



Full wwPDB EM Validation Report ⓘ

Sep 23, 2024 – 12:35 PM JST

PDB ID : 8YMP
EMDB ID : EMD-39402
Title : OSCA1.1-F516A nanodisc in LPC
Authors : Zhang, M.F.
Deposited on : 2024-03-09
Resolution : 2.60 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.dev112
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.38.2

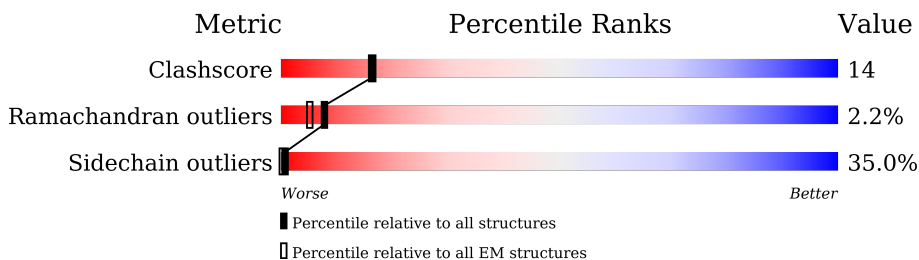
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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 $\leq 5\%$. 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	772	
1	B	772	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9570 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.

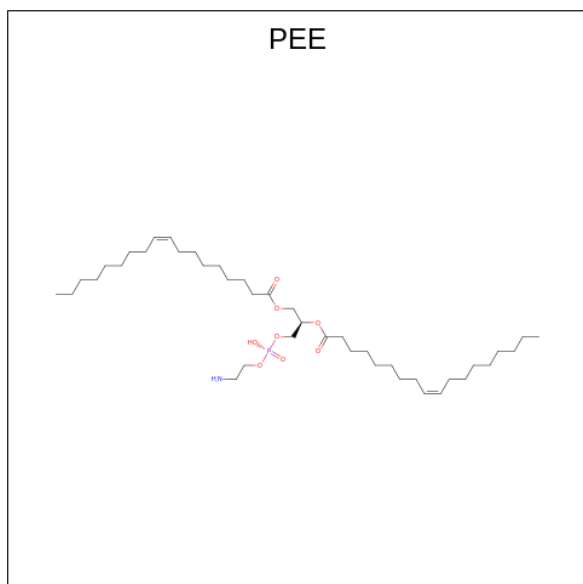
- Molecule 1 is a protein called Protein OSCA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	592	4776	3149	780	822	25	0	0
1	B	592	4776	3149	780	822	25	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ALA	PHE	engineered mutation	UNP Q9XEA1
B	516	ALA	PHE	engineered mutation	UNP Q9XEA1

- Molecule 2 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C 9 9	0

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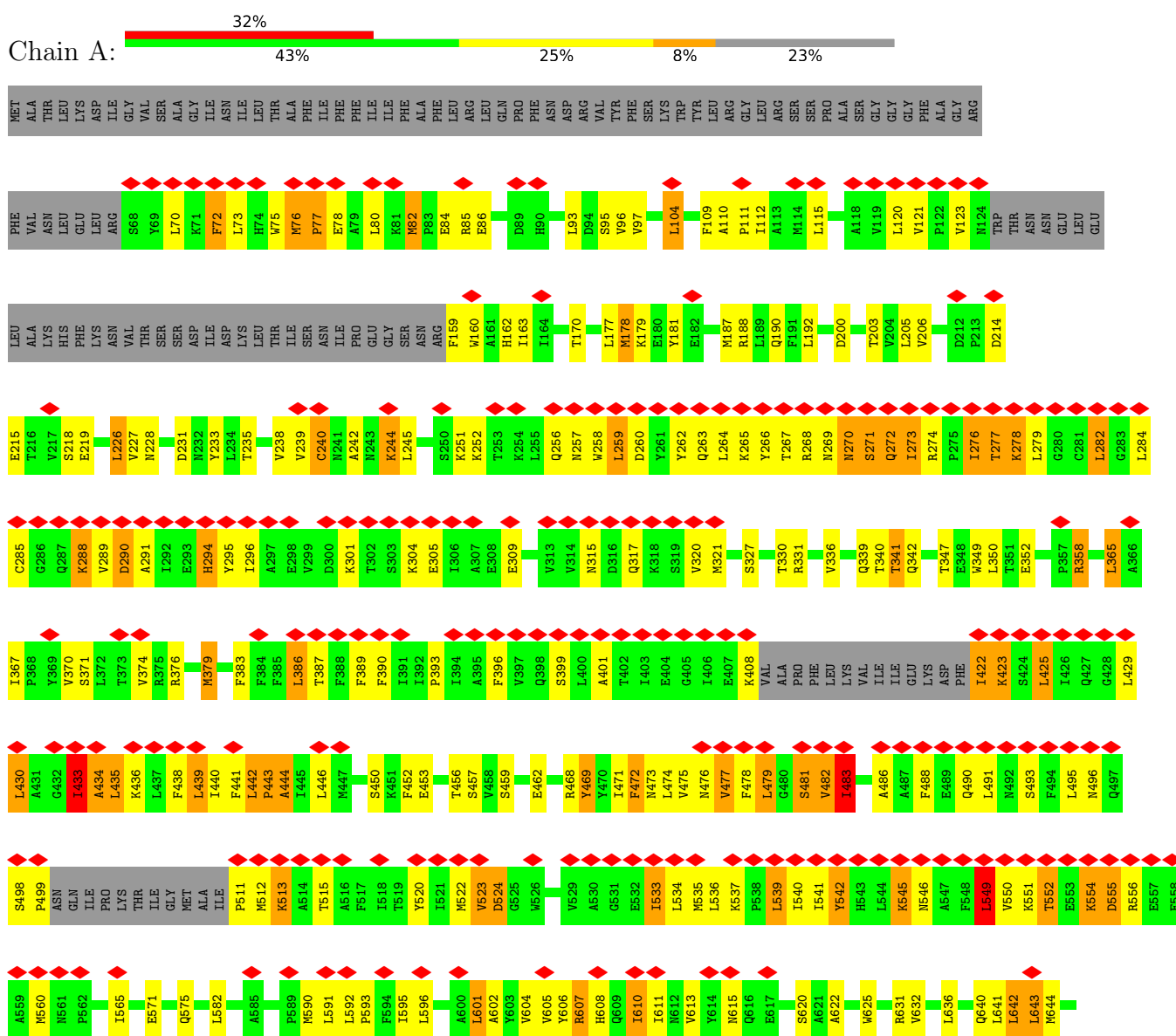
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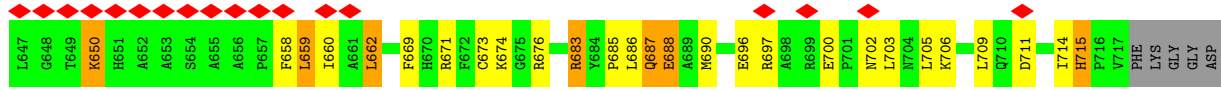
Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	C	0
			9	9	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein OSCA1





ASN	ASP	ASP	ASP	GLY	ASP	MET	ILE	GLY	LYS	LEU	GLY	ASN	VAL	ILE	ILE	VAL	PRO	THR	LYS	ARG	GLN	ARG	ASN	PRO	ALA	ARG	ILE	ASP	GLY	GLY	LEU	LEU	ALA	ASN	ILE	GLY	LYS	ARG	VAL	VAL	ALA	LEU	GLY	GLY	ALA	THR	THR	THR	GLY	GLY	ASP
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● Molecule 1: Protein OSCA1



