



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:39 AM UTC

PDB ID : 8T1D / pdb_00008t1d
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

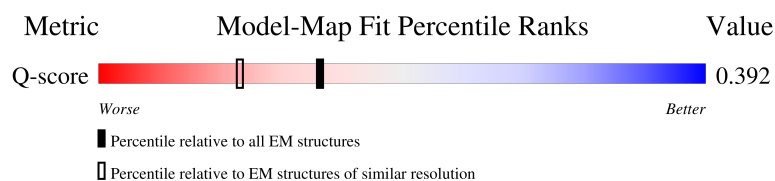
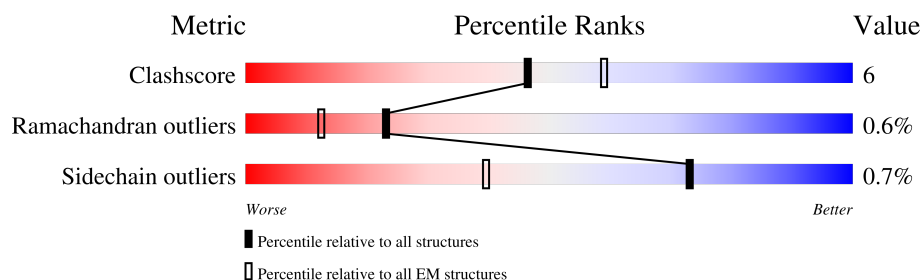
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14390 (2.85 - 3.85)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1132	14% 46% 9% 44%
1	B	1132	12% 44% 10% 45%
1	C	1132	15% 46% 9% 44%
1	D	1132	13% 44% 10% 45%

2 Entry composition [i](#)

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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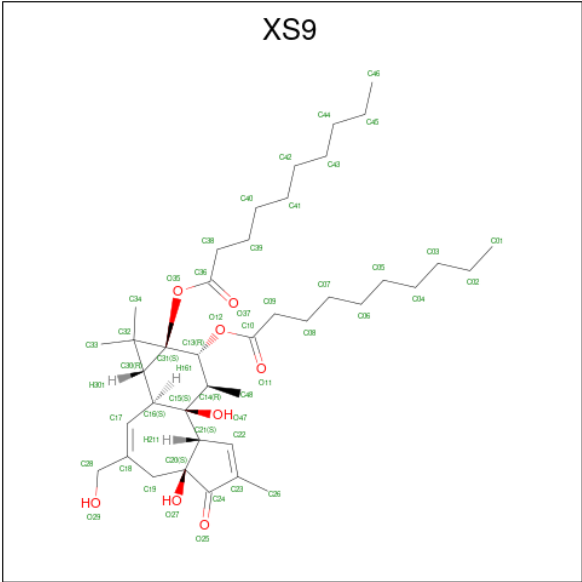
Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	PHE	-	expression tag	UNP C5MKY7
A	1131	GLU	-	expression tag	UNP C5MKY7
A	1132	LYS	-	expression tag	UNP C5MKY7
B	872	LEU	-	linker	UNP Q9HBA0
B	873	VAL	-	linker	UNP Q9HBA0
B	874	PRO	-	linker	UNP Q9HBA0
B	875	ARG	-	linker	UNP Q9HBA0
B	876	GLY	-	linker	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
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C	1120	SER	-	expression tag	UNP C5MKY7
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C	1122	LEU	-	expression tag	UNP C5MKY7
C	1123	ARG	-	expression tag	UNP C5MKY7

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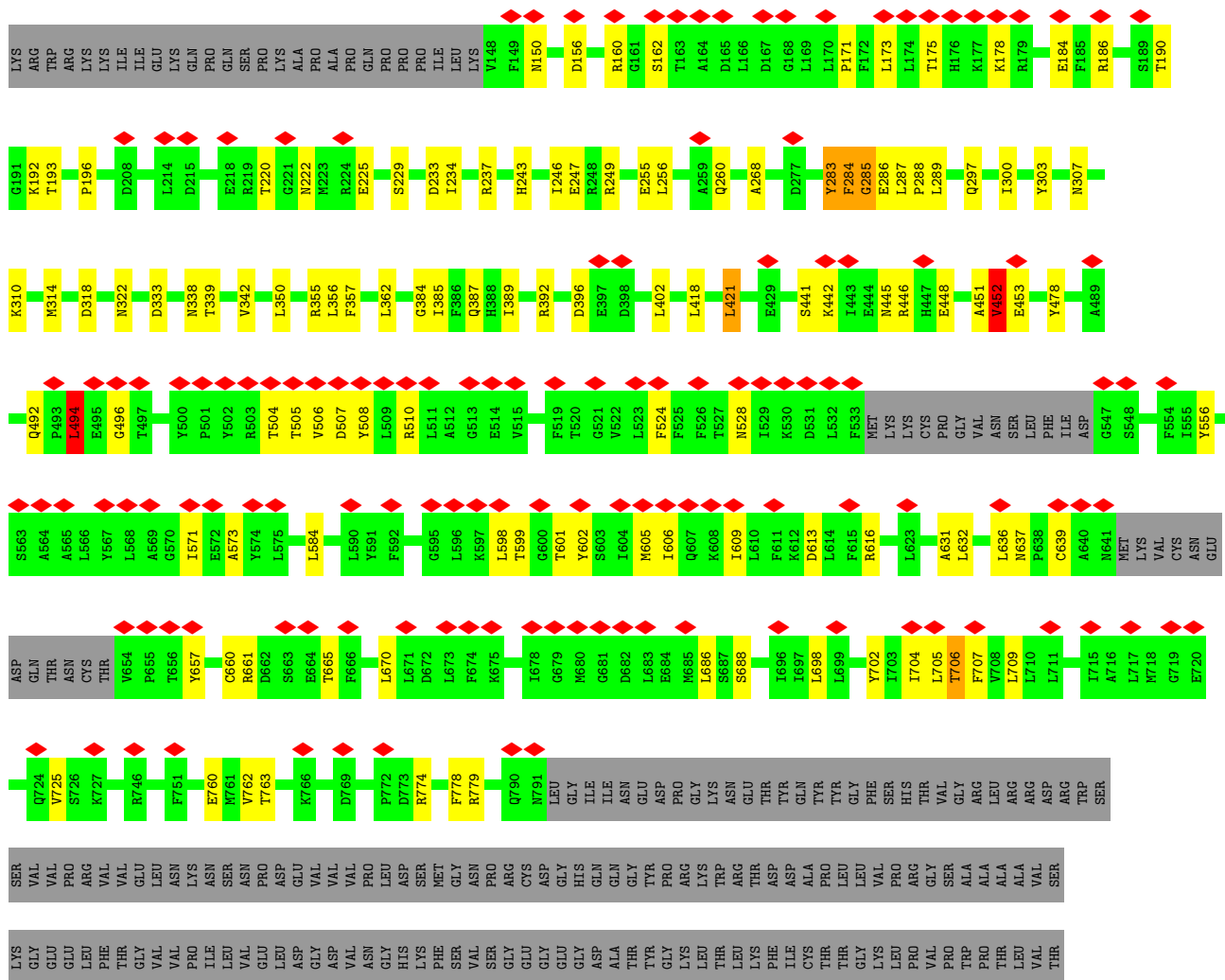
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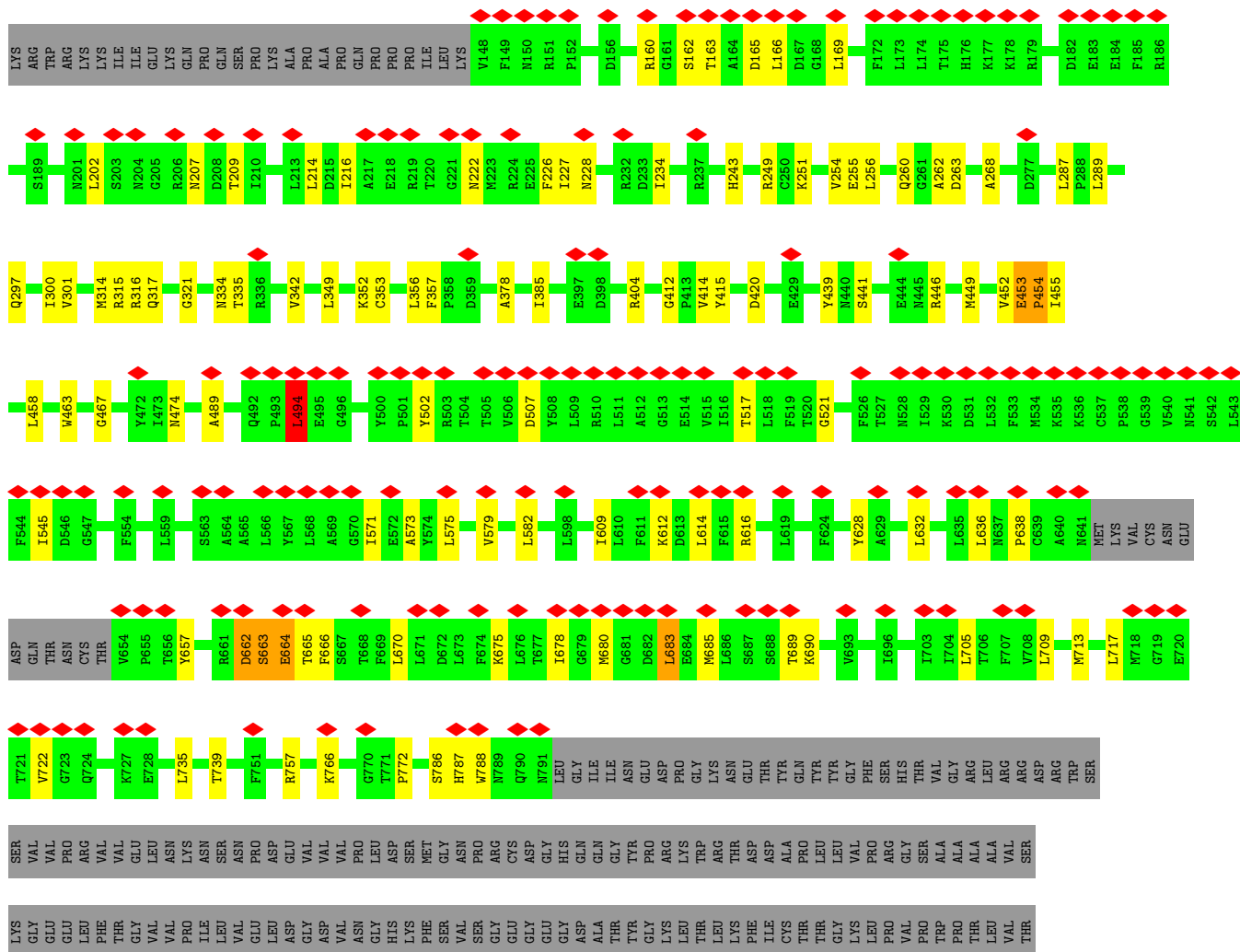
Chain	Residue	Modelled	Actual	Comment	Reference
C	1124	SER	-	expression tag	UNP C5MKY7
C	1125	TRP	-	expression tag	UNP C5MKY7
C	1126	SER	-	expression tag	UNP C5MKY7
C	1127	HIS	-	expression tag	UNP C5MKY7
C	1128	PRO	-	expression tag	UNP C5MKY7
C	1129	GLN	-	expression tag	UNP C5MKY7
C	1130	PHE	-	expression 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 (CCD ID: XS9) (formula: C₄₀H₆₄O₈) (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	





