



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2025 – 02:15 PM JST

PDB ID : 9W4M / pdb\_00009w4m  
EMDB ID : EMD-65638  
Title : ratTRPV1 bound with antagonist AMG517  
Authors : Gao, Y.H.; Li, Z.X.  
Deposited on : 2025-07-31  
Resolution : 2.70 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.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

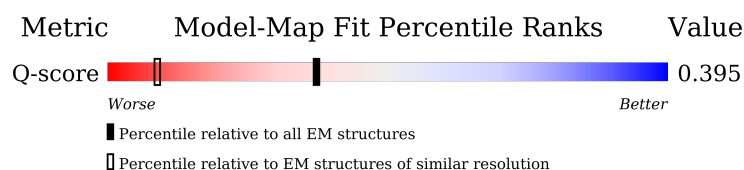
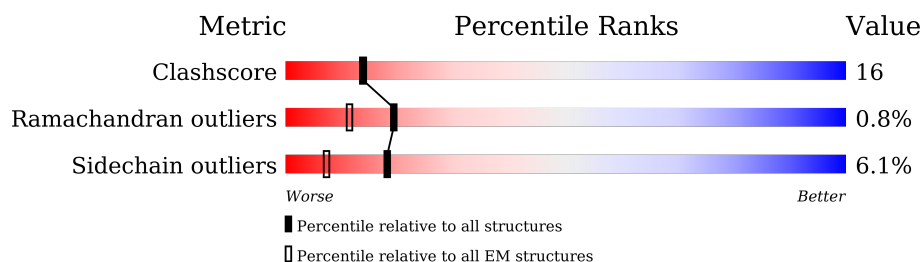
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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	1252	
1	B	1252	
1	C	1252	
1	D	1252	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35110 atoms, of which 17564 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 Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	537	Total	C	H	N	O	S	0	0
			8747	2851	4391	707	773	25		
1	B	537	Total	C	H	N	O	S	0	0
			8747	2851	4391	707	773	25		
1	C	537	Total	C	H	N	O	S	0	0
			8747	2851	4391	707	773	25		
1	D	537	Total	C	H	N	O	S	0	0
			8747	2851	4391	707	773	25		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-413	MET	-	initiating methionine	UNP P0AEX9
A	-46	ASN	-	linker	UNP P0AEX9
A	-45	SER	-	linker	UNP P0AEX9
A	-44	GLY	-	linker	UNP P0AEX9
A	-43	THR	-	linker	UNP P0AEX9
A	-42	GLY	-	linker	UNP P0AEX9
A	-41	GLY	-	linker	UNP P0AEX9
A	-40	GLY	-	linker	UNP P0AEX9
A	-39	SER	-	linker	UNP P0AEX9
A	-38	GLY	-	linker	UNP P0AEX9
A	-37	ASP	-	linker	UNP P0AEX9
A	-36	ASP	-	linker	UNP P0AEX9
A	-35	ASP	-	linker	UNP P0AEX9
A	-34	ASP	-	linker	UNP P0AEX9
A	-33	LYS	-	linker	UNP P0AEX9
A	-32	SER	-	linker	UNP P0AEX9
A	-31	PRO	-	linker	UNP P0AEX9
A	-30	MET	-	linker	UNP P0AEX9
A	-29	GLY	-	linker	UNP P0AEX9
A	-28	SER	-	linker	UNP P0AEX9
A	-27	HIS	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	HIS	-	linker	UNP P0AEX9
A	-25	HIS	-	linker	UNP P0AEX9
A	-24	HIS	-	linker	UNP P0AEX9
A	-23	HIS	-	linker	UNP P0AEX9
A	-22	HIS	-	linker	UNP P0AEX9
A	-21	HIS	-	linker	UNP P0AEX9
A	-20	HIS	-	linker	UNP P0AEX9
A	-19	GLY	-	linker	UNP P0AEX9
A	-18	SER	-	linker	UNP P0AEX9
A	-17	ASP	-	linker	UNP P0AEX9
A	-16	TYR	-	linker	UNP P0AEX9
A	-15	ASP	-	linker	UNP P0AEX9
A	-14	ILE	-	linker	UNP P0AEX9
A	-13	PRO	-	linker	UNP P0AEX9
A	-12	THR	-	linker	UNP P0AEX9
A	-11	THR	-	linker	UNP P0AEX9
A	-10	GLU	-	linker	UNP P0AEX9
A	-9	ASN	-	linker	UNP P0AEX9
A	-8	LEU	-	linker	UNP P0AEX9
A	-7	TYR	-	linker	UNP P0AEX9
A	-6	PHE	-	linker	UNP P0AEX9
A	-5	GLN	-	linker	UNP P0AEX9
A	-4	GLY	-	linker	UNP P0AEX9
A	-3	ALA	-	linker	UNP P0AEX9
A	-2	MET	-	linker	UNP P0AEX9
A	-1	ASP	-	linker	UNP P0AEX9
A	0	PRO	-	linker	UNP P0AEX9
B	-413	MET	-	initiating methionine	UNP P0AEX9
B	-46	ASN	-	linker	UNP P0AEX9
B	-45	SER	-	linker	UNP P0AEX9
B	-44	GLY	-	linker	UNP P0AEX9
B	-43	THR	-	linker	UNP P0AEX9
B	-42	GLY	-	linker	UNP P0AEX9
B	-41	GLY	-	linker	UNP P0AEX9
B	-40	GLY	-	linker	UNP P0AEX9
B	-39	SER	-	linker	UNP P0AEX9
B	-38	GLY	-	linker	UNP P0AEX9
B	-37	ASP	-	linker	UNP P0AEX9
B	-36	ASP	-	linker	UNP P0AEX9
B	-35	ASP	-	linker	UNP P0AEX9
B	-34	ASP	-	linker	UNP P0AEX9
B	-33	LYS	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	SER	-	linker	UNP P0AEX9
B	-31	PRO	-	linker	UNP P0AEX9
B	-30	MET	-	linker	UNP P0AEX9
B	-29	GLY	-	linker	UNP P0AEX9
B	-28	SER	-	linker	UNP P0AEX9
B	-27	HIS	-	linker	UNP P0AEX9
B	-26	HIS	-	linker	UNP P0AEX9
B	-25	HIS	-	linker	UNP P0AEX9
B	-24	HIS	-	linker	UNP P0AEX9
B	-23	HIS	-	linker	UNP P0AEX9
B	-22	HIS	-	linker	UNP P0AEX9
B	-21	HIS	-	linker	UNP P0AEX9
B	-20	HIS	-	linker	UNP P0AEX9
B	-19	GLY	-	linker	UNP P0AEX9
B	-18	SER	-	linker	UNP P0AEX9
B	-17	ASP	-	linker	UNP P0AEX9
B	-16	TYR	-	linker	UNP P0AEX9
B	-15	ASP	-	linker	UNP P0AEX9
B	-14	ILE	-	linker	UNP P0AEX9
B	-13	PRO	-	linker	UNP P0AEX9
B	-12	THR	-	linker	UNP P0AEX9
B	-11	THR	-	linker	UNP P0AEX9
B	-10	GLU	-	linker	UNP P0AEX9
B	-9	ASN	-	linker	UNP P0AEX9
B	-8	LEU	-	linker	UNP P0AEX9
B	-7	TYR	-	linker	UNP P0AEX9
B	-6	PHE	-	linker	UNP P0AEX9
B	-5	GLN	-	linker	UNP P0AEX9
B	-4	GLY	-	linker	UNP P0AEX9
B	-3	ALA	-	linker	UNP P0AEX9
B	-2	MET	-	linker	UNP P0AEX9
B	-1	ASP	-	linker	UNP P0AEX9
B	0	PRO	-	linker	UNP P0AEX9
C	-413	MET	-	initiating methionine	UNP P0AEX9
C	-46	ASN	-	linker	UNP P0AEX9
C	-45	SER	-	linker	UNP P0AEX9
C	-44	GLY	-	linker	UNP P0AEX9
C	-43	THR	-	linker	UNP P0AEX9
C	-42	GLY	-	linker	UNP P0AEX9
C	-41	GLY	-	linker	UNP P0AEX9
C	-40	GLY	-	linker	UNP P0AEX9
C	-39	SER	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-38	GLY	-	linker	UNP P0AEX9
C	-37	ASP	-	linker	UNP P0AEX9
C	-36	ASP	-	linker	UNP P0AEX9
C	-35	ASP	-	linker	UNP P0AEX9
C	-34	ASP	-	linker	UNP P0AEX9
C	-33	LYS	-	linker	UNP P0AEX9
C	-32	SER	-	linker	UNP P0AEX9
C	-31	PRO	-	linker	UNP P0AEX9
C	-30	MET	-	linker	UNP P0AEX9
C	-29	GLY	-	linker	UNP P0AEX9
C	-28	SER	-	linker	UNP P0AEX9
C	-27	HIS	-	linker	UNP P0AEX9
C	-26	HIS	-	linker	UNP P0AEX9
C	-25	HIS	-	linker	UNP P0AEX9
C	-24	HIS	-	linker	UNP P0AEX9
C	-23	HIS	-	linker	UNP P0AEX9
C	-22	HIS	-	linker	UNP P0AEX9
C	-21	HIS	-	linker	UNP P0AEX9
C	-20	HIS	-	linker	UNP P0AEX9
C	-19	GLY	-	linker	UNP P0AEX9
C	-18	SER	-	linker	UNP P0AEX9
C	-17	ASP	-	linker	UNP P0AEX9
C	-16	TYR	-	linker	UNP P0AEX9
C	-15	ASP	-	linker	UNP P0AEX9
C	-14	ILE	-	linker	UNP P0AEX9
C	-13	PRO	-	linker	UNP P0AEX9
C	-12	THR	-	linker	UNP P0AEX9
C	-11	THR	-	linker	UNP P0AEX9
C	-10	GLU	-	linker	UNP P0AEX9
C	-9	ASN	-	linker	UNP P0AEX9
C	-8	LEU	-	linker	UNP P0AEX9
C	-7	TYR	-	linker	UNP P0AEX9
C	-6	PHE	-	linker	UNP P0AEX9
C	-5	GLN	-	linker	UNP P0AEX9
C	-4	GLY	-	linker	UNP P0AEX9
C	-3	ALA	-	linker	UNP P0AEX9
C	-2	MET	-	linker	UNP P0AEX9
C	-1	ASP	-	linker	UNP P0AEX9
C	0	PRO	-	linker	UNP P0AEX9
D	-413	MET	-	initiating methionine	UNP P0AEX9
D	-46	ASN	-	linker	UNP P0AEX9
D	-45	SER	-	linker	UNP P0AEX9

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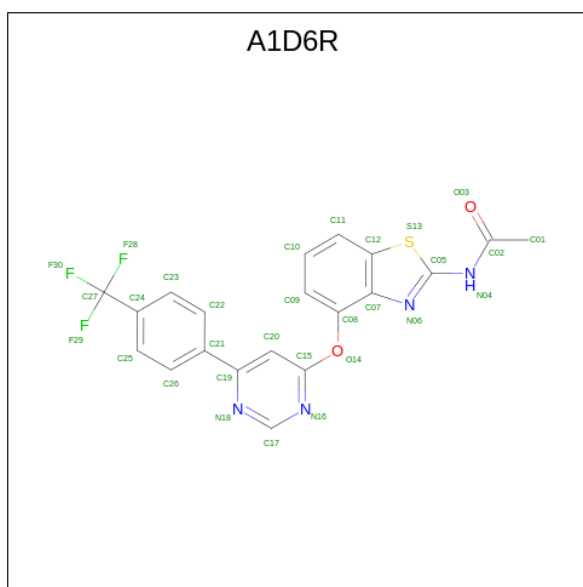
Chain	Residue	Modelled	Actual	Comment	Reference
D	-44	GLY	-	linker	UNP P0AEX9
D	-43	THR	-	linker	UNP P0AEX9
D	-42	GLY	-	linker	UNP P0AEX9
D	-41	GLY	-	linker	UNP P0AEX9
D	-40	GLY	-	linker	UNP P0AEX9
D	-39	SER	-	linker	UNP P0AEX9
D	-38	GLY	-	linker	UNP P0AEX9
D	-37	ASP	-	linker	UNP P0AEX9
D	-36	ASP	-	linker	UNP P0AEX9
D	-35	ASP	-	linker	UNP P0AEX9
D	-34	ASP	-	linker	UNP P0AEX9
D	-33	LYS	-	linker	UNP P0AEX9
D	-32	SER	-	linker	UNP P0AEX9
D	-31	PRO	-	linker	UNP P0AEX9
D	-30	MET	-	linker	UNP P0AEX9
D	-29	GLY	-	linker	UNP P0AEX9
D	-28	SER	-	linker	UNP P0AEX9
D	-27	HIS	-	linker	UNP P0AEX9
D	-26	HIS	-	linker	UNP P0AEX9
D	-25	HIS	-	linker	UNP P0AEX9
D	-24	HIS	-	linker	UNP P0AEX9
D	-23	HIS	-	linker	UNP P0AEX9
D	-22	HIS	-	linker	UNP P0AEX9
D	-21	HIS	-	linker	UNP P0AEX9
D	-20	HIS	-	linker	UNP P0AEX9
D	-19	GLY	-	linker	UNP P0AEX9
D	-18	SER	-	linker	UNP P0AEX9
D	-17	ASP	-	linker	UNP P0AEX9
D	-16	TYR	-	linker	UNP P0AEX9
D	-15	ASP	-	linker	UNP P0AEX9
D	-14	ILE	-	linker	UNP P0AEX9
D	-13	PRO	-	linker	UNP P0AEX9
D	-12	THR	-	linker	UNP P0AEX9
D	-11	THR	-	linker	UNP P0AEX9
D	-10	GLU	-	linker	UNP P0AEX9
D	-9	ASN	-	linker	UNP P0AEX9
D	-8	LEU	-	linker	UNP P0AEX9
D	-7	TYR	-	linker	UNP P0AEX9
D	-6	PHE	-	linker	UNP P0AEX9
D	-5	GLN	-	linker	UNP P0AEX9
D	-4	GLY	-	linker	UNP P0AEX9
D	-3	ALA	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	linker	UNP P0AEX9
D	-1	ASP	-	linker	UNP P0AEX9
D	0	PRO	-	linker	UNP P0AEX9

- Molecule 2 is {N}-[4-[6-[4-(trifluoromethyl)phenyl]pyrimidin-4-yl]oxy-1,3-benzothiazol-2-yl] ethanamide (CCD ID: A1D6R) (formula: C<sub>20</sub>H<sub>13</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 30	C 20	F 3	N 4	O 2	S 1	0
2	B	1	Total 30	C 20	F 3	N 4	O 2	S 1	0
2	C	1	Total 30	C 20	F 3	N 4	O 2	S 1	0
2	D	1	Total 30	C 20	F 3	N 4	O 2	S 1	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