MET	ALA	THR	LEU	LYS	ASP	LYS	ILE	GLY	VAL	SER	ALA	GLY	ASN	ILE	ILE	THR	ALA	PHE	ILE	PHE	ILE	PHE	LEU	LEU	ALA	GLN	PRO	PRO	ARG	ASN	PRO	GLN	PRO	PRO	ASN	ASP	ARG	VAL	TYR	PHE	LYS	TRP	TRP	LEU	VAL	ARG	LEU	GLY	GLY	GLY	PHE	ALA	ALA	ARG
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PHE	VAL	ASN	LEU	PHE	LEU	ARG	S68	Y69	K71	F72	L73	H74	W75	M76	P77	E78	A79	L80	K81	M82	P83	E84	R85	E86	D89	H90	L93	D94	V96	V97	L104	F109	A110	P111	I112	A113	M114	L115	A118	V119	L120	V121	P122	V123	N124	TRP	THR	ASN	ASN	GLU	LEU	GLU
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LEU	ALA	LYS	HIS	PHE	ASN	VAL	THR	SER	SER	ASP	ASP	LEU	THR	ILE	ILE	THR	ILE	SER	ASN	ILE	ARG	F159	V160	A161	H162	I163	T170	L177	S95	M178	K179	E180	Y181	E182	M187	R188	L189	Q190	F191	L192	D200	T203	V204	L205	V206	D212	P213	D214
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E216	T216	S218	E219	L226	V227	N228	D231	H232	Y233	T235	V238	V239	C240	N241	A242	N243	K244	L245	S250	F159	K251	K252	T253	K254	L255	Q256	N257	K258	L259	D260	E261	Y262	Q263	L264	K265	Y266	T267	R268	N269	N270	S271	Q272	L273	R274	P275	I276	T277	K278	L279	G280	C281	G283	L284
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C285	Q286	Q287	K288	D289	V289	A291	I292	E293	H294	Y295	I296	A297	E298	V299	D300	K301	T302	S303	K304	E305	I306	A307	E308	E309	W313	V314	N315	D316	Q317	K318	S319	V320	N321	S327	T330	R331	V336	Q339	T340	T341	Q342	T347	E348	K349	E352	P357	R358	L365	A366	I367
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F368	Y369	V370	S371	L372	V374	R375	R376	K379	F383	F384	F385	L386	T387	F388	F389	F390	I391	I392	P393	I394	A395	F396	V397	I398	S399	L400	A401	T402	L403	E404	G405	L406	E407	K408	VAL	ALA	PRO	PHE	LEU	LYS	VAL	ILE	GLU	LYS	ASP	PHE	L422	K423	S424	L425	L426	Q427	G428	L429	L430
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A431	G432	L433	A434	L435	K436	L437	F438	L439	I440	F441	L442	P443	A444	I445	L446	H447	S450	K451	F452	E453	T456	S457	A458	S459	E462	R468	Y469	V470	I471	F472	M473	L474	N475	V477	F478	L479	G480	S481	V482	I483	A486	A487	F488	E489	Q490	L491	M492	S493	F494	L495	M496	Q497	S498
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P499	ASN	GLN	ILE	PRO	THR	LYS	GLY	MET	ALA	ILE	P511	M512	K513	A514	T515	A516	F517	I518	T519	Y520	I521	M522	V523	D524	G525	W526	V529	A530	G531	E532	I533	L534	M535	L536	K537	P538	L539	I540	I541	Y542	H543	L544	K545	M546	A547	F548	L549	V550	K551	T552	E553	K554	D555	R556	E557	E558	A559
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M560	M561	P562	L565	E571	Q575	L582	A585	P589	M590	L591	P593	F594	I595	L596	A600	L601	A602	Y603	V604	V605	R607	H608	Q609	L610	I611	N612	V613	F614	M615	Q616	E617	S620	A621	A622	V625	R631	V632	L636	Q640	L641	L642	L643	N644	L647
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G648	T649	K650	H651	A652	A653	S654	A655	A656	P657	F658	L659	I660	A661	L662	F669	H670	R671	F672	C673	K674	G675	R676	R683	Y684	P685	L686	Q687	E688	M689	E696	R697	A698	R699	E700	P701	N702	L703	N704	K706	L709	Q710	D711	I714	H715	V717
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ASP	ASP	GLY	ASP	MET	ILE	GLY	LEU	LEU	GLU	ASN	VAL	ILE	VAL	PRO	LYS	ARG	GLN	SER	ARG	ASN	THR	THR	PRO	ALA	SER	ARG	ILE	SER	GLY	GLU	SER	SER	PRO	SER	LEU	ALA	VAL	ILE	ASN	LYS	GLY	GLU	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	-0.419	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	291.84, 291.84, 291.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.57, 0.57, 0.57	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/4906	0.60	5/6673 (0.1%)
1	B	0.38	0/4906	0.60	5/6673 (0.1%)
All	All	0.38	0/9812	0.60	10/13346 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	MET	C-N-CD	11.28	152.08	128.40
1	B	76	MET	C-N-CD	11.28	152.08	128.40
1	A	443	PRO	CA-N-CD	-8.60	99.45	111.50
1	B	443	PRO	CA-N-CD	-8.60	99.45	111.50
1	A	77	PRO	CA-N-CD	-8.56	99.52	111.50
1	B	77	PRO	CA-N-CD	-8.56	99.52	111.50
1	A	549	LEU	CA-CB-CG	6.00	129.10	115.30
1	B	549	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	549	LEU	N-CA-C	5.65	126.27	111.00
1	B	549	LEU	N-CA-C	5.65	126.27	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4776	0	4841	166	0
1	B	4776	0	4841	160	0
2	A	9	0	17	1	0
2	B	9	0	17	2	0
All	All	9570	0	9716	270	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 14.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:THR:CG2	1:B:683:ARG:HG2	1.79	1.12
1:A:683:ARG:HG2	1:B:341:THR:CG2	1.79	1.12
1:A:340:THR:CG2	1:B:686:LEU:HD13	1.81	1.11
1:A:686:LEU:HD13	1:B:340:THR:CG2	1.81	1.11
1:B:386:LEU:HD13	1:B:472:PHE:HZ	1.17	1.07
1:A:386:LEU:HD13	1:A:472:PHE:HZ	1.17	1.06
1:A:683:ARG:HG2	1:B:341:THR:HG22	1.34	1.06
1:A:341:THR:HG22	1:B:683:ARG:HG2	1.34	1.04
1:A:358:ARG:CG	1:A:358:ARG:O	2.06	1.03
1:B:358:ARG:O	1:B:358:ARG:CG	2.06	1.02
1:B:386:LEU:HD13	1:B:472:PHE:CZ	1.94	1.02
1:A:340:THR:HG21	1:B:686:LEU:CD2	1.91	1.01
1:A:386:LEU:HD13	1:A:472:PHE:CZ	1.94	1.01
1:A:686:LEU:CD2	1:B:340:THR:HG21	1.91	0.99
1:A:340:THR:HG21	1:B:686:LEU:CD1	1.96	0.96
1:A:686:LEU:CD1	1:B:340:THR:HG21	1.96	0.95
1:A:73:LEU:O	1:A:77:PRO:HD3	1.69	0.93
1:B:73:LEU:O	1:B:77:PRO:HD3	1.69	0.92
1:A:358:ARG:O	1:A:358:ARG:HG2	1.71	0.91
1:A:686:LEU:CD1	1:B:340:THR:CG2	2.48	0.91
1:A:340:THR:CG2	1:B:686:LEU:CD1	2.48	0.91
1:B:386:LEU:HD11	1:B:442:LEU:HD21	1.55	0.89
1:A:386:LEU:HD11	1:A:442:LEU:HD21	1.55	0.88
1:A:486:ALA:O	1:A:490:GLN:HG2	1.73	0.87
1:B:390:PHE:HE1	1:B:438:PHE:HB3	1.39	0.87
1:B:486:ALA:O	1:B:490:GLN:HG2	1.73	0.87
1:A:390:PHE:HE1	1:A:438:PHE:HB3	1.39	0.86
1:B:358:ARG:O	1:B:358:ARG:HG2	1.71	0.86
1:A:683:ARG:HG2	1:B:341:THR:HG21	1.59	0.85
1:A:341:THR:CG2	1:B:683:ARG:CG	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ARG:CG	1:B:341:THR:CG2	2.55	0.84
1:A:341:THR:HG21	1:B:683:ARG:HG2	1.59	0.83
1:A:687:GLN:HA	1:B:228:ASN:ND2	1.94	0.83
1:A:686:LEU:HD22	1:B:340:THR:HG21	1.62	0.81
1:A:228:ASN:ND2	1:B:687:GLN:HA	1.94	0.81
1:A:687:GLN:HA	1:B:228:ASN:HD21	1.45	0.81
1:A:228:ASN:HD21	1:B:687:GLN:HA	1.45	0.81
1:A:340:THR:HG21	1:B:686:LEU:HD22	1.62	0.80
1:A:341:THR:HG21	1:B:683:ARG:CG	2.12	0.80
1:A:358:ARG:O	1:A:358:ARG:HG3	1.82	0.80
1:A:686:LEU:HD22	1:B:340:THR:CG2	2.14	0.78
1:A:683:ARG:CG	1:B:341:THR:HG21	2.12	0.78
1:B:358:ARG:O	1:B:358:ARG:HG3	1.82	0.78
1:A:228:ASN:HD21	1:B:687:GLN:CA	1.97	0.77
1:A:340:THR:CG2	1:B:686:LEU:HD22	2.14	0.77
1:A:687:GLN:CA	1:B:228:ASN:HD21	1.97	0.76
1:A:511:PRO:HB3	1:A:642:LEU:HD21	1.67	0.75
1:B:511:PRO:HB3	1:B:642:LEU:HD21	1.67	0.75
1:B:386:LEU:CD1	1:B:472:PHE:CZ	2.71	0.74
1:A:240:CYS:HA	1:A:320:VAL:HA	1.70	0.74
1:A:386:LEU:CD1	1:A:472:PHE:CZ	2.71	0.73
1:B:240:CYS:HA	1:B:320:VAL:HA	1.70	0.73
1:A:690:MET:HG2	1:B:227:VAL:O	1.90	0.72
1:B:389:PHE:O	1:B:393:PRO:HD2	1.90	0.72
1:A:227:VAL:O	1:B:690:MET:HG2	1.90	0.71
1:A:389:PHE:O	1:A:393:PRO:HD2	1.90	0.71
1:B:390:PHE:CE1	1:B:438:PHE:HB3	2.24	0.71
1:A:339:GLN:HE21	1:B:340:THR:HG23	1.56	0.71
1:B:259:LEU:HG	1:B:262:TYR:HB2	1.74	0.70
1:A:390:PHE:CE1	1:A:438:PHE:HB3	2.24	0.70
1:A:72:PHE:HE1	1:A:76:MET:CE	2.04	0.70
1:A:340:THR:HG23	1:B:339:GLN:NE2	2.07	0.69
1:A:339:GLN:NE2	1:B:340:THR:HG23	2.07	0.69
1:B:72:PHE:HE1	1:B:76:MET:CE	2.04	0.69
1:A:259:LEU:HG	1:A:262:TYR:HB2	1.74	0.69
1:A:340:THR:HG23	1:B:339:GLN:HE21	1.56	0.68
1:A:439:LEU:O	1:A:443:PRO:HD2	1.94	0.68
1:B:439:LEU:O	1:B:443:PRO:HD2	1.94	0.68
1:A:228:ASN:HD21	1:B:687:GLN:CB	2.07	0.68
1:A:341:THR:HG22	1:B:683:ARG:CG	2.19	0.67
1:A:341:THR:HG21	1:B:683:ARG:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ARG:HB3	1:B:341:THR:HG21	1.76	0.67
1:A:72:PHE:HE1	1:A:76:MET:HE2	1.59	0.66
1:B:72:PHE:CE1	1:B:76:MET:CE	2.79	0.66
1:A:72:PHE:CE1	1:A:76:MET:CE	2.79	0.66
1:A:687:GLN:CB	1:B:228:ASN:HD21	2.07	0.65
1:A:340:THR:HG22	1:B:686:LEU:HD13	1.76	0.64
1:B:575:GLN:HE21	1:B:631:ARG:HB2	1.64	0.62
1:A:575:GLN:HE21	1:A:631:ARG:HB2	1.64	0.62
1:B:72:PHE:HE1	1:B:76:MET:HE2	1.65	0.61
1:B:433:ILE:O	1:B:435:LEU:N	2.33	0.61
1:A:340:THR:CG2	1:B:686:LEU:CD2	2.71	0.61
1:A:433:ILE:O	1:A:435:LEU:N	2.33	0.61
1:A:683:ARG:CB	1:B:341:THR:HG21	2.29	0.61
1:A:686:LEU:HD13	1:B:340:THR:HG22	1.76	0.61
1:A:341:THR:HG21	1:B:683:ARG:CB	2.29	0.61
1:B:439:LEU:HA	1:B:442:LEU:HB2	1.83	0.60
1:A:439:LEU:HA	1:A:442:LEU:HB2	1.83	0.59