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

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

[illegible]

F707	M637	F554	Y478	G191	LYS
V708	P638	I555	I484	M314	ARG
L709	P639	Y556		T192	TRP
L710	A640			D318	ARG
L711	M641		A489	P196	LYS
	NET	I561	Q492	N322	LYS
I715	LYS	A564	P493	D333	ILE
A716	VAL	A565	L494	N338	GLU
L717	CYS	L566	E495	T339	LYS
L718	ASN	L567	G496	V342	GLN
G719	GLU	L568	T497	E218	PRO
E720	ASP	A569		R219	GLN
	THR	G570	Y500	T220	SER
	ASN	I571	F501	G221	PRO
Q724	CYS	E572	Y502	R224	LYS
W725	THR	A573	R503	E225	ALA
S726	V654	P655	T504	S229	PRO
K727	P656	L574	T505	D233	ALA
E745	T656	L575	G384	I234	PRO
R746	P657	F580	V506	R237	GLN
	C660	V583	D507	H243	PRO
F751	R661	L584	Y508	I246	PRO
E760	D662	F592	R510	E247	ILE
M761	S663	G595	L511	R249	ILE
W762	E664	L596	A512	E255	LYS
T763	T665	A597	G513	L256	V148
	P666	L598	V515	A259	F149
K766	L670	G600	L518	Q260	N150
	L671	T601	F519	L402	
D769	D672	F602	L523	L418	D156
G770	L673	S603	F524	L421	
R774	L674	M605	G525	E429	R160
F778	R675	L606	F526	D277	G161
R779	L676	Q607	T527	Y281	S162
Q790	P679	X608	N528	F282	T163
N791	M680	L609	F529	S441	A164
LEU	G681	L610	K530	K442	D165
GLY	D682	F611	D531	F283	L166
ILE	L683	K612	L532	F284	D167
ILE		D613	R446	E285	G168
ASN	L686	L614	H447	P288	L170
GLU	S687	F615	E448	L289	P171
PRO	S688	R616	LYS	Q297	F172
PRO	P692	GLY	LYS	I300	L173
GLY	L696	THR	CYS	Y303	T175
GLY	L698	TYR	PRO	K177	H176
LYS	L699	GLN	GLY	K178	K179
ASN	L699	TYR	VAL	R179	E184
GLU	Y702	TYR	ASN	K462	F185
THR	I703	GLY	LEU		R186
PHE	W704	THR	SER	K311	
SER	L705	PHE	ILE		S189
	T706	TYR	ASP		T190
			G547		
			S548		
			F549		

[illegible]

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

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	252.416, 252.416, 252.416	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.31	1/5206 (0.0%)	0.84	8/7061 (0.1%)
1	B	0.30	0/5104	0.79	5/6923 (0.1%)
1	C	0.31	1/5206 (0.0%)	0.84	8/7061 (0.1%)
1	D	0.30	0/5104	0.79	5/6923 (0.1%)
All	All	0.31	2/20620 (0.0%)	0.82	26/27968 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	657	TYR	C-N	6.39	1.40	1.34
1	A	657	TYR	C-N	6.38	1.40	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	SER	CA-C-N	7.87	136.57	121.54
1	A	663	SER	C-N-CA	7.87	136.57	121.54
1	C	663	SER	CA-C-N	7.86	136.55	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	663	SER	C-N-CA	7.86	136.55	121.54
1	C	662	ASP	CA-C-N	6.49	133.93	121.54
1	C	662	ASP	C-N-CA	6.49	133.93	121.54
1	A	662	ASP	CA-C-N	6.48	133.91	121.54
1	A	662	ASP	C-N-CA	6.48	133.91	121.54
1	B	494	LEU	CA-CB-CG	6.30	138.35	116.30
1	D	494	LEU	CA-CB-CG	6.30	138.34	116.30
1	C	234	ILE	N-CA-C	-6.08	105.44	111.88
1	A	234	ILE	N-CA-C	-6.07	105.44	111.88
1	A	494	LEU	CA-CB-CG	5.64	136.05	116.30
1	C	494	LEU	CA-CB-CG	5.64	136.03	116.30
1	D	285	GLY	CA-C-N	5.58	130.56	122.36
1	D	285	GLY	C-N-CA	5.58	130.56	122.36
1	B	285	GLY	CA-C-N	5.58	130.56	122.36
1	B	285	GLY	C-N-CA	5.58	130.56	122.36
1	C	452	VAL	CA-C-N	5.15	134.36	121.80
1	C	452	VAL	C-N-CA	5.15	134.36	121.80
1	A	452	VAL	CA-C-N	5.14	134.35	121.80
1	A	452	VAL	C-N-CA	5.14	134.35	121.80
1	D	706	THR	CA-C-N	5.09	131.25	121.54
1	D	706	THR	C-N-CA	5.09	131.25	121.54
1	B	706	THR	CA-C-N	5.08	131.25	121.54
1	B	706	THR	C-N-CA	5.08	131.25	121.54

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

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Mol	Chain	Res	Type	Group
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	61	0
1	B	4987	0	5042	69	0
1	C	5086	0	5148	61	0
1	D	4987	0	5042	72	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	247	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 (247) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:713:MET:HE2	1:D:606:ILE:HG12	1.98	0.46
1:B:356:LEU:HB3	1:B:357:PHE:H	1.63	0.46
1:B:601:THR:HG22	1:B:605:MET:HE3	1.98	0.46
1:D:246:ILE:HG23	1:D:300:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASN:ND2	1:A:262:ALA:O	2.49	0.45
1:D:601:THR:HG22	1:D:605:MET:HE3	1.98	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:A:378:ALA:HA	1:A:449:MET:HE1	1.97	0.45
1:C:378:ALA:HA	1:C:449:MET:HE1	1.97	0.45
1:D:283:TYR:OH	1:D:322:ASN:ND2	2.38	0.45
1:C:314:MET:HE1	1:C:352:LYS:HB3	1.99	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
1:A:314:MET:HE1	1:A:352:LYS:HB3	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:606:ILE:HG12	1:C:713:MET:HE2	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:462:LYS:NZ	1:D:745:GLU:OE2	2.48	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: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
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:D:297:GLN:N	1:D:345:MET:HE1	2.37	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

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	628/1132 (56%)	529 (84%)	95 (15%)	4 (1%)	21	49
1	B	613/1132 (54%)	553 (90%)	56 (9%)	4 (1%)	18	46
1	C	628/1132 (56%)	529 (84%)	95 (15%)	4 (1%)	21	49
1	D	613/1132 (54%)	552 (90%)	57 (9%)	4 (1%)	18	46
All	All	2482/4528 (55%)	2163 (87%)	303 (12%)	16 (1%)	23	49

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
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

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%)	556 (100%)	2 (0%)	84	82
1	B	546/987 (55%)	540 (99%)	6 (1%)	65	73
1	C	558/987 (56%)	556 (100%)	2 (0%)	84	82
1	D	546/987 (55%)	540 (99%)	6 (1%)	65	73
All	All	2208/3948 (56%)	2192 (99%)	16 (1%)	73	77

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

Mol	Chain	Res	Type
1	A	494	LEU
1	A	683	LEU
1	B	150	ASN
1	B	362	LEU
1	B	421	LEU
1	B	494	LEU
1	B	670	LEU
1	B	686	LEU
1	C	494	LEU
1	C	683	LEU
1	D	150	ASN
1	D	362	LEU
1	D	421	LEU
1	D	494	LEU
1	D	670	LEU
1	D	686	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	228	ASN
1	A	260	GLN
1	A	297	GLN
1	A	401	HIS
1	A	456	ASN
1	A	474	ASN
1	A	712	ASN
1	A	784	ASN

