



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:43 AM UTC

PDB ID : 6MAT / pdb_00006mat
EMDB ID : EMD-9063
Title : Cryo-EM structure of the essential ribosome assembly AAA-ATPase Rix7
Authors : Lo, Y.H.; Sobhany, M.; Hsu, A.L.; Ford, B.L.; Krahm, J.M.; Borgnia, M.J.; Stanley, R.E.
Deposited on : 2018-08-28
Resolution : 4.50 Å(reported)
Based on initial model : 5FTK

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

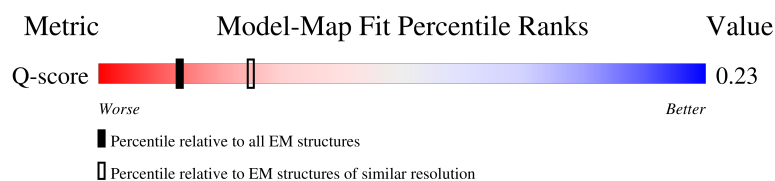
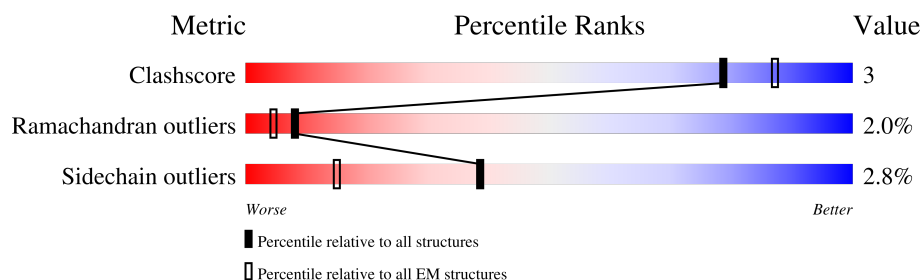
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	813	14% 61% 9% • 29%
1	B	813	10% 61% 9% • 29%
1	C	813	10% 61% 9% • 29%
1	D	813	10% 61% 9% • 29%

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Mol	Chain	Length	Quality of chain
1	E	813	22% 61% 8% 30%
1	F	813	34% 61% 8% 30%
2	G	27	33% 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27030 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 mutant.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	B	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	C	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	D	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	E	568	Total	C	N	O	S	0	0
			4369	2734	781	834	20		
1	F	568	Total	C	N	O	S	0	0
			4369	2734	781	834	20		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	GLN	GLU	engineered mutation	UNP G0RZG1
A	602	GLN	GLU	engineered mutation	UNP G0RZG1
A	803	ALA	-	expression tag	UNP G0RZG1
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	303	GLN	GLU	engineered mutation	UNP G0RZG1
B	602	GLN	GLU	engineered mutation	UNP G0RZG1
B	803	ALA	-	expression tag	UNP G0RZG1
B	804	ALA	-	expression tag	UNP G0RZG1
B	805	ALA	-	expression tag	UNP G0RZG1

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Chain	Residue	Modelled	Actual	Comment	Reference
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	303	GLN	GLU	engineered mutation	UNP G0RZG1
C	602	GLN	GLU	engineered mutation	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	303	GLN	GLU	engineered mutation	UNP G0RZG1
D	602	GLN	GLU	engineered mutation	UNP G0RZG1
D	803	ALA	-	expression tag	UNP G0RZG1
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	303	GLN	GLU	engineered mutation	UNP G0RZG1
E	602	GLN	GLU	engineered mutation	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

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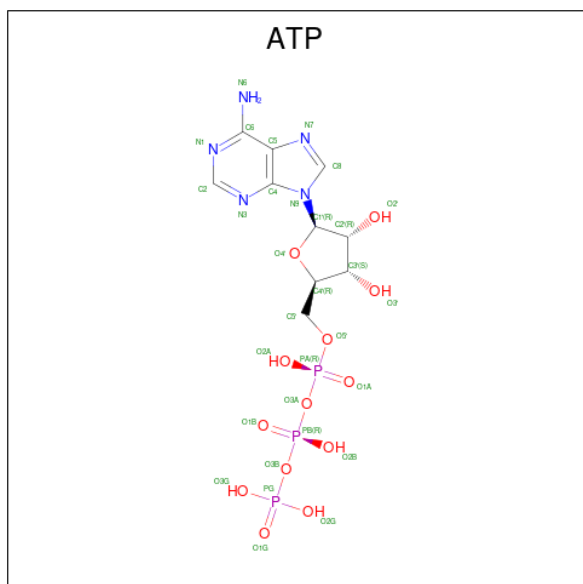
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Chain	Residue	Modelled	Actual	Comment	Reference
E	809	HIS	-	expression tag	UNP G0RZG1
E	810	HIS	-	expression tag	UNP G0RZG1
E	811	HIS	-	expression tag	UNP G0RZG1
E	812	HIS	-	expression tag	UNP G0RZG1
E	813	HIS	-	expression tag	UNP G0RZG1
F	303	GLN	GLU	engineered mutation	UNP G0RZG1
F	602	GLN	GLU	engineered mutation	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 unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

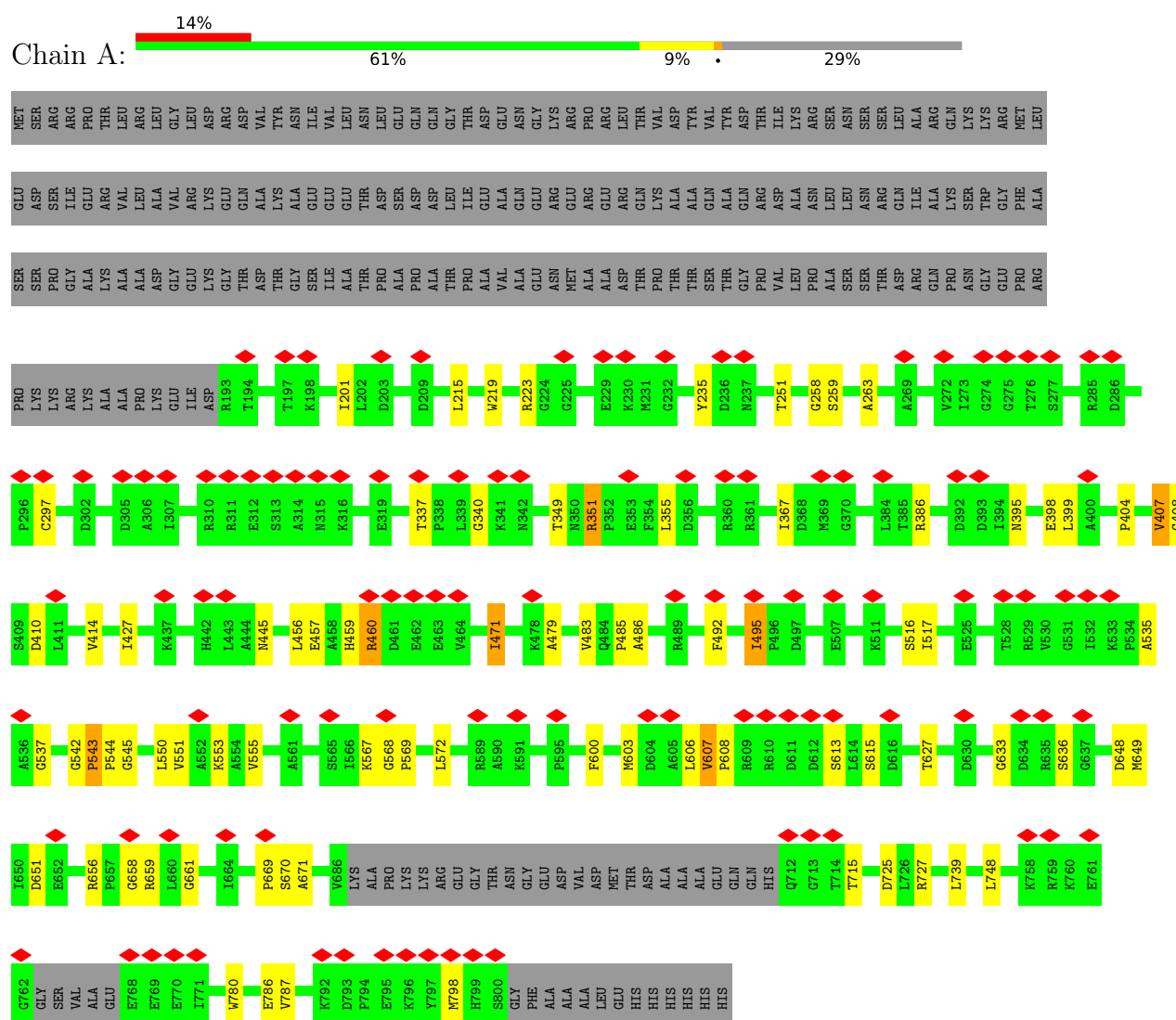


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10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

3 Residue-property plots

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.

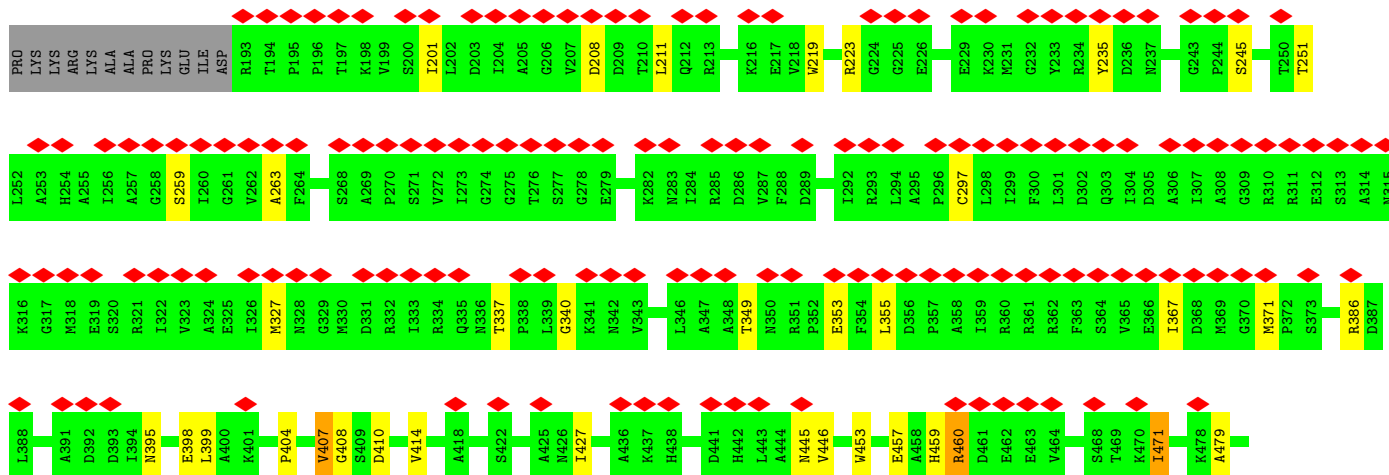
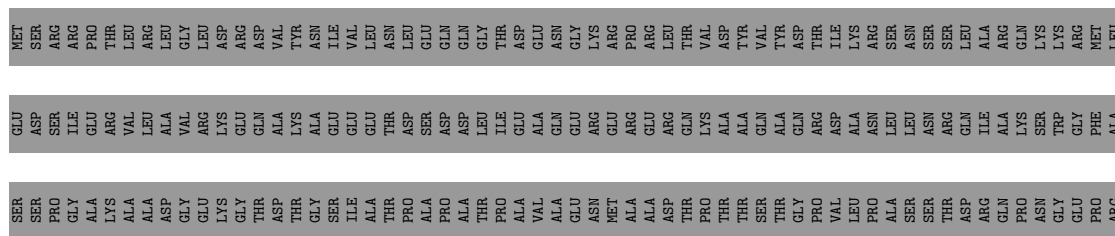
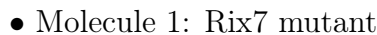
• Molecule 1: Rix7 mutant

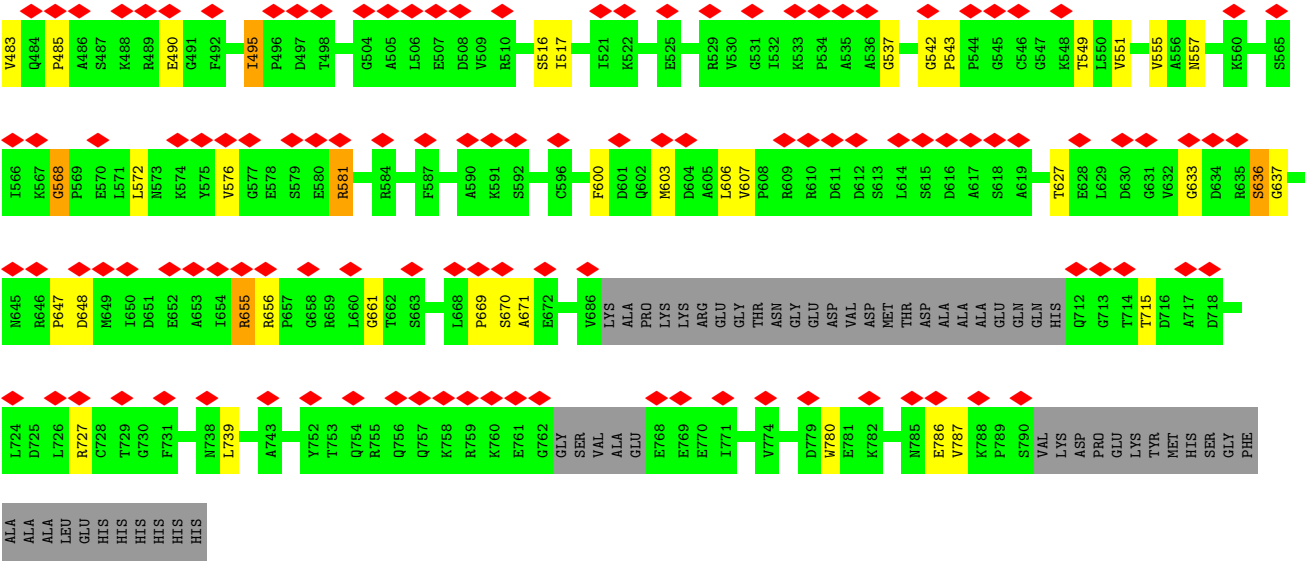


• Molecule 1: Rix7 mutant

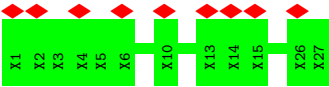








● Molecule 2: unknown protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64386	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1200	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.311	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0796	Depositor
Map size (Å)	266.88, 266.88, 266.88	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	2/4527 (0.0%)	1.25	26/6120 (0.4%)
1	B	0.73	2/4527 (0.0%)	1.24	28/6120 (0.5%)
1	C	0.73	2/4527 (0.0%)	1.24	25/6120 (0.4%)
1	D	0.73	2/4527 (0.0%)	1.25	26/6120 (0.4%)
1	E	0.76	1/4439 (0.0%)	1.28	28/6002 (0.5%)
1	F	0.79	1/4439 (0.0%)	1.27	26/6002 (0.4%)
All	All	0.75	10/26986 (0.0%)	1.25	159/36484 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	PRO	CA-C	7.72	1.56	1.51
1	D	543	PRO	CA-C	7.51	1.56	1.51
1	B	543	PRO	CA-C	7.26	1.55	1.51
1	A	659	ARG	CA-C	6.79	1.55	1.52
1	C	543	PRO	CA-C	6.70	1.55	1.51
1	C	337	THR	CA-CB	6.37	1.59	1.54
1	E	337	THR	CA-CB	6.23	1.59	1.54
1	D	337	THR	CA-CB	6.22	1.59	1.54
1	B	337	THR	CA-CB	6.17	1.59	1.54
1	F	543	PRO	CA-C	5.13	1.55	1.52