1:B:73:LEU:O	1:B:76:MET:HB2	2.02	0.59
1:A:73:LEU:O	1:A:76:MET:HB2	2.02	0.59
1:A:72:PHE:CE1	1:A:76:MET:HE2	2.37	0.59
1:A:109:PHE:HA	1:A:112:ILE:HG12	1.85	0.59
1:A:683:ARG:CG	1:B:341:THR:HG22	2.19	0.59
1:B:109:PHE:HA	1:B:112:ILE:HG12	1.85	0.58
1:A:340:THR:HG21	1:B:686:LEU:CG	2.33	0.58
1:A:686:LEU:CG	1:B:340:THR:HG21	2.33	0.58
1:A:686:LEU:HD21	1:B:340:THR:HG21	1.82	0.58
1:B:72:PHE:HA	1:B:75:TRP:CD1	2.39	0.57
1:A:72:PHE:HA	1:A:75:TRP:CD1	2.39	0.57
1:A:686:LEU:HD13	1:B:340:THR:HG23	1.81	0.57
1:B:379:MET:HG2	1:B:452:PHE:HD2	1.71	0.56
1:B:72:PHE:CE1	1:B:76:MET:HE3	2.41	0.56
1:B:277:THR:HG23	1:B:282:LEU:HD11	1.87	0.56
1:A:277:THR:HG23	1:A:282:LEU:HD11	1.87	0.56
1:A:340:THR:HG21	1:B:686:LEU:HD21	1.82	0.56
1:A:687:GLN:CA	1:B:228:ASN:ND2	2.62	0.56
1:A:340:THR:HG23	1:B:686:LEU:HD13	1.81	0.55
1:A:433:ILE:O	1:A:436:LYS:N	2.27	0.55
1:A:340:THR:HG21	1:B:686:LEU:HD11	1.88	0.55
1:A:546:ASN:O	1:A:549:LEU:HB3	2.07	0.55
1:A:686:LEU:CD2	1:B:340:THR:CG2	2.71	0.55
1:B:546:ASN:O	1:B:549:LEU:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:HG13	1:B:336:VAL:HG13	1.88	0.55
1:A:379:MET:HG2	1:A:452:PHE:HD2	1.71	0.54
1:A:228:ASN:ND2	1:B:687:GLN:CA	2.62	0.54
1:A:178:MET:HB2	1:A:669:PHE:HE1	1.74	0.53
1:B:178:MET:HB2	1:B:669:PHE:HE1	1.74	0.53
1:A:473:ASN:HA	1:A:477:VAL:HG23	1.92	0.52
1:B:383:PHE:CE1	1:B:472:PHE:CD1	2.97	0.52
1:B:473:ASN:HA	1:B:477:VAL:HG23	1.92	0.52
1:B:110:ALA:HB3	1:B:111:PRO:HD3	1.92	0.52
1:A:110:ALA:HB3	1:A:111:PRO:HD3	1.92	0.52
1:A:443:PRO:HG3	1:A:469:TYR:HE2	1.74	0.52
1:B:72:PHE:CE1	1:B:76:MET:HE2	2.43	0.52
1:B:443:PRO:HG3	1:B:469:TYR:HE2	1.74	0.52
1:A:486:ALA:O	1:A:490:GLN:CG	2.54	0.52
1:B:644:MET:HG3	1:B:659:LEU:HB3	1.92	0.52
1:A:383:PHE:CE1	1:A:472:PHE:CD1	2.97	0.51
1:B:441:PHE:O	1:B:444:ALA:HB3	2.11	0.51
1:A:644:MET:HG3	1:A:659:LEU:HB3	1.92	0.51
1:B:433:ILE:O	1:B:436:LYS:N	2.27	0.51
1:A:496:ASN:O	1:A:499:PRO:HD3	2.11	0.51
1:B:486:ALA:O	1:B:490:GLN:CG	2.54	0.51
1:A:441:PHE:O	1:A:444:ALA:HB3	2.11	0.50
1:A:383:PHE:CE1	1:A:472:PHE:HD1	2.30	0.50
1:A:226:LEU:HD13	1:A:233:TYR:HD2	1.77	0.50
1:B:383:PHE:CE1	1:B:472:PHE:HD1	2.30	0.50
1:B:476:ASN:O	1:B:481:SER:HB3	2.13	0.49
1:B:177:LEU:HD11	1:B:632:VAL:HG11	1.94	0.49
1:B:496:ASN:O	1:B:499:PRO:HD3	2.11	0.49
1:A:177:LEU:HD11	1:A:632:VAL:HG11	1.94	0.49
1:B:97:VAL:HG21	1:B:622:ALA:HB2	1.94	0.49
1:B:75:TRP:HB2	1:B:608:HIS:CD2	2.48	0.49
1:A:75:TRP:HB2	1:A:608:HIS:CD2	2.48	0.49
1:A:390:PHE:HE1	1:A:438:PHE:CB	2.19	0.49
1:A:439:LEU:O	1:A:443:PRO:CD	2.61	0.49
1:A:476:ASN:O	1:A:481:SER:HB3	2.13	0.49
1:B:226:LEU:HD13	1:B:233:TYR:HD2	1.77	0.49
1:A:97:VAL:HG21	1:A:622:ALA:HB2	1.94	0.49
1:B:206:VAL:HG21	1:B:349:TRP:HE3	1.78	0.49
1:A:533:ILE:HD12	1:A:533:ILE:HA	1.67	0.48
1:A:539:LEU:HD13	1:A:539:LEU:HA	1.69	0.48
1:A:259:LEU:CB	1:A:294:HIS:H	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:CE1	1:A:76:MET:HE3	2.47	0.48
1:A:554:LYS:HB3	1:A:555:ASP:H	1.53	0.47
1:B:259:LEU:CB	1:B:294:HIS:H	2.27	0.47
1:A:206:VAL:HG21	1:A:349:TRP:HE3	1.78	0.47
1:B:554:LYS:HB3	1:B:555:ASP:H	1.53	0.47
1:B:339:GLN:HB2	1:B:683:ARG:HH21	1.81	0.46
1:B:662:LEU:HD12	1:B:662:LEU:HA	1.77	0.46
1:B:422:ILE:HG13	1:B:425:LEU:HB2	1.98	0.46
1:A:339:GLN:HB2	1:A:683:ARG:HH21	1.81	0.46
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.80	0.46
1:B:685:PRO:HB2	1:B:688:GLU:HB2	1.97	0.46
1:A:483:ILE:H	1:A:483:ILE:HG13	1.21	0.46
1:B:439:LEU:O	1:B:443:PRO:CD	2.61	0.46
1:B:545:LYS:HD3	1:B:545:LYS:HA	1.52	0.46
1:A:685:PRO:HB2	1:A:688:GLU:HB2	1.97	0.45
1:A:270:ASN:O	1:A:271:SER:C	2.55	0.45
1:A:662:LEU:HD12	1:A:662:LEU:HA	1.77	0.45
1:B:93:LEU:HD11	1:B:187:MET:HB3	1.99	0.45
1:B:95:SER:HB2	1:B:610:ILE:HG12	1.98	0.45
1:B:270:ASN:O	1:B:271:SER:C	2.55	0.45
1:B:602:ALA:O	1:B:606:TYR:HB2	2.17	0.45
1:A:95:SER:HB2	1:A:610:ILE:HG12	1.98	0.45
1:B:401:ALA:HB1	1:B:430:LEU:HD21	1.98	0.45
1:A:442:LEU:O	1:A:443:PRO:C	2.54	0.45
1:A:93:LEU:HD11	1:A:187:MET:HB3	1.99	0.45
1:B:276:ILE:H	1:B:276:ILE:HG13	1.46	0.45
1:A:601:LEU:HD12	1:A:601:LEU:HA	1.75	0.45
1:A:602:ALA:O	1:A:606:TYR:HB2	2.17	0.45
1:A:401:ALA:HB1	1:A:430:LEU:HD21	1.98	0.44
1:A:422:ILE:HG13	1:A:425:LEU:HB2	1.98	0.44
1:B:288:LYS:H	1:B:288:LYS:HG3	1.53	0.44
1:A:244:LYS:HB3	1:A:309:GLU:HG2	1.98	0.44
1:A:479:LEU:H	1:A:479:LEU:HG	1.69	0.44
1:A:650:LYS:HB2	1:A:650:LYS:HE2	1.35	0.44
1:A:686:LEU:HD11	1:B:340:THR:HG21	1.88	0.44
1:A:481:SER:HB2	1:A:482:VAL:H	1.47	0.44
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.61	0.44
1:B:72:PHE:HE1	1:B:76:MET:HE3	1.74	0.44
1:A:541:ILE:HD13	1:A:541:ILE:HA	1.82	0.44
1:B:244:LYS:HB3	1:B:309:GLU:HG2	1.98	0.44
1:B:268:ARG:HB2	1:B:269:ASN:H	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:PEE:H71	2:B:801:PEE:H77	1.90	0.44
1:B:523:VAL:O	1:B:524:ASP:C	2.56	0.44
1:A:443:PRO:O	1:A:444:ALA:C	2.56	0.44
1:B:442:LEU:O	1:B:443:PRO:C	2.54	0.44
1:A:242:ALA:HB3	1:A:715:HIS:CD2	2.53	0.43
1:A:512:MET:HB3	1:A:513:LYS:H	1.59	0.43
1:B:443:PRO:O	1:B:444:ALA:C	2.56	0.43
1:A:170:THR:HG21	1:A:640:GLN:HE21	1.83	0.43
1:A:607:ARG:O	1:A:611:ILE:HG13	2.18	0.43
1:A:443:PRO:HD3	1:A:469:TYR:CE2	2.54	0.43
1:A:545:LYS:HA	1:A:545:LYS:HD3	1.52	0.43
1:A:523:VAL:O	1:A:524:ASP:C	2.56	0.43
1:A:549:LEU:HD12	1:A:552:THR:HA	2.01	0.43
1:B:423:LYS:HA	1:B:423:LYS:HD3	1.61	0.43
1:B:607:ARG:O	1:B:611:ILE:HG13	2.18	0.43
1:A:443:PRO:HG3	1:A:469:TYR:CE2	2.53	0.43
1:B:276:ILE:HG22	1:B:282:LEU:HD12	2.01	0.43
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.89	0.43
1:B:170:THR:HG21	1:B:640:GLN:HE21	1.83	0.43
1:B:242:ALA:HB3	1:B:715:HIS:CD2	2.53	0.43
1:A:259:LEU:HB2	1:A:294:HIS:H	1.84	0.43
1:A:481:SER:O	1:A:482:VAL:C	2.57	0.42
1:B:245:LEU:HD13	1:B:309:GLU:HB3	2.02	0.42
1:B:443:PRO:HG3	1:B:469:TYR:CE2	2.53	0.42
1:A:442:LEU:HD22	1:A:442:LEU:HA	1.53	0.42
1:B:110:ALA:HA	1:B:596:LEU:HD11	2.00	0.42
1:B:592:LEU:HB2	1:B:593:PRO:HD3	2.01	0.42
1:A:110:ALA:HA	1:A:596:LEU:HD11	2.00	0.42
1:B:365:LEU:HD22	1:B:456:THR:HB	2.01	0.42
1:B:443:PRO:HD3	1:B:469:TYR:CE2	2.54	0.42
1:B:481:SER:O	1:B:482:VAL:C	2.57	0.42
1:B:539:LEU:HD13	1:B:539:LEU:HA	1.69	0.42
1:B:259:LEU:HB2	1:B:294:HIS:H	1.84	0.42
2:B:801:PEE:H73	2:B:801:PEE:H67	1.67	0.42
1:A:276:ILE:HG22	1:A:282:LEU:HD12	2.01	0.42
1:B:77:PRO:HA	1:B:80:LEU:HB2	2.00	0.42
1:B:365:LEU:HD13	1:B:365:LEU:HA	1.84	0.42
1:A:408:LYS:HE2	1:A:408:LYS:HB2	1.67	0.42
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.90	0.42
1:A:251:LYS:HB3	1:A:251:LYS:HE3	1.79	0.42
1:A:288:LYS:H	1:A:288:LYS:HG3	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASP:HB3	1:A:291:ALA:H	1.62	0.42
1:A:365:LEU:HD22	1:A:456:THR:HB	2.01	0.42
1:A:77:PRO:HA	1:A:80:LEU:HB2	2.00	0.42
1:A:433:ILE:HG23	1:A:434:ALA:H	1.85	0.42
1:A:245:LEU:HD13	1:A:309:GLU:HB3	2.02	0.41
1:B:549:LEU:HD12	1:B:552:THR:HA	2.01	0.41
1:A:273:ILE:H	1:A:273:ILE:HG13	1.37	0.41
1:B:433:ILE:HG23	1:B:434:ALA:H	1.85	0.41
1:A:272:GLN:H	1:A:272:GLN:HG2	1.66	0.41
1:B:390:PHE:HE1	1:B:438:PHE:CB	2.19	0.41
1:B:601:LEU:HD12	1:B:601:LEU:HA	1.75	0.41
1:A:82:MET:HE2	1:A:82:MET:HB3	1.84	0.41
1:A:542:TYR:HD1	1:A:542:TYR:HA	1.67	0.41
1:A:592:LEU:HB2	1:A:593:PRO:HD3	2.01	0.41
1:B:273:ILE:H	1:B:273:ILE:HG13	1.37	0.41
1:B:542:TYR:HD1	1:B:542:TYR:HA	1.67	0.41
1:A:440:ILE:O	1:A:441:PHE:C	2.59	0.41
2:A:801:PEE:H73	2:A:801:PEE:H67	1.67	0.41
1:B:75:TRP:HZ3	1:B:604:VAL:HG22	1.86	0.41
1:A:278:LYS:HD2	1:A:278:LYS:HA	1.74	0.41
1:B:440:ILE:O	1:B:441:PHE:C	2.59	0.41
1:B:512:MET:HB3	1:B:513:LYS:H	1.59	0.41
1:B:643:LEU:HD13	1:B:643:LEU:HA	1.74	0.41
1:A:643:LEU:HD13	1:A:643:LEU:HA	1.74	0.41
1:B:650:LYS:HB2	1:B:650:LYS:HE2	1.35	0.41
1:A:75:TRP:HZ3	1:A:604:VAL:HG22	1.86	0.40
1:A:75:TRP:HH2	1:A:605:VAL:HG12	1.86	0.40
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.89	0.40
1:B:392:ILE:H	1:B:392:ILE:HG13	1.70	0.40
1:A:342:GLN:O	1:B:687:GLN:HB2	2.21	0.40
1:B:82:MET:HE2	1:B:82:MET:HB3	1.78	0.40
1:B:97:VAL:HG21	1:B:622:ALA:CB	2.51	0.40
1:B:596:LEU:HD23	1:B:596:LEU:HA	1.90	0.40
1:A:687:GLN:HB2	1:B:342:GLN:O	2.21	0.40
1:B:408:LYS:HE2	1:B:408:LYS:HB2	1.67	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	584/772 (76%)	509 (87%)	62 (11%)	13 (2%)	5	10
1	B	584/772 (76%)	509 (87%)	62 (11%)	13 (2%)	5	10
All	All	1168/1544 (76%)	1018 (87%)	124 (11%)	26 (2%)	8	10

