



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:22 AM UTC

PDB ID : 9UGJ / pdb\_00009ugj  
EMDB ID : EMD-64139  
Title : Structure of SARM1 bound to SIR3-ADPR  
Authors : Zhang, J.; Zheng, S.; Wang, X.  
Deposited on : 2025-04-12  
Resolution : 3.85 Å(reported)

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

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

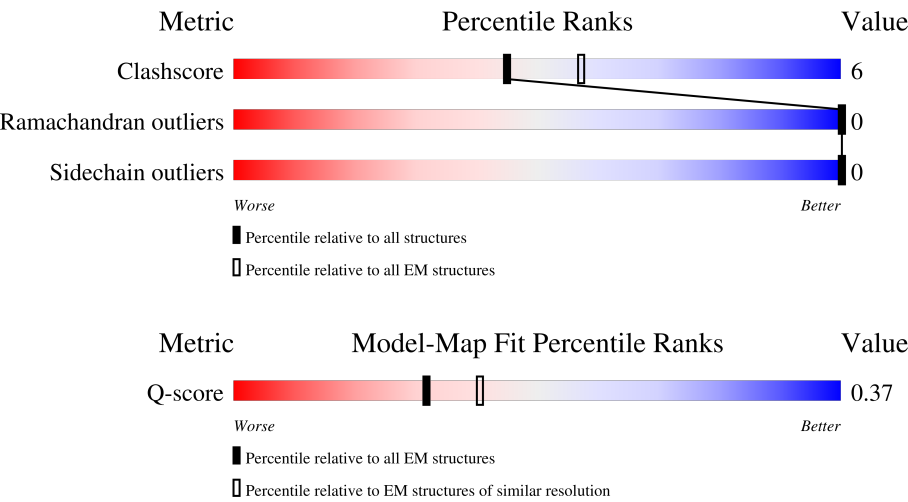
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.85 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	8989 ( 3.35 - 4.35 )

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	761	<div><div></div><div>15% . 82%</div></div>
1	B	761	<div><div></div><div>15% . 82%</div></div>
1	C	761	<div><div></div><div>15% . 82%</div></div>
1	D	761	<div><div></div><div>16% . 82%</div></div>

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Mol	Chain	Length	Quality of chain
1	E	761	 15% . 82%
1	F	761	 15% . 82%
1	G	761	 16% . 82%
1	H	761	 15% . 82%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8542 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	139	Total	C	N	O	S	0	0
			1029	670	171	183	5		
1	B	139	Total	C	N	O	S	0	0
			1017	662	167	183	5		
1	C	139	Total	C	N	O	S	0	0
			1053	679	175	193	6		
1	D	139	Total	C	N	O	S	0	0
			1032	668	171	188	5		
1	E	139	Total	C	N	O	S	0	0
			1028	669	169	187	3		
1	F	138	Total	C	N	O	S	0	0
			1014	659	167	183	5		
1	G	135	Total	C	N	O	S	0	0
			946	610	158	174	4		
1	H	138	Total	C	N	O	S	0	0
			1007	657	168	177	5		

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	CYS	SER	conflict	UNP Q6SZW1
A	423	CYS	GLN	conflict	UNP Q6SZW1
A	725	TYR	-	expression tag	UNP Q6SZW1
A	726	PRO	-	expression tag	UNP Q6SZW1
A	727	TYR	-	expression tag	UNP Q6SZW1
A	728	ASP	-	expression tag	UNP Q6SZW1
A	729	VAL	-	expression tag	UNP Q6SZW1
A	730	PRO	-	expression tag	UNP Q6SZW1
A	731	ASP	-	expression tag	UNP Q6SZW1
A	732	TYR	-	expression tag	UNP Q6SZW1
A	733	ALA	-	expression tag	UNP Q6SZW1
A	734	THR	-	expression tag	UNP Q6SZW1
A	735	ARG	-	expression tag	UNP Q6SZW1
A	736	GLY	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	737	THR	-	expression tag	UNP Q6SZW1
A	738	SER	-	expression tag	UNP Q6SZW1
A	739	ARG	-	expression tag	UNP Q6SZW1
A	740	ASP	-	expression tag	UNP Q6SZW1
A	741	TYR	-	expression tag	UNP Q6SZW1
A	742	LYS	-	expression tag	UNP Q6SZW1
A	743	ASP	-	expression tag	UNP Q6SZW1
A	744	HIS	-	expression tag	UNP Q6SZW1
A	745	ASP	-	expression tag	UNP Q6SZW1
A	746	GLY	-	expression tag	UNP Q6SZW1
A	747	ASP	-	expression tag	UNP Q6SZW1
A	748	TYR	-	expression tag	UNP Q6SZW1
A	749	LYS	-	expression tag	UNP Q6SZW1
A	750	ASP	-	expression tag	UNP Q6SZW1
A	751	HIS	-	expression tag	UNP Q6SZW1
A	752	ASP	-	expression tag	UNP Q6SZW1
A	753	ILE	-	expression tag	UNP Q6SZW1
A	754	ASP	-	expression tag	UNP Q6SZW1
A	755	TYR	-	expression tag	UNP Q6SZW1
A	756	LYS	-	expression tag	UNP Q6SZW1
A	757	ASP	-	expression tag	UNP Q6SZW1
A	758	ASP	-	expression tag	UNP Q6SZW1
A	759	ASP	-	expression tag	UNP Q6SZW1
A	760	ASP	-	expression tag	UNP Q6SZW1
A	761	LYS	-	expression tag	UNP Q6SZW1
B	379	CYS	SER	conflict	UNP Q6SZW1
B	423	CYS	GLN	conflict	UNP Q6SZW1
B	725	TYR	-	expression tag	UNP Q6SZW1
B	726	PRO	-	expression tag	UNP Q6SZW1
B	727	TYR	-	expression tag	UNP Q6SZW1
B	728	ASP	-	expression tag	UNP Q6SZW1
B	729	VAL	-	expression tag	UNP Q6SZW1
B	730	PRO	-	expression tag	UNP Q6SZW1
B	731	ASP	-	expression tag	UNP Q6SZW1
B	732	TYR	-	expression tag	UNP Q6SZW1
B	733	ALA	-	expression tag	UNP Q6SZW1
B	734	THR	-	expression tag	UNP Q6SZW1
B	735	ARG	-	expression tag	UNP Q6SZW1
B	736	GLY	-	expression tag	UNP Q6SZW1
B	737	THR	-	expression tag	UNP Q6SZW1
B	738	SER	-	expression tag	UNP Q6SZW1
B	739	ARG	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	740	ASP	-	expression tag	UNP Q6SZW1
B	741	TYR	-	expression tag	UNP Q6SZW1
B	742	LYS	-	expression tag	UNP Q6SZW1
B	743	ASP	-	expression tag	UNP Q6SZW1
B	744	HIS	-	expression tag	UNP Q6SZW1
B	745	ASP	-	expression tag	UNP Q6SZW1
B	746	GLY	-	expression tag	UNP Q6SZW1
B	747	ASP	-	expression tag	UNP Q6SZW1
B	748	TYR	-	expression tag	UNP Q6SZW1
B	749	LYS	-	expression tag	UNP Q6SZW1
B	750	ASP	-	expression tag	UNP Q6SZW1
B	751	HIS	-	expression tag	UNP Q6SZW1
B	752	ASP	-	expression tag	UNP Q6SZW1
B	753	ILE	-	expression tag	UNP Q6SZW1
B	754	ASP	-	expression tag	UNP Q6SZW1
B	755	TYR	-	expression tag	UNP Q6SZW1
B	756	LYS	-	expression tag	UNP Q6SZW1
B	757	ASP	-	expression tag	UNP Q6SZW1
B	758	ASP	-	expression tag	UNP Q6SZW1
B	759	ASP	-	expression tag	UNP Q6SZW1
B	760	ASP	-	expression tag	UNP Q6SZW1
B	761	LYS	-	expression tag	UNP Q6SZW1
C	379	CYS	SER	conflict	UNP Q6SZW1
C	423	CYS	GLN	conflict	UNP Q6SZW1
C	725	TYR	-	expression tag	UNP Q6SZW1
C	726	PRO	-	expression tag	UNP Q6SZW1
C	727	TYR	-	expression tag	UNP Q6SZW1
C	728	ASP	-	expression tag	UNP Q6SZW1
C	729	VAL	-	expression tag	UNP Q6SZW1
C	730	PRO	-	expression tag	UNP Q6SZW1
C	731	ASP	-	expression tag	UNP Q6SZW1
C	732	TYR	-	expression tag	UNP Q6SZW1
C	733	ALA	-	expression tag	UNP Q6SZW1
C	734	THR	-	expression tag	UNP Q6SZW1
C	735	ARG	-	expression tag	UNP Q6SZW1
C	736	GLY	-	expression tag	UNP Q6SZW1
C	737	THR	-	expression tag	UNP Q6SZW1
C	738	SER	-	expression tag	UNP Q6SZW1
C	739	ARG	-	expression tag	UNP Q6SZW1
C	740	ASP	-	expression tag	UNP Q6SZW1
C	741	TYR	-	expression tag	UNP Q6SZW1
C	742	LYS	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	743	ASP	-	expression tag	UNP Q6SZW1
C	744	HIS	-	expression tag	UNP Q6SZW1
C	745	ASP	-	expression tag	UNP Q6SZW1
C	746	GLY	-	expression tag	UNP Q6SZW1
C	747	ASP	-	expression tag	UNP Q6SZW1
C	748	TYR	-	expression tag	UNP Q6SZW1
C	749	LYS	-	expression tag	UNP Q6SZW1
C	750	ASP	-	expression tag	UNP Q6SZW1
C	751	HIS	-	expression tag	UNP Q6SZW1
C	752	ASP	-	expression tag	UNP Q6SZW1
C	753	ILE	-	expression tag	UNP Q6SZW1
C	754	ASP	-	expression tag	UNP Q6SZW1
C	755	TYR	-	expression tag	UNP Q6SZW1
C	756	LYS	-	expression tag	UNP Q6SZW1
C	757	ASP	-	expression tag	UNP Q6SZW1
C	758	ASP	-	expression tag	UNP Q6SZW1
C	759	ASP	-	expression tag	UNP Q6SZW1
C	760	ASP	-	expression tag	UNP Q6SZW1
C	761	LYS	-	expression tag	UNP Q6SZW1
D	379	CYS	SER	conflict	UNP Q6SZW1
D	423	CYS	GLN	conflict	UNP Q6SZW1
D	725	TYR	-	expression tag	UNP Q6SZW1
D	726	PRO	-	expression tag	UNP Q6SZW1
D	727	TYR	-	expression tag	UNP Q6SZW1
D	728	ASP	-	expression tag	UNP Q6SZW1
D	729	VAL	-	expression tag	UNP Q6SZW1
D	730	PRO	-	expression tag	UNP Q6SZW1
D	731	ASP	-	expression tag	UNP Q6SZW1
D	732	TYR	-	expression tag	UNP Q6SZW1
D	733	ALA	-	expression tag	UNP Q6SZW1
D	734	THR	-	expression tag	UNP Q6SZW1
D	735	ARG	-	expression tag	UNP Q6SZW1
D	736	GLY	-	expression tag	UNP Q6SZW1
D	737	THR	-	expression tag	UNP Q6SZW1
D	738	SER	-	expression tag	UNP Q6SZW1
D	739	ARG	-	expression tag	UNP Q6SZW1
D	740	ASP	-	expression tag	UNP Q6SZW1
D	741	TYR	-	expression tag	UNP Q6SZW1
D	742	LYS	-	expression tag	UNP Q6SZW1
D	743	ASP	-	expression tag	UNP Q6SZW1
D	744	HIS	-	expression tag	UNP Q6SZW1
D	745	ASP	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	746	GLY	-	expression tag	UNP Q6SZW1
D	747	ASP	-	expression tag	UNP Q6SZW1
D	748	TYR	-	expression tag	UNP Q6SZW1
D	749	LYS	-	expression tag	UNP Q6SZW1
D	750	ASP	-	expression tag	UNP Q6SZW1
D	751	HIS	-	expression tag	UNP Q6SZW1
D	752	ASP	-	expression tag	UNP Q6SZW1
D	753	ILE	-	expression tag	UNP Q6SZW1
D	754	ASP	-	expression tag	UNP Q6SZW1
D	755	TYR	-	expression tag	UNP Q6SZW1
D	756	LYS	-	expression tag	UNP Q6SZW1
D	757	ASP	-	expression tag	UNP Q6SZW1
D	758	ASP	-	expression tag	UNP Q6SZW1
D	759	ASP	-	expression tag	UNP Q6SZW1
D	760	ASP	-	expression tag	UNP Q6SZW1
D	761	LYS	-	expression tag	UNP Q6SZW1
E	379	CYS	SER	conflict	UNP Q6SZW1
E	423	CYS	GLN	conflict	UNP Q6SZW1
E	725	TYR	-	expression tag	UNP Q6SZW1
E	726	PRO	-	expression tag	UNP Q6SZW1
E	727	TYR	-	expression tag	UNP Q6SZW1
E	728	ASP	-	expression tag	UNP Q6SZW1
E	729	VAL	-	expression tag	UNP Q6SZW1
E	730	PRO	-	expression tag	UNP Q6SZW1
E	731	ASP	-	expression tag	UNP Q6SZW1
E	732	TYR	-	expression tag	UNP Q6SZW1
E	733	ALA	-	expression tag	UNP Q6SZW1
E	734	THR	-	expression tag	UNP Q6SZW1
E	735	ARG	-	expression tag	UNP Q6SZW1
E	736	GLY	-	expression tag	UNP Q6SZW1
E	737	THR	-	expression tag	UNP Q6SZW1
E	738	SER	-	expression tag	UNP Q6SZW1
E	739	ARG	-	expression tag	UNP Q6SZW1
E	740	ASP	-	expression tag	UNP Q6SZW1
E	741	TYR	-	expression tag	UNP Q6SZW1
E	742	LYS	-	expression tag	UNP Q6SZW1
E	743	ASP	-	expression tag	UNP Q6SZW1
E	744	HIS	-	expression tag	UNP Q6SZW1
E	745	ASP	-	expression tag	UNP Q6SZW1
E	746	GLY	-	expression tag	UNP Q6SZW1
E	747	ASP	-	expression tag	UNP Q6SZW1
E	748	TYR	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	749	LYS	-	expression tag	UNP Q6SZW1
E	750	ASP	-	expression tag	UNP Q6SZW1
E	751	HIS	-	expression tag	UNP Q6SZW1
E	752	ASP	-	expression tag	UNP Q6SZW1
E	753	ILE	-	expression tag	UNP Q6SZW1
E	754	ASP	-	expression tag	UNP Q6SZW1
E	755	TYR	-	expression tag	UNP Q6SZW1
E	756	LYS	-	expression tag	UNP Q6SZW1
E	757	ASP	-	expression tag	UNP Q6SZW1
E	758	ASP	-	expression tag	UNP Q6SZW1
E	759	ASP	-	expression tag	UNP Q6SZW1
E	760	ASP	-	expression tag	UNP Q6SZW1
E	761	LYS	-	expression tag	UNP Q6SZW1
F	379	CYS	SER	conflict	UNP Q6SZW1
F	423	CYS	GLN	conflict	UNP Q6SZW1
F	725	TYR	-	expression tag	UNP Q6SZW1
F	726	PRO	-	expression tag	UNP Q6SZW1
F	727	TYR	-	expression tag	UNP Q6SZW1
F	728	ASP	-	expression tag	UNP Q6SZW1
F	729	VAL	-	expression tag	UNP Q6SZW1
F	730	PRO	-	expression tag	UNP Q6SZW1
F	731	ASP	-	expression tag	UNP Q6SZW1
F	732	TYR	-	expression tag	UNP Q6SZW1
F	733	ALA	-	expression tag	UNP Q6SZW1
F	734	THR	-	expression tag	UNP Q6SZW1
F	735	ARG	-	expression tag	UNP Q6SZW1
F	736	GLY	-	expression tag	UNP Q6SZW1
F	737	THR	-	expression tag	UNP Q6SZW1
F	738	SER	-	expression tag	UNP Q6SZW1
F	739	ARG	-	expression tag	UNP Q6SZW1
F	740	ASP	-	expression tag	UNP Q6SZW1
F	741	TYR	-	expression tag	UNP Q6SZW1
F	742	LYS	-	expression tag	UNP Q6SZW1
F	743	ASP	-	expression tag	UNP Q6SZW1
F	744	HIS	-	expression tag	UNP Q6SZW1
F	745	ASP	-	expression tag	UNP Q6SZW1
F	746	GLY	-	expression tag	UNP Q6SZW1
F	747	ASP	-	expression tag	UNP Q6SZW1
F	748	TYR	-	expression tag	UNP Q6SZW1
F	749	LYS	-	expression tag	UNP Q6SZW1
F	750	ASP	-	expression tag	UNP Q6SZW1
F	751	HIS	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	752	ASP	-	expression tag	UNP Q6SZW1
F	753	ILE	-	expression tag	UNP Q6SZW1
F	754	ASP	-	expression tag	UNP Q6SZW1
F	755	TYR	-	expression tag	UNP Q6SZW1
F	756	LYS	-	expression tag	UNP Q6SZW1
F	757	ASP	-	expression tag	UNP Q6SZW1
F	758	ASP	-	expression tag	UNP Q6SZW1
F	759	ASP	-	expression tag	UNP Q6SZW1
F	760	ASP	-	expression tag	UNP Q6SZW1
F	761	LYS	-	expression tag	UNP Q6SZW1
G	379	CYS	SER	conflict	UNP Q6SZW1
G	423	CYS	GLN	conflict	UNP Q6SZW1
G	725	TYR	-	expression tag	UNP Q6SZW1
G	726	PRO	-	expression tag	UNP Q6SZW1
G	727	TYR	-	expression tag	UNP Q6SZW1
G	728	ASP	-	expression tag	UNP Q6SZW1
G	729	VAL	-	expression tag	UNP Q6SZW1
G	730	PRO	-	expression tag	UNP Q6SZW1
G	731	ASP	-	expression tag	UNP Q6SZW1
G	732	TYR	-	expression tag	UNP Q6SZW1
G	733	ALA	-	expression tag	UNP Q6SZW1
G	734	THR	-	expression tag	UNP Q6SZW1
G	735	ARG	-	expression tag	UNP Q6SZW1
G	736	GLY	-	expression tag	UNP Q6SZW1
G	737	THR	-	expression tag	UNP Q6SZW1
G	738	SER	-	expression tag	UNP Q6SZW1
G	739	ARG	-	expression tag	UNP Q6SZW1
G	740	ASP	-	expression tag	UNP Q6SZW1
G	741	TYR	-	expression tag	UNP Q6SZW1
G	742	LYS	-	expression tag	UNP Q6SZW1
G	743	ASP	-	expression tag	UNP Q6SZW1
G	744	HIS	-	expression tag	UNP Q6SZW1
G	745	ASP	-	expression tag	UNP Q6SZW1
G	746	GLY	-	expression tag	UNP Q6SZW1
G	747	ASP	-	expression tag	UNP Q6SZW1
G	748	TYR	-	expression tag	UNP Q6SZW1
G	749	LYS	-	expression tag	UNP Q6SZW1
G	750	ASP	-	expression tag	UNP Q6SZW1
G	751	HIS	-	expression tag	UNP Q6SZW1
G	752	ASP	-	expression tag	UNP Q6SZW1
G	753	ILE	-	expression tag	UNP Q6SZW1
G	754	ASP	-	expression tag	UNP Q6SZW1