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	543	PRO	CA-C-N	-13.08	103.49	119.84
1	E	543	PRO	C-N-CA	-13.08	103.49	119.84
1	F	446	VAL	N-CA-C	-10.71	103.13	112.12
1	D	446	VAL	N-CA-C	-10.37	103.41	112.12
1	B	517	ILE	N-CA-C	8.28	119.15	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	517	ILE	N-CA-C	8.15	119.03	111.45
1	A	517	ILE	N-CA-C	8.03	118.91	111.45
1	D	517	ILE	N-CA-C	7.90	118.80	111.45
1	E	517	ILE	N-CA-C	7.90	118.80	111.45
1	F	517	ILE	N-CA-C	7.81	118.71	111.45
1	E	568	GLY	N-CA-C	7.51	127.67	112.34
1	F	606	LEU	N-CA-C	7.45	119.47	111.36
1	A	606	LEU	N-CA-C	7.41	119.44	111.36
1	B	337	THR	N-CA-C	7.33	123.44	113.77
1	C	337	THR	N-CA-C	7.25	123.34	113.77
1	E	606	LEU	N-CA-C	7.18	119.19	111.36
1	E	337	THR	N-CA-C	7.17	123.24	113.77
1	D	337	THR	N-CA-C	7.16	123.23	113.77
1	C	606	LEU	N-CA-C	7.11	119.11	111.36
1	C	537	GLY	N-CA-C	7.04	121.41	110.91
1	F	542	GLY	CA-C-N	7.03	124.72	119.66
1	F	542	GLY	C-N-CA	7.03	124.72	119.66
1	F	537	GLY	N-CA-C	7.02	120.77	110.38
1	A	670	SER	N-CA-C	7.01	120.93	109.72
1	D	606	LEU	N-CA-C	6.99	118.98	111.36
1	E	535	ALA	N-CA-C	6.95	119.30	110.33
1	C	670	SER	N-CA-C	6.92	120.79	109.72
1	F	490	GLU	N-CA-C	-6.91	103.75	112.93
1	C	786	GLU	N-CA-C	6.87	118.56	111.14
1	B	786	GLU	N-CA-C	6.83	118.52	111.14
1	E	542	GLY	CA-C-N	6.83	127.41	120.38
1	E	542	GLY	C-N-CA	6.83	127.41	120.38
1	B	537	GLY	N-CA-C	6.82	121.06	110.91
1	B	606	LEU	N-CA-C	6.81	118.78	111.36
1	D	786	GLU	N-CA-C	6.79	118.48	111.14
1	F	786	GLU	N-CA-C	6.76	118.44	111.14
1	D	670	SER	N-CA-C	6.75	120.69	109.95
1	B	670	SER	N-CA-C	6.75	120.68	109.95
1	A	786	GLU	N-CA-C	6.73	118.40	111.14
1	D	537	GLY	N-CA-C	6.68	120.87	110.91
1	E	786	GLU	N-CA-C	6.67	118.34	111.14
1	C	630	ASP	N-CA-C	6.64	121.60	112.90
1	B	607	VAL	N-CA-C	6.62	123.17	108.88
1	A	607	VAL	N-CA-C	6.61	123.16	108.88
1	D	572	LEU	N-CA-C	6.59	119.79	110.23
1	F	516	SER	N-CA-C	6.53	118.06	111.07
1	D	607	VAL	N-CA-C	6.50	122.92	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ASN	N-CA-C	6.44	119.40	108.90
1	E	537	GLY	N-CA-C	6.44	120.51	110.91
1	E	607	VAL	N-CA-C	6.44	122.78	108.88
1	E	516	SER	N-CA-C	6.43	117.95	111.07
1	D	516	SER	N-CA-C	6.42	117.94	111.07
1	A	535	ALA	N-CA-C	6.41	118.60	110.33
1	E	671	ALA	N-CA-C	6.39	117.91	111.07
1	C	607	VAL	N-CA-C	6.38	122.67	108.88
1	A	787	VAL	N-CA-C	6.37	117.97	109.37
1	A	516	SER	N-CA-C	6.37	117.89	111.07
1	A	537	GLY	N-CA-C	6.36	120.39	110.91
1	D	445	ASN	N-CA-C	6.35	119.26	108.90
1	F	607	VAL	N-CA-C	6.33	122.55	108.88
1	C	787	VAL	N-CA-C	6.32	117.89	109.37
1	A	445	ASN	N-CA-C	6.31	119.19	108.90
1	B	787	VAL	N-CA-C	6.29	117.86	109.37
1	F	445	ASN	N-CA-C	6.29	119.15	108.90
1	B	572	LEU	N-CA-C	6.28	119.33	110.23
1	B	516	SER	N-CA-C	6.25	117.76	111.07
1	D	787	VAL	N-CA-C	6.23	117.78	109.37
1	F	576	VAL	N-CA-C	6.22	117.58	111.67
1	F	670	SER	N-CA-C	6.21	120.39	109.96
1	E	787	VAL	N-CA-C	6.19	117.72	109.37
1	F	787	VAL	N-CA-C	6.18	117.72	109.37
1	C	445	ASN	N-CA-C	6.18	118.97	108.90
1	C	516	SER	N-CA-C	6.16	117.66	111.07
1	C	637	GLY	N-CA-C	-6.15	106.26	114.25
1	A	337	THR	N-CA-C	6.11	123.31	109.81
1	E	544	PRO	N-CA-C	6.11	125.06	112.47
1	A	615	SER	N-CA-C	6.10	118.23	109.14
1	F	337	THR	N-CA-C	6.07	123.23	109.81
1	F	459	HIS	N-CA-C	6.07	117.56	111.07
1	A	572	LEU	N-CA-C	6.06	119.02	110.23
1	B	631	GLY	N-CA-C	6.06	127.53	113.18
1	E	668	LEU	N-CA-C	6.05	123.18	109.81
1	E	445	ASN	N-CA-C	6.03	118.73	108.90
1	F	568	GLY	N-CA-C	6.03	124.64	112.34
1	A	671	ALA	N-CA-C	6.02	117.51	111.07
1	C	572	LEU	N-CA-C	6.01	118.95	110.23
1	C	671	ALA	N-CA-C	6.00	117.50	111.07
1	D	630	ASP	N-CA-C	6.00	120.76	112.90
1	B	671	ALA	N-CA-C	5.95	117.44	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	637	GLY	N-CA-C	-5.94	106.52	114.25
1	A	613	SER	N-CA-C	5.94	117.70	109.15
1	B	637	GLY	N-CA-C	-5.93	106.54	114.25
1	A	661	GLY	N-CA-C	5.93	122.75	113.86
1	B	491	GLY	N-CA-C	5.85	121.05	113.27
1	D	671	ALA	N-CA-C	5.74	117.21	111.07
1	D	459	HIS	N-CA-C	5.73	117.22	110.97
1	D	542	GLY	CA-C-N	5.73	123.84	119.66
1	D	542	GLY	C-N-CA	5.73	123.84	119.66
1	B	630	ASP	N-CA-C	5.71	120.38	112.90
1	C	459	HIS	N-CA-C	5.71	117.18	111.07
1	A	542	GLY	CA-C-N	5.70	123.82	119.66
1	A	542	GLY	C-N-CA	5.70	123.82	119.66
1	D	798	MET	N-CA-C	5.69	117.29	111.14
1	A	656	ARG	N-CA-C	5.66	116.11	109.60
1	E	370	GLY	N-CA-C	5.61	121.73	112.30
1	C	798	MET	N-CA-C	5.55	117.13	111.14
1	C	542	GLY	CA-C-N	5.54	123.71	119.66
1	C	542	GLY	C-N-CA	5.54	123.71	119.66
1	D	235	TYR	N-CA-C	5.54	118.30	109.65
1	A	459	HIS	N-CA-C	5.49	116.95	110.97
1	E	235	TYR	N-CA-C	5.49	118.21	109.65
1	F	235	TYR	N-CA-C	5.49	118.21	109.65
1	B	235	TYR	N-CA-C	5.48	118.20	109.65
1	F	656	ARG	N-CA-C	5.47	115.89	109.60
1	A	725	ASP	N-CA-C	5.43	117.30	110.24
1	A	235	TYR	N-CA-C	5.43	118.12	109.65
1	B	459	HIS	N-CA-C	5.42	116.87	111.07
1	D	371	MET	N-CA-C	5.41	116.49	109.72
1	A	798	MET	N-CA-C	5.41	116.98	111.14
1	E	459	HIS	N-CA-C	5.41	116.86	110.97
1	E	577	GLY	N-CA-C	5.40	125.98	113.18
1	B	798	MET	N-CA-C	5.39	116.84	111.07
1	E	541	TRP	N-CA-C	5.39	117.87	108.76
1	E	669	PRO	N-CA-C	5.36	123.51	112.47
1	B	542	GLY	CA-C-N	5.35	123.56	119.66
1	B	542	GLY	C-N-CA	5.35	123.56	119.66
1	E	572	LEU	N-CA-C	5.34	117.98	110.23
1	F	572	LEU	N-CA-C	5.34	117.98	110.23
1	F	671	ALA	N-CA-C	5.34	116.79	111.07
1	C	235	TYR	N-CA-C	5.34	117.98	109.65
1	C	658	GLY	N-CA-C	-5.33	107.65	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	658	GLY	N-CA-C	-5.31	107.67	114.37
1	F	208	ASP	N-CA-C	5.23	116.67	110.97
1	B	658	GLY	N-CA-C	-5.22	107.68	113.79
1	F	647	PRO	N-CA-C	5.19	123.16	112.47
1	C	219	TRP	N-CA-C	5.18	116.61	111.07
1	F	655	ARG	N-CA-C	5.17	117.66	111.71
1	C	223	ARG	N-CA-C	5.17	118.04	111.69
1	C	208	ASP	N-CA-C	5.14	116.58	110.97
1	F	219	TRP	N-CA-C	5.13	116.56	111.07
1	D	219	TRP	N-CA-C	5.13	116.56	111.07
1	E	219	TRP	N-CA-C	5.13	116.56	111.07
1	B	208	ASP	N-CA-C	5.13	116.56	110.97
1	F	223	ARG	N-CA-C	5.12	117.99	111.69
1	A	223	ARG	N-CA-C	5.11	117.98	111.69
1	B	527	PHE	N-CA-C	5.10	116.84	111.28
1	D	208	ASP	N-CA-C	5.10	116.53	110.97
1	B	219	TRP	N-CA-C	5.09	116.52	111.07
1	C	725	ASP	N-CA-C	5.09	117.42	110.24
1	C	527	PHE	N-CA-C	5.09	116.83	111.28
1	B	223	ARG	N-CA-C	5.06	117.91	111.69
1	D	527	PHE	N-CA-C	5.05	116.79	111.28
1	A	658	GLY	N-CA-C	-5.04	108.02	114.37
1	E	223	ARG	N-CA-C	5.04	117.88	111.69
1	E	527	PHE	N-CA-C	5.03	116.76	111.28
1	D	725	ASP	N-CA-C	5.03	117.33	110.24
1	B	725	ASP	N-CA-C	5.02	117.32	110.24
1	A	219	TRP	N-CA-C	5.01	116.43	111.07
1	B	724	LEU	N-CA-C	5.00	116.73	111.28

