



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:06 PM UTC

PDB ID : 8GFT / pdb_00008gft
EMDB ID : EMD-29984
Title : Hsp90 provides platform for CRaf dephosphorylation by PP5
Authors : Jaime-Garza, M.; Nowotny, C.A.; Coutandin, D.; Wang, F.; Tabios, M.;
Agard, D.A.
Deposited on : 2023-03-08
Resolution : 3.80 Å (reported)
Based on initial models : 1S95, 5FWL, 1WAO

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

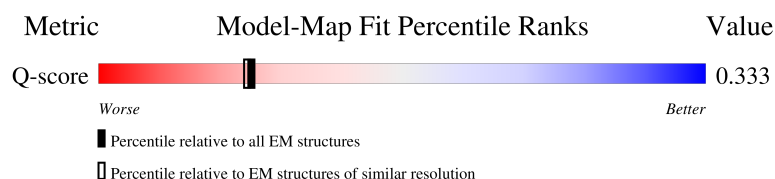
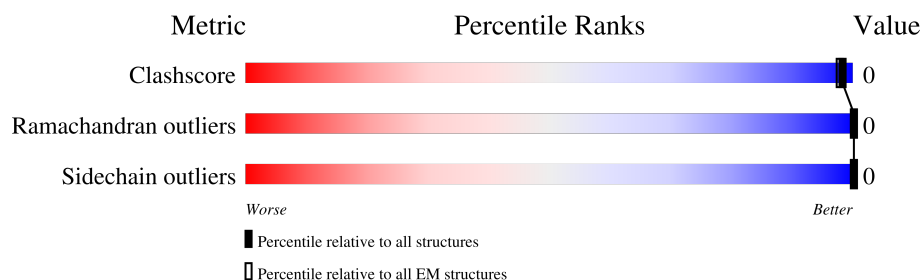
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	727	 83% • 12%
1	B	727	 83% • 13%
2	C	384	 11% 65% • 33%
3	D	304	 61% • 37%

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Mol	Chain	Length	Quality of chain
4	E	503	33% 83% 6% 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35507 atoms, of which 17710 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 Heat shock protein HSP 90-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	639	Total	C	H	N	O	S	0	0
			10411	3284	5230	871	1003	23		
1	B	633	Total	C	H	N	O	S	0	0
			10284	3249	5155	859	998	23		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P08238
A	-1	PRO	-	expression tag	UNP P08238
A	0	GLY	-	expression tag	UNP P08238
B	-1	GLY	-	expression tag	UNP P08238
B	0	PRO	-	expression tag	UNP P08238
B	1	GLY	-	expression tag	UNP P08238

- Molecule 2 is a protein called Hsp90 co-chaperone Cdc37, N-terminally processed.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	C	259	Total	C	H	N	O	P	S	0	0
			4307	1358	2125	383	425	1	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	379	LEU	-	expression tag	UNP Q16543
C	380	GLU	-	expression tag	UNP Q16543
C	381	VAL	-	expression tag	UNP Q16543
C	382	LEU	-	expression tag	UNP Q16543
C	383	PHE	-	expression tag	UNP Q16543
C	384	GLN	-	expression tag	UNP Q16543

- Molecule 3 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	191	Total	C	H	N	O	S	0	0
			3101	995	1553	262	278	13		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	334	GLY	-	expression tag	UNP P04049
D	335	GLY	-	expression tag	UNP P04049
D	619	LEU	-	expression tag	UNP P04049
D	620	PRO	-	expression tag	UNP P04049
D	621	GLU	-	expression tag	UNP P04049
D	622	SER	-	expression tag	UNP P04049
D	623	GLY	-	expression tag	UNP P04049
D	624	TRP	-	expression tag	UNP P04049
D	625	SER	-	expression tag	UNP P04049
D	626	HIS	-	expression tag	UNP P04049
D	627	PRO	-	expression tag	UNP P04049
D	628	GLN	-	expression tag	UNP P04049
D	629	PHE	-	expression tag	UNP P04049
D	630	GLU	-	expression tag	UNP P04049
D	631	LYS	-	expression tag	UNP P04049
D	632	LEU	-	expression tag	UNP P04049
D	633	GLU	-	expression tag	UNP P04049
D	634	VAL	-	expression tag	UNP P04049
D	635	LEU	-	expression tag	UNP P04049
D	636	PHE	-	expression tag	UNP P04049
D	637	GLN	-	expression tag	UNP P04049

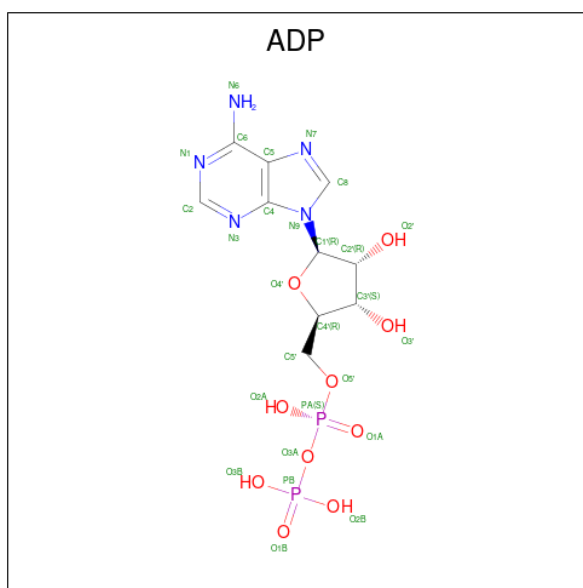
- Molecule 4 is a protein called Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	459	Total	C	H	N	O	S	0	0
			7316	2347	3623	628	699	19		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P53041
E	-2	PRO	-	expression tag	UNP P53041
E	-1	GLY	-	expression tag	UNP P53041
E	0	SER	-	expression tag	UNP P53041
E	304	ALA	HIS	engineered mutation	UNP P53041

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	P
			39	10	12	5	10	2
								0

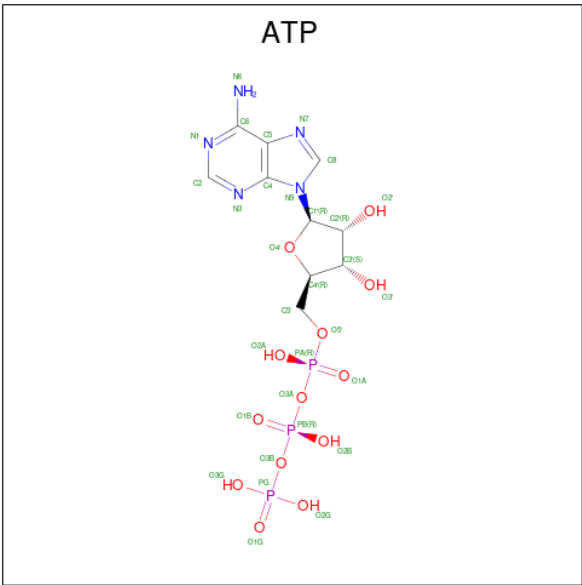
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	K	0
			1	1	
7	B	1	Total	K	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
8	B	1	43	10	12	5	13	3	0

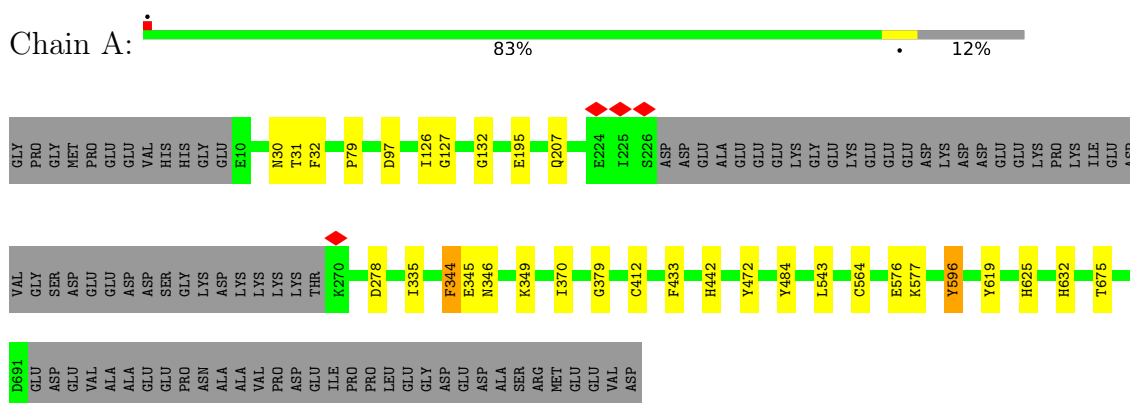
- Molecule 9 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
9	E	2	Total	Mn	0
			2	2	

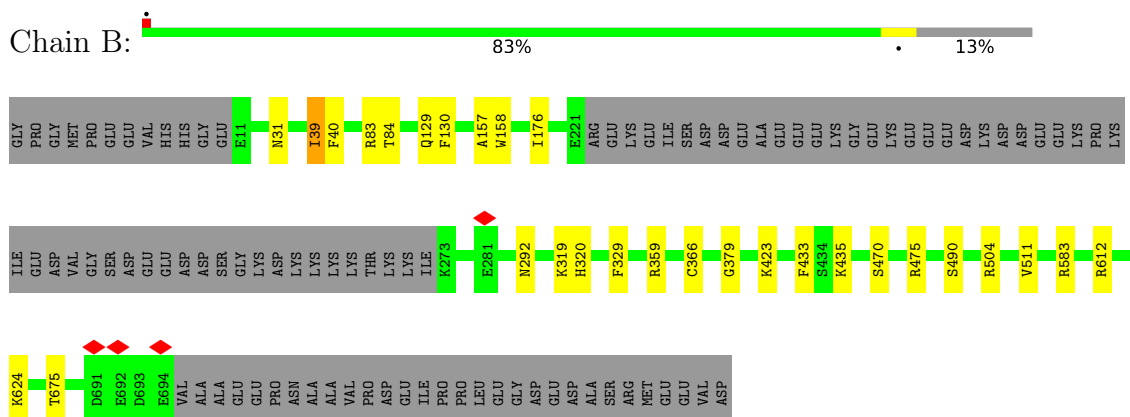
3 Residue-property plots

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.

