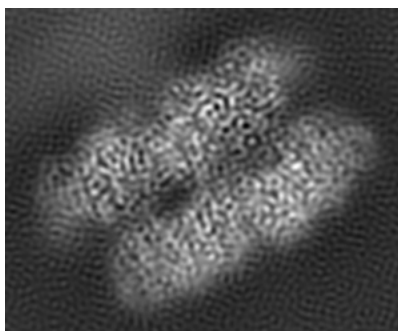
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

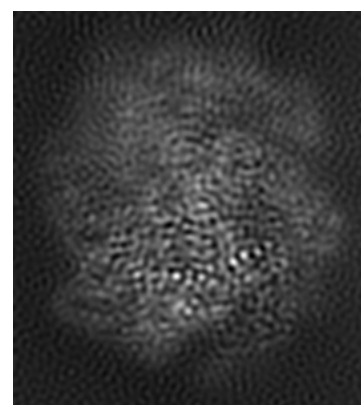
#### 6.1.1 Primary map



X



Y

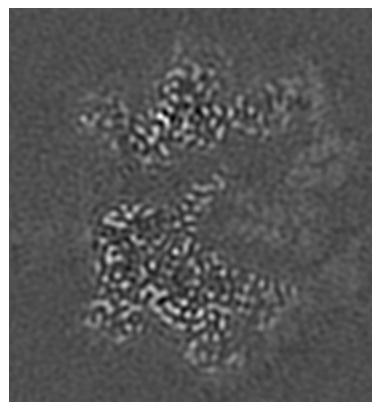


Z

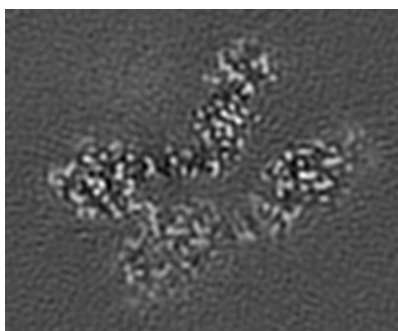
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

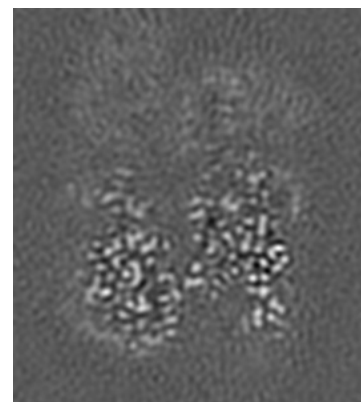
#### 6.2.1 Primary map



X Index: 63



Y Index: 70

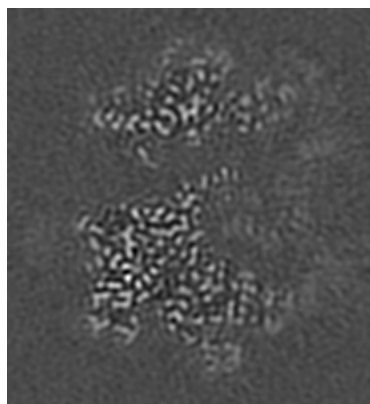


Z Index: 77

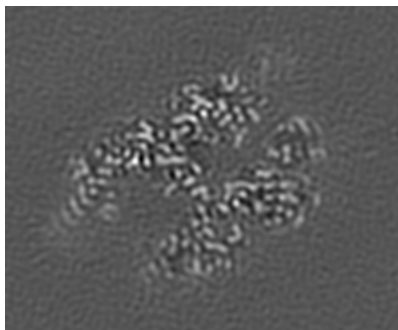
The images above show central slices of the map in three orthogonal directions.