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	4454	0	4506	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4454	0	4506	40	0
1	C	4454	0	4506	31	0
1	D	4454	0	4506	32	0
1	E	4369	0	4424	23	0
1	F	4369	0	4424	24	0
2	G	135	0	32	0	0
3	A	62	0	24	8	0
3	B	62	0	24	6	0
3	C	62	0	24	2	0
3	D	62	0	24	2	0
3	E	31	0	12	1	0
3	F	62	0	24	2	0
All	All	27030	0	27036	153	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 (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:SER:O	1:F:407:VAL:HG11	1.86	0.76
1:A:351:ARG:HH22	1:B:311:ARG:HB2	1.52	0.74
1:B:607:VAL:HG12	1:B:651:ASP:H	1.52	0.72
1:E:544:PRO:HB3	1:E:645:ASN:ND2	2.06	0.71
1:C:607:VAL:HG12	1:C:651:ASP:H	1.56	0.70
1:D:404:PRO:HB3	1:D:595:PRO:HD2	1.75	0.68
1:C:495:ILE:H	1:C:495:ILE:HD13	1.59	0.67
1:D:495:ILE:HD13	1:D:495:ILE:H	1.60	0.67
1:E:495:ILE:H	1:E:495:ILE:HD13	1.58	0.66
1:D:607:VAL:HG12	1:D:651:ASP:H	1.61	0.66
1:F:495:ILE:H	1:F:495:ILE:HD13	1.58	0.66
1:B:495:ILE:H	1:B:495:ILE:HD13	1.60	0.65
3:A:901:ATP:H5'1	1:B:656:ARG:HH12	1.60	0.65
1:A:495:ILE:H	1:A:495:ILE:HD13	1.61	0.63
1:B:607:VAL:HG13	1:B:654:ILE:HD13	1.80	0.63
1:D:567:LYS:HD3	1:E:627:THR:HG23	1.80	0.62
1:A:251:THR:HG21	3:A:902:ATP:H3'	1.81	0.62
1:C:251:THR:HG21	3:C:902:ATP:H3'	1.82	0.62
1:D:251:THR:HG21	3:D:902:ATP:H3'	1.83	0.60
1:F:251:THR:HG21	3:F:902:ATP:H3'	1.84	0.60
1:E:251:THR:HG21	3:E:901:ATP:H3'	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:VAL:HG13	1:D:654:ILE:HD13	1.84	0.59
1:C:607:VAL:HG13	1:C:654:ILE:HD13	1.85	0.59
1:B:251:THR:HG21	3:B:902:ATP:H3'	1.84	0.59
1:F:655:ARG:O	1:F:661:GLY:HA2	2.02	0.58
1:E:479:ALA:O	1:E:483:VAL:HG23	2.03	0.58
1:A:607:VAL:HG12	1:A:651:ASP:H	1.69	0.58
1:A:479:ALA:O	1:A:483:VAL:HG23	2.03	0.58
1:D:488:LYS:NZ	1:E:360:ARG:HH22	2.02	0.57
1:F:353:GLU:HG2	1:F:581:ARG:HG2	1.87	0.56
1:A:351:ARG:NH2	1:B:311:ARG:HB2	2.21	0.56
3:A:901:ATP:H5'1	1:B:656:ARG:NH1	2.21	0.56
1:A:550:LEU:HD11	3:A:901:ATP:H2'	1.88	0.55
1:E:607:VAL:HG13	1:E:654:ILE:HD13	1.87	0.55
1:F:471:ILE:H	1:F:471:ILE:HD13	1.70	0.55
1:A:407:VAL:HG12	1:A:408:GLY:H	1.73	0.54
1:C:479:ALA:O	1:C:483:VAL:HG23	2.08	0.54
1:F:479:ALA:O	1:F:483:VAL:HG23	2.07	0.54
1:B:479:ALA:O	1:B:483:VAL:HG23	2.07	0.54
1:A:258:GLY:O	1:F:460:ARG:NH2	2.41	0.53
1:D:407:VAL:HG12	1:D:408:GLY:H	1.74	0.53
1:E:471:ILE:H	1:E:471:ILE:HD13	1.73	0.53
1:D:479:ALA:O	1:D:483:VAL:HG23	2.08	0.53
1:A:395:ASN:HD22	1:A:398:GLU:HG3	1.72	0.53
1:B:407:VAL:HG12	1:B:408:GLY:H	1.72	0.53
1:E:453:TRP:NE1	1:F:211:LEU:HG	2.24	0.53
1:E:414:VAL:HG22	1:E:483:VAL:HG21	1.91	0.52
1:A:471:ILE:H	1:A:471:ILE:HD13	1.74	0.52
1:C:407:VAL:HG12	1:C:408:GLY:H	1.74	0.52
1:B:395:ASN:HD22	1:B:398:GLU:HG3	1.75	0.52
1:E:607:VAL:HG12	1:E:651:ASP:H	1.74	0.52
1:D:656:ARG:HH21	1:D:659:ARG:HG3	1.75	0.52
1:D:471:ILE:HD13	1:D:471:ILE:H	1.74	0.51
1:F:395:ASN:HD22	1:F:398:GLU:HG3	1.75	0.51
1:C:567:LYS:HD3	1:D:627:THR:HG23	1.93	0.51
1:C:551:VAL:O	1:C:555:VAL:HG23	2.11	0.51
1:D:395:ASN:HD22	1:D:398:GLU:HG3	1.76	0.51
1:E:546:CYS:SG	1:E:732:SER:HB2	2.51	0.51
1:B:550:LEU:HD11	3:B:901:ATP:H2'	1.92	0.51
1:C:373:SER:H	1:C:376:ALA:HB3	1.76	0.50
1:C:471:ILE:HD13	1:C:471:ILE:H	1.76	0.50
1:D:550:LEU:HD11	3:D:901:ATP:H2'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ASP:O	1:F:414:VAL:HG23	2.11	0.50
1:C:395:ASN:HD22	1:C:398:GLU:HG3	1.76	0.50
1:E:407:VAL:HG12	1:E:408:GLY:H	1.78	0.49
1:C:748:LEU:HD21	1:D:530:VAL:HG11	1.93	0.49
1:C:550:LEU:HD11	3:C:901:ATP:H2'	1.94	0.49
1:D:490:GLU:HG2	1:D:491:GLY:H	1.77	0.49
1:B:646:ARG:HH12	1:C:611:ASP:HA	1.78	0.48
1:A:201:ILE:H	1:A:201:ILE:HD12	1.78	0.48
1:B:551:VAL:O	1:B:555:VAL:HG23	2.14	0.48
1:E:263:ALA:HB3	1:E:297:CYS:SG	2.53	0.48
1:A:553:LYS:HZ1	1:B:632:VAL:HA	1.77	0.48
1:B:263:ALA:HB3	1:B:297:CYS:SG	2.53	0.48
1:D:485:PRO:C	1:D:487:SER:H	2.22	0.48
1:F:263:ALA:HB3	1:F:297:CYS:SG	2.53	0.48
1:A:263:ALA:HB3	1:A:297:CYS:SG	2.53	0.48
1:E:206:GLY:HA2	1:E:379:GLN:NE2	2.29	0.48
1:E:635:ARG:HD3	1:E:635:ARG:H	1.79	0.48
1:B:656:ARG:HH21	1:B:659:ARG:HG3	1.77	0.48
1:F:407:VAL:HG12	1:F:408:GLY:H	1.78	0.48
3:A:901:ATP:C5'	1:B:656:ARG:HH12	2.26	0.48
1:B:471:ILE:H	1:B:471:ILE:HD13	1.77	0.47
1:B:270:PRO:HG2	1:C:325:GLU:HG2	1.96	0.47
1:F:600:PHE:HB3	1:F:603:MET:SD	2.54	0.47
1:B:373:SER:H	1:B:376:ALA:HB3	1.80	0.47
1:E:544:PRO:HB3	1:E:645:ASN:HD21	1.80	0.47
1:B:632:VAL:HG12	1:B:633:GLY:H	1.81	0.46
1:E:395:ASN:HD22	1:E:398:GLU:HG3	1.80	0.46
1:A:456:LEU:HD13	1:B:219:TRP:NE1	2.31	0.46
1:A:600:PHE:HB3	1:A:603:MET:SD	2.56	0.45
1:C:201:ILE:HD12	1:C:201:ILE:H	1.82	0.45
1:C:263:ALA:HB3	1:C:297:CYS:SG	2.57	0.45
1:D:263:ALA:HB3	1:D:297:CYS:SG	2.57	0.45
1:E:410:ASP:O	1:E:414:VAL:HG23	2.16	0.45
3:A:901:ATP:PG	1:B:659:ARG:NH2	2.90	0.45
1:B:567:LYS:HD3	1:C:627:THR:HG23	1.98	0.45
1:D:551:VAL:O	1:D:555:VAL:HG23	2.16	0.45
1:E:201:ILE:HD12	1:E:201:ILE:H	1.81	0.45
3:B:901:ATP:PG	1:C:659:ARG:NH2	2.90	0.44
1:B:456:LEU:HD13	1:C:219:TRP:NE1	2.32	0.44
1:F:495:ILE:HB	1:F:557:ASN:HD22	1.82	0.44
1:C:456:LEU:HD13	1:D:219:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HH22	1:B:311:ARG:CB	2.24	0.44
1:C:656:ARG:HH21	1:C:659:ARG:HG3	1.82	0.44
1:D:273:ILE:HG13	1:E:321:ARG:HD3	1.99	0.44
1:A:608:PRO:HB3	1:A:649:MET:HB3	2.00	0.43
1:B:410:ASP:O	1:B:414:VAL:HG23	2.18	0.43
1:A:259:SER:HB2	1:F:457:GLU:HG2	2.00	0.43
1:F:414:VAL:HG22	1:F:483:VAL:HG21	2.01	0.43
1:A:567:LYS:HD3	1:B:627:THR:HG23	1.99	0.43
1:B:600:PHE:HB3	1:B:603:MET:SD	2.59	0.43
1:D:201:ILE:H	1:D:201:ILE:HD12	1.83	0.43
1:D:373:SER:H	1:D:376:ALA:HB3	1.82	0.43
1:A:215:LEU:HB2	1:F:453:TRP:CZ2	2.54	0.43
1:C:607:VAL:HG11	1:C:650:ILE:HG23	2.01	0.43
1:C:270:PRO:HG2	1:D:325:GLU:HG2	2.01	0.43
1:A:748:LEU:HD21	1:B:530:VAL:HG11	2.00	0.42
1:A:545:GLY:HA3	1:B:656:ARG:HD2	2.00	0.42
1:E:457:GLU:HG2	1:F:259:SER:HB2	2.02	0.42
1:B:457:GLU:O	1:B:460:ARG:HG2	2.20	0.42
1:E:547:GLY:O	1:E:551:VAL:HG23	2.20	0.42
1:A:551:VAL:O	1:A:555:VAL:HG23	2.18	0.42
1:D:476:PHE:O	1:D:480:VAL:HG23	2.20	0.42
1:A:543:PRO:HA	1:A:544:PRO:HD3	1.94	0.42
1:A:349:THR:HG21	1:A:355:LEU:HD11	2.02	0.41
1:C:600:PHE:HB3	1:C:603:MET:SD	2.59	0.41
1:A:410:ASP:O	1:A:414:VAL:HG23	2.20	0.41
1:D:600:PHE:HB3	1:D:603:MET:SD	2.60	0.41
1:B:201:ILE:HD12	1:B:201:ILE:H	1.84	0.41
1:D:371:MET:HA	1:D:372:PRO:HD3	1.85	0.41
1:B:632:VAL:HG12	1:B:633:GLY:N	2.35	0.41
1:C:485:PRO:C	1:C:487:SER:H	2.28	0.41
1:D:648:ASP:HB3	1:D:800:SER:HB3	2.03	0.41
3:A:901:ATP:O3G	1:B:659:ARG:NH2	2.50	0.41
1:B:646:ARG:NH1	1:C:610:ARG:O	2.54	0.41
3:B:901:ATP:PG	1:C:659:ARG:HH22	2.44	0.41
1:A:457:GLU:O	1:A:460:ARG:HG2	2.21	0.41
1:F:349:THR:HG21	1:F:355:LEU:HD11	2.02	0.41
3:A:901:ATP:PG	1:B:659:ARG:HH22	2.44	0.41
1:D:349:THR:HG21	1:D:355:LEU:HD11	2.03	0.41
1:F:551:VAL:O	1:F:555:VAL:HG23	2.20	0.41
1:F:636:SER:HB3	1:F:637:GLY:H	1.71	0.41
1:D:410:ASP:O	1:D:414:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:PRO:HA	1:D:544:PRO:HD3	1.93	0.40
1:C:410:ASP:O	1:C:414:VAL:HG23	2.21	0.40
1:C:490:GLU:HG3	1:C:589:ARG:HD3	2.04	0.40
1:D:457:GLU:O	1:D:460:ARG:HG2	2.21	0.40
1:F:201:ILE:H	1:F:201:ILE:HD12	1.85	0.40
1:A:351:ARG:NH2	1:B:311:ARG:NE	2.70	0.40
3:B:901:ATP:O1G	1:C:659:ARG:NH2	2.49	0.40
1:F:251:THR:CG2	3:F:902:ATP:H3'	2.51	0.40
1:B:251:THR:CG2	3:B:902:ATP:H3'	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	572/813 (70%)	521 (91%)	38 (7%)	13 (2%)	5	28
1	B	572/813 (70%)	527 (92%)	32 (6%)	13 (2%)	5	28
1	C	572/813 (70%)	521 (91%)	38 (7%)	13 (2%)	5	28
1	D	572/813 (70%)	528 (92%)	35 (6%)	9 (2%)	7	37
1	E	562/813 (69%)	513 (91%)	39 (7%)	10 (2%)	6	33
1	F	562/813 (69%)	516 (92%)	35 (6%)	11 (2%)	6	31
All	All	3412/4878 (70%)	3126 (92%)	217 (6%)	69 (2%)	8	31

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	636	SER
1	A	669	PRO
1	B	490	GLU

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Mol	Chain	Res	Type
1	B	631	GLY
1	B	669	PRO
1	C	669	PRO
1	D	669	PRO
1	E	544	PRO
1	A	404	PRO
1	A	460	ARG
1	A	485	PRO
1	A	486	ALA
1	A	568	GLY
1	A	648	ASP
1	A	715	THR
1	B	404	PRO
1	B	460	ARG
1	B	568	GLY
1	B	632	VAL
1	B	648	ASP
1	B	715	THR
1	C	404	PRO
1	C	460	ARG
1	C	568	GLY
1	C	636	SER
1	C	648	ASP
1	C	715	THR
1	D	404	PRO
1	D	460	ARG
1	D	648	ASP
1	D	715	THR
1	E	404	PRO
1	E	460	ARG
1	E	493	SER
1	E	568	GLY
1	E	715	THR
1	F	404	PRO
1	F	460	ARG
1	F	568	GLY
1	F	648	ASP
1	F	669	PRO
1	F	715	THR
1	A	340	GLY
1	A	386	ARG
1	A	633	GLY

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Mol	Chain	Res	Type
1	B	340	GLY
1	B	386	ARG
1	C	340	GLY
1	C	386	ARG
1	C	491	GLY
1	C	569	PRO
1	D	340	GLY
1	D	386	ARG
1	E	340	GLY
1	E	648	ASP
1	F	340	GLY
1	F	386	ARG
1	F	633	GLY
1	F	636	SER
1	B	569	PRO
1	E	386	ARG
1	F	485	PRO
1	A	569	PRO
1	E	789	PRO
1	D	270	PRO
1	D	569	PRO
1	B	270	PRO
1	C	270	PRO
1	C	632	VAL

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	481/671 (72%)	469 (98%)	12 (2%)	42	62
1	B	481/671 (72%)	468 (97%)	13 (3%)	39	59
1	C	481/671 (72%)	468 (97%)	13 (3%)	39	59
1	D	481/671 (72%)	467 (97%)	14 (3%)	37	58
1	E	471/671 (70%)	457 (97%)	14 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	471/671 (70%)	457 (97%)	14 (3%)	36 57
All	All	2866/4026 (71%)	2786 (97%)	80 (3%)	38 59

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	ARG
1	A	367	ILE
1	A	399	LEU
1	A	407	VAL
1	A	427	ILE
1	A	471	ILE
1	A	492	PHE
1	A	495	ILE
1	A	627	THR
1	A	727	ARG
1	A	739	LEU
1	A	780	TRP
1	B	325	GLU
1	B	367	ILE
1	B	399	LEU
1	B	407	VAL
1	B	427	ILE
1	B	471	ILE
1	B	488	LYS
1	B	495	ILE
1	B	627	THR
1	B	656	ARG
1	B	727	ARG
1	B	739	LEU
1	B	780	TRP
1	C	325	GLU
1	C	367	ILE
1	C	399	LEU
1	C	407	VAL
1	C	427	ILE
1	C	471	ILE
1	C	495	ILE
1	C	624	THR
1	C	627	THR
1	C	656	ARG
1	C	727	ARG

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Mol	Chain	Res	Type
1	C	739	LEU
1	C	780	TRP
1	D	325	GLU
1	D	367	ILE
1	D	399	LEU
1	D	407	VAL
1	D	427	ILE
1	D	471	ILE
1	D	488	LYS
1	D	495	ILE
1	D	624	THR
1	D	627	THR
1	D	648	ASP
1	D	727	ARG
1	D	739	LEU
1	D	780	TRP
1	E	325	GLU
1	E	367	ILE
1	E	399	LEU
1	E	407	VAL
1	E	427	ILE
1	E	471	ILE
1	E	484	GLN
1	E	495	ILE
1	E	624	THR
1	E	627	THR
1	E	635	ARG
1	E	727	ARG
1	E	739	LEU
1	E	780	TRP
1	F	327	MET
1	F	367	ILE
1	F	371	MET
1	F	399	LEU
1	F	407	VAL
1	F	427	ILE
1	F	471	ILE
1	F	495	ILE
1	F	549	THR
1	F	581	ARG
1	F	627	THR
1	F	727	ARG

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Mol	Chain	Res	Type
1	F	739	LEU
1	F	780	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	303	GLN
1	A	379	GLN
1	A	395	ASN
1	A	424	GLN
1	A	445	ASN
1	A	450	GLN
1	A	502	HIS
1	A	557	ASN
1	A	602	GLN
1	A	756	GLN
1	A	785	ASN
1	B	242	HIS
1	B	379	GLN
1	B	424	GLN
1	B	445	ASN
1	B	450	GLN
1	B	557	ASN
1	B	756	GLN
1	B	785	ASN
1	C	379	GLN
1	C	424	GLN
1	C	445	ASN
1	C	450	GLN
1	C	502	HIS
1	C	557	ASN
1	C	756	GLN
1	C	785	ASN
1	D	303	GLN
1	D	379	GLN
1	D	424	GLN
1	D	445	ASN
1	D	450	GLN
1	D	502	HIS
1	D	557	ASN
1	D	602	GLN

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Mol	Chain	Res	Type
1	D	756	GLN
1	D	785	ASN
1	E	379	GLN
1	E	424	GLN
1	E	445	ASN
1	E	562	ASN
1	E	756	GLN
1	E	785	ASN
1	F	342	ASN
1	F	395	ASN
1	F	424	GLN
1	F	445	ASN
1	F	557	ASN
1	F	585	GLN
1	F	756	GLN
1	F	785	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](#)

11 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	ATP	C	901	-	32,33,33	1.36	4 (12%)	48,52,52	1.84	14 (29%)
3	ATP	A	901	-	32,33,33	1.34	3 (9%)	48,52,52	1.86	13 (27%)
3	ATP	C	902	-	32,33,33	1.37	4 (12%)	48,52,52	1.88	9 (18%)
3	ATP	B	901	-	32,33,33	1.35	3 (9%)	48,52,52	1.90	15 (31%)
3	ATP	E	901	-	32,33,33	1.34	4 (12%)	48,52,52	1.82	10 (20%)
3	ATP	A	902	-	32,33,33	1.38	3 (9%)	48,52,52	1.86	11 (22%)
3	ATP	B	902	-	32,33,33	1.47	3 (9%)	48,52,52	1.91	11 (22%)
3	ATP	D	901	-	32,33,33	1.36	4 (12%)	48,52,52	1.84	15 (31%)
3	ATP	F	901	-	32,33,33	1.46	7 (21%)	48,52,52	1.79	9 (18%)
3	ATP	D	902	-	32,33,33	1.38	3 (9%)	48,52,52	1.91	11 (22%)
3	ATP	F	902	-	32,33,33	1.36	4 (12%)	48,52,52	1.81	9 (18%)

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	901	-	-	4/22/38/38	0/3/3/3
3	ATP	A	901	-	-	5/22/38/38	0/3/3/3
3	ATP	C	902	-	-	3/22/38/38	0/3/3/3
3	ATP	B	901	-	-	4/22/38/38	0/3/3/3
3	ATP	E	901	-	-	3/22/38/38	0/3/3/3
3	ATP	A	902	-	-	3/22/38/38	0/3/3/3
3	ATP	B	902	-	-	3/22/38/38	0/3/3/3
3	ATP	D	901	-	-	4/22/38/38	0/3/3/3
3	ATP	F	901	-	-	5/22/38/38	0/3/3/3
3	ATP	D	902	-	-	3/22/38/38	0/3/3/3
3	ATP	F	902	-	-	3/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	ATP	C5-C4	5.13	1.48	1.39
3	C	901	ATP	C5-C4	4.92	1.47	1.39
3	D	901	ATP	C5-C4	4.91	1.47	1.39
3	A	901	ATP	C5-C4	4.87	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	ATP	C5-C4	4.86	1.47	1.39
3	D	902	ATP	C5-C4	4.84	1.47	1.39
3	A	902	ATP	C5-C4	4.83	1.47	1.39
3	B	901	ATP	C5-C4	4.80	1.47	1.39
3	F	901	ATP	C5-C4	4.77	1.47	1.39
3	E	901	ATP	C5-C4	4.75	1.47	1.39
3	F	902	ATP	C5-C4	4.73	1.47	1.39
3	B	902	ATP	C5-C6	3.34	1.50	1.41
3	D	902	ATP	C5-C6	3.18	1.49	1.41
3	A	902	ATP	C5-C6	3.07	1.49	1.41
3	C	902	ATP	C5-C6	2.97	1.49	1.41
3	F	902	ATP	C5-C6	2.81	1.48	1.41
3	F	901	ATP	C5-C6	2.81	1.48	1.41
3	D	901	ATP	C5-C6	2.80	1.48	1.41
3	E	901	ATP	C5-C6	2.79	1.48	1.41
3	A	901	ATP	C5-C6	2.77	1.48	1.41
3	B	901	ATP	C5-C6	2.76	1.48	1.41
3	C	901	ATP	C5-C6	2.71	1.48	1.41
3	F	901	ATP	C8-N7	2.40	1.36	1.31
3	C	901	ATP	C8-N7	2.30	1.36	1.31
3	F	902	ATP	C8-N7	2.29	1.36	1.31
3	A	901	ATP	C8-N7	2.27	1.36	1.31
3	C	902	ATP	C8-N7	2.26	1.36	1.31
3	D	902	ATP	C8-N7	2.25	1.36	1.31
3	D	901	ATP	C8-N7	2.25	1.36	1.31
3	B	901	ATP	C8-N7	2.24	1.36	1.31
3	E	901	ATP	C8-N7	2.23	1.36	1.31
3	B	902	ATP	C8-N7	2.21	1.35	1.31
3	F	902	ATP	C5-N7	-2.21	1.35	1.39
3	F	901	ATP	C5-N7	-2.21	1.35	1.39
3	A	902	ATP	C8-N7	2.20	1.35	1.31
3	F	901	ATP	PB-O3A	2.20	1.61	1.59
3	F	901	ATP	PA-O3A	2.17	1.61	1.59
3	E	901	ATP	C5-N7	-2.17	1.35	1.39
3	C	901	ATP	C5-N7	-2.13	1.35	1.39
3	C	902	ATP	C5-N7	-2.04	1.35	1.39
3	D	901	ATP	C5-N7	-2.03	1.35	1.39
3	F	901	ATP	PB-O3B	2.03	1.61	1.59