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ILE
1	A	433	ILE
1	A	434	ALA
1	A	475	VAL
1	B	296	ILE
1	B	433	ILE
1	B	434	ALA
1	B	475	VAL
1	A	482	VAL
1	A	483	ILE
1	A	524	ASP
1	A	549	LEU
1	B	482	VAL
1	B	483	ILE
1	B	524	ASP
1	B	549	LEU
1	A	271	SER
1	A	444	ALA
1	A	474	LEU
1	B	271	SER
1	B	444	ALA
1	B	474	LEU
1	A	523	VAL
1	B	523	VAL
1	A	498	SER

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Mol	Chain	Res	Type
1	B	498	SER

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	511/665 (77%)	332 (65%)	179 (35%)	0	0
1	B	511/665 (77%)	332 (65%)	179 (35%)	0	0
All	All	1022/1330 (77%)	664 (65%)	358 (35%)	1	0

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	72	PHE
1	A	78	GLU
1	A	82	MET
1	A	84	GLU
1	A	85	ARG
1	A	86	GLU
1	A	96	VAL
1	A	104	LEU
1	A	115	LEU
1	A	120	LEU
1	A	121	VAL
1	A	123	VAL
1	A	159	PHE
1	A	160	TRP
1	A	162	HIS
1	A	163	ILE
1	A	178	MET
1	A	179	LYS
1	A	181	TYR
1	A	188	ARG
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	200	ASP
1	A	203	THR
1	A	205	LEU
1	A	214	ASP
1	A	215	GLU
1	A	218	SER
1	A	219	GLU
1	A	226	LEU
1	A	231	ASP
1	A	235	THR
1	A	238	VAL
1	A	239	VAL
1	A	240	CYS
1	A	244	LYS
1	A	252	LYS
1	A	256	GLN
1	A	257	ASN
1	A	258	TRP
1	A	259	LEU
1	A	260	ASP
1	A	263	GLN
1	A	264	LEU
1	A	265	LYS
1	A	266	TYR
1	A	267	THR
1	A	268	ARG
1	A	269	ASN
1	A	270	ASN
1	A	272	GLN
1	A	273	ILE
1	A	274	ARG
1	A	276	ILE
1	A	277	THR
1	A	278	LYS
1	A	279	LEU
1	A	282	LEU
1	A	284	LEU
1	A	285	CYS
1	A	288	LYS
1	A	289	VAL
1	A	290	ASP

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Mol	Chain	Res	Type
1	A	294	HIS
1	A	295	TYR
1	A	301	LYS
1	A	304	LYS
1	A	305	GLU
1	A	315	ASN
1	A	317	GLN
1	A	321	MET
1	A	327	SER
1	A	330	THR
1	A	331	ARG
1	A	341	THR
1	A	347	THR
1	A	352	GLU
1	A	358	ARG
1	A	365	LEU
1	A	367	ILE
1	A	370	VAL
1	A	371	SER
1	A	374	VAL
1	A	376	ARG
1	A	379	MET
1	A	386	LEU
1	A	387	THR
1	A	396	PHE
1	A	399	SER
1	A	422	ILE
1	A	423	LYS
1	A	425	LEU
1	A	429	LEU
1	A	430	LEU
1	A	433	ILE
1	A	435	LEU
1	A	439	LEU
1	A	442	LEU
1	A	446	LEU
1	A	450	SER
1	A	453	GLU
1	A	457	SER
1	A	459	SER
1	A	462	GLU
1	A	468	ARG

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Mol	Chain	Res	Type
1	A	469	TYR
1	A	471	ILE
1	A	472	PHE
1	A	477	VAL
1	A	478	PHE
1	A	479	LEU
1	A	481	SER
1	A	483	ILE
1	A	488	PHE
1	A	491	LEU
1	A	493	SER
1	A	495	LEU
1	A	513	LYS
1	A	515	THR
1	A	520	TYR
1	A	522	MET
1	A	533	ILE
1	A	534	LEU
1	A	535	MET
1	A	536	LEU
1	A	537	LYS
1	A	539	LEU
1	A	540	ILE
1	A	542	TYR
1	A	545	LYS
1	A	549	LEU
1	A	550	VAL
1	A	551	LYS
1	A	552	THR
1	A	554	LYS
1	A	555	ASP
1	A	556	ARG
1	A	560	MET
1	A	565	ILE
1	A	571	GLU
1	A	582	LEU
1	A	590	MET
1	A	591	LEU
1	A	595	ILE
1	A	601	LEU
1	A	607	ARG
1	A	610	ILE

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Mol	Chain	Res	Type
1	A	613	VAL
1	A	615	ASN
1	A	620	SER
1	A	625	TRP
1	A	636	LEU
1	A	641	LEU
1	A	642	LEU
1	A	643	LEU
1	A	650	LYS
1	A	658	PHE
1	A	659	LEU
1	A	660	ILE
1	A	662	LEU
1	A	671	ARG
1	A	673	CYS
1	A	674	LYS
1	A	676	ARG
1	A	683	ARG
1	A	687	GLN
1	A	688	GLU
1	A	696	GLU
1	A	697	ARG
1	A	700	GLU
1	A	702	ASN
1	A	703	LEU
1	A	705	LEU
1	A	706	LYS
1	A	709	LEU
1	A	711	ASP
1	A	714	ILE
1	A	715	HIS
1	B	70	LEU
1	B	72	PHE
1	B	78	GLU
1	B	82	MET
1	B	84	GLU
1	B	85	ARG
1	B	86	GLU
1	B	96	VAL
1	B	104	LEU
1	B	115	LEU
1	B	120	LEU

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Mol	Chain	Res	Type
1	B	121	VAL
1	B	123	VAL
1	B	159	PHE
1	B	160	TRP
1	B	162	HIS
1	B	163	ILE
1	B	178	MET
1	B	179	LYS
1	B	181	TYR
1	B	188	ARG
1	B	190	GLN
1	B	192	LEU
1	B	200	ASP
1	B	203	THR
1	B	205	LEU
1	B	214	ASP
1	B	215	GLU
1	B	218	SER
1	B	219	GLU
1	B	226	LEU
1	B	231	ASP
1	B	235	THR
1	B	238	VAL
1	B	239	VAL
1	B	240	CYS
1	B	244	LYS
1	B	252	LYS
1	B	256	GLN
1	B	257	ASN
1	B	258	TRP
1	B	259	LEU
1	B	260	ASP
1	B	263	GLN
1	B	264	LEU
1	B	265	LYS
1	B	266	TYR
1	B	267	THR
1	B	268	ARG
1	B	269	ASN
1	B	270	ASN
1	B	272	GLN
1	B	273	ILE

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Mol	Chain	Res	Type
1	B	274	ARG
1	B	276	ILE
1	B	277	THR
1	B	278	LYS
1	B	279	LEU
1	B	282	LEU
1	B	284	LEU
1	B	285	CYS
1	B	288	LYS
1	B	289	VAL
1	B	290	ASP
1	B	294	HIS
1	B	295	TYR
1	B	301	LYS
1	B	304	LYS
1	B	305	GLU
1	B	315	ASN
1	B	317	GLN
1	B	321	MET
1	B	327	SER
1	B	330	THR
1	B	331	ARG
1	B	341	THR
1	B	347	THR
1	B	352	GLU
1	B	358	ARG
1	B	365	LEU
1	B	367	ILE
1	B	370	VAL
1	B	371	SER
1	B	374	VAL
1	B	376	ARG
1	B	379	MET
1	B	386	LEU
1	B	387	THR
1	B	396	PHE
1	B	399	SER
1	B	422	ILE
1	B	423	LYS
1	B	425	LEU
1	B	429	LEU
1	B	430	LEU

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Mol	Chain	Res	Type
1	B	433	ILE
1	B	435	LEU
1	B	439	LEU
1	B	442	LEU
1	B	446	LEU
1	B	450	SER
1	B	453	GLU
1	B	457	SER
1	B	459	SER
1	B	462	GLU
1	B	468	ARG
1	B	469	TYR
1	B	471	ILE
1	B	472	PHE
1	B	477	VAL
1	B	478	PHE
1	B	479	LEU
1	B	481	SER
1	B	483	ILE
1	B	488	PHE
1	B	491	LEU
1	B	493	SER
1	B	495	LEU
1	B	513	LYS
1	B	515	THR
1	B	520	TYR
1	B	522	MET
1	B	533	ILE
1	B	534	LEU
1	B	535	MET
1	B	536	LEU
1	B	537	LYS
1	B	539	LEU
1	B	540	ILE
1	B	542	TYR
1	B	545	LYS
1	B	549	LEU
1	B	550	VAL
1	B	551	LYS
1	B	552	THR
1	B	554	LYS
1	B	555	ASP

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Mol	Chain	Res	Type
1	B	556	ARG
1	B	560	MET
1	B	565	ILE
1	B	571	GLU
1	B	582	LEU
1	B	590	MET
1	B	591	LEU
1	B	595	ILE
1	B	601	LEU
1	B	607	ARG
1	B	610	ILE
1	B	613	VAL
1	B	615	ASN
1	B	620	SER
1	B	625	TRP
1	B	636	LEU
1	B	641	LEU
1	B	642	LEU
1	B	643	LEU
1	B	650	LYS
1	B	658	PHE
1	B	659	LEU
1	B	660	ILE
1	B	662	LEU
1	B	671	ARG
1	B	673	CYS
1	B	674	LYS
1	B	676	ARG
1	B	683	ARG
1	B	687	GLN
1	B	688	GLU
1	B	696	GLU
1	B	697	ARG
1	B	700	GLU
1	B	702	ASN
1	B	703	LEU
1	B	705	LEU
1	B	706	LYS
1	B	709	LEU
1	B	711	ASP
1	B	714	ILE
1	B	715	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	237	GLN
1	A	339	GLN
1	A	427	GLN
1	A	497	GLN
1	A	546	ASN
1	A	575	GLN
1	A	608	HIS
1	A	687	GLN
1	B	228	ASN
1	B	237	GLN
1	B	339	GLN
1	B	427	GLN
1	B	497	GLN
1	B	546	ASN
1	B	575	GLN
1	B	608	HIS
1	B	687	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](#)