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

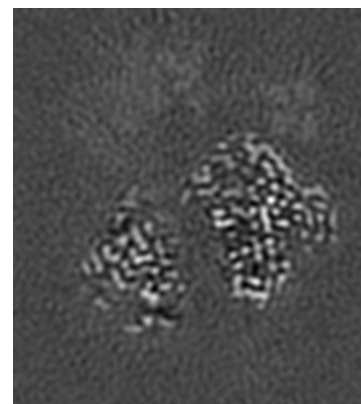
### 6.3.1 Primary map



X Index: 66



Y Index: 46

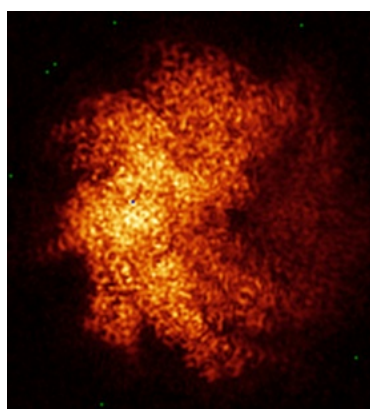


Z Index: 87

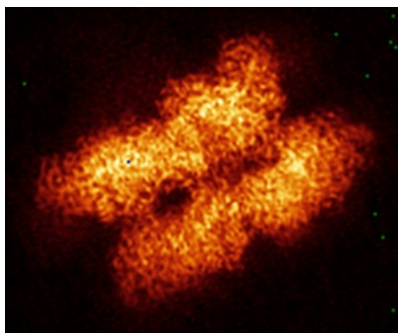
The images above show the largest variance slices of the map in three orthogonal directions.

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

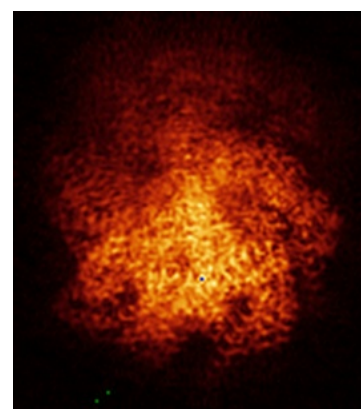
### 6.4.1 Primary map



X



Y



Z

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 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

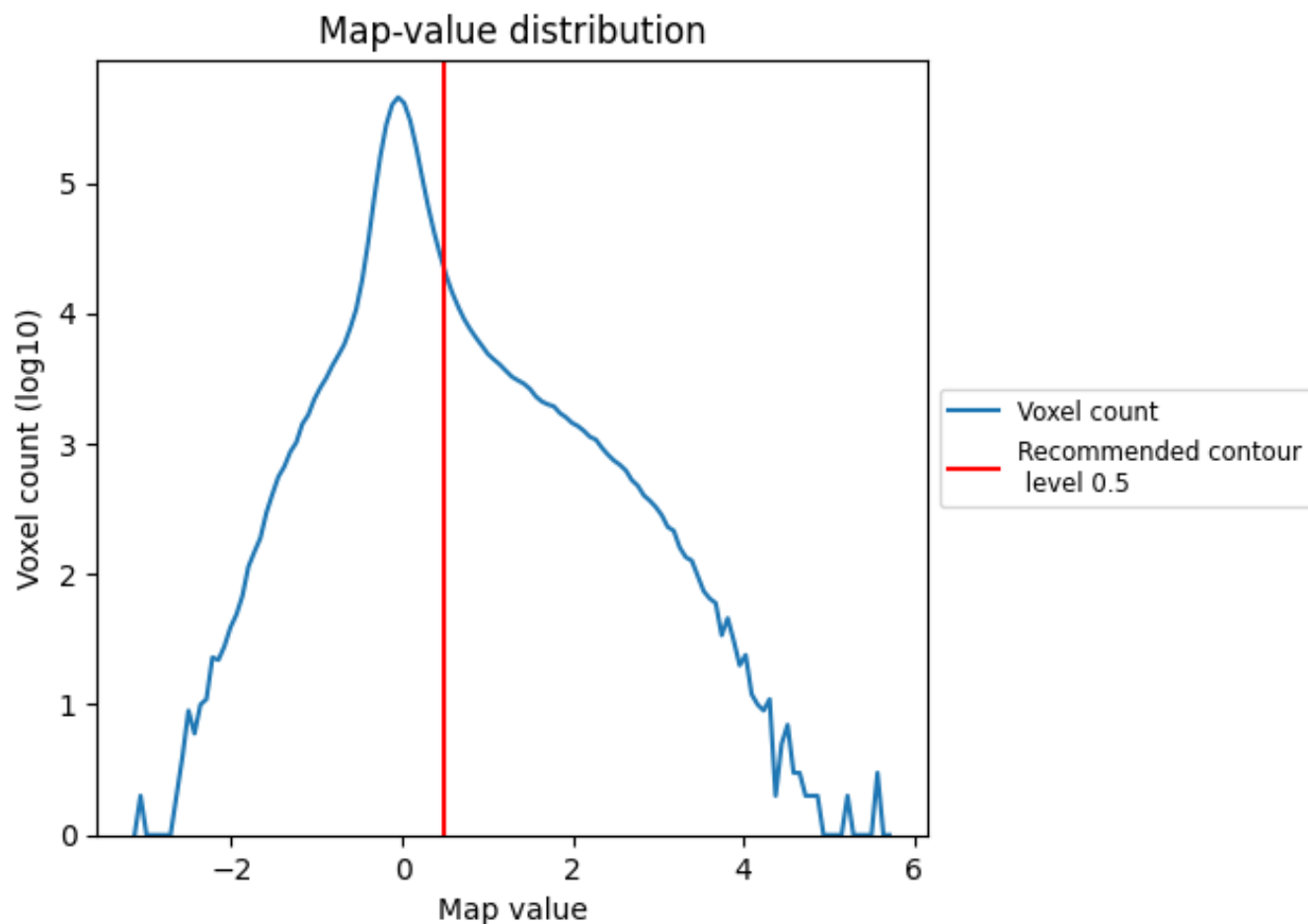
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

