



## Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 02:59 PM EDT

PDB ID : 8EVB  
EMDB ID : EMD-28625  
Title : Cryo-EM structure of cGMP bound truncated human CNGA3/CNGB3 channel in lipid nanodisc, pre-open state  
Authors : Hu, Z.; Yang, J.  
Deposited on : 2022-10-20  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

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

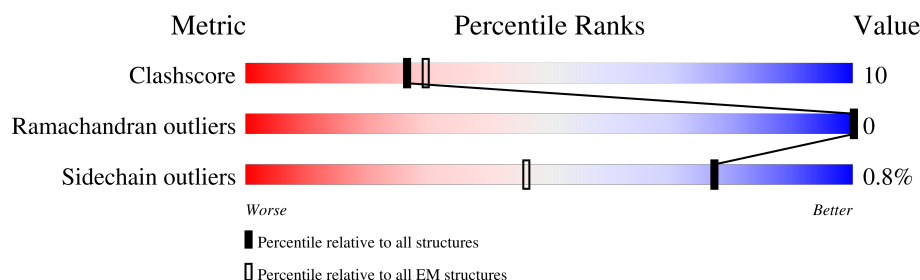
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




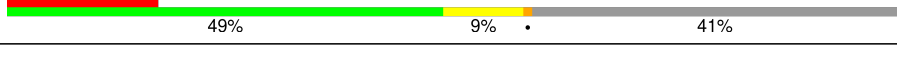
The reported resolution of this entry is 3.60 Å.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	
1	B	552	
1	C	552	
2	D	740	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PCG	B	802	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14456 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 Cyclic nucleotide-gated cation channel alpha-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	444	Total	C	N	O	S	1	0
			3629	2368	591	655	15		
1	B	432	Total	C	N	O	S	0	0
			3532	2308	575	635	14		
1	C	438	Total	C	N	O	S	0	0
			3576	2337	581	643	15		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP Q16281
A	144	ASP	-	expression tag	UNP Q16281
A	145	TYR	-	expression tag	UNP Q16281
A	146	LYS	-	expression tag	UNP Q16281
A	147	ASP	-	expression tag	UNP Q16281
A	148	ASP	-	expression tag	UNP Q16281
A	149	ASP	-	expression tag	UNP Q16281
A	150	ASP	-	expression tag	UNP Q16281
B	143	MET	-	initiating methionine	UNP Q16281
B	144	ASP	-	expression tag	UNP Q16281
B	145	TYR	-	expression tag	UNP Q16281
B	146	LYS	-	expression tag	UNP Q16281
B	147	ASP	-	expression tag	UNP Q16281
B	148	ASP	-	expression tag	UNP Q16281
B	149	ASP	-	expression tag	UNP Q16281
B	150	ASP	-	expression tag	UNP Q16281
C	143	MET	-	initiating methionine	UNP Q16281
C	144	ASP	-	expression tag	UNP Q16281
C	145	TYR	-	expression tag	UNP Q16281
C	146	LYS	-	expression tag	UNP Q16281
C	147	ASP	-	expression tag	UNP Q16281
C	148	ASP	-	expression tag	UNP Q16281
C	149	ASP	-	expression tag	UNP Q16281
C	150	ASP	-	expression tag	UNP Q16281

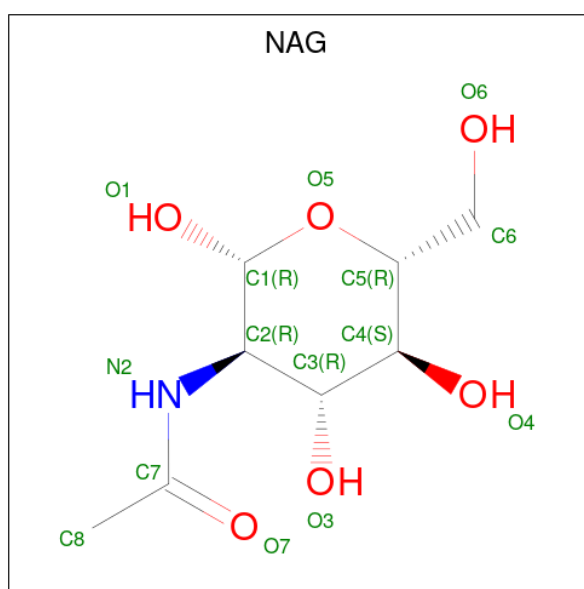
- Molecule 2 is a protein called Cyclic nucleotide-gated cation channel beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	437	3585	2350	584	630	21	0	0

There are 9 discrepancies between the modelled and reference sequences:

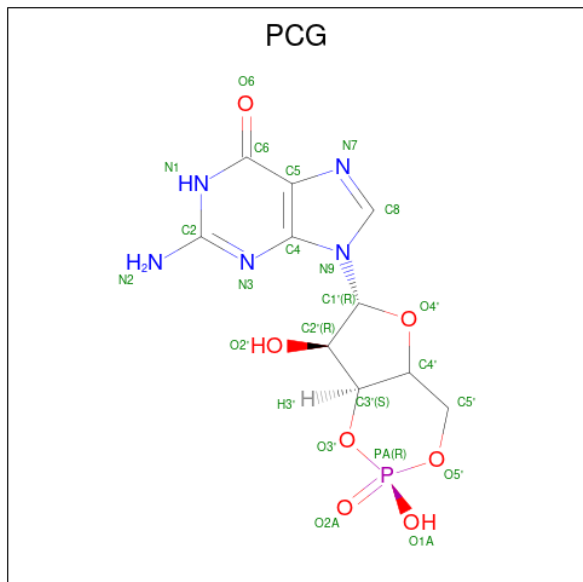
Chain	Residue	Modelled	Actual	Comment	Reference
D	70	MET	-	initiating methionine	UNP Q9NQW8
D	71	ASP	-	expression tag	UNP Q9NQW8
D	72	TYR	-	expression tag	UNP Q9NQW8
D	73	LYS	-	expression tag	UNP Q9NQW8
D	74	ASP	-	expression tag	UNP Q9NQW8
D	75	ASP	-	expression tag	UNP Q9NQW8
D	76	ASP	-	expression tag	UNP Q9NQW8
D	77	ASP	-	expression tag	UNP Q9NQW8
D	78	LYS	-	expression tag	UNP Q9NQW8

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	C	1	14	8	1	5	0

- Molecule 4 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (formula:  $C_{10}H_{12}N_5O_7P$ ) (labeled as "Ligand of Interest" by depositor).

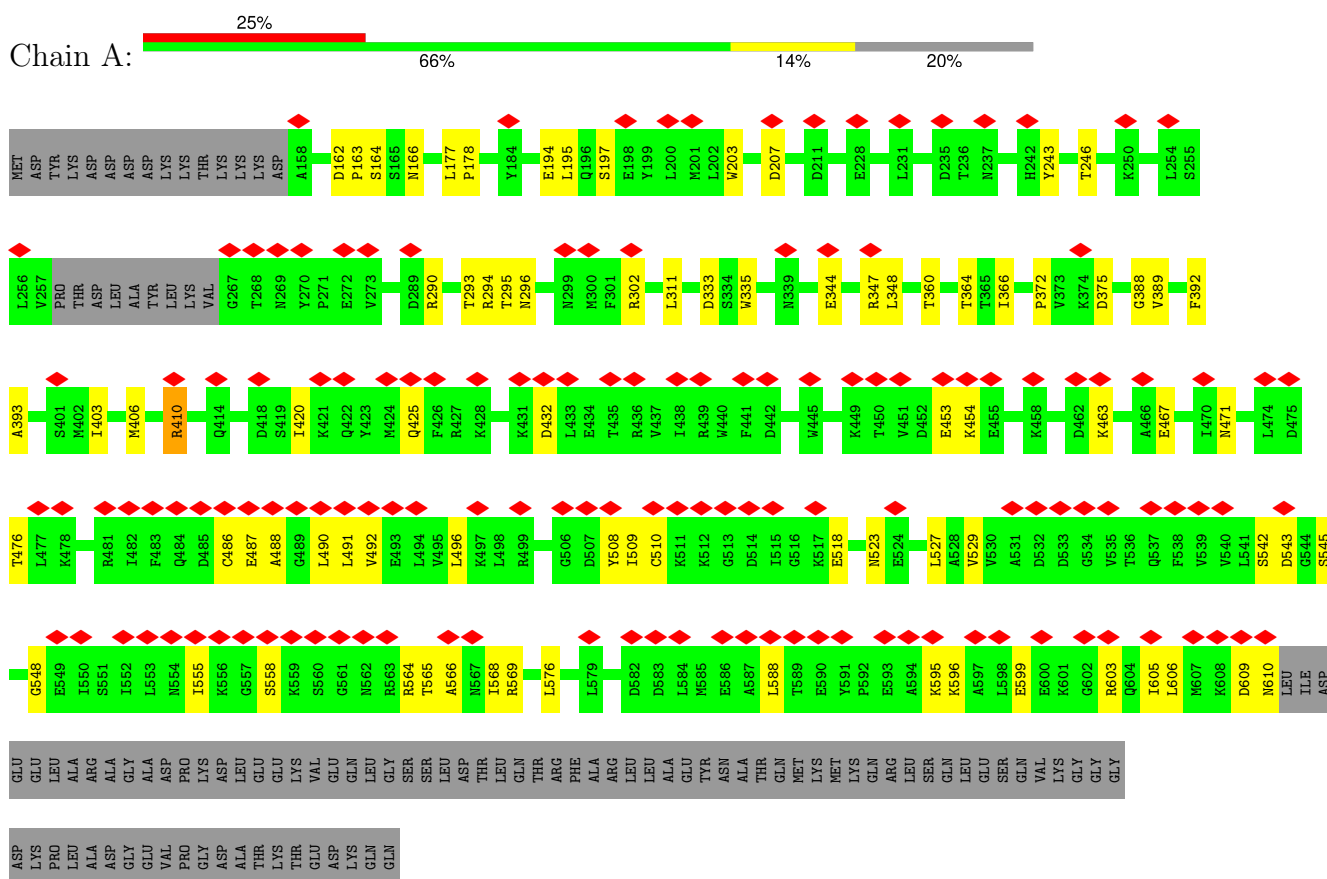


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
4	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
4	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
4	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

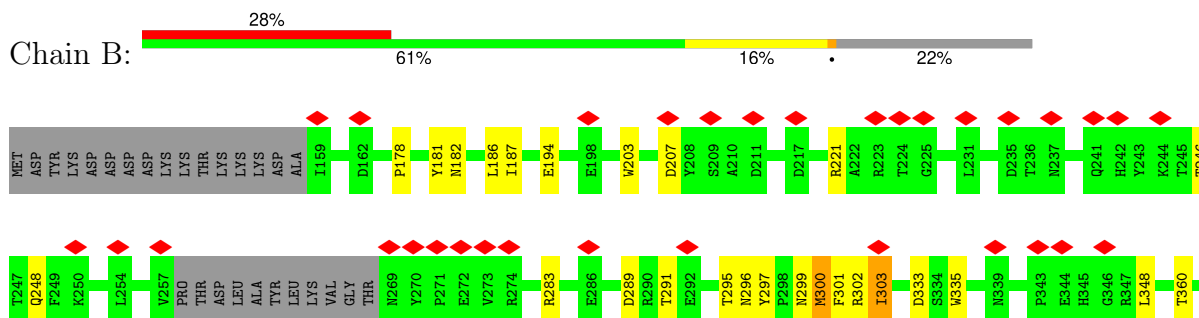
### 3 Residue-property plots

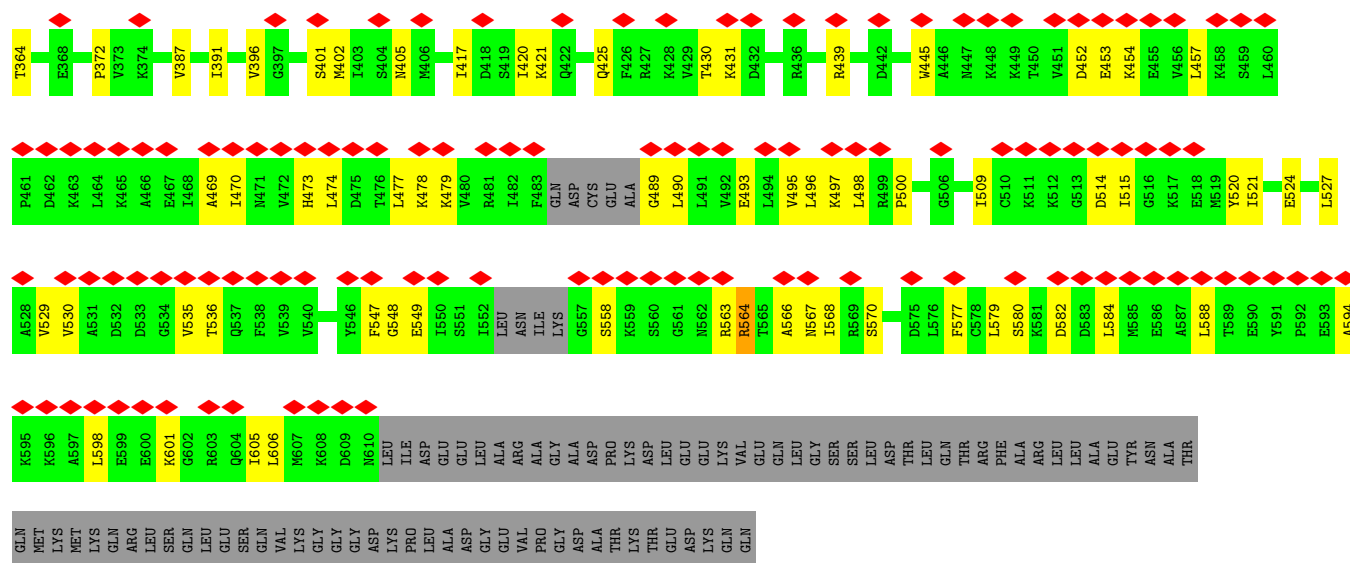
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cyclic nucleotide-gated cation channel alpha-3

