



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:45 PM UTC

PDB ID : 8UXF / pdb_00008uxf
EMDB ID : EMD-42762
Title : Structure of PKA phosphorylated human RyR2-R420W in the primed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.13 Å(reported)
Based on initial model : 7UA5

This is a wwPDB EM Validation Summary 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:

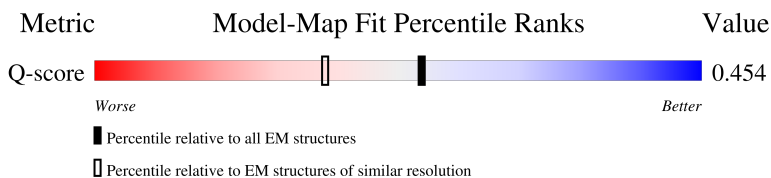
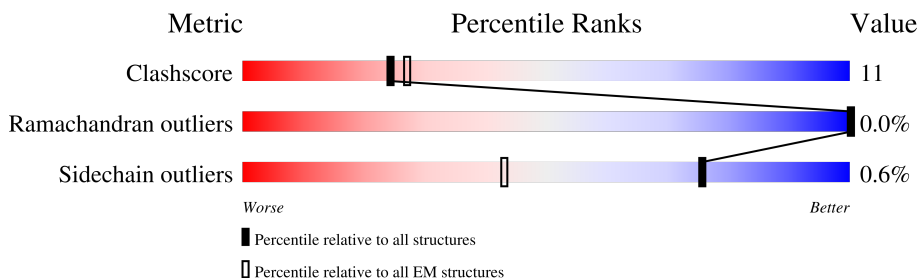
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.13 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	14478 (2.63 - 3.63)

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	4967	 5% 65% 20% 15%
1	B	4967	 5% 65% 20% 15%
1	C	4967	 5% 65% 20% 15%
1	D	4967	 5% 65% 20% 15%

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Mol	Chain	Length	Quality of chain
2	E	108	 77%21%..
2	F	108	 73%24%..
2	G	108	 75%22%..
2	H	108	 74%24%..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138620 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	B	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	C	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	D	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

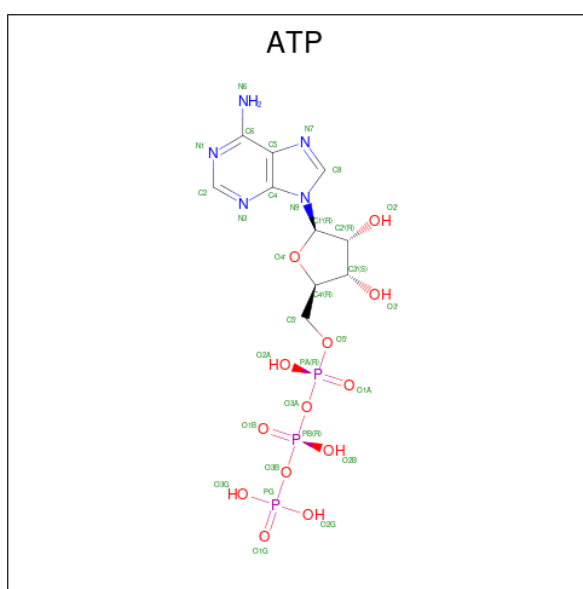
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	F	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	G	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	H	107	Total 818	C 516	N 144	O 154	S 4	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

3 Residue-property plots

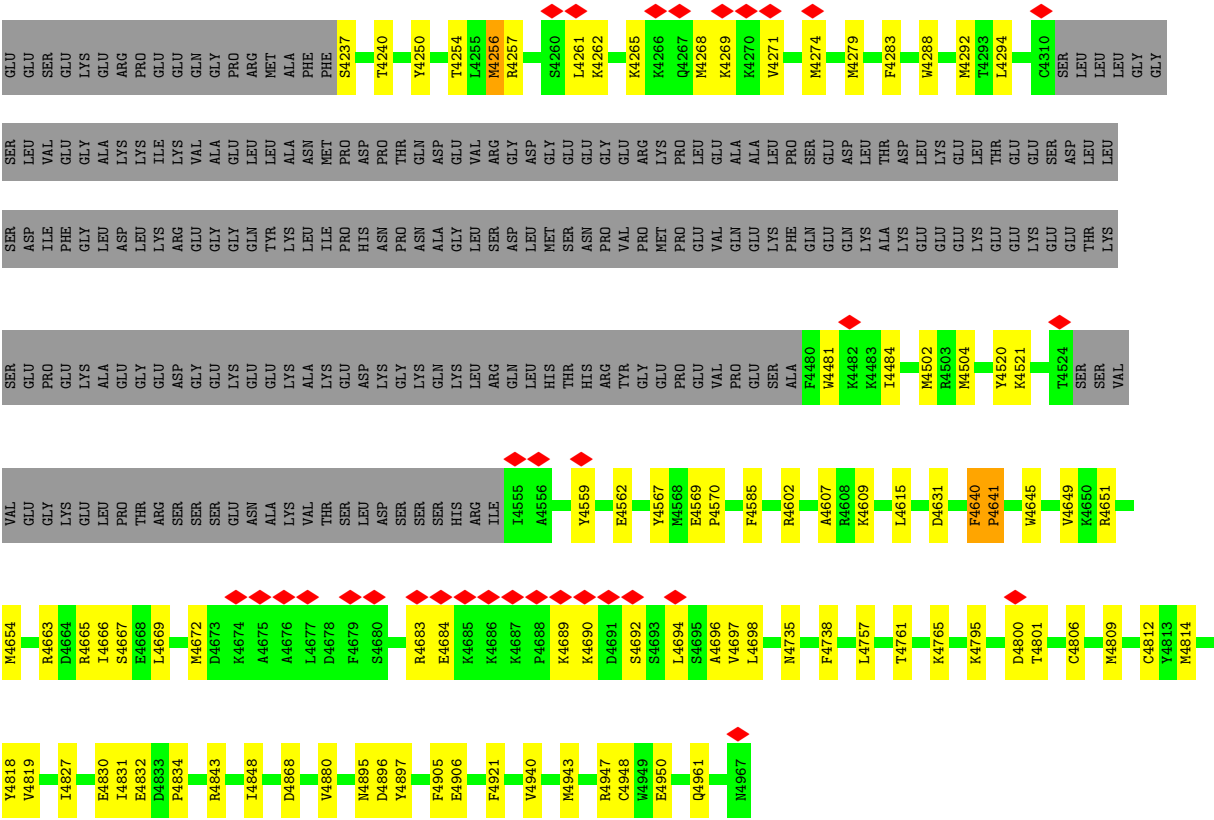
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 2

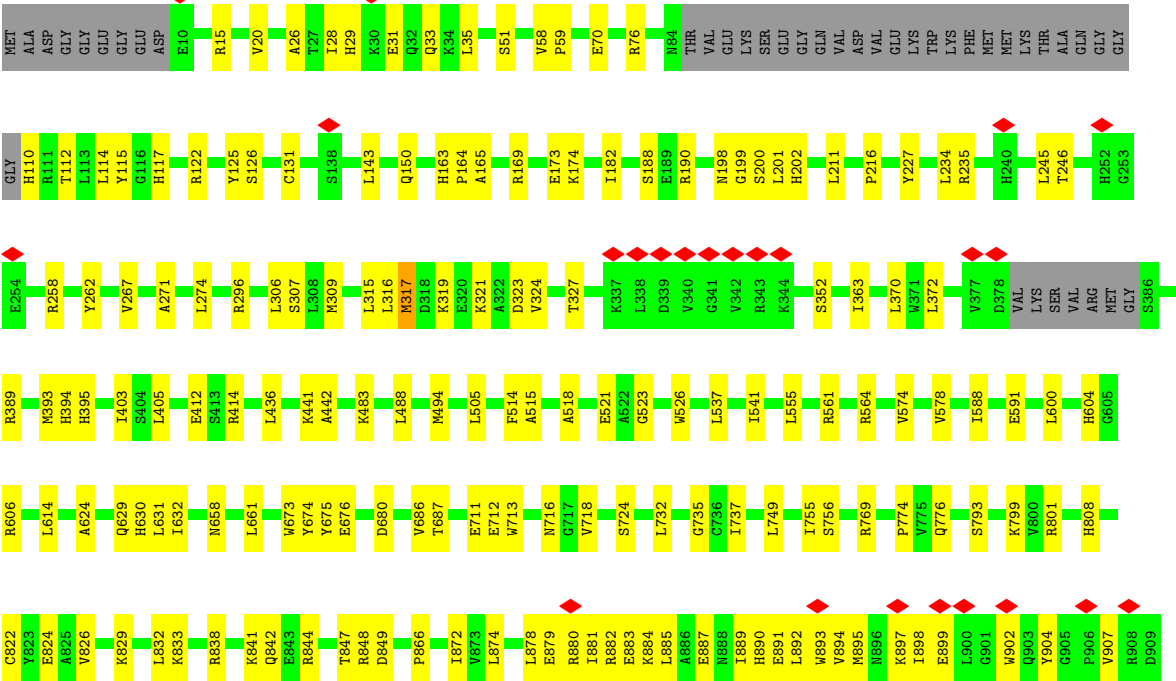






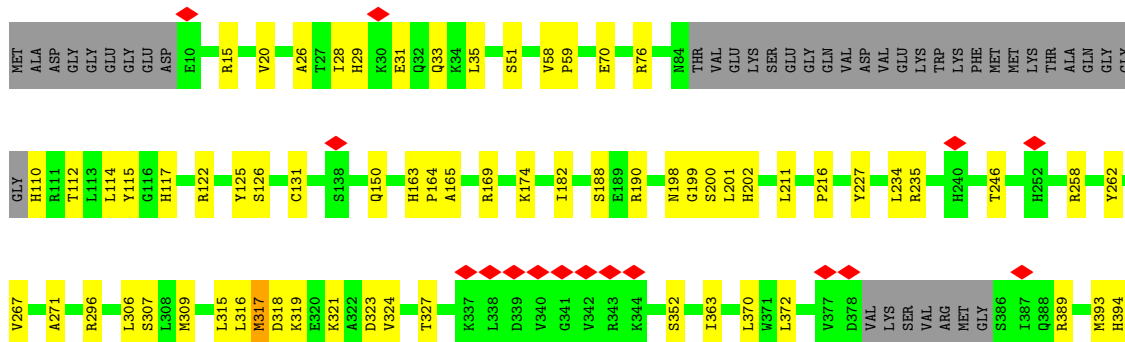
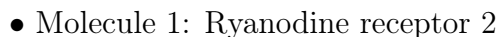


