



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 12:33 AM JST

PDB ID : 24VW / pdb_000024vw
EMDB ID : EMD-69854
Title : Cryo-EM structure of the human KCNQ2/KCNQ3 heterotetramer (1:3 stoichiometry) with CLM142 (M2333 CLM142, with symmetry expansion)
Authors : Wang, Y.F.; Yang, H.; Qu, Y.N.; Shen, H.Z.
Deposited on : 2026-03-22
Resolution : 3.93 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

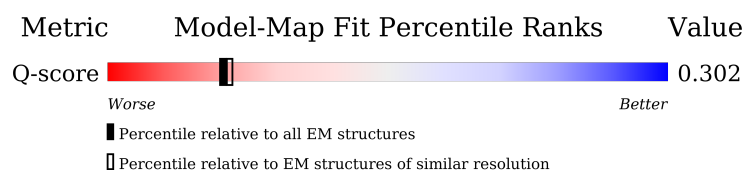
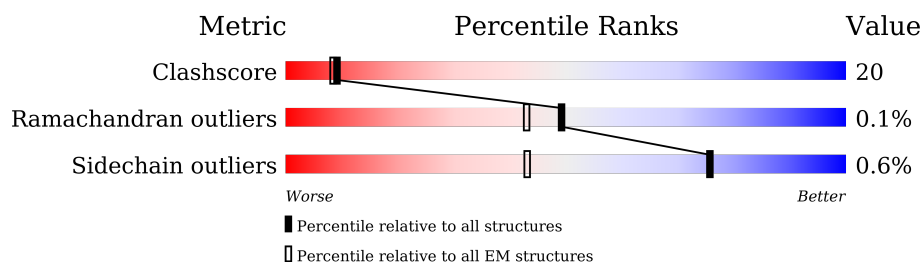
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	620	10% 21% 17% 61%
1	B	620	10% 23% 15% 61%
1	C	620	12% 23% 15% 61%
2	D	753	8% 20% 13% 67%

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
5	YJ0	D	1203	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7966 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 Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		
1	B	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		
1	C	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	MET	-	initiating methionine	UNP O43525
A	73	ALA	-	expression tag	UNP O43525
A	74	SER	-	expression tag	UNP O43525
A	75	ASP	-	expression tag	UNP O43525
A	76	TYR	-	expression tag	UNP O43525
A	77	LYS	-	expression tag	UNP O43525
A	78	ASP	-	expression tag	UNP O43525
A	79	HIS	-	expression tag	UNP O43525
A	80	ASP	-	expression tag	UNP O43525
A	81	ILE	-	expression tag	UNP O43525
A	82	ASP	-	expression tag	UNP O43525
A	83	TYR	-	expression tag	UNP O43525
A	84	LYS	-	expression tag	UNP O43525
A	85	ASP	-	expression tag	UNP O43525
A	86	ASP	-	expression tag	UNP O43525
A	87	ASP	-	expression tag	UNP O43525
A	88	ASP	-	expression tag	UNP O43525
A	89	LYS	-	expression tag	UNP O43525
A	90	GLY	-	expression tag	UNP O43525
A	91	THR	-	expression tag	UNP O43525
A	92	MET	-	expression tag	UNP O43525
B	72	MET	-	initiating methionine	UNP O43525
B	73	ALA	-	expression tag	UNP O43525
B	74	SER	-	expression tag	UNP O43525