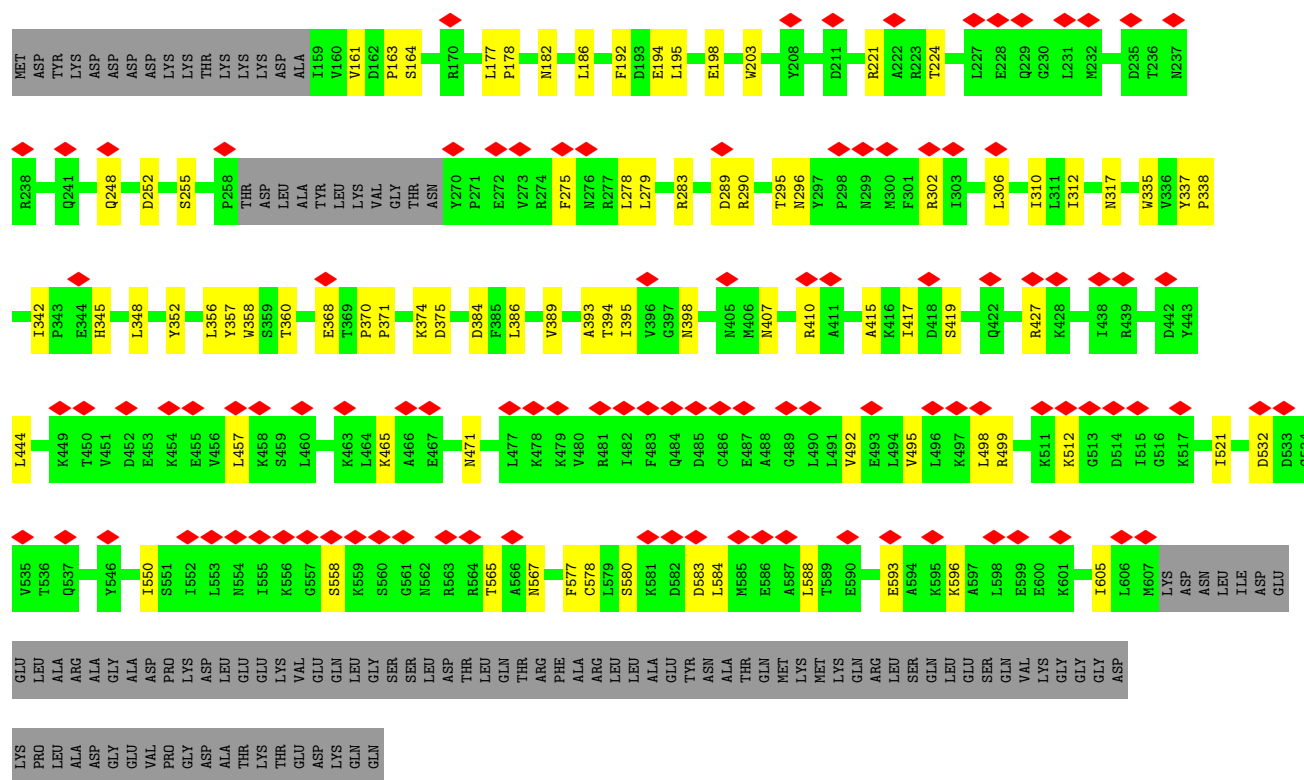


- Molecule 1: Cyclic nucleotide-gated cation channel alpha-3

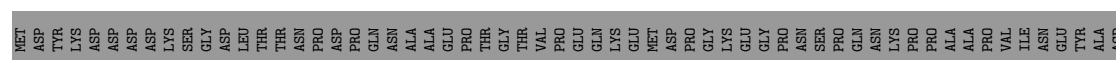




• Molecule 1: Cyclic nucleotide-gated cation channel alpha-3



• Molecule 2: Cyclic nucleotide-gated cation channel beta-3



ALA	GLN	LEU	HIS	ASN	LEU	VAL	LYS	ARG	MET	GLU	THR	ILE	LEU	LYS	TYR	LYS	LYS	LEU	VAL	GLU	GLY	ASP	LEU	SER	SER	PRO	GLU	PRO	ALA	ALA	SER	PRO	GLN	THR	GLN	ALA	LYS	LYS	PRO	THR	THR	ALA	ALA	LYS	PRO	VAL	LYS	GLU	SER	ASP	LYS	PRO	THR	GLU	HIS	TYR	TYR	ARG	LEU	LEU	TRP				
PHE	LYS	VAL	LYS	LYS	MET	PRO	LEU	THR	THR	GLU	TYR	LEU	LYS	ARG	ILE	LYS	L206	S209	I210	D211	S212	Y213	T214	D215	R216	V221	L222	V225	T226	L227	F235	L238	R239	L240	V241	F242	T246	A247	D248	H251	L254	D257	C260	D261	Y264	D267	Q272																		
P273	R279	D282	I283	I284	V285	E289	I290	R291	K292	H293	Y294	R295	T296	S297	T298	K299	F300	Q301	L302	A305	I308	D311	I312	C313	Y314	L315	F316	F317	G318	F319	N320	F321	N322	F323	R324	A325	N326	R327	E336	H339	D346	R352	R396	Y399	R403																				
I406	C410	E413	T416	L417	L424	I438	R442	Q446	R453	R456	D460	D461	R467	S470	R477	R480	E484	Y485	T486	Q490	R491	M492	L493	D494	E495	S496	D497	L498	L499	K500	T501	L502	P503	T504	T505	V506	Q507	A509	I512	F516																									
S517	I518	I519	S520	K521	V522	D523	K526	G527	C528	D529	T530	Q531	M532	I533	Y534	D535	M536	L537	L538	R539	L544	Y545	V551	K554	G555	E556	K559	E560	M561	Y562	I563	I564	K565	H566	V571	L572	G573	G574	P575	D576	G577	K579	V580	L581	V582	K585	G591	E592	I593	S594															
L595	L596	A597	ALA	GLY	GLY	N602	R603	R604	T605	A606	N607	V608	L619	D620	K621	K622	Q625	E626	I627	L628	V629	H630	H631	P632	D633	S634	E635	R636	M639	R640	K641	A642	R643	R644	L645	L646	LYS	GLN	LYS	LYS	ALA	LYS	THR	ALA	ALA	PRO	PRO	ARG	LYS	ASP	LEU	ALA	LEU	LEU											
PHE	PRO	PRO	LYS	GLU	ASN	GLU	THR	PRO	LYS	LYS	PHE	PHE	LYS	ASN	LYS	THR	LEU	LEU	GLY	GLY	LYS	LYS	GLY	THR	GLY	GLY	ARG	GLU	LYS	PRO	ALA	ALA	SER	GLU	LYS	ALA	LYS	ALA	LYS	LYS	GLU	ASN	GLU	GLY	ASP	GLN	GLY	THR	LYS	ASN	GLU	GLU	LEU	LEU	ASP										
LYS	GLN	LYS	GLU	ALA	ASN	GLU	GLY	ASP	LYS	GLY	LYS	GLY	LYS	GLY	ARG	GLY	GLU	PRO	LYS	ALA	ALA	GLU	LYS	PRO	LYS	GLU	GLY	LYS	PRO	ALA	ALA	ILE	GLN	LYS	LYS	VAL	GLU	ASN	GLU	SER	GLU	PRO	HIS	GLY	GLY	VAL	ARG	GLU	GLU	THR	VAL	LYS	LEU	PRO	ARG	GLY	THR	LYS	ASN	GLN	ARG	GLY	LEU	LEU	ILE
ILE	SER	MET	ALA	PRO	PRO	SER	SER	ALA	GLU	GLY	GLY	GLY	GLY	GLY	VAL	VAL	LYS	GLU	LYS	LYS	ALA	ALA	LYS	GLN																																									



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15177	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 ( $e^-/\text{\AA}^2$ )	61.05	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.681	Depositor
Minimum map value	-0.441	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.167	Depositor
Map size ( $\text{\AA}$ )	258.96, 258.96, 258.96	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	0/3711	0.65	0/5028
1	B	0.40	0/3611	0.63	0/4890
1	C	0.41	0/3658	0.63	0/4958
2	D	0.42	0/3675	0.65	0/4988
All	All	0.42	0/14655	0.64	0/19864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3629	0	3674	67	0
1	B	3532	0	3580	81	0
1	C	3576	0	3629	75	0
2	D	3585	0	3601	66	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
4	A	23	0	10	6	0
4	B	23	0	10	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	23	0	10	6	0
4	D	23	0	10	6	0
All	All	14456	0	14563	283	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 10.

