



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:48 PM UTC

PDB ID : 6YW7 / pdb_00006yw7
EMDB ID : EMD-10960
Title : Cryo-EM structure of the ARP2/3 1A5C isoform complex.
Authors : von Loeffelholz, O.; Moores, C.; Purkiss, A.
Deposited on : 2020-04-29
Resolution : 4.50 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:

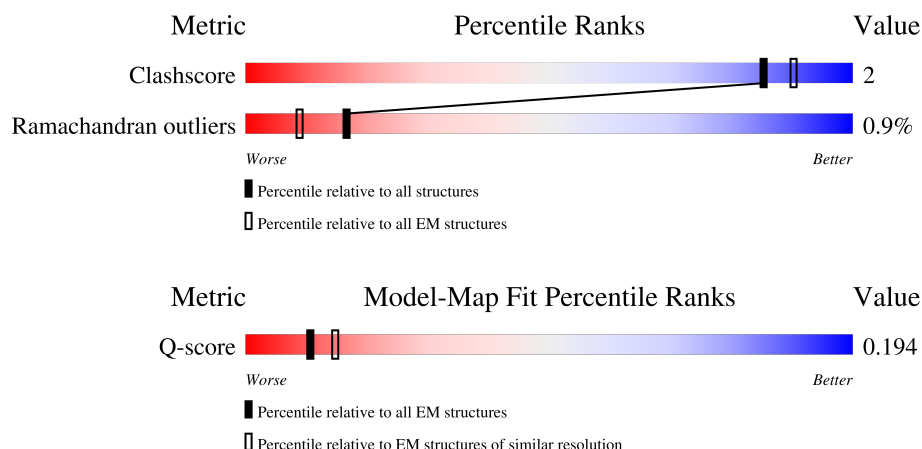
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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	-
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	418	11% 84% 9% 5%
2	D	300	8% 91% 5%
3	E	178	33% 82% 13%
4	B	394	27% 60% 11% 27%
5	F	168	5% 98%

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Mol	Chain	Length	Quality of chain
6	G	151	14% 89% • 8%
7	C	370	22% 84% 10% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5426 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms			AltConf	Trace
1	A	396	Total	C	N	0	0
			1188	792	396		

- Molecule 2 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms			AltConf	Trace
2	D	284	Total	C	N	0	0
			852	568	284		

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms			AltConf	Trace
3	E	170	Total	C	N	0	0
			510	340	170		

- Molecule 4 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms			AltConf	Trace
4	B	286	Total	C	N	0	0
			858	572	286		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	35	ILE	LEU	conflict	UNP P61160

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms			AltConf	Trace
5	F	165	Total	C	N	0	0
			495	330	165		

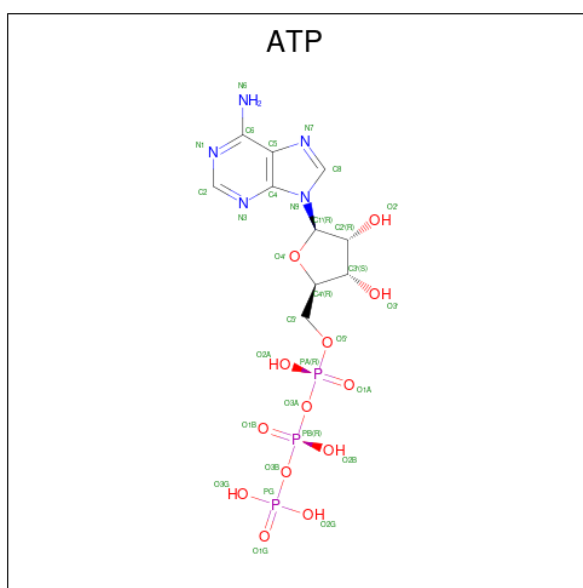
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	G	139	Total	C	N	0	0
			417	278	139		

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 1A.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	C	348	Total	C	N	0	0
			1044	696	348		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

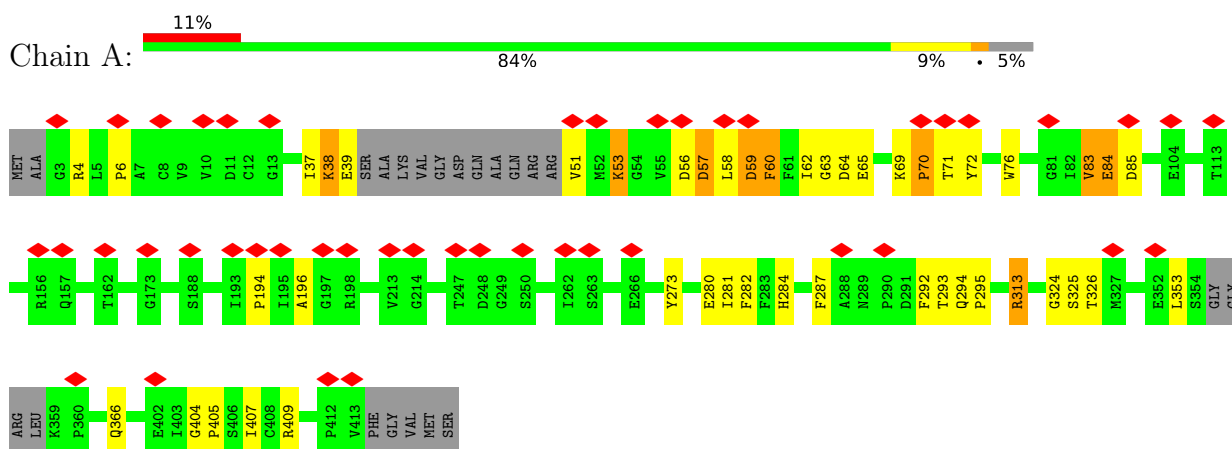


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

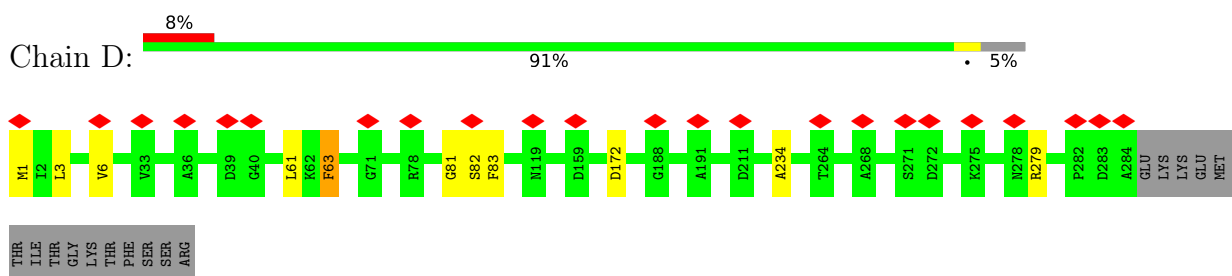
3 Residue-property plots

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.