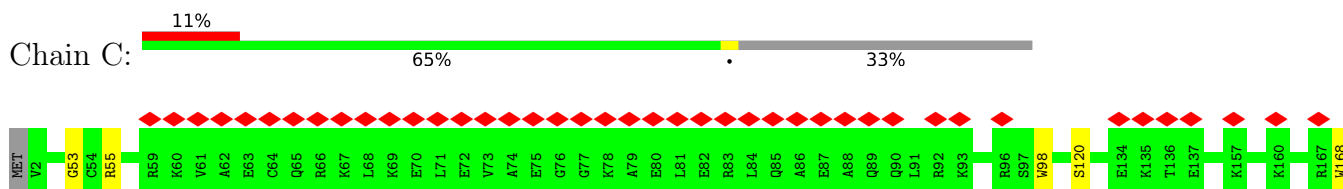
- Molecule 1: Heat shock protein HSP 90-beta



- Molecule 1: Heat shock protein HSP 90-beta



- Molecule 2: Hsp90 co-chaperone Cdc37, N-terminally processed



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	545237	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 ($e^-/\text{\AA}^2$)	69.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00576	Depositor
Map size (Å)	267.19998, 267.19998, 267.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8349999, 0.8349999, 0.8349999	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: MN, ADP, K, ATP, MG, SEP

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	0.99	4/5265 (0.1%)	1.32	35/7073 (0.5%)
1	B	0.97	9/5213 (0.2%)	1.36	34/7007 (0.5%)
2	C	0.92	2/2209 (0.1%)	1.26	6/2955 (0.2%)
3	D	0.98	1/1582 (0.1%)	1.33	9/2132 (0.4%)
4	E	1.02	9/3774 (0.2%)	1.56	52/5088 (1.0%)
All	All	0.98	25/18043 (0.1%)	1.38	136/24255 (0.6%)

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	4
1	B	0	2
4	E	0	3
All	All	0	9

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	490	SER	CB-OG	-15.92	1.10	1.42
4	E	205	HIS	CE1-NE2	-12.84	1.19	1.32
1	B	612	ARG	CZ-NH2	-11.79	1.18	1.33
1	A	127	GLY	N-CA	-9.75	1.32	1.45
2	C	189	TYR	N-CA	-8.53	1.36	1.46
4	E	205	HIS	CG-CD2	-8.49	1.26	1.35
1	B	435	LYS	C-N	-8.47	1.23	1.33
4	E	205	HIS	ND1-CE1	-8.18	1.24	1.32
4	E	101	ARG	CZ-NH2	-7.71	1.23	1.33
1	B	583	ARG	CZ-NH2	-7.34	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	TRP	N-CA	-6.95	1.37	1.46
3	D	406	LEU	C-O	-6.85	1.15	1.24
1	B	320	HIS	N-CA	-6.79	1.37	1.46
4	E	296	HIS	CB-CG	-6.78	1.40	1.50
4	E	205	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	126	ILE	C-N	-6.30	1.24	1.33
1	A	442	HIS	CB-CG	-6.20	1.41	1.50
4	E	480	PRO	C-N	-5.83	1.25	1.33
2	C	188	ASN	C-N	-5.76	1.26	1.33
1	B	612	ARG	CZ-NH1	-5.39	1.25	1.32
4	E	303	ASN	CG-ND2	-5.27	1.22	1.33
1	B	84	THR	CB-OG1	-5.16	1.35	1.43
1	A	345	GLU	C-N	-5.05	1.26	1.33
1	B	157	ALA	C-N	-5.01	1.26	1.33
4	E	402	VAL	CB-CG1	-5.01	1.36	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	402	VAL	CA-CB-CG1	16.27	138.06	110.40
1	B	435	LYS	CA-C-N	12.37	136.98	120.65
1	B	435	LYS	C-N-CA	12.37	136.98	120.65
1	B	319	LYS	CA-C-N	11.93	138.63	122.77
1	B	319	LYS	C-N-CA	11.93	138.63	122.77
1	B	157	ALA	CA-C-N	11.21	138.19	122.72
1	B	157	ALA	C-N-CA	11.21	138.19	122.72
1	A	126	ILE	CA-C-N	10.72	139.45	121.87
1	A	126	ILE	C-N-CA	10.72	139.45	121.87
4	E	402	VAL	N-CA-C	10.63	123.63	108.42
4	E	446	PHE	CA-CB-CG	10.54	124.34	113.80
2	C	188	ASN	CA-C-N	10.44	137.79	121.19
2	C	188	ASN	C-N-CA	10.44	137.79	121.19
1	A	32	PHE	CA-CB-CG	9.48	123.28	113.80
4	E	375	PRO	CA-C-N	9.35	129.78	120.52
4	E	375	PRO	C-N-CA	9.35	129.78	120.52
4	E	190	PHE	CA-CB-CG	-9.12	104.68	113.80
1	A	127	GLY	N-CA-C	8.64	123.88	112.65
3	D	508	SER	N-CA-C	-8.53	102.07	111.36
1	A	127	GLY	CA-C-N	8.24	134.54	121.44
1	A	127	GLY	C-N-CA	8.24	134.54	121.44
1	B	319	LYS	O-C-N	-8.19	113.77	123.27
1	A	79	PRO	CA-C-N	7.93	131.55	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	PRO	C-N-CA	7.93	131.55	120.29
4	E	303	ASN	OD1-CG-ND2	-7.91	114.69	122.60
4	E	303	ASN	CA-CB-CG	7.90	120.50	112.60
1	B	435	LYS	O-C-N	-7.72	113.93	122.12
4	E	393	ASN	N-CA-C	7.41	119.00	111.07
1	B	366	CYS	CA-CB-SG	-7.39	97.41	114.40
4	E	473	PHE	N-CA-C	7.37	121.14	109.50
3	D	596	ARG	CA-C-N	7.03	126.99	120.03
3	D	596	ARG	C-N-CA	7.03	126.99	120.03
2	C	188	ASN	O-C-N	-6.98	114.72	122.12
4	E	112	PHE	N-CA-C	6.98	118.97	111.36
4	E	406	PHE	N-CA-C	6.87	119.77	108.99
4	E	304	ALA	CA-C-N	6.84	134.55	123.33
4	E	304	ALA	C-N-CA	6.84	134.55	123.33
4	E	480	PRO	CA-C-N	6.66	133.69	121.70
4	E	480	PRO	C-N-CA	6.66	133.69	121.70
1	A	132	GLY	N-CA-C	6.64	122.19	114.16
1	B	83	ARG	CA-C-N	6.58	133.15	122.81
1	B	83	ARG	C-N-CA	6.58	133.15	122.81
1	B	624	LYS	CA-C-N	6.45	132.28	122.93
1	B	624	LYS	C-N-CA	6.45	132.28	122.93
4	E	100	TYR	O-C-N	-6.40	115.48	122.07
1	B	129	GLN	N-CA-C	6.39	118.25	111.28
1	A	335	ILE	CA-C-N	6.35	126.31	120.03
1	A	335	ILE	C-N-CA	6.35	126.31	120.03
4	E	293	TYR	CA-C-N	6.33	125.95	119.56
4	E	293	TYR	C-N-CA	6.33	125.95	119.56
4	E	379	GLY	CA-C-N	6.26	126.46	119.32
4	E	379	GLY	C-N-CA	6.26	126.46	119.32
4	E	446	PHE	N-CA-C	6.25	118.57	109.07
4	E	480	PRO	N-CA-C	-6.23	102.10	111.57
1	B	511	VAL	O-C-N	-6.09	116.04	122.67
1	A	576	GLU	CB-CG-CD	5.99	122.78	112.60
1	B	31	ASN	N-CA-C	5.91	120.77	113.50
2	C	120	SER	N-CA-C	5.90	117.21	108.60
1	B	157	ALA	O-C-N	-5.85	116.38	123.29
1	A	349	LYS	N-CA-C	5.78	119.40	111.54
1	A	278	ASP	CA-CB-CG	5.77	118.37	112.60
4	E	259	LEU	CA-C-N	5.77	127.05	119.84
4	E	259	LEU	C-N-CA	5.77	127.05	119.84
4	E	281	GLU	CA-C-N	5.74	127.88	120.70
4	E	281	GLU	C-N-CA	5.74	127.88	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	306	THR	CA-CB-CG2	5.74	120.26	110.50
4	E	352	HIS	CA-CB-CG	-5.72	108.08	113.80
4	E	398	SER	N-CA-C	5.72	118.00	109.59
1	B	176	ILE	N-CA-C	-5.72	100.16	108.17
2	C	189	TYR	N-CA-CB	5.68	119.38	109.72
4	E	205	HIS	CB-CG-CD2	-5.68	123.81	131.20
4	E	381	MET	O-C-N	-5.68	115.28	122.27
4	E	352	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	B	511	VAL	CA-C-N	5.67	130.22	122.84
1	B	511	VAL	C-N-CA	5.67	130.22	122.84
4	E	109	LEU	N-CA-C	5.62	119.84	112.92
4	E	401	GLY	CA-C-N	5.62	130.32	122.23
4	E	401	GLY	C-N-CA	5.62	130.32	122.23
4	E	304	ALA	O-C-N	-5.49	115.11	122.19
1	A	596	TYR	CA-CB-CG	5.45	123.70	113.90
1	A	543	LEU	N-CA-C	-5.43	102.58	110.08
1	A	126	ILE	O-C-N	-5.43	115.80	122.97
3	D	466	HIS	CB-CG-CD2	-5.40	124.18	131.20
4	E	428	GLU	CA-C-N	5.39	127.79	120.63
4	E	428	GLU	C-N-CA	5.39	127.79	120.63
3	D	406	LEU	CA-C-N	5.38	129.11	121.42
3	D	406	LEU	C-N-CA	5.38	129.11	121.42
4	E	411	THR	CA-CB-CG2	5.37	119.62	110.50
1	A	675	THR	N-CA-C	-5.37	105.09	111.69
1	B	470	SER	CA-C-N	5.36	129.75	120.58
1	B	470	SER	C-N-CA	5.36	129.75	120.58
1	B	292	ASN	CA-C-N	5.34	125.16	119.28
1	B	292	ASN	C-N-CA	5.34	125.16	119.28
4	E	251	LEU	N-CA-C	-5.34	105.35	111.07
1	A	564	CYS	CA-C-N	5.32	127.41	120.28
1	A	564	CYS	C-N-CA	5.32	127.41	120.28
1	B	423	LYS	CA-C-N	5.32	127.35	120.44
1	B	423	LYS	C-N-CA	5.32	127.35	120.44
1	B	359	ARG	N-CA-C	5.31	119.71	113.23
1	A	412	CYS	CA-CB-SG	-5.31	102.19	114.40
1	A	97	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	195	GLU	CB-CG-CD	5.27	121.56	112.60
3	D	569	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	346	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	632	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	A	472	TYR	N-CA-C	-5.22	105.49	111.07
1	A	207	GLN	OE1-CD-NE2	-5.22	117.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	310	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	379	GLY	N-CA-C	5.21	118.18	110.42
3	D	529	SER	N-CA-C	-5.19	105.70	111.36
1	A	30	ASN	N-CA-C	5.19	119.88	113.50
1	A	433	PHE	N-CA-C	5.18	119.15	112.41
3	D	447	ASP	CA-CB-CG	-5.18	107.42	112.60
4	E	404	CYS	CA-C-N	5.17	130.70	121.75
4	E	404	CYS	C-N-CA	5.17	130.70	121.75
4	E	451	TYR	CA-CB-CG	5.17	123.20	113.90
1	A	31	THR	O-C-N	-5.16	116.00	122.35
4	E	402	VAL	CB-CA-C	-5.16	101.89	111.18
1	B	130	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	379	GLY	N-CA-C	5.10	118.19	110.75
1	A	127	GLY	CA-C-O	-5.09	117.65	122.39
4	E	133	LYS	CA-C-O	-5.09	114.12	119.97
1	A	344	PHE	O-C-N	-5.08	115.50	122.46
1	B	433	PHE	N-CA-C	5.08	119.02	112.41
4	E	278	PHE	CA-C-N	5.07	127.49	120.29
4	E	278	PHE	C-N-CA	5.07	127.49	120.29
1	A	370	ILE	CA-C-N	5.07	125.00	119.78
1	A	370	ILE	C-N-CA	5.07	125.00	119.78
1	B	329	PHE	CA-CB-CG	5.07	118.87	113.80
4	E	252	ASN	CA-C-N	-5.05	112.02	120.30
4	E	252	ASN	C-N-CA	-5.05	112.02	120.30
1	B	39	ILE	CA-C-N	-5.03	113.04	120.28
1	B	39	ILE	C-N-CA	-5.03	113.04	120.28
2	C	55	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	B	675	THR	N-CA-C	-5.01	105.89	111.36
4	E	451	TYR	O-C-N	-5.01	116.88	122.09