2 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	PEE	A	801	-	8,8,50	0.23	0	7,7,55	0.55	0
2	PEE	B	801	-	8,8,50	0.23	0	7,7,55	0.55	0

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	PEE	A	801	-	-	3/6/6/54	-
2	PEE	B	801	-	-	3/6/6/54	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PEE	C40-C41-C42-C43
2	B	801	PEE	C40-C41-C42-C43
2	A	801	PEE	C42-C43-C44-C45
2	B	801	PEE	C42-C43-C44-C45
2	A	801	PEE	C43-C44-C45-C46
2	B	801	PEE	C43-C44-C45-C46

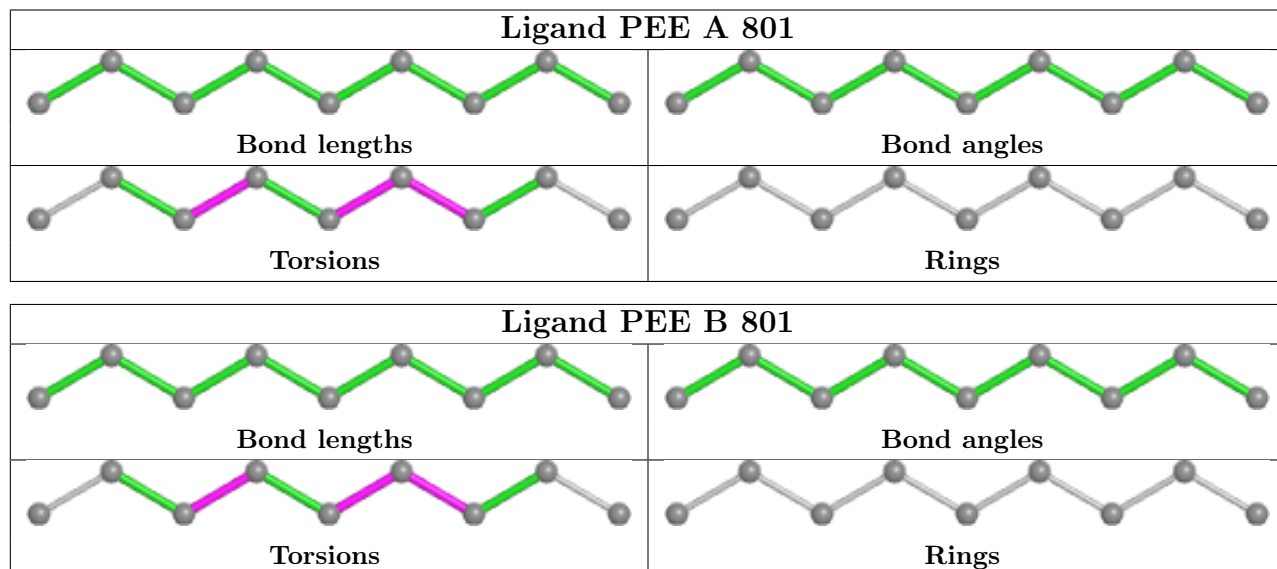
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PEE	1	0
2	B	801	PEE	2	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.

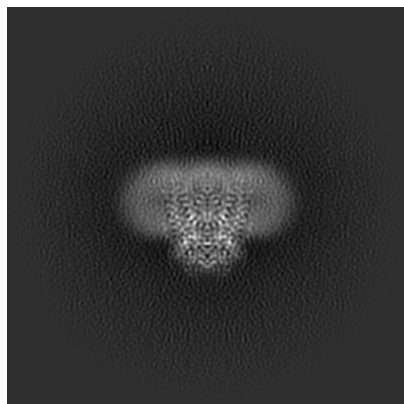
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39402. These allow visual inspection of the internal detail of the map and identification of artifacts.

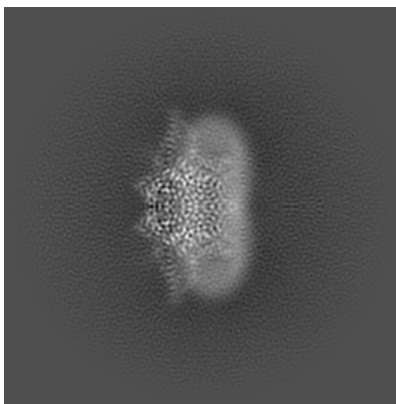
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

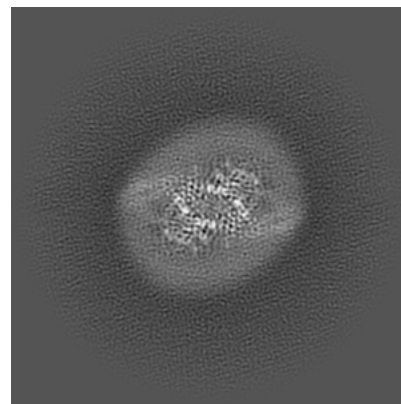
6.1.1 Primary map



X

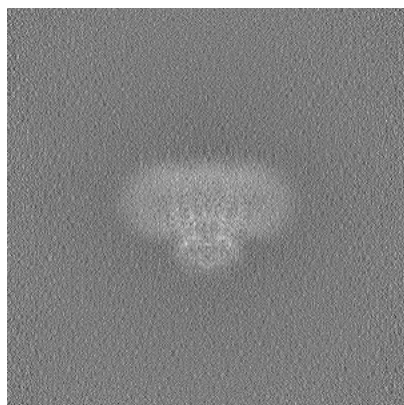


Y

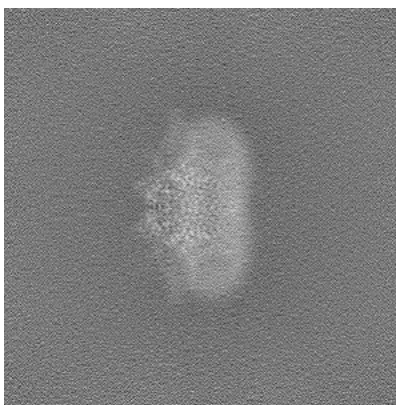


Z

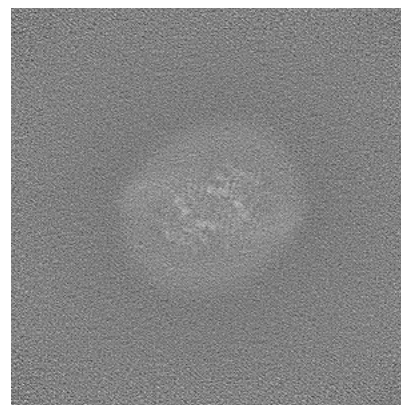
6.1.2 Raw map



X



Y

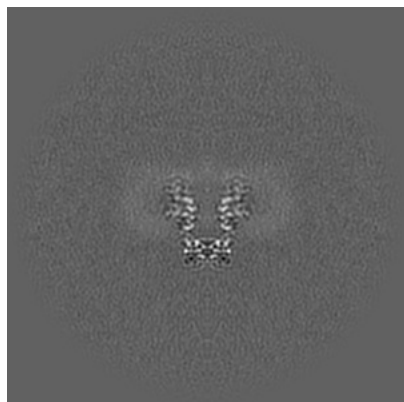


Z

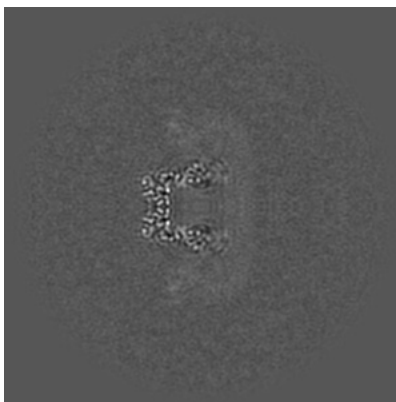
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

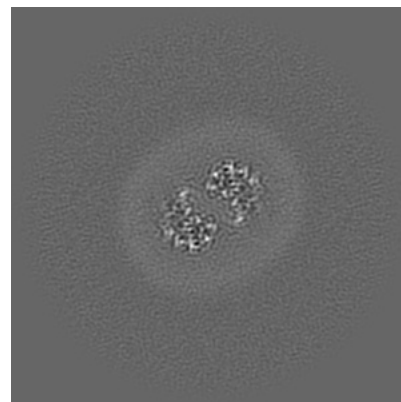
6.2.1 Primary map



X Index: 256

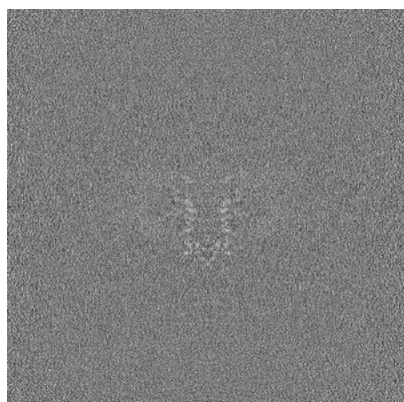


Y Index: 256

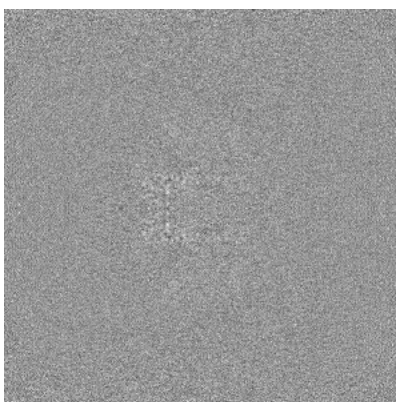


Z Index: 256

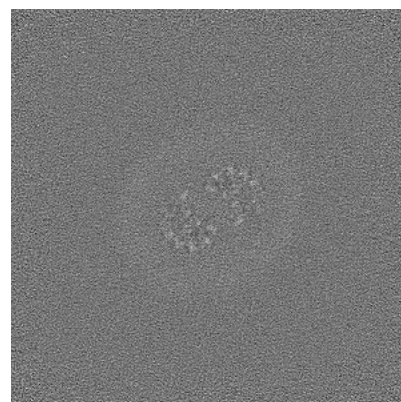
6.2.2 Raw map



X Index: 256



Y Index: 256

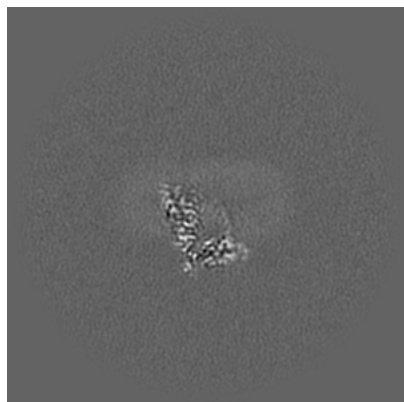


Z Index: 256

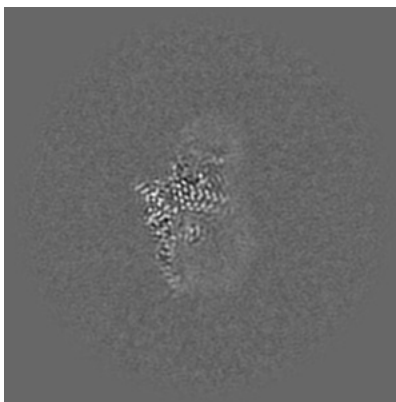
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