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Mol	Chain	Res	Type
1	B	150	ASN
1	B	228	ASN
1	B	239	GLN
1	B	297	GLN
1	B	309	HIS
1	B	361	ASN
1	B	401	HIS
1	B	456	ASN
1	B	492	GLN
1	B	724	GLN
1	C	207	ASN
1	C	228	ASN
1	C	260	GLN
1	C	297	GLN
1	C	401	HIS
1	C	456	ASN
1	C	474	ASN
1	C	712	ASN
1	C	784	ASN
1	D	150	ASN
1	D	228	ASN
1	D	239	GLN
1	D	260	GLN
1	D	297	GLN
1	D	309	HIS
1	D	326	HIS
1	D	361	ASN
1	D	401	HIS
1	D	456	ASN
1	D	492	GLN
1	D	724	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	B	1201	-	46,51,51	0.53	1 (2%)	39,76,76	0.68	2 (5%)
2	XS9	C	1201	-	46,51,51	0.48	0	39,76,76	1.09	3 (7%)
2	XS9	A	1201	-	46,51,51	0.48	0	39,76,76	1.09	3 (7%)
2	XS9	D	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	B	1201	-	-	15/29/108/108	0/4/4/4
2	XS9	C	1201	-	-	15/29/108/108	0/4/4/4
2	XS9	A	1201	-	-	14/29/108/108	0/4/4/4
2	XS9	D	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(°)	Ideal(°)
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

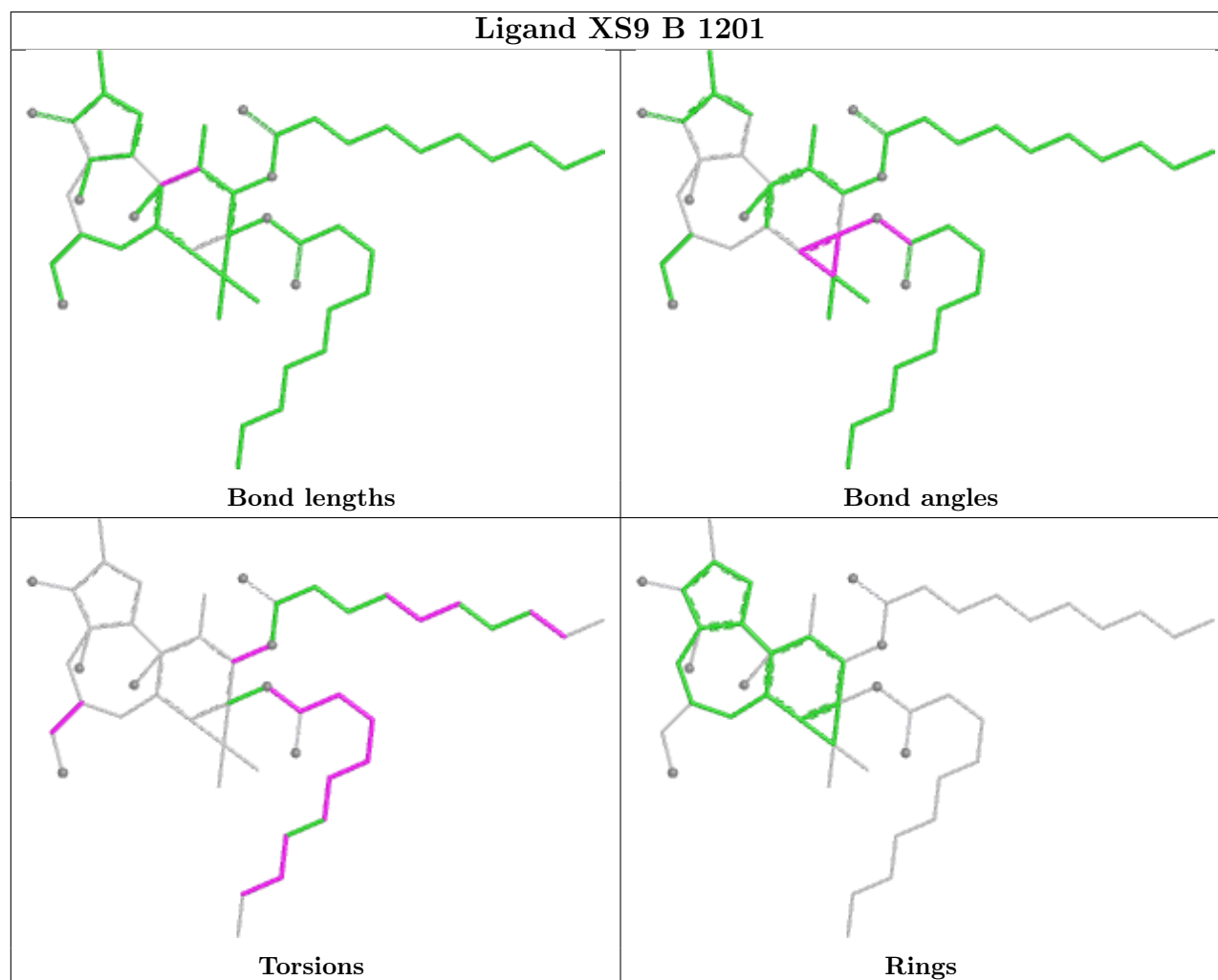
There are no ring outliers.

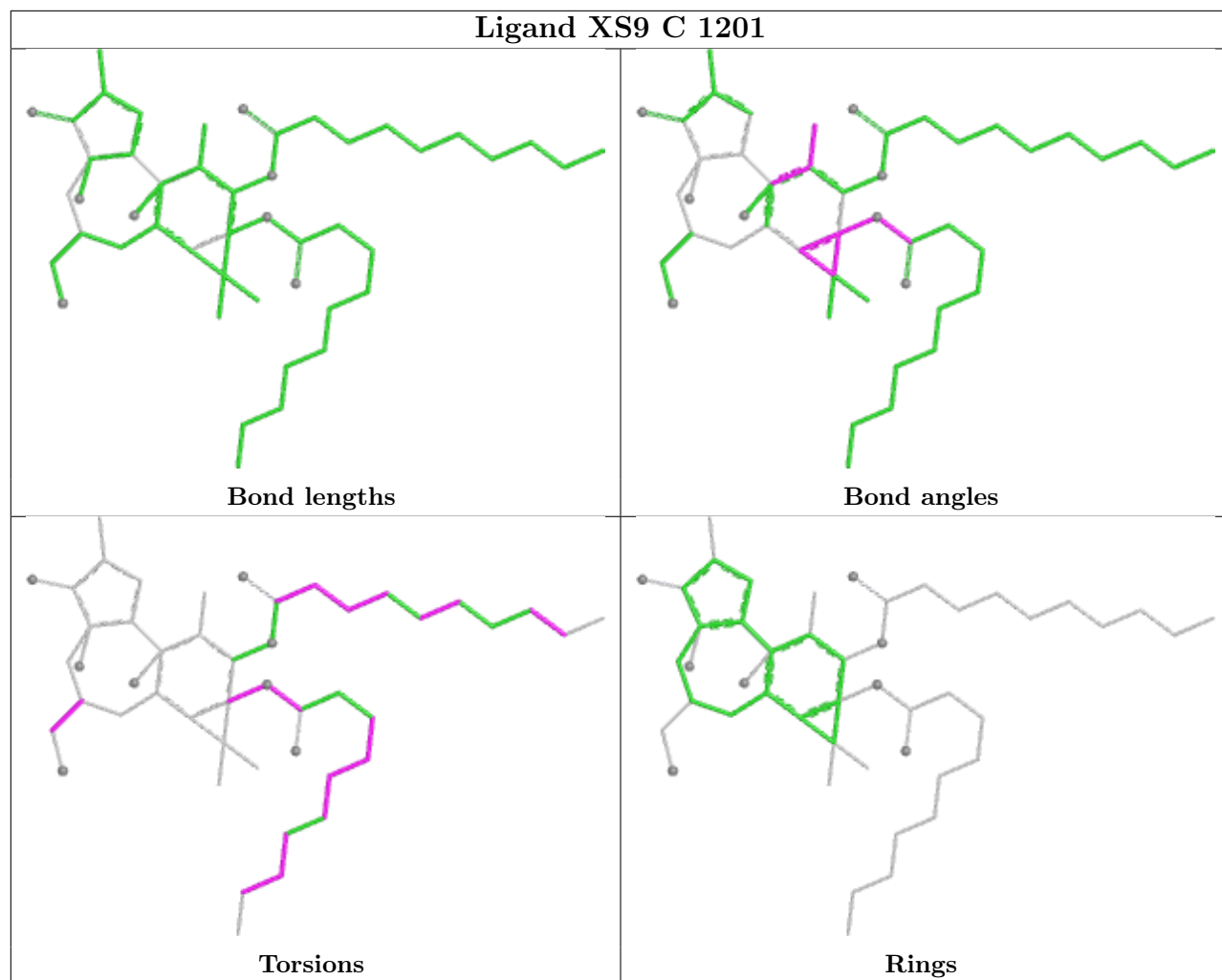
4 monomers are involved in 10 short contacts:

