



# Preliminary Full wwPDB EM Validation Report ⓘ

Mar 25, 2023 – 06:45 PM EDT

**This wwPDB validation report is NOT for manuscript review**

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.  
**The structure in question has not been deposited to the wwPDB.**  
**This report should not be submitted to journals.**

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

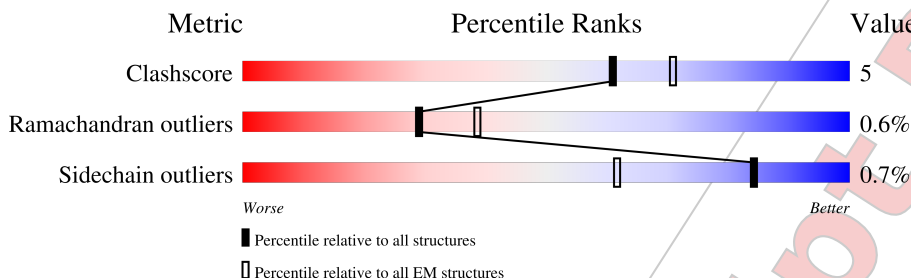
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	644	<div> <div>22%</div> <div>85%</div> <div>14%</div> </div>
1	B	644	<div> <div>21%</div> <div>85%</div> <div>14%</div> </div>
1	C	644	<div> <div>21%</div> <div>87%</div> <div>13%</div> </div>
1	D	644	<div> <div>21%</div> <div>85%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47748 atoms, of which 24568 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	644	Total	C	H	N	O	S	0	0
			10415	3364	5239	859	926	27		
1	B	644	Total	C	H	N	O	S	0	0
			10415	3364	5239	859	926	27		
1	C	644	Total	C	H	N	O	S	0	0
			10415	3364	5239	859	926	27		
1	D	644	Total	C	H	N	O	S	0	0
			10415	3364	5239	859	926	27		

- Molecule 2 is a ligand with the chemical component id POV but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for POV. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			110	34	66	1	8	1	
2	A	1	Total	C	H				0
			38	13	25				
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			144	46	88	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 115	C 36	H 69	N 1	O 8	P 1	0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 110	C 34	H 66	N 1	O 8	P 1	0
2	B	1	Total 38	C 13	H 25				0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	B	1	Total 115	C 36	H 69	N 1	O 8	P 1	0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 110	C 34	H 66	N 1	O 8	P 1	0
2	C	1	Total 38	C 13	H 25				0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 144	C 46	H 88	N 1	O 8	P 1	0
2	C	1	Total 115	C 36	H 69	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			110	34	66	1	8	1
2	D	1	Total	C	H			
			38	13	25			
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			144	46	88	1	8	1
2	D	1	Total	C	H	N	O	P
			115	36	69	1	8	1

- Molecule 3 is a ligand with the chemical component id GDN but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for GDN. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			151	50	81	20	
3	A	1	Total	C	H	O	0
			81	32	46	3	
3	B	1	Total	C	H	O	0
			151	50	81	20	
3	B	1	Total	C	H	O	0
			81	32	46	3	
3	C	1	Total	C	H	O	0
			151	50	81	20	
3	C	1	Total	C	H	O	0
			81	32	46	3	
3	D	1	Total	C	H	O	0
			151	50	81	20	
3	D	1	Total	C	H	O	0
			81	32	46	3	

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
4	I	1	Total	Na	0
			1	1	
4	I	1	Total	Na	0
			1	1	
4	I	1	Total	Na	0
			1	1	
4	I	1	Total	Na	0
			1	1	

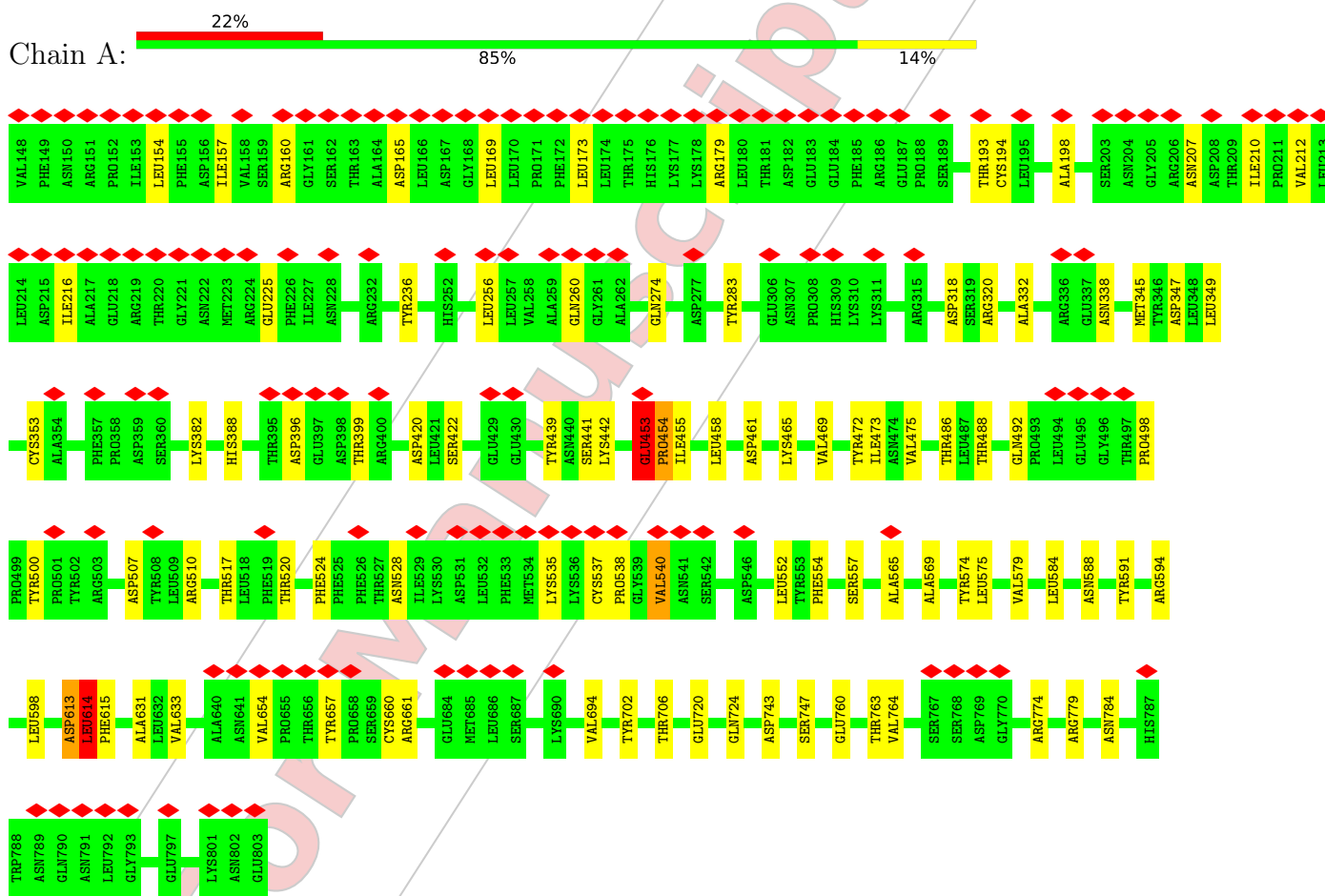
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	18	Total	O	0
			18	18	
5	B	18	Total	O	0
			18	18	
5	C	18	Total	O	0
			18	18	
5	D	18	Total	O	0
			18	18	

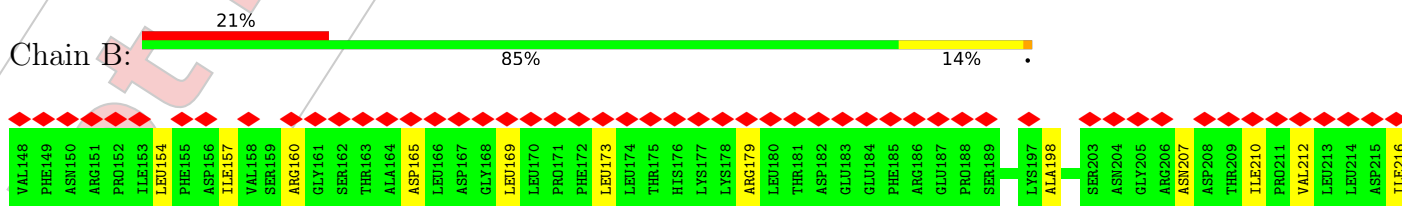
### 3 Residue-property plots

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:

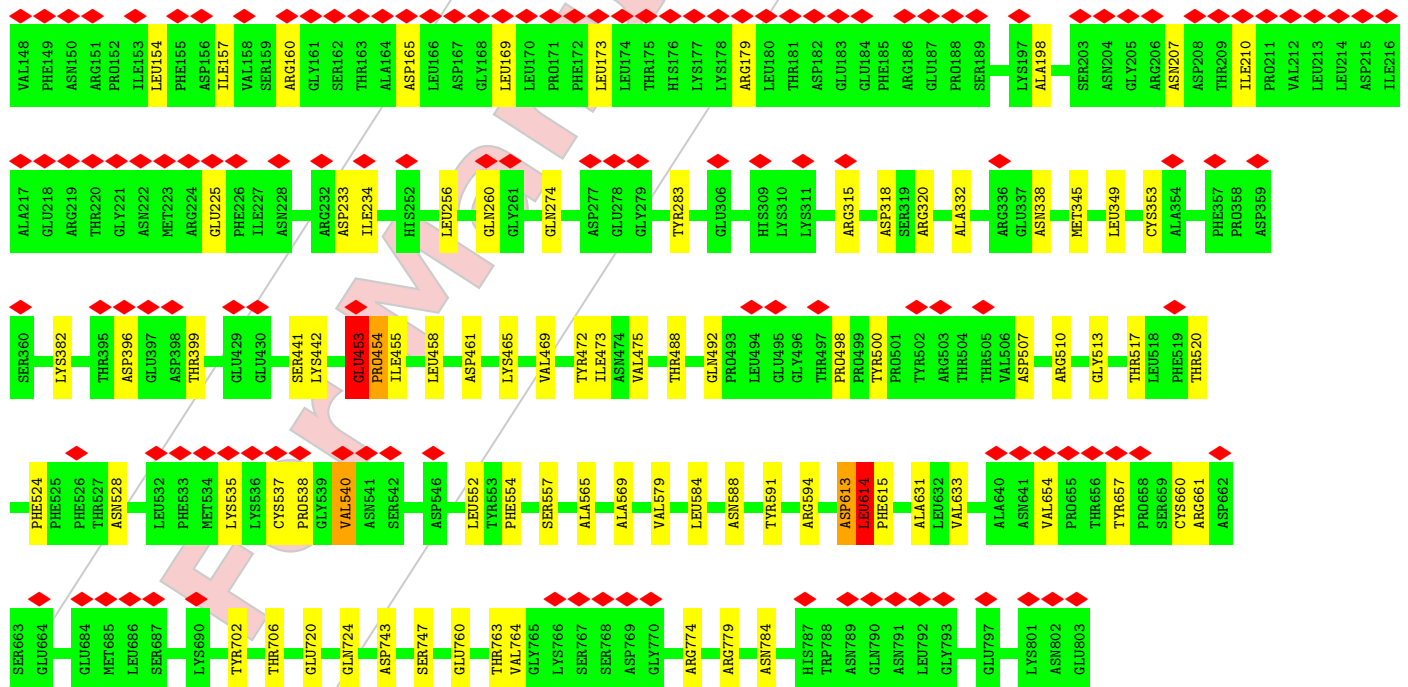
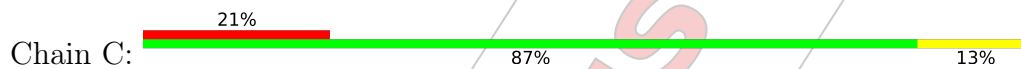


#### • Molecule 1:

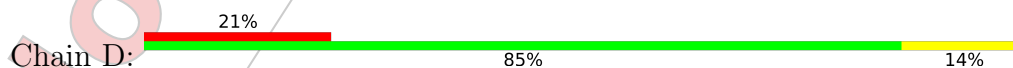




## ● Molecule 1:



## ● Molecule 1:





ASP798	GLU800	LYS801	ASN802	GLU803	PRO655	THR656	TYR657	PRO658	SER659	CYS660	ARG661	ASP662	SER663	GLU664	GLU664	MET685	LEU686	SER687	LYS690	TYR702	THR706	GLU720	GLN724	VAL725	SER729	ASP743	SER747	GLU760	THR763	VAL764	GLY765	LYS766	SER767	SER768	ASP769	GLY770	ARG774	ARG775	ARG779	ASN784	HIS787	TRP788	ASN789	GLN790	ASN791	LEU792	GLY793	GLU797	VAL148	PHE149	ASN150	ARG151	PRO152	ILE153	LEU154	PHE155	ASP156	ILE157	VAL158	SER159	ARG160	GLY161	SER162	THR163	ALA164	ASP165	LEU166	ASP167	GLY168	LEU169	LEU170	PRO171	PHE172	LEU173	LEU174	THR175	HIS176	LYS177	LYS178	ARG179	LEU180	THR181	ASP182	GLU183	GLU184	PHE185	ARG186	GLU187	PRO188	SER189	THR193	CYS194	LYS197	ALA198	SER203	ASN204	GLY205	ARG206	ASN207	ASP208	THR209	ILE210	PRO211	VAL212	LEU213	LEU214	ASP215	ILE216	ALA217	GLU218	ARG219	THR220	GLY221	ASN222	MET223	ARG224	GLU225	PHE226	ILE227	ASN228	ARG232	ASP233	ILE234	HIS252	LEU256	GLN260	GLY261	GLN274	ASP277	GLU278	GLY279	TYR283	GLU306	HIS309	LYS310	LYS311	ARG315	ASP318	SER319	ARG320	ALA332	ARG336	GLU337	ASN338	MET345	LEU349	CYS353	ALA354	PHE357	PRO358	ASP359	SER360	LYS382	THR395	ASP396	GLU397	ASP398	THR399	SER403	GLU429	GLU430	TYR439	ASN440	SER441	LYS442	GLU463	PRO464	ILE465	LEU468	ASP461	LYS465	VAL469	TYR472	ILE473	ASN474	VAL475	THR488	GLU492	PRO493	LEU494	GLU495	GLY496	THR497	PRO498	PRO499	TYR500	PRO501	TYR502	ARG503	THR504	THR505	VAL506	ASP507	ARG510	THR517	LEU518	PHE519	THR520	PHE524	PHE525	PHE526	THR527	ASN528	LEU532	PHE533	MET534	LYS535	LYS536	CYS537	PRO538	GLY539	VAL540	ASN541	SER542	ASP546	LEU552	TYR553	PHE554	SER557	ALA565	ALA569	TYR574	VAL579	PHE580	LEU584	ASN588	TYR591	ARG594	ASP613	LEU614	PHE615	ALA631	LEU632	VAL633	ALA640	ASN641	VAL654
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## 4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	1.386	Depositor
Minimum map value	-0.975	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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: GDN, POV, NA