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Chain	Residue	Modelled	Actual	Comment	Reference
B	75	ASP	-	expression tag	UNP O43525
B	76	TYR	-	expression tag	UNP O43525
B	77	LYS	-	expression tag	UNP O43525
B	78	ASP	-	expression tag	UNP O43525
B	79	HIS	-	expression tag	UNP O43525
B	80	ASP	-	expression tag	UNP O43525
B	81	ILE	-	expression tag	UNP O43525
B	82	ASP	-	expression tag	UNP O43525
B	83	TYR	-	expression tag	UNP O43525
B	84	LYS	-	expression tag	UNP O43525
B	85	ASP	-	expression tag	UNP O43525
B	86	ASP	-	expression tag	UNP O43525
B	87	ASP	-	expression tag	UNP O43525
B	88	ASP	-	expression tag	UNP O43525
B	89	LYS	-	expression tag	UNP O43525
B	90	GLY	-	expression tag	UNP O43525
B	91	THR	-	expression tag	UNP O43525
B	92	MET	-	expression tag	UNP O43525
C	72	MET	-	initiating methionine	UNP O43525
C	73	ALA	-	expression tag	UNP O43525
C	74	SER	-	expression tag	UNP O43525
C	75	ASP	-	expression tag	UNP O43525
C	76	TYR	-	expression tag	UNP O43525
C	77	LYS	-	expression tag	UNP O43525
C	78	ASP	-	expression tag	UNP O43525
C	79	HIS	-	expression tag	UNP O43525
C	80	ASP	-	expression tag	UNP O43525
C	81	ILE	-	expression tag	UNP O43525
C	82	ASP	-	expression tag	UNP O43525
C	83	TYR	-	expression tag	UNP O43525
C	84	LYS	-	expression tag	UNP O43525
C	85	ASP	-	expression tag	UNP O43525
C	86	ASP	-	expression tag	UNP O43525
C	87	ASP	-	expression tag	UNP O43525
C	88	ASP	-	expression tag	UNP O43525
C	89	LYS	-	expression tag	UNP O43525
C	90	GLY	-	expression tag	UNP O43525
C	91	THR	-	expression tag	UNP O43525
C	92	MET	-	expression tag	UNP O43525

- Molecule 2 is a protein called Green fluorescent protein,Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	247	Total 2006	C 1333	N 336	O 328	S 9	0	0

There are 63 discrepancies between the modelled and reference sequences:

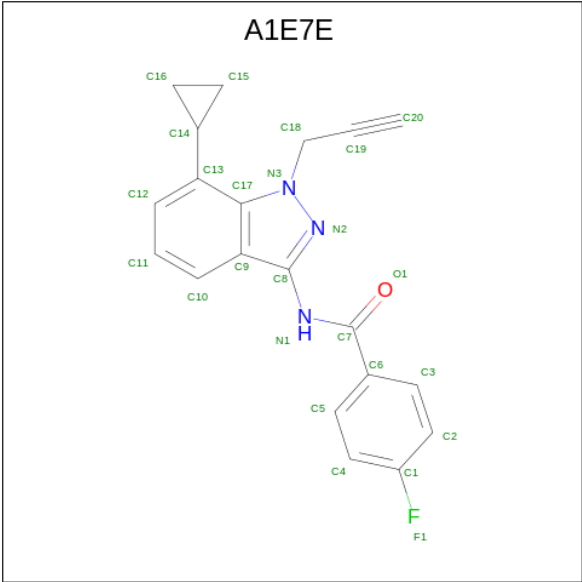
Chain	Residue	Modelled	Actual	Comment	Reference
D	-208	MET	-	initiating methionine	UNP P42212
D	-207	ALA	-	expression tag	UNP P42212
D	-206	MET	-	expression tag	UNP P42212
D	-205	HIS	-	expression tag	UNP P42212
D	-204	HIS	-	expression tag	UNP P42212
D	-203	HIS	-	expression tag	UNP P42212
D	-202	HIS	-	expression tag	UNP P42212
D	-201	HIS	-	expression tag	UNP P42212
D	-200	HIS	-	expression tag	UNP P42212
D	-199	HIS	-	expression tag	UNP P42212
D	-198	HIS	-	expression tag	UNP P42212
D	-197	GLY	-	expression tag	UNP P42212
D	-196	GLY	-	expression tag	UNP P42212
D	-195	SER	-	expression tag	UNP P42212
D	-194	MET	-	expression tag	UNP P42212
D	-193	VAL	-	expression tag	UNP P42212
D	-130	LEU	PHE	conflict	UNP P42212
D	-129	THR	SER	conflict	UNP P42212
D	-87	THR	LYS	conflict	UNP P42212
D	12	LYS	ALA	conflict	UNP P42212
D	37	LEU	HIS	conflict	UNP P42212
D	45	SER	-	linker	UNP P42212
D	46	GLY	-	linker	UNP P42212
D	47	LEU	-	linker	UNP P42212
D	48	ARG	-	linker	UNP P42212
D	49	SER	-	linker	UNP P42212
D	50	GLY	-	linker	UNP P42212
D	51	LEU	-	linker	UNP P42212
D	52	GLU	-	linker	UNP P42212
D	53	VAL	-	linker	UNP P42212
D	54	LEU	-	linker	UNP P42212
D	55	PHE	-	linker	UNP P42212
D	56	GLN	-	linker	UNP P42212
D	57	GLY	-	linker	UNP P42212
D	58	PRO	-	linker	UNP P42212
D	59	GLY	-	linker	UNP P42212
D	60	GLY	-	linker	UNP P42212