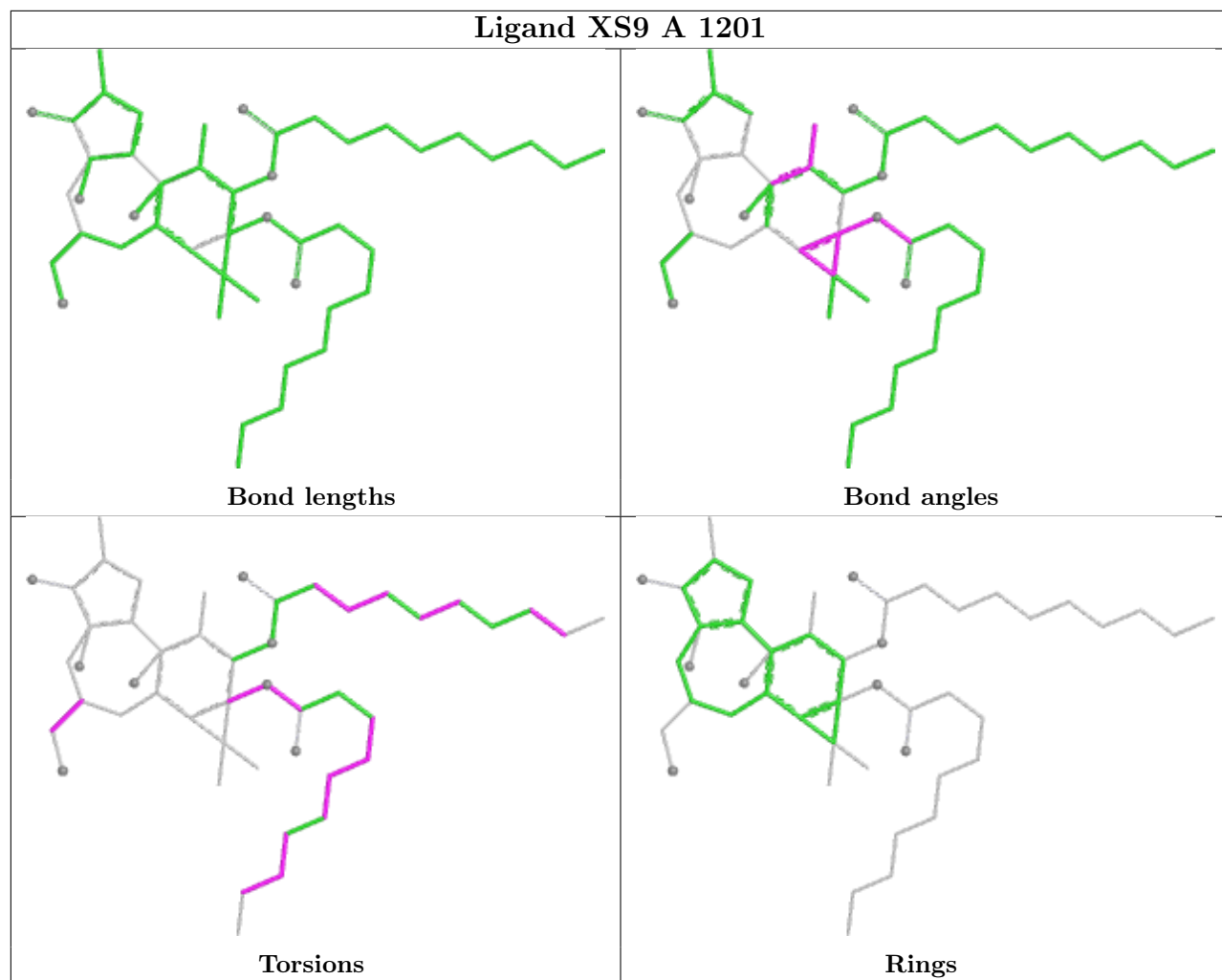
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	XS9	3	0
2	C	1201	XS9	2	0
2	A	1201	XS9	2	0
2	D	1201	XS9	3	0

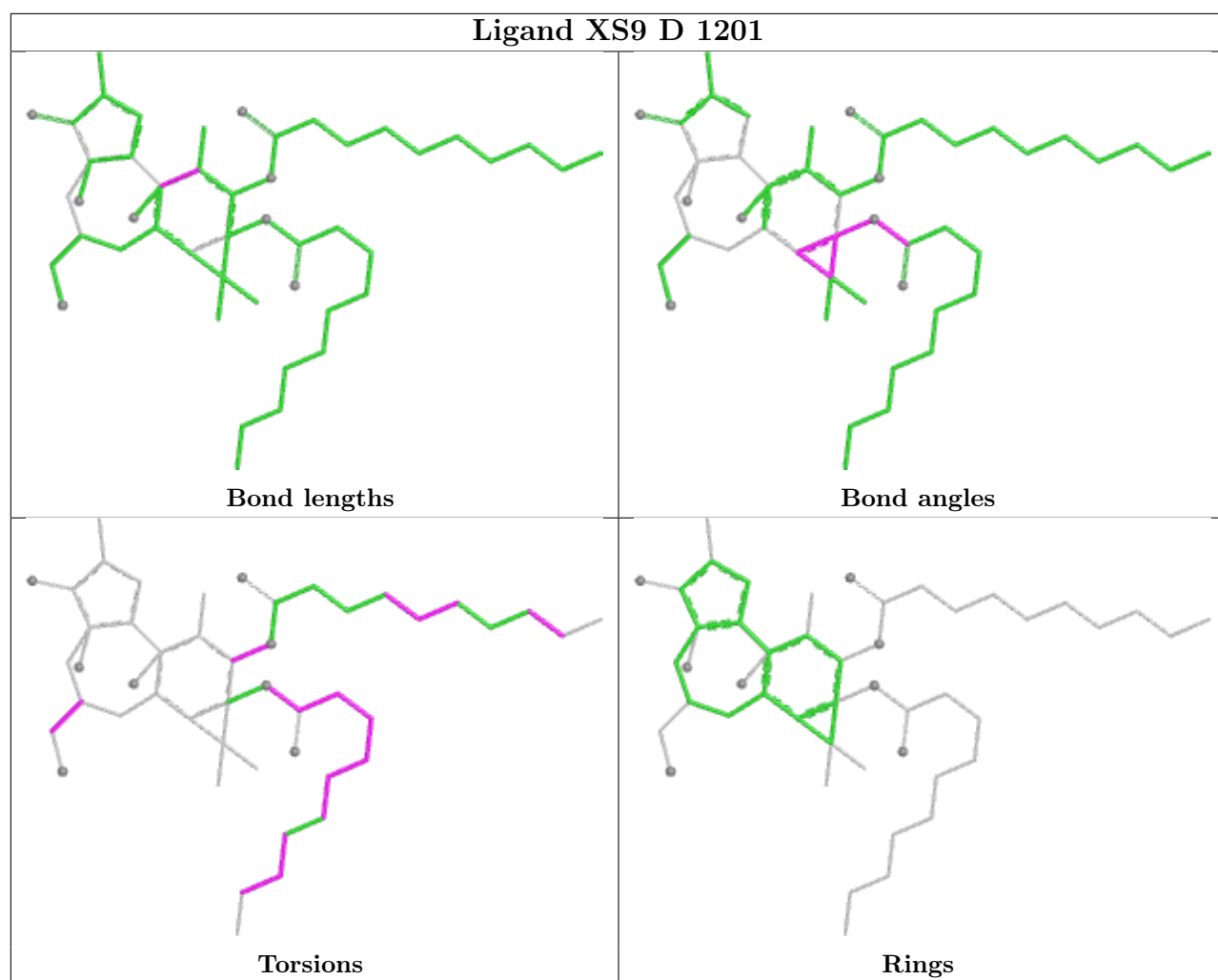
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

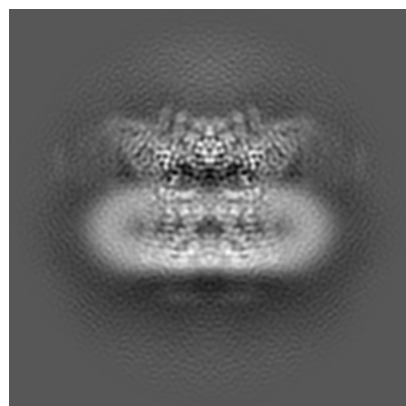
6 Map visualisation [i](#)

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

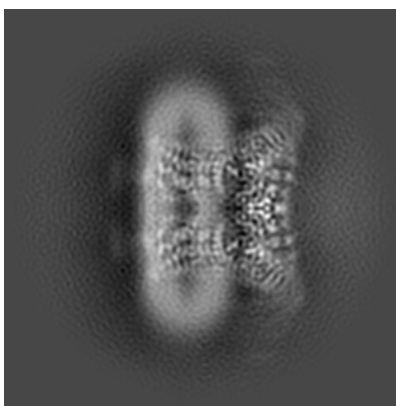
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

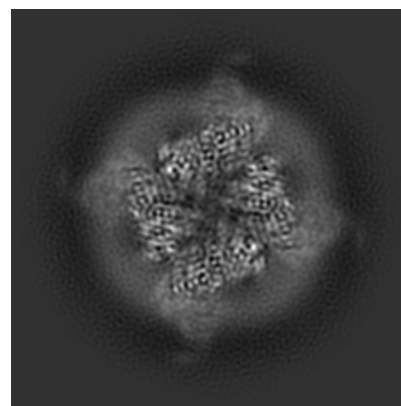
6.1.1 Primary map



X

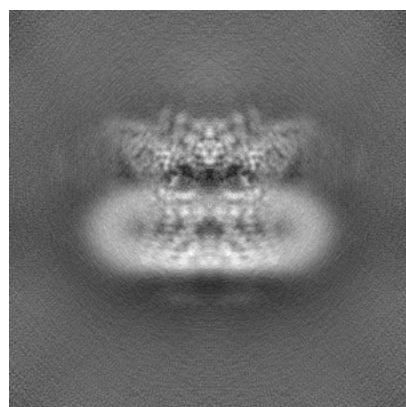


Y

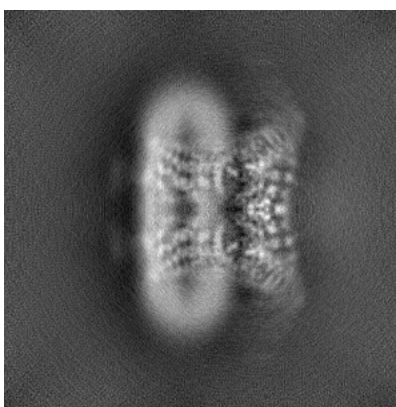


Z

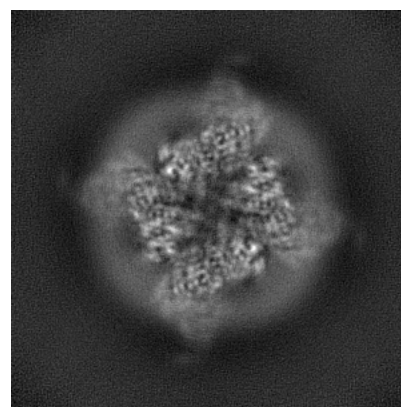
6.1.2 Raw map



X



Y



Z

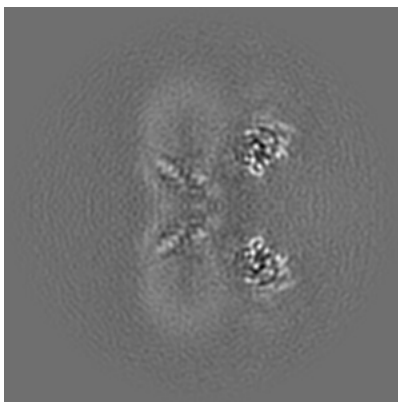
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