All (127) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	ATP	C5-C4-N3	-6.11	118.31	126.72
3	F	901	ATP	C5-C4-N3	-6.01	118.44	126.72
3	F	902	ATP	C5-C4-N3	-6.00	118.46	126.72
3	D	902	ATP	C5-C4-N3	-5.87	118.64	126.72
3	E	901	ATP	C5-C4-N3	-5.81	118.71	126.72
3	A	902	ATP	C5-C4-N3	-5.79	118.74	126.72
3	B	902	ATP	C5-C4-N3	-5.56	119.07	126.72
3	D	901	ATP	C5-C4-N3	-5.37	119.32	126.72
3	B	901	ATP	C5-C4-N3	-5.33	119.38	126.72
3	A	901	ATP	C5-C4-N3	-5.31	119.40	126.72
3	C	901	ATP	C5-C4-N3	-5.24	119.51	126.72
3	C	902	ATP	N3-C4-N9	5.23	136.06	127.17
3	B	902	ATP	N3-C4-N9	5.21	136.02	127.17
3	D	902	ATP	N3-C4-N9	4.95	135.59	127.17
3	F	902	ATP	N3-C4-N9	4.93	135.55	127.17
3	E	901	ATP	N3-C4-N9	4.86	135.44	127.17
3	A	902	ATP	N3-C4-N9	4.81	135.36	127.17
3	A	901	ATP	N3-C4-N9	4.71	135.17	127.17
3	D	901	ATP	N3-C4-N9	4.68	135.12	127.17
3	B	901	ATP	N3-C4-N9	4.63	135.04	127.17
3	F	901	ATP	N3-C4-N9	4.61	135.01	127.17
3	C	901	ATP	N3-C4-N9	4.56	134.93	127.17
3	B	902	ATP	C4-N9-C8	4.50	110.46	105.74
3	F	901	ATP	C2-N3-C4	3.84	121.21	111.83
3	A	902	ATP	C2-N3-C4	3.81	121.13	111.83
3	D	902	ATP	C4-C5-N7	-3.79	106.25	110.58
3	D	902	ATP	C2-N3-C4	3.78	121.05	111.83
3	C	902	ATP	C2-N3-C4	3.75	121.00	111.83
3	F	902	ATP	C2-N3-C4	3.74	120.98	111.83
3	D	902	ATP	C4-N9-C8	3.66	109.58	105.74
3	E	901	ATP	C2-N3-C4	3.64	120.72	111.83
3	B	901	ATP	C4-N9-C8	3.59	109.51	105.74
3	A	901	ATP	C4-N9-C8	3.59	109.50	105.74
3	F	901	ATP	C4-C5-N7	-3.58	106.48	110.58
3	A	902	ATP	C4-C5-N7	-3.54	106.53	110.58
3	C	902	ATP	C4-N9-C8	3.49	109.40	105.74
3	E	901	ATP	C4-C5-N7	-3.47	106.61	110.58
3	B	902	ATP	C2-N3-C4	3.47	120.31	111.83
3	F	902	ATP	C4-C5-N7	-3.47	106.62	110.58
3	B	902	ATP	C4-C5-N7	-3.43	106.66	110.58
3	D	901	ATP	C2-N3-C4	3.42	120.18	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	901	ATP	N3-C2-N1	-3.39	123.45	128.58
3	C	902	ATP	C4-C5-N7	-3.39	106.71	110.58
3	A	901	ATP	C2-N3-C4	3.36	120.03	111.83
3	C	901	ATP	C2-N3-C4	3.35	120.02	111.83
3	B	901	ATP	C2-N3-C4	3.34	119.98	111.83
3	D	901	ATP	C4-N9-C8	3.32	109.22	105.74
3	B	901	ATP	C4-C5-N7	-3.30	106.81	110.58
3	A	902	ATP	N3-C2-N1	-3.30	123.59	128.58
3	E	901	ATP	C4-N9-C8	3.22	109.12	105.74
3	C	901	ATP	C4-N9-C8	3.21	109.11	105.74
3	F	902	ATP	N3-C2-N1	-3.16	123.80	128.58
3	A	902	ATP	C4-N9-C8	3.15	109.04	105.74
3	A	901	ATP	C4-C5-N7	-3.14	106.99	110.58
3	D	902	ATP	N3-C2-N1	-3.13	123.84	128.58
3	E	901	ATP	N3-C2-N1	-3.11	123.88	128.58
3	D	901	ATP	C4-C5-N7	-3.11	107.03	110.58
3	C	901	ATP	N3-C2-N1	-3.07	123.94	128.58
3	A	901	ATP	N3-C2-N1	-3.05	123.96	128.58
3	C	901	ATP	C4-C5-N7	-3.03	107.12	110.58
3	D	901	ATP	N3-C2-N1	-3.02	124.01	128.58
3	C	902	ATP	N3-C2-N1	-2.97	124.09	128.58
3	B	902	ATP	C5-N7-C8	2.96	108.10	103.45
3	D	902	ATP	C5-N7-C8	2.96	108.10	103.45
3	B	901	ATP	N3-C2-N1	-2.92	124.16	128.58
3	F	902	ATP	C4-N9-C8	2.90	108.79	105.74
3	B	902	ATP	N9-C8-N7	-2.87	109.86	113.94
3	B	901	ATP	O3B-PB-O1B	-2.80	102.29	110.70
3	B	902	ATP	N3-C2-N1	-2.75	124.41	128.58
3	A	902	ATP	C5-N7-C8	2.75	107.77	103.45
3	E	901	ATP	C5-N7-C8	2.71	107.71	103.45
3	F	902	ATP	C5-N7-C8	2.71	107.71	103.45
3	C	902	ATP	C5-N7-C8	2.70	107.69	103.45
3	B	901	ATP	O3B-PG-O1G	-2.60	97.38	111.04
3	B	901	ATP	C5-N7-C8	2.58	107.51	103.45
3	D	901	ATP	O3B-PB-O1B	-2.57	102.96	110.70
3	C	901	ATP	O3B-PB-O1B	-2.57	102.97	110.70
3	C	901	ATP	C3'-C2'-C1'	2.56	106.31	101.46
3	D	902	ATP	N9-C8-N7	-2.56	110.30	113.94
3	F	901	ATP	C5-N7-C8	2.56	107.47	103.45
3	C	901	ATP	O3G-PG-O2G	2.56	117.40	107.80
3	F	901	ATP	C3'-C2'-C1'	2.55	106.30	101.46
3	D	901	ATP	C3'-C2'-C1'	2.53	106.25	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ATP	O2B-PB-O1B	2.53	124.19	112.44
3	B	901	ATP	C3'-C2'-C1'	2.52	106.24	101.46
3	A	901	ATP	O3A-PB-O1B	-2.51	103.17	110.70
3	A	901	ATP	C5-N7-C8	2.50	107.38	103.45
3	A	901	ATP	O2B-PB-O1B	2.46	123.88	112.44
3	A	901	ATP	O3B-PB-O1B	-2.44	103.35	110.70
3	D	901	ATP	C5-N7-C8	2.40	107.23	103.45
3	D	902	ATP	C6-C5-N7	2.39	136.70	132.09
3	C	902	ATP	N9-C8-N7	-2.37	110.57	113.94
3	C	901	ATP	C5-N7-C8	2.36	107.16	103.45
3	B	901	ATP	N9-C8-N7	-2.35	110.60	113.94
3	C	902	ATP	C2'-C1'-N9	-2.34	107.49	113.30
3	A	901	ATP	C3'-C2'-C1'	2.33	105.87	101.46
3	C	901	ATP	O2B-PB-O1B	2.31	123.21	112.44
3	A	902	ATP	C6-C5-N7	2.30	136.53	132.09
3	F	901	ATP	C4-N9-C8	2.29	108.14	105.74
3	A	901	ATP	N9-C8-N7	-2.28	110.70	113.94
3	C	901	ATP	O3A-PB-O1B	-2.28	103.84	110.70
3	D	901	ATP	O3A-PB-O1B	-2.28	103.86	110.70
3	A	902	ATP	C3'-C2'-C1'	2.27	105.77	101.46
3	E	901	ATP	N9-C8-N7	-2.27	110.71	113.94
3	D	901	ATP	O2B-PB-O1B	2.27	122.98	112.44
3	C	901	ATP	O3B-PG-O1G	-2.25	99.18	111.04
3	A	902	ATP	N9-C8-N7	-2.24	110.76	113.94
3	B	902	ATP	C6-C5-N7	2.20	136.33	132.09
3	B	901	ATP	O3A-PB-O1B	-2.17	104.17	110.70
3	D	902	ATP	C2'-C1'-N9	-2.16	107.95	113.30
3	A	902	ATP	O4'-C4'-C3'	2.15	109.42	105.15
3	F	902	ATP	N9-C8-N7	-2.14	110.89	113.94
3	D	901	ATP	O3G-PG-O2G	2.14	115.83	107.80
3	E	901	ATP	O4'-C1'-N9	-2.14	103.98	108.09
3	B	902	ATP	O4'-C1'-N9	-2.13	103.99	108.09
3	B	902	ATP	O4'-C4'-C3'	2.13	109.37	105.15
3	D	901	ATP	O3B-PG-O1G	-2.12	99.87	111.04
3	F	901	ATP	C6-C5-N7	2.10	136.15	132.09
3	D	901	ATP	N9-C8-N7	-2.09	110.97	113.94
3	E	901	ATP	C6-C5-N7	2.08	136.10	132.09
3	F	902	ATP	C6-C5-N7	2.05	136.04	132.09
3	C	901	ATP	N9-C8-N7	-2.04	111.05	113.94
3	B	901	ATP	C6-C5-N7	2.04	136.01	132.09
3	A	901	ATP	C6-C5-N7	2.03	136.01	132.09
3	D	901	ATP	C6-C5-N7	2.03	136.00	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	ATP	O4'-C4'-C3'	2.01	109.13	105.15
3	B	901	ATP	O4'-C4'-C3'	2.00	109.13	105.15

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	PB-O3B-PG-O2G
3	A	901	ATP	PB-O3B-PG-O3G
3	B	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O2G
3	D	901	ATP	PB-O3B-PG-O2G
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C5'-O5'-PA-O3A
3	C	902	ATP	O4'-C4'-C5'-O5'
3	D	902	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PA-O3A-PB-O1B
3	B	901	ATP	PA-O3A-PB-O1B
3	C	901	ATP	PA-O3A-PB-O1B
3	D	901	ATP	PA-O3A-PB-O1B
3	A	902	ATP	O4'-C4'-C5'-O5'
3	B	902	ATP	O4'-C4'-C5'-O5'
3	F	902	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	F	901	ATP	C2'-C1'-N9-C8
3	A	901	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PA-O3A-PB-O2B
3	C	901	ATP	PA-O3A-PB-O2B
3	C	902	ATP	PA-O3A-PB-O1B
3	D	901	ATP	PA-O3A-PB-O2B
3	F	902	ATP	PA-O3A-PB-O1B
3	F	901	ATP	C2'-C1'-N9-C4
3	A	902	ATP	PA-O3A-PB-O1B
3	B	902	ATP	PA-O3A-PB-O1B
3	C	902	ATP	PA-O3A-PB-O2B
3	D	902	ATP	PA-O3A-PB-O1B
3	E	901	ATP	PA-O3A-PB-O1B
3	F	902	ATP	PA-O3A-PB-O2B
3	F	901	ATP	O4'-C1'-N9-C8
3	A	901	ATP	PB-O3B-PG-O1G
3	A	902	ATP	PA-O3A-PB-O2B
3	B	902	ATP	PA-O3A-PB-O2B

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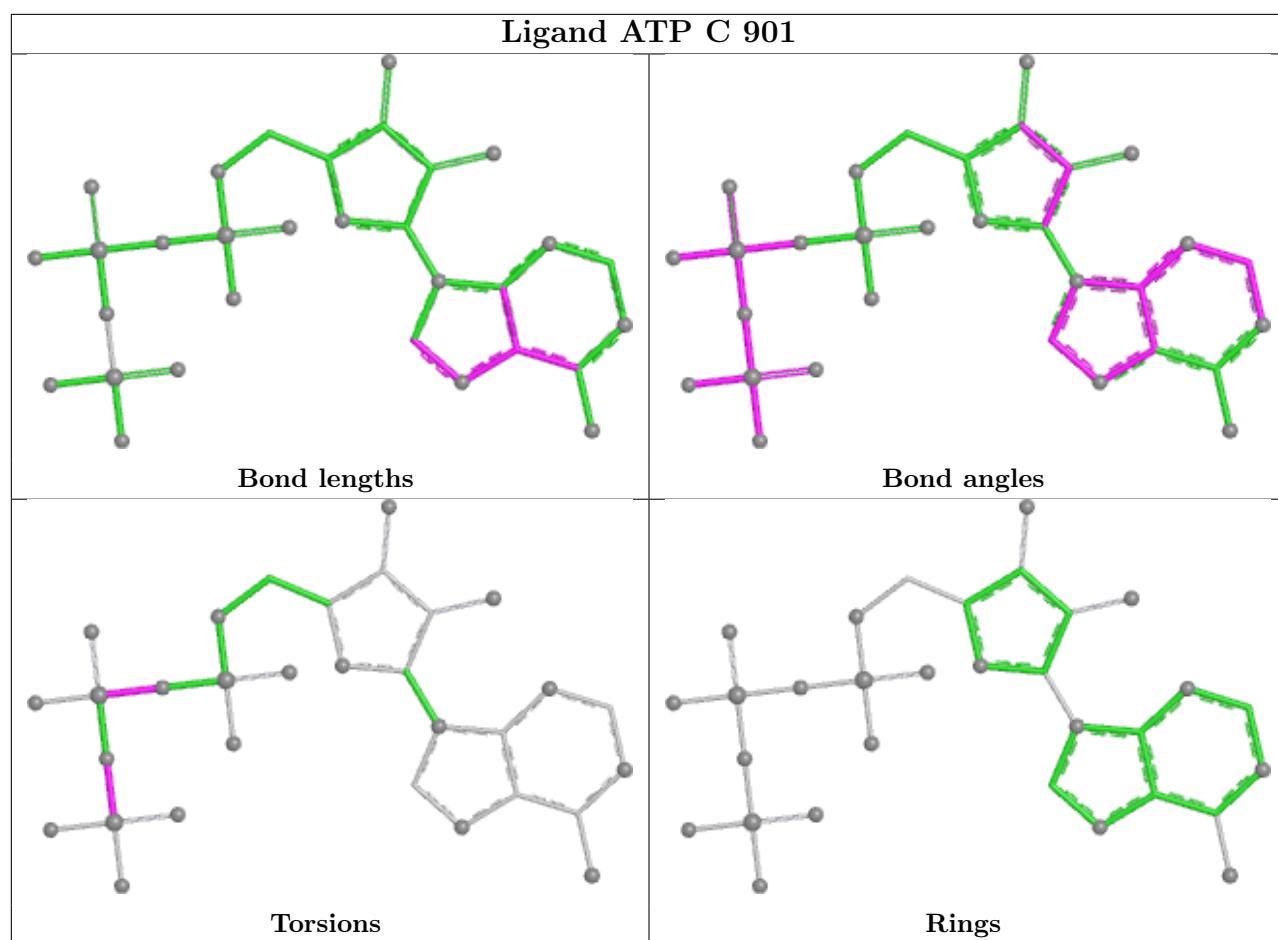
Mol	Chain	Res	Type	Atoms
3	D	902	ATP	PA-O3A-PB-O2B
3	E	901	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PB-O3B-PG-O1G
3	C	901	ATP	PB-O3B-PG-O1G
3	D	901	ATP	PB-O3B-PG-O1G