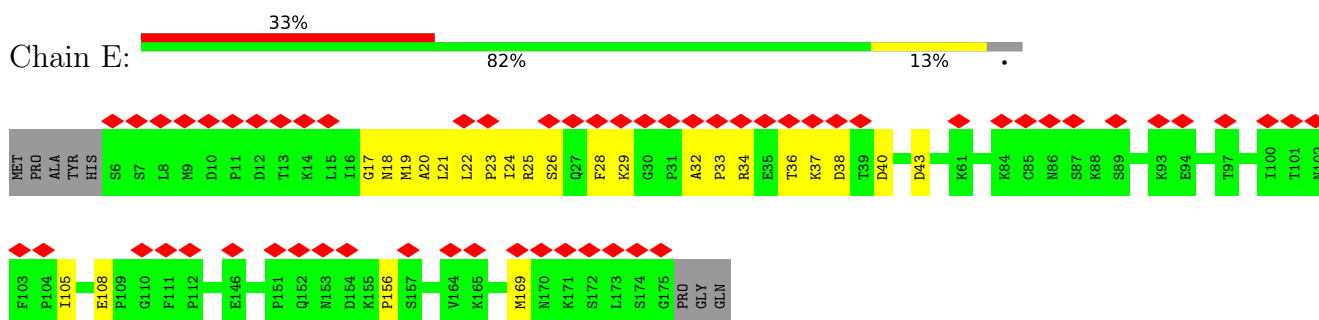
- Molecule 1: Actin-related protein 3



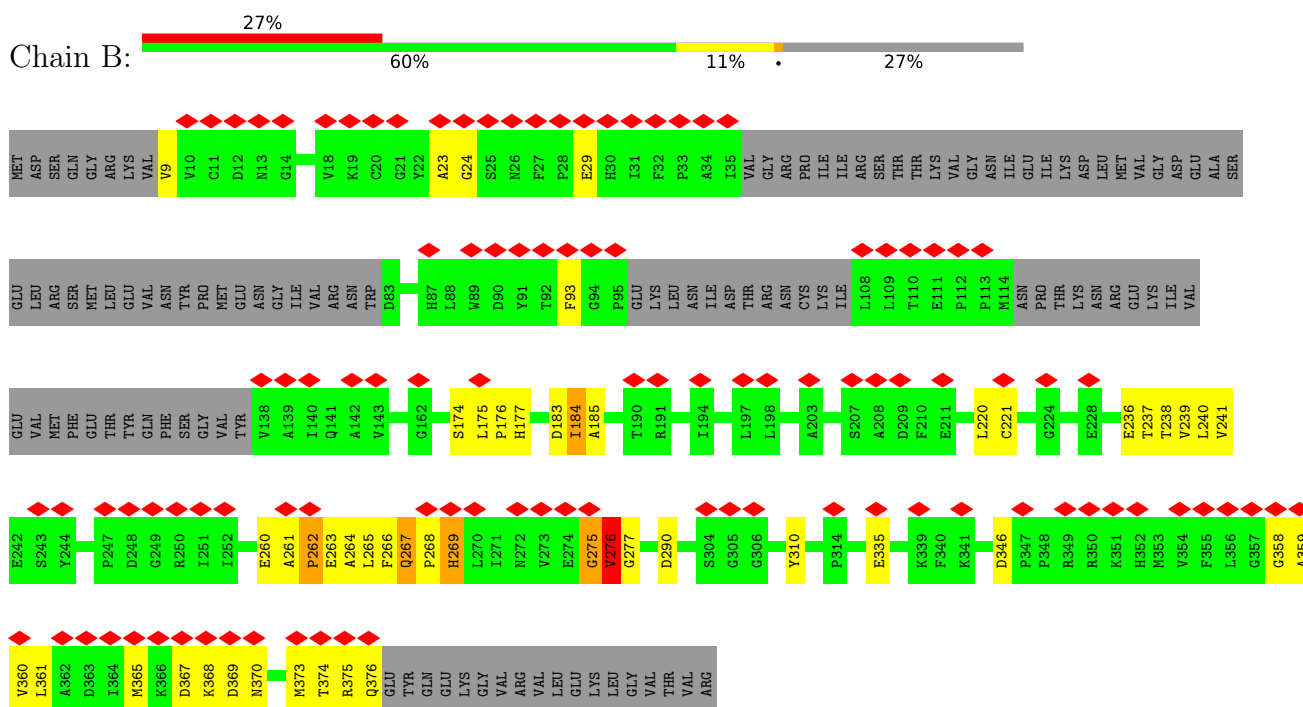
- Molecule 2: Actin-related protein 2/3 complex subunit 2



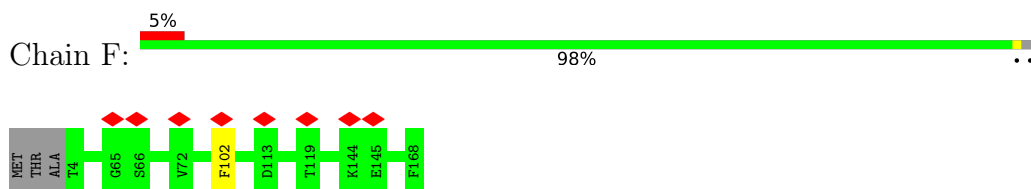
- Molecule 3: Actin-related protein 2/3 complex subunit 3



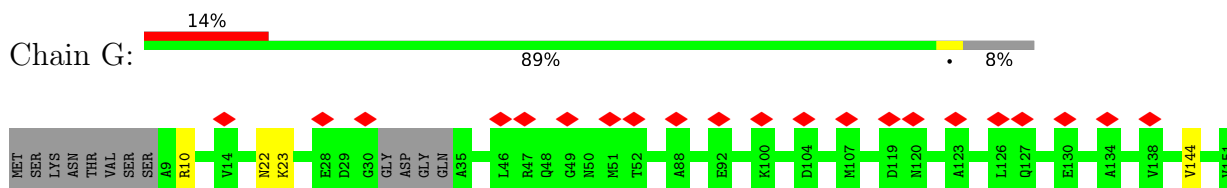
- Molecule 4: Actin-related protein 2



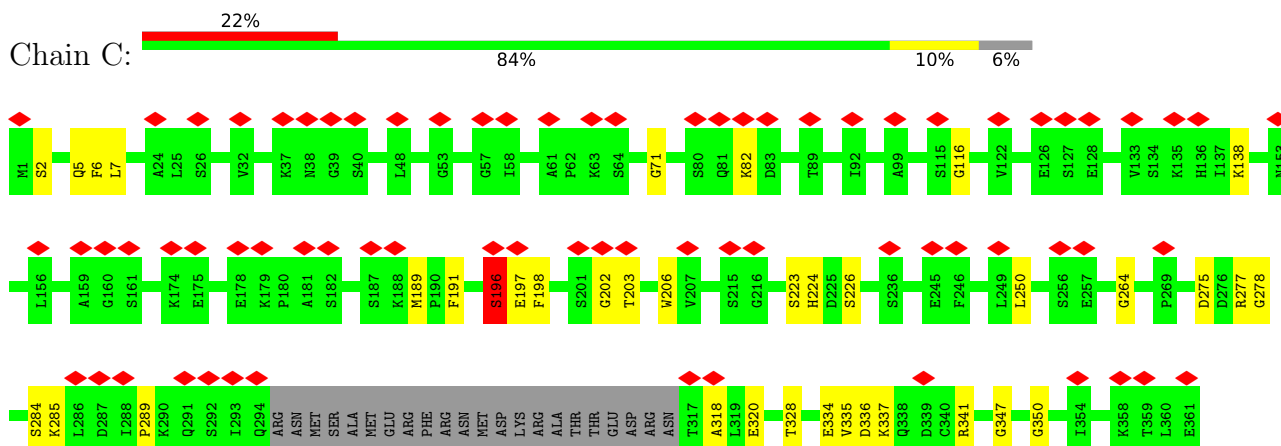
- Molecule 5: Actin-related protein 2/3 complex subunit 4



- Molecule 6: Actin-related protein 2/3 complex subunit 5



- Molecule 7: Actin-related protein 2/3 complex subunit 1A



S362	S363	I364	Q365	G366	L367	R368	I369	K370
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	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	0.077	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0174	Depositor
Map size (Å)	279.04, 279.04, 279.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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	1.92	31/1185 (2.6%)	2.83	61/1182 (5.2%)
2	D	0.87	5/851 (0.6%)	1.90	19/850 (2.2%)
3	E	1.61	13/508 (2.6%)	2.60	34/506 (6.7%)
4	B	2.09	32/854 (3.7%)	3.23	74/850 (8.7%)
5	F	0.81	0/494	1.30	1/493 (0.2%)
6	G	0.57	0/415	1.10	1/413 (0.2%)
7	C	1.70	1/1042 (0.1%)	2.29	39/1040 (3.8%)
All	All	1.59	82/5349 (1.5%)	2.44	229/5334 (4.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
2	D	0	1
4	B	0	4
7	C	0	1
All	All	0	15

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	VAL	C-N	31.37	1.73	1.33
1	A	280	GLU	C-N	-17.21	1.16	1.34
4	B	184	ILE	C-N	15.80	1.53	1.33
4	B	261	ALA	CA-C	14.51	1.71	1.52
4	B	310	TYR	C-N	14.38	1.50	1.33
1	A	313	ARG	C-N	14.37	1.51	1.34
4	B	237	THR	N-CA	13.66	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	LEU	CA-C	-12.04	1.36	1.52
3	E	20	ALA	CA-C	-11.93	1.36	1.52
4	B	185	ALA	N-CA	11.63	1.60	1.46
1	A	63	GLY	C-N	-10.93	1.19	1.33
4	B	264	ALA	CA-C	-10.55	1.39	1.52
1	A	69	LYS	C-N	-10.30	1.20	1.34
4	B	269	HIS	N-CA	-10.00	1.35	1.46
4	B	241	VAL	N-CA	-9.98	1.33	1.46
3	E	34	ARG	C-N	-9.52	1.20	1.33
4	B	359	ALA	CA-C	9.23	1.64	1.52
4	B	221	CYS	CA-C	9.01	1.64	1.53
4	B	277	GLY	CA-C	-8.82	1.39	1.51
4	B	373	MET	CA-C	-8.51	1.41	1.52
1	A	39	GLU	CA-C	8.43	1.70	1.52
4	B	277	GLY	N-CA	-8.25	1.33	1.45
4	B	23	ALA	CA-C	-8.19	1.43	1.52
4	B	237	THR	C-N	8.01	1.45	1.33
3	E	25	ARG	CA-C	-7.99	1.42	1.52
1	A	62	ILE	C-N	7.88	1.43	1.33
1	A	282	PHE	CA-C	-7.63	1.43	1.52
4	B	238	THR	N-CA	7.57	1.56	1.46
1	A	53	LYS	N-CA	-7.51	1.35	1.45
3	E	20	ALA	N-CA	-7.49	1.36	1.45
4	B	370	ASN	N-CA	7.34	1.55	1.46
3	E	34	ARG	CA-C	7.33	1.62	1.52
4	B	239	VAL	CA-C	7.27	1.63	1.52
4	B	368	LYS	CA-C	-7.27	1.42	1.52
1	A	366	GLN	N-CA	7.24	1.55	1.46
1	A	38	LYS	N-CA	7.24	1.54	1.45
1	A	59	ASP	C-N	6.96	1.42	1.33
3	E	21	LEU	CA-C	-6.96	1.43	1.53
3	E	19	MET	CA-C	-6.95	1.43	1.52
1	A	70	PRO	C-N	6.84	1.43	1.33
1	A	353	LEU	C-N	6.82	1.43	1.33
4	B	240	LEU	CA-C	-6.79	1.44	1.52
1	A	71	THR	N-CA	6.71	1.54	1.46
7	C	196	SER	CA-C	-6.62	1.44	1.52
3	E	23	PRO	CA-C	-6.41	1.45	1.52
4	B	221	CYS	C-N	6.37	1.40	1.33
1	A	76	TRP	C-N	6.26	1.42	1.33
4	B	375	ARG	CA-C	-6.24	1.44	1.52
4	B	185	ALA	CA-C	6.22	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	267	GLN	CA-C	-6.21	1.46	1.53
4	B	236	GLU	C-N	6.18	1.41	1.33
4	B	361	LEU	CA-C	6.16	1.60	1.52
1	A	38	LYS	C-N	6.06	1.41	1.33
1	A	84	GLU	N-CA	5.96	1.53	1.46
4	B	374	THR	N-CA	-5.91	1.39	1.46
2	D	82	SER	CA-C	5.86	1.61	1.52
3	E	33	PRO	N-CA	-5.86	1.39	1.47
1	A	70	PRO	N-CA	-5.85	1.40	1.47
3	E	26	SER	N-CA	-5.81	1.37	1.45
1	A	69	LYS	CA-C	-5.78	1.45	1.52
4	B	262	PRO	N-CA	5.76	1.54	1.47
1	A	76	TRP	N-CA	-5.72	1.40	1.46
2	D	63	PHE	C-N	-5.72	1.26	1.33
3	E	22	LEU	CA-C	-5.69	1.48	1.52
3	E	24	ILE	CA-C	5.54	1.60	1.53
1	A	295	PRO	CA-C	-5.52	1.46	1.52
4	B	277	GLY	C-N	5.48	1.38	1.33
1	A	366	GLN	C-N	5.45	1.40	1.33
1	A	196	ALA	C-N	5.43	1.40	1.33
4	B	238	THR	C-N	5.35	1.39	1.33
1	A	284	HIS	C-N	-5.32	1.27	1.33
2	D	61	LEU	C-N	5.29	1.41	1.33
2	D	82	SER	C-N	5.26	1.41	1.33
1	A	53	LYS	CA-C	-5.24	1.46	1.53
1	A	281	ILE	CA-C	-5.23	1.45	1.52
3	E	19	MET	N-CA	-5.19	1.39	1.46
4	B	367	ASP	C-N	5.19	1.41	1.33
1	A	56	ASP	C-N	5.18	1.41	1.33
1	A	404	GLY	C-N	-5.17	1.28	1.34
1	A	85	ASP	CA-C	-5.17	1.46	1.52
2	D	1	MET	N-CA	5.12	1.55	1.46
4	B	263	GLU	N-CA	-5.08	1.39	1.45