● Molecule 1: Ryanodine receptor 2











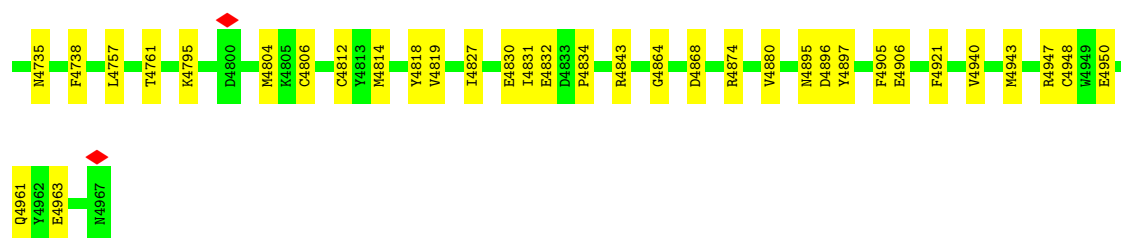
ASN	GLN	ASP	A3294	K3215	L3134	L3057	K2965	E2881	D2796	S2728	I2445	G2273	E2114
ASN	ASN	GLU	W3295	E3216	T3135	R3058	K2966	K2882	S2797	K2731	V2451	E2296	P2115
PHE	VAL	THR	M3296	E3217	S3136	A3059	V2967	A2883	M2798	W2732	D2455	R2303	L2119
VAL	VAL	THR	R3298	V3219	L3137	F3060	L2970	K2885	W2802	M2734	K2456	N2318	R2127
GLN	LEU	THR	L3140		L3140	D3062	Q2973	R2886	THR	D2735	S2457		S2128
ASN	ALA	ARG	S3145		S3145	N3063	F2975	E2887	ARG	K2736	E2658	R2322	L2129
ASN	ASN	LEU	E3149		E3149	E3066	H2978	A2889	ILE	L2737	V2475	R2326	L2130
ASN	ASN	TYR	Q3230		Q3230	D3067	R2979	Q2890	SER	A2738			E2137
MET	PHE	ALA	M3231		M3231	L3068		Q2891	GLN	W2739	Q2481	G2332	E2138
ALA	PHE	THR	R3232		R3232	E3069	L2983	K2894	SER	G2740	L2488	R2336	L2141
ALA	THR	THR	V3234		V3234	T3070	A2986	F2895	GLN	W2741	L2488	G2337	M2142
LEU	LEU	PRO	M3235		M3235	T3071	S2987	L2896	VAL	L2742	G2491	E2338	L2146
LEU	LEU	LEU	P3312		P3312	M3072	K2987	Q2897	SER	Y2743	L2666	N2341	N2152
THR	THR	LEU	Q3313		Q3313	N3073	S2987	VAL	VAL	G2744	L2496	G2342	F2155
ASP	ASP	ILE	L3314		L3314	L3075	P2988	ASP	ALA	L2745	L2502	I2353	
THR	THR	ARG	L3239		L3239	K3076	L2990	ALA	ALA	G2674	M2512	R2359	M2162
LYS	LYS	PHE	P3240		P3240	Q3077	K2999	HIS	HIS	Y2747	L2820	P2364	N2167
SER	VAL	VAL	M3241		M3241	G3078	E3002	G2820	G2820	S2748	G2537	ASN	H2168
LYS	ASP	ASP	M3246		M3246	Q3079	M3003	Y2821	Y2821	S2750	E2570	SER	E2172
LYS	TYR	TYR				F3080	K3010	P2823	P2823	S2751	R2548	GLY	E2173
SER	ASN	ASN	W3250		W3250	T3081	S3013	A2825	A2825	K2752	R2554	SER	
ALA	ALA	ALA					V3015	I2826	I2826	M2688		LYS	G2181
LYS	LYS	LYS	N3256		N3256	THR	V3015	D2827	D2827	K2691	E2570	THR	G2182
VAL	TRP	TRP	E3259		E3259	ARG	R3016	N2830	N2830	Q2692	L2573	ASP	E2183
SER	LEU	LEU	R3260		R3260	ASN	R3018	F2925	F2925	S2694	R2581	THR	S2184
ASP	ASP	ASP	A3261		A3261	GLN	S3020	L2926	L2926	M2695		GLU	K2185
GLN	GLU	GLU	K3262		K3262	PRO	L3021	Q2927	Q2927	D2696	E2377	GLU	E2186
GLU	PRO	PRO	M3263		M3263		D3025	Q2928	Q2928	S2697	E2377		
ARG	ASN	ASN	K3328		K3328	K3088	A3026	L2929	L2929	E2698	M2584	E2378	F2199
LYS	PRO	PRO	A3330		A3330	G3089	T3027	I2930	I2930	G2699	Q2586	D2379	
LYS	LYS	GLU	T3266		T3266	V3090	I3029	H2937	H2937	N2700	L2589	D2380	Y2202
MET	ALA	ALA	A3267		A3267		I3035	D2944	D2944	F2701	I2382	I2206	
LYS	GLU	GLU	L3268		L3268		I3036	G2945	G2945	N2702		F2215	
ARG	GLU	GLU	N3269		N3269		T3039	Q2946	Q2946	P2703		P2232	
LYS	LEU	LEU	S3270		S3270		L3040	R2947	R2947	Q2704		P2233	
GLY	PHE	PHE	E3271		E3271		A3042	R2948	R2948	P2705		N2401	
ASP	ARG	ARG	M3272		M3272		Q3041	Q2949	Q2949	N2706		R2402	
ASP	MET	MET	K3273		K3273		R3043	K2950	K2950	T2707		A2403	
TYR	VAL	VAL	N3274		N3274		V3044	E2951	E2951	T2708		N2251	
ALA	ALA	ALA	T3275		T3275		V3045	E2952	E2952	N2710		E2252	
MET	GLU	GLU	L3276		L3276		R3128	H2953	H2953	I2711		L2253	
GLN	VAL	VAL	L3277		L3277		V3128	Q2954	Q2954	K2716		R2258	
THR	PHE	PHE	G3278		G3278		G3129	P2955	P2955	F2720		E2259	
SER	ILE	ILE	N3279		N3279		K3046	Y2956	Y2956			Q2441	
LEU	LEU	LEU	I3280		I3280		R3132	E2957	E2957	K2723		M2442	
VAL	VAL	VAL	T3283		T3283		I3133	Q2958	Q2958	Y2724		P2443	
ALA	ALA	ALA	L3284		L3284			I2960	I2960			T2444	
ALA	LYS	LYS	Y3285		Y3285								
ALA	ASP	ASP											
MET	ASN	ASN	L3288		L3288								
ARG	PHE	PHE	G3289		G3289								
LEU	LYS	LYS	L3290		L3290								
LEU	ARG	ARG	D3291		D3291								
PRO	GLU	GLU	E3292		E3292								
ILE	ILE	ILE	G3293		G3293								





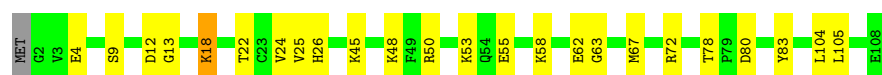






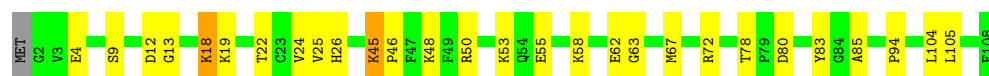
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: ..



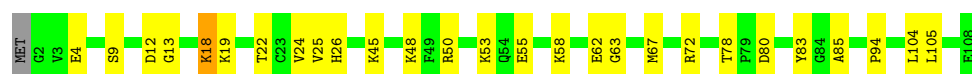
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	102478	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.646	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	430.848, 430.848, 430.848	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8415, 0.8415, 0.8415	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/34516	0.41	4/46623 (0.0%)
1	B	0.19	0/34516	0.41	4/46623 (0.0%)
1	C	0.19	0/34516	0.41	4/46623 (0.0%)
1	D	0.19	0/34516	0.41	4/46623 (0.0%)
2	E	0.20	0/834	0.41	0/1123
2	F	0.20	0/834	0.41	0/1123
2	G	0.20	0/834	0.41	0/1123
2	H	0.20	0/834	0.41	0/1123
All	All	0.19	0/141400	0.41	16/190984 (0.0%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3215	MET	CB-CG-SD	5.48	129.15	112.70
1	C	3215	MET	CB-CG-SD	5.48	129.14	112.70
1	B	3215	MET	CB-CG-SD	5.47	129.12	112.70
1	D	3215	MET	CB-CG-SD	5.47	129.12	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3310	VAL	CA-C-N	5.12	128.46	120.68

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3926	GLY	Peptide
1	A	4640	PHE	Peptide
1	B	3926	GLY	Peptide
1	B	4640	PHE	Peptide
1	C	3926	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33774	0	33452	740	0
1	B	33774	0	33452	737	0
1	C	33774	0	33452	724	0
1	D	33774	0	33452	740	0
2	E	818	0	821	15	0
2	F	818	0	821	18	0
2	G	818	0	821	17	0
2	H	818	0	821	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
All	All	138620	0	137188	2938	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 11.