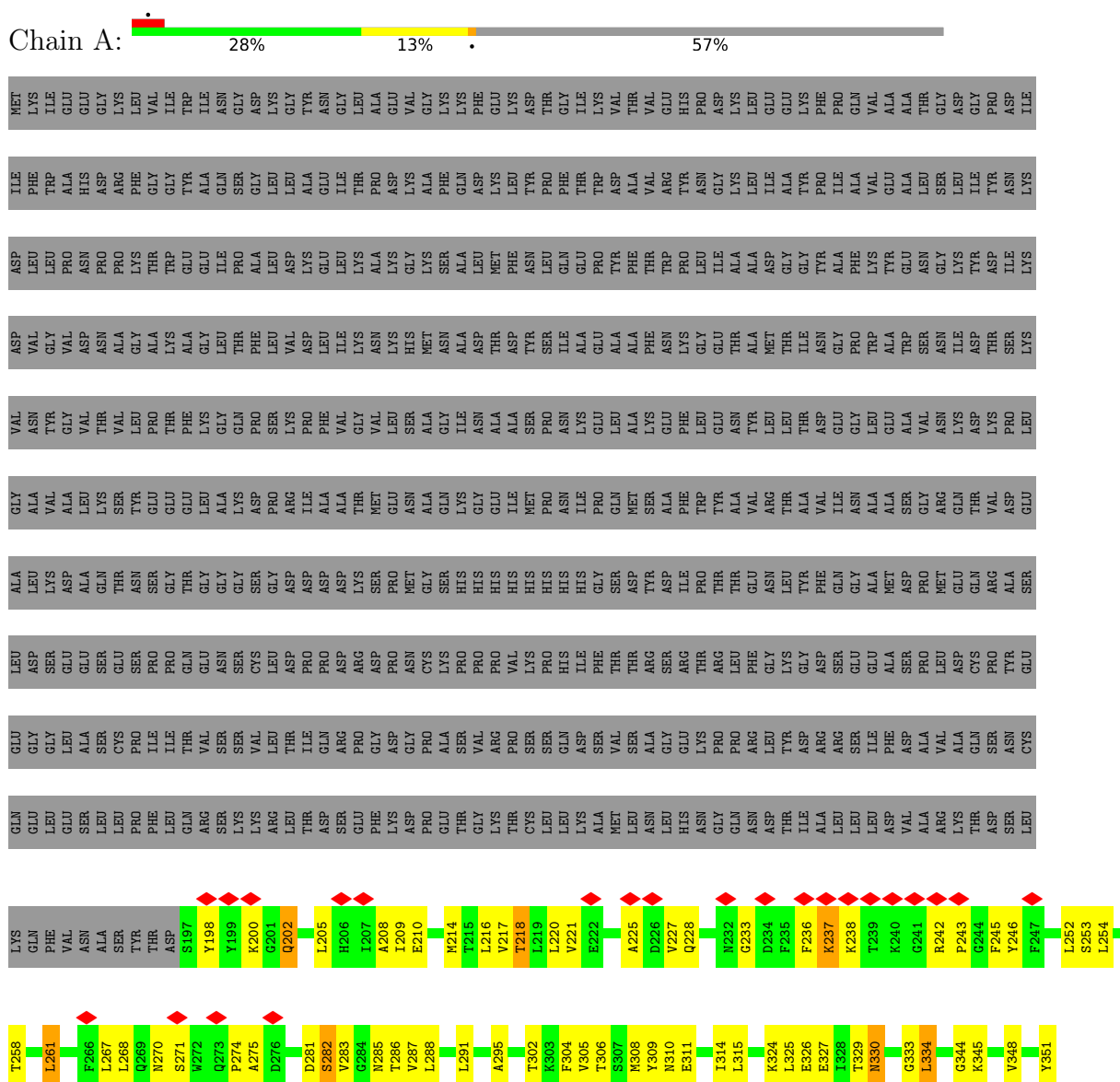
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Na	0
			2	2	



### 3 Residue-property plots

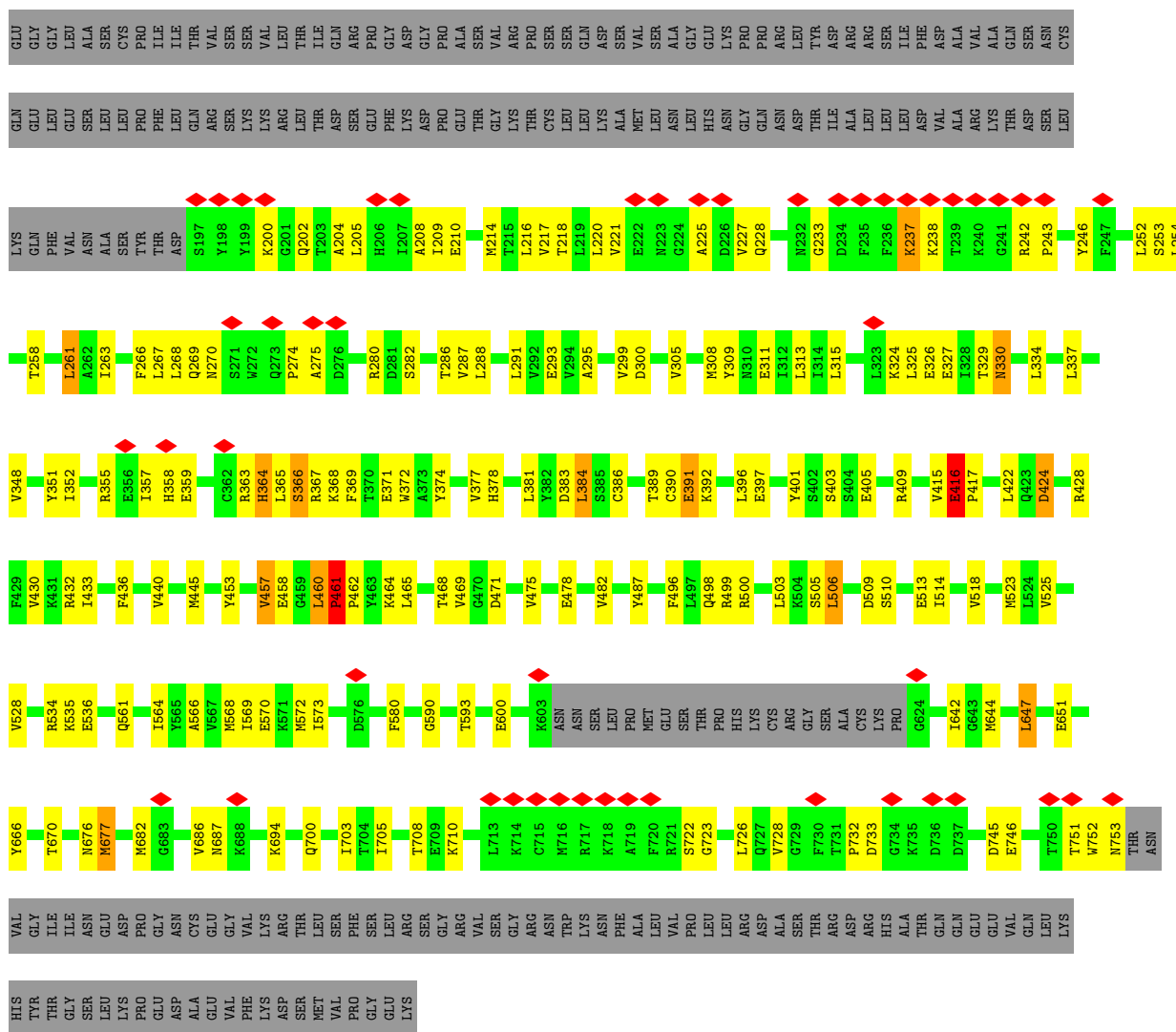
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily V member 1



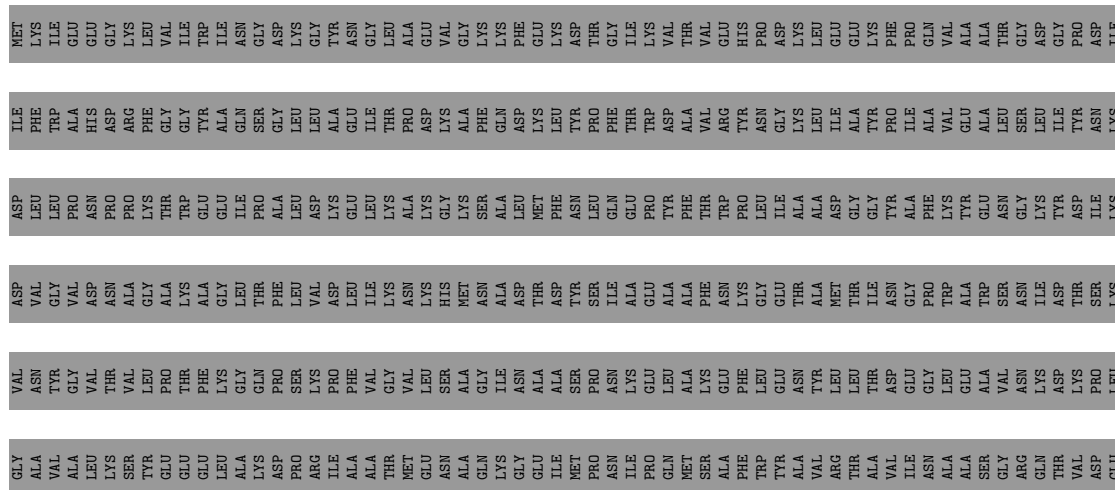






- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Transient receptor potential cation channel subfamily V member 1

Chain D: 29% 13% 57%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368794	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.589	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.0913	Depositor
Map size (Å)	245.76, 245.76, 245.76	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1D6R, 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	0.32	0/4460	0.58	4/6037 (0.1%)
1	B	0.32	0/4460	0.54	2/6037 (0.0%)
1	C	0.32	0/4460	0.56	2/6037 (0.0%)
1	D	0.33	0/4460	0.56	3/6037 (0.0%)
All	All	0.32	0/17840	0.56	11/24148 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	PRO	N-CA-CB	-14.94	88.58	103.08
1	A	461	PRO	N-CA-C	14.79	128.75	110.70
1	D	461	PRO	N-CA-CB	-14.75	88.77	103.08
1	B	461	PRO	N-CA-C	13.05	126.63	110.70
1	C	461	PRO	N-CA-C	12.58	126.04	110.70
1	D	461	PRO	N-CA-C	11.08	124.22	110.70
1	C	461	PRO	N-CD-CG	-6.92	92.83	103.20
1	D	459	GLY	CA-C-O	-6.71	117.62	122.45
1	A	459	GLY	CA-C-O	-6.55	117.73	122.45
1	B	461	PRO	N-CD-CG	-6.46	93.51	103.20
1	A	461	PRO	CA-C-O	-5.01	113.29	120.56

There are no chirality outliers.

There are no planarity outliers.