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	0.42	0/5297	0.67	6/7184 (0.1%)
1	B	0.42	0/5297	0.67	6/7184 (0.1%)
1	C	0.42	0/5297	0.67	6/7184 (0.1%)
1	D	0.42	0/5297	0.67	6/7184 (0.1%)
All	All	0.42	0/21188	0.67	24/28736 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	764	VAL	CG1-CB-CG2	7.22	122.45	110.90
1	C	764	VAL	CG1-CB-CG2	7.22	122.45	110.90
1	D	764	VAL	CG1-CB-CG2	7.21	122.44	110.90
1	B	764	VAL	CG1-CB-CG2	7.19	122.40	110.90
1	D	540	VAL	CG1-CB-CG2	7.06	122.20	110.90
1	B	540	VAL	CG1-CB-CG2	7.03	122.14	110.90
1	C	540	VAL	CG1-CB-CG2	7.02	122.13	110.90
1	A	540	VAL	CG1-CB-CG2	7.02	122.13	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	633	VAL	CG1-CB-CG2	6.99	122.08	110.90
1	C	633	VAL	CG1-CB-CG2	6.97	122.06	110.90
1	B	633	VAL	CG1-CB-CG2	6.97	122.05	110.90
1	A	633	VAL	CG1-CB-CG2	6.96	122.04	110.90
1	B	654	VAL	CG1-CB-CG2	6.14	120.73	110.90
1	A	654	VAL	CG1-CB-CG2	6.12	120.69	110.90
1	D	654	VAL	CG1-CB-CG2	6.11	120.68	110.90
1	C	654	VAL	CG1-CB-CG2	6.09	120.65	110.90
1	A	614	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	654	VAL	CA-CB-CG2	5.53	119.19	110.90
1	C	614	LEU	CA-CB-CG	5.53	128.01	115.30
1	D	614	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	614	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	654	VAL	CA-CB-CG2	5.51	119.17	110.90
1	B	654	VAL	CA-CB-CG2	5.50	119.14	110.90
1	D	654	VAL	CA-CB-CG2	5.49	119.13	110.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	GLU	Peptide
1	A	537	CYS	Peptide
1	A	614	LEU	Peptide
1	B	453	GLU	Peptide
1	B	537	CYS	Peptide
1	B	614	LEU	Peptide
1	C	453	GLU	Peptide
1	C	537	CYS	Peptide
1	C	614	LEU	Peptide
1	D	453	GLU	Peptide
1	D	537	CYS	Peptide
1	D	614	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5176	5239	5235	51	0
1	B	5176	5239	5235	52	0
1	C	5176	5239	5235	42	0
1	D	5176	5239	5235	48	0
2	A	495	776	36	2	0
2	B	495	776	36	2	0
2	C	495	776	36	3	0
2	D	495	776	36	3	0
3	A	105	127	0	4	0
3	B	105	127	0	4	0
3	C	105	127	0	4	0
3	D	105	127	0	4	0
4	I	4	0	0	0	0
5	A	18	0	0	1	0
5	B	18	0	0	1	0
5	C	18	0	0	1	0
5	D	18	0	0	1	0
All	All	23180	24568	21084	205	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (205) 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)
3:A:911:GDN:C15	3:A:911:GDN:C14	1.79	1.61
3:C:911:GDN:C15	3:C:911:GDN:C14	1.79	1.60
3:D:911:GDN:C15	3:D:911:GDN:C14	1.79	1.59
3:B:911:GDN:C15	3:B:911:GDN:C14	1.79	1.59
3:A:903:GDN:C14	3:A:903:GDN:C15	1.81	1.58
3:D:903:GDN:C15	3:D:903:GDN:C14	1.80	1.54
3:B:903:GDN:C15	3:B:903:GDN:C14	1.81	1.54
3:C:903:GDN:C15	3:C:903:GDN:C14	1.81	1.53
1:A:283:TYR:OH	1:A:318:ASP:OD2	2.02	0.77
1:D:283:TYR:OH	1:D:318:ASP:OD2	2.03	0.76
1:C:283:TYR:OH	1:C:318:ASP:OD2	2.02	0.76
1:B:283:TYR:OH	1:B:318:ASP:OD2	2.02	0.76
1:D:660:CYS:SG	1:D:661:ARG:N	2.59	0.75
1:C:660:CYS:SG	1:C:661:ARG:N	2.59	0.75
1:C:591:TYR:O	1:C:594:ARG:NH1	2.20	0.74
1:A:660:CYS:SG	1:A:661:ARG:N	2.60	0.74
1:D:591:TYR:O	1:D:594:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:TYR:O	1:A:594:ARG:NH1	2.20	0.74
1:B:591:TYR:O	1:B:594:ARG:NH1	2.20	0.74
1:A:631:ALA:HB1	1:D:579:VAL:HG13	1.71	0.72
1:B:660:CYS:SG	1:B:661:ARG:N	2.60	0.72
3:A:911:GDN:C14	3:A:911:GDN:C20	2.66	0.70
3:D:911:GDN:C14	3:D:911:GDN:C20	2.67	0.70
1:A:702:TYR:O	1:A:706:THR:OG1	2.07	0.69
3:B:911:GDN:C14	3:B:911:GDN:C20	2.67	0.69
1:A:720:GLU:OE2	1:A:724:GLN:NE2	2.27	0.68
1:B:720:GLU:OE2	1:B:724:GLN:NE2	2.27	0.68
3:C:911:GDN:C14	3:C:911:GDN:C20	2.67	0.68
1:D:720:GLU:OE2	1:D:724:GLN:NE2	2.27	0.68
1:B:657:TYR:O	1:B:660:CYS:N	2.28	0.67
1:C:720:GLU:OE2	1:C:724:GLN:NE2	2.27	0.67
1:B:274:GLN:OE1	1:B:320:ARG:NH2	2.28	0.67
1:C:274:GLN:OE1	1:C:320:ARG:NH2	2.28	0.67
1:D:657:TYR:O	1:D:660:CYS:N	2.28	0.67
1:C:657:TYR:O	1:C:660:CYS:N	2.28	0.66
1:A:657:TYR:O	1:A:660:CYS:N	2.28	0.66
1:D:702:TYR:O	1:D:706:THR:OG1	2.07	0.66
1:D:274:GLN:OE1	1:D:320:ARG:NH2	2.28	0.66
1:C:517:THR:O	1:C:520:THR:OG1	2.14	0.66
1:A:274:GLN:OE1	1:A:320:ARG:NH2	2.28	0.65
1:C:579:VAL:HG13	1:D:631:ALA:HB1	1.79	0.65
1:D:160:ARG:NH1	1:D:165:ASP:OD2	2.30	0.65
1:A:160:ARG:NH1	1:A:165:ASP:OD2	2.30	0.65
1:B:160:ARG:NH1	1:B:165:ASP:OD2	2.30	0.65
1:C:160:ARG:NH1	1:C:165:ASP:OD2	2.30	0.64
1:B:256:LEU:O	1:B:260:GLN:NE2	2.32	0.63
1:A:256:LEU:O	1:A:260:GLN:NE2	2.32	0.63
1:D:256:LEU:O	1:D:260:GLN:NE2	2.32	0.62
1:C:256:LEU:O	1:C:260:GLN:NE2	2.32	0.62
1:B:702:TYR:O	1:B:706:THR:OG1	2.07	0.61
3:C:903:GDN:C14	3:C:903:GDN:C20	2.73	0.61
1:D:524:PHE:O	1:D:528:ASN:ND2	2.34	0.61
1:D:453:GLU:O	1:D:455:ILE:N	2.34	0.61
3:B:903:GDN:C14	3:B:903:GDN:C20	2.73	0.61
1:C:554:PHE:O	1:C:557:SER:OG	2.17	0.61
1:B:524:PHE:O	1:B:528:ASN:ND2	2.34	0.61
1:B:453:GLU:O	1:B:455:ILE:N	2.34	0.60
1:C:453:GLU:O	1:C:455:ILE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:PHE:O	1:C:528:ASN:ND2	2.34	0.60
3:A:903:GDN:C14	3:A:903:GDN:C20	2.73	0.60
1:C:702:TYR:O	1:C:706:THR:OG1	2.07	0.60
1:A:524:PHE:O	1:A:528:ASN:ND2	2.34	0.60
1:A:453:GLU:O	1:A:455:ILE:N	2.34	0.60
1:B:725:VAL:O	1:B:729:SER:OG	2.19	0.60
1:A:574:TYR:OH	5:A:932:HOH:O	2.17	0.57
1:D:554:PHE:O	1:D:557:SER:OG	2.17	0.57
3:D:903:GDN:C14	3:D:903:GDN:C20	2.72	0.57
1:B:579:VAL:HG13	1:C:631:ALA:HB1	1.86	0.57
1:C:169:LEU:O	1:C:173:LEU:N	2.37	0.57
1:B:554:PHE:O	1:B:557:SER:OG	2.17	0.56
1:D:760:GLU:OE1	1:D:779:ARG:NH2	2.39	0.56
1:C:760:GLU:OE1	1:C:779:ARG:NH2	2.39	0.56
1:A:517:THR:O	1:A:520:THR:OG1	2.14	0.56
1:A:760:GLU:OE1	1:A:779:ARG:NH2	2.39	0.56
1:D:169:LEU:O	1:D:173:LEU:N	2.37	0.56
1:B:169:LEU:O	1:B:173:LEU:N	2.37	0.56
1:B:760:GLU:OE1	1:B:779:ARG:NH2	2.39	0.56
1:A:554:PHE:O	1:A:557:SER:OG	2.17	0.55
1:A:236:TYR:OH	1:D:799:PRO:O	2.21	0.55
1:A:332:ALA:O	1:A:382:LYS:NZ	2.33	0.55
1:B:535:LYS:NZ	1:B:743:ASP:OD1	2.40	0.54
1:D:439:TYR:OH	1:D:743:ASP:OD1	2.23	0.54
1:C:535:LYS:NZ	1:C:743:ASP:OD1	2.40	0.54