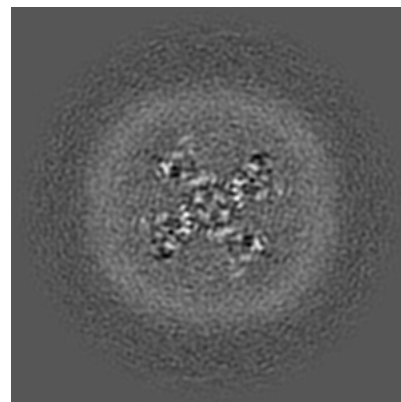
6.2.1 Primary map



X Index: 160

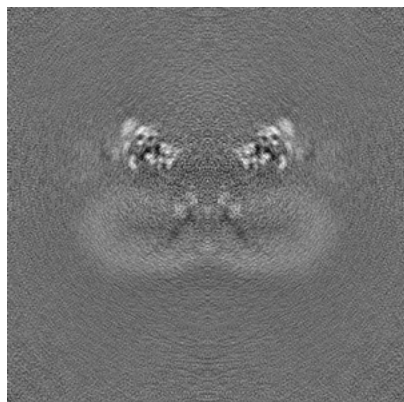


Y Index: 160

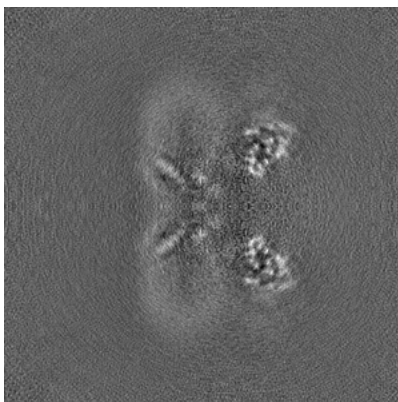


Z Index: 160

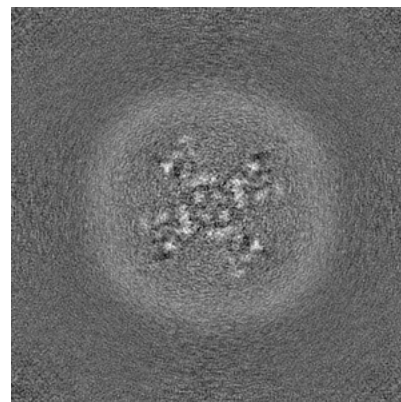
6.2.2 Raw map



X Index: 160



Y Index: 160

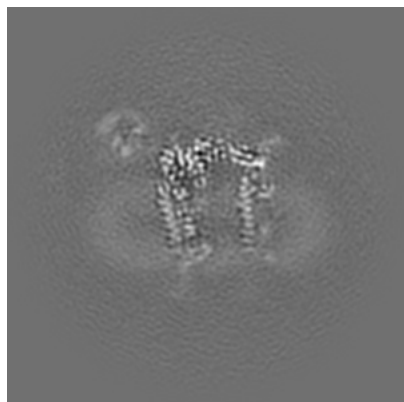


Z Index: 160

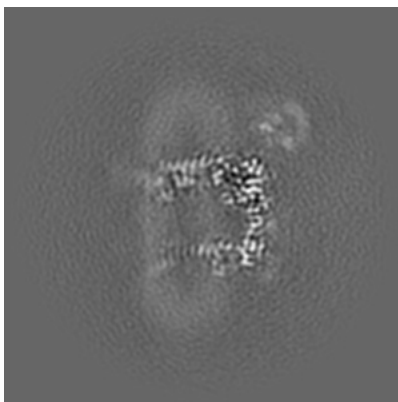
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

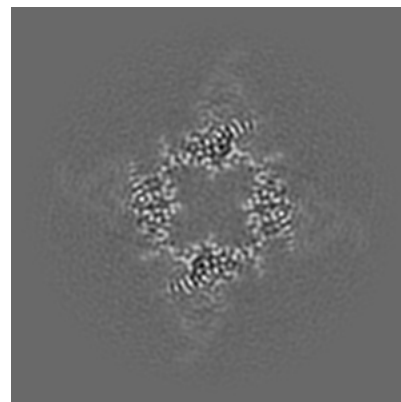
6.3.1 Primary map



X Index: 125

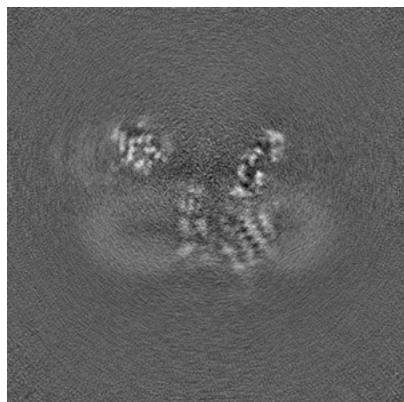


Y Index: 126

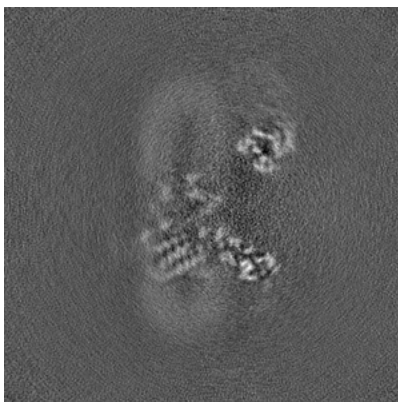


Z Index: 205

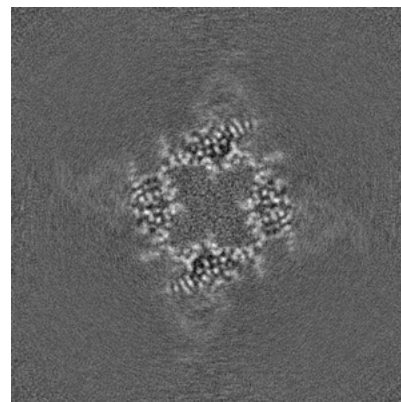
6.3.2 Raw map



X Index: 142



Y Index: 148

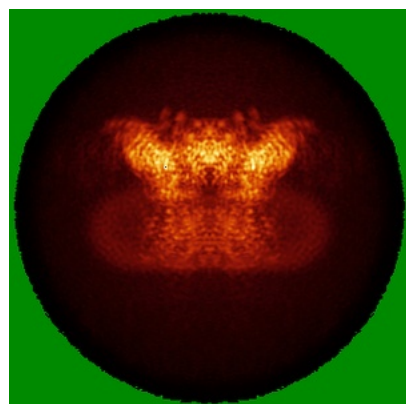


Z Index: 205

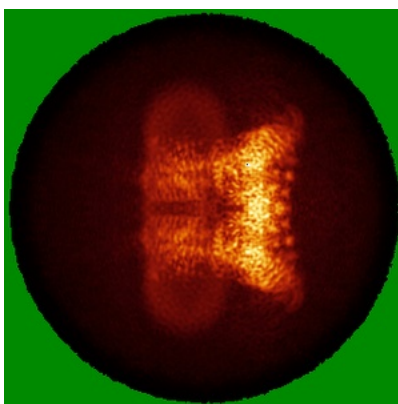
The images above show the largest variance slices of the map in three orthogonal directions.