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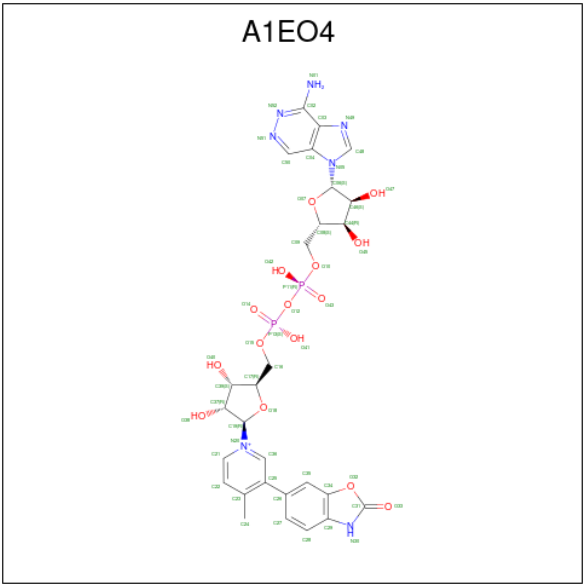
Chain	Residue	Modelled	Actual	Comment	Reference
G	755	TYR	-	expression tag	UNP Q6SZW1
G	756	LYS	-	expression tag	UNP Q6SZW1
G	757	ASP	-	expression tag	UNP Q6SZW1
G	758	ASP	-	expression tag	UNP Q6SZW1
G	759	ASP	-	expression tag	UNP Q6SZW1
G	760	ASP	-	expression tag	UNP Q6SZW1
G	761	LYS	-	expression tag	UNP Q6SZW1
H	379	CYS	SER	conflict	UNP Q6SZW1
H	423	CYS	GLN	conflict	UNP Q6SZW1
H	725	TYR	-	expression tag	UNP Q6SZW1
H	726	PRO	-	expression tag	UNP Q6SZW1
H	727	TYR	-	expression tag	UNP Q6SZW1
H	728	ASP	-	expression tag	UNP Q6SZW1
H	729	VAL	-	expression tag	UNP Q6SZW1
H	730	PRO	-	expression tag	UNP Q6SZW1
H	731	ASP	-	expression tag	UNP Q6SZW1
H	732	TYR	-	expression tag	UNP Q6SZW1
H	733	ALA	-	expression tag	UNP Q6SZW1
H	734	THR	-	expression tag	UNP Q6SZW1
H	735	ARG	-	expression tag	UNP Q6SZW1
H	736	GLY	-	expression tag	UNP Q6SZW1
H	737	THR	-	expression tag	UNP Q6SZW1
H	738	SER	-	expression tag	UNP Q6SZW1
H	739	ARG	-	expression tag	UNP Q6SZW1
H	740	ASP	-	expression tag	UNP Q6SZW1
H	741	TYR	-	expression tag	UNP Q6SZW1
H	742	LYS	-	expression tag	UNP Q6SZW1
H	743	ASP	-	expression tag	UNP Q6SZW1
H	744	HIS	-	expression tag	UNP Q6SZW1
H	745	ASP	-	expression tag	UNP Q6SZW1
H	746	GLY	-	expression tag	UNP Q6SZW1
H	747	ASP	-	expression tag	UNP Q6SZW1
H	748	TYR	-	expression tag	UNP Q6SZW1
H	749	LYS	-	expression tag	UNP Q6SZW1
H	750	ASP	-	expression tag	UNP Q6SZW1
H	751	HIS	-	expression tag	UNP Q6SZW1
H	752	ASP	-	expression tag	UNP Q6SZW1
H	753	ILE	-	expression tag	UNP Q6SZW1
H	754	ASP	-	expression tag	UNP Q6SZW1
H	755	TYR	-	expression tag	UNP Q6SZW1
H	756	LYS	-	expression tag	UNP Q6SZW1
H	757	ASP	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	758	ASP	-	expression tag	UNP Q6SZW1
H	759	ASP	-	expression tag	UNP Q6SZW1
H	760	ASP	-	expression tag	UNP Q6SZW1
H	761	LYS	-	expression tag	UNP Q6SZW1

- Molecule 2 is [[(2 {S},3 {R},4 {S},5 {S})-5-(4-azanylimidazo[4,5-d]pyridazin-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},5 {R})-5-[4-methyl-3-(2-oxidanylidene-3 {H}-1,3-benzoxazol-6-yl)pyridin-1-ium-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (CCD ID: A1EO4) (formula: C<sub>28</sub>H<sub>32</sub>N<sub>7</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			52	28	7	15	2	
2	C	1	Total	C	N	O	P	0
			52	28	7	15	2	
2	D	1	Total	C	N	O	P	0
			52	28	7	15	2	
2	E	1	Total	C	N	O	P	0
			52	28	7	15	2	
2	E	1	Total	C	N	O	P	0
			52	28	7	15	2	
2	F	1	Total	C	N	O	P	0
			52	28	7	15	2	
2	H	1	Total	C	N	O	P	0
			52	28	7	15	2	

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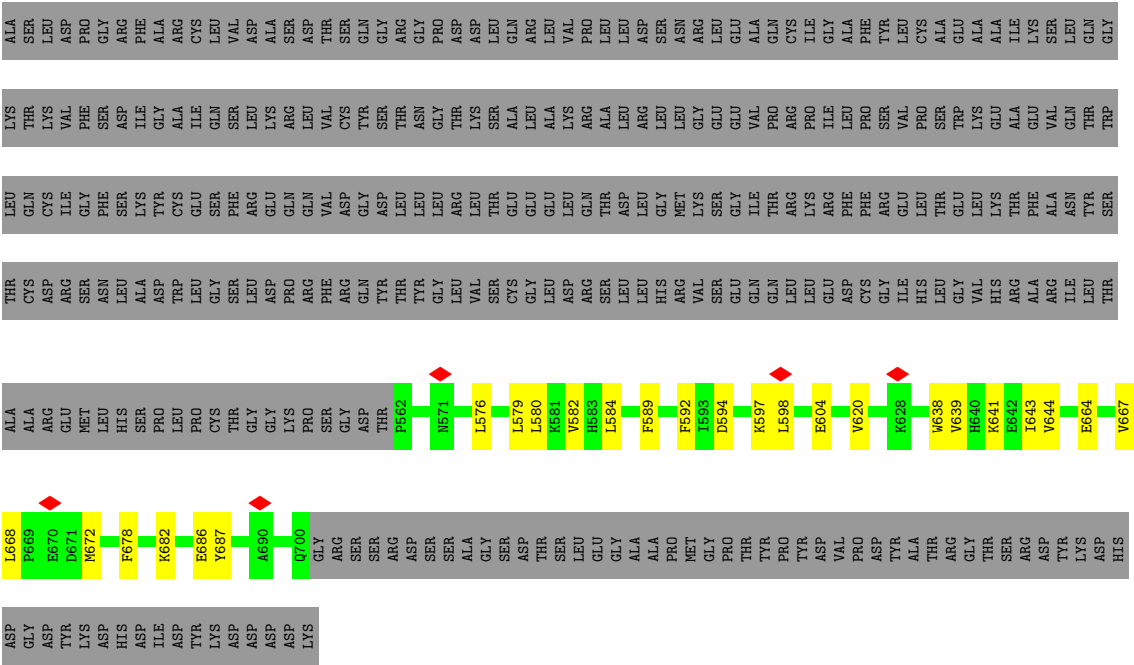
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	H	1	52	28	7	15	2	0

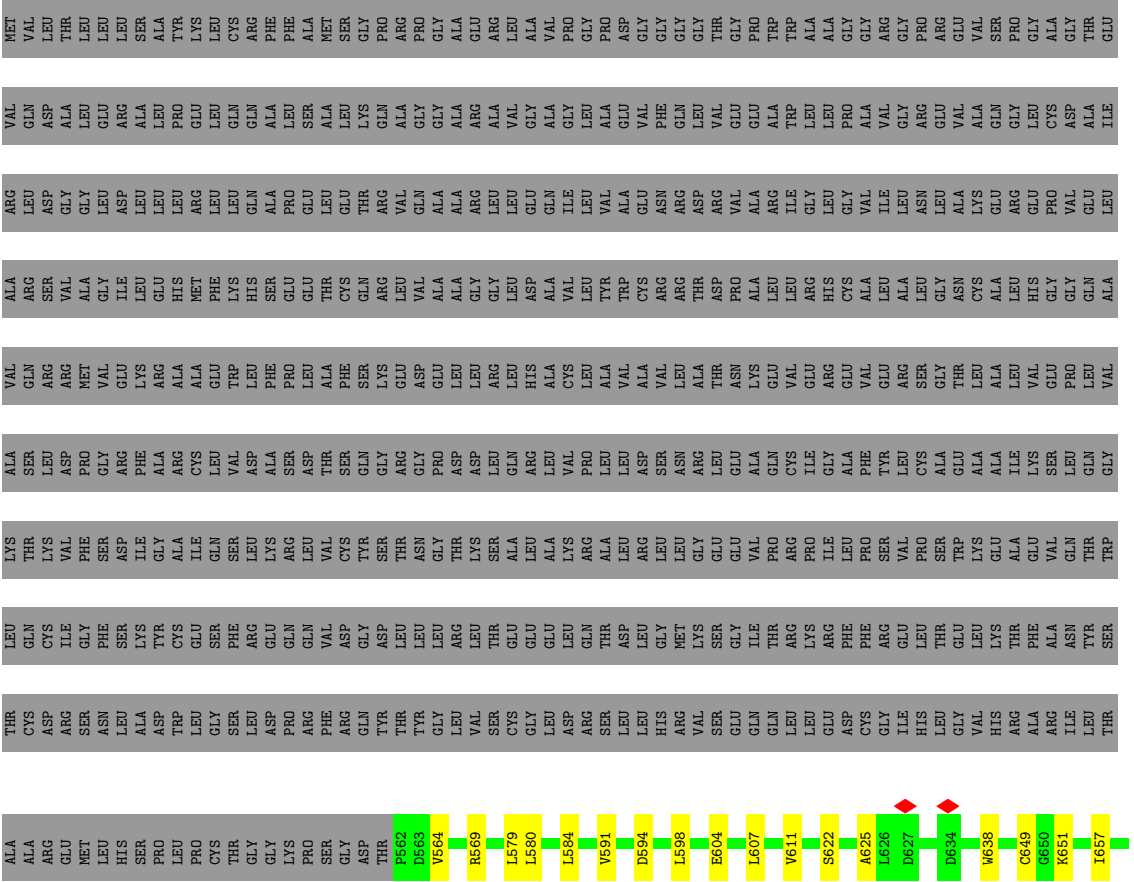


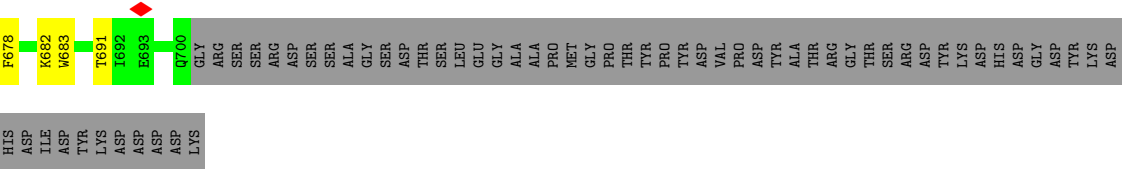
- Molecule 1: NAD(+) hydrolase SARM1

[illegible]

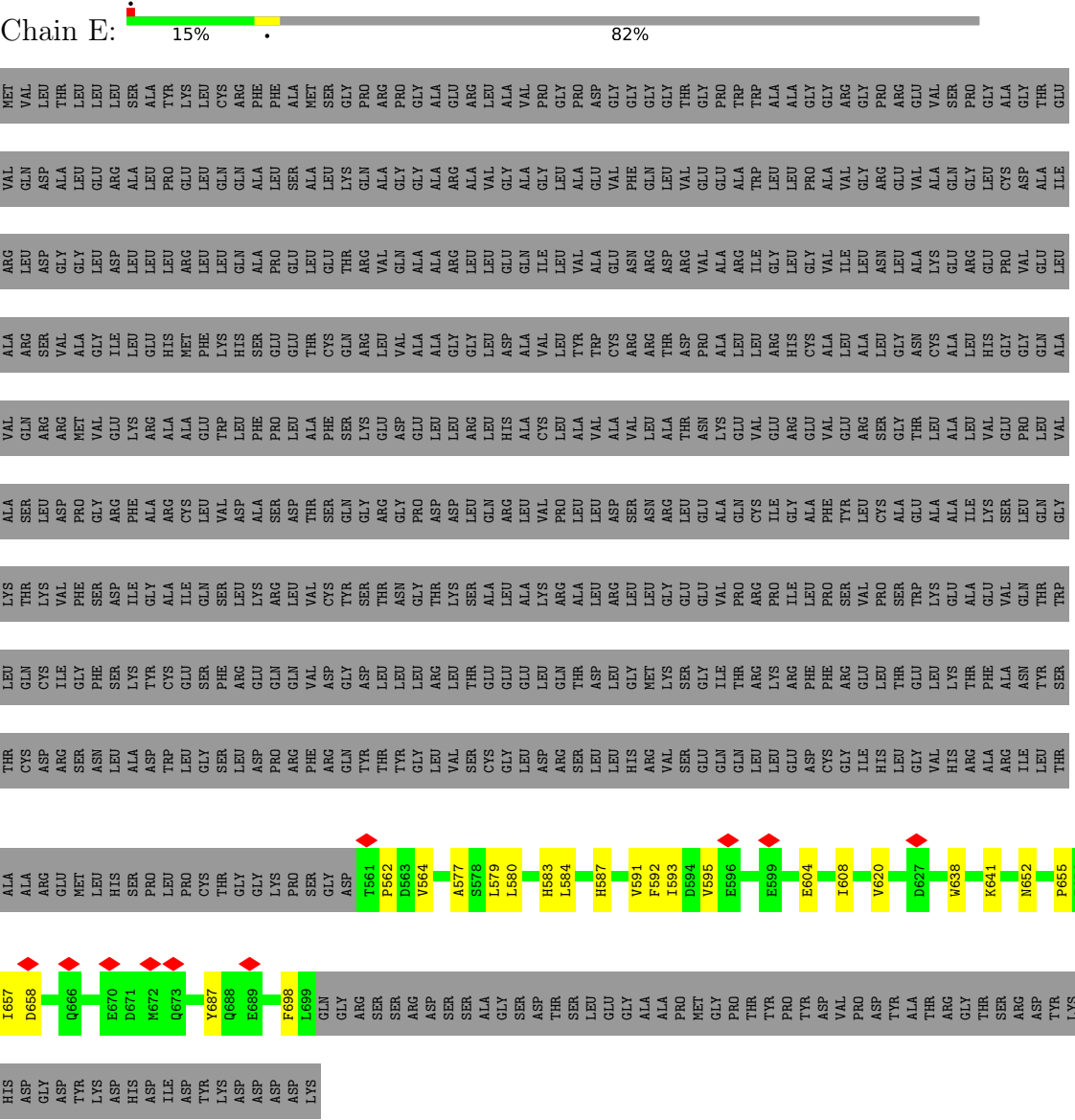


● Molecule 1: NAD(+) hydrolase SARM1

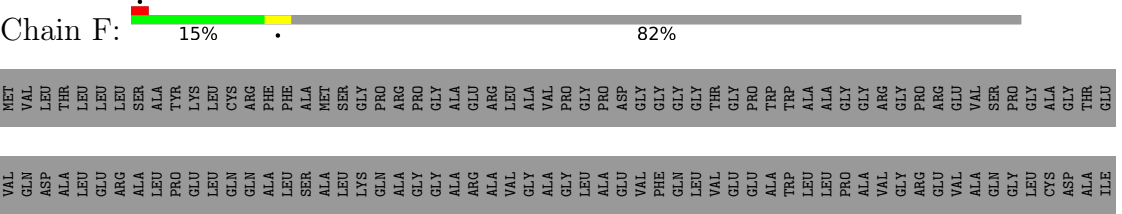




• Molecule 1: NAD(+) hydrolase SARM1



• Molecule 1: NAD(+) hydrolase SARM1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28854	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.932	Depositor
Minimum map value	-1.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.249	Depositor
Map size (Å)	404.0, 404.0, 404.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EO4

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	0.12	0/1054	0.39	0/1439
1	B	0.12	0/1041	0.38	0/1424
1	C	0.14	0/1077	0.38	0/1465
1	D	0.13	0/1056	0.37	0/1440
1	E	0.13	0/1054	0.42	0/1439
1	F	0.11	0/1036	0.35	0/1412
1	G	0.12	0/966	0.38	0/1322
1	H	0.13	0/1031	0.41	0/1406
All	All	0.13	0/8315	0.39	0/11347

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1029	0	967	17	0
1	B	1017	0	955	16	0
1	C	1053	0	1004	18	0
1	D	1032	0	972	13	0
1	E	1028	0	954	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1014	0	961	14	0
1	G	946	0	839	7	0
1	H	1007	0	937	14	0
2	B	52	0	0	2	0
2	C	52	0	0	1	0
2	D	52	0	0	1	0
2	E	104	0	0	1	0
2	F	52	0	0	0	0
2	H	104	0	0	0	0
All	All	8542	0	7589	101	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 6.

