



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 06:29 PM JST

PDB ID : 9L2D
EMDB ID : EMD-62772
Title : Structure of SARM1 bound to M1 in the intermediate state 1
Authors : Huang, Y.; Zhang, J.; Zheng, S.; Wang, X.
Deposited on : 2024-12-17
Resolution : 2.83 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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<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.dev117
Mogul : 1.8.5 (274361), 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) : 2.41.2

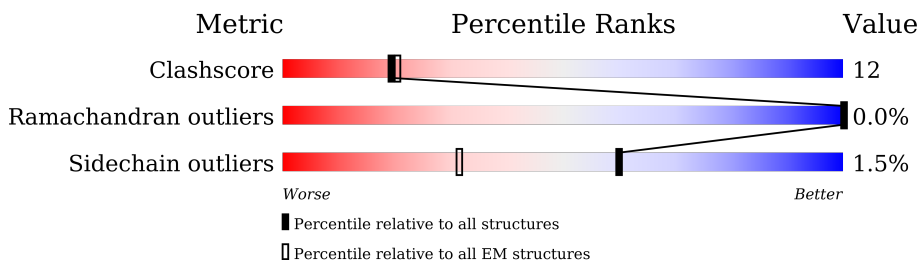
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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 ≥ 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	732	<div> <div>30%</div> <div>56%</div> <div>25%</div> <div>•</div> <div>18%</div> </div>
1	B	732	<div> <div>29%</div> <div>57%</div> <div>24%</div> <div>•</div> <div>18%</div> </div>
1	C	732	<div> <div>30%</div> <div>56%</div> <div>25%</div> <div>•</div> <div>18%</div> </div>
1	D	732	<div> <div>29%</div> <div>57%</div> <div>24%</div> <div>•</div> <div>18%</div> </div>
1	E	732	<div> <div>29%</div> <div>56%</div> <div>25%</div> <div>•</div> <div>18%</div> </div>
1	F	732	<div> <div>29%</div> <div>56%</div> <div>25%</div> <div>•</div> <div>18%</div> </div>
1	G	732	<div> <div>30%</div> <div>56%</div> <div>25%</div> <div>•</div> <div>18%</div> </div>
1	H	732	<div> <div>29%</div> <div>58%</div> <div>23%</div> <div>•</div> <div>18%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37836 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 NAD(+) hydrolase SARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	B	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	C	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	D	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	E	600	Total	C	N	O	S	0	0
			4708	2977	847	862	22		
1	F	599	Total	C	N	O	S	0	0
			4704	2975	846	861	22		
1	G	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	H	601	Total	C	N	O	S	0	0
			4714	2980	848	863	23		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	725	ASP	-	expression tag	UNP Q6SZW1
A	726	TYR	-	expression tag	UNP Q6SZW1
A	727	LYS	-	expression tag	UNP Q6SZW1
A	728	ASP	-	expression tag	UNP Q6SZW1
A	729	ASP	-	expression tag	UNP Q6SZW1
A	730	ASP	-	expression tag	UNP Q6SZW1
A	731	ASP	-	expression tag	UNP Q6SZW1
A	732	LYS	-	expression tag	UNP Q6SZW1
B	725	ASP	-	expression tag	UNP Q6SZW1
B	726	TYR	-	expression tag	UNP Q6SZW1
B	727	LYS	-	expression tag	UNP Q6SZW1
B	728	ASP	-	expression tag	UNP Q6SZW1
B	729	ASP	-	expression tag	UNP Q6SZW1
B	730	ASP	-	expression tag	UNP Q6SZW1

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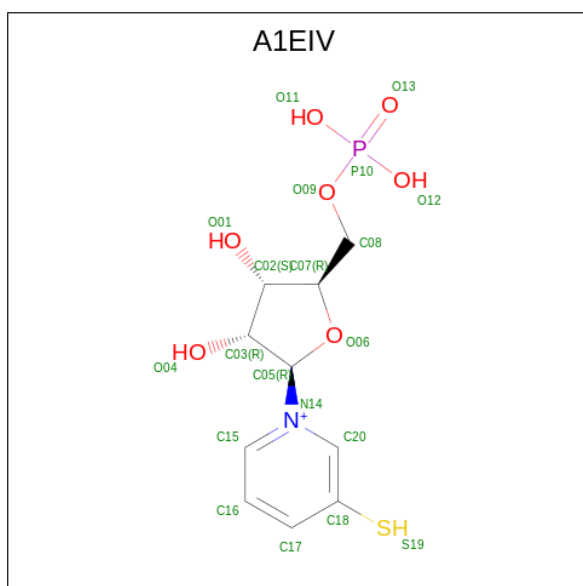
Chain	Residue	Modelled	Actual	Comment	Reference
B	731	ASP	-	expression tag	UNP Q6SZW1
B	732	LYS	-	expression tag	UNP Q6SZW1
C	725	ASP	-	expression tag	UNP Q6SZW1
C	726	TYR	-	expression tag	UNP Q6SZW1
C	727	LYS	-	expression tag	UNP Q6SZW1
C	728	ASP	-	expression tag	UNP Q6SZW1
C	729	ASP	-	expression tag	UNP Q6SZW1
C	730	ASP	-	expression tag	UNP Q6SZW1
C	731	ASP	-	expression tag	UNP Q6SZW1
C	732	LYS	-	expression tag	UNP Q6SZW1
D	725	ASP	-	expression tag	UNP Q6SZW1
D	726	TYR	-	expression tag	UNP Q6SZW1
D	727	LYS	-	expression tag	UNP Q6SZW1
D	728	ASP	-	expression tag	UNP Q6SZW1
D	729	ASP	-	expression tag	UNP Q6SZW1
D	730	ASP	-	expression tag	UNP Q6SZW1
D	731	ASP	-	expression tag	UNP Q6SZW1
D	732	LYS	-	expression tag	UNP Q6SZW1
E	725	ASP	-	expression tag	UNP Q6SZW1
E	726	TYR	-	expression tag	UNP Q6SZW1
E	727	LYS	-	expression tag	UNP Q6SZW1
E	728	ASP	-	expression tag	UNP Q6SZW1
E	729	ASP	-	expression tag	UNP Q6SZW1
E	730	ASP	-	expression tag	UNP Q6SZW1
E	731	ASP	-	expression tag	UNP Q6SZW1
E	732	LYS	-	expression tag	UNP Q6SZW1
F	725	ASP	-	expression tag	UNP Q6SZW1
F	726	TYR	-	expression tag	UNP Q6SZW1
F	727	LYS	-	expression tag	UNP Q6SZW1
F	728	ASP	-	expression tag	UNP Q6SZW1
F	729	ASP	-	expression tag	UNP Q6SZW1
F	730	ASP	-	expression tag	UNP Q6SZW1
F	731	ASP	-	expression tag	UNP Q6SZW1
F	732	LYS	-	expression tag	UNP Q6SZW1
G	725	ASP	-	expression tag	UNP Q6SZW1
G	726	TYR	-	expression tag	UNP Q6SZW1
G	727	LYS	-	expression tag	UNP Q6SZW1
G	728	ASP	-	expression tag	UNP Q6SZW1
G	729	ASP	-	expression tag	UNP Q6SZW1
G	730	ASP	-	expression tag	UNP Q6SZW1
G	731	ASP	-	expression tag	UNP Q6SZW1
G	732	LYS	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	725	ASP	-	expression tag	UNP Q6SZW1
H	726	TYR	-	expression tag	UNP Q6SZW1
H	727	LYS	-	expression tag	UNP Q6SZW1
H	728	ASP	-	expression tag	UNP Q6SZW1
H	729	ASP	-	expression tag	UNP Q6SZW1
H	730	ASP	-	expression tag	UNP Q6SZW1
H	731	ASP	-	expression tag	UNP Q6SZW1
H	732	LYS	-	expression tag	UNP Q6SZW1

- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-3,4-bis(oxidanyl)-5-(3-sulfanylpurin-1-yl)oxolan-2-yl]methyl dihydrogen phosphate (three-letter code: A1EIV) (formula: C₁₀H₁₅NO₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	B	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	C	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	D	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	E	1	Total 20	C 10	N 1	O 7	P 1	S 1	0
2	F	1	Total 20	C 10	N 1	O 7	P 1	S 1	0

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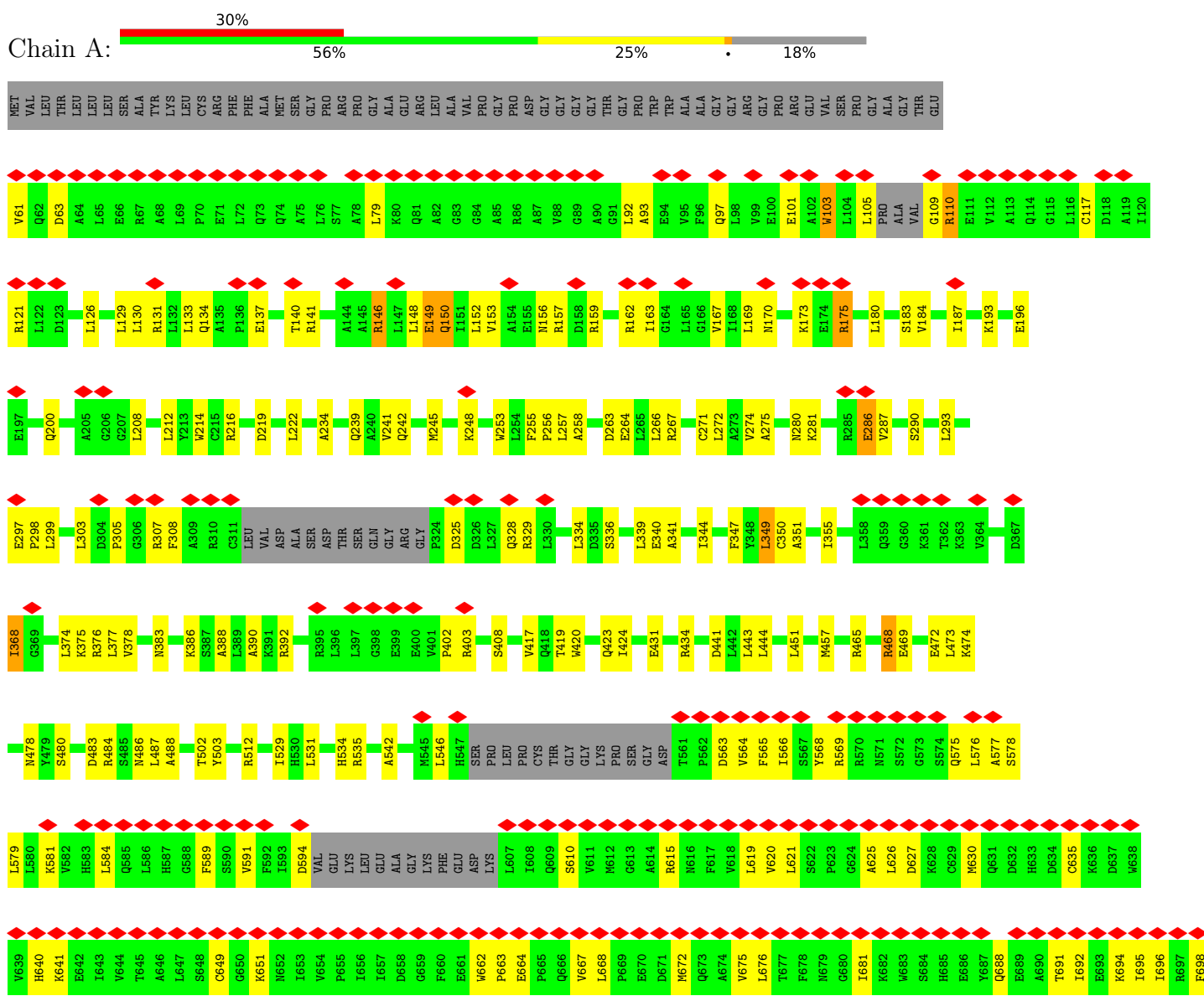
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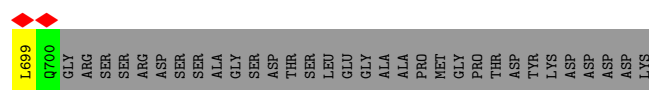
Mol	Chain	Residues	Atoms						AltConf
2	G	1	Total	C	N	O	P	S	0
			20	10	1	7	1	1	
2	H	1	Total	C	N	O	P	S	0
			20	10	1	7	1	1	