All (283) 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:C:278:LEU:O	1:C:278:LEU:HD12	1.26	1.31
1:C:186:LEU:HD21	1:C:278:LEU:HD23	1.21	1.18
1:C:186:LEU:CD2	1:C:278:LEU:HD23	1.79	1.13
1:C:407:ASN:HA	1:C:410:ARG:NH1	1.76	1.00
2:D:512:ILE:O	2:D:516:PHE:HB3	1.64	0.96
1:A:488:ALA:HA	1:A:491:LEU:CD2	1.96	0.96
1:C:278:LEU:O	1:C:278:LEU:CD1	2.12	0.96
1:B:182:ASN:O	1:B:186:LEU:HB2	1.67	0.95
2:D:545:TYR:CZ	2:D:551:VAL:HG23	2.04	0.92
1:B:299:ASN:OD1	1:B:402:MET:CE	2.20	0.89
1:B:514:ASP:O	1:B:563:ARG:HG2	1.73	0.88
1:B:493:GLU:O	1:B:496:LEU:HD23	1.75	0.86
1:C:584:LEU:O	1:C:588:LEU:HB2	1.75	0.86
1:B:291:THR:HB	1:B:301:PHE:CZ	2.12	0.84
1:B:584:LEU:O	1:B:588:LEU:HB2	1.77	0.83
1:C:182:ASN:O	1:C:186:LEU:CB	2.26	0.83
1:A:488:ALA:HA	1:A:491:LEU:HD21	1.61	0.82
1:B:297:TYR:HB3	1:B:300:MET:HB2	1.60	0.81
1:C:186:LEU:CD2	1:C:278:LEU:CD2	2.57	0.81
1:C:550:ILE:HG13	4:C:802:PCG:O3'	1.81	0.80
1:A:388:GLY:O	1:A:392[B]:PHE:HB3	1.81	0.80
2:D:272:GLN:HG3	2:D:294:TYR:CE1	2.16	0.80
1:A:488:ALA:O	1:A:491:LEU:HG	1.82	0.79
1:B:291:THR:HG21	1:B:301:PHE:CE1	2.18	0.79
1:B:548:GLY:HA2	4:B:802:PCG:O2A	1.84	0.78
1:C:407:ASN:HA	1:C:410:ARG:HH11	1.48	0.78
1:C:182:ASN:O	1:C:186:LEU:HB2	1.82	0.78
1:B:299:ASN:OD1	1:B:402:MET:HE3	1.86	0.74
2:D:605:THR:HG22	4:D:901:PCG:O1A	1.88	0.74
1:B:566:ALA:HB2	4:B:802:PCG:C2	2.18	0.73
2:D:605:THR:HG23	2:D:606:ALA:N	2.03	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LEU:HD23	1:C:278:LEU:CD2	2.18	0.72
1:A:410:ARG:HH21	1:A:410:ARG:HG3	1.54	0.72
1:A:360:THR:O	1:A:364:THR:HB	1.90	0.71
1:A:410:ARG:HG3	1:A:410:ARG:NH2	2.03	0.71
1:B:564:ARG:HG2	1:B:564:ARG:HH11	1.54	0.71
1:B:564:ARG:HG2	1:B:564:ARG:NH1	2.06	0.69
1:C:550:ILE:CG1	4:C:802:PCG:O3'	2.40	0.69
2:D:456:ARG:O	2:D:456:ARG:HD3	1.92	0.69
1:B:299:ASN:OD1	1:B:402:MET:HE1	1.93	0.69
1:B:453:GLU:O	1:B:457:LEU:HB2	1.92	0.69
1:B:530:VAL:HG23	1:B:567:ASN:HB3	1.73	0.68
1:B:564:ARG:HA	4:B:802:PCG:O1A	1.93	0.68
2:D:545:TYR:CZ	2:D:551:VAL:CG2	2.77	0.68
1:B:490:LEU:HG	1:B:490:LEU:O	1.93	0.67
2:D:545:TYR:OH	2:D:551:VAL:HG23	1.93	0.67
2:D:272:GLN:HG3	2:D:294:TYR:CZ	2.29	0.67
1:C:407:ASN:HA	1:C:410:ARG:HH12	1.59	0.67
1:A:496:LEU:HD23	1:A:496:LEU:O	1.95	0.66
1:C:186:LEU:HD23	1:C:278:LEU:HD23	1.73	0.66
1:C:356:LEU:HD23	2:D:424:LEU:HD11	1.77	0.66
1:B:291:THR:CG2	1:B:301:PHE:CE1	2.80	0.65
1:B:246:THR:HG22	1:B:248:GLN:H	1.61	0.64
1:C:182:ASN:O	1:C:186:LEU:HB3	1.96	0.64
2:D:486:THR:O	2:D:490:GLN:HB2	1.97	0.64
1:A:488:ALA:HA	1:A:491:LEU:HD23	1.78	0.64
2:D:512:ILE:HD11	2:D:534:TYR:CE1	2.33	0.64
1:C:360:THR:HG21	2:D:424:LEU:HG	1.80	0.63
1:B:496:LEU:HD12	1:B:497:LYS:HB2	1.80	0.63
1:A:410:ARG:HD2	1:A:410:ARG:O	1.99	0.63
2:D:424:LEU:C	2:D:424:LEU:HD23	2.19	0.63
1:C:177:LEU:HB2	1:C:178:PRO:HD3	1.81	0.62
2:D:564:ILE:HD11	2:D:585:LYS:O	2.00	0.61
2:D:641:LYS:O	2:D:645:LEU:HB2	2.00	0.61
2:D:260:CYS:SG	2:D:324:ARG:NH1	2.74	0.60
2:D:456:ARG:O	2:D:460:ASP:HB2	2.01	0.60
1:A:566:ALA:HB2	4:A:802:PCG:C2	2.32	0.60
1:B:203:TRP:O	1:B:207:ASP:HB2	2.01	0.59
1:C:302:ARG:O	1:C:306:LEU:HG	2.01	0.59
1:C:356:LEU:CD2	2:D:424:LEU:HD11	2.32	0.59
1:C:221:ARG:HH21	1:C:283:ARG:HH21	1.49	0.59
1:B:598:LEU:HD23	1:B:601:LYS:HE2	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ILE:HD12	1:C:395:ILE:HG21	1.85	0.58
1:A:177:LEU:CB	1:A:178:PRO:HD3	2.34	0.58
1:C:521:ILE:HB	1:C:577:PHE:HB2	1.85	0.58
1:A:164:SER:HA	1:A:290:ARG:HH22	1.69	0.57
1:B:566:ALA:HB2	4:B:802:PCG:N2	2.20	0.57
1:A:566:ALA:HB2	4:A:802:PCG:N2	2.19	0.57
1:C:192:PHE:CZ	1:C:352:TYR:HD1	2.23	0.57
1:B:291:THR:HB	1:B:301:PHE:CE2	2.39	0.57
2:D:605:THR:CG2	2:D:606:ALA:N	2.68	0.56
1:B:221:ARG:HH11	1:B:283:ARG:HD3	1.71	0.56
1:B:509:ILE:HD13	1:B:568:ILE:HG22	1.88	0.55
1:B:520:TYR:HB2	1:B:547:PHE:HB2	1.87	0.55
1:A:393:ALA:HB1	2:D:438:ILE:HG23	1.87	0.55
1:B:495:VAL:HA	1:B:498:LEU:HD13	1.88	0.55
1:B:564:ARG:HH11	1:B:564:ARG:CG	2.19	0.55
2:D:516:PHE:HA	2:D:519:ILE:HG22	1.89	0.55
1:B:333:ASP:OD1	1:B:333:ASP:N	2.39	0.55
1:B:594:ALA:O	1:B:598:LEU:HG	2.05	0.55
1:A:388:GLY:O	1:A:392[A]:PHE:HB2	2.07	0.55
1:C:375:ASP:N	1:C:375:ASP:OD1	2.40	0.54
1:C:335:TRP:HE1	1:C:358:TRP:HZ2	1.54	0.54
1:B:291:THR:CB	1:B:301:PHE:CZ	2.87	0.54
1:B:387:VAL:O	1:B:391:ILE:HB	2.07	0.54
1:C:550:ILE:HG21	1:C:565:THR:CG2	2.38	0.53
2:D:238:LEU:O	2:D:242:PHE:HB2	2.08	0.53
1:A:375:ASP:OD1	2:D:396:ARG:NH2	2.41	0.53
1:A:595:LYS:HD2	1:A:596:LYS:HD2	1.90	0.53
2:D:572:LEU:HB2	2:D:607:ASN:HB2	1.91	0.53
1:A:518:GLU:O	1:A:564:ARG:NH2	2.38	0.53
1:B:527:LEU:HD22	1:B:570:SER:HA	1.91	0.53
1:B:396:VAL:HG12	1:C:393:ALA:HB2	1.90	0.53
2:D:561:MET:HB3	2:D:619:LEU:HB3	1.91	0.52
1:A:432:ASP:OD2	1:A:432:ASP:N	2.42	0.52
1:A:163:PRO:O	1:A:290:ARG:NH1	2.39	0.52
1:A:565:THR:OG1	4:A:802:PCG:N2	2.37	0.52
1:A:333:ASP:OD1	1:A:333:ASP:N	2.42	0.52
4:C:802:PCG:C3'	4:C:802:PCG:N3	2.73	0.52
4:B:802:PCG:N3	4:B:802:PCG:C3'	2.73	0.52
4:D:901:PCG:N3	4:D:901:PCG:C2'	2.73	0.52
1:C:186:LEU:HD23	1:C:278:LEU:HD22	1.90	0.52
1:B:529:VAL:HG12	1:B:568:ILE:HD13	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:PCG:N3	4:A:802:PCG:C3'	2.73	0.51
1:B:473:HIS:O	1:B:477:LEU:HB2	2.11	0.51
2:D:509:ALA:HA	2:D:512:ILE:HG22	1.93	0.51
1:B:469:ALA:O	1:B:473:HIS:HB2	2.10	0.51
1:B:439:ARG:HD2	1:C:164:SER:HB2	1.93	0.51
2:D:605:THR:HG23	2:D:606:ALA:H	1.73	0.51
1:C:178:PRO:O	1:C:182:ASN:HB2	2.11	0.51
4:D:901:PCG:N3	4:D:901:PCG:C3'	2.73	0.51
1:C:163:PRO:O	1:C:290:ARG:NH1	2.43	0.51
2:D:502:LEU:O	2:D:507:GLN:NE2	2.44	0.50
2:D:554:LYS:HA	2:D:604:ARG:HB2	1.93	0.50
1:A:162:ASP:OD1	1:A:162:ASP:N	2.42	0.50
2:D:563:ILE:O	2:D:563:ILE:HG13	2.11	0.50
1:A:195:LEU:HG	1:A:348:LEU:HD21	1.93	0.50
4:A:802:PCG:N3	4:A:802:PCG:C2'	2.73	0.50
1:B:524:GLU:O	1:B:524:GLU:HG3	2.12	0.50
2:D:311:ASP:HA	2:D:314:TYR:HB2	1.94	0.50
1:A:542:SER:OG	1:A:543:ASP:N	2.44	0.49
1:C:194:GLU:HB3	1:C:348:LEU:HD13	1.95	0.49
1:B:515:ILE:HD12	1:B:563:ARG:HG3	1.95	0.49
4:C:802:PCG:N3	4:C:802:PCG:C2'	2.73	0.49
1:B:421:LYS:NZ	1:C:295:THR:O	2.44	0.49
1:A:425:GLN:NE2	1:B:296:ASN:HD21	2.11	0.49
1:B:430:THR:HG22	1:B:431:LYS:N	2.28	0.49
1:A:467:GLU:OE2	1:A:471:ASN:ND2	2.46	0.49
1:A:529:VAL:HG23	1:A:568:ILE:HG13	1.95	0.49
1:C:558:SER:OG	1:C:605:ILE:O	2.31	0.49
1:A:509:ILE:HD12	1:A:510:CYS:N	2.28	0.48
2:D:591:GLY:O	4:D:901:PCG:O2A	2.30	0.48
4:B:802:PCG:N3	4:B:802:PCG:C2'	2.73	0.48
2:D:561:MET:HG3	2:D:591:GLY:HA3	1.93	0.48
1:A:606:LEU:HA	1:A:609:ASP:HB3	1.95	0.48
2:D:485:TYR:HD2	2:D:544:LEU:HD21	1.79	0.48
1:A:293:THR:O	2:D:480:ARG:NH2	2.46	0.48
2:D:533:ILE:O	2:D:537:LEU:HD23	2.14	0.48
1:A:476:THR:OG1	1:A:523:ASN:ND2	2.47	0.48
1:C:194:GLU:O	1:C:198:GLU:HB2	2.13	0.48
2:D:508:LEU:O	2:D:512:ILE:HG22	2.13	0.48
1:B:478:LYS:NZ	1:B:489:GLY:O	2.47	0.48
1:A:203:TRP:O	1:A:207:ASP:HB2	2.14	0.47
1:A:295:THR:OG1	1:A:296:ASN:N	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:HA	1:B:563:ARG:CG	2.45	0.47
2:D:555:GLY:O	2:D:603:ARG:NH2	2.45	0.47
2:D:605:THR:CG2	2:D:606:ALA:H	2.27	0.47
1:B:529:VAL:HG12	1:B:568:ILE:CD1	2.45	0.47
1:C:427:ARG:NH2	2:D:490:GLN:OE1	2.42	0.47
1:A:492:VAL:O	1:A:496:LEU:HB2	2.15	0.47
1:B:401:SER:O	1:B:405:ASN:HB2	2.15	0.47
1:B:535:VAL:HG23	1:B:536:THR:HG23	1.96	0.47
1:C:161:VAL:HG12	1:C:224:THR:HA	1.96	0.47
1:C:357:TYR:HA	2:D:424:LEU:HD12	1.97	0.47
2:D:497:ASP:OD1	2:D:497:ASP:N	2.45	0.47
1:C:192:PHE:CZ	1:C:352:TYR:CD1	3.03	0.47
1:A:166:ASN:OD1	1:A:294:ARG:NH1	2.45	0.47
1:A:486:CYS:HB2	1:A:490:LEU:HD23	1.97	0.47
1:B:335:TRP:HB2	1:B:372:PRO:HA	1.97	0.47
1:B:470:ILE:O	1:B:474:LEU:HB2	2.15	0.47
1:A:410:ARG:HH21	1:A:410:ARG:CG	2.21	0.46
1:B:498:LEU:HD12	1:B:579:LEU:HD21	1.97	0.46
1:A:527:LEU:HD21	1:A:576:LEU:HD11	1.97	0.46
1:C:275:PHE:O	1:C:278:LEU:HG	2.15	0.46
1:A:508:TYR:OH	1:A:569:ARG:NH2	2.49	0.46
1:A:599:GLU:HG2	1:A:603:ARG:HH21	1.81	0.46
1:C:593:GLU:HA	1:C:596:LYS:HB2	1.97	0.46
1:C:495:VAL:HA	1:C:498:LEU:HG	1.98	0.46
1:A:605:ILE:O	1:A:609:ASP:CB	2.64	0.46
2:D:403:ARG:HH11	2:D:410:GLY:HA3	1.81	0.46
1:A:195:LEU:HD22	1:A:203:TRP:HZ2	1.80	0.46
1:B:303:ILE:HD13	1:B:303:ILE:HA	1.72	0.45
1:C:342:ILE:HD11	1:C:345:HIS:HD2	1.81	0.45
1:B:558:SER:OG	1:B:606:LEU:HD13	2.15	0.45
1:B:178:PRO:HA	1:B:181:TYR:HB3	1.99	0.45
1:B:360:THR:O	1:B:364:THR:OG1	2.34	0.45
1:B:564:ARG:HB3	4:B:802:PCG:PA	2.56	0.45
2:D:571:VAL:HG12	2:D:608:VAL:HG12	1.98	0.45
1:B:194:GLU:HG3	1:B:348:LEU:HD22	1.98	0.45
2:D:574:GLY:HA3	2:D:579:LYS:HB2	1.99	0.45
1:A:403:ILE:HA	1:A:406:MET:HG2	1.99	0.45
1:C:394:THR:O	1:C:398:ASN:HB2	2.16	0.45
1:A:588:LEU:HD13	1:A:595:LYS:HE2	1.99	0.44
2:D:633:ASP:OD1	2:D:633:ASP:N	2.47	0.44
1:B:580:SER:OG	1:B:582:ASP:OD2	2.35	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:THR:OG1	2:D:417:LEU:N	2.49	0.44
1:B:445:TRP:NE1	1:C:289:ASP:OD2	2.50	0.44
1:B:479:LYS:HD2	1:B:479:LYS:HA	1.84	0.44
2:D:272:GLN:CB	2:D:273:PRO:HD3	2.47	0.44
2:D:564:ILE:O	2:D:564:ILE:HG13	2.17	0.44
1:C:499:ARG:HB2	1:C:578:CYS:HB2	1.99	0.44
1:B:521:ILE:HG12	1:B:577:PHE:HB2	1.99	0.44
1:B:548:GLY:CA	4:B:802:PCG:O2A	2.61	0.44
1:A:177:LEU:CB	1:A:178:PRO:CD	2.96	0.44
1:C:471:ASN:N	1:C:471:ASN:OD1	2.49	0.44
1:C:492:VAL:HA	1:C:495:VAL:HG22	1.99	0.44
2:D:399:TYR:OH	2:D:403:ARG:NH2	2.51	0.44
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.89	0.43
1:C:580:SER:OG	1:C:583:ASP:OD2	2.36	0.43
1:A:463:LYS:HE2	1:A:463:LYS:HB3	1.77	0.43
1:B:549:GLU:OE2	1:B:598:LEU:O	2.35	0.43
1:C:498:LEU:HD22	1:C:577:PHE:HB3	2.00	0.43
1:A:243:TYR:O	1:A:246:THR:OG1	2.35	0.43
1:A:335:TRP:HB2	1:A:372:PRO:HA	2.00	0.43
1:A:177:LEU:HB3	1:A:178:PRO:HD3	1.99	0.43
4:C:802:PCG:N3	4:C:802:PCG:H3'	2.33	0.43
1:A:420:ILE:HD13	1:A:420:ILE:HA	1.93	0.43
1:A:453:GLU:OE1	1:A:454:LYS:NZ	2.43	0.43
1:C:186:LEU:CD2	1:C:278:LEU:HB3	2.48	0.43
1:C:248:GLN:O	1:C:252:ASP:HB2	2.18	0.43
1:A:487:GLU:O	1:A:491:LEU:HD23	2.19	0.43
1:B:478:LYS:HD2	1:B:478:LYS:HA	1.86	0.43
1:B:490:LEU:H	1:B:490:LEU:HD23	1.84	0.43
1:B:520:TYR:O	1:B:547:PHE:N	2.51	0.43
1:C:275:PHE:HD1	1:C:278:LEU:CD2	2.32	0.43
1:C:195:LEU:HD22	1:C:203:TRP:HZ2	1.84	0.43
1:B:430:THR:CG2	1:B:431:LYS:N	2.82	0.43
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.93	0.43
1:A:344:GLU:O	1:A:347:ARG:NH2	2.52	0.42
1:C:317:ASN:ND2	1:C:384:ASP:OD1	2.52	0.42
2:D:209:SER:O	2:D:209:SER:OG	2.35	0.42
2:D:582:VAL:HG21	4:D:901:PCG:C8	2.49	0.42
1:B:417:ILE:HG22	1:B:421:LYS:HE2	2.02	0.42
1:C:255:SER:HB3	1:C:279:LEU:HB3	1.99	0.42
1:A:555:ILE:HB	1:A:558:SER:HB3	2.01	0.42
1:B:497:LYS:HG3	1:B:497:LYS:O	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:802:PCG:N3	4:B:802:PCG:H3'	2.34	0.42
1:C:337:TYR:HA	1:C:338:PRO:HD3	1.90	0.42
1:B:295:THR:HG23	1:B:297:TYR:H	1.85	0.42
2:D:490:GLN:HB3	2:D:492:MET:HG2	2.01	0.42
2:D:519:ILE:HG21	2:D:537:LEU:HD21	2.00	0.42
1:A:364:THR:HG22	1:A:366:ILE:HG13	2.02	0.42
4:A:802:PCG:N3	4:A:802:PCG:H3'	2.34	0.42
1:B:564:ARG:HB3	4:B:802:PCG:O1A	2.19	0.42
1:A:548:GLY:HA2	1:A:564:ARG:NH1	2.34	0.42
1:B:291:THR:CG2	1:B:301:PHE:CZ	3.02	0.42
2:D:246:THR:OG1	2:D:247:ALA:N	2.53	0.42
4:D:901:PCG:N3	4:D:901:PCG:H3'	2.34	0.42
1:A:389:VAL:HG21	2:D:406:ILE:HD12	2.00	0.42
2:D:235:PHE:O	2:D:239:ARG:NH1	2.52	0.42
1:A:389:VAL:O	1:A:393:ALA:HB2	2.20	0.42
1:A:543:ASP:N	1:A:543:ASP:OD1	2.50	0.41
1:B:425:GLN:HE22	1:C:296:ASN:HB3	1.85	0.41
1:C:312:ILE:HD13	1:C:312:ILE:HA	1.94	0.41
2:D:222:LEU:HA	2:D:225:VAL:HG12	2.01	0.41
1:C:192:PHE:CZ	1:C:352:TYR:HA	2.54	0.41
1:C:370:PRO:HA	1:C:371:PRO:HD3	1.84	0.41
1:C:374:LYS:HE2	1:C:374:LYS:HB3	1.89	0.41
1:C:417:ILE:HD13	1:C:417:ILE:HA	1.91	0.41
1:C:532:ASP:HA	1:C:567:ASN:HD22	1.85	0.41
2:D:261:ASP:OD1	2:D:327:ARG:NE	2.53	0.41
1:A:302:ARG:NH1	2:D:456:ARG:HD2	2.35	0.41
1:C:415:ALA:O	1:C:419:SER:HB2	2.21	0.41
1:C:192:PHE:HZ	1:C:352:TYR:HD1	1.64	0.41
1:A:194:GLU:HB3	1:A:348:LEU:HD22	2.01	0.41
1:A:194:GLU:HA	1:A:197:SER:HB3	2.03	0.41
1:B:500:PRO:HA	1:B:577:PHE:HA	2.01	0.41
1:B:601:LYS:O	1:B:605:ILE:HG13	2.21	0.41
1:A:606:LEU:O	1:A:610:ASN:C	2.58	0.41
1:B:420:ILE:HD13	1:B:420:ILE:HA	1.95	0.41
1:C:386:LEU:HD23	1:C:386:LEU:HA	1.94	0.41
2:D:221:TRP:NE1	2:D:267:ASP:OD1	2.47	0.41
1:A:542:SER:O	1:A:545:SER:OG	2.37	0.41
1:B:452:ASP:OD1	1:B:452:ASP:N	2.40	0.41
1:C:550:ILE:HG21	1:C:565:THR:HG23	2.02	0.41
2:D:222:LEU:HA	2:D:222:LEU:HD12	1.95	0.41
1:B:396:VAL:HG11	1:C:389:VAL:HG22	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:GLU:OE1	2:D:410:GLY:N	2.54	0.41
1:C:550:ILE:HG13	4:C:802:PCG:C3'	2.51	0.41
2:D:227:LEU:HD23	2:D:227:LEU:HA	1.92	0.41
2:D:272:GLN:OE1	2:D:272:GLN:HA	2.20	0.41
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.96	0.40
1:C:457:LEU:HB3	1:C:465:LYS:HG3	2.03	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	441/552 (80%)	418 (95%)	23 (5%)	0	100	100
1	B	424/552 (77%)	404 (95%)	20 (5%)	0	100	100
1	C	434/552 (79%)	417 (96%)	17 (4%)	0	100	100
2	D	433/740 (58%)	415 (96%)	18 (4%)	0	100	100
All	All	1732/2396 (72%)	1654 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	400/491 (82%)	399 (100%)	1 (0%)	91	96
1	B	390/491 (79%)	384 (98%)	6 (2%)	60	78
1	C	395/491 (80%)	394 (100%)	1 (0%)	91	96
2	D	391/651 (60%)	386 (99%)	5 (1%)	65	81
All	All	1576/2124 (74%)	1563 (99%)	13 (1%)	77	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	ARG
1	B	289	ASP
1	B	300	MET
1	B	302	ARG
1	B	303	ILE
1	B	454	LYS
1	B	564	ARG
1	C	512	LYS
2	D	260	CYS
2	D	264	TYR
2	D	272	GLN
2	D	438	ILE
2	D	537	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	425	GLN
1	A	471	ASN
1	A	523	ASN
1	B	317	ASN
1	B	414	GLN
1	B	425	GLN
1	C	241	GLN
1	C	248	GLN
1	C	276	ASN
1	C	345	HIS
2	D	367	ASN
2	D	426	ASN
2	D	515	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

