



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:13 PM UTC

PDB ID : 6PPJ / pdb_00006ppj
EMDB ID : EMD-20440
Title : Cryo-EM structure of AdnA(D934A)-AdnB(D1014A) in complex with AMPPNP
Authors : Jia, N.; Unciuleac, M.; Shuman, S.; Patel, D.J.
Deposited on : 2019-07-07
Resolution : 3.50 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

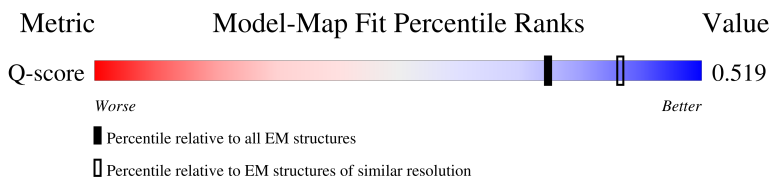
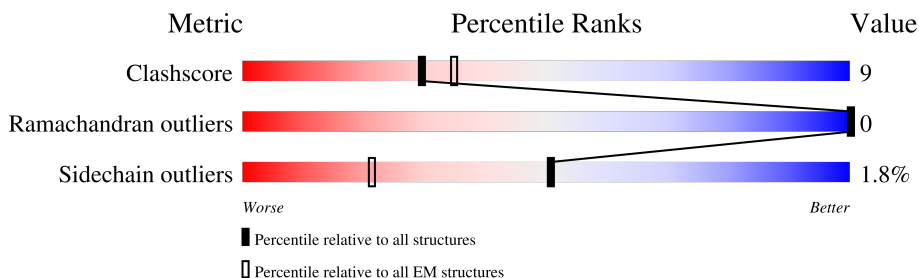
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	B	1095	 68% 9% 23%
2	A	1045	 75% 11% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12004 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 UvrD/REP helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	848	Total	C	N	O	S	0	0
			5756	3668	1063	1011	14		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	537	THR	SER	conflict	UNP A0A0D6HIW1
B	540	VAL	LEU	conflict	UNP A0A0D6HIW1
B	559	GLU	GLN	conflict	UNP A0A0D6HIW1
B	599	ALA	VAL	conflict	UNP A0A0D6HIW1
B	627	GLY	SER	conflict	UNP A0A0D6HIW1
B	1014	ALA	ASP	engineered mutation	UNP A0A0D6HIW1

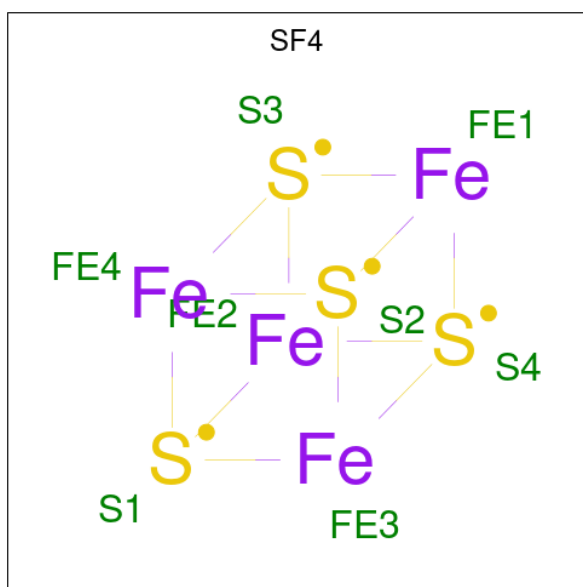
- Molecule 2 is a protein called ATP-dependent DNA helicase (UvrD/REP).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	901	Total	C	N	O	S	0	0
			6209	3943	1161	1086	19		

There is a discrepancy between the modelled and reference sequences:

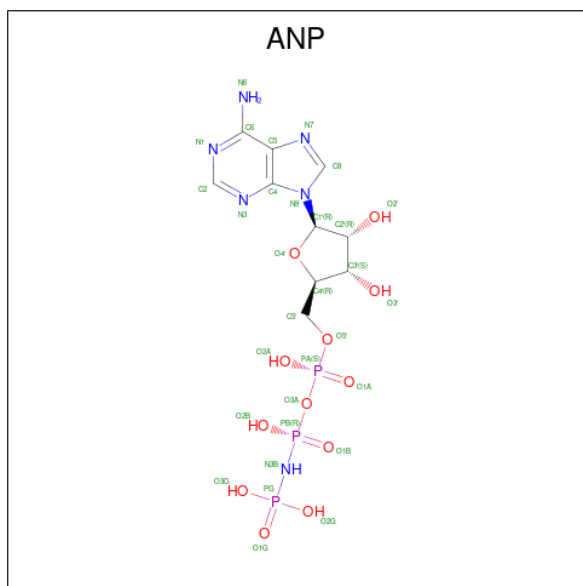
Chain	Residue	Modelled	Actual	Comment	Reference
A	934	ALA	ASP	engineered mutation	UNP A0A0D6HKQ2

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	Fe	S	0
			8	4	4	

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

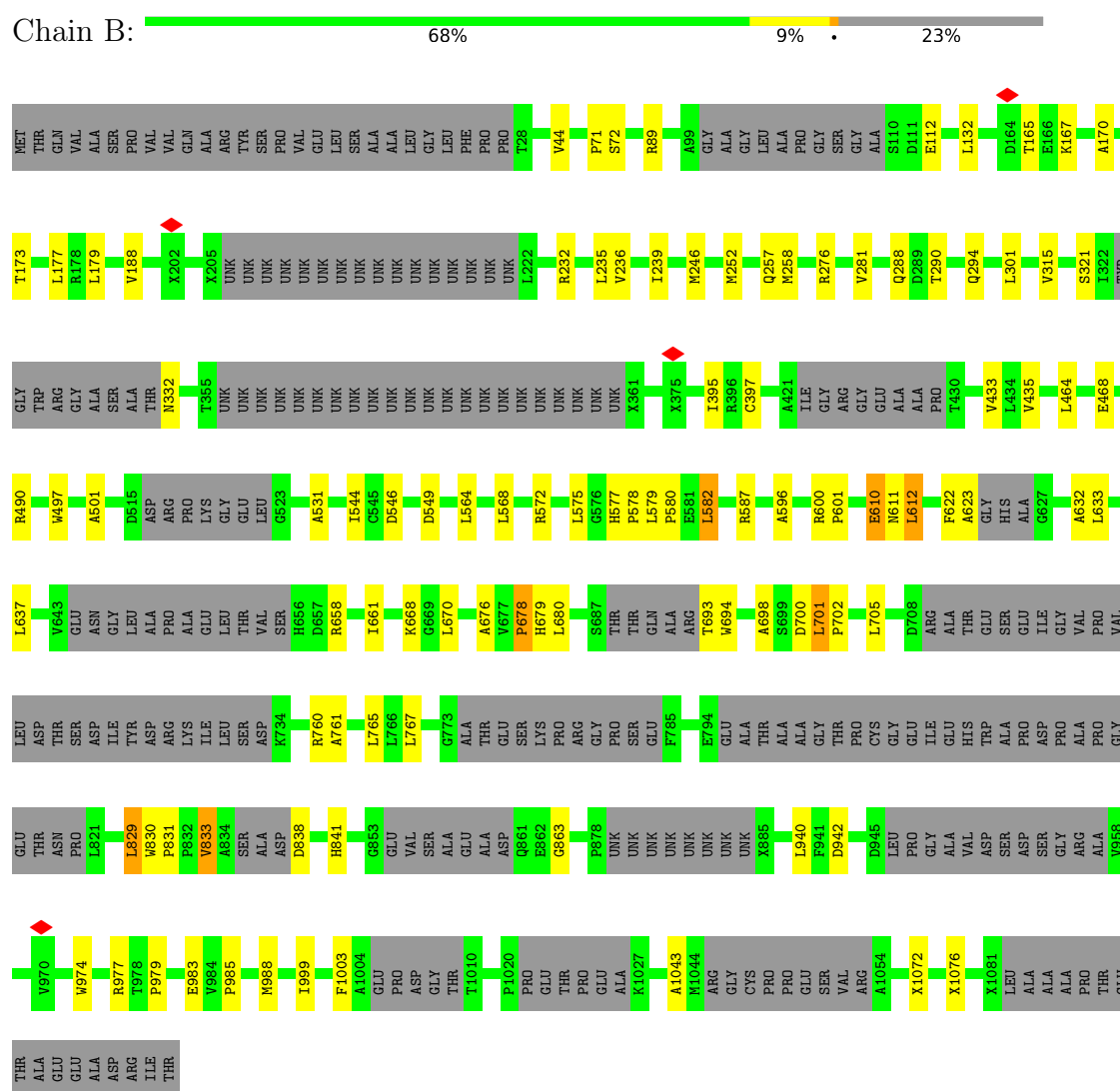


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

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: UvrD/REP helicase



• Molecule 2: ATP-dependent DNA helicase (UvrD/REP)