3 Residue-property plots

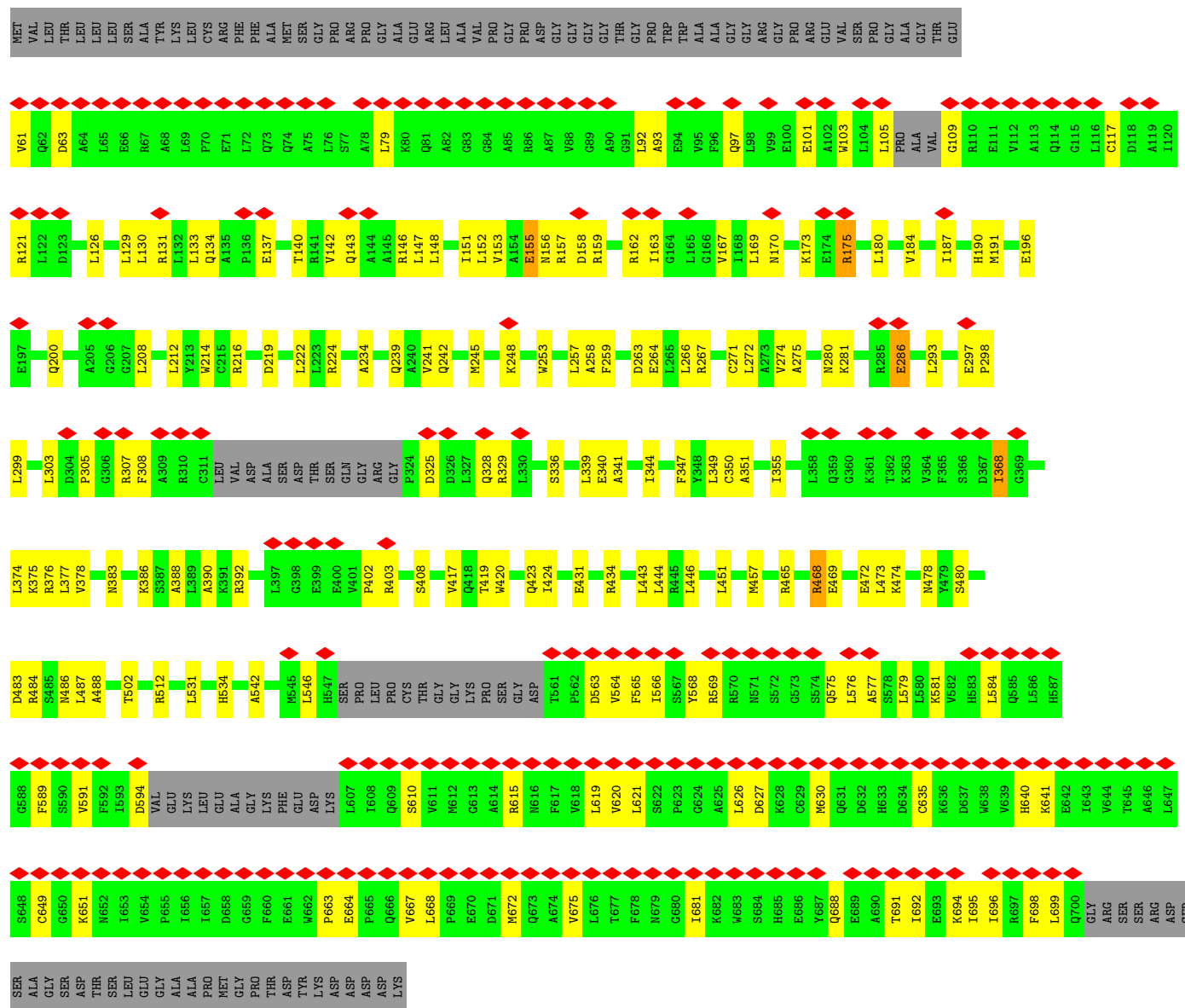
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NAD(+) hydrolase SARM1

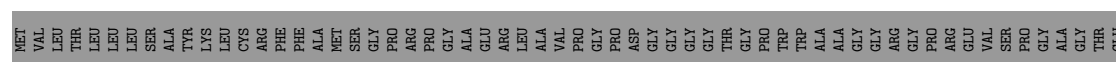


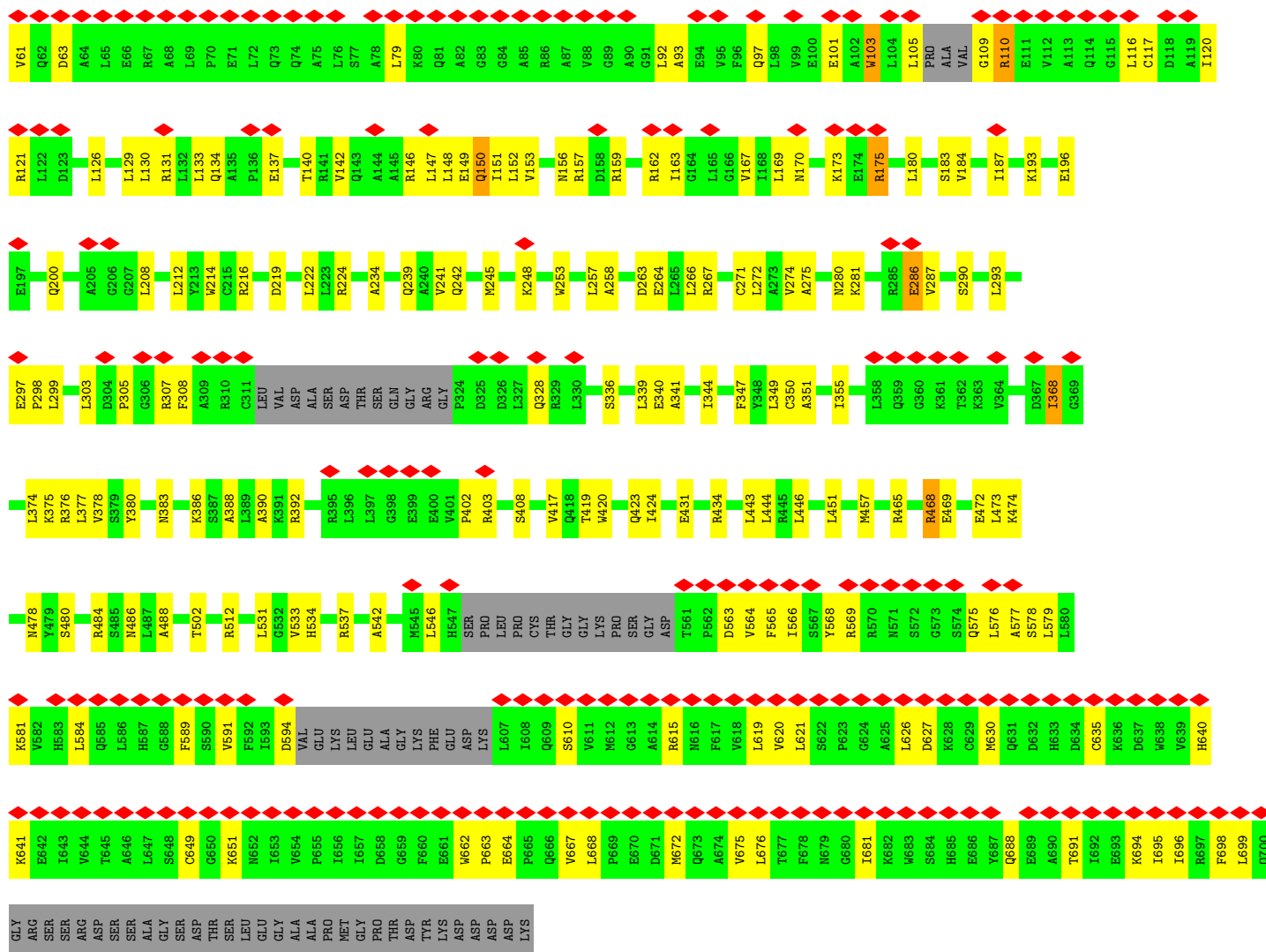


• Molecule 1: NAD(+) hydrolase SARM1

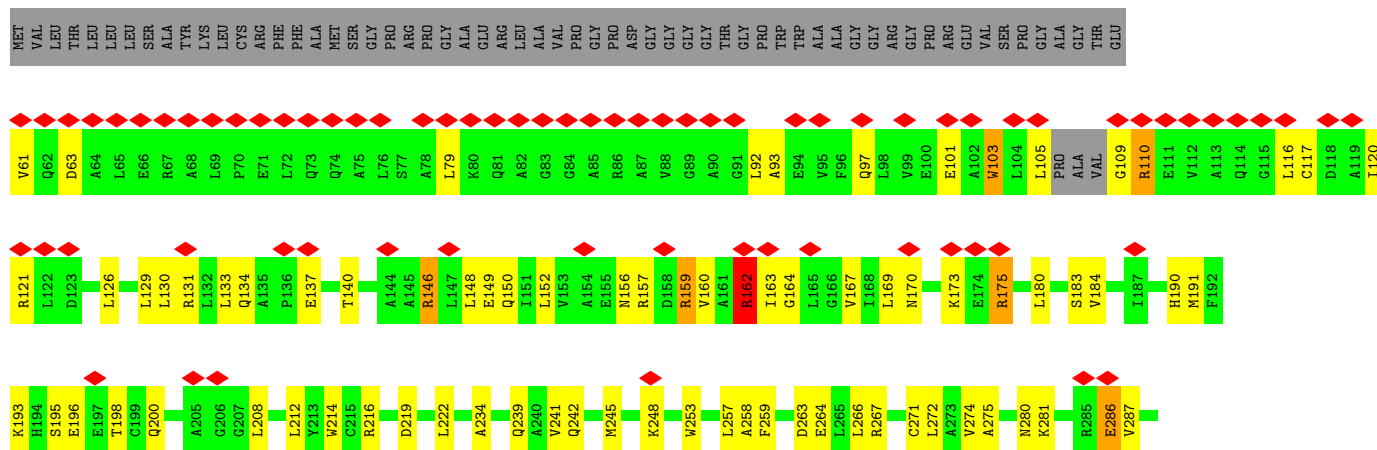


• Molecule 1: NAD(+) hydrolase SARM1

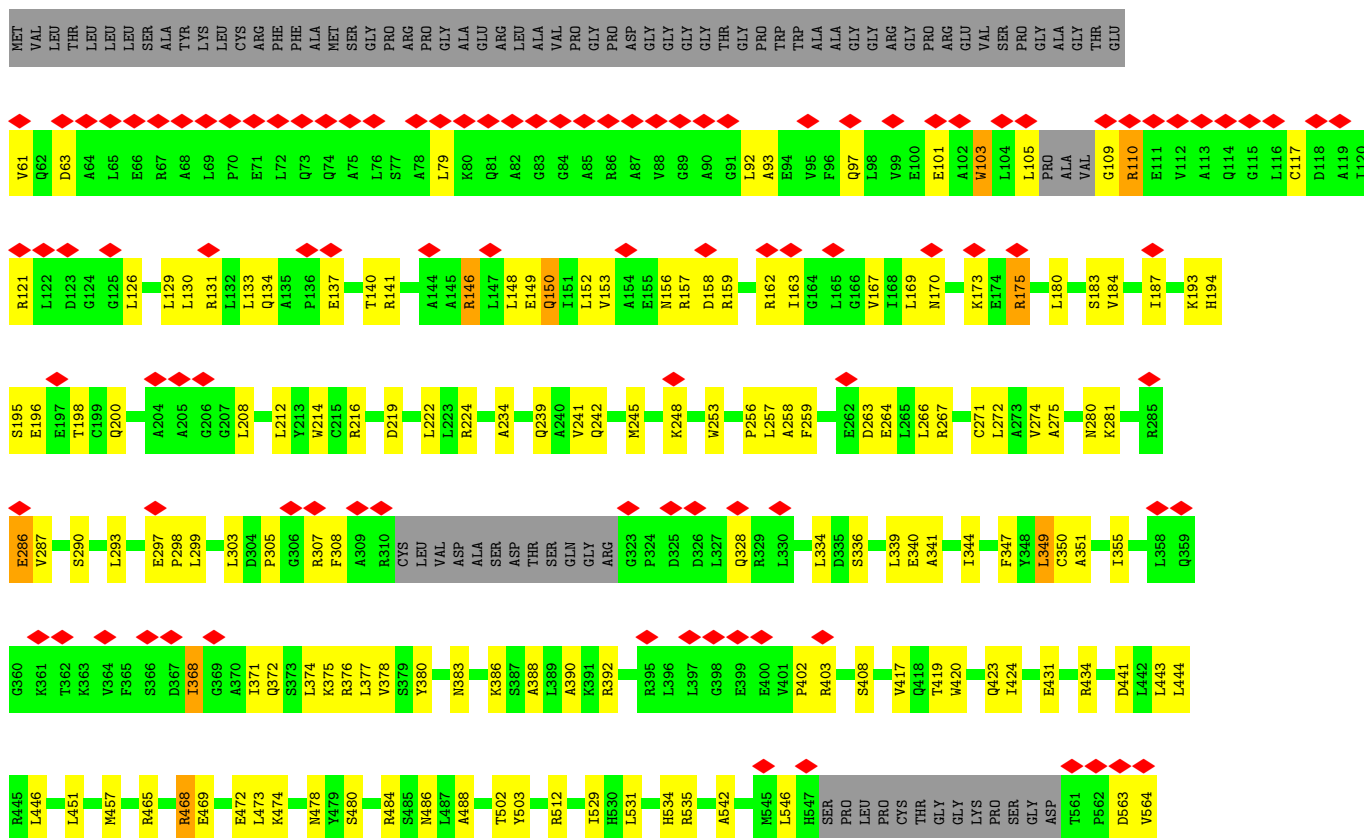




• Molecule 1: NAD(+)-hydrolase SARM1

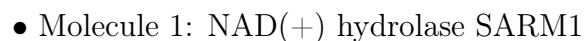


- Molecule 1: NAD(+) hydrolase SARM1

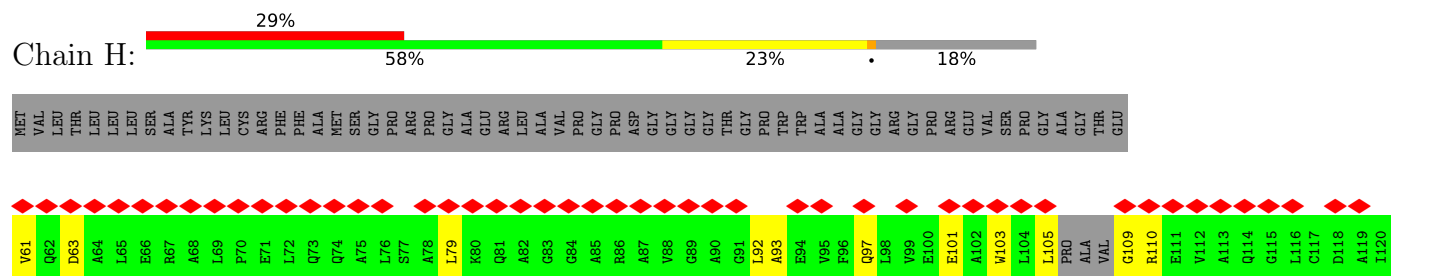




Chain G:



Chain H:



ALA	GLY	SER	ASP	THR	SER	LEU	LEU	GLY	ALA	ALA	PRO	MET	GLY	PRO	THR	ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS																																					
C649	G650	K651	N652	I653	V654	P655	T656	I657	D658	G659	F660	E661	N662	P663	E664	P665	Q666	V667	L668	P669	E670	D671	N672	Q673	A674	V675	L676	T677	P678	N679	G680	I681	K682	N683	S684	H685	E686	T687	Q688	E689	A690	T691	I692	E693	K694	I695	I696	N697	F698	L699	Q700	GLY	ARG	SER	SER	ARG	ASP	SER	SER	
F889	S890	V891	F892	I893	D894	VAL	GLU	LYS	LEU	GLU	ALA	ALA	GLY	LYS	GLY	LYS	GLU	ASP	L867	I868	Q869	S870	V871	N872	F873	A874	V875	L876	T877	P878	N879	G880	P823	P823	G824	A825	L826	L826	D827	K828	C829	M830	Q831	D832	H833	D834	C835	K836	D837	V838	V839	H840	K841	E842	I843	V844	T845	A846	L847	S848
T502	R512	I529	H530	L531	G532	H533	H534	R535	A536	R537	A542	H545	L546	H547	SER	PRO	LEU	PRO	CYS	THR	GLY	GLY	LYS	PRO	PRO	GLY	ASP	T561	P562	D563	V564	F565	I566	S567	Y568	R569	R570	N571	S572	G573	S574	Q575	L576	A577	S578	L579	L580	K581	L584	Q585	L586	H587	G588							
L377	V378	N383	K386	S387	A388	L389	A390	K391	R392	L397	G398	E400	V401	R403	S408	V417	Q418	T419	W420	Q423	I424	E431	R434	L443	L444	L451	M457	R465	R468	E469	E472	L473	K474	N478	Y479	S480	R484	S485	N486	L487	A488																			
D304	P305	G306	R307	F308	A309	R310	C311	LEU	VAL	ASP	ALA	SER	ASP	THR	SER	GLN	GLY	ARG	G323	P324	D325	D326	L327	Q328	R329	L330	L334	D335	S336	L339	E340	A341	I344	F347	Y348	L349	C350	A351	I355	L358	Q359	G360	K361	T362	S366	D367	I368	G369	L374	K375	R376									
G206	G207	L208	L212	Y213	W214	C215	R216	D219	L222	L223	R224	A234	Q239	A240	V241	Q242	W245	K248	W253	L254	P255	P256	L257	A258	F259	D263	E264	L265	L266	R267	C271	L272	A273	V274	A275	N280	K281	R285	E286	L293	E297	P298	L299	L303																
R121	L122	D123	L126	L130	R131	L132	L133	Q134	A135	P136	E137	T140	A144	A145	R146	E149	Q150	I151	L152	V153	A154	E155	N156	R157	D158	R159	R162	I163	G164	L165	G166	V167	I168	L169	N170	K173	E174	R175	S183	I187	H194	S195	E196	E197	Q200	A204	A205													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42713	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 ($e^-/\text{\AA}^2$)	52.73	Depositor
Minimum defocus (nm)	710	Depositor
Maximum defocus (nm)	2240	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.128	Depositor
Minimum map value	-2.341	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.365	Depositor
Map size (Å)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EIV

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	0.29	0/4786	0.56	1/6466 (0.0%)
1	B	0.27	0/4786	0.53	1/6466 (0.0%)
1	C	0.28	0/4786	0.56	1/6466 (0.0%)
1	D	0.29	0/4786	0.56	1/6466 (0.0%)
1	E	0.28	0/4784	0.55	1/6464 (0.0%)
1	F	0.28	0/4780	0.55	1/6458 (0.0%)
1	G	0.28	0/4786	0.55	1/6466 (0.0%)
1	H	0.28	0/4790	0.54	2/6472 (0.0%)
All	All	0.28	0/38284	0.55	9/51724 (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	3
1	C	0	1
1	D	0	4
1	E	0	3
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	155	GLU	CA-CB-CG	5.86	126.28	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	SER	C-N-CA	5.21	134.74	121.70
1	C	336	SER	C-N-CA	5.20	134.70	121.70
1	F	336	SER	C-N-CA	5.20	134.70	121.70
1	H	336	SER	C-N-CA	5.20	134.70	121.70

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	141	ARG	Sidechain
1	A	146	ARG	Sidechain
1	C	110	ARG	Sidechain
1	D	110	ARG	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	4710	0	4791	122	0
1	B	4710	0	4791	119	0
1	C	4710	0	4791	125	0
1	D	4710	0	4791	123	0
1	E	4708	0	4788	124	0
1	F	4704	0	4786	124	0
1	G	4710	0	4791	128	0
1	H	4714	0	4793	115	0
2	A	20	0	0	0	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	20	0	0	0	0
2	E	20	0	0	1	0
2	F	20	0	0	0	0
2	G	20	0	0	1	0
2	H	20	0	0	3	0
All	All	37836	0	38322	945	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 12.

The worst 5 of 945 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:H:155:GLU:OE1	1:H:155:GLU:N	2.03	0.92
1:A:121:ARG:HA	1:A:126:LEU:HD22	1.56	0.88
1:H:121:ARG:HA	1:H:126:LEU:HD22	1.56	0.88
1:B:121:ARG:HA	1:B:126:LEU:HD22	1.56	0.87
1:C:121:ARG:HA	1:C:126:LEU:HD22	1.56	0.87

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	590/732 (81%)	582 (99%)	8 (1%)	0	100	100
1	B	590/732 (81%)	582 (99%)	8 (1%)	0	100	100
1	C	590/732 (81%)	582 (99%)	8 (1%)	0	100	100
1	D	590/732 (81%)	583 (99%)	7 (1%)	0	100	100
1	E	590/732 (81%)	582 (99%)	8 (1%)	0	100	100
1	F	589/732 (80%)	581 (99%)	8 (1%)	0	100	100
1	G	590/732 (81%)	582 (99%)	8 (1%)	0	100	100
1	H	591/732 (81%)	582 (98%)	8 (1%)	1 (0%)	44	63
All	All	4720/5856 (81%)	4656 (99%)	63 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	152	LEU

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	502/598 (84%)	493 (98%)	9 (2%)	54	76
1	B	502/598 (84%)	495 (99%)	7 (1%)	62	82
1	C	502/598 (84%)	494 (98%)	8 (2%)	58	79
1	D	502/598 (84%)	495 (99%)	7 (1%)	62	82
1	E	501/598 (84%)	493 (98%)	8 (2%)	58	79
1	F	501/598 (84%)	494 (99%)	7 (1%)	62	82
1	G	502/598 (84%)	493 (98%)	9 (2%)	54	76
1	H	502/598 (84%)	495 (99%)	7 (1%)	62	82
All	All	4014/4784 (84%)	3952 (98%)	62 (2%)	60	81

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	349	LEU
1	H	155	GLU
1	E	286	GLU
1	G	468	ARG
1	H	349	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	280	ASN
1	G	575	GLN
1	H	575	GLN
1	C	575	GLN
1	C	280	ASN

5.3.3 RNA ⓘ

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1EIV	A	801	-	20,21,21	2.12	4 (20%)	25,31,31	1.29	4 (16%)
2	A1EIV	G	801	-	20,21,21	2.07	4 (20%)	25,31,31	1.26	4 (16%)
2	A1EIV	H	801	-	20,21,21	2.06	5 (25%)	25,31,31	1.20	3 (12%)
2	A1EIV	F	801	-	20,21,21	1.93	6 (30%)	25,31,31	1.38	3 (12%)
2	A1EIV	E	801	-	20,21,21	2.09	3 (15%)	25,31,31	1.27	3 (12%)
2	A1EIV	C	801	-	20,21,21	2.13	4 (20%)	25,31,31	1.22	2 (8%)
2	A1EIV	B	801	-	20,21,21	2.19	7 (35%)	25,31,31	1.32	4 (16%)
2	A1EIV	D	801	-	20,21,21	2.09	3 (15%)	25,31,31	1.22	2 (8%)

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	A1EIV	A	801	-	-	4/10/26/26	0/2/2/2
2	A1EIV	G	801	-	-	5/10/26/26	0/2/2/2
2	A1EIV	H	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	F	801	-	-	4/10/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EIV	E	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	C	801	-	-	5/10/26/26	0/2/2/2
2	A1EIV	B	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	D	801	-	-	5/10/26/26	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	A1EIV	P10-O09	6.88	1.82	1.60
2	A	801	A1EIV	P10-O09	6.81	1.82	1.60
2	B	801	A1EIV	P10-O09	6.78	1.82	1.60
2	D	801	A1EIV	P10-O09	6.68	1.81	1.60
2	E	801	A1EIV	P10-O09	6.60	1.81	1.60

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1EIV	O12-P10-O09	-3.49	97.45	106.73
2	A	801	A1EIV	C15-N14-C20	-3.15	119.10	121.97
2	E	801	A1EIV	C15-N14-C20	-3.10	119.15	121.97
2	C	801	A1EIV	C15-N14-C20	-3.03	119.21	121.97
2	D	801	A1EIV	C15-N14-C20	-3.01	119.23	121.97

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1EIV	C08-O09-P10-O11
2	A	801	A1EIV	C08-O09-P10-O12
2	B	801	A1EIV	C08-O09-P10-O11
2	B	801	A1EIV	C08-O09-P10-O12
2	C	801	A1EIV	C08-O09-P10-O11

There are no ring outliers.

5 monomers are involved in 9 short contacts:

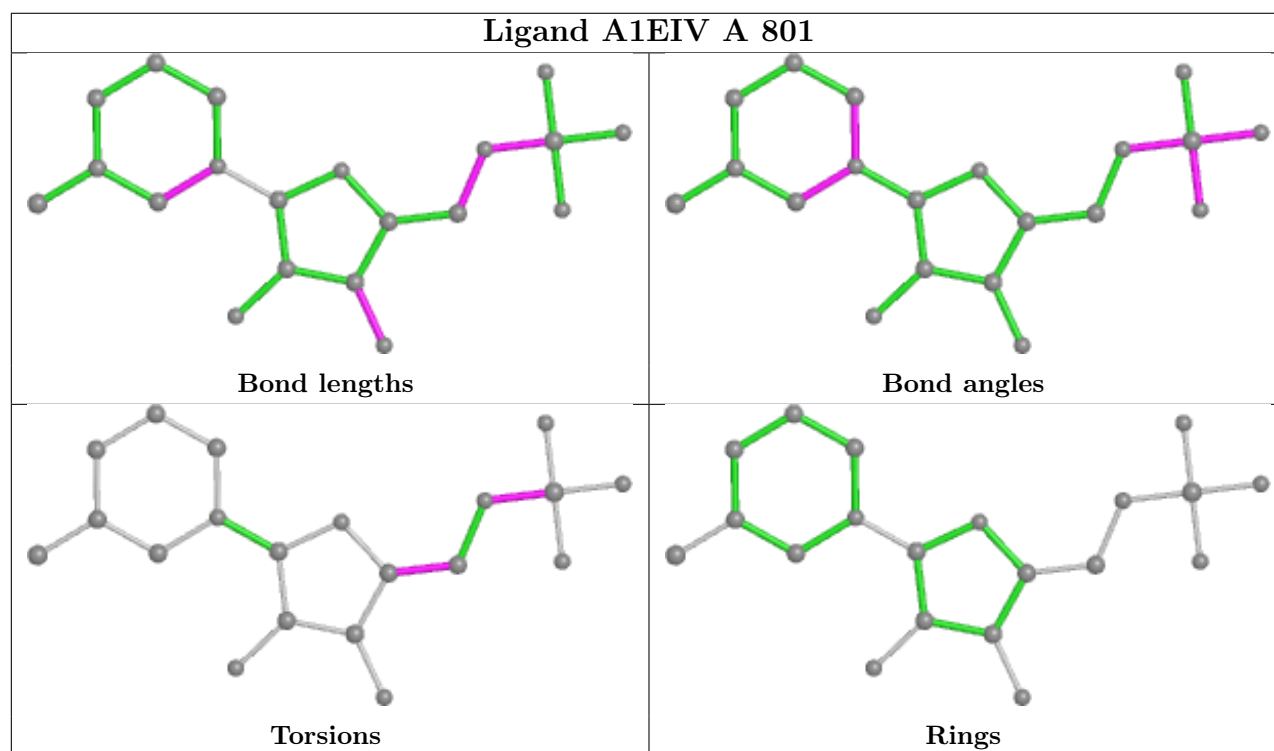
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	801	A1EIV	1	0
2	H	801	A1EIV	3	0
2	E	801	A1EIV	1	0