1:A:169:LEU:O	1:A:173:LEU:N	2.37	0.54
1:D:535:LYS:NZ	1:D:743:ASP:OD1	2.40	0.54
1:A:535:LYS:NZ	1:A:743:ASP:OD1	2.40	0.53
1:D:332:ALA:O	1:D:382:LYS:NZ	2.33	0.53
1:D:517:THR:O	1:D:520:THR:OG1	2.14	0.53
1:B:613:ASP:O	1:B:615:PHE:N	2.37	0.53
1:B:584:LEU:O	1:B:588:ASN:N	2.42	0.53
1:C:498:PRO:O	1:C:500:TYR:N	2.42	0.52
1:B:507:ASP:OD1	1:B:510:ARG:NH1	2.41	0.52
1:C:332:ALA:O	1:C:382:LYS:NZ	2.33	0.52
1:A:498:PRO:O	1:A:500:TYR:N	2.42	0.52
1:C:584:LEU:O	1:C:588:ASN:N	2.42	0.52
1:D:498:PRO:O	1:D:500:TYR:N	2.42	0.52
1:B:517:THR:O	1:B:520:THR:OG1	2.14	0.52
1:B:498:PRO:O	1:B:500:TYR:N	2.42	0.52
1:C:613:ASP:O	1:C:615:PHE:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:LEU:O	1:D:588:ASN:N	2.42	0.52
1:C:507:ASP:OD1	1:C:510:ARG:NH1	2.41	0.51
1:D:613:ASP:O	1:D:615:PHE:N	2.37	0.51
1:B:332:ALA:O	1:B:382:LYS:NZ	2.33	0.51
1:A:584:LEU:O	1:A:588:ASN:N	2.42	0.51
1:A:486:THR:HG23	1:B:630:SER:HB3	1.91	0.51
1:A:507:ASP:OD1	1:A:510:ARG:NH1	2.41	0.51
1:B:454:PRO:O	1:B:458:LEU:N	2.44	0.51
1:A:469:VAL:O	1:A:473:ILE:HD12	2.13	0.48
1:D:507:ASP:OD1	1:D:510:ARG:NH1	2.41	0.48
1:D:454:PRO:O	1:D:458:LEU:N	2.44	0.48
1:A:613:ASP:O	1:A:615:PHE:N	2.37	0.48
1:C:469:VAL:O	1:C:473:ILE:HD12	2.13	0.48
1:D:574:TYR:OH	5:D:932:HOH:O	2.20	0.48
1:B:469:VAL:O	1:B:473:ILE:HD12	2.13	0.47
1:D:469:VAL:O	1:D:473:ILE:HD12	2.13	0.47
1:A:565:ALA:O	1:A:569:ALA:N	2.46	0.47
1:B:349:LEU:O	1:B:353:CYS:N	2.47	0.47
1:A:598:LEU:O	1:B:616:ARG:NH1	2.45	0.47
1:C:454:PRO:O	1:C:458:LEU:N	2.44	0.47
2:B:909:POV:H37	2:B:909:POV:O32	2.15	0.47
1:D:565:ALA:O	1:D:569:ALA:N	2.46	0.47
1:D:763:THR:OG1	1:D:774:ARG:NH1	2.45	0.46
1:A:454:PRO:O	1:A:458:LEU:N	2.44	0.46
1:A:763:THR:OG1	1:A:774:ARG:NH1	2.45	0.46
1:A:349:LEU:O	1:A:353:CYS:N	2.47	0.46
1:D:472:TYR:HA	1:D:475:VAL:HG12	1.97	0.46
1:C:565:ALA:O	1:C:569:ALA:N	2.46	0.46
1:C:763:THR:OG1	1:C:774:ARG:NH1	2.45	0.46
1:D:349:LEU:O	1:D:353:CYS:N	2.47	0.46
1:B:565:ALA:O	1:B:569:ALA:N	2.46	0.46
1:D:747:SER:OG	2:D:910:POV:H37A	2.16	0.46
1:B:472:TYR:HA	1:B:475:VAL:HG12	1.97	0.45
1:C:472:TYR:HA	1:C:475:VAL:HG12	1.97	0.45
1:C:747:SER:OG	2:C:910:POV:H37A	2.16	0.45
1:A:439:TYR:OH	1:A:743:ASP:OD1	2.23	0.45
2:A:909:POV:O32	2:A:909:POV:H37	2.17	0.45
1:A:472:TYR:HA	1:A:475:VAL:HG12	1.97	0.45
1:C:396:ASP:OD1	1:C:399:THR:OG1	2.35	0.45
1:D:396:ASP:OD1	1:D:399:THR:OG1	2.35	0.45
1:B:441:SER:OG	1:B:442:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:SER:OG	2:B:910:POV:H37A	2.17	0.45
1:A:579:VAL:HG13	1:B:631:ALA:HB1	1.98	0.45
1:D:725:VAL:O	1:D:729:SER:OG	2.19	0.45
1:A:396:ASP:OD1	1:A:399:THR:OG1	2.35	0.45
1:C:552:LEU:HB3	1:C:588:ASN:HD21	1.81	0.45
1:D:552:LEU:HB3	1:D:588:ASN:HD21	1.81	0.45
1:C:441:SER:OG	1:C:442:LYS:N	2.50	0.44
1:A:552:LEU:HB3	1:A:588:ASN:HD21	1.81	0.44
1:B:552:LEU:HB3	1:B:588:ASN:HD21	1.81	0.44
1:C:349:LEU:O	1:C:353:CYS:N	2.47	0.44
1:B:396:ASP:OD1	1:B:399:THR:OG1	2.35	0.44
1:D:154:LEU:O	1:D:157:ILE:N	2.50	0.44
2:C:909:POV:O32	2:C:909:POV:H37	2.16	0.44
1:A:420:ASP:OD1	1:A:422:SER:OG	2.32	0.44
1:A:747:SER:OG	2:A:910:POV:H37A	2.16	0.44
1:B:154:LEU:O	1:B:157:ILE:N	2.50	0.44
1:C:154:LEU:O	1:C:157:ILE:N	2.50	0.44
1:A:154:LEU:O	1:A:157:ILE:N	2.50	0.44
1:B:763:THR:OG1	1:B:774:ARG:NH1	2.45	0.43
1:B:488:THR:O	1:B:492:GLN:N	2.52	0.43
2:D:909:POV:O32	2:D:909:POV:H37	2.18	0.43
1:B:633:VAL:O	1:B:661:ARG:NH2	2.49	0.43
1:D:441:SER:OG	1:D:442:LYS:N	2.50	0.43
1:C:488:THR:O	1:C:492:GLN:N	2.52	0.43
1:A:441:SER:OG	1:A:442:LYS:N	2.50	0.43
1:A:488:THR:O	1:A:492:GLN:N	2.52	0.43
1:D:233:ASP:OD1	1:D:234:ILE:N	2.52	0.43
1:D:488:THR:O	1:D:492:GLN:N	2.52	0.43
1:B:574:TYR:OH	5:B:932:HOH:O	2.20	0.43
1:B:439:TYR:OH	1:B:743:ASP:OD1	2.23	0.42
1:B:461:ASP:OD2	1:B:465:LYS:NZ	2.52	0.42
1:C:233:ASP:OD1	1:C:234:ILE:N	2.52	0.42
1:B:513:GLY:O	1:B:517:THR:OG1	2.30	0.42
1:A:461:ASP:OD2	1:A:465:LYS:NZ	2.52	0.42
1:D:179:ARG:NH2	1:D:225:GLU:OE1	2.50	0.42
1:C:461:ASP:OD2	1:C:465:LYS:NZ	2.52	0.42
1:D:538:PRO:O	1:D:540:VAL:N	2.53	0.42
1:C:315:ARG:NH2	5:C:924:HOH:O	2.42	0.42
1:A:538:PRO:O	1:A:540:VAL:N	2.53	0.41
1:B:420:ASP:OD1	1:B:422:SER:OG	2.32	0.41
2:D:909:POV:H37	2:D:909:POV:O30	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ALA:HB1	1:A:210:ILE:HD11	2.03	0.41
1:B:233:ASP:OD1	1:B:234:ILE:N	2.52	0.41
1:C:513:GLY:O	1:C:517:THR:OG1	2.30	0.41
1:A:179:ARG:NH2	1:A:225:GLU:OE1	2.50	0.41
1:B:538:PRO:O	1:B:540:VAL:N	2.53	0.41
1:C:198:ALA:HB1	1:C:210:ILE:HD11	2.03	0.41
1:B:198:ALA:HB1	1:B:210:ILE:HD11	2.03	0.41
1:C:538:PRO:O	1:C:540:VAL:N	2.53	0.41
1:D:461:ASP:OD2	1:D:465:LYS:NZ	2.52	0.41
1:A:193:THR:HG22	1:A:194:CYS:N	2.36	0.41
1:A:212:VAL:O	1:A:216:ILE:HD12	2.21	0.41
1:B:212:VAL:O	1:B:216:ILE:HD12	2.21	0.41
1:C:179:ARG:NH2	1:C:225:GLU:OE1	2.50	0.41
1:D:193:THR:HG22	1:D:194:CYS:N	2.36	0.41
1:D:198:ALA:HB1	1:D:210:ILE:HD11	2.03	0.41
1:A:631:ALA:HB1	1:D:579:VAL:CG1	2.44	0.40
1:B:347:ASP:CG	1:B:388:HIS:HE2	2.24	0.40
1:B:179:ARG:NH2	1:B:225:GLU:OE1	2.50	0.40
1:A:575:LEU:HD21	1:B:635:LEU:HD23	2.03	0.40
1:A:694:VAL:HG23	1:D:580:PHE:CZ	2.56	0.40
1:A:347:ASP:CG	1:A:388:HIS:HE2	2.24	0.40
1:B:630:SER:O	1:B:634:SER:OG	2.33	0.40
2:C:909:POV:H37	2:C:909:POV:O30	2.22	0.40
1:D:403:SER:O	1:D:775:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	640/644 (99%)	563 (88%)	73 (11%)	4 (1%)	25 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	640/644 (99%)	563 (88%)	73 (11%)	4 (1%)	25	25
1	C	640/644 (99%)	562 (88%)	74 (12%)	4 (1%)	25	25
1	D	640/644 (99%)	563 (88%)	73 (11%)	4 (1%)	25	25
All	All	2560/2576 (99%)	2251 (88%)	293 (11%)	16 (1%)	29	25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	LEU
1	B	614	LEU
1	C	614	LEU
1	D	614	LEU
1	A	613	ASP
1	B	613	ASP
1	C	613	ASP
1	D	613	ASP
1	A	453	GLU
1	B	453	GLU
1	C	453	GLU
1	D	453	GLU
1	A	454	PRO
1	B	454	PRO
1	C	454	PRO
1	D	454	PRO