The worst 5 of 2938 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:B:3235:MET:HA	1:B:3239:LEU:HD13	1.41	1.03
1:D:3235:MET:HA	1:D:3239:LEU:HD13	1.41	1.02
1:C:3235:MET:HA	1:C:3239:LEU:HD13	1.41	1.02
1:A:3235:MET:HA	1:A:3239:LEU:HD13	1.41	1.02
1:B:1564:MET:HE3	1:B:1565:PRO:HD2	1.51	0.93

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	4198/4967 (84%)	4097 (98%)	99 (2%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4098 (98%)	98 (2%)	2 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17212/20300 (85%)	16802 (98%)	402 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG
1	A	4641	PRO
1	B	2988	ARG
1	B	4641	PRO

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Mol	Chain	Res	Type
1	C	2988	ARG

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	3708/4358 (85%)	3688 (100%)	20 (0%)	81	82
1	B	3708/4358 (85%)	3688 (100%)	20 (0%)	81	82
1	C	3708/4358 (85%)	3688 (100%)	20 (0%)	81	82
1	D	3708/4358 (85%)	3688 (100%)	20 (0%)	81	82
2	E	88/89 (99%)	86 (98%)	2 (2%)	44	66
2	F	88/89 (99%)	86 (98%)	2 (2%)	44	66
2	G	88/89 (99%)	86 (98%)	2 (2%)	44	66
2	H	88/89 (99%)	86 (98%)	2 (2%)	44	66
All	All	15184/17788 (85%)	15096 (99%)	88 (1%)	76	80

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3241	MET
1	D	2884	LYS
1	C	4002	MET
1	D	1300	MET
1	D	3190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1294	ASN
1	C	4178	ASN
2	F	26	HIS
1	C	1581	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3111	HIS

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
4	ATP	D	5002	-	32,33,33	0.34	0	48,52,52	0.36	0
4	ATP	C	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	B	5002	-	32,33,33	0.33	0	48,52,52	0.36	0
4	ATP	D	5003	-	32,33,33	0.26	0	48,52,52	0.28	0
4	ATP	A	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	B	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.34	0	48,52,52	0.36	0
4	ATP	A	5002	-	32,33,33	0.34	0	48,52,52	0.36	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
4	ATP	D	5002	-	-	10/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	10/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	10/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	10/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

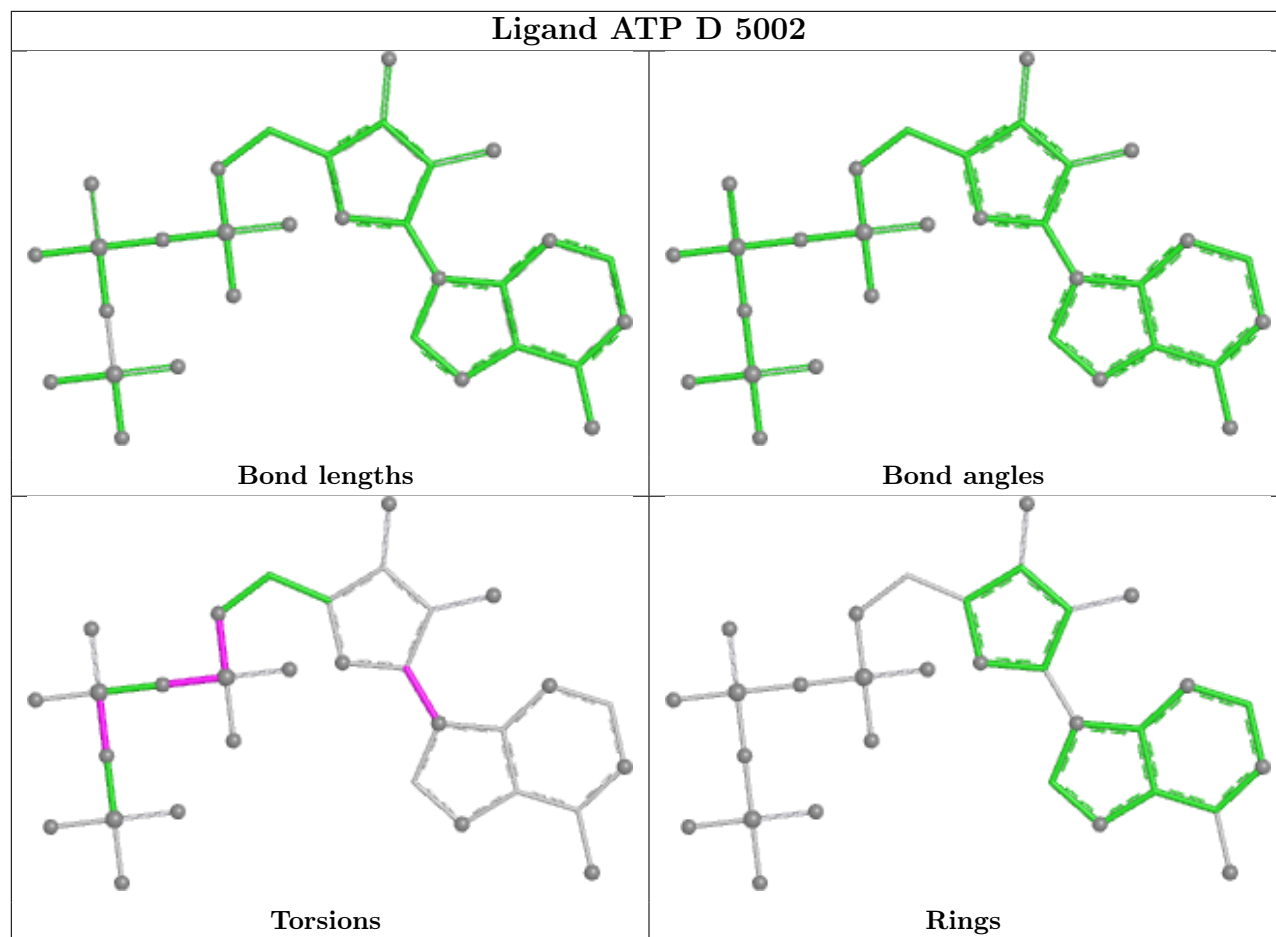
5 of 68 torsion outliers are listed below:

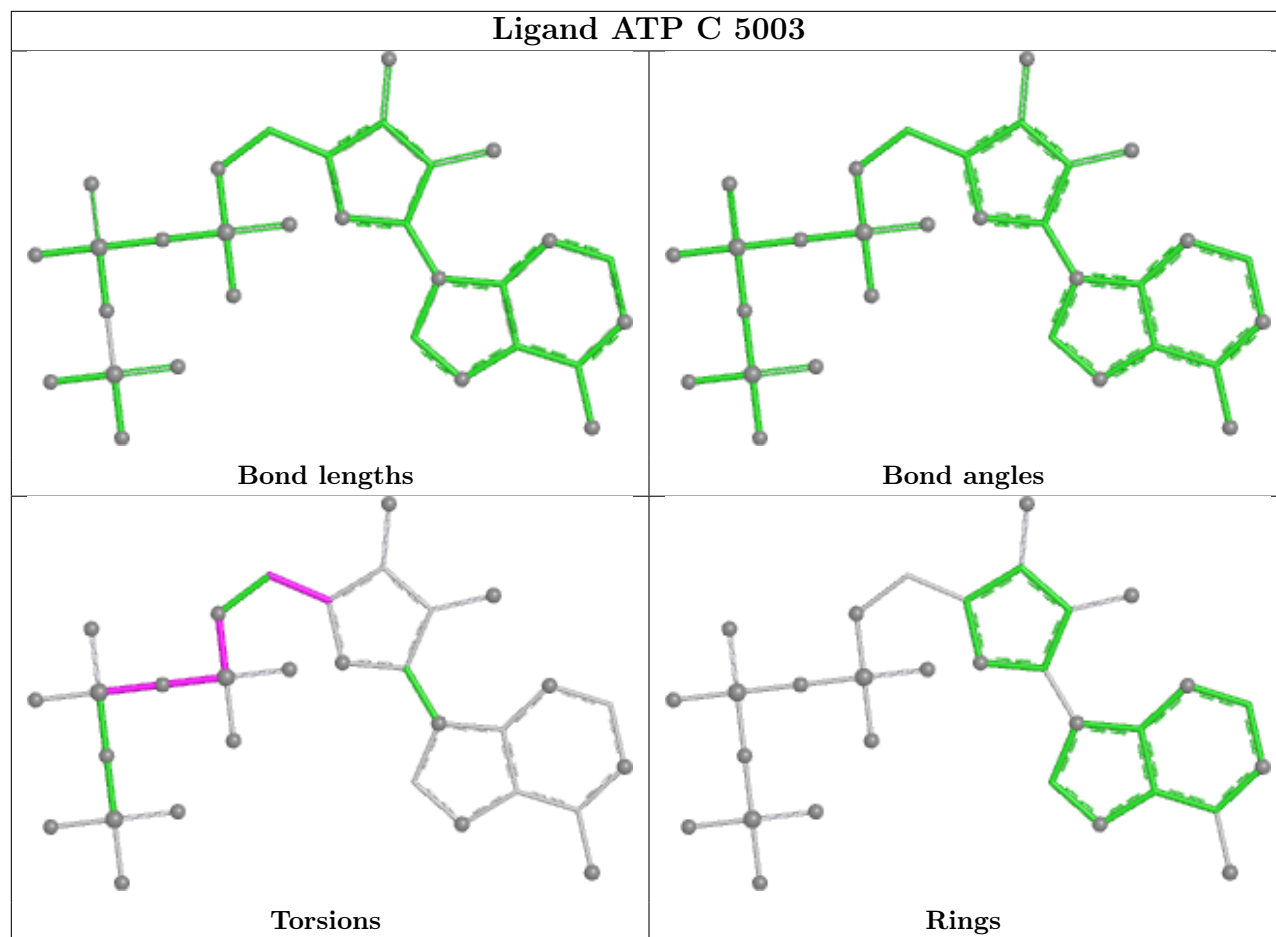
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A