7 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$
3	NAG	B	801	1	14,14,15	0.63	0	17,19,21	0.67	1 (5%)
3	NAG	C	801	1	14,14,15	0.91	1 (7%)	17,19,21	0.84	1 (5%)
4	PCG	D	901	-	22,26,26	2.26	4 (18%)	25,41,41	3.61	16 (64%)
3	NAG	A	801	1	14,14,15	0.68	1 (7%)	17,19,21	0.81	1 (5%)
4	PCG	C	802	-	22,26,26	2.26	4 (18%)	25,41,41	3.60	17 (68%)
4	PCG	A	802	-	22,26,26	2.26	4 (18%)	25,41,41	3.60	17 (68%)
4	PCG	B	802	-	22,26,26	2.26	4 (18%)	25,41,41	3.61	16 (64%)

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
3	NAG	B	801	1	-	2/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	801	1	-	2/6/23/26	0/1/1/1
4	PCG	D	901	-	-	0/0/31/31	0/4/4/4
3	NAG	A	801	1	-	2/6/23/26	0/1/1/1
4	PCG	C	802	-	-	0/0/31/31	0/4/4/4
4	PCG	A	802	-	-	0/0/31/31	0/4/4/4
4	PCG	B	802	-	-	0/0/31/31	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	PCG	PA-O5'	-7.26	1.49	1.57
4	A	802	PCG	PA-O5'	-7.25	1.49	1.57
4	B	802	PCG	PA-O5'	-7.24	1.49	1.57
4	C	802	PCG	PA-O5'	-7.16	1.49	1.57
4	D	901	PCG	PA-O3'	-3.76	1.51	1.57
4	C	802	PCG	PA-O3'	-3.76	1.51	1.57
4	B	802	PCG	PA-O3'	-3.73	1.51	1.57
4	A	802	PCG	PA-O3'	-3.70	1.51	1.57
3	C	801	NAG	O5-C1	2.87	1.48	1.43
4	C	802	PCG	C6-N1	2.80	1.42	1.37
4	D	901	PCG	C6-N1	2.76	1.42	1.37
4	A	802	PCG	C6-N1	2.75	1.42	1.37
4	B	802	PCG	C6-N1	2.74	1.42	1.37
4	B	802	PCG	C8-N7	-2.59	1.30	1.34
4	C	802	PCG	C8-N7	-2.56	1.30	1.34
4	D	901	PCG	C8-N7	-2.55	1.30	1.34
4	A	802	PCG	C8-N7	-2.49	1.30	1.34
3	A	801	NAG	O5-C1	2.26	1.47	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	PCG	C5'-C4'-C3'	8.31	128.17	112.56
4	C	802	PCG	C5'-C4'-C3'	8.27	128.11	112.56
4	A	802	PCG	C5'-C4'-C3'	8.27	128.10	112.56
4	B	802	PCG	C5'-C4'-C3'	8.26	128.09	112.56
4	A	802	PCG	O4'-C1'-N9	-6.61	99.98	108.75
4	D	901	PCG	O4'-C1'-N9	-6.59	100.01	108.75
4	B	802	PCG	O4'-C1'-N9	-6.58	100.02	108.75
4	C	802	PCG	O4'-C1'-N9	-6.58	100.02	108.75
4	D	901	PCG	O3'-C3'-C4'	-6.56	105.76	110.71
4	C	802	PCG	O3'-C3'-C4'	-6.51	105.79	110.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	PCG	O3'-C3'-C4'	-6.51	105.79	110.71
4	B	802	PCG	O3'-C3'-C4'	-6.49	105.81	110.71
4	D	901	PCG	C4'-O4'-C1'	-5.17	105.19	109.92
4	B	802	PCG	C4'-O4'-C1'	-5.17	105.19	109.92
4	A	802	PCG	C4'-O4'-C1'	-5.15	105.21	109.92
4	C	802	PCG	C4'-O4'-C1'	-5.13	105.22	109.92
4	D	901	PCG	O5'-PA-O3'	4.90	112.26	105.70
4	B	802	PCG	O5'-PA-O3'	4.89	112.25	105.70
4	C	802	PCG	O5'-PA-O3'	4.86	112.21	105.70
4	A	802	PCG	O5'-PA-O3'	4.85	112.20	105.70
4	B	802	PCG	O5'-PA-O2A	-4.58	99.87	110.44
4	D	901	PCG	O5'-PA-O2A	-4.58	99.88	110.44
4	A	802	PCG	O5'-PA-O2A	-4.58	99.88	110.44
4	C	802	PCG	O5'-PA-O2A	-4.58	99.88	110.44
4	D	901	PCG	O1A-PA-O5'	4.41	117.93	107.16
4	A	802	PCG	O1A-PA-O5'	4.41	117.92	107.16
4	B	802	PCG	O1A-PA-O5'	4.41	117.92	107.16
4	C	802	PCG	O1A-PA-O5'	4.38	117.86	107.16
4	D	901	PCG	O3'-C3'-C2'	3.47	119.01	115.61
4	C	802	PCG	O3'-C3'-C2'	3.47	119.00	115.61
4	B	802	PCG	O3'-C3'-C2'	3.44	118.98	115.61
4	A	802	PCG	O3'-C3'-C2'	3.42	118.96	115.61
3	C	801	NAG	C1-O5-C5	3.14	116.40	112.19
4	B	802	PCG	C2'-C3'-C4'	-3.03	97.94	103.24
4	C	802	PCG	C2'-C3'-C4'	-3.00	97.98	103.24
4	D	901	PCG	C2'-C3'-C4'	-3.00	97.98	103.24
4	A	802	PCG	C2'-C3'-C4'	-3.00	97.99	103.24
3	A	801	NAG	C1-O5-C5	2.90	116.07	112.19
4	B	802	PCG	C5-C6-N1	-2.76	108.80	114.07
4	C	802	PCG	C5-C6-N1	-2.75	108.82	114.07
4	D	901	PCG	C5-C6-N1	-2.73	108.86	114.07
4	A	802	PCG	C5-C6-N1	-2.72	108.86	114.07
4	C	802	PCG	O3'-PA-O2A	2.68	116.14	110.39
4	B	802	PCG	O3'-PA-O2A	2.66	116.09	110.39
4	A	802	PCG	O3'-PA-O2A	2.66	116.08	110.39
4	D	901	PCG	O3'-PA-O2A	2.65	116.06	110.39
4	D	901	PCG	C3'-C2'-C1'	2.62	105.65	99.89
4	B	802	PCG	C3'-C2'-C1'	2.62	105.64	99.89
4	C	802	PCG	C3'-C2'-C1'	2.62	105.64	99.89
4	A	802	PCG	C3'-C2'-C1'	2.61	105.62	99.89
4	A	802	PCG	O4'-C4'-C5'	2.42	119.69	112.38
4	C	802	PCG	O4'-C4'-C5'	2.41	119.67	112.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	PCG	O4'-C4'-C3'	2.40	109.97	104.92
4	B	802	PCG	O4'-C4'-C5'	2.39	119.60	112.38
4	D	901	PCG	O4'-C4'-C5'	2.38	119.59	112.38
4	D	901	PCG	O4'-C4'-C3'	2.37	109.92	104.92
4	C	802	PCG	O4'-C4'-C3'	2.36	109.91	104.92
4	A	802	PCG	O4'-C4'-C3'	2.36	109.90	104.92
4	B	802	PCG	O6-C6-N1	2.22	123.25	120.62
4	C	802	PCG	O6-C6-N1	2.20	123.22	120.62
4	A	802	PCG	O6-C6-N1	2.19	123.22	120.62
3	B	801	NAG	C1-O5-C5	2.19	115.12	112.19
4	D	901	PCG	O6-C6-N1	2.18	123.21	120.62
4	A	802	PCG	N2-C2-N1	-2.03	112.48	116.76
4	B	802	PCG	O1A-PA-O3'	-2.03	102.32	107.04
4	A	802	PCG	O1A-PA-O3'	-2.02	102.33	107.04
4	D	901	PCG	O1A-PA-O3'	-2.01	102.36	107.04
4	C	802	PCG	N2-C2-N1	-2.01	112.52	116.76
4	C	802	PCG	O1A-PA-O3'	-2.01	102.37	107.04

