



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:43 PM UTC

PDB ID : 8SWK / pdb_00008swk
EMDB ID : EMD-40820
Title : Cryo-EM structure of NLRP3 closed hexamer
Authors : Yu, X.; Matico, R.E.; Miller, R.; Schoubroeck, B.V.; Grauwen, K.; Suarez, J.; Pietrak, B.; Haloi, N.; Yin, Y.; Tresadern, G.J.; Perez-Benito, L.; Lindahl, E.; Bottelbergs, A.; Oehlrich, D.; Opdenbosch, N.V.; Sharma, S.
Deposited on : 2023-05-18
Resolution : 4.32 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

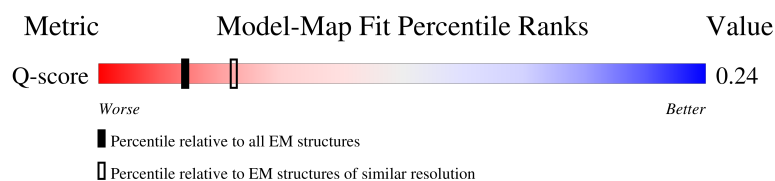
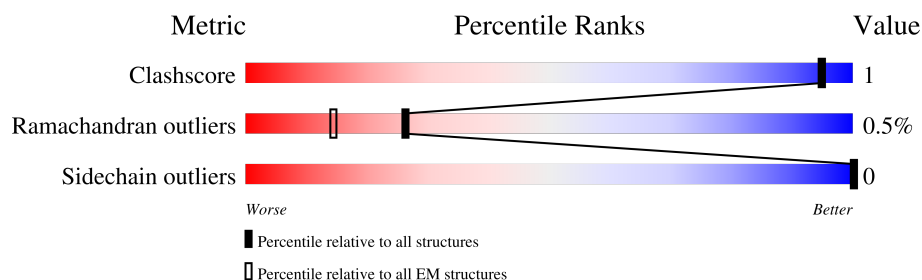
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.32 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	3853 (3.83 - 4.82)

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	910	13% 85% 5% 10%
1	B	910	13% 85% 5% 10%
1	C	910	14% 85% 5% 10%
1	D	910	14% 85% 5% 10%

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Mol	Chain	Length	Quality of chain
1	E	910	14% 85% 5% 10%
1	F	910	13% 85% 5% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39510 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 NACHT, LRR and PYD domains-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	818	Total	C	N	O	S	0	0
			6526	4162	1105	1203	56		
1	B	818	Total	C	N	O	S	0	0
			6526	4162	1105	1203	56		
1	C	818	Total	C	N	O	S	0	0
			6526	4162	1105	1203	56		
1	D	818	Total	C	N	O	S	0	0
			6526	4162	1105	1203	56		
1	E	818	Total	C	N	O	S	0	0
			6526	4162	1105	1203	56		
1	F	818	Total	C	N	O	S	0	0
			6526	4162	1105	1203	56		

There are 36 discrepancies between the modelled and reference sequences:

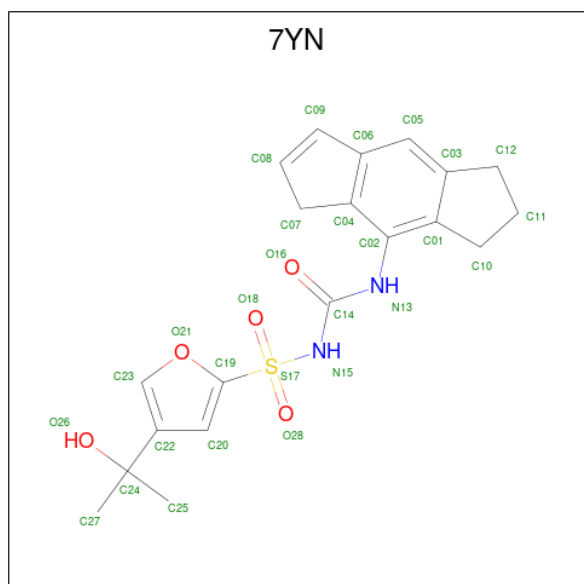
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	-	expression tag	UNP Q96P20
A	128	GLU	-	expression tag	UNP Q96P20
A	129	TYR	-	expression tag	UNP Q96P20
A	130	CYS	-	expression tag	UNP Q96P20
A	131	PHE	-	expression tag	UNP Q96P20
A	132	ASN	-	expression tag	UNP Q96P20
B	127	ALA	-	expression tag	UNP Q96P20
B	128	GLU	-	expression tag	UNP Q96P20
B	129	TYR	-	expression tag	UNP Q96P20
B	130	CYS	-	expression tag	UNP Q96P20
B	131	PHE	-	expression tag	UNP Q96P20
B	132	ASN	-	expression tag	UNP Q96P20
C	127	ALA	-	expression tag	UNP Q96P20
C	128	GLU	-	expression tag	UNP Q96P20
C	129	TYR	-	expression tag	UNP Q96P20
C	130	CYS	-	expression tag	UNP Q96P20
C	131	PHE	-	expression tag	UNP Q96P20
C	132	ASN	-	expression tag	UNP Q96P20

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Chain	Residue	Modelled	Actual	Comment	Reference
D	127	ALA	-	expression tag	UNP Q96P20
D	128	GLU	-	expression tag	UNP Q96P20
D	129	TYR	-	expression tag	UNP Q96P20
D	130	CYS	-	expression tag	UNP Q96P20
D	131	PHE	-	expression tag	UNP Q96P20
D	132	ASN	-	expression tag	UNP Q96P20
E	127	ALA	-	expression tag	UNP Q96P20
E	128	GLU	-	expression tag	UNP Q96P20
E	129	TYR	-	expression tag	UNP Q96P20
E	130	CYS	-	expression tag	UNP Q96P20
E	131	PHE	-	expression tag	UNP Q96P20
E	132	ASN	-	expression tag	UNP Q96P20
F	127	ALA	-	expression tag	UNP Q96P20
F	128	GLU	-	expression tag	UNP Q96P20
F	129	TYR	-	expression tag	UNP Q96P20
F	130	CYS	-	expression tag	UNP Q96P20
F	131	PHE	-	expression tag	UNP Q96P20
F	132	ASN	-	expression tag	UNP Q96P20

- Molecule 2 is 1-[4-(2-oxidanylpropan-2-yl)furan-2-yl]sulfonyl-3-(1,2,3,5-tetrahydro-s-indacen-4-yl)urea (CCD ID: 7YN) (formula: C₂₀H₂₂N₂O₅S) (labeled as "Ligand of Interest" by depositor).



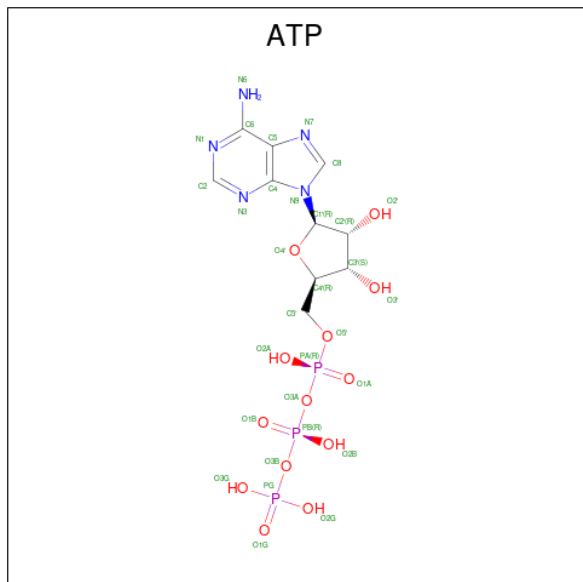
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			28	20	2	5	1	

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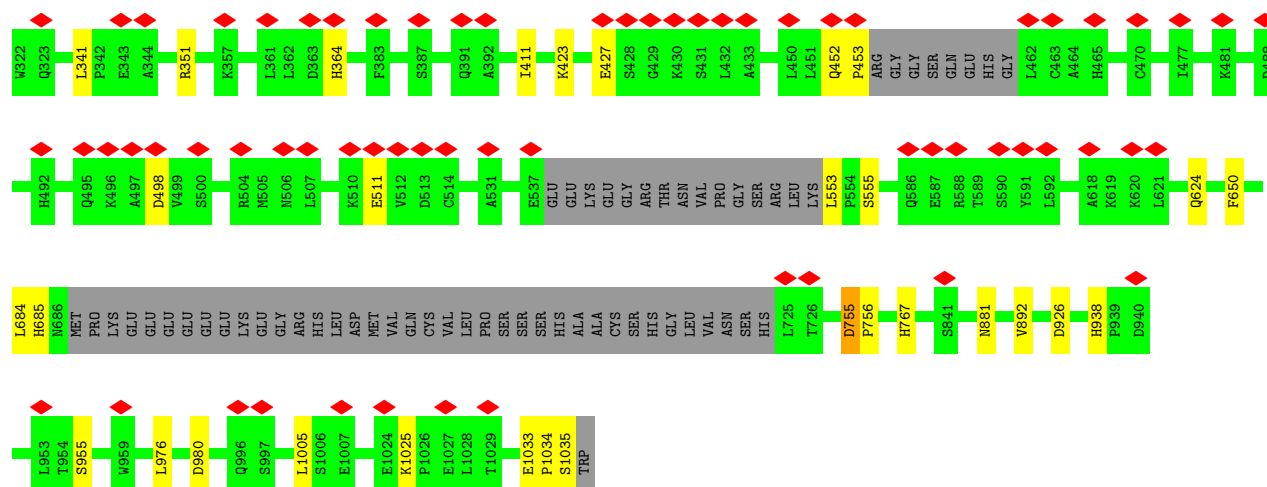
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	S	0
			28	20	2	5	1	
2	C	1	Total	C	N	O	S	0
			28	20	2	5	1	
2	D	1	Total	C	N	O	S	0
			28	20	2	5	1	
2	E	1	Total	C	N	O	S	0
			28	20	2	5	1	
2	F	1	Total	C	N	O	S	0
			28	20	2	5	1	

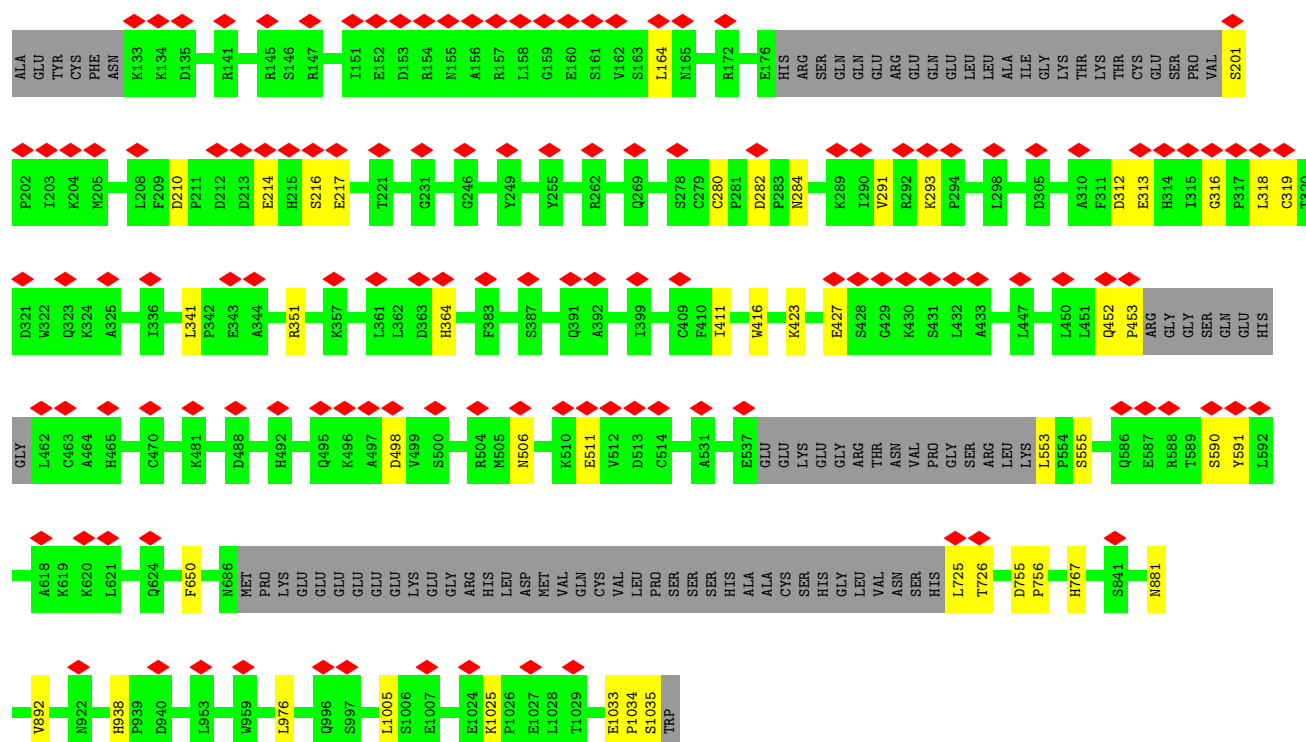
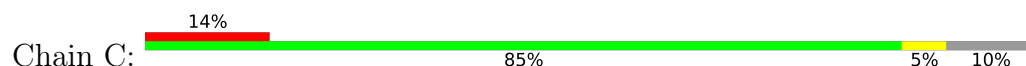
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



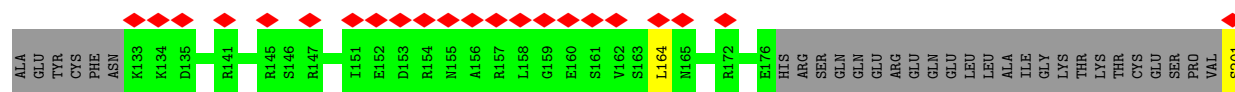
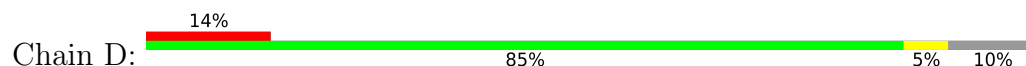
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

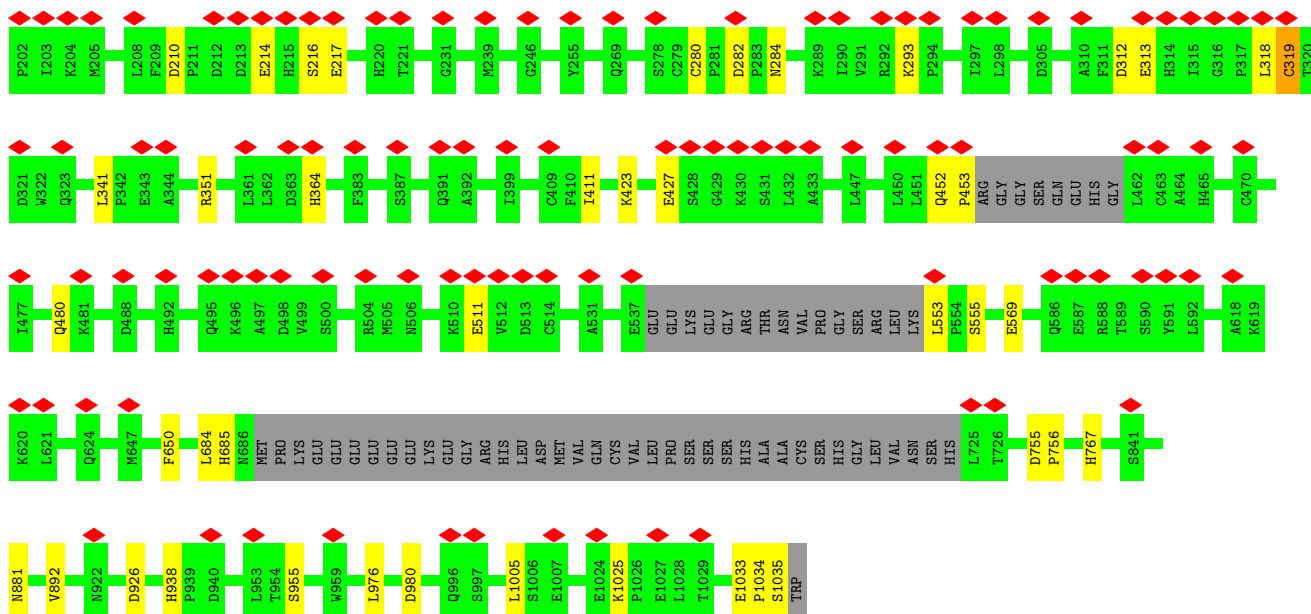


- Molecule 1: NACHT, LRR and PYD domains-containing protein 3

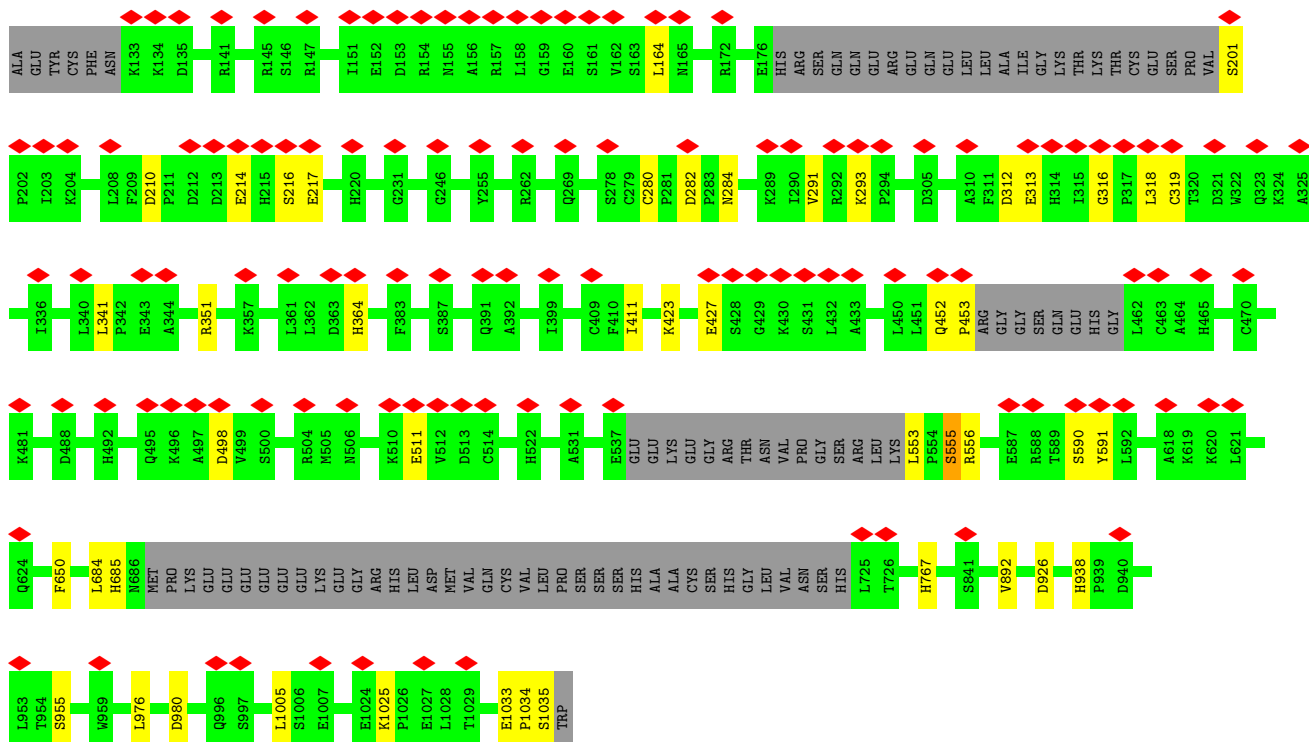
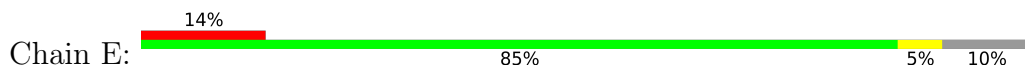