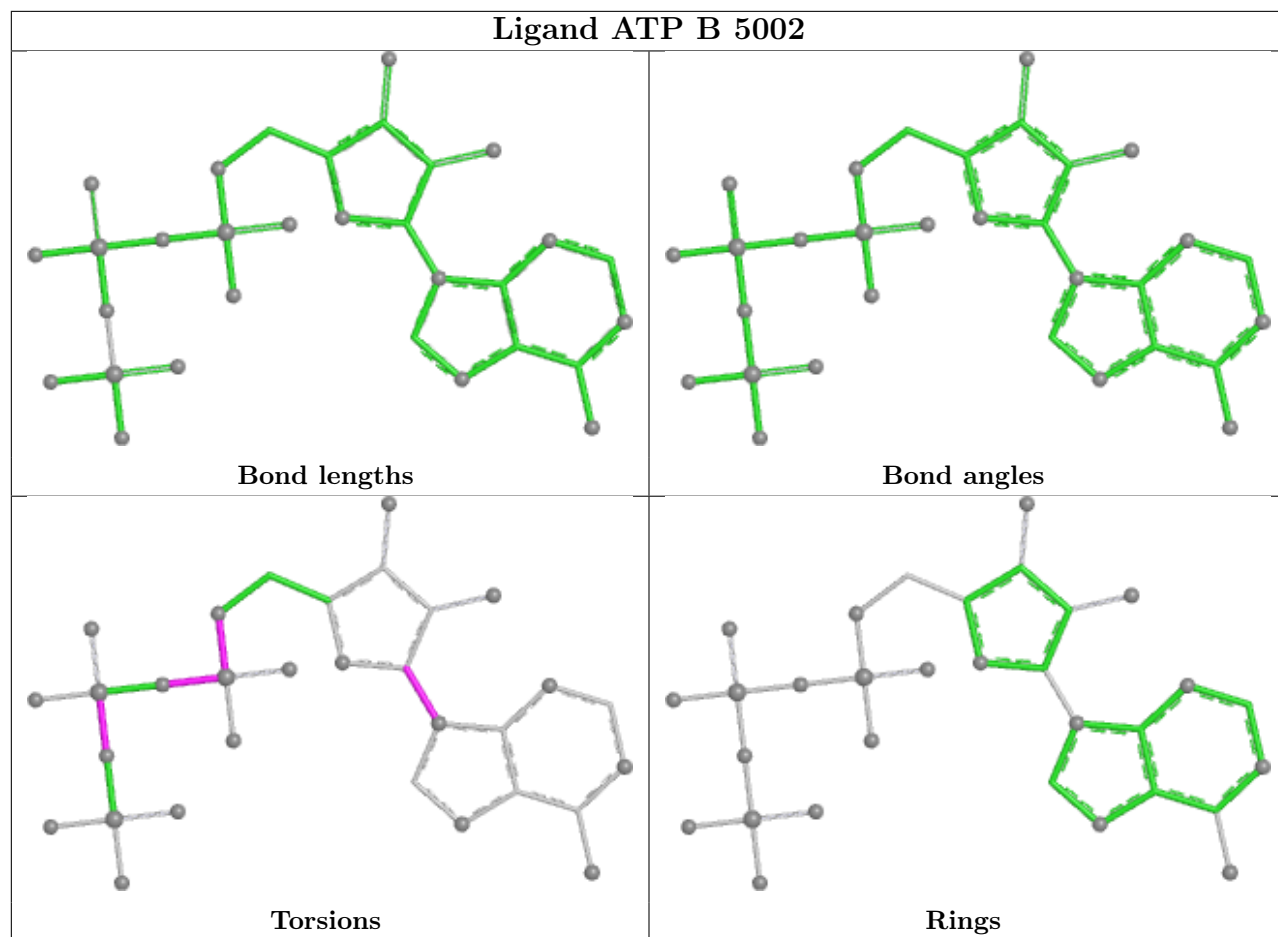
There are no ring outliers.

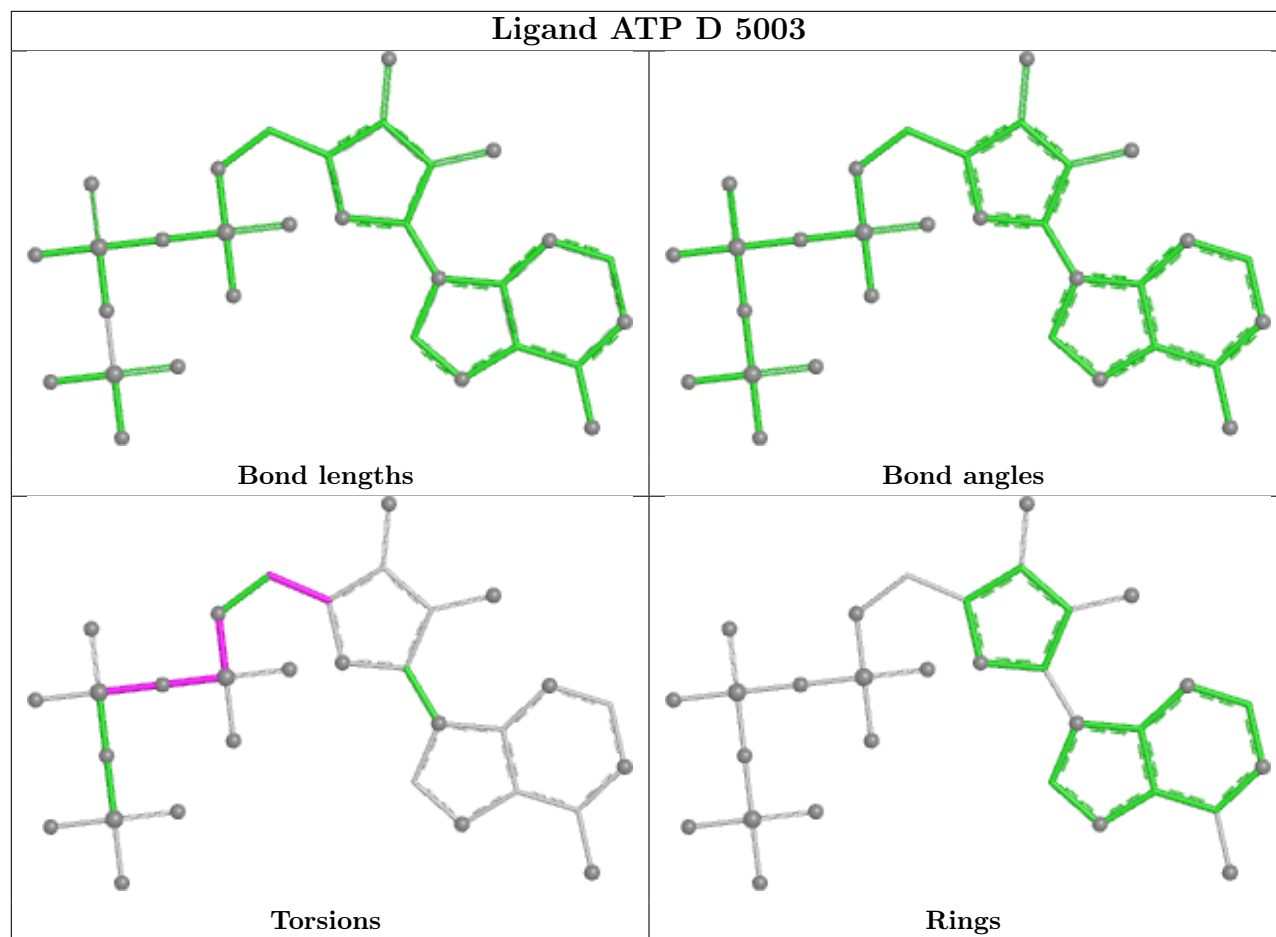
No monomer is involved in short contacts.

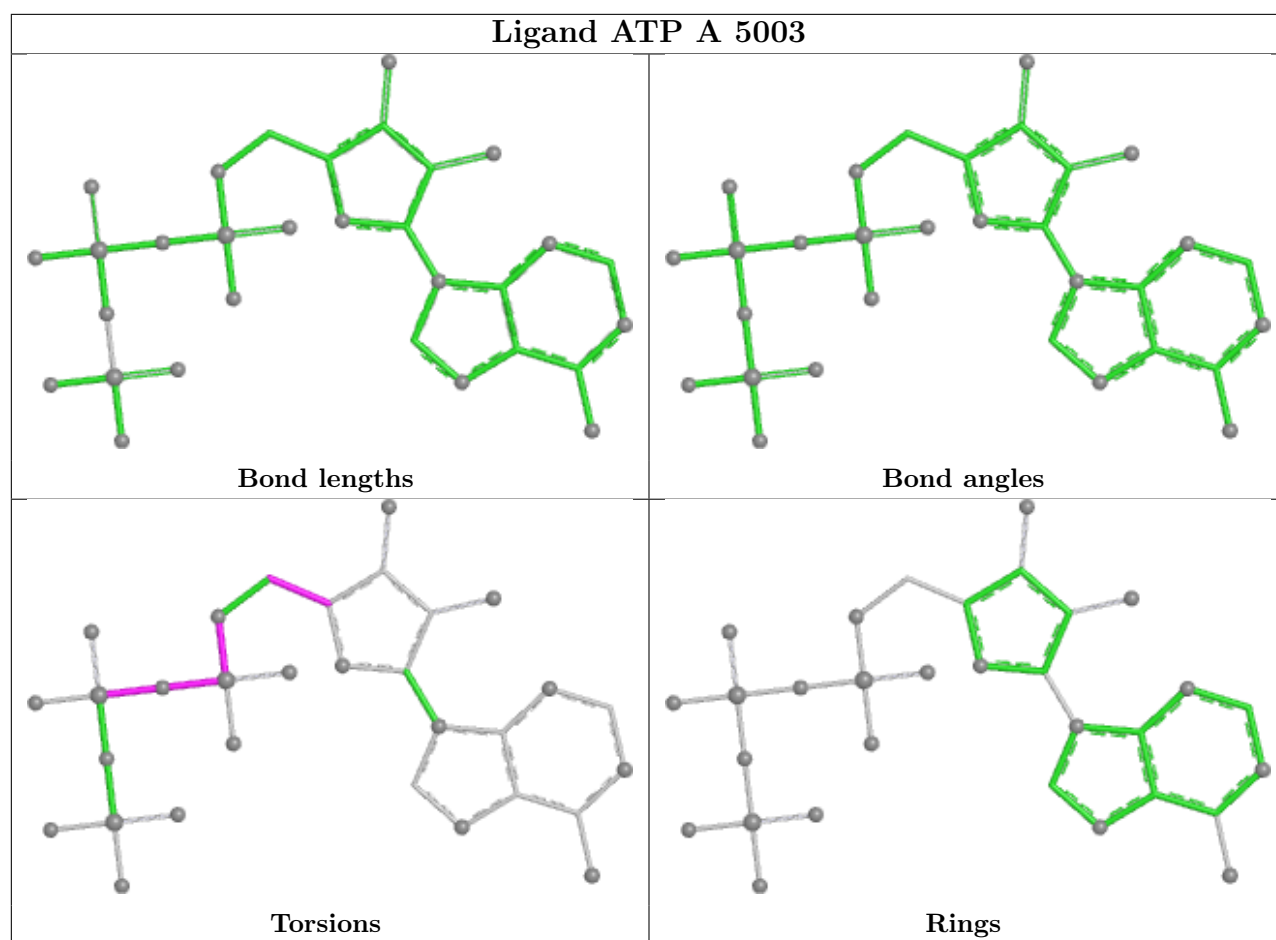
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