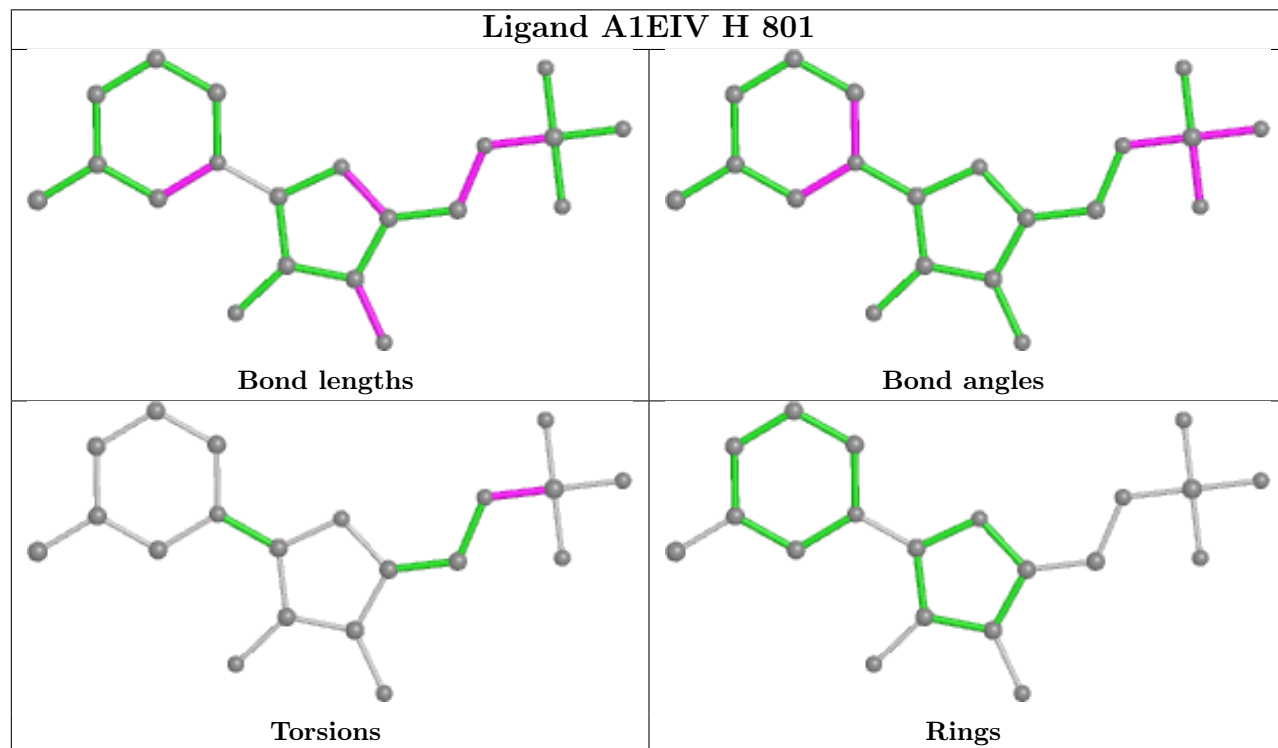
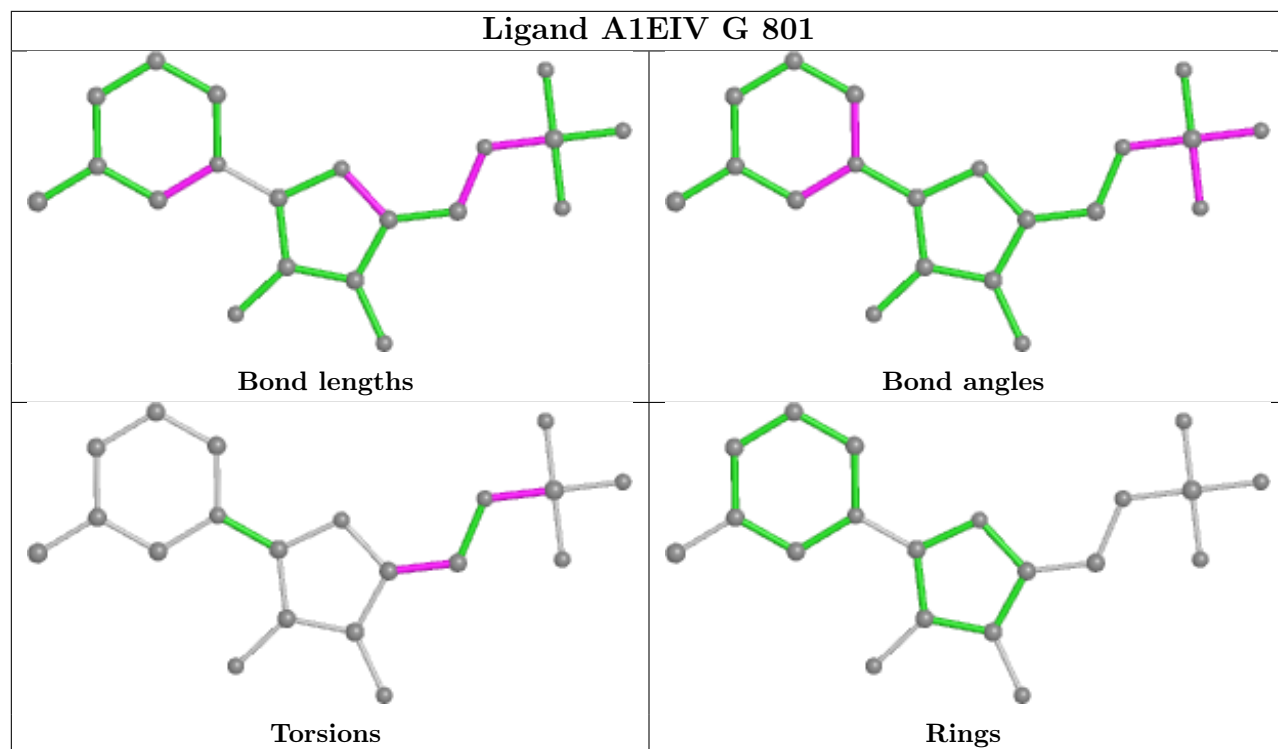
Continued on next page...

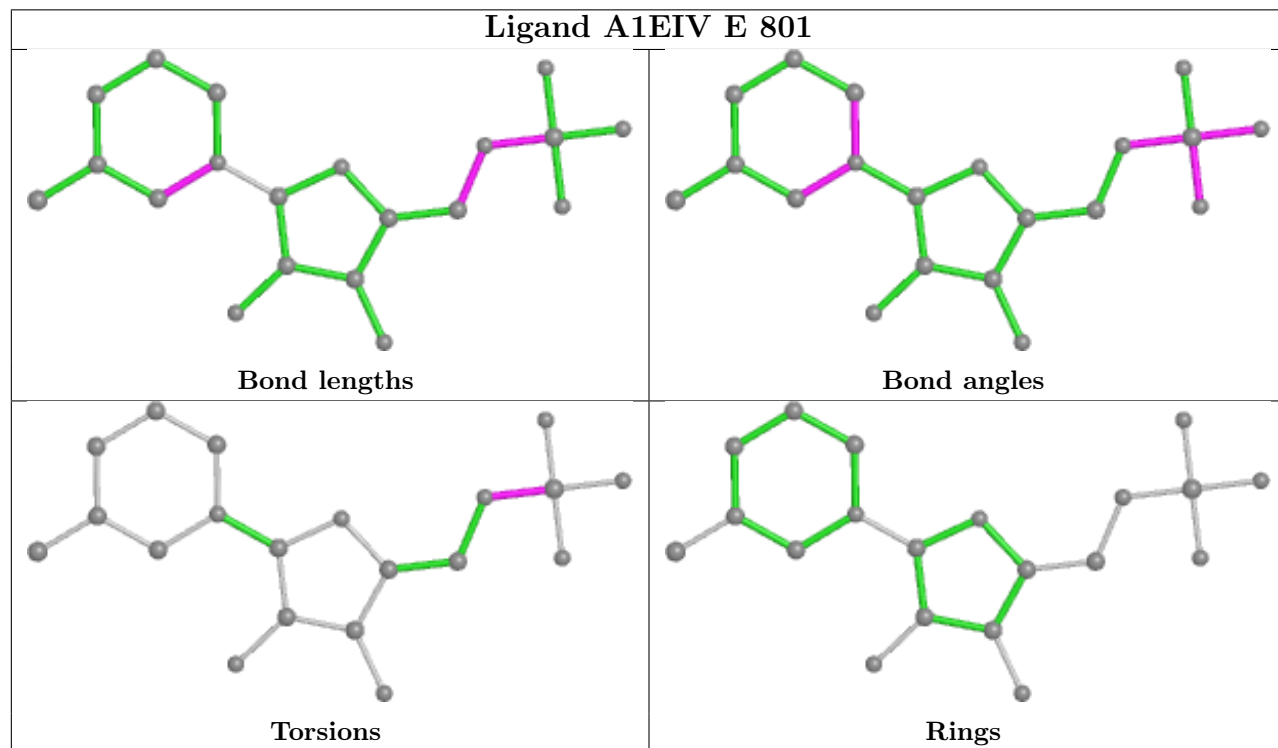
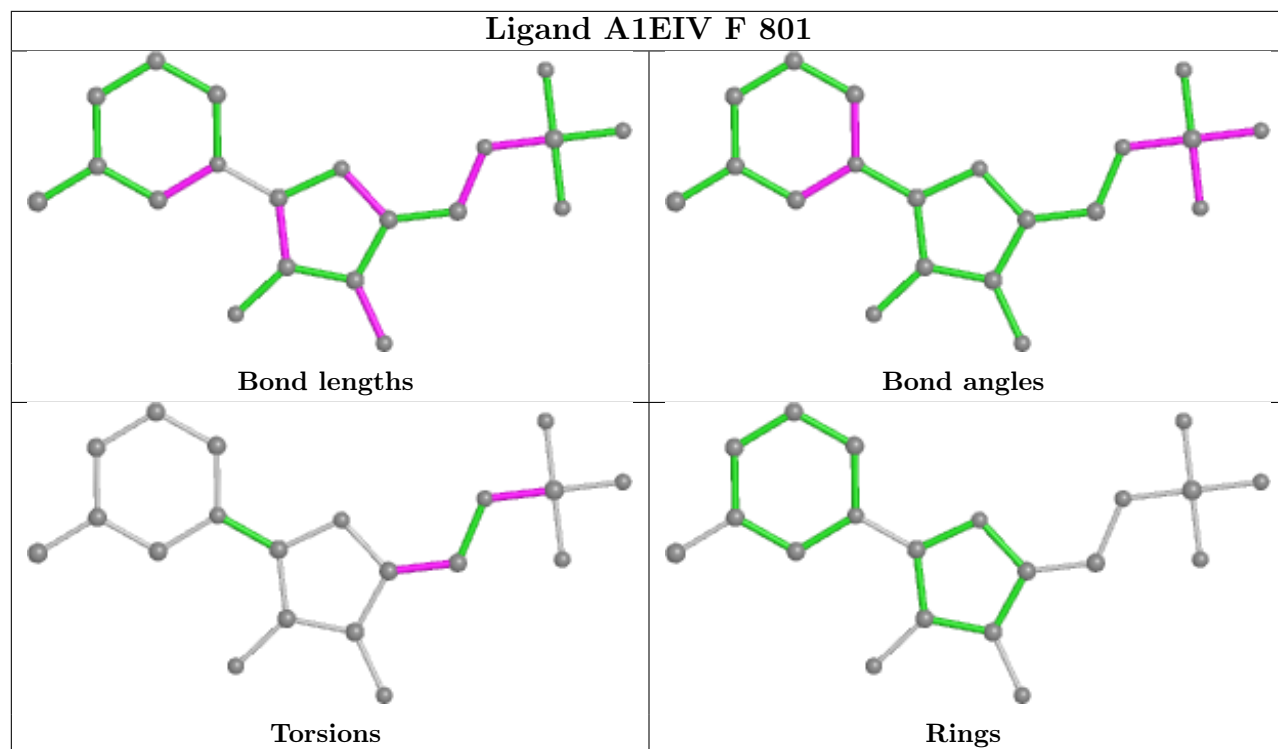
Continued from previous page...