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	GLU	N-CA-C	-21.78	50.01	111.00
1	A	58	LEU	N-CA-C	-19.03	90.20	113.41
4	B	264	ALA	N-CA-C	-16.49	93.42	111.07
1	A	71	THR	CA-C-N	15.85	143.45	122.84
1	A	71	THR	C-N-CA	15.85	143.45	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	CA-C-N	15.73	136.00	118.85
1	A	313	ARG	C-N-CA	15.73	136.00	118.85
4	B	93	PHE	CA-C-N	-15.59	97.39	121.87
4	B	93	PHE	C-N-CA	-15.59	97.39	121.87
1	A	366	GLN	CA-C-N	-15.49	102.98	123.12
1	A	366	GLN	C-N-CA	-15.49	102.98	123.12
3	E	20	ALA	N-CA-C	-15.46	85.74	110.32
4	B	310	TYR	CA-C-N	15.38	136.39	119.93
4	B	310	TYR	C-N-CA	15.38	136.39	119.93
3	E	25	ARG	CA-C-N	-14.67	93.12	123.20
3	E	25	ARG	C-N-CA	-14.67	93.12	123.20
2	D	82	SER	N-CA-C	14.56	130.35	112.87
4	B	238	THR	CA-C-N	14.49	145.31	121.54
4	B	238	THR	C-N-CA	14.49	145.31	121.54
4	B	185	ALA	N-CA-C	14.17	132.97	108.75
1	A	70	PRO	CA-C-N	14.04	140.23	120.29
1	A	70	PRO	C-N-CA	14.04	140.23	120.29
1	A	282	PHE	CA-C-N	13.96	138.98	120.28
1	A	282	PHE	C-N-CA	13.96	138.98	120.28
1	A	65	GLU	CA-C-N	13.60	138.50	120.28
1	A	65	GLU	C-N-CA	13.60	138.50	120.28
4	B	359	ALA	CA-C-N	13.54	143.11	120.64
4	B	359	ALA	C-N-CA	13.54	143.11	120.64
1	A	284	HIS	CA-C-N	13.39	133.22	119.56
1	A	284	HIS	C-N-CA	13.39	133.22	119.56
4	B	275	GLY	CA-C-N	13.20	145.73	121.97
4	B	275	GLY	C-N-CA	13.20	145.73	121.97
4	B	268	PRO	CA-C-N	-13.09	101.25	120.89
4	B	268	PRO	C-N-CA	-13.09	101.25	120.89
2	D	81	GLY	CA-C-N	13.02	145.21	120.99
2	D	81	GLY	C-N-CA	13.02	145.21	120.99
1	A	38	LYS	CA-C-N	-12.62	98.98	121.70
1	A	38	LYS	C-N-CA	-12.62	98.98	121.70
1	A	37	ILE	CA-C-N	12.30	146.75	122.03
1	A	37	ILE	C-N-CA	12.30	146.75	122.03
4	B	276	VAL	CA-C-N	-12.20	97.51	121.41
4	B	276	VAL	C-N-CA	-12.20	97.51	121.41
4	B	184	ILE	CA-C-N	12.11	143.25	121.94
4	B	184	ILE	C-N-CA	12.11	143.25	121.94
4	B	267	GLN	CA-C-N	12.08	132.44	119.87
4	B	267	GLN	C-N-CA	12.08	132.44	119.87
1	A	51	VAL	N-CA-C	12.03	144.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	TRP	CA-C-N	11.31	131.72	119.28
1	A	76	TRP	C-N-CA	11.31	131.72	119.28
7	C	197	GLU	N-CA-C	-10.88	97.42	111.02
1	A	53	LYS	CA-C-N	-10.79	100.27	121.41
1	A	53	LYS	C-N-CA	-10.79	100.27	121.41
4	B	240	LEU	N-CA-C	-10.55	99.86	111.36
4	B	277	GLY	CA-C-N	-10.32	110.17	122.35
4	B	277	GLY	C-N-CA	-10.32	110.17	122.35
1	A	281	ILE	CA-C-N	-10.15	105.88	120.29
1	A	281	ILE	C-N-CA	-10.15	105.88	120.29
4	B	262	PRO	N-CA-C	10.12	126.35	114.20
4	B	239	VAL	CA-C-N	10.05	134.56	120.29
4	B	239	VAL	C-N-CA	10.05	134.56	120.29
3	E	34	ARG	N-CA-C	9.79	125.88	110.32
1	A	405	PRO	N-CA-C	9.65	127.30	114.27
3	E	20	ALA	CA-C-N	-9.49	101.13	121.45
3	E	20	ALA	C-N-CA	-9.49	101.13	121.45
4	B	367	ASP	CA-C-N	9.49	137.75	121.14
4	B	367	ASP	C-N-CA	9.49	137.75	121.14
7	C	334	GLU	CA-C-N	9.20	138.54	121.97
7	C	334	GLU	C-N-CA	9.20	138.54	121.97
2	D	1	MET	CA-C-N	-9.14	113.85	123.08
2	D	1	MET	C-N-CA	-9.14	113.85	123.08
2	D	82	SER	CA-C-N	9.13	138.05	122.26
2	D	82	SER	C-N-CA	9.13	138.05	122.26
1	A	85	ASP	CA-C-N	-9.01	108.20	120.28
1	A	85	ASP	C-N-CA	-9.01	108.20	120.28
2	D	61	LEU	CA-C-N	8.98	134.96	120.60
2	D	61	LEU	C-N-CA	8.98	134.96	120.60
4	B	369	ASP	CA-C-N	8.93	138.99	121.58
4	B	369	ASP	C-N-CA	8.93	138.99	121.58
4	B	221	CYS	N-CA-C	8.86	125.08	107.62
1	A	59	ASP	CA-C-N	8.81	141.61	121.87
1	A	59	ASP	C-N-CA	8.81	141.61	121.87
3	E	17	GLY	CA-C-N	-8.74	109.08	120.44
3	E	17	GLY	C-N-CA	-8.74	109.08	120.44
7	C	196	SER	N-CA-C	-8.72	92.22	110.80
4	B	266	PHE	CA-C-N	8.72	132.51	120.65
4	B	266	PHE	C-N-CA	8.72	132.51	120.65
4	B	360	VAL	CA-C-N	-8.63	108.79	120.79
4	B	360	VAL	C-N-CA	-8.63	108.79	120.79
7	C	363	SER	CA-C-N	-8.48	111.58	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	363	SER	C-N-CA	-8.48	111.58	123.11
3	E	40	ASP	CA-C-N	8.43	132.00	120.46
3	E	40	ASP	C-N-CA	8.43	132.00	120.46
4	B	263	GLU	N-CA-C	-8.32	103.32	113.97
7	C	341	ARG	N-CA-C	8.29	120.00	110.97
4	B	374	THR	N-CA-C	-8.26	101.86	111.03
7	C	203	THR	CA-C-N	-8.26	112.84	121.35
7	C	203	THR	C-N-CA	-8.26	112.84	121.35
1	A	407	ILE	N-CA-C	-8.24	102.67	110.42
7	C	197	GLU	CA-C-N	-7.94	109.31	122.17
7	C	197	GLU	C-N-CA	-7.94	109.31	122.17
3	E	26	SER	CA-C-N	7.91	131.53	120.29
3	E	26	SER	C-N-CA	7.91	131.53	120.29
1	A	59	ASP	N-CA-C	7.90	121.87	110.10
1	A	4	ARG	N-CA-C	-7.83	102.71	111.71
4	B	361	LEU	CA-C-N	7.82	136.48	121.54
4	B	361	LEU	C-N-CA	7.82	136.48	121.54
1	A	84	GLU	CA-C-N	7.71	134.61	122.74
1	A	84	GLU	C-N-CA	7.71	134.61	122.74
1	A	69	LYS	N-CA-C	-7.68	100.12	109.72
4	B	261	ALA	N-CA-C	7.66	126.73	109.81
2	D	1	MET	N-CA-C	7.58	132.24	111.00
2	D	6	VAL	CA-C-N	7.44	131.37	120.95
2	D	6	VAL	C-N-CA	7.44	131.37	120.95