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

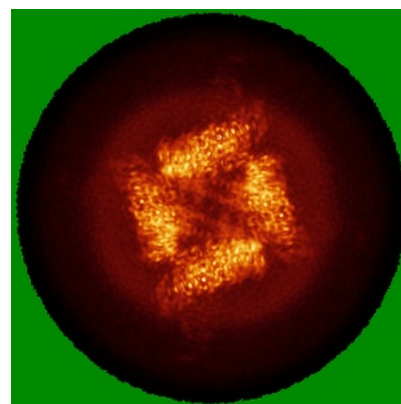
6.4.1 Primary map



X

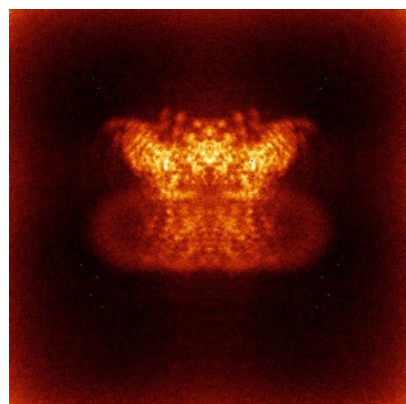


Y

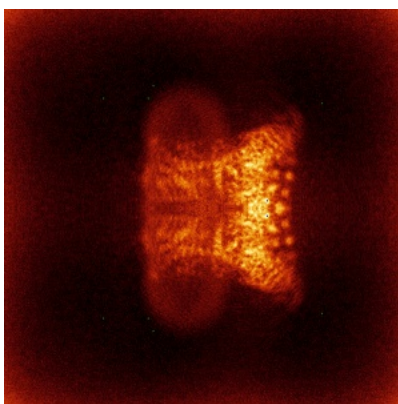


Z

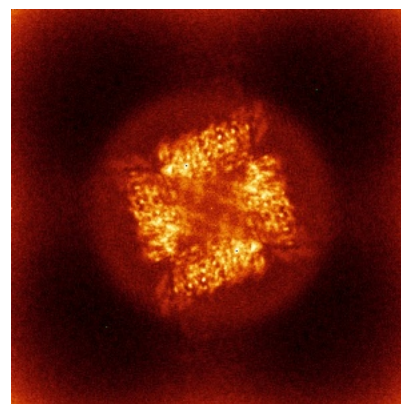
6.4.2 Raw map



X



Y

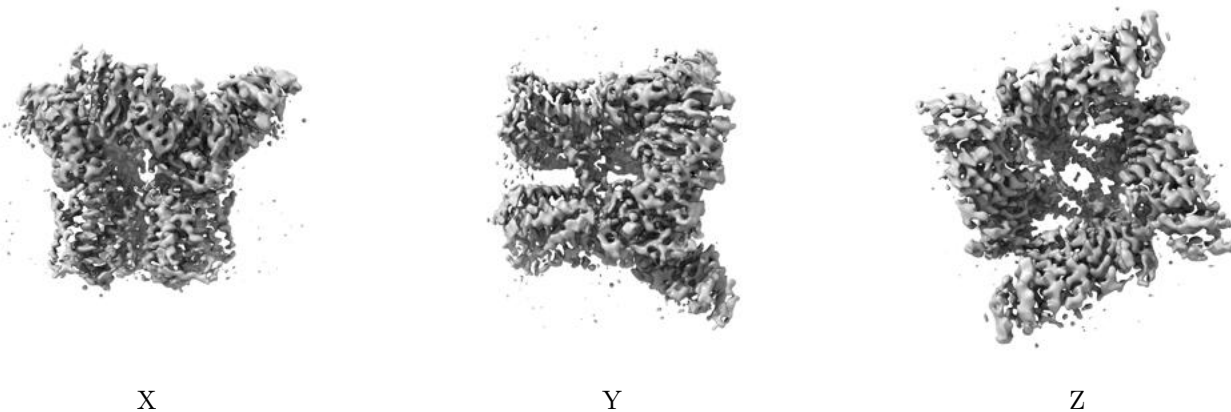


Z

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.

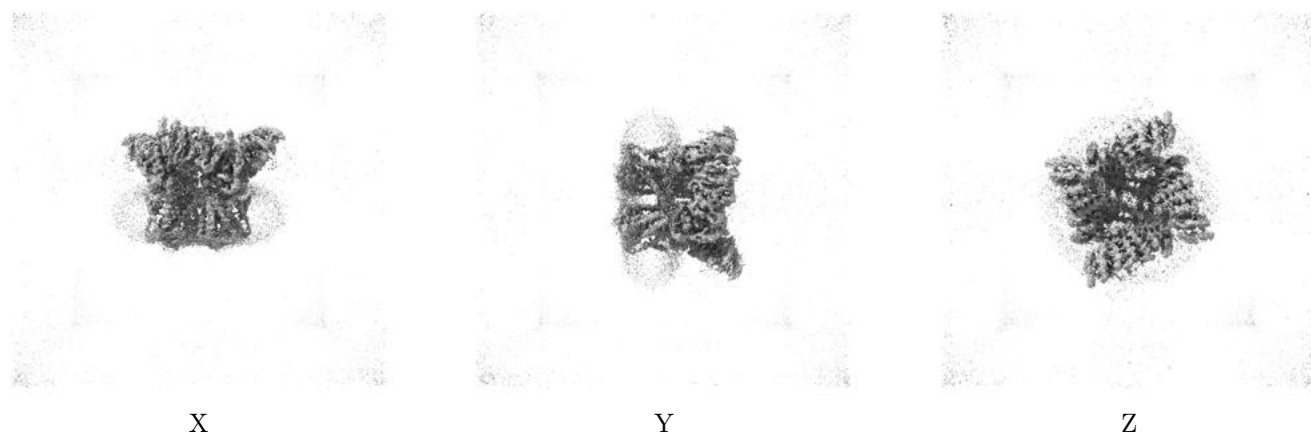
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

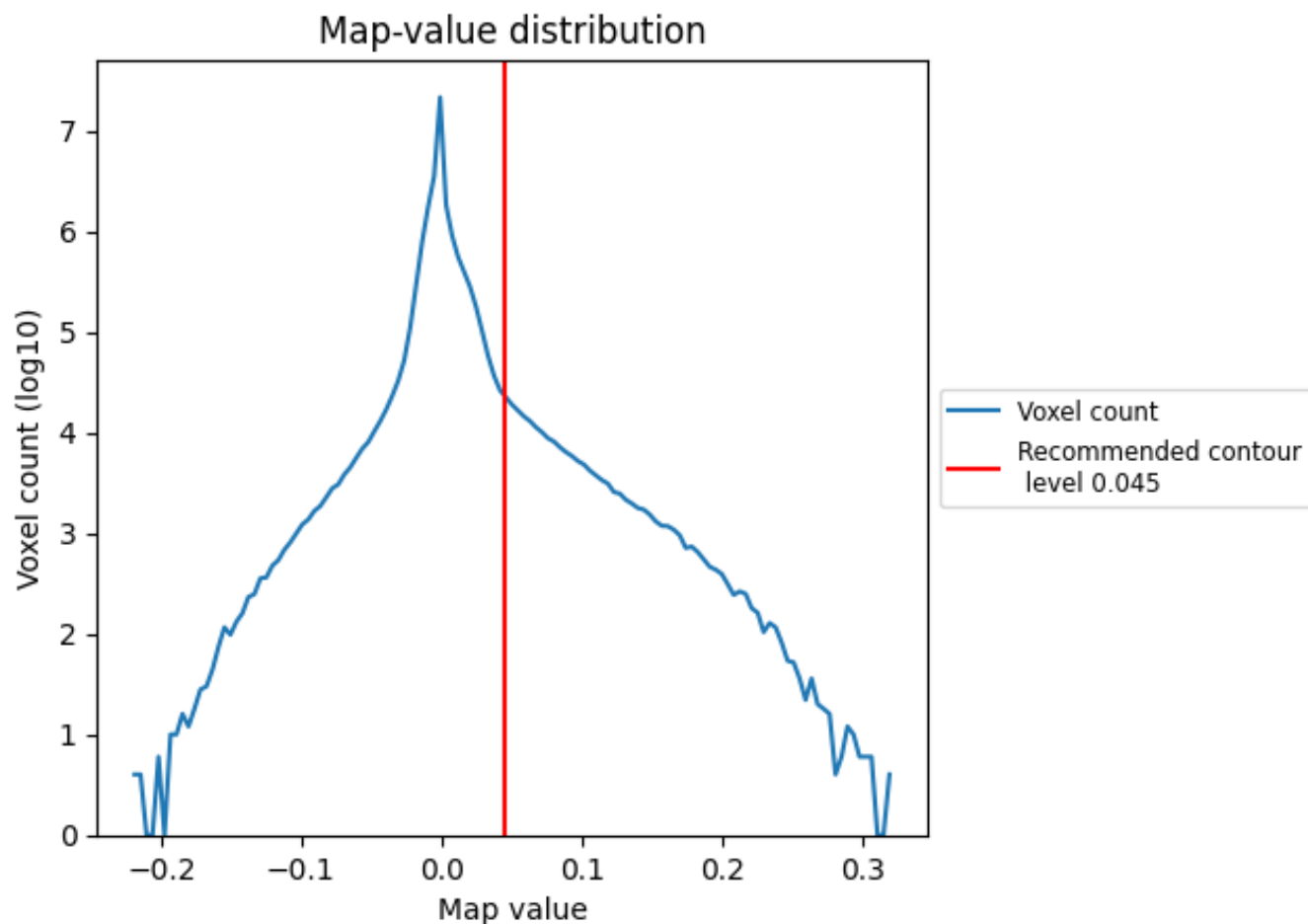
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

