Full wwPDB EM Validation Report

Oct 27, 2024 – 11:51 PM EDT

PDB ID	:	8T1D
EMDB ID	:	EMD-40960
Title	:	Open-state cryo-EM structure of full-length human TRPV4 in complex with agonist 4a-PDD
Authors	:	Talyzina, I.A.; Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2023-06-02
Resolution	:	3.35 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

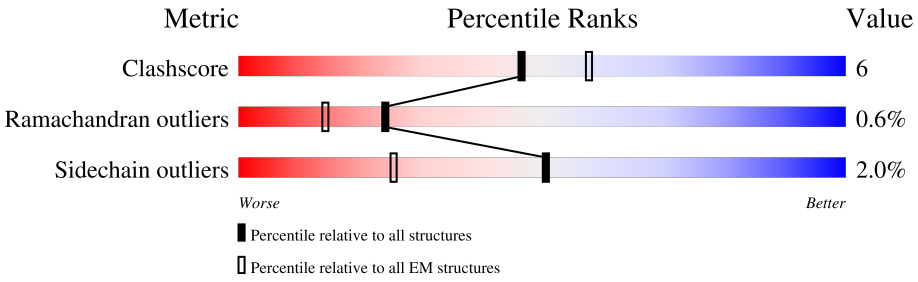
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1132	14% 46% 9% · 44%
1	B	1132	12% 43% 11% 45%
1	C	1132	15% 46% 9% · 44%
1	D	1132	13% 44% 10% 45%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20338 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	632	Total	C	N	O	S	0	0
			5086	3309	844	906	27		
1	B	619	Total	C	N	O	S	0	0
			4987	3245	828	889	25		
1	C	632	Total	C	N	O	S	0	0
			5086	3309	844	906	27		
1	D	619	Total	C	N	O	S	0	0
			4987	3245	828	889	25		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	872	LEU	-	linker	UNP Q9HBA0
A	873	VAL	-	linker	UNP Q9HBA0
A	874	PRO	-	linker	UNP Q9HBA0
A	875	ARG	-	linker	UNP Q9HBA0
A	876	GLY	-	linker	UNP Q9HBA0
A	877	SER	-	linker	UNP Q9HBA0
A	878	ALA	-	linker	UNP Q9HBA0
A	879	ALA	-	linker	UNP Q9HBA0
A	880	ALA	-	linker	UNP Q9HBA0
A	881	ALA	-	linker	UNP Q9HBA0
A	1087	LYS	ALA	engineered mutation	UNP C5MKY7
A	1120	SER	-	expression tag	UNP C5MKY7
A	1121	GLY	-	expression tag	UNP C5MKY7
A	1122	LEU	-	expression tag	UNP C5MKY7
A	1123	ARG	-	expression tag	UNP C5MKY7
A	1124	SER	-	expression tag	UNP C5MKY7
A	1125	TRP	-	expression tag	UNP C5MKY7
A	1126	SER	-	expression tag	UNP C5MKY7
A	1127	HIS	-	expression tag	UNP C5MKY7
A	1128	PRO	-	expression tag	UNP C5MKY7
A	1129	GLN	-	expression tag	UNP C5MKY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	PHE	-	expression tag	UNP C5MKY7
A	1131	GLU	-	expression tag	UNP C5MKY7
A	1132	LYS	-	expression tag	UNP C5MKY7
B	872	LEU	-	linker	UNP Q9HBA0
B	873	VAL	-	linker	UNP Q9HBA0
B	874	PRO	-	linker	UNP Q9HBA0
B	875	ARG	-	linker	UNP Q9HBA0
B	876	GLY	-	linker	UNP Q9HBA0
B	877	SER	-	linker	UNP Q9HBA0
B	878	ALA	-	linker	UNP Q9HBA0
B	879	ALA	-	linker	UNP Q9HBA0
B	880	ALA	-	linker	UNP Q9HBA0
B	881	ALA	-	linker	UNP Q9HBA0
B	1087	LYS	ALA	engineered mutation	UNP C5MKY7
B	1120	SER	-	expression tag	UNP C5MKY7
B	1121	GLY	-	expression tag	UNP C5MKY7
B	1122	LEU	-	expression tag	UNP C5MKY7
B	1123	ARG	-	expression tag	UNP C5MKY7
B	1124	SER	-	expression tag	UNP C5MKY7
B	1125	TRP	-	expression tag	UNP C5MKY7
B	1126	SER	-	expression tag	UNP C5MKY7
B	1127	HIS	-	expression tag	UNP C5MKY7
B	1128	PRO	-	expression tag	UNP C5MKY7
B	1129	GLN	-	expression tag	UNP C5MKY7
B	1130	PHE	-	expression tag	UNP C5MKY7
B	1131	GLU	-	expression tag	UNP C5MKY7
B	1132	LYS	-	expression tag	UNP C5MKY7
C	872	LEU	-	linker	UNP Q9HBA0
C	873	VAL	-	linker	UNP Q9HBA0
C	874	PRO	-	linker	UNP Q9HBA0
C	875	ARG	-	linker	UNP Q9HBA0
C	876	GLY	-	linker	UNP Q9HBA0
C	877	SER	-	linker	UNP Q9HBA0
C	878	ALA	-	linker	UNP Q9HBA0
C	879	ALA	-	linker	UNP Q9HBA0
C	880	ALA	-	linker	UNP Q9HBA0
C	881	ALA	-	linker	UNP Q9HBA0
C	1087	LYS	ALA	engineered mutation	UNP C5MKY7
C	1120	SER	-	expression tag	UNP C5MKY7
C	1121	GLY	-	expression tag	UNP C5MKY7
C	1122	LEU	-	expression tag	UNP C5MKY7
C	1123	ARG	-	expression tag	UNP C5MKY7

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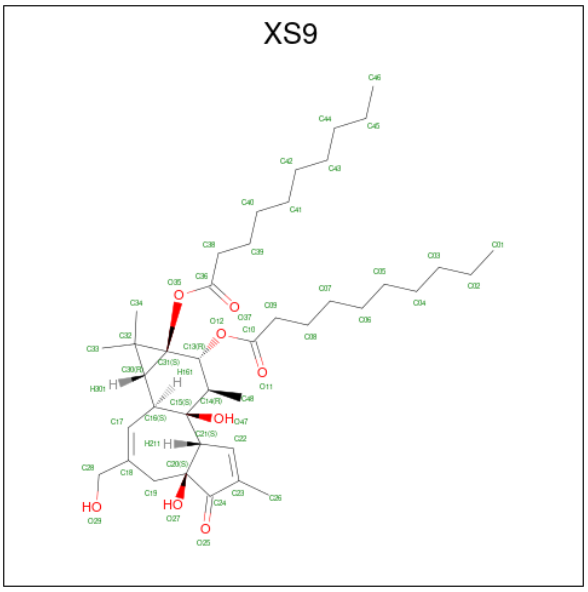
Chain	Residue	Modelled	Actual	Comment	Reference
C	1124	SER	-	expression tag	UNP C5MKY7
C	1125	TRP	-	expression tag	UNP C5MKY7
C	1126	SER	-	expression tag	UNP C5MKY7
C	1127	HIS	-	expression tag	UNP C5MKY7
C	1128	PRO	-	expression tag	UNP C5MKY7
C	1129	GLN	-	expression tag	UNP C5MKY7
C	1130	PHE	-	expression tag	UNP C5MKY7
C	1131	GLU	-	expression tag	UNP C5MKY7
C	1132	LYS	-	expression tag	UNP C5MKY7
D	872	LEU	-	linker	UNP Q9HBA0
D	873	VAL	-	linker	UNP Q9HBA0
D	874	PRO	-	linker	UNP Q9HBA0
D	875	ARG	-	linker	UNP Q9HBA0
D	876	GLY	-	linker	UNP Q9HBA0
D	877	SER	-	linker	UNP Q9HBA0
D	878	ALA	-	linker	UNP Q9HBA0
D	879	ALA	-	linker	UNP Q9HBA0
D	880	ALA	-	linker	UNP Q9HBA0
D	881	ALA	-	linker	UNP Q9HBA0
D	1087	LYS	ALA	engineered mutation	UNP C5MKY7
D	1120	SER	-	expression tag	UNP C5MKY7
D	1121	GLY	-	expression tag	UNP C5MKY7
D	1122	LEU	-	expression tag	UNP C5MKY7
D	1123	ARG	-	expression tag	UNP C5MKY7
D	1124	SER	-	expression tag	UNP C5MKY7
D	1125	TRP	-	expression tag	UNP C5MKY7
D	1126	SER	-	expression tag	UNP C5MKY7
D	1127	HIS	-	expression tag	UNP C5MKY7
D	1128	PRO	-	expression tag	UNP C5MKY7
D	1129	GLN	-	expression tag	UNP C5MKY7
D	1130	PHE	-	expression tag	UNP C5MKY7
D	1131	GLU	-	expression tag	UNP C5MKY7
D	1132	LYS	-	expression tag	UNP C5MKY7

- Molecule 2 is (1aR,1bS,4aS,7aS,7bS,8R,9R,9aS)-9a-(decanoyloxy)-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-1H-cyclopropa[3,4]benzo[1,2-e]azulen-9-yl decanoate (three-letter code: XS9) (formula: $C_{40}H_{64}O_8$) (labeled as "Ligand of Interest" by depositor).



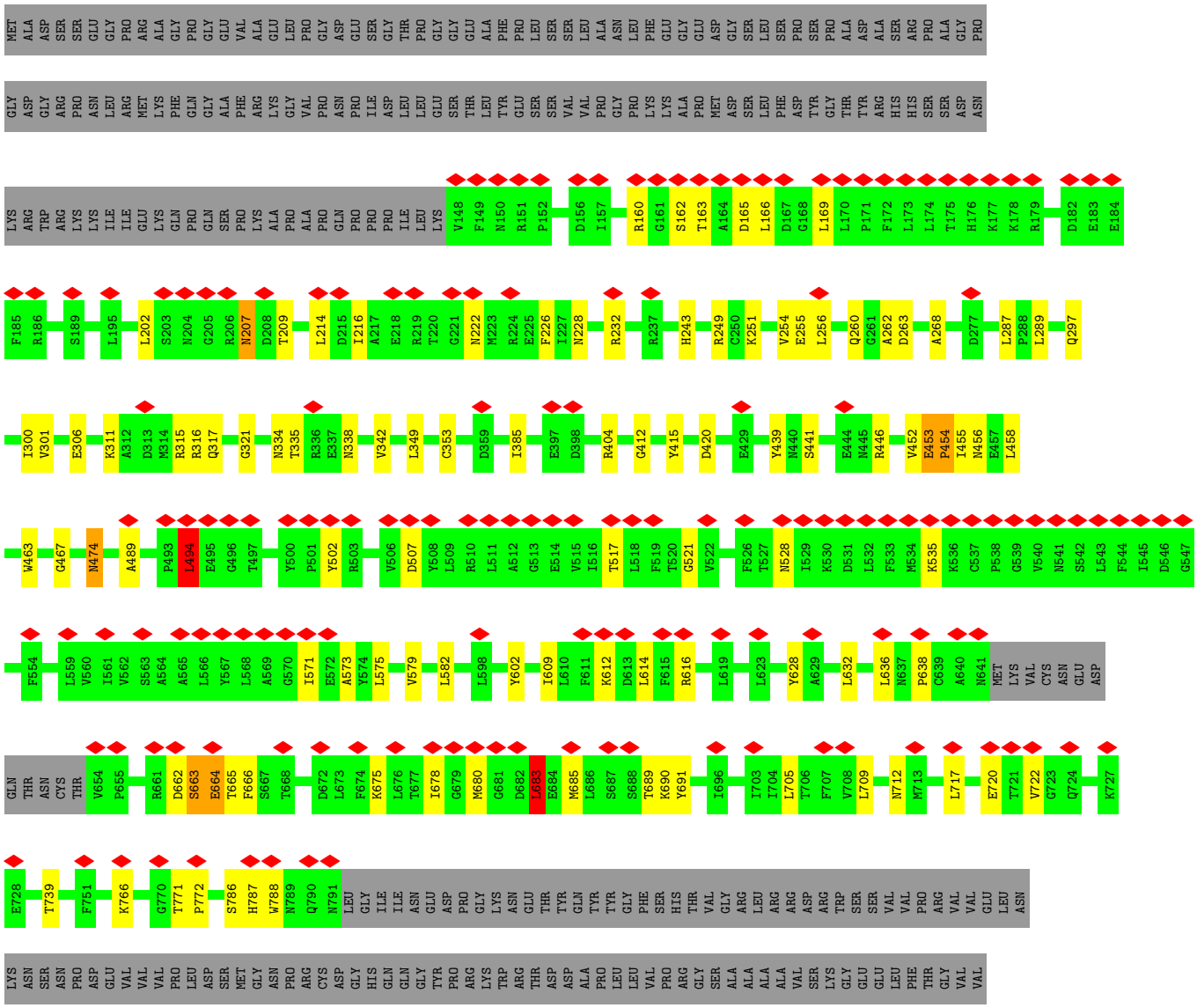
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			48	40	8	
2	B	1	Total	C	O	0
			48	40	8	
2	C	1	Total	C	O	0
			48	40	8	
2	D	1	Total	C	O	0
			48	40	8	

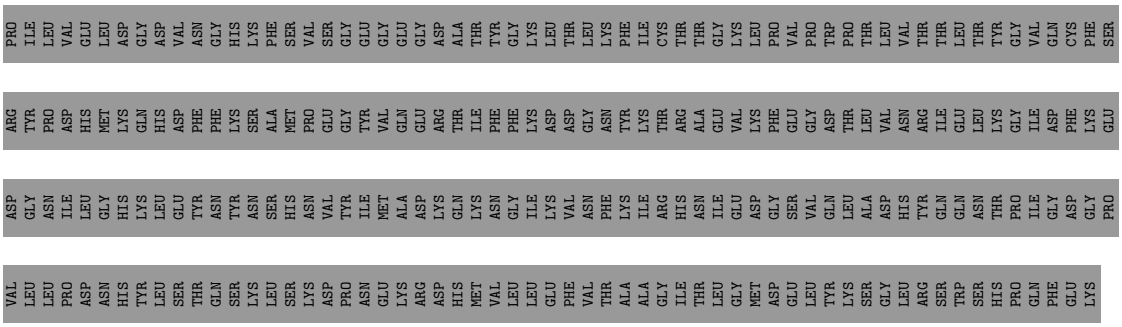
3 Residue-property plots (i)