3	E	33	PRO	N-CA-C	-7.43	97.16	112.47
4	B	265	LEU	N-CA-C	-7.42	103.49	112.54
1	A	6	PRO	CA-C-N	7.34	131.13	120.71
1	A	6	PRO	C-N-CA	7.34	131.13	120.71
3	E	21	LEU	CA-C-N	7.28	135.37	122.48
3	E	21	LEU	C-N-CA	7.28	135.37	122.48
1	A	409	ARG	CA-C-N	-7.25	110.08	123.05
1	A	409	ARG	C-N-CA	-7.25	110.08	123.05
7	C	284	SER	CA-C-N	7.24	135.36	121.54
7	C	284	SER	C-N-CA	7.24	135.36	121.54
4	B	9	VAL	CA-C-N	7.17	132.08	123.19
4	B	9	VAL	C-N-CA	7.17	132.08	123.19
7	C	275	ASP	CA-C-N	7.09	130.49	120.28
7	C	275	ASP	C-N-CA	7.09	130.49	120.28
4	B	268	PRO	N-CA-C	-7.07	105.34	114.03
4	B	261	ALA	CA-C-N	7.02	127.92	120.12
4	B	261	ALA	C-N-CA	7.02	127.92	120.12
1	A	293	THR	CA-C-N	-6.96	111.11	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	THR	C-N-CA	-6.96	111.11	122.65
4	B	260	GLU	CA-C-N	-6.95	104.83	121.80
4	B	260	GLU	C-N-CA	-6.95	104.83	121.80
4	B	346	ASP	CA-C-N	6.75	127.33	120.38
4	B	346	ASP	C-N-CA	6.75	127.33	120.38
7	C	6	PHE	N-CA-C	6.67	121.38	111.04
1	A	366	GLN	N-CA-C	6.66	120.38	109.06
7	C	82	LYS	N-CA-C	-6.48	100.87	110.46
7	C	71	GLY	CA-C-N	6.45	129.56	120.28
7	C	71	GLY	C-N-CA	6.45	129.56	120.28
4	B	263	GLU	CA-C-N	6.43	128.80	120.44
4	B	263	GLU	C-N-CA	6.43	128.80	120.44
1	A	292	PHE	CA-C-N	6.33	129.93	120.31
1	A	292	PHE	C-N-CA	6.33	129.93	120.31
1	A	405	PRO	CA-C-N	6.31	128.73	120.28
1	A	405	PRO	C-N-CA	6.31	128.73	120.28
4	B	269	HIS	N-CA-C	-6.29	101.28	111.04
2	D	83	PHE	CA-C-N	-6.29	113.33	122.19
2	D	83	PHE	C-N-CA	-6.29	113.33	122.19
4	B	29	GLU	N-CA-C	-6.26	104.90	112.54
4	B	359	ALA	N-CA-C	6.25	118.65	111.02
4	B	183	ASP	CA-C-N	6.25	129.11	120.49
4	B	183	ASP	C-N-CA	6.25	129.11	120.49
4	B	267	GLN	N-CA-C	-6.25	100.48	109.48
2	D	279	ARG	N-CA-C	-6.24	104.39	111.07
4	B	376	GLN	N-CA-C	6.23	128.43	111.00
1	A	58	LEU	CA-C-N	6.21	129.57	120.82
1	A	58	LEU	C-N-CA	6.21	129.57	120.82
3	E	37	LYS	N-CA-C	6.20	119.25	110.14
3	E	29	LYS	N-CA-C	-6.14	100.00	109.76
1	A	57	ASP	CA-C-N	-6.14	111.11	122.09
1	A	57	ASP	C-N-CA	-6.14	111.11	122.09
3	E	36	THR	CA-C-N	-6.13	112.08	123.05
3	E	36	THR	C-N-CA	-6.13	112.08	123.05
3	E	156	PRO	N-CA-C	-6.07	101.11	110.95
3	E	40	ASP	N-CA-C	-6.06	101.51	110.48
7	C	278	GLY	N-CA-C	-6.06	105.14	115.08
7	C	206	TRP	N-CA-C	-6.05	101.33	110.28
1	A	294	GLN	CA-C-N	6.03	126.37	119.92
1	A	294	GLN	C-N-CA	6.03	126.37	119.92
2	D	3	LEU	N-CA-C	-6.02	100.69	110.20
4	B	335	GLU	N-CA-C	5.97	117.79	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	18	ASN	CA-C-N	5.96	130.92	122.09
3	E	18	ASN	C-N-CA	5.96	130.92	122.09
4	B	24	GLY	CA-C-N	5.96	132.92	121.54
4	B	24	GLY	C-N-CA	5.96	132.92	121.54
3	E	28	PHE	CA-C-N	-5.94	113.00	121.50
3	E	28	PHE	C-N-CA	-5.94	113.00	121.50
7	C	289	PRO	N-CA-C	-5.93	102.55	111.57
7	C	363	SER	N-CA-C	5.91	118.96	111.69
3	E	24	ILE	CA-C-N	-5.88	113.68	122.74
3	E	24	ILE	C-N-CA	-5.88	113.68	122.74
3	E	32	ALA	N-CA-C	5.84	113.27	108.07
7	C	223	SER	CA-C-N	5.84	129.18	120.31
7	C	223	SER	C-N-CA	5.84	129.18	120.31
4	B	220	LEU	N-CA-C	5.81	120.87	113.55
7	C	320	GLU	N-CA-C	-5.80	104.95	111.28
3	E	37	LYS	CA-C-N	5.80	129.13	120.31
3	E	37	LYS	C-N-CA	5.80	129.13	120.31
7	C	277	ARG	N-CA-C	-5.80	105.31	112.38
2	D	234	ALA	CA-C-N	-5.77	112.10	120.29
2	D	234	ALA	C-N-CA	-5.77	112.10	120.29
3	E	21	LEU	N-CA-C	-5.75	103.11	110.53
2	D	172	ASP	N-CA-C	5.74	120.84	111.37
4	B	358	GLY	CA-C-N	5.65	128.64	120.79
4	B	358	GLY	C-N-CA	5.65	128.64	120.79
7	C	5	GLN	CA-C-N	5.64	129.35	120.89
7	C	5	GLN	C-N-CA	5.64	129.35	120.89
7	C	196	SER	CA-C-N	-5.64	114.21	122.78
7	C	196	SER	C-N-CA	-5.64	114.21	122.78
4	B	174	SER	CA-C-N	-5.57	115.95	123.46
4	B	174	SER	C-N-CA	-5.57	115.95	123.46
4	B	262	PRO	CA-C-N	-5.56	113.00	122.11
4	B	262	PRO	C-N-CA	-5.56	113.00	122.11
4	B	365	MET	CA-C-N	5.55	128.04	120.54
4	B	365	MET	C-N-CA	5.55	128.04	120.54
7	C	202	GLY	CA-C-N	5.49	130.74	121.14
7	C	202	GLY	C-N-CA	5.49	130.74	121.14
7	C	189	MET	N-CA-C	5.48	121.92	109.81
6	G	144	VAL	N-CA-C	-5.36	105.30	110.72
3	E	43	ASP	N-CA-C	-5.31	105.49	111.28
4	B	9	VAL	N-CA-C	-5.25	96.29	111.00
1	A	64	ASP	CA-C-N	5.25	127.27	120.44
1	A	64	ASP	C-N-CA	5.25	127.27	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	337	LYS	N-CA-C	-5.20	105.61	111.28
7	C	116	GLY	CA-C-N	5.19	131.45	121.18
7	C	116	GLY	C-N-CA	5.19	131.45	121.18
1	A	85	ASP	N-CA-C	5.19	117.53	108.76
1	A	70	PRO	N-CA-C	5.17	120.86	113.47
3	E	38	ASP	CA-C-N	-5.15	113.82	122.17
3	E	38	ASP	C-N-CA	-5.15	113.82	122.17
1	A	60	PHE	N-CA-C	5.13	116.31	108.52
7	C	335	VAL	N-CA-C	5.09	119.92	109.34
1	A	273	TYR	N-CA-C	5.05	117.44	111.33
4	B	269	HIS	CA-C-N	5.05	127.04	120.28
4	B	269	HIS	C-N-CA	5.05	127.04	120.28
7	C	138	LYS	N-CA-C	5.05	119.28	111.56
5	F	102	PHE	N-CA-C	5.01	121.46	110.80