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	801	NAG	C4-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
3	B	801	NAG	C4-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6

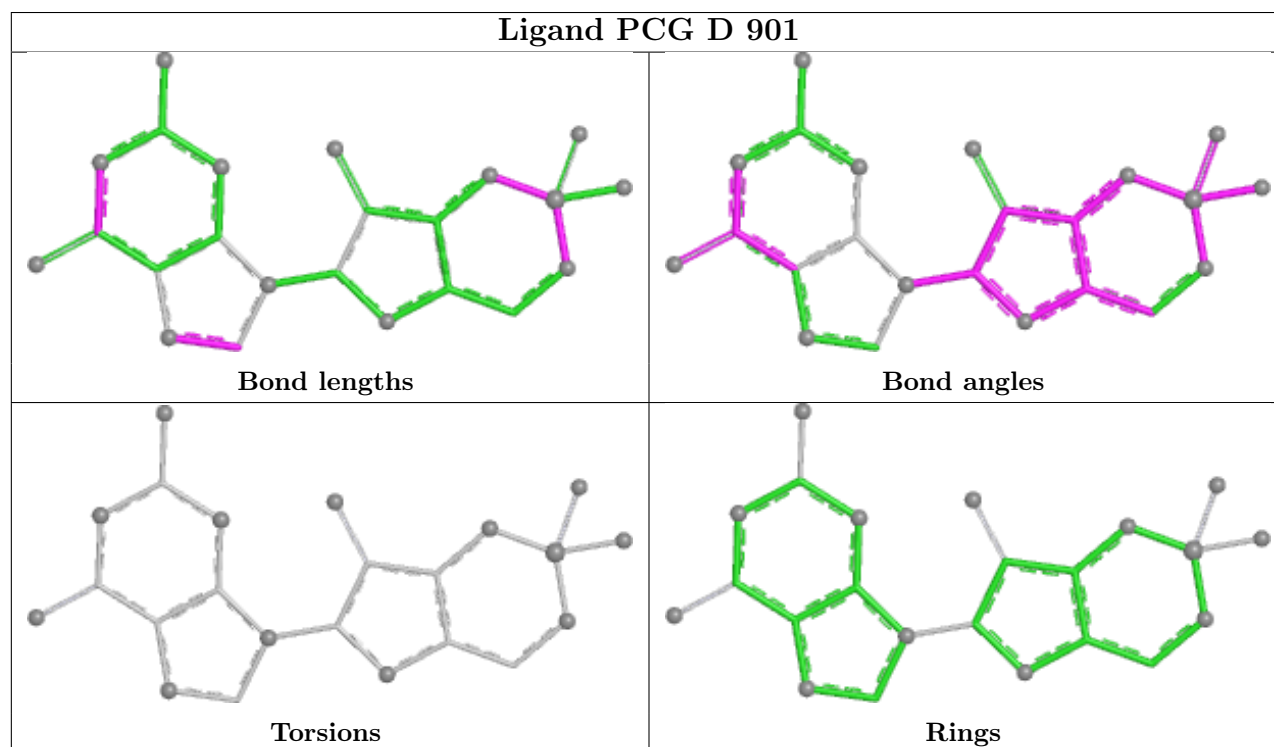
There are no ring outliers.

4 monomers are involved in 28 short contacts:

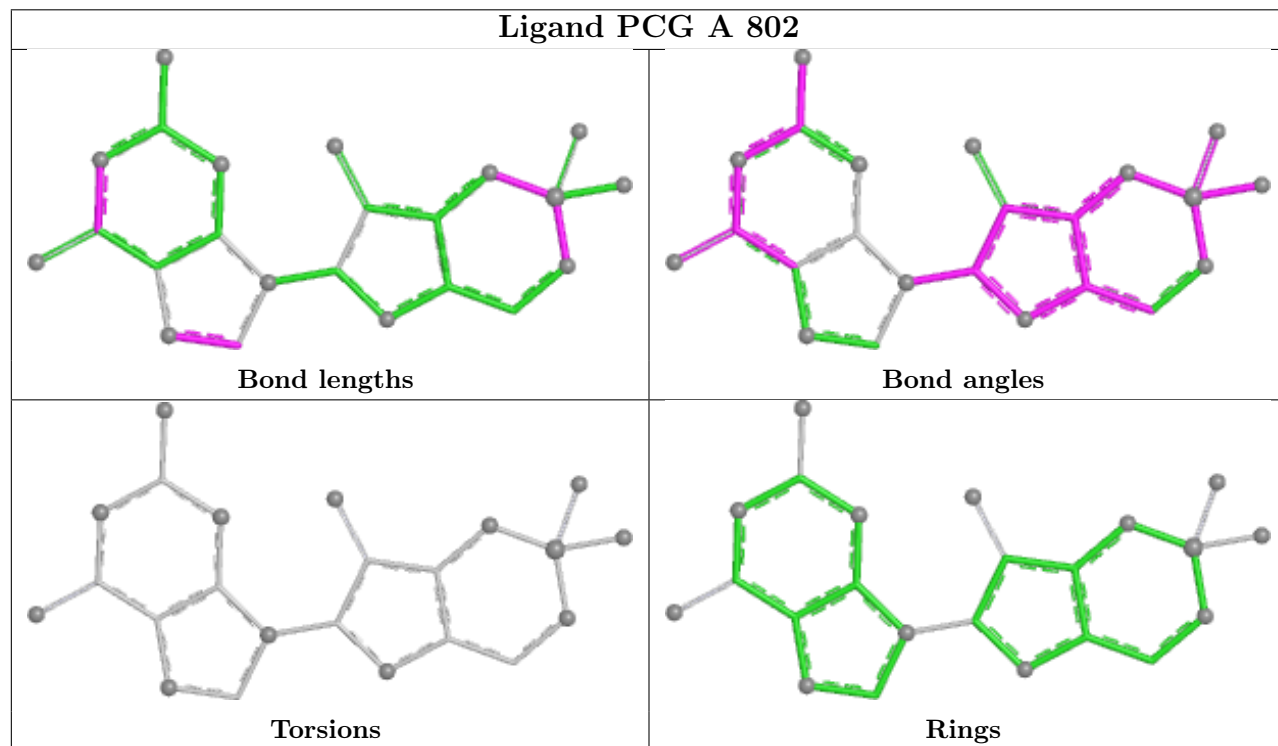
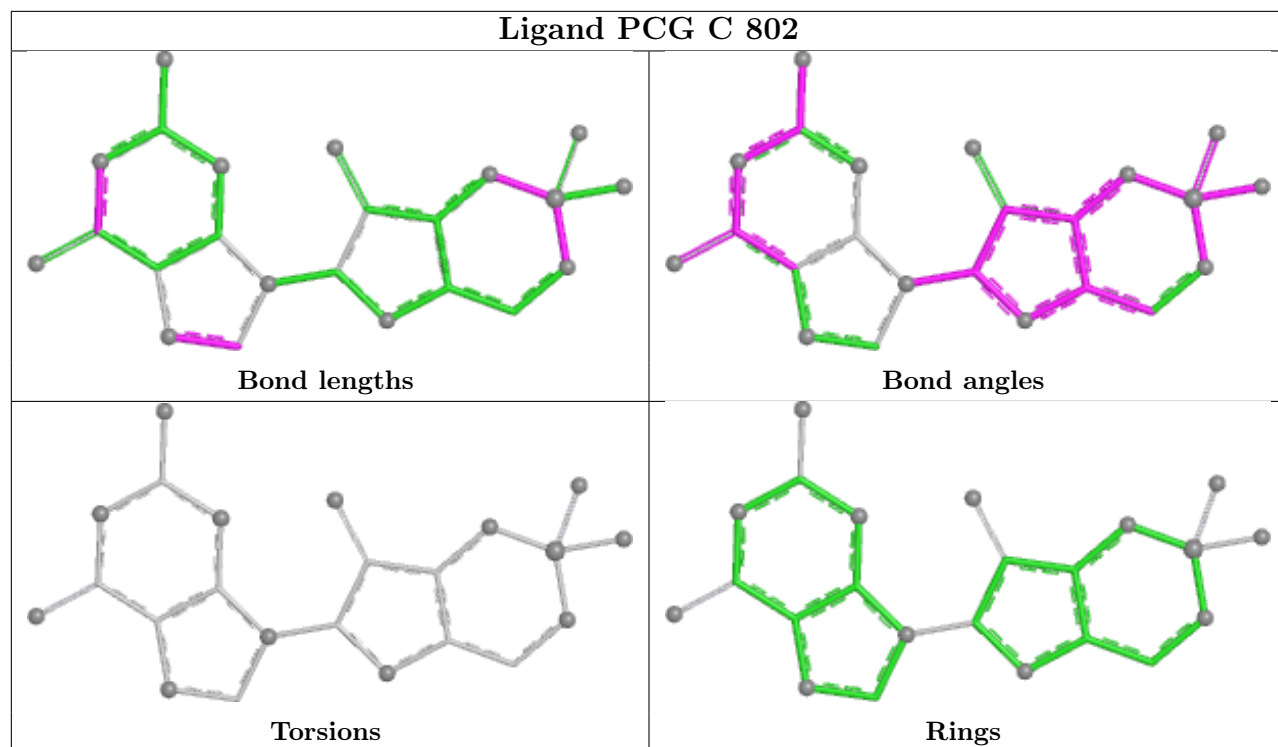
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	PCG	6	0
4	C	802	PCG	6	0
4	A	802	PCG	6	0
4	B	802	PCG	10	0

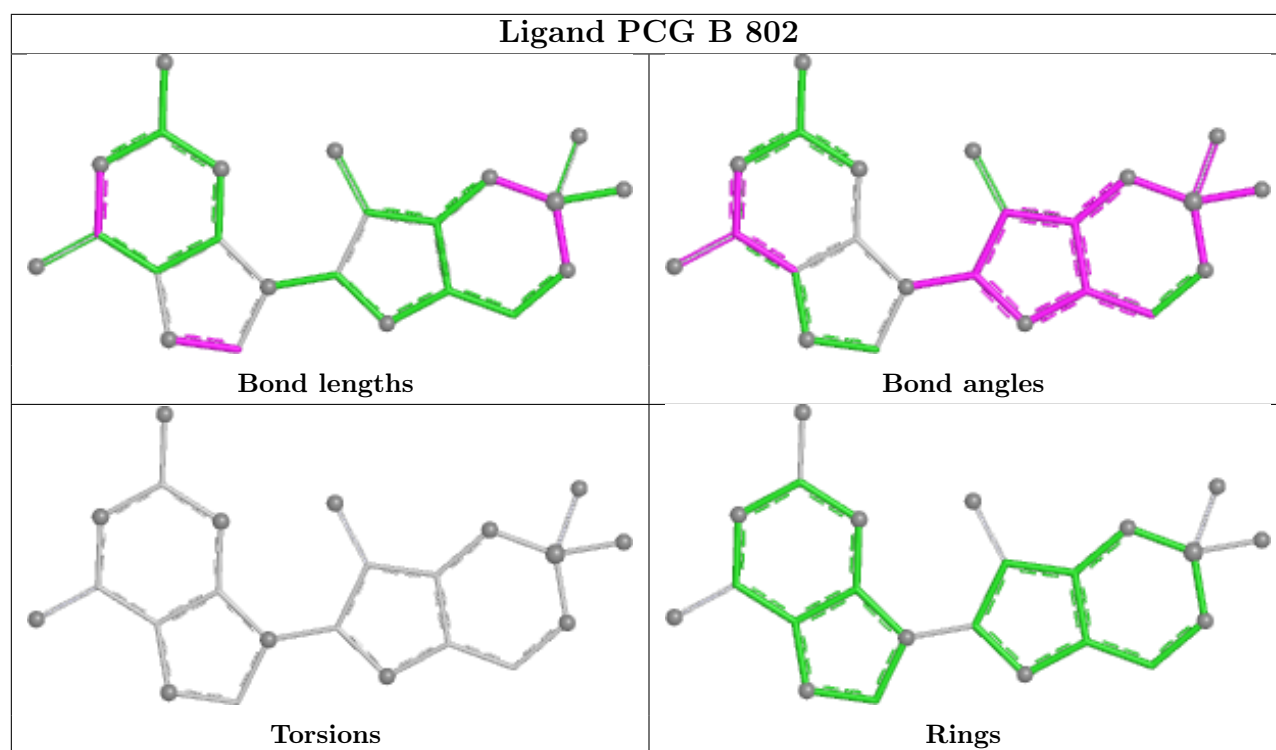
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

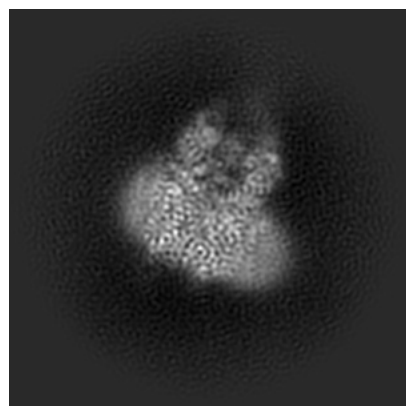
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28625. These allow visual inspection of the internal detail of the map and identification of artifacts.