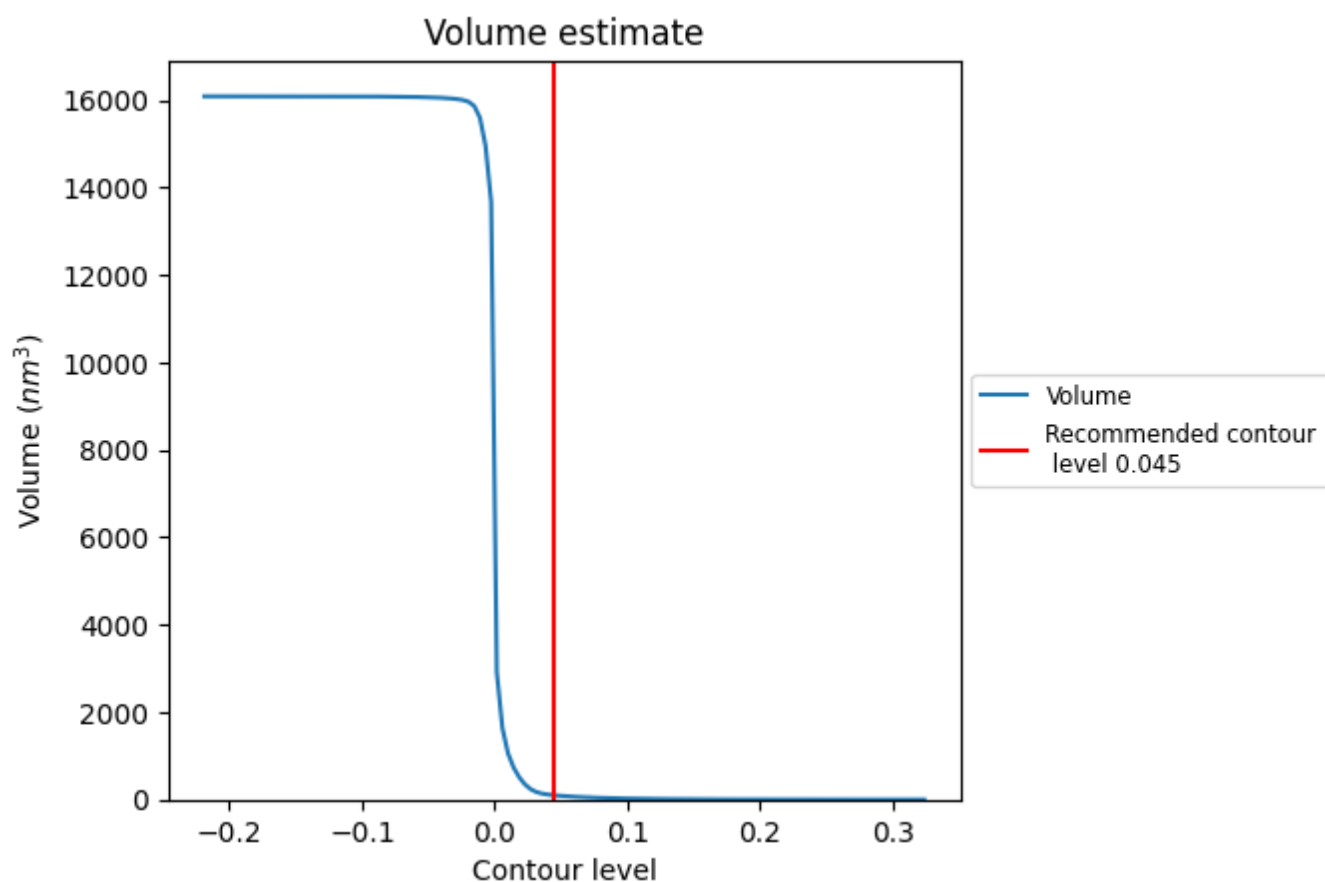
This section contains the results of statistical analysis of the map.

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.

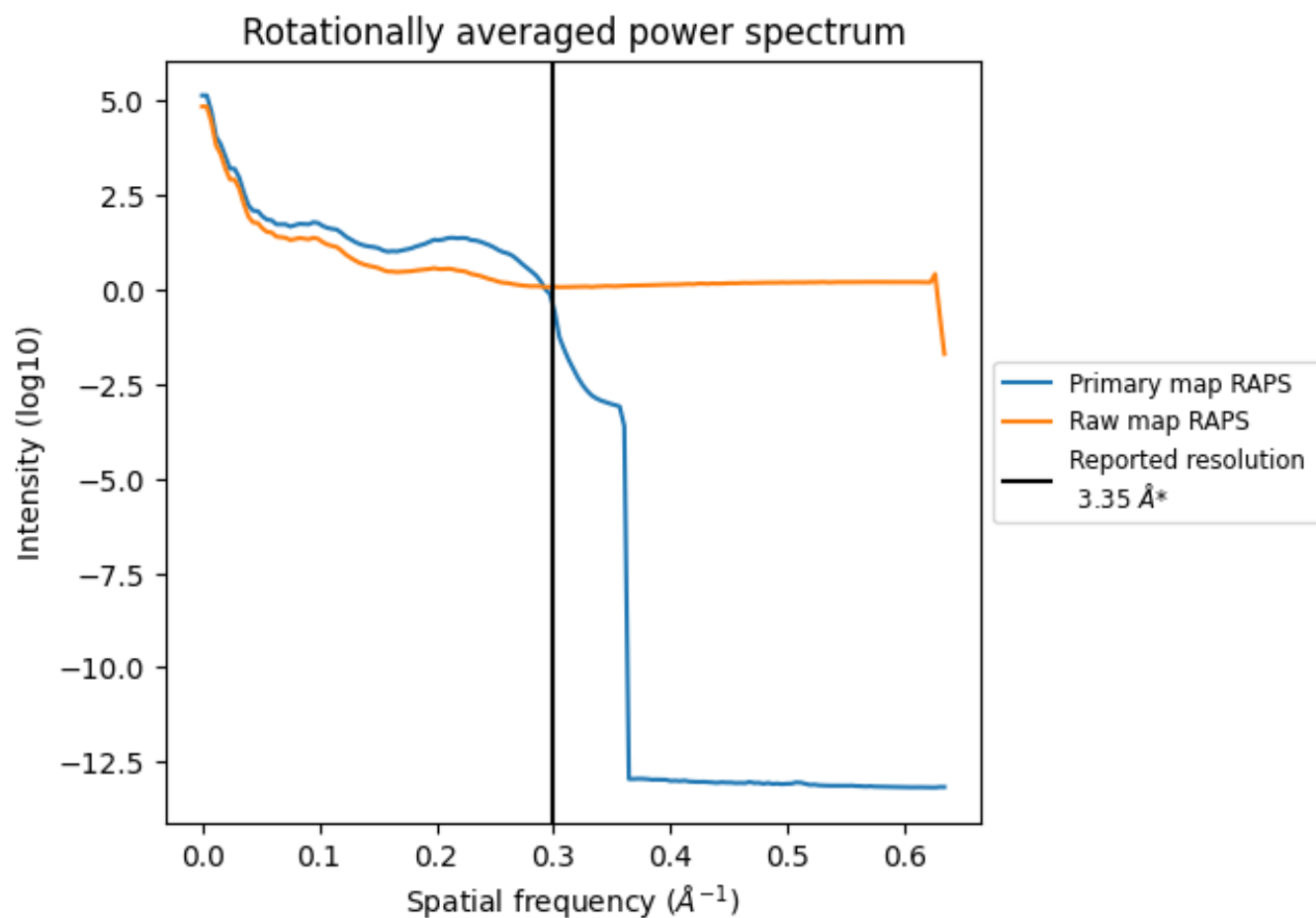
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; 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 ⓘ

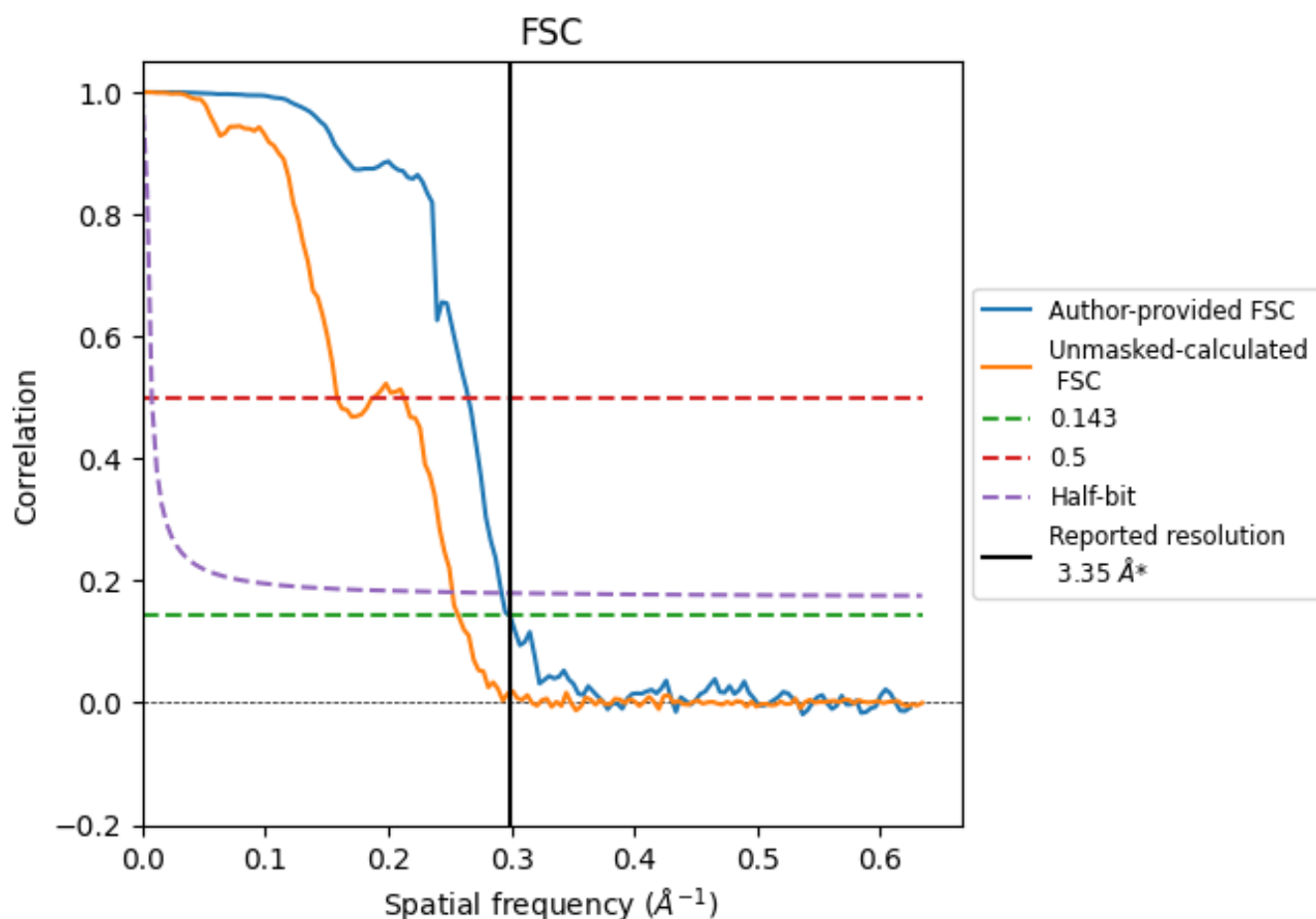


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.299 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