V932	W787	W629	GLN	A306	ASN	MET
Y956	S788	P634	P473	A312	GLY	THR
V960	E789	V638	F477	S312	THR	THR
L964	PRO	H792	L481	Y313	ARG	ARG
LEU	GLY	L796	S493	R314	ALA	ALA
ASP	L801	H643	A497	L326	GLU	GLU
ASP	Q802	L644	S513	L330	SER	SER
ASP	M803	D646	ASP	P331	ALA	ALA
GLU	L804	A652	VAL	GLY	GLN	GLN
PRO	T805	S660	SER	VAL	THR	THR
GLY	L809	T661	ALA	SER	ALA	ALA
G973	R810	R662	GLY	ASP	S14	S14
K981	R821	R670	ASP	T336	L17	L17
ALA	ARG	R671	PE20	R171	G23	G23
GLY	D823	R679	L524	R167	V24	V24
ALA	T827	A680	S541	R167	V25	V25
GLY	E838	R683	GLU	R167	R26	R26
A987	PRO	S691	ARG	R167	L27	L27
P994	GLY	ASP	GLY	R167	L28	L28
LEU	LYS	THR	GLY	R167	T33	T33
THR	T842	GLY	GLY	R167	G34	G34
PRO	N867	GLY	GLY	R167	T42	T42
ASP	E892	L699	GLY	R167	L48	L48
K999	G901	I707	SER	R167	ALA	ALA
A1010	V904	T712	L577	R167	GLY	GLY
A1011	E905	GLU	L587	R167	ALA	ALA
T1014	P906	PRO	GLY	R167	D52	D52
A1015	GLY	VAL	ALA	R167	P53	P53
G1016	GLU	ALA	ALA	R167	E54	E54
P1017	ASN	ALA	VAL	R167	S55	S55
R1018	THR	GLU	ALA	R167	V56	V56
F1019	P911	P718	ALA	R167	L57	L57
V1020	G912	R724	ARG	R167	L58	L58
A1021	V913	V739	THR	R167	L77	L77
S1034	R914	A741	ALA	R167	LEU	LEU
P1037	R918	P742	ARG	R167	GLY	GLY
A1038	L919	ASP	GLU	R167	ALA	ALA
Q1039	D920	GLY	THR	R167	GLY	GLY
ALA	R921	A745	ALA	R167	THR	THR
ASN	D925	R751	A600	R167	VAL	VAL
GLY	GLU	E784	L606	R167	G84	G84
ASP	ALA	L786	F618	R167	V85	V85
ARG	GLY	V931	V619	R167	V86	V86
PRO	ARG		V624	R167	R87	R87
	L930			R167	P89	P89
	V931			R167	V91	V91
				R167	R92	R92
				R167	Q107	Q107
				R167	ARG	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80396	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 ($e^-/\text{\AA}^2$)	2.16	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	241.164, 241.164, 241.164	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8613, 0.8613, 0.8613	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: SF4, ANP