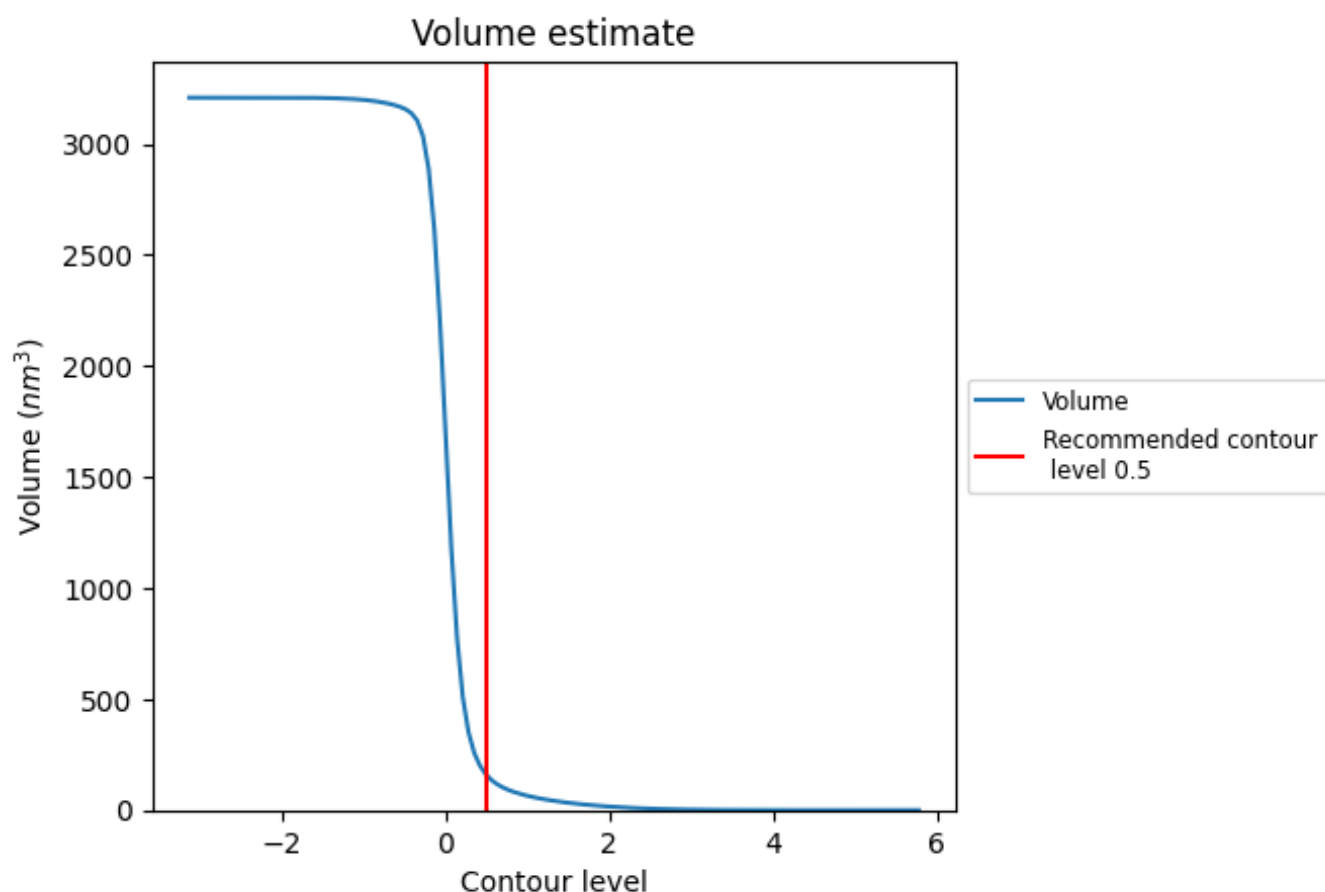
This section contains the results of statistical analysis of the map.