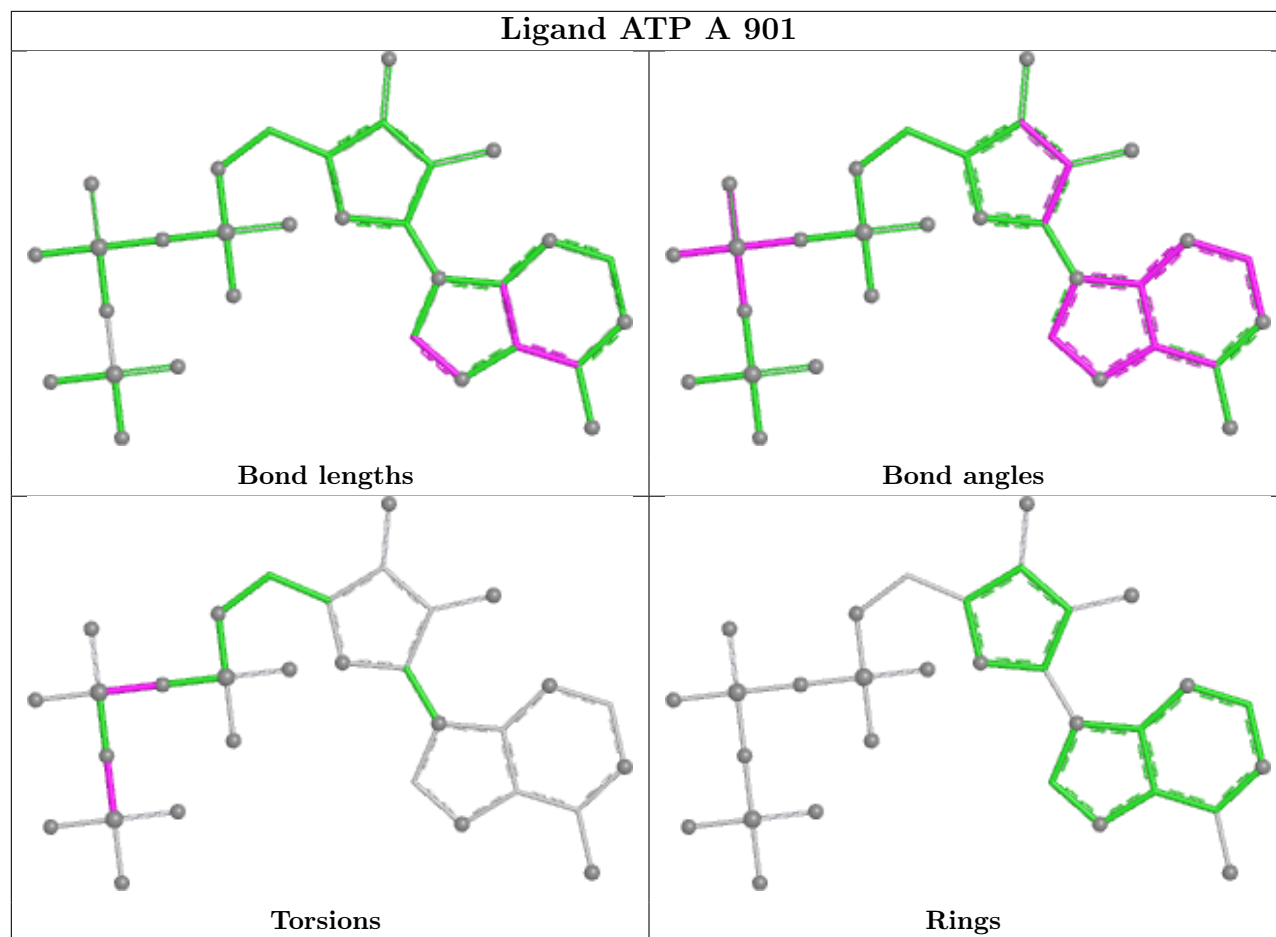
There are no ring outliers.

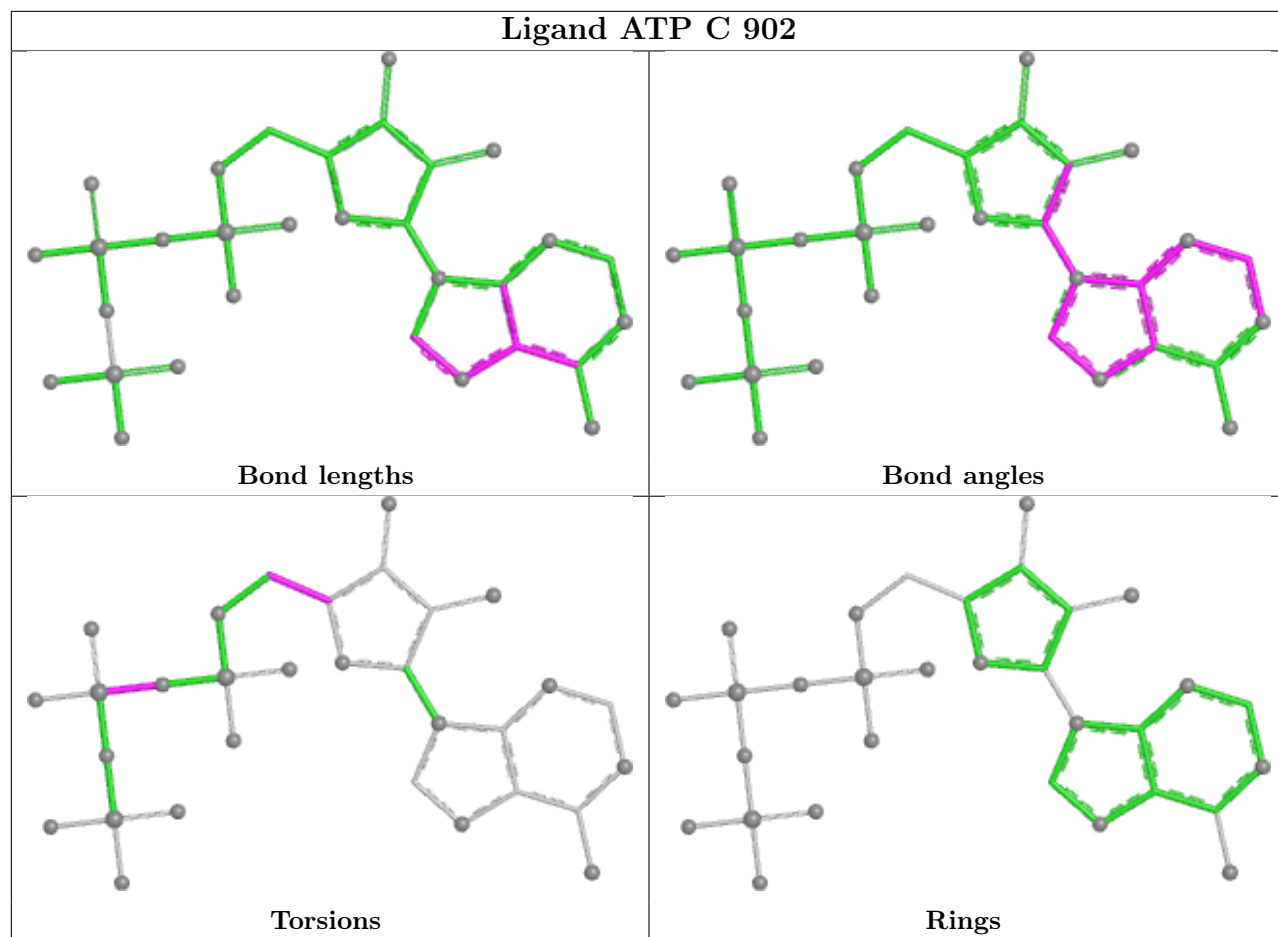
10 monomers are involved in 21 short contacts:

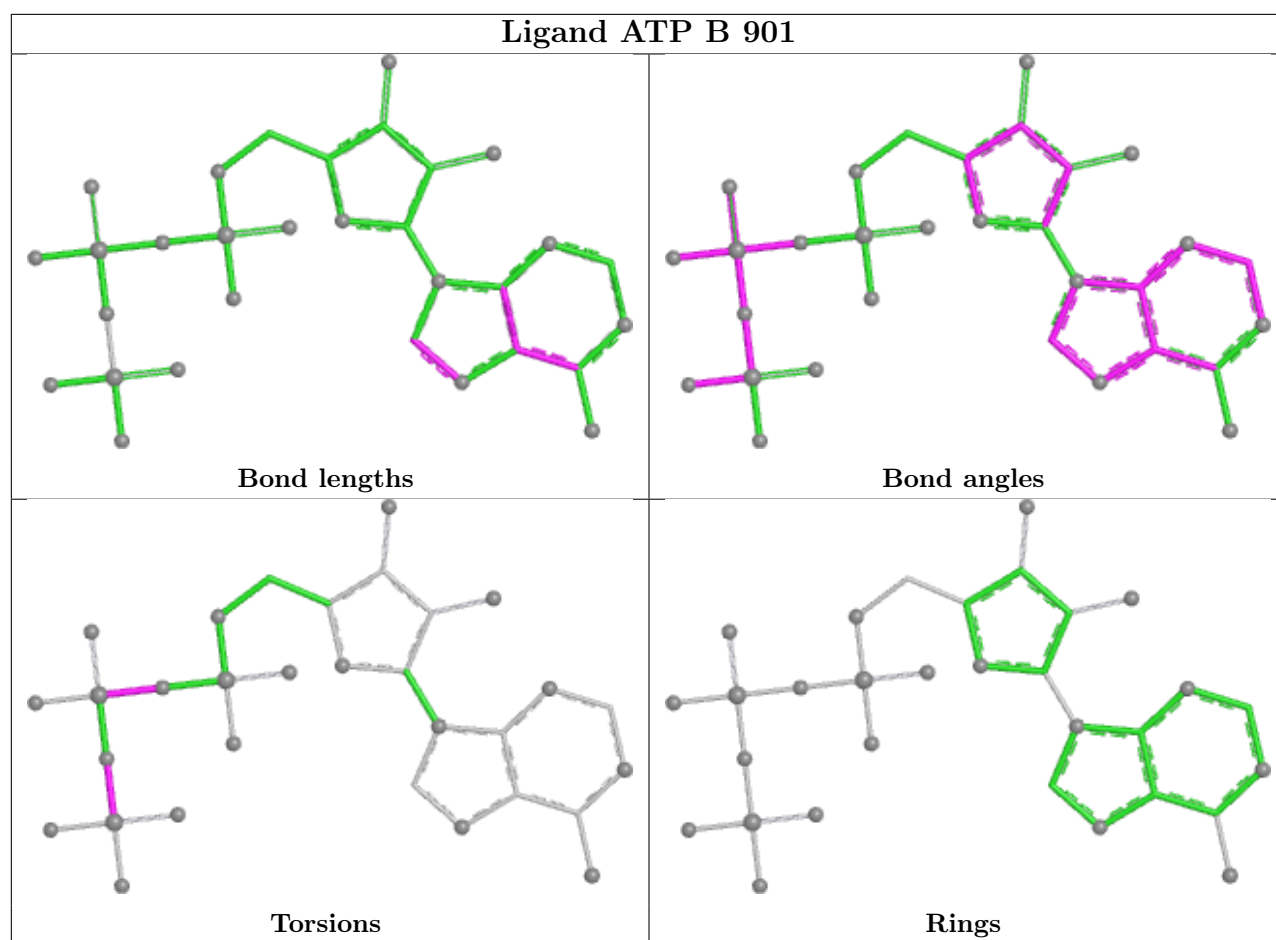
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	ATP	1	0
3	A	901	ATP	7	0
3	C	902	ATP	1	0
3	B	901	ATP	4	0
3	E	901	ATP	1	0
3	A	902	ATP	1	0
3	B	902	ATP	2	0
3	D	901	ATP	1	0
3	D	902	ATP	1	0
3	F	902	ATP	2	0

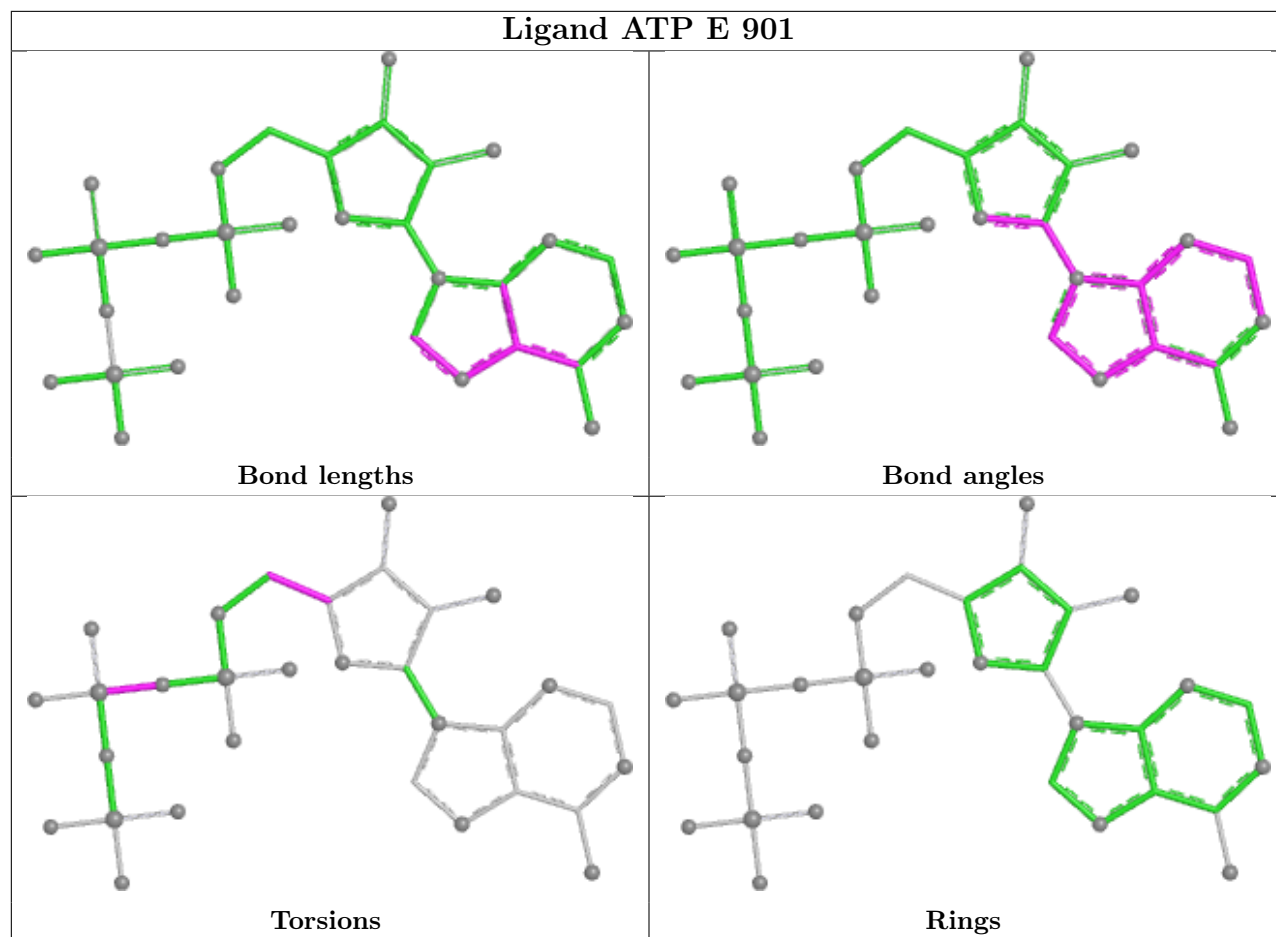
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