- Molecule 1: NACHT, LRR and PYD domains-containing protein 3

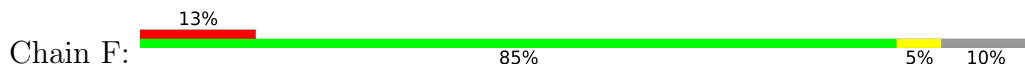


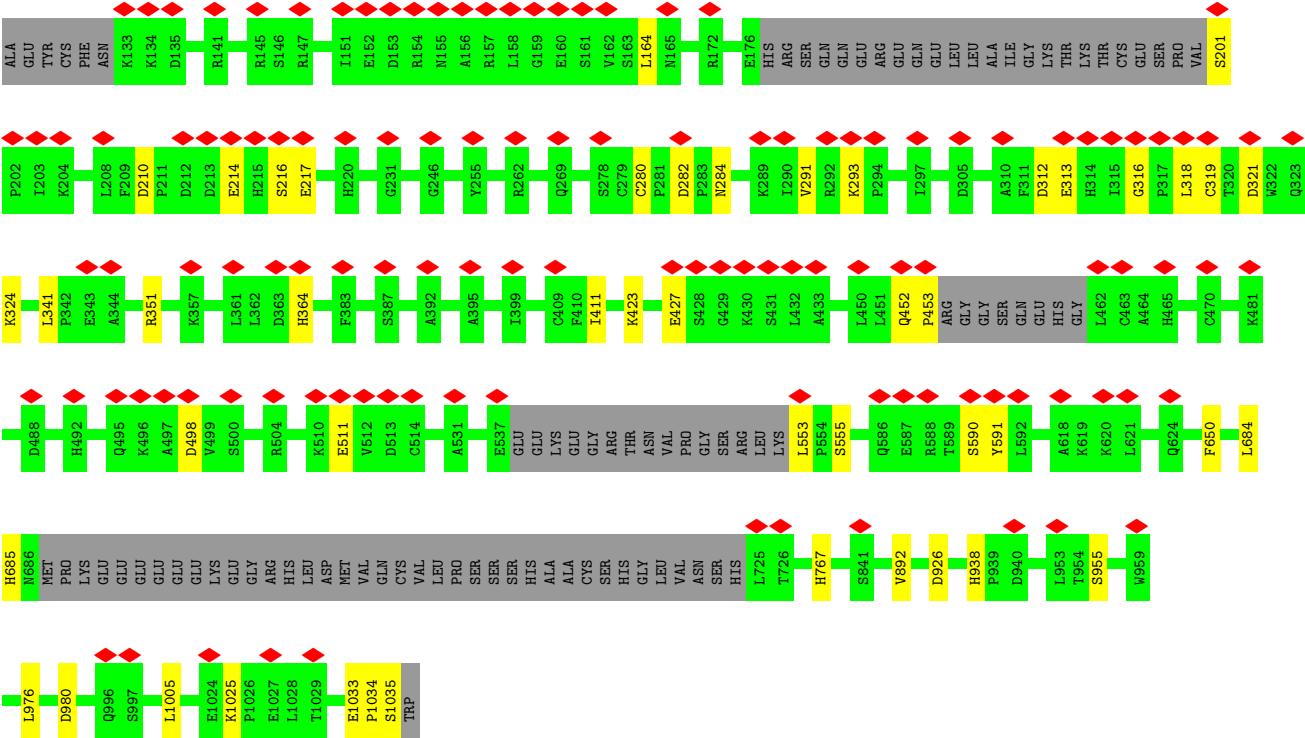


- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



- Molecule 1: NACHT, LRR and PYD domains-containing protein 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72861	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.239	Depositor
Minimum map value	-0.860	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.181	Depositor
Map size (Å)	299.52002, 299.52002, 299.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7YN, 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	0.60	0/6647	0.86	40/8962 (0.4%)
1	B	0.60	0/6647	0.85	42/8962 (0.5%)
1	C	0.59	0/6647	0.85	38/8962 (0.4%)
1	D	0.59	0/6647	0.85	36/8962 (0.4%)
1	E	0.60	0/6647	0.86	36/8962 (0.4%)
1	F	0.59	0/6647	0.85	36/8962 (0.4%)
All	All	0.60	0/39882	0.85	228/53772 (0.4%)

There are no bond length outliers.

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1025	LYS	CA-C-N	8.29	128.02	119.56
1	C	1025	LYS	C-N-CA	8.29	128.02	119.56
1	F	1025	LYS	CA-C-N	8.28	128.01	119.56
1	F	1025	LYS	C-N-CA	8.28	128.01	119.56
1	B	1025	LYS	CA-C-N	8.25	127.97	119.56
1	B	1025	LYS	C-N-CA	8.25	127.97	119.56
1	D	1025	LYS	CA-C-N	8.24	127.97	119.56
1	D	1025	LYS	C-N-CA	8.24	127.97	119.56
1	E	1025	LYS	CA-C-N	8.22	127.94	119.56
1	E	1025	LYS	C-N-CA	8.22	127.94	119.56
1	A	1025	LYS	CA-C-N	8.20	127.92	119.56
1	A	1025	LYS	C-N-CA	8.20	127.92	119.56
1	C	201	SER	CA-C-N	7.54	127.47	119.85
1	C	201	SER	C-N-CA	7.54	127.47	119.85
1	B	201	SER	CA-C-N	7.49	127.41	119.85
1	B	201	SER	C-N-CA	7.49	127.41	119.85
1	D	201	SER	CA-C-N	7.45	127.38	119.85
1	D	201	SER	C-N-CA	7.45	127.38	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	201	SER	CA-C-N	7.44	127.36	119.85
1	F	201	SER	C-N-CA	7.44	127.36	119.85
1	A	201	SER	CA-C-N	7.42	127.35	119.85
1	A	201	SER	C-N-CA	7.42	127.35	119.85
1	E	201	SER	CA-C-N	7.42	127.35	119.85
1	E	201	SER	C-N-CA	7.42	127.35	119.85
1	E	280	CYS	CA-C-N	7.28	126.98	119.56
1	E	280	CYS	C-N-CA	7.28	126.98	119.56
1	F	553	LEU	CA-C-N	7.26	126.89	119.56
1	F	553	LEU	C-N-CA	7.26	126.89	119.56
1	A	280	CYS	CA-C-N	7.21	126.91	119.56
1	A	280	CYS	C-N-CA	7.21	126.91	119.56
1	C	553	LEU	CA-C-N	7.20	126.83	119.56
1	C	553	LEU	C-N-CA	7.20	126.83	119.56
1	E	364	HIS	CA-C-N	7.15	127.31	120.31
1	E	364	HIS	C-N-CA	7.15	127.31	120.31
1	B	364	HIS	CA-C-N	7.13	127.30	120.31
1	B	364	HIS	C-N-CA	7.13	127.30	120.31
1	F	364	HIS	CA-C-N	7.08	127.25	120.31
1	F	364	HIS	C-N-CA	7.08	127.25	120.31
1	A	553	LEU	CA-C-N	7.07	126.70	119.56
1	A	553	LEU	C-N-CA	7.07	126.70	119.56
1	D	553	LEU	CA-C-N	7.04	126.67	119.56
1	D	553	LEU	C-N-CA	7.04	126.67	119.56
1	E	217	GLU	CA-C-N	7.00	126.97	120.03
1	E	217	GLU	C-N-CA	7.00	126.97	120.03
1	D	217	GLU	CA-C-N	7.00	126.96	120.03
1	D	217	GLU	C-N-CA	7.00	126.96	120.03
1	B	553	LEU	CA-C-N	6.95	126.58	119.56
1	B	553	LEU	C-N-CA	6.95	126.58	119.56
1	C	364	HIS	CA-C-N	6.94	127.11	120.31
1	C	364	HIS	C-N-CA	6.94	127.11	120.31
1	C	341	LEU	CA-C-N	6.92	126.89	120.03
1	C	341	LEU	C-N-CA	6.92	126.89	120.03
1	A	217	GLU	CA-C-N	6.91	126.87	120.03
1	A	217	GLU	C-N-CA	6.91	126.87	120.03
1	F	217	GLU	CA-C-N	6.91	126.87	120.03
1	F	217	GLU	C-N-CA	6.91	126.87	120.03
1	E	553	LEU	CA-C-N	6.90	126.53	119.56
1	E	553	LEU	C-N-CA	6.90	126.53	119.56
1	B	217	GLU	CA-C-N	6.89	126.86	120.03
1	B	217	GLU	C-N-CA	6.89	126.86	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	GLU	CA-C-N	6.87	126.83	120.03
1	C	217	GLU	C-N-CA	6.87	126.83	120.03
1	D	210	ASP	CA-C-N	6.82	126.80	119.78
1	D	210	ASP	C-N-CA	6.82	126.80	119.78
1	B	210	ASP	CA-C-N	6.82	126.80	119.78
1	B	210	ASP	C-N-CA	6.82	126.80	119.78
1	D	364	HIS	CA-C-N	6.77	127.31	120.14
1	D	364	HIS	C-N-CA	6.77	127.31	120.14
1	A	364	HIS	CA-C-N	6.71	127.25	120.14
1	A	364	HIS	C-N-CA	6.71	127.25	120.14
1	D	282	ASP	CA-C-N	6.71	126.85	119.87
1	D	282	ASP	C-N-CA	6.71	126.85	119.87
1	B	282	ASP	CA-C-N	6.71	126.84	119.87
1	B	282	ASP	C-N-CA	6.71	126.84	119.87
1	B	650	PHE	CA-C-N	6.68	126.31	119.56
1	B	650	PHE	C-N-CA	6.68	126.31	119.56
1	C	282	ASP	CA-C-N	6.67	126.81	119.87
1	C	282	ASP	C-N-CA	6.67	126.81	119.87
1	F	650	PHE	CA-C-N	6.67	126.30	119.56
1	F	650	PHE	C-N-CA	6.67	126.30	119.56
1	F	411	ILE	CA-C-N	6.65	126.90	119.32
1	F	411	ILE	C-N-CA	6.65	126.90	119.32
1	E	210	ASP	CA-C-N	6.65	126.62	119.78
1	E	210	ASP	C-N-CA	6.65	126.62	119.78
1	F	341	LEU	CA-C-N	6.64	126.62	119.78
1	F	341	LEU	C-N-CA	6.64	126.62	119.78
1	A	650	PHE	CA-C-N	6.63	126.25	119.56
1	A	650	PHE	C-N-CA	6.63	126.25	119.56
1	D	411	ILE	CA-C-N	6.61	126.85	119.32
1	D	411	ILE	C-N-CA	6.61	126.85	119.32
1	E	1033	GLU	CA-C-N	6.60	126.29	119.56
1	E	1033	GLU	C-N-CA	6.60	126.29	119.56
1	D	1033	GLU	CA-C-N	6.59	126.28	119.56
1	D	1033	GLU	C-N-CA	6.59	126.28	119.56
1	A	282	ASP	CA-C-N	6.58	126.71	119.87
1	A	282	ASP	C-N-CA	6.58	126.71	119.87
1	C	1033	GLU	CA-C-N	6.58	126.27	119.56
1	C	1033	GLU	C-N-CA	6.58	126.27	119.56
1	E	282	ASP	CA-C-N	6.55	126.68	119.87
1	E	282	ASP	C-N-CA	6.55	126.68	119.87
1	F	282	ASP	CA-C-N	6.54	126.67	119.87
1	F	282	ASP	C-N-CA	6.54	126.67	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1033	GLU	CA-C-N	6.54	126.23	119.56
1	A	1033	GLU	C-N-CA	6.54	126.23	119.56
1	C	411	ILE	CA-C-N	6.51	126.75	119.32
1	C	411	ILE	C-N-CA	6.51	126.75	119.32
1	A	210	ASP	CA-C-N	6.48	126.45	119.78
1	A	210	ASP	C-N-CA	6.48	126.45	119.78
1	E	411	ILE	CA-C-N	6.47	126.70	119.32
1	E	411	ILE	C-N-CA	6.47	126.70	119.32
1	D	341	LEU	CA-C-N	6.46	126.83	119.92
1	D	341	LEU	C-N-CA	6.46	126.83	119.92
1	F	1033	GLU	CA-C-N	6.46	126.15	119.56
1	F	1033	GLU	C-N-CA	6.46	126.15	119.56
1	A	341	LEU	CA-C-N	6.43	126.80	119.92
1	A	341	LEU	C-N-CA	6.43	126.80	119.92
1	F	210	ASP	CA-C-N	6.43	126.40	119.78
1	F	210	ASP	C-N-CA	6.43	126.40	119.78
1	B	1033	GLU	CA-C-N	6.41	126.10	119.56
1	B	1033	GLU	C-N-CA	6.41	126.10	119.56
1	E	650	PHE	CA-C-N	6.39	126.02	119.56
1	E	650	PHE	C-N-CA	6.39	126.02	119.56
1	C	210	ASP	CA-C-N	6.38	126.35	119.78
1	C	210	ASP	C-N-CA	6.38	126.35	119.78
1	B	341	LEU	CA-C-N	6.36	126.73	119.92
1	B	341	LEU	C-N-CA	6.36	126.73	119.92
1	C	650	PHE	CA-C-N	6.35	125.97	119.56
1	C	650	PHE	C-N-CA	6.35	125.97	119.56
1	E	351	ARG	CA-C-N	6.34	126.55	119.32
1	E	351	ARG	C-N-CA	6.34	126.55	119.32
1	D	650	PHE	CA-C-N	6.29	125.91	119.56
1	D	650	PHE	C-N-CA	6.29	125.91	119.56
1	F	351	ARG	CA-C-N	6.27	126.46	119.32
1	F	351	ARG	C-N-CA	6.27	126.46	119.32
1	B	351	ARG	CA-C-N	6.24	126.44	119.32
1	B	351	ARG	C-N-CA	6.24	126.44	119.32
1	C	293	LYS	CA-C-N	6.21	126.12	119.85
1	C	293	LYS	C-N-CA	6.21	126.12	119.85
1	B	293	LYS	CA-C-N	6.19	126.10	119.85
1	B	293	LYS	C-N-CA	6.19	126.10	119.85
1	E	767	HIS	CA-C-N	6.19	125.88	119.56
1	E	767	HIS	C-N-CA	6.19	125.88	119.56
1	F	280	CYS	CA-C-N	6.19	127.58	119.84
1	F	280	CYS	C-N-CA	6.19	127.58	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	767	HIS	CA-C-N	6.19	125.87	119.56
1	F	767	HIS	C-N-CA	6.19	125.87	119.56
1	B	938	HIS	CA-C-N	6.17	126.63	119.47
1	B	938	HIS	C-N-CA	6.17	126.63	119.47
1	C	767	HIS	CA-C-N	6.16	125.84	119.56
1	C	767	HIS	C-N-CA	6.16	125.84	119.56
1	B	767	HIS	CA-C-N	6.14	125.82	119.56
1	B	767	HIS	C-N-CA	6.14	125.82	119.56
1	A	351	ARG	CA-C-N	6.14	126.32	119.32
1	A	351	ARG	C-N-CA	6.14	126.32	119.32
1	A	411	ILE	CA-C-N	6.13	126.31	119.32
1	A	411	ILE	C-N-CA	6.13	126.31	119.32
1	B	411	ILE	CA-C-N	6.12	126.30	119.32
1	B	411	ILE	C-N-CA	6.12	126.30	119.32
1	C	351	ARG	CA-C-N	6.12	126.57	119.47
1	C	351	ARG	C-N-CA	6.12	126.57	119.47
1	D	767	HIS	CA-C-N	6.12	125.80	119.56
1	D	767	HIS	C-N-CA	6.12	125.80	119.56
1	A	293	LYS	CA-C-N	6.10	126.02	119.85
1	A	293	LYS	C-N-CA	6.10	126.02	119.85
1	A	767	HIS	CA-C-N	6.09	125.77	119.56
1	A	767	HIS	C-N-CA	6.09	125.77	119.56
1	D	351	ARG	CA-C-N	6.08	125.97	119.28
1	D	351	ARG	C-N-CA	6.08	125.97	119.28
1	B	280	CYS	CA-C-N	6.07	127.42	119.84
1	B	280	CYS	C-N-CA	6.07	127.42	119.84
1	D	280	CYS	CA-C-N	6.04	127.39	119.84
1	D	280	CYS	C-N-CA	6.04	127.39	119.84
1	C	938	HIS	CA-C-N	6.02	126.45	119.47
1	C	938	HIS	C-N-CA	6.02	126.45	119.47
1	E	341	LEU	CA-C-N	6.02	125.98	119.78
1	E	341	LEU	C-N-CA	6.02	125.98	119.78
1	F	938	HIS	CA-C-N	6.00	126.43	119.47
1	F	938	HIS	C-N-CA	6.00	126.43	119.47
1	C	280	CYS	CA-C-N	5.99	127.33	119.84
1	C	280	CYS	C-N-CA	5.99	127.33	119.84
1	D	293	LYS	CA-C-N	5.99	125.90	119.85
1	D	293	LYS	C-N-CA	5.99	125.90	119.85
1	F	293	LYS	CA-C-N	5.96	125.88	119.85
1	F	293	LYS	C-N-CA	5.96	125.88	119.85
1	E	293	LYS	CA-C-N	5.90	125.81	119.85
1	E	293	LYS	C-N-CA	5.90	125.81	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	938	HIS	CA-C-N	5.89	126.31	119.47
1	E	938	HIS	C-N-CA	5.89	126.31	119.47
1	D	938	HIS	CA-C-N	5.87	126.28	119.47
1	D	938	HIS	C-N-CA	5.87	126.28	119.47
1	A	938	HIS	CA-C-N	5.87	126.27	119.47
1	A	938	HIS	C-N-CA	5.87	126.27	119.47
1	D	284	ASN	CA-C-N	5.80	126.35	120.38
1	D	284	ASN	C-N-CA	5.80	126.35	120.38
1	C	284	ASN	CA-C-N	5.72	126.27	120.38
1	C	284	ASN	C-N-CA	5.72	126.27	120.38
1	A	284	ASN	CA-C-N	5.71	126.26	120.38
1	A	284	ASN	C-N-CA	5.71	126.26	120.38
1	B	284	ASN	CA-C-N	5.69	126.24	120.38
1	B	284	ASN	C-N-CA	5.69	126.24	120.38
1	B	881	ASN	CA-C-N	5.65	125.32	119.56
1	B	881	ASN	C-N-CA	5.65	125.32	119.56
1	D	881	ASN	CA-C-N	5.65	126.03	119.47
1	D	881	ASN	C-N-CA	5.65	126.03	119.47
1	F	284	ASN	CA-C-N	5.64	126.19	120.38
1	F	284	ASN	C-N-CA	5.64	126.19	120.38
1	A	881	ASN	CA-C-N	5.62	125.30	119.56
1	A	881	ASN	C-N-CA	5.62	125.30	119.56
1	E	284	ASN	CA-C-N	5.50	126.05	120.38
1	E	284	ASN	C-N-CA	5.50	126.05	120.38
1	A	316	GLY	CA-C-N	5.27	126.42	119.84
1	A	316	GLY	C-N-CA	5.27	126.42	119.84
1	F	316	GLY	CA-C-N	5.26	126.41	119.84
1	F	316	GLY	C-N-CA	5.26	126.41	119.84
1	B	316	GLY	CA-C-N	5.23	126.38	119.84
1	B	316	GLY	C-N-CA	5.23	126.38	119.84
1	C	316	GLY	CA-C-N	5.21	126.36	119.84
1	C	316	GLY	C-N-CA	5.21	126.36	119.84
1	E	316	GLY	CA-C-N	5.13	126.26	119.84
1	E	316	GLY	C-N-CA	5.13	126.26	119.84
1	A	755	ASP	CA-C-N	5.13	125.17	119.32
1	A	755	ASP	C-N-CA	5.13	125.17	119.32
1	B	755	ASP	CA-C-N	5.13	125.16	119.32
1	B	755	ASP	C-N-CA	5.13	125.16	119.32
1	B	624	GLN	CA-C-N	5.06	125.34	119.93
1	B	624	GLN	C-N-CA	5.06	125.34	119.93
1	C	881	ASN	CA-C-N	5.02	126.12	119.84
1	C	881	ASN	C-N-CA	5.02	126.12	119.84