### 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 158 nm<sup>3</sup>; this corresponds to an approximate mass of 142 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

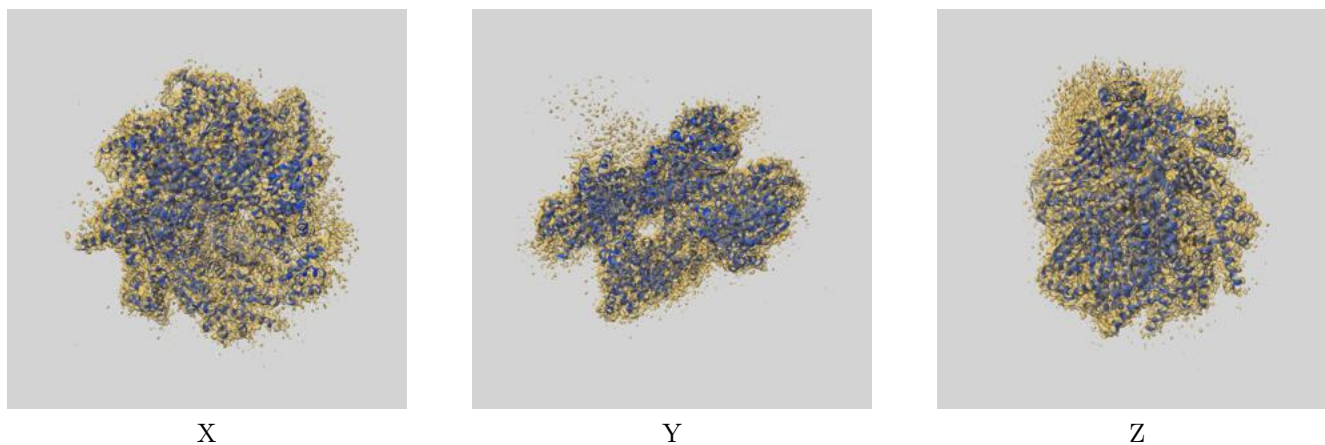
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