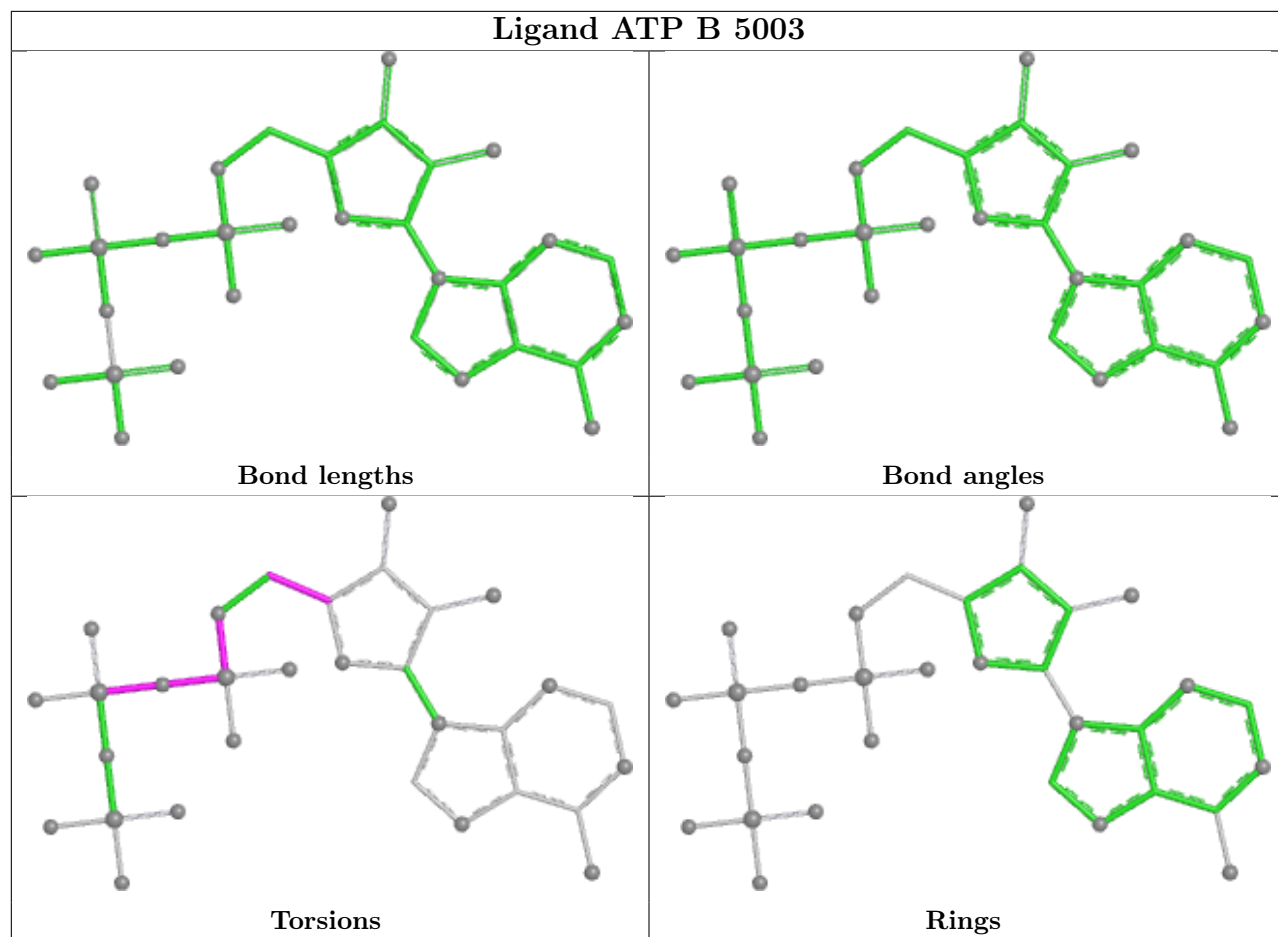


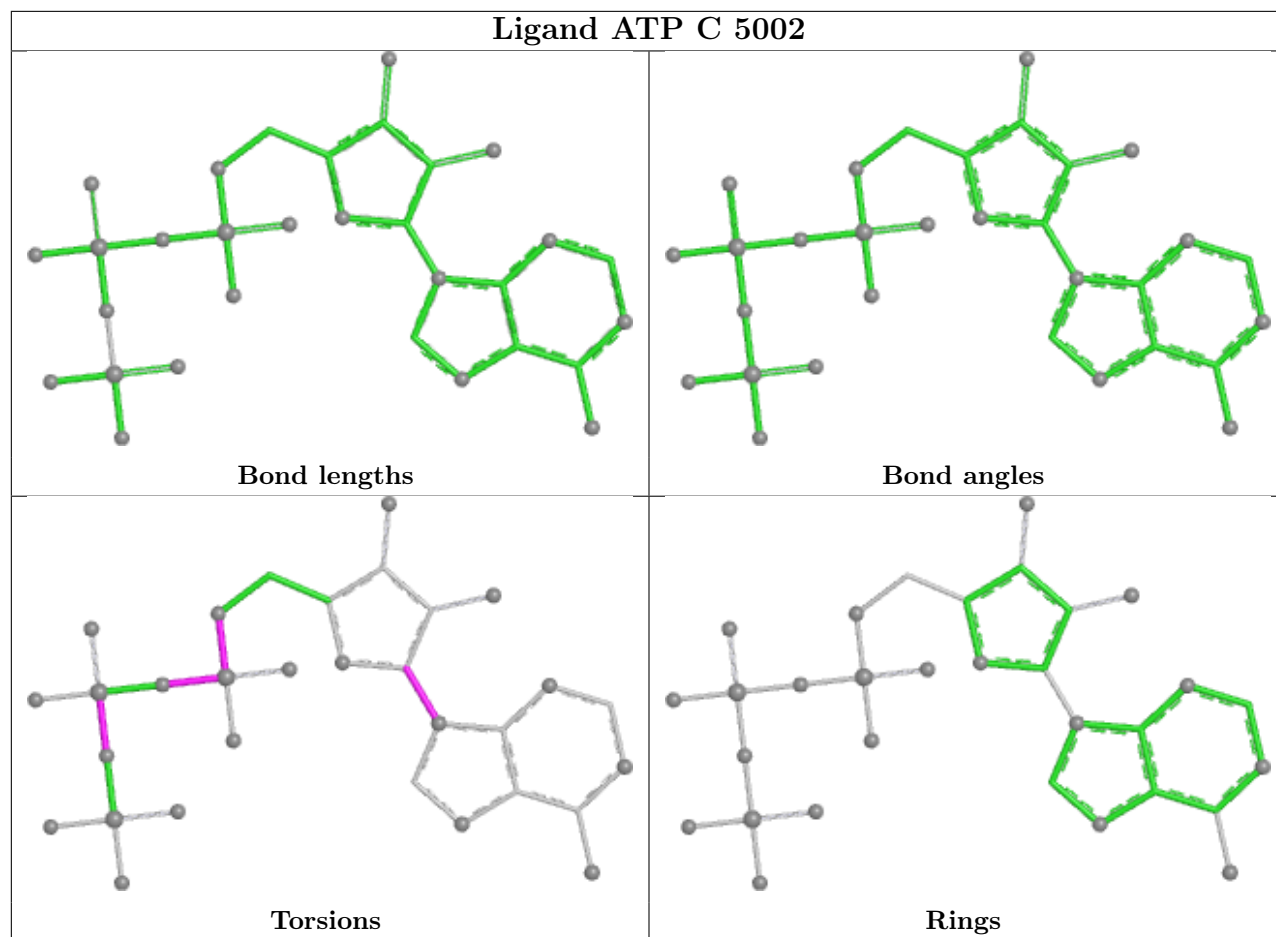


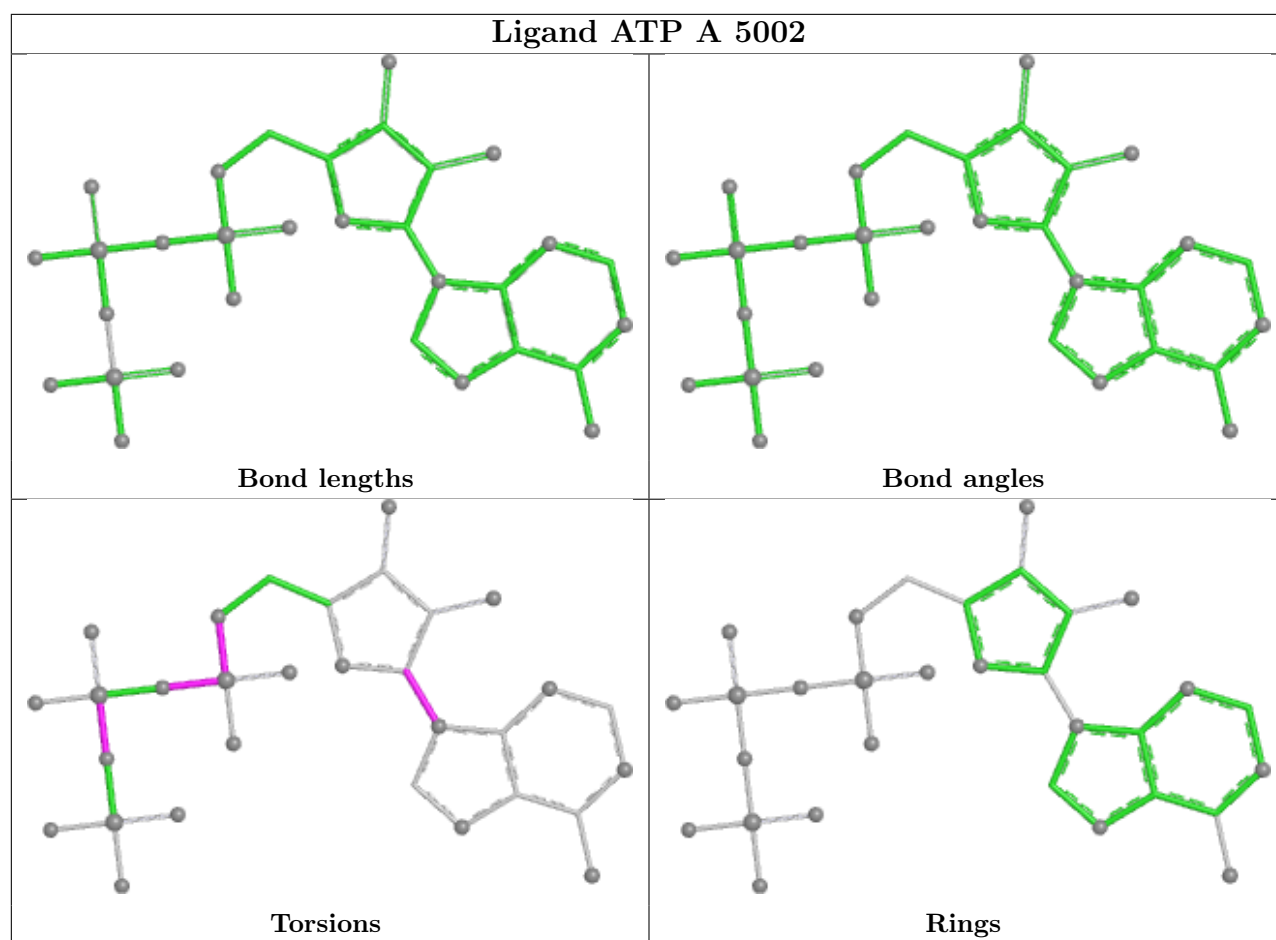












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42762. These allow visual inspection of the internal detail of the map and identification of artifacts.

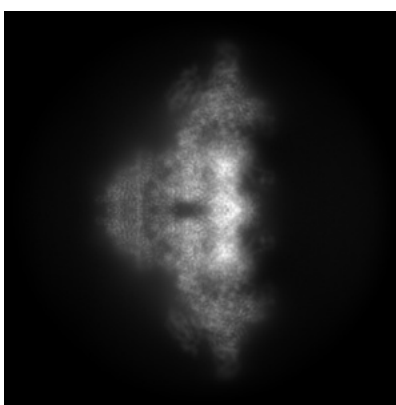
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

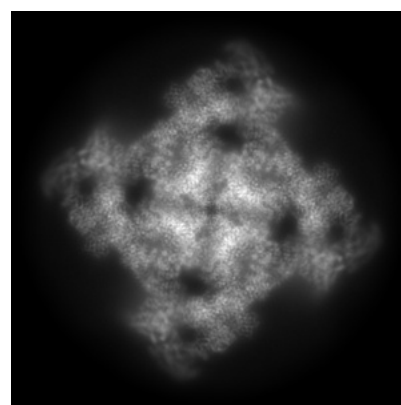
6.1.1 Primary map



X



Y

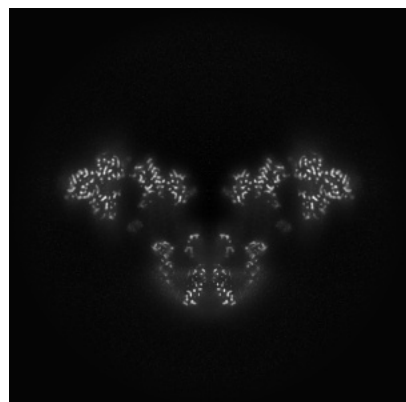


Z

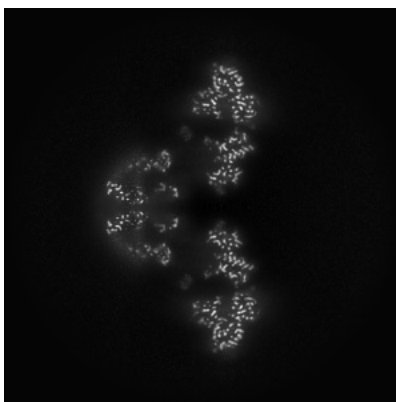