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	PRO	Peptide
1	A	287	PHE	Peptide
1	A	38	LYS	Peptide
1	A	53	LYS	Peptide
1	A	57	ASP	Peptide
1	A	59	ASP	Peptide
1	A	60	PHE	Peptide
1	A	70	PRO	Peptide
1	A	72	TYR	Peptide
4	B	184	ILE	Peptide
4	B	262	PRO	Peptide
4	B	275	GLY	Peptide
4	B	276	VAL	Peptide
7	C	196	SER	Peptide
2	D	63	PHE	Peptide

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	1188	0	419	3	0
2	D	852	0	303	0	0
3	E	510	0	174	4	0
4	B	858	0	316	3	0
5	F	495	0	164	0	0
6	G	417	0	153	0	0
7	C	1044	0	380	6	0
8	A	31	0	12	0	0
8	B	31	0	12	0	0
All	All	5426	0	1933	16	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 2.

All (16) 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:A:83:VAL:C	1:A:84:GLU:N	1.73	1.46
3:E:105:ILE:C	3:E:108:GLU:CA	2.29	1.06
7:C:7:LEU:H	7:C:350:GLY:HA2	1.37	0.87
7:C:7:LEU:H	7:C:350:GLY:CA	1.95	0.80
7:C:250:LEU:H	7:C:264:GLY:HA3	1.57	0.70
7:C:328:THR:H	7:C:347:GLY:HA2	1.61	0.66
3:E:105:ILE:C	3:E:108:GLU:C	2.65	0.64
3:E:105:ILE:C	3:E:108:GLU:N	2.56	0.62
3:E:105:ILE:C	3:E:108:GLU:H	2.15	0.53
7:C:224:HIS:C	7:C:226:SER:H	2.18	0.51
7:C:196:SER:H	7:C:198:PHE:N	2.09	0.50
4:B:267:GLN:C	4:B:269:HIS:H	2.23	0.45
1:A:324:GLY:C	1:A:326:THR:N	2.74	0.45
1:A:324:GLY:C	1:A:326:THR:H	2.25	0.44
4:B:267:GLN:C	4:B:269:HIS:N	2.73	0.42
4:B:175:LEU:C	4:B:177:HIS:H	2.28	0.41

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	390/418 (93%)	372 (95%)	16 (4%)	2 (0%)	24	63
2	D	282/300 (94%)	278 (99%)	4 (1%)	0	100	100
3	E	166/178 (93%)	161 (97%)	4 (2%)	1 (1%)	21	58
4	B	278/394 (71%)	245 (88%)	30 (11%)	3 (1%)	11	45
5	F	163/168 (97%)	158 (97%)	5 (3%)	0	100	100
6	G	135/151 (89%)	130 (96%)	2 (2%)	3 (2%)	5	29
7	C	344/370 (93%)	320 (93%)	18 (5%)	6 (2%)	7	35
All	All	1758/1979 (89%)	1664 (95%)	79 (4%)	15 (1%)	16	49

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	290	ASP
6	G	10	ARG
6	G	22	ASN
7	C	191	PHE
7	C	196	SER
7	C	2	SER
7	C	285	LYS
7	C	336	ASP
3	E	169	MET
7	C	318	ALA
1	A	313	ARG
1	A	325	SER
4	B	276	VAL
6	G	23	LYS
4	B	176	PRO

5.3.2 Protein sidechains [i](#)

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

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](#)

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
8	ATP	B	401	-	32,33,33	1.40	5 (15%)	48,52,52	1.74	9 (18%)
8	ATP	A	501	-	32,33,33	1.41	6 (18%)	48,52,52	1.87	12 (25%)

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
8	ATP	B	401	-	-	9/22/38/38	0/3/3/3
8	ATP	A	501	-	-	3/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	401	ATP	C5-C4	4.55	1.47	1.39
8	A	501	ATP	C5-C4	4.45	1.47	1.39
8	A	501	ATP	C5-C6	2.80	1.48	1.41
8	B	401	ATP	C5-C6	2.73	1.48	1.41
8	A	501	ATP	C8-N7	2.50	1.36	1.31
8	B	401	ATP	PB-O3B	2.40	1.62	1.59
8	B	401	ATP	C5-N7	-2.32	1.34	1.39
8	B	401	ATP	C8-N7	2.29	1.36	1.31
8	A	501	ATP	C5-N7	-2.29	1.34	1.39
8	A	501	ATP	C4-N9	-2.04	1.33	1.37
8	A	501	ATP	C1'-N9	2.01	1.51	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	401	ATP	C5-C4-N3	-5.88	118.62	126.72
8	A	501	ATP	C5-C4-N3	-5.63	118.96	126.72
8	B	401	ATP	N3-C4-N9	4.61	135.00	127.17
8	A	501	ATP	C4-C5-N7	-4.00	106.01	110.58
8	A	501	ATP	N3-C4-N9	3.94	133.87	127.17
8	A	501	ATP	O4'-C1'-N9	3.82	115.43	108.09
8	B	401	ATP	C2-N3-C4	3.72	120.92	111.83
8	A	501	ATP	C2-N3-C4	3.68	120.83	111.83
8	B	401	ATP	C4-C5-N7	-3.54	106.53	110.58
8	A	501	ATP	N3-C2-N1	-3.27	123.63	128.58
8	B	401	ATP	N3-C2-N1	-3.18	123.78	128.58
8	A	501	ATP	C4-N9-C1'	-2.81	120.07	126.63
8	A	501	ATP	C5-N7-C8	2.66	107.62	103.45
8	B	401	ATP	C4-N9-C8	2.64	108.51	105.74
8	B	401	ATP	C5-N7-C8	2.56	107.48	103.45
8	A	501	ATP	C6-C5-N7	2.54	136.99	132.09
8	A	501	ATP	C3'-C2'-C1'	2.19	105.61	101.46
8	A	501	ATP	C4-N9-C8	2.19	108.04	105.74
8	B	401	ATP	C3'-C2'-C1'	2.17	105.58	101.46
8	B	401	ATP	C6-C5-N7	2.11	136.16	132.09
8	A	501	ATP	N9-C8-N7	-2.06	111.02	113.94

There are no chirality outliers.

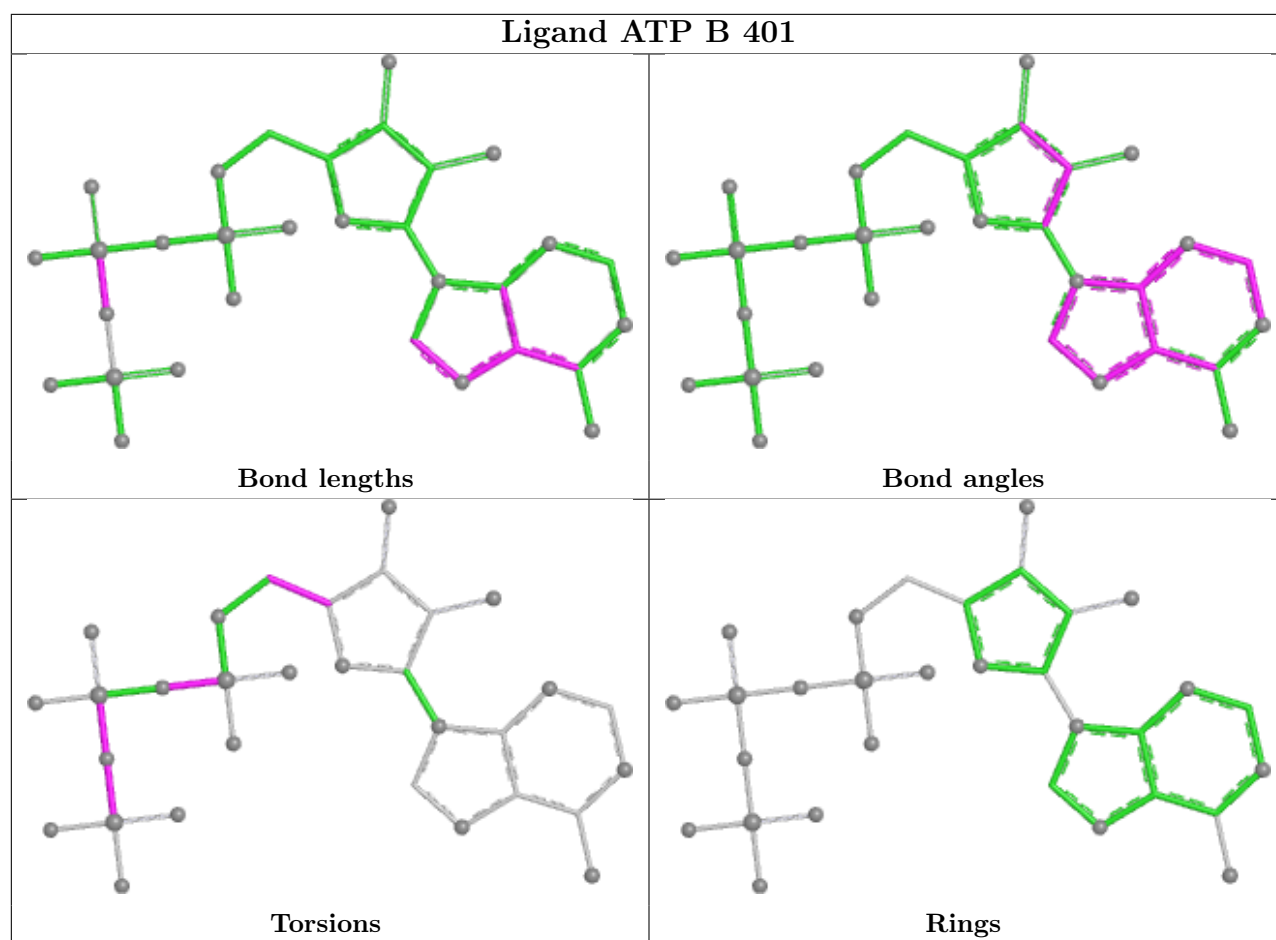
All (12) torsion outliers are listed below:

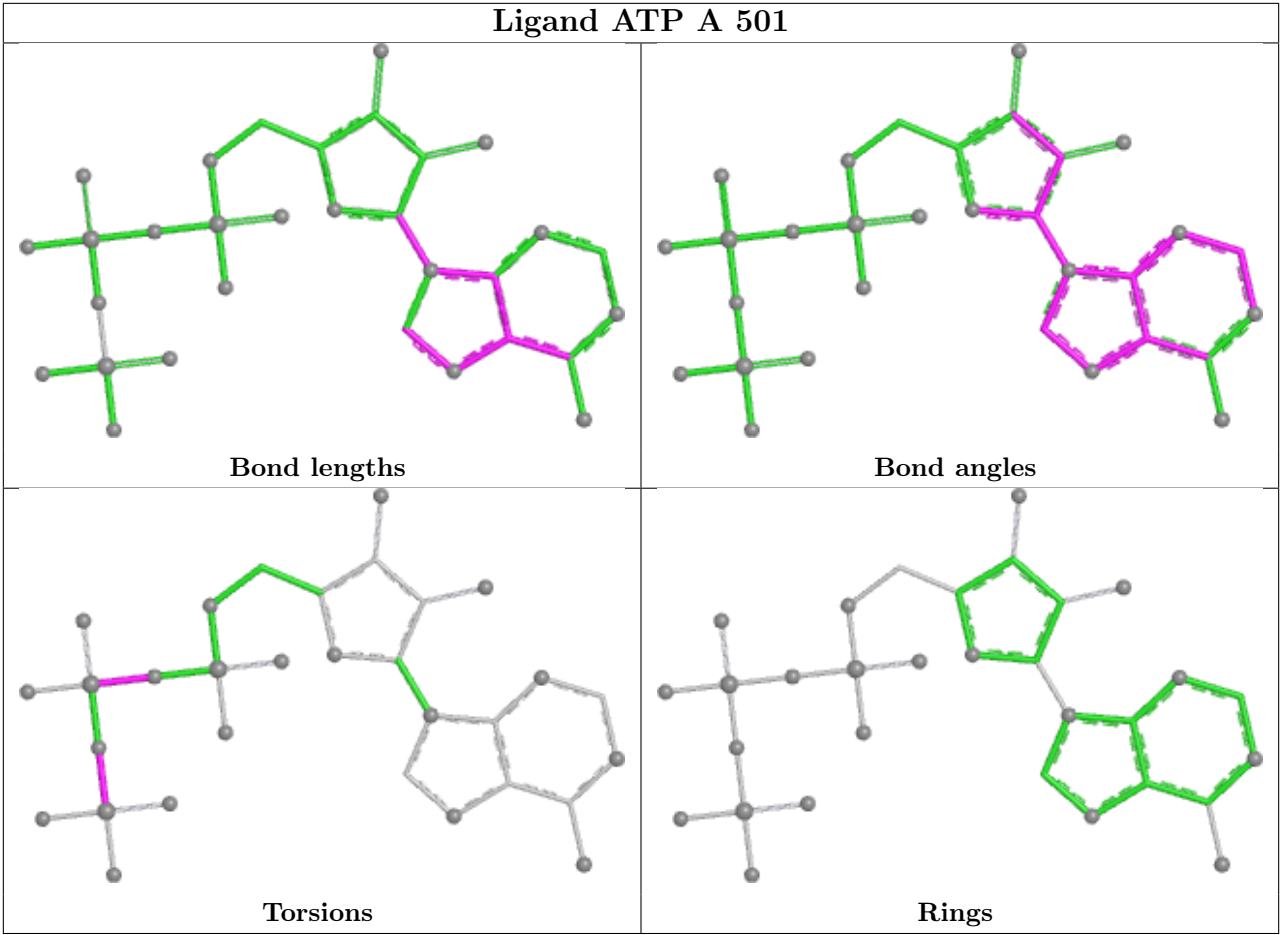
Mol	Chain	Res	Type	Atoms
8	B	401	ATP	PB-O3B-PG-O2G
8	B	401	ATP	O4'-C4'-C5'-O5'
8	B	401	ATP	C3'-C4'-C5'-O5'
8	B	401	ATP	PB-O3A-PA-O2A
8	A	501	ATP	PB-O3B-PG-O3G
8	B	401	ATP	PB-O3B-PG-O3G
8	B	401	ATP	PB-O3A-PA-O1A
8	A	501	ATP	PB-O3B-PG-O1G
8	B	401	ATP	PB-O3B-PG-O1G
8	A	501	ATP	PA-O3A-PB-O2B
8	B	401	ATP	PG-O3B-PB-O1B
8	B	401	ATP	PG-O3B-PB-O2B

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 ⓘ

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	A	3
3	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	105:ILE	C	106:PRO	N	4.37
1	A	83:VAL	C	84:GLU	N	1.73
1	E	34:ARG	C	35:GLU	N	1.20
1	A	63:GLY	C	64:ASP	N	1.19

Continued on next page...

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	280:GLU	C	281:ILE	N	1.15

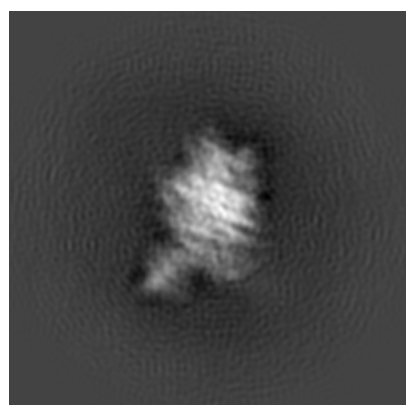
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10960. These allow visual inspection of the internal detail of the map and identification of artifacts.

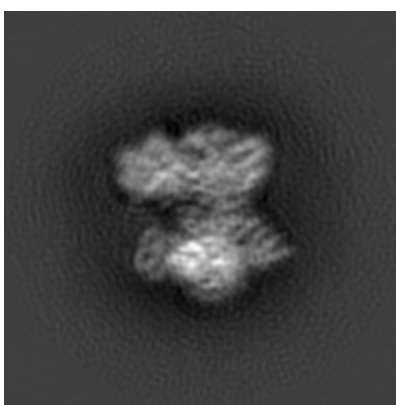
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

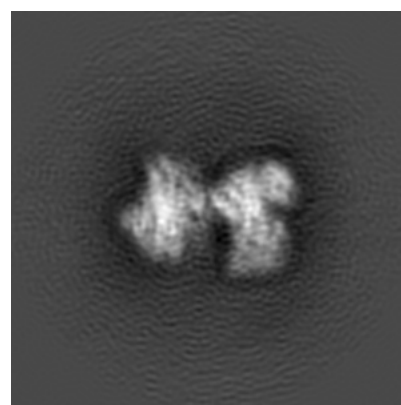
6.1.1 Primary map



X



Y

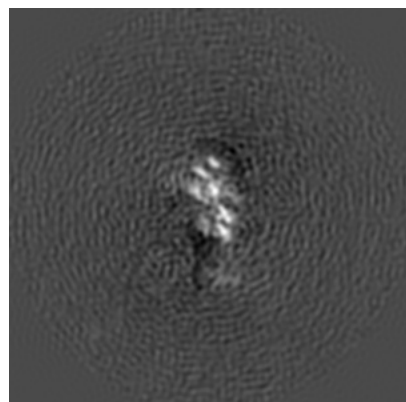


Z

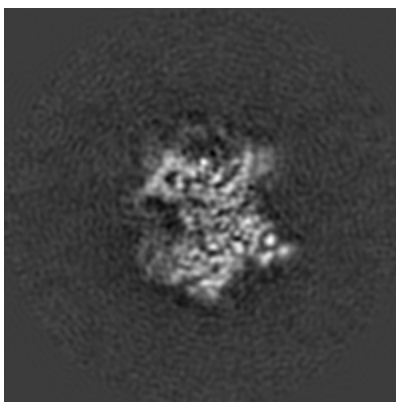
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

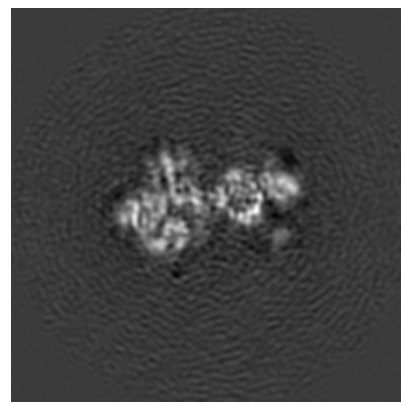
6.2.1 Primary map



X Index: 128



Y Index: 128

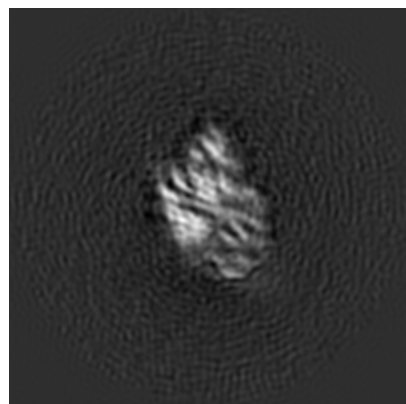


Z Index: 128

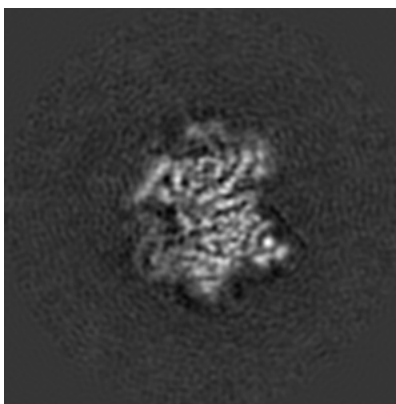
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

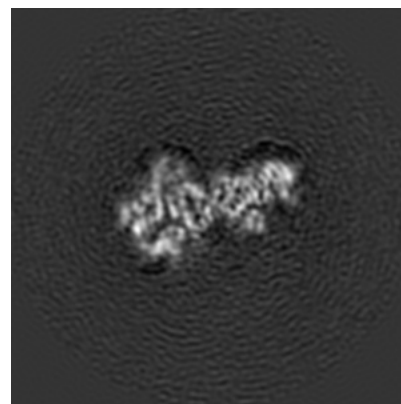
6.3.1 Primary map



X Index: 95



Y Index: 131

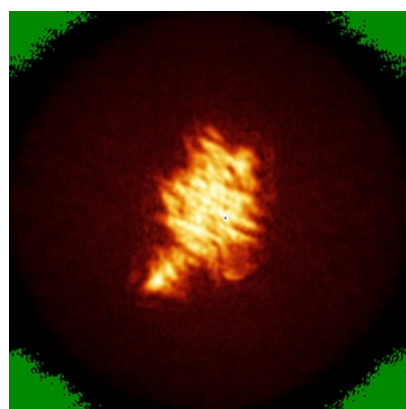


Z Index: 135

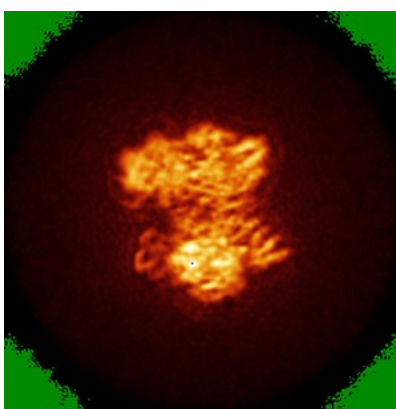
The images above show the largest variance slices of the map in three orthogonal directions.

