



## Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 09:43 pm BST

PDB ID : 7OIM  
EMDB ID : EMD-12932  
Title : Mouse RNF213, with mixed nucleotides bound  
Authors : Grabarczyk, D.; Ahel, J.; Clausen, T.  
Deposited on : 2021-05-11  
Resolution : 4.00 Å(reported)  
Based on initial model : 6TAX

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

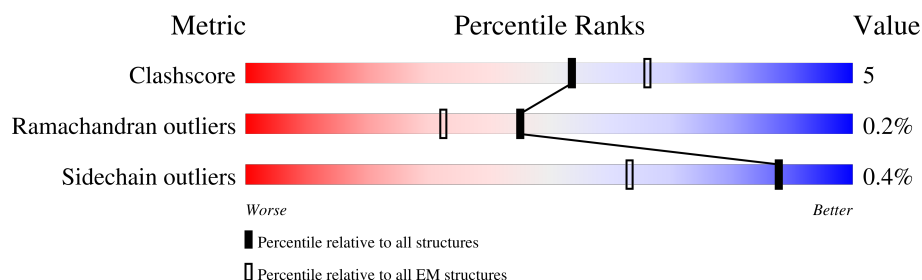
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	4836	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35597 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4426	Total	C	N	O	S	0	0
			35505	22641	6093	6561	210		

There are 30 discrepancies between the modelled and reference sequences:

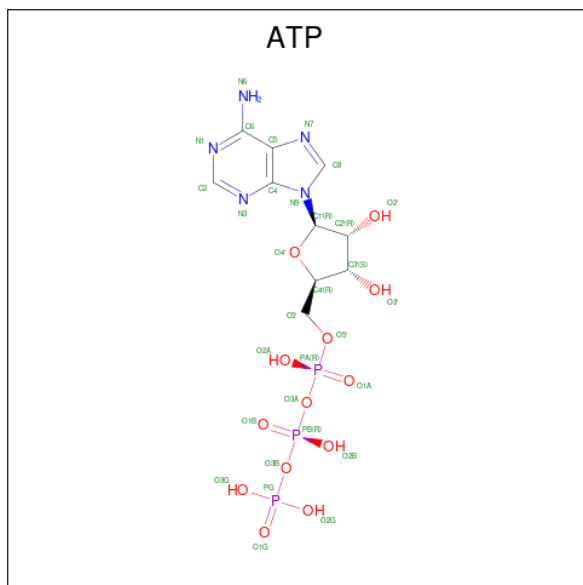
Chain	Residue	Modelled	Actual	Comment	Reference
A	326	MET	-	initiating methionine	UNP E9Q555
A	327	ALA	-	expression tag	UNP E9Q555
A	328	SER	-	expression tag	UNP E9Q555
A	329	TRP	-	expression tag	UNP E9Q555
A	330	SER	-	expression tag	UNP E9Q555
A	331	HIS	-	expression tag	UNP E9Q555
A	332	PRO	-	expression tag	UNP E9Q555
A	333	GLN	-	expression tag	UNP E9Q555
A	334	PHE	-	expression tag	UNP E9Q555
A	335	GLU	-	expression tag	UNP E9Q555
A	336	LYS	-	expression tag	UNP E9Q555
A	337	GLY	-	expression tag	UNP E9Q555
A	338	SER	-	expression tag	UNP E9Q555
A	?	-	VAL	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	?	-	ASN	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

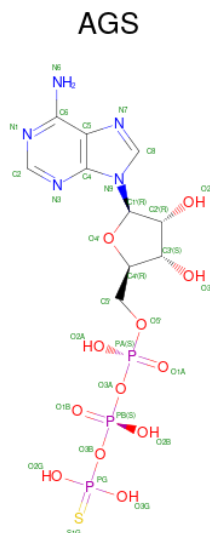
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$ ) (labeled as "Ligand of Interest" by depositor).

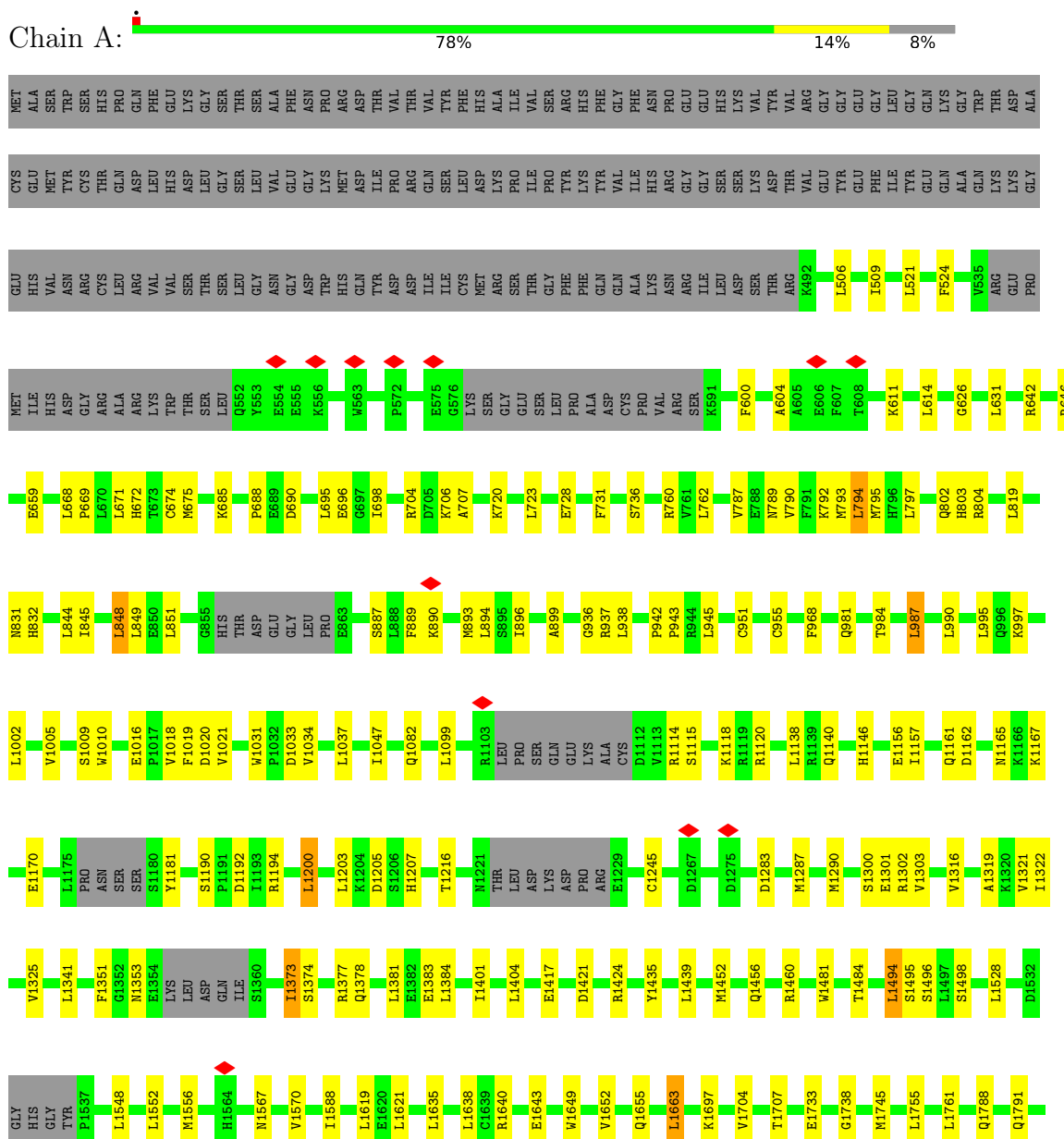


Mol	Chain	Residues	Atoms					AltConf	
6	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

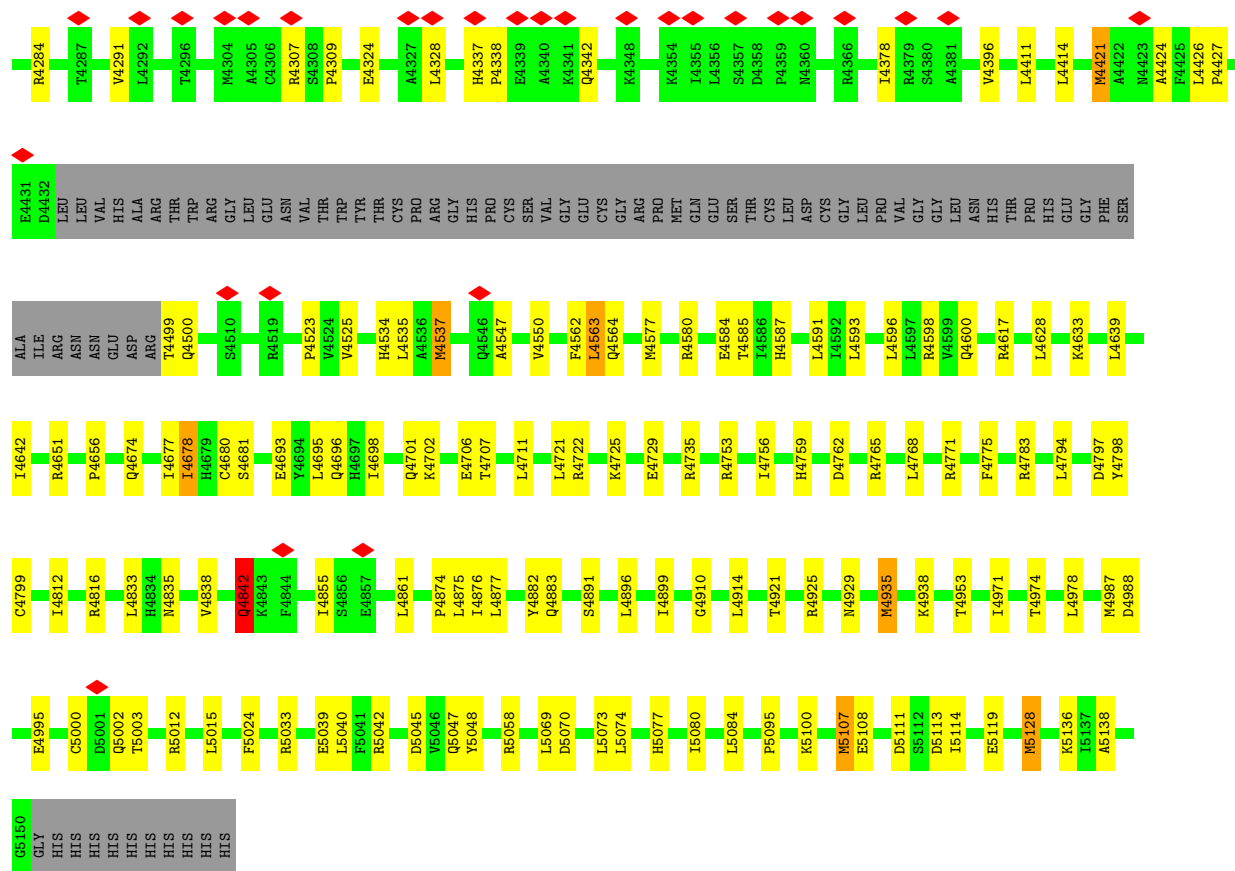
### 3 Residue-property plots

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: E3 ubiquitin-protein ligase RNF213



D4116	E3849	L3124	L2878	R2590	G2299	Q2139	Y2040	L1807
K4117	G3850	F3125	D2887	C2594	K2303	D2142	L2041	L2041
L4122	Y3851	R3126	D2887	G2595	K2303	V2151	M2042	T1820
S4126	S3855	L3133	L2914	D2601	V2306	V2151	L2048	F1821
C4127	R3860	D3134	L2935	C2605	M2307	L2159	W2049	D1822
L4128	I3863	M3135	Q2938	D2624	L2311	F2162	Y2057	L1826
E4129	Q3864	V3138	D2939	C2608	F2326	W2173	P2062	T1845
D4130	R3867	L3139	I2940	D2628	L2329	L2176	Q2063	D1860
V4132	R3867	Q3140	T2941	H2628	K2334	R2177	GLY	E1865
A4138	R3872	W3142	H2942	H2628	L2339	F2182	LEU	Q1869
N4142	A3877	K3143	Y2984	D2632	L2356	L2183	VAL	H1882
L4143	K3691	V3147	L2994	E2660	M2369	Q2186	GLN	R1883
K3992	T3692	K3161	D2995	A2708	R2370	D2189	PRG	E1884
F3993	P3693	K3164	G2996	A2708	R2372	F2208	LYS	R1896
S3994	V3696	C3185	S2999	V2717	V2377	F2208	LEU	L1925
P3995	Q3700	Q3185	R3000	E2721	T2406	W2219	ALA	R1934
K4007	Q3720	V3188	T3006	L2722	Y2422	D2222	ARG	S1937
H4008	K3723	E3194	A3011	P2725	T2443	T2225	ALA	A1938
A4009	S3726	R3199	L3012	L2728	F2447	L2227	L2081	F1942
R4012	R3727	D3200	Q3017	G2733	HIS	LEU	L2085	L1946
H4013	E3728	E3203	E3021	I2742	THR	THR	R2094	L1956
D4021	M3731	L3205	I3028	A2746	ASP	ASP	P2095	L1975
I4039	L3592	Y3206	V3059	G2808	GLN	GLN	K2097	E2098
L4042	G3593	R3207	L3062	K2815	SER	SER	E2098	R1976
L4043	N3594	P3223	L3063	I2830	I2462	GLY	I2100	D1977
L4046	L3595	A3225	L3064	E2831	GLY	ARG	E2103	P1981
L4049	L3598	V3226	Y3068	D2832	THR	THR	LEU	R1986
K4050	L3598	F3237	Q3077	F2842	ILE	GLU	THR	L1987
L4053	H3785	S3254	G3091	I2845	GLU	GLU	ARG	T1988
ARG	V3788	H3268	R3096	N2847	VAL	VAL	HIS	L1992
ASP	S3790	F3274	V3109	W2848	ASP	ASP	THR	V2014
ALA	S3793	S3281	V3115	A2853	T2513	K2257	D2019	D2019
SER	K3798	R3282	Q3119	R2863	V2529	R2258	S2021	T2022
LYS	L3808	L3292	F3120	P2866	P2534	F2269	F2033	F2033
P3946	D3809	L3296	V3121	T2872	Q2556	D2272	K2034	L2035
V3958	K3821	S3472	V3122		V2559	T2294	L2038	L2038
L3960	G3822						Q2137	Q2137
H3964	L3825						Q2138	Q2138
R3969	K3826							
C3970	P3827							
I3971	L3833							
Q3972								
T3973	GLU							
W3974	MET							
L3975	S3637							
T3976	N3645							
P3977	M3646							
G3978	L3647							
C3982	P3656							
L3986	F3657							
T3987	S3658							
D3988	R3662							
L3989	E3687							
P3990	K3691							
D3991	T3692							
K3992	P3693							
F3993	V3696							
S3994	Q3700							
P3995	Q3720							
K4007	K3723							
H4008	S3726							
I4009	R3727							
R4012	E3728							
H4013	M3731							
D4021	L3592							
I4039	G3593							
L4042	N3594							
L4043	L3595							
L4046	L3598							
L4049	H3785							
K4050	V3788							
L4053	S3790							
ARG	S3793							
ASP	K3937							
ALA	K3938							
SER	F3942							
GLN	P3946							
LYS	V3958							
H4060	L3960							
R4061	H3964							
P4069	R3969							
D4072	C3970							
L4084	I3971							
L4098	Q3972							
L4113								
T4114								
E4115								