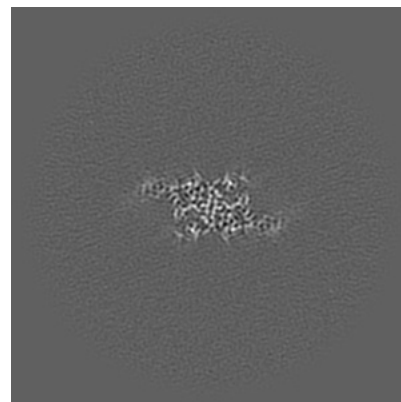
6.3.1 Primary map



X Index: 236

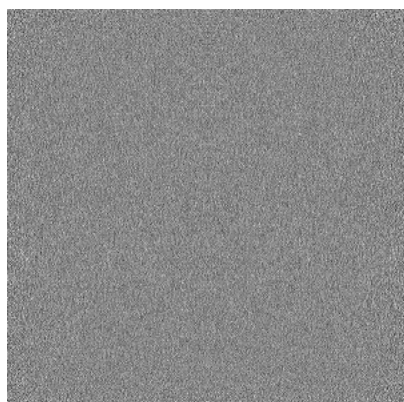


Y Index: 279

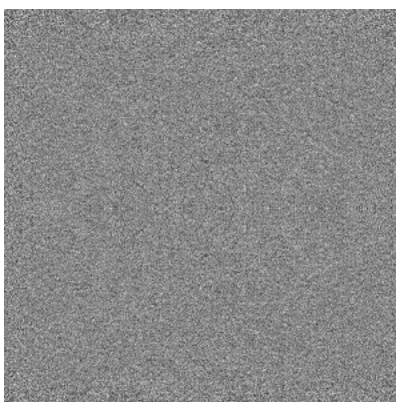


Z Index: 208

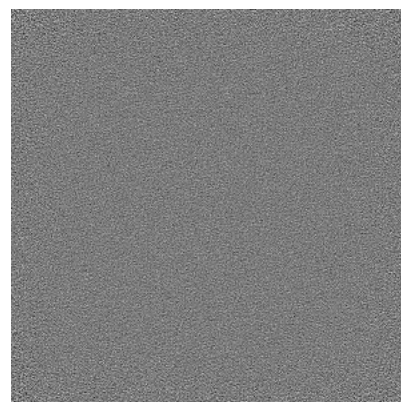
6.3.2 Raw map



X Index: 0



Y Index: 0

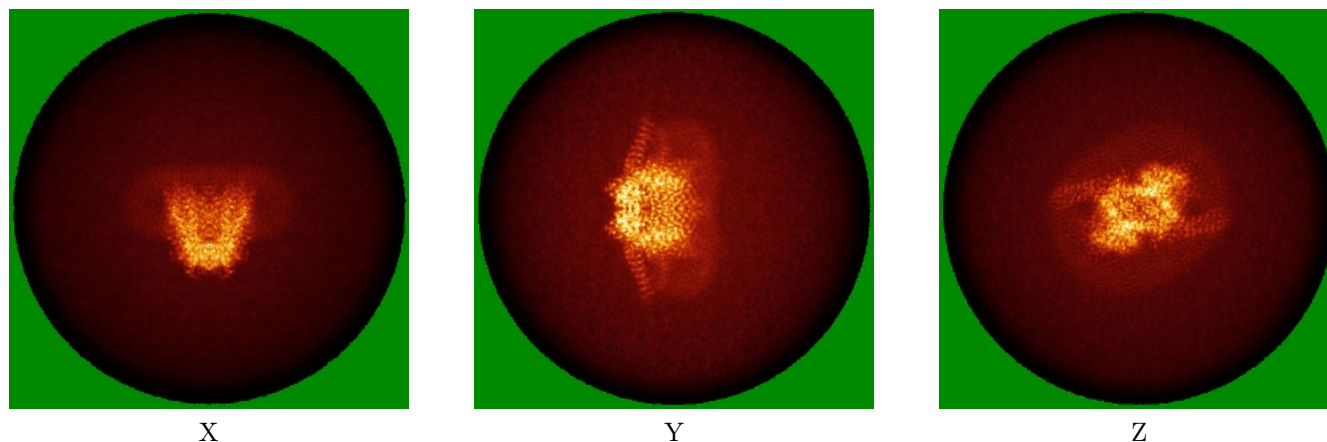


Z Index: 0

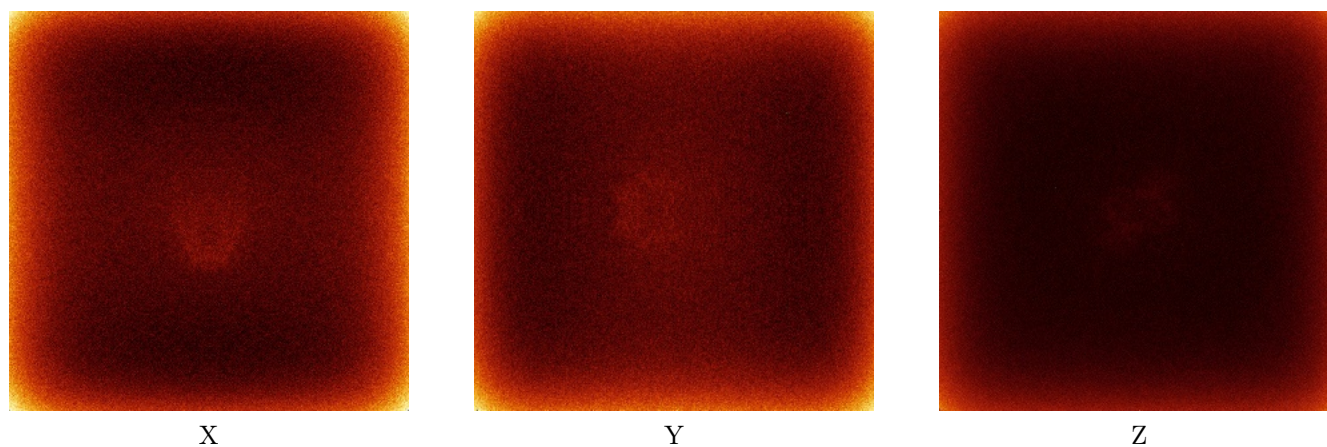
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



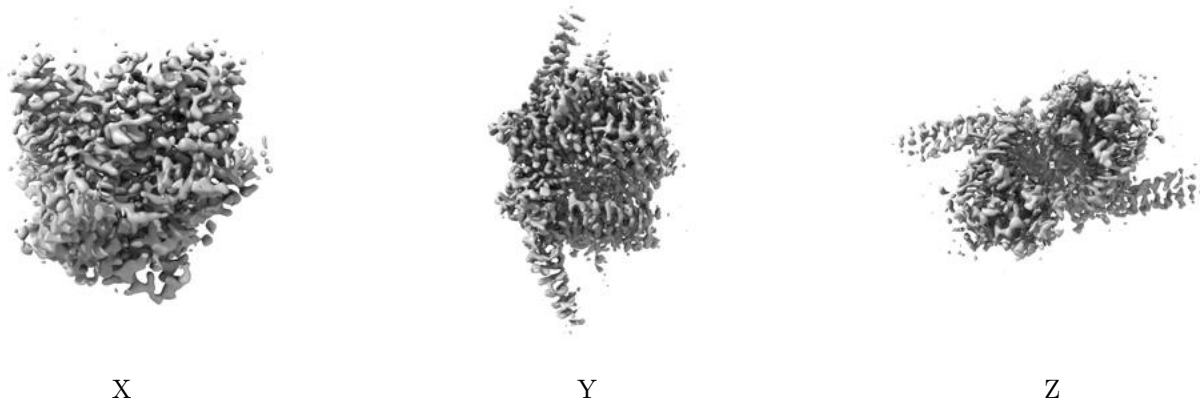
6.4.2 Raw map



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

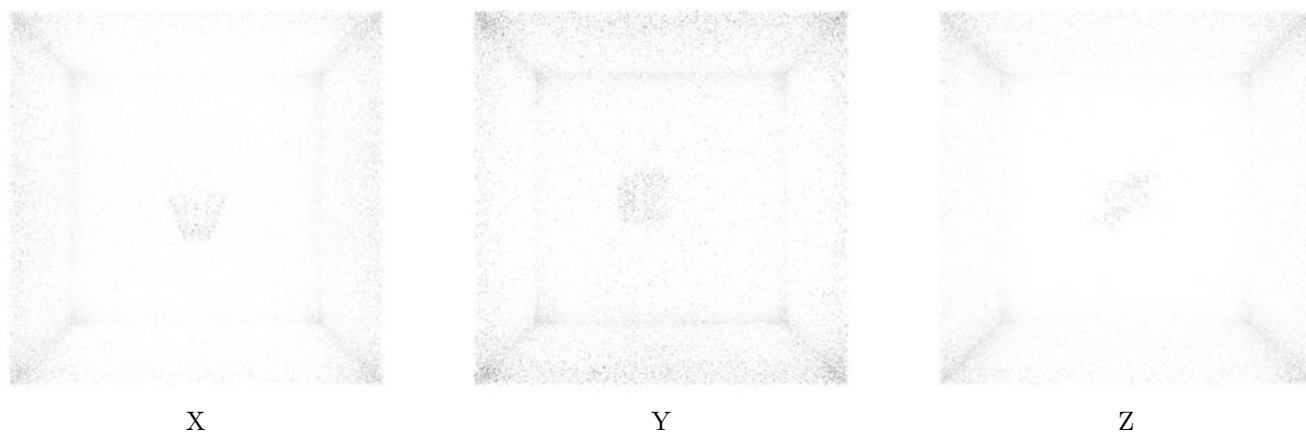
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