### 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	4356	4391	4389	146	0
1	B	4356	4391	4389	139	0
1	C	4356	4391	4389	145	0
1	D	4356	4391	4389	143	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	A	2	0	0	0	0
All	All	17546	17564	17556	549	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 16.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASP:OD1	1:B:389:THR:N	2.05	0.89
1:D:354:GLN:OE1	1:D:416:GLU:HG2	1.71	0.89
1:C:536:GLU:N	1:C:536:GLU:OE2	2.08	0.86
1:D:354:GLN:CD	1:D:416:GLU:HG3	2.03	0.83
1:D:388:ASP:OD1	1:D:389:THR:N	2.14	0.81
1:D:415:VAL:O	1:D:416:GLU:HG2	1.84	0.78
1:D:388:ASP:OD1	1:D:389:THR:OG1	2.00	0.77
1:D:416:GLU:HB2	1:D:417:PRO:HD3	1.65	0.77
1:D:536:GLU:OE2	1:D:536:GLU:N	2.18	0.77
1:D:367:ARG:NH1	1:D:383:ASP:OD2	2.20	0.75
1:D:415:VAL:O	1:D:416:GLU:CG	2.37	0.73
1:D:354:GLN:OE1	1:D:416:GLU:CG	2.36	0.73
1:A:561:GLN:O	1:B:579:ARG:NH1	2.22	0.72
1:C:397:GLU:OE2	1:C:710:LYS:NZ	2.20	0.72
1:C:396:LEU:HD21	1:C:422:LEU:HD21	1.71	0.72
1:B:396:LEU:HD21	1:B:422:LEU:HD21	1.72	0.71
1:B:388:ASP:OD1	1:B:389:THR:OG1	2.06	0.71
1:D:326:GLU:OE2	1:D:355:ARG:NH2	2.23	0.71
1:A:445:MET:HE2	1:A:445:MET:HA	1.72	0.71
1:A:355:ARG:NH1	1:A:365:LEU:O	2.25	0.70
1:B:745:ASP:OD1	1:B:746:GLU:N	2.25	0.70
1:D:354:GLN:CD	1:D:416:GLU:CG	2.64	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:GLN:O	1:D:579:ARG:NH1	2.25	0.69
1:A:396:LEU:HD21	1:A:422:LEU:HD21	1.74	0.69
1:A:465:LEU:HD21	1:A:475:VAL:HG21	1.75	0.69
1:B:355:ARG:NH1	1:B:365:LEU:O	2.25	0.69
1:D:396:LEU:HD21	1:D:422:LEU:HD21	1.75	0.69
1:A:367:ARG:NH1	1:A:383:ASP:OD2	2.26	0.69
1:B:397:GLU:OE2	1:B:710:LYS:NZ	2.21	0.68
1:C:355:ARG:NH1	1:C:365:LEU:O	2.26	0.68
1:C:465:LEU:HD21	1:C:475:VAL:HG21	1.76	0.68
1:C:445:MET:HE2	1:C:445:MET:HA	1.75	0.68
1:B:288:LEU:HD23	1:B:325:LEU:HD21	1.76	0.68
1:A:745:ASP:OD1	1:A:746:GLU:N	2.27	0.67
1:D:355:ARG:NH1	1:D:365:LEU:O	2.27	0.67
1:A:288:LEU:HD23	1:A:325:LEU:HD21	1.76	0.67
1:D:209:ILE:HD12	1:D:263:ILE:HD13	1.77	0.67
1:B:445:MET:HE2	1:B:445:MET:HA	1.77	0.67
1:D:208:ALA:HB1	1:D:216:LEU:HD22	1.77	0.67
1:B:208:ALA:HB1	1:B:216:LEU:HD22	1.76	0.66
1:C:288:LEU:HD23	1:C:325:LEU:HD21	1.77	0.66
1:C:498:GLN:OE1	1:C:499:ARG:N	2.28	0.66
1:C:523:MET:HE2	1:C:523:MET:HA	1.78	0.66
1:D:288:LEU:HD23	1:D:325:LEU:HD21	1.78	0.66
1:C:745:ASP:OD1	1:C:746:GLU:N	2.28	0.65
1:D:445:MET:HE2	1:D:445:MET:HA	1.79	0.65
1:C:700:GLN:O	1:C:703:ILE:HG22	1.96	0.65
1:A:288:LEU:HD12	1:A:309:TYR:CE2	2.33	0.64
1:A:267:LEU:O	1:A:267:LEU:HD23	1.98	0.63
1:D:267:LEU:O	1:D:267:LEU:HD23	1.97	0.63
1:B:295:ALA:CB	1:B:305:VAL:HG21	2.29	0.62
1:D:745:ASP:OD1	1:D:746:GLU:N	2.33	0.62
1:A:217:VAL:O	1:A:221:VAL:HG12	1.99	0.62
1:B:465:LEU:HD21	1:B:475:VAL:HG21	1.80	0.62
1:C:288:LEU:HD12	1:C:309:TYR:CE2	2.34	0.62
1:A:295:ALA:CB	1:A:305:VAL:HG21	2.30	0.62
1:B:536:GLU:OE2	1:B:536:GLU:N	2.32	0.62
1:C:295:ALA:CB	1:C:305:VAL:HG21	2.29	0.62
1:D:465:LEU:HD21	1:D:475:VAL:HG21	1.82	0.62
1:B:682:MET:HE1	1:C:676:ASN:HB2	1.81	0.62
1:C:214:MET:HE3	1:C:214:MET:O	2.00	0.62
1:C:401:TYR:CD1	1:C:703:ILE:HD11	2.35	0.62
1:C:460:LEU:HD23	1:C:461:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ARG:HB2	1:C:500:ARG:NH1	2.15	0.62
1:A:348:VAL:HG12	1:A:352:ILE:HD11	1.80	0.61
1:D:415:VAL:O	1:D:416:GLU:CD	2.44	0.61
1:C:267:LEU:HD23	1:C:267:LEU:O	2.00	0.61
1:B:288:LEU:HD12	1:B:309:TYR:CE2	2.35	0.61
1:A:208:ALA:HB1	1:A:216:LEU:HD22	1.82	0.61
1:D:295:ALA:CB	1:D:305:VAL:HG21	2.30	0.61
1:A:383:ASP:C	1:A:383:ASP:OD1	2.43	0.61
1:A:579:ARG:NH1	1:D:561:GLN:O	2.33	0.61
1:A:676:ASN:HB2	1:D:682:MET:HE1	1.82	0.61
1:C:208:ALA:HB1	1:C:216:LEU:HD22	1.82	0.61
1:B:217:VAL:O	1:B:221:VAL:HG12	2.01	0.61
1:C:401:TYR:CE1	1:C:703:ILE:HD11	2.36	0.61
1:D:416:GLU:HB2	1:D:417:PRO:CD	2.31	0.61
1:D:461:PRO:O	1:D:462:PRO:C	2.44	0.61
1:D:288:LEU:HD12	1:D:309:TYR:CE2	2.36	0.60
1:D:422:LEU:HD22	1:D:705:ILE:HG21	1.84	0.60
1:A:457:VAL:O	1:A:457:VAL:HG13	2.01	0.60
1:C:217:VAL:O	1:C:221:VAL:HG12	2.02	0.60
1:D:383:ASP:OD1	1:D:383:ASP:C	2.44	0.60
1:A:281:ASP:OD2	1:A:285:ASN:N	2.34	0.59
1:D:514:ILE:O	1:D:518:VAL:HG23	2.01	0.59
1:B:267:LEU:HD23	1:B:267:LEU:O	2.01	0.59
1:D:214:MET:O	1:D:218:THR:OG1	2.20	0.59
1:A:381:LEU:HD12	1:A:728:VAL:HG21	1.84	0.59
1:D:217:VAL:O	1:D:221:VAL:HG12	2.02	0.58
1:C:295:ALA:HB2	1:C:305:VAL:HG21	1.85	0.57
1:C:357:ILE:HG23	1:C:363:ARG:HG3	1.87	0.57
1:A:324:LYS:N	1:A:324:LYS:HD2	2.20	0.57
1:B:647:LEU:HD23	1:B:647:LEU:O	2.04	0.57
1:A:422:LEU:HD22	1:A:705:ILE:HG21	1.86	0.57
1:A:514:ILE:O	1:A:518:VAL:HG23	2.05	0.57
1:B:514:ILE:O	1:B:518:VAL:HG23	2.04	0.57
1:C:205:LEU:O	1:C:209:ILE:HD13	2.05	0.57
1:D:381:LEU:HD12	1:D:728:VAL:HG21	1.88	0.56
1:A:430:VAL:HG13	1:A:708:THR:HG21	1.88	0.56
1:C:324:LYS:HD2	1:C:324:LYS:N	2.20	0.56
1:A:499:ARG:NH2	1:A:509:ASP:OD2	2.37	0.56
1:C:205:LEU:HD21	1:C:225:ALA:HB1	1.88	0.56
1:D:205:LEU:HD21	1:D:225:ALA:HB1	1.88	0.56
1:A:523:MET:HE2	1:A:523:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:MET:HE1	1:D:572:MET:HE2	1.88	0.56
1:D:513:GLU:N	1:D:513:GLU:OE1	2.39	0.56
1:A:677:MET:CE	1:D:572:MET:HE2	2.36	0.55
1:B:381:LEU:HD12	1:B:728:VAL:HG21	1.89	0.55
1:A:205:LEU:HD21	1:A:225:ALA:HB1	1.88	0.55
1:A:666:TYR:CE1	1:A:670:THR:HG21	2.42	0.55
1:C:514:ILE:O	1:C:518:VAL:HG23	2.07	0.55
1:A:687:ASN:C	1:A:687:ASN:OD1	2.50	0.55
1:B:205:LEU:O	1:B:209:ILE:HD13	2.07	0.55
1:A:427:ASP:OD1	1:A:431:LYS:NZ	2.20	0.55
1:C:644:MET:HG3	1:C:644:MET:O	2.06	0.55
1:B:295:ALA:HB2	1:B:305:VAL:HG21	1.88	0.55
1:B:535:LYS:HG2	1:B:535:LYS:O	2.06	0.55
1:A:503:LEU:HD13	1:A:503:LEU:O	2.08	0.54
1:C:752:TRP:CH2	1:D:258:THR:HG23	2.42	0.54
1:A:205:LEU:O	1:A:209:ILE:HD13	2.08	0.54
1:A:295:ALA:HB2	1:A:305:VAL:HG21	1.89	0.54
1:C:405:GLU:N	1:C:405:GLU:OE1	2.40	0.54
1:B:205:LEU:HD21	1:B:225:ALA:HB1	1.90	0.54
1:B:383:ASP:OD1	1:B:385:SER:N	2.38	0.54
1:D:324:LYS:HD2	1:D:324:LYS:N	2.23	0.54
1:B:396:LEU:HD13	1:B:418:LEU:HD22	1.90	0.54
1:D:399:ILE:HD13	1:D:412:MET:HE2	1.89	0.54
1:B:357:ILE:HG23	1:B:363:ARG:HG3	1.90	0.53
1:C:647:LEU:HD23	1:C:647:LEU:O	2.08	0.53
1:D:425:LYS:NZ	1:D:709:GLU:OE1	2.35	0.53
1:D:647:LEU:HD23	1:D:647:LEU:O	2.07	0.53
1:B:324:LYS:HD2	1:B:324:LYS:N	2.23	0.53
1:D:354:GLN:CG	1:D:416:GLU:HG3	2.39	0.53
1:A:258:THR:HG23	1:D:752:TRP:CH2	2.43	0.53
1:C:227:VAL:HG23	1:C:228:GLN:OE1	2.08	0.53
1:C:422:LEU:HD22	1:C:705:ILE:HG21	1.91	0.53
1:D:461:PRO:CB	1:D:462:PRO:CD	2.87	0.53
1:A:496:PHE:HZ	1:A:514:ILE:HD13	1.74	0.53
1:D:357:ILE:HG23	1:D:363:ARG:HG3	1.91	0.53
1:D:369:PHE:HB3	1:D:728:VAL:HG11	1.90	0.53
1:D:246:TYR:O	1:D:246:TYR:CG	2.62	0.52
1:D:460:LEU:HD12	1:D:461:PRO:HD2	1.91	0.52
1:D:666:TYR:CE1	1:D:670:THR:HG21	2.44	0.52
1:D:227:VAL:HG23	1:D:228:GLN:OE1	2.09	0.52
1:B:509:ASP:OD1	1:B:509:ASP:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:ASP:OD1	1:B:733:ASP:C	2.53	0.52
1:D:503:LEU:HD13	1:D:503:LEU:O	2.09	0.52
1:A:214:MET:O	1:A:218:THR:OG1	2.27	0.52
1:B:254:LEU:C	1:B:254:LEU:HD13	2.34	0.52
1:B:326:GLU:O	1:B:326:GLU:HG2	2.08	0.52
1:C:381:LEU:HD12	1:C:728:VAL:HG21	1.92	0.52
1:B:415:VAL:HG12	1:B:416:GLU:N	2.24	0.52
1:B:422:LEU:HD22	1:B:705:ILE:HG21	1.91	0.52
1:B:424:ASP:C	1:B:424:ASP:OD1	2.53	0.52
1:C:254:LEU:HD13	1:C:254:LEU:C	2.34	0.52
1:A:381:LEU:HD13	1:A:726:LEU:HD13	1.92	0.52
1:C:214:MET:O	1:C:217:VAL:HG22	2.09	0.52
1:C:261:LEU:HD13	1:C:261:LEU:O	2.10	0.52
1:C:424:ASP:OD1	1:C:424:ASP:C	2.53	0.52
1:C:432:ARG:HG3	1:C:433:ILE:HD12	1.90	0.52
1:C:572:MET:HE2	1:D:677:MET:HE1	1.91	0.52
1:A:357:ILE:HG23	1:A:363:ARG:HG3	1.91	0.51
1:B:461:PRO:HB2	1:B:462:PRO:HD3	1.93	0.51
1:C:348:VAL:O	1:C:352:ILE:HG12	2.09	0.51
1:C:430:VAL:HG13	1:C:708:THR:HG21	1.93	0.51
1:D:311:GLU:OE1	1:D:315:LEU:HD11	2.10	0.51
1:B:261:LEU:HD13	1:B:261:LEU:O	2.10	0.51
1:D:399:ILE:HD13	1:D:412:MET:CE	2.40	0.51
1:A:227:VAL:HG23	1:A:228:GLN:OE1	2.10	0.51
1:B:288:LEU:CD2	1:B:325:LEU:HD21	2.40	0.51
1:C:733:ASP:C	1:C:733:ASP:OD1	2.53	0.51
1:B:246:TYR:O	1:B:246:TYR:CG	2.64	0.51
1:D:523:MET:O	1:D:527:VAL:HG23	2.10	0.51
1:C:568:MET:HE1	1:D:681:LEU:HD21	1.93	0.51
1:C:666:TYR:CE1	1:C:670:THR:HG21	2.45	0.51
1:D:415:VAL:O	1:D:416:GLU:OE2	2.29	0.51
1:D:348:VAL:O	1:D:352:ILE:HG12	2.11	0.51
1:A:369:PHE:HB3	1:A:728:VAL:HG11	1.92	0.51
1:B:214:MET:O	1:B:217:VAL:HG22	2.11	0.51
1:B:500:ARG:HB2	1:B:500:ARG:CZ	2.41	0.51
1:C:722:SER:OG	1:C:723:GLY:N	2.44	0.51
1:D:733:ASP:OD1	1:D:733:ASP:C	2.53	0.51
1:B:348:VAL:O	1:B:352:ILE:HG12	2.11	0.51
1:B:666:TYR:CE1	1:B:670:THR:HG21	2.46	0.51
1:B:387:ILE:HD11	1:B:418:LEU:HD21	1.93	0.50
1:C:357:ILE:HG22	1:C:366:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:TRP:CD1	1:A:431:LYS:HZ3	2.28	0.50
1:C:415:VAL:HG12	1:C:416:GLU:N	2.25	0.50
1:D:295:ALA:HB2	1:D:305:VAL:HG21	1.92	0.50
1:C:460:LEU:HD23	1:C:461:PRO:CG	2.40	0.50
1:A:499:ARG:HD2	1:A:499:ARG:C	2.37	0.50
1:A:722:SER:OG	1:A:723:GLY:N	2.43	0.50
1:B:371:GLU:O	1:B:372:TRP:C	2.55	0.50
1:B:752:TRP:CH2	1:C:258:THR:HG23	2.47	0.50
1:D:252:LEU:HD21	1:D:268:LEU:HD11	1.93	0.50
1:D:261:LEU:HD13	1:D:261:LEU:O	2.11	0.50
1:D:722:SER:OG	1:D:723:GLY:N	2.44	0.50
1:A:461:PRO:CB	1:A:462:PRO:CD	2.89	0.50
1:C:384:LEU:O	1:C:384:LEU:HG	2.10	0.50
1:D:384:LEU:HG	1:D:384:LEU:O	2.12	0.50
1:A:383:ASP:OD1	1:A:385:SER:N	2.44	0.50
1:A:384:LEU:HG	1:A:384:LEU:O	2.11	0.50
1:B:384:LEU:HD12	1:B:387:ILE:HG22	1.94	0.50
1:C:371:GLU:O	1:C:372:TRP:C	2.54	0.50
1:A:572:MET:HE2	1:B:677:MET:SD	2.52	0.49
1:B:283:VAL:HG23	1:B:285:ASN:OD1	2.11	0.49
1:C:461:PRO:HG3	1:C:534:ARG:N	2.28	0.49
1:A:682:MET:O	1:A:686:VAL:HG23	2.12	0.49
1:B:208:ALA:HB1	1:B:216:LEU:CD2	2.42	0.49
1:B:357:ILE:HG22	1:B:366:SER:HB2	1.93	0.49
1:C:428:ARG:HH11	1:C:428:ARG:HG3	1.77	0.49
1:B:722:SER:OG	1:B:723:GLY:N	2.44	0.49
1:D:430:VAL:HG12	1:D:430:VAL:O	2.12	0.49
1:B:399:ILE:HD13	1:B:412:MET:HE2	1.94	0.49
1:D:487:TYR:CD1	1:D:487:TYR:C	2.90	0.49
1:B:416:GLU:HB3	1:B:417:PRO:HD3	1.94	0.49
1:C:311:GLU:OE1	1:C:315:LEU:HD11	2.12	0.49
1:D:415:VAL:HG12	1:D:416:GLU:N	2.28	0.49
1:A:368:LYS:NZ	1:A:368:LYS:HB2	2.28	0.49
1:B:286:THR:OG1	1:B:287:VAL:N	2.46	0.49
1:B:381:LEU:HD13	1:B:726:LEU:HD13	1.95	0.49
1:C:461:PRO:HB2	1:C:462:PRO:HD3	1.94	0.49
1:A:351:TYR:CD1	1:A:351:TYR:C	2.91	0.48
1:A:682:MET:HE1	1:B:676:ASN:HB2	1.95	0.48
1:B:291:LEU:O	1:B:291:LEU:HD23	2.13	0.48
1:C:561:GLN:OE1	1:C:561:GLN:HA	2.11	0.48
1:D:430:VAL:HG13	1:D:708:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:PRO:HB2	1:A:462:PRO:HD2	1.95	0.48
1:C:233:GLY:O	1:C:237:LYS:N	2.46	0.48
1:D:209:ILE:HD12	1:D:263:ILE:HG21	1.95	0.48
1:B:478:GLU:O	1:B:482:VAL:HG23	2.13	0.48
1:C:416:GLU:HB3	1:C:417:PRO:HD3	1.96	0.48
1:D:432:ARG:HG3	1:D:433:ILE:HD12	1.94	0.48
1:B:416:GLU:CB	1:B:417:PRO:HD3	2.44	0.48
1:C:498:GLN:OE1	1:C:499:ARG:HB2	2.12	0.48
1:C:535:LYS:O	1:C:535:LYS:HG2	2.14	0.48
1:C:246:TYR:CG	1:C:246:TYR:O	2.64	0.48
1:C:252:LEU:HD21	1:C:268:LEU:HD11	1.96	0.48
1:A:651:GLU:C	1:A:651:GLU:OE2	2.57	0.48
1:D:288:LEU:CD2	1:D:325:LEU:HD21	2.43	0.48
1:D:381:LEU:HD13	1:D:726:LEU:HD13	1.95	0.48
1:D:524:LEU:O	1:D:528:VAL:HG23	2.14	0.48
1:A:288:LEU:CD2	1:A:325:LEU:HD21	2.41	0.48
1:B:365:LEU:O	1:B:365:LEU:HD12	2.14	0.48
1:D:208:ALA:HB1	1:D:216:LEU:CD2	2.44	0.48
1:A:233:GLY:O	1:A:236:PHE:N	2.47	0.48
1:A:286:THR:OG1	1:A:287:VAL:N	2.47	0.48
1:B:365:LEU:O	1:B:365:LEU:CD1	2.62	0.48
1:C:288:LEU:CD2	1:C:325:LEU:HD21	2.42	0.48
1:C:383:ASP:C	1:C:383:ASP:OD1	2.56	0.48
1:B:384:LEU:O	1:B:384:LEU:HG	2.13	0.47
1:A:348:VAL:HG12	1:A:352:ILE:CD1	2.43	0.47
1:A:498:GLN:OE1	1:A:499:ARG:N	2.46	0.47
1:C:313:LEU:O	1:C:313:LEU:HD12	2.13	0.47
1:C:401:TYR:HE2	1:C:710:LYS:HZ1	1.63	0.47
1:C:478:GLU:O	1:C:482:VAL:HG23	2.14	0.47
1:A:457:VAL:HG21	1:B:600:GLU:OE1	2.13	0.47
1:A:478:GLU:O	1:A:482:VAL:HG23	2.14	0.47
1:B:214:MET:SD	1:B:218:THR:OG1	2.72	0.47
1:B:430:VAL:HG12	1:B:430:VAL:O	2.14	0.47
1:C:293:GLU:O	1:C:293:GLU:OE2	2.32	0.47
1:C:564:ILE:HD12	1:C:694:LYS:HA	1.96	0.47
1:D:233:GLY:O	1:D:237:LYS:N	2.48	0.47
1:A:430:VAL:HG12	1:A:430:VAL:O	2.13	0.47
1:A:468:THR:HG22	1:A:469:VAL:N	2.29	0.47
1:A:498:GLN:OE1	1:A:499:ARG:HB2	2.15	0.47
1:B:369:PHE:HB3	1:B:728:VAL:HG11	1.96	0.47
1:C:430:VAL:HG12	1:C:430:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:MET:HE1	1:D:676:ASN:HB2	1.95	0.47
1:D:648:GLU:O	1:D:648:GLU:HG3	2.14	0.47
1:A:261:LEU:HD13	1:A:261:LEU:O	2.13	0.47