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	336000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45, 40.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	370.656, 370.656, 370.656	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	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, ZN, MG, ADP, AGS

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	0.32	0/36242	0.75	71/49026 (0.1%)

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	6

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	671	LEU	CA-CB-CG	9.41	136.93	115.30
1	A	4421	MET	CA-CB-CG	9.06	128.69	113.30
1	A	762	LEU	CA-CB-CG	9.05	136.12	115.30
1	A	1494	LEU	O-C-N	8.98	137.07	122.70
1	A	1975	LEU	CA-CB-CG	8.69	135.29	115.30
1	A	4701	GLN	CA-CB-CG	8.47	132.05	113.40
1	A	1205	ASP	CB-CG-OD1	7.77	125.30	118.30
1	A	2994	LEU	CA-CB-CG	7.71	133.03	115.30
1	A	4877	LEU	CA-CB-CG	7.39	132.29	115.30
1	A	4987	MET	CA-CB-CG	7.39	125.86	113.30
1	A	4861	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	1138	LEU	CA-CB-CG	7.20	131.87	115.30
1	A	4042	LEU	CA-CB-CG	7.13	131.69	115.30
1	A	4537	MET	CA-CB-CG	6.91	125.05	113.30
1	A	987	LEU	CA-CB-CG	6.76	130.85	115.30
1	A	3825	LEU	CA-CB-CG	6.76	130.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4833	LEU	CA-CB-CG	6.71	130.74	115.30
1	A	3602	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	797	LEU	CB-CG-CD1	6.49	122.03	111.00
1	A	4122	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	2878	ILE	CG1-CB-CG2	-6.36	97.41	111.40
1	A	1494	LEU	CA-C-N	-6.29	103.37	117.20
1	A	951	CYS	CA-CB-SG	6.12	125.02	114.00
1	A	3909	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	4426	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	4309	PRO	C-N-CA	5.98	136.64	121.70
1	A	5108	GLU	CA-CB-CG	5.97	126.55	113.40
1	A	3121	PRO	C-N-CA	5.89	136.42	121.70
1	A	5108	GLU	N-CA-CB	5.87	121.17	110.60
1	A	4701	GLN	N-CA-CB	5.84	121.11	110.60
1	A	2369	MET	CB-CG-SD	5.83	129.90	112.40
1	A	4128	LEU	CB-CG-CD1	5.81	120.87	111.00
1	A	945	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	794	LEU	CB-CG-CD2	5.76	120.80	111.00
1	A	819	LEU	CB-CG-CD1	5.75	120.78	111.00
1	A	4721	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	4274	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	1452	MET	CA-CB-CG	5.62	122.85	113.30
1	A	1383	GLU	N-CA-CB	5.60	120.68	110.60
1	A	4593	LEU	CB-CG-CD1	5.60	120.51	111.00
1	A	4797	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	1745	MET	CA-CB-CG	5.53	122.70	113.30
1	A	4875	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	1663	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	4591	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	3731	MET	CA-CB-CG	5.48	122.61	113.30
1	A	4563	LEU	CB-CG-CD2	5.47	120.30	111.00
1	A	4842	GLN	CA-CB-CG	5.46	125.41	113.40
1	A	4043	LEU	CA-CB-CG	5.45	127.82	115.30
1	A	3905	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	5107	MET	CA-CB-CG	5.43	122.54	113.30
1	A	894	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	4935	MET	CB-CG-SD	5.40	128.61	112.40
1	A	3910	GLU	CA-CB-CG	5.39	125.25	113.40
1	A	3864	GLN	N-CA-CB	5.37	120.26	110.60
1	A	4596	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	3570	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	5073	LEU	CA-CB-CG	5.26	127.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	848	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	797	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	3135	MET	CB-CG-SD	-5.23	96.70	112.40
1	A	4995	GLU	CA-CB-CG	5.22	124.89	113.40
1	A	1934	ARG	CA-CB-CG	5.21	124.86	113.40
1	A	3491	MET	CA-CB-CG	5.20	122.13	113.30
1	A	1452	MET	CB-CG-SD	5.17	127.91	112.40
1	A	1377	ARG	CA-CB-CG	5.15	124.73	113.40
1	A	3833	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	4721	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	1099	LEU	CB-CG-CD2	5.07	119.62	111.00
1	A	4678	ILE	CG1-CB-CG2	-5.04	100.32	111.40
1	A	1200	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1170	GLU	Peptide
1	A	1373	ILE	Peptide
1	A	4165	GLU	Peptide
1	A	659	GLU	Peptide
1	A	688	PRO	Peptide

## 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	A	35505	0	35642	355	0
2	A	31	0	12	3	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	27	0	12	0	0
6	A	31	0	12	2	0
All	All	35597	0	35678	355	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 5.