All (101) 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:594:ASP:HA	1:A:598:LEU:HD23	1.75	0.68
1:D:594:ASP:HA	1:D:598:LEU:HD23	1.75	0.68
1:F:582:VAL:HG11	1:H:582:VAL:HG11	1.76	0.67
1:H:668:LEU:HD13	1:H:672:MET:HE2	1.78	0.66
1:E:562:PRO:HG2	1:E:592:PHE:HD2	1.63	0.63
1:A:619:LEU:HD22	1:A:643:ILE:HD11	1.82	0.62
1:F:581:LYS:HG3	1:F:591:VAL:HG21	1.81	0.61
1:D:657:ILE:HB	1:D:682:LYS:HA	1.82	0.61
1:A:580:LEU:O	1:A:584:LEU:HD23	2.00	0.61
1:E:652:ASN:ND2	1:E:698:PHE:O	2.30	0.61
1:F:562:PRO:HG2	1:F:592:PHE:HB2	1.83	0.60
1:D:682:LYS:O	1:E:687:TYR:OH	2.16	0.60
1:B:685:HIS:O	1:B:688:GLN:NE2	2.32	0.59
1:B:694:LYS:NZ	1:C:686:GLU:OE2	2.35	0.59
1:E:564:VAL:HB	1:E:591:VAL:HG22	1.84	0.59
1:C:594:ASP:HA	1:C:598:LEU:HD23	1.85	0.58
1:E:608:ILE:HD11	1:E:641:LYS:HG2	1.85	0.58
1:D:678:PHE:O	2:D:801:A1EO4:N01	2.36	0.58
1:H:569:ARG:NH2	1:H:629:CYS:SG	2.76	0.58
1:H:564:VAL:HB	1:H:591:VAL:HG12	1.86	0.58
1:F:644:VAL:HA	1:F:647:LEU:HD12	1.86	0.58
1:H:683:TRP:HA	1:H:691:THR:HG21	1.87	0.57
1:E:580:LEU:O	1:E:584:LEU:HD23	2.05	0.57
1:H:583:HIS:O	1:H:587:HIS:ND1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:LEU:HD12	1:C:589:PHE:HD2	1.73	0.54
1:G:654:VAL:HG13	1:G:698:PHE:HD2	1.72	0.53
1:B:622:SER:H	1:B:625:ALA:HB2	1.74	0.53
1:C:580:LEU:O	1:C:584:LEU:HD23	2.09	0.53
1:F:561:THR:HG21	1:F:613:GLY:HA3	1.91	0.53
1:H:674:ALA:O	1:H:677:THR:OG1	2.28	0.52
1:E:579:LEU:HA	1:G:579:LEU:HD13	1.92	0.52
1:B:687:TYR:OH	1:C:682:LYS:O	2.27	0.51
1:H:653:ILE:HG22	1:H:655:PRO:HD3	1.92	0.51
1:D:607:LEU:O	1:D:611:VAL:HG23	2.10	0.51
1:B:565:PHE:HD1	1:B:592:PHE:HB3	1.76	0.51
1:D:604:GLU:HG2	1:D:638:TRP:HZ2	1.75	0.51
1:H:577:ALA:O	1:H:581:LYS:N	2.39	0.51
1:E:658:ASP:OD2	1:G:575:GLN:NE2	2.43	0.51
1:B:579:LEU:HA	1:D:579:LEU:HD13	1.93	0.51
1:B:679:ASN:OD1	2:B:801:A1EO4:N30	2.44	0.51
1:A:579:LEU:HA	1:C:579:LEU:HD13	1.92	0.50
1:B:597:LYS:O	1:B:598:LEU:HG	2.11	0.50
1:B:569:ARG:NH1	2:E:801:A1EO4:O41	2.45	0.50
1:D:580:LEU:O	1:D:584:LEU:HD23	2.12	0.50
1:C:639:VAL:O	1:C:643:ILE:HG12	2.12	0.49
1:C:641:LYS:O	1:C:644:VAL:HG12	2.11	0.49
1:A:668:LEU:HD13	1:A:672:MET:HE2	1.95	0.49
1:F:579:LEU:HD13	1:H:579:LEU:HA	1.94	0.49
1:G:580:LEU:HD23	1:G:584:LEU:HD23	1.95	0.49
1:B:564:VAL:HG21	1:B:584:LEU:HD11	1.95	0.48
1:F:630:MET:HE1	1:F:667:VAL:HB	1.96	0.48
1:B:682:LYS:O	1:C:687:TYR:OH	2.27	0.48
1:C:668:LEU:HD13	1:C:672:MET:HE2	1.96	0.47
1:A:576:LEU:HD23	1:A:620:VAL:HG13	1.97	0.47
1:A:604:GLU:HA	1:A:638:TRP:HH2	1.79	0.47
1:F:579:LEU:O	1:F:582:VAL:HG12	2.15	0.46
1:E:562:PRO:HG2	1:E:592:PHE:CD2	2.49	0.46
1:C:664:GLU:O	1:C:667:VAL:HG22	2.17	0.45
1:E:583:HIS:O	1:E:587:HIS:ND1	2.38	0.45
1:C:604:GLU:HA	1:C:638:TRP:CH2	2.51	0.45
1:A:669:PRO:HD2	1:A:672:MET:SD	2.57	0.45
1:G:583:HIS:O	1:G:587:HIS:ND1	2.44	0.45
1:C:592:PHE:HA	1:C:597:LYS:HG3	1.98	0.45
1:H:581:LYS:HG2	1:H:591:VAL:HG21	1.99	0.45
1:D:683:TRP:HA	1:D:691:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:OG	1:A:687:TYR:O	2.34	0.44
1:H:669:PRO:HG2	1:H:672:MET:HG2	2.00	0.44
1:F:580:LEU:O	1:F:584:LEU:HD23	2.18	0.43
1:C:672:MET:HE3	1:C:672:MET:HB2	1.94	0.43
1:F:607:LEU:O	1:F:611:VAL:HG23	2.18	0.43
1:H:692:ILE:O	1:H:695:ILE:HG22	2.19	0.43
1:B:665:PRO:HA	1:B:676:LEU:HD12	2.00	0.43
1:A:582:VAL:HG11	1:C:582:VAL:HG11	2.01	0.43
1:D:622:SER:H	1:D:625:ALA:HB2	1.84	0.43
1:A:584:LEU:HD12	1:A:589:PHE:HD2	1.84	0.43
1:E:604:GLU:HA	1:E:638:TRP:HH2	1.83	0.43
1:G:580:LEU:HD11	1:G:618:VAL:HG11	2.01	0.43
1:A:579:LEU:O	1:A:582:VAL:HG12	2.19	0.43
1:A:682:LYS:O	1:H:687:TYR:OH	2.32	0.43
1:C:576:LEU:HD23	1:C:620:VAL:HG13	2.00	0.43
1:B:664:GLU:O	1:B:667:VAL:HG22	2.20	0.42
1:B:678:PHE:O	2:B:801:A1EO4:N01	2.53	0.42
1:D:564:VAL:HB	1:D:591:VAL:HG12	2.02	0.42
1:D:569:ARG:HG3	1:D:625:ALA:HA	2.00	0.42
1:F:564:VAL:O	1:F:591:VAL:HA	2.19	0.42
1:C:678:PHE:O	2:C:801:A1EO4:N01	2.52	0.42
1:D:649:CYS:SG	1:D:651:LYS:HE2	2.60	0.42
1:B:604:GLU:HA	1:B:638:TRP:HH2	1.83	0.42
1:E:577:ALA:HB2	1:E:620:VAL:HG21	2.02	0.42
1:A:594:ASP:N	1:A:594:ASP:OD1	2.53	0.42
1:B:604:GLU:HA	1:B:638:TRP:CH2	2.55	0.42
1:A:622:SER:H	1:A:625:ALA:HB2	1.85	0.41
1:E:593:ILE:HG12	1:E:595:VAL:HG22	2.02	0.41
1:G:653:ILE:HG22	1:G:655:PRO:HD3	2.02	0.41
1:E:655:PRO:O	1:E:657:ILE:HG13	2.21	0.41
1:F:634:ASP:OD1	1:F:634:ASP:N	2.46	0.41
1:F:691:THR:O	1:F:695:ILE:HG12	2.21	0.41
1:A:681:ILE:HD11	1:A:698:PHE:CG	2.56	0.40
1:A:564:VAL:HB	1:A:591:VAL:HG12	2.03	0.40
1:C:579:LEU:O	1:C:582:VAL:HG12	2.21	0.40
1:F:594:ASP:OD1	1:F:595:VAL:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	137/761 (18%)	133 (97%)	4 (3%)	0	100	100
1	B	137/761 (18%)	127 (93%)	10 (7%)	0	100	100
1	C	137/761 (18%)	129 (94%)	8 (6%)	0	100	100
1	D	137/761 (18%)	132 (96%)	5 (4%)	0	100	100
1	E	137/761 (18%)	130 (95%)	7 (5%)	0	100	100
1	F	134/761 (18%)	128 (96%)	6 (4%)	0	100	100
1	G	129/761 (17%)	126 (98%)	3 (2%)	0	100	100
1	H	136/761 (18%)	130 (96%)	6 (4%)	0	100	100
All	All	1084/6088 (18%)	1035 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	102/624 (16%)	102 (100%)	0	100	100
1	B	101/624 (16%)	101 (100%)	0	100	100
1	C	109/624 (18%)	109 (100%)	0	100	100
1	D	104/624 (17%)	104 (100%)	0	100	100
1	E	101/624 (16%)	101 (100%)	0	100	100
1	F	102/624 (16%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	87/624 (14%)	87 (100%)	0	100	100
1	H	96/624 (15%)	96 (100%)	0	100	100
All	All	802/4992 (16%)	802 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	GLN
1	B	616	ASN
1	E	685	HIS
1	F	685	HIS
1	G	583	HIS
1	G	685	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](#)

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	A1EO4	H	801	-	56,58,58	2.68	24 (42%)	76,89,89	2.06	19 (25%)
2	A1EO4	B	801	-	56,58,58	2.68	24 (42%)	76,89,89	2.07	19 (25%)
2	A1EO4	E	801	-	56,58,58	2.68	25 (44%)	76,89,89	2.07	19 (25%)
2	A1EO4	H	802	-	56,58,58	2.69	25 (44%)	76,89,89	2.06	19 (25%)
2	A1EO4	D	801	-	56,58,58	2.69	25 (44%)	76,89,89	2.08	19 (25%)
2	A1EO4	C	801	-	56,58,58	2.69	25 (44%)	76,89,89	2.07	19 (25%)
2	A1EO4	E	802	-	56,58,58	2.69	24 (42%)	76,89,89	2.05	19 (25%)
2	A1EO4	F	801	-	56,58,58	2.68	25 (44%)	76,89,89	2.07	19 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EO4	H	801	-	-	15/30/62/62	0/7/7/7
2	A1EO4	B	801	-	-	18/30/62/62	0/7/7/7
2	A1EO4	E	801	-	-	17/30/62/62	0/7/7/7
2	A1EO4	H	802	-	-	16/30/62/62	0/7/7/7
2	A1EO4	D	801	-	-	18/30/62/62	0/7/7/7
2	A1EO4	C	801	-	-	17/30/62/62	0/7/7/7
2	A1EO4	E	802	-	-	17/30/62/62	0/7/7/7
2	A1EO4	F	801	-	-	13/30/62/62	0/7/7/7