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

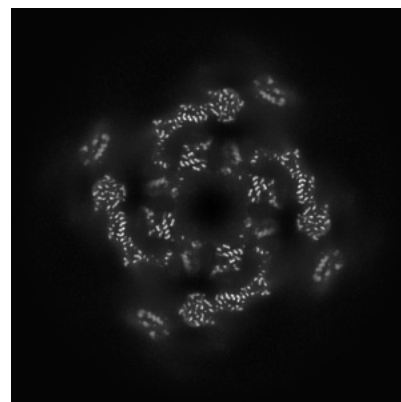
6.2.1 Primary map



X Index: 256



Y Index: 256

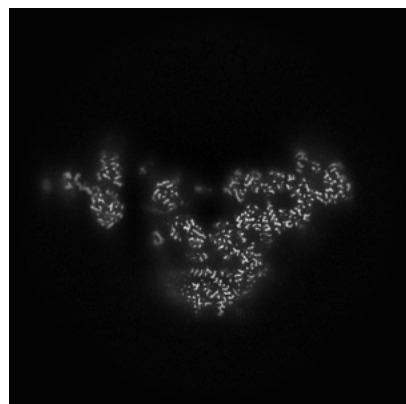


Z Index: 256

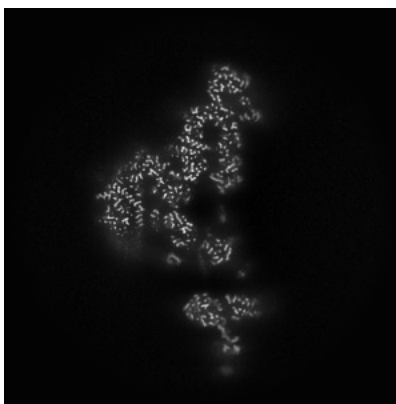
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

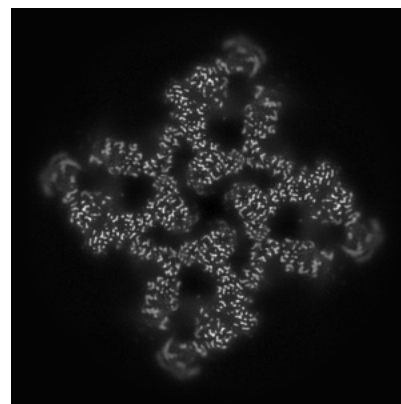
6.3.1 Primary map



X Index: 238



Y Index: 274

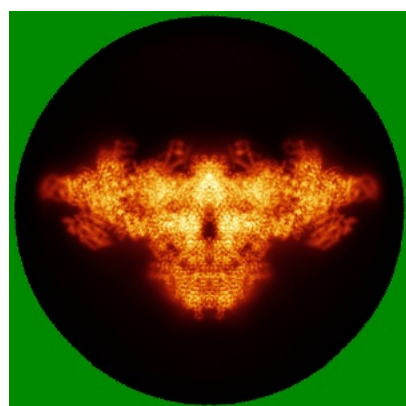


Z Index: 282

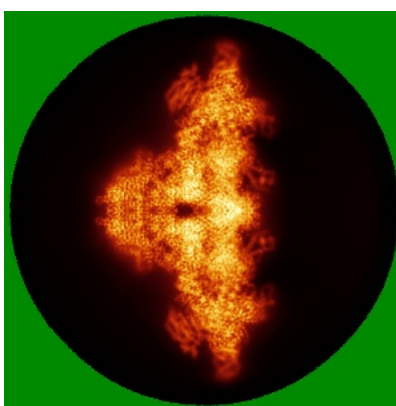
The images above show the largest variance slices of the map in three orthogonal directions.