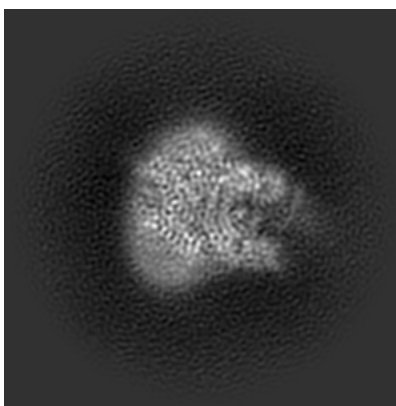
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

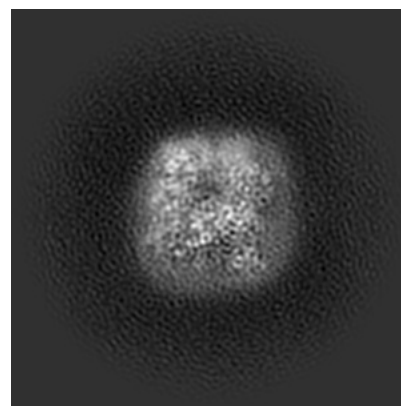
#### 6.1.1 Primary map



X

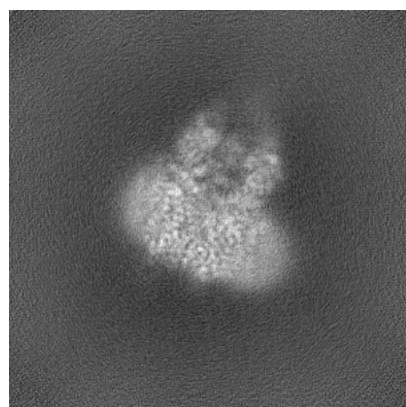


Y

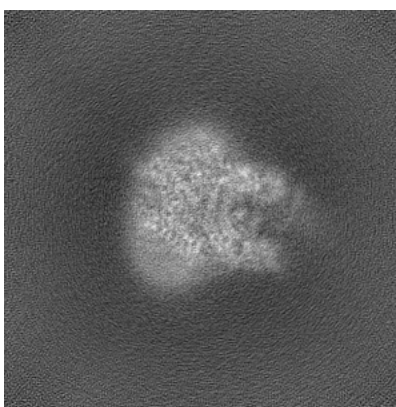


Z

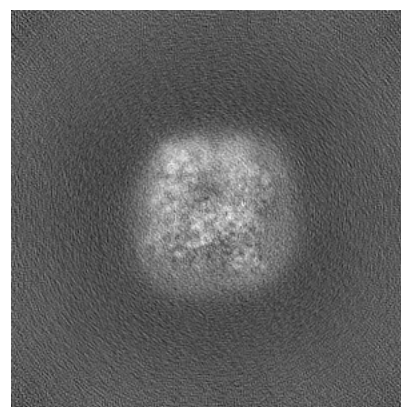
#### 6.1.2 Raw map



X



Y

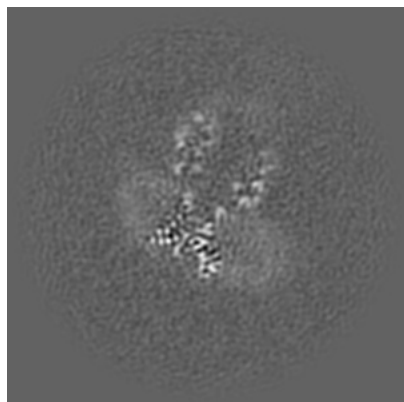


Z

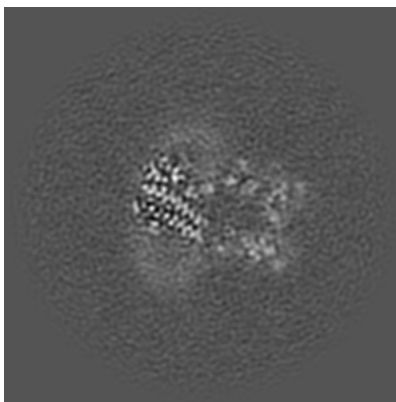
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

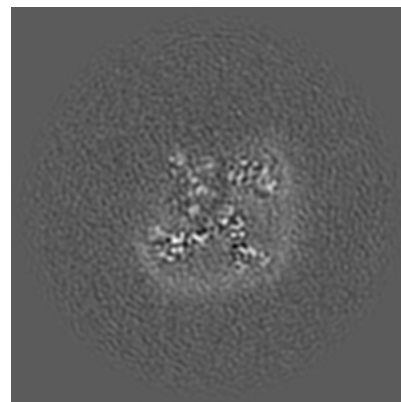
### 6.2.1 Primary map



X Index: 156

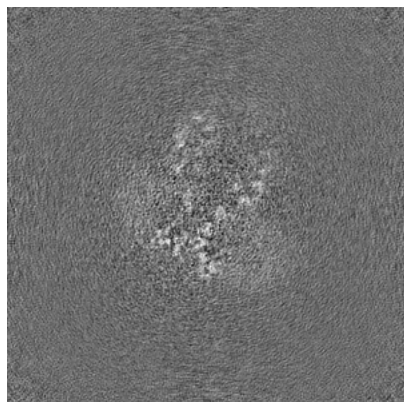


Y Index: 156

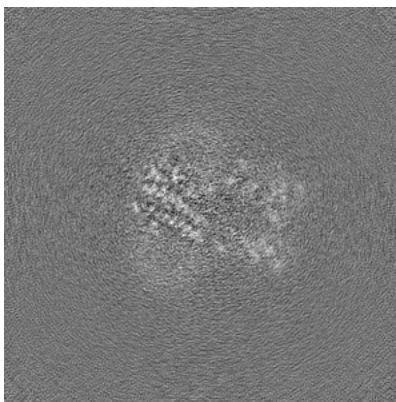


Z Index: 156

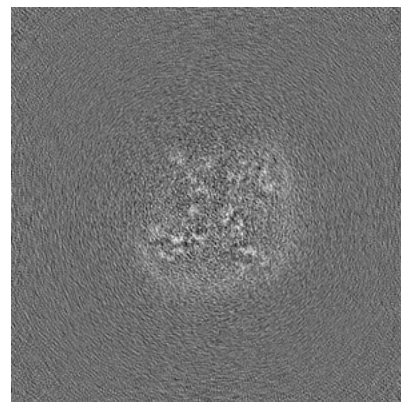
### 6.2.2 Raw map



X Index: 156



Y Index: 156

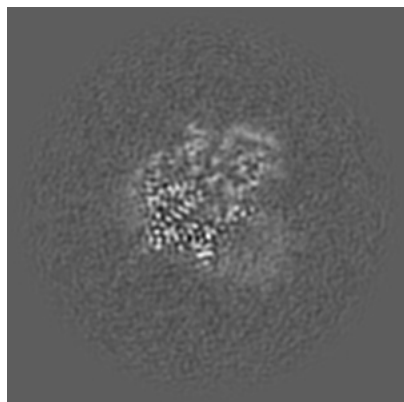


Z Index: 156

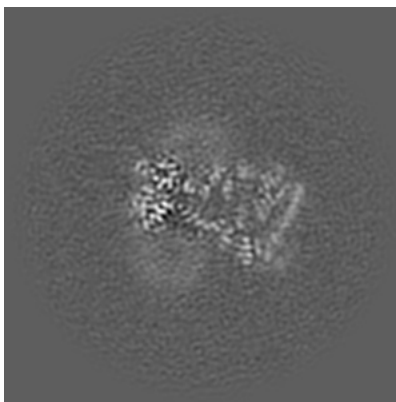
The images above show central slices of the map in three orthogonal directions.

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

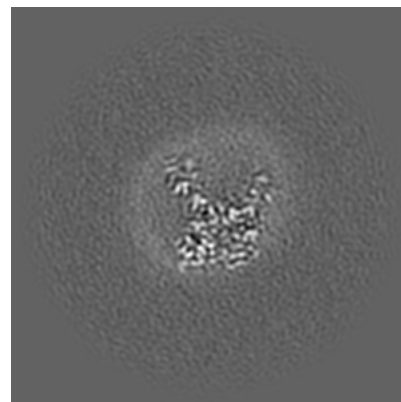
### 6.3.1 Primary map



X Index: 178

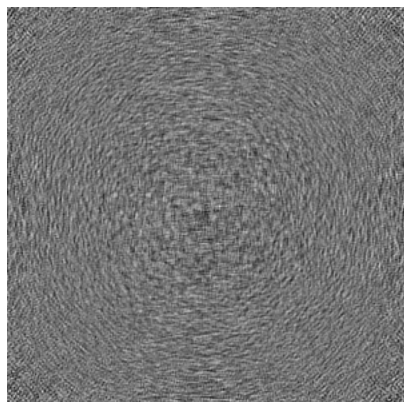


Y Index: 151

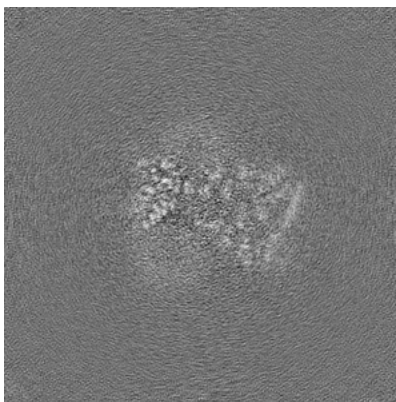


Z Index: 129

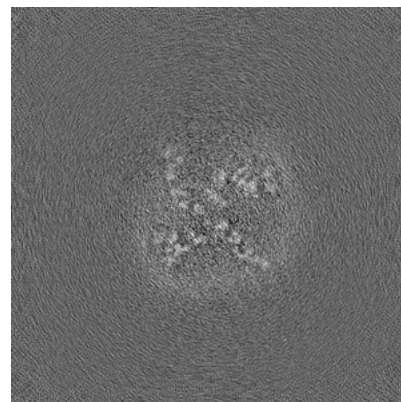
### 6.3.2 Raw map



X Index: 0



Y Index: 150



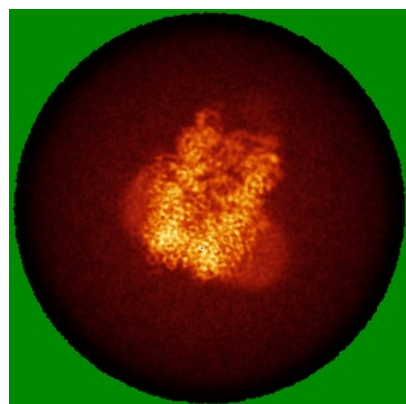
Z Index: 150

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

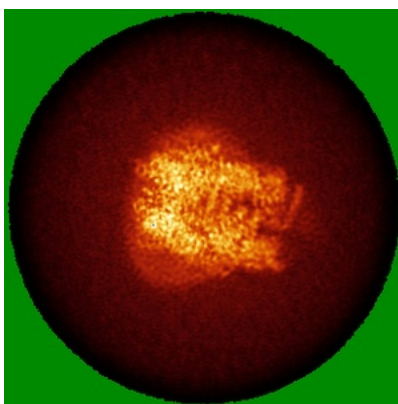


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

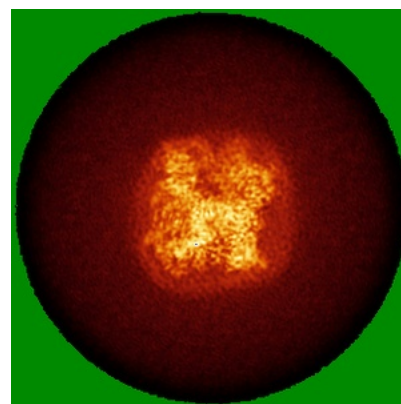
### 6.4.1 Primary map



X

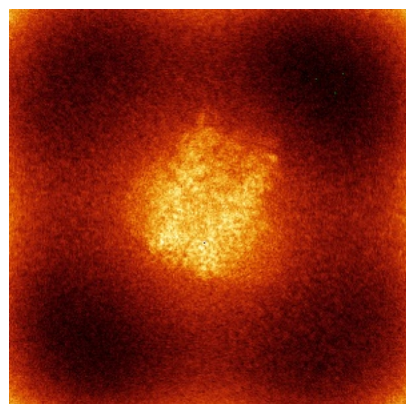


Y

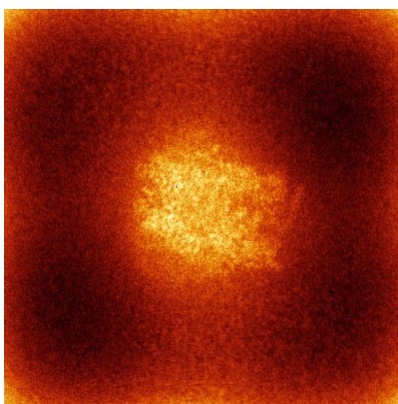


Z

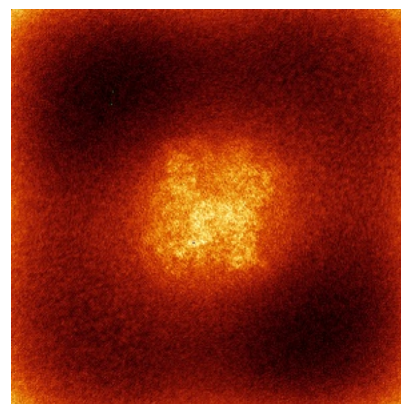
### 6.4.2 Raw map



X



Y

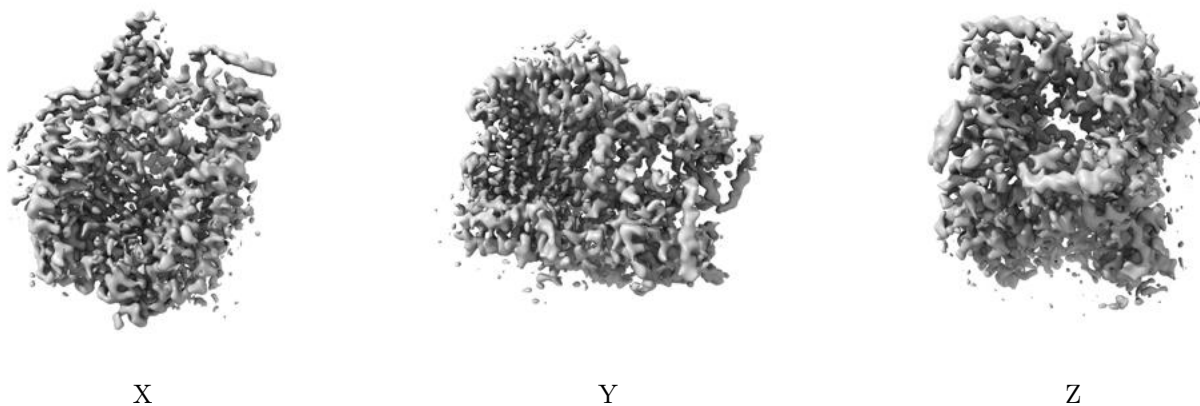


Z

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.