1:A:415:VAL:O	1:A:416:GLU:HG2	2.15	0.47
1:B:369:PHE:CD1	1:B:369:PHE:N	2.83	0.47
1:B:560:GLN:HG2	1:B:697:TRP:CH2	2.50	0.47
1:B:682:MET:O	1:B:686:VAL:HG23	2.15	0.47
1:D:286:THR:OG1	1:D:287:VAL:N	2.45	0.47
1:D:561:GLN:HA	1:D:561:GLN:OE1	2.15	0.47
1:B:430:VAL:HG13	1:B:708:THR:HG21	1.95	0.47
1:A:291:LEU:HD23	1:A:291:LEU:O	2.14	0.47
1:B:308:MET:O	1:B:309:TYR:C	2.58	0.47
1:A:752:TRP:CH2	1:B:258:THR:HG23	2.50	0.47
1:B:329:THR:HG22	1:B:330:ASN:N	2.30	0.47
1:B:600:GLU:O	1:B:600:GLU:OE2	2.33	0.47
1:A:252:LEU:HD21	1:A:268:LEU:HD11	1.98	0.46
1:A:401:TYR:CE1	1:A:703:ILE:HD13	2.51	0.46
1:A:436:PHE:O	1:A:440:VAL:HG23	2.16	0.46
1:A:460:LEU:HD12	1:A:461:PRO:HD2	1.97	0.46
1:A:570:GLU:O	1:A:573:ILE:HG22	2.14	0.46
1:A:651:GLU:OE2	1:A:651:GLU:O	2.33	0.46
1:B:233:GLY:O	1:B:237:LYS:N	2.48	0.46
1:B:511:TYR:CE2	1:B:570:GLU:OE2	2.68	0.46
1:D:291:LEU:HD23	1:D:291:LEU:O	2.14	0.46
1:D:566:ALA:O	1:D:569:ILE:HG22	2.15	0.46
1:B:252:LEU:HD21	1:B:268:LEU:HD11	1.98	0.46
1:C:369:PHE:HB3	1:C:728:VAL:HG11	1.96	0.46
1:D:281:ASP:OD1	1:D:282:SER:N	2.48	0.46
1:A:461:PRO:HB2	1:A:462:PRO:CD	2.45	0.46
1:B:751:THR:HG22	1:B:753:ASN:OD1	2.16	0.46
1:C:327:GLU:O	1:C:327:GLU:OE2	2.32	0.46
1:C:416:GLU:CB	1:C:417:PRO:HD3	2.45	0.46
1:D:368:LYS:O	1:D:368:LYS:HG2	2.15	0.46
1:D:751:THR:HG22	1:D:753:ASN:OD1	2.15	0.46
1:B:496:PHE:HZ	1:B:514:ILE:HD13	1.81	0.46
1:C:363:ARG:O	1:C:363:ARG:HG2	2.16	0.46
1:C:580:PHE:CD1	1:C:580:PHE:C	2.94	0.46
1:D:600:GLU:OE1	1:D:600:GLU:O	2.33	0.46
1:D:682:MET:O	1:D:686:VAL:HG23	2.16	0.46
1:A:363:ARG:O	1:A:363:ARG:HG2	2.16	0.46
1:B:254:LEU:HD13	1:B:254:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:GLN:OE1	1:D:499:ARG:HB2	2.15	0.46
1:B:457:VAL:HG11	1:C:600:GLU:OE1	2.16	0.46
1:D:369:PHE:N	1:D:369:PHE:CD1	2.82	0.46
1:D:564:ILE:HD12	1:D:694:LYS:HA	1.98	0.46
1:A:564:ILE:HD12	1:A:694:LYS:HA	1.98	0.46
1:A:600:GLU:OE2	1:A:600:GLU:O	2.33	0.46
1:C:359:GLU:OE2	1:C:359:GLU:O	2.33	0.46
1:C:651:GLU:O	1:C:651:GLU:OE2	2.33	0.46
1:D:564:ILE:HG23	1:D:693:SER:OG	2.15	0.46
1:B:233:GLY:O	1:B:236:PHE:N	2.48	0.46
1:C:308:MET:O	1:C:309:TYR:C	2.59	0.46
1:C:600:GLU:OE2	1:C:600:GLU:HA	2.16	0.46
1:D:198:TYR:O	1:D:202:GLN:OE1	2.34	0.46
1:B:344:GLY:O	1:B:345:LYS:HD2	2.15	0.46
1:C:751:THR:HG22	1:C:753:ASN:OD1	2.15	0.46
1:A:564:ILE:HG23	1:A:693:SER:OG	2.16	0.46
1:D:397:GLU:C	1:D:397:GLU:OE2	2.59	0.46
1:A:676:ASN:CB	1:D:682:MET:HE1	2.46	0.45
1:B:209:ILE:HG23	1:B:263:ILE:HD13	1.97	0.45
1:D:360:PRO:O	1:D:361:GLU:C	2.59	0.45
1:D:461:PRO:HB3	1:D:462:PRO:HD3	1.99	0.45
1:C:291:LEU:HD23	1:C:291:LEU:O	2.16	0.45
1:A:329:THR:HG22	1:A:330:ASN:N	2.32	0.45
1:B:227:VAL:HG23	1:B:228:GLN:OE1	2.16	0.45
1:B:436:PHE:O	1:B:440:VAL:HG23	2.16	0.45
1:C:570:GLU:O	1:C:573:ILE:HG22	2.15	0.45
1:B:311:GLU:OE1	1:B:315:LEU:HD11	2.17	0.45
1:C:369:PHE:N	1:C:369:PHE:CD1	2.81	0.45
1:A:487:TYR:CD1	1:A:487:TYR:C	2.94	0.45
1:A:751:THR:HG22	1:A:753:ASN:OD1	2.16	0.45
1:B:566:ALA:O	1:B:569:ILE:HG22	2.17	0.45
1:B:687:ASN:OD1	1:B:687:ASN:C	2.60	0.45
1:C:280:ARG:HG3	1:C:280:ARG:HH11	1.82	0.45
1:D:363:ARG:HG2	1:D:363:ARG:O	2.17	0.45
1:B:439:PHE:CD1	1:B:439:PHE:C	2.94	0.45
1:D:266:PHE:O	1:D:270:ASN:N	2.48	0.45
1:A:233:GLY:O	1:A:237:LYS:N	2.50	0.45
1:A:577:LEU:HD22	1:B:673:LEU:HD13	1.99	0.45
1:B:288:LEU:HD12	1:B:309:TYR:CZ	2.51	0.45
1:D:651:GLU:OE2	1:D:651:GLU:O	2.34	0.45
1:A:344:GLY:O	1:A:345:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:HIS:HB2	1:B:359:GLU:OE2	2.17	0.45
1:B:395:VAL:O	1:B:399:ILE:HG13	2.17	0.45
1:B:523:MET:HE3	1:B:523:MET:O	2.17	0.45
1:A:363:ARG:HH11	1:A:363:ARG:HB3	1.82	0.45
1:B:368:LYS:HG2	1:B:368:LYS:O	2.17	0.45
1:C:274:PRO:O	1:C:275:ALA:C	2.60	0.45
1:D:535:LYS:O	1:D:535:LYS:CG	2.65	0.45
1:A:360:PRO:O	1:A:361:GLU:C	2.58	0.45
1:C:286:THR:OG1	1:C:287:VAL:N	2.47	0.45
1:C:436:PHE:O	1:C:440:VAL:HG23	2.17	0.45
1:D:498:GLN:OE1	1:D:499:ARG:N	2.50	0.45
1:A:461:PRO:O	1:A:462:PRO:C	2.60	0.44
1:B:250:LEU:H	1:B:250:LEU:HD22	1.80	0.44
1:B:337:LEU:O	1:B:338:ALA:C	2.60	0.44
1:B:572:MET:HE2	1:C:677:MET:HE1	1.99	0.44
1:C:677:MET:HE2	1:C:677:MET:HB2	1.84	0.44
1:D:358:HIS:C	1:D:359:GLU:OE2	2.59	0.44
1:A:351:TYR:CE1	1:A:355:ARG:HD3	2.52	0.44
1:B:564:ILE:HG23	1:B:693:SER:OG	2.17	0.44
1:A:281:ASP:OD1	1:A:282:SER:N	2.50	0.44
1:C:381:LEU:HD13	1:C:726:LEU:HD13	1.99	0.44
1:A:378:HIS:O	1:A:378:HIS:CD2	2.71	0.44
1:B:425:LYS:NZ	1:B:709:GLU:OE2	2.47	0.44
1:C:386:CYS:HA	1:C:391:GLU:OE2	2.18	0.44
1:C:396:LEU:HD21	1:C:422:LEU:CD2	2.44	0.44
1:D:383:ASP:OD1	1:D:385:SER:N	2.51	0.44
1:C:505:SER:O	1:C:506:LEU:C	2.60	0.44
1:D:651:GLU:OE2	1:D:651:GLU:C	2.61	0.44
1:A:369:PHE:CD1	1:A:369:PHE:N	2.82	0.44
1:C:288:LEU:HD12	1:C:309:TYR:CZ	2.51	0.44
1:C:525:VAL:O	1:C:528:VAL:HG12	2.18	0.44
1:D:371:GLU:O	1:D:372:TRP:C	2.61	0.44
1:D:396:LEU:HD21	1:D:422:LEU:CD2	2.46	0.44
1:B:274:PRO:O	1:B:275:ALA:C	2.61	0.44
1:C:254:LEU:HD13	1:C:254:LEU:O	2.18	0.44
1:C:498:GLN:CD	1:C:498:GLN:C	2.85	0.44
1:D:436:PHE:O	1:D:440:VAL:HG23	2.17	0.44
1:D:478:GLU:O	1:D:482:VAL:HG23	2.17	0.44
1:D:496:PHE:HZ	1:D:514:ILE:HD13	1.81	0.44
1:A:415:VAL:HG12	1:A:416:GLU:N	2.33	0.44
1:A:566:ALA:O	1:A:569:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:HG12	1:A:285:ASN:OD1	2.18	0.43
1:A:677:MET:HE2	1:A:677:MET:HB2	1.85	0.43
1:A:712:PHE:N	1:A:712:PHE:CD1	2.86	0.43
1:B:363:ARG:HB3	1:B:363:ARG:HH11	1.82	0.43
1:C:505:SER:O	1:C:509:ASP:OD1	2.36	0.43
1:C:566:ALA:O	1:C:569:ILE:HG22	2.17	0.43
1:D:274:PRO:O	1:D:275:ALA:C	2.60	0.43
1:A:246:TYR:CG	1:A:246:TYR:O	2.70	0.43
1:B:386:CYS:HA	1:B:390:CYS:SG	2.58	0.43
1:B:416:GLU:CB	1:B:417:PRO:CD	2.96	0.43
1:C:209:ILE:O	1:C:210:GLU:C	2.61	0.43
1:C:371:GLU:OE1	1:C:372:TRP:CD1	2.71	0.43
1:D:329:THR:HG22	1:D:330:ASN:N	2.33	0.43
1:D:369:PHE:HD2	1:D:728:VAL:HB	1.83	0.43
1:A:208:ALA:HB1	1:A:216:LEU:CD2	2.46	0.43
1:A:288:LEU:HD12	1:A:309:TYR:CZ	2.53	0.43
1:C:351:TYR:CD1	1:C:351:TYR:C	2.94	0.43
1:D:710:LYS:O	1:D:713:LEU:N	2.47	0.43
1:B:364:HIS:HB3	1:B:730:PHE:O	2.19	0.43
1:D:308:MET:O	1:D:309:TYR:C	2.60	0.43
1:A:371:GLU:HG2	1:A:372:TRP:H	1.83	0.43
1:B:401:TYR:CE1	1:B:703:ILE:HD13	2.54	0.43
1:B:461:PRO:HG3	1:B:534:ARG:N	2.32	0.43
1:A:384:LEU:O	1:A:384:LEU:CG	2.66	0.43
1:A:710:LYS:O	1:A:713:LEU:N	2.46	0.43
1:B:487:TYR:C	1:B:487:TYR:CD1	2.94	0.43
1:A:525:VAL:O	1:A:528:VAL:HG12	2.18	0.43
1:A:647:LEU:HD23	1:A:647:LEU:O	2.19	0.43
1:B:329:THR:HG22	1:B:330:ASN:H	1.82	0.43
1:B:564:ILE:HD12	1:B:694:LYS:HA	1.99	0.43
1:C:329:THR:HG22	1:C:330:ASN:N	2.34	0.43
1:D:313:LEU:O	1:D:313:LEU:HD23	2.18	0.43
1:A:310:ASN:O	1:A:314:ILE:HG12	2.19	0.43
1:C:209:ILE:HG23	1:C:263:ILE:HD13	2.00	0.43
1:C:378:HIS:ND1	1:C:378:HIS:N	2.66	0.43
1:C:384:LEU:O	1:C:384:LEU:CG	2.65	0.43
1:C:468:THR:OG1	1:C:469:VAL:N	2.52	0.43
1:C:214:MET:O	1:C:217:VAL:CG2	2.67	0.43
1:C:358:HIS:O	1:C:359:GLU:HG3	2.18	0.43
1:D:288:LEU:HD12	1:D:309:TYR:CZ	2.53	0.43
1:A:389:THR:O	1:A:390:CYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ALA:HB1	1:C:216:LEU:CD2	2.47	0.42
1:A:371:GLU:O	1:A:372:TRP:C	2.62	0.42
1:A:416:GLU:HB2	1:A:417:PRO:HD3	2.01	0.42
1:A:518:VAL:HG12	1:A:547:MET:HE1	2.01	0.42
1:B:378:HIS:ND1	1:B:378:HIS:N	2.67	0.42
1:B:701:ARG:HA	1:B:704:THR:HG22	2.02	0.42
1:C:242:ARG:HE	1:C:243:PRO:HD2	1.84	0.42
1:A:274:PRO:O	1:A:275:ALA:C	2.61	0.42
1:D:677:MET:HE2	1:D:677:MET:HB2	1.90	0.42
1:A:396:LEU:HD21	1:A:422:LEU:CD2	2.46	0.42
1:D:384:LEU:O	1:D:384:LEU:CG	2.68	0.42
1:D:384:LEU:HD12	1:D:387:ILE:HG22	2.01	0.42
1:A:357:ILE:HG22	1:A:366:SER:HB2	2.01	0.42
1:A:378:HIS:O	1:A:378:HIS:HD2	2.02	0.42
1:B:209:ILE:O	1:B:210:GLU:C	2.61	0.42
1:B:313:LEU:HD11	1:B:365:LEU:HD22	2.02	0.42
1:C:389:THR:O	1:C:390:CYS:HB3	2.19	0.42
1:C:682:MET:O	1:C:686:VAL:HG23	2.19	0.42
1:D:281:ASP:OD2	1:D:285:ASN:N	2.52	0.42
1:D:357:ILE:HG22	1:D:366:SER:HB2	2.01	0.42
1:D:399:ILE:CD1	1:D:412:MET:HE2	2.49	0.42
1:A:304:PHE:CD1	1:A:304:PHE:C	2.95	0.42
1:B:359:GLU:O	1:B:361:GLU:N	2.52	0.42
1:C:358:HIS:O	1:C:359:GLU:CG	2.68	0.42
1:D:570:GLU:O	1:D:573:ILE:HG22	2.19	0.42
1:D:580:PHE:CD1	1:D:580:PHE:C	2.97	0.42
1:B:242:ARG:HE	1:B:243:PRO:HD2	1.84	0.42
1:B:360:PRO:O	1:B:361:GLU:C	2.61	0.42
1:C:368:LYS:O	1:C:368:LYS:HG2	2.19	0.42
1:C:403:SER:O	1:C:409:ARG:NH1	2.52	0.42
1:C:487:TYR:CD1	1:C:487:TYR:C	2.96	0.42
1:C:651:GLU:OE2	1:C:651:GLU:C	2.63	0.42
1:C:703:ILE:HD12	1:C:703:ILE:HA	1.91	0.42
1:A:424:ASP:OD1	1:A:424:ASP:C	2.62	0.42
1:B:505:SER:O	1:B:506:LEU:C	2.62	0.42
1:D:242:ARG:HE	1:D:243:PRO:HD2	1.84	0.42
1:A:242:ARG:HE	1:A:243:PRO:HD2	1.85	0.42
1:A:311:GLU:OE1	1:A:315:LEU:HD11	2.20	0.42
1:B:384:LEU:HD11	1:B:388:ASP:OD2	2.20	0.42
1:C:687:ASN:OD1	1:C:687:ASN:C	2.62	0.42
1:A:209:ILE:O	1:A:210:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:HIS:CD2	1:A:365:LEU:N	2.88	0.42
1:B:513:GLU:OE2	1:B:513:GLU:HA	2.20	0.42
1:B:570:GLU:O	1:B:573:ILE:HG22	2.20	0.42
1:D:386:CYS:HA	1:D:390:CYS:SG	2.59	0.42
1:A:285:ASN:N	1:A:285:ASN:OD1	2.52	0.41
1:A:326:GLU:OE2	1:A:355:ARG:NH2	2.52	0.41
1:C:416:GLU:CB	1:C:417:PRO:CD	2.98	0.41
1:C:496:PHE:HZ	1:C:514:ILE:HD13	1.85	0.41
1:C:590:GLY:O	1:C:593:THR:HG22	2.20	0.41
1:D:365:LEU:O	1:D:365:LEU:CD1	2.68	0.41
1:B:351:TYR:CZ	1:B:355:ARG:HD3	2.55	0.41
1:B:461:PRO:HG2	1:B:533:GLN:HA	2.01	0.41
1:C:217:VAL:O	1:C:218:THR:C	2.63	0.41
1:C:266:PHE:O	1:C:270:ASN:N	2.52	0.41
1:A:416:GLU:CB	1:A:417:PRO:CD	2.99	0.41
1:C:367:ARG:NH1	1:C:383:ASP:OD2	2.53	0.41
1:C:453:TYR:CD1	1:C:453:TYR:C	2.99	0.41
1:C:572:MET:HE2	1:D:677:MET:CE	2.50	0.41
1:D:498:GLN:C	1:D:498:GLN:CD	2.88	0.41
1:A:390:CYS:O	1:A:391:GLU:HB2	2.21	0.41
1:B:327:GLU:CD	1:B:327:GLU:O	2.63	0.41
1:C:503:LEU:O	1:C:503:LEU:HD13	2.19	0.41
1:D:313:LEU:HD22	1:D:365:LEU:HD22	2.02	0.41
1:D:571:LYS:CA	1:D:571:LYS:HE2	2.50	0.41
1:A:359:GLU:O	1:A:361:GLU:N	2.53	0.41
1:B:572:MET:HE2	1:C:677:MET:CE	2.51	0.41
1:D:590:GLY:O	1:D:593:THR:HG22	2.20	0.41
1:A:399:ILE:HD13	1:A:412:MET:HE2	2.02	0.41
1:A:600:GLU:OE2	1:A:600:GLU:C	2.64	0.41
1:B:559:PHE:CD1	1:B:559:PHE:N	2.87	0.41
1:C:390:CYS:SG	1:C:391:GLU:OE2	2.76	0.41
1:D:268:LEU:O	1:D:274:PRO:HB3	2.19	0.41
1:A:302:THR:O	1:A:306:THR:OG1	2.31	0.41
1:A:416:GLU:CB	1:A:417:PRO:HD3	2.51	0.41
1:B:572:MET:HE3	1:B:682:MET:HG2	2.02	0.41
1:A:369:PHE:HD2	1:A:728:VAL:HB	1.84	0.41
1:A:644:MET:O	1:A:644:MET:CG	2.69	0.41
1:B:536:GLU:N	1:B:536:GLU:CD	2.78	0.41
1:C:299:VAL:HG23	1:C:300:ASP:N	2.35	0.41
1:C:327:GLU:OE2	1:C:327:GLU:C	2.64	0.41
1:D:378:HIS:HD2	1:D:378:HIS:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLY:O	1:A:334:LEU:HD12	2.21	0.41
1:A:535:LYS:O	1:A:535:LYS:CG	2.68	0.41
1:A:687:ASN:OD1	1:A:688:LYS:N	2.54	0.41
1:B:396:LEU:HD21	1:B:422:LEU:CD2	2.47	0.41
1:B:460:LEU:HD23	1:B:461:PRO:CG	2.51	0.41
1:B:468:THR:OG1	1:B:469:VAL:N	2.53	0.41
1:B:653:TYR:CE1	1:B:656:LYS:HA	2.55	0.41
1:D:351:TYR:CZ	1:D:355:ARG:HD3	2.55	0.41
1:B:266:PHE:O	1:B:270:ASN:N	2.53	0.41
1:B:363:ARG:O	1:B:363:ARG:HG2	2.20	0.41
1:B:590:GLY:O	1:B:593:THR:HG22	2.21	0.41
1:D:218:THR:H	1:D:218:THR:HG1	1.59	0.41
1:A:198:TYR:O	1:A:202:GLN:OE1	2.38	0.40
1:B:384:LEU:O	1:B:384:LEU:CG	2.69	0.40
1:A:308:MET:O	1:A:309:TYR:C	2.63	0.40
1:A:511:TYR:HD2	1:A:570:GLU:CG	2.34	0.40
1:A:562:MET:HE2	1:A:562:MET:HB3	1.87	0.40
1:D:337:LEU:HD23	1:D:337:LEU:HA	1.94	0.40
1:D:701:ARG:HA	1:D:704:THR:HG22	2.02	0.40
1:A:327:GLU:C	1:A:327:GLU:CD	2.89	0.40
1:C:261:LEU:HD11	1:C:311:GLU:OE2	2.21	0.40
1:C:364:HIS:CE1	1:C:732:PRO:HD2	2.55	0.40
1:C:374:TYR:O	1:C:377:VAL:HG22	2.22	0.40
1:C:457:VAL:O	1:C:457:VAL:HG22	2.20	0.40
1:D:461:PRO:HB3	1:D:462:PRO:CD	2.50	0.40
1:D:715:CYS:C	1:D:716:MET:SD	3.04	0.40
1:A:270:ASN:O	1:A:271:SER:C	2.64	0.40
1:A:752:TRP:HH2	1:B:258:THR:HG23	1.87	0.40
1:D:600:GLU:OE1	1:D:600:GLU:C	2.64	0.40
1:A:408:ASN:O	1:A:412:MET:HG3	2.22	0.40
1:A:499:ARG:HD2	1:A:499:ARG:O	2.22	0.40
1:A:590:GLY:O	1:A:593:THR:HG22	2.21	0.40
1:C:204:ALA:O	1:C:208:ALA:HB2	2.22	0.40
1:C:326:GLU:OE1	1:C:355:ARG:NH2	2.55	0.40
1:C:351:TYR:CZ	1:C:355:ARG:HD3	2.56	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	533/1252 (43%)	486 (91%)	42 (8%)	5 (1%)	14	35
1	B	533/1252 (43%)	483 (91%)	48 (9%)	2 (0%)	30	55
1	C	533/1252 (43%)	491 (92%)	38 (7%)	4 (1%)	16	38
1	D	533/1252 (43%)	490 (92%)	38 (7%)	5 (1%)	14	35
All	All	2132/5008 (43%)	1950 (92%)	166 (8%)	16 (1%)	19	38