All (355) 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:731:PHE:HB3	1:A:760:ARG:HH21	1.47	0.78
1:A:4935:MET:SD	1:A:4938:LYS:NZ	2.60	0.74
1:A:942:PRO:HB3	1:A:3207:ARG:HE	1.54	0.72
1:A:3292:LEU:O	1:A:3296:LEU:HB2	1.91	0.70
1:A:942:PRO:HB3	1:A:3207:ARG:HH21	1.56	0.70
1:A:1216:THR:HG21	1:A:1245:CYS:HB2	1.77	0.66
1:A:4695:LEU:HD11	1:A:4876:ILE:HG12	1.78	0.66
1:A:646:ARG:NH2	1:A:674:CYS:SG	2.69	0.65
1:A:1301:GLU:OE2	1:A:1302:ARG:NH1	2.29	0.65
1:A:2186:GLN:NE2	1:A:2369:MET:SD	2.70	0.65
1:A:4427:PRO:HA	1:A:4617:ARG:HE	1.61	0.64
1:A:728:GLU:O	1:A:760:ARG:NH2	2.30	0.64
1:A:981:GLN:NE2	1:A:3206:TYR:OH	2.30	0.64
1:A:942:PRO:HB3	1:A:3207:ARG:NH2	2.11	0.64
1:A:4185:LEU:HD22	1:A:4228:LEU:HD12	1.80	0.63
1:A:5040:LEU:HD21	1:A:5136:LYS:HE2	1.81	0.63
1:A:4009:ALA:O	1:A:4013:HIS:ND1	2.28	0.63
1:A:4842:GLN:HE21	1:A:4842:GLN:HA	1.65	0.62
1:A:3605:ALA:O	1:A:3609:ASP:HB2	1.99	0.62
1:A:4525:VAL:HG13	1:A:4628:LEU:HD12	1.82	0.62
1:A:2594:CYS:SG	1:A:2595:GLY:N	2.73	0.61
1:A:3780:ARG:NH2	1:A:4910:GLY:O	2.33	0.61
1:A:794:LEU:HD22	1:A:844:LEU:HD11	1.81	0.61
1:A:3064:LEU:HD22	1:A:3109:VAL:HG11	1.83	0.61
1:A:1417:GLU:OE1	1:A:1496:SER:OG	2.07	0.61
1:A:3658:SER:HB3	1:A:3720:LEU:HD11	1.82	0.61
1:A:3091:GLY:HA3	1:A:3096:ARG:HD3	1.83	0.61
1:A:3897:LEU:HB2	1:A:3938:LYS:HE3	1.83	0.61
1:A:4200:GLU:HA	1:A:4206:ARG:HH21	1.65	0.61
1:A:942:PRO:HB3	1:A:3207:ARG:NE	2.15	0.61
1:A:3937:LYS:HG3	1:A:3942:PHE:HA	1.83	0.61
1:A:887:SER:O	1:A:890:LYS:NZ	2.34	0.60
1:A:2294:ILE:HD11	1:A:2299:GLY:HA2	1.82	0.60
1:A:2334:LYS:HD3	1:A:2356:LEU:HD22	1.84	0.59
1:A:4735:ARG:NH2	1:A:4855:ILE:O	2.36	0.59
1:A:2128:PRO:HB3	1:A:2183:LEU:HD23	1.84	0.59
1:A:3530:ARG:HH12	1:A:3618:ILE:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1384:LEU:HD11	1:A:1439:LEU:HD11	1.84	0.58
1:A:3882:HIS:NE2	1:A:4021:ASP:OD2	2.36	0.58
1:A:3006:THR:HG21	1:A:3011:ALA:HB2	1.86	0.58
1:A:3501:ARG:HH12	1:A:3593:GLY:HA2	1.68	0.58
1:A:942:PRO:CB	1:A:3207:ARG:HH21	2.16	0.58
1:A:4411:LEU:HD23	1:A:4414:LEU:HD12	1.86	0.58
1:A:2459:ILE:HA	1:A:2462:ILE:HD12	1.85	0.58
1:A:893:MET:SD	1:A:937:ARG:NH2	2.78	0.57
1:A:4221:ASN:O	1:A:4224:HIS:ND1	2.36	0.57
1:A:4971:ILE:HA	1:A:4974:THR:HG22	1.85	0.57
1:A:704:ARG:NH2	1:A:736:SER:O	2.37	0.57
1:A:845:ILE:HA	1:A:848:LEU:HG	1.87	0.57
1:A:611:LYS:HA	1:A:614:LEU:HD13	1.87	0.56
1:A:987:LEU:HA	1:A:990:LEU:HD13	1.86	0.56
1:A:2100:ILE:HD13	1:A:2159:LEU:HD23	1.86	0.56
1:A:4759:HIS:O	1:A:4765:ARG:NH1	2.33	0.56
1:A:4142:ASN:ND2	1:A:4144:GLU:OE2	2.38	0.56
1:A:4768:LEU:HD22	1:A:4771:ARG:HH21	1.70	0.56
1:A:2601:ASP:O	1:A:2605:CYS:HB2	2.05	0.56
1:A:4378:ILE:O	1:A:4564:GLN:NE2	2.38	0.56
1:A:2474:HIS:HB2	1:A:2477:SER:HB3	1.87	0.55
1:A:3696:VAL:O	1:A:3700:GLN:NE2	2.30	0.55
1:A:4117:LYS:HZ3	1:A:4168:ARG:HD3	1.72	0.55
1:A:2590:ARG:NH1	1:A:2660:GLU:OE2	2.40	0.55
1:A:3127:ARG:NH2	6:A:5206:AGS:S1G	2.80	0.55
1:A:936:GLY:O	1:A:3238:THR:OG1	2.25	0.54
1:A:2021:SER:OG	1:A:2022:THR:N	2.40	0.54
1:A:1845:THR:O	1:A:1883:ARG:NH1	2.39	0.54
1:A:4117:LYS:HE3	1:A:4677:ILE:HG12	1.90	0.54
1:A:831:ASN:O	1:A:832:HIS:ND1	2.40	0.54
1:A:1435:TYR:HB3	1:A:1439:LEU:HD13	1.90	0.54
1:A:3479:ARG:NH2	1:A:5000:CYS:SG	2.76	0.54
1:A:5077:HIS:HA	1:A:5080:ILE:HG12	1.89	0.54
1:A:3891:ILE:HG21	1:A:4007:LYS:HG2	1.89	0.54
1:A:3728:GLU:HA	1:A:3731:MET:HG3	1.89	0.53
1:A:4164:GLN:HG2	1:A:4171:SER:H	1.73	0.53
1:A:4835:ASN:ND2	1:A:4914:LEU:O	2.41	0.53
1:A:1162:ASP:O	1:A:1165:ASN:ND2	2.42	0.53
1:A:803:HIS:HB3	1:A:851:LEU:HG	1.91	0.53
1:A:1494:LEU:HG	1:A:1498:SER:OG	2.09	0.53
1:A:2222:ASP:HA	1:A:2258:ARG:HH22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HD22	1:A:698:ILE:HD12	1.91	0.53
1:A:1321:VAL:HG11	1:A:1378:GLN:HG3	1.90	0.53
1:A:4729:GLU:HG3	1:A:4771:ARG:HG2	1.91	0.53
1:A:1181:TYR:OH	1:A:1194:ARG:NH2	2.43	0.52
1:A:3281:SER:OG	1:A:3282:ARG:N	2.42	0.52
1:A:2370:ARG:HB3	1:A:2377:VAL:HG22	1.91	0.52
1:A:2708:ALA:HA	1:A:2863:ARG:HH22	1.74	0.52
1:A:4378:ILE:HG13	1:A:4564:GLN:HE21	1.74	0.52
1:A:2733:GLY:HA3	1:A:2914:LEU:HB2	1.92	0.52
1:A:984:THR:HG21	1:A:3203:GLU:HG3	1.90	0.52
1:A:2162:PHE:HB3	1:A:2176:LEU:HD11	1.90	0.52
1:A:2306:VAL:HG23	1:A:2307:MET:HG3	1.91	0.52
1:A:4783:ARG:NH1	1:A:4799:CYS:O	2.42	0.52
1:A:4842:GLN:HE21	1:A:4842:GLN:CA	2.22	0.52
1:A:1316:VAL:HA	1:A:1341:LEU:HD21	1.92	0.51
1:A:3017:GLN:NE2	1:A:3394:GLY:O	2.42	0.51
1:A:4978:LEU:HD22	1:A:5015:LEU:HD22	1.92	0.51
1:A:4175:LEU:HA	1:A:4178:VAL:HG22	1.90	0.51
1:A:2225:THR:O	1:A:2258:ARG:NH1	2.43	0.51
1:A:2142:ASP:OD1	1:A:2142:ASP:N	2.42	0.51
1:A:3960:LEU:HB2	1:A:3964:HIS:HB2	1.92	0.51
1:A:4988:ASP:N	1:A:4988:ASP:OD1	2.43	0.51
1:A:3224:ASP:OD2	1:A:3381:ARG:NH1	2.43	0.51
1:A:4328:LEU:HD13	1:A:4337:HIS:HB3	1.91	0.51
1:A:1156:GLU:HG2	1:A:1157:ILE:HG12	1.92	0.51
1:A:3403:ASP:OD2	1:A:3567:ARG:HD3	2.11	0.51
1:A:2042:MET:HG3	1:A:2048:ILE:HG12	1.93	0.51
1:A:1567:ASN:HA	1:A:1570:VAL:HG22	1.93	0.51
1:A:787:VAL:HA	1:A:790:VAL:HG12	1.92	0.50
1:A:2528:ARG:HG3	1:A:2853:ALA:HB3	1.94	0.50
1:A:5048:TYR:HE1	1:A:5095:PRO:HB3	1.76	0.50
1:A:1300:SER:HA	1:A:1303:VAL:HG12	1.92	0.50
1:A:3012:LEU:HD21	1:A:3062:LEU:HD21	1.92	0.50
1:A:3254:SER:OG	1:A:3404:LEU:O	2.29	0.50
1:A:2450:ALA:HB1	1:A:2459:ILE:HD13	1.94	0.50
1:A:3115:VAL:O	1:A:3119:GLN:HB2	2.10	0.50
1:A:3958:VAL:HG11	1:A:3971:ILE:HG21	1.93	0.50
1:A:4794:LEU:HD12	1:A:4798:TYR:HD2	1.75	0.50
1:A:1421:ASP:HA	1:A:1424:ARG:HE	1.77	0.50
1:A:3645:MET:HB2	1:A:3647:LEU:HD23	1.93	0.49
1:A:4547:ALA:HA	1:A:4550:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:SER:HA	1:A:1118:LYS:HG2	1.93	0.49
1:A:4164:GLN:HG3	1:A:4169:ILE:HG22	1.93	0.49
1:A:3693:PRO:HA	1:A:3696:VAL:HG22	1.93	0.49
1:A:5069:LEU:HD11	1:A:5138:ALA:HB1	1.95	0.49
1:A:942:PRO:HB3	1:A:3207:ARG:CZ	2.42	0.49
1:A:1704:VAL:HA	1:A:1707:THR:HG22	1.93	0.49
1:A:955:CYS:O	1:A:997:LYS:NZ	2.38	0.49
1:A:4775:PHE:HE2	1:A:4812:ILE:HG22	1.78	0.49
1:A:2189:ASP:HB3	1:A:2269:PHE:HB2	1.94	0.49
1:A:3505:ARG:NE	1:A:3590:ASP:OD2	2.45	0.49
1:A:2608:VAL:HG22	1:A:2722:LEU:HG	1.93	0.49
1:A:4113:LEU:O	1:A:4168:ARG:NH1	2.45	0.49
1:A:995:LEU:HD22	1:A:1047:ILE:HG12	1.95	0.49
1:A:1322:ILE:HA	1:A:1325:VAL:HG12	1.95	0.49
1:A:2022:THR:HG22	1:A:2062:PRO:HG3	1.94	0.49
1:A:4835:ASN:HA	1:A:4838:VAL:HG22	1.95	0.49
1:A:3982:CYS:HB3	1:A:3987:THR:H	1.78	0.49
1:A:4271:ASP:HB3	1:A:4651:ARG:HH22	1.77	0.49
1:A:5095:PRO:HA	1:A:5128:MET:HB3	1.94	0.49
1:A:1146:HIS:NE2	1:A:2872:ILE:HG21	2.28	0.48
1:A:5033:ARG:NH2	1:A:5039:GLU:O	2.45	0.48
1:A:4165:GLU:OE2	1:A:4674:GLN:NE2	2.46	0.48
1:A:1860:ASP:O	1:A:1896:ARG:NH1	2.46	0.48
1:A:3610:LEU:HD23	1:A:3656:PRO:HD2	1.96	0.48
1:A:1031:TRP:HE3	1:A:1034:VAL:HG13	1.77	0.48
1:A:1140:GLN:HG3	1:A:1200:LEU:HD12	1.95	0.48
1:A:4816:ARG:HE	1:A:4921:THR:HG21	1.78	0.48
1:A:4953:THR:OG1	1:A:5012:ARG:NH2	2.46	0.48
1:A:3928:LEU:HD23	1:A:4069:PRO:HG3	1.95	0.48
1:A:1788:GLN:HG3	1:A:1791:GLN:HB2	1.95	0.48
1:A:2509:SER:O	1:A:2513:THR:OG1	2.31	0.48
1:A:669:PRO:HG2	1:A:723:LEU:HD23	1.96	0.48
1:A:3028:ILE:HD13	1:A:3059:VAL:HG13	1.96	0.48
1:A:3223:PRO:HA	1:A:3226:VAL:HG12	1.95	0.48
1:A:5070:ASP:OD1	1:A:5070:ASP:N	2.46	0.48
1:A:506:LEU:HD23	1:A:509:ILE:HD11	1.95	0.48
1:A:1325:VAL:HG11	1:A:1381:LEU:HD12	1.94	0.48
1:A:3687:GLU:OE2	1:A:3691:LYS:NZ	2.47	0.48
1:A:3849:GLU:OE2	1:A:3867:ARG:NH2	2.44	0.48
1:A:1619:LEU:HB3	1:A:1621:LEU:HD23	1.96	0.47
1:A:3365:GLN:NE2	1:A:3369:ASP:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4225:ARG:HH11	1:A:4256:PRO:HA	1.79	0.47
1:A:4499:THR:OG1	1:A:4500:GLN:N	2.46	0.47
1:A:2486:ASN:HB2	1:A:2529:VAL:HG11	1.96	0.47
1:A:2808:GLY:HA3	1:A:2848:TRP:HB2	1.97	0.47
1:A:3860:ARG:HA	1:A:3863:ILE:HG12	1.96	0.47
1:A:4138:ALA:HB2	1:A:4874:PRO:HG3	1.96	0.47
1:A:600:PHE:O	1:A:604:ALA:HB2	2.14	0.47
1:A:889:PHE:HB3	1:A:937:ARG:HH22	1.80	0.47
1:A:2038:LEU:HD23	1:A:2040:TYR:HE1	1.78	0.47
1:A:2369:MET:HA	1:A:2372:ARG:HB3	1.95	0.47
1:A:3144:LYS:HA	1:A:3147:VAL:HG12	1.95	0.47
1:A:3662:ARG:HD2	1:A:3720:LEU:HD13	1.95	0.47
1:A:4639:LEU:HA	1:A:4642:ILE:HG22	1.96	0.47
1:A:1031:TRP:CZ3	1:A:1033:ASP:HB2	2.49	0.47
1:A:3200:ASP:N	1:A:3200:ASP:OD1	2.48	0.47
1:A:2094:ARG:HB3	1:A:2098:GLU:HB2	1.96	0.47
1:A:4722:ARG:O	1:A:4725:LYS:NZ	2.46	0.47
1:A:4762:ASP:N	1:A:4762:ASP:OD1	2.45	0.47
1:A:4130:ASP:OD2	1:A:4882:TYR:OH	2.28	0.47
1:A:4896:LEU:HA	1:A:4899:ILE:HG22	1.97	0.47
1:A:4039:ILE:HA	1:A:4042:LEU:HG	1.97	0.47
1:A:1495:SER:HB3	1:A:1498:SER:H	1.80	0.46
1:A:2866:PRO:HG3	1:A:2914:LEU:HD21	1.97	0.46
1:A:1002:LEU:HD22	1:A:1037:LEU:HD12	1.97	0.46
1:A:2847:ASN:ND2	6:A:5206:AGS:S1G	2.83	0.46
1:A:3185:CYS:HA	1:A:3188:VAL:HG12	1.98	0.46
1:A:3726:SER:OG	1:A:3728:GLU:OE1	2.32	0.46
1:A:3785:HIS:HD2	1:A:3788:VAL:HB	1.79	0.46
1:A:642:ARG:HD2	1:A:4765:ARG:HH22	1.79	0.46
1:A:2728:LEU:HD12	1:A:2845:ILE:HG12	1.97	0.46
1:A:2999:SER:O	1:A:3077:GLN:NE2	2.48	0.46
1:A:1865:GLU:OE2	1:A:1869:GLN:NE2	2.48	0.46
1:A:4050:LYS:HD2	1:A:4061:ARG:HH11	1.81	0.46
1:A:626:GLY:HA2	1:A:631:LEU:HD23	1.96	0.46
1:A:720:LYS:HB3	1:A:723:LEU:HD13	1.98	0.46
1:A:1942:PHE:HD2	1:A:1946:LEU:HB2	1.79	0.46
1:A:3006:THR:HG22	1:A:3134:ASP:HA	1.96	0.46
1:A:1020:ASP:OD1	1:A:1021:VAL:N	2.44	0.46
1:A:1203:LEU:HD11	1:A:1290:MET:HG3	1.98	0.46
1:A:2422:TYR:OH	1:A:2458:CYS:SG	2.70	0.46
1:A:3014:ILE:HD11	1:A:3138:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3958:VAL:HG21	1:A:3993:PHE:HB2	1.97	0.46
1:A:4396:VAL:HG11	1:A:4535:LEU:HB3	1.97	0.46
1:A:1937:SER:OG	1:A:1938:ALA:N	2.49	0.46
1:A:2406:THR:O	1:A:2443:THR:OG1	2.28	0.46
1:A:1986:ARG:NH1	1:A:2019:ASP:OD2	2.50	0.45
1:A:2227:THR:HA	1:A:2257:LYS:HG3	1.97	0.45
1:A:3418:GLN:HE22	1:A:3551:THR:HG1	1.57	0.45
1:A:3946:PRO:HG2	1:A:4072:ASP:HB2	1.97	0.45
1:A:4126:SER:HA	1:A:4129:GLU:HG2	1.96	0.45
1:A:2182:PHE:HZ	1:A:2219:MET:HG3	1.81	0.45
1:A:2272:ASP:N	1:A:2272:ASP:OD1	2.48	0.45
1:A:2303:LYS:HD2	1:A:2303:LYS:HA	1.84	0.45
1:A:4114:THR:HG23	1:A:4168:ARG:HH22	1.81	0.45
1:A:5107:MET:HG3	1:A:5111:ASP:HB3	1.99	0.45
1:A:1981:PRO:HD2	1:A:2014:VAL:HG22	1.99	0.45
1:A:3880:VAL:HG23	1:A:3884:LEU:HD12	1.99	0.45
1:A:1456:GLN:HG3	1:A:1460:ARG:HH21	1.82	0.45
1:A:1663:LEU:HD11	1:A:1761:LEU:HD12	1.99	0.45
1:A:1826:LEU:HD11	1:A:2033:PHE:HD2	1.82	0.45
1:A:2624:ASP:O	1:A:2628:HIS:HB2	2.17	0.45
1:A:646:ARG:HD3	1:A:646:ARG:HA	1.62	0.45
1:A:1082:GLN:OE1	1:A:1082:GLN:N	2.48	0.45
1:A:3194:GLU:HG2	1:A:3199:ARG:HH22	1.82	0.45
1:A:3519:ARG:HD2	1:A:3598:LEU:HD12	1.98	0.45
1:A:4577:MET:HG2	1:A:4693:GLU:HB3	1.99	0.45
1:A:706:LYS:NZ	1:A:707:ALA:O	2.42	0.45
1:A:849:LEU:HD23	1:A:849:LEU:HA	1.84	0.45
1:A:2935:LEU:HB3	1:A:2940:ILE:HD11	1.98	0.45
1:A:3140:GLN:OE1	1:A:3142:TRP:NE1	2.40	0.45
1:A:3809:ASP:OD2	1:A:3851:TYR:OH	2.30	0.45
1:A:1988:THR:OG1	1:A:2457:SER:OG	2.28	0.44
1:A:2830:ILE:HG22	1:A:2831:GLU:HG3	1.99	0.44
1:A:1481:TRP:HA	1:A:1484:THR:HG22	1.98	0.44
1:A:3904:LEU:HD23	1:A:3907:LYS:HZ3	1.82	0.44
1:A:4046:LEU:HD11	1:A:4084:LEU:HD12	1.99	0.44
1:A:4167:VAL:HG23	1:A:4168:ARG:HG2	1.98	0.44
1:A:5002:GLN:HG2	1:A:5003:THR:H	1.82	0.44
1:A:4201:LEU:HB3	1:A:4205:LYS:HB2	1.98	0.44
1:A:4706:GLU:HG2	1:A:4707:THR:HG23	1.98	0.44
1:A:896:ILE:HD11	1:A:899:ALA:HA	2.00	0.44
1:A:1207:HIS:NE2	1:A:2887:ASP:OD2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4753:ARG:HA	1:A:4756:ILE:HG22	1.99	0.44
1:A:2938:GLN:O	1:A:2942:HIS:ND1	2.46	0.44
1:A:1619:LEU:HD21	1:A:1755:LEU:HD13	2.00	0.44
1:A:1733:GLU:HG2	1:A:1738:GLY:HA3	1.99	0.44
1:A:1807:LEU:HD21	1:A:1925:LEU:HD21	1.99	0.44
1:A:5080:ILE:HA	1:A:5084:LEU:HD13	2.00	0.44
1:A:3481:VAL:O	1:A:3485:VAL:HG13	2.18	0.44
1:A:3508:ILE:HG21	1:A:3595:LEU:HB3	1.99	0.44
1:A:1018:VAL:HG23	1:A:1019:PHE:H	1.82	0.44
1:A:1640:ARG:NH1	1:A:1643:GLU:OE1	2.51	0.43
1:A:2326:PHE:HA	1:A:2329:LEU:HD13	2.00	0.43
1:A:2815:LYS:HB2	1:A:2815:LYS:HE2	1.87	0.43
1:A:3224:ASP:OD1	1:A:3224:ASP:N	2.51	0.43
1:A:802:GLN:HB3	1:A:804:ARG:H	1.82	0.43
1:A:1652:VAL:HA	1:A:1655:GLN:HG2	1.99	0.43
1:A:3877:ALA:HA	1:A:3880:VAL:HG12	2.00	0.43
1:A:4421:MET:SD	1:A:4424:ALA:HB3	2.58	0.43
1:A:2119:GLU:OE2	2:A:5201:ATP:O2'	2.36	0.43
1:A:2725:PRO:HB3	1:A:2842:PHE:HB3	2.01	0.43
1:A:2832:ASP:OD1	1:A:2832:ASP:N	2.51	0.43
1:A:5113:ASP:HB3	1:A:5114:ILE:H	1.58	0.43
1:A:1384:LEU:HD12	1:A:1384:LEU:HA	1.88	0.43
1:A:4523:PRO:HG3	1:A:4696:GLN:HE21	1.83	0.43
1:A:1987:LEU:HD23	1:A:1992:LEU:HD11	2.00	0.43
1:A:3611:TRP:HD1	1:A:3656:PRO:HB3	1.83	0.43
1:A:4695:LEU:HA	1:A:4698:ILE:HG22	2.01	0.43
1:A:789:ASN:O	1:A:793:MET:HG2	2.19	0.43
1:A:2137:GLN:HG2	1:A:2139:GLN:HE22	1.83	0.43
1:A:2177:ARG:HH21	2:A:5201:ATP:H4'	1.82	0.43
1:A:1820:THR:OG1	1:A:1822:ASP:OD1	2.28	0.42
1:A:2035:LEU:HD11	1:A:2057:TYR:HE2	1.84	0.42
1:A:2632:ASP:OD1	1:A:2632:ASP:N	2.48	0.42
1:A:3516:ASP:N	1:A:3516:ASP:OD1	2.52	0.42
1:A:2096:PRO:HG3	1:A:2173:TRP:CE2	2.54	0.42
1:A:2717:VAL:O	1:A:2721:GLU:HG2	2.19	0.42
1:A:1956:ALA:HB3	1:A:2534:PRO:HB2	2.01	0.42
1:A:2081:LEU:HB3	1:A:2085:LEU:HD23	2.00	0.42
1:A:2447:PHE:HB3	1:A:2450:ALA:HB2	2.01	0.42
1:A:4291:VAL:HG21	1:A:4324:GLU:HB3	2.01	0.42
1:A:4680:CYS:SG	1:A:4681:SER:N	2.92	0.42
1:A:1552:LEU:O	1:A:1556:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3790:SER:O	1:A:3793:SER:HB2	2.19	0.42
1:A:4677:ILE:HG23	1:A:4678:ILE:HD12	2.01	0.42
1:A:646:ARG:HH12	1:A:675:MET:HB3	1.84	0.42
1:A:2041:LEU:HB2	1:A:2049:TRP:HB3	2.01	0.42
1:A:3855:SER:O	1:A:3860:ARG:NH1	2.52	0.42
1:A:668:LEU:O	1:A:672:HIS:ND1	2.53	0.42
1:A:1822:ASP:OD1	1:A:1822:ASP:N	2.53	0.42
1:A:2130:GLN:HE22	1:A:2151:VAL:HB	1.85	0.42
1:A:2473:LEU:HD23	1:A:2473:LEU:HA	1.89	0.42
1:A:5045:ASP:OD2	1:A:5047:GLN:NE2	2.52	0.42
1:A:685:LYS:HE2	1:A:685:LYS:HB3	1.82	0.42
1:A:3000:ARG:NH1	1:A:3126:ASN:O	2.53	0.42
1:A:2984:TYR:OH	1:A:3021:GLU:O	2.36	0.42
1:A:1528:LEU:HD23	1:A:1548:LEU:HD21	2.01	0.41
1:A:3592:ASP:OD1	1:A:3592:ASP:N	2.53	0.41
1:A:1161:GLN:OE1	1:A:1165:ASN:ND2	2.50	0.41
1:A:1190:SER:HB2	1:A:1192:ASP:OD1	2.21	0.41
1:A:4116:ASP:N	1:A:4116:ASP:OD1	2.53	0.41
1:A:600:PHE:O	1:A:604:ALA:CB	2.69	0.41
1:A:792:LYS:HA	1:A:795:MET:HG2	2.02	0.41
1:A:3274:PHE:HD1	1:A:3373:VAL:HB	1.85	0.41
1:A:690:ASP:HB3	1:A:696:GLU:HA	2.01	0.41
1:A:2208:PHE:HD1	1:A:2311:LEU:HD21	1.85	0.41
1:A:4098:ASP:N	1:A:4098:ASP:OD1	2.53	0.41
1:A:4129:GLU:HA	1:A:4132:VAL:HG12	2.01	0.41
1:A:1351:PHE:HD2	1:A:1353:ASN:H	1.67	0.41
1:A:3068:TYR:HB2	1:A:3124:LEU:HD11	2.03	0.41
1:A:521:LEU:HA	1:A:524:PHE:HD2	1.86	0.41
1:A:1120:ARG:HD2	1:A:1167:LYS:NZ	2.36	0.41
1:A:1319:ALA:HA	1:A:1322:ILE:HG22	2.01	0.41
1:A:1882:HIS:NE2	1:A:1884:GLU:OE1	2.50	0.41
1:A:3200:ASP:H	1:A:3205:LEU:HD13	1.84	0.41
1:A:937:ARG:NH1	1:A:3237:PHE:CE1	2.89	0.41
1:A:1649:TRP:HA	1:A:1652:VAL:HG12	2.01	0.41
1:A:3736:ALA:HB2	1:A:3808:LEU:HD12	2.02	0.41
1:A:4562:PHE:HD2	1:A:4563:LEU:HD22	1.85	0.41
1:A:4580:ARG:HB3	1:A:4584:GLU:HB2	2.02	0.41
1:A:1283:ASP:O	1:A:1287:MET:HB2	2.21	0.41
1:A:2556:GLN:HA	1:A:2559:VAL:HG12	2.01	0.41
1:A:3558:ASP:OD2	1:A:5042:ARG:NH1	2.53	0.41
1:A:3726:SER:OG	1:A:3727:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3821:LYS:HZ1	1:A:3872:ARG:HH22	1.68	0.41
1:A:3960:LEU:HG	1:A:3989:LEU:HD12	2.03	0.41
1:A:4534:HIS:HA	1:A:4537:MET:HG3	2.03	0.41
1:A:942:PRO:HA	1:A:943:PRO:HD3	1.91	0.41
1:A:2177:ARG:NE	2:A:5201:ATP:O3'	2.53	0.41
1:A:3133:LEU:HD11	1:A:3138:VAL:HB	2.03	0.41
1:A:4338:PRO:HA	1:A:4342:GLN:HB2	2.02	0.41
1:A:4698:ILE:O	1:A:4702:LYS:HG2	2.21	0.41
1:A:4883:GLN:HB3	1:A:4891:SER:OG	2.21	0.41
1:A:1005:VAL:O	1:A:1009:SER:HB3	2.21	0.40
1:A:1635:LEU:HD13	1:A:1638:LEU:HD23	2.03	0.40
1:A:1697:LYS:HD2	1:A:1697:LYS:HA	1.89	0.40
1:A:2742:ILE:O	1:A:2746:ALA:CB	2.69	0.40
1:A:3015:LEU:HD23	1:A:3015:LEU:HA	1.93	0.40
1:A:1494:LEU:O	1:A:1495:SER:HB2	2.22	0.40
1:A:1010:TRP:HE1	1:A:1018:VAL:HG11	1.86	0.40
1:A:1120:ARG:HD2	1:A:1167:LYS:HZ1	1.86	0.40
1:A:1401:ILE:HD12	1:A:1404:LEU:HD12	2.02	0.40
1:A:3282:ARG:HD2	1:A:3282:ARG:HA	1.83	0.40
1:A:4009:ALA:HA	1:A:4012:ARG:HG2	2.03	0.40
1:A:4259:VAL:HG23	1:A:4656:PRO:HB2	2.04	0.40
1:A:4281:LYS:HA	1:A:4284:ARG:HG2	2.04	0.40
1:A:4580:ARG:HB2	1:A:4585:THR:HG23	2.04	0.40
1:A:4711:LEU:HD21	1:A:4899:ILE:HG23	2.03	0.40
1:A:5024:PHE:HA	1:A:5074:LEU:HD11	2.04	0.40
1:A:5100:LYS:HE2	1:A:5119:GLU:HA	2.04	0.40
1:A:938:LEU:HD11	1:A:968:PHE:CE1	2.56	0.40
1:A:1588:ILE:HD12	1:A:1588:ILE:HA	1.88	0.40
1:A:3922:VAL:HA	1:A:3925:MET:HG2	2.02	0.40
1:A:3975:LEU:HD23	1:A:3993:PHE:HD1	1.86	0.40
1:A:4925:ARG:HH22	1:A:4929:ASN:HB3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4394/4836 (91%)	4028 (92%)	358 (8%)	8 (0%)	44 76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3122	VAL
1	A	4600	GLN
1	A	1374	SER
1	A	3496	ASN
1	A	4166	PRO
1	A	5128	MET
1	A	4049	GLN
1	A	1373	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3970/4342 (91%)	3955 (100%)	15 (0%)	89 91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1114	ARG
1	A	1934	ARG
1	A	3161	LYS
1	A	3405	ARG
1	A	3552	ARG
1	A	3619	LYS
1	A	3723	LYS
1	A	3798	LYS
1	A	3919	ARG
1	A	4307	ARG
1	A	4587	HIS