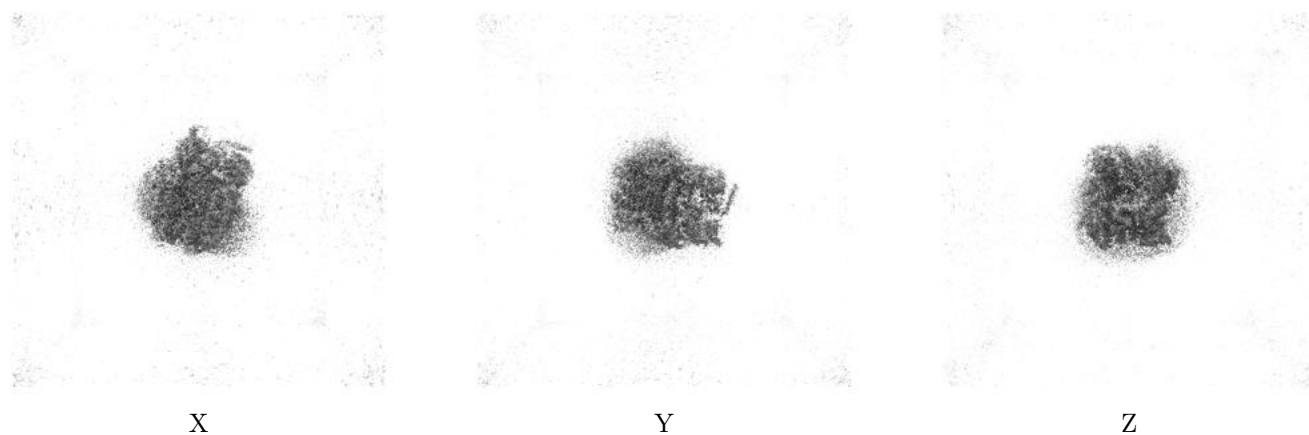
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.167. 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.

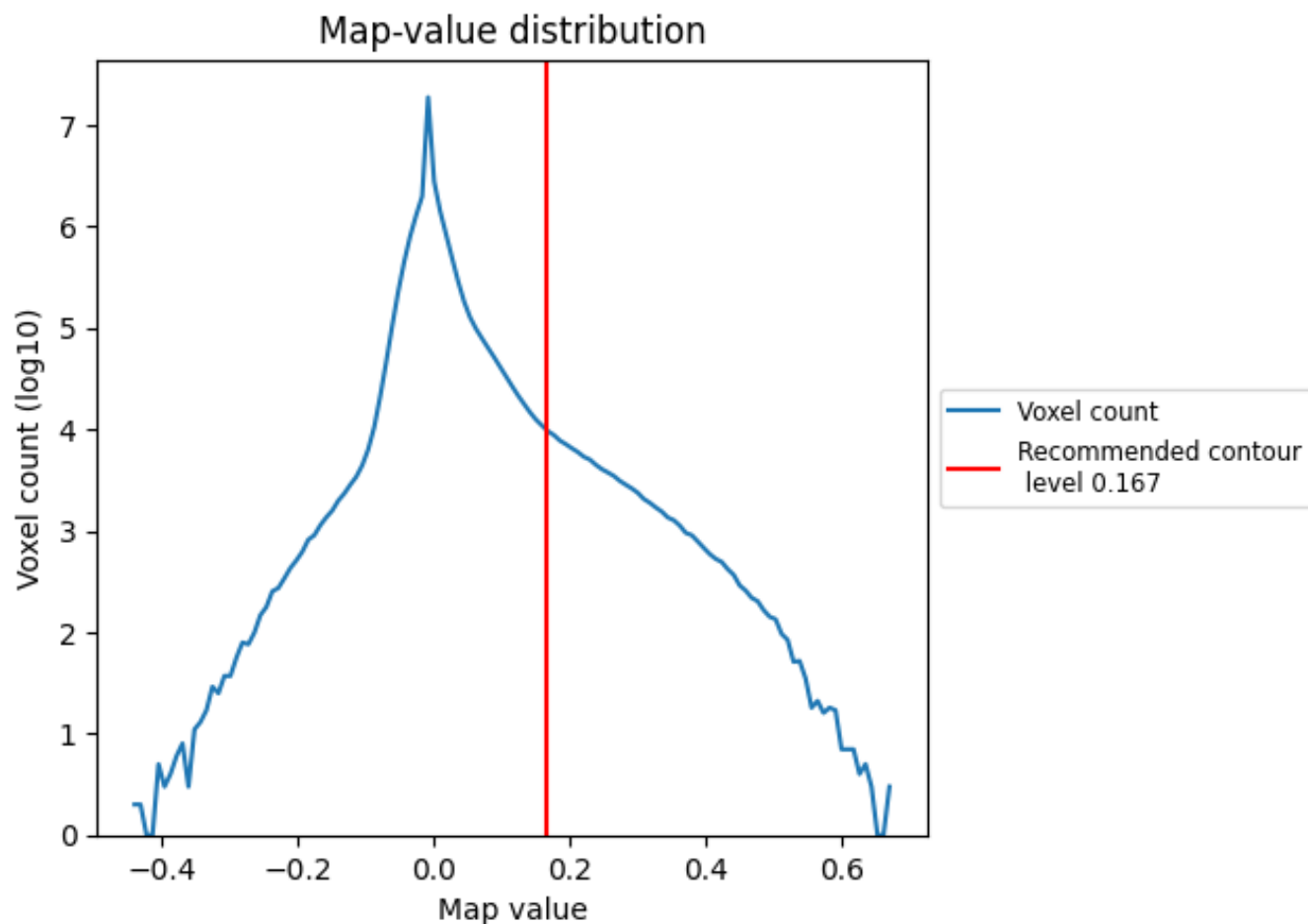
## 6.6 Mask visualisation [i](#)

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.

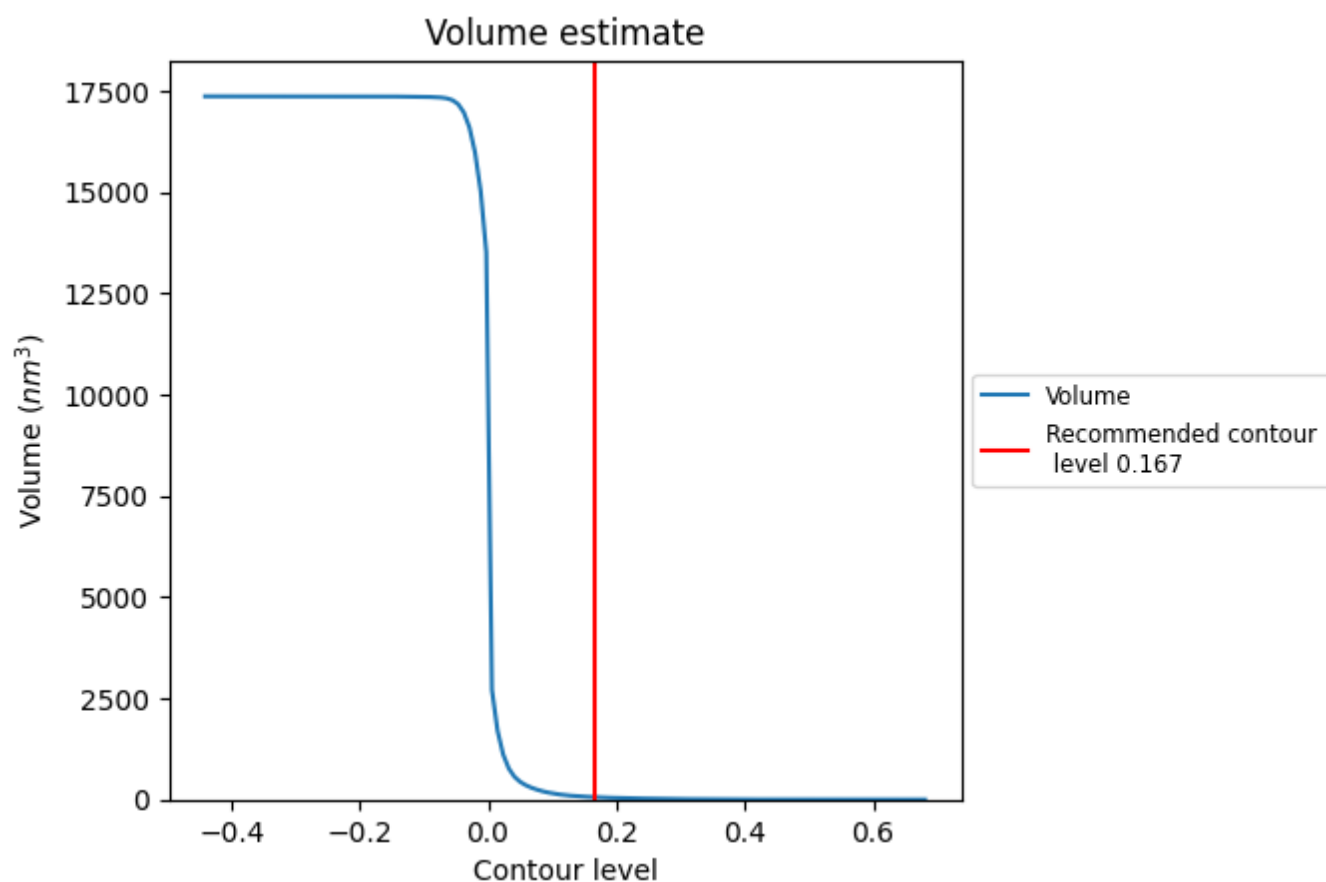
### 7.1 Map-value distribution [i](#)



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.



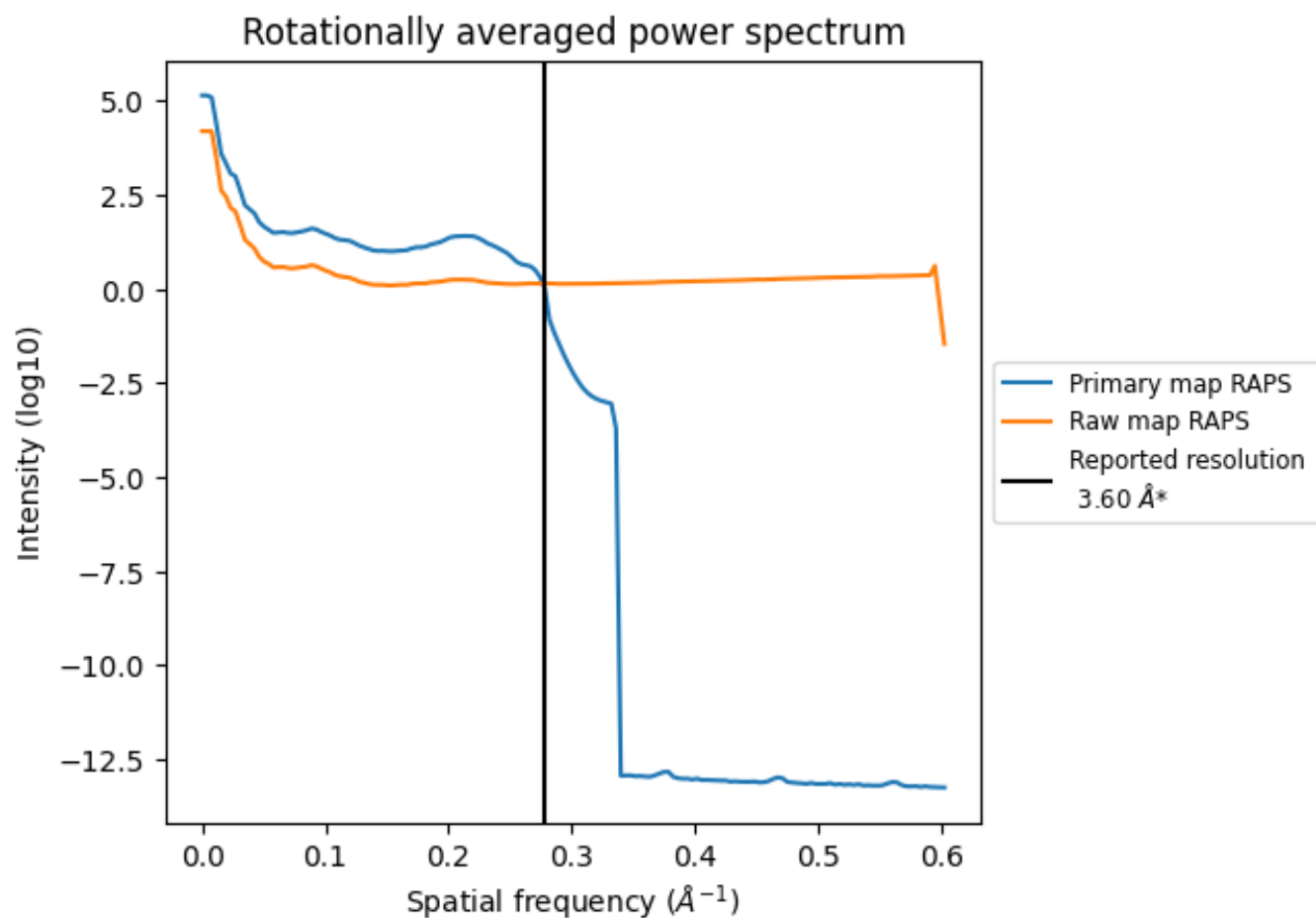
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm<sup>3</sup>; this corresponds to an approximate mass of 53 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 ⓘ