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	PHE	Mainchain
1	A	484	TYR	Sidechain
1	A	596	TYR	Sidechain
1	A	619	TYR	Sidechain
1	B	475	ARG	Sidechain
1	B	504	ARG	Sidechain
4	E	101	ARG	Sidechain
4	E	446	PHE	Sidechain

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Mol	Chain	Res	Type	Group
4	E	451	TYR	Sidechain

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	5181	5230	5227	1	0
1	B	5129	5155	5153	2	0
2	C	2182	2125	2124	2	0
3	D	1548	1553	1551	0	0
4	E	3693	3623	3622	7	0
5	A	27	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	31	12	12	0	0
9	E	2	0	0	0	0
All	All	17797	17710	17701	12	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 0.

All (12) 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)
4:E:382:CYS:HB3	4:E:401:GLY:O	1.98	0.62
4:E:399:LYS:O	4:E:402:VAL:HB	2.01	0.60
4:E:382:CYS:CB	4:E:401:GLY:O	2.57	0.52
4:E:429:VAL:O	4:E:429:VAL:HG23	2.13	0.48
4:E:408:PRO:O	4:E:411:THR:HG22	2.14	0.47
4:E:377:ASP:HA	4:E:401:GLY:C	2.40	0.47
1:B:40:PHE:CD2	1:B:40:PHE:C	2.92	0.46
2:C:168:TRP:CZ3	2:C:238:PHE:CD2	3.05	0.44
2:C:53:GLY:HA3	2:C:98:TRP:CH2	2.54	0.43
4:E:375:PRO:HB2	4:E:382:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LYS:HE2	1:A:625:HIS:CE1	2.54	0.43
1:B:39:ILE:O	1:B:40:PHE:C	2.61	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	635/727 (87%)	632 (100%)	3 (0%)	0	100	100
1	B	629/727 (86%)	622 (99%)	7 (1%)	0	100	100
2	C	256/384 (67%)	249 (97%)	7 (3%)	0	100	100
3	D	187/304 (62%)	181 (97%)	6 (3%)	0	100	100
4	E	457/503 (91%)	446 (98%)	11 (2%)	0	100	100
All	All	2164/2645 (82%)	2130 (98%)	34 (2%)	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	A	578/653 (88%)	578 (100%)	0	100	100
1	B	572/653 (88%)	572 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	238/346 (69%)	238 (100%)	0	100	100
3	D	172/271 (64%)	172 (100%)	0	100	100
4	E	397/431 (92%)	397 (100%)	0	100	100
All	All	1957/2354 (83%)	1957 (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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	396	GLN
1	A	436	ASN
1	A	609	GLN
1	A	614	ASN
1	B	190	GLN
1	B	279	GLN
1	B	436	ASN
2	C	22	ASN
2	C	89	GLN
2	C	90	GLN
2	C	172	GLN
2	C	211	HIS
3	D	422	GLN
3	D	454	GLN
3	D	477	HIS
4	E	211	GLN
4	E	264	ASN
4	E	310	ASN
4	E	374	GLN
4	E	463	HIS
4	E	465	GLN
4	E	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	SEP	C	13	2	8,9,10	1.07	0	7,12,14	1.15	0

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
2	SEP	C	13	2	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	13	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	ATP	B	802	6	32,33,33	2.08	4 (12%)	48,52,52	1.24	6 (12%)
5	ADP	A	801	6	28,29,29	1.19	2 (7%)	43,45,45	1.24	7 (16%)

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	802	6	-	3/22/38/38	0/3/3/3
5	ADP	A	801	6	-	0/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	802	ATP	PA-O3A	-7.36	1.51	1.59
8	B	802	ATP	PB-O3A	-6.34	1.52	1.59
5	A	801	ADP	PA-O3A	-3.74	1.55	1.59
8	B	802	ATP	C5-C4	-2.39	1.34	1.39
8	B	802	ATP	PB-O3B	-2.37	1.56	1.59
5	A	801	ADP	C5-C4	-2.22	1.35	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	802	ATP	C4-C5-N7	3.05	114.06	110.58
5	A	801	ADP	O2A-PA-O3A	3.00	115.37	107.27
5	A	801	ADP	C4-C5-N7	2.87	113.86	110.58
8	B	802	ATP	O2B-PB-O3B	2.86	115.01	107.27
5	A	801	ADP	C5-C4-N3	-2.79	122.87	126.72
8	B	802	ATP	O2A-PA-O3A	2.52	114.07	107.27
8	B	802	ATP	C5-C4-N3	-2.24	123.63	126.72
5	A	801	ADP	C2-N1-C6	-2.21	115.10	118.73
8	B	802	ATP	C5-C6-N1	2.19	123.07	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	ADP	C5-C6-N1	2.12	122.89	117.51
5	A	801	ADP	O2B-PB-O3A	2.03	111.45	104.64
5	A	801	ADP	N3-C4-N9	2.02	130.61	127.17
8	B	802	ATP	N6-C6-N1	-2.00	113.91	118.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