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

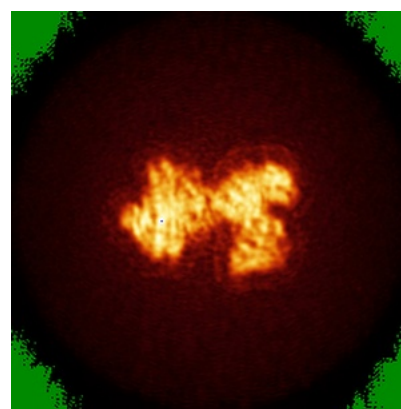
6.4.1 Primary map



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 0.0174. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

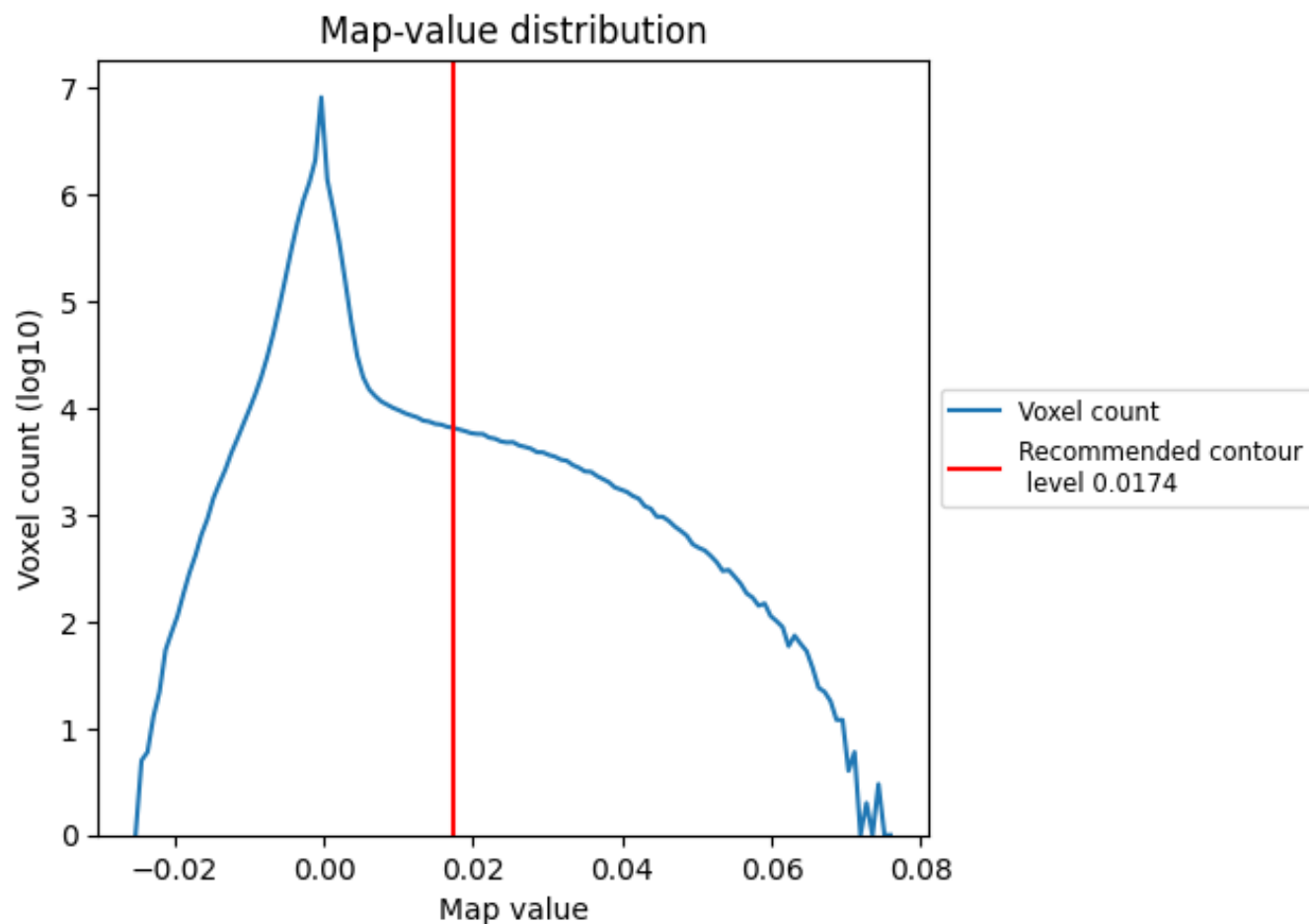
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

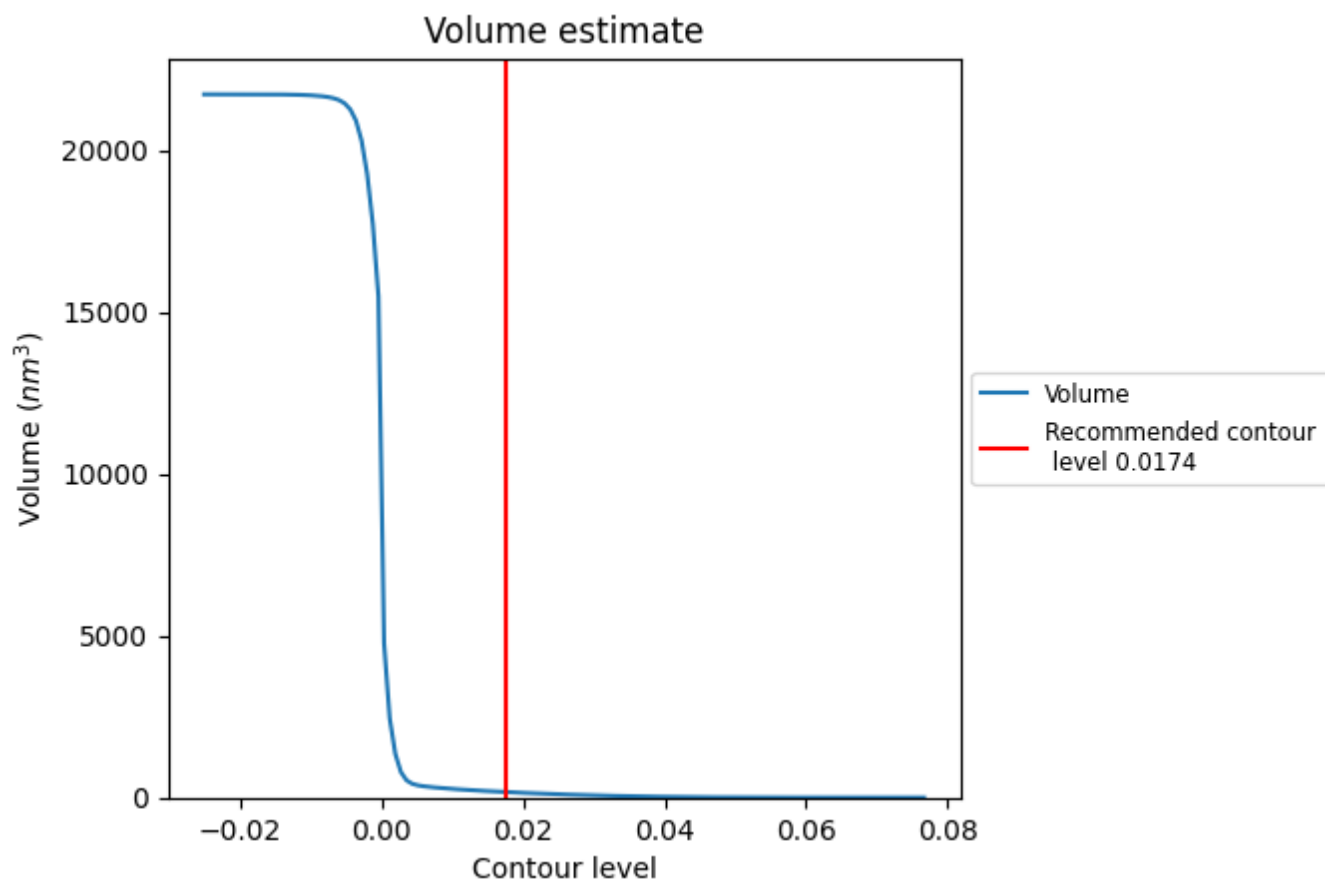
This section contains the results of statistical analysis of the map.

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.