### 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	568/568 (100%)	564 (99%)	4 (1%)	84	84
1	B	568/568 (100%)	564 (99%)	4 (1%)	84	84
1	C	568/568 (100%)	564 (99%)	4 (1%)	84	84
1	D	568/568 (100%)	564 (99%)	4 (1%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2272/2272 (100%)	2256 (99%)	16 (1%)	84 84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	338	ASN
1	A	345	MET
1	A	784	ASN
1	B	207	ASN
1	B	338	ASN
1	B	345	MET
1	B	784	ASN
1	C	207	ASN
1	C	338	ASN
1	C	345	MET
1	C	784	ASN
1	D	207	ASN
1	D	338	ASN
1	D	345	MET
1	D	784	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	207	ASN
1	A	243	HIS
1	A	492	GLN
1	A	724	GLN
1	A	784	ASN
1	B	201	ASN
1	B	207	ASN
1	B	243	HIS
1	B	260	GLN
1	B	492	GLN
1	B	724	GLN
1	B	784	ASN
1	C	201	ASN
1	C	207	ASN
1	C	243	HIS

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Mol	Chain	Res	Type
1	C	492	GLN
1	C	724	GLN
1	C	784	ASN
1	D	201	ASN
1	D	207	ASN
1	D	243	HIS
1	D	260	GLN
1	D	492	GLN
1	D	724	GLN
1	D	784	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 48 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	641:ASN	C	654:VAL	N	8.04
1	B	641:ASN	C	654:VAL	N	8.04
1	C	641:ASN	C	654:VAL	N	8.04
1	D	641:ASN	C	654:VAL	N	8.04

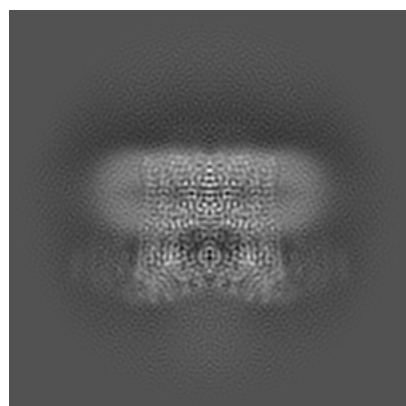
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D\_9100078173. These allow visual inspection of the internal detail of the map and identification of artifacts.

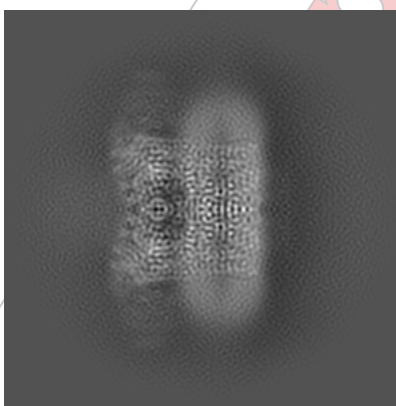
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

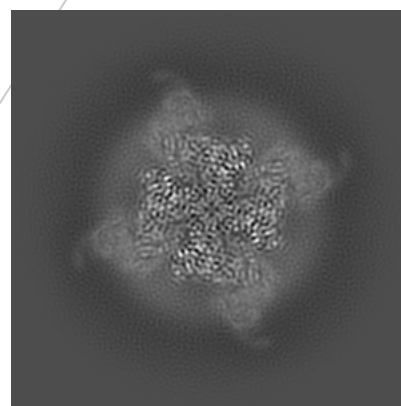
#### 6.1.1 Primary map



X



Y

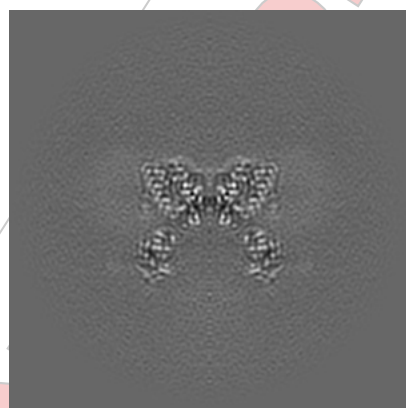


Z

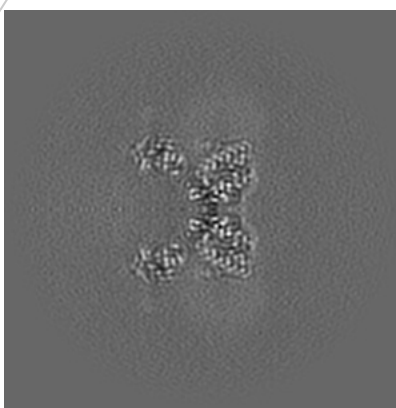
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