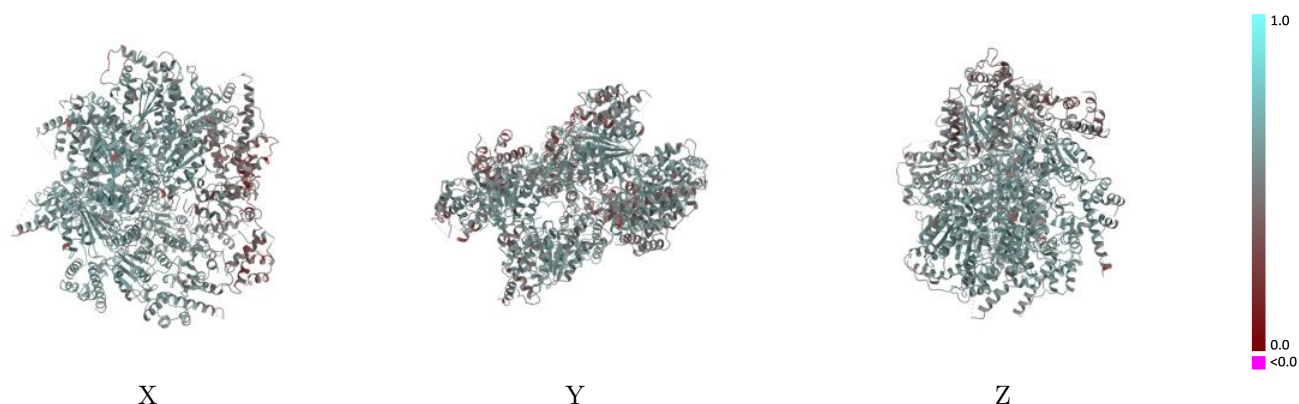
This section contains information regarding the fit between EMDB map EMD-25474 and PDB model 7SWL. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



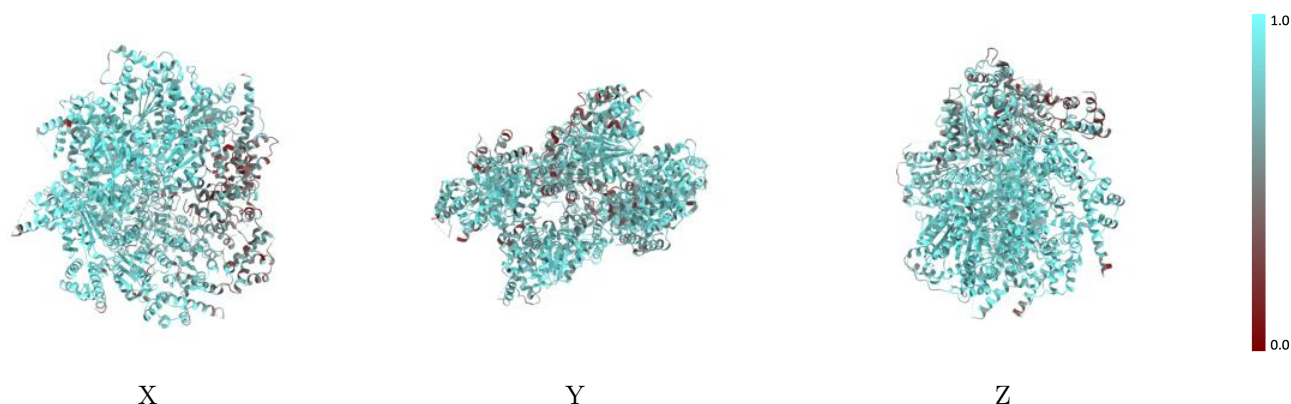
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