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	PRO
1	D	461	PRO
1	A	416	GLU
1	B	416	GLU
1	C	416	GLU
1	D	416	GLU
1	D	462	PRO
1	A	391	GLU
1	A	458	GLU
1	B	461	PRO
1	C	461	PRO
1	D	458	GLU
1	C	391	GLU
1	C	458	GLU
1	A	372	TRP
1	D	391	GLU

### 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	474/1074 (44%)	445 (94%)	29 (6%)	15	36
1	B	474/1074 (44%)	448 (94%)	26 (6%)	18	41
1	C	474/1074 (44%)	446 (94%)	28 (6%)	16	38
1	D	474/1074 (44%)	441 (93%)	33 (7%)	12	31
All	All	1896/4296 (44%)	1780 (94%)	116 (6%)	18	36

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LYS
1	A	202	GLN
1	A	218	THR
1	A	220	LEU
1	A	237	LYS
1	A	238	LYS
1	A	245	PHE
1	A	253	SER
1	A	254	LEU
1	A	261	LEU
1	A	282	SER
1	A	330	ASN
1	A	334	LEU
1	A	363	ARG
1	A	378	HIS
1	A	392	LYS
1	A	394	SER
1	A	414	LEU
1	A	447	ILE
1	A	461	PRO
1	A	464	LYS
1	A	506	LEU
1	A	508	VAL
1	A	510	SER
1	A	524	LEU
1	A	647	LEU
1	A	700	GLN
1	A	703	ILE
1	A	710	LYS
1	B	200	LYS

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Mol	Chain	Res	Type
1	B	218	THR
1	B	220	LEU
1	B	237	LYS
1	B	238	LYS
1	B	253	SER
1	B	261	LEU
1	B	269	GLN
1	B	282	SER
1	B	334	LEU
1	B	363	ARG
1	B	371	GLU
1	B	392	LYS
1	B	410	HIS
1	B	416	GLU
1	B	424	ASP
1	B	445	MET
1	B	460	LEU
1	B	471	ASP
1	B	506	LEU
1	B	510	SER
1	B	629	SER
1	B	647	LEU
1	B	648	GLU
1	B	677	MET
1	B	703	ILE
1	C	200	LYS
1	C	202	GLN
1	C	220	LEU
1	C	237	LYS
1	C	238	LYS
1	C	253	SER
1	C	261	LEU
1	C	269	GLN
1	C	282	SER
1	C	330	ASN
1	C	334	LEU
1	C	337	LEU
1	C	364	HIS
1	C	366	SER
1	C	384	LEU
1	C	392	LYS
1	C	416	GLU

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Mol	Chain	Res	Type
1	C	424	ASP
1	C	457	VAL
1	C	460	LEU
1	C	464	LYS
1	C	471	ASP
1	C	506	LEU
1	C	510	SER
1	C	513	GLU
1	C	642	ILE
1	C	647	LEU
1	C	677	MET
1	D	202	GLN
1	D	218	THR
1	D	220	LEU
1	D	237	LYS
1	D	238	LYS
1	D	245	PHE
1	D	253	SER
1	D	254	LEU
1	D	261	LEU
1	D	269	GLN
1	D	281	ASP
1	D	282	SER
1	D	313	LEU
1	D	322	THR
1	D	330	ASN
1	D	334	LEU
1	D	366	SER
1	D	378	HIS
1	D	384	LEU
1	D	392	LYS
1	D	410	HIS
1	D	427	ASP
1	D	431	LYS
1	D	445	MET
1	D	457	VAL
1	D	461	PRO
1	D	462	PRO
1	D	493	ILE
1	D	506	LEU
1	D	510	SER
1	D	552	MET

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Mol	Chain	Res	Type
1	D	647	LEU
1	D	677	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	364	HIS
1	A	378	HIS
1	A	560	GLN
1	B	467	ASN
1	C	364	HIS
1	C	467	ASN
1	C	560	GLN
1	D	301	ASN
1	D	364	HIS
1	D	378	HIS
1	D	419	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1D6R	D	901	-	29,33,33	2.06	5 (17%)	37,48,48	2.14	11 (29%)
2	A1D6R	B	901	-	29,33,33	2.07	5 (17%)	37,48,48	2.15	10 (27%)
2	A1D6R	A	901	-	29,33,33	2.07	5 (17%)	37,48,48	2.13	11 (29%)
2	A1D6R	C	901	-	29,33,33	2.05	5 (17%)	37,48,48	2.13	11 (29%)

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	A1D6R	D	901	-	-	0/16/18/18	0/4/4/4
2	A1D6R	B	901	-	-	0/16/18/18	0/4/4/4
2	A1D6R	A	901	-	-	0/16/18/18	0/4/4/4
2	A1D6R	C	901	-	-	0/16/18/18	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	A1D6R	C02-N04	5.55	1.46	1.36
2	A	901	A1D6R	C02-N04	5.53	1.46	1.36
2	B	901	A1D6R	C02-N04	5.52	1.46	1.36
2	C	901	A1D6R	C02-N04	5.45	1.46	1.36
2	D	901	A1D6R	C05-N04	5.36	1.46	1.36
2	B	901	A1D6R	C05-N04	5.29	1.45	1.36
2	A	901	A1D6R	C05-N04	5.28	1.45	1.36
2	C	901	A1D6R	C05-N04	5.27	1.45	1.36
2	A	901	A1D6R	O14-C15	4.92	1.42	1.36
2	D	901	A1D6R	O14-C15	4.89	1.42	1.36
2	B	901	A1D6R	O14-C15	4.84	1.42	1.36
2	C	901	A1D6R	O14-C15	4.80	1.42	1.36
2	C	901	A1D6R	C21-C19	3.91	1.55	1.48
2	A	901	A1D6R	C21-C19	3.81	1.54	1.48
2	B	901	A1D6R	C21-C19	3.78	1.54	1.48
2	D	901	A1D6R	C21-C19	3.77	1.54	1.48
2	A	901	A1D6R	O03-C02	-2.38	1.17	1.23
2	C	901	A1D6R	O03-C02	-2.35	1.17	1.23
2	B	901	A1D6R	O03-C02	-2.35	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	A1D6R	O03-C02	-2.32	1.18	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	A1D6R	C17-N16-C15	6.80	119.60	114.48
2	C	901	A1D6R	C17-N16-C15	6.69	119.51	114.48
2	A	901	A1D6R	C17-N16-C15	6.53	119.39	114.48
2	D	901	A1D6R	C17-N16-C15	6.48	119.35	114.48
2	B	901	A1D6R	N18-C17-N16	-3.85	122.57	128.60
2	C	901	A1D6R	N18-C17-N16	-3.84	122.60	128.60
2	C	901	A1D6R	C07-C12-S13	-3.84	106.43	112.46
2	A	901	A1D6R	C07-C12-S13	-3.83	106.44	112.46
2	D	901	A1D6R	C07-C12-S13	-3.80	106.48	112.46
2	B	901	A1D6R	C07-C12-S13	-3.80	106.49	112.46
2	D	901	A1D6R	N18-C17-N16	-3.75	122.74	128.60
2	B	901	A1D6R	C01-C02-N04	3.68	120.38	114.98
2	A	901	A1D6R	N18-C17-N16	-3.67	122.86	128.60
2	A	901	A1D6R	C01-C02-N04	3.64	120.32	114.98
2	C	901	A1D6R	C01-C02-N04	3.49	120.11	114.98
2	B	901	A1D6R	C08-O14-C15	-3.49	111.11	118.51
2	D	901	A1D6R	C01-C02-N04	3.48	120.08	114.98
2	A	901	A1D6R	C08-O14-C15	-3.34	111.42	118.51
2	A	901	A1D6R	C20-C15-N16	-3.18	120.10	124.57
2	D	901	A1D6R	C20-C15-N16	-3.11	120.20	124.57
2	C	901	A1D6R	C17-N18-C19	3.10	119.94	115.74
2	C	901	A1D6R	C20-C15-N16	-3.08	120.23	124.57
2	B	901	A1D6R	C20-C15-N16	-3.07	120.25	124.57
2	B	901	A1D6R	C17-N18-C19	3.07	119.90	115.74
2	D	901	A1D6R	C17-N18-C19	3.01	119.82	115.74
2	A	901	A1D6R	C17-N18-C19	2.99	119.79	115.74
2	D	901	A1D6R	C20-C19-C21	-2.79	118.14	121.85
2	C	901	A1D6R	C08-O14-C15	-2.74	112.70	118.51
2	D	901	A1D6R	C21-C19-N18	2.73	122.17	116.84
2	C	901	A1D6R	O03-C02-N04	-2.64	119.57	123.04
2	D	901	A1D6R	C08-O14-C15	-2.60	112.99	118.51
2	B	901	A1D6R	O03-C02-N04	-2.54	119.71	123.04
2	D	901	A1D6R	O03-C02-N04	-2.52	119.73	123.04
2	A	901	A1D6R	O03-C02-N04	-2.44	119.83	123.04
2	C	901	A1D6R	C21-C19-N18	2.41	121.54	116.84
2	A	901	A1D6R	C21-C19-N18	2.38	121.48	116.84
2	C	901	A1D6R	C20-C19-C21	-2.31	118.78	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	A1D6R	C20-C19-C21	-2.28	118.82	121.85
2	D	901	A1D6R	C19-C20-C15	2.25	118.21	116.73
2	A	901	A1D6R	C19-C20-C15	2.19	118.17	116.73
2	B	901	A1D6R	C21-C19-N18	2.17	121.07	116.84
2	B	901	A1D6R	C20-C19-C21	-2.10	119.06	121.85
2	C	901	A1D6R	C19-C20-C15	2.00	118.05	116.73

There are no chirality outliers.