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Mol	Chain	Res	Type
1	A	4598	ARG
1	A	4633	LYS
1	A	4842	GLN
1	A	5058	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4564	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
2	ATP	A	5201	3	26,33,33	0.60	0	31,52,52	0.79	2 (6%)
5	ADP	A	5205	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
6	AGS	A	5206	-	26,33,33	0.71	1 (3%)	26,52,52	1.18	2 (7%)

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	ATP	A	5201	3	-	6/18/38/38	0/3/3/3
5	ADP	A	5205	-	-	5/12/32/32	0/3/3/3
6	AGS	A	5206	-	-	4/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5205	ADP	C5-C4	2.43	1.47	1.40
6	A	5206	AGS	PG-S1G	2.10	1.95	1.90

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5206	AGS	PA-O3A-PB	-4.64	116.90	132.83
5	A	5205	ADP	N3-C2-N1	-3.36	123.43	128.68
5	A	5205	ADP	PA-O3A-PB	-2.98	122.60	132.83
5	A	5205	ADP	C4-C5-N7	-2.77	106.51	109.40
5	A	5205	ADP	C3'-C2'-C1'	2.53	104.78	100.98
2	A	5201	ATP	C5-C6-N6	2.31	123.86	120.35
6	A	5206	AGS	C5-C6-N6	2.24	123.75	120.35
2	A	5201	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5201	ATP	C5'-O5'-PA-O1A
2	A	5201	ATP	C5'-O5'-PA-O2A
2	A	5201	ATP	O4'-C4'-C5'-O5'
5	A	5205	ADP	C5'-O5'-PA-O3A
5	A	5205	ADP	O4'-C4'-C5'-O5'
5	A	5205	ADP	C3'-C4'-C5'-O5'
6	A	5206	AGS	C5'-O5'-PA-O3A
6	A	5206	AGS	C4'-C5'-O5'-PA
2	A	5201	ATP	C3'-C4'-C5'-O5'
5	A	5205	ADP	C5'-O5'-PA-O1A
5	A	5205	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	A	5206	AGS	C5'-O5'-PA-O2A
2	A	5201	ATP	PA-O3A-PB-O2B
6	A	5206	AGS	PG-O3B-PB-O2B
2	A	5201	ATP	C5'-O5'-PA-O3A