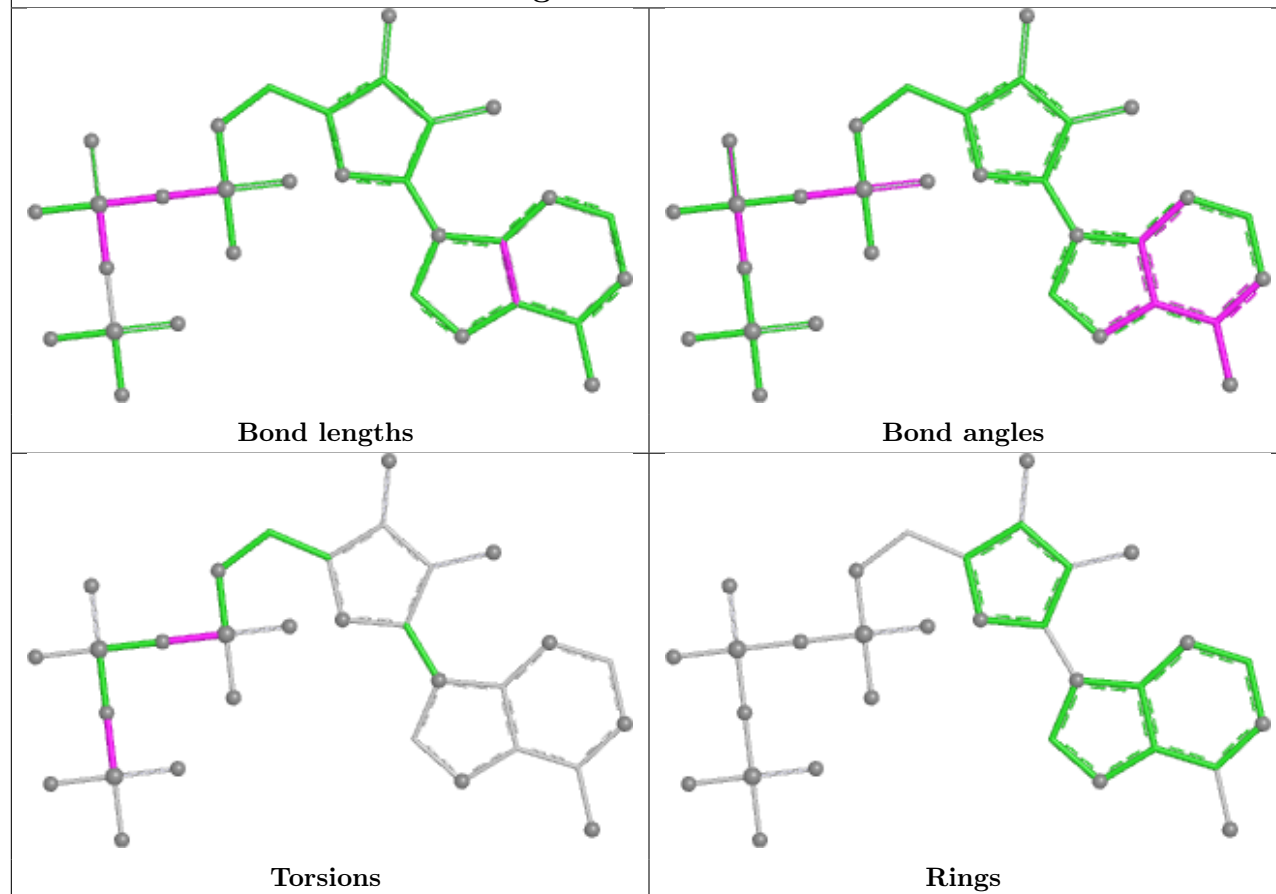
Mol	Chain	Res	Type	Atoms
8	B	802	ATP	PB-O3B-PG-O3G
8	B	802	ATP	PB-O3B-PG-O1G
8	B	802	ATP	PB-O3A-PA-O5'

There are no ring outliers.

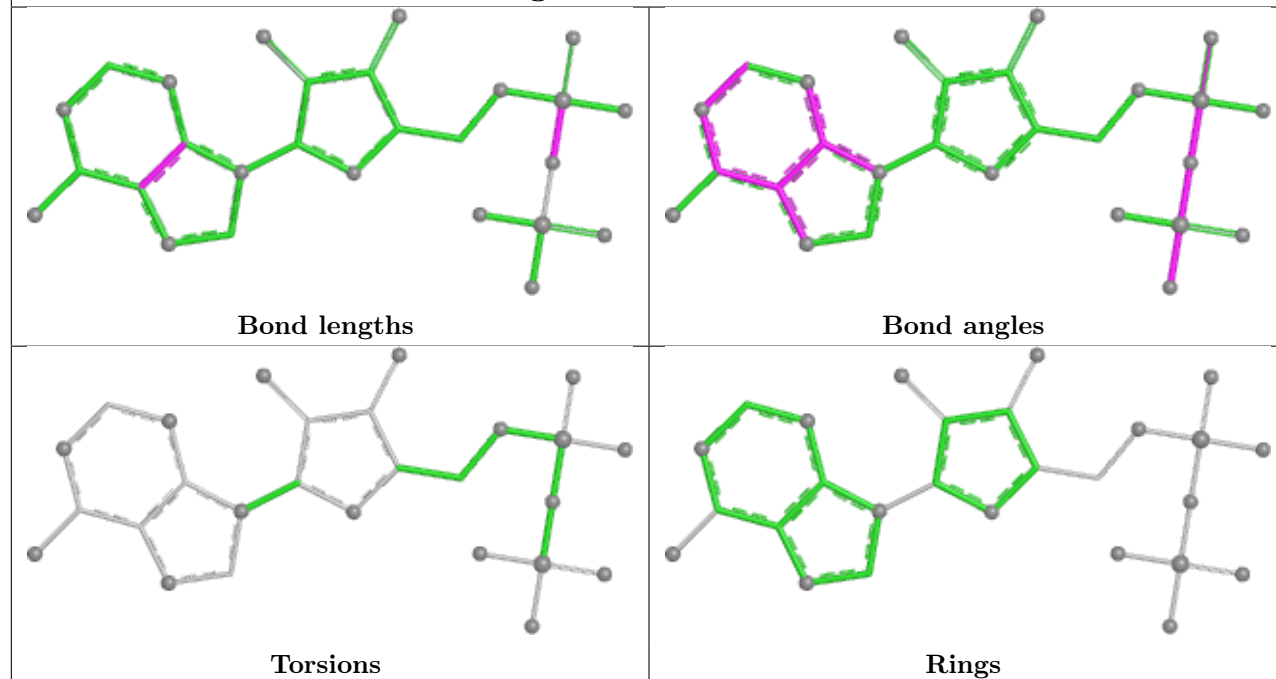
No monomer is involved in short contacts.

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.

Ligand ATP B 802



Ligand ADP A 801



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

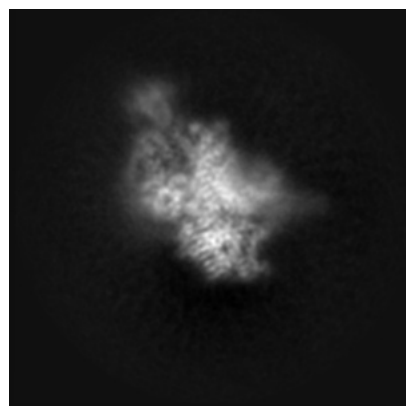
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29984. These allow visual inspection of the internal detail of the map and identification of artifacts.

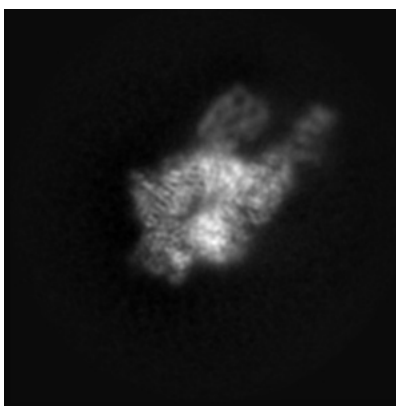
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