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: Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera

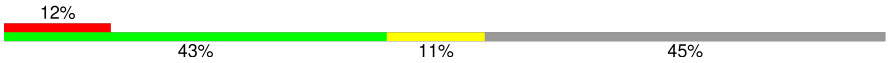
Chain A:

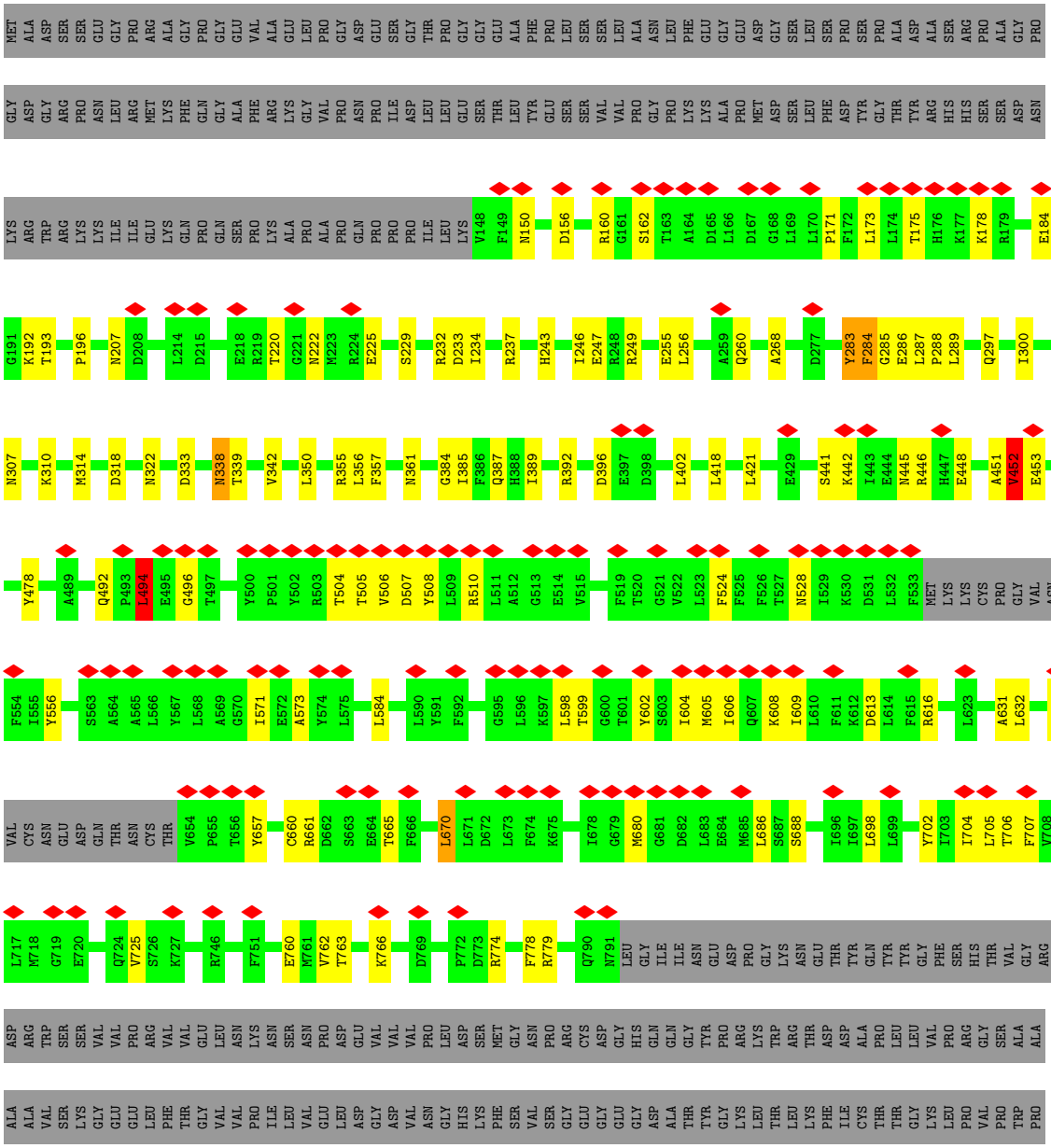


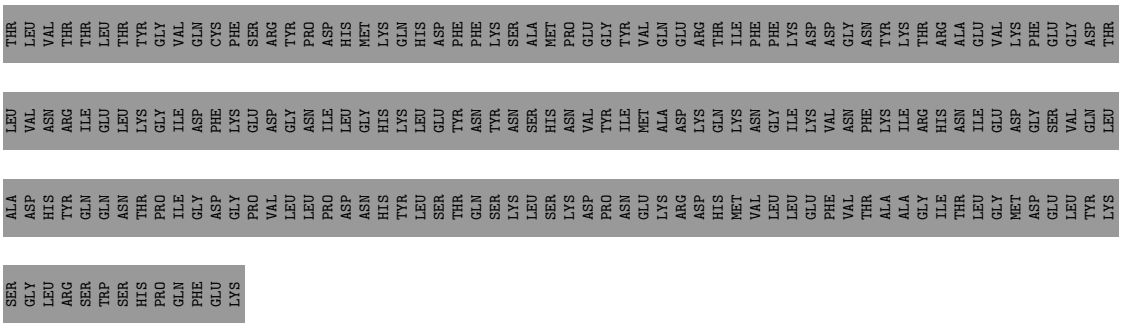


• Molecule 1: Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera

Chain B:

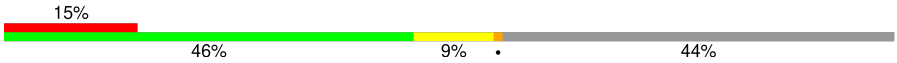


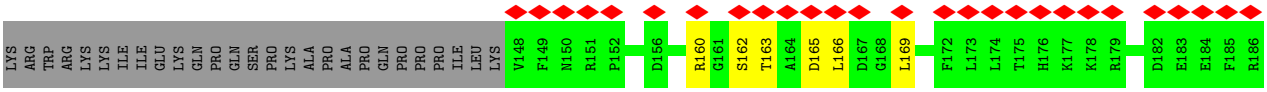


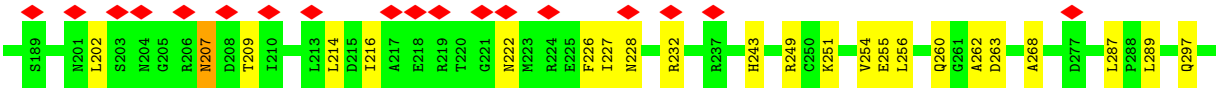


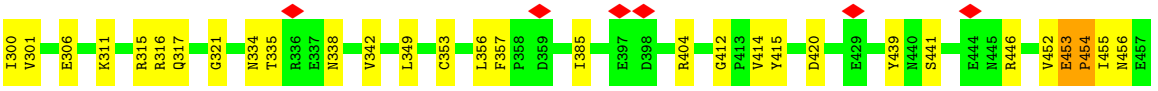
• Molecule 1: Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera

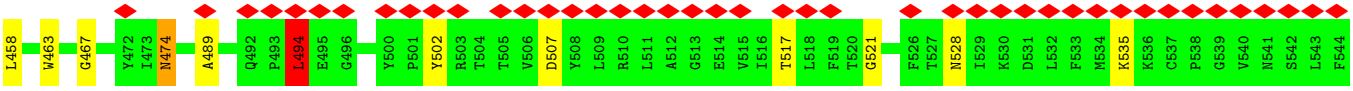
Chain C:

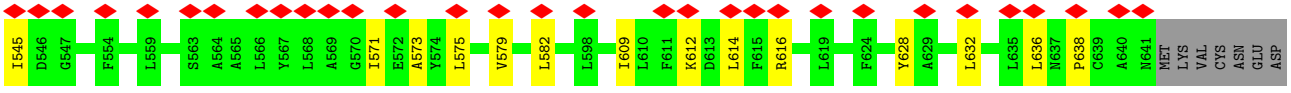


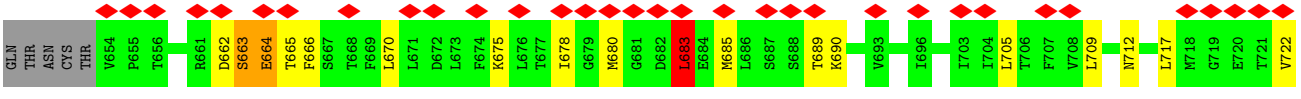


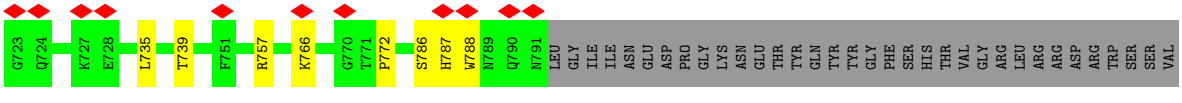


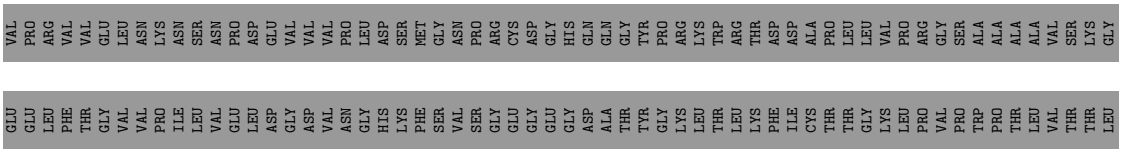


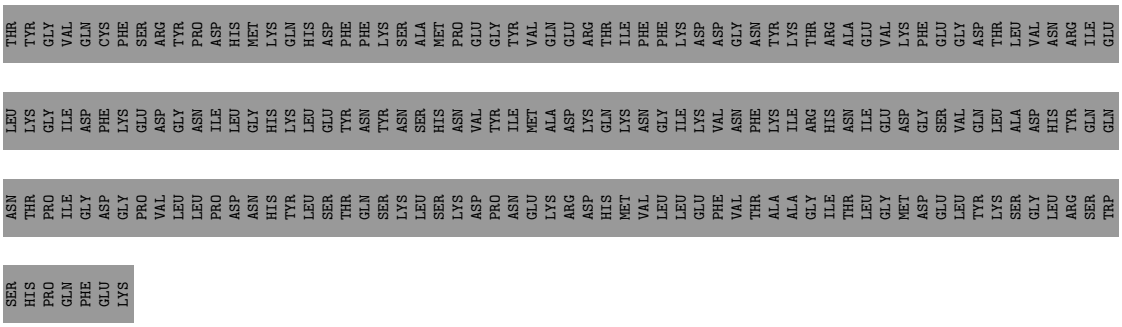






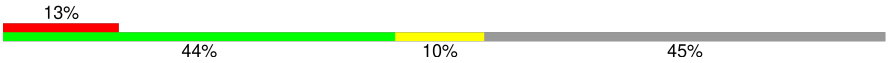


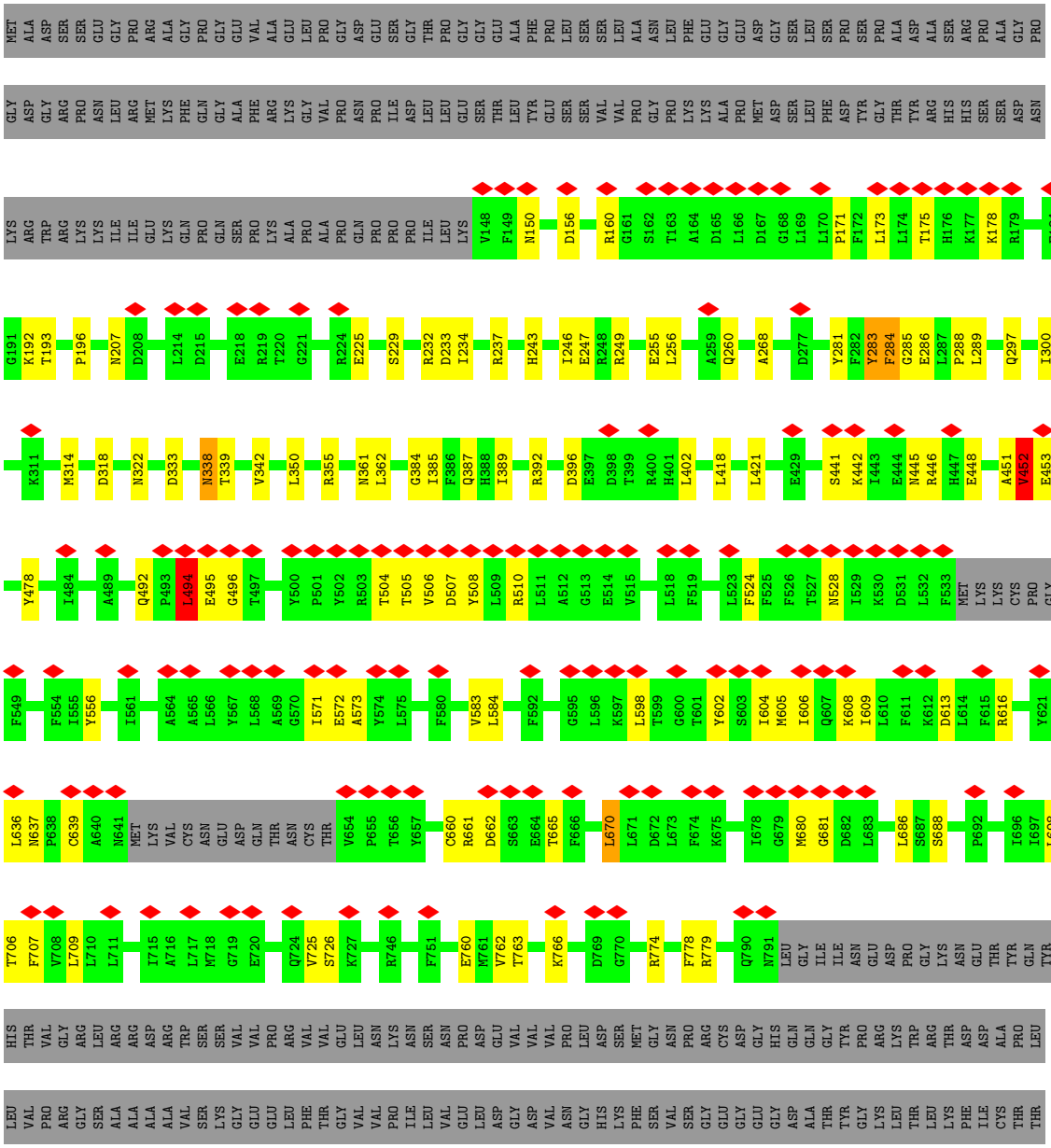




• Molecule 1: Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera

Chain D:





GLY LYS LEU PRO VAL PRO TRP PRO THR LEU VAL THR THR LEU THR TYR GLY VAL GLN CYS PHE SER ARG TYR PRO ASP HIS MET LYS GLN HIS ASP PHE PHE LYS SER ALA MET PRO GLU GLY TYR VAL GLN GLU ARG THR ILE PHE PHE LYS ASP ASP GLY ASN TYR LYS THR ARG ALA

GLU VAL LYS PHE GLU GLY ASP THR LEU VAL ASN ARG ILE GLU LEU LYS GLY ILE ASP PHE LYS GLU ASP GLY ASN ILE LEU GLY HIS LYS LEU GLU SER THR ASN TYR ASN SER HIS ASN VAL TYR ILE MET ALA ASP LYS GLN LYS ASN GLY ILE LYS VAL ASN PHE LYS ILE ARG HIS ASN

ILE GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL LEU LEU PRO ASP ASN HIS TYR LEU SER THR GLN SER LYS LEU SER LYS ASP PRO ASN GLU LYS ARG ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR

LEU GLY MET ASP GLU LEU TYR LYS SER GLY LEU ARG SER TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.323	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	252.416, 252.416, 252.416	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7888, 0.7888, 0.7888	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XS9

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	0.34	0/5206	0.65	5/7061 (0.1%)
1	B	0.32	0/5104	0.63	4/6923 (0.1%)
1	C	0.33	0/5206	0.65	5/7061 (0.1%)
1	D	0.32	0/5104	0.63	4/6923 (0.1%)
All	All	0.33	0/20620	0.64	18/27968 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	494	LEU	CA-CB-CG	10.02	138.35	115.30
1	D	494	LEU	CA-CB-CG	10.02	138.34	115.30
1	A	494	LEU	CA-CB-CG	9.02	136.05	115.30
1	C	494	LEU	CA-CB-CG	9.01	136.03	115.30
1	C	683	LEU	CA-CB-CG	7.83	133.32	115.30
1	A	683	LEU	CA-CB-CG	7.82	133.30	115.30
1	D	670	LEU	CA-CB-CG	7.57	132.70	115.30
1	B	670	LEU	CA-CB-CG	7.56	132.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	494	LEU	CB-CG-CD1	6.26	121.65	111.00
1	D	494	LEU	CB-CG-CD1	6.26	121.64	111.00
1	A	663	SER	C-N-CA	5.95	136.57	121.70
1	C	663	SER	C-N-CA	5.94	136.55	121.70
1	D	604	ILE	CG1-CB-CG2	-5.29	99.76	111.40
1	B	604	ILE	CG1-CB-CG2	-5.29	99.77	111.40
1	C	494	LEU	CB-CG-CD1	5.07	119.61	111.00
1	C	452	VAL	C-N-CA	5.06	134.36	121.70
1	A	452	VAL	C-N-CA	5.06	134.35	121.70
1	A	494	LEU	CB-CG-CD1	5.05	119.59	111.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ASN	Peptide
1	A	453	GLU	Peptide
1	A	662	ASP	Peptide
1	A	664	GLU	Peptide
1	A	680	MET	Peptide
1	B	283	TYR	Peptide
1	B	284	PHE	Peptide
1	B	442	LYS	Peptide
1	B	451	ALA	Peptide
1	B	452	VAL	Peptide
1	C	334	ASN	Peptide
1	C	453	GLU	Peptide
1	C	662	ASP	Peptide
1	C	664	GLU	Peptide
1	C	680	MET	Peptide
1	D	283	TYR	Peptide
1	D	284	PHE	Peptide
1	D	442	LYS	Peptide
1	D	451	ALA	Peptide
1	D	452	VAL	Peptide

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5086	0	5148	59	0
1	B	4987	0	5042	67	0
1	C	5086	0	5148	59	0
1	D	4987	0	5042	68	0
2	A	48	0	0	2	0
2	B	48	0	0	3	0
2	C	48	0	0	2	0
2	D	48	0	0	3	0
All	All	20338	0	20380	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (239) 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:D:441:SER:HB3	1:D:446:ARG:HE	1.55	0.72
1:B:441:SER:HB3	1:B:446:ARG:HE	1.55	0.71
1:C:404:ARG:HG3	1:C:420:ASP:HB3	1.76	0.68
1:A:404:ARG:HG3	1:A:420:ASP:HB3	1.76	0.67
1:B:494:LEU:HD13	1:B:496:GLY:H	1.62	0.65
1:D:494:LEU:HD13	1:D:496:GLY:H	1.62	0.63
1:A:638:PRO:HG3	1:D:495:GLU:HG2	1.81	0.63
1:B:702:TYR:O	1:B:706:THR:OG1	2.17	0.62
1:D:702:TYR:O	1:D:706:THR:OG1	2.17	0.61
1:D:660:CYS:SG	1:D:661:ARG:N	2.73	0.61
1:B:660:CYS:SG	1:B:661:ARG:N	2.73	0.60
1:C:571:ILE:HG22	1:C:573:ALA:H	1.66	0.60
1:D:284:PHE:O	1:D:286:GLU:N	2.33	0.60
1:B:763:THR:OG1	1:B:774:ARG:NH2	2.35	0.59
1:A:571:ILE:HG22	1:A:573:ALA:H	1.66	0.59
1:D:763:THR:OG1	1:D:774:ARG:NH2	2.35	0.59
1:B:637:ASN:ND2	1:B:688:SER:OG	2.35	0.59
1:D:605:MET:HG2	1:D:725:VAL:HG21	1.85	0.59
1:A:301:VAL:HG11	1:A:349:LEU:HD11	1.85	0.58
1:B:605:MET:HG2	1:B:725:VAL:HG21	1.85	0.58
1:D:507:ASP:OD1	1:D:510:ARG:NH2	2.37	0.58
1:C:301:VAL:HG11	1:C:349:LEU:HD11	1.85	0.57
1:C:675:LYS:NZ	1:D:681:GLY:O	2.32	0.57
1:D:637:ASN:ND2	1:D:688:SER:OG	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ASN:HB3	1:B:448:GLU:HB2	1.86	0.57
1:C:412:GLY:N	1:D:247:GLU:OE2	2.38	0.57
1:B:507:ASP:OD1	1:B:510:ARG:NH2	2.37	0.57
1:B:284:PHE:O	1:B:286:GLU:N	2.33	0.57
1:D:445:ASN:HB3	1:D:448:GLU:HB2	1.86	0.56
1:D:156:ASP:OD2	1:D:160:ARG:NH1	2.38	0.56
1:C:169:LEU:HD23	1:C:216:ILE:HG21	1.88	0.56
1:A:166:LEU:HB2	1:A:169:LEU:HB2	1.88	0.55
1:A:256:LEU:O	1:A:260:GLN:NE2	2.39	0.55
1:B:524:PHE:CE1	2:B:1201:XS9:C17	2.89	0.55
1:D:524:PHE:CE1	2:D:1201:XS9:C17	2.89	0.55
1:C:256:LEU:O	1:C:260:GLN:NE2	2.39	0.55
1:B:478:TYR:HB2	2:B:1201:XS9:C39	2.37	0.55
1:D:478:TYR:HB2	2:D:1201:XS9:C39	2.37	0.55
1:B:156:ASP:OD2	1:B:160:ARG:NH1	2.38	0.55
1:C:614:LEU:HG	1:D:709:LEU:HD21	1.89	0.55
1:B:598:LEU:HB3	1:C:717:LEU:HD21	1.89	0.55
1:C:166:LEU:HB2	1:C:169:LEU:HB2	1.88	0.55
1:A:169:LEU:HD23	1:A:216:ILE:HG21	1.88	0.54
1:A:705:LEU:HA	1:A:709:LEU:HB2	1.90	0.54
1:C:705:LEU:HA	1:C:709:LEU:HB2	1.90	0.54
1:D:421:LEU:HD21	1:D:778:PHE:HB2	1.90	0.53
1:A:251:LYS:NZ	1:A:255:GLU:OE2	2.41	0.53
1:C:251:LYS:NZ	1:C:255:GLU:OE2	2.41	0.53
1:A:717:LEU:HD21	1:D:598:LEU:HB3	1.90	0.53
1:B:186:ARG:NH1	1:B:193:THR:OG1	2.42	0.53
1:A:453:GLU:O	1:A:455:ILE:N	2.42	0.53
1:C:453:GLU:O	1:C:455:ILE:N	2.42	0.53
1:D:186:ARG:NH1	1:D:193:THR:OG1	2.42	0.53
1:D:418:LEU:HD21	1:D:762:VAL:HG11	1.91	0.53
1:C:636:LEU:HA	1:C:689:THR:HG22	1.91	0.52
1:A:636:LEU:HA	1:A:689:THR:HG22	1.91	0.52
1:C:163:THR:HB	1:C:209:THR:HG22	1.91	0.52
1:A:222:ASN:O	1:A:226:PHE:N	2.42	0.52
1:A:163:THR:HB	1:A:209:THR:HG22	1.91	0.52
1:B:421:LEU:HD21	1:B:778:PHE:HB2	1.90	0.52
1:B:418:LEU:HD21	1:B:762:VAL:HG11	1.91	0.52
1:C:222:ASN:O	1:C:226:PHE:N	2.42	0.52
1:D:225:GLU:O	1:D:229:SER:OG	2.28	0.51
1:A:316:ARG:NH1	1:A:317:GLN:O	2.44	0.51
1:C:315:ARG:NH2	1:C:353:CYS:SG	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ARG:NH1	1:C:317:GLN:O	2.44	0.51
1:C:441:SER:O	1:C:446:ARG:NH2	2.44	0.51
1:D:606:ILE:HA	1:D:609:ILE:HG22	1.93	0.51
1:B:225:GLU:O	1:B:229:SER:OG	2.28	0.51
1:A:315:ARG:NH2	1:A:353:CYS:SG	2.84	0.51
1:A:412:GLY:N	1:B:247:GLU:OE2	2.44	0.51
1:A:160:ARG:NE	1:A:162:SER:OG	2.45	0.50
1:A:441:SER:O	1:A:446:ARG:NH2	2.44	0.50
1:C:494:LEU:HD23	1:C:575:LEU:HD13	1.93	0.50
1:A:494:LEU:HD23	1:A:575:LEU:HD13	1.93	0.49
1:C:579:VAL:HG13	1:D:631:ALA:HB1	1.94	0.49
1:B:606:ILE:HA	1:B:609:ILE:HG22	1.93	0.49
1:D:492:GLN:HE21	1:D:494:LEU:HG	1.77	0.49
1:B:249:ARG:HG2	1:B:297:GLN:HE21	1.78	0.49
1:D:249:ARG:HG2	1:D:297:GLN:HE21	1.78	0.49
1:A:287:LEU:HD23	1:A:289:LEU:H	1.77	0.49
1:A:463:TRP:HA	1:A:467:GLY:HA3	1.94	0.49
1:B:492:GLN:HE21	1:B:494:LEU:HG	1.77	0.49
1:A:454:PRO:O	1:A:458:LEU:N	2.38	0.48
1:B:760:GLU:OE2	1:B:779:ARG:NE	2.44	0.48
1:C:287:LEU:HD23	1:C:289:LEU:H	1.77	0.48
1:D:256:LEU:O	1:D:260:GLN:NE2	2.47	0.48
1:C:160:ARG:NE	1:C:162:SER:OG	2.45	0.48
1:C:254:VAL:HG11	1:C:300:ILE:HG23	1.95	0.48
1:B:256:LEU:O	1:B:260:GLN:NE2	2.47	0.48
1:C:342:VAL:HG12	1:C:385:ILE:HD13	1.96	0.48
1:A:683:LEU:HD13	1:A:685:MET:HB2	1.95	0.48
1:B:342:VAL:HG12	1:B:385:ILE:HD13	1.96	0.48
1:A:160:ARG:NH1	1:A:165:ASP:OD2	2.44	0.48
1:B:636:LEU:O	1:B:661:ARG:NH1	2.44	0.48
1:C:160:ARG:NH1	1:C:165:ASP:OD2	2.44	0.48
1:C:463:TRP:HA	1:C:467:GLY:HA3	1.94	0.48
1:C:502:TYR:HD1	1:C:507:ASP:HB3	1.78	0.48
1:D:342:VAL:HG12	1:D:385:ILE:HD13	1.96	0.48
1:B:613:ASP:OD1	1:B:616:ARG:NH1	2.47	0.48
1:C:683:LEU:HD13	1:C:685:MET:HB2	1.95	0.48
1:D:524:PHE:HE1	2:D:1201:XS9:C17	2.27	0.48
1:A:691:TYR:OH	1:D:572:GLU:OE1	2.32	0.48
1:D:613:ASP:OD1	1:D:616:ARG:NH1	2.47	0.47
1:A:342:VAL:HG12	1:A:385:ILE:HD13	1.95	0.47
1:B:504:THR:HG22	1:B:506:VAL:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:PHE:HE1	2:B:1201:XS9:C17	2.27	0.47
1:B:333:ASP:N	1:B:338:ASN:OD1	2.46	0.47
1:A:439:TYR:HE1	1:A:739:THR:HG23	1.80	0.47
1:A:502:TYR:HD1	1:A:507:ASP:HB3	1.79	0.47
1:C:439:TYR:HE1	1:C:739:THR:HG23	1.80	0.47
1:D:504:THR:HG22	1:D:506:VAL:H	1.79	0.47
1:D:556:TYR:HB2	1:D:584:LEU:HD12	1.97	0.47
1:A:664:GLU:O	1:A:666:PHE:N	2.41	0.47
1:A:766:LYS:HA	1:A:772:PRO:HA	1.96	0.47
1:C:766:LYS:HA	1:C:772:PRO:HA	1.96	0.47
1:D:333:ASP:N	1:D:338:ASN:OD1	2.46	0.47
1:D:636:LEU:O	1:D:661:ARG:NH1	2.44	0.47
1:A:638:PRO:HD3	1:A:690:LYS:HD2	1.96	0.46
1:B:441:SER:H	1:B:446:ARG:HH21	1.63	0.46
1:D:441:SER:H	1:D:446:ARG:HH21	1.63	0.46
1:B:556:TYR:HB2	1:B:584:LEU:HD12	1.97	0.46
1:D:760:GLU:OE2	1:D:779:ARG:NE	2.44	0.46
1:A:254:VAL:HG11	1:A:300:ILE:HG23	1.96	0.46
1:C:441:SER:HB3	1:C:446:ARG:HE	1.81	0.46
1:A:243:HIS:CE1	1:A:268:ALA:HB2	2.51	0.46
1:C:454:PRO:O	1:C:458:LEU:N	2.38	0.46
1:C:638:PRO:HD3	1:C:690:LYS:HD2	1.96	0.46
1:B:356:LEU:HB3	1:B:357:PHE:H	1.63	0.46
1:D:246:ILE:HG23	1:D:300:ILE:HG21	1.98	0.46
1:A:228:ASN:ND2	1:A:262:ALA:O	2.49	0.45
1:A:317:GLN:HB3	1:A:321:GLY:HA2	1.98	0.45
1:A:441:SER:HB3	1:A:446:ARG:HE	1.80	0.45
1:A:579:VAL:HG13	1:B:631:ALA:HB1	1.98	0.45
1:B:283:TYR:OH	1:B:322:ASN:ND2	2.38	0.45
1:B:246:ILE:HG23	1:B:300:ILE:HG21	1.98	0.45
1:D:318:ASP:OD1	1:D:322:ASN:N	2.49	0.45
1:D:283:TYR:OH	1:D:322:ASN:ND2	2.38	0.45
1:C:228:ASN:ND2	1:C:262:ALA:O	2.49	0.45
1:C:356:LEU:HB3	1:C:357:PHE:H	1.70	0.45
1:A:786:SER:OG	1:A:787:HIS:N	2.49	0.45
1:B:192:LYS:HG3	1:B:196:PRO:HB2	1.98	0.45
1:A:609:ILE:HG12	1:A:722:VAL:HG21	1.99	0.45
1:C:609:ILE:HG12	1:C:722:VAL:HG21	1.99	0.45
1:D:192:LYS:HG3	1:D:196:PRO:HB2	1.98	0.45
1:C:317:GLN:HB3	1:C:321:GLY:HA2	1.98	0.44
1:B:243:HIS:CE1	1:B:268:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:HD21	2:A:1201:XS9:C39	2.31	0.44
1:C:243:HIS:CE1	1:C:268:ALA:HB2	2.51	0.44
1:C:786:SER:OG	1:C:787:HIS:N	2.49	0.44
1:D:704:ILE:HG13	1:D:705:LEU:HD22	2.00	0.44
1:A:249:ARG:HG2	1:A:297:GLN:HE21	1.83	0.44
1:B:704:ILE:HG13	1:B:705:LEU:HD22	2.00	0.44
1:D:243:HIS:CE1	1:D:268:ALA:HB2	2.53	0.44
1:C:664:GLU:O	1:C:666:PHE:N	2.41	0.44
1:C:474:ASN:HD21	2:C:1201:XS9:C39	2.31	0.44
1:B:318:ASP:OD1	1:B:322:ASN:N	2.49	0.44
1:A:614:LEU:HG	1:B:709:LEU:HD21	1.99	0.44
1:C:414:VAL:HG21	1:D:281:TYR:HB3	1.98	0.44
1:D:389:ILE:HG23	1:D:392:ARG:HH12	1.83	0.44
1:B:178:LYS:NZ	1:B:184:GLU:OE1	2.40	0.43
1:C:249:ARG:HG2	1:C:297:GLN:HE21	1.83	0.43
1:D:387:GLN:HG2	1:D:452:VAL:HG13	2.00	0.43
1:B:387:GLN:HG2	1:B:452:VAL:HG13	2.01	0.43
1:C:489:ALA:HB2	1:C:582:LEU:HD21	2.00	0.43
1:C:675:LYS:HD3	1:C:678:ILE:HD11	2.00	0.43
1:A:489:ALA:HB2	1:A:582:LEU:HD21	2.00	0.43
1:A:675:LYS:HD3	1:A:678:ILE:HD11	2.00	0.43
1:B:173:LEU:HA	1:B:178:LYS:HB2	2.01	0.43
1:B:571:ILE:HG22	1:B:573:ALA:H	1.84	0.43
1:D:234:ILE:HG22	1:D:237:ARG:HH21	1.84	0.43
1:A:289:LEU:HD11	1:A:301:VAL:HG13	2.01	0.43
1:B:289:LEU:HD21	1:B:314:MET:HG2	2.01	0.43
2:A:1201:XS9:C48	2:A:1201:XS9:C22	2.97	0.43
1:B:255:GLU:HG2	1:B:303:TYR:CZ	2.54	0.42
1:B:339:THR:HG21	1:B:384:GLY:HA3	2.01	0.42
1:B:389:ILE:HG23	1:B:392:ARG:HH12	1.83	0.42
1:D:339:THR:HG21	1:D:384:GLY:HA3	2.01	0.42
1:B:639:CYS:N	1:B:660:CYS:SG	2.92	0.42
1:C:214:LEU:HD11	1:C:256:LEU:HD21	2.01	0.42
1:C:289:LEU:HD11	1:C:301:VAL:HG13	2.01	0.42
1:D:255:GLU:HG2	1:D:303:TYR:CZ	2.54	0.42
1:A:628:TYR:CE1	1:D:583:VAL:HG23	2.54	0.42
1:A:720:GLU:HB2	1:D:726:SER:HB2	2.01	0.42
1:A:214:LEU:HD11	1:A:256:LEU:HD21	2.01	0.42
1:A:771:THR:HA	1:A:772:PRO:HD3	1.90	0.42
1:D:662:ASP:N	1:D:665:THR:OG1	2.44	0.42
1:C:757:ARG:HA	1:C:757:ARG:HD2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:THR:HA	1:D:233:ASP:HB2	2.02	0.42
1:D:632:LEU:HD11	1:D:698:LEU:HB3	2.02	0.42
1:D:639:CYS:N	1:D:660:CYS:SG	2.92	0.42
1:B:505:THR:HA	1:B:508:TYR:HB2	2.00	0.42
1:C:612:LYS:O	1:C:616:ARG:NH2	2.53	0.42
2:C:1201:XS9:C22	2:C:1201:XS9:C48	2.97	0.42
1:D:289:LEU:HD21	1:D:314:MET:HG2	2.01	0.42
1:D:505:THR:HA	1:D:508:TYR:HB2	2.00	0.42
1:A:602:TYR:HB2	1:B:616:ARG:HD2	2.01	0.42
1:A:612:LYS:O	1:A:616:ARG:NH2	2.53	0.42
1:A:717:LEU:HD22	1:D:602:TYR:HD1	1.85	0.42
1:B:234:ILE:HG22	1:B:237:ARG:HH21	1.84	0.42
1:A:628:TYR:HB3	1:A:632:LEU:HD13	2.01	0.41
1:B:190:THR:HA	1:B:233:ASP:HB2	2.02	0.41
1:C:517:THR:O	1:C:521:GLY:N	2.49	0.41
1:C:306:GLU:HA	1:C:311:LYS:HZ1	1.85	0.41
1:D:173:LEU:O	1:D:178:LYS:N	2.50	0.41
1:B:243:HIS:CD2	1:B:288:PRO:HG3	2.55	0.41
1:C:202:LEU:HD12	1:C:207:ASN:HB2	2.01	0.41
1:D:173:LEU:HA	1:D:178:LYS:HB2	2.01	0.41
1:D:243:HIS:CD2	1:D:288:PRO:HG3	2.55	0.41
1:D:362:LEU:HD22	1:D:362:LEU:HA	1.91	0.41
1:D:571:ILE:HG22	1:D:573:ALA:H	1.84	0.41
1:A:202:LEU:HD12	1:A:207:ASN:HB2	2.01	0.41
1:A:517:THR:O	1:A:521:GLY:N	2.49	0.41
1:B:632:LEU:HD11	1:B:698:LEU:HB3	2.02	0.41
1:D:524:PHE:O	1:D:528:ASN:ND2	2.54	0.41
1:B:171:PRO:O	1:B:175:THR:N	2.54	0.41
1:C:628:TYR:HB3	1:C:632:LEU:HD13	2.01	0.41
1:D:355:ARG:NH2	1:D:396:ASP:OD2	2.54	0.41
1:C:228:ASN:ND2	1:C:263:ASP:HB2	2.36	0.41
1:C:415:TYR:HE2	1:C:788:TRP:HB3	1.86	0.41
1:D:171:PRO:O	1:D:175:THR:N	2.54	0.41
1:B:355:ARG:NH2	1:B:396:ASP:OD2	2.54	0.41
1:B:524:PHE:O	1:B:528:ASN:ND2	2.54	0.41
1:A:306:GLU:HA	1:A:311:LYS:HZ1	1.86	0.41
1:B:307:ASN:ND2	1:B:310:LYS:O	2.46	0.41
1:B:160:ARG:HG3	1:B:162:SER:H	1.86	0.40
1:A:228:ASN:ND2	1:A:263:ASP:HB2	2.36	0.40
1:B:173:LEU:O	1:B:178:LYS:N	2.50	0.40
1:C:227:ILE:HD12	1:C:262:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:LEU:HG	1:D:402:LEU:HD13	2.03	0.40
1:A:415:TYR:HE2	1:A:788:TRP:HB3	1.86	0.40
1:B:220:THR:OG1	1:B:222:ASN:OD1	2.28	0.40
1:B:287:LEU:HD23	1:B:289:LEU:H	1.86	0.40
1:B:350:LEU:HG	1:B:402:LEU:HD13	2.03	0.40
1:C:670:LEU:HD13	1:C:670:LEU:HA	1.94	0.40
1:D:606:ILE:H	1:D:606:ILE:HG13	1.70	0.40
1:B:657:TYR:HE1	1:B:665:THR:HG23	1.87	0.40
1:C:545:ILE:HD13	1:C:735:LEU:HD22	2.03	0.40
1:B:599:THR:HA	1:B:602:TYR:CE1	2.57	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	628/1132 (56%)	529 (84%)	95 (15%)	4 (1%)	22	50
1	B	613/1132 (54%)	553 (90%)	56 (9%)	4 (1%)	19	47
1	C	628/1132 (56%)	529 (84%)	95 (15%)	4 (1%)	22	50
1	D	613/1132 (54%)	552 (90%)	57 (9%)	4 (1%)	19	47
All	All	2482/4528 (55%)	2163 (87%)	303 (12%)	16 (1%)	24	50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	SER
1	A	665	THR
1	C	663	SER
1	C	665	THR
1	A	335	THR