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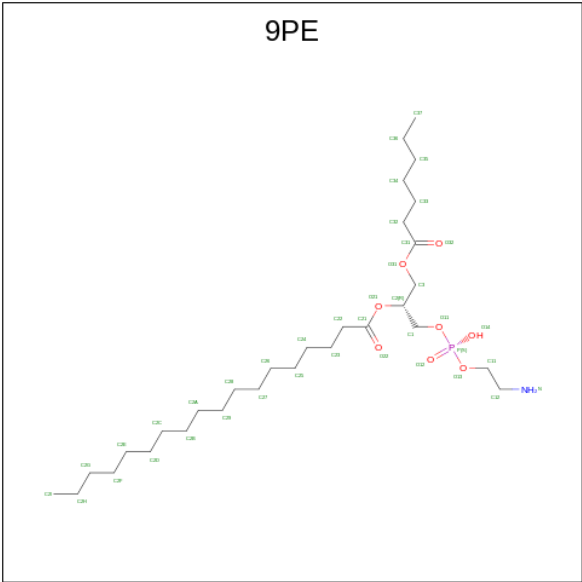
Chain	Residue	Modelled	Actual	Comment	Reference
D	61	ARG	-	linker	UNP P42212
D	62	MET	-	linker	UNP P42212
D	953	GLY	-	linker	UNP O43526
D	954	GLY	-	linker	UNP O43526
D	955	GLY	-	linker	UNP O43526
D	956	SER	-	linker	UNP O43526
D	957	GLY	-	linker	UNP O43526
D	958	GLY	-	linker	UNP O43526
D	959	GLY	-	linker	UNP O43526
D	960	SER	-	linker	UNP O43526
D	1130	VAL	-	expression tag	UNP O43526
D	1131	GLU	-	expression tag	UNP O43526
D	1132	GLY	-	expression tag	UNP O43526
D	1133	GLY	-	expression tag	UNP O43526
D	1134	SER	-	expression tag	UNP O43526
D	1135	SER	-	expression tag	UNP O43526
D	1136	GLY	-	expression tag	UNP O43526
D	1137	GLY	-	expression tag	UNP O43526
D	1138	TRP	-	expression tag	UNP O43526
D	1139	SER	-	expression tag	UNP O43526
D	1140	HIS	-	expression tag	UNP O43526
D	1141	PRO	-	expression tag	UNP O43526
D	1142	GLN	-	expression tag	UNP O43526
D	1143	PHE	-	expression tag	UNP O43526
D	1144	GLU	-	expression tag	UNP O43526
D	1145	LYS	-	expression tag	UNP O43526

- Molecule 3 is {N}-(7-cyclopropyl-1-prop-2-ynyl-indazol-3-yl)-4-fluoranyl-benzamide (CCD ID: A1E7E) (formula: C₂₀H₁₆FN₃O) (labeled as "Ligand of Interest" by depositor).