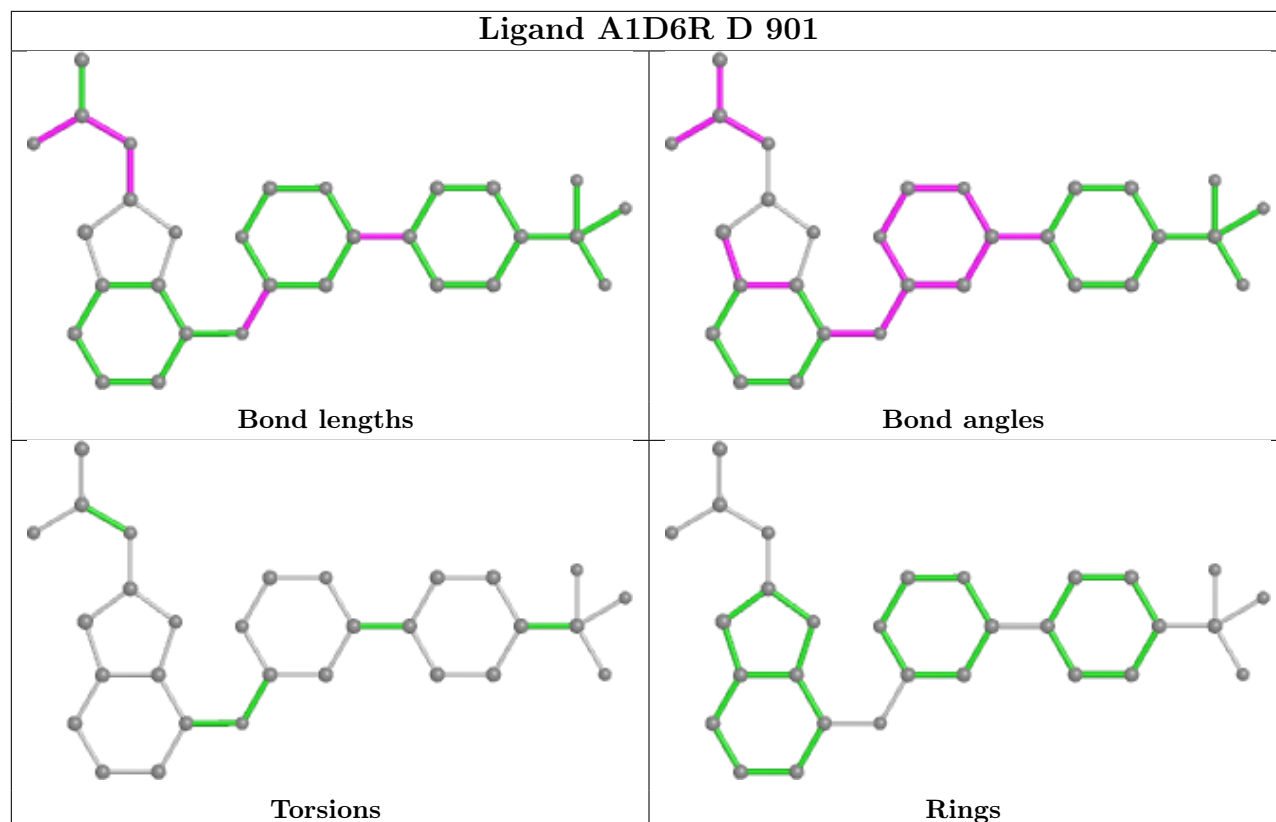
There are no torsion outliers.

There are no ring outliers.

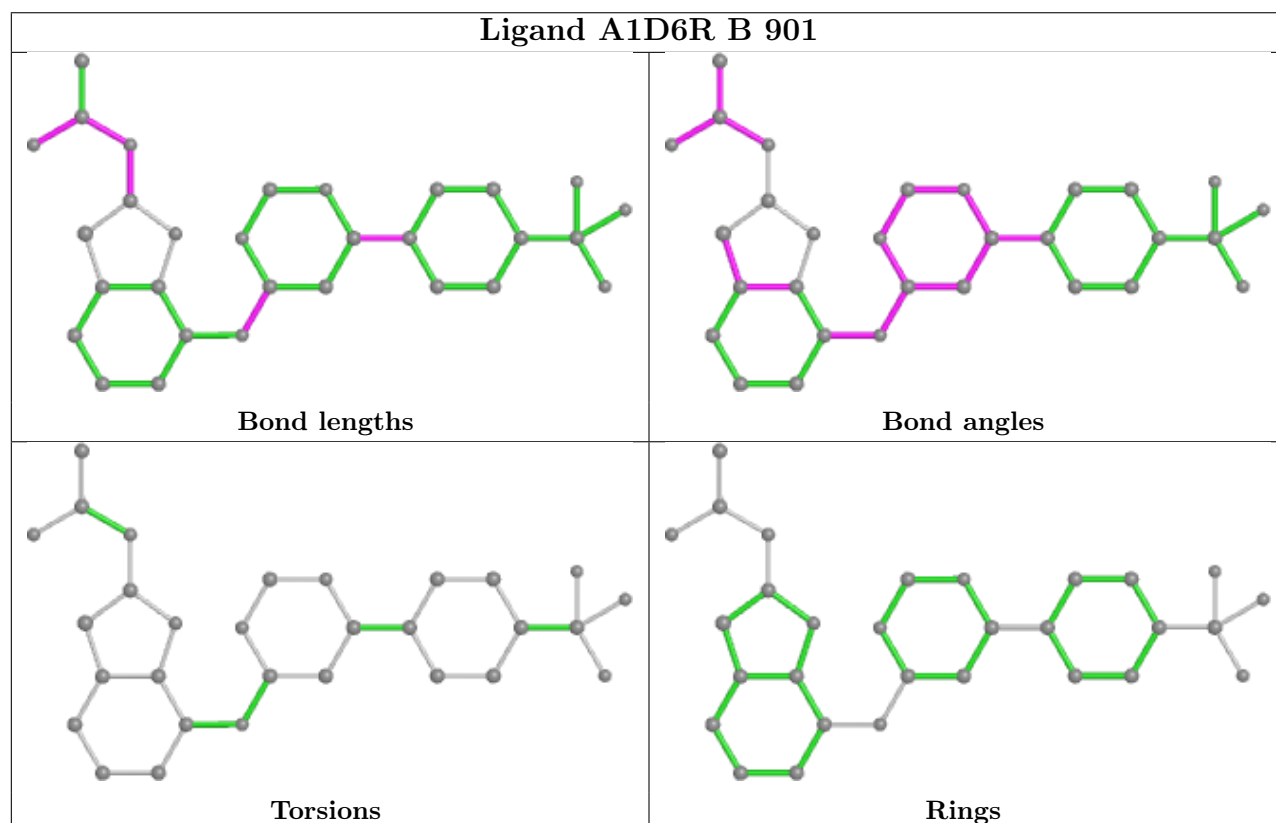
No monomer is involved in short contacts.

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

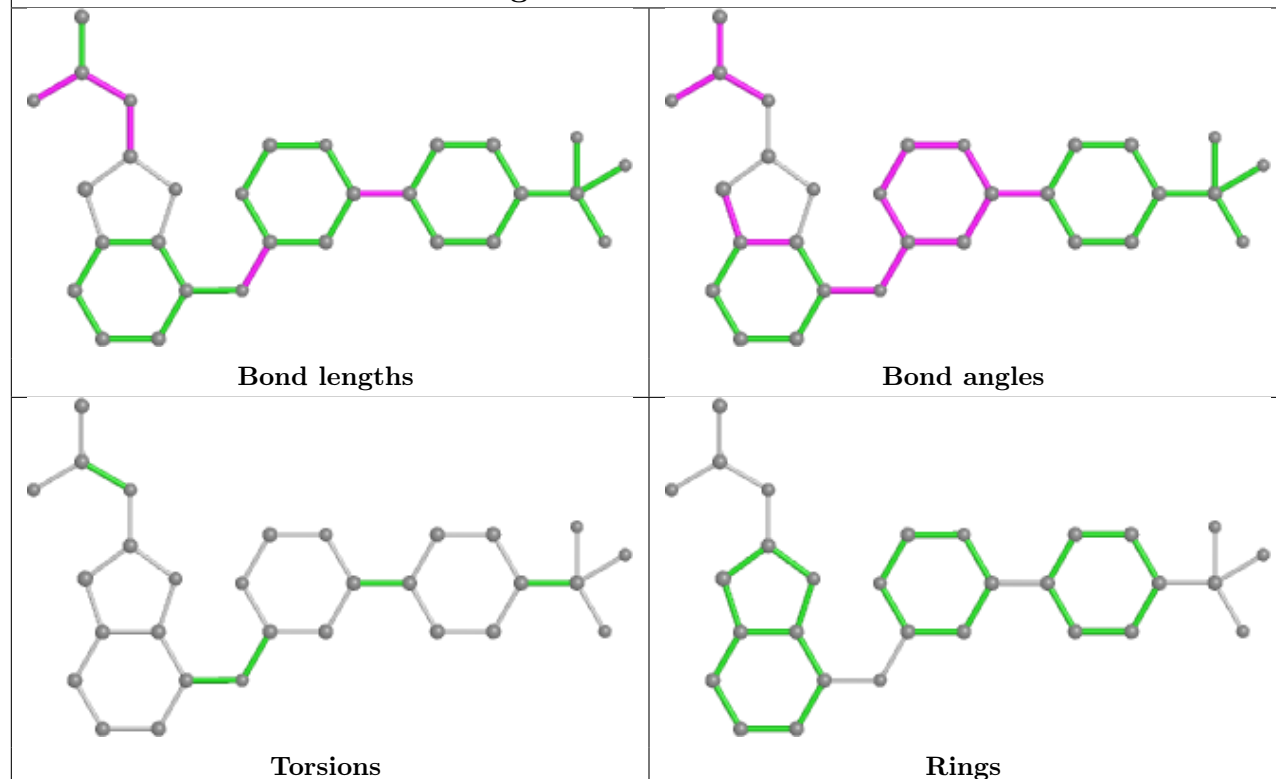
## Ligand A1D6R D 901



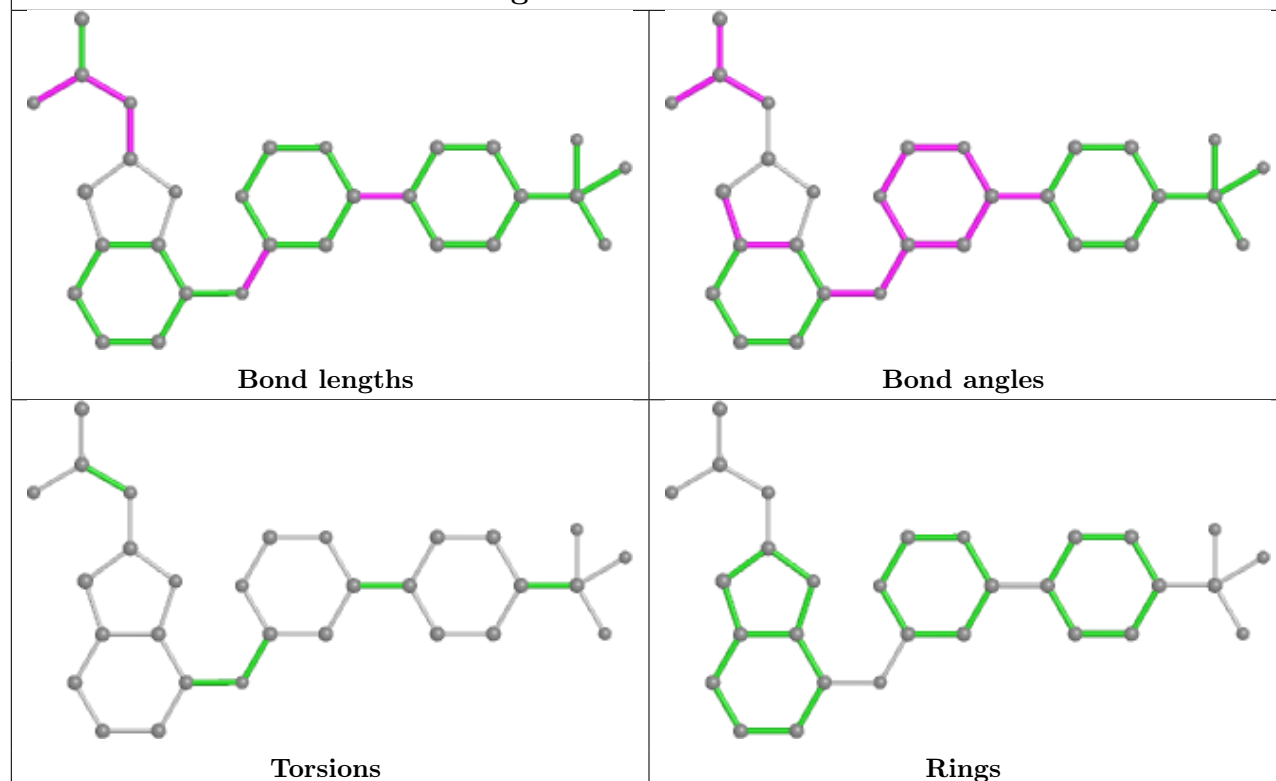
## Ligand A1D6R B 901



## Ligand A1D6R A 901



## Ligand A1D6R C 901



## 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.



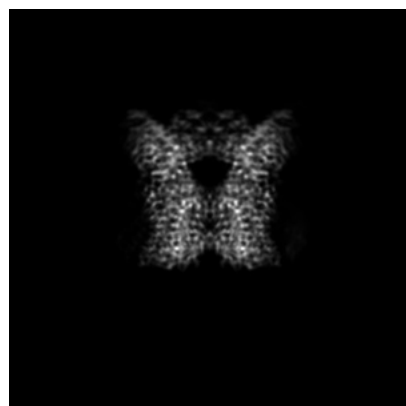
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65638. These allow visual inspection of the internal detail of the map and identification of artifacts.

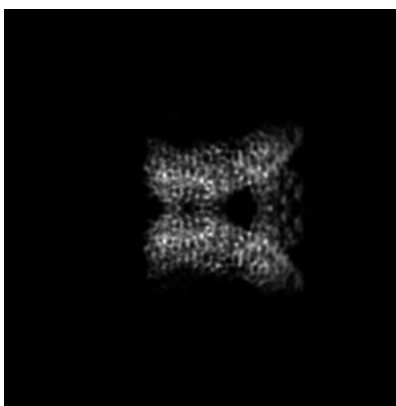
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

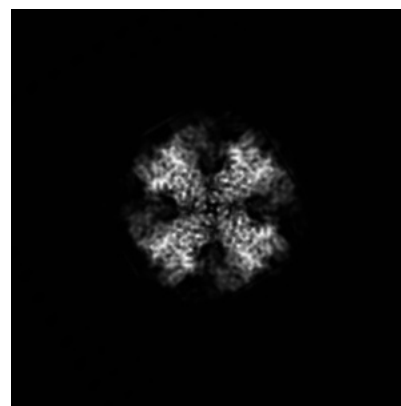
#### 6.1.1 Primary map



X

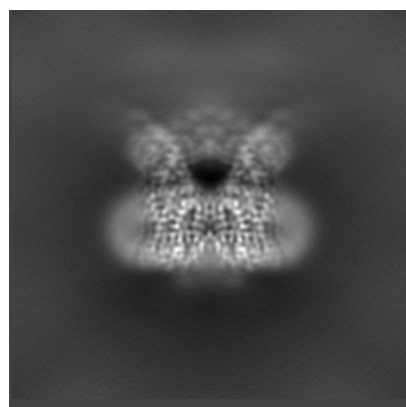


Y

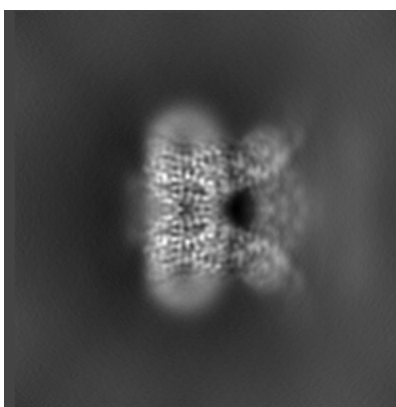


Z

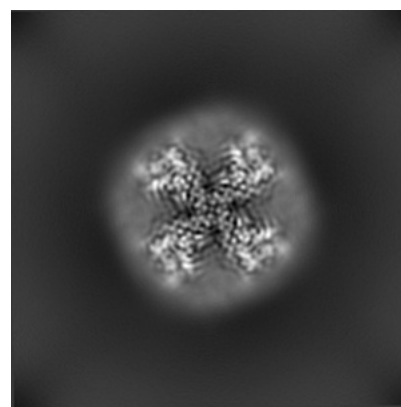
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