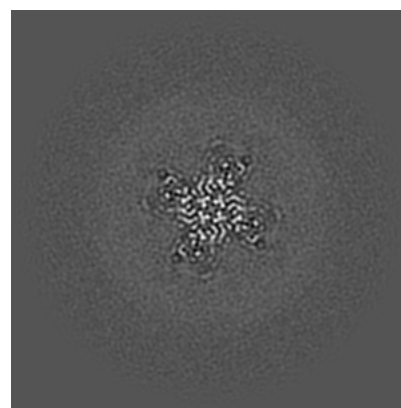
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



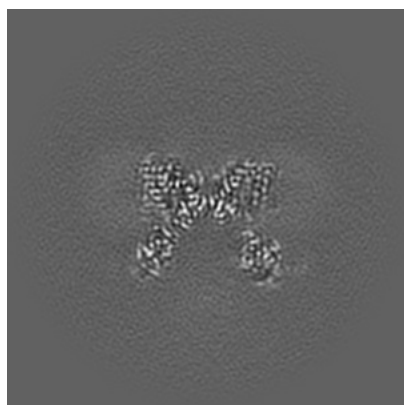
Z Index: 160



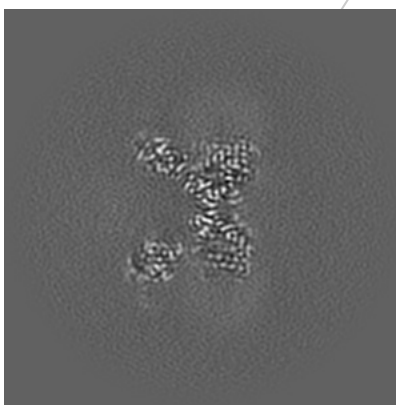
The images above show central slices of the map in three orthogonal directions.

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

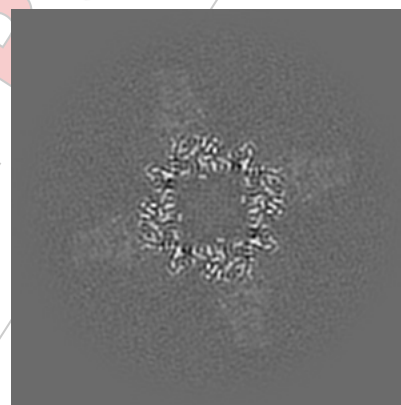
### 6.3.1 Primary map



X Index: 157



Y Index: 157

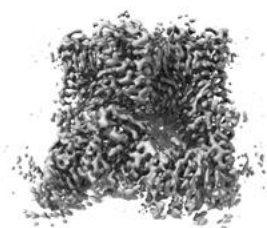


Z Index: 123

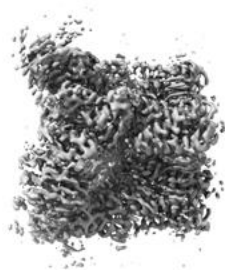
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation

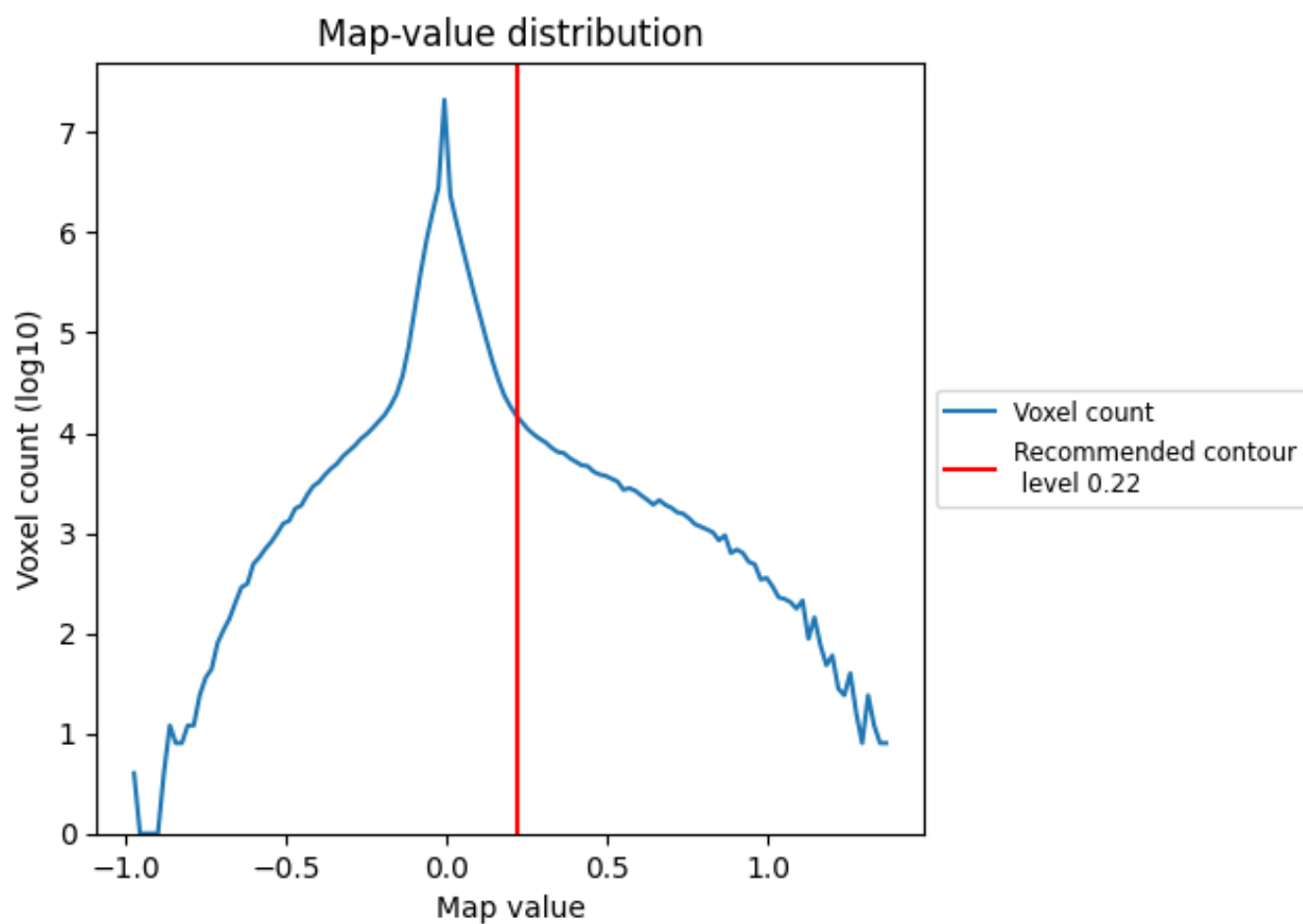
This section was not generated. No masks/segmentation were deposited.