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	6526	0	6590	14	0
1	B	6526	0	6590	13	0
1	C	6526	0	6590	14	0
1	D	6526	0	6590	14	0
1	E	6526	0	6590	15	0
1	F	6526	0	6590	15	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
2	D	28	0	0	0	0
2	E	28	0	0	0	0
2	F	28	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
All	All	39510	0	39612	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:LYS:NZ	1:D:427:GLU:OE2	2.42	0.51
1:B:926:ASP:N	1:B:926:ASP:OD1	2.43	0.51
1:C:416:TRP:HE1	1:C:506:ASN:HD21	1.58	0.50
1:A:423:LYS:NZ	1:A:427:GLU:OE2	2.43	0.49
1:E:926:ASP:OD1	1:E:926:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:LYS:NZ	1:E:427:GLU:OE2	2.45	0.47
1:F:423:LYS:NZ	1:F:427:GLU:OE2	2.46	0.47
1:B:684:LEU:O	1:B:685:HIS:C	2.57	0.47
1:C:312:ASP:OD1	1:C:313:GLU:N	2.48	0.47
1:D:318:LEU:O	1:D:319:CYS:HB3	2.14	0.47
1:D:452:GLN:N	1:D:453:PRO:CD	2.78	0.47
1:D:312:ASP:OD1	1:D:313:GLU:N	2.48	0.47
1:F:312:ASP:OD1	1:F:313:GLU:N	2.48	0.47
1:A:312:ASP:OD1	1:A:313:GLU:N	2.48	0.46
1:E:312:ASP:OD1	1:E:313:GLU:N	2.47	0.46
1:F:452:GLN:N	1:F:453:PRO:CD	2.78	0.46
1:B:423:LYS:NZ	1:B:427:GLU:OE2	2.45	0.46
1:F:498:ASP:N	1:F:498:ASP:OD1	2.46	0.46
1:A:452:GLN:N	1:A:453:PRO:CD	2.77	0.46
1:C:318:LEU:O	1:C:319:CYS:HB3	2.16	0.46
1:B:452:GLN:N	1:B:453:PRO:CD	2.78	0.46
1:D:684:LEU:O	1:D:685:HIS:C	2.59	0.46
1:B:312:ASP:OD1	1:B:313:GLU:N	2.48	0.46
1:C:423:LYS:NZ	1:C:427:GLU:OE2	2.46	0.45
1:C:452:GLN:N	1:C:453:PRO:CD	2.78	0.45
1:E:452:GLN:N	1:E:453:PRO:CD	2.78	0.45
1:B:1034:PRO:O	1:B:1035:SER:CB	2.64	0.45
1:C:976:LEU:O	1:C:1005:LEU:N	2.49	0.45
1:F:318:LEU:O	1:F:319:CYS:HB3	2.17	0.45
1:F:684:LEU:O	1:F:685:HIS:C	2.60	0.45
1:A:498:ASP:OD1	1:A:498:ASP:N	2.46	0.44
1:A:684:LEU:O	1:A:685:HIS:C	2.59	0.44
1:A:318:LEU:O	1:A:319:CYS:HB3	2.18	0.44
1:B:318:LEU:O	1:B:319:CYS:HB3	2.18	0.44
1:B:498:ASP:OD1	1:B:498:ASP:N	2.47	0.44
1:B:1034:PRO:O	1:B:1035:SER:HB2	2.18	0.43
1:E:684:LEU:O	1:E:685:HIS:C	2.60	0.43
1:B:955:SER:N	1:B:980:ASP:O	2.51	0.43
1:E:590:SER:OG	1:E:591:TYR:N	2.51	0.43
1:C:725:LEU:O	1:C:726:THR:C	2.60	0.43
1:E:555:SER:OG	1:E:556:ARG:N	2.51	0.43
1:F:976:LEU:O	1:F:1005:LEU:N	2.51	0.43
1:E:1034:PRO:O	1:E:1035:SER:HB2	2.19	0.43
1:F:1034:PRO:O	1:F:1035:SER:HB2	2.19	0.43
1:D:214:GLU:C	1:D:216:SER:H	2.27	0.43
1:F:926:ASP:OD1	1:F:926:ASP:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:PRO:O	1:A:1035:SER:CB	2.67	0.43
1:C:498:ASP:OD1	1:C:498:ASP:N	2.46	0.43
1:C:1034:PRO:O	1:C:1035:SER:HB2	2.19	0.43
1:A:1034:PRO:O	1:A:1035:SER:HB2	2.18	0.42
1:B:976:LEU:O	1:B:1005:LEU:N	2.52	0.42
1:D:480:GLN:NE2	1:D:569:GLU:O	2.52	0.42
1:E:955:SER:N	1:E:980:ASP:O	2.52	0.42
1:E:498:ASP:OD1	1:E:498:ASP:N	2.46	0.42
1:F:1034:PRO:O	1:F:1035:SER:CB	2.67	0.42
1:E:1034:PRO:O	1:E:1035:SER:CB	2.68	0.42
1:F:955:SER:N	1:F:980:ASP:O	2.53	0.42
1:A:590:SER:OG	1:A:591:TYR:N	2.52	0.42
1:C:1034:PRO:O	1:C:1035:SER:CB	2.68	0.42
1:D:1034:PRO:O	1:D:1035:SER:HB2	2.19	0.42
1:E:318:LEU:O	1:E:319:CYS:HB3	2.19	0.42
1:A:214:GLU:C	1:A:216:SER:H	2.27	0.41
1:C:214:GLU:C	1:C:216:SER:H	2.27	0.41
1:F:321:ASP:OD2	1:F:324:LYS:NZ	2.53	0.41
1:B:214:GLU:C	1:B:216:SER:H	2.27	0.41
1:D:1034:PRO:O	1:D:1035:SER:CB	2.69	0.41
1:F:214:GLU:C	1:F:216:SER:H	2.28	0.41
1:C:755:ASP:N	1:C:756:PRO:CD	2.83	0.41
1:E:214:GLU:C	1:E:216:SER:H	2.28	0.41
1:E:976:LEU:O	1:E:1005:LEU:N	2.53	0.41
1:D:955:SER:N	1:D:980:ASP:O	2.53	0.41
1:B:755:ASP:N	1:B:756:PRO:CD	2.84	0.41
1:C:291:VAL:O	1:C:291:VAL:HG12	2.21	0.41
1:C:590:SER:OG	1:C:591:TYR:N	2.52	0.41
1:D:926:ASP:OD1	1:D:926:ASP:N	2.44	0.41
1:F:590:SER:OG	1:F:591:TYR:N	2.52	0.41
1:F:291:VAL:O	1:F:291:VAL:HG12	2.21	0.40
1:D:755:ASP:HB2	1:D:756:PRO:HD3	2.03	0.40
1:D:976:LEU:O	1:D:1005:LEU:N	2.53	0.40
1:A:291:VAL:O	1:A:291:VAL:HG12	2.21	0.40
1:A:321:ASP:OD2	1:A:324:LYS:NZ	2.50	0.40
1:A:755:ASP:N	1:A:756:PRO:CD	2.84	0.40
1:A:976:LEU:O	1:A:1005:LEU:N	2.53	0.40
1:D:755:ASP:N	1:D:756:PRO:CD	2.85	0.40
1:E:291:VAL:O	1:E:291:VAL:HG12	2.22	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	808/910 (89%)	773 (96%)	31 (4%)	4 (0%)	24	62
1	B	808/910 (89%)	773 (96%)	31 (4%)	4 (0%)	24	62
1	C	808/910 (89%)	775 (96%)	29 (4%)	4 (0%)	24	62
1	D	808/910 (89%)	774 (96%)	29 (4%)	5 (1%)	21	58
1	E	808/910 (89%)	778 (96%)	26 (3%)	4 (0%)	24	62
1	F	808/910 (89%)	774 (96%)	30 (4%)	4 (0%)	24	62
All	All	4848/5460 (89%)	4647 (96%)	176 (4%)	25 (0%)	26	62

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	GLU
1	A	555	SER
1	A	892	VAL
1	B	511	GLU
1	B	555	SER
1	B	892	VAL
1	C	511	GLU
1	C	555	SER
1	C	892	VAL
1	D	511	GLU
1	D	555	SER
1	D	892	VAL
1	E	511	GLU
1	E	555	SER
1	E	892	VAL
1	F	511	GLU
1	F	555	SER
1	F	892	VAL
1	A	164	LEU
1	B	164	LEU

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Mol	Chain	Res	Type
1	C	164	LEU
1	D	164	LEU
1	D	319	CYS
1	E	164	LEU
1	F	164	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	742/822 (90%)	742 (100%)	0	100	100
1	B	742/822 (90%)	742 (100%)	0	100	100
1	C	742/822 (90%)	742 (100%)	0	100	100
1	D	742/822 (90%)	742 (100%)	0	100	100
1	E	742/822 (90%)	742 (100%)	0	100	100
1	F	742/822 (90%)	742 (100%)	0	100	100
All	All	4452/4932 (90%)	4452 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	215	HIS
1	A	522	HIS
1	A	798	GLN
1	B	215	HIS
1	B	400	GLN
1	B	522	HIS
1	B	798	GLN
1	C	215	HIS
1	C	465	HIS
1	C	506	ASN
1	C	526	GLN

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Mol	Chain	Res	Type
1	C	644	GLN
1	C	672	ASN
1	C	798	GLN
1	D	215	HIS
1	D	465	HIS
1	D	644	GLN
1	D	672	ASN
1	D	798	GLN
1	E	215	HIS
1	E	798	GLN
1	E	887	GLN
1	F	215	HIS
1	F	465	HIS
1	F	644	GLN
1	F	672	ASN
1	F	798	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	1102	-	32,33,33	1.24	4 (12%)	48,52,52	1.79	8 (16%)
3	ATP	A	1102	-	32,33,33	1.26	4 (12%)	48,52,52	1.79	8 (16%)
3	ATP	C	1102	-	32,33,33	1.28	4 (12%)	48,52,52	1.80	8 (16%)
3	ATP	D	1102	-	32,33,33	1.28	4 (12%)	48,52,52	1.79	8 (16%)
3	ATP	E	1102	-	32,33,33	1.24	3 (9%)	48,52,52	1.79	8 (16%)
3	ATP	F	1102	-	32,33,33	1.27	4 (12%)	48,52,52	1.78	8 (16%)
2	7YN	A	1101	-	28,31,31	2.79	15 (53%)	33,48,48	2.57	13 (39%)
2	7YN	F	1101	-	28,31,31	2.42	14 (50%)	33,48,48	2.47	9 (27%)
2	7YN	D	1101	-	28,31,31	2.72	13 (46%)	33,48,48	2.62	11 (33%)
2	7YN	C	1101	-	28,31,31	2.59	15 (53%)	33,48,48	2.49	11 (33%)
2	7YN	E	1101	-	28,31,31	2.52	14 (50%)	33,48,48	2.48	10 (30%)
2	7YN	B	1101	-	28,31,31	2.69	15 (53%)	33,48,48	2.46	13 (39%)

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	B	1102	-	-	1/22/38/38	0/3/3/3
3	ATP	A	1102	-	-	1/22/38/38	0/3/3/3
3	ATP	C	1102	-	-	1/22/38/38	0/3/3/3
3	ATP	D	1102	-	-	0/22/38/38	0/3/3/3
3	ATP	E	1102	-	-	0/22/38/38	0/3/3/3
3	ATP	F	1102	-	-	0/22/38/38	0/3/3/3
2	7YN	A	1101	-	-	8/19/33/33	0/4/4/4
2	7YN	F	1101	-	-	9/19/33/33	0/4/4/4
2	7YN	D	1101	-	-	8/19/33/33	0/4/4/4
2	7YN	C	1101	-	-	4/19/33/33	0/4/4/4
2	7YN	E	1101	-	-	3/19/33/33	0/4/4/4
2	7YN	B	1101	-	-	6/19/33/33	0/4/4/4

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	7YN	S17-N15	7.42	1.71	1.64
2	D	1101	7YN	S17-N15	7.26	1.71	1.64
2	A	1101	7YN	S17-N15	7.25	1.71	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	7YN	S17-N15	6.30	1.70	1.64
2	C	1101	7YN	S17-N15	5.96	1.69	1.64
2	A	1101	7YN	C24-C22	4.88	1.56	1.52
2	F	1101	7YN	O21-C19	-4.68	1.33	1.37
2	A	1101	7YN	C14-N13	4.61	1.47	1.37
2	D	1101	7YN	C14-N13	4.58	1.47	1.37
2	D	1101	7YN	C24-C22	4.54	1.56	1.52
2	B	1101	7YN	C14-N13	4.50	1.47	1.37
2	F	1101	7YN	S17-N15	4.49	1.68	1.64
2	C	1101	7YN	C14-N13	4.37	1.47	1.37
2	B	1101	7YN	C02-C04	4.35	1.45	1.40
2	D	1101	7YN	C07-C04	4.02	1.57	1.50
2	C	1101	7YN	C02-C04	3.92	1.44	1.40
2	D	1101	7YN	C06-C09	3.74	1.54	1.43
2	B	1101	7YN	C07-C04	3.72	1.56	1.50
2	A	1101	7YN	C02-C04	3.67	1.44	1.40
2	E	1101	7YN	O26-C24	-3.65	1.39	1.43
2	E	1101	7YN	C06-C09	3.64	1.54	1.43
2	E	1101	7YN	C14-N13	3.62	1.45	1.37
2	F	1101	7YN	C14-N13	3.61	1.45	1.37
2	F	1101	7YN	C07-C04	3.60	1.56	1.50
2	A	1101	7YN	C06-C09	3.54	1.54	1.43
2	D	1101	7YN	C02-C04	3.52	1.44	1.40
2	C	1101	7YN	C07-C04	3.41	1.56	1.50
2	B	1101	7YN	C06-C09	3.40	1.53	1.43
2	E	1101	7YN	C07-C04	3.36	1.56	1.50
2	A	1101	7YN	C07-C04	3.34	1.56	1.50
2	B	1101	7YN	C24-C22	3.33	1.55	1.52
2	C	1101	7YN	O26-C24	-3.31	1.40	1.43
2	F	1101	7YN	C06-C09	3.31	1.53	1.43
2	A	1101	7YN	C14-N15	3.29	1.46	1.39
2	F	1101	7YN	C14-N15	3.28	1.46	1.39
2	C	1101	7YN	C06-C09	3.25	1.53	1.43
2	E	1101	7YN	C24-C22	3.15	1.55	1.52
2	D	1101	7YN	C10-C01	3.15	1.57	1.51
3	C	1102	ATP	PB-O3A	3.10	1.62	1.59
2	C	1101	7YN	C14-N15	3.04	1.46	1.39
2	E	1101	7YN	C02-C01	3.04	1.43	1.40
2	A	1101	7YN	C10-C01	3.03	1.56	1.51
3	D	1102	ATP	PB-O3A	3.00	1.62	1.59
2	E	1101	7YN	C02-C04	2.99	1.43	1.40
3	F	1102	ATP	PB-O3A	2.98	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	ATP	PB-O3A	2.96	1.62	1.59
2	F	1101	7YN	O16-C14	-2.95	1.17	1.23
2	C	1101	7YN	C24-C22	2.94	1.54	1.52
2	B	1101	7YN	C09-C08	2.93	1.52	1.36
2	D	1101	7YN	C09-C08	2.91	1.52	1.36
2	C	1101	7YN	C09-C08	2.91	1.52	1.36
2	A	1101	7YN	C09-C08	2.88	1.52	1.36
2	E	1101	7YN	C09-C08	2.86	1.52	1.36
2	F	1101	7YN	C24-C22	2.84	1.54	1.52
2	B	1101	7YN	O16-C14	-2.84	1.17	1.23
3	E	1102	ATP	PB-O3A	2.82	1.62	1.59
2	A	1101	7YN	O21-C19	-2.81	1.34	1.37
2	E	1101	7YN	C14-N15	2.77	1.45	1.39
2	B	1101	7YN	C14-N15	2.77	1.45	1.39
3	B	1102	ATP	PB-O3A	2.77	1.62	1.59
2	F	1101	7YN	C09-C08	2.76	1.51	1.36
2	B	1101	7YN	C10-C01	2.74	1.56	1.51
2	F	1101	7YN	C02-C04	2.68	1.43	1.40
2	D	1101	7YN	C14-N15	2.67	1.45	1.39
2	F	1101	7YN	O21-C23	-2.64	1.32	1.37
2	C	1101	7YN	O16-C14	-2.64	1.17	1.23
2	C	1101	7YN	C10-C01	2.62	1.56	1.51
2	D	1101	7YN	O16-C14	-2.57	1.17	1.23
2	D	1101	7YN	O26-C24	-2.51	1.40	1.43
2	A	1101	7YN	O26-C24	-2.50	1.40	1.43
2	A	1101	7YN	C02-C01	2.46	1.43	1.40
2	C	1101	7YN	O18-S17	2.46	1.47	1.43
2	F	1101	7YN	C10-C01	2.42	1.55	1.51
2	C	1101	7YN	O21-C19	-2.42	1.35	1.37
2	E	1101	7YN	C10-C01	2.41	1.55	1.51
2	A	1101	7YN	O16-C14	-2.39	1.18	1.23
2	E	1101	7YN	O16-C14	-2.39	1.18	1.23
2	B	1101	7YN	O18-S17	2.35	1.46	1.43
2	B	1101	7YN	O21-C19	-2.35	1.35	1.37
2	B	1101	7YN	C02-C01	2.34	1.42	1.40
3	C	1102	ATP	C5-C4	2.33	1.43	1.39
3	F	1102	ATP	PA-O3A	2.32	1.62	1.59
2	D	1101	7YN	O18-S17	2.31	1.46	1.43
3	B	1102	ATP	C5-C4	2.30	1.43	1.39
3	D	1102	ATP	C5-C4	2.27	1.43	1.39
2	C	1101	7YN	O28-S17	2.27	1.46	1.43
3	A	1102	ATP	C5-C4	2.26	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1102	ATP	C5-C4	2.24	1.43	1.39
2	B	1101	7YN	C12-C03	2.23	1.54	1.51
2	F	1101	7YN	C05-C03	2.21	1.43	1.39
3	D	1102	ATP	PB-O3B	2.20	1.61	1.59
3	A	1102	ATP	PB-O3B	2.19	1.61	1.59
2	A	1101	7YN	C05-C03	2.18	1.42	1.39
2	E	1101	7YN	O18-S17	2.18	1.46	1.43
3	F	1102	ATP	C5-C4	2.17	1.43	1.39
3	D	1102	ATP	PA-O3A	2.17	1.61	1.59
2	E	1101	7YN	O28-S17	2.15	1.46	1.43
3	A	1102	ATP	PA-O3A	2.14	1.61	1.59
2	A	1101	7YN	O21-C23	-2.14	1.33	1.37
3	C	1102	ATP	PA-O3A	2.13	1.61	1.59
2	D	1101	7YN	O21-C23	-2.13	1.33	1.37
3	B	1102	ATP	PB-O3B	2.11	1.61	1.59
3	C	1102	ATP	PB-O3B	2.09	1.61	1.59
3	F	1102	ATP	PB-O3B	2.08	1.61	1.59
2	B	1101	7YN	O26-C24	-2.08	1.41	1.43
3	E	1102	ATP	PA-O3A	2.07	1.61	1.59
2	F	1101	7YN	C02-N13	2.03	1.47	1.43
3	B	1102	ATP	PA-O3A	2.02	1.61	1.59
2	C	1101	7YN	C02-N13	2.01	1.47	1.43