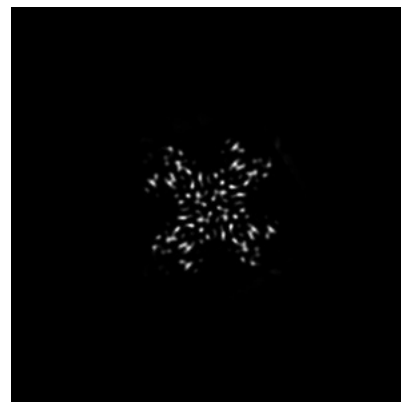
### 6.2.1 Primary map



X Index: 128

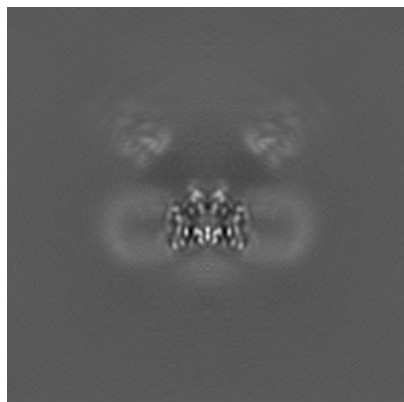


Y Index: 128

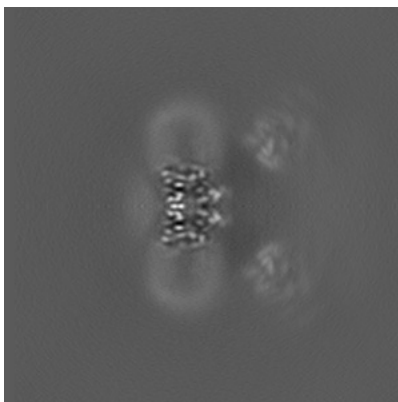


Z Index: 128

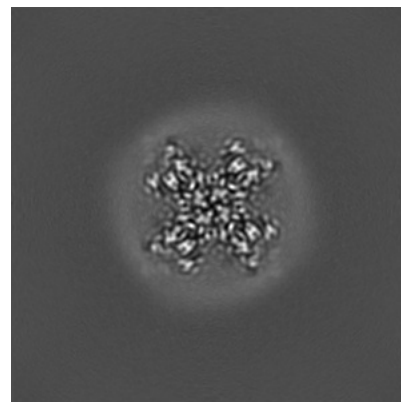
### 6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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: 145

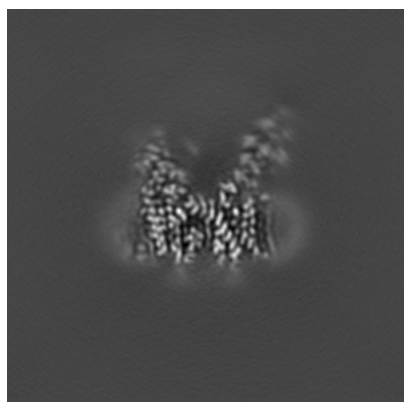


Y Index: 145

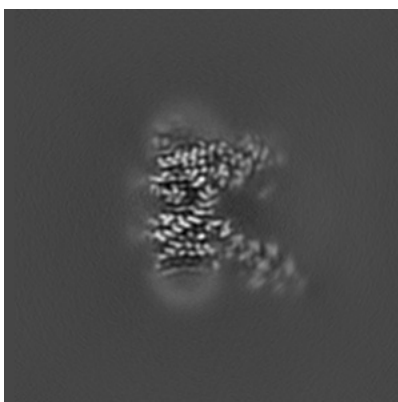


Z Index: 102

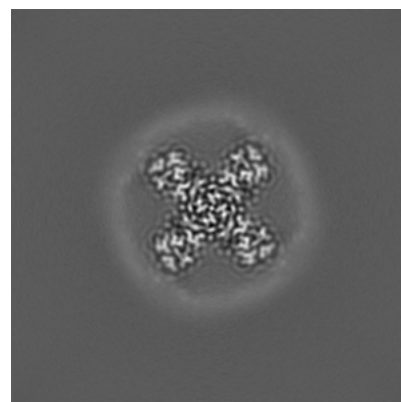
### 6.3.2 Raw map



X Index: 110



Y Index: 110

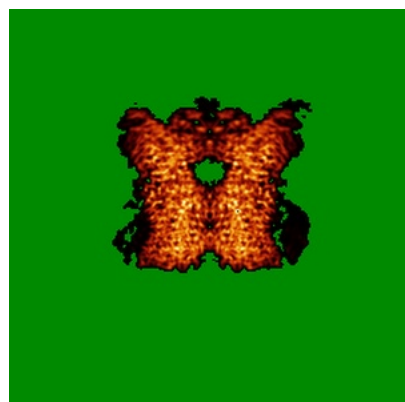


Z Index: 112

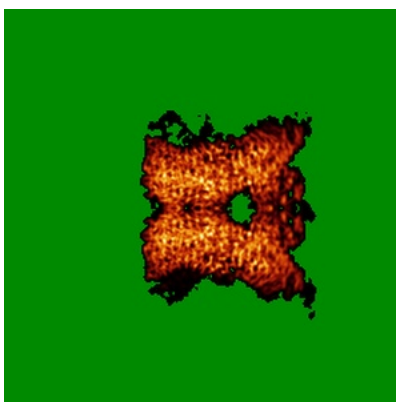
The images above show the largest variance slices of the map in three orthogonal directions.

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

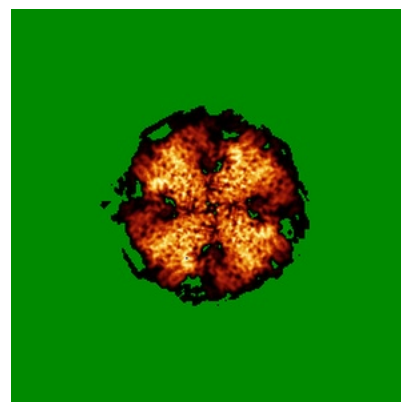
### 6.4.1 Primary map



X

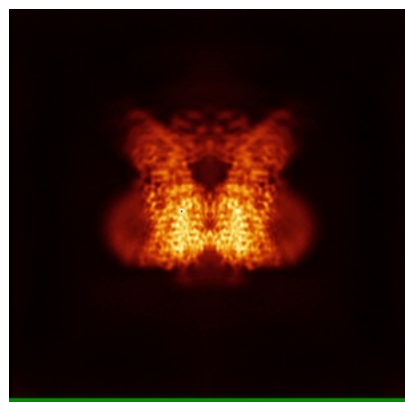


Y

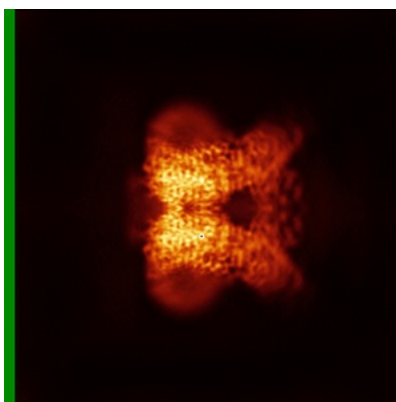


Z

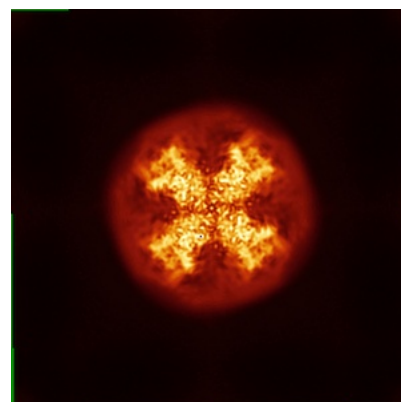
### 6.4.2 Raw map



X



Y

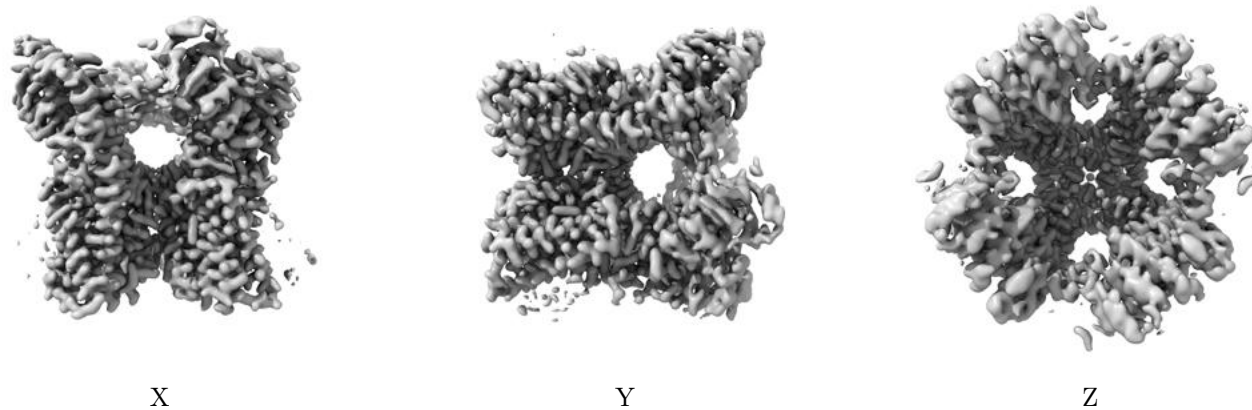


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0913. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

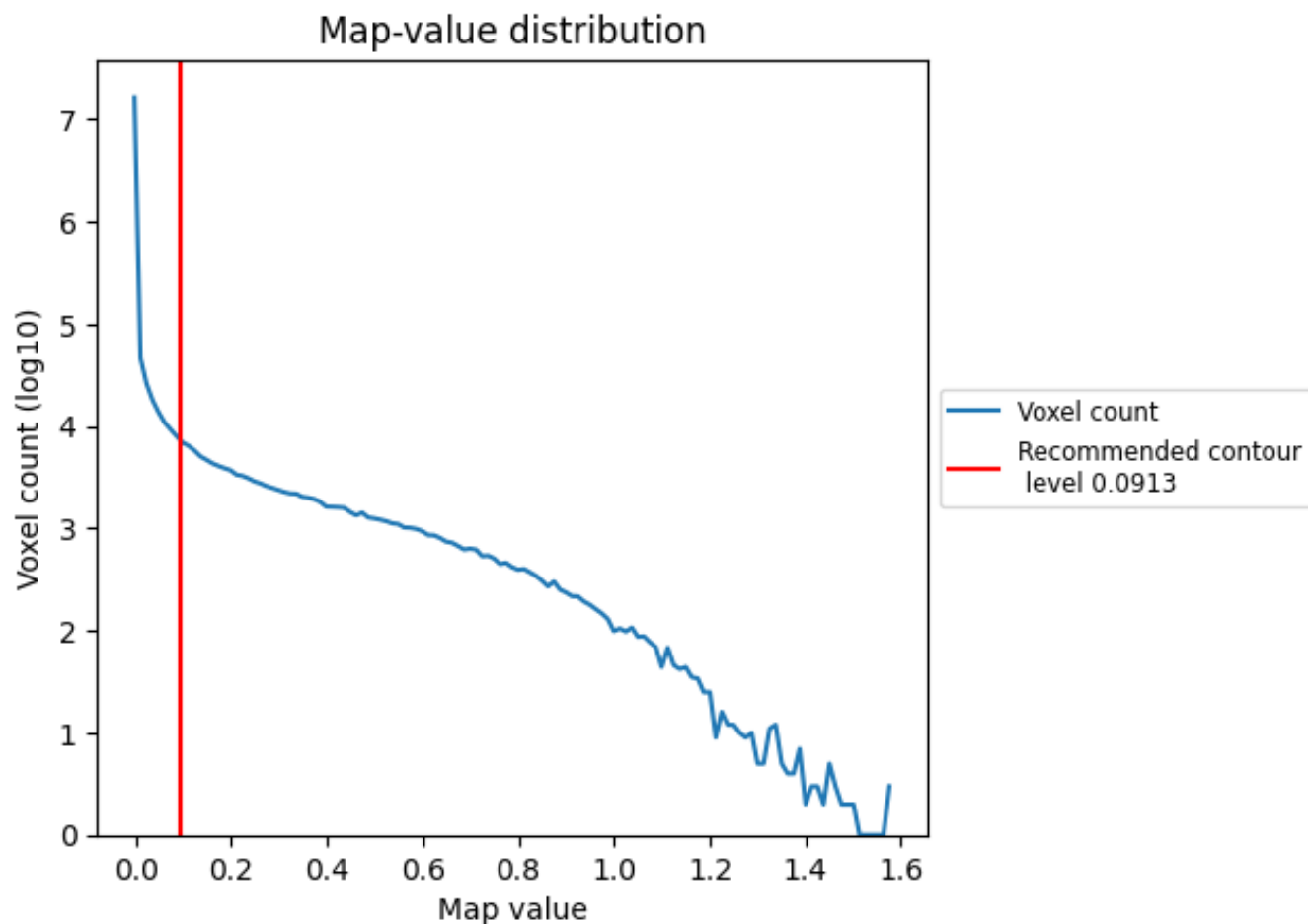
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

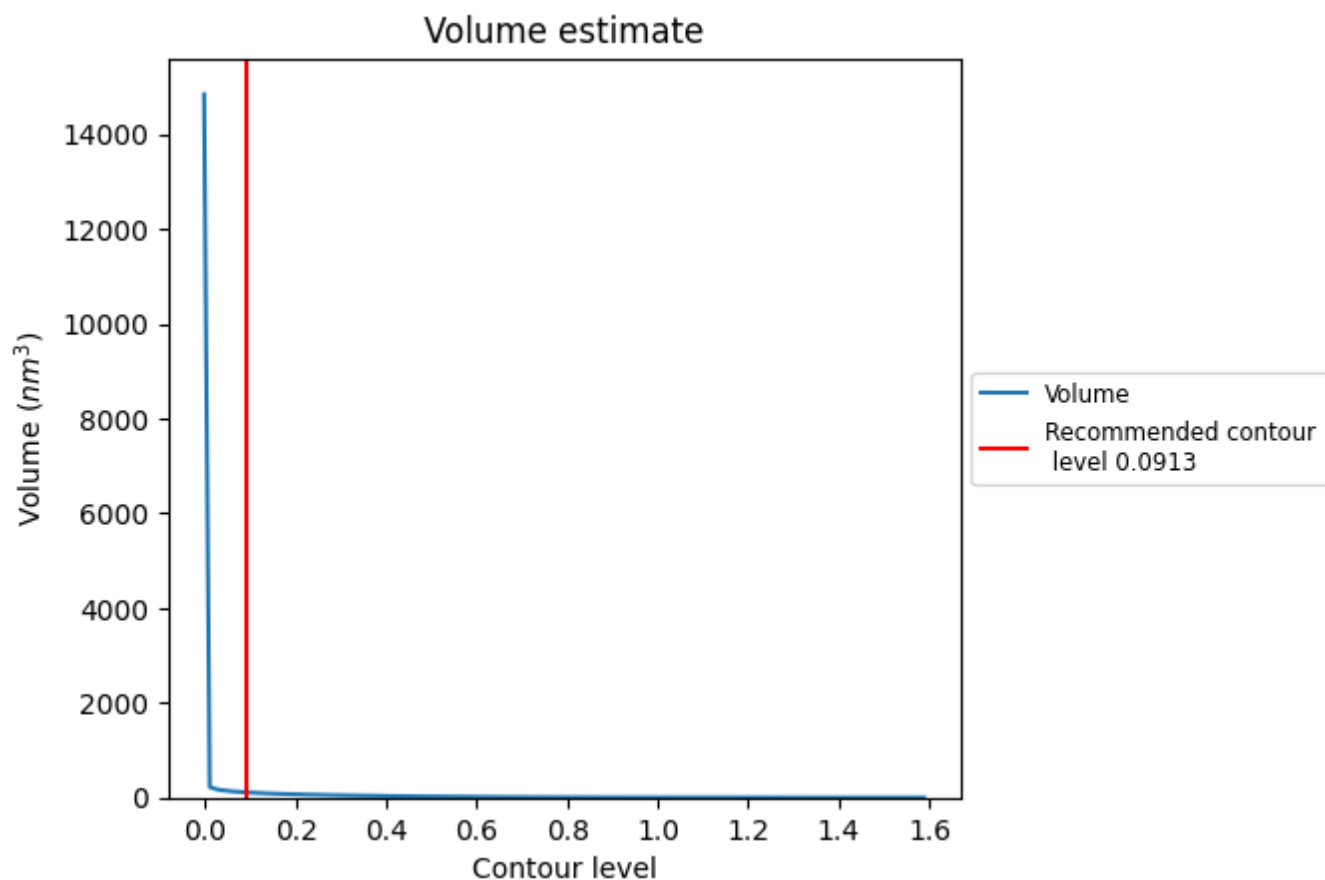
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