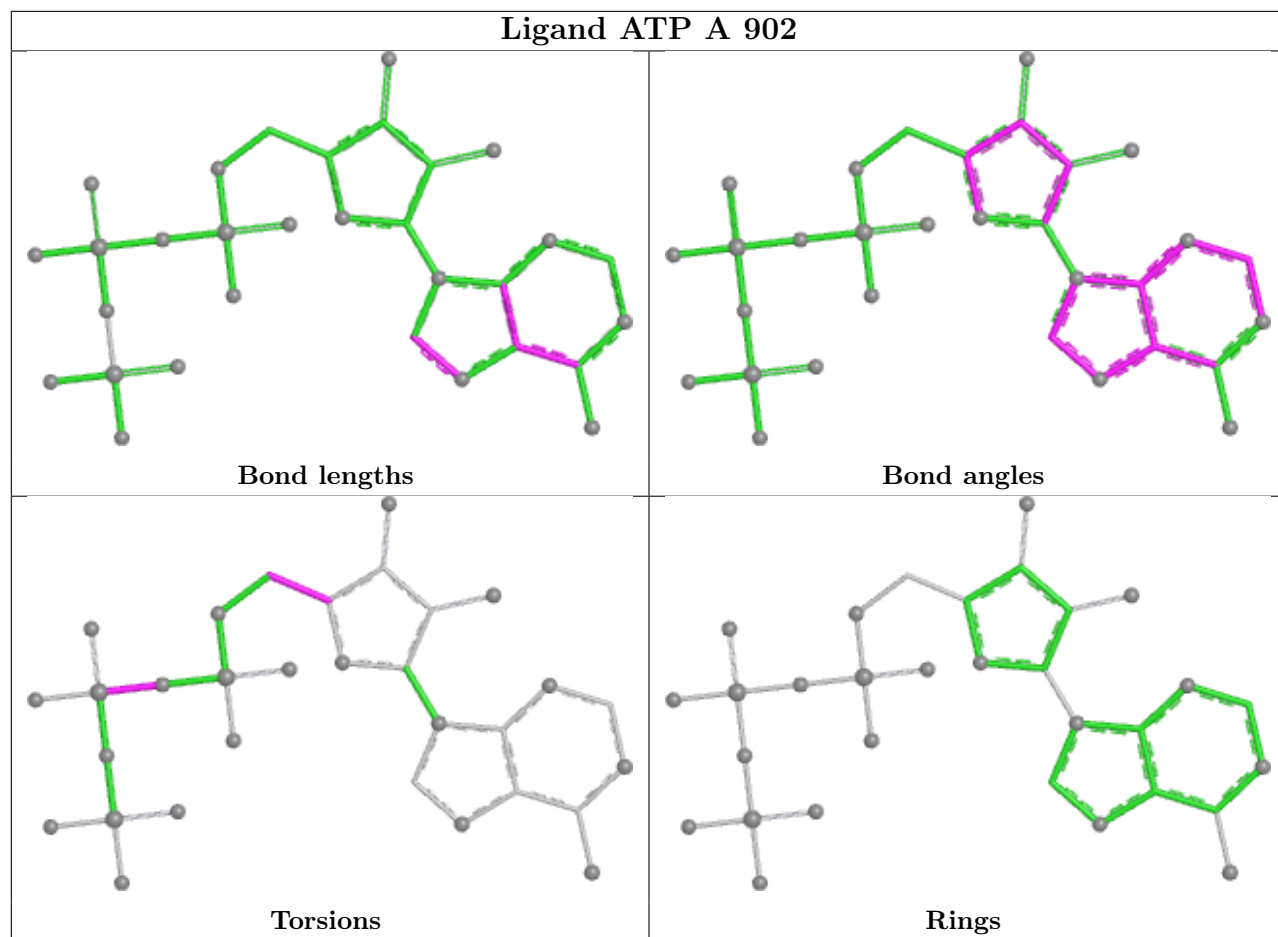


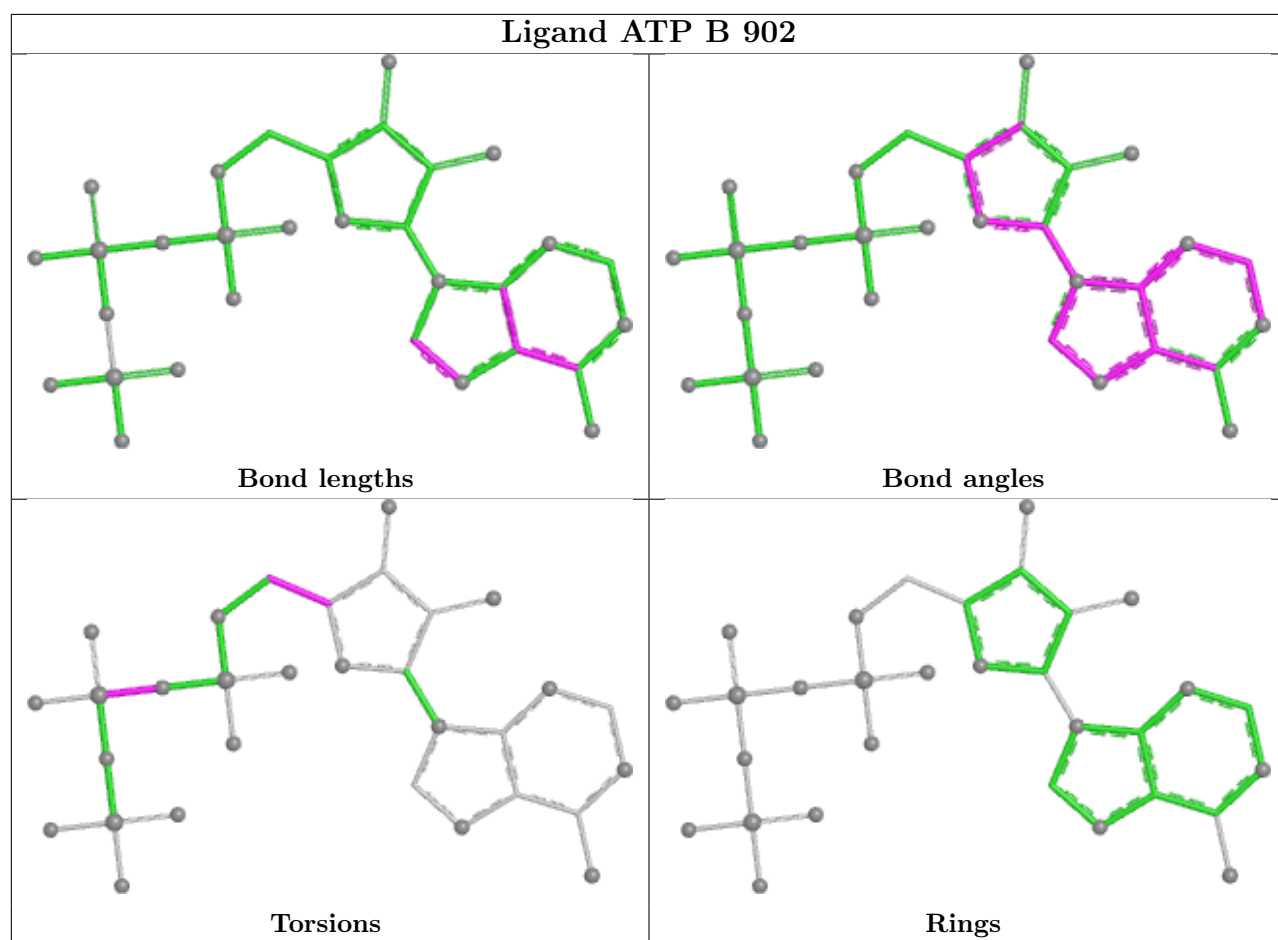


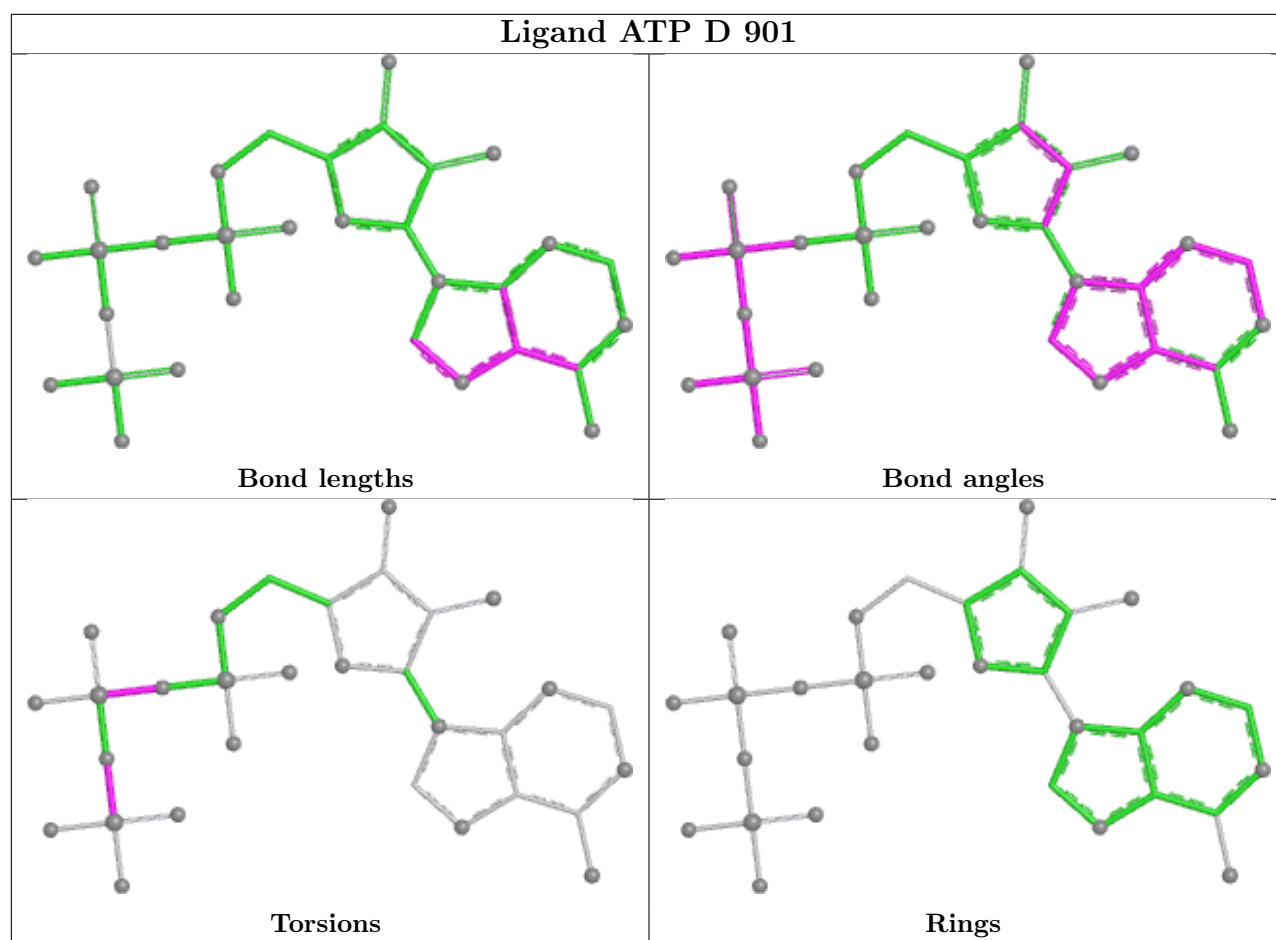


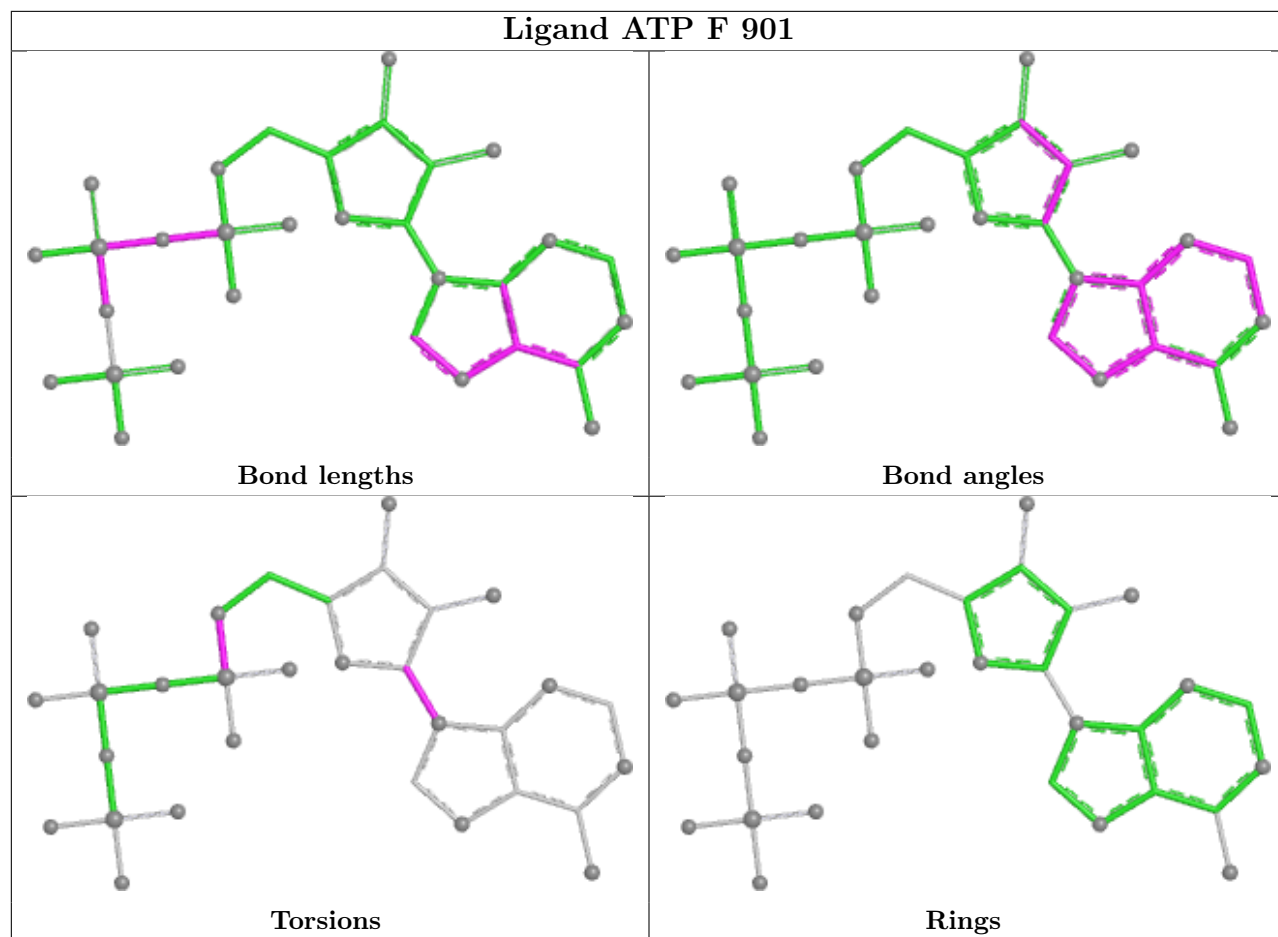


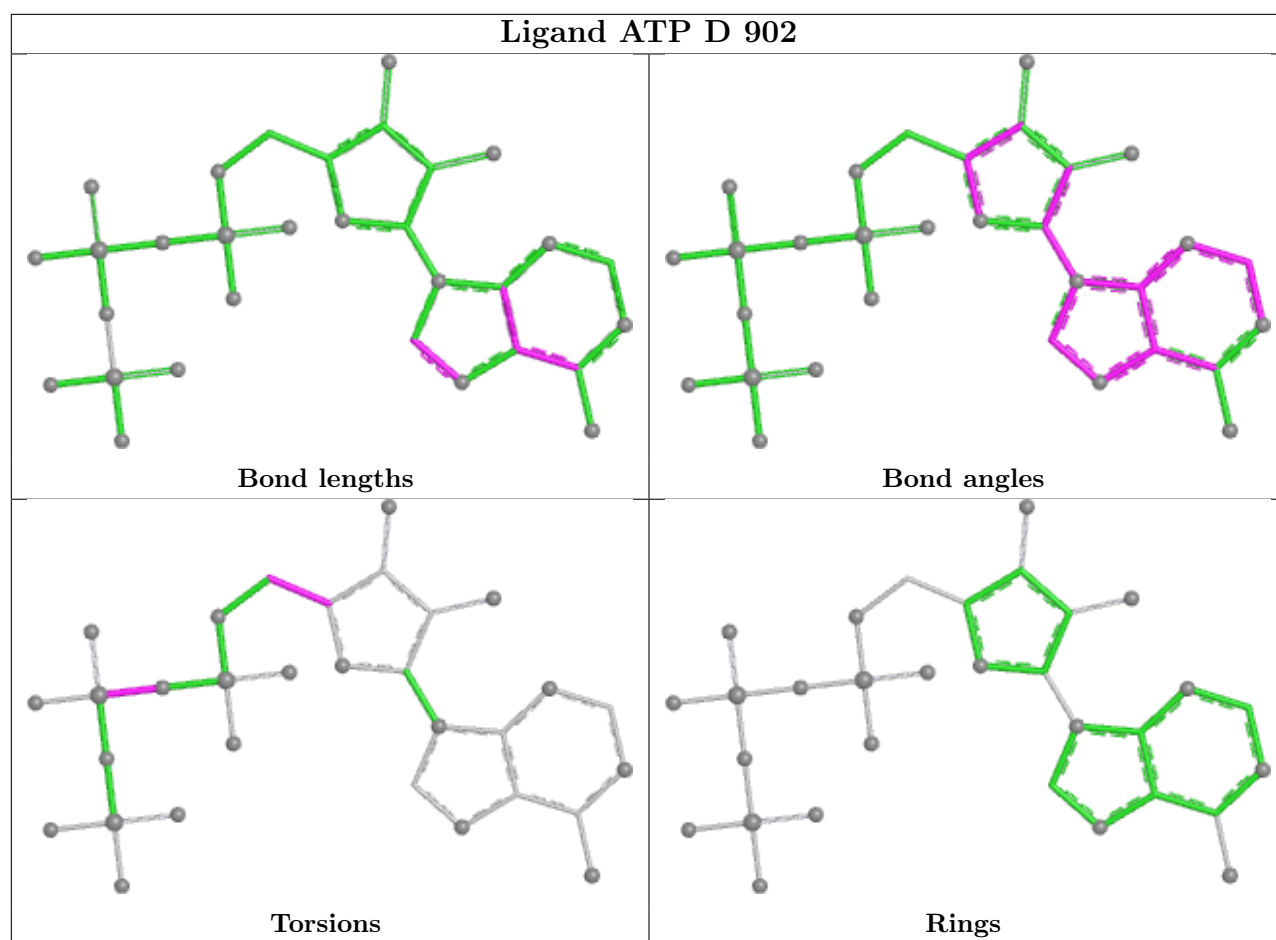


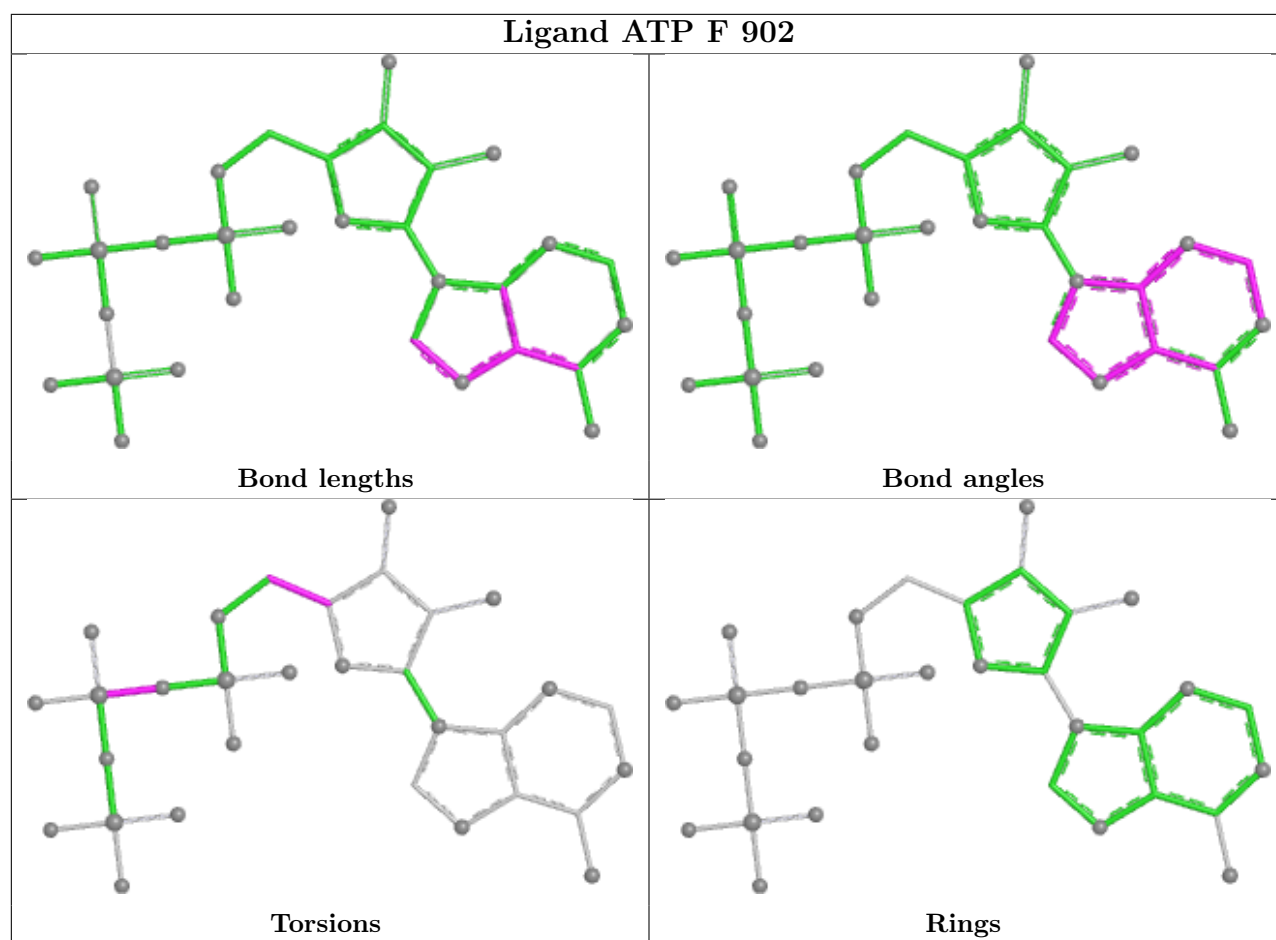












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

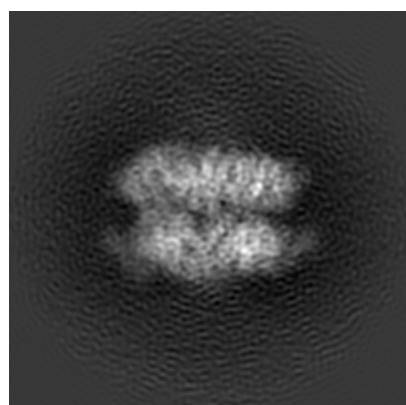
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9063. These allow visual inspection of the internal detail of the map and identification of artifacts.

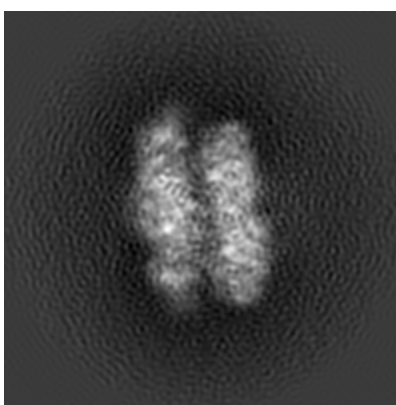
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

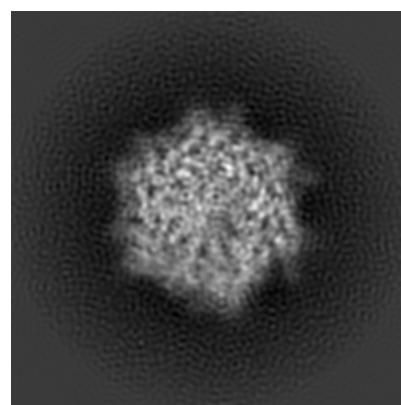
6.1.1 Primary map



X



Y

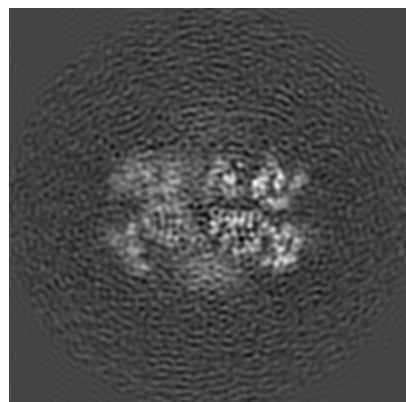


Z

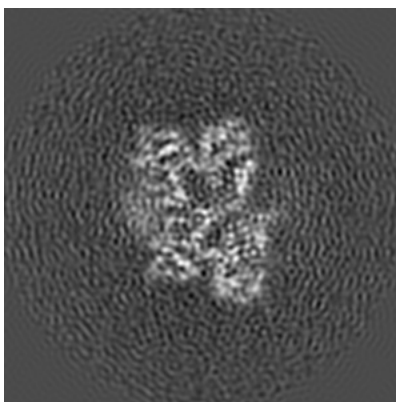