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	B	0.48	0/5466	0.73	1/7494 (0.0%)
2	A	0.42	0/6302	0.68	1/8626 (0.0%)
All	All	0.45	0/11768	0.70	2/16120 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	918	ARG	N-CA-C	7.27	121.42	111.17
1	B	678	PRO	N-CA-C	7.03	123.53	113.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	B	5756	0	5147	119	0
2	A	6209	0	5972	113	0
3	A	8	0	0	0	0
4	A	31	0	13	2	0
All	All	12004	0	11132	212	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 9.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:787:TRP:NE1	2:A:1015:ALA:HA	1.37	1.40
2:A:787:TRP:HE1	2:A:1015:ALA:CA	1.43	1.29
1:B:579:LEU:HD23	1:B:633:LEU:CD1	1.71	1.19
1:B:188:VAL:CG1	1:B:705:LEU:HD21	1.78	1.14
1:B:579:LEU:HD23	1:B:633:LEU:HD11	1.25	1.11
2:A:784:GLU:HG2	2:A:785:PRO:CD	1.81	1.10
2:A:784:GLU:HG2	2:A:785:PRO:HD2	1.33	1.10
1:B:761:ALA:HB3	1:B:765:LEU:HD21	1.29	1.09
2:A:27:LEU:O	2:A:281:ALA:HA	1.54	1.07
1:B:579:LEU:CD2	1:B:633:LEU:HD13	1.87	1.04
1:B:579:LEU:CD2	1:B:633:LEU:CD1	2.36	1.03
1:B:580:PRO:HD3	1:B:623:ALA:HB1	1.40	1.01
1:B:188:VAL:HG21	1:B:705:LEU:CD2	1.97	0.93
1:B:188:VAL:HG11	1:B:705:LEU:HD21	1.51	0.92
2:A:784:GLU:CG	2:A:785:PRO:CD	2.49	0.91
1:B:188:VAL:CG2	1:B:705:LEU:CD2	2.50	0.90
2:A:787:TRP:CZ2	2:A:1015:ALA:HB2	2.08	0.88
1:B:579:LEU:HD21	1:B:633:LEU:HD13	1.54	0.87
1:B:188:VAL:CG2	1:B:705:LEU:HD21	2.04	0.86
1:B:761:ALA:HB3	1:B:765:LEU:CD2	2.10	0.81
1:B:188:VAL:HG13	1:B:705:LEU:HD21	1.63	0.79
1:B:705:LEU:HD23	1:B:705:LEU:O	1.81	0.79
2:A:784:GLU:CG	2:A:785:PRO:HD3	2.13	0.78
1:B:761:ALA:CB	1:B:765:LEU:HD21	2.10	0.77
2:A:787:TRP:HE1	2:A:1015:ALA:HA	0.64	0.77
2:A:787:TRP:HZ2	2:A:1015:ALA:HB2	1.49	0.76
2:A:804:LEU:HD12	2:A:1010:ALA:HB1	1.69	0.74
1:B:974:TRP:CD1	1:B:977:ARG:NH1	2.56	0.73
2:A:785:PRO:HA	2:A:1017:PRO:HD3	1.71	0.73
1:B:580:PRO:HD3	1:B:623:ALA:CB	2.16	0.73
1:B:564:LEU:HD13	1:B:564:LEU:O	1.90	0.71
2:A:787:TRP:CD1	2:A:787:TRP:H	2.08	0.71
1:B:572:ARG:HA	1:B:575:LEU:CD2	2.22	0.69
2:A:25:VAL:HG23	2:A:277:LEU:HD21	1.74	0.69
1:B:544:ILE:HG21	1:B:564:LEU:HD12	1.72	0.69
2:A:804:LEU:C	2:A:804:LEU:HD13	2.18	0.69
2:A:904:VAL:HG12	2:A:913:VAL:HG22	1.74	0.69
2:A:784:GLU:HG3	2:A:785:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:787:TRP:CD1	2:A:1015:ALA:HA	2.24	0.68
1:B:435:VAL:HG12	1:B:678:PRO:HG3	1.75	0.68
2:A:27:LEU:O	2:A:281:ALA:CA	2.40	0.68
1:B:188:VAL:HG11	1:B:705:LEU:CD2	2.24	0.67
1:B:564:LEU:HD13	1:B:564:LEU:C	2.19	0.67
1:B:830:TRP:HB2	2:A:809:LEU:CD1	2.23	0.67
2:A:787:TRP:NE1	2:A:1015:ALA:CA	2.20	0.66
1:B:1072:UNK:CB	1:B:1076:UNK:CB	2.74	0.66
2:A:786:LEU:HB2	2:A:1015:ALA:O	1.97	0.65
2:A:55:SER:CB	2:A:250:LYS:HB2	2.26	0.65
1:B:693:THR:O	1:B:700:ASP:CB	2.44	0.65
1:B:942:ASP:HB3	2:A:92:ARG:HE	1.62	0.65
1:B:979:PRO:HA	1:B:1003:PHE:HB3	1.79	0.64
1:B:165:THR:O	2:A:867:ASN:ND2	2.29	0.64
1:B:587:ARG:HD2	1:B:612:LEU:HD22	1.76	0.64
1:B:72:SER:HB3	1:B:112:GLU:HB3	1.79	0.64
2:A:786:LEU:CB	2:A:1015:ALA:O	2.45	0.64
2:A:803:MET:CE	2:A:810:ARG:HG2	2.28	0.64
1:B:761:ALA:CB	1:B:765:LEU:CD2	2.73	0.64
1:B:830:TRP:HB2	2:A:809:LEU:HD12	1.81	0.63
1:B:694:TRP:HB2	1:B:701:LEU:O	1.99	0.62
1:B:694:TRP:HA	1:B:700:ASP:CB	2.30	0.62
1:B:829:LEU:HD12	1:B:831:PRO:HD2	1.81	0.61
2:A:90:LEU:HD22	2:A:92:ARG:HH12	1.64	0.61
2:A:787:TRP:NE1	2:A:1015:ALA:CB	2.64	0.61
1:B:188:VAL:CG2	1:B:705:LEU:HD23	2.31	0.60
2:A:330:LEU:HD11	2:A:671:ARG:HE	1.66	0.60
2:A:904:VAL:O	2:A:904:VAL:HG13	2.01	0.60
1:B:579:LEU:N	1:B:580:PRO:HD2	2.16	0.60
1:B:974:TRP:CD1	1:B:977:ARG:HH11	2.17	0.60
1:B:564:LEU:HD11	1:B:568:LEU:HD11	1.84	0.60
1:B:165:THR:CG2	1:B:167:LYS:H	2.15	0.59
1:B:833:VAL:HG12	1:B:833:VAL:O	2.01	0.59
1:B:694:TRP:CB	1:B:701:LEU:O	2.50	0.59
2:A:804:LEU:HD13	2:A:804:LEU:O	2.03	0.59
2:A:56:VAL:HG12	2:A:56:VAL:O	2.02	0.58
1:B:863:GLY:O	2:A:724:ARG:NH1	2.36	0.58
2:A:387:ARG:HB2	2:A:629:TRP:CE3	2.37	0.58
1:B:831:PRO:HG2	2:A:1018:ARG:HD2	1.85	0.58
2:A:23:GLY:O	2:A:277:LEU:HA	2.03	0.58
1:B:188:VAL:CB	1:B:705:LEU:HD21	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ARG:HH12	1:B:658:ARG:HH21	1.52	0.57
1:B:600:ARG:HD3	1:B:601:PRO:HD2	1.86	0.57
2:A:330:LEU:HD23	2:A:670:ARG:HD2	1.86	0.57
1:B:165:THR:HG22	1:B:167:LYS:H	1.67	0.57
1:B:610:GLU:H	1:B:610:GLU:CD	2.12	0.57
2:A:277:LEU:C	2:A:277:LEU:HD13	2.30	0.56
1:B:71:PRO:HG2	1:B:112:GLU:HG3	1.87	0.55
1:B:188:VAL:HG22	1:B:705:LEU:CD2	2.34	0.55
1:B:572:ARG:O	1:B:575:LEU:HD23	2.05	0.55
1:B:132:LEU:HB2	2:A:638:VAL:HG21	1.88	0.55
2:A:801:LEU:O	2:A:805:THR:HG23	2.07	0.55
2:A:634:PRO:HA	2:A:662:ARG:O	2.07	0.54
2:A:787:TRP:CZ2	2:A:1015:ALA:CB	2.87	0.54
1:B:89:ARG:HE	2:A:699:LEU:HD21	1.72	0.54
2:A:429:LEU:HD11	2:A:524:LEU:HD12	1.90	0.54
2:A:26:ARG:HH21	2:A:306:ALA:HB2	1.73	0.54
2:A:787:TRP:H	2:A:787:TRP:HD1	1.55	0.54
2:A:787:TRP:CE3	2:A:792:HIS:ND1	2.76	0.53
2:A:164:LEU:HD11	2:A:644:LEU:HD13	1.91	0.53
1:B:580:PRO:CD	1:B:623:ALA:HB1	2.27	0.53
1:B:232:ARG:HG3	1:B:698:ALA:O	2.09	0.53
1:B:701:LEU:HD12	1:B:701:LEU:C	2.34	0.53
2:A:919:LEU:HD11	2:A:932:VAL:HG13	1.91	0.53
2:A:618:PHE:HD1	2:A:683:ARG:HG3	1.74	0.52
1:B:170:ALA:HA	1:B:173:THR:HG22	1.90	0.52
2:A:33:THR:O	4:A:1102:ANP:O2A	2.27	0.52
1:B:501:ALA:HB2	1:B:830:TRP:HZ3	1.74	0.52
2:A:786:LEU:HB3	2:A:1015:ALA:O	2.10	0.52
2:A:787:TRP:CE2	2:A:1015:ALA:CB	2.93	0.52
1:B:258:MET:HE2	1:B:294:GLN:HG2	1.92	0.52
1:B:983:GLU:HA	1:B:999:ILE:O	2.10	0.52
1:B:497:TRP:CZ2	1:B:564:LEU:HD23	2.45	0.51
1:B:670:LEU:O	1:B:760:ARG:NH1	2.43	0.51
1:B:830:TRP:HA	2:A:1037:PRO:HG3	1.92	0.51
1:B:397:CYS:HA	1:B:767:LEU:O	2.11	0.51
2:A:17:LEU:HD13	2:A:42:THR:HG21	1.92	0.51
2:A:369:ARG:NH2	2:A:403:ALA:O	2.44	0.51
1:B:668:LYS:O	1:B:760:ARG:NH1	2.42	0.51
1:B:830:TRP:HB2	2:A:809:LEU:HD11	1.90	0.51
2:A:904:VAL:CG1	2:A:913:VAL:HG13	2.41	0.51
2:A:803:MET:HE2	2:A:810:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:PRO:HG2	2:A:1018:ARG:HA	1.93	0.50
1:B:188:VAL:HG21	1:B:705:LEU:HD23	1.86	0.50
1:B:701:LEU:C	1:B:701:LEU:CD1	2.85	0.50
2:A:58:LEU:HD12	2:A:91:VAL:HG22	1.93	0.50
1:B:464:LEU:HD11	1:B:637:LEU:HD22	1.93	0.50
2:A:809:LEU:HD13	2:A:1021:ALA:HB2	1.94	0.49
1:B:577:HIS:HB3	1:B:578:PRO:HD2	1.95	0.49
2:A:459:ARG:HG2	2:A:462:ARG:HH21	1.78	0.49
2:A:787:TRP:CE2	2:A:1015:ALA:HB2	2.48	0.49
1:B:610:GLU:OE1	1:B:658:ARG:NH2	2.46	0.48
2:A:55:SER:CB	2:A:250:LYS:N	2.76	0.48
1:B:564:LEU:C	1:B:564:LEU:CD1	2.85	0.48
2:A:25:VAL:CG2	2:A:277:LEU:HD21	2.43	0.48
2:A:901:GLY:O	2:A:914:ARG:HG3	2.14	0.48
1:B:838:ASP:HB3	1:B:841:HIS:HD2	1.78	0.48
1:B:572:ARG:HA	1:B:575:LEU:HD21	1.93	0.48
1:B:940:LEU:HD12	2:A:248:ARG:HH11	1.79	0.48
2:A:804:LEU:C	2:A:804:LEU:CD1	2.85	0.48
1:B:678:PRO:HB2	1:B:679:HIS:CD2	2.49	0.48
2:A:369:ARG:HD2	2:A:373:LEU:HD22	1.96	0.47
1:B:252:MET:SD	1:B:257:GLN:NE2	2.87	0.47
2:A:53:PRO:CB	2:A:87:ARG:HB2	2.44	0.47
1:B:490:ARG:HH11	2:A:1034:SER:HB2	1.80	0.47
2:A:28:LEU:HA	2:A:282:GLY:O	2.13	0.47
2:A:803:MET:HE3	2:A:810:ARG:HG2	1.97	0.47
1:B:236:VAL:HA	1:B:239:ILE:HG12	1.95	0.47
1:B:701:LEU:HB2	1:B:702:PRO:HD2	1.95	0.47
2:A:342:ASN:HD22	2:A:343:PRO:HD2	1.80	0.47
2:A:55:SER:CB	2:A:250:LYS:CB	2.93	0.47
1:B:622:PHE:HE2	1:B:632:ALA:HB1	1.80	0.46
2:A:804:LEU:HD21	2:A:1014:THR:HG22	1.97	0.46
1:B:579:LEU:HD21	1:B:633:LEU:CD1	2.26	0.46
1:B:290:THR:O	1:B:332:ASN:ND2	2.48	0.46
1:B:579:LEU:CD2	1:B:633:LEU:HD11	2.14	0.46
2:A:331:PRO:O	2:A:337:ARG:NH2	2.40	0.46
2:A:646:ASP:HB2	2:A:652:ALA:HB3	1.97	0.46
1:B:468:GLU:HG2	1:B:596:ALA:HB2	1.97	0.46
2:A:804:LEU:CD1	2:A:1010:ALA:HB1	2.42	0.46
1:B:188:VAL:HG22	1:B:705:LEU:HD21	1.93	0.46
1:B:188:VAL:HG22	1:B:705:LEU:HD23	1.97	0.46
2:A:892:GLU:OE2	2:A:921:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ALA:HB2	2:A:827:THR:HG21	1.98	0.45
1:B:44:VAL:HB	1:B:315:VAL:HG12	1.97	0.45
1:B:582:LEU:O	1:B:582:LEU:HD23	2.16	0.45
1:B:831:PRO:CD	2:A:1018:ARG:HA	2.47	0.45
2:A:619:VAL:HB	2:A:680:ALA:HB2	1.98	0.45
1:B:232:ARG:NH2	1:B:694:TRP:O	2.46	0.45
2:A:34:GLY:HA2	4:A:1102:ANP:O2A	2.15	0.45
1:B:572:ARG:CA	1:B:575:LEU:CD2	2.95	0.45
2:A:57:LEU:HD22	2:A:252:LEU:HD23	1.98	0.44
1:B:1003:PHE:O	1:B:1003:PHE:CD2	2.70	0.44
1:B:433:VAL:HB	1:B:661:ILE:HG12	1.98	0.44
1:B:276:ARG:NH1	1:B:301:LEU:O	2.50	0.44
2:A:314:ARG:O	2:A:345:ARG:NH1	2.48	0.44
2:A:312:SER:O	2:A:313:TYR:HB2	2.16	0.44
1:B:1003:PHE:O	1:B:1003:PHE:HD2	2.01	0.43
1:B:179:LEU:HD12	1:B:235:LEU:HD11	2.01	0.43
2:A:739:VAL:O	2:A:751:ARG:NH1	2.51	0.43
2:A:25:VAL:HG23	2:A:277:LEU:CD2	2.46	0.43
1:B:288:GLN:HB2	1:B:321:SER:HB2	2.00	0.43
2:A:326:LEU:HD11	2:A:707:ILE:HD11	1.99	0.43
1:B:165:THR:CG2	1:B:167:LYS:HB2	2.49	0.43
1:B:246:MET:HE2	1:B:246:MET:HB3	1.87	0.43
1:B:694:TRP:HB3	1:B:701:LEU:O	2.18	0.43
2:A:741:ALA:O	2:A:751:ARG:NH2	2.44	0.43
2:A:796:LEU:HD11	2:A:1011:ALA:HB2	2.00	0.43
2:A:235:LEU:HD12	2:A:242:LEU:HD23	2.01	0.42
2:A:643:HIS:HB2	2:A:660:SER:CB	2.49	0.42
2:A:167:ARG:O	2:A:171:ARG:NH1	2.48	0.42
1:B:549:ASP:OD1	1:B:549:ASP:N	2.53	0.42
1:B:1043:ALA:HB3	2:A:85:VAL:HG22	2.02	0.42
2:A:493:SER:HA	2:A:497:ALA:HB2	2.01	0.42
2:A:784:GLU:CG	2:A:785:PRO:HD2	2.19	0.42
1:B:433:VAL:HA	1:B:676:ALA:O	2.20	0.42
2:A:786:LEU:HB3	2:A:787:TRP:H	1.67	0.42
1:B:985:PRO:HB2	2:A:88:GLU:HG3	2.01	0.42
1:B:988:MET:HA	2:A:85:VAL:HG12	2.01	0.42
2:A:786:LEU:HB3	2:A:787:TRP:HD1	1.84	0.42
1:B:165:THR:HG22	1:B:167:LYS:N	2.35	0.41
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.85	0.41
1:B:546:ASP:OD1	1:B:546:ASP:N	2.54	0.41
2:A:462:ARG:HG2	2:A:477:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:ARG:HA	1:B:575:LEU:HD22	2.03	0.41
2:A:787:TRP:CD1	2:A:787:TRP:N	2.81	0.41
2:A:956:TYR:O	2:A:960:VAL:HG23	2.20	0.41
1:B:831:PRO:CG	2:A:1018:ARG:HA	2.50	0.41
2:A:446:LEU:HD12	2:A:481:LEU:HD11	2.02	0.41
2:A:679:ARG:HA	2:A:679:ARG:HD3	1.85	0.41
1:B:395:ILE:HG22	1:B:765:LEU:HB2	2.03	0.40
1:B:564:LEU:CD1	1:B:568:LEU:CD1	3.00	0.40
1:B:829:LEU:HD13	2:A:1019:PHE:O	2.21	0.40
2:A:787:TRP:CE3	2:A:792:HIS:CE1	3.10	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	B	733/1095 (67%)	684 (93%)	49 (7%)	0	100	100
2	A	849/1045 (81%)	783 (92%)	66 (8%)	0	100	100
All	All	1582/2140 (74%)	1467 (93%)	115 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	B	451/743 (61%)	442 (98%)	9 (2%)	48	67
2	A	540/796 (68%)	531 (98%)	9 (2%)	53	70
All	All	991/1539 (64%)	973 (98%)	18 (2%)	51	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	281	VAL
1	B	582	LEU
1	B	610	GLU
1	B	611	ASN
1	B	612	LEU
1	B	680	LEU
1	B	701	LEU
1	B	829	LEU
1	B	833	VAL
2	A	258	GLN
2	A	277	LEU
2	A	313	TYR
2	A	385	ILE
2	A	389	VAL
2	A	606	LEU
2	A	624	VAL
2	A	786	LEU
2	A	964	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	257	GLN
1	B	413	HIS
1	B	577	HIS
1	B	679	HIS
1	B	770	HIS
1	B	841	HIS
2	A	46	HIS
2	A	95	HIS
2	A	263	GLN
2	A	342	ASN
2	A	381	GLN