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

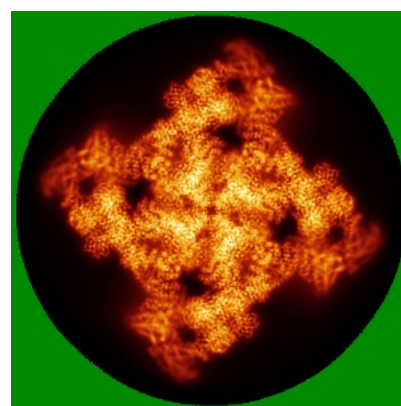
6.4.1 Primary map



X



Y

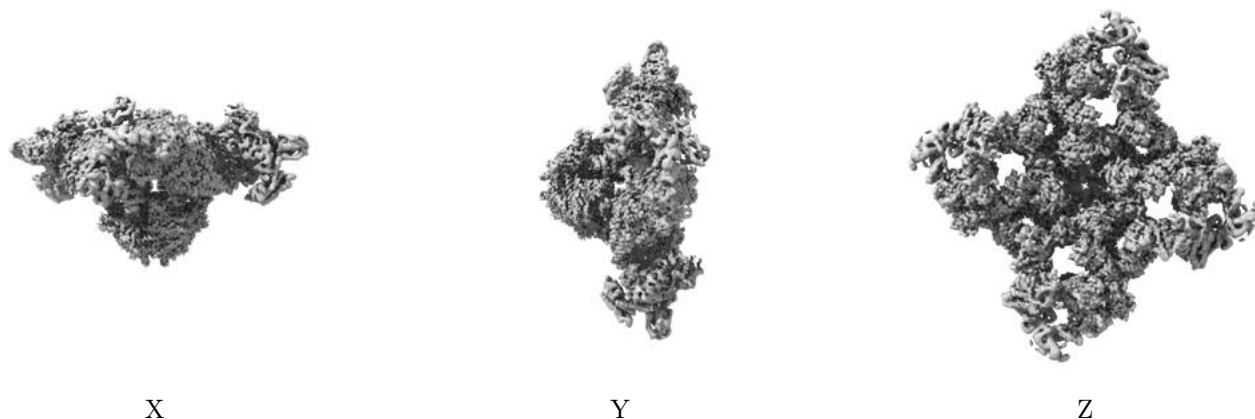


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

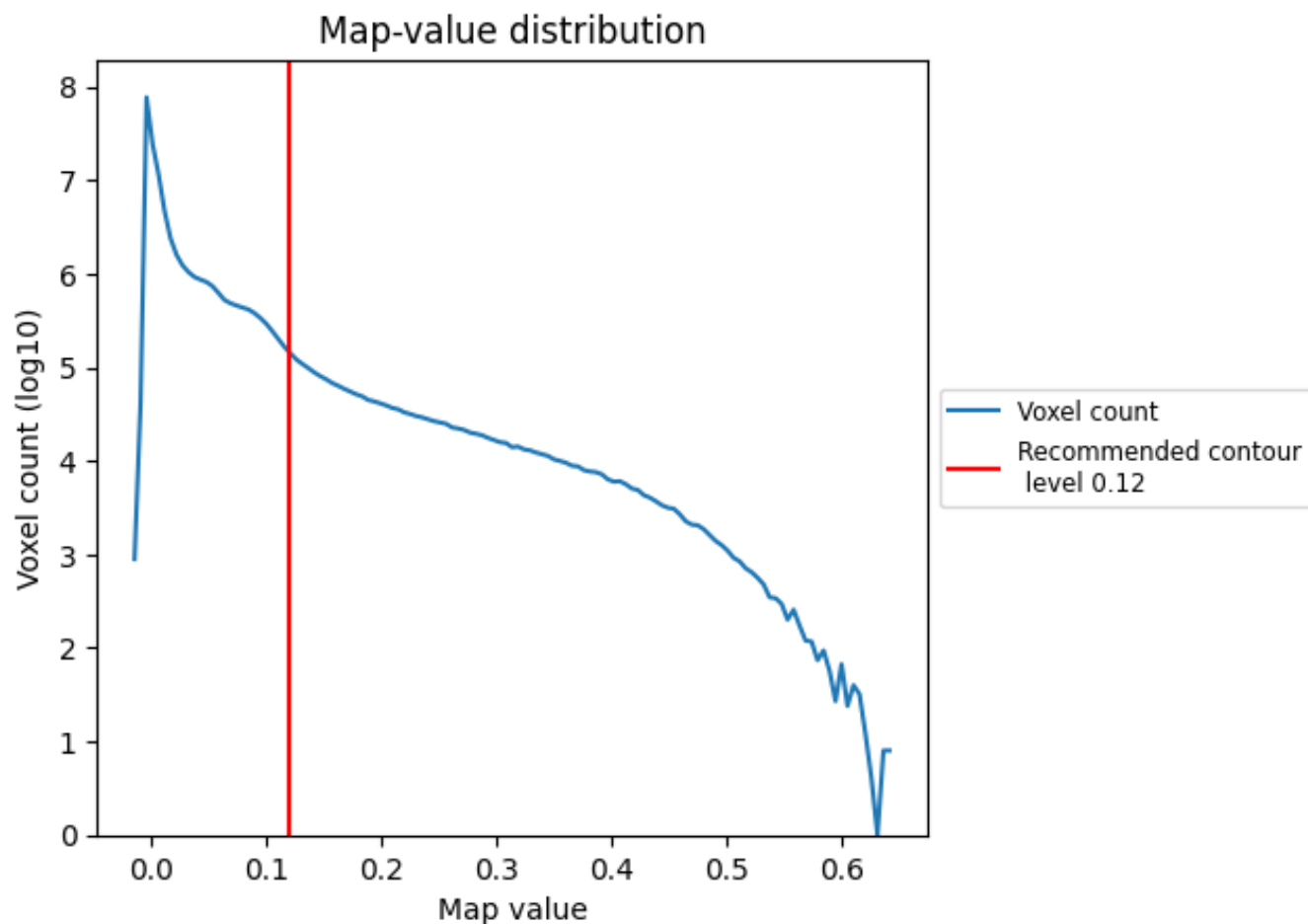
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

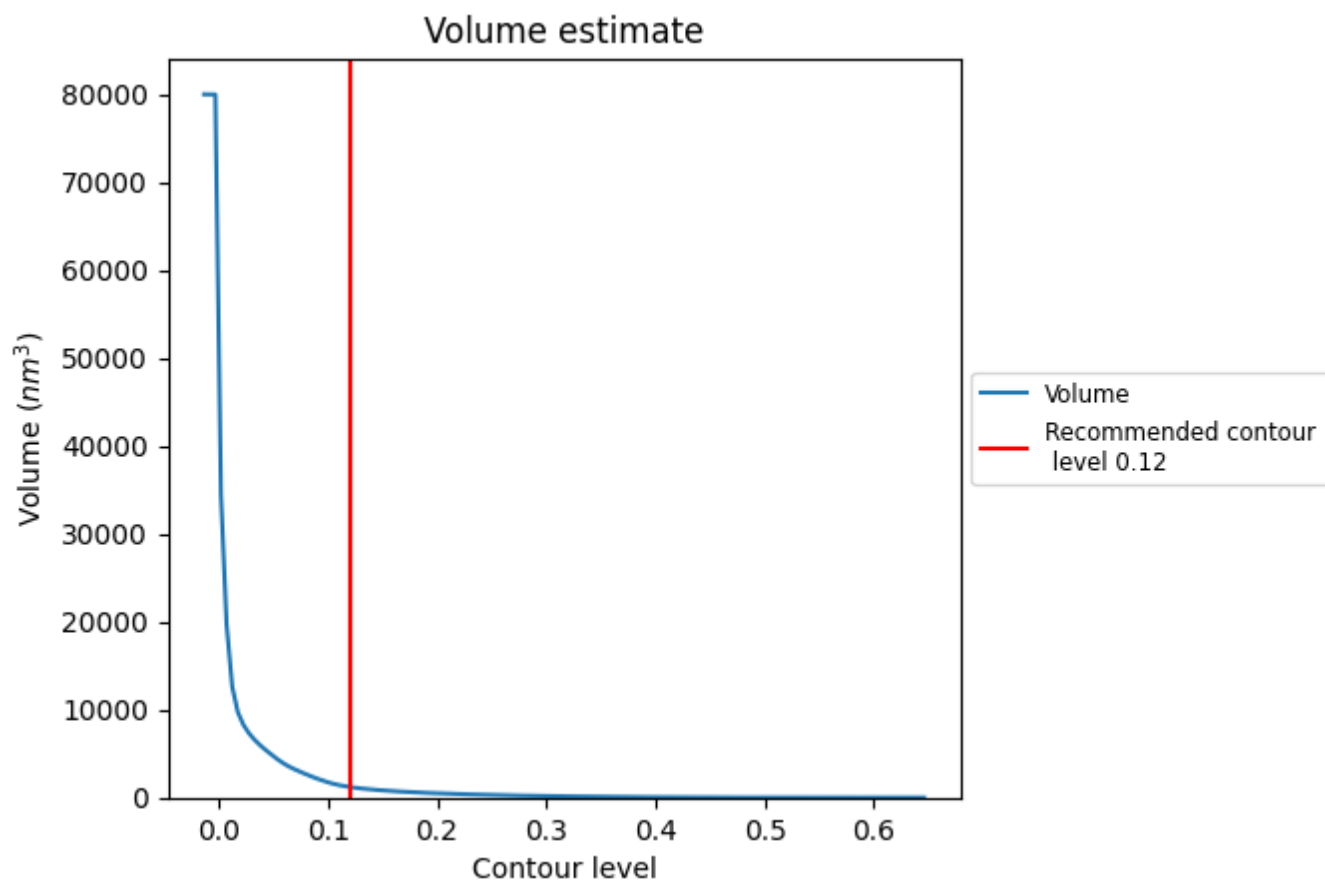
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