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	7YN	O28-S17-O18	-10.38	100.79	119.82
2	C	1101	7YN	O28-S17-O18	-10.26	101.01	119.82
2	B	1101	7YN	O28-S17-O18	-10.06	101.38	119.82
2	E	1101	7YN	O28-S17-O18	-9.91	101.66	119.82
2	F	1101	7YN	O28-S17-O18	-9.87	101.73	119.82
2	A	1101	7YN	O28-S17-O18	-9.70	102.04	119.82
3	C	1102	ATP	C5-C4-N3	-5.74	118.81	126.72
3	E	1102	ATP	C5-C4-N3	-5.74	118.82	126.72
3	D	1102	ATP	C5-C4-N3	-5.73	118.83	126.72
3	F	1102	ATP	C5-C4-N3	-5.66	118.92	126.72
3	B	1102	ATP	C5-C4-N3	-5.64	118.95	126.72
3	A	1102	ATP	C5-C4-N3	-5.62	118.98	126.72
3	B	1102	ATP	N3-C4-N9	5.00	135.68	127.17
3	D	1102	ATP	N3-C4-N9	4.99	135.65	127.17
3	A	1102	ATP	N3-C4-N9	4.97	135.62	127.17
3	C	1102	ATP	N3-C4-N9	4.94	135.57	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1102	ATP	N3-C4-N9	4.93	135.55	127.17
3	F	1102	ATP	N3-C4-N9	4.85	135.42	127.17
3	A	1102	ATP	N3-C2-N1	-4.48	121.81	128.58
3	E	1102	ATP	N3-C2-N1	-4.45	121.85	128.58
3	B	1102	ATP	N3-C2-N1	-4.43	121.88	128.58
3	F	1102	ATP	N3-C2-N1	-4.42	121.89	128.58
3	D	1102	ATP	N3-C2-N1	-4.42	121.89	128.58
3	C	1102	ATP	N3-C2-N1	-4.39	121.94	128.58
2	A	1101	7YN	C20-C22-C23	4.17	107.43	105.23
2	A	1101	7YN	O18-S17-C19	4.15	113.33	107.07
2	E	1101	7YN	C23-O21-C19	4.04	109.70	106.07
2	E	1101	7YN	O18-S17-C19	4.03	113.14	107.07
2	D	1101	7YN	C23-O21-C19	3.97	109.64	106.07
2	C	1101	7YN	C23-O21-C19	3.94	109.62	106.07
2	F	1101	7YN	C23-O21-C19	3.94	109.61	106.07
2	B	1101	7YN	C23-O21-C19	3.90	109.58	106.07
2	D	1101	7YN	O18-S17-C19	3.89	112.94	107.07
2	D	1101	7YN	C20-C22-C23	3.77	107.22	105.23
3	C	1102	ATP	C5-N7-C8	3.76	109.37	103.45
3	F	1102	ATP	C5-N7-C8	3.76	109.36	103.45
3	D	1102	ATP	C5-N7-C8	3.72	109.30	103.45
3	E	1102	ATP	C5-N7-C8	3.71	109.28	103.45
3	E	1102	ATP	C2-N3-C4	3.71	120.89	111.83
3	A	1102	ATP	C2-N3-C4	3.71	120.89	111.83
3	A	1102	ATP	C5-N7-C8	3.70	109.27	103.45
3	D	1102	ATP	C2-N3-C4	3.70	120.87	111.83
3	B	1102	ATP	C5-N7-C8	3.70	109.27	103.45
3	B	1102	ATP	C2-N3-C4	3.69	120.83	111.83
3	C	1102	ATP	C2-N3-C4	3.69	120.83	111.83
3	F	1102	ATP	C2-N3-C4	3.68	120.82	111.83
2	A	1101	7YN	C23-O21-C19	3.68	109.38	106.07
2	A	1101	7YN	C10-C01-C03	-3.26	107.41	110.78
2	E	1101	7YN	O28-S17-C19	3.21	111.90	107.07
2	F	1101	7YN	C20-C22-C23	3.15	106.89	105.23
2	F	1101	7YN	O28-S17-C19	3.13	111.78	107.07
2	B	1101	7YN	O28-S17-C19	3.06	111.68	107.07
2	B	1101	7YN	C04-C02-C01	-3.00	118.04	122.56
2	C	1101	7YN	C10-C01-C03	-2.99	107.69	110.78
2	C	1101	7YN	O18-S17-C19	2.97	111.55	107.07
2	E	1101	7YN	C12-C03-C01	-2.96	107.79	110.27
2	D	1101	7YN	O28-S17-C19	2.96	111.53	107.07
3	C	1102	ATP	C4-C5-N7	-2.91	107.25	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	7YN	C12-C03-C01	-2.91	107.83	110.27
2	B	1101	7YN	O18-S17-C19	2.90	111.44	107.07
3	E	1102	ATP	C4-C5-N7	-2.86	107.31	110.58
3	F	1102	ATP	C4-C5-N7	-2.86	107.32	110.58
3	D	1102	ATP	C4-C5-N7	-2.80	107.38	110.58
3	A	1102	ATP	C4-C5-N7	-2.78	107.41	110.58
2	C	1101	7YN	C12-C03-C01	-2.76	107.96	110.27
3	B	1102	ATP	C4-C5-N7	-2.76	107.43	110.58
2	B	1101	7YN	C12-C03-C01	-2.69	108.02	110.27
2	F	1101	7YN	C10-C01-C03	-2.68	108.02	110.78
2	F	1101	7YN	C12-C03-C01	-2.66	108.04	110.27
2	A	1101	7YN	C04-C02-C01	-2.64	118.59	122.56
2	A	1101	7YN	C25-C24-C22	-2.62	106.86	110.88
2	A	1101	7YN	O18-S17-N15	2.59	112.97	106.66
2	C	1101	7YN	O28-S17-C19	2.58	110.96	107.07
2	B	1101	7YN	C07-C08-C09	-2.58	103.40	111.78
2	F	1101	7YN	C07-C08-C09	-2.57	103.42	111.78
2	E	1101	7YN	C10-C01-C03	-2.57	108.13	110.78
2	C	1101	7YN	C07-C08-C09	-2.55	103.49	111.78
2	A	1101	7YN	O28-S17-C19	2.53	110.88	107.07
2	D	1101	7YN	C10-C01-C03	-2.53	108.17	110.78
2	E	1101	7YN	C04-C02-C01	-2.50	118.80	122.56
2	A	1101	7YN	C02-N13-C14	2.46	125.85	121.95
2	B	1101	7YN	C10-C01-C03	-2.44	108.26	110.78
2	A	1101	7YN	C07-C08-C09	-2.41	103.93	111.78
2	F	1101	7YN	O18-S17-C19	2.41	110.70	107.07
2	E	1101	7YN	C07-C08-C09	-2.39	104.00	111.78
2	D	1101	7YN	C07-C08-C09	-2.38	104.04	111.78
2	F	1101	7YN	O18-S17-N15	2.33	112.33	106.66
2	D	1101	7YN	C06-C09-C08	-2.32	103.48	108.91
2	D	1101	7YN	C04-C02-C01	-2.27	119.14	122.56
2	A	1101	7YN	C06-C05-C03	-2.27	118.99	122.25
3	C	1102	ATP	O2G-PG-O3B	2.27	112.25	104.64
2	D	1101	7YN	C12-C11-C10	-2.26	102.69	107.08
3	E	1102	ATP	O2G-PG-O3B	2.25	112.17	104.64
3	F	1102	ATP	O2G-PG-O3B	2.23	112.13	104.64
3	F	1102	ATP	N9-C8-N7	-2.23	110.77	113.94
3	B	1102	ATP	O2G-PG-O3B	2.21	112.06	104.64
2	B	1101	7YN	C06-C09-C08	-2.21	103.74	108.91
3	A	1102	ATP	O2G-PG-O3B	2.21	112.04	104.64
2	C	1101	7YN	C06-C09-C08	-2.18	103.80	108.91
2	B	1101	7YN	C20-C22-C23	2.17	106.37	105.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	ATP	N9-C8-N7	-2.16	110.88	113.94
2	B	1101	7YN	C06-C05-C03	-2.14	119.18	122.25
2	A	1101	7YN	C12-C03-C01	-2.13	108.49	110.27
2	E	1101	7YN	C12-C11-C10	-2.13	102.94	107.08
3	D	1102	ATP	N9-C8-N7	-2.13	110.92	113.94
3	A	1102	ATP	N9-C8-N7	-2.12	110.92	113.94
3	E	1102	ATP	N9-C8-N7	-2.12	110.93	113.94
3	C	1102	ATP	N9-C8-N7	-2.11	110.94	113.94
2	C	1101	7YN	N15-C14-N13	2.11	118.22	114.87
2	C	1101	7YN	C04-C02-C01	-2.07	119.45	122.56
3	D	1102	ATP	O2G-PG-O3B	2.05	111.53	104.64
2	E	1101	7YN	C06-C09-C08	-2.04	104.14	108.91
2	B	1101	7YN	N15-C14-N13	2.01	118.06	114.87
2	C	1101	7YN	C12-C11-C10	-2.00	103.18	107.08
2	B	1101	7YN	C12-C11-C10	-2.00	103.19	107.08

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	7YN	C23-C22-C24-C27
2	A	1101	7YN	C23-C22-C24-O26
2	A	1101	7YN	O21-C19-S17-O18
2	A	1101	7YN	O21-C19-S17-O28
2	B	1101	7YN	C23-C22-C24-C27
2	B	1101	7YN	C23-C22-C24-O26
2	C	1101	7YN	C23-C22-C24-C27
2	C	1101	7YN	C23-C22-C24-O26
2	D	1101	7YN	C23-C22-C24-C27
2	D	1101	7YN	C23-C22-C24-O26
2	D	1101	7YN	O21-C19-S17-O28
2	E	1101	7YN	C23-C22-C24-C27
2	E	1101	7YN	C23-C22-C24-O26
2	F	1101	7YN	C23-C22-C24-C25
2	F	1101	7YN	C23-C22-C24-O26
2	F	1101	7YN	O21-C19-S17-O18
2	F	1101	7YN	C14-N15-S17-O28
2	B	1101	7YN	C23-C22-C24-C25
2	C	1101	7YN	C23-C22-C24-C25
2	E	1101	7YN	C23-C22-C24-C25
2	F	1101	7YN	C14-N15-S17-C19
3	A	1102	ATP	C5'-O5'-PA-O1A

Continued on next page...

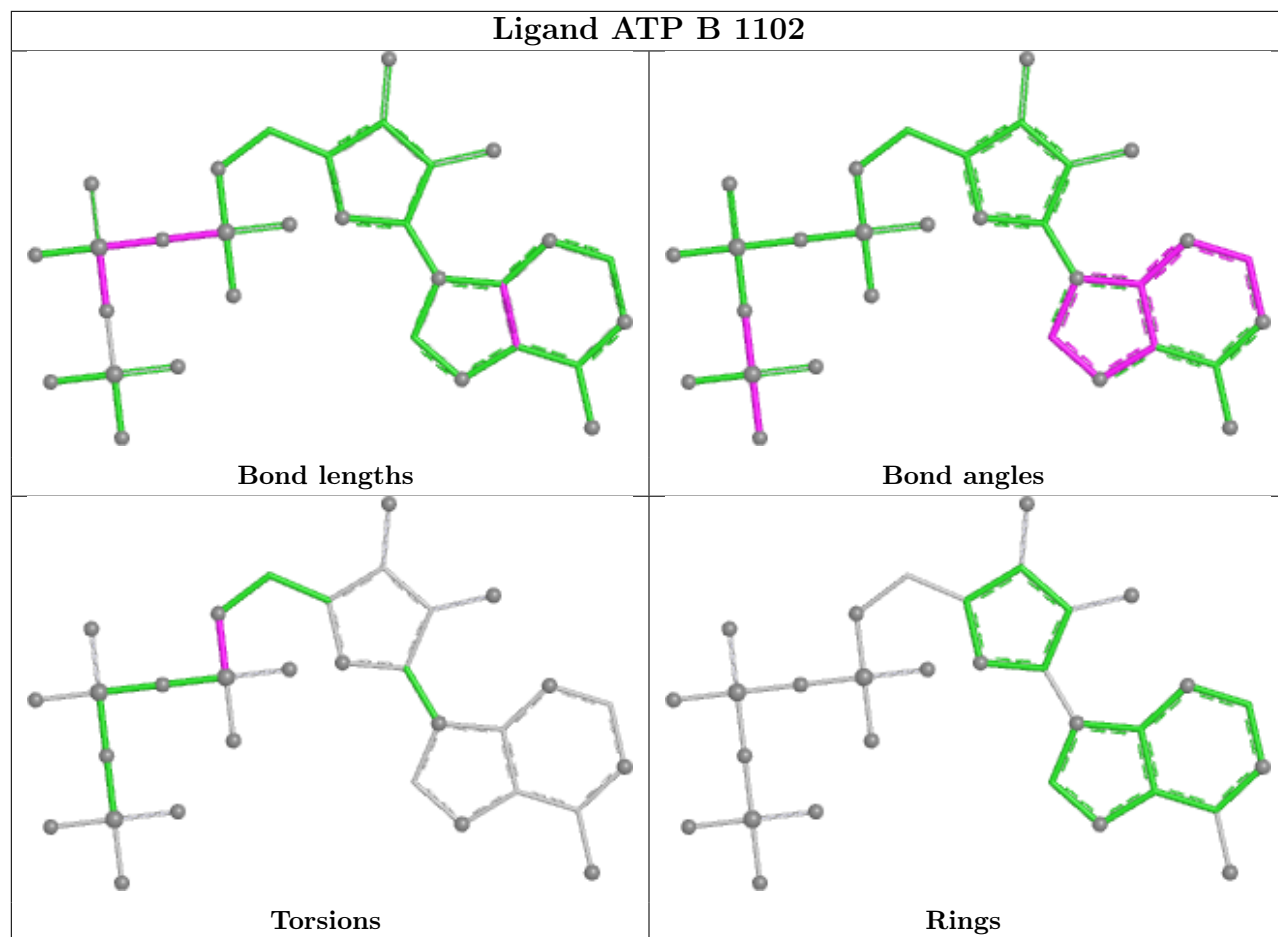
Continued from previous page...