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	802	A1EO4	P11-O12	7.53	1.67	1.59
2	D	801	A1EO4	P11-O12	7.51	1.67	1.59
2	F	801	A1EO4	P11-O12	7.50	1.67	1.59
2	H	801	A1EO4	P11-O12	7.48	1.67	1.59
2	C	801	A1EO4	P11-O12	7.48	1.67	1.59
2	E	802	A1EO4	P11-O12	7.47	1.67	1.59
2	E	801	A1EO4	P11-O12	7.47	1.67	1.59
2	B	801	A1EO4	P11-O12	7.38	1.67	1.59
2	D	801	A1EO4	C31-N30	7.20	1.41	1.35
2	B	801	A1EO4	C31-N30	7.17	1.41	1.35
2	C	801	A1EO4	C31-N30	7.15	1.41	1.35
2	E	801	A1EO4	C31-N30	7.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	A1EO4	C31-N30	7.11	1.41	1.35
2	H	802	A1EO4	C31-N30	7.11	1.41	1.35
2	H	801	A1EO4	C31-N30	7.10	1.41	1.35
2	E	802	A1EO4	C31-N30	7.04	1.41	1.35
2	H	802	A1EO4	P13-O15	6.25	1.83	1.59
2	D	801	A1EO4	P13-O15	6.24	1.83	1.59
2	E	802	A1EO4	P13-O15	6.24	1.83	1.59
2	H	801	A1EO4	P13-O15	6.23	1.83	1.59
2	F	801	A1EO4	P13-O15	6.23	1.83	1.59
2	E	801	A1EO4	P13-O15	6.23	1.83	1.59
2	B	801	A1EO4	P13-O15	6.23	1.83	1.59
2	C	801	A1EO4	P13-O15	6.22	1.83	1.59
2	H	802	A1EO4	P11-O10	5.01	1.79	1.59
2	H	801	A1EO4	P11-O10	5.00	1.79	1.59
2	C	801	A1EO4	P11-O10	4.99	1.78	1.59
2	B	801	A1EO4	P11-O10	4.99	1.78	1.59
2	F	801	A1EO4	P11-O10	4.99	1.78	1.59
2	E	801	A1EO4	P11-O10	4.99	1.78	1.59
2	D	801	A1EO4	P11-O10	4.98	1.78	1.59
2	E	802	A1EO4	P11-O10	4.98	1.78	1.59
2	E	802	A1EO4	C25-C26	4.85	1.58	1.49
2	E	801	A1EO4	C25-C26	4.84	1.58	1.49
2	H	802	A1EO4	C25-C26	4.84	1.58	1.49
2	H	801	A1EO4	C25-C26	4.83	1.58	1.49
2	F	801	A1EO4	C25-C26	4.82	1.58	1.49
2	C	801	A1EO4	C25-C26	4.82	1.58	1.49
2	B	801	A1EO4	C25-C26	4.78	1.58	1.49
2	D	801	A1EO4	C25-C26	4.78	1.58	1.49
2	H	802	A1EO4	C02-N52	4.42	1.40	1.34
2	E	802	A1EO4	C02-N52	4.38	1.40	1.34
2	F	801	A1EO4	C02-N52	4.37	1.40	1.34
2	C	801	A1EO4	C02-N52	4.35	1.40	1.34
2	B	801	A1EO4	C02-N52	4.35	1.40	1.34
2	D	801	A1EO4	C02-N52	4.32	1.40	1.34
2	E	801	A1EO4	C02-N52	4.31	1.40	1.34
2	H	801	A1EO4	C02-N52	4.31	1.40	1.34
2	C	801	A1EO4	C36-N20	4.02	1.39	1.35
2	E	802	A1EO4	C36-N20	4.01	1.39	1.35
2	F	801	A1EO4	C36-N20	3.99	1.39	1.35
2	H	801	A1EO4	C36-N20	3.98	1.39	1.35
2	D	801	A1EO4	C36-N20	3.97	1.39	1.35
2	H	802	A1EO4	C36-N20	3.95	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	A1EO4	C36-N20	3.93	1.39	1.35
2	B	801	A1EO4	C36-N20	3.88	1.39	1.35
2	C	801	A1EO4	C06-N05	3.72	1.56	1.46
2	H	802	A1EO4	C06-N05	3.71	1.56	1.46
2	D	801	A1EO4	C06-N05	3.71	1.56	1.46
2	F	801	A1EO4	C06-N05	3.71	1.56	1.46
2	E	801	A1EO4	C06-N05	3.70	1.56	1.46
2	B	801	A1EO4	C06-N05	3.70	1.56	1.46
2	E	802	A1EO4	C06-N05	3.70	1.56	1.46
2	H	801	A1EO4	C06-N05	3.68	1.56	1.46
2	B	801	A1EO4	C04-C03	3.67	1.45	1.40
2	E	802	A1EO4	C04-C03	3.65	1.45	1.40
2	H	801	A1EO4	C04-C03	3.64	1.45	1.40
2	D	801	A1EO4	C04-C03	3.64	1.45	1.40
2	H	802	A1EO4	C04-C03	3.63	1.45	1.40
2	C	801	A1EO4	C04-C03	3.62	1.45	1.40
2	E	801	A1EO4	C04-C03	3.61	1.45	1.40
2	F	801	A1EO4	C04-C03	3.58	1.45	1.40
2	C	801	A1EO4	P13-O12	3.27	1.63	1.59
2	B	801	A1EO4	P13-O12	3.27	1.63	1.59
2	E	802	A1EO4	P13-O12	3.27	1.63	1.59
2	D	801	A1EO4	P13-O12	3.26	1.63	1.59
2	H	801	A1EO4	P13-O12	3.25	1.63	1.59
2	H	802	A1EO4	P13-O12	3.24	1.63	1.59
2	E	801	A1EO4	P13-O12	3.23	1.63	1.59
2	F	801	A1EO4	P13-O12	3.22	1.63	1.59
2	H	801	A1EO4	C09-C08	3.04	1.60	1.51
2	E	801	A1EO4	C09-C08	3.03	1.60	1.51
2	C	801	A1EO4	C09-C08	3.03	1.60	1.51
2	H	802	A1EO4	C09-C08	3.03	1.60	1.51
2	E	802	A1EO4	C09-C08	3.03	1.60	1.51
2	F	801	A1EO4	C09-C08	3.03	1.60	1.51
2	B	801	A1EO4	C09-C08	3.02	1.60	1.51
2	D	801	A1EO4	C09-C08	3.01	1.60	1.51
2	H	802	A1EO4	N51-N52	-3.00	1.30	1.34
2	E	802	A1EO4	N51-N52	-2.99	1.30	1.34
2	F	801	A1EO4	N51-N52	-2.99	1.30	1.34
2	B	801	A1EO4	N51-N52	-2.98	1.30	1.34
2	H	801	A1EO4	C16-C17	2.97	1.60	1.51
2	D	801	A1EO4	N51-N52	-2.96	1.30	1.34
2	F	801	A1EO4	C16-C17	2.96	1.60	1.51
2	C	801	A1EO4	N51-N52	-2.96	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	802	A1EO4	C16-C17	2.96	1.60	1.51
2	E	801	A1EO4	C16-C17	2.96	1.60	1.51
2	E	801	A1EO4	N51-N52	-2.96	1.30	1.34
2	C	801	A1EO4	C16-C17	2.95	1.60	1.51
2	E	802	A1EO4	C16-C17	2.95	1.60	1.51
2	D	801	A1EO4	C16-C17	2.94	1.60	1.51
2	H	801	A1EO4	N51-N52	-2.94	1.30	1.34
2	B	801	A1EO4	C16-C17	2.94	1.60	1.51
2	F	801	A1EO4	C29-N30	2.94	1.44	1.38
2	E	802	A1EO4	C29-N30	2.93	1.44	1.38
2	E	801	A1EO4	C29-N30	2.92	1.44	1.38
2	H	802	A1EO4	C29-N30	2.92	1.44	1.38
2	B	801	A1EO4	C29-N30	2.92	1.44	1.38
2	D	801	A1EO4	C29-N30	2.92	1.44	1.38
2	C	801	A1EO4	C29-N30	2.91	1.44	1.38
2	H	801	A1EO4	C29-N30	2.90	1.44	1.38
2	D	801	A1EO4	C48-N05	2.65	1.42	1.37
2	H	802	A1EO4	C48-N05	2.65	1.42	1.37
2	F	801	A1EO4	C48-N05	2.64	1.42	1.37
2	E	801	A1EO4	C48-N05	2.64	1.42	1.37
2	E	802	A1EO4	C48-N05	2.64	1.42	1.37
2	B	801	A1EO4	C48-N05	2.63	1.42	1.37
2	H	801	A1EO4	C48-N05	2.62	1.42	1.37
2	C	801	A1EO4	C48-N05	2.62	1.42	1.37
2	E	802	A1EO4	C27-C28	2.58	1.43	1.38
2	C	801	A1EO4	C27-C28	2.57	1.43	1.38
2	F	801	A1EO4	C27-C28	2.56	1.42	1.38
2	E	802	A1EO4	O15-C16	-2.54	1.35	1.44
2	H	802	A1EO4	O15-C16	-2.53	1.35	1.44
2	B	801	A1EO4	C27-C28	2.53	1.42	1.38
2	D	801	A1EO4	O15-C16	-2.53	1.35	1.44
2	C	801	A1EO4	O15-C16	-2.53	1.35	1.44
2	E	801	A1EO4	C27-C28	2.53	1.42	1.38
2	H	801	A1EO4	C27-C28	2.53	1.42	1.38
2	B	801	A1EO4	O15-C16	-2.53	1.35	1.44
2	E	801	A1EO4	O15-C16	-2.52	1.35	1.44
2	H	801	A1EO4	O15-C16	-2.52	1.35	1.44
2	D	801	A1EO4	C27-C28	2.52	1.42	1.38
2	F	801	A1EO4	O15-C16	-2.51	1.35	1.44
2	H	802	A1EO4	C27-C28	2.50	1.42	1.38
2	D	801	A1EO4	C25-C23	2.46	1.45	1.40
2	E	802	A1EO4	C25-C23	2.43	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	A1EO4	C25-C23	2.43	1.44	1.40
2	H	802	A1EO4	C25-C23	2.43	1.44	1.40
2	C	801	A1EO4	C25-C23	2.43	1.44	1.40
2	B	801	A1EO4	C35-C26	2.43	1.44	1.39
2	E	802	A1EO4	C35-C26	2.42	1.44	1.39
2	F	801	A1EO4	C35-C26	2.42	1.44	1.39
2	H	802	A1EO4	C35-C26	2.42	1.44	1.39
2	H	801	A1EO4	C25-C23	2.41	1.44	1.40
2	B	801	A1EO4	C25-C23	2.39	1.44	1.40
2	C	801	A1EO4	C35-C26	2.39	1.43	1.39
2	D	801	A1EO4	C35-C26	2.39	1.43	1.39
2	F	801	A1EO4	C25-C23	2.39	1.44	1.40
2	H	801	A1EO4	C35-C26	2.37	1.43	1.39
2	E	801	A1EO4	C35-C26	2.36	1.43	1.39
2	H	801	A1EO4	C48-N49	2.31	1.36	1.31
2	E	801	A1EO4	C02-N01	2.30	1.40	1.34
2	C	801	A1EO4	C48-N49	2.29	1.36	1.31
2	D	801	A1EO4	C02-N01	2.29	1.40	1.34
2	E	802	A1EO4	C02-N01	2.28	1.40	1.34
2	E	802	A1EO4	C48-N49	2.28	1.36	1.31
2	H	801	A1EO4	C02-N01	2.28	1.40	1.34
2	H	802	A1EO4	C02-N01	2.28	1.40	1.34
2	C	801	A1EO4	C02-N01	2.28	1.40	1.34
2	F	801	A1EO4	C48-N49	2.27	1.36	1.31
2	E	801	A1EO4	C48-N49	2.26	1.36	1.31
2	H	802	A1EO4	C48-N49	2.26	1.36	1.31
2	F	801	A1EO4	C02-N01	2.26	1.40	1.34
2	D	801	A1EO4	C48-N49	2.25	1.36	1.31
2	B	801	A1EO4	C02-N01	2.25	1.40	1.34
2	B	801	A1EO4	C48-N49	2.24	1.36	1.31
2	F	801	A1EO4	C35-C34	2.19	1.42	1.38
2	H	801	A1EO4	O32-C31	2.19	1.40	1.38
2	H	802	A1EO4	C35-C34	2.18	1.42	1.38
2	C	801	A1EO4	C35-C34	2.18	1.42	1.38
2	E	802	A1EO4	C35-C34	2.18	1.42	1.38
2	D	801	A1EO4	C35-C34	2.17	1.42	1.38
2	E	801	A1EO4	C35-C34	2.16	1.42	1.38
2	H	801	A1EO4	C35-C34	2.16	1.42	1.38
2	B	801	A1EO4	C35-C34	2.13	1.42	1.38
2	H	802	A1EO4	O32-C31	2.13	1.40	1.38
2	C	801	A1EO4	O32-C31	2.11	1.40	1.38
2	D	801	A1EO4	O32-C31	2.11	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1EO4	O32-C31	2.09	1.40	1.38
2	H	802	A1EO4	O10-C09	-2.09	1.36	1.44
2	E	802	A1EO4	O32-C31	2.08	1.40	1.38
2	F	801	A1EO4	O10-C09	-2.08	1.36	1.44
2	D	801	A1EO4	O10-C09	-2.08	1.36	1.44
2	E	801	A1EO4	O32-C31	2.07	1.40	1.38
2	E	801	A1EO4	O10-C09	-2.07	1.36	1.44
2	B	801	A1EO4	O10-C09	-2.07	1.36	1.44
2	C	801	A1EO4	O10-C09	-2.06	1.36	1.44
2	H	801	A1EO4	O10-C09	-2.06	1.36	1.44
2	E	802	A1EO4	O10-C09	-2.06	1.36	1.44
2	F	801	A1EO4	C50-C04	2.05	1.42	1.39
2	H	802	A1EO4	C50-C04	2.03	1.42	1.39
2	D	801	A1EO4	C50-C04	2.02	1.42	1.39
2	F	801	A1EO4	O32-C31	2.02	1.40	1.38
2	C	801	A1EO4	C50-C04	2.01	1.42	1.39
2	E	801	A1EO4	C50-C04	2.01	1.42	1.39

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	A1EO4	C03-C04-N05	9.02	108.68	105.24
2	D	801	A1EO4	C03-C04-N05	8.99	108.66	105.24
2	C	801	A1EO4	C03-C04-N05	8.98	108.66	105.24
2	H	802	A1EO4	C03-C04-N05	8.97	108.66	105.24
2	B	801	A1EO4	C03-C04-N05	8.93	108.64	105.24
2	E	802	A1EO4	C03-C04-N05	8.91	108.63	105.24
2	E	801	A1EO4	C03-C04-N05	8.91	108.63	105.24
2	H	801	A1EO4	C03-C04-N05	8.83	108.60	105.24
2	H	802	A1EO4	C36-C25-C23	-4.93	113.73	119.47
2	D	801	A1EO4	C36-C25-C23	-4.91	113.75	119.47
2	E	802	A1EO4	C36-C25-C23	-4.90	113.77	119.47
2	E	801	A1EO4	C36-C25-C23	-4.89	113.77	119.47
2	F	801	A1EO4	C36-C25-C23	-4.89	113.78	119.47
2	B	801	A1EO4	C36-C25-C23	-4.87	113.80	119.47
2	C	801	A1EO4	C36-C25-C23	-4.87	113.81	119.47
2	H	801	A1EO4	C36-C25-C23	-4.84	113.83	119.47
2	E	802	A1EO4	C50-N51-N52	4.67	125.92	119.17
2	C	801	A1EO4	C50-N51-N52	4.67	125.91	119.17
2	D	801	A1EO4	C50-N51-N52	4.65	125.89	119.17
2	E	801	A1EO4	C50-N51-N52	4.65	125.89	119.17
2	H	802	A1EO4	C50-N51-N52	4.64	125.87	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	A1EO4	C50-N51-N52	4.63	125.86	119.17
2	H	801	A1EO4	C50-N51-N52	4.63	125.85	119.17
2	B	801	A1EO4	C50-N51-N52	4.62	125.85	119.17
2	B	801	A1EO4	C04-C03-N49	-3.97	107.48	110.44
2	F	801	A1EO4	C04-C03-N49	-3.97	107.48	110.44
2	H	802	A1EO4	C04-C03-N49	-3.96	107.48	110.44
2	D	801	A1EO4	C04-C03-N49	-3.95	107.49	110.44
2	C	801	A1EO4	C04-C03-N49	-3.94	107.49	110.44
2	E	802	A1EO4	C04-C03-N49	-3.92	107.51	110.44
2	E	801	A1EO4	C04-C03-N49	-3.92	107.51	110.44
2	B	801	A1EO4	C29-N30-C31	-3.91	107.80	109.90
2	H	802	A1EO4	C29-N30-C31	-3.89	107.80	109.90
2	D	801	A1EO4	C29-N30-C31	-3.89	107.81	109.90
2	H	801	A1EO4	C04-C03-N49	-3.88	107.54	110.44
2	F	801	A1EO4	C29-N30-C31	-3.88	107.81	109.90
2	C	801	A1EO4	C29-N30-C31	-3.83	107.84	109.90
2	E	801	A1EO4	C29-N30-C31	-3.83	107.84	109.90
2	H	801	A1EO4	C29-N30-C31	-3.78	107.86	109.90
2	E	802	A1EO4	C29-N30-C31	-3.76	107.88	109.90
2	H	802	A1EO4	C28-C29-C34	-3.50	117.25	120.75
2	H	801	A1EO4	C28-C29-C34	-3.48	117.27	120.75
2	D	801	A1EO4	C28-C29-C34	-3.47	117.28	120.75
2	E	801	A1EO4	C28-C29-C34	-3.47	117.28	120.75
2	B	801	A1EO4	C28-C29-C34	-3.47	117.28	120.75
2	F	801	A1EO4	C28-C29-C34	-3.47	117.28	120.75
2	E	802	A1EO4	C28-C29-C34	-3.46	117.30	120.75
2	C	801	A1EO4	C28-C29-C34	-3.44	117.31	120.75
2	B	801	A1EO4	C04-N05-C48	-3.30	103.27	106.26
2	D	801	A1EO4	C04-N05-C48	-3.29	103.28	106.26
2	E	802	A1EO4	C04-N05-C48	-3.27	103.29	106.26
2	C	801	A1EO4	C04-N05-C48	-3.27	103.30	106.26
2	H	802	A1EO4	C04-N05-C48	-3.25	103.31	106.26
2	E	801	A1EO4	C04-N05-C48	-3.25	103.31	106.26
2	H	801	A1EO4	C04-N05-C48	-3.24	103.32	106.26
2	F	801	A1EO4	C04-N05-C48	-3.23	103.33	106.26
2	E	801	A1EO4	C34-O32-C31	3.22	108.93	107.00
2	H	801	A1EO4	C34-O32-C31	3.18	108.91	107.00
2	D	801	A1EO4	C34-O32-C31	3.15	108.89	107.00
2	H	802	A1EO4	C34-O32-C31	3.10	108.86	107.00
2	C	801	A1EO4	C34-O32-C31	3.10	108.86	107.00
2	F	801	A1EO4	C34-O32-C31	3.08	108.85	107.00
2	B	801	A1EO4	C34-O32-C31	3.08	108.85	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	802	A1EO4	C34-O32-C31	3.08	108.85	107.00
2	F	801	A1EO4	C04-N05-C06	3.02	130.52	125.41
2	H	802	A1EO4	C04-N05-C06	3.01	130.51	125.41
2	C	801	A1EO4	C04-N05-C06	3.01	130.50	125.41
2	D	801	A1EO4	C04-N05-C06	3.00	130.48	125.41
2	B	801	A1EO4	C04-N05-C06	2.99	130.47	125.41
2	E	802	A1EO4	C04-N05-C06	2.99	130.47	125.41
2	E	801	A1EO4	C04-N05-C06	2.99	130.47	125.41
2	H	801	A1EO4	C04-N05-C06	2.99	130.46	125.41
2	D	801	A1EO4	O07-C06-N05	2.61	113.11	108.09
2	F	801	A1EO4	O07-C06-N05	2.61	113.10	108.09
2	B	801	A1EO4	O07-C06-N05	2.61	113.10	108.09
2	B	801	A1EO4	O41-P13-O12	2.58	114.26	107.27
2	C	801	A1EO4	O41-P13-O12	2.58	114.24	107.27
2	F	801	A1EO4	O41-P13-O12	2.58	114.24	107.27
2	E	802	A1EO4	O41-P13-O12	2.58	114.24	107.27
2	H	802	A1EO4	O41-P13-O12	2.57	114.23	107.27
2	H	801	A1EO4	O41-P13-O12	2.57	114.23	107.27
2	C	801	A1EO4	O07-C06-N05	2.57	113.02	108.09
2	E	801	A1EO4	O07-C06-N05	2.57	113.02	108.09
2	H	801	A1EO4	O07-C06-N05	2.56	113.01	108.09
2	E	801	A1EO4	O41-P13-O12	2.56	114.19	107.27
2	D	801	A1EO4	O41-P13-O12	2.56	114.18	107.27
2	H	802	A1EO4	C03-C02-N52	-2.54	114.92	118.93
2	E	802	A1EO4	O07-C06-N05	2.54	112.96	108.09
2	F	801	A1EO4	C03-C02-N52	-2.54	114.93	118.93
2	B	801	A1EO4	C03-C02-N52	-2.52	114.95	118.93
2	H	802	A1EO4	O07-C06-N05	2.51	112.91	108.09
2	H	801	A1EO4	C03-C02-N52	-2.51	114.97	118.93
2	D	801	A1EO4	C03-C02-N52	-2.51	114.97	118.93
2	E	802	A1EO4	C03-C02-N52	-2.50	114.98	118.93
2	E	801	A1EO4	C03-C02-N52	-2.50	114.99	118.93
2	C	801	A1EO4	C03-C02-N52	-2.50	114.99	118.93
2	H	802	A1EO4	C44-C46-C06	2.44	106.08	101.46
2	F	801	A1EO4	C44-C46-C06	2.44	106.08	101.46
2	E	802	A1EO4	C28-C29-N30	2.44	135.76	130.83
2	E	802	A1EO4	C44-C46-C06	2.44	106.07	101.46
2	F	801	A1EO4	C28-C29-N30	2.43	135.74	130.83
2	H	801	A1EO4	C28-C29-N30	2.42	135.73	130.83
2	B	801	A1EO4	C28-C29-N30	2.41	135.71	130.83
2	H	802	A1EO4	C28-C29-N30	2.41	135.70	130.83
2	E	801	A1EO4	C28-C29-N30	2.41	135.69	130.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1EO4	C28-C29-N30	2.40	135.69	130.83
2	C	801	A1EO4	C28-C29-N30	2.40	135.69	130.83
2	C	801	A1EO4	C44-C46-C06	2.35	105.92	101.46
2	D	801	A1EO4	C27-C26-C35	-2.35	115.00	118.23
2	B	801	A1EO4	C27-C26-C35	-2.34	115.01	118.23
2	H	801	A1EO4	C27-C26-C35	-2.34	115.01	118.23
2	B	801	A1EO4	C44-C46-C06	2.34	105.89	101.46
2	E	801	A1EO4	O32-C34-C35	2.34	129.87	124.95
2	D	801	A1EO4	C44-C46-C06	2.34	105.89	101.46
2	E	801	A1EO4	C27-C26-C35	-2.33	115.02	118.23
2	H	802	A1EO4	C27-C26-C35	-2.33	115.02	118.23
2	E	802	A1EO4	C27-C26-C35	-2.33	115.02	118.23
2	F	801	A1EO4	C27-C26-C35	-2.32	115.03	118.23
2	H	801	A1EO4	O32-C34-C35	2.32	129.83	124.95
2	D	801	A1EO4	O32-C34-C35	2.31	129.81	124.95
2	C	801	A1EO4	C27-C26-C35	-2.30	115.06	118.23
2	B	801	A1EO4	O32-C34-C35	2.30	129.79	124.95
2	H	802	A1EO4	O32-C34-C35	2.30	129.78	124.95
2	C	801	A1EO4	O32-C34-C35	2.29	129.77	124.95
2	F	801	A1EO4	O32-C34-C35	2.28	129.75	124.95
2	E	801	A1EO4	C44-C46-C06	2.28	105.77	101.46
2	E	802	A1EO4	O32-C34-C35	2.28	129.74	124.95
2	H	801	A1EO4	C44-C46-C06	2.26	105.74	101.46
2	D	801	A1EO4	C28-C27-C26	2.25	124.01	121.12
2	H	802	A1EO4	C28-C27-C26	2.25	124.00	121.12
2	B	801	A1EO4	C28-C27-C26	2.24	123.99	121.12
2	E	802	A1EO4	C28-C27-C26	2.22	123.97	121.12
2	E	801	A1EO4	C28-C27-C26	2.22	123.97	121.12
2	F	801	A1EO4	C28-C27-C26	2.21	123.96	121.12
2	C	801	A1EO4	C28-C27-C26	2.21	123.96	121.12
2	H	801	A1EO4	C28-C27-C26	2.20	123.95	121.12
2	E	801	A1EO4	C04-C50-N51	-2.15	117.97	122.52
2	C	801	A1EO4	C04-C50-N51	-2.14	118.00	122.52
2	E	802	A1EO4	C04-C50-N51	-2.14	118.00	122.52
2	D	801	A1EO4	C04-C50-N51	-2.13	118.01	122.52
2	H	801	A1EO4	C04-C50-N51	-2.13	118.01	122.52
2	F	801	A1EO4	C04-C50-N51	-2.13	118.02	122.52
2	B	801	A1EO4	C04-C50-N51	-2.12	118.05	122.52
2	H	802	A1EO4	C04-C50-N51	-2.11	118.05	122.52
2	E	802	A1EO4	O38-C37-C39	-2.07	105.19	111.82
2	D	801	A1EO4	O38-C37-C39	-2.06	105.20	111.82
2	B	801	A1EO4	O38-C37-C39	-2.06	105.21	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	A1EO4	O38-C37-C39	-2.06	105.23	111.82
2	E	801	A1EO4	O38-C37-C39	-2.05	105.24	111.82
2	H	801	A1EO4	O38-C37-C39	-2.05	105.25	111.82
2	F	801	A1EO4	O38-C37-C39	-2.04	105.26	111.82
2	H	802	A1EO4	O38-C37-C39	-2.04	105.27	111.82