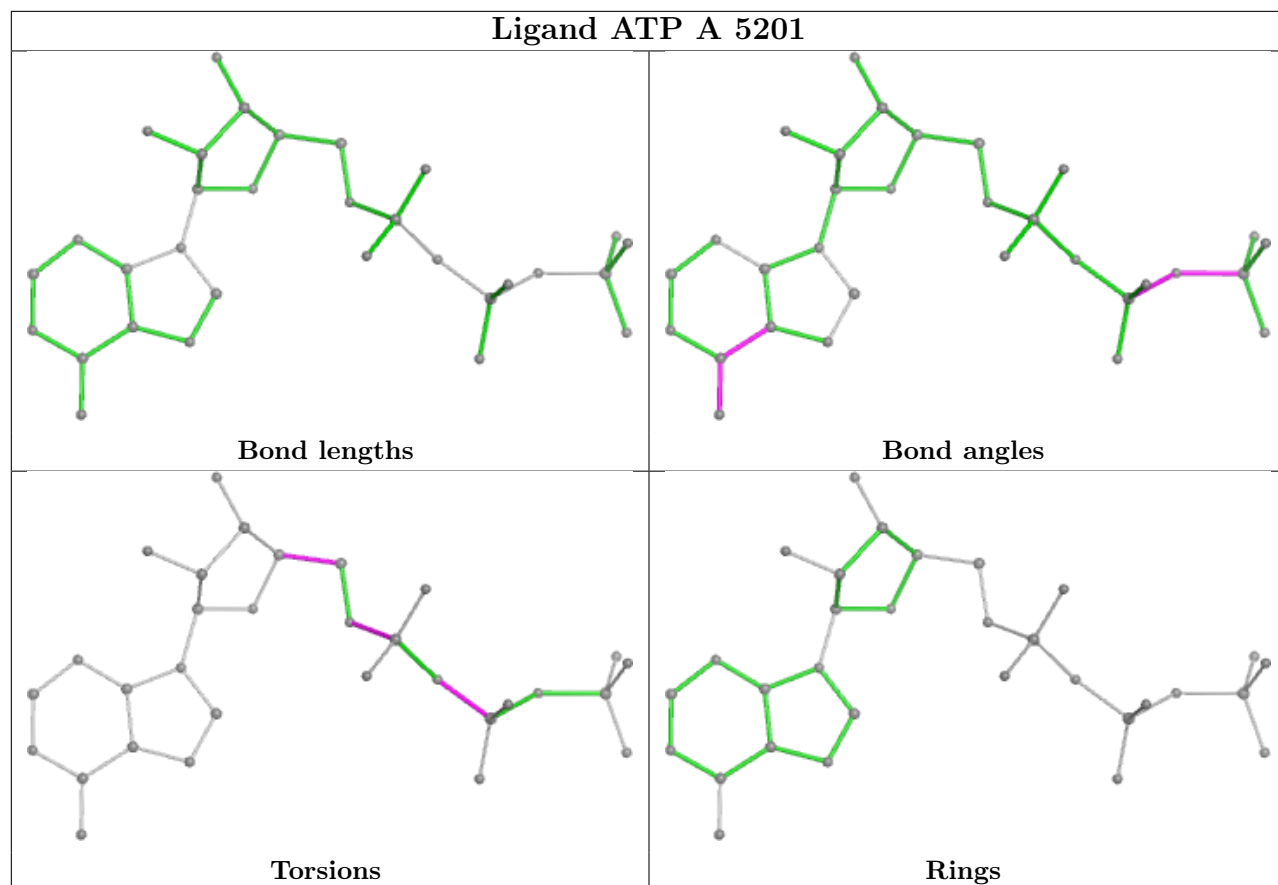
There are no ring outliers.

2 monomers are involved in 5 short contacts:

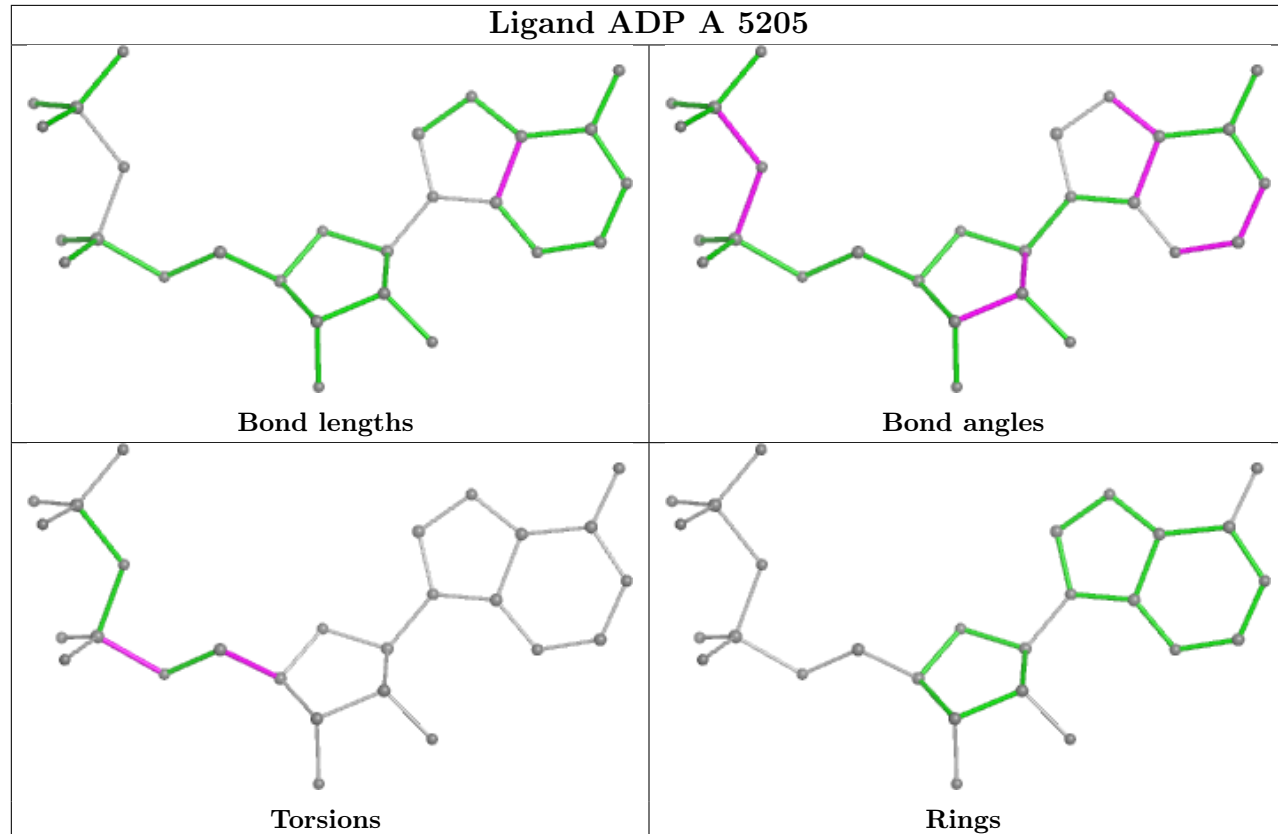
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5201	ATP	3	0
6	A	5206	AGS	2	0

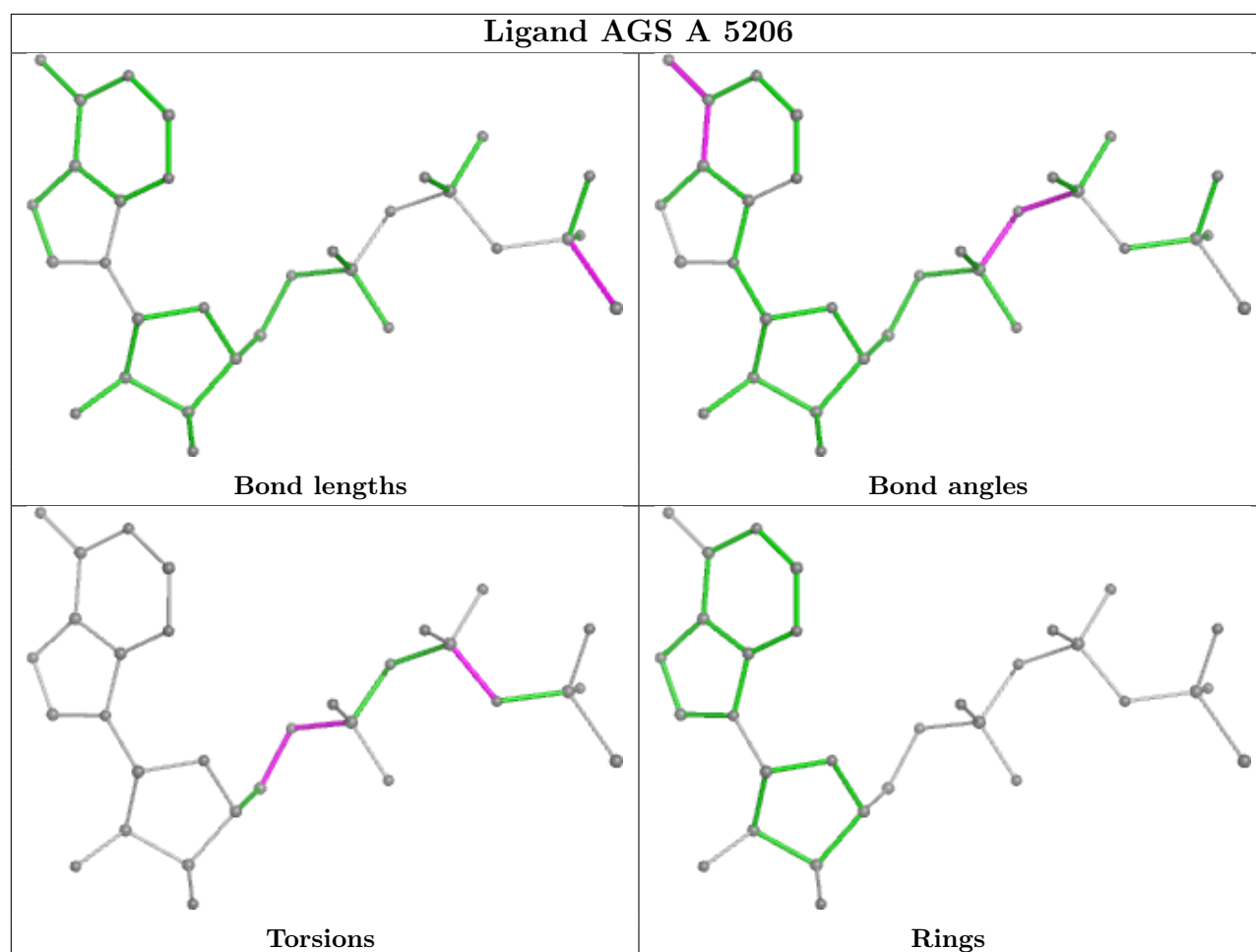
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand ATP A 5201



## Ligand ADP A 5205





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

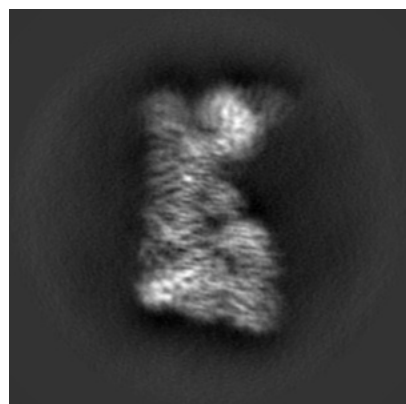
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12932. These allow visual inspection of the internal detail of the map and identification of artifacts.

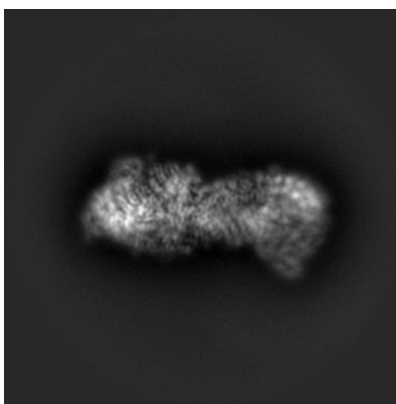
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