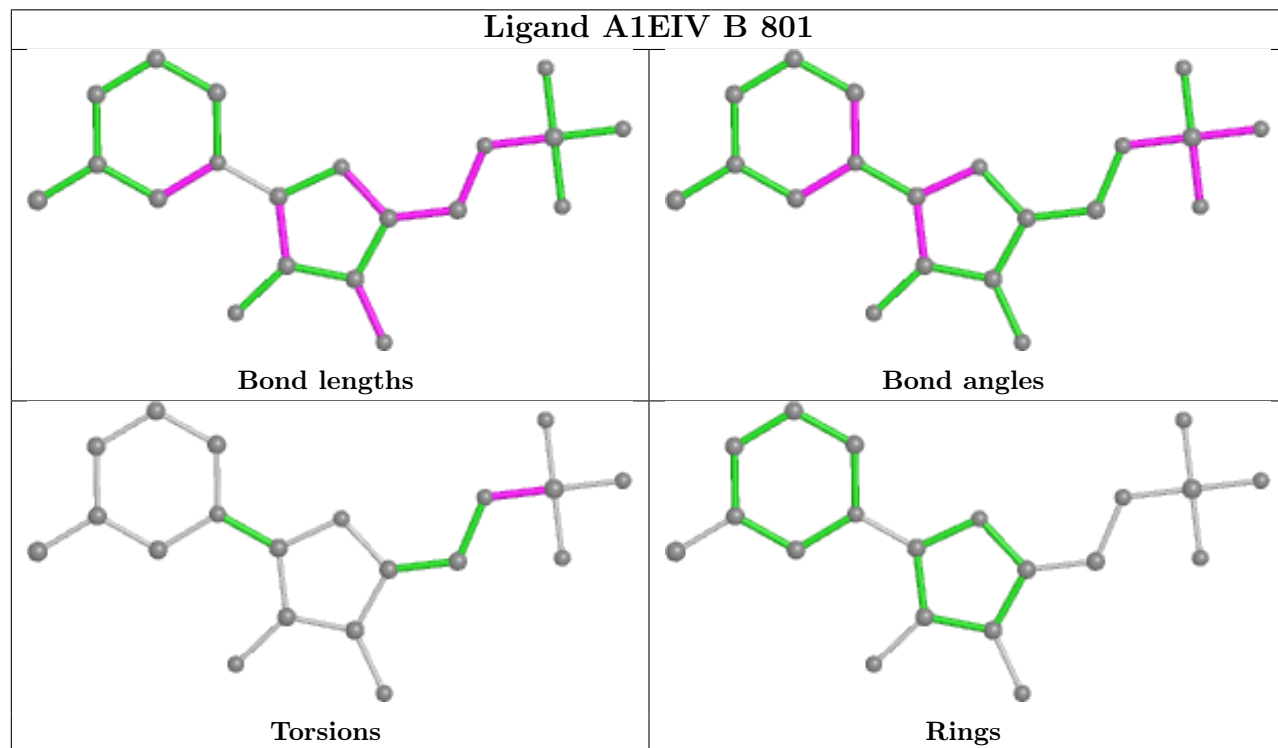
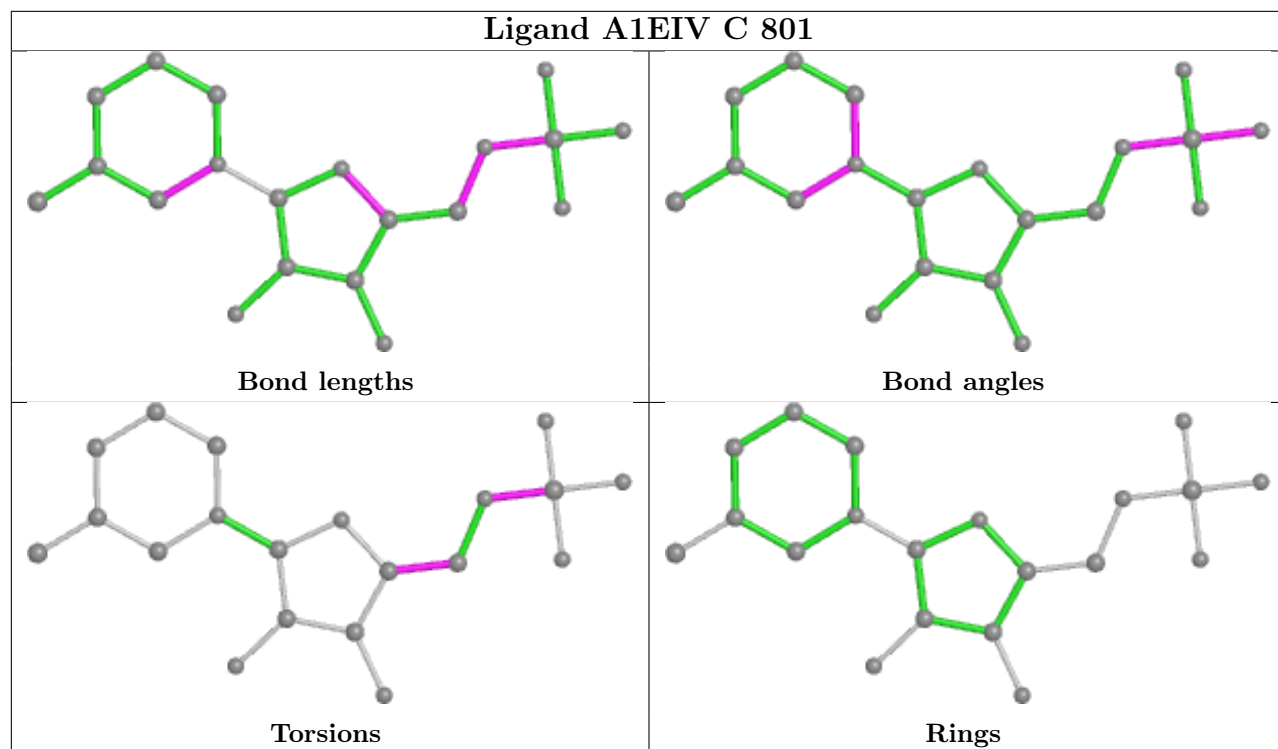
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	A1EIV	1	0
2	B	801	A1EIV	3	0

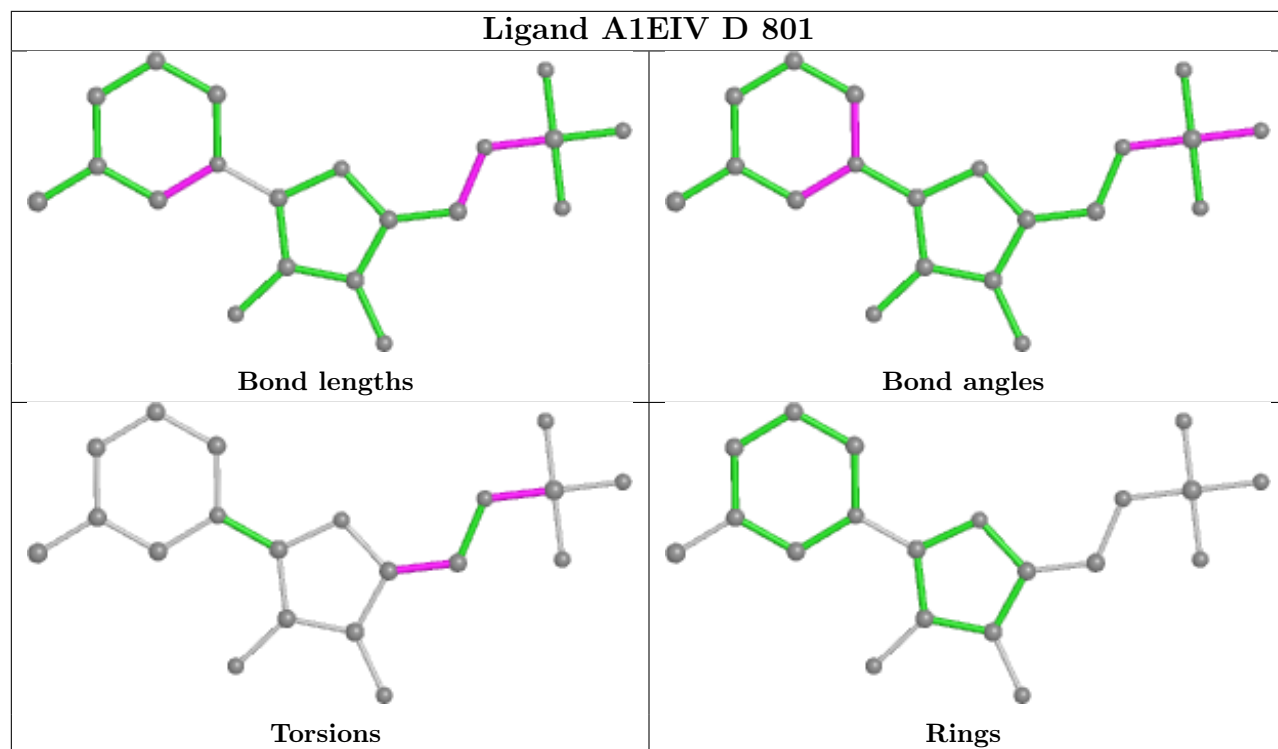
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

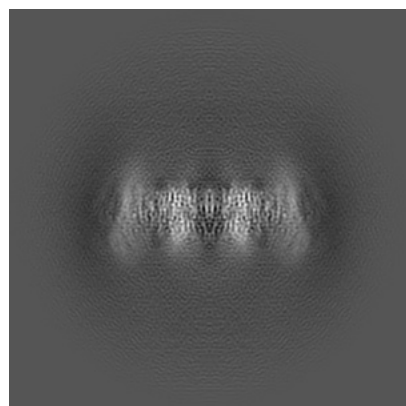
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62772. These allow visual inspection of the internal detail of the map and identification of artifacts.

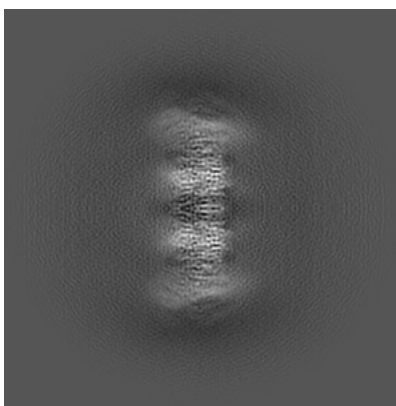
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

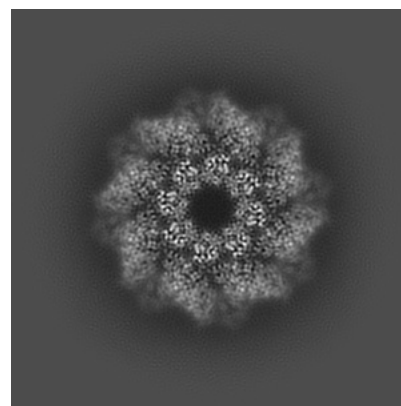
6.1.1 Primary map



X

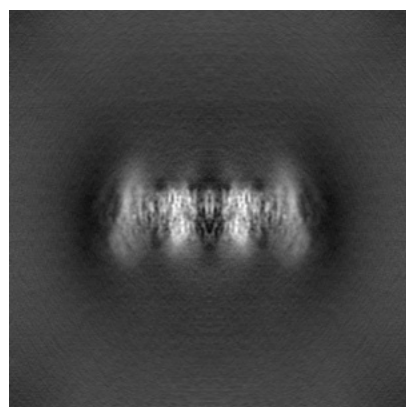


Y

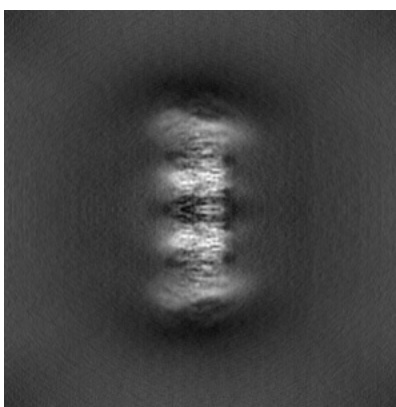


Z

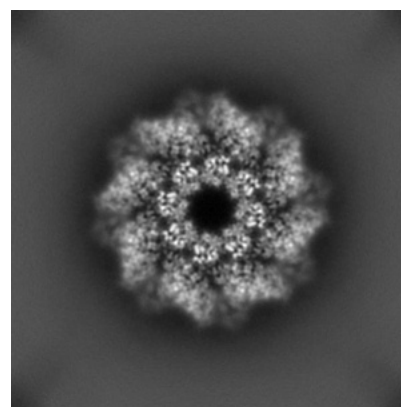
6.1.2 Raw map



X



Y

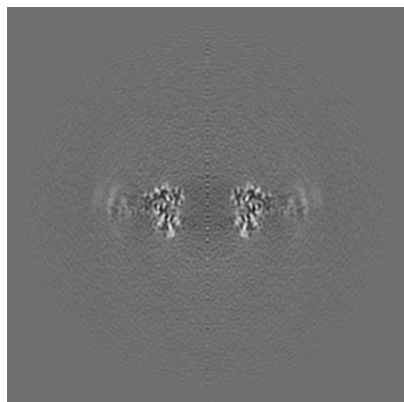


Z

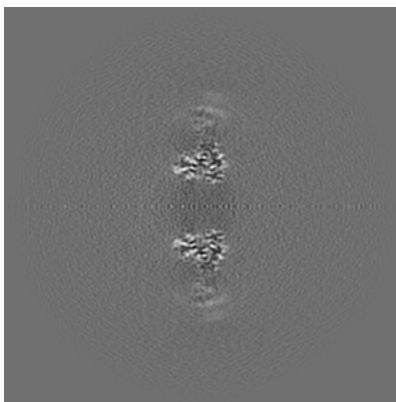
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