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	A1EO4	C37-C19-N20-C21
2	B	801	A1EO4	C37-C19-N20-C36
2	B	801	A1EO4	C09-O10-P11-O12
2	B	801	A1EO4	C09-O10-P11-O42
2	B	801	A1EO4	C09-O10-P11-O43
2	B	801	A1EO4	C16-O15-P13-O41
2	C	801	A1EO4	C37-C19-N20-C21
2	C	801	A1EO4	C37-C19-N20-C36
2	C	801	A1EO4	C09-O10-P11-O12
2	C	801	A1EO4	C09-O10-P11-O42
2	C	801	A1EO4	C09-O10-P11-O43
2	C	801	A1EO4	C16-O15-P13-O14
2	C	801	A1EO4	C16-O15-P13-O41
2	D	801	A1EO4	C37-C19-N20-C21
2	D	801	A1EO4	C37-C19-N20-C36
2	D	801	A1EO4	C09-O10-P11-O12
2	D	801	A1EO4	C09-O10-P11-O42
2	D	801	A1EO4	C09-O10-P11-O43
2	D	801	A1EO4	C16-O15-P13-O12
2	D	801	A1EO4	C16-O15-P13-O14
2	D	801	A1EO4	C16-O15-P13-O41
2	E	801	A1EO4	C37-C19-N20-C21
2	E	801	A1EO4	C37-C19-N20-C36
2	E	801	A1EO4	C09-O10-P11-O12
2	E	801	A1EO4	C09-O10-P11-O42
2	E	801	A1EO4	C09-O10-P11-O43
2	E	801	A1EO4	C16-O15-P13-O41
2	E	802	A1EO4	O15-C16-C17-C39
2	E	802	A1EO4	O15-C16-C17-O18
2	E	802	A1EO4	O07-C08-C09-O10
2	E	802	A1EO4	C37-C19-N20-C21
2	E	802	A1EO4	C09-O10-P11-O12

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Mol	Chain	Res	Type	Atoms
2	E	802	A1EO4	C09-O10-P11-O43
2	E	802	A1EO4	C16-O15-P13-O12
2	E	802	A1EO4	C16-O15-P13-O14
2	E	802	A1EO4	C16-O15-P13-O41
2	F	801	A1EO4	C37-C19-N20-C21
2	F	801	A1EO4	C37-C19-N20-C36
2	F	801	A1EO4	C09-O10-P11-O12
2	F	801	A1EO4	C09-O10-P11-O42
2	F	801	A1EO4	C16-O15-P13-O14
2	H	801	A1EO4	C37-C19-N20-C21
2	H	801	A1EO4	C37-C19-N20-C36
2	H	801	A1EO4	C09-O10-P11-O12
2	H	801	A1EO4	C09-O10-P11-O42
2	H	801	A1EO4	C09-O10-P11-O43
2	H	801	A1EO4	C16-O15-P13-O12
2	H	801	A1EO4	C16-O15-P13-O41
2	H	802	A1EO4	C37-C19-N20-C21
2	H	802	A1EO4	C37-C19-N20-C36
2	H	802	A1EO4	C09-O10-P11-O12
2	H	802	A1EO4	C09-O10-P11-O42
2	H	802	A1EO4	C09-O10-P11-O43
2	H	802	A1EO4	C16-O15-P13-O12
2	H	802	A1EO4	C16-O15-P13-O14
2	H	802	A1EO4	C16-O15-P13-O41
2	B	801	A1EO4	O15-C16-C17-C39
2	C	801	A1EO4	O15-C16-C17-C39
2	D	801	A1EO4	O15-C16-C17-C39
2	E	801	A1EO4	O15-C16-C17-C39
2	F	801	A1EO4	O15-C16-C17-C39
2	F	801	A1EO4	O15-C16-C17-O18
2	H	801	A1EO4	O15-C16-C17-C39
2	H	802	A1EO4	O15-C16-C17-C39
2	H	802	A1EO4	O15-C16-C17-O18
2	H	802	A1EO4	O07-C08-C09-O10
2	C	801	A1EO4	O15-C16-C17-O18
2	D	801	A1EO4	O15-C16-C17-O18
2	E	801	A1EO4	O15-C16-C17-O18
2	E	802	A1EO4	C44-C08-C09-O10
2	H	801	A1EO4	O15-C16-C17-O18
2	H	801	A1EO4	C08-C09-O10-P11
2	B	801	A1EO4	O15-C16-C17-O18
2	H	802	A1EO4	C44-C08-C09-O10

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Mol	Chain	Res	Type	Atoms
2	E	801	A1EO4	C08-C09-O10-P11
2	F	801	A1EO4	C44-C08-C09-O10
2	B	801	A1EO4	C08-C09-O10-P11
2	C	801	A1EO4	C08-C09-O10-P11
2	B	801	A1EO4	C46-C06-N05-C04
2	C	801	A1EO4	C46-C06-N05-C04
2	D	801	A1EO4	C46-C06-N05-C04
2	E	801	A1EO4	C46-C06-N05-C04
2	E	802	A1EO4	C46-C06-N05-C04
2	F	801	A1EO4	C46-C06-N05-C04
2	H	801	A1EO4	C46-C06-N05-C04
2	H	802	A1EO4	C46-C06-N05-C04
2	F	801	A1EO4	O07-C08-C09-O10
2	E	802	A1EO4	C17-C16-O15-P13
2	F	801	A1EO4	C08-C09-O10-P11
2	E	802	A1EO4	P13-O12-P11-O43
2	H	801	A1EO4	O07-C08-C09-O10
2	D	801	A1EO4	C36-C25-C26-C27
2	D	801	A1EO4	C08-C09-O10-P11
2	H	801	A1EO4	C17-C16-O15-P13
2	B	801	A1EO4	C16-O15-P13-O12
2	B	801	A1EO4	C16-O15-P13-O14
2	C	801	A1EO4	C16-O15-P13-O12
2	E	801	A1EO4	C16-O15-P13-O12
2	E	801	A1EO4	C16-O15-P13-O14
2	E	802	A1EO4	C09-O10-P11-O42
2	F	801	A1EO4	C09-O10-P11-O43
2	E	801	A1EO4	C17-C16-O15-P13
2	B	801	A1EO4	C36-C25-C26-C27
2	B	801	A1EO4	C36-C25-C26-C35
2	C	801	A1EO4	C36-C25-C26-C27
2	C	801	A1EO4	C36-C25-C26-C35
2	B	801	A1EO4	C17-C16-O15-P13
2	E	802	A1EO4	C37-C19-N20-C36
2	E	801	A1EO4	O07-C08-C09-O10
2	C	801	A1EO4	C23-C25-C26-C27
2	H	802	A1EO4	C08-C09-O10-P11
2	E	801	A1EO4	C36-C25-C26-C35
2	B	801	A1EO4	C23-C25-C26-C27
2	D	801	A1EO4	O07-C08-C09-O10
2	C	801	A1EO4	C23-C25-C26-C35
2	C	801	A1EO4	C17-C16-O15-P13

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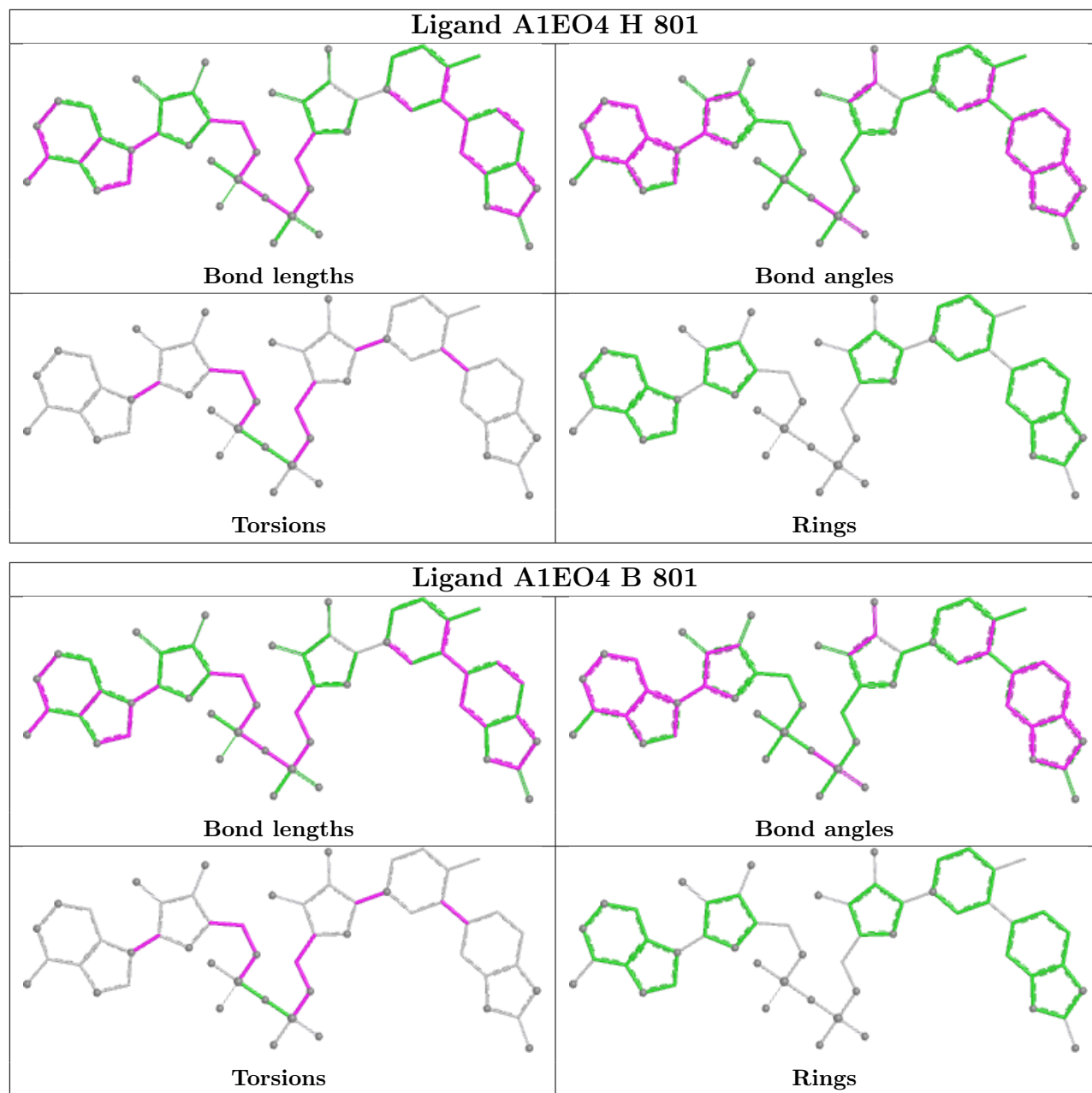
Mol	Chain	Res	Type	Atoms
2	H	802	A1EO4	C17-C16-O15-P13
2	D	801	A1EO4	C23-C25-C26-C27
2	D	801	A1EO4	C36-C25-C26-C35
2	H	801	A1EO4	C36-C25-C26-C35
2	B	801	A1EO4	C23-C25-C26-C35
2	D	801	A1EO4	C23-C25-C26-C35
2	D	801	A1EO4	O07-C06-N05-C04
2	B	801	A1EO4	O07-C08-C09-O10
2	E	801	A1EO4	C36-C25-C26-C27
2	E	802	A1EO4	P13-O12-P11-O42
2	E	801	A1EO4	C23-C25-C26-C35
2	E	802	A1EO4	C36-C25-C26-C35
2	H	801	A1EO4	C36-C25-C26-C27
2	F	801	A1EO4	P11-O12-P13-O41
2	H	802	A1EO4	P13-O12-P11-O42