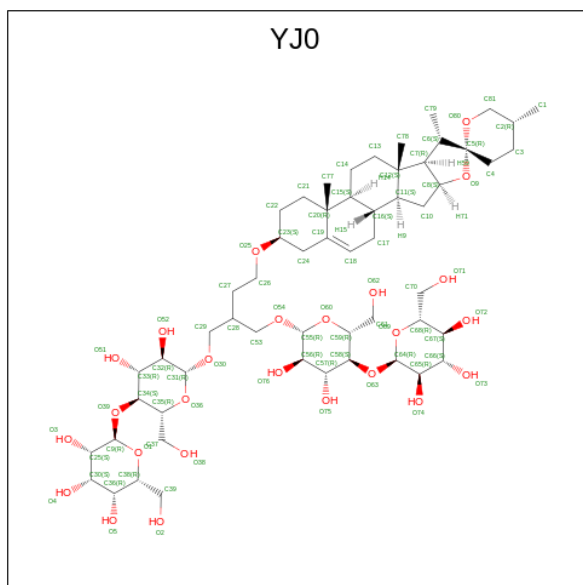
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	F	N	O	0
			25	20	1	3	1	
3	B	1	Total	C	F	N	O	0
			25	20	1	3	1	
3	C	1	Total	C	F	N	O	0
			25	20	1	3	1	
3	D	1	Total	C	F	N	O	0
			25	20	1	3	1	

- Molecule 4 is (1R)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P) (labeled as "Ligand of Interest" by depositor).

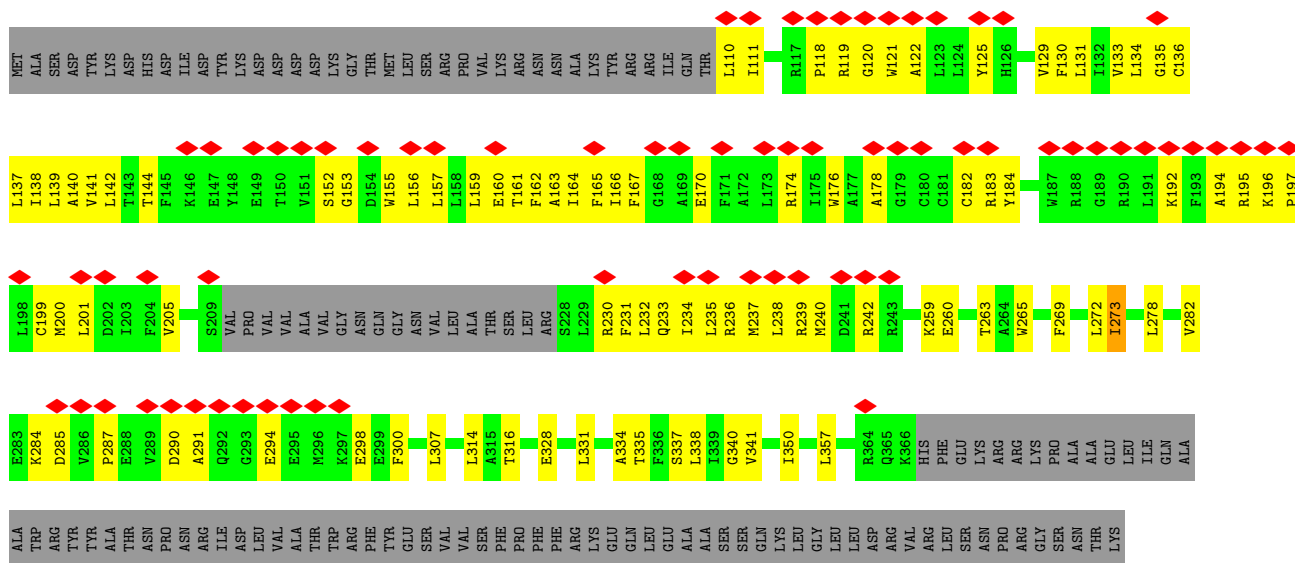


Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 5 is (2R)-2-{[(4-O-hexopyranosyl-beta-D-glucopyranosyl)oxy]methyl}-4-{[(25R)-5beta,14beta,17beta-spirostan-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: YJ0) (formula: C₅₆H₉₂O₂₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	D	1	Total	C	O	0
			81	56	25	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.112	Depositor
Minimum map value	-1.024	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.371	Depositor
Map size (Å)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9PE, A1E7E, YJ0