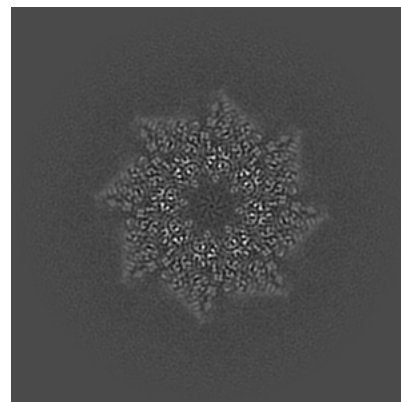
6.2.1 Primary map



X Index: 200

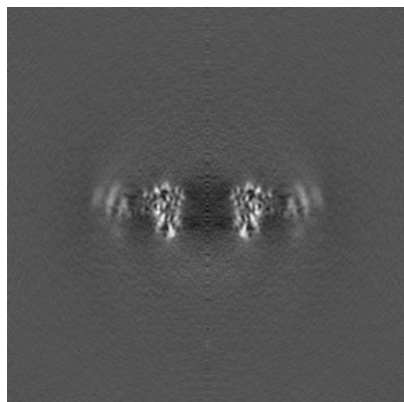


Y Index: 200

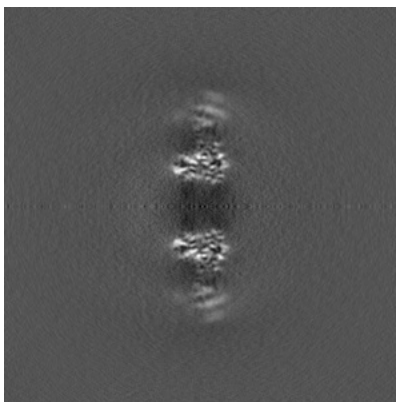


Z Index: 200

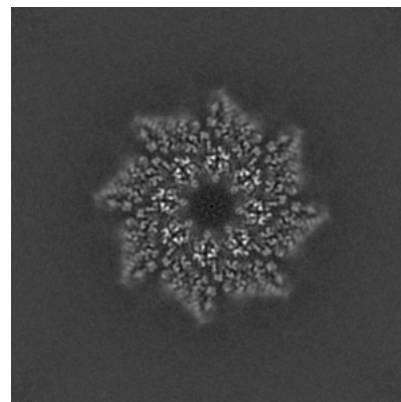
6.2.2 Raw map



X Index: 200



Y Index: 200

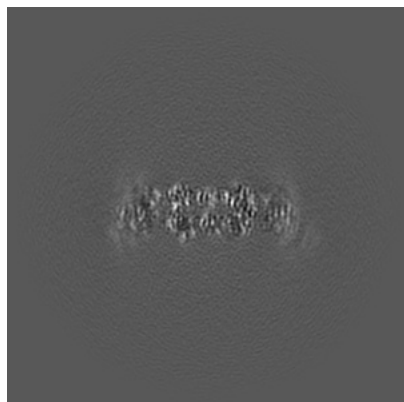


Z Index: 200

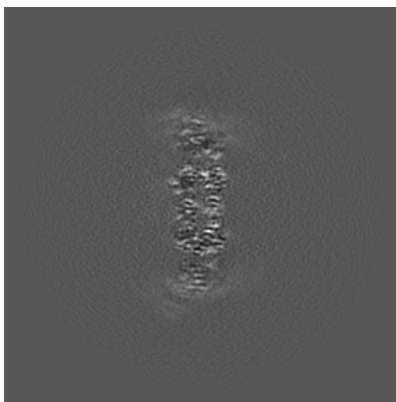
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

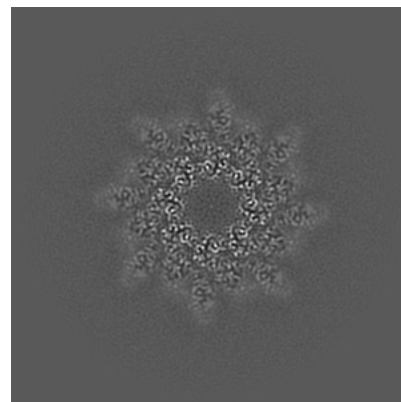
6.3.1 Primary map



X Index: 170

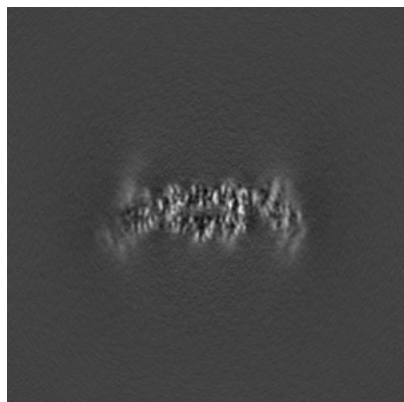


Y Index: 170

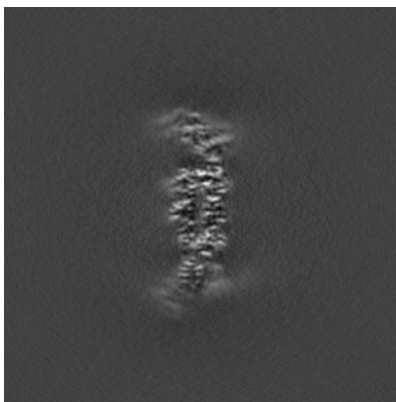


Z Index: 203

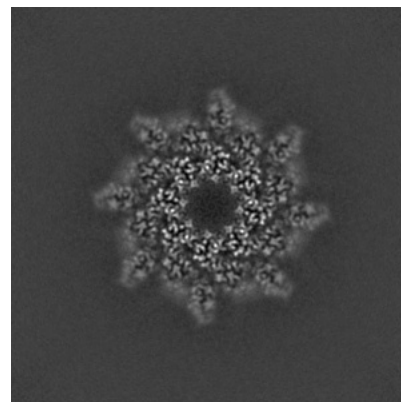
6.3.2 Raw map



X Index: 235



Y Index: 165

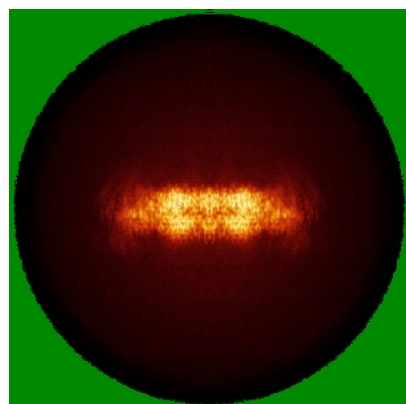


Z Index: 204

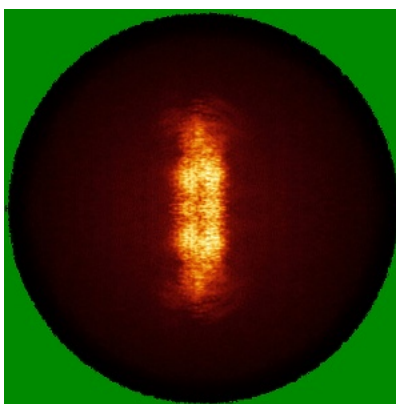
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

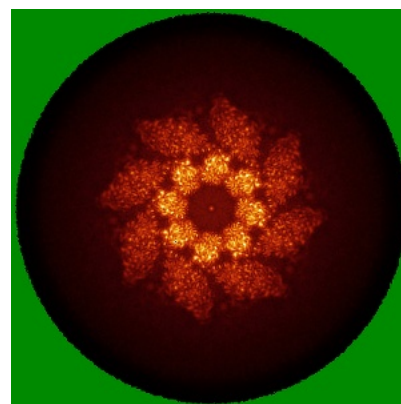
6.4.1 Primary map



X

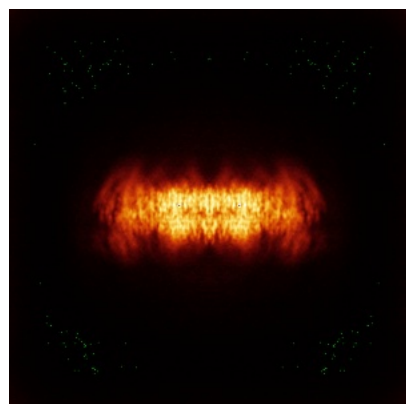


Y

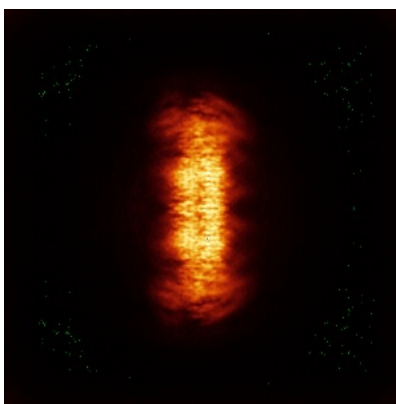


Z

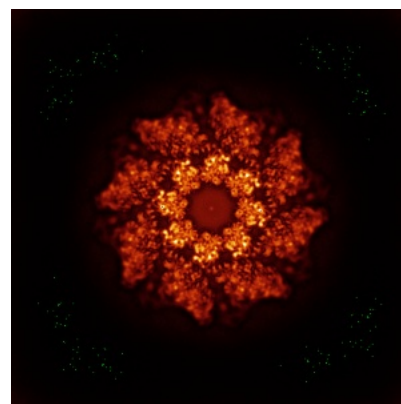
6.4.2 Raw map



X



Y

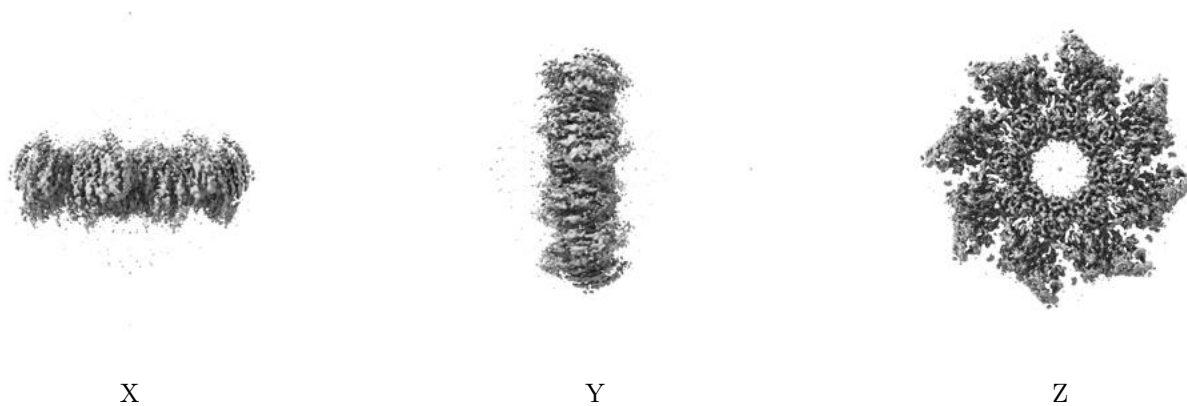


Z

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.

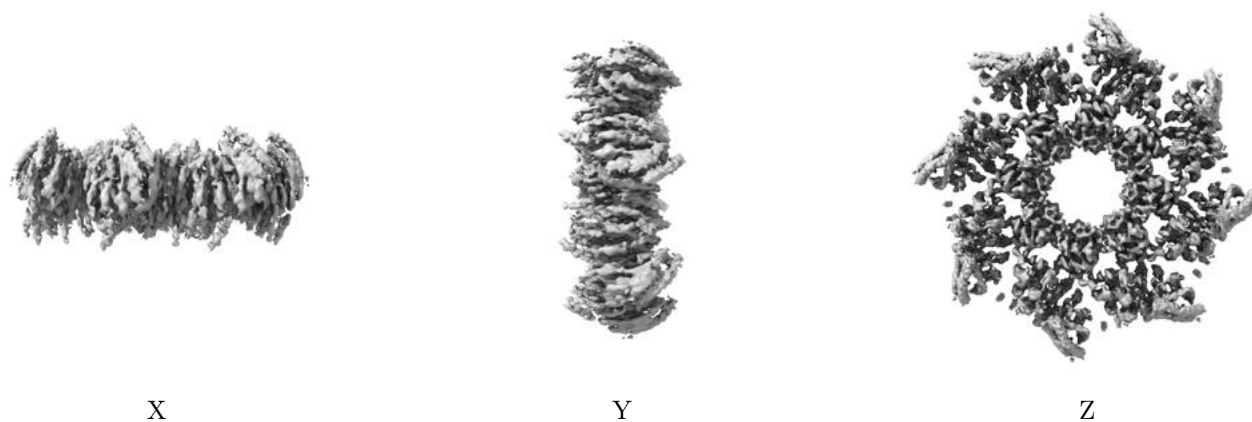
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.365. 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.