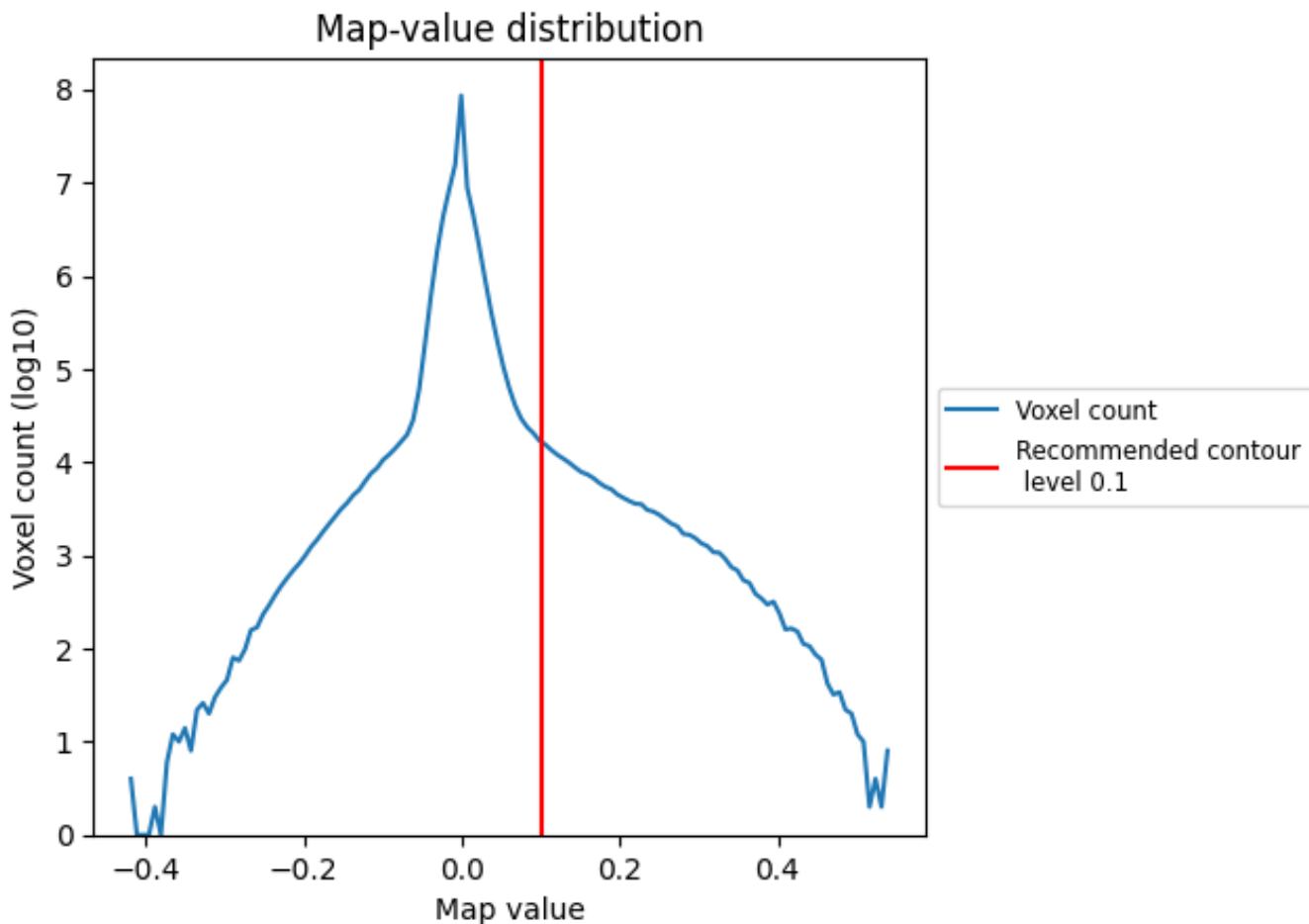
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

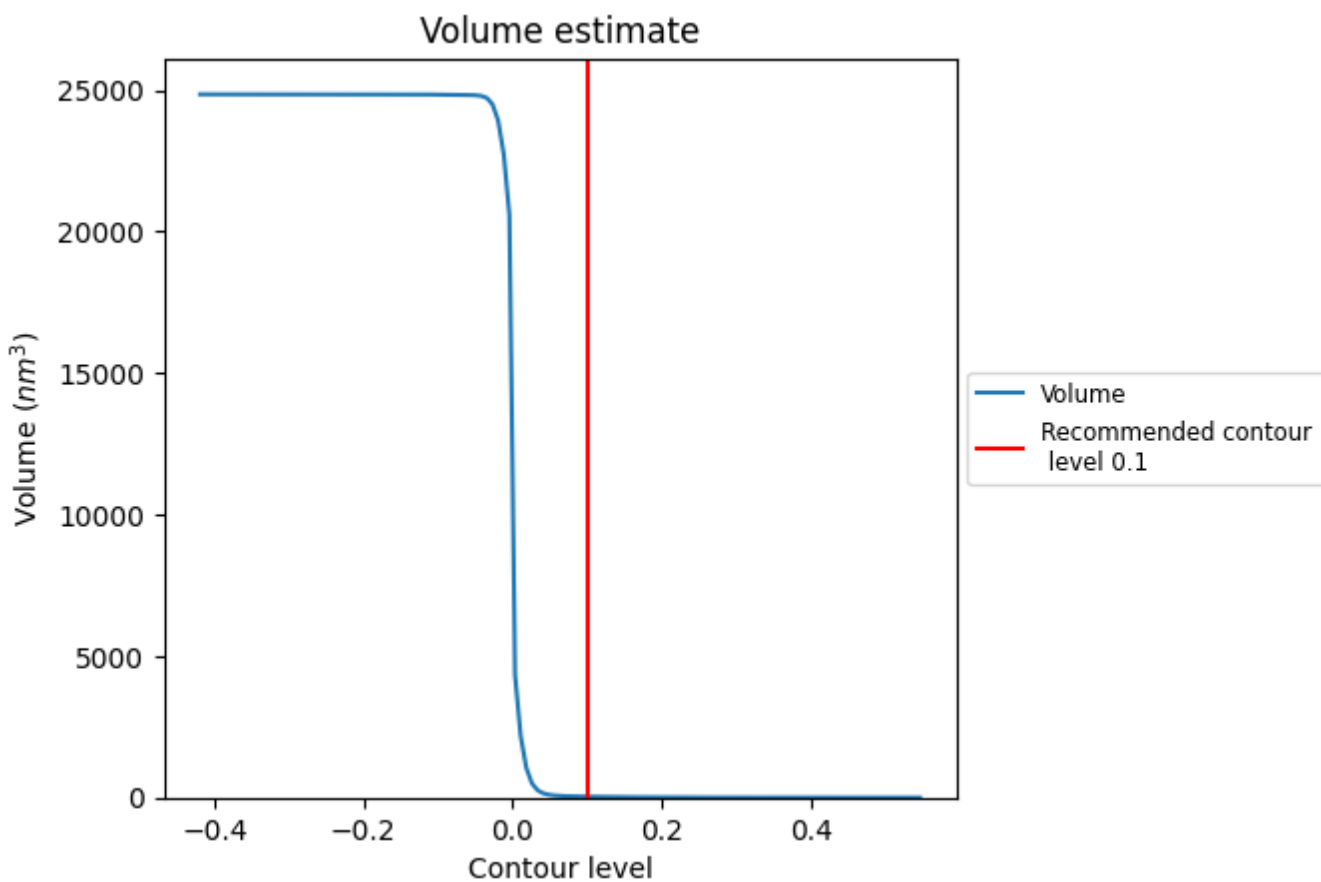
This section contains the results of statistical analysis of the map.

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.

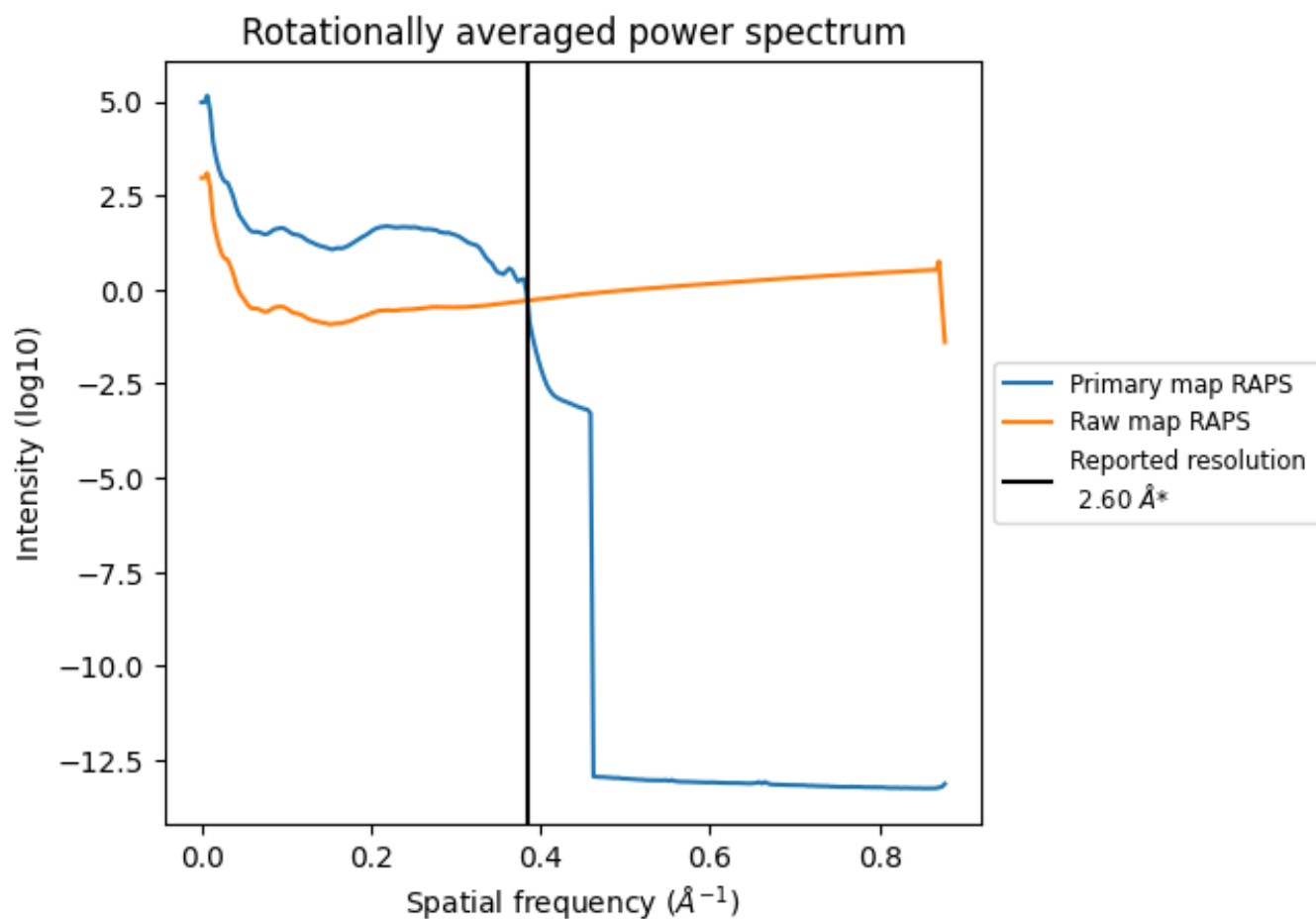
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm^3 ; this corresponds to an approximate mass of 29 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](#)