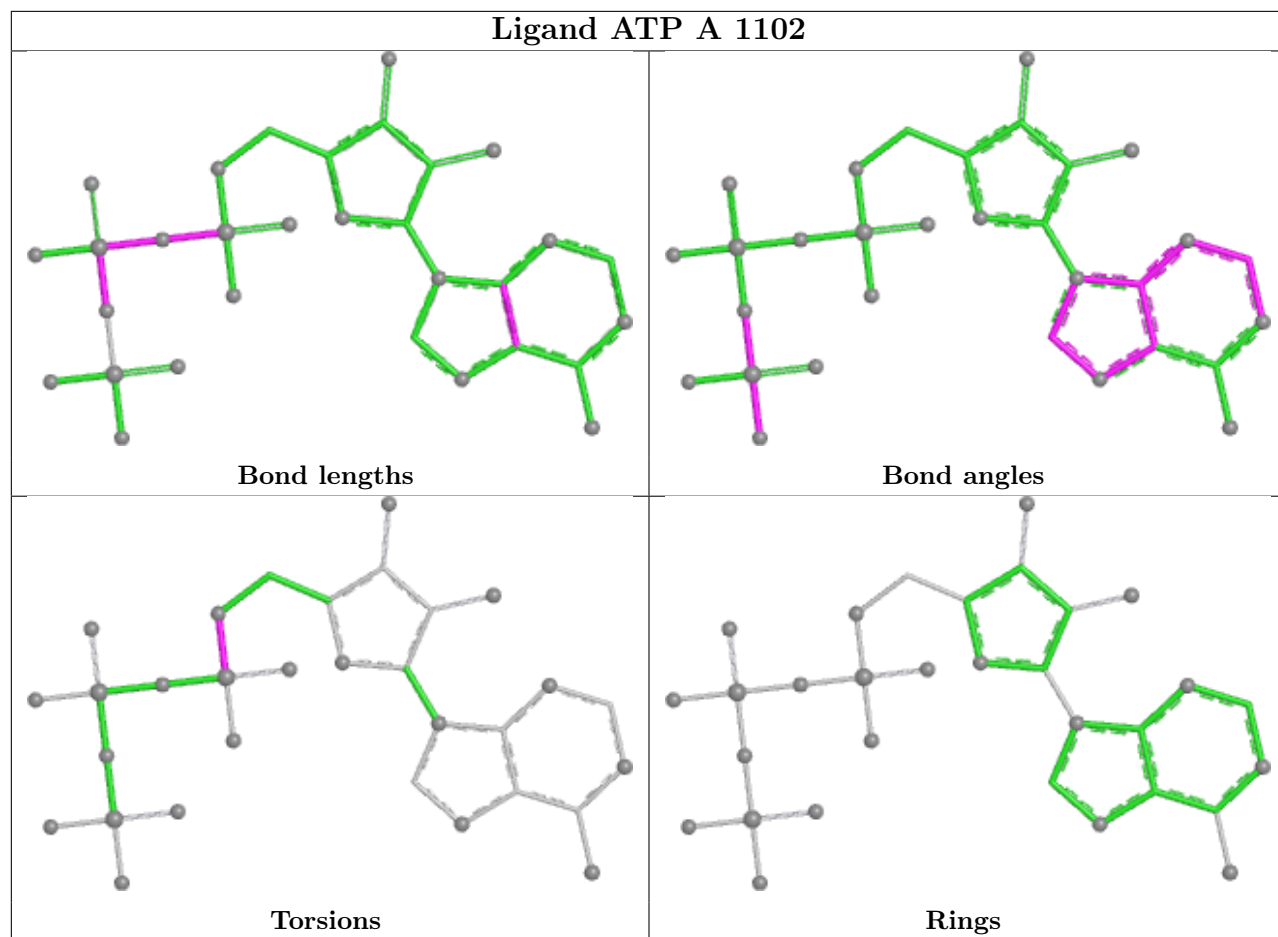
Mol	Chain	Res	Type	Atoms
3	B	1102	ATP	C5'-O5'-PA-O1A
2	A	1101	7YN	C20-C22-C24-C27
2	D	1101	7YN	C20-C22-C24-C27
2	A	1101	7YN	C20-C22-C24-C25
2	D	1101	7YN	C20-C22-C24-C25
2	F	1101	7YN	C20-C22-C24-C27
2	F	1101	7YN	C14-N15-S17-O18
2	A	1101	7YN	C20-C19-S17-O28
2	D	1101	7YN	C20-C19-S17-O28
2	F	1101	7YN	C20-C19-S17-O18
2	B	1101	7YN	C20-C22-C24-C27
3	C	1102	ATP	C2'-C1'-N9-C4
2	B	1101	7YN	C20-C22-C24-C25
2	F	1101	7YN	C20-C22-C24-C25
2	B	1101	7YN	O21-C19-S17-O28
2	C	1101	7YN	O21-C19-S17-O28
2	D	1101	7YN	O21-C19-S17-O18
2	A	1101	7YN	C23-C22-C24-C25
2	D	1101	7YN	C23-C22-C24-C25

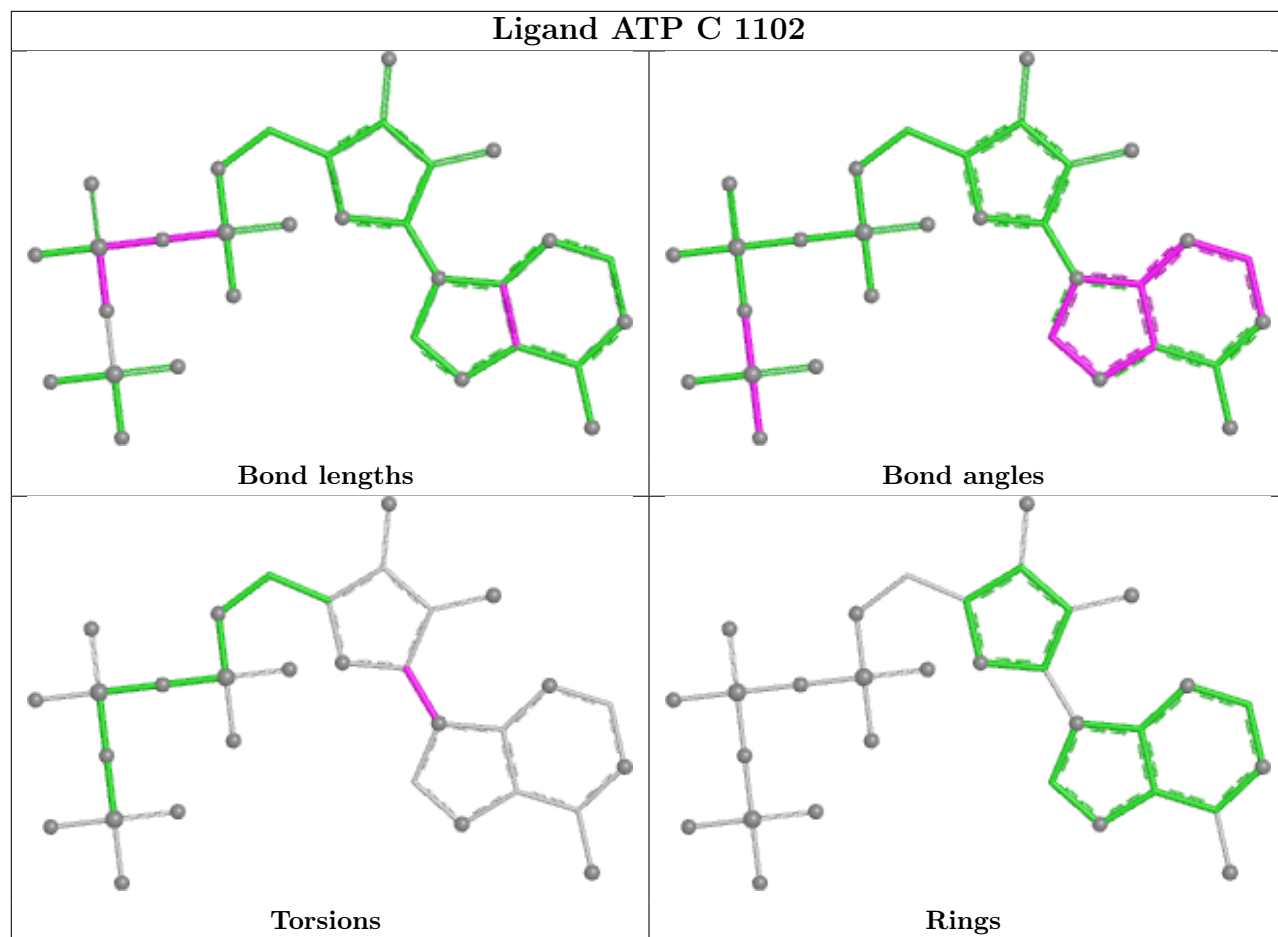
There are no ring outliers.

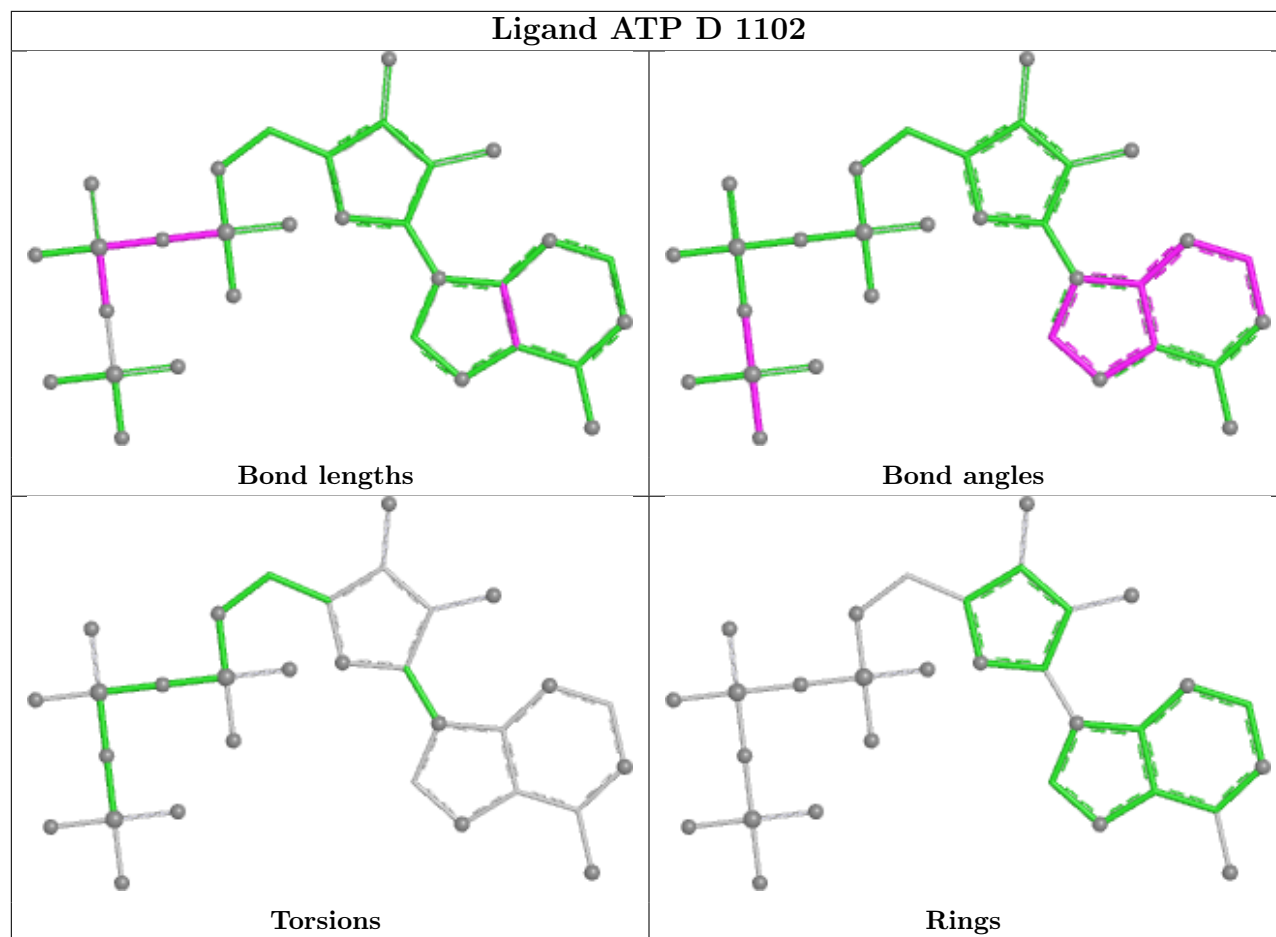
No monomer is involved in short contacts.

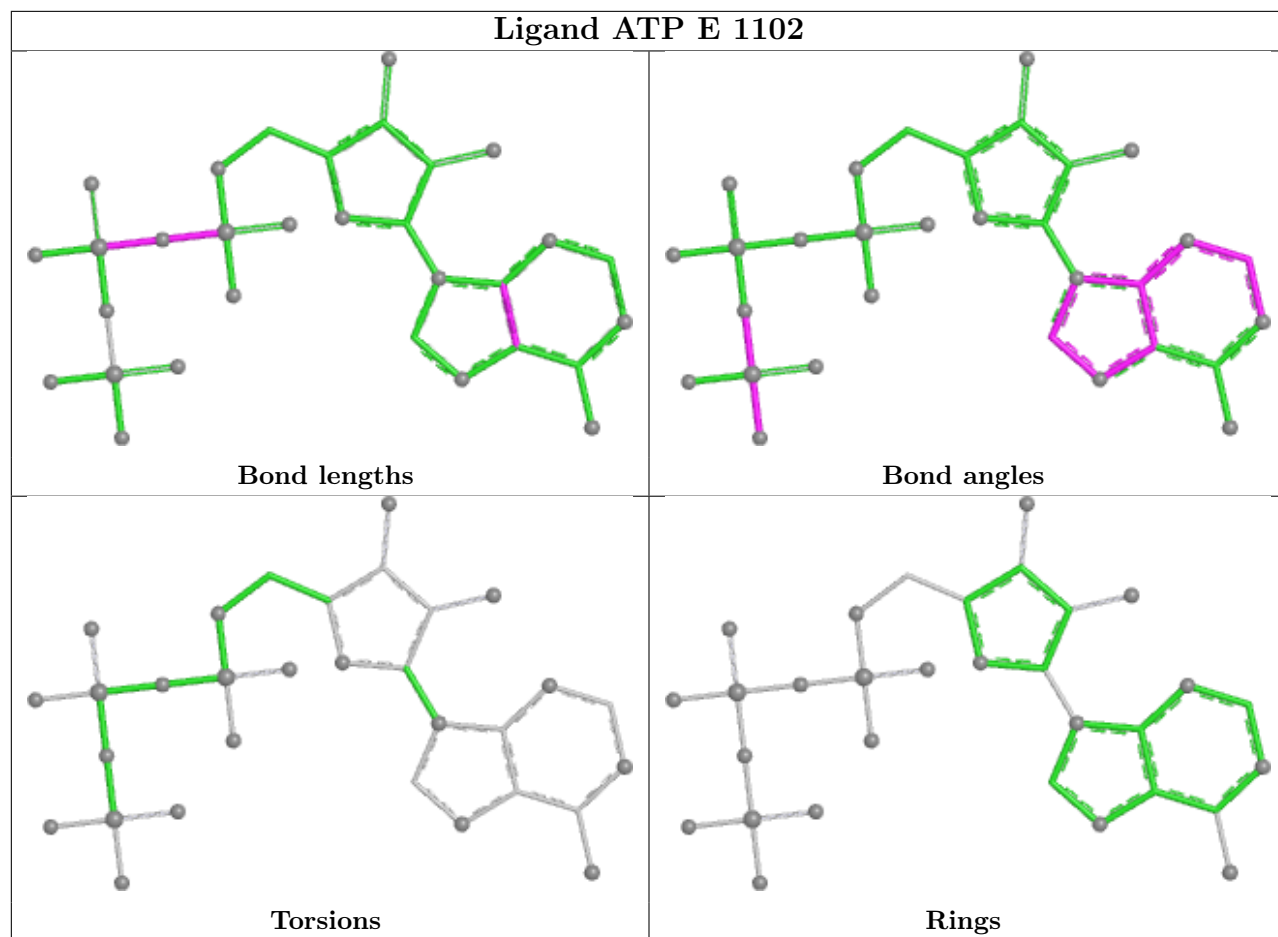
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