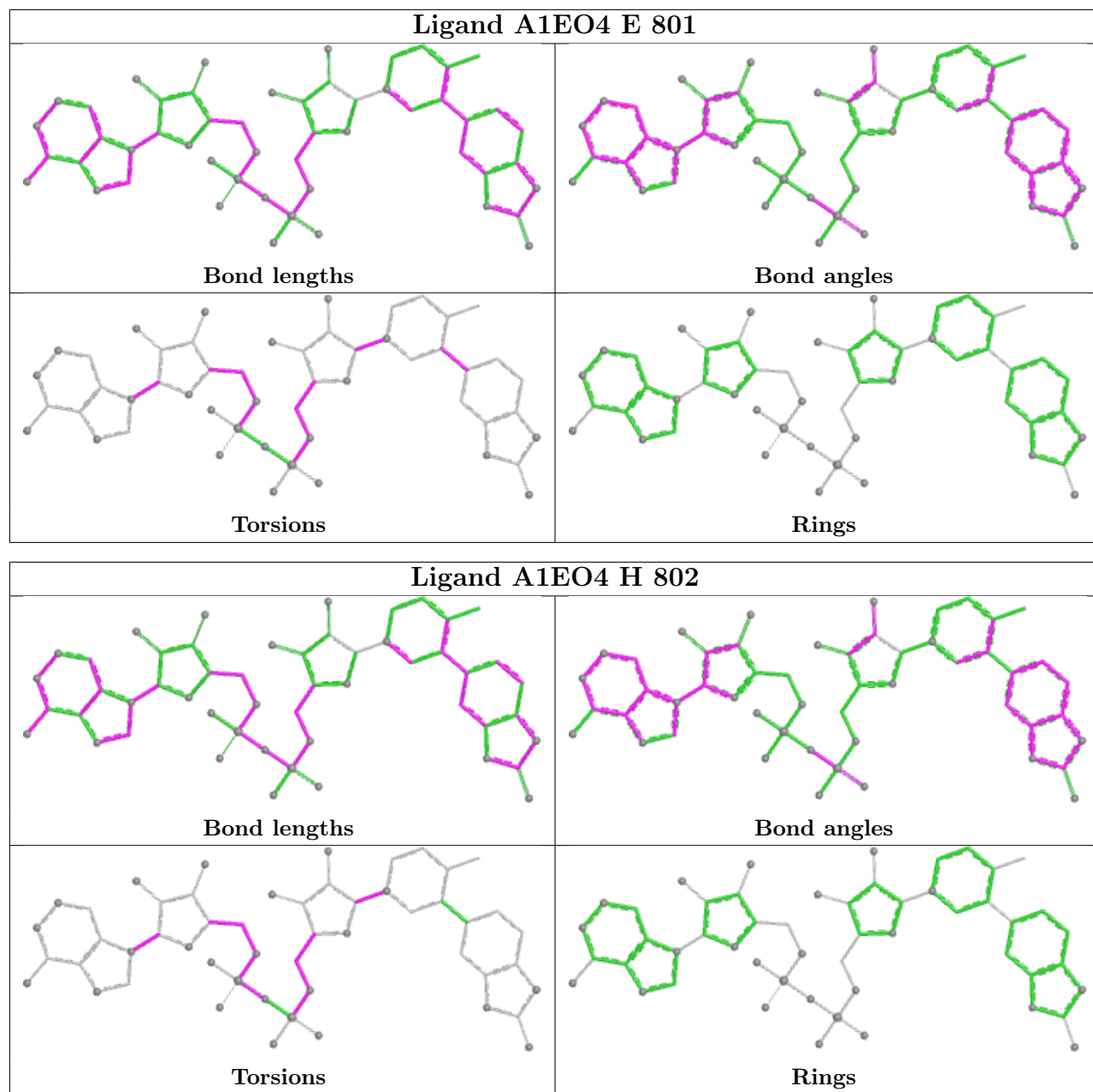
There are no ring outliers.

4 monomers are involved in 5 short contacts:

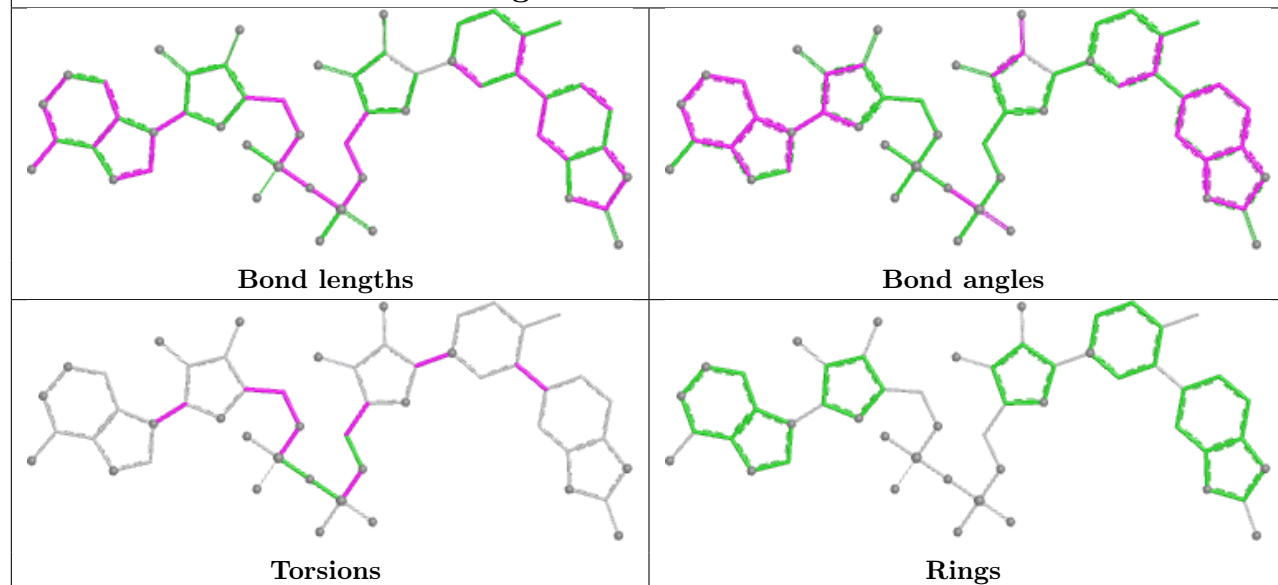
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	A1EO4	2	0
2	E	801	A1EO4	1	0
2	D	801	A1EO4	1	0
2	C	801	A1EO4	1	0

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.

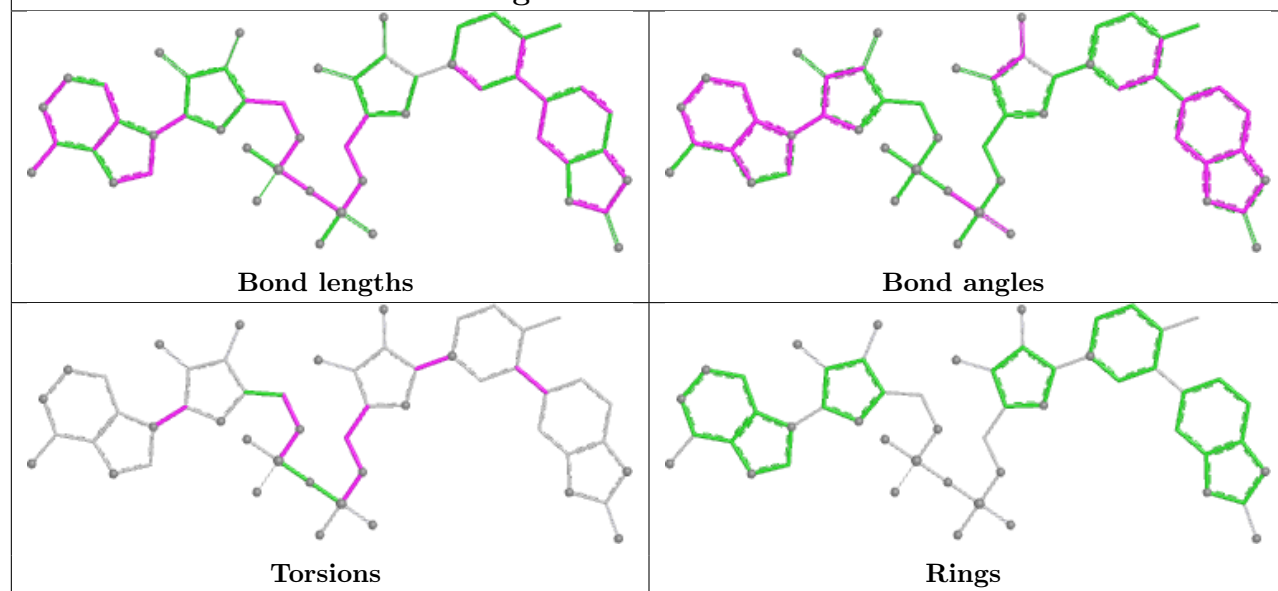


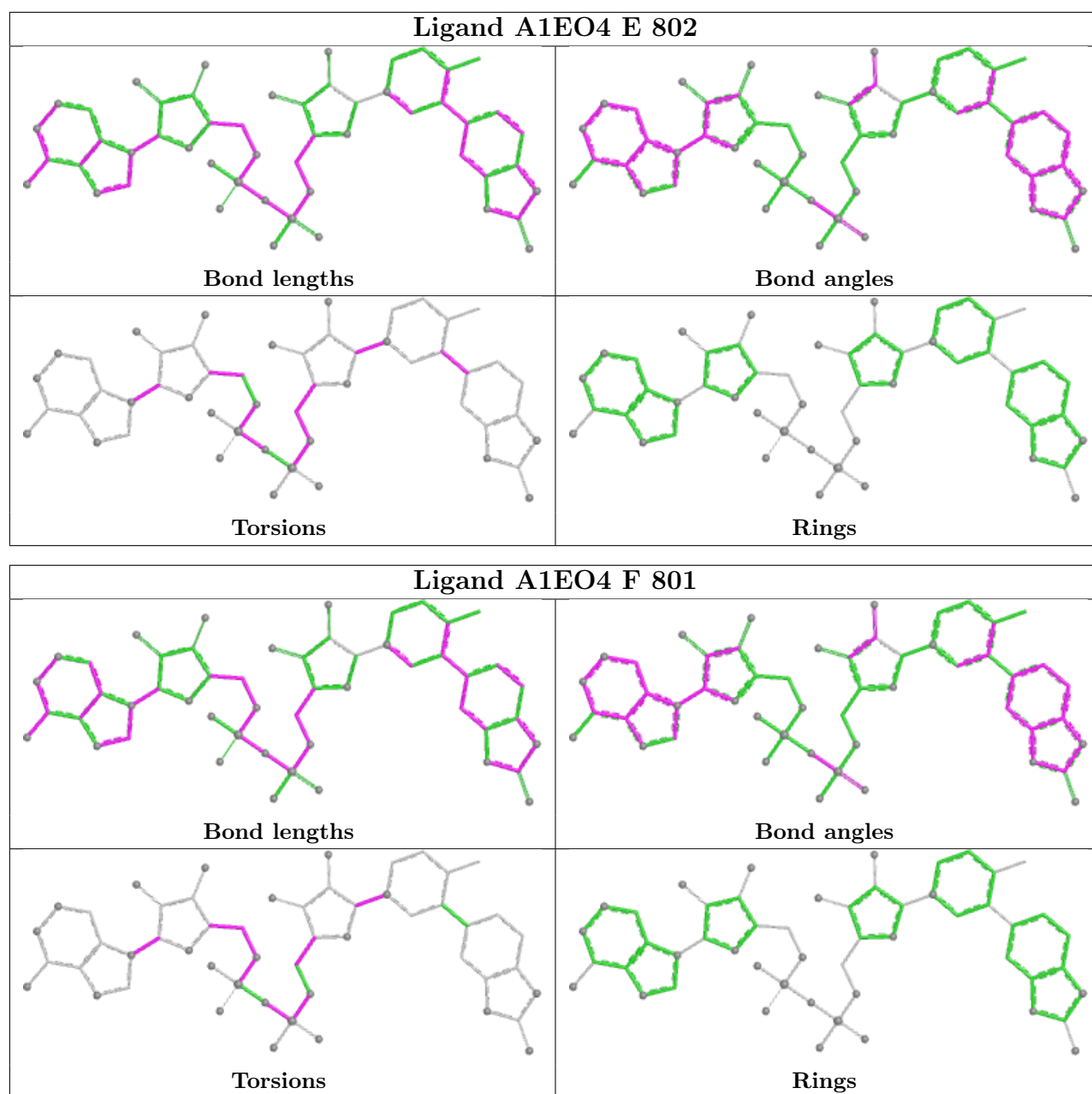


## Ligand A1EO4 D 801



## Ligand A1EO4 C 801





## 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.

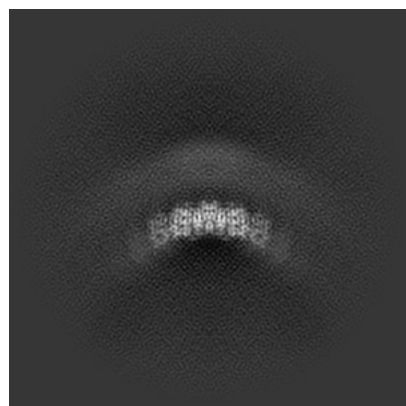
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64139. These allow visual inspection of the internal detail of the map and identification of artifacts.

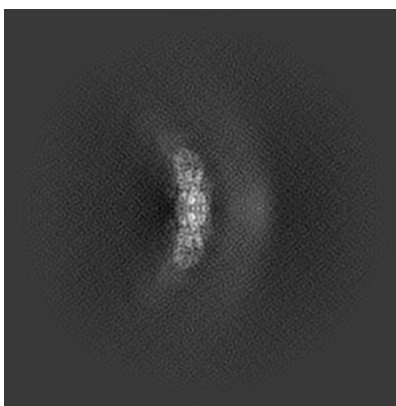
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

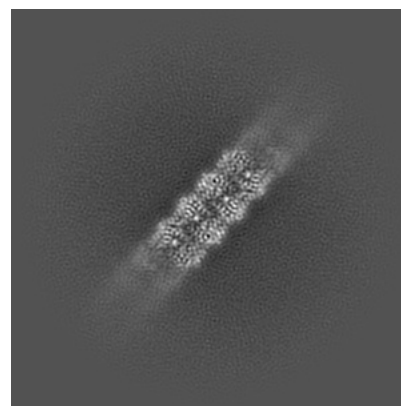
#### 6.1.1 Primary map



X

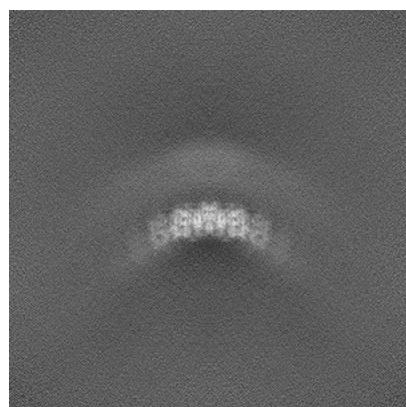


Y

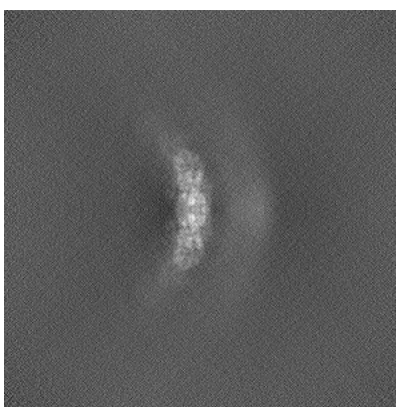


Z

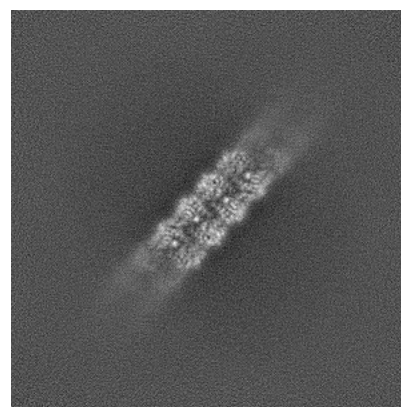
#### 6.1.2 Raw map



X



Y

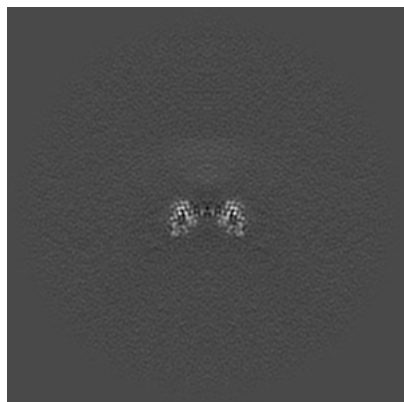


Z

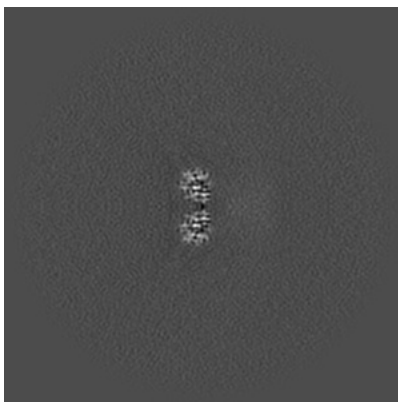
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