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Mol	Chain	Res	Type
1	B	707	PHE
1	C	335	THR
1	D	707	PHE
1	A	454	PRO
1	B	452	VAL
1	B	453	GLU
1	C	454	PRO
1	D	452	VAL
1	D	453	GLU
1	B	285	GLY
1	D	285	GLY

5.3.2 Protein sidechains (i)

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	558/987 (56%)	548 (98%)	10 (2%)	54	73
1	B	546/987 (55%)	534 (98%)	12 (2%)	47	68
1	C	558/987 (56%)	548 (98%)	10 (2%)	54	73
1	D	546/987 (55%)	534 (98%)	12 (2%)	47	68
All	All	2208/3948 (56%)	2164 (98%)	44 (2%)	50	71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	232	ARG
1	A	338	ASN
1	A	456	ASN
1	A	474	ASN
1	A	494	LEU
1	A	528	ASN
1	A	535	LYS
1	A	683	LEU
1	A	712	ASN

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Mol	Chain	Res	Type
1	B	150	ASN
1	B	207	ASN
1	B	232	ARG
1	B	338	ASN
1	B	361	ASN
1	B	456	ASN
1	B	494	LEU
1	B	608	LYS
1	B	670	LEU
1	B	680	MET
1	B	686	LEU
1	B	766	LYS
1	C	207	ASN
1	C	232	ARG
1	C	338	ASN
1	C	456	ASN
1	C	474	ASN
1	C	494	LEU
1	C	528	ASN
1	C	535	LYS
1	C	683	LEU
1	C	712	ASN
1	D	150	ASN
1	D	207	ASN
1	D	232	ARG
1	D	338	ASN
1	D	361	ASN
1	D	456	ASN
1	D	494	LEU
1	D	608	LYS
1	D	670	LEU
1	D	680	MET
1	D	686	LEU
1	D	766	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	207	ASN
1	A	260	GLN
1	A	456	ASN

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Mol	Chain	Res	Type
1	A	474	ASN
1	A	550	GLN
1	A	712	ASN
1	B	150	ASN
1	B	207	ASN
1	B	228	ASN
1	B	260	GLN
1	B	326	HIS
1	B	361	ASN
1	B	456	ASN
1	B	492	GLN
1	B	550	GLN
1	B	787	HIS
1	B	791	ASN
1	C	201	ASN
1	C	207	ASN
1	C	260	GLN
1	C	456	ASN
1	C	474	ASN
1	C	550	GLN
1	C	712	ASN
1	D	150	ASN
1	D	207	ASN
1	D	228	ASN
1	D	260	GLN
1	D	326	HIS
1	D	361	ASN
1	D	456	ASN
1	D	492	GLN
1	D	550	GLN

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	XS9	D	1201	-	46,51,51	0.53	1 (2%)	39,76,76	0.68	2 (5%)
2	XS9	A	1201	-	46,51,51	0.48	0	39,76,76	1.09	3 (7%)
2	XS9	C	1201	-	46,51,51	0.48	0	39,76,76	1.09	3 (7%)
2	XS9	B	1201	-	46,51,51	0.53	1 (2%)	39,76,76	0.68	2 (5%)

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	XS9	D	1201	-	-	15/29/108/108	0/4/4/4
2	XS9	A	1201	-	-	14/29/108/108	0/4/4/4
2	XS9	C	1201	-	-	15/29/108/108	0/4/4/4
2	XS9	B	1201	-	-	15/29/108/108	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	XS9	C15-C14	-2.88	1.49	1.55
2	D	1201	XS9	C15-C14	-2.86	1.49	1.55

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1201	XS9	C48-C14-C15	4.64	118.59	113.34
2	A	1201	XS9	C48-C14-C15	4.61	118.56	113.34
2	A	1201	XS9	C31-O35-C36	3.69	128.15	119.93
2	C	1201	XS9	C31-O35-C36	3.68	128.13	119.93
2	D	1201	XS9	C31-O35-C36	3.11	126.86	119.93
2	B	1201	XS9	C31-O35-C36	3.10	126.83	119.93
2	A	1201	XS9	C31-C30-C32	2.21	60.83	59.74
2	C	1201	XS9	C31-C30-C32	2.18	60.82	59.74
2	B	1201	XS9	C31-C30-C32	2.13	60.80	59.74
2	D	1201	XS9	C31-C30-C32	2.09	60.78	59.74