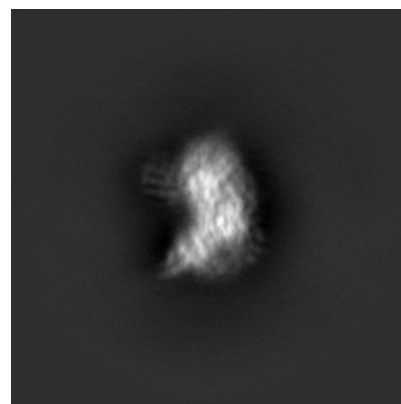
#### 6.1.1 Primary map



X

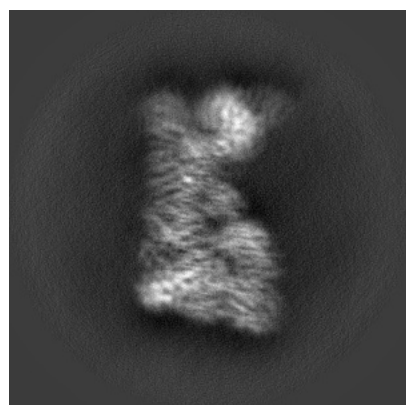


Y

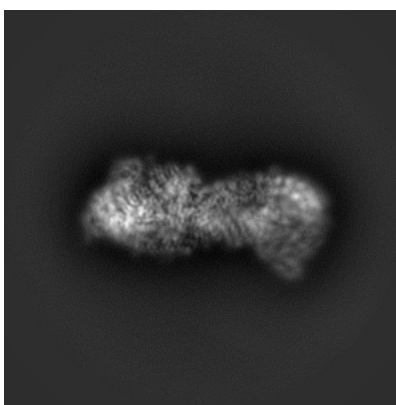


Z

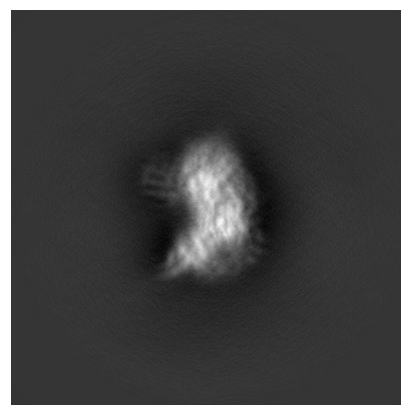
#### 6.1.2 Raw map



X



Y

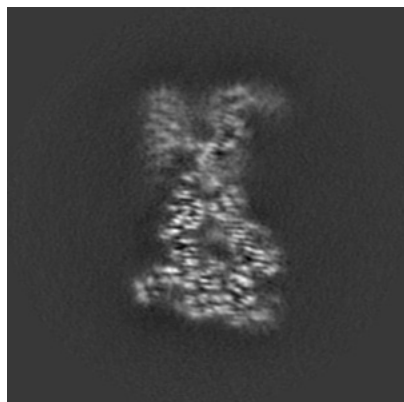


Z

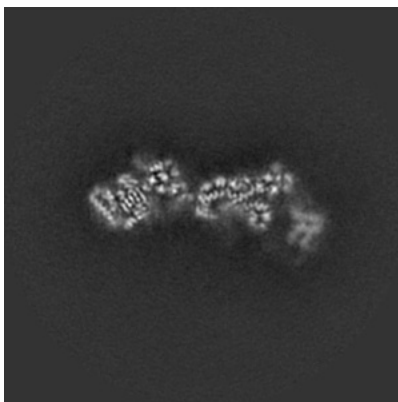
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

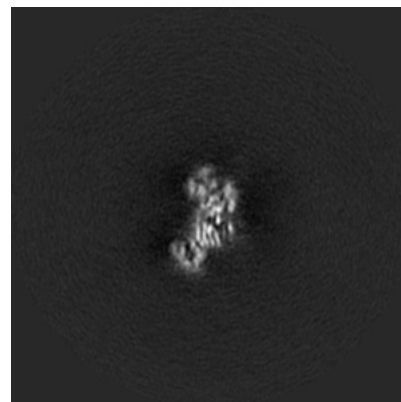
### 6.2.1 Primary map



X Index: 176

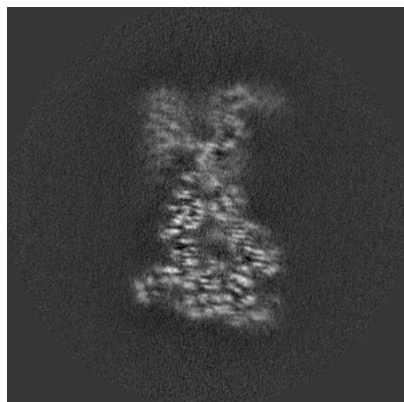


Y Index: 176

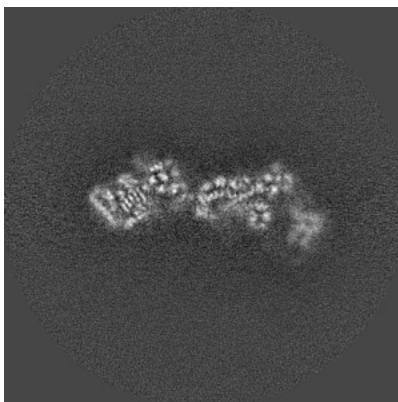


Z Index: 176

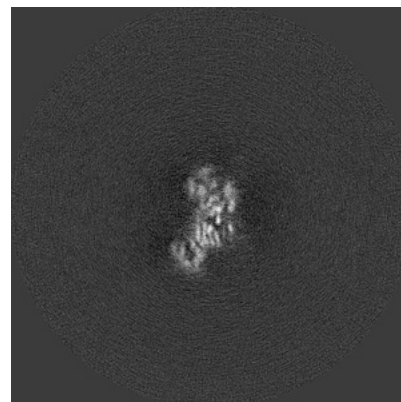
### 6.2.2 Raw map



X Index: 176



Y Index: 176

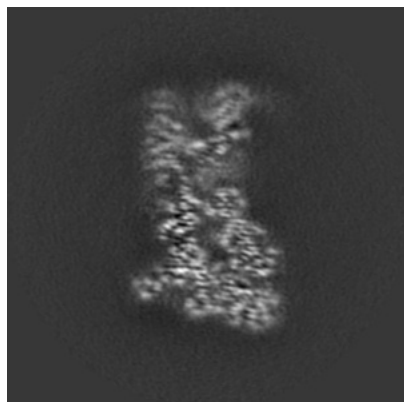


Z Index: 176

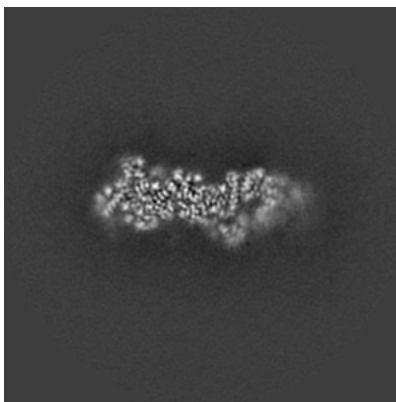
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

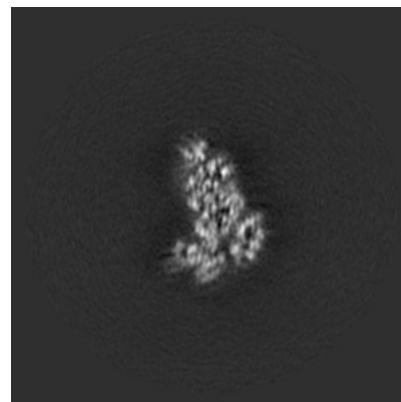
### 6.3.1 Primary map



X Index: 172

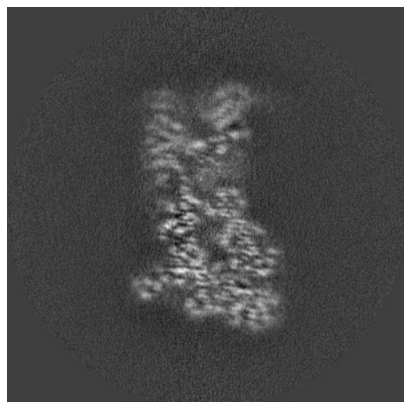


Y Index: 159

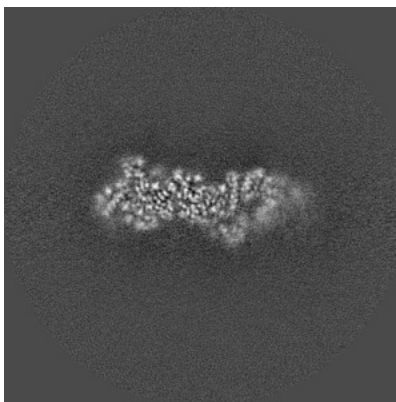


Z Index: 109

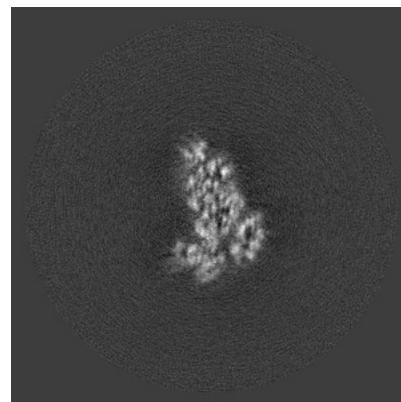
### 6.3.2 Raw map



X Index: 172



Y Index: 159



Z Index: 109

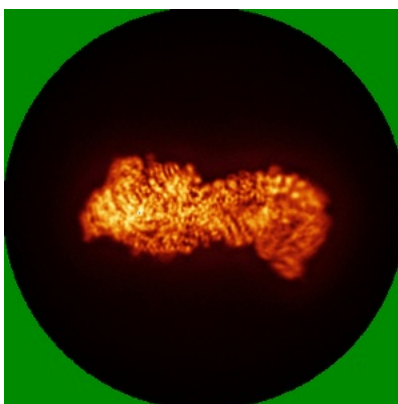
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

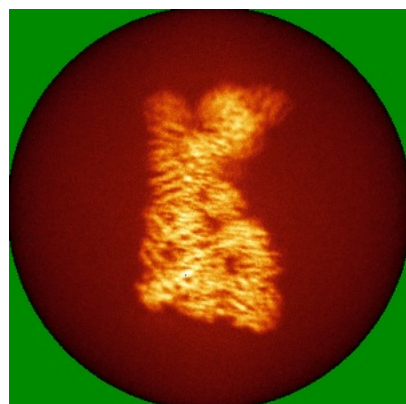


Y

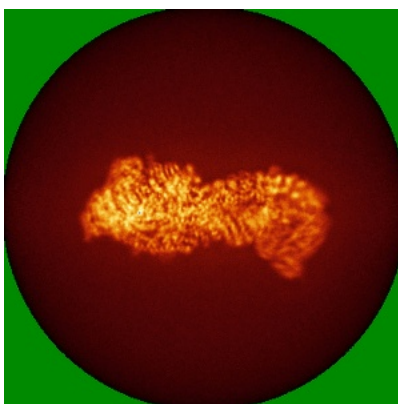


Z

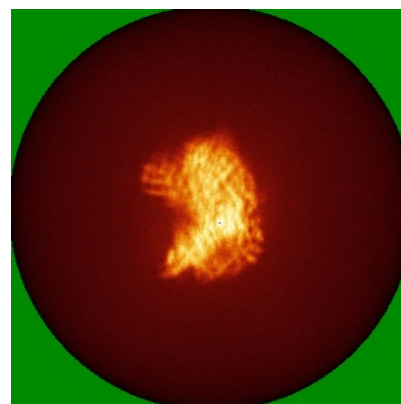
### 6.4.2 Raw map



X



Y



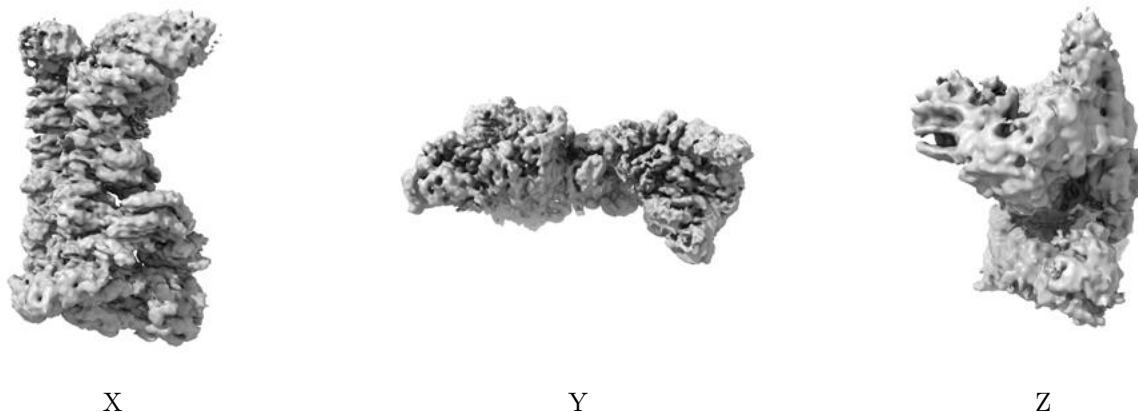
Z

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.



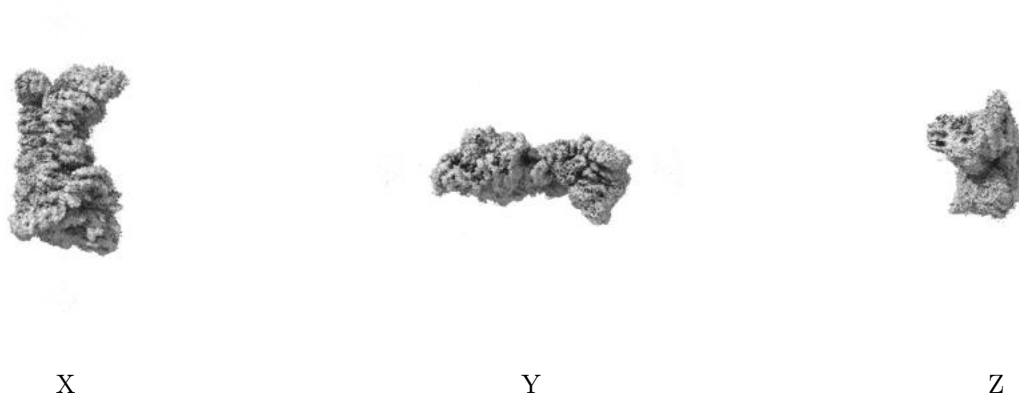
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.