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Mol	Chain	Res	Type
2	A	496	HIS
2	A	526	GLN
2	A	816	HIS
2	A	848	ASN
2	A	950	HIS
2	A	957	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	SF4	A	1101	-	0,12,12	-	-	-		
4	ANP	A	1102	-	33,33,33	1.08	5 (15%)	45,52,52	0.84	1 (2%)

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
4	ANP	A	1102	-	-	7/18/38/38	0/3/3/3
3	SF4	A	1101	-	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	ANP	PG-O1G	3.10	1.50	1.46
4	A	1102	ANP	PB-O1B	2.95	1.50	1.46
4	A	1102	ANP	PB-O2B	-2.33	1.50	1.56
4	A	1102	ANP	PG-O2G	-2.20	1.51	1.56
4	A	1102	ANP	PG-O3G	-2.18	1.51	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	ANP	O2B-PB-O1B	4.09	118.65	109.87

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	ANP	PB-N3B-PG-O1G
4	A	1102	ANP	PG-N3B-PB-O1B
4	A	1102	ANP	C5'-O5'-PA-O2A
4	A	1102	ANP	C5'-O5'-PA-O3A
4	A	1102	ANP	O4'-C4'-C5'-O5'
4	A	1102	ANP	C3'-C4'-C5'-O5'
4	A	1102	ANP	C5'-O5'-PA-O1A