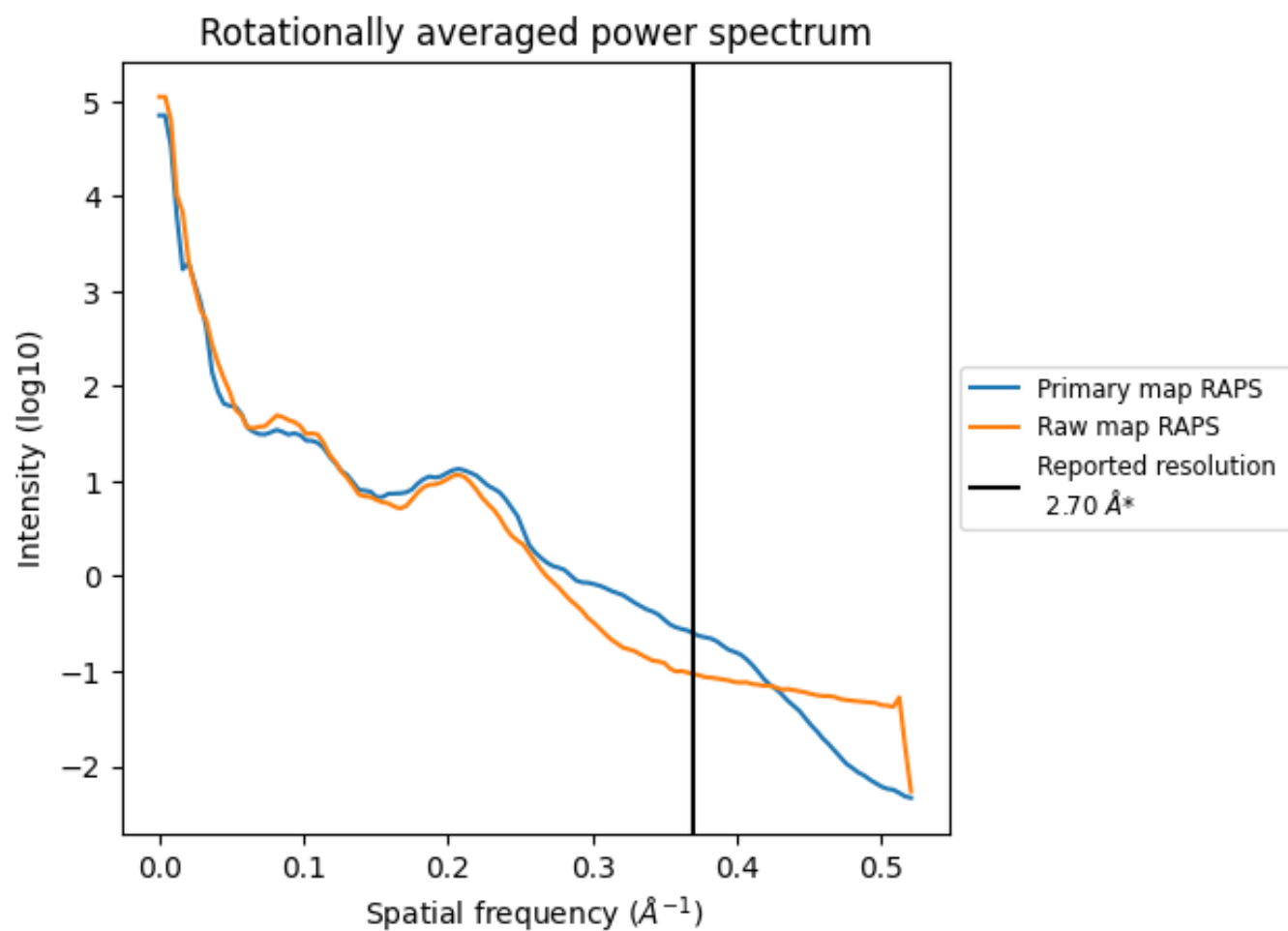
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm<sup>3</sup>; this corresponds to an approximate mass of 98 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



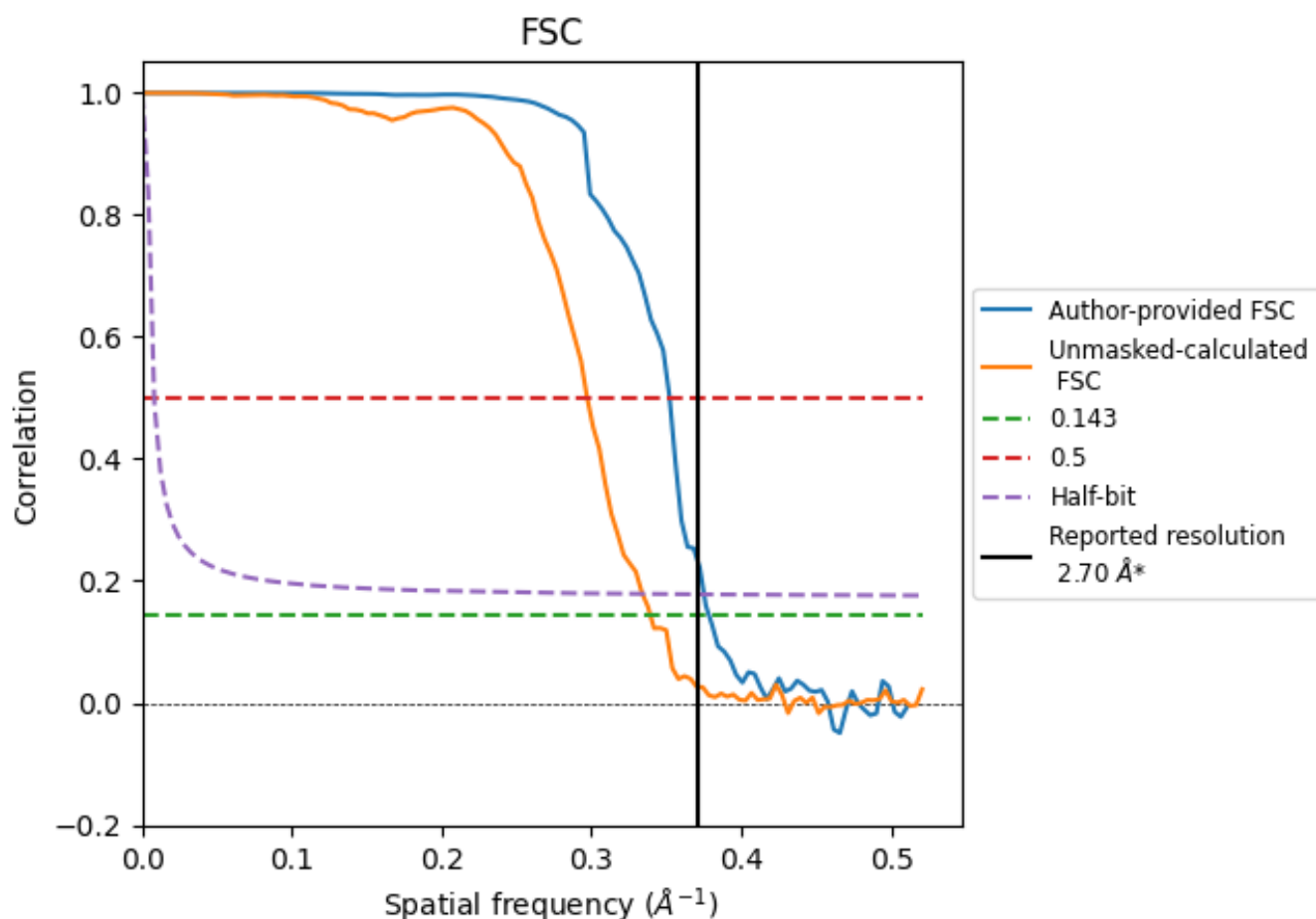
\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

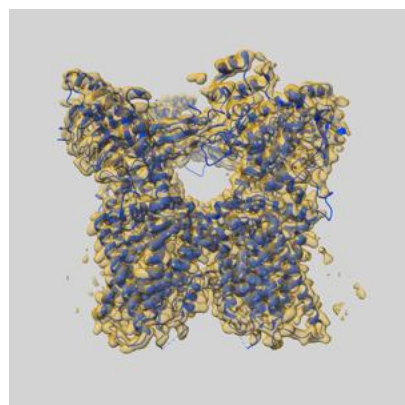
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.64	2.84	2.67
Unmasked-calculated*	2.95	3.36	2.99

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

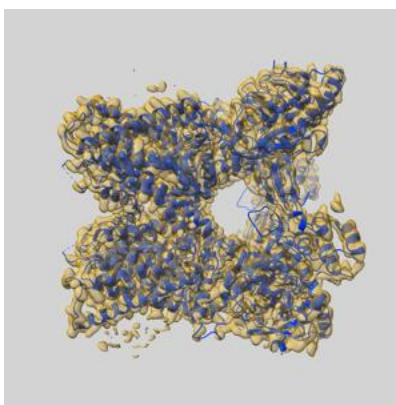
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65638 and PDB model 9W4M. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

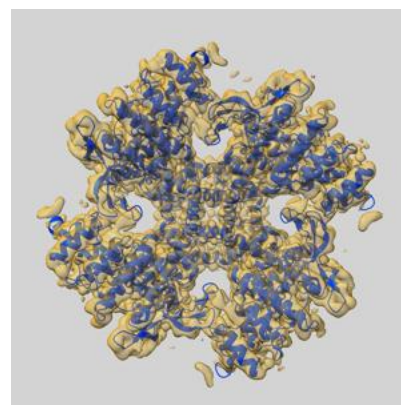
### 9.1 Map-model overlay [i](#)



X



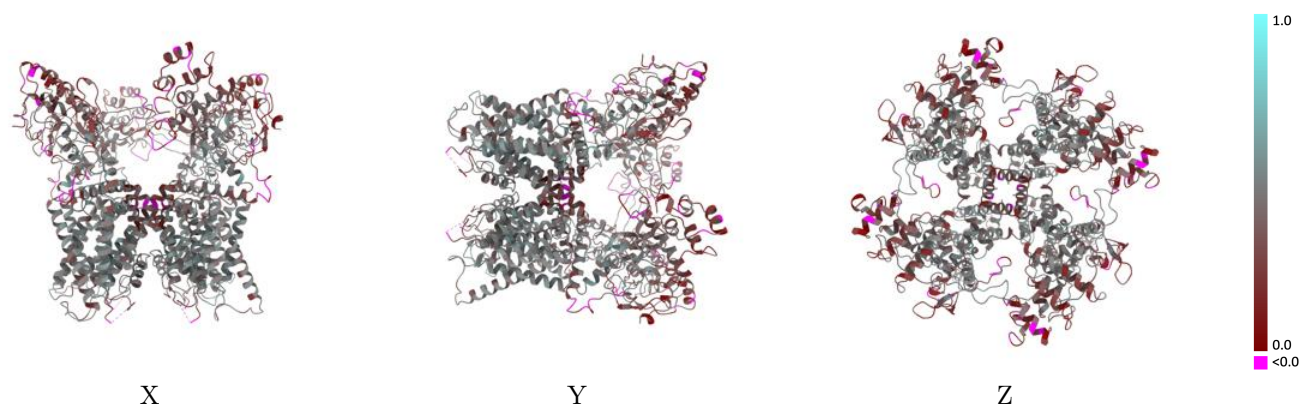
Y



Z

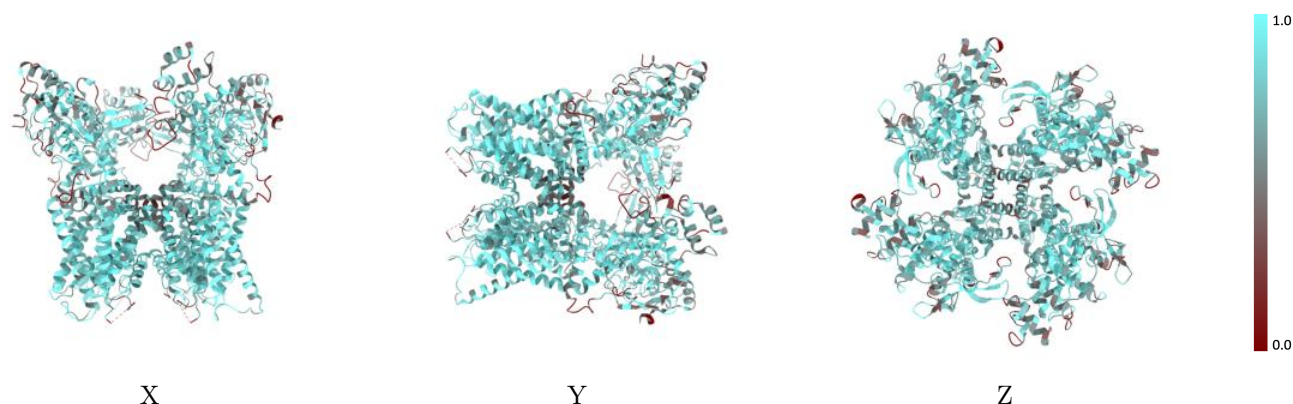
The images above show the 3D surface view of the map at the recommended contour level 0.0913 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



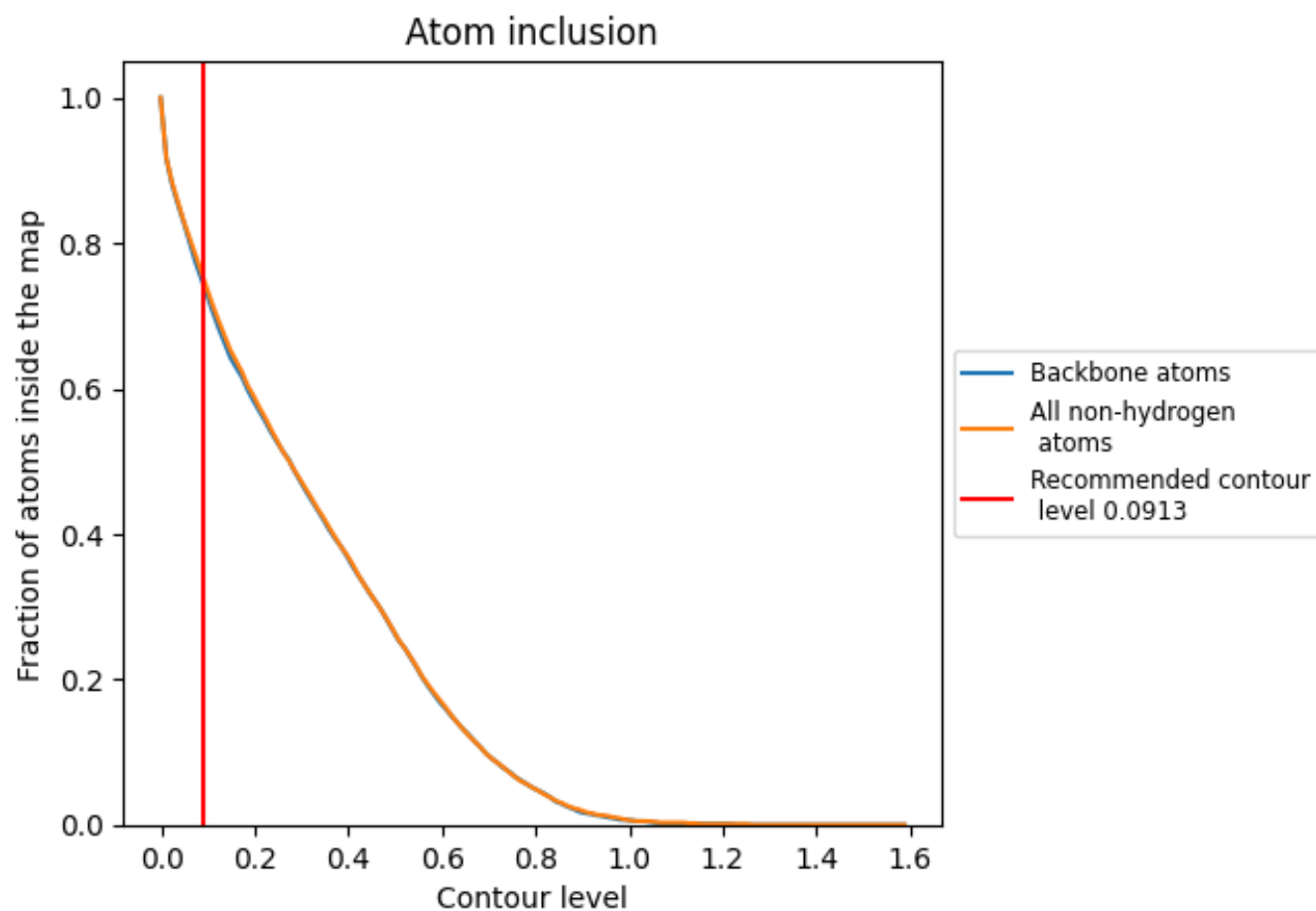
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0913).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 75% 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 (0.0913) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7480	<div></div> 0.3950
A	<div></div> 0.7630	<div></div> 0.3940
B	<div></div> 0.7470	<div></div> 0.3930
C	<div></div> 0.7530	<div></div> 0.3950
D	<div></div> 0.7650	<div></div> 0.3990