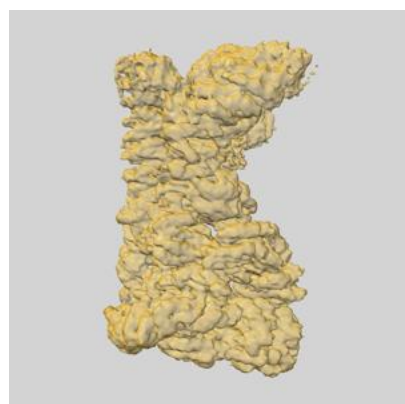
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

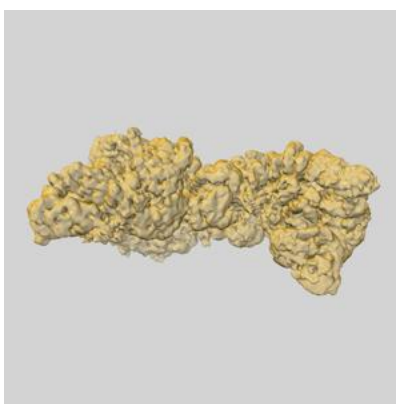
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

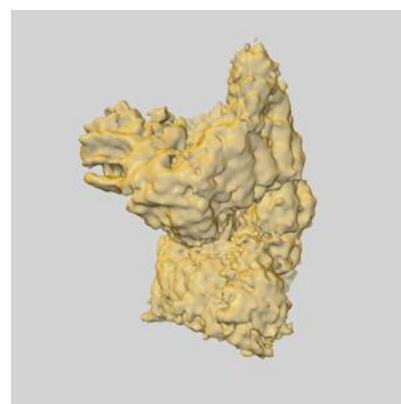
### 6.6.1 emd\_12932\_msk\_2.map [i](#)



X

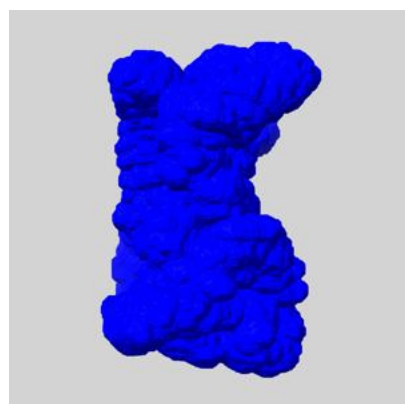


Y

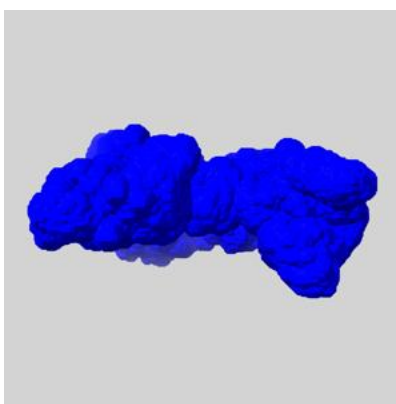


Z

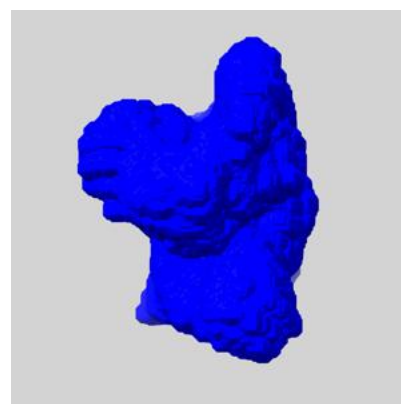
### 6.6.2 emd\_12932\_msk\_1.map [i](#)



X



Y

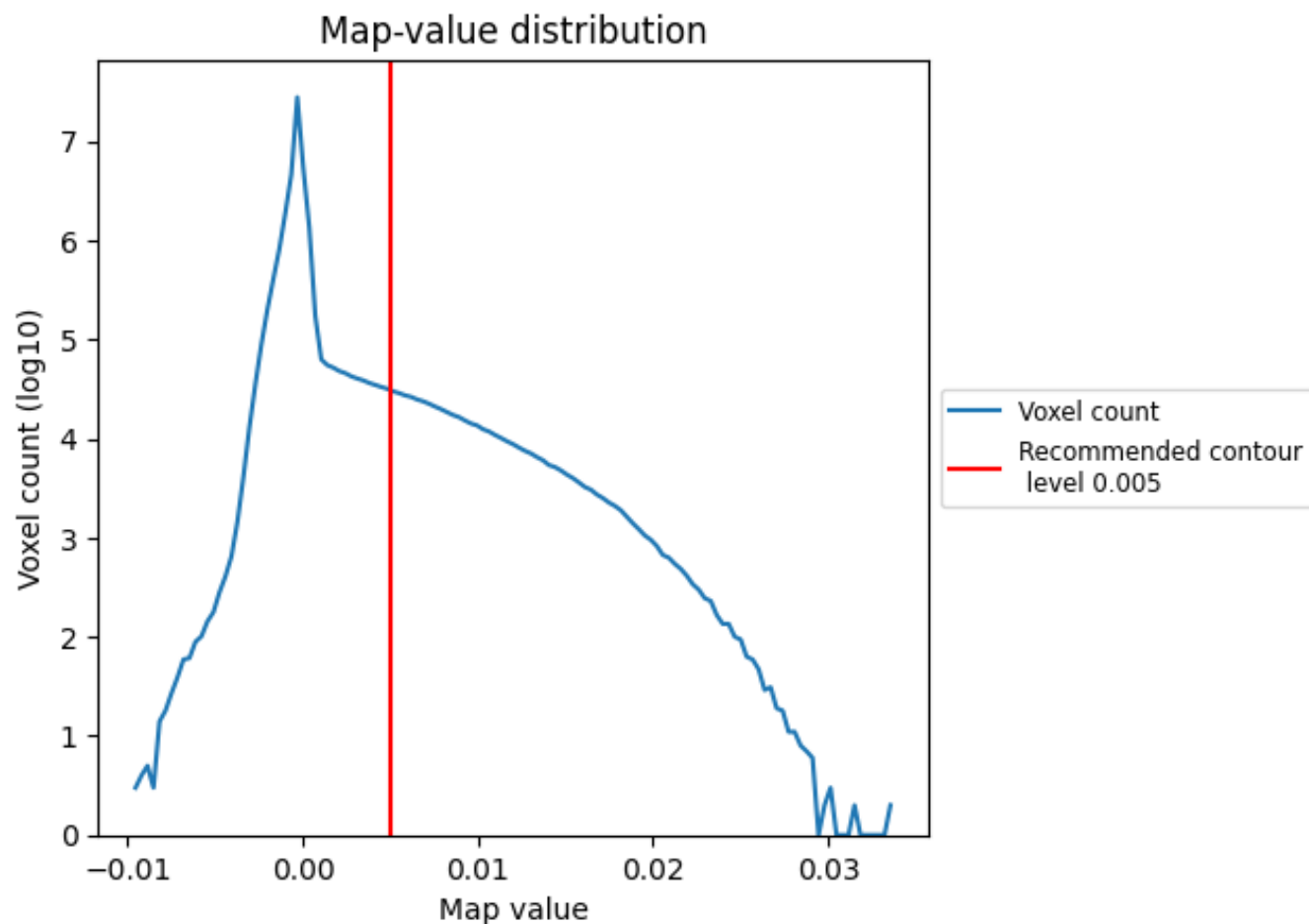


Z

## 7 Map analysis [i](#)

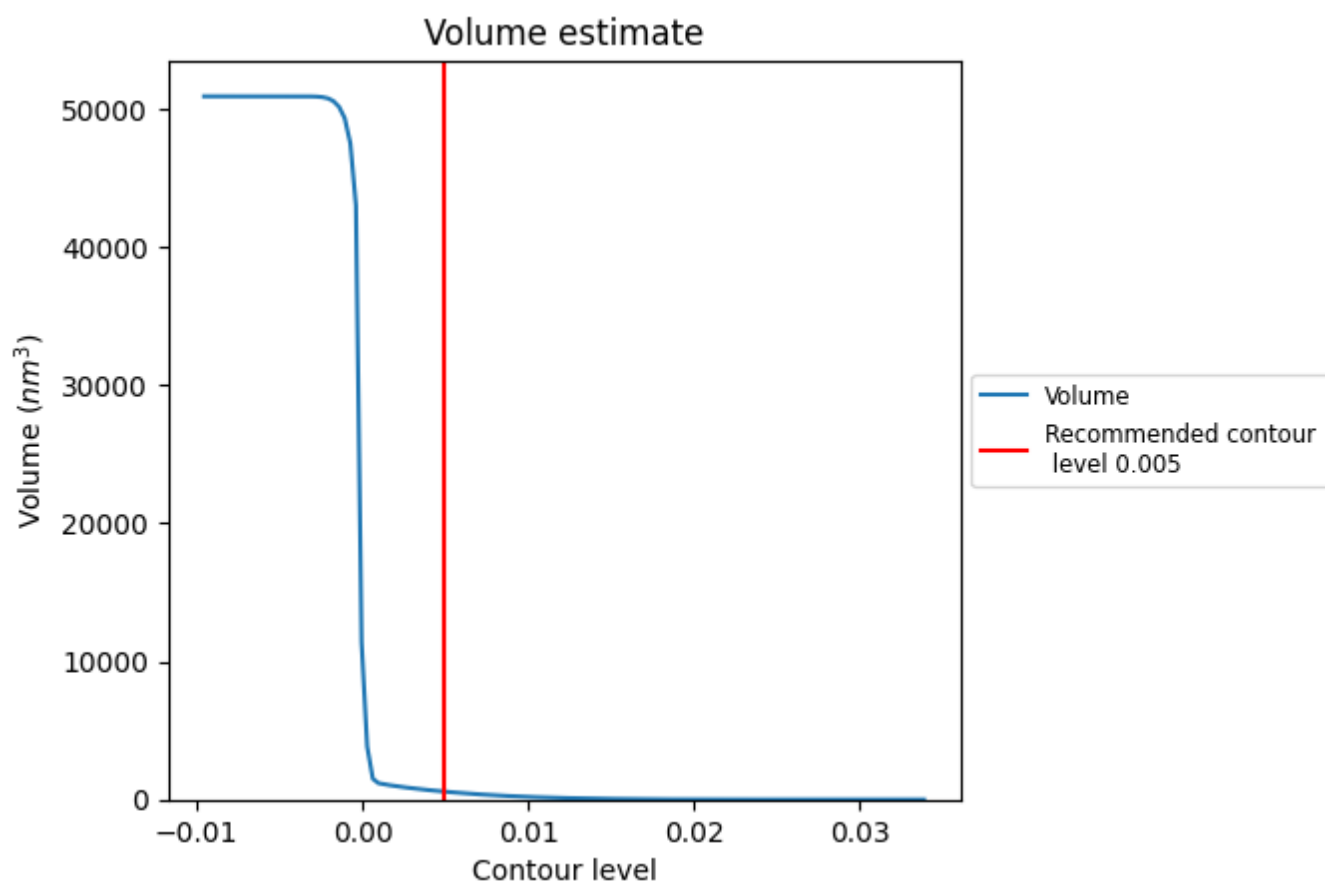
This section contains the results of statistical analysis of the map.

### 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.

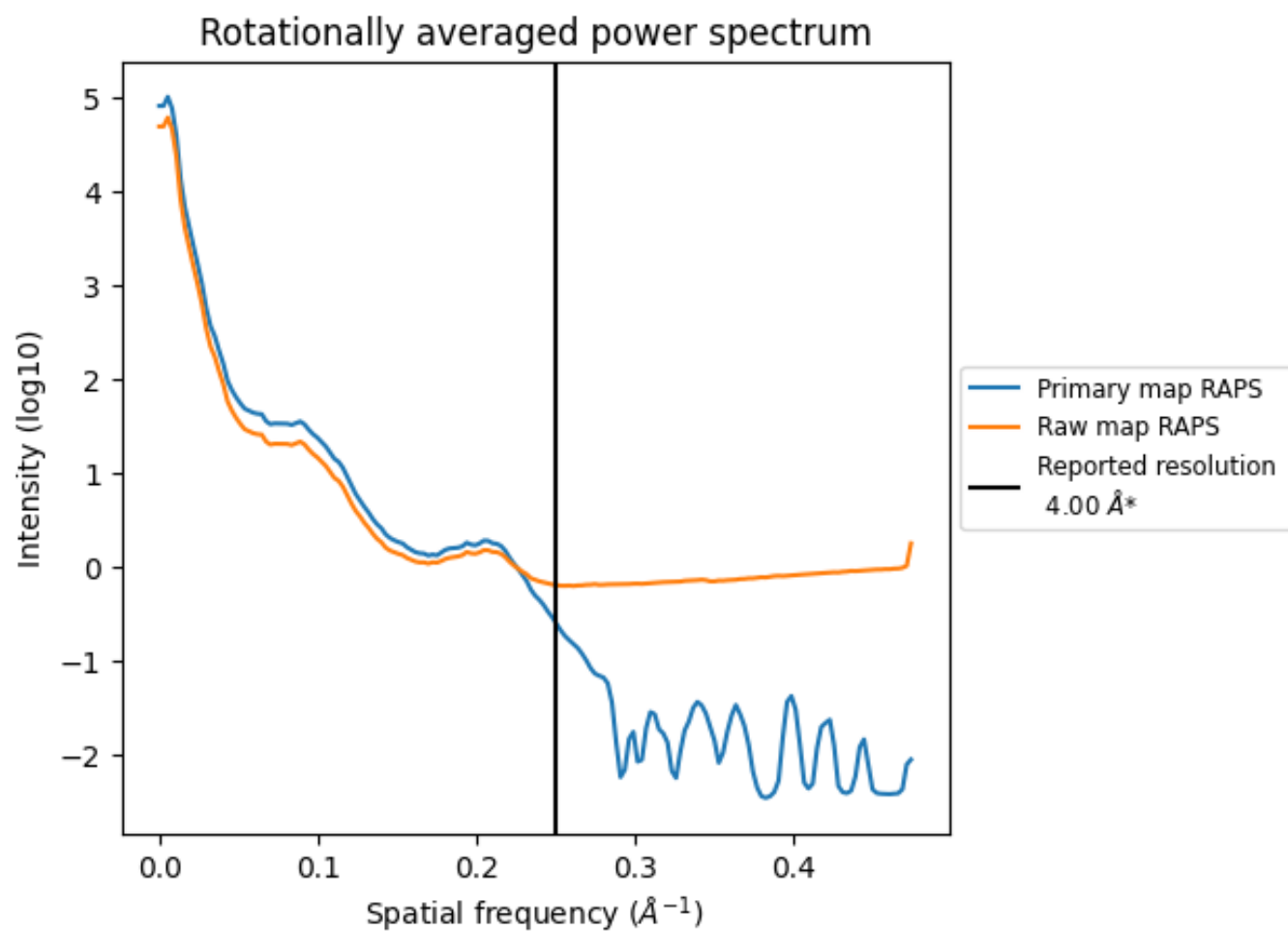
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 572  $\text{nm}^3$ ; this corresponds to an approximate mass of 517 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 [i](#)