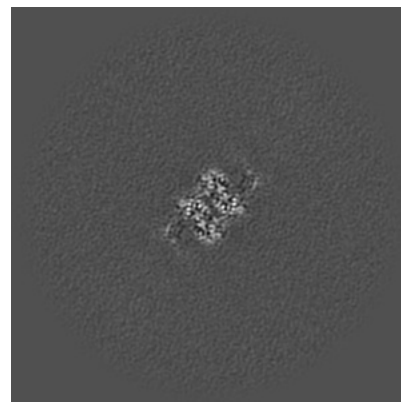
### 6.2.1 Primary map



X Index: 250

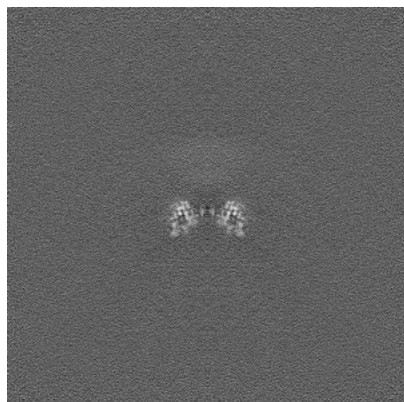


Y Index: 250

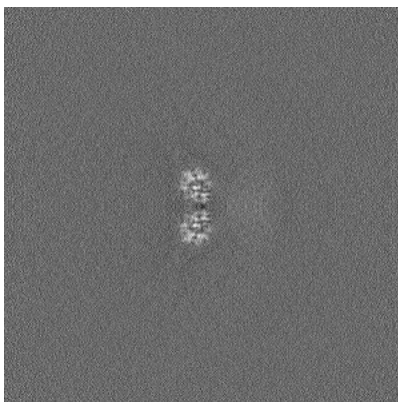


Z Index: 250

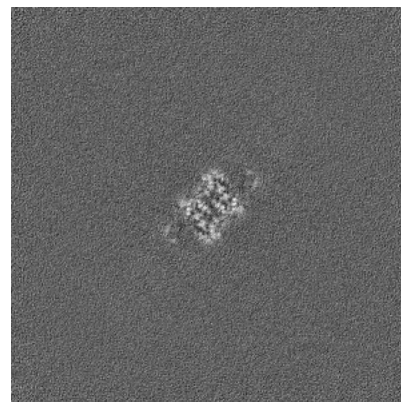
### 6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

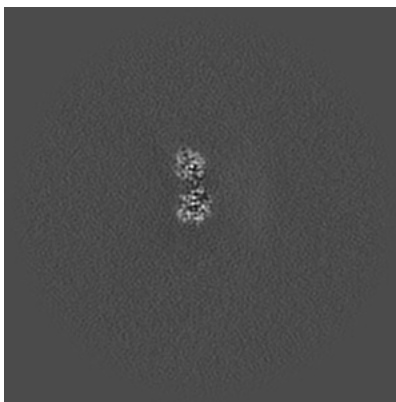
The images above show central slices of the map in three orthogonal directions.

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

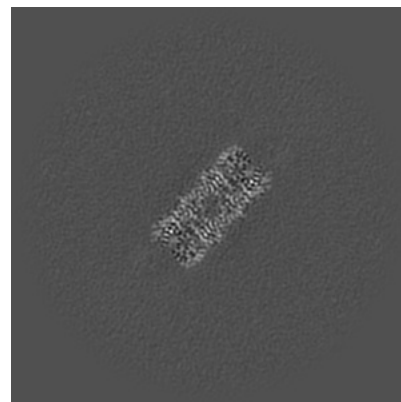
### 6.3.1 Primary map



X Index: 234

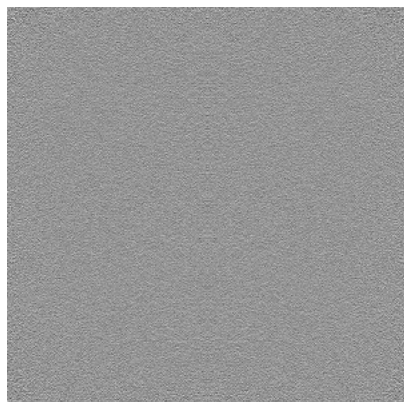


Y Index: 280

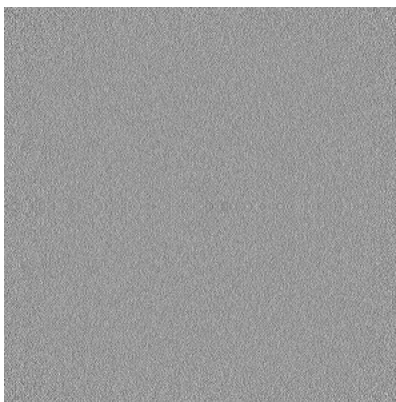


Z Index: 235

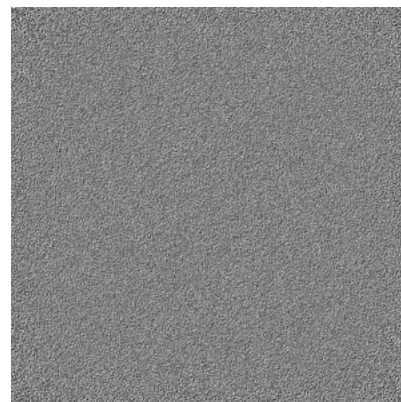
### 6.3.2 Raw map



X Index: 0



Y Index: 0

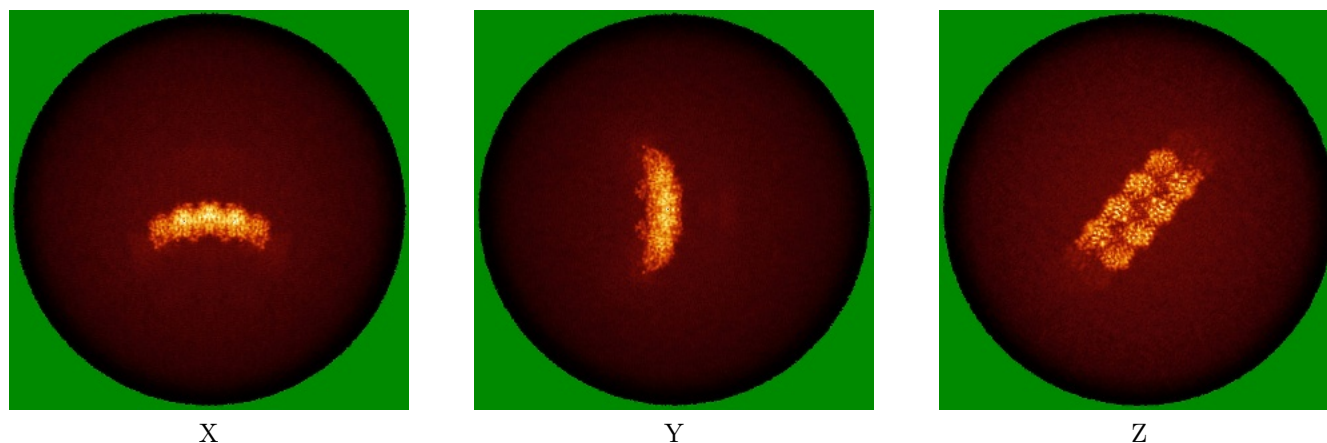


Z Index: 0

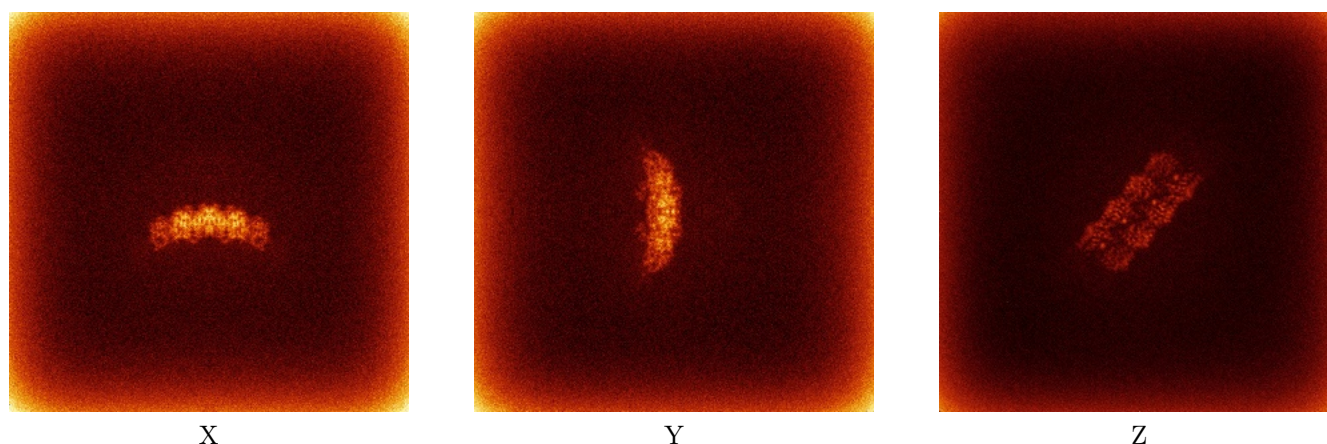
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

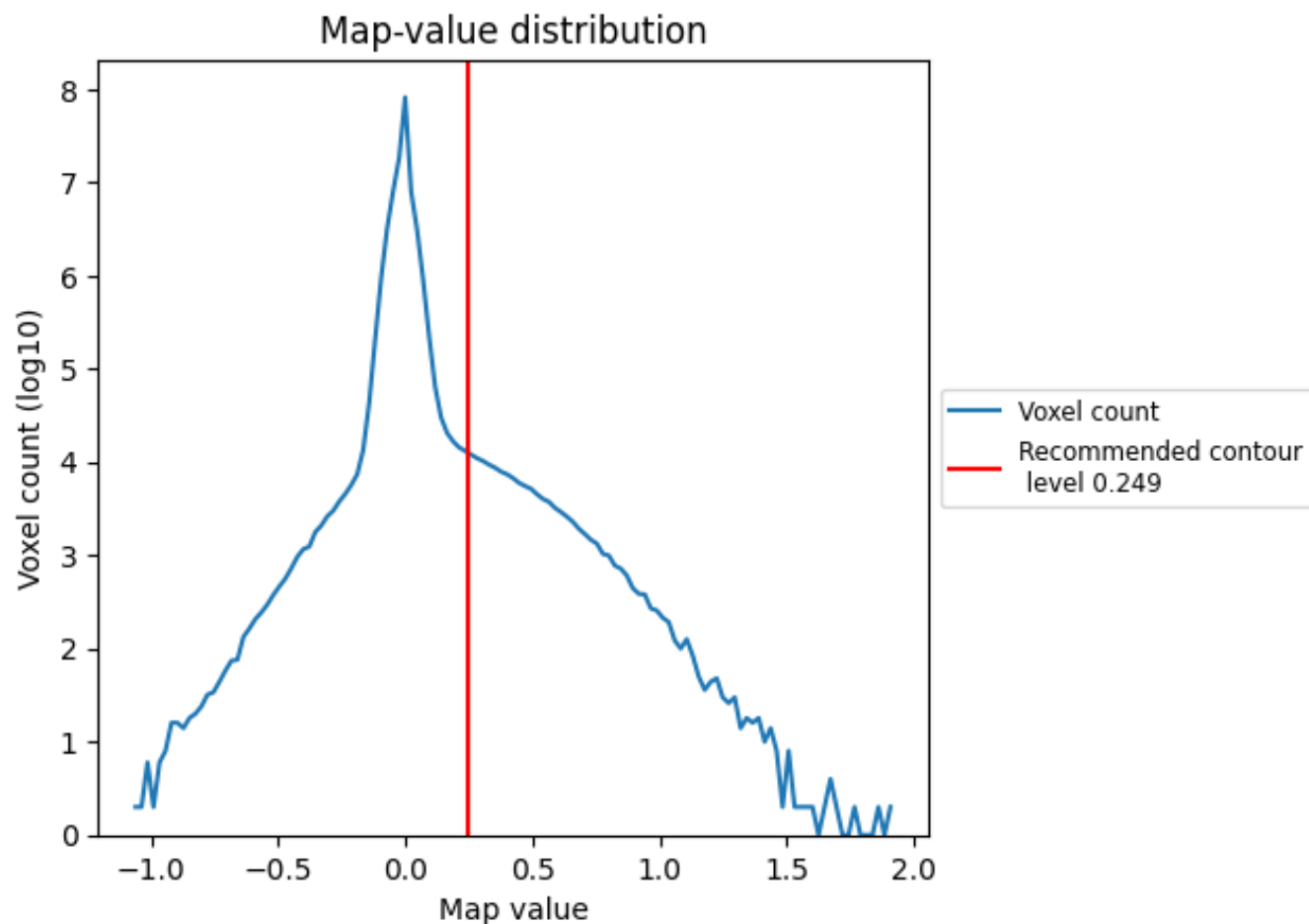
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

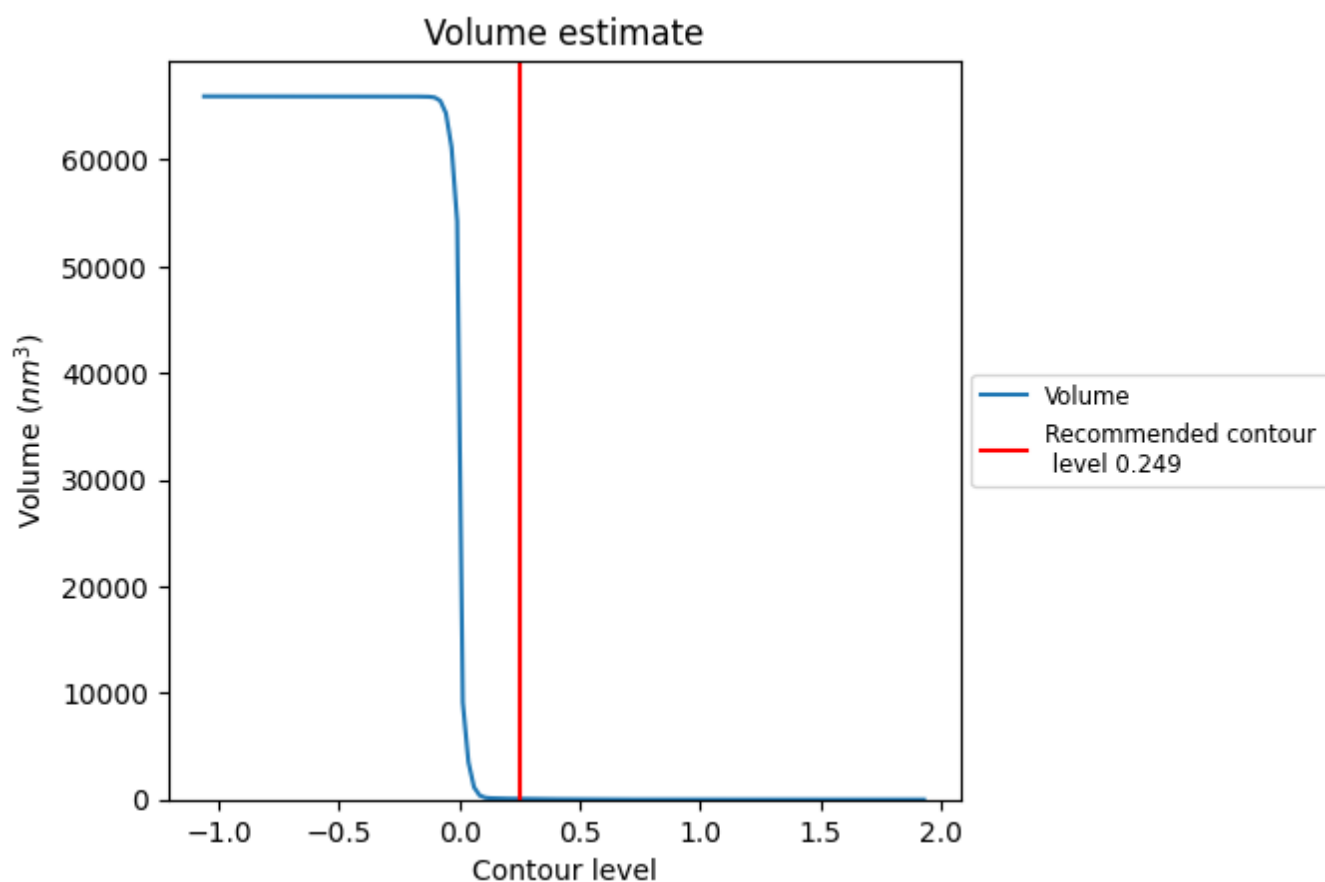
This section contains the results of statistical analysis of the map.