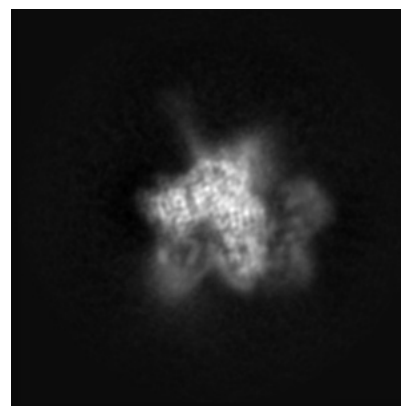
6.1.1 Primary map



X

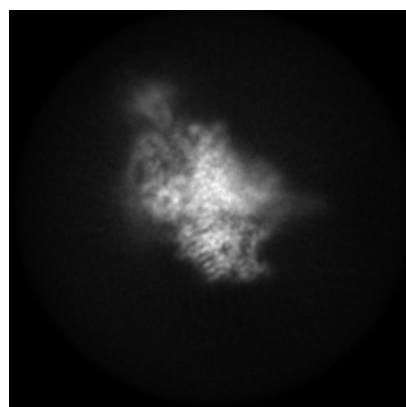


Y

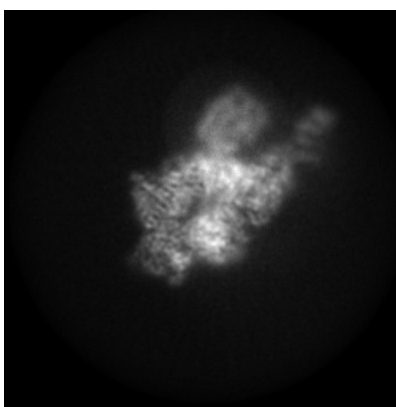


Z

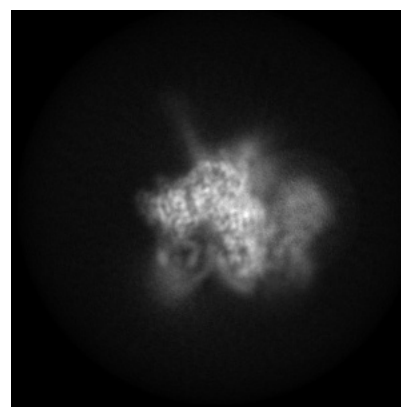
6.1.2 Raw map



X



Y

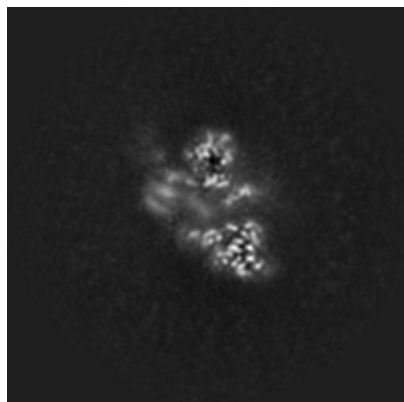


Z

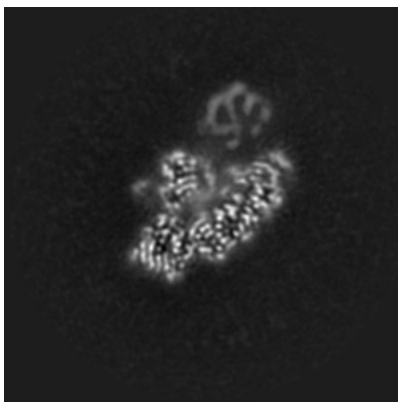
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

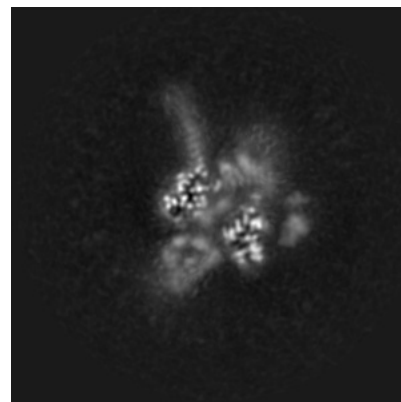
6.2.1 Primary map



X Index: 160

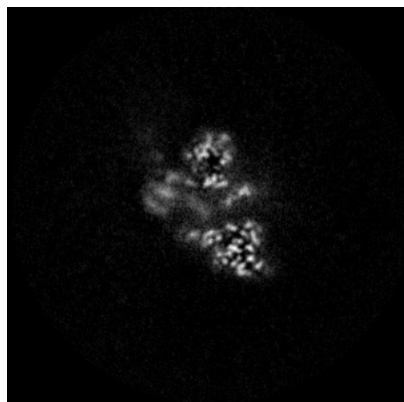


Y Index: 160

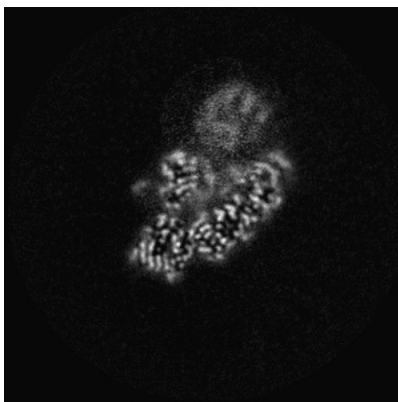


Z Index: 160

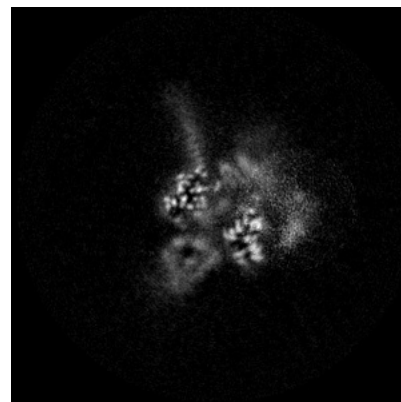
6.2.2 Raw map



X Index: 160



Y Index: 160

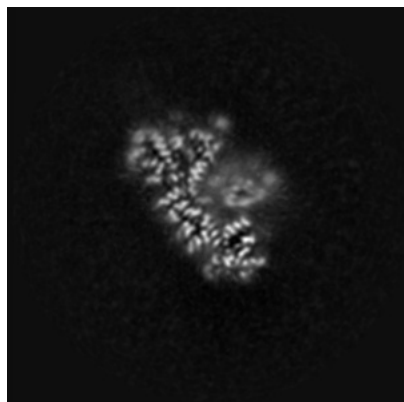


Z Index: 160

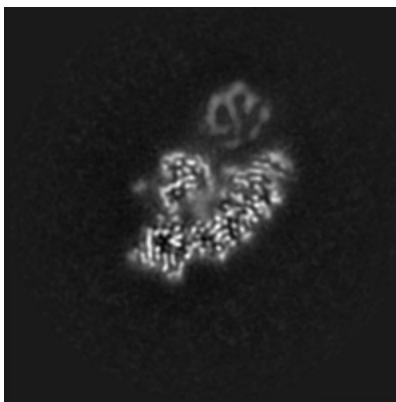
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