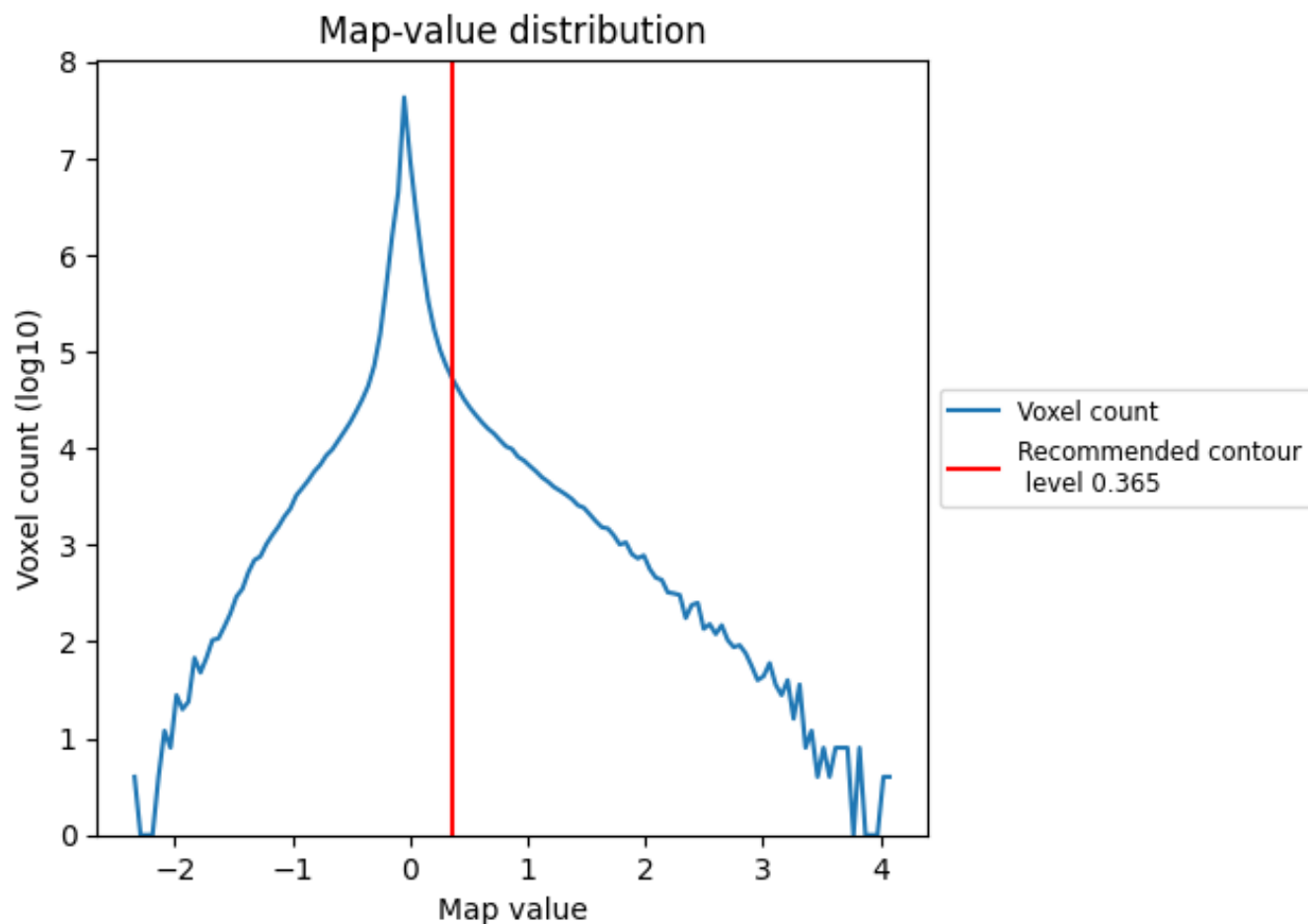
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

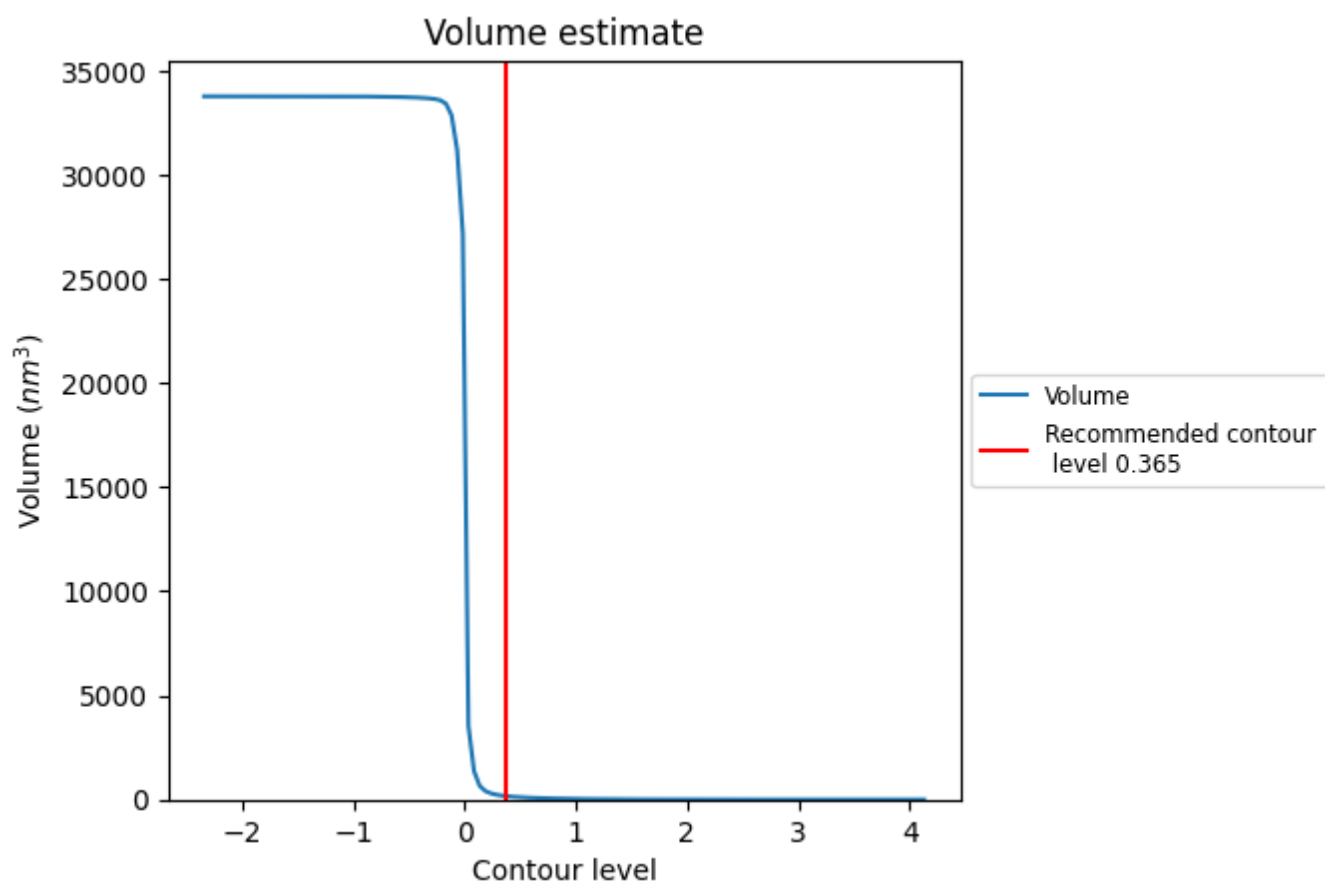
This section contains the results of statistical analysis of the map.

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.

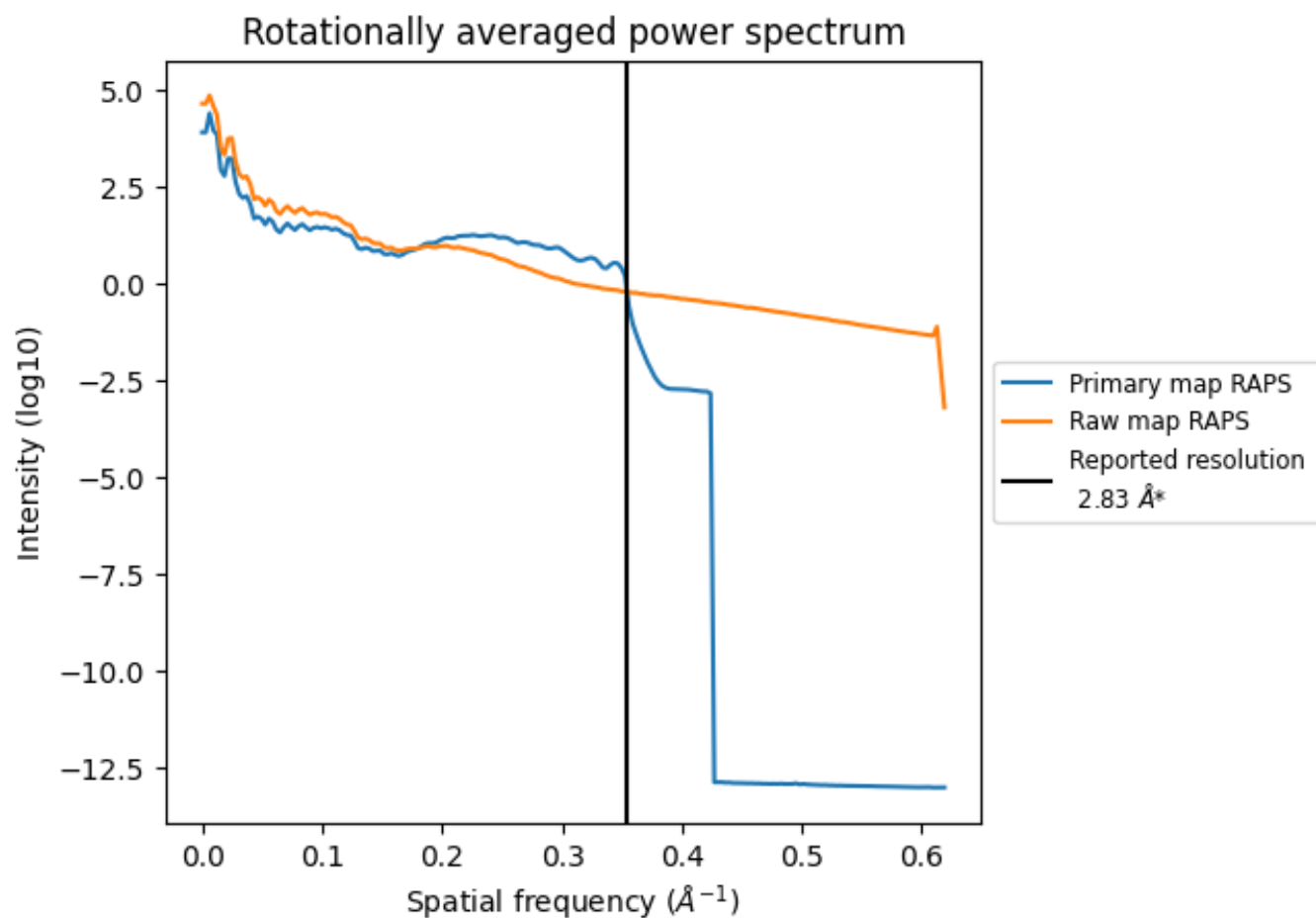
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm³; this corresponds to an approximate mass of 154 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 ⓘ