### 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.

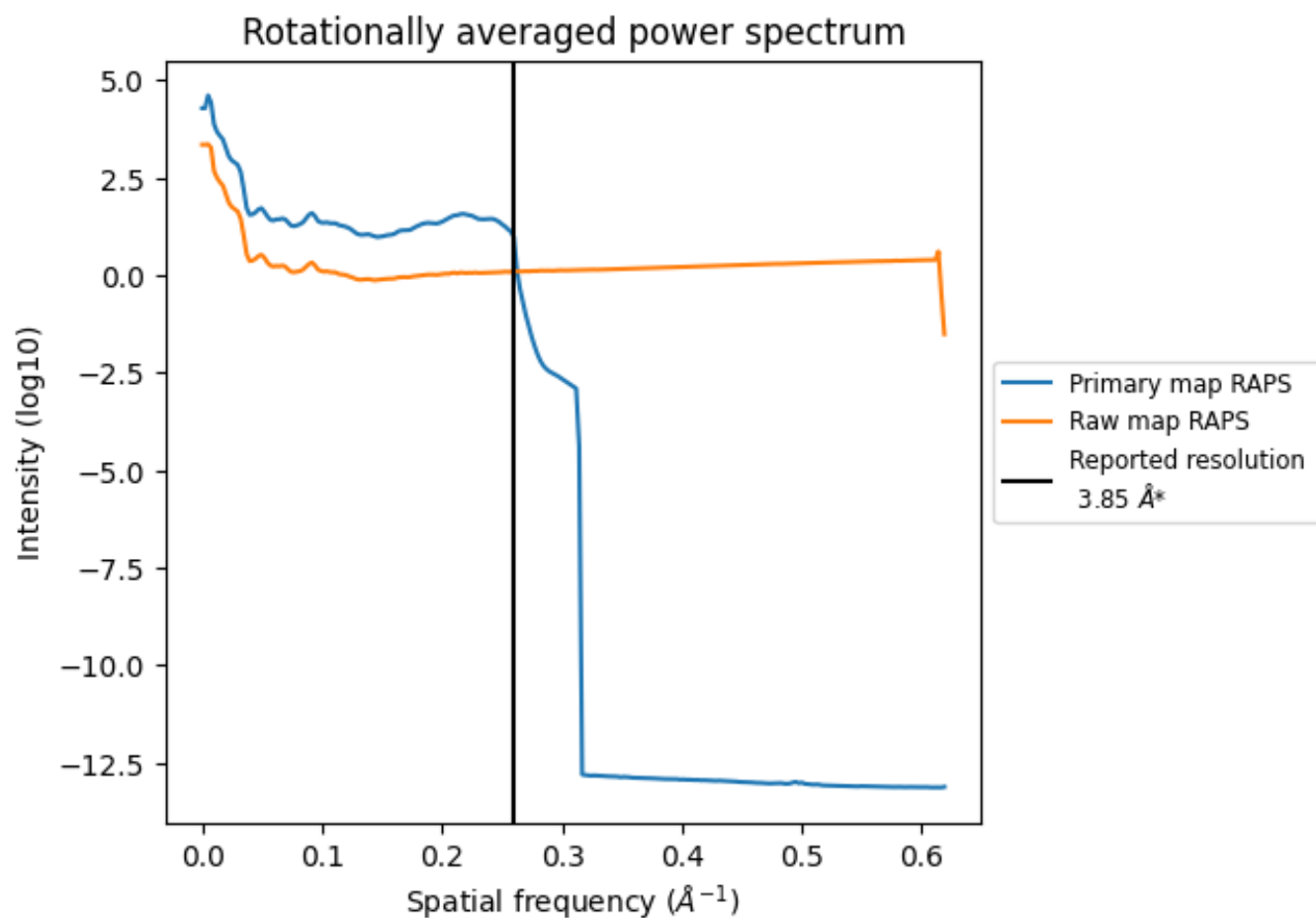
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm<sup>3</sup>; this corresponds to an approximate mass of 63 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 ⓘ

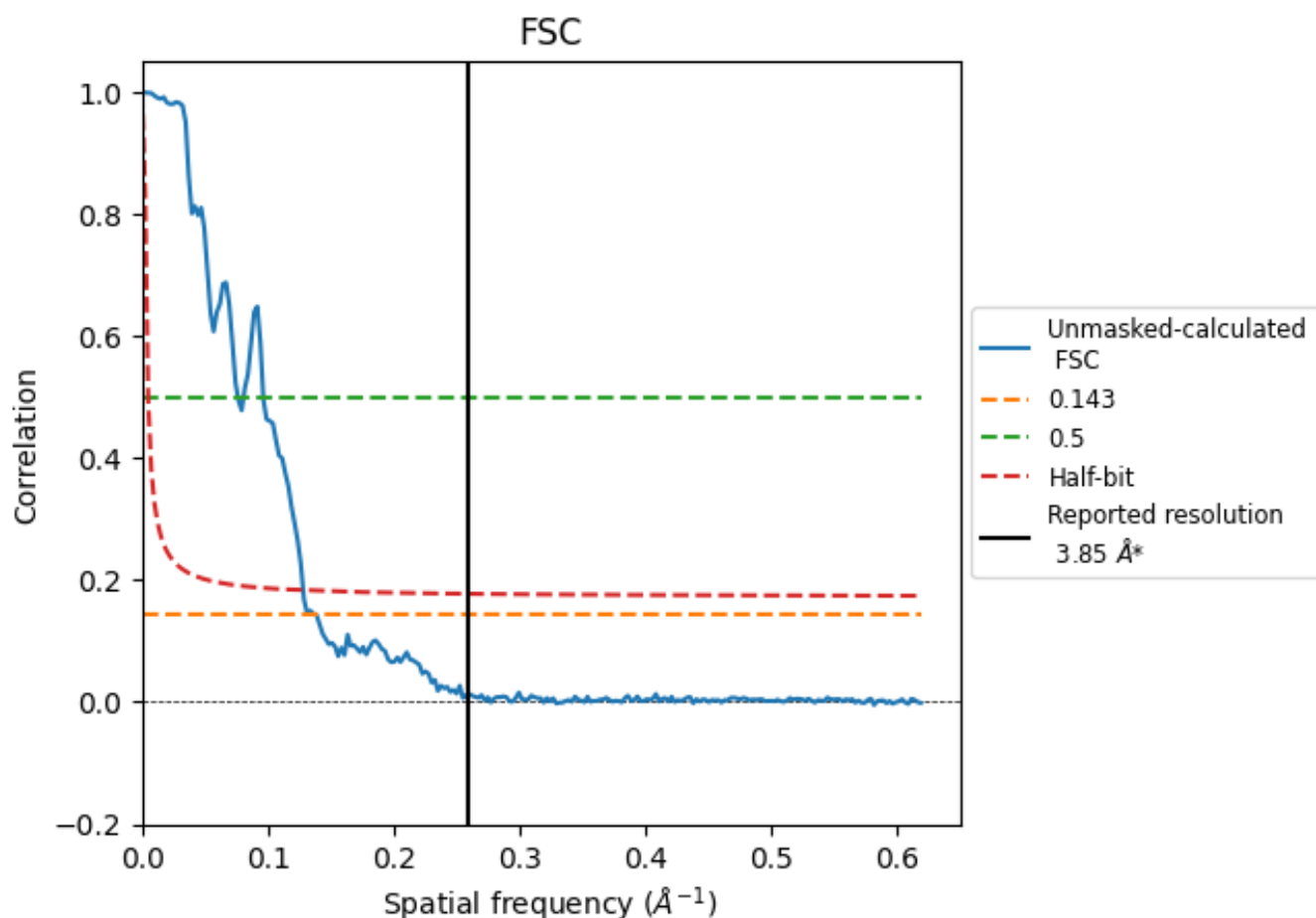


\*Reported resolution corresponds to spatial frequency of 0.260 Å<sup>-1</sup>

## 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  $0.260 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

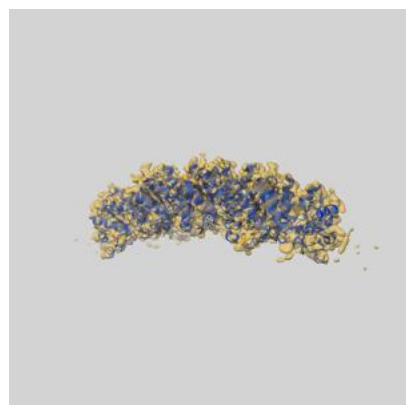
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.22	13.12	7.81

\*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 7.22 differs from the reported value 3.85 by more than 10 %

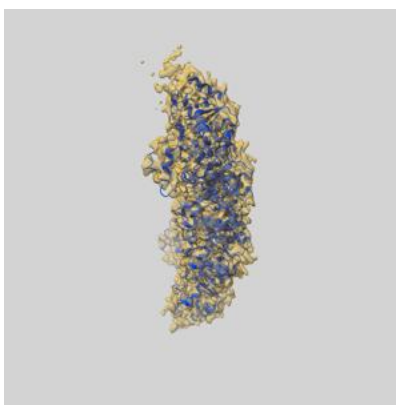
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64139 and PDB model 9UGJ. Per-residue inclusion information can be found in section 3 on page 14.

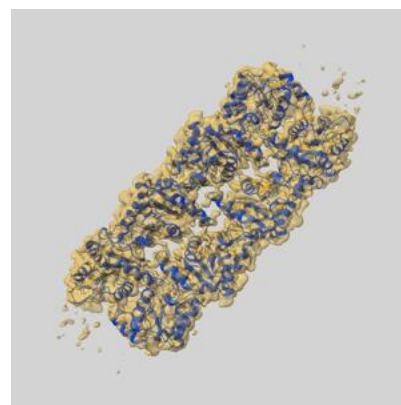
### 9.1 Map-model overlay [i](#)



X



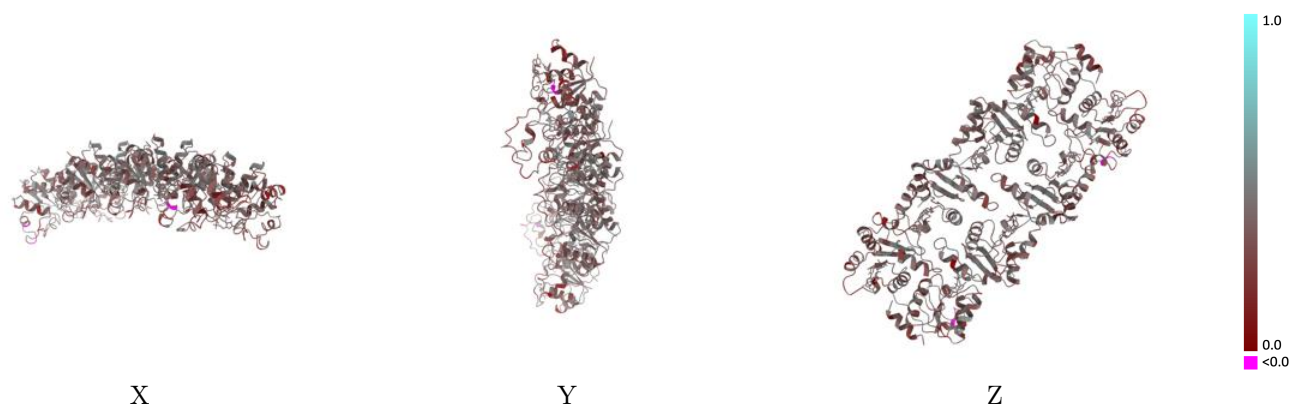
Y



Z

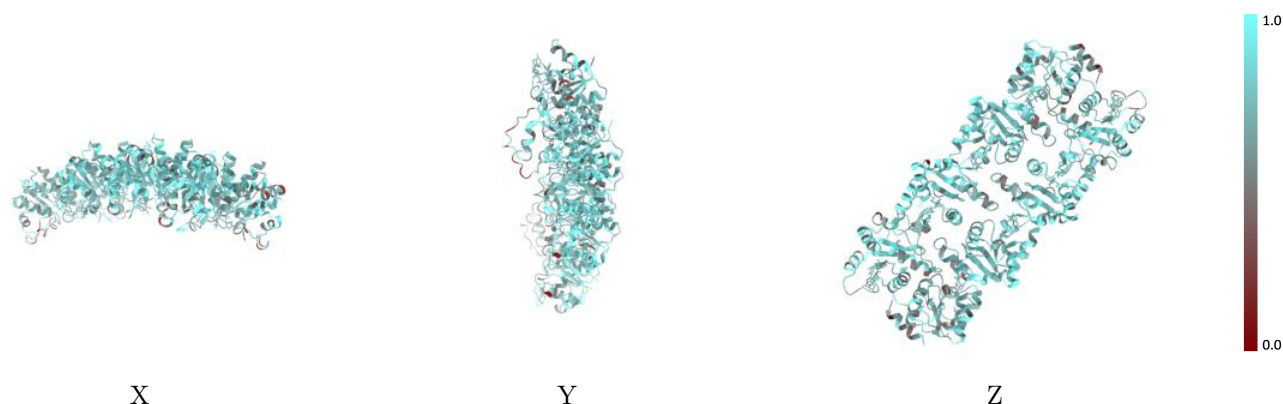
The images above show the 3D surface view of the map at the recommended contour level 0.249 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



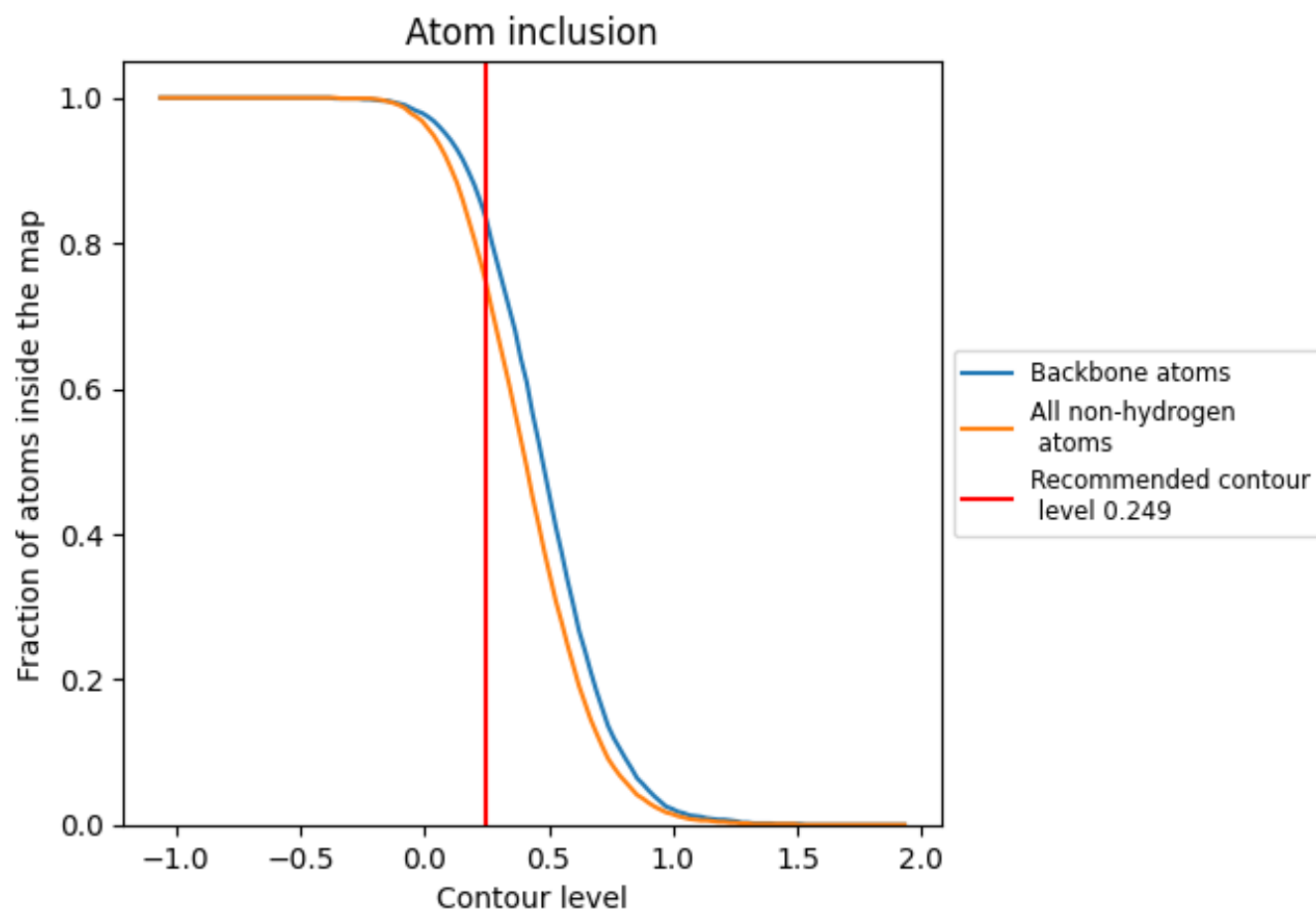
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.249).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 74% 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 (0.249) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7440	<div></div> 0.3700
A	<div></div> 0.7690	<div></div> 0.3890
B	<div></div> 0.7790	<div></div> 0.3930
C	<div></div> 0.7730	<div></div> 0.3910
D	<div></div> 0.7740	<div></div> 0.4000
E	<div></div> 0.7400	<div></div> 0.3460
F	<div></div> 0.6630	<div></div> 0.3430
G	<div></div> 0.6880	<div></div> 0.3500
H	<div></div> 0.7580	<div></div> 0.3490