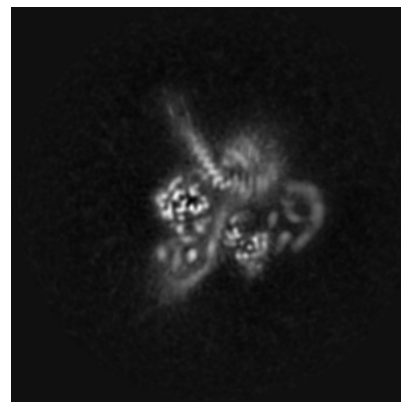
6.3.1 Primary map



X Index: 177

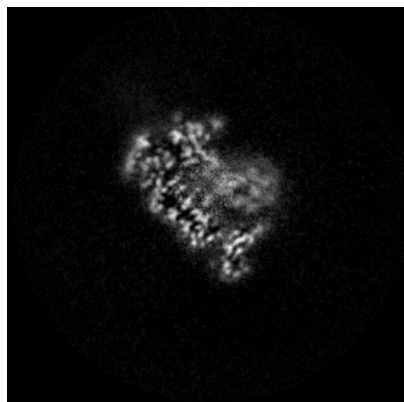


Y Index: 158

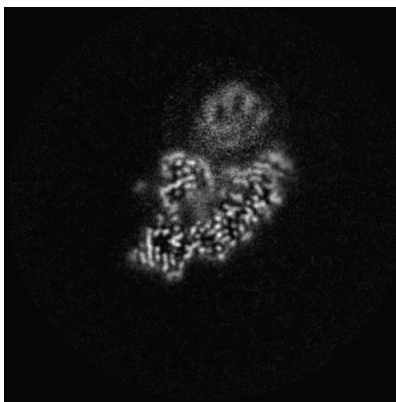


Z Index: 171

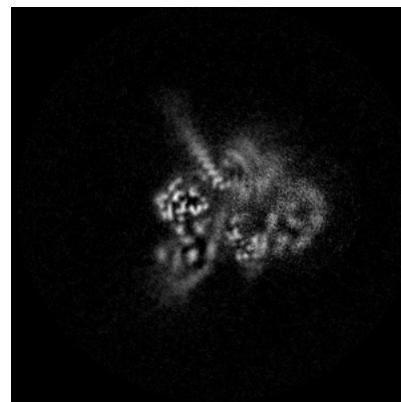
6.3.2 Raw map



X Index: 183



Y Index: 158

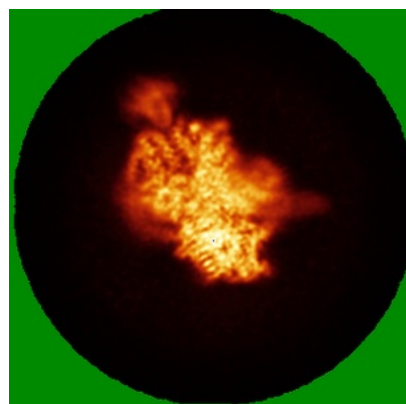


Z Index: 171

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

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

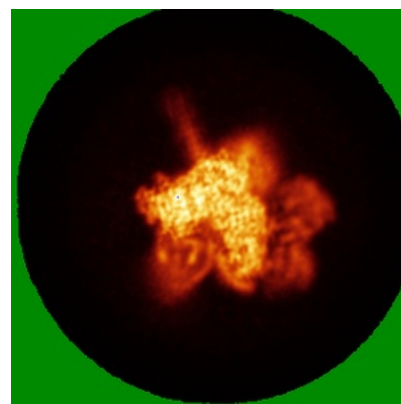
6.4.1 Primary map



X

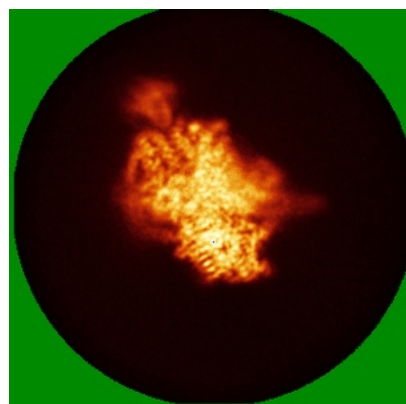


Y



Z

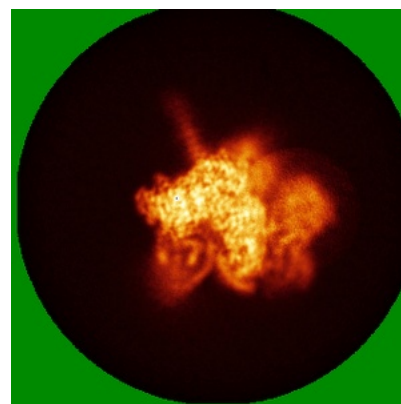
6.4.2 Raw map



X



Y

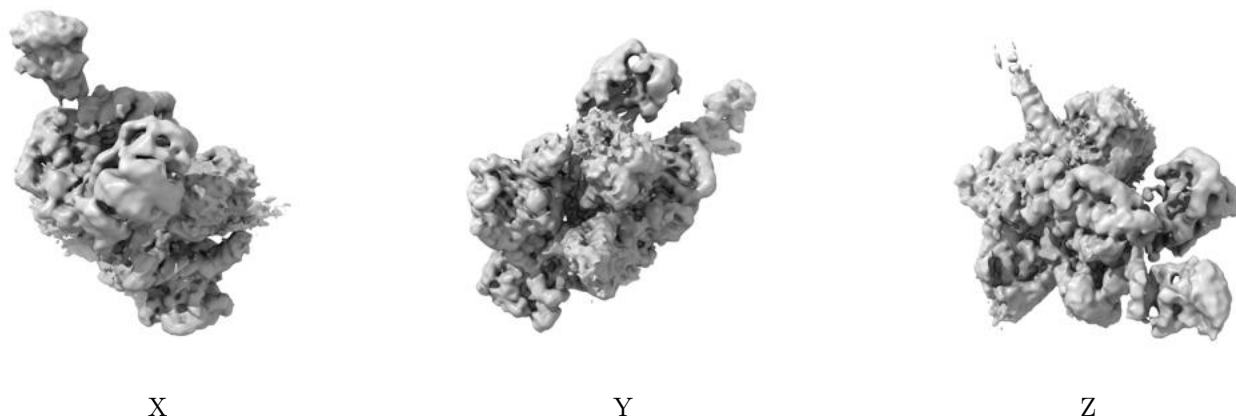


Z

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.

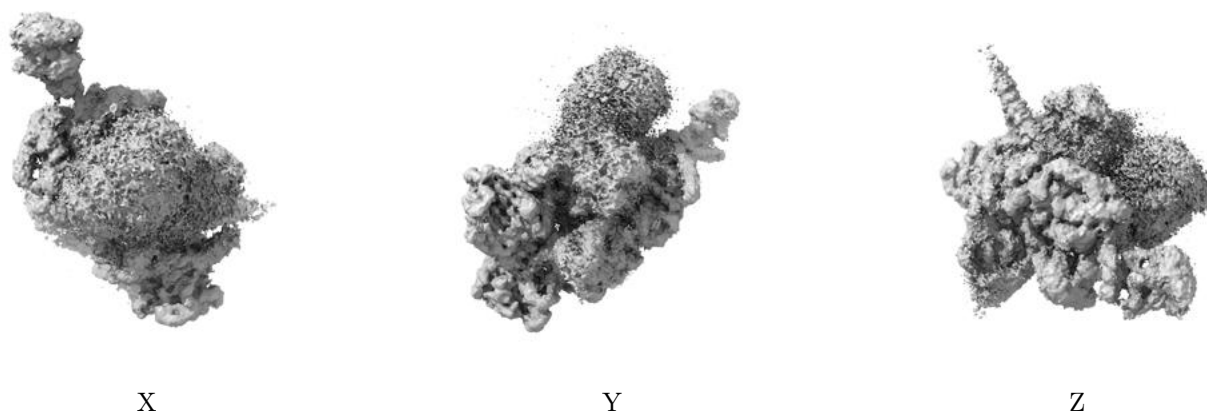
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00576. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

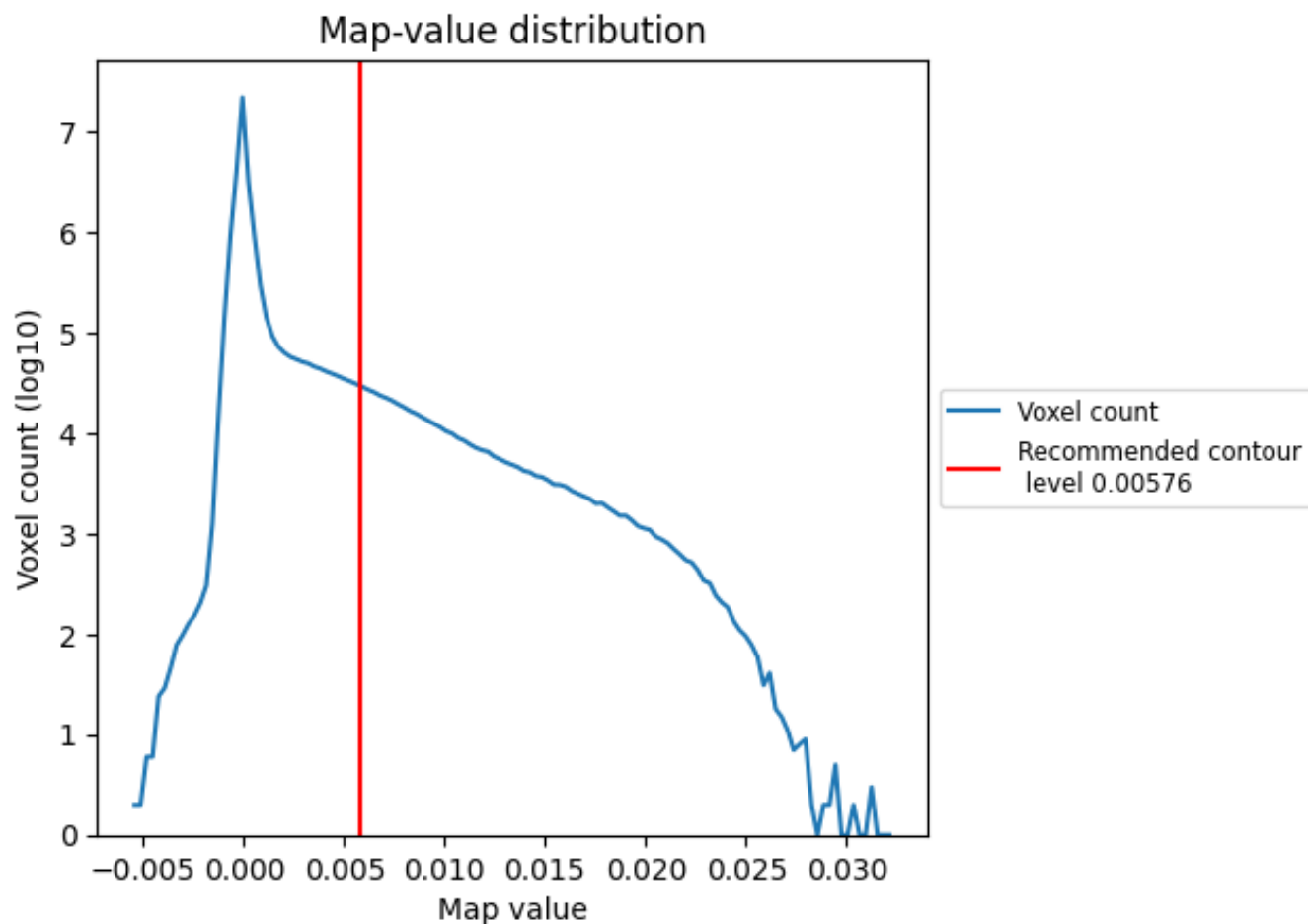
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

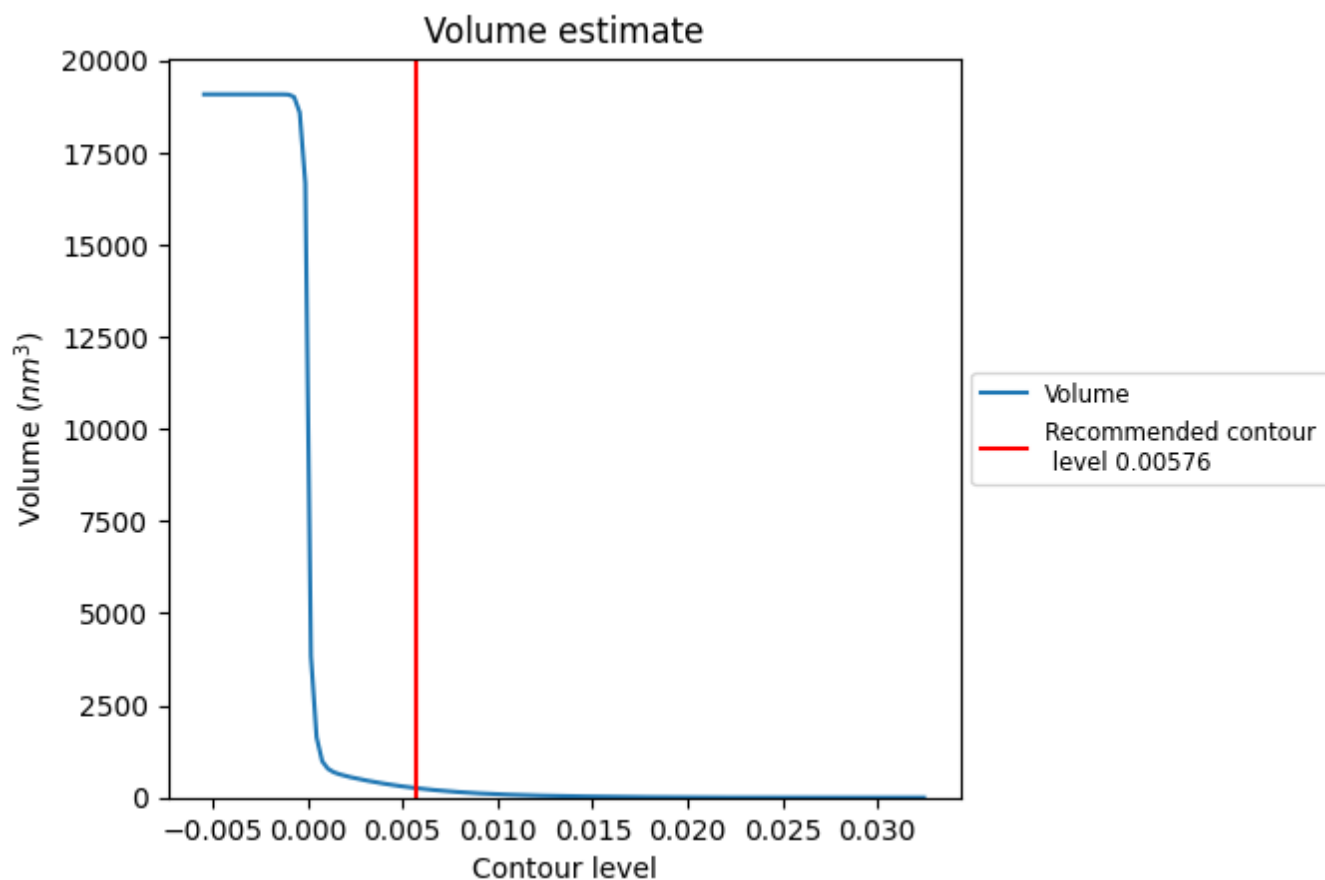
This section contains the results of statistical analysis of the map.