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	XS9	C17-C18-C28-O29
2	A	1201	XS9	C19-C18-C28-O29
2	A	1201	XS9	O37-C36-O35-C31
2	A	1201	XS9	C38-C36-O35-C31
2	B	1201	XS9	C17-C18-C28-O29
2	B	1201	XS9	C19-C18-C28-O29
2	B	1201	XS9	O37-C36-O35-C31
2	B	1201	XS9	C38-C36-O35-C31
2	C	1201	XS9	C17-C18-C28-O29
2	C	1201	XS9	C19-C18-C28-O29
2	C	1201	XS9	O37-C36-O35-C31
2	C	1201	XS9	C38-C36-O35-C31
2	D	1201	XS9	C17-C18-C28-O29
2	D	1201	XS9	C19-C18-C28-O29
2	D	1201	XS9	O37-C36-O35-C31
2	D	1201	XS9	C38-C36-O35-C31
2	A	1201	XS9	C07-C08-C09-C10
2	C	1201	XS9	C07-C08-C09-C10
2	A	1201	XS9	C04-C05-C06-C07
2	C	1201	XS9	C04-C05-C06-C07
2	A	1201	XS9	C39-C40-C41-C42
2	C	1201	XS9	C39-C40-C41-C42
2	A	1201	XS9	C42-C43-C44-C45
2	B	1201	XS9	C42-C43-C44-C45
2	C	1201	XS9	C42-C43-C44-C45
2	D	1201	XS9	C42-C43-C44-C45
2	B	1201	XS9	C04-C05-C06-C07
2	D	1201	XS9	C04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
2	B	1201	XS9	C43-C44-C45-C46
2	D	1201	XS9	C43-C44-C45-C46
2	A	1201	XS9	C38-C39-C40-C41
2	C	1201	XS9	C38-C39-C40-C41
2	A	1201	XS9	C40-C41-C42-C43
2	C	1201	XS9	C40-C41-C42-C43
2	B	1201	XS9	C40-C41-C42-C43
2	D	1201	XS9	C40-C41-C42-C43
2	D	1201	XS9	C38-C39-C40-C41
2	B	1201	XS9	C38-C39-C40-C41
2	A	1201	XS9	C43-C44-C45-C46
2	C	1201	XS9	C43-C44-C45-C46
2	B	1201	XS9	C36-C38-C39-C40
2	D	1201	XS9	C36-C38-C39-C40
2	B	1201	XS9	C01-C02-C03-C04
2	D	1201	XS9	C01-C02-C03-C04
2	B	1201	XS9	C05-C06-C07-C08
2	D	1201	XS9	C05-C06-C07-C08
2	D	1201	XS9	C39-C40-C41-C42
2	B	1201	XS9	C39-C40-C41-C42
2	A	1201	XS9	C13-C31-O35-C36
2	C	1201	XS9	C13-C31-O35-C36
2	A	1201	XS9	C01-C02-C03-C04
2	C	1201	XS9	C01-C02-C03-C04
2	C	1201	XS9	C06-C07-C08-C09
2	A	1201	XS9	C06-C07-C08-C09
2	B	1201	XS9	C31-C13-O12-C10
2	D	1201	XS9	C31-C13-O12-C10
2	B	1201	XS9	O35-C36-C38-C39
2	D	1201	XS9	O35-C36-C38-C39
2	C	1201	XS9	C08-C09-C10-O12

There are no ring outliers.

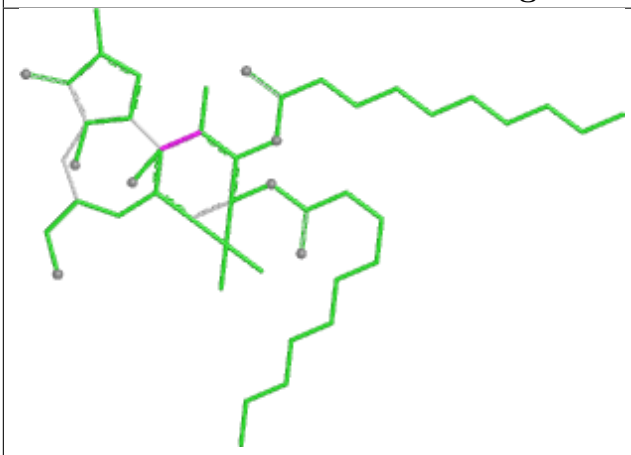
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1201	XS9	3	0
2	A	1201	XS9	2	0
2	C	1201	XS9	2	0
2	B	1201	XS9	3	0

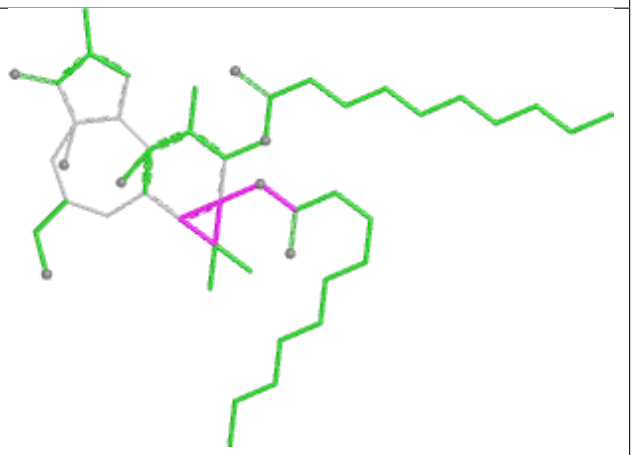
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