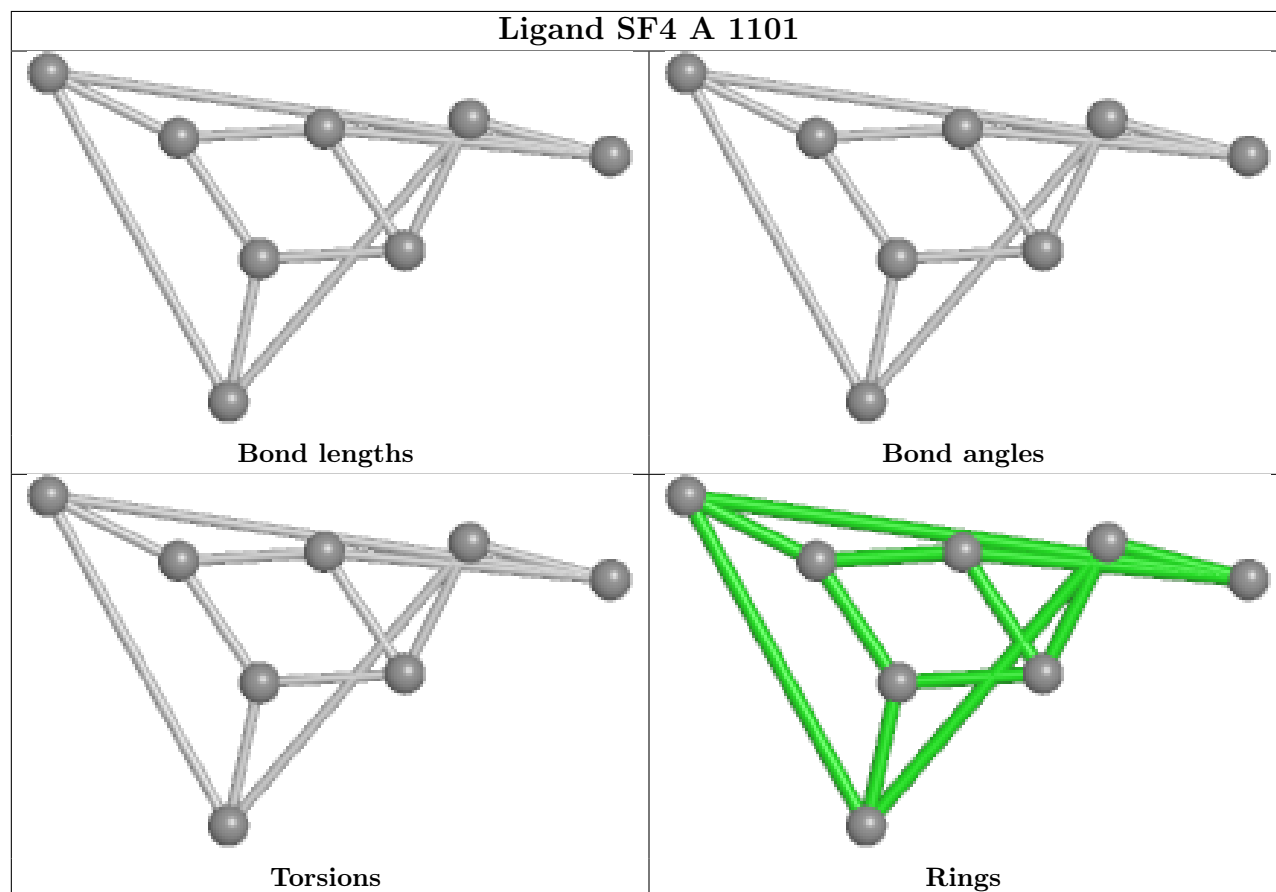
There are no ring outliers.

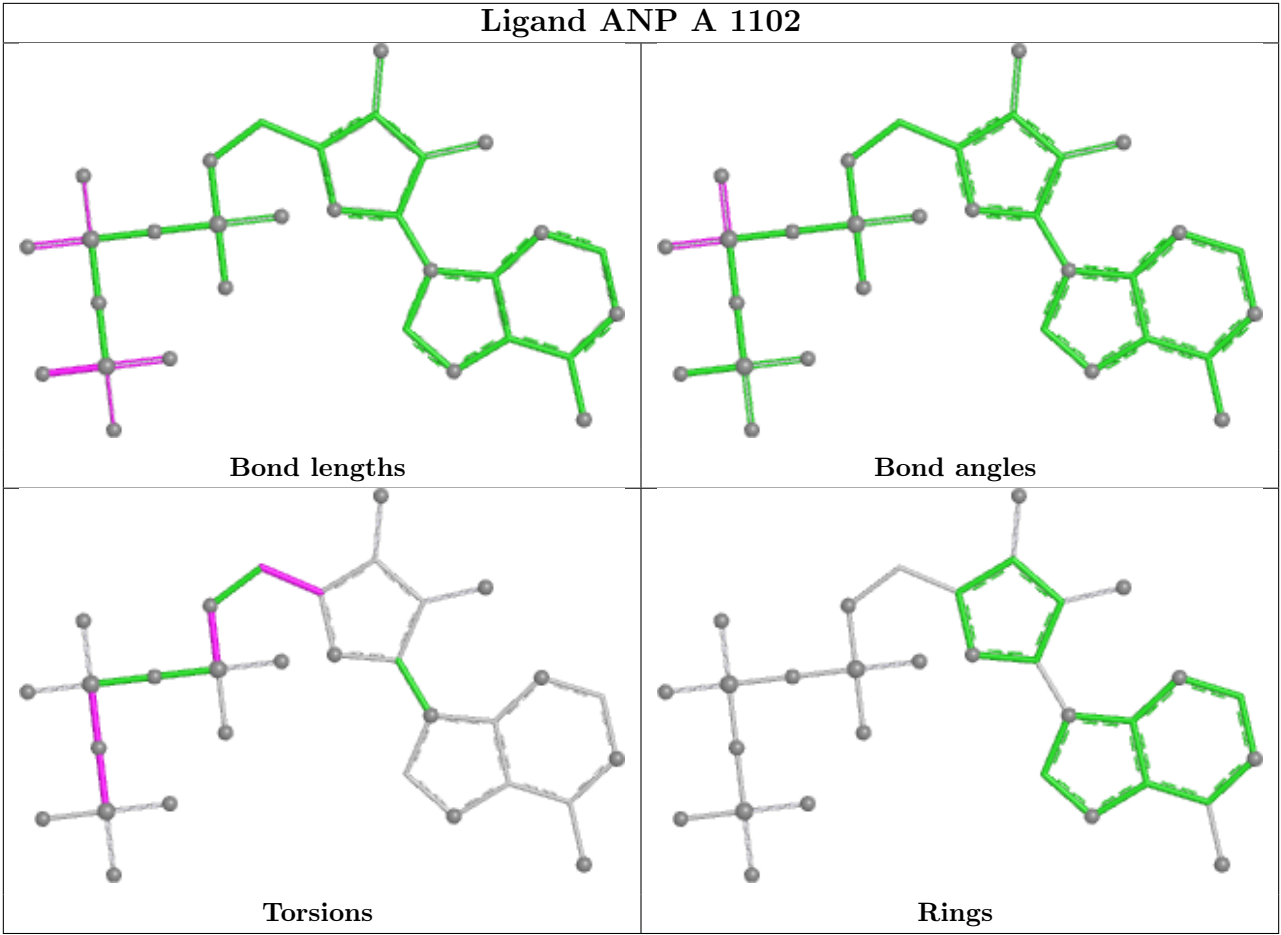
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	ANP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	376:UNK	C	394:THR	N	25.56
1	B	917:UNK	C	920:HIS	N	10.39
1	B	1067:UNK	C	1070:UNK	N	5.56

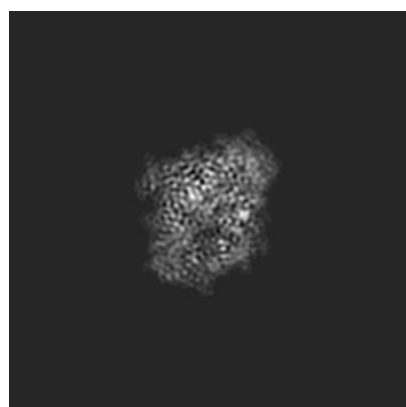
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20440. These allow visual inspection of the internal detail of the map and identification of artifacts.

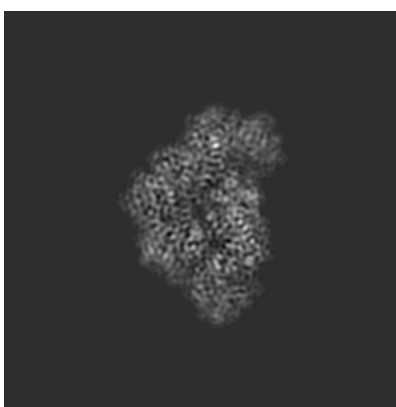
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

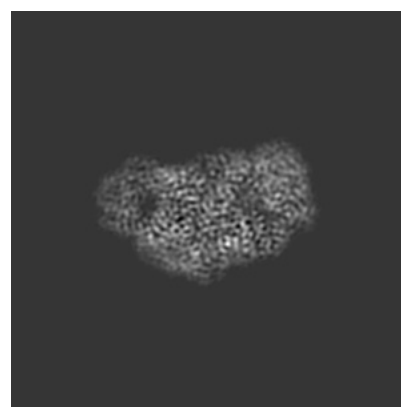
6.1.1 Primary map



X



Y



Z

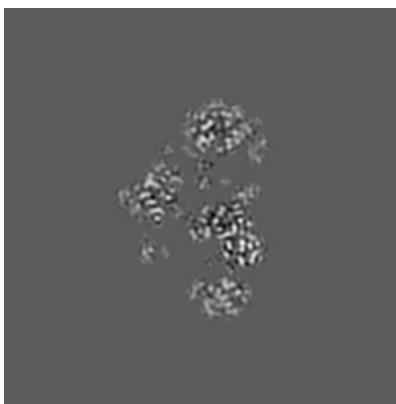
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