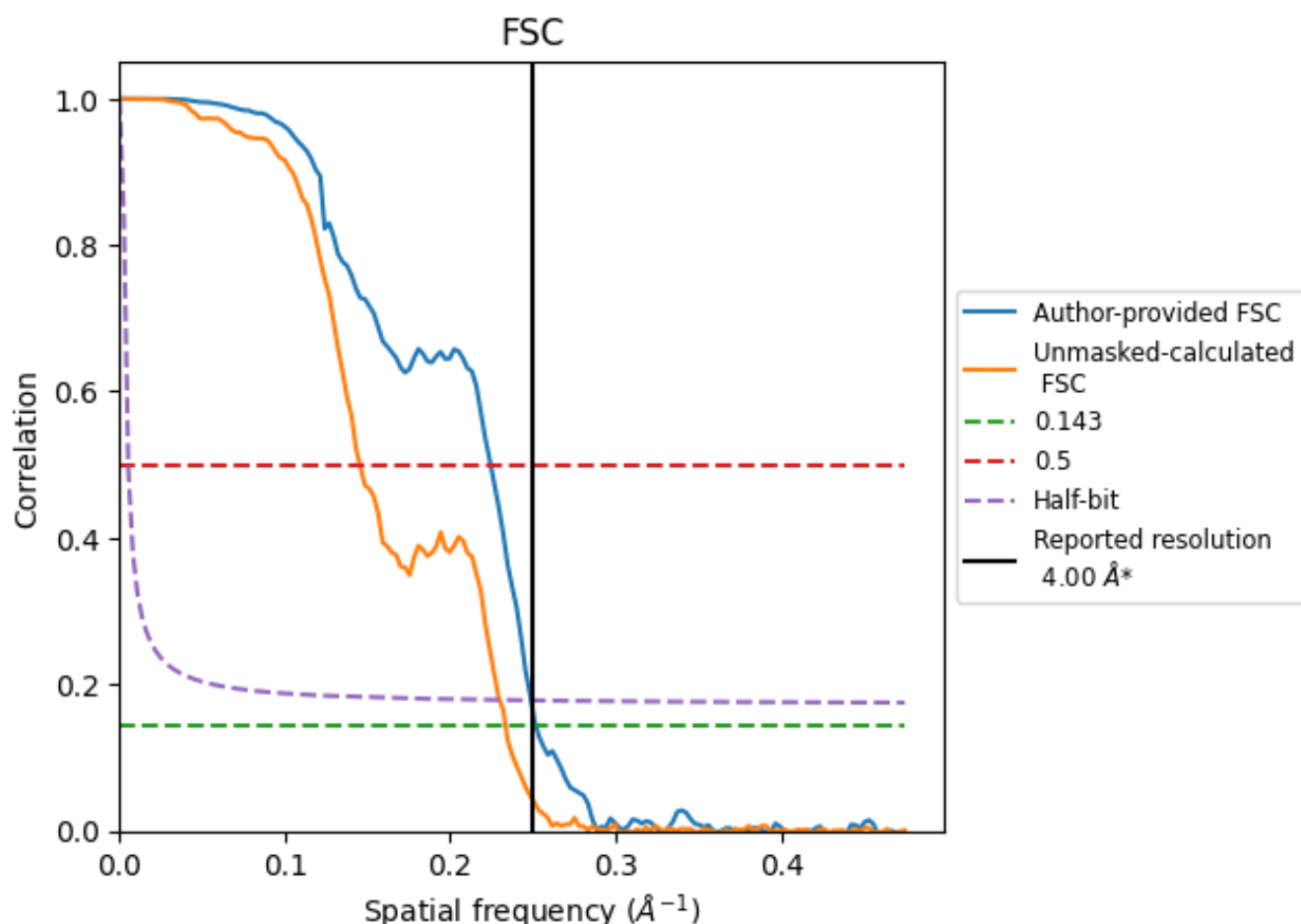


\*Reported resolution corresponds to spatial frequency of 0.250  $\text{\AA}^{-1}$

## 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 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

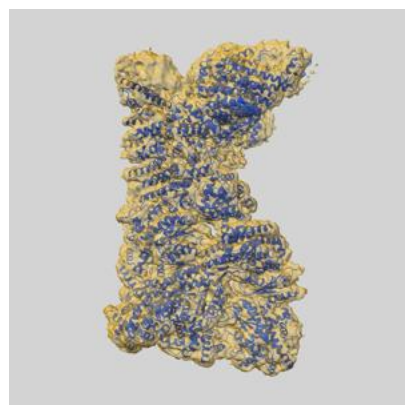
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.46	4.02
Unmasked-calculated*	4.28	6.88	4.35

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

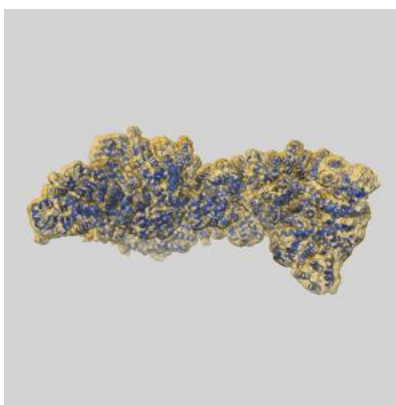
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12932 and PDB model 7OIM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

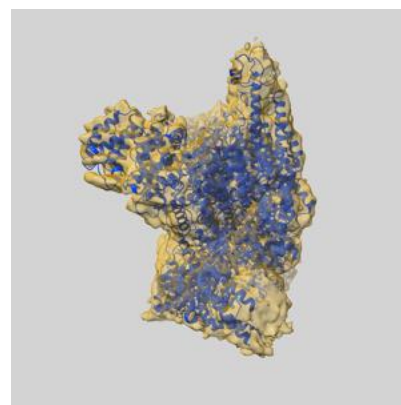
### 9.1 Map-model overlay [i](#)



X



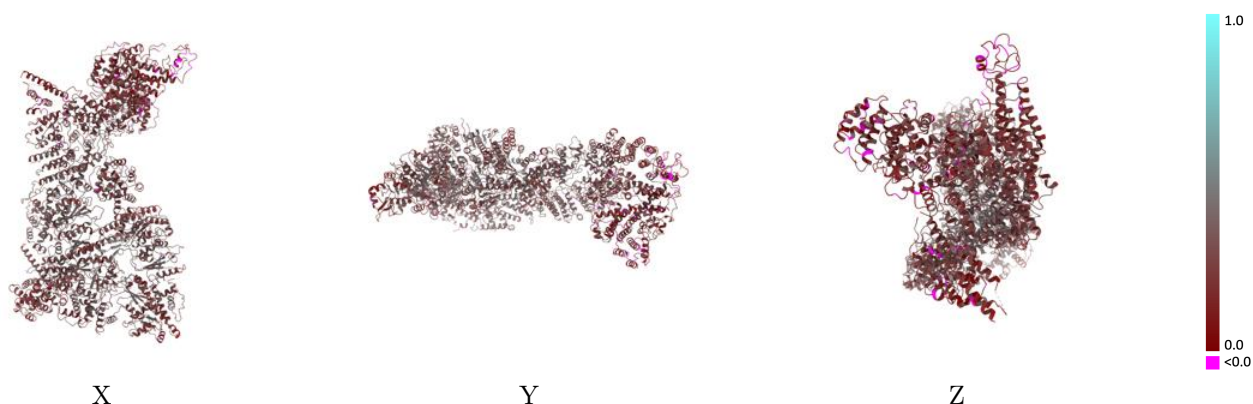
Y



Z

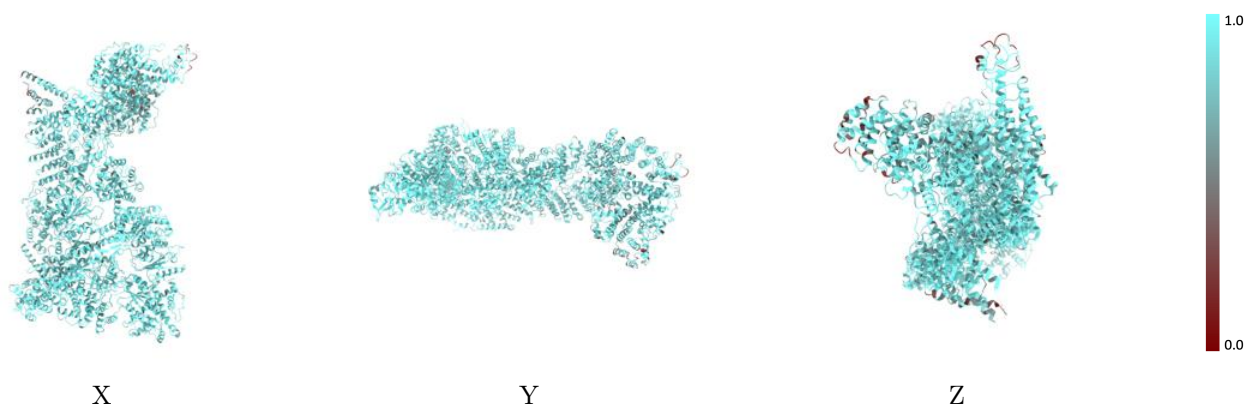
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

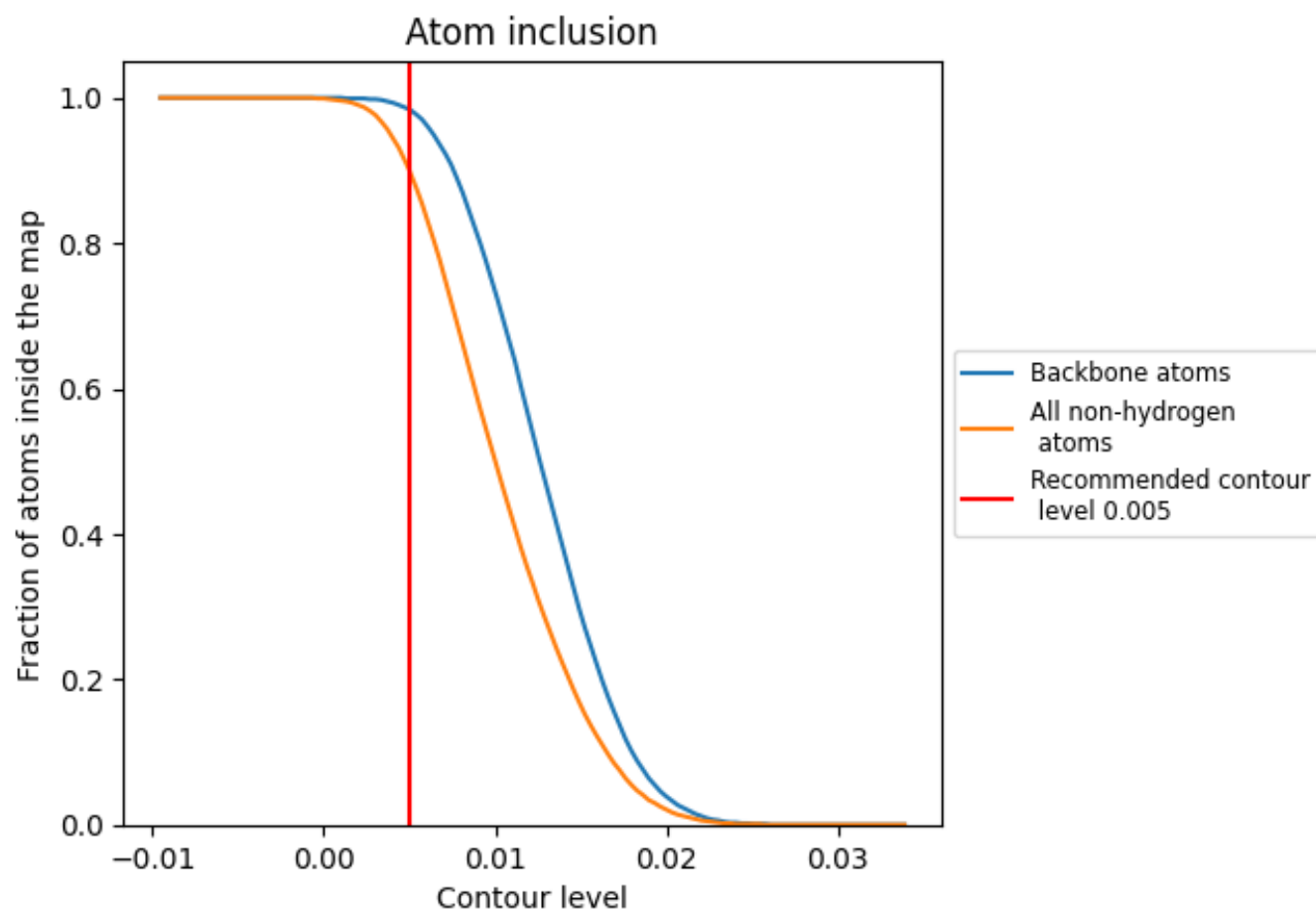
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.005).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 90% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9000	<div><div></div></div> 0.2870
A	<div><div></div></div> 0.9000	<div><div></div></div> 0.2870