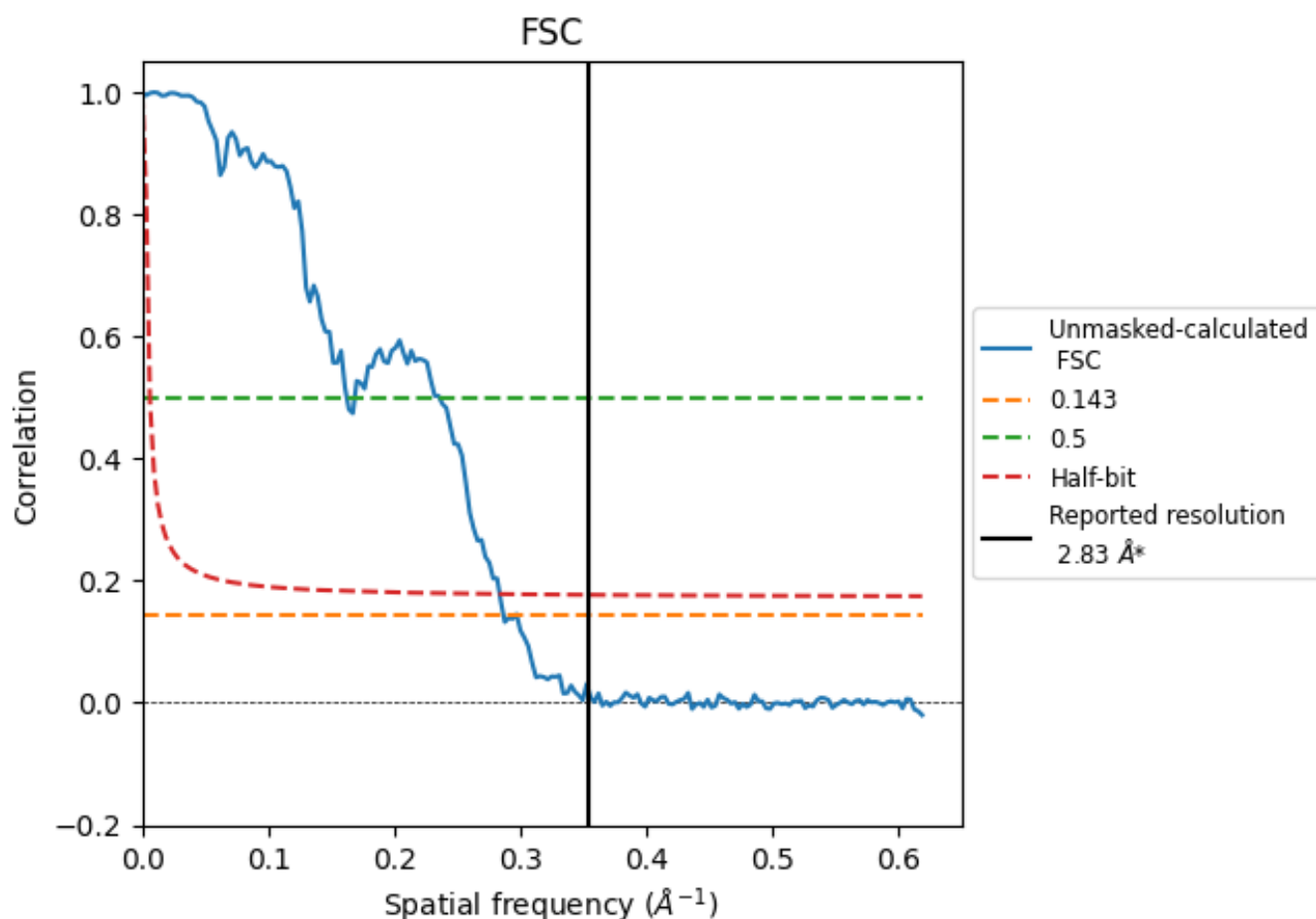


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

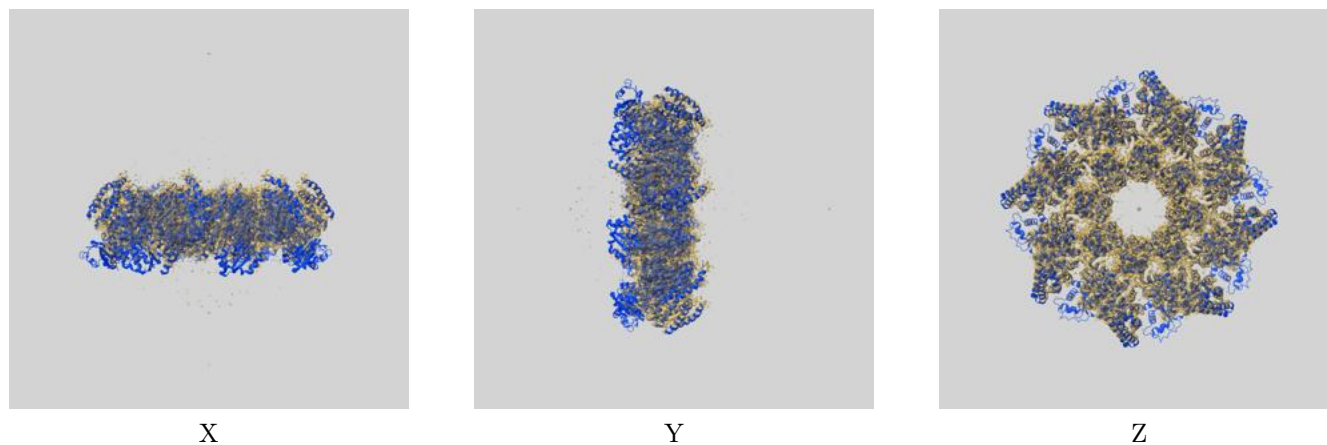
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	6.16	3.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

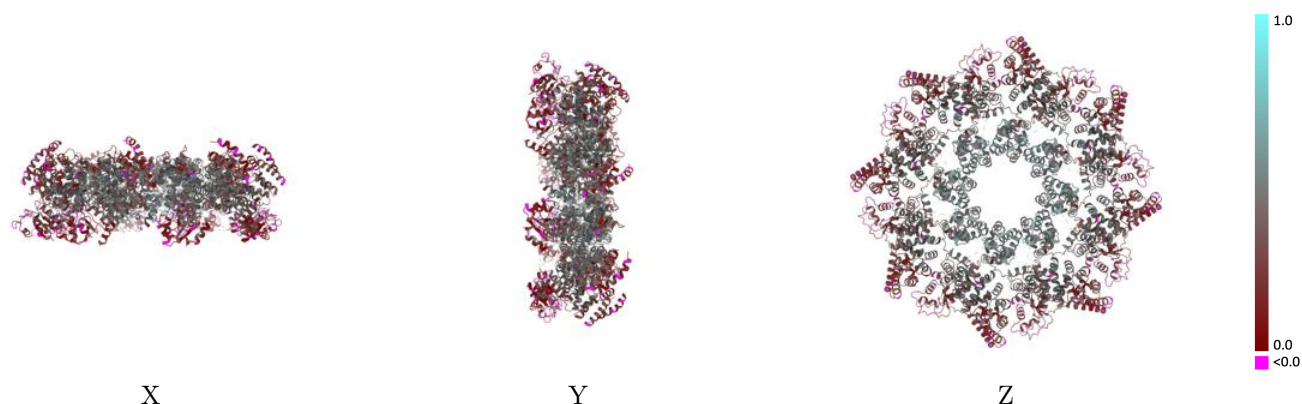
This section contains information regarding the fit between EMDB map EMD-62772 and PDB model 9L2D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



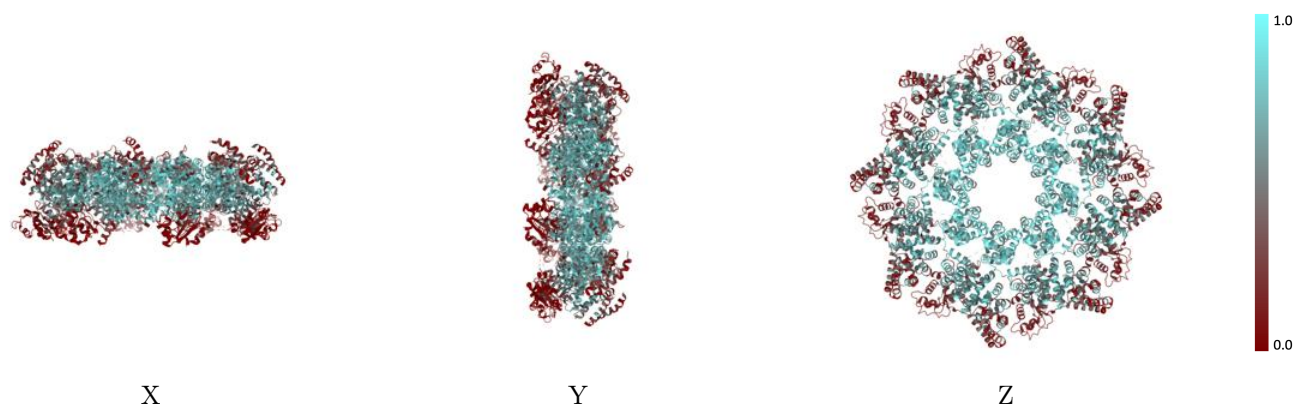
The images above show the 3D surface view of the map at the recommended contour level 0.365 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



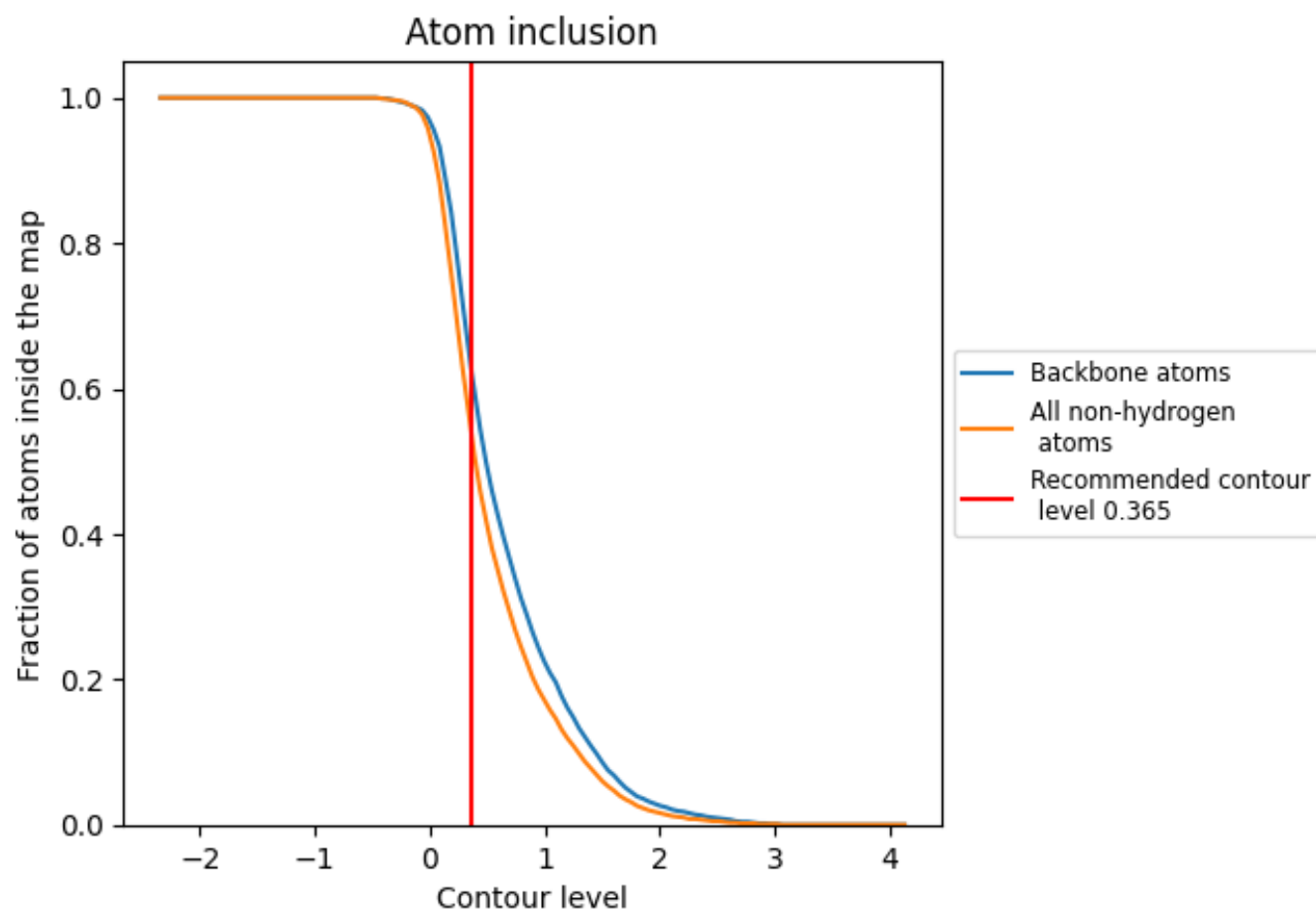
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.365).

9.4 Atom inclusion ⓘ



At the recommended contour level, 62% of all backbone atoms, 53% 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 (0.365) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5330	<div><div></div></div> 0.3530
A	<div><div></div></div> 0.5320	<div><div></div></div> 0.3530
B	<div><div></div></div> 0.5320	<div><div></div></div> 0.3510
C	<div><div></div></div> 0.5320	<div><div></div></div> 0.3530
D	<div><div></div></div> 0.5330	<div><div></div></div> 0.3540
E	<div><div></div></div> 0.5330	<div><div></div></div> 0.3530
F	<div><div></div></div> 0.5320	<div><div></div></div> 0.3530
G	<div><div></div></div> 0.5340	<div><div></div></div> 0.3530
H	<div><div></div></div> 0.5320	<div><div></div></div> 0.3520

1.0

0.0

<0.0