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.

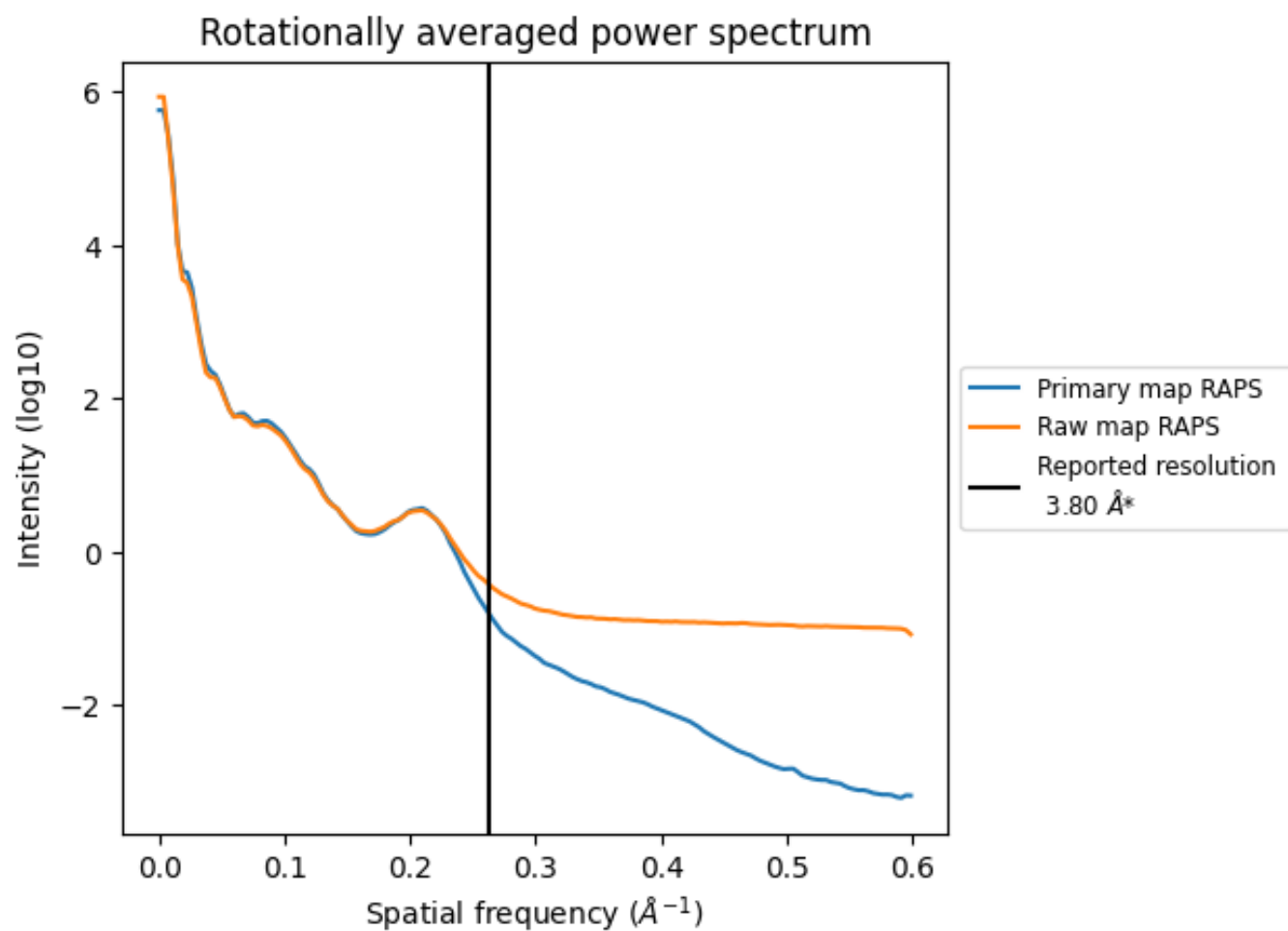
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm^3 ; this corresponds to an approximate mass of 230 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 ⓘ

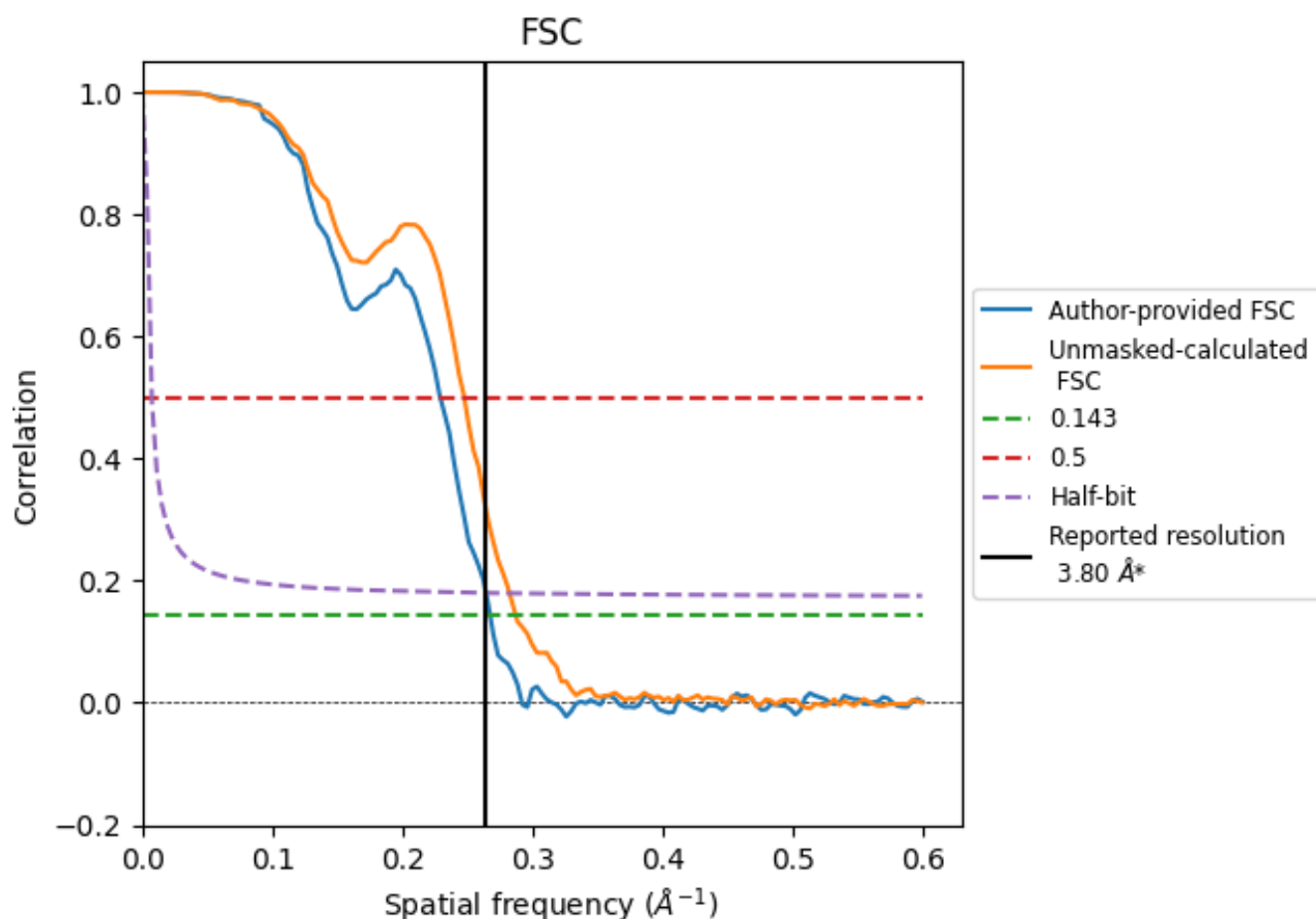


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

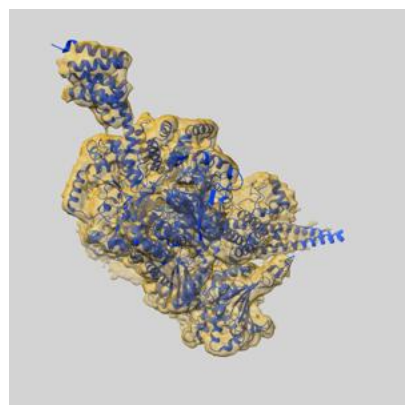
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.74	4.37	3.79
Unmasked-calculated*	3.49	4.04	3.55