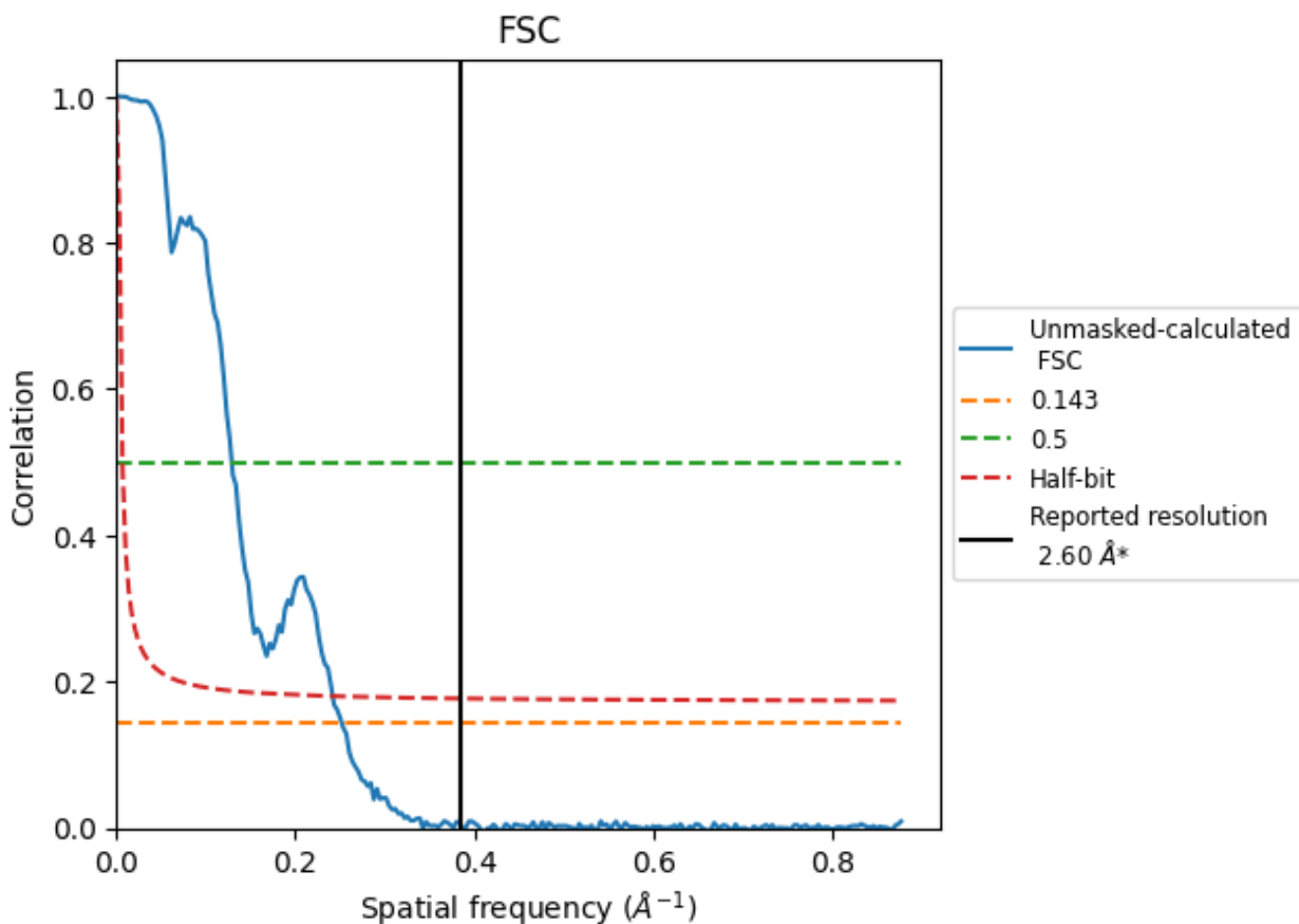


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

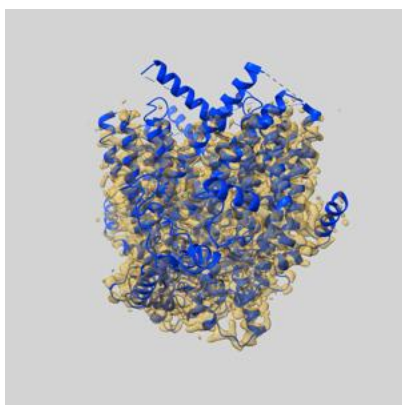
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	7.76	4.14

*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 3.97 differs from the reported value 2.6 by more than 10 %

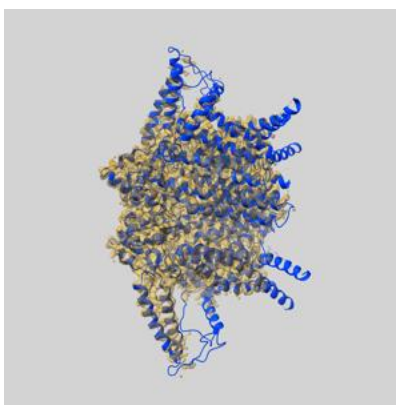
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39402 and PDB model 8YMP. Per-residue inclusion information can be found in section [3](#) on page [5](#).

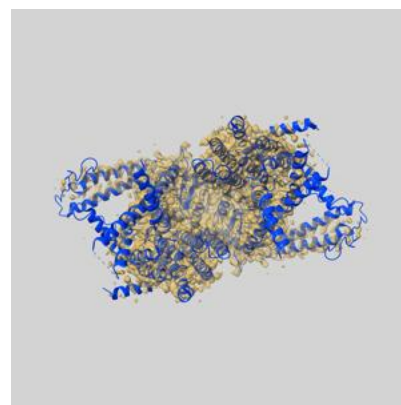
9.1 Map-model overlay [i](#)



X



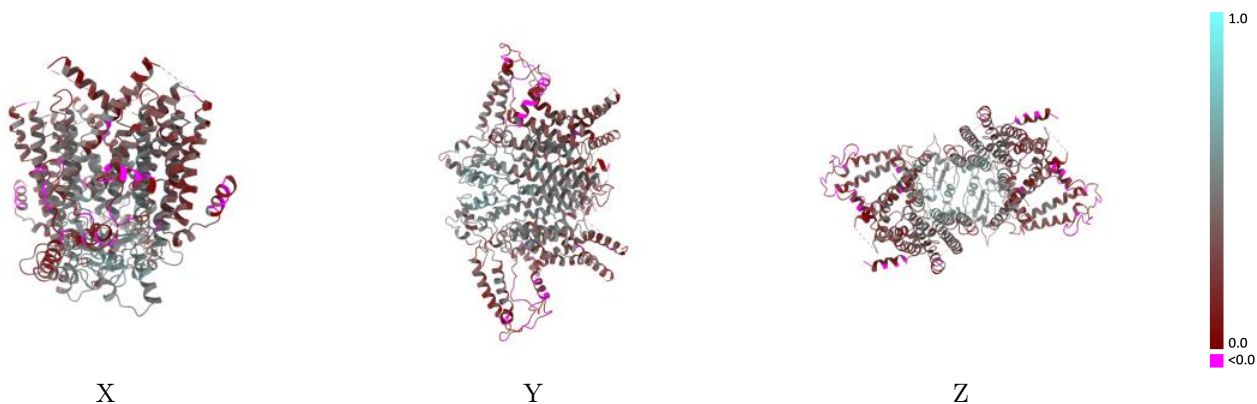
Y



Z

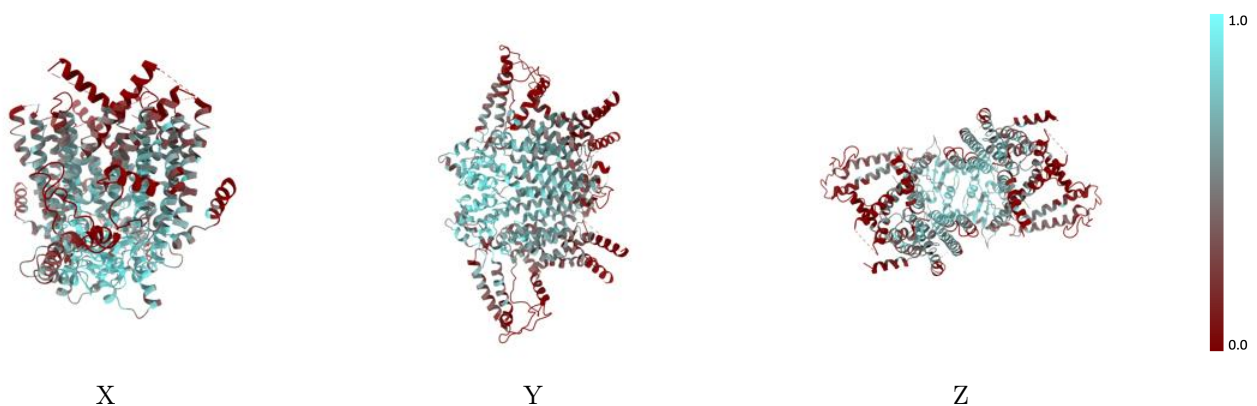
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



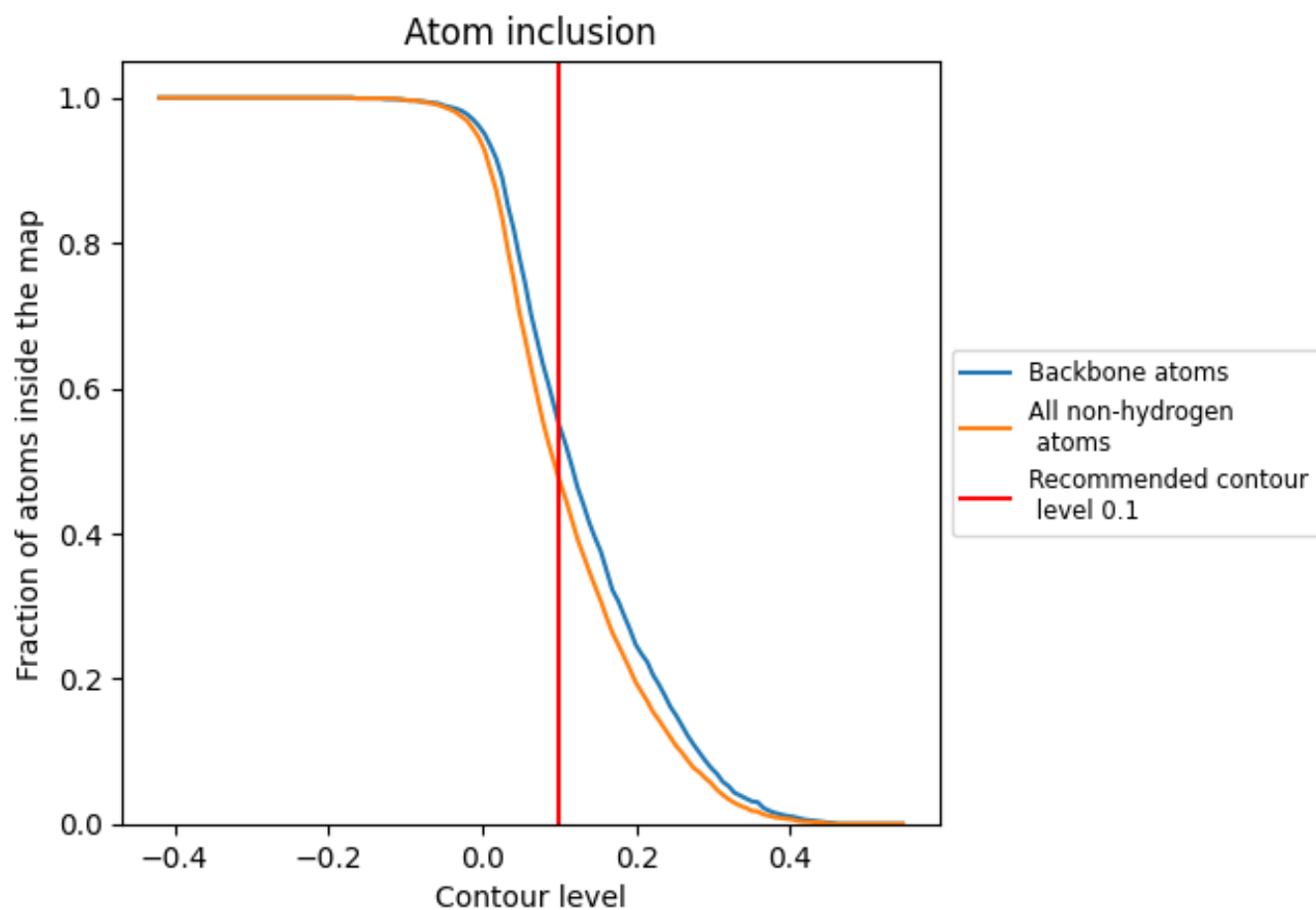
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.4740	■ 0.3470
A	■ 0.4740	■ 0.3480
B	■ 0.4740	■ 0.3470