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	0.20	0/1960	0.58	1/2653 (0.0%)
1	B	0.19	0/1960	0.56	1/2653 (0.0%)
1	C	0.20	0/1960	0.53	1/2653 (0.0%)
2	D	0.18	0/2060	0.47	0/2790
All	All	0.19	0/7940	0.54	3/10749 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ALA	CB-CA-C	-5.16	110.61	116.54
1	B	291	ALA	CB-CA-C	-5.09	110.68	116.54
1	C	291	ALA	CB-CA-C	-5.00	110.79	116.54

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	1913	0	1970	95	0
1	B	1913	0	1970	87	0
1	C	1913	0	1970	81	0
2	D	2006	0	2046	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	0	1	0
3	B	25	0	0	1	0
3	C	25	0	0	1	0
3	D	25	0	0	0	0
4	D	40	0	59	2	0
5	D	81	0	0	2	0
All	All	7966	0	8015	327	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 20.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PHE:HE2	1:C:230:ARG:HB2	1.32	0.94
1:A:233:GLN:HA	1:A:236:ARG:HE	1.40	0.87
1:C:139:LEU:HD22	1:C:156:LEU:HD13	1.61	0.81
1:C:196:LYS:HD2	1:C:197:PRO:HD2	1.62	0.81
1:B:303:TYR:H	1:C:144:THR:HG21	1.45	0.80
1:B:136:CYS:SG	1:B:236:ARG:NH2	2.55	0.79
1:C:233:GLN:HA	1:C:236:ARG:HE	1.47	0.79
2:D:127:ILE:HD12	2:D:130:ILE:HD11	1.65	0.78
1:C:182:CYS:SG	1:C:183:ARG:NH1	2.60	0.74
1:B:117:ARG:HH12	1:B:124:LEU:HB3	1.52	0.74
1:B:157:LEU:O	1:B:161:THR:HG23	1.88	0.73
1:A:134:LEU:O	1:A:138:ILE:HG12	1.90	0.72
1:C:337:SER:O	1:C:341:VAL:HG23	1.90	0.71
1:C:136:CYS:SG	1:C:236:ARG:NH2	2.63	0.71
1:A:231:PHE:O	1:A:235:LEU:HD12	1.90	0.70
1:A:350:ILE:HD11	1:B:355:LEU:HD12	1.73	0.70
1:B:260:GLU:N	1:B:260:GLU:OE2	2.24	0.70
1:A:260:GLU:OE2	1:A:260:GLU:N	2.25	0.69
1:A:239:ARG:O	1:A:239:ARG:NH1	2.21	0.69
1:A:197:PRO:HA	1:A:200:MET:HE3	1.72	0.68
1:C:157:LEU:O	1:C:161:THR:HG23	1.92	0.68
1:B:363:HIS:HA	1:B:366:LYS:HZ3	1.57	0.68
1:B:277:PHE:CE2	1:C:230:ARG:HB2	2.23	0.68
1:A:184:TYR:HD1	1:A:192:LYS:HZ2	1.43	0.66
1:B:314:LEU:HG	1:B:340:GLY:HA3	1.77	0.66
1:A:195:ARG:O	1:A:195:ARG:NH1	2.29	0.66
1:C:314:LEU:HG	1:C:340:GLY:HA3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD11	1:B:351:LEU:HB2	1.76	0.66
2:D:76:LEU:O	2:D:80:LEU:HG	1.96	0.65
1:B:337:SER:O	1:B:341:VAL:HG23	1.97	0.65
1:A:136:CYS:SG	1:A:236:ARG:NH2	2.69	0.65
1:A:242:ARG:O	1:A:242:ARG:NH1	2.30	0.64