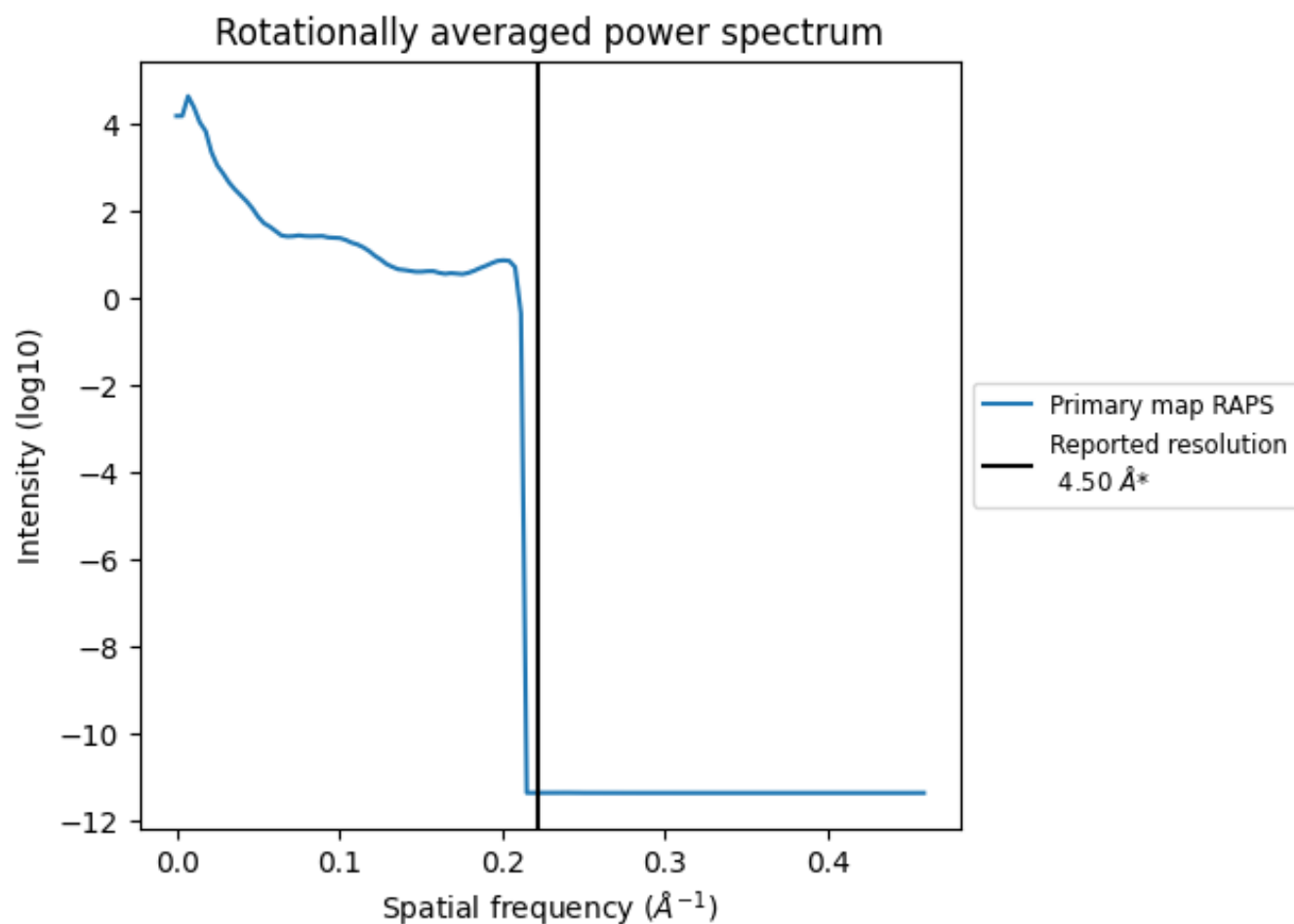
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 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 ⓘ

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

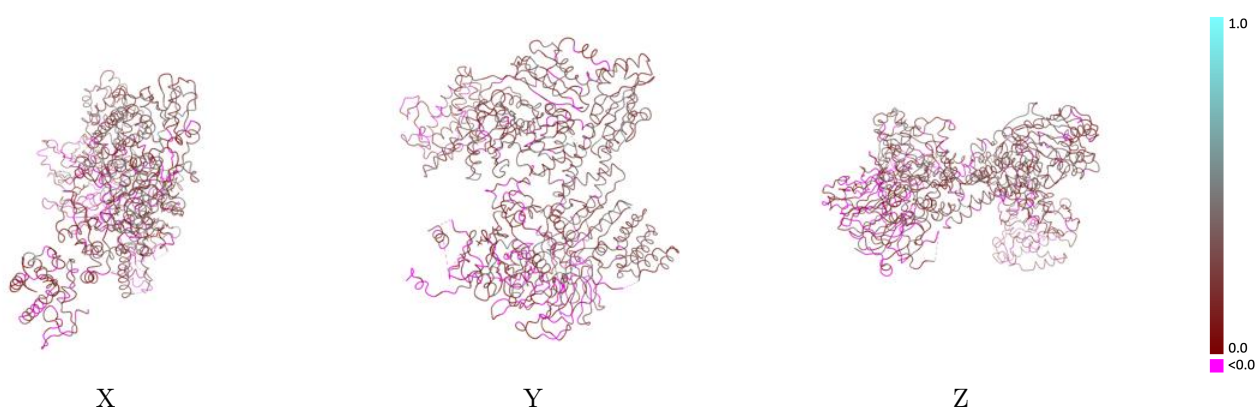
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-10960 and PDB model 6YW7. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

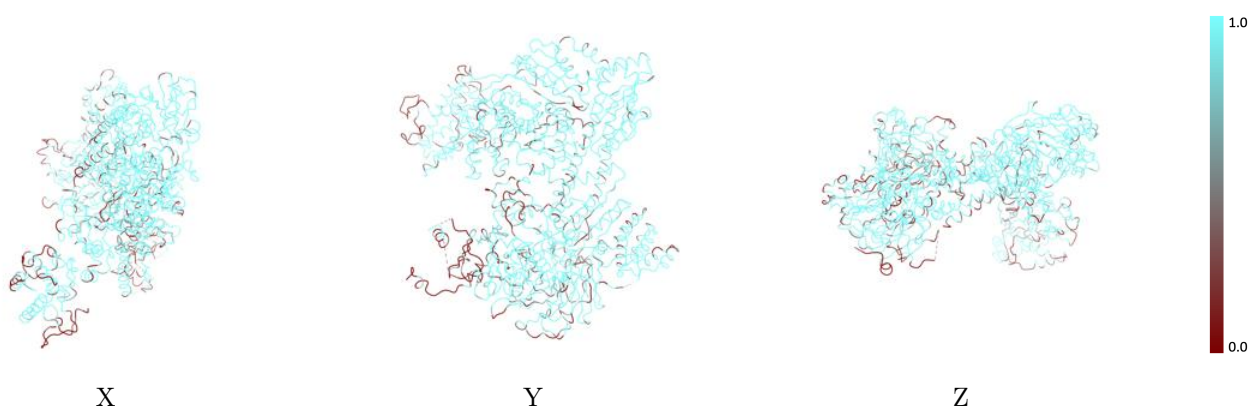
This section was not generated.

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



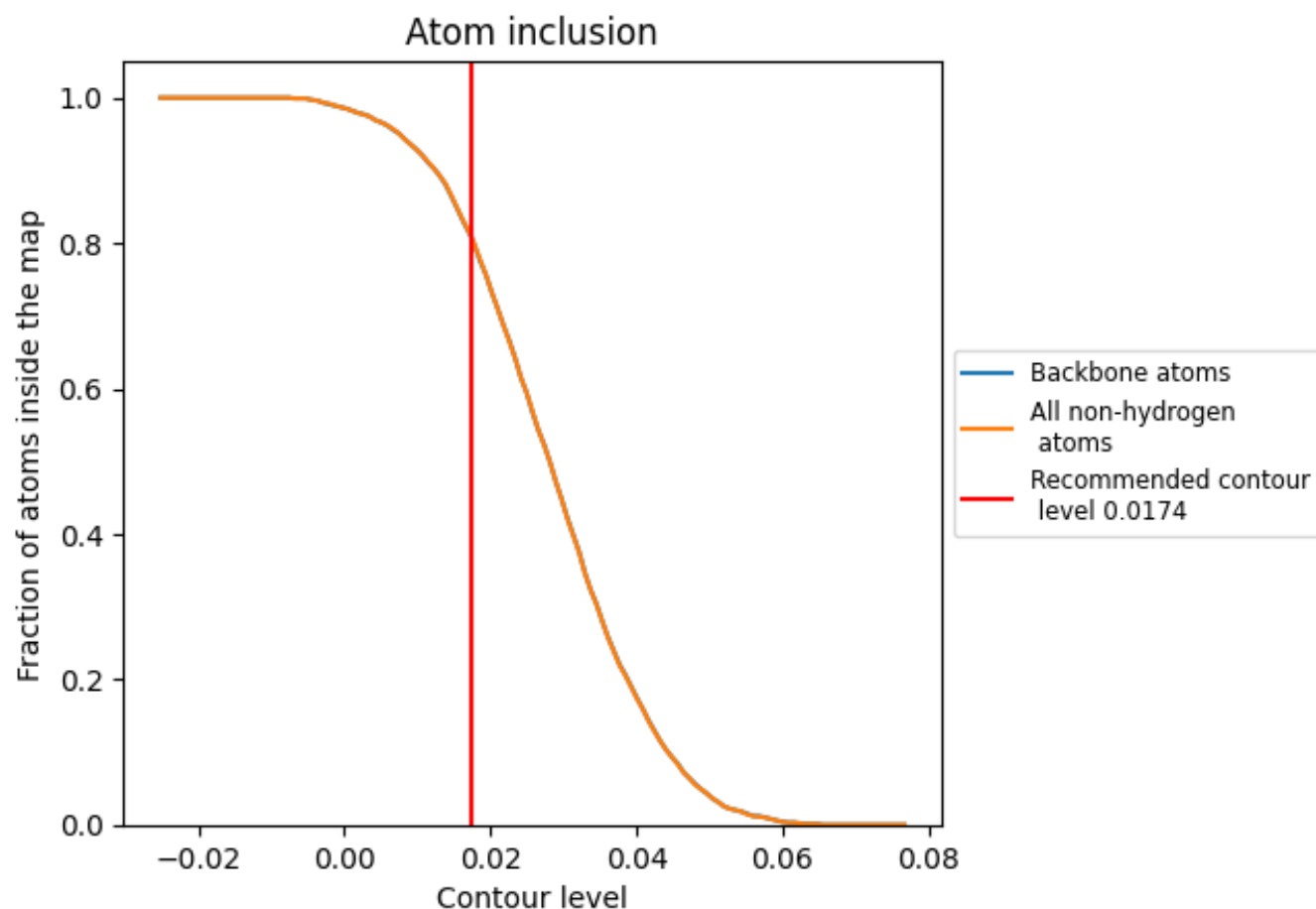
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0174).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.0174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.1940
A	0.8820	0.2390
B	0.6390	0.1590
C	0.7650	0.0670
D	0.9200	0.2640
E	0.6590	0.1330
F	0.9410	0.2880
G	0.8660	0.2700

1.0

0.0

<0.0