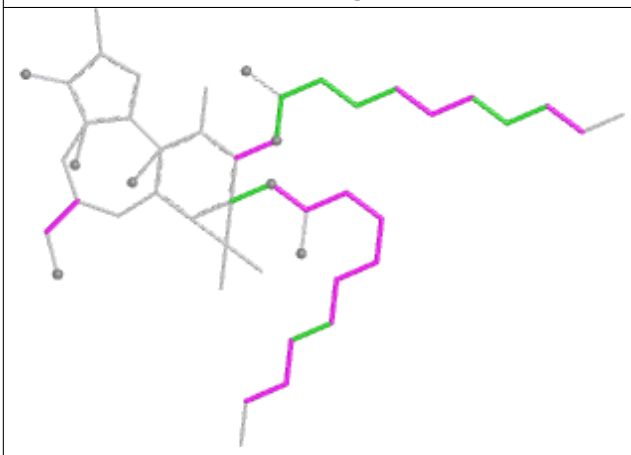
Ligand XS9 D 1201



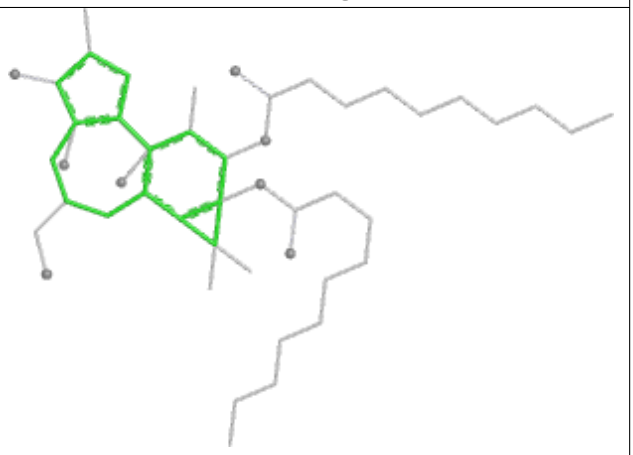
Bond lengths



Bond angles

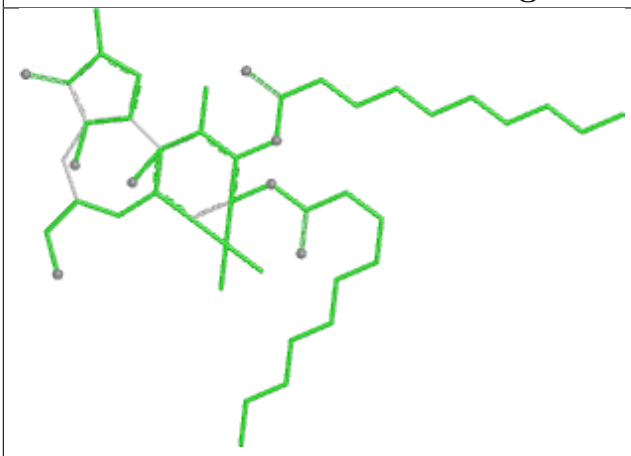


Torsions

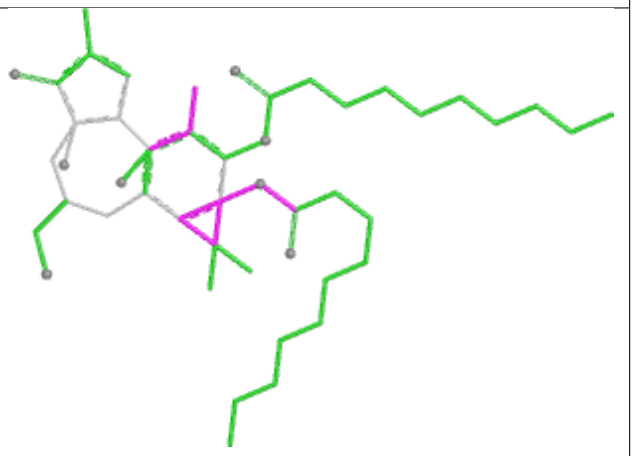


Rings

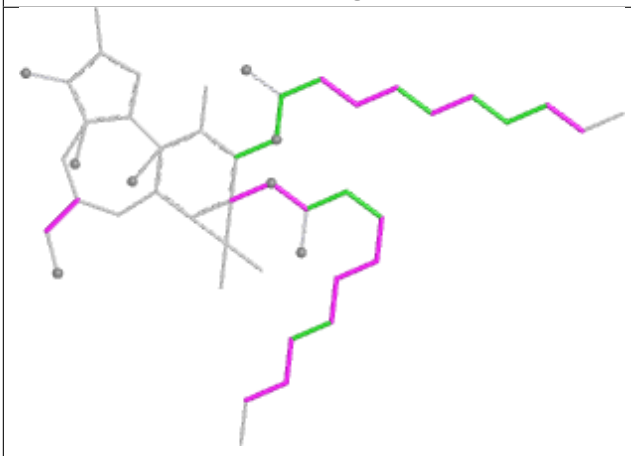
Ligand XS9 A 1201



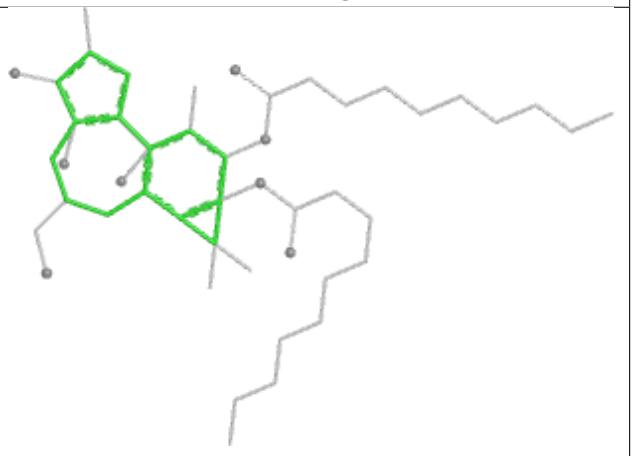
Bond lengths



Bond angles

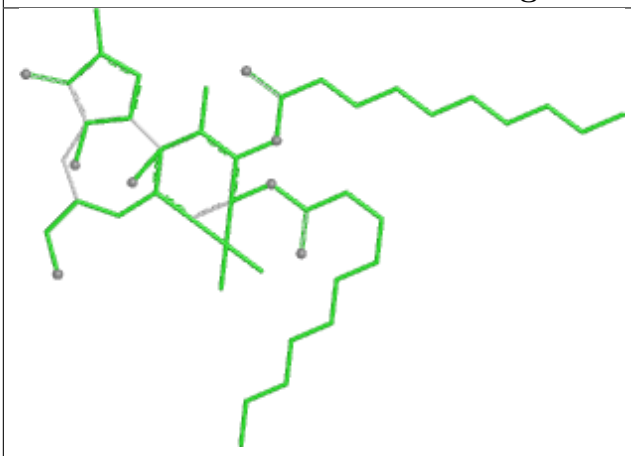


Torsions

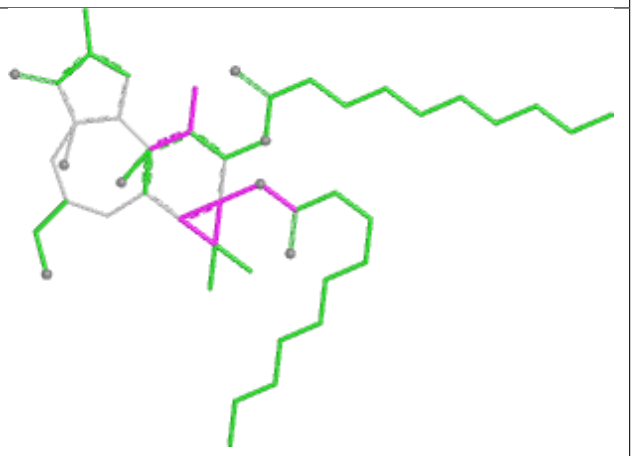


Rings

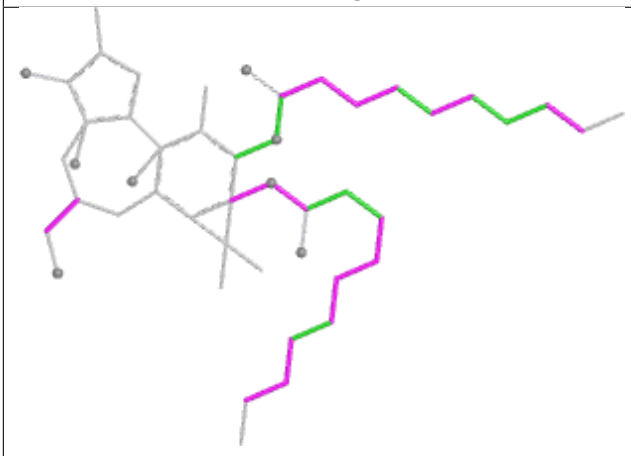
Ligand XS9 C 1201



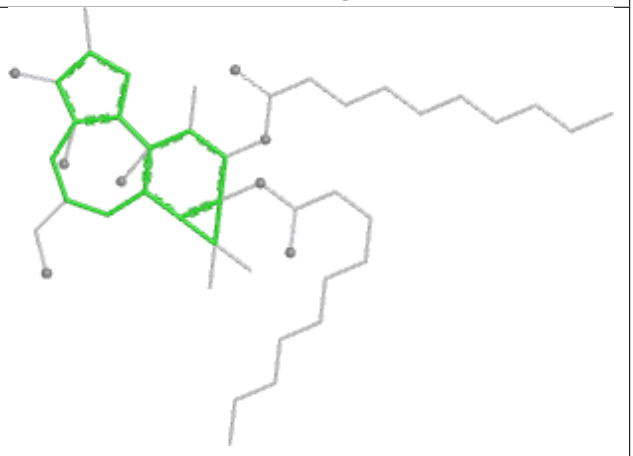
Bond lengths



Bond angles

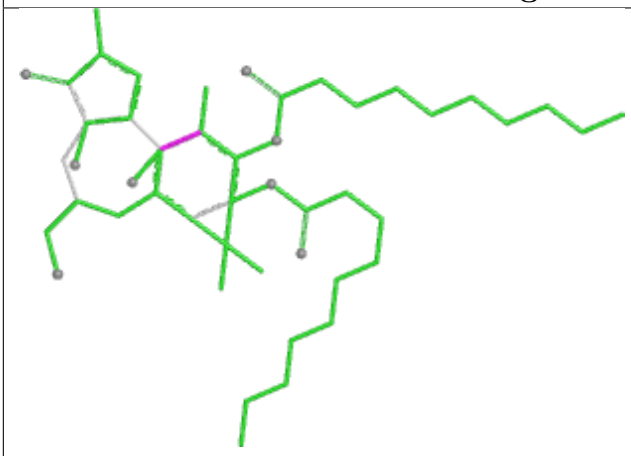


Torsions

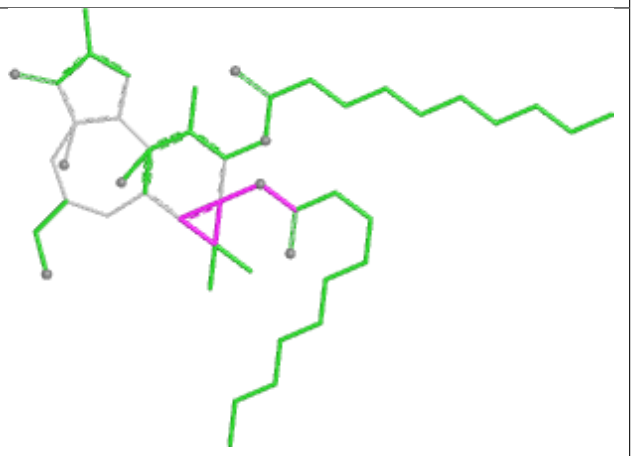


Rings

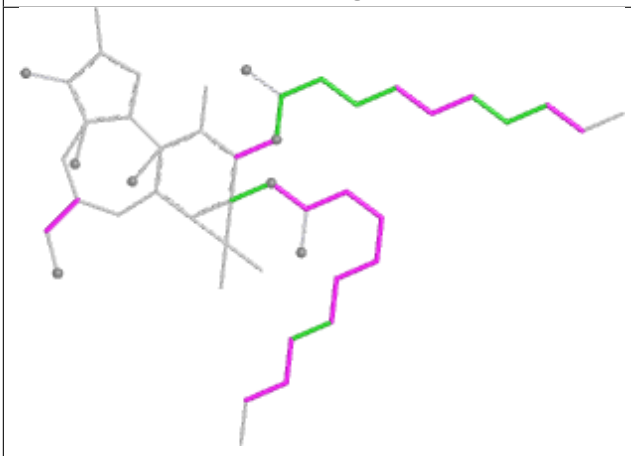
Ligand XS9 B 1201



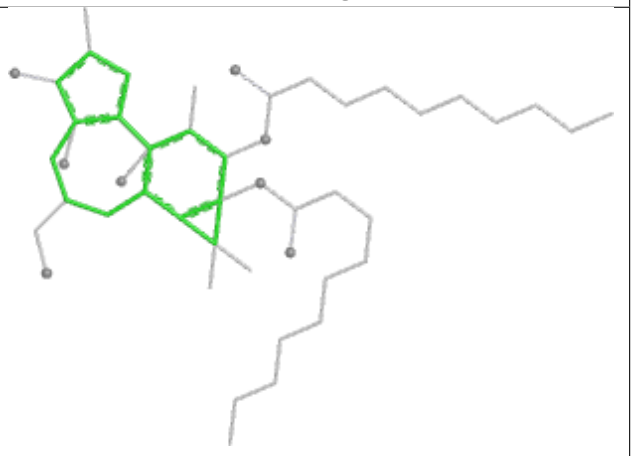
Bond lengths



Bond angles



Torsions



Rings

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.

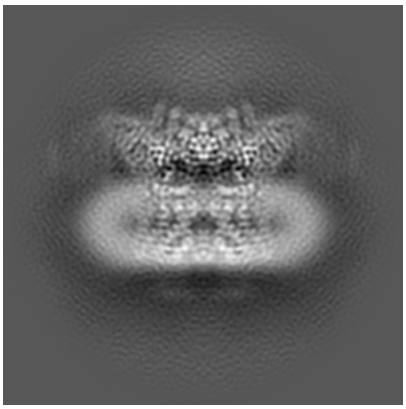
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40960. These allow visual inspection of the internal detail of the map and identification of artifacts.

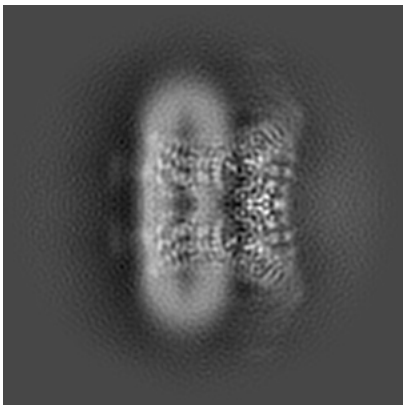
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

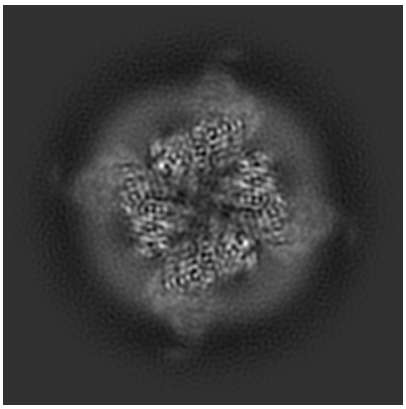
6.1.1 Primary map



X

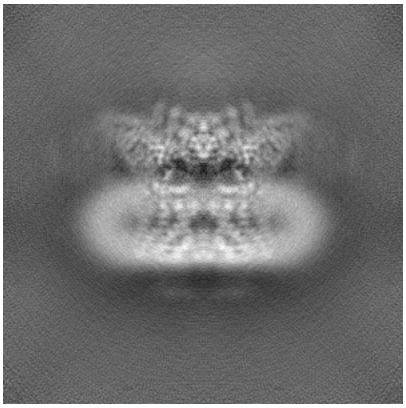


Y

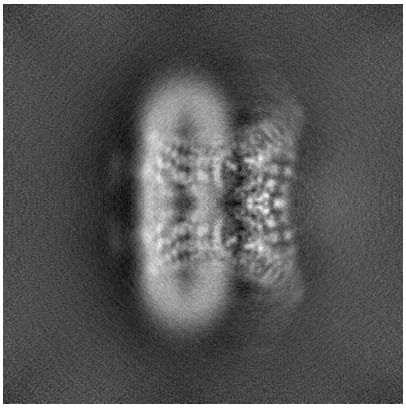


Z

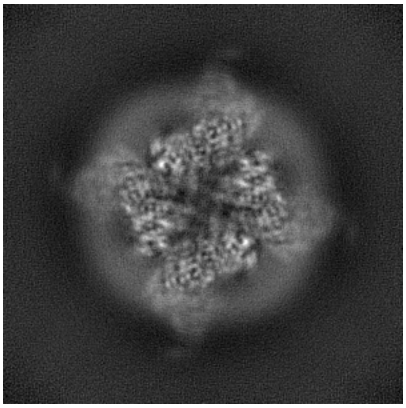
6.1.2 Raw map



X



Y

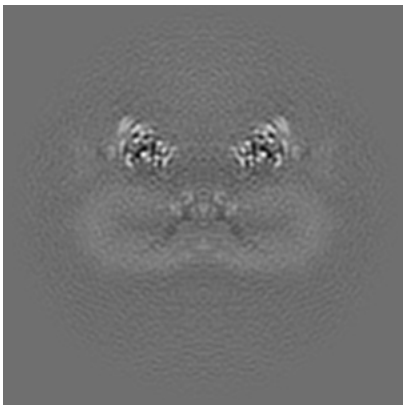


Z

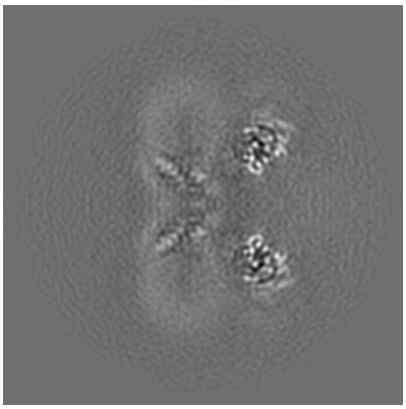
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

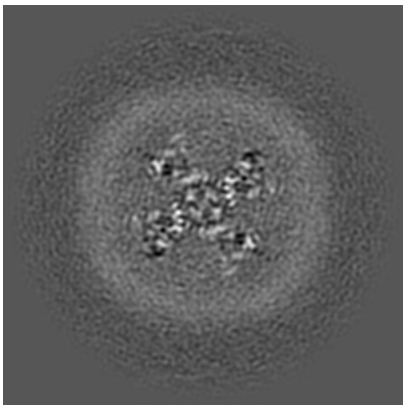
6.2.1 Primary map



X Index: 160

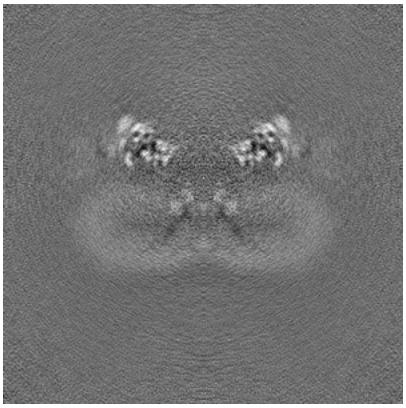


Y Index: 160

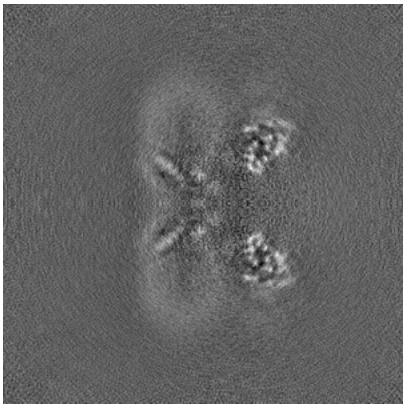


Z Index: 160

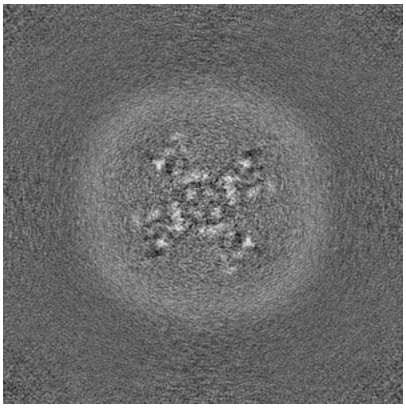
6.2.2 Raw map



X Index: 160



Y Index: 160

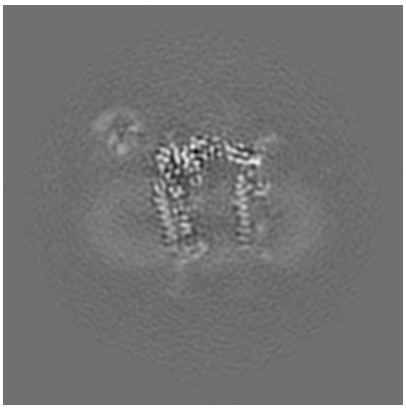


Z Index: 160

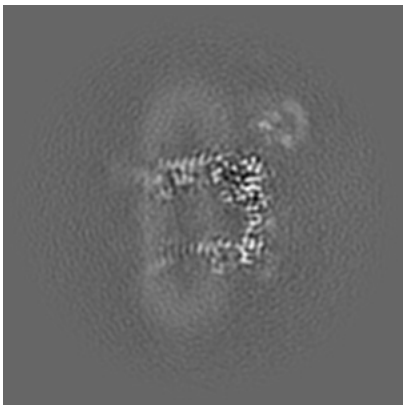
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