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## 7 Map analysis ⓘ

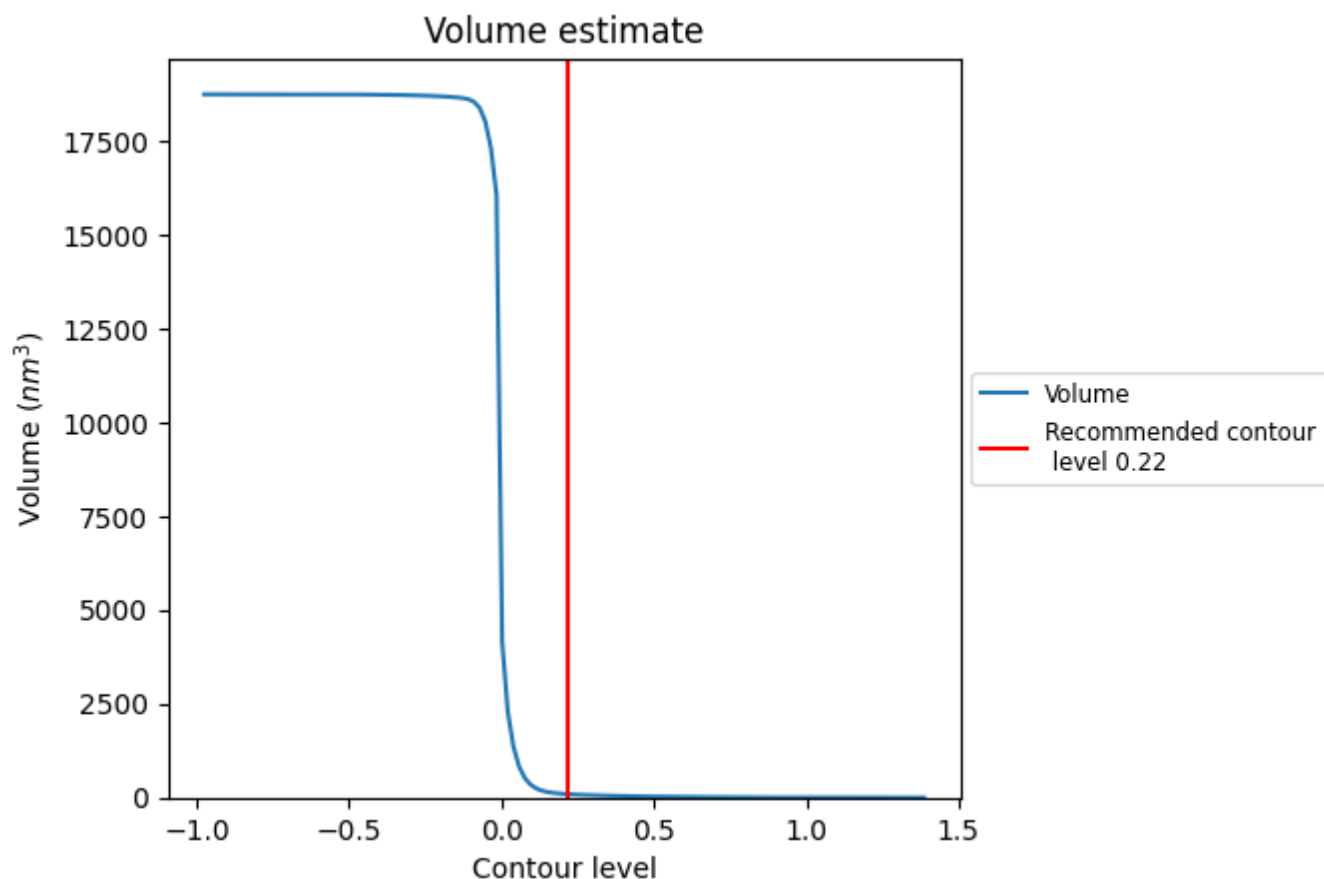
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ



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.

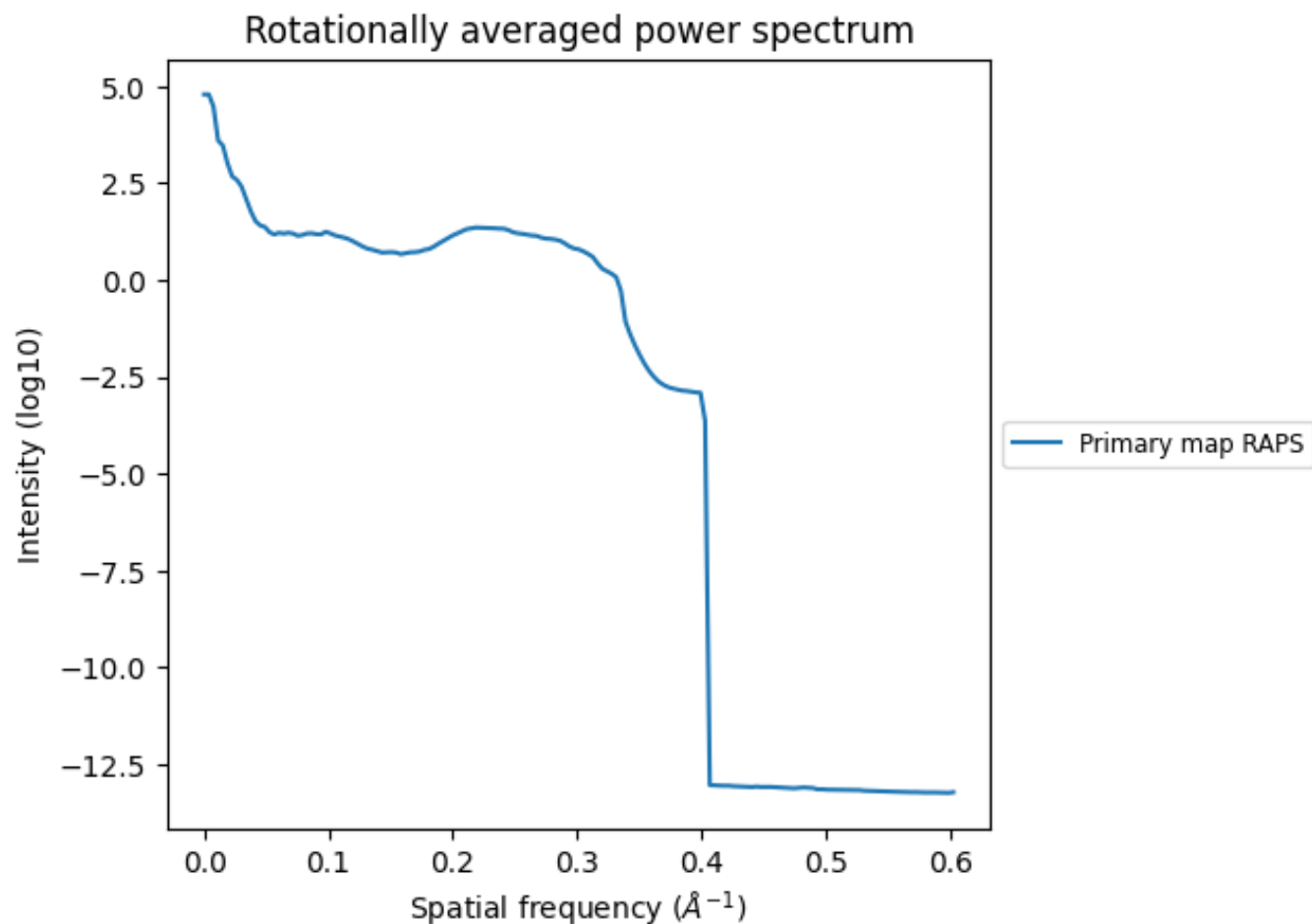
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89  $\text{nm}^3$ ; this corresponds to an approximate mass of 81 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 ⓘ



## 8 Fourier-Shell correlation ⓘ

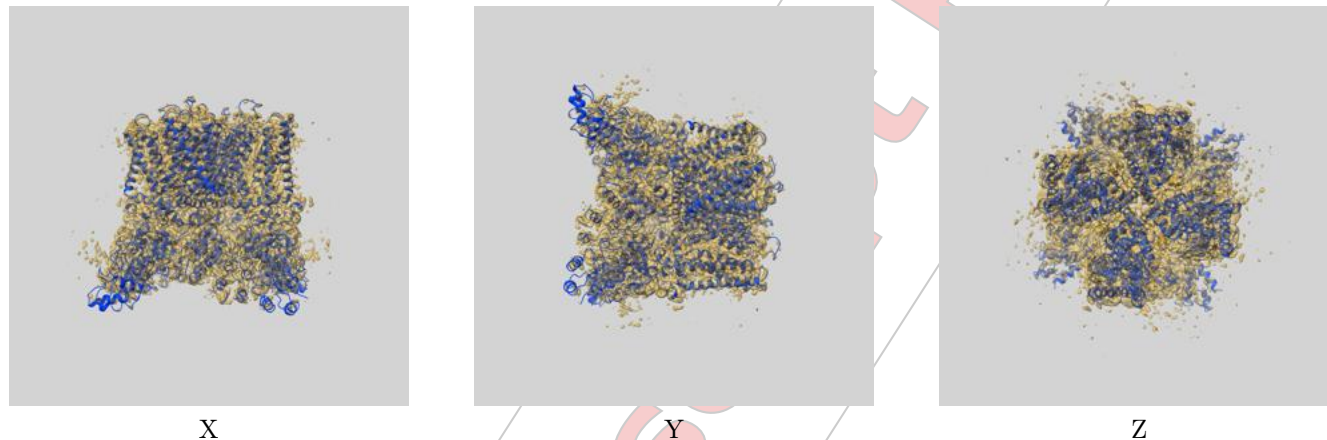
This section was not generated. No FSC curve or half-maps provided.