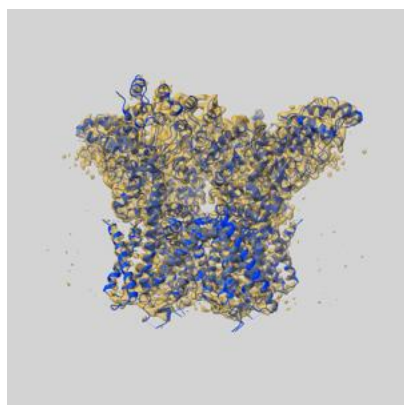
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.78	3.42
Unmasked-calculated*	3.89	6.32	3.97

*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 %

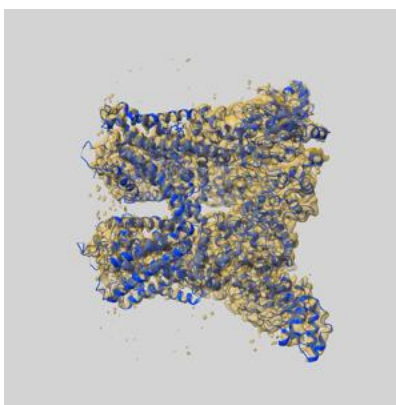
9 Map-model fit [i](#)

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](#).

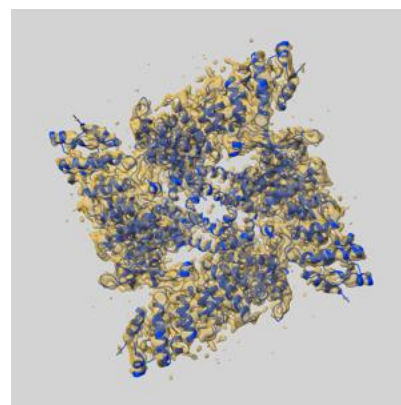
9.1 Map-model overlay [i](#)



X



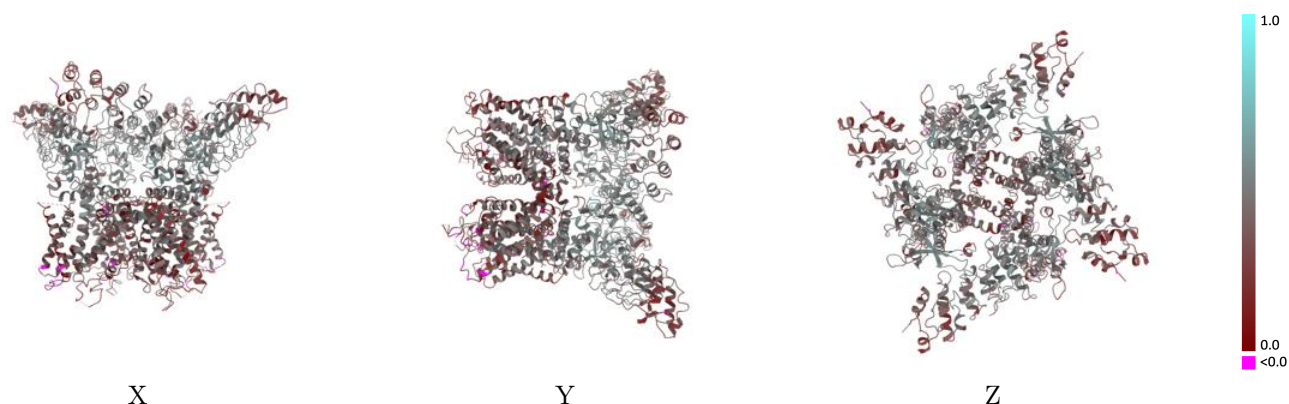
Y



Z

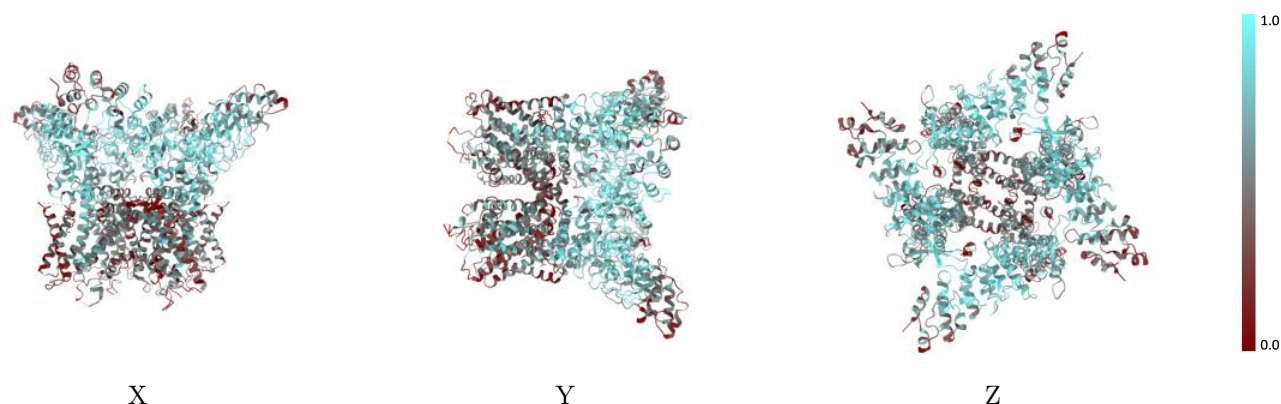
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



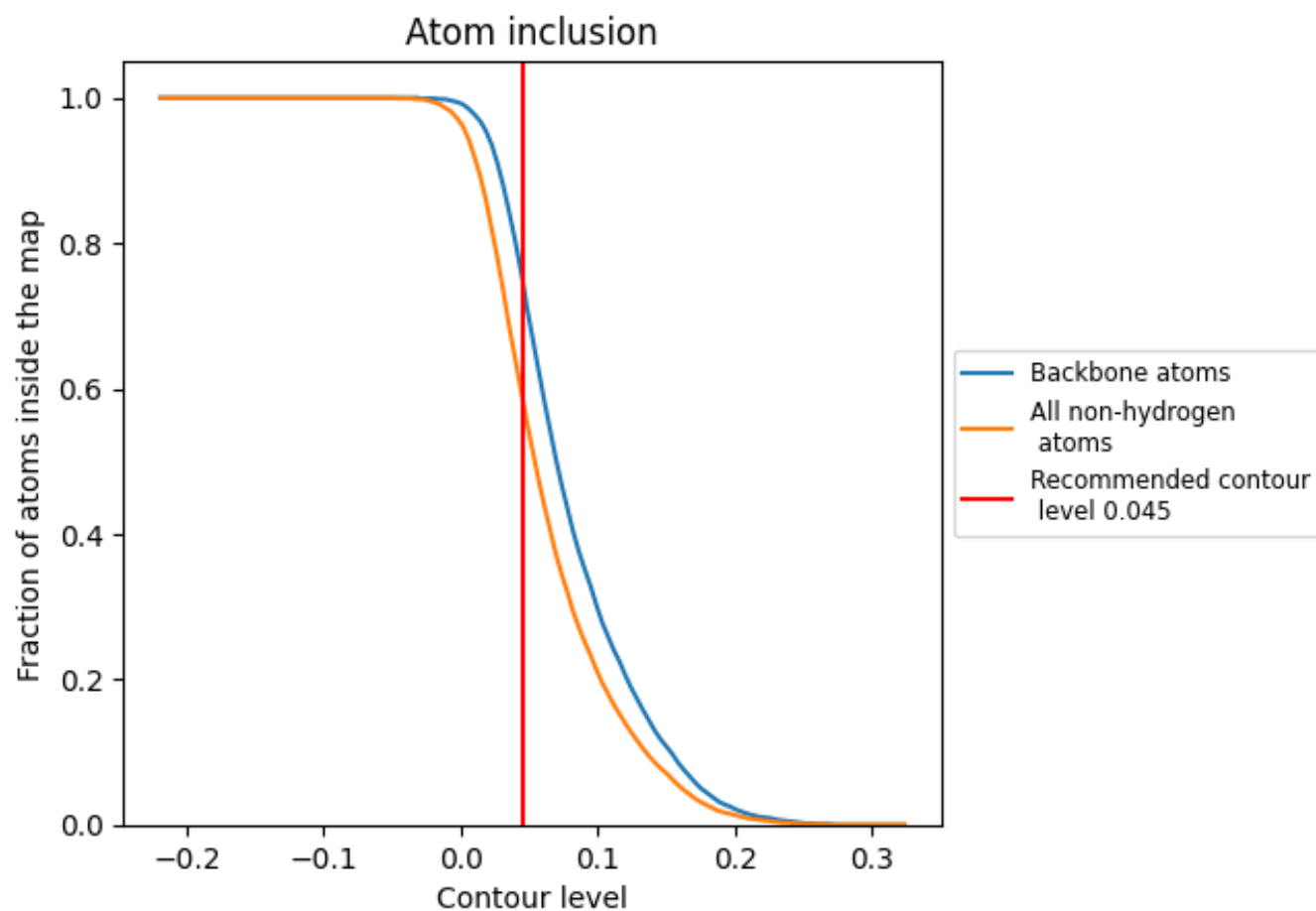
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

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