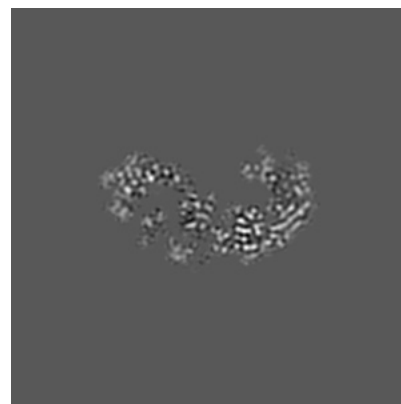
6.2.1 Primary map



X Index: 140



Y Index: 140



Z Index: 140

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

6.3 Largest variance slices [i](#)

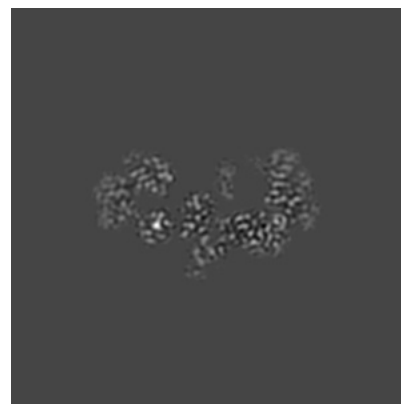
6.3.1 Primary map



X Index: 121



Y Index: 127

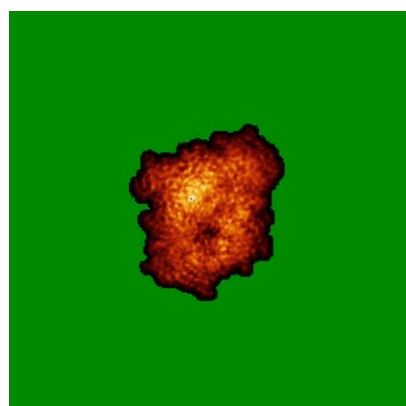


Z Index: 148

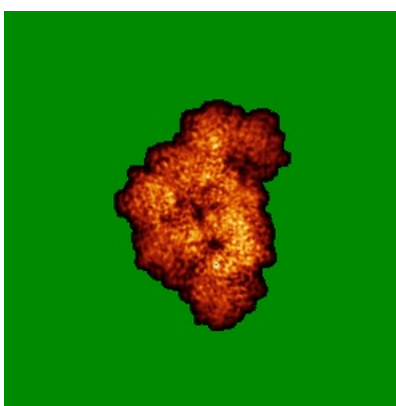
The images above show the largest variance slices of the map in three orthogonal directions.

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

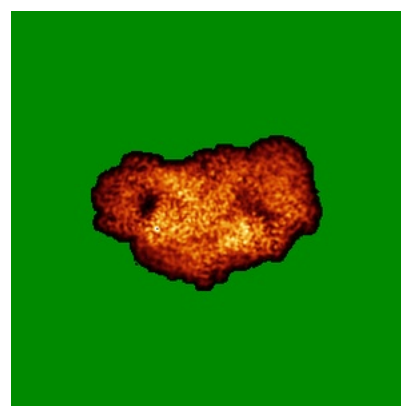
6.4.1 Primary map



X



Y

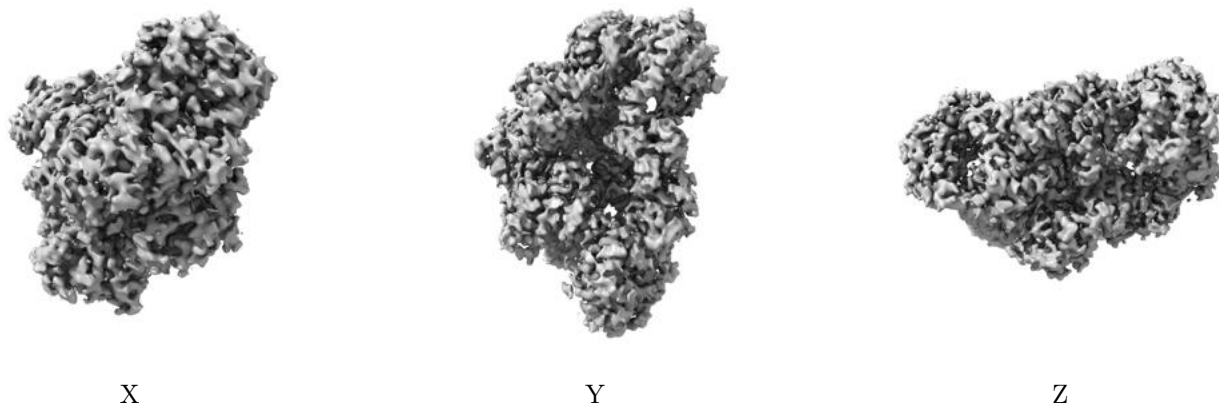


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

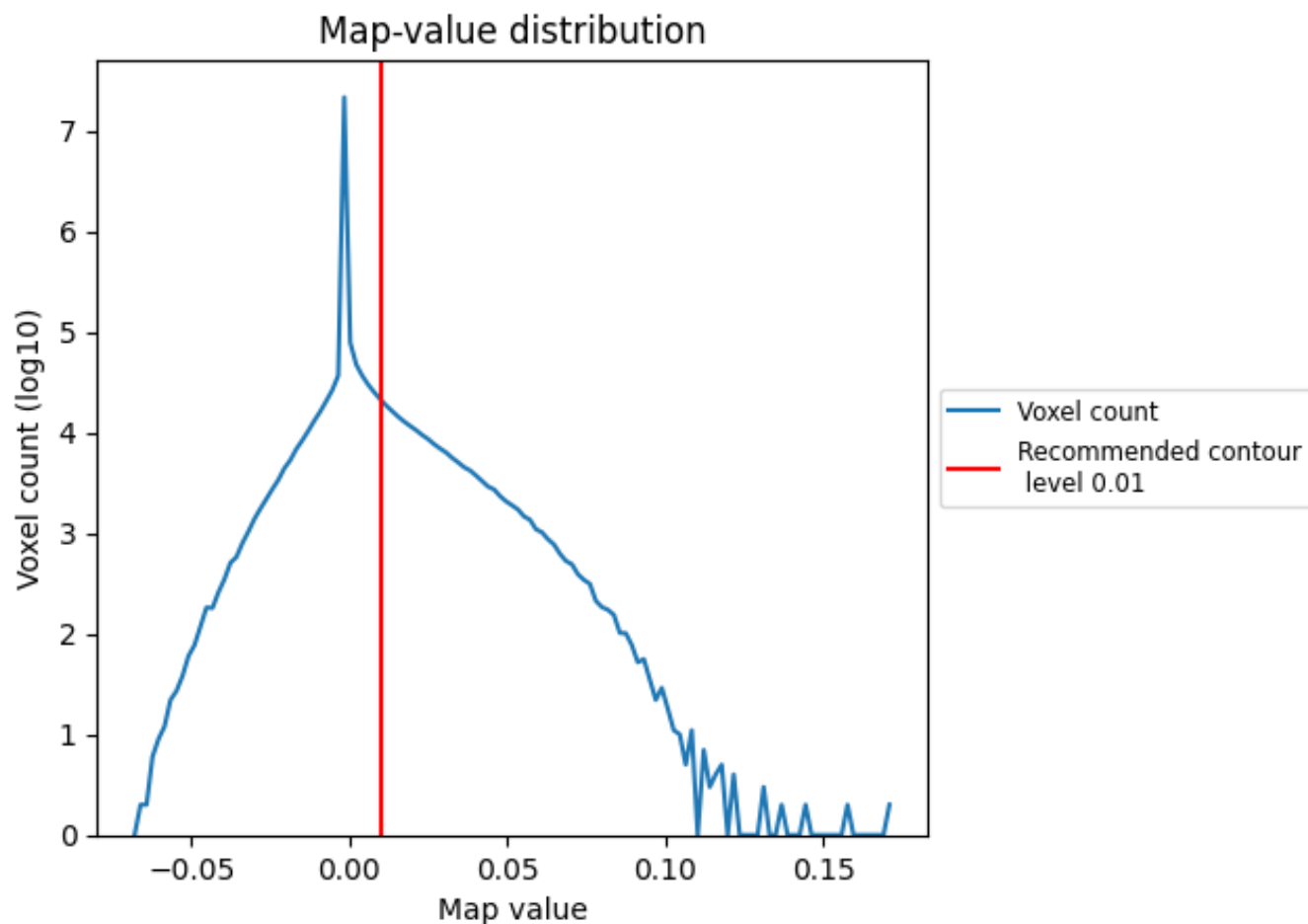
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