1:A:309:TRP:HD1	1:A:322:LYS:HB2	1.62	0.64
1:C:233:GLN:O	1:C:237:MET:HE2	1.98	0.64
1:A:129:VAL:O	1:A:133:VAL:HG22	1.97	0.64
1:B:233:GLN:OE1	1:B:233:GLN:N	2.31	0.63
2:D:178:SER:O	2:D:182:LEU:HG	1.99	0.63
1:B:200:MET:HA	1:B:203:ILE:HG12	1.80	0.63
1:A:303:TYR:H	1:B:144:THR:HG21	1.64	0.63
2:D:77:GLN:NE2	2:D:146:ALA:O	2.32	0.62
1:A:357:LEU:HD21	1:B:360:GLN:HG3	1.82	0.62
1:B:277:PHE:CD2	1:C:234:ILE:HD11	2.35	0.62
1:A:149:GLU:HG2	1:A:150:THR:HG23	1.80	0.62
1:A:328:GLU:O	1:A:332:ILE:HG12	1.99	0.62
1:C:232:LEU:O	1:C:236:ARG:HG3	2.00	0.62
1:B:357:LEU:HD21	1:C:357:LEU:HD12	1.80	0.61
1:A:125:TYR:O	1:A:129:VAL:HG22	2.00	0.61
1:C:129:VAL:O	1:C:133:VAL:HG22	2.01	0.61
1:A:142:LEU:HA	1:A:145:PHE:CE2	2.36	0.61
1:A:139:LEU:HD13	1:A:142:LEU:HD23	1.83	0.60
1:C:233:GLN:OE1	1:C:233:GLN:N	2.31	0.60
1:A:233:GLN:HB3	1:A:236:ARG:HH21	1.65	0.60
1:A:196:LYS:HD2	1:A:197:PRO:HD2	1.83	0.60
1:C:140:ALA:HB1	1:C:230:ARG:HE	1.66	0.60
1:A:351:LEU:HB3	2:D:907:LEU:HD21	1.84	0.59
1:C:137:LEU:O	1:C:141:VAL:HG23	2.03	0.59
1:A:194:ALA:HA	1:A:199:CYS:SG	2.43	0.58
1:B:182:CYS:SG	1:B:183:ARG:N	2.75	0.58
1:C:231:PHE:HA	1:C:234:ILE:HD12	1.85	0.58
2:D:286:THR:HG23	2:D:289:GLY:H	1.67	0.58
1:A:274:LEU:HG	1:A:336:PHE:HE2	1.69	0.58
2:D:201:PHE:HA	2:D:204:ILE:HG22	1.85	0.58
1:B:302:THR:OG1	1:B:305:ASP:OD2	2.21	0.57
1:B:363:HIS:HA	1:B:366:LYS:NZ	2.18	0.57
1:B:163:ALA:O	1:B:166:ILE:HG22	2.04	0.57
1:A:182:CYS:SG	1:A:183:ARG:N	2.77	0.57
2:D:143:ARG:NH1	5:D:1203:YJ0:O51	2.37	0.57
1:B:142:LEU:HA	1:B:145:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:O	1:B:133:VAL:HG13	2.04	0.57
1:B:139:LEU:O	1:B:143:THR:OG1	2.22	0.57
1:A:240:MET:SD	1:A:240:MET:N	2.77	0.57
1:C:119:ARG:HG3	1:C:120:GLY:H	1.69	0.57
2:D:167:PHE:HB3	2:D:209:ARG:CZ	2.34	0.57
1:A:200:MET:O	1:A:203:ILE:HG22	2.05	0.56
1:A:314:LEU:HD11	1:A:340:GLY:HA3	1.87	0.56
2:D:174:VAL:HG13	2:D:202:LEU:HG	1.87	0.56
1:A:130:PHE:O	1:A:134:LEU:HG	2.05	0.56
1:A:181:CYS:HA	1:A:185:LYS:HD3	1.87	0.56
2:D:132:THR:HA	2:D:135:VAL:HG12	1.87	0.56
1:A:196:LYS:HE3	1:A:198:LEU:HB2	1.88	0.56
1:C:328:GLU:HA	1:C:331:LEU:HD12	1.88	0.56
2:D:257:ASN:OD1	2:D:258:ASP:N	2.38	0.56
2:D:168:CYS:O	2:D:172:ILE:HG12	2.06	0.55