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

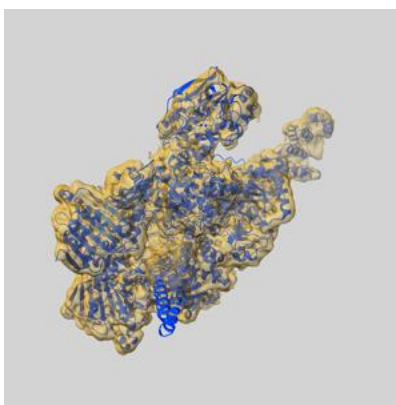
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29984 and PDB model 8GFT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

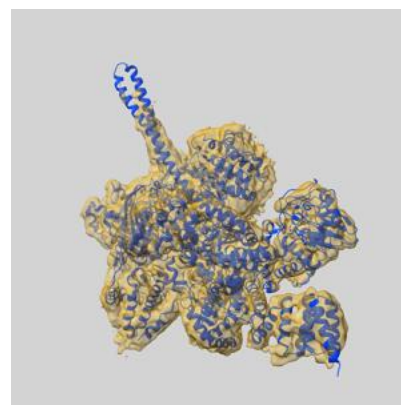
9.1 Map-model overlay [i](#)



X



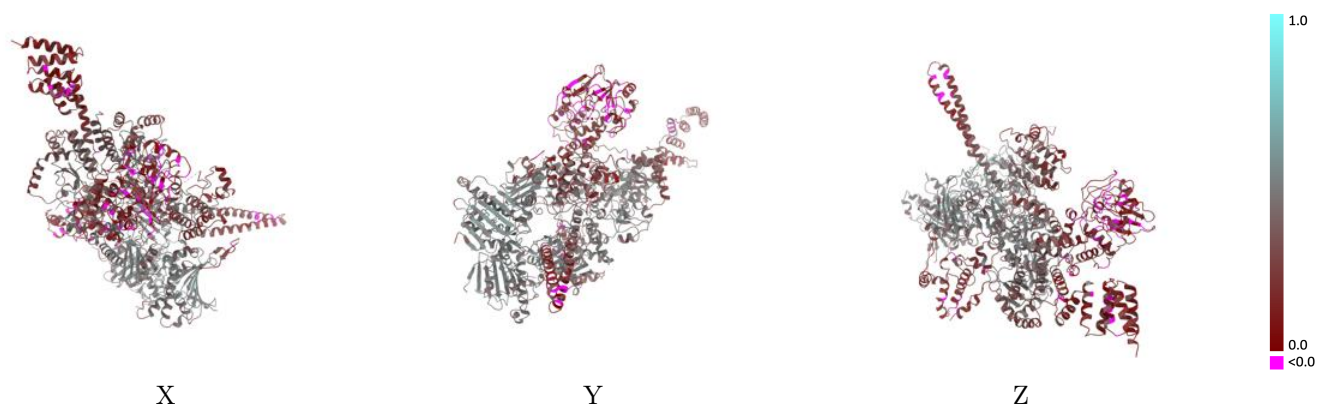
Y



Z

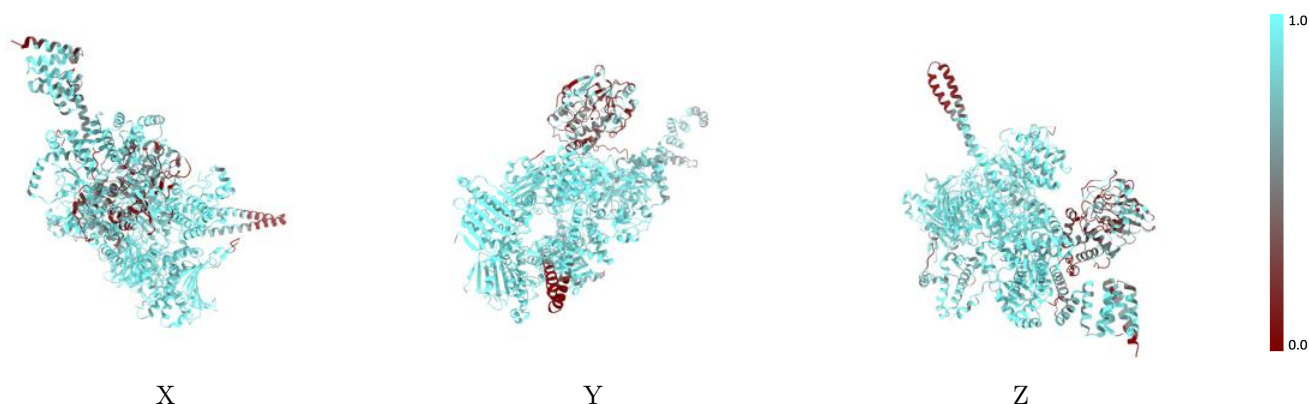
The images above show the 3D surface view of the map at the recommended contour level 0.00576 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



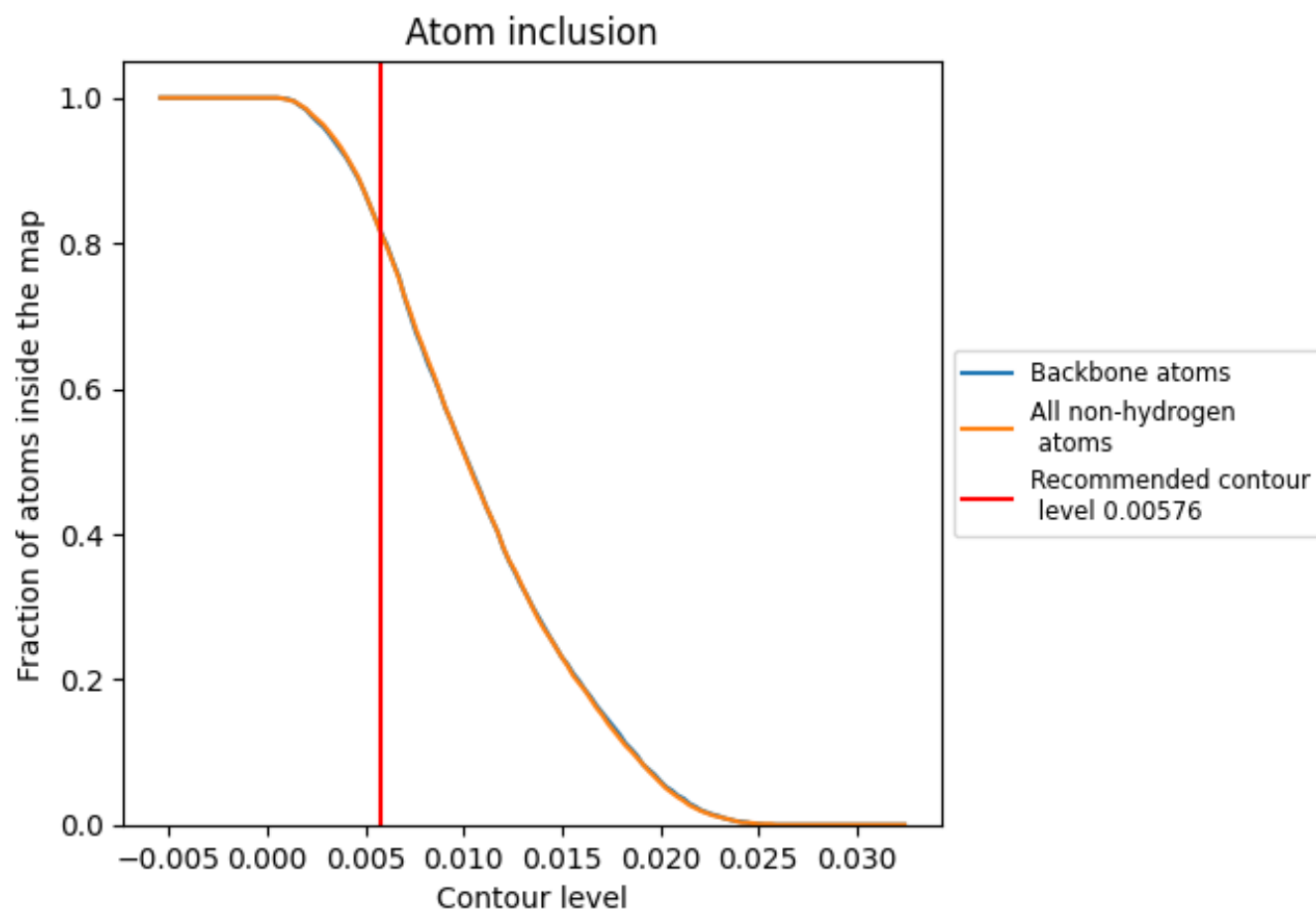
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00576).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00576) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.3330
A	0.9350	0.4280
B	0.9320	0.4350
C	0.7330	0.2300
D	0.9570	0.2810
E	0.5080	0.1410