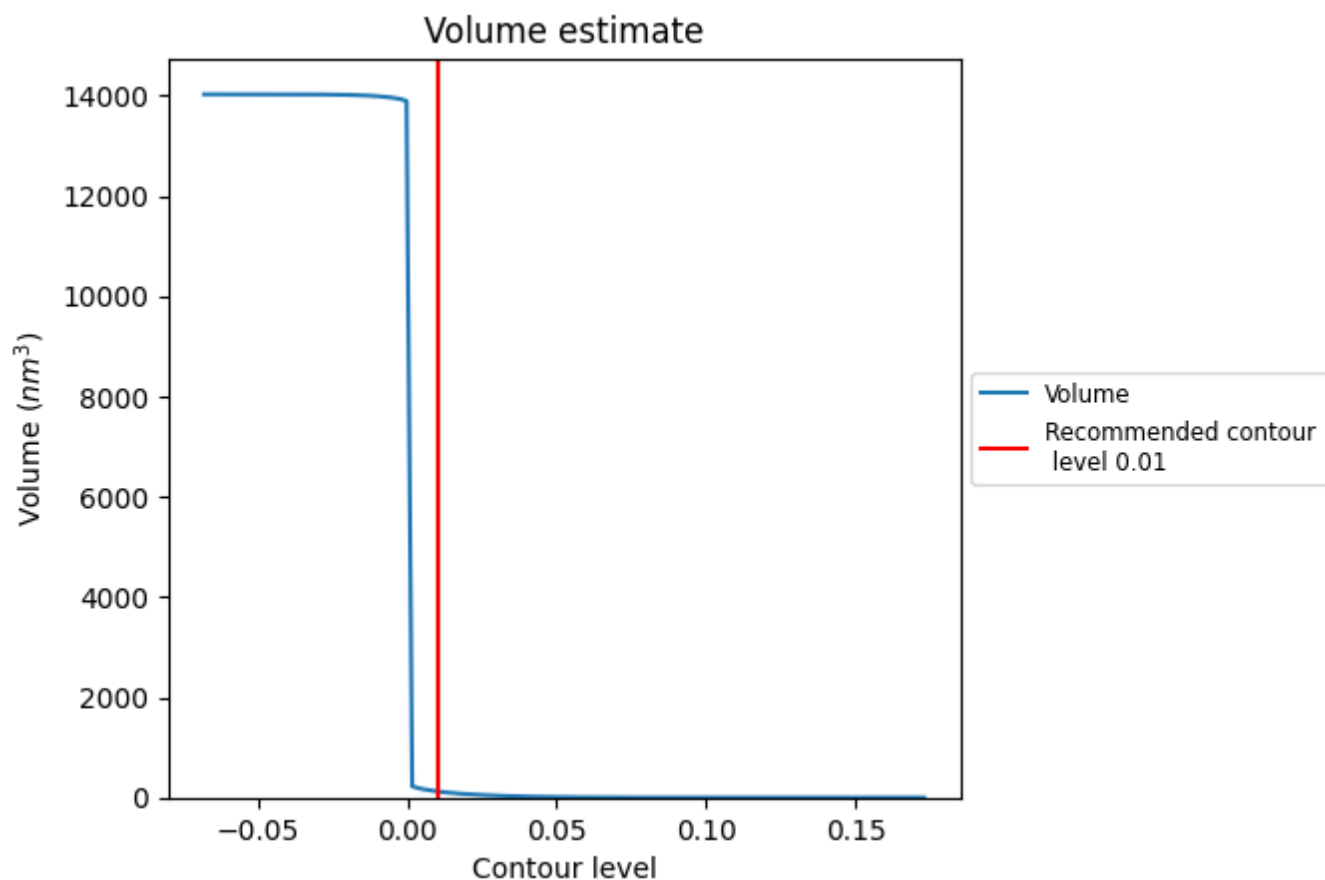
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

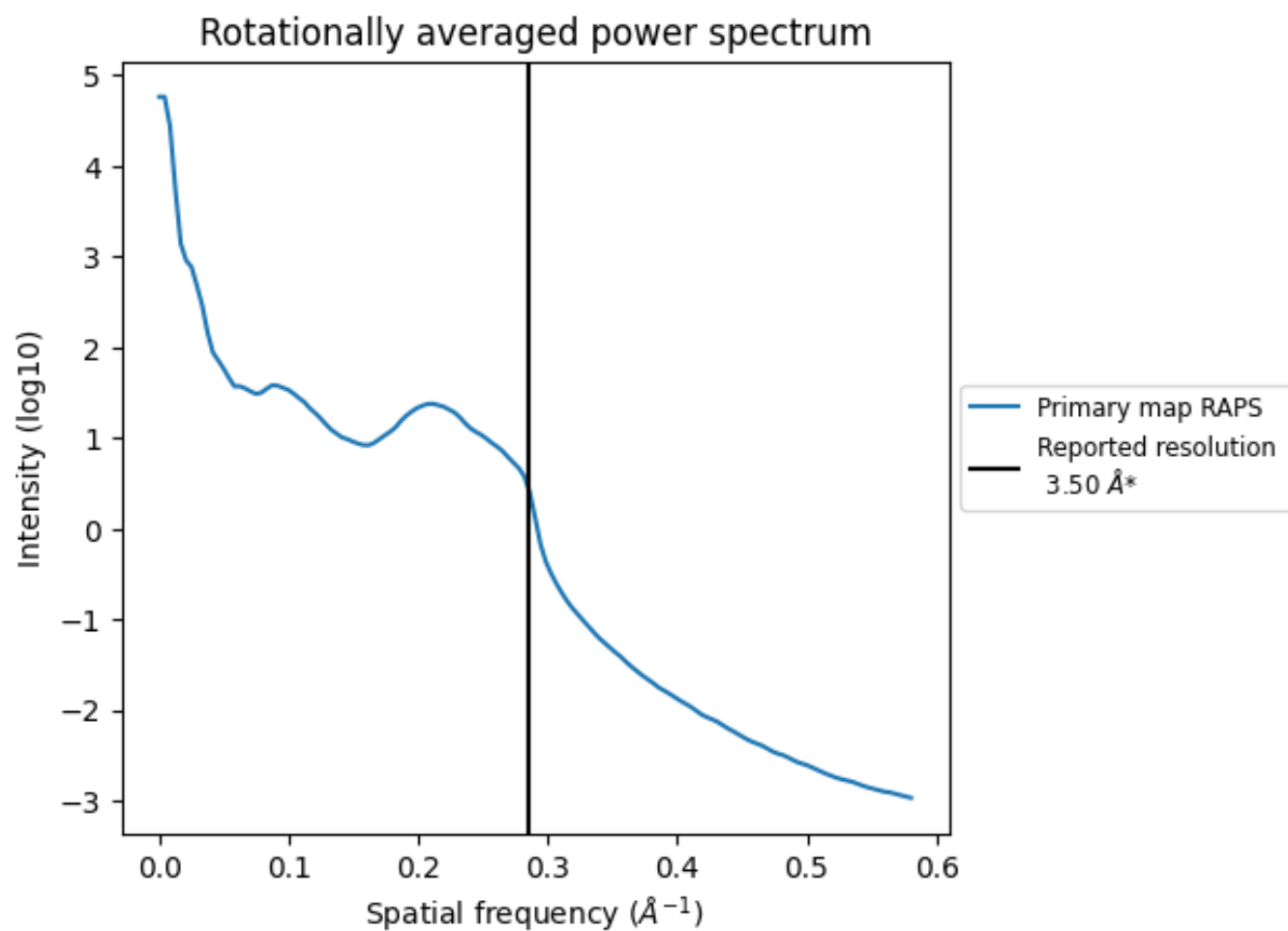
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm^3 ; this corresponds to an approximate mass of 111 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 ⓘ