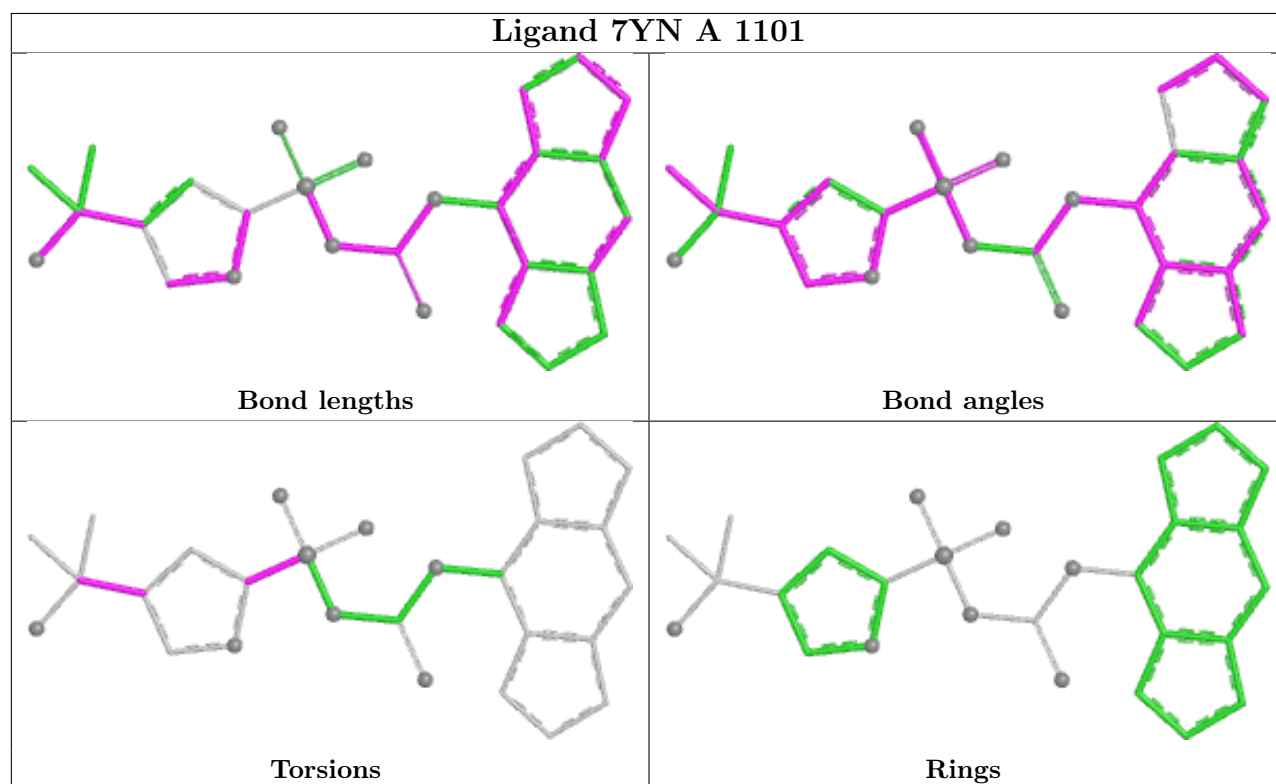
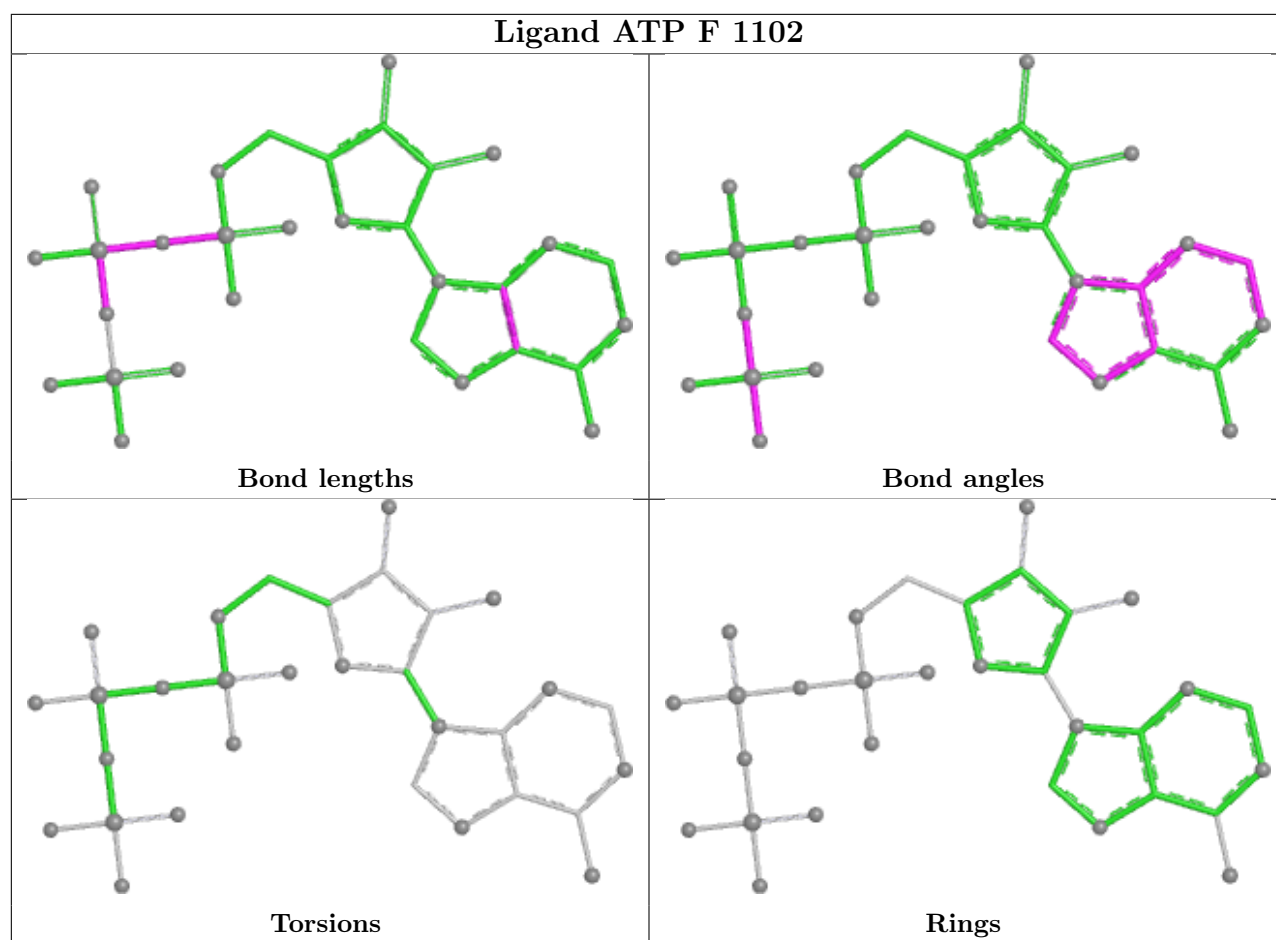


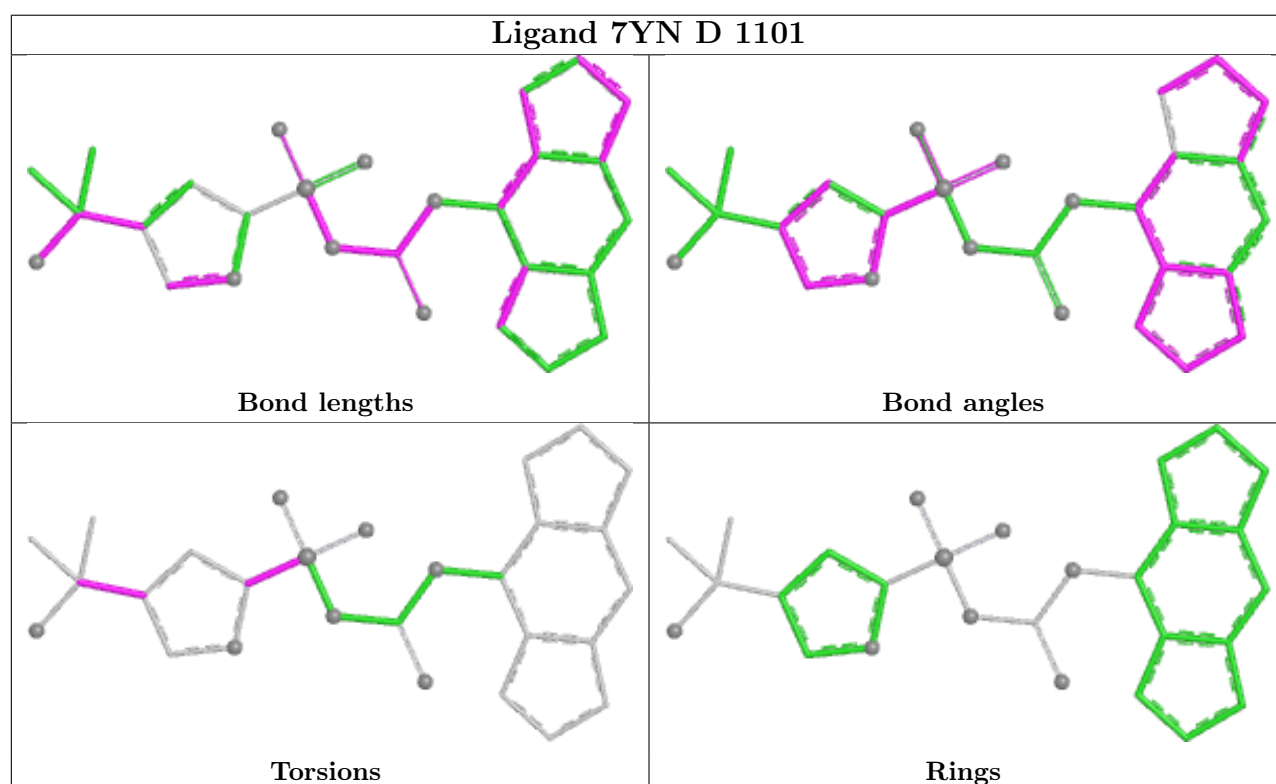
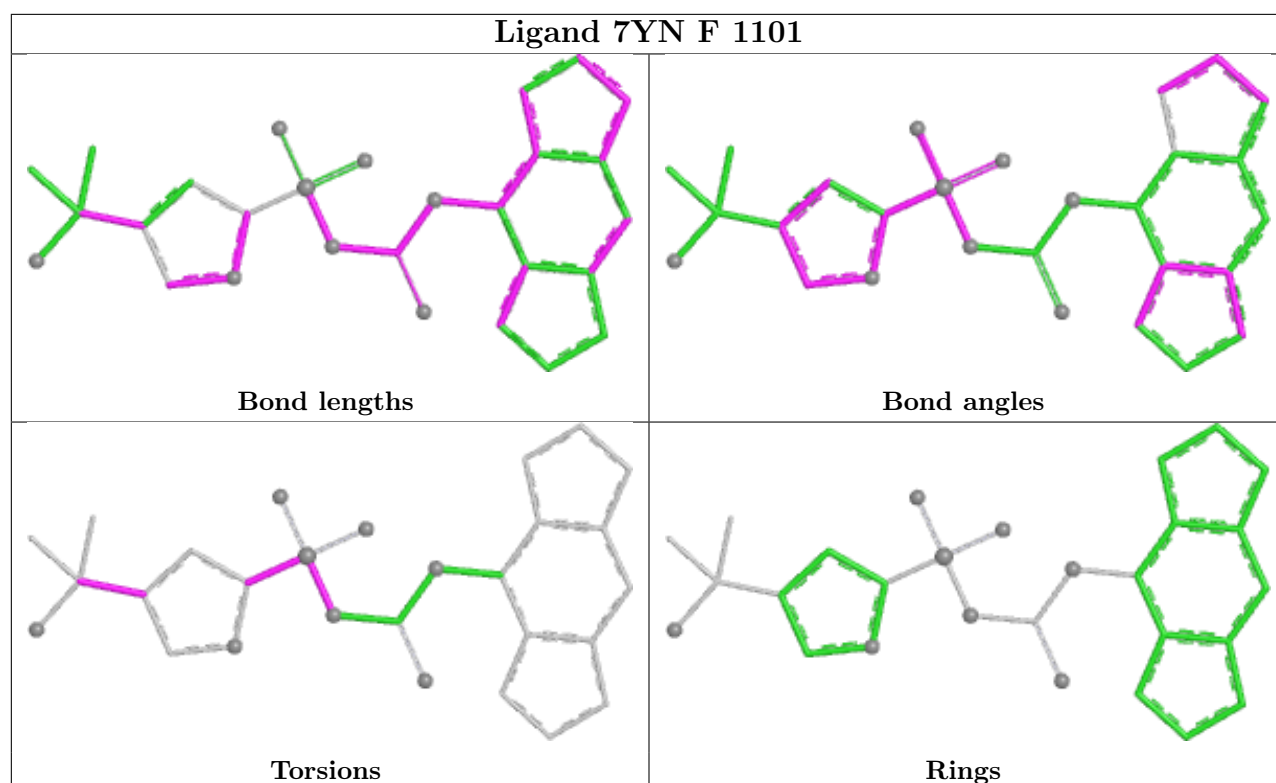


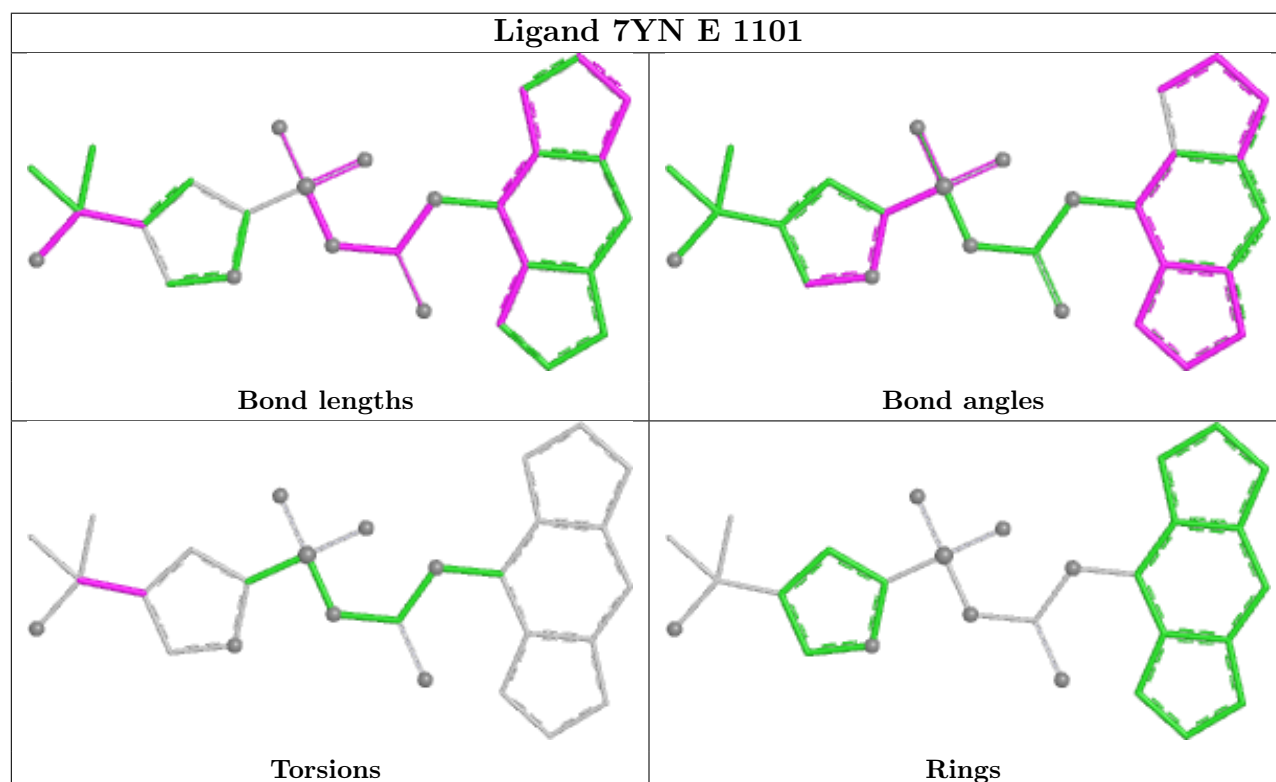
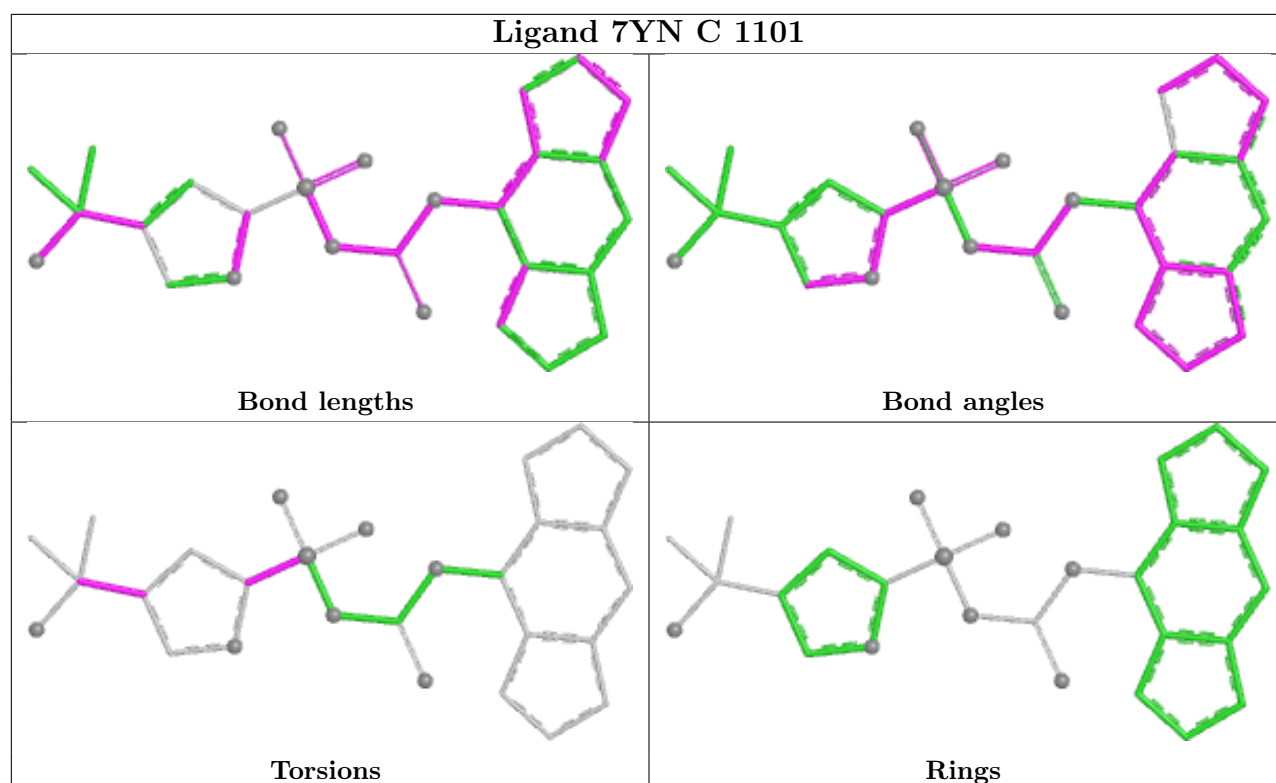


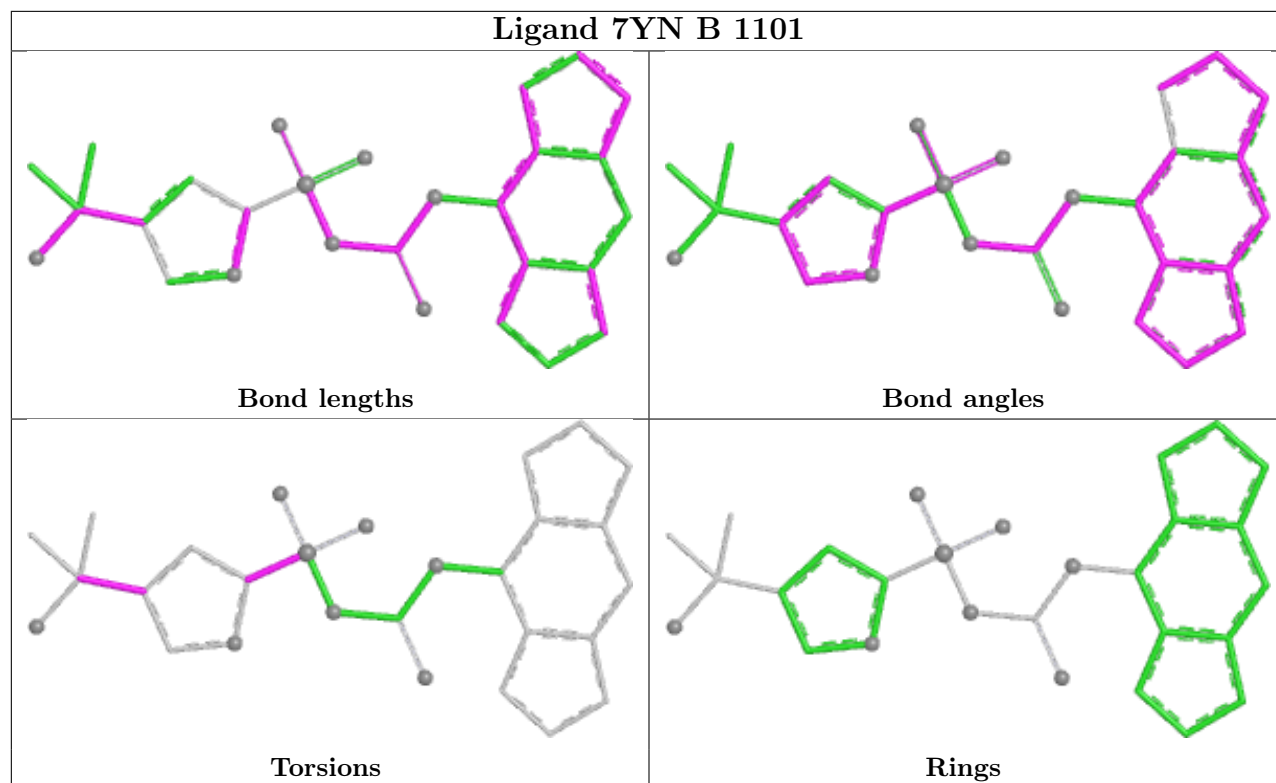












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

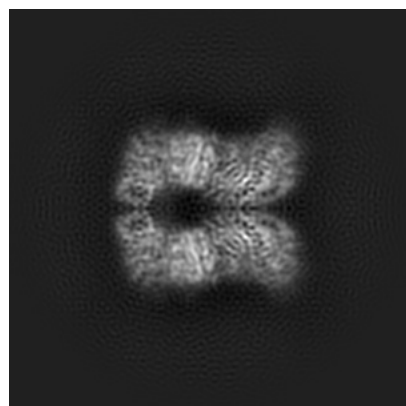
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40820. These allow visual inspection of the internal detail of the map and identification of artifacts.