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

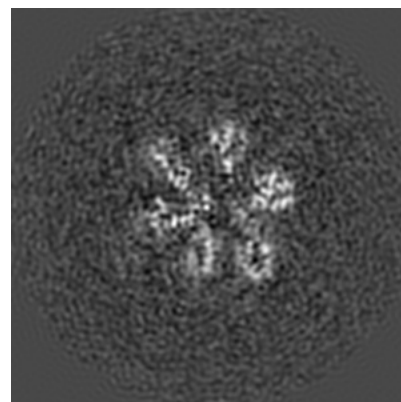
6.2.1 Primary map



X Index: 96



Y Index: 96

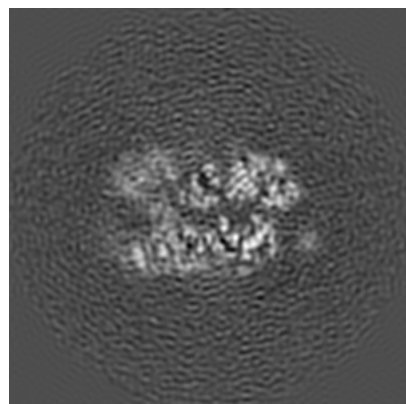


Z Index: 96

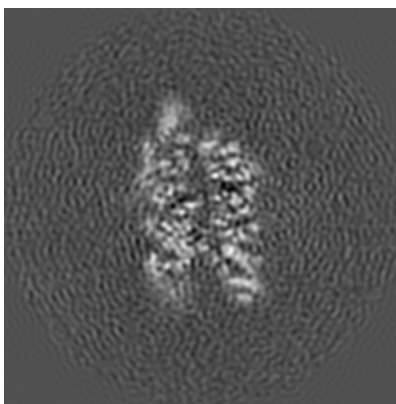
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

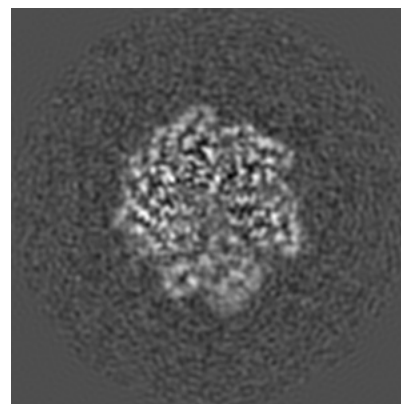
6.3.1 Primary map



X Index: 110



Y Index: 111

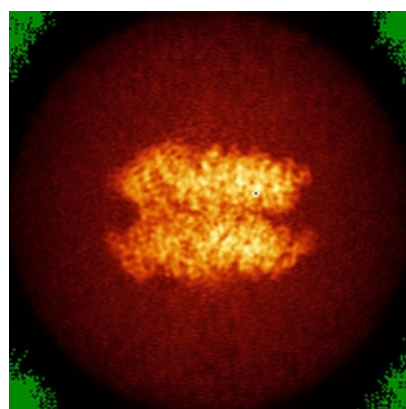


Z Index: 109

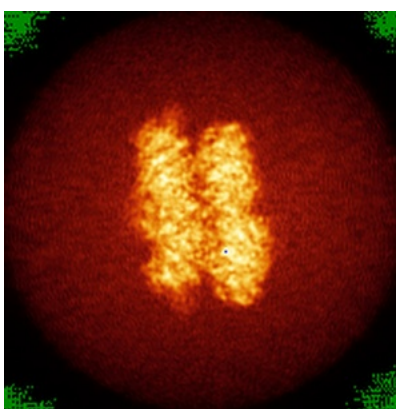
The images above show the largest variance slices of the map in three orthogonal directions.

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

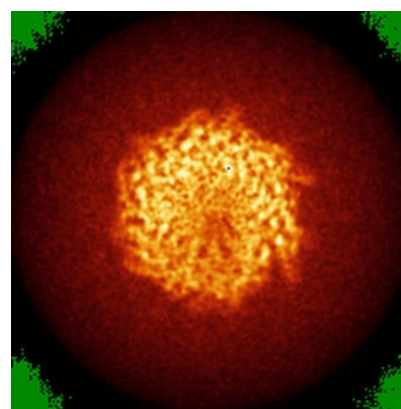
6.4.1 Primary map



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

This section was not generated.