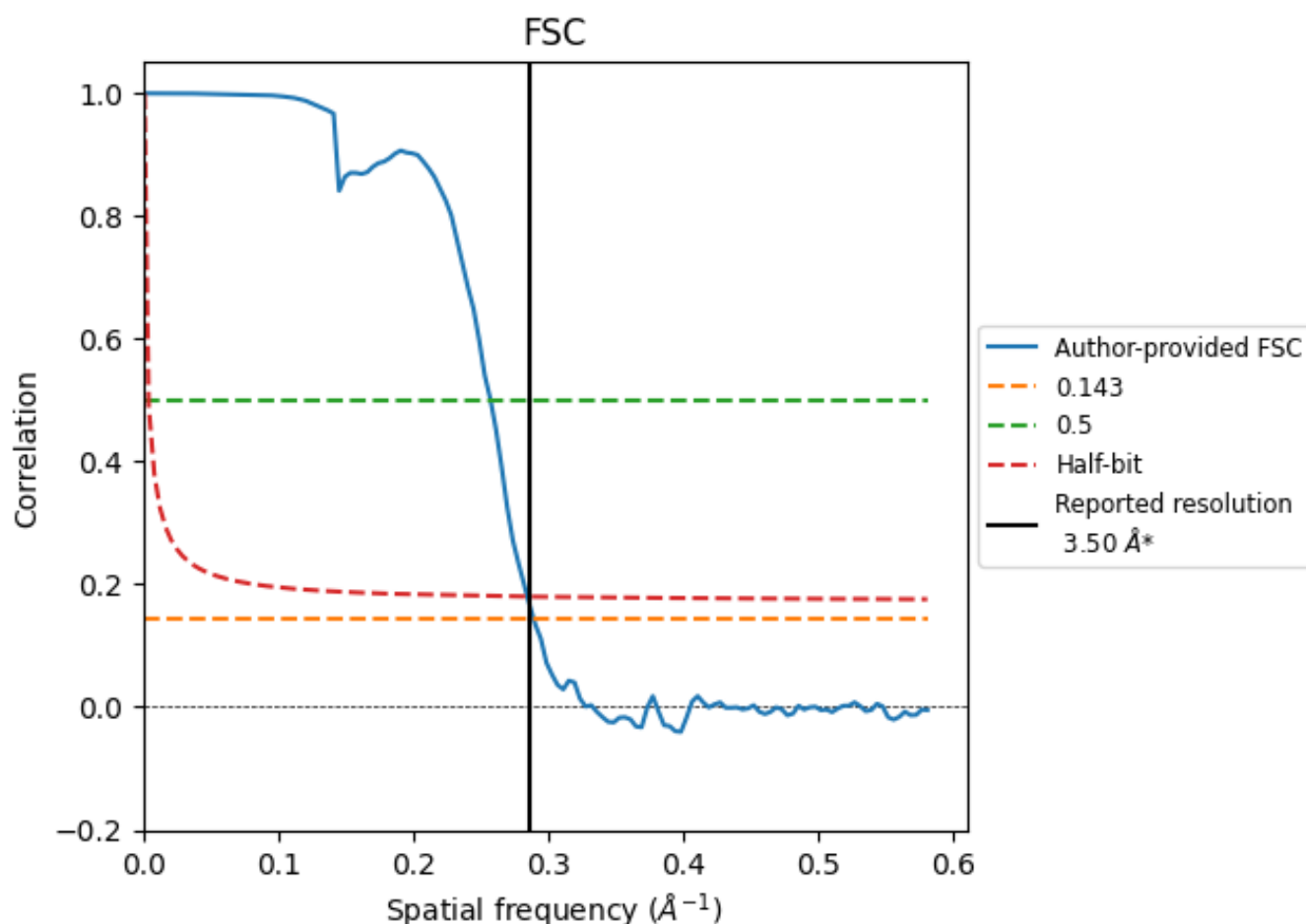


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.89	3.52
Unmasked-calculated*	-	-	-

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

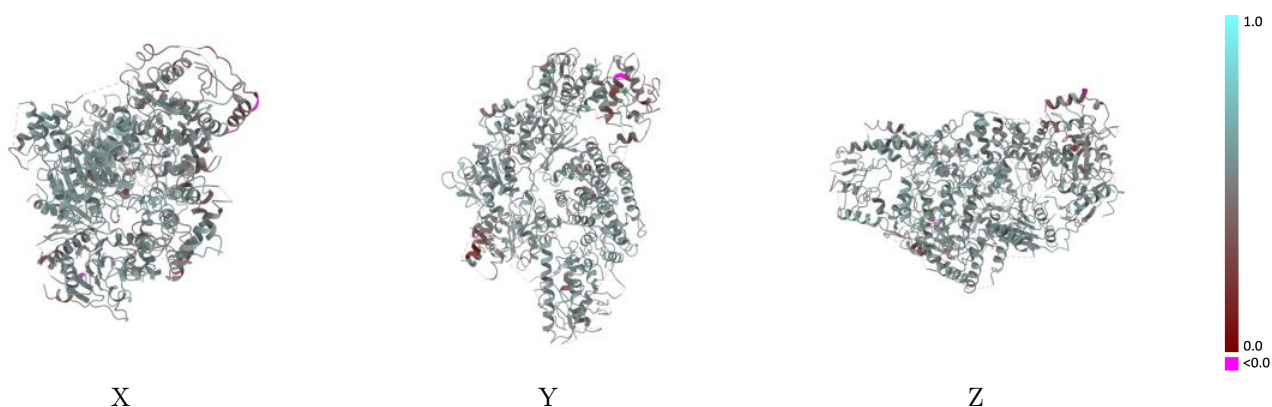
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20440 and PDB model 6PPJ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

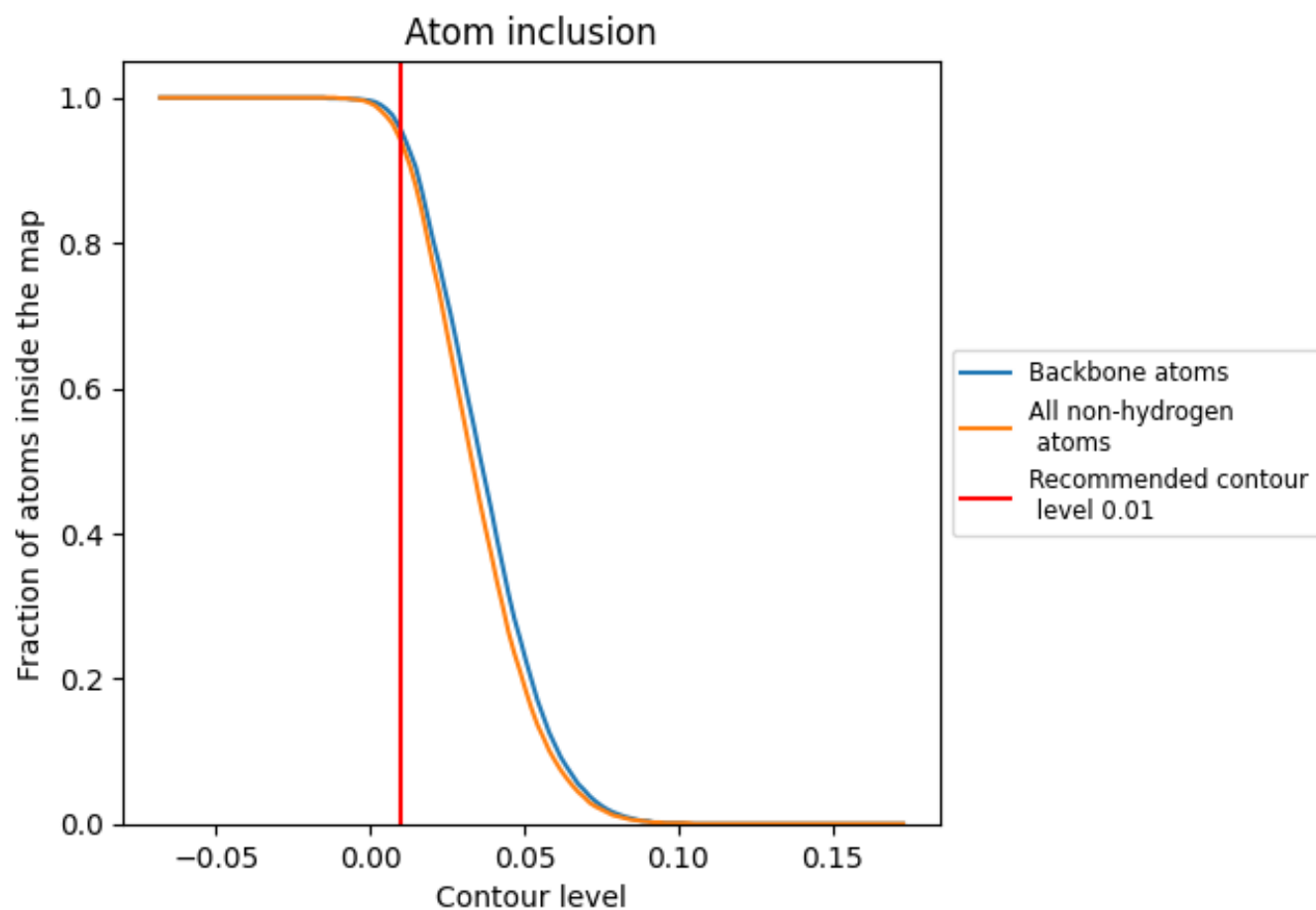


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 94% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.5190
A	0.9500	0.5270
B	0.9320	0.5100