1:A:278:LEU:O	1:A:282:VAL:HG12	2.05	0.55
1:C:155:TRP:O	1:C:159:LEU:HG	2.05	0.55
1:C:201:LEU:O	1:C:205:VAL:HG22	2.07	0.55
1:A:128:LEU:O	1:A:132:ILE:HG12	2.06	0.55
1:A:246:THR:HB	2:D:233:THR:HG22	1.87	0.55
1:A:119:ARG:HG3	1:A:120:GLY:H	1.72	0.55
2:D:256:GLU:CD	2:D:256:GLU:H	2.14	0.55
1:A:196:LYS:HE2	1:A:242:ARG:HH12	1.72	0.55
2:D:129:GLU:HG2	2:D:182:LEU:HD11	1.89	0.55
1:A:200:MET:HB2	1:A:204:PHE:CZ	2.42	0.55
1:B:196:LYS:HD2	1:B:197:PRO:HD2	1.88	0.54
1:C:121:TRP:CG	1:C:122:ALA:H	2.26	0.54
1:A:232:LEU:O	1:A:236:ARG:HG3	2.07	0.54
1:C:284:LYS:O	1:C:287:PRO:HD2	2.08	0.54
1:C:338:LEU:HD21	2:D:271:LEU:HD11	1.89	0.54
1:B:232:LEU:O	1:B:236:ARG:HG3	2.07	0.54
1:A:144:THR:HB	2:D:262:THR:HG23	1.90	0.54
1:A:167:PHE:HE2	1:A:236:ARG:HD2	1.72	0.53
1:A:237:MET:HA	1:A:237:MET:HE2	1.89	0.53
2:D:912:LEU:HB3	2:D:916:PHE:HE1	1.73	0.53
1:C:272:LEU:HD23	1:C:273:ILE:HD13	1.90	0.53
1:C:125:TYR:OH	1:C:242:ARG:NH2	2.42	0.53
2:D:223:VAL:HG22	2:D:919:LYS:HE3	1.90	0.53
2:D:230:GLU:O	2:D:233:THR:OG1	2.27	0.53
1:A:155:TRP:O	1:A:159:LEU:HG	2.09	0.52
2:D:162:PHE:HA	2:D:165:LYS:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PRO:HA	1:B:200:MET:CE	2.38	0.52
1:C:139:LEU:HD11	1:C:155:TRP:HB3	1.91	0.52
2:D:136:PHE:CZ	2:D:206:ARG:HD3	2.44	0.52
2:D:262:THR:HG22	2:D:264:ALA:H	1.74	0.52
1:B:141:VAL:HG12	1:B:142:LEU:HD12	1.92	0.52
1:B:181:CYS:HA	1:B:185:LYS:HD2	1.92	0.52
1:A:196:LYS:HG2	1:A:242:ARG:HH22	1.75	0.52
1:A:334:ALA:HB1	1:B:311:LEU:HD21	1.91	0.52
1:B:134:LEU:O	1:B:138:ILE:HG12	2.09	0.52
1:B:147:GLU:OE2	1:B:147:GLU:N	2.35	0.52
2:D:96:ALA:O	2:D:100:LEU:HD22	2.10	0.52
2:D:167:PHE:HD1	2:D:209:ARG:HD2	1.74	0.52
1:A:309:TRP:CD1	1:A:322:LYS:HB2	2.45	0.51
1:B:197:PRO:HA	1:B:200:MET:HE1	1.92	0.51
1:C:182:CYS:SG	1:C:183:ARG:N	2.83	0.51
1:B:133:VAL:HA	1:B:136:CYS:SG	2.50	0.51
1:B:162:PHE:HA	1:B:165:PHE:CD2	2.45	0.51
1:C:162:PHE:HA	1:C:165:PHE:CD2	2.45	0.51
2:D:160:LEU:HD13	2:D:164:ARG:HH12	1.76	0.51
2:D:291:LEU:O	2:D:295:THR:HG23	2.11	0.51
1:B:233:GLN:O	1:B:237:MET:HE2	2.10	0.51
1:A:134:LEU:O	1:A:137:LEU:HD12	2.11	0.51
1:C:139:LEU:HD21	1:C:152:SER:O	2.11	0.51
2:D:257:ASN:HD21	2:D:259:HIS:CD2	2.28	0.51