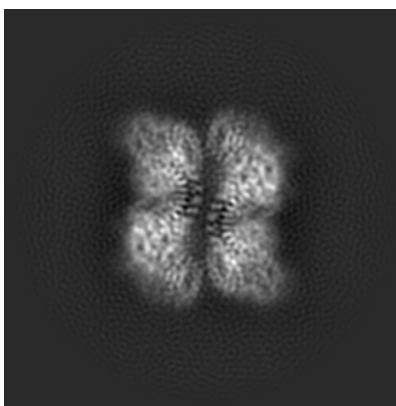
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

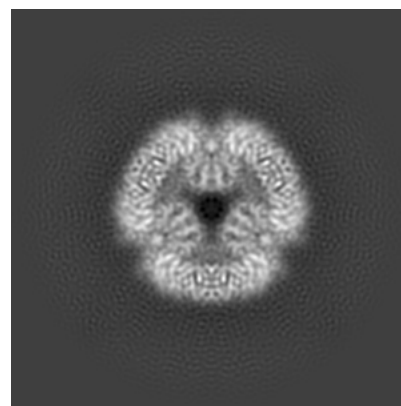
6.1.1 Primary map



X

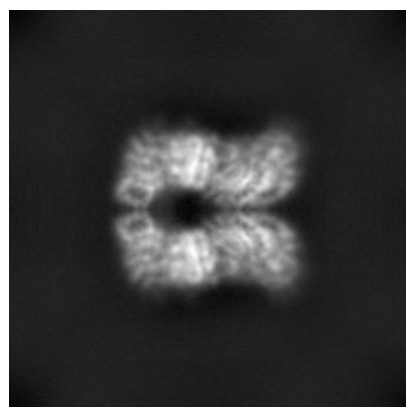


Y

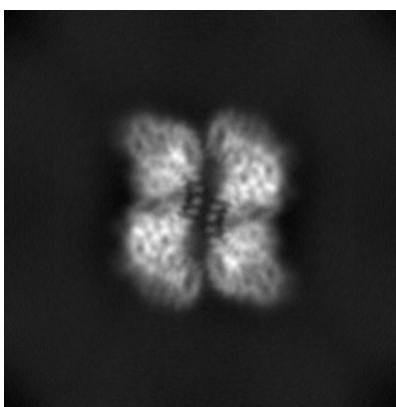


Z

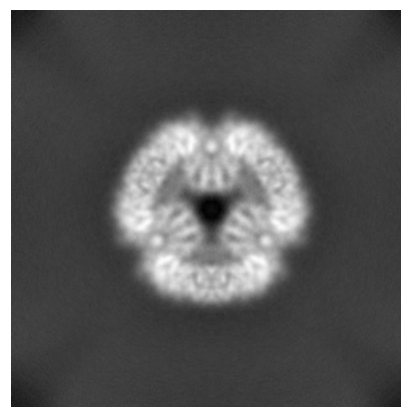
6.1.2 Raw map



X



Y

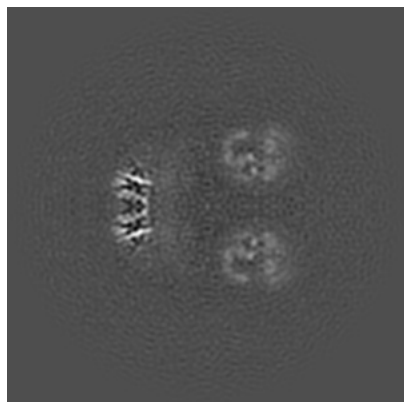


Z

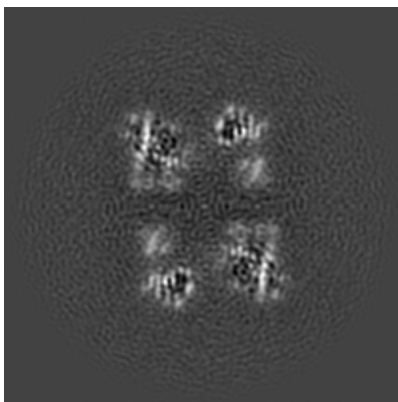
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

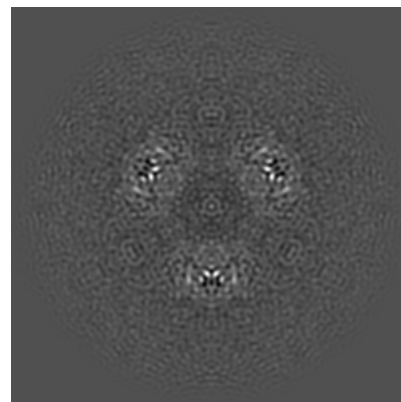
6.2.1 Primary map



X Index: 180

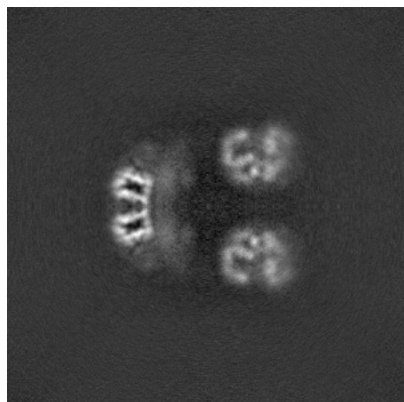


Y Index: 180

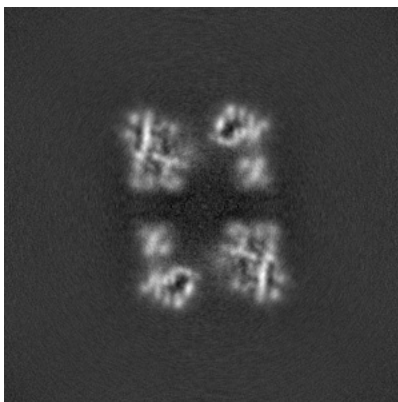


Z Index: 180

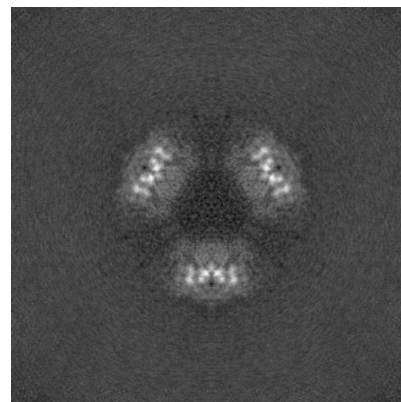
6.2.2 Raw map



X Index: 180



Y Index: 180

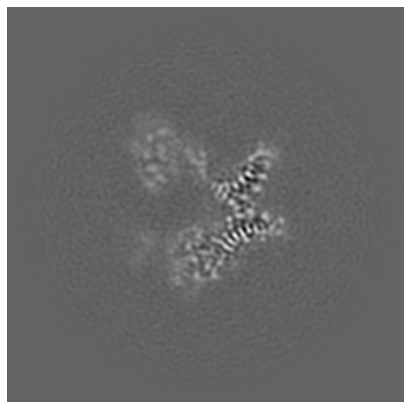


Z Index: 180

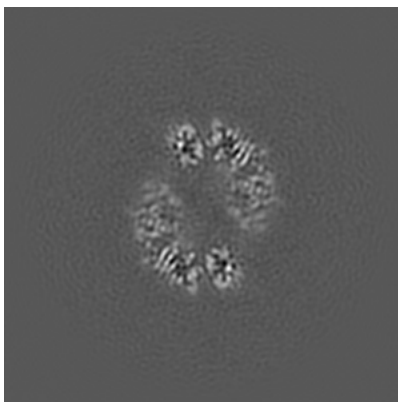
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

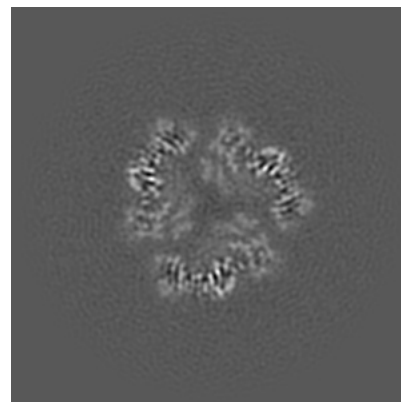
6.3.1 Primary map



X Index: 234

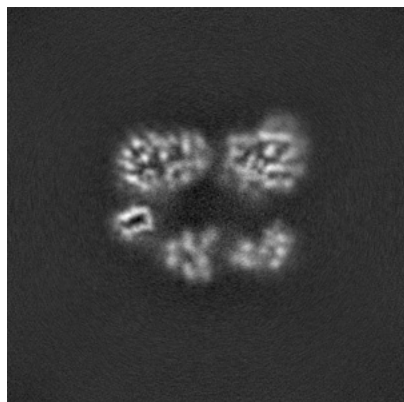


Y Index: 218

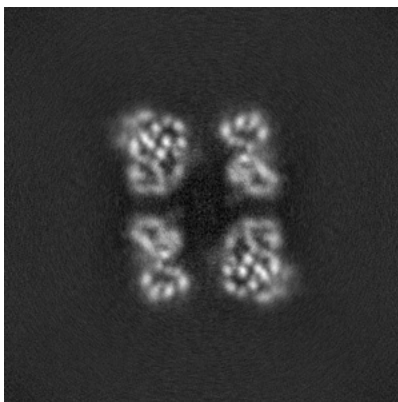


Z Index: 206

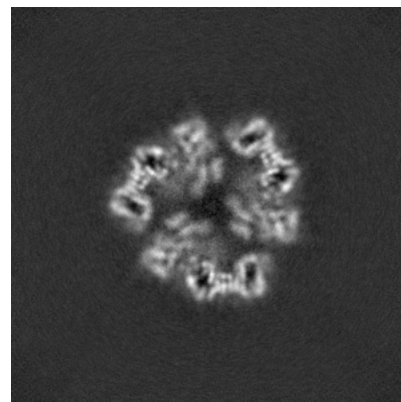
6.3.2 Raw map



X Index: 199



Y Index: 169

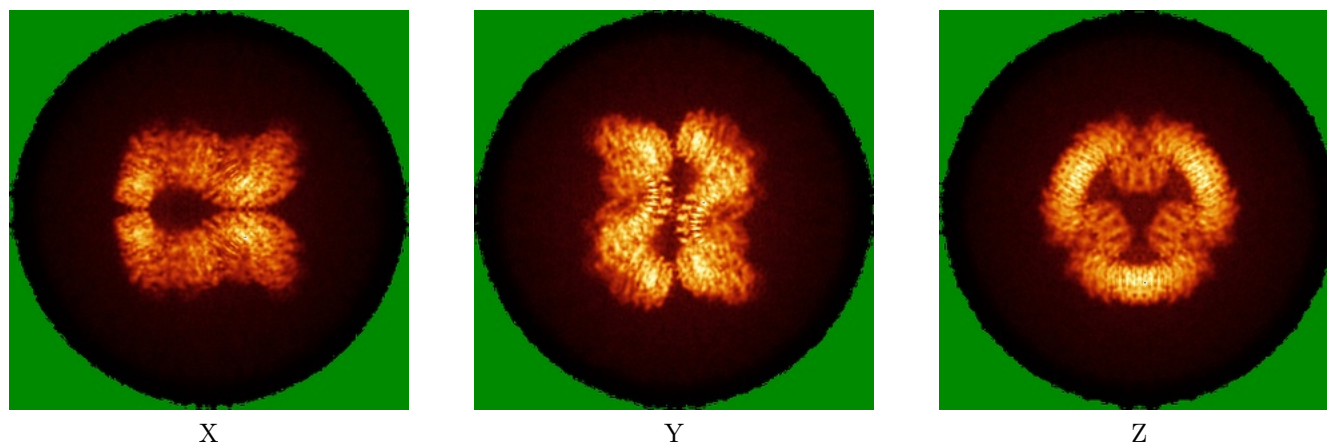


Z Index: 156

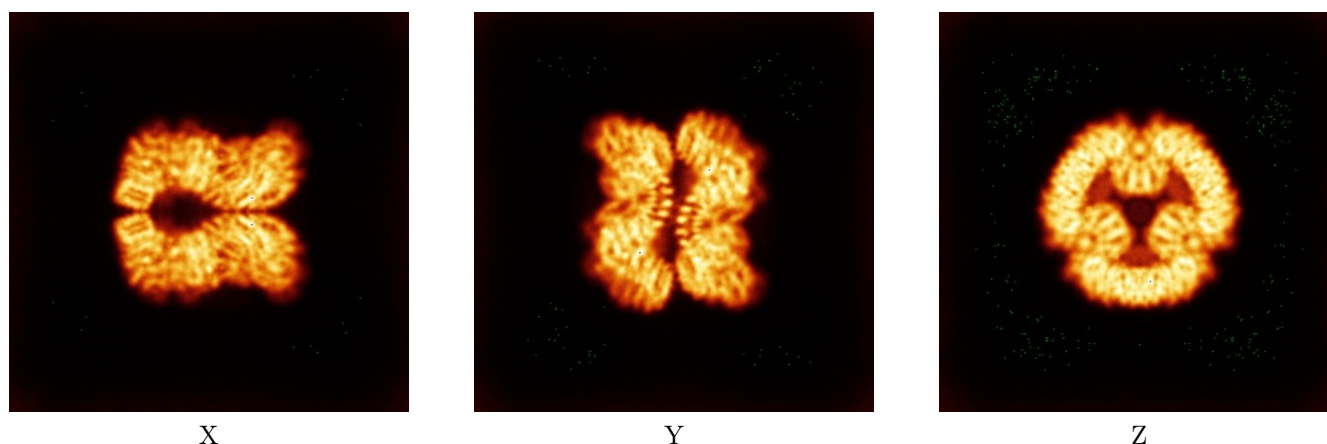
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

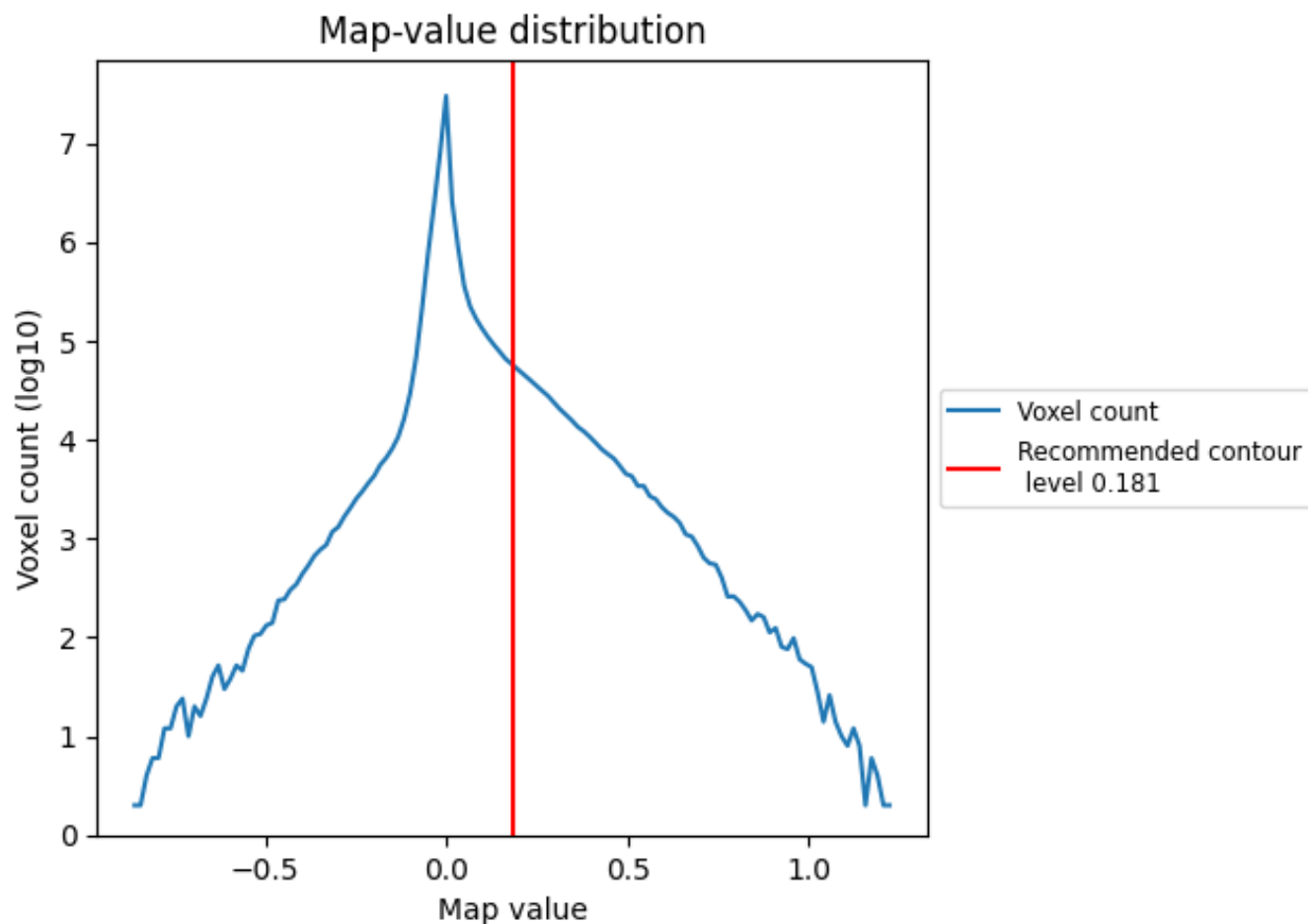
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