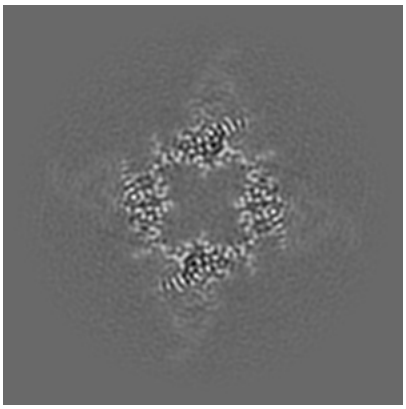
6.3.1 Primary map



X Index: 125

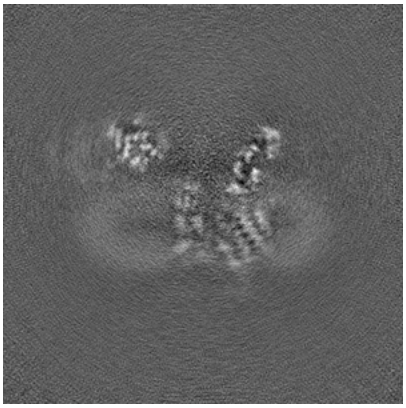


Y Index: 126

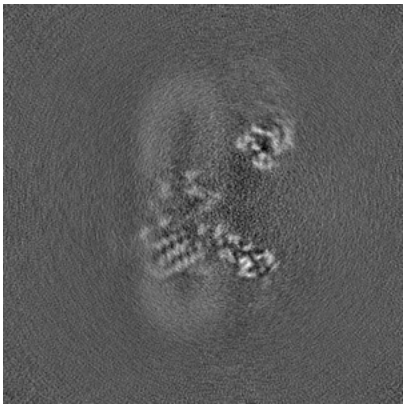


Z Index: 205

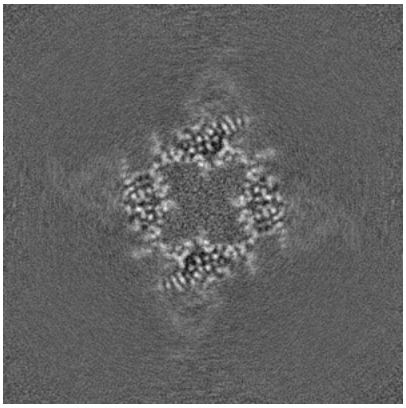
6.3.2 Raw map



X Index: 142



Y Index: 148

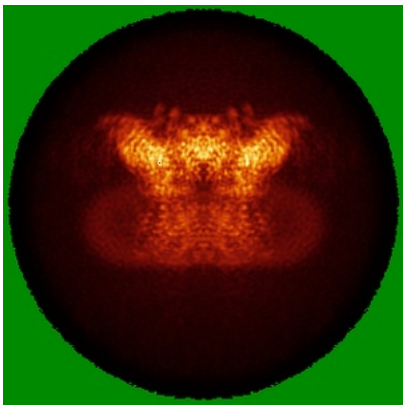


Z Index: 205

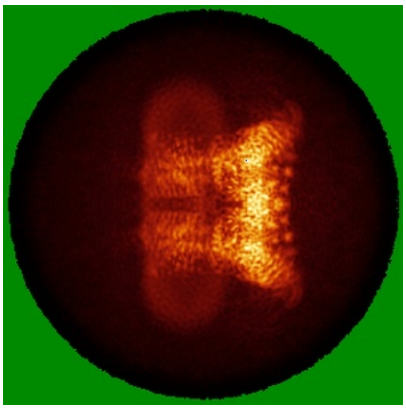
The images above show the largest variance slices of the map in three orthogonal directions.

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

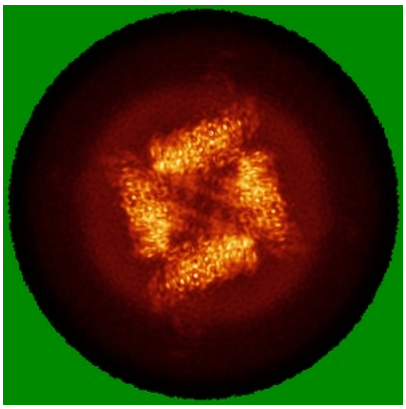
6.4.1 Primary map



X

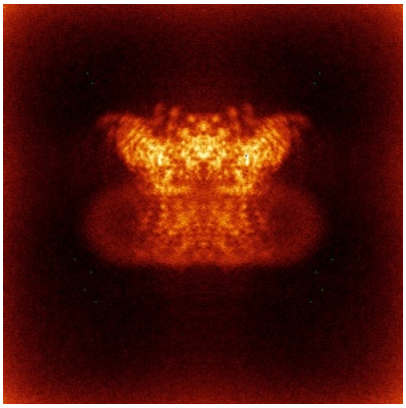


Y

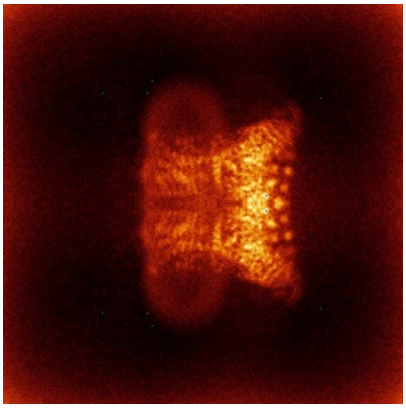


Z

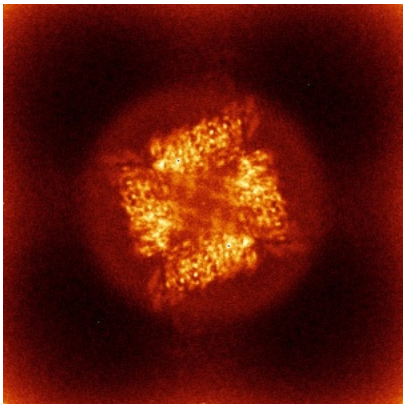
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. 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

X Y Z

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.

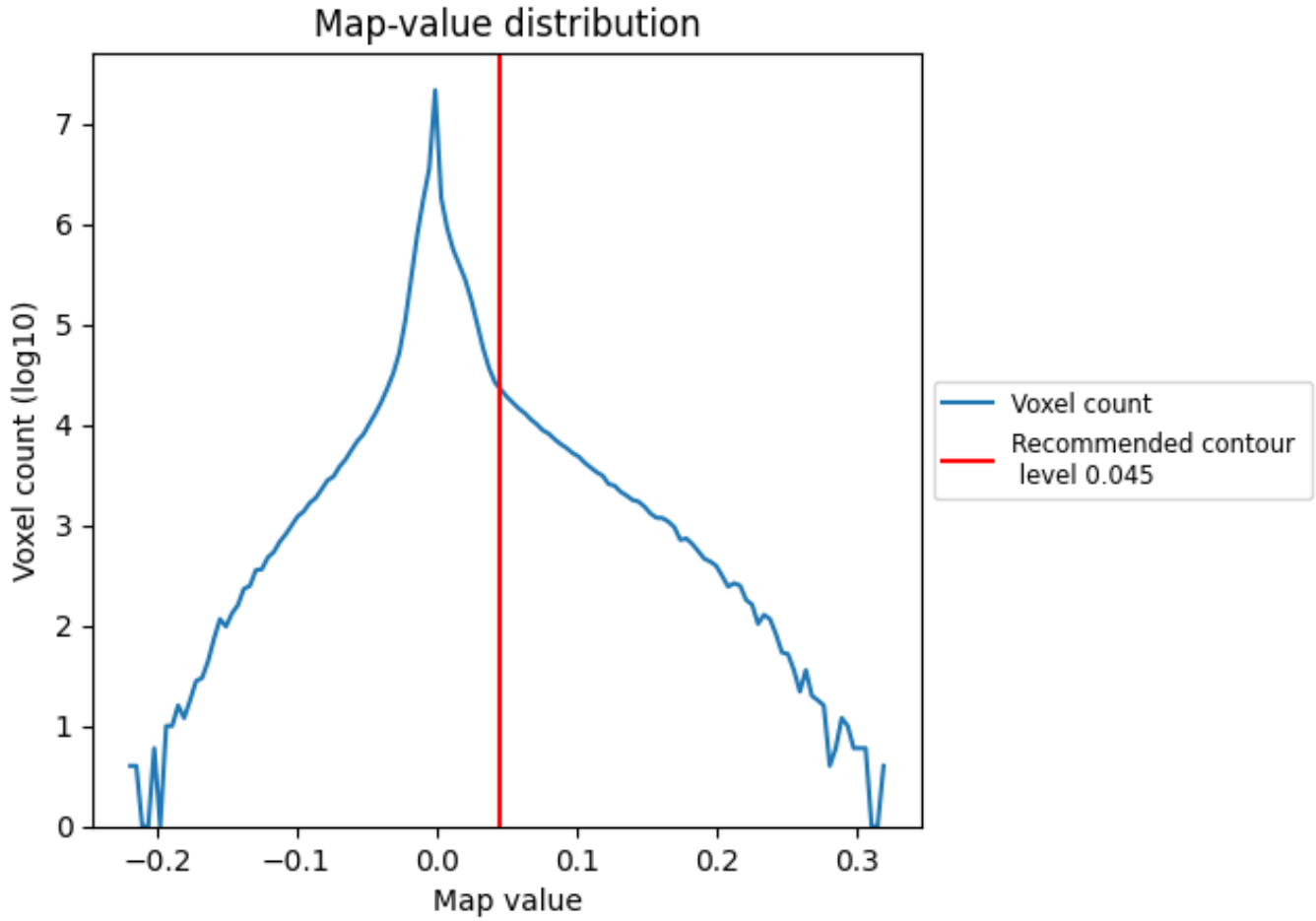
6.6 Mask visualisation (i)

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

7 Map analysis

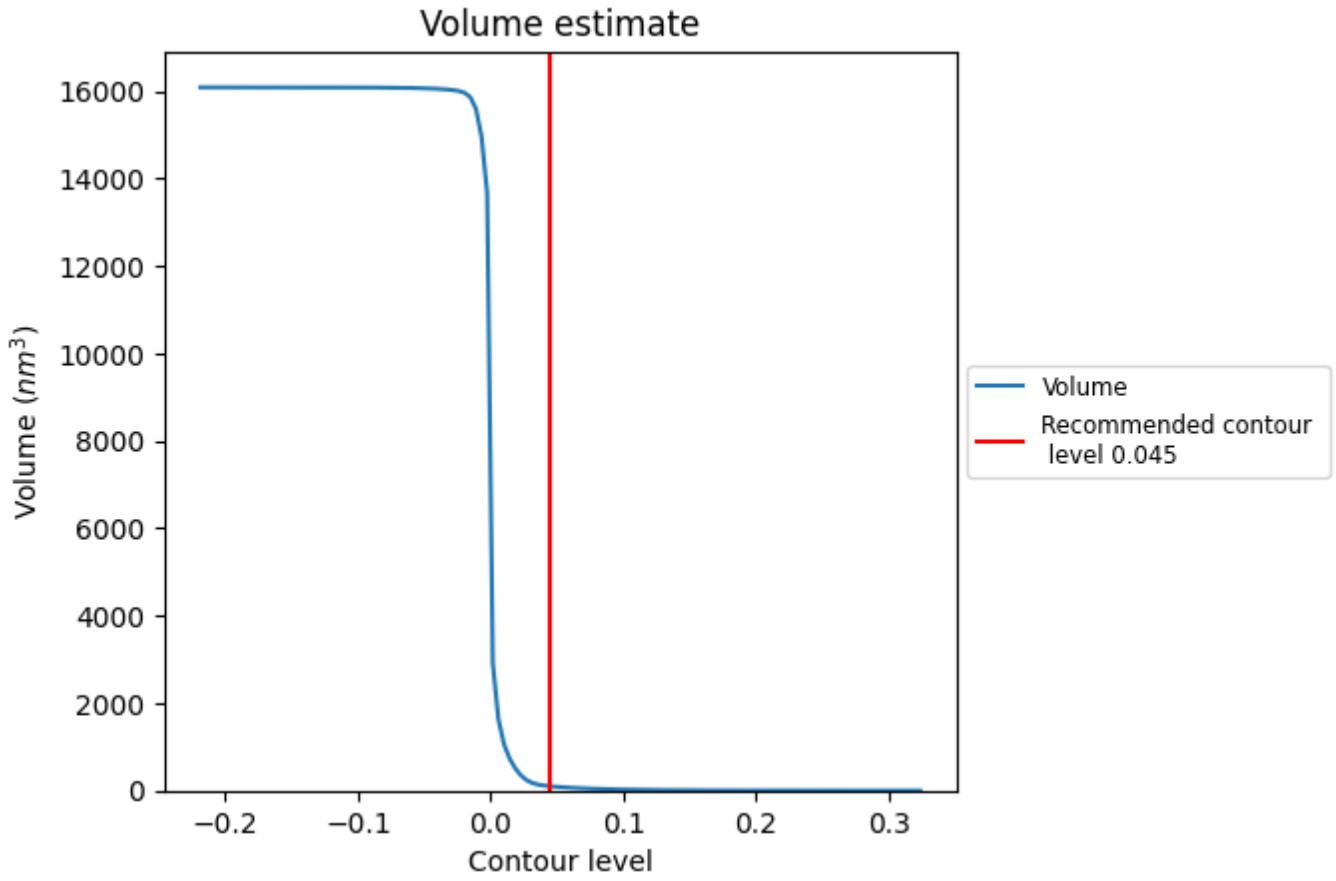
This section contains the results of statistical analysis of the map.

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.