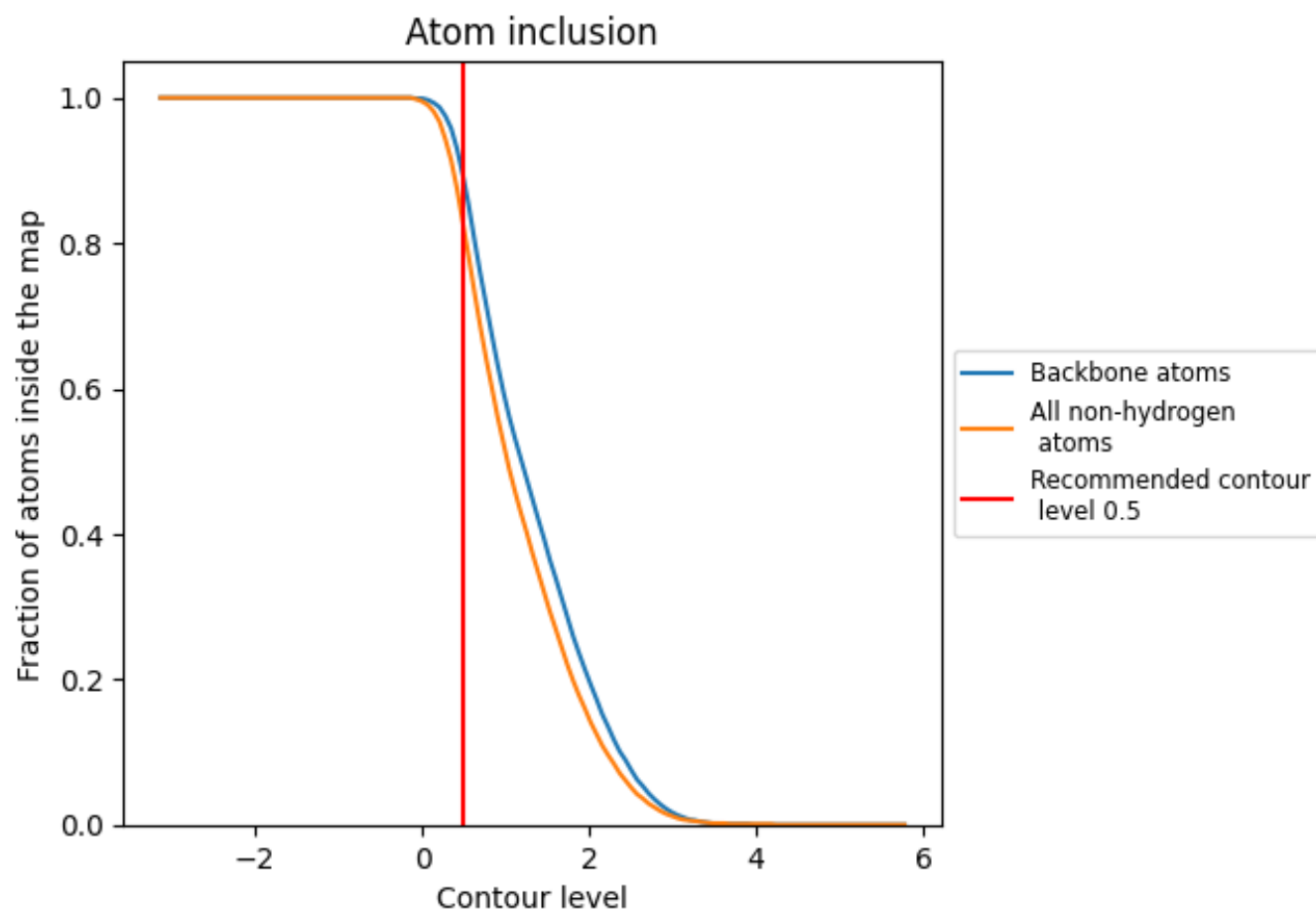
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8200	<div><div></div></div> 0.5460
A	<div><div></div></div> 0.8350	<div><div></div></div> 0.5460
B	<div><div></div></div> 0.9110	<div><div></div></div> 0.5860
C	<div><div></div></div> 0.9020	<div><div></div></div> 0.5850
D	<div><div></div></div> 0.8750	<div><div></div></div> 0.5660
E	<div><div></div></div> 0.7520	<div><div></div></div> 0.5180
F	<div><div></div></div> 0.5330	<div><div></div></div> 0.4300
G	<div><div></div></div> 0.6720	<div><div></div></div> 0.5080

1.0

0.0

<0.0