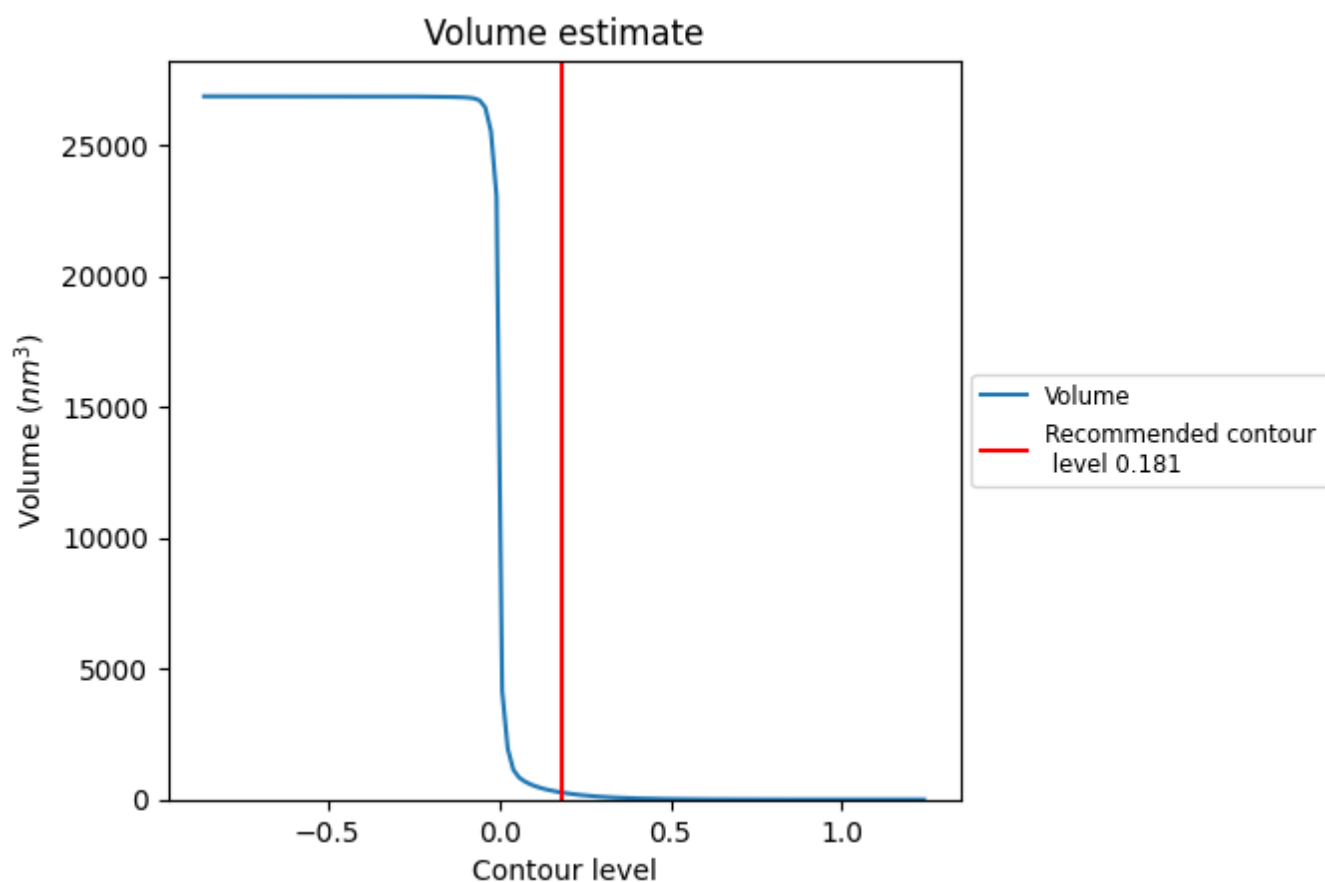
This section contains the results of statistical analysis of the map.

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.

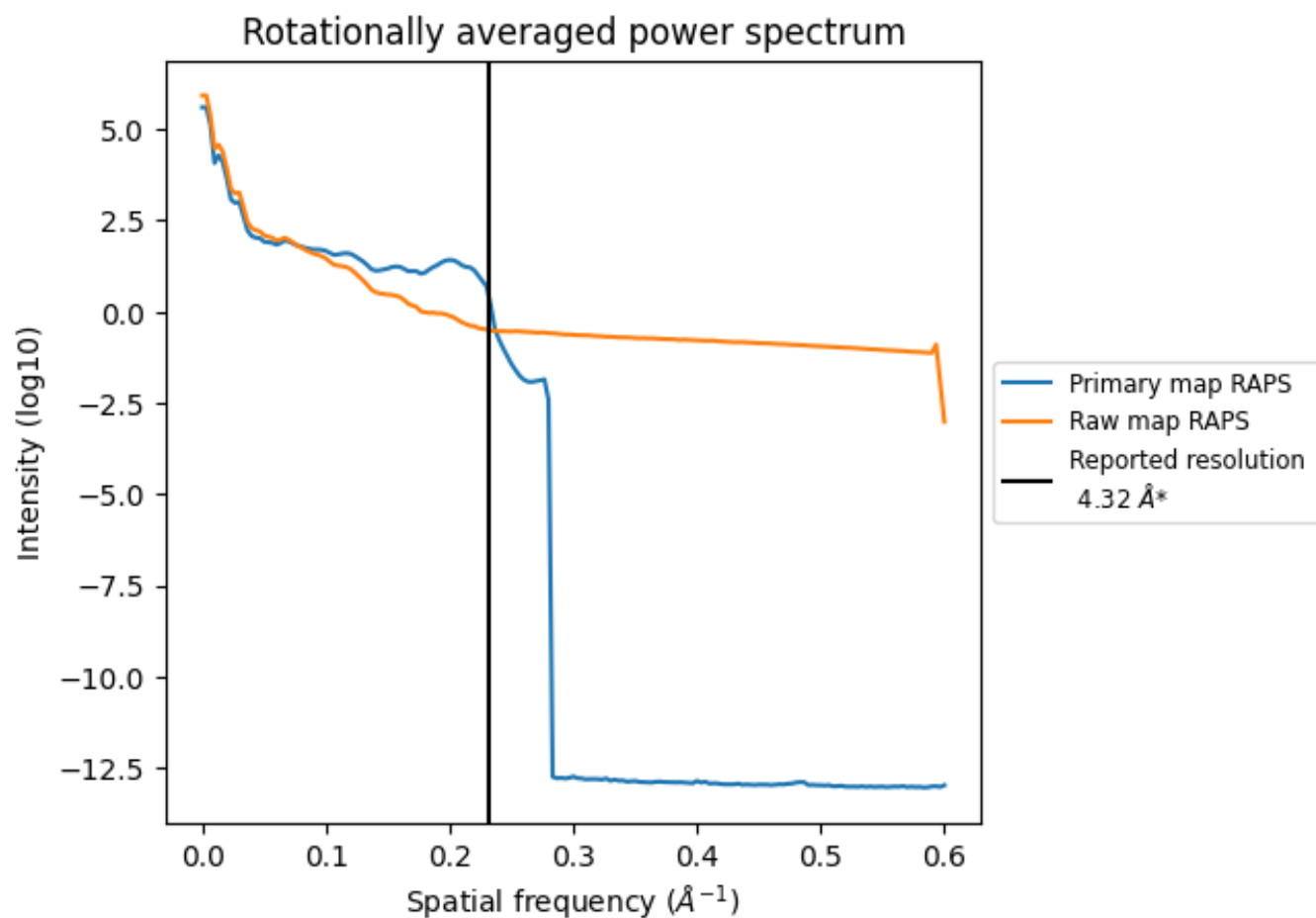
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 247 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 ⓘ

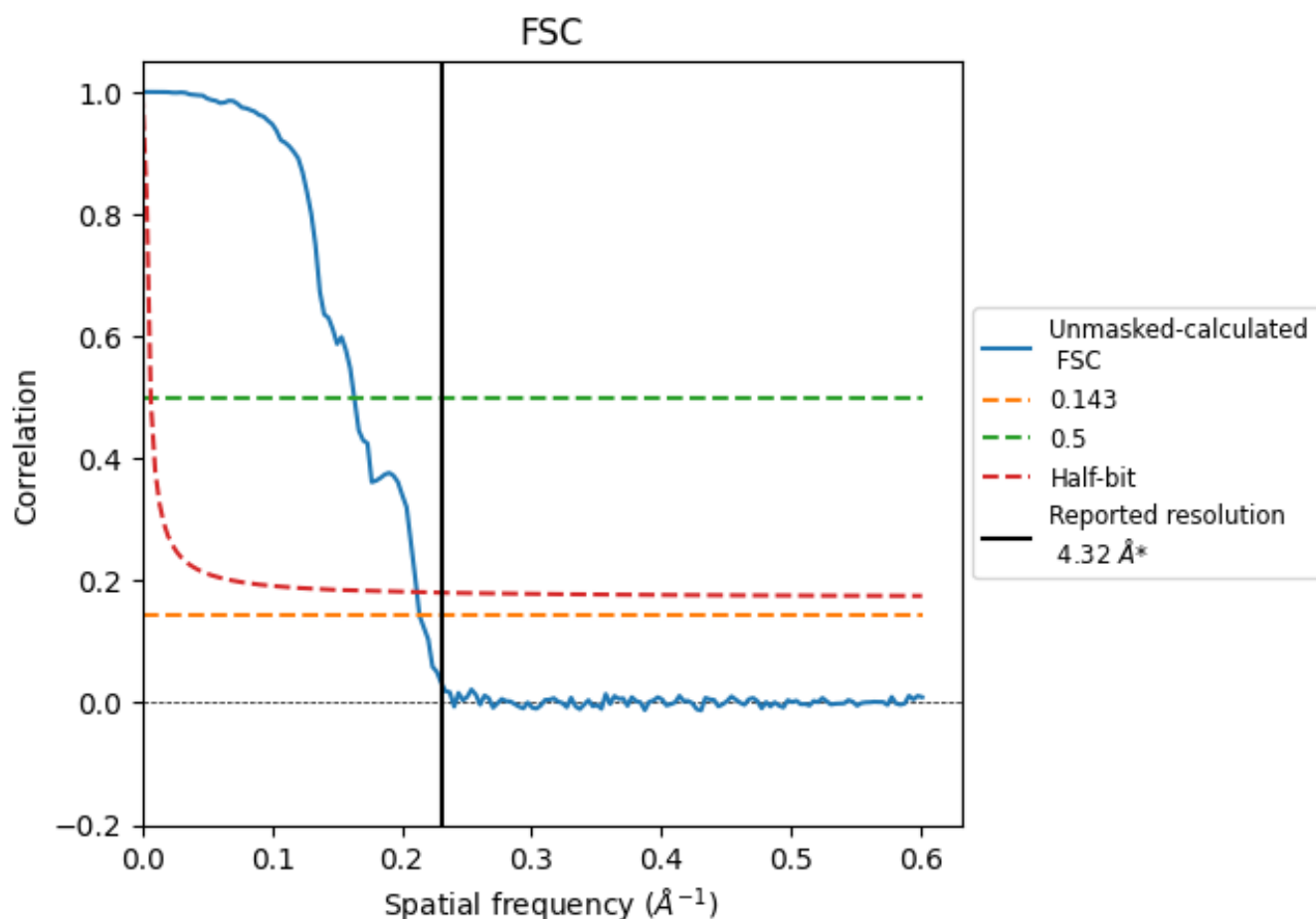


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

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 0.231 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	6.12	4.73

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

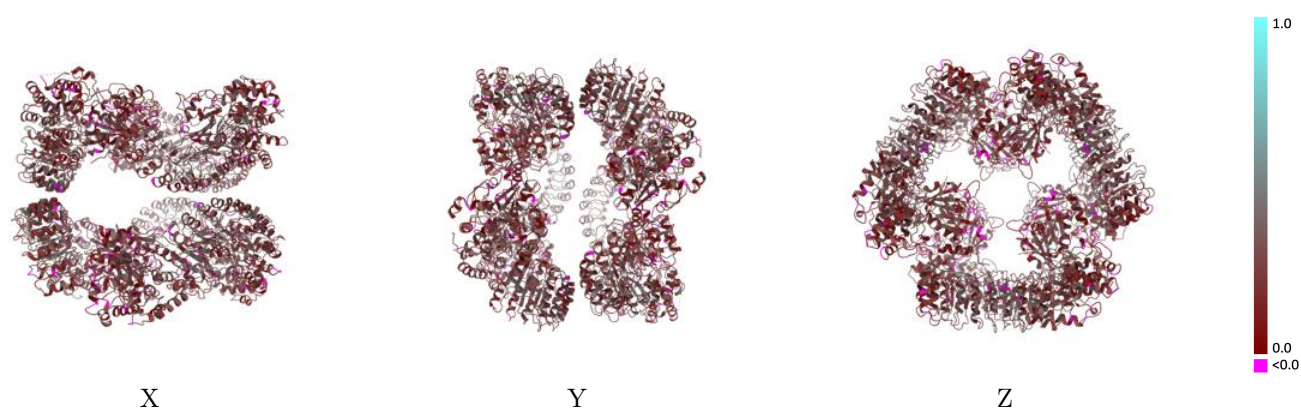
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40820 and PDB model 8SWK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)

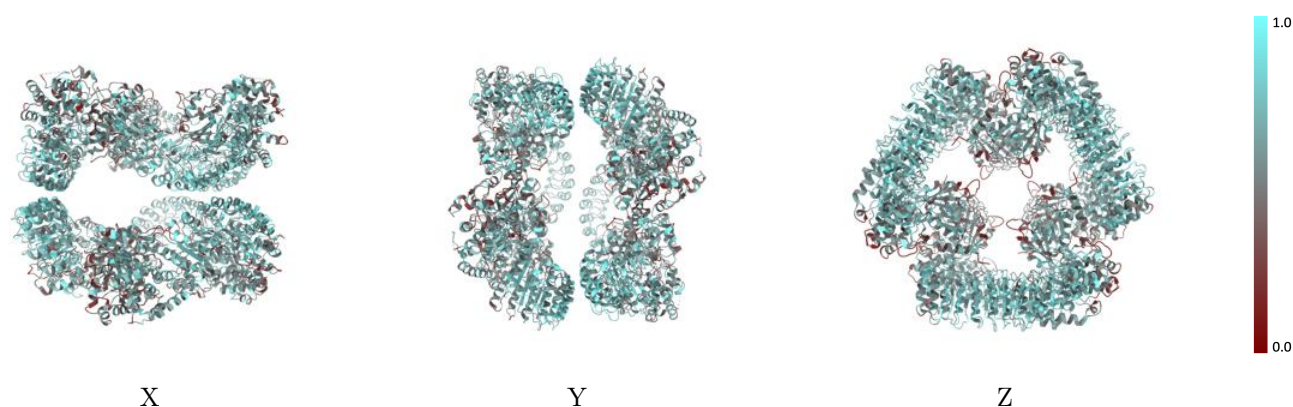
This section was not generated.

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



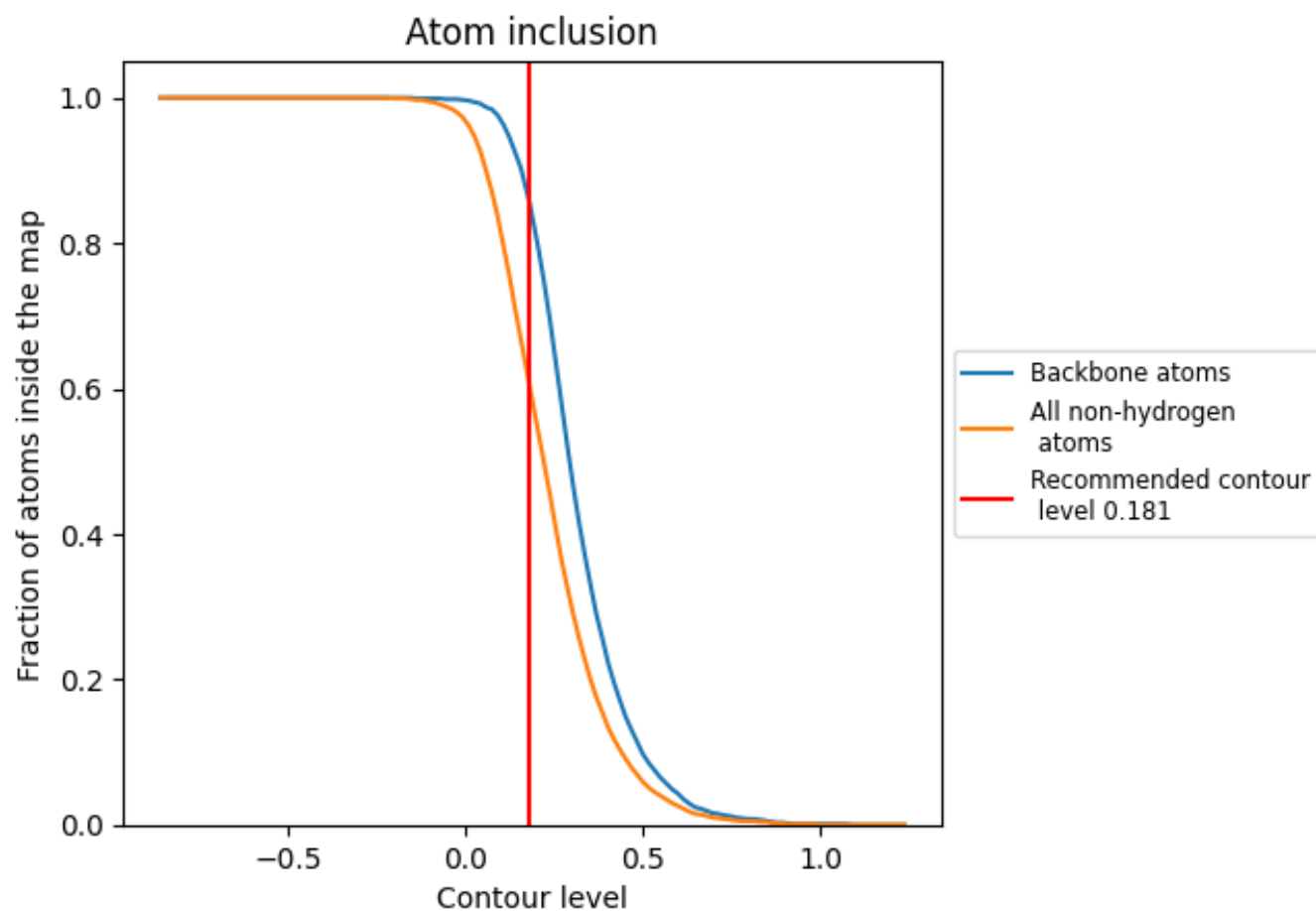
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.181).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 60% 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 (0.181) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.2400
A	0.6030	0.2410
B	0.6020	0.2410
C	0.6020	0.2400
D	0.6020	0.2390
E	0.6010	0.2380
F	0.6030	0.2390

1.0

0.0

<0.0