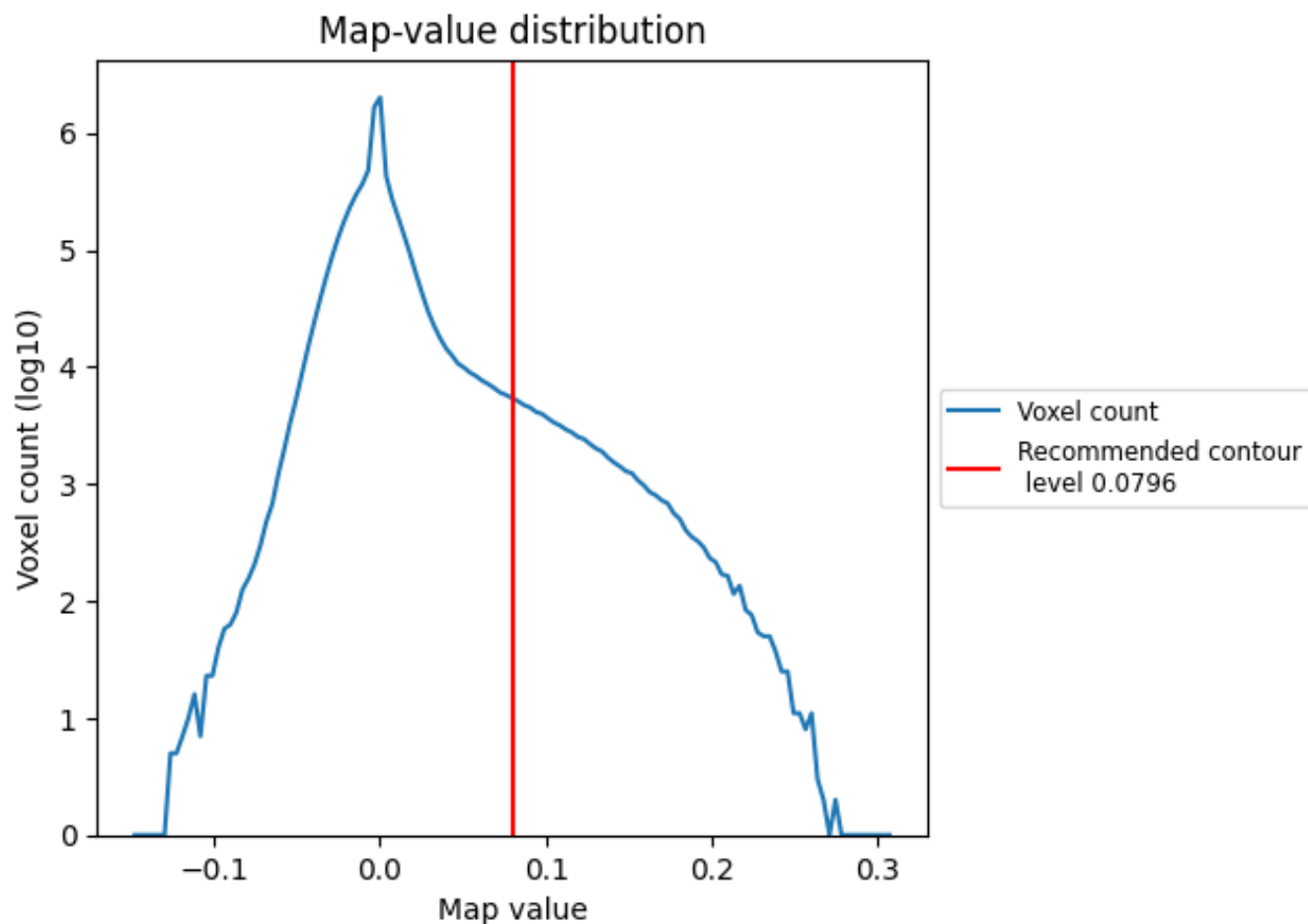
6.6 Mask visualisation

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

7 Map analysis [i](#)

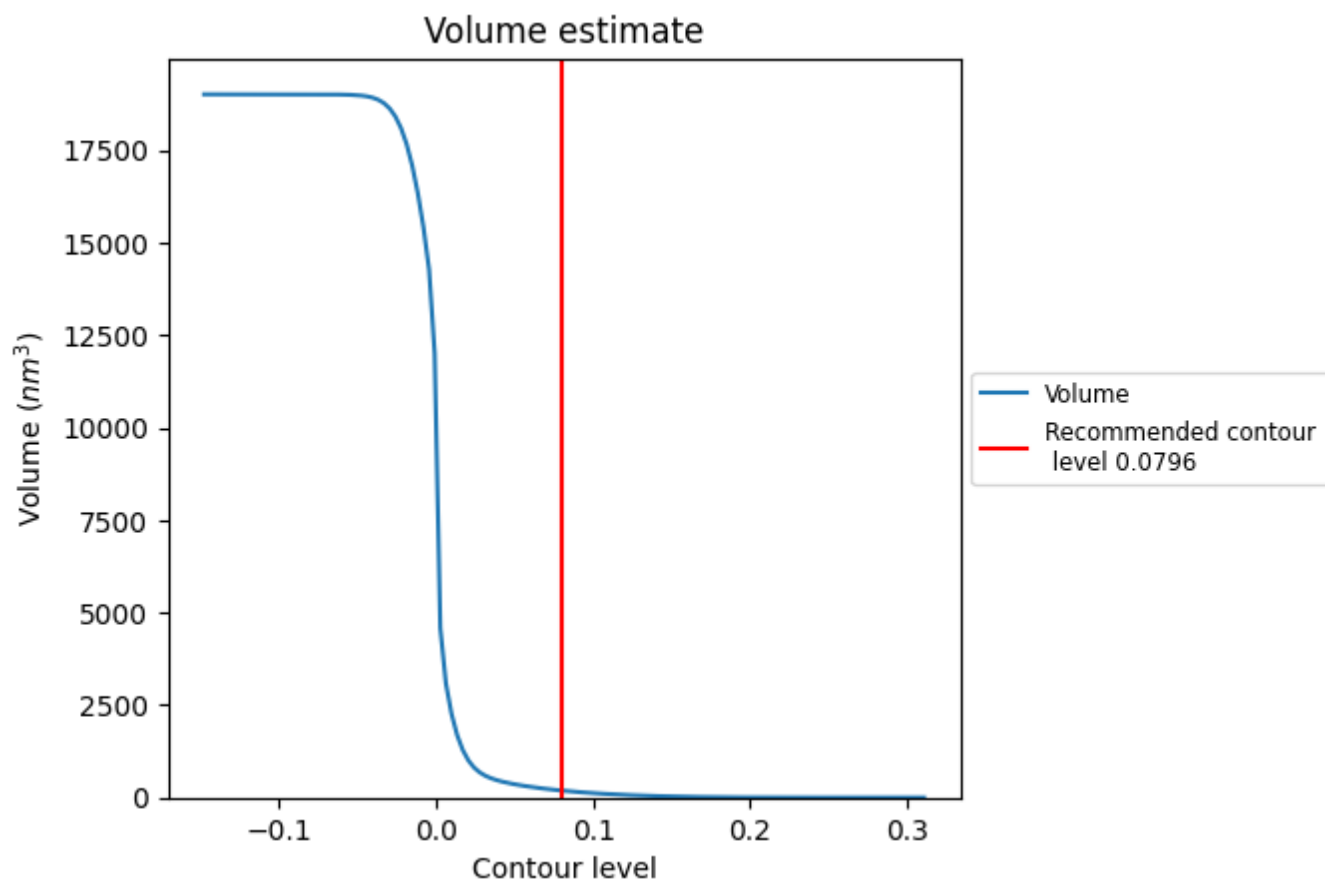
This section contains the results of statistical analysis of the map.

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.

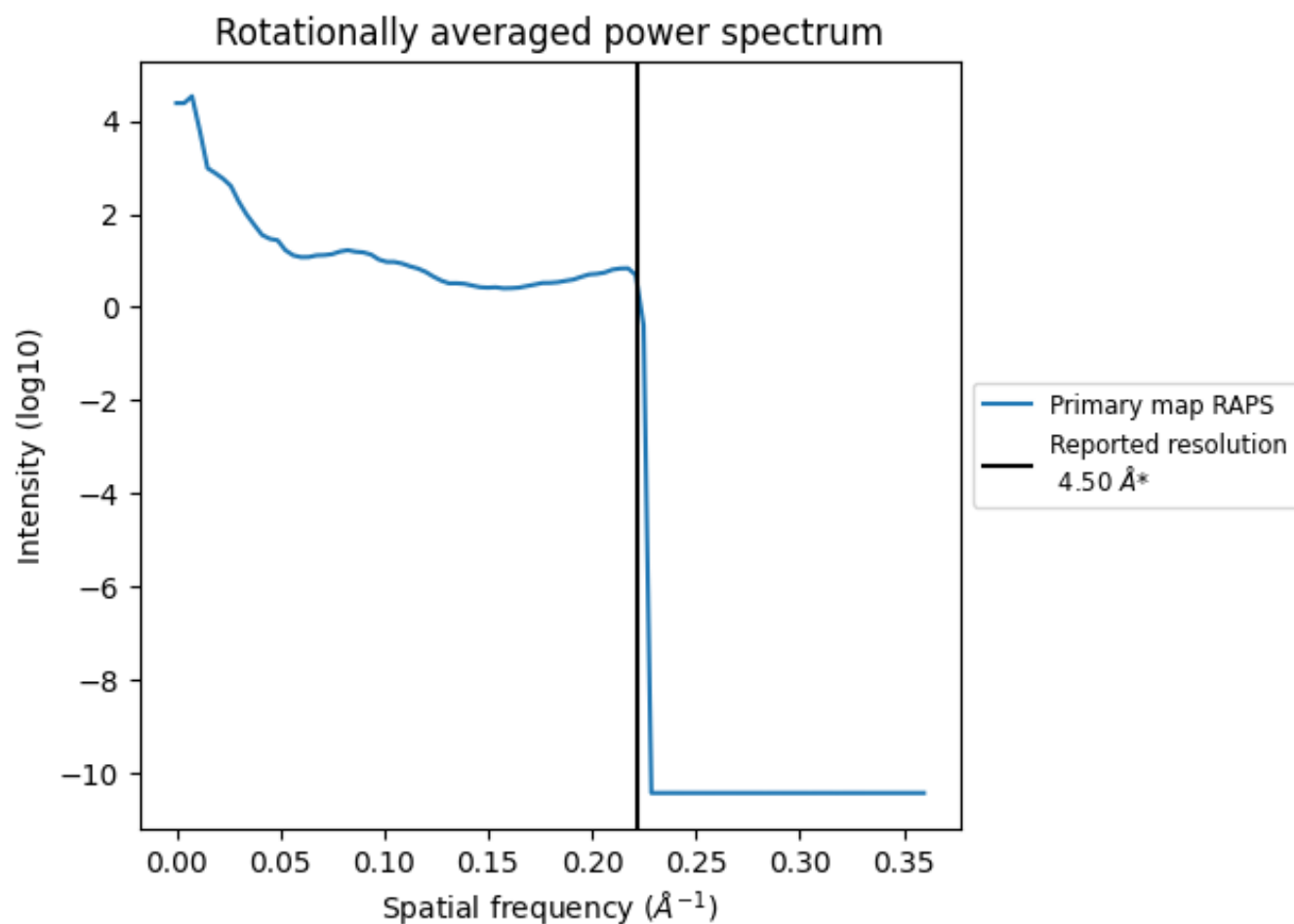
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

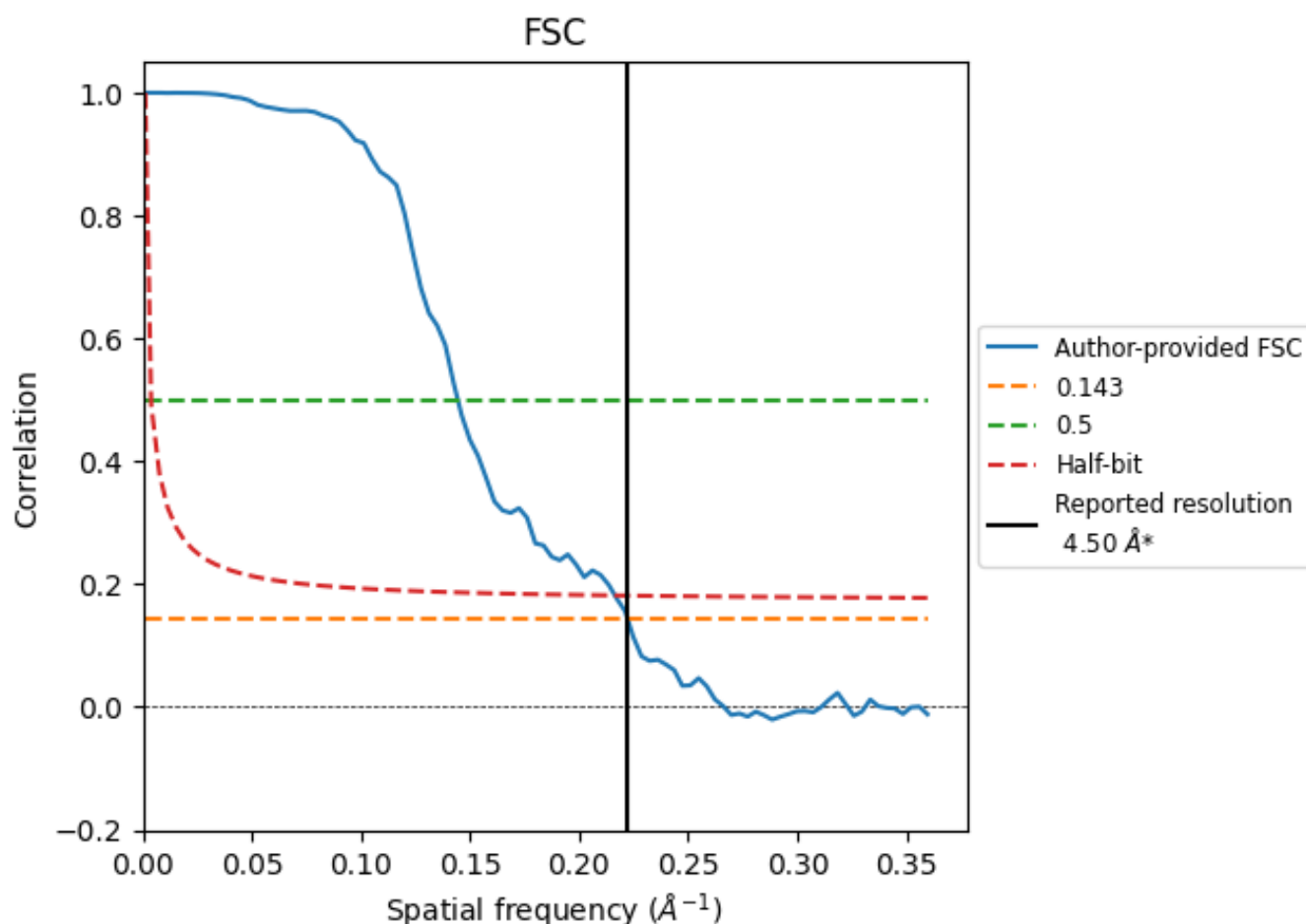


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.93	4.62
Unmasked-calculated*	-	-	-

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

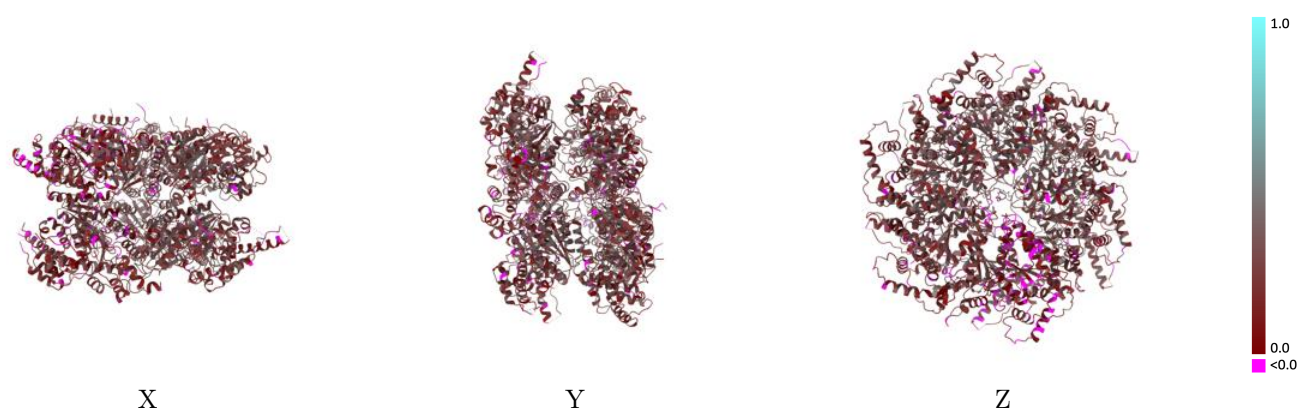
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9063 and PDB model 6MAT. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

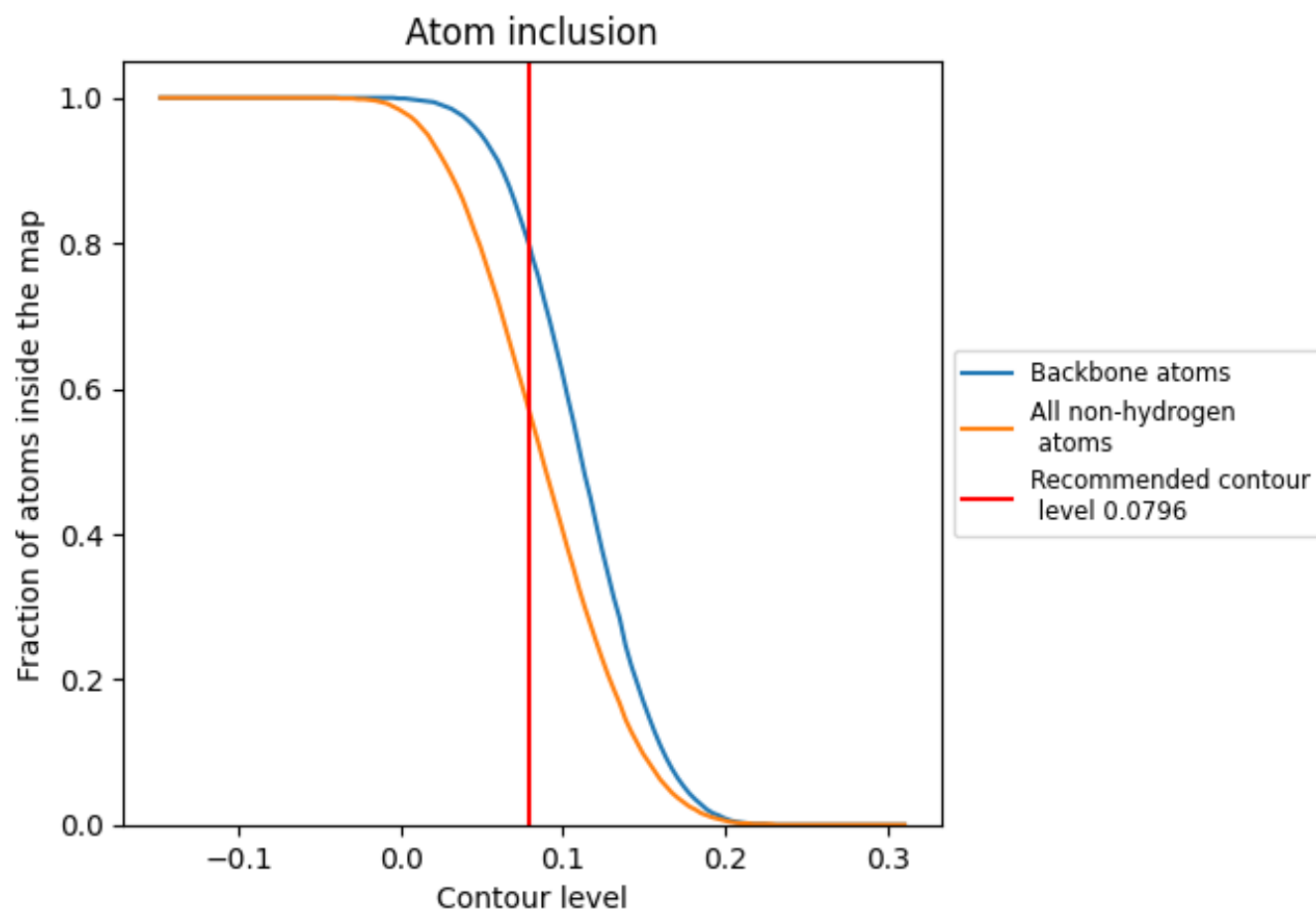


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 57% 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 (0.0796) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5680	0.2300
A	0.5960	0.2380
B	0.6330	0.2570
C	0.6290	0.2560
D	0.6150	0.2550
E	0.5180	0.2130
F	0.4150	0.1560
G	0.6150	0.3040

1.0

0.0

<0.0