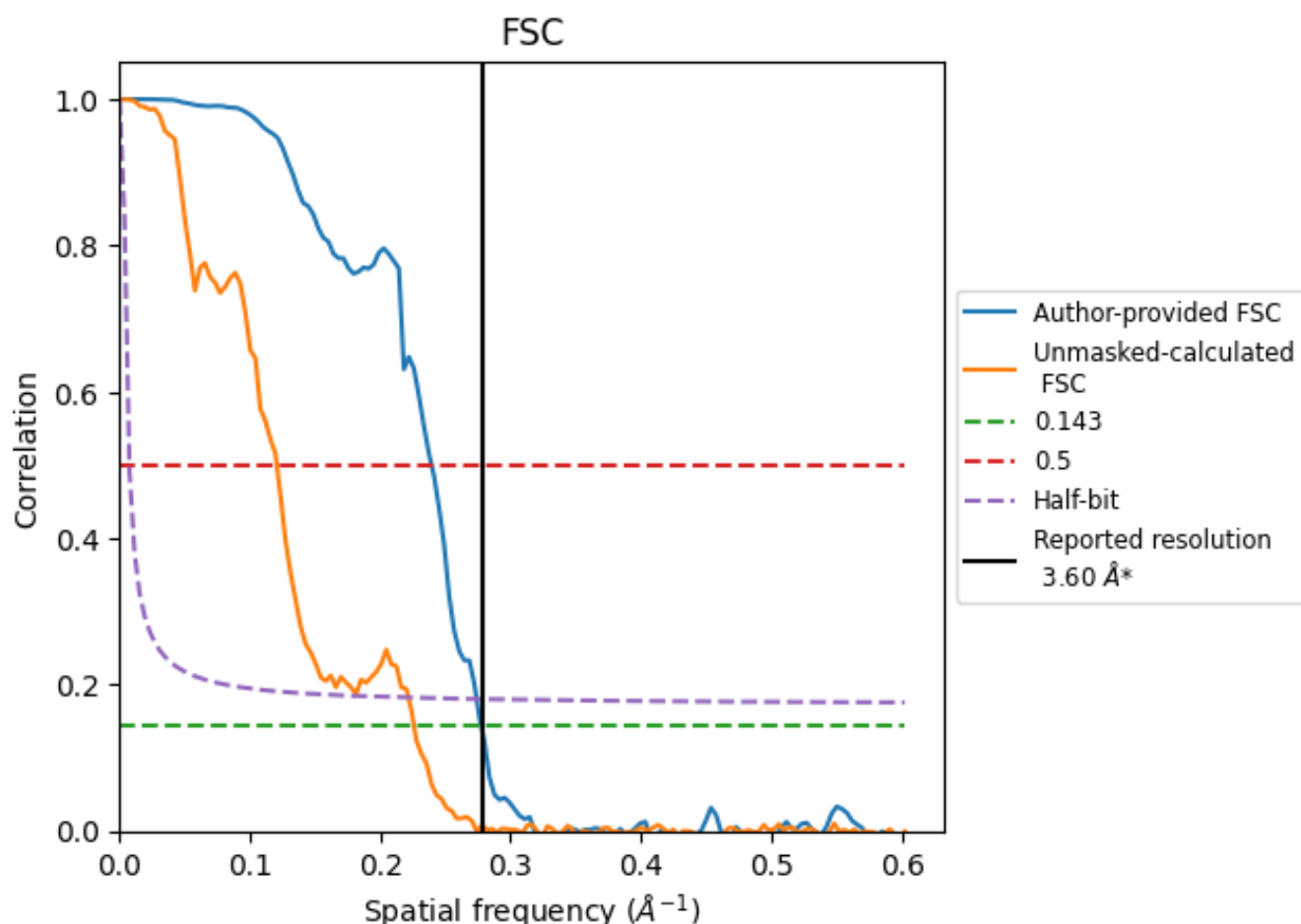


\*Reported resolution corresponds to spatial frequency of 0.278  $\text{\AA}^{-1}$

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

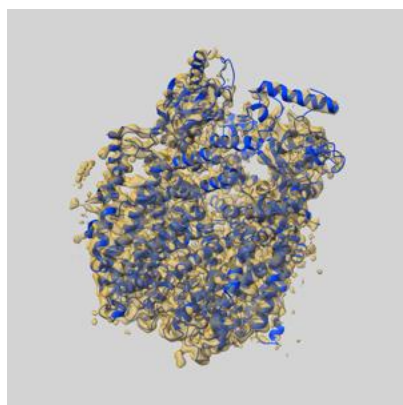
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.18	3.65
Unmasked-calculated*	4.43	8.29	4.51

\*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 4.43 differs from the reported value 3.6 by more than 10 %

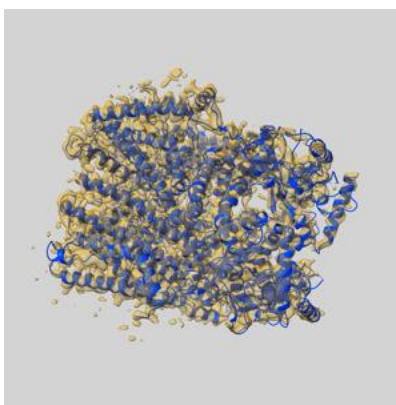
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28625 and PDB model 8EVB. Per-residue inclusion information can be found in section 3 on page 6.

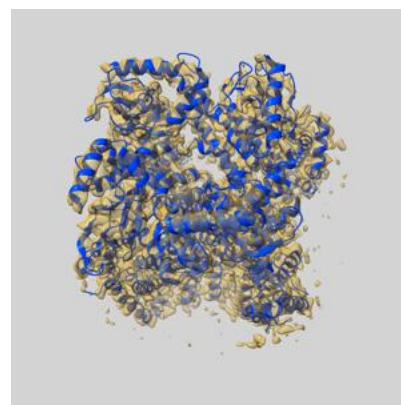
### 9.1 Map-model overlay [i](#)



X



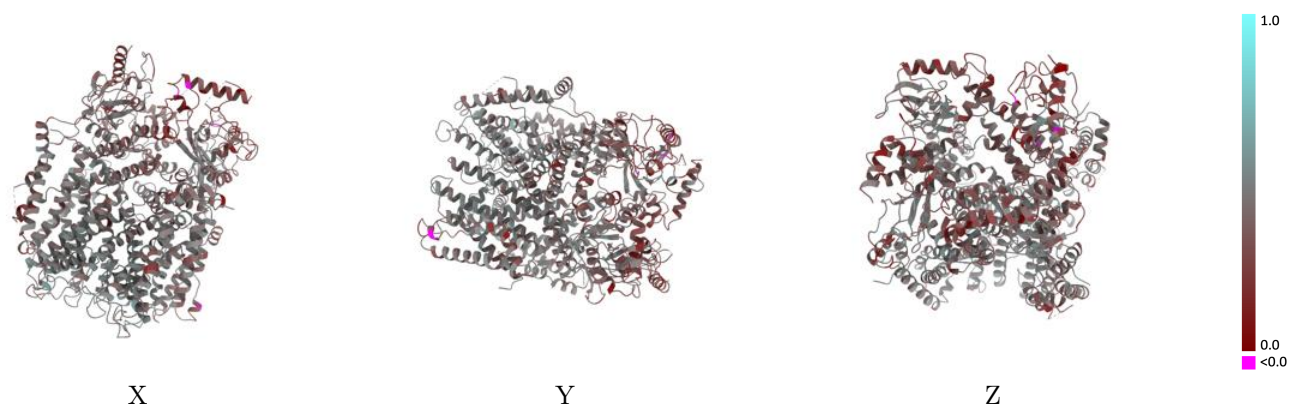
Y



Z

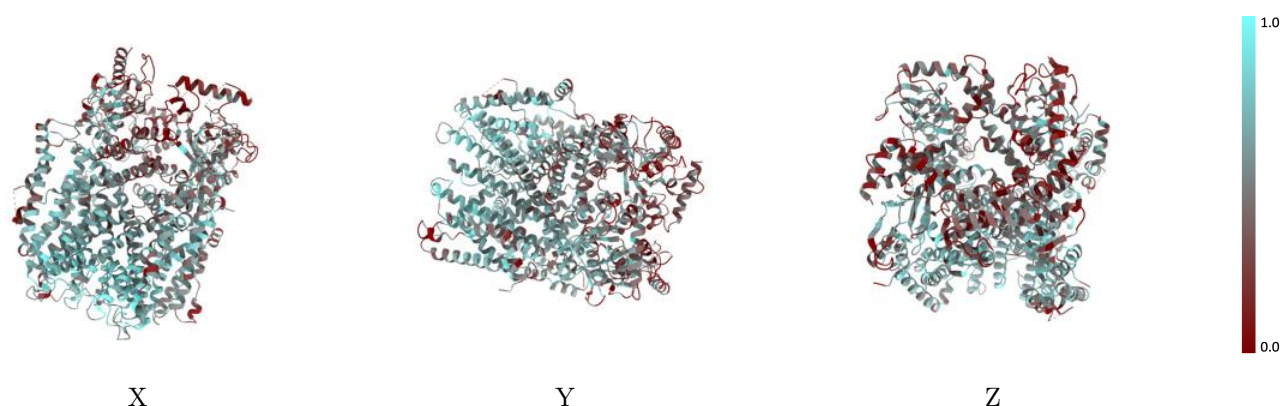
The images above show the 3D surface view of the map at the recommended contour level 0.167 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



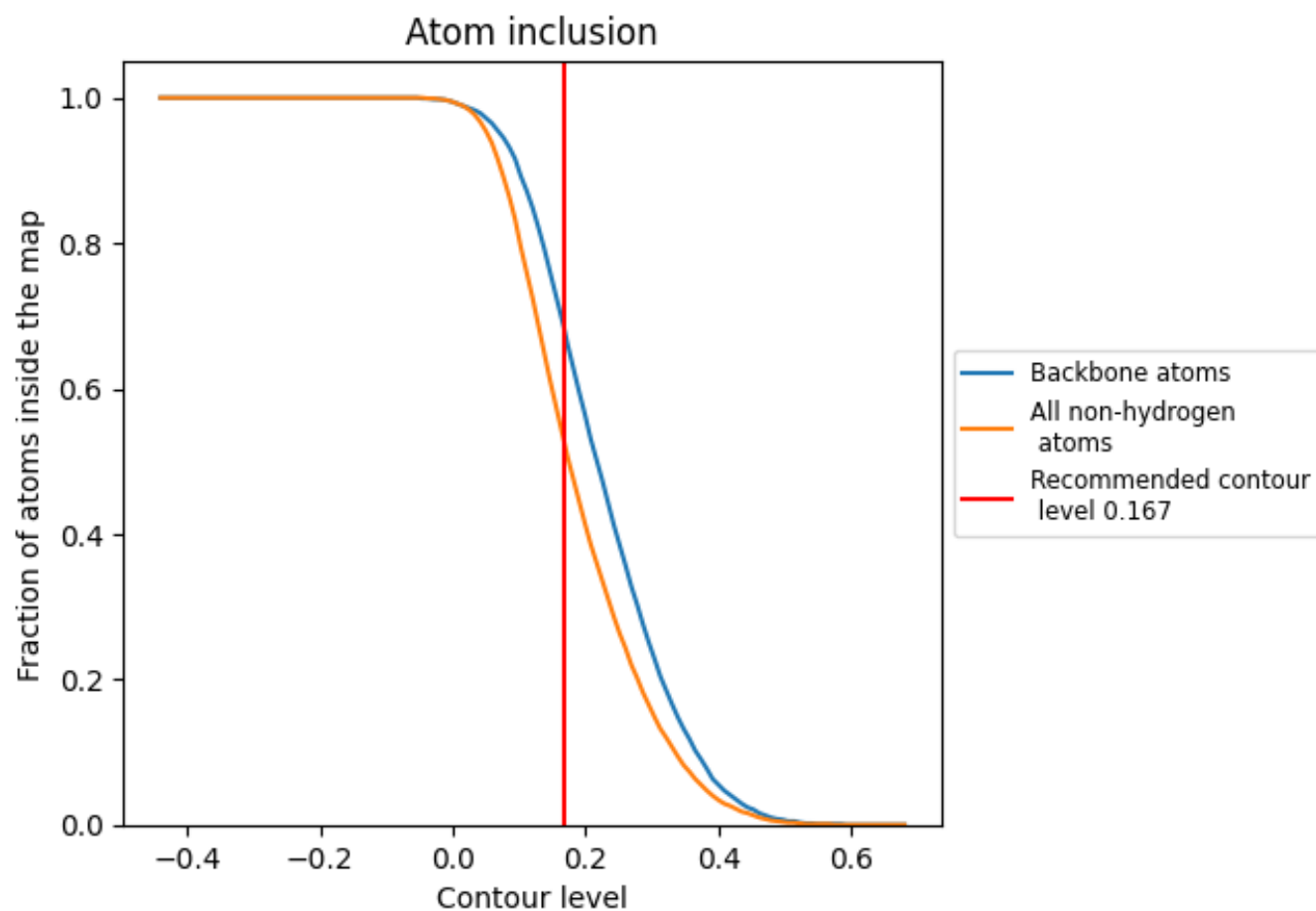
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.167).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 53% 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 (0.167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5300	<div></div> 0.4140
A	<div></div> 0.5260	<div></div> 0.4170
B	<div></div> 0.4880	<div></div> 0.3920
C	<div></div> 0.5620	<div></div> 0.4250
D	<div></div> 0.5420	<div></div> 0.4200