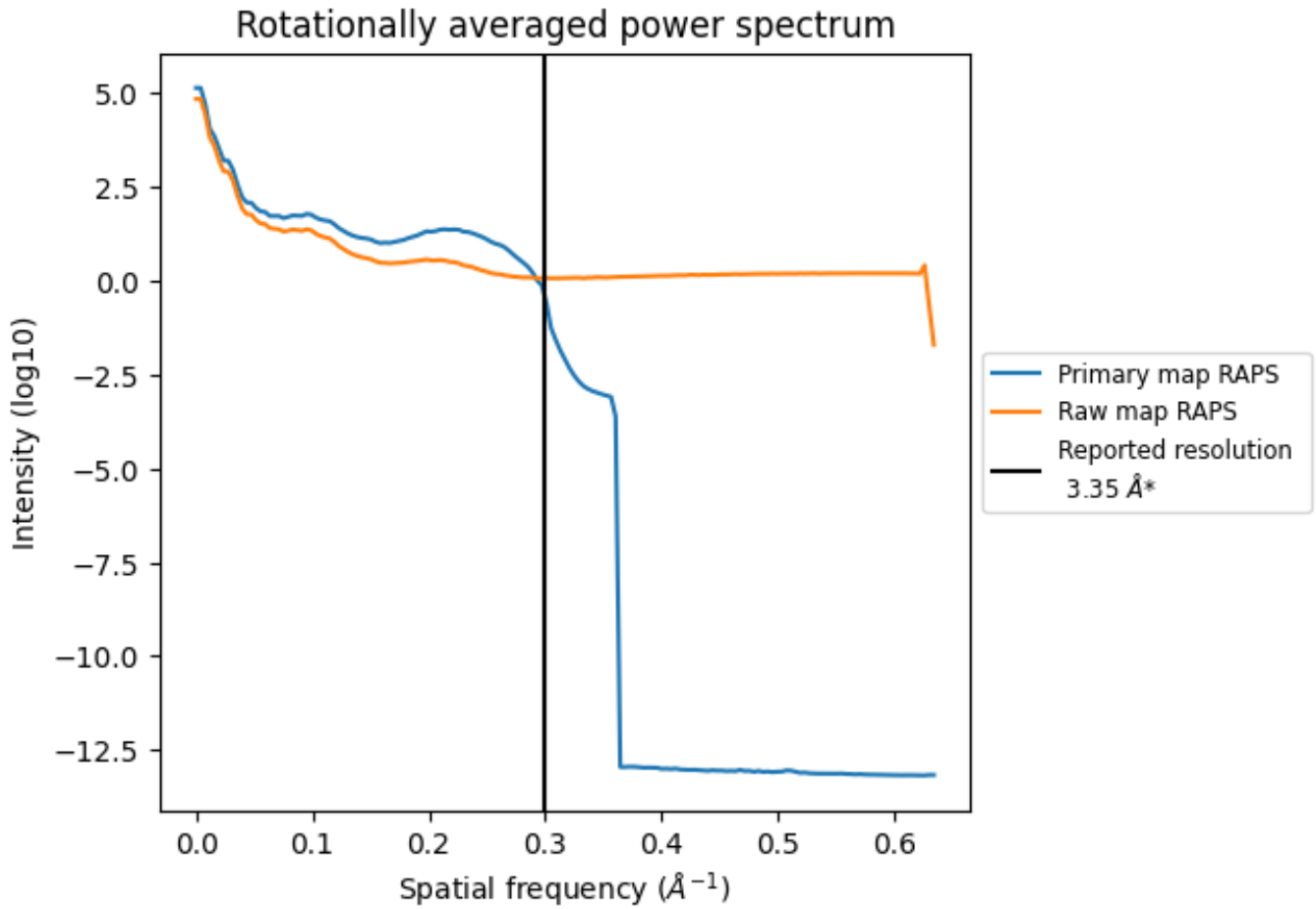
7.2 Volume estimate



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 88 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)

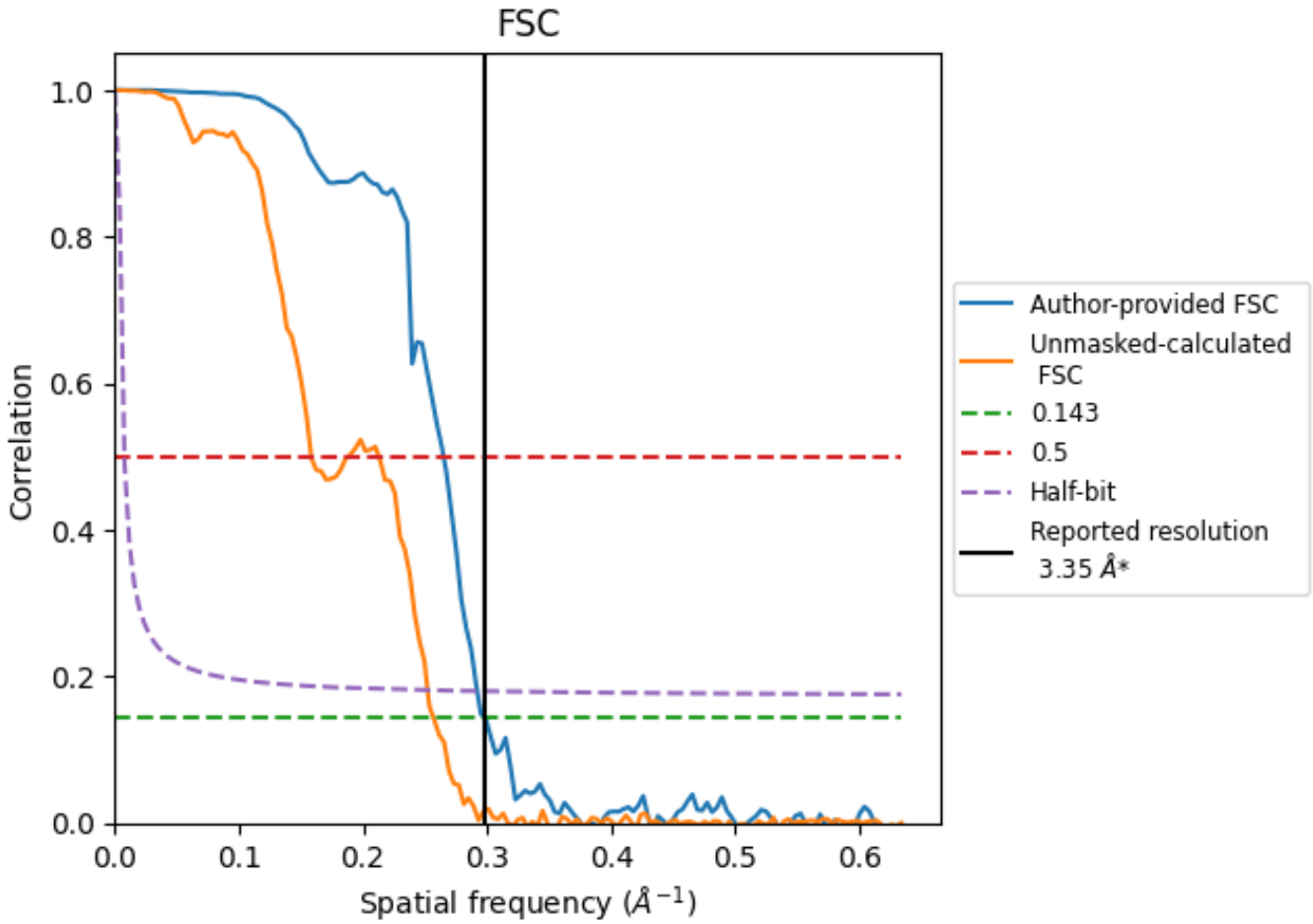


*Reported resolution corresponds to spatial frequency of 0.299 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8.2 Resolution estimates (i)

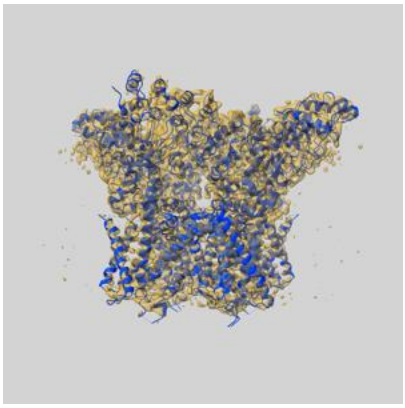
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.78	3.42
Unmasked-calculated*	3.89	6.32	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.35 by more than 10 %

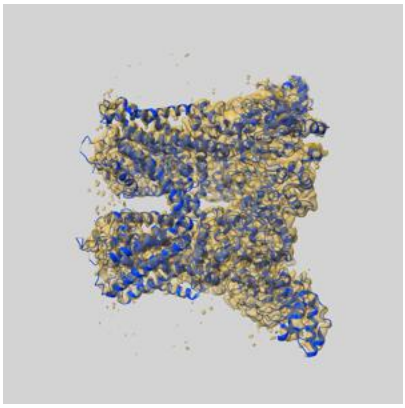
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40960 and PDB model 8T1D. Per-residue inclusion information can be found in section 3 on page 7.

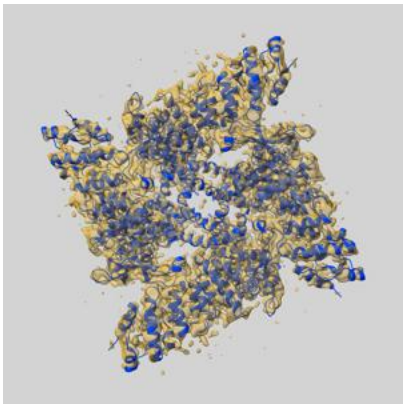
9.1 Map-model overlay



X



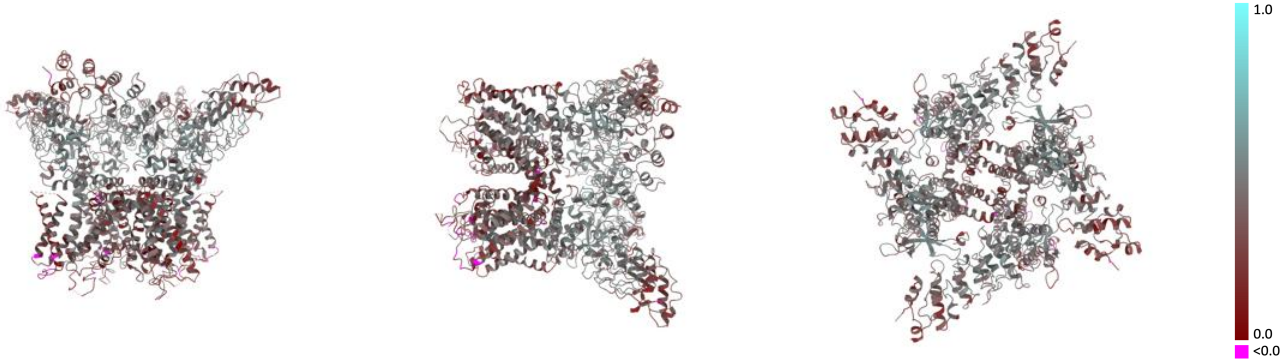
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

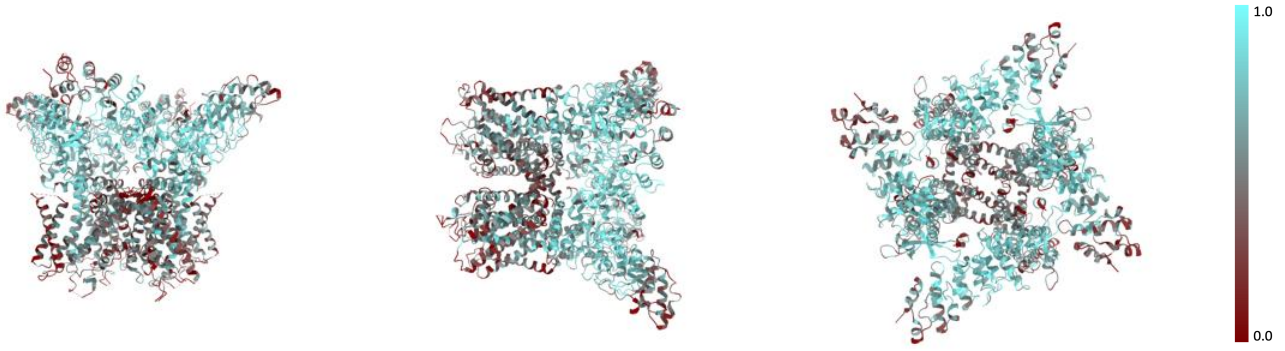
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

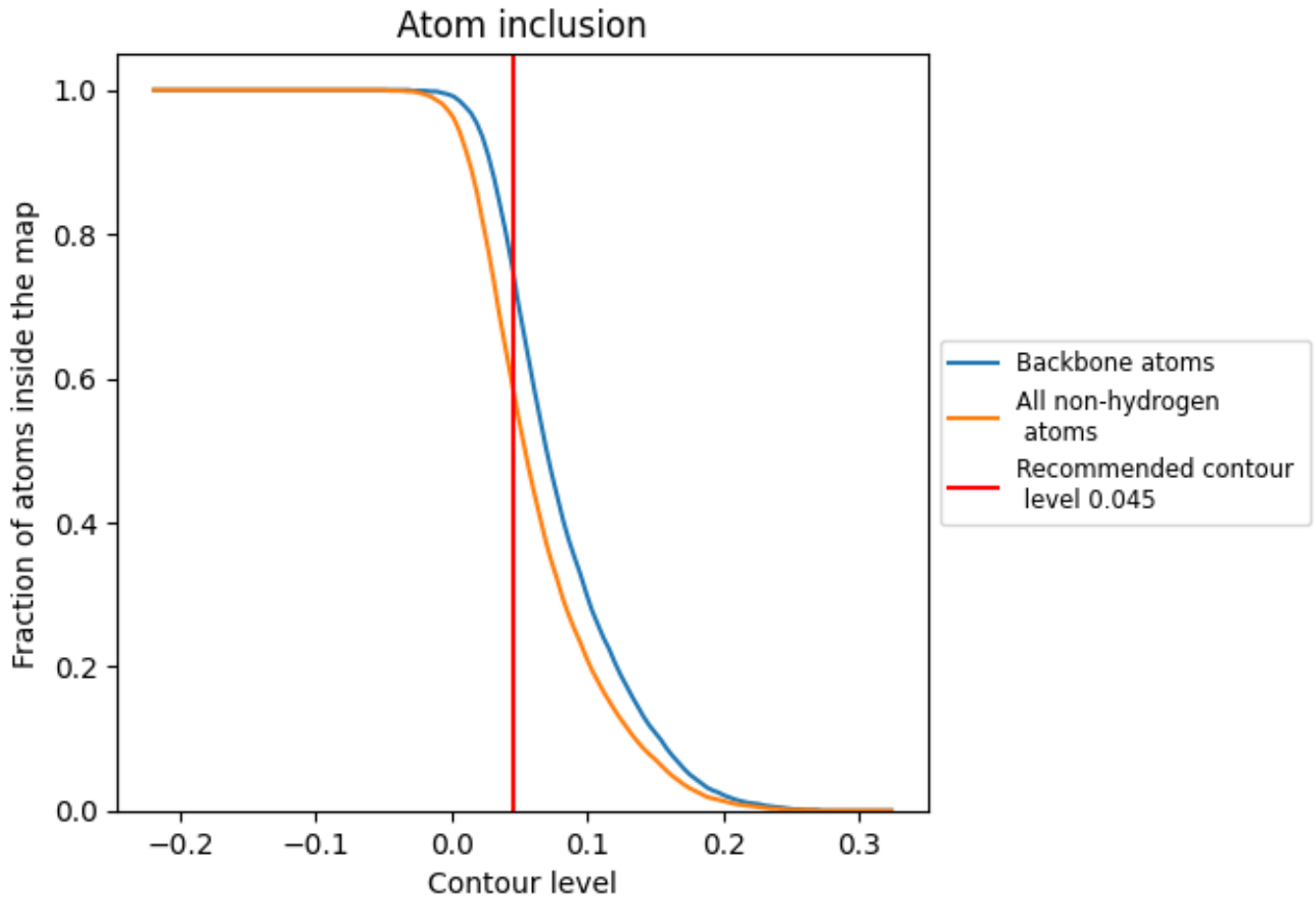
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 75% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5880	0.3920
A	0.5780	0.3940
B	0.6060	0.3990
C	0.5720	0.3880
D	0.5970	0.3880