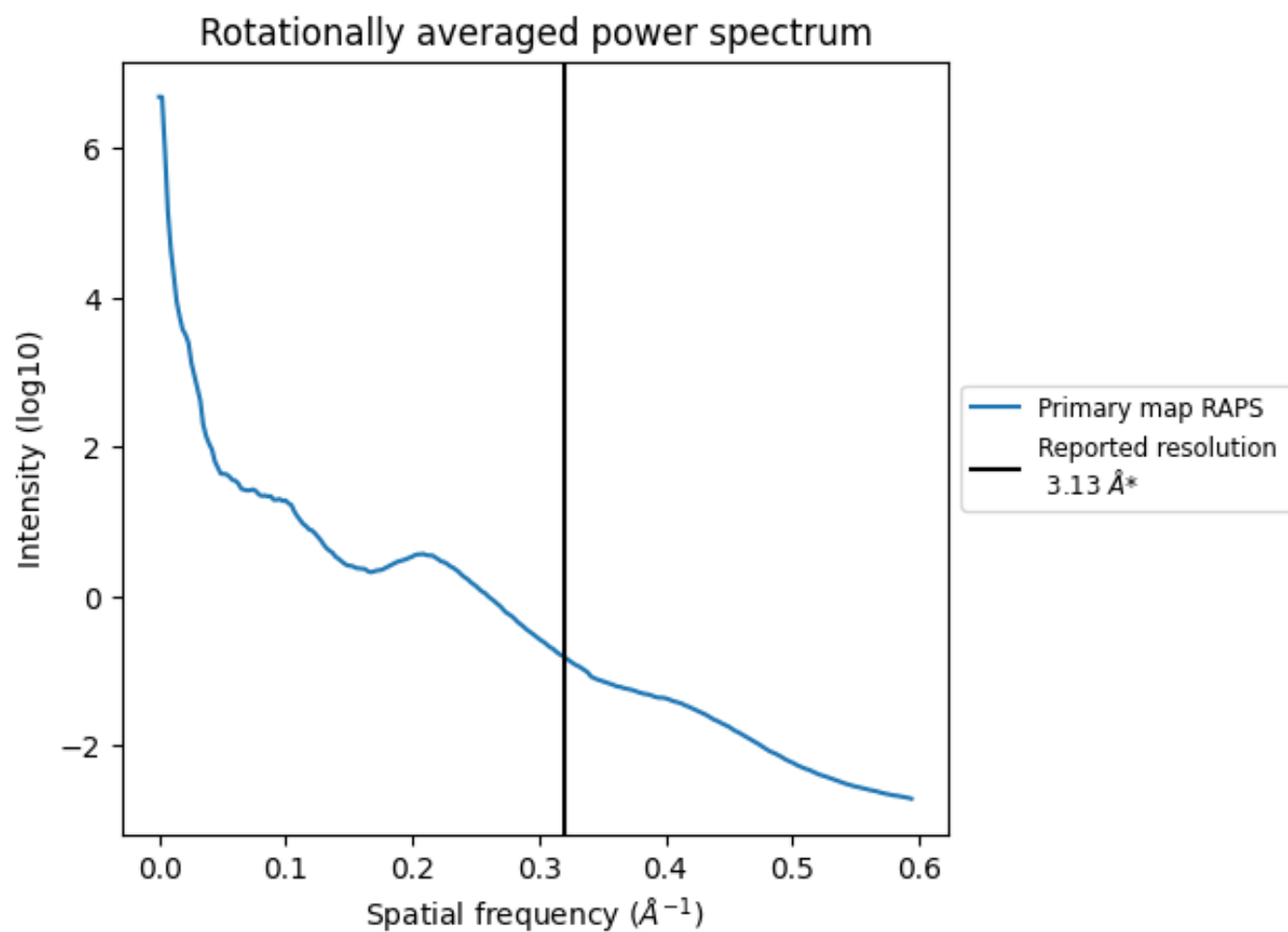
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1200 nm^3 ; this corresponds to an approximate mass of 1084 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 0.319 Å⁻¹

8 Fourier-Shell correlation

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

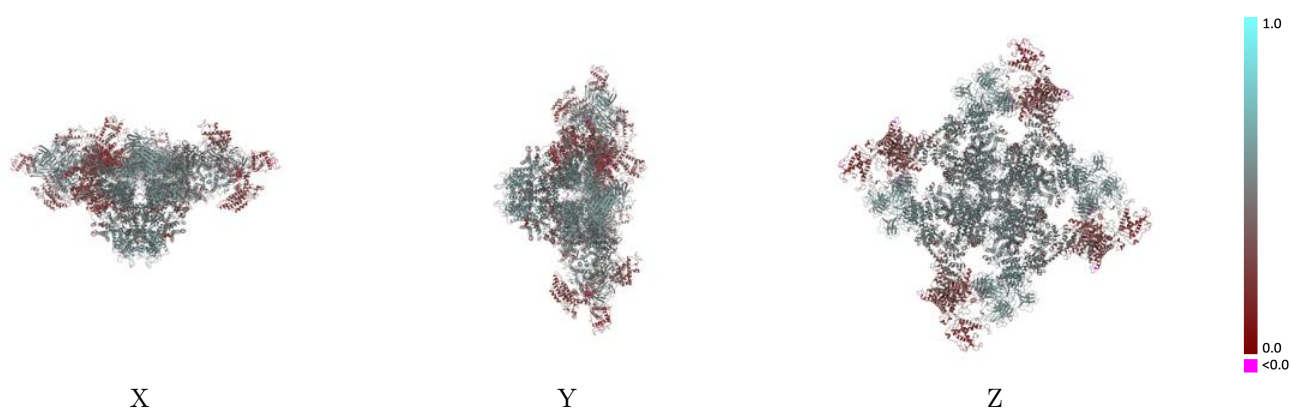
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42762 and PDB model 8UXF. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

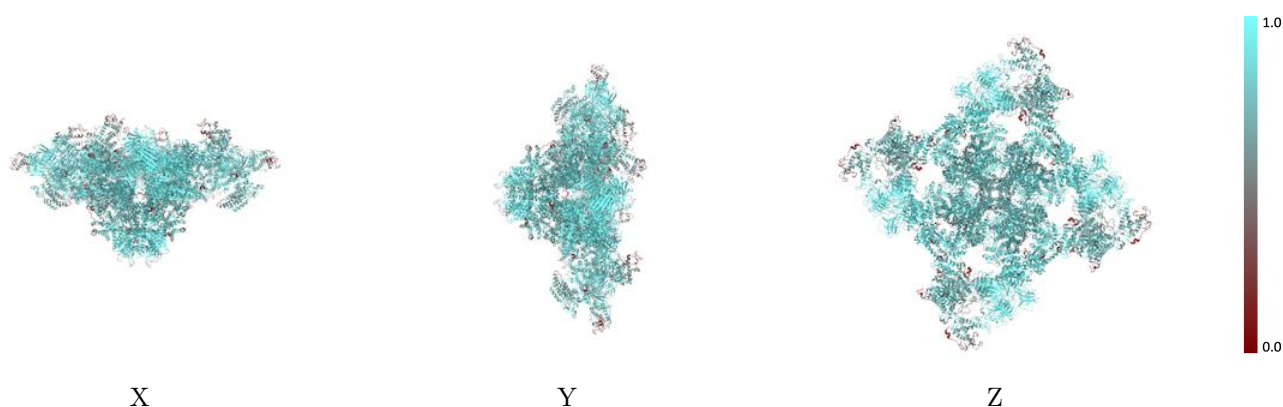
This section was not generated.

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



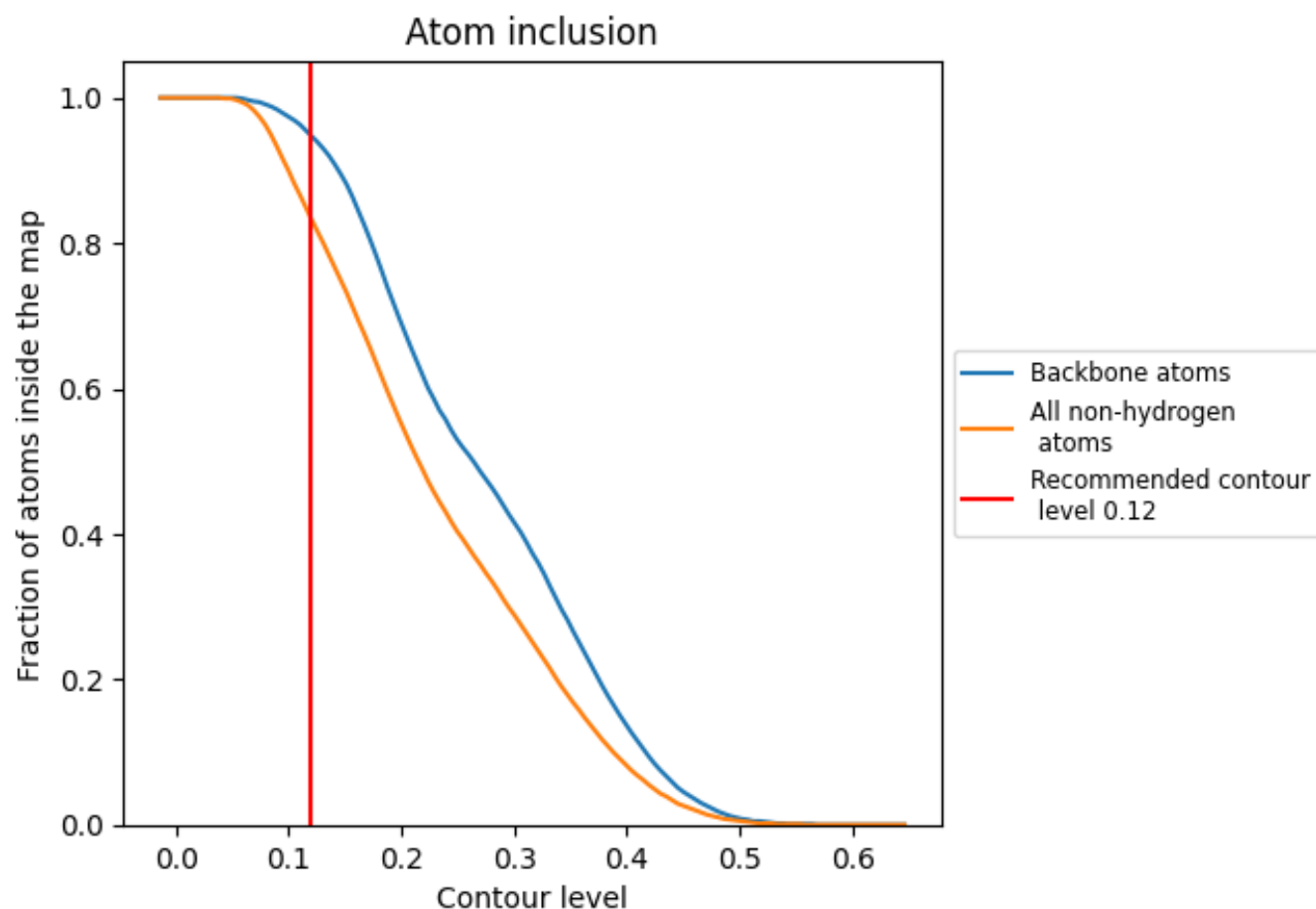
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 83% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.4540
A	0.8300	0.4510
B	0.8300	0.4510
C	0.8310	0.4530
D	0.8310	0.4520
E	0.9430	0.5530
F	0.9420	0.5530
G	0.9430	0.5540
H	0.9440	0.5540

1.0

0.0

<0.0