Not For Manuscript Review

## 9 Map-model fit ⓘ

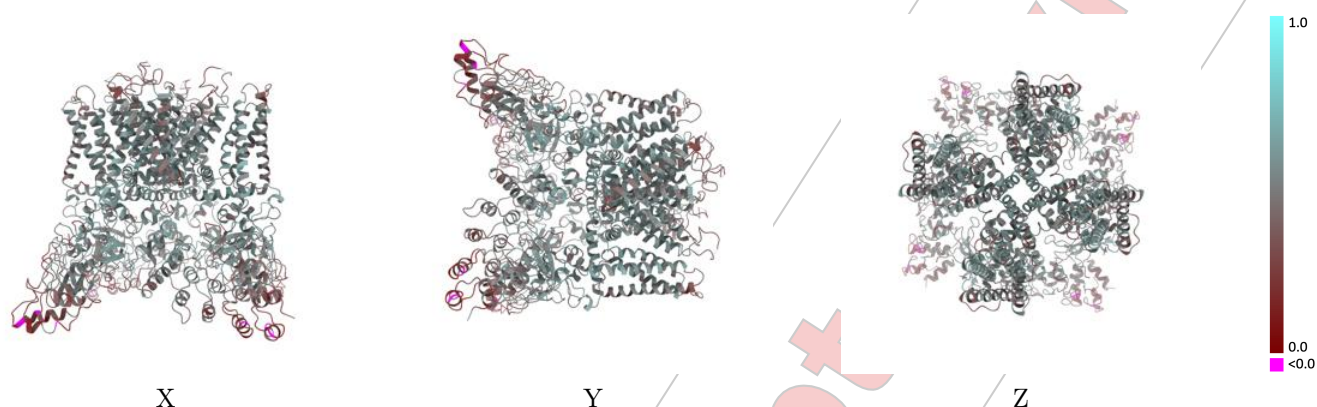
This section contains information regarding the fit between EMDB map D\_9100078173 and PDB model D\_9100078173. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay ⓘ



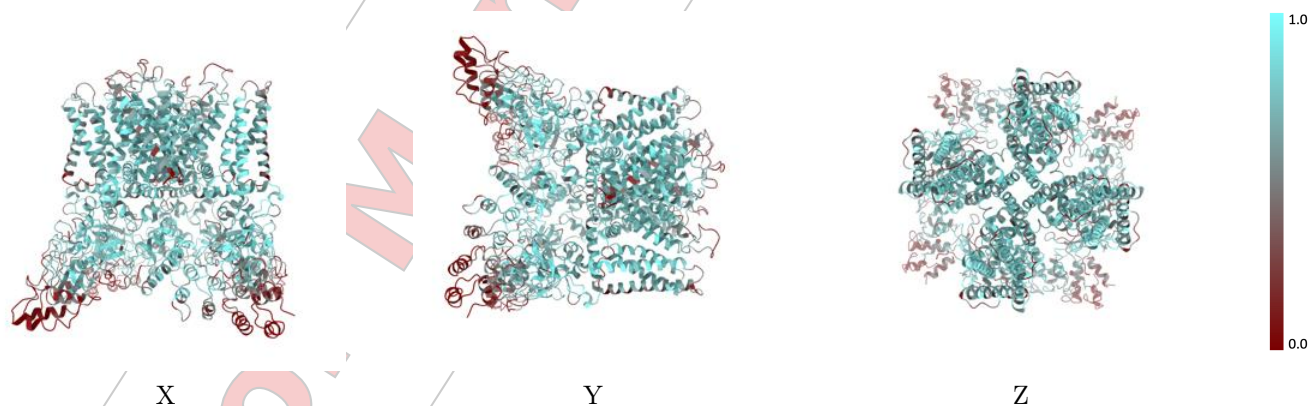
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



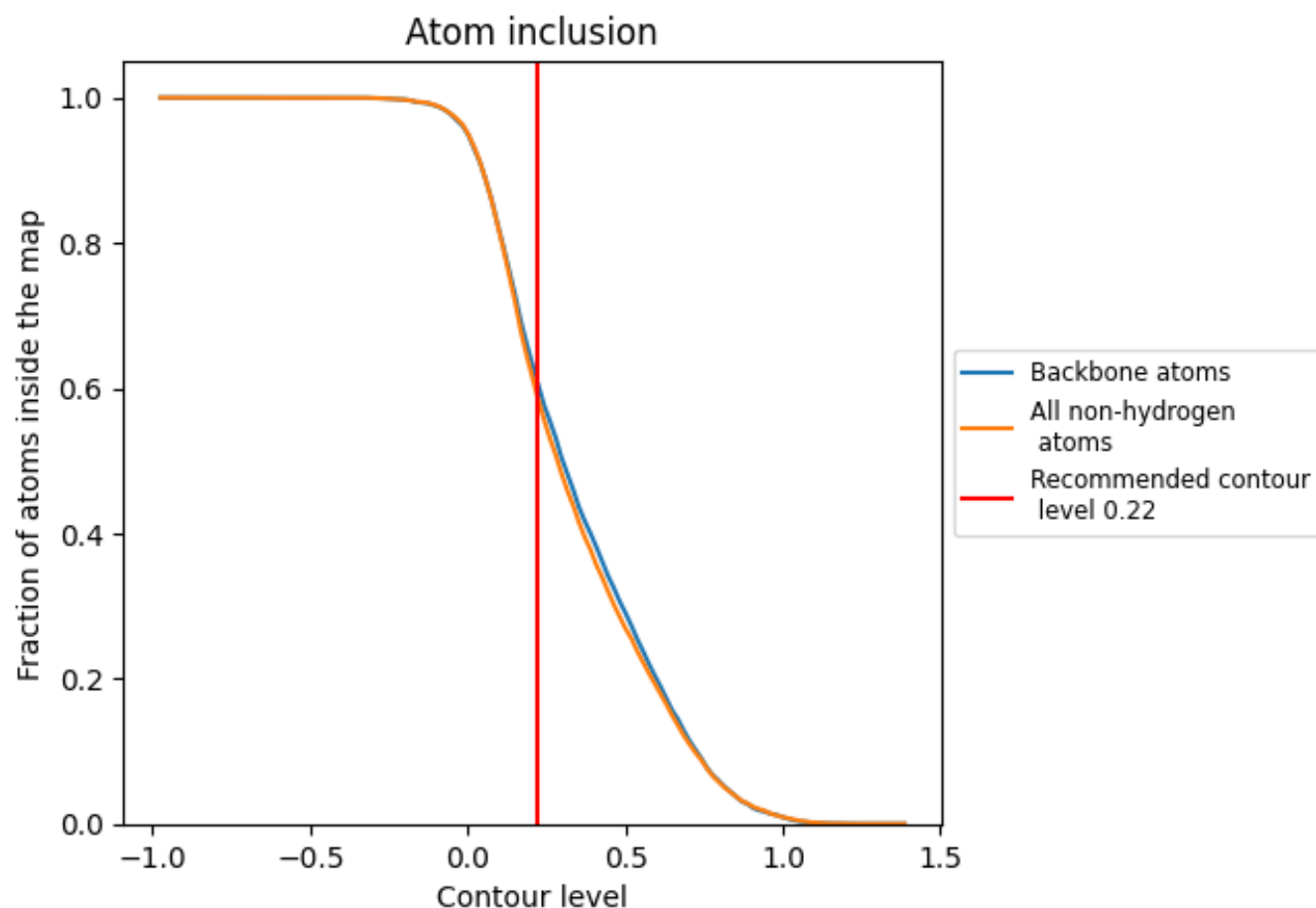
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

## 9.4 Atom inclusion ⓘ















At the recommended contour level, 61% of all backbone atoms, 59% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5900	 0.4670
A	 0.5881	 0.4660
B	 0.5881	 0.4650
C	 0.5899	 0.4660
D	 0.5883	 0.4680
I	 0.7500	 0.7200