1:A:334:ALA:O	1:A:338:LEU:HG	2.11	0.51
1:B:198:LEU:HD23	1:B:201:LEU:HD11	1.93	0.51
2:D:918:LEU:O	2:D:922:GLU:HG2	2.10	0.51
1:B:328:GLU:OE2	1:B:328:GLU:N	2.29	0.50
1:C:194:ALA:O	1:C:200:MET:HE2	2.11	0.50
2:D:101:LEU:HD21	2:D:132:THR:OG1	2.11	0.50
2:D:134:VAL:O	2:D:138:VAL:HG13	2.11	0.50
1:A:117:ARG:HB2	1:A:174:ARG:HH12	1.76	0.50
1:A:231:PHE:O	1:A:234:ILE:HG13	2.11	0.50
2:D:172:ILE:HA	2:D:175:LEU:HG	1.93	0.50
1:B:235:LEU:HD23	1:B:238:LEU:HD21	1.94	0.50
2:D:165:LYS:O	2:D:169:VAL:HG23	2.12	0.50
2:D:239:PHE:O	2:D:243:ILE:HG23	2.11	0.50
1:A:275:SER:O	1:A:279:VAL:HG23	2.12	0.49
1:C:316:THR:HG22	1:C:341:VAL:HG13	1.94	0.49
2:D:201:PHE:O	2:D:205:LEU:HG	2.12	0.49
1:A:167:PHE:CE2	1:A:236:ARG:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:O	1:C:142:LEU:HG	2.12	0.49
2:D:156:TRP:O	2:D:159:ARG:HG3	2.13	0.49
2:D:227:HIS:O	2:D:231:LEU:HD13	2.13	0.49
1:A:265:TRP:NE1	3:A:701:A1E7E:O1	2.46	0.49
1:B:201:LEU:HA	1:B:204:PHE:CD2	2.47	0.49
1:C:118:PRO:HA	1:C:242:ARG:HE	1.78	0.49
1:A:137:LEU:O	1:A:141:VAL:HG13	2.13	0.49
1:A:236:ARG:O	1:A:239:ARG:HB3	2.13	0.49
1:B:157:LEU:O	1:B:160:GLU:HG2	2.13	0.49
1:C:259:LYS:NZ	5:D:1203:YJ0:O72	2.46	0.48
1:C:278:LEU:O	1:C:282:VAL:HG12	2.14	0.48
1:A:358:LYS:O	1:A:361:GLU:HG3	2.14	0.48
1:B:239:ARG:O	1:B:239:ARG:HG2	2.14	0.48
1:C:121:TRP:CG	1:C:122:ALA:N	2.81	0.48
1:B:141:VAL:O	1:B:144:THR:HG22	2.14	0.48
1:C:197:PRO:HA	1:C:200:MET:HE3	1.95	0.48
1:C:284:LYS:HG2	1:C:285:ASP:H	1.78	0.48
2:D:139:GLU:HA	2:D:142:VAL:HG12	1.96	0.48
1:A:121:TRP:HE3	1:A:122:ALA:H	1.61	0.47
2:D:129:GLU:HA	2:D:132:THR:HG22	1.96	0.47
1:A:197:PRO:O	1:A:200:MET:HG2	2.14	0.47
1:A:241:ASP:OD2	1:A:246:THR:HG23	2.14	0.47
1:B:138:ILE:O	1:B:142:LEU:HD13	2.14	0.47
1:B:167:PHE:HZ	1:B:236:ARG:HH11	1.61	0.47
1:A:201:LEU:O	1:A:205:VAL:HG22	2.14	0.47
1:B:201:LEU:O	1:B:205:VAL:HG22	2.13	0.47
1:B:269:PHE:O	1:B:273:ILE:HG22	2.14	0.47
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.63	0.47
1:B:233:GLN:HA	1:B:236:ARG:HE	1.79	0.47
1:B:298:GLU:OE1	1:B:298:GLU:N	2.47	0.47
1:C:334:ALA:HB1	2:D:271:LEU:HD21	1.96	0.47
2:D:112:SER:O	2:D:115:LYS:NZ	2.48	0.47
1:B:296:MET:HE1	1:B:299:GLU:HG3	1.97	0.47
1:A:162:PHE:O	1:A:166:ILE:HG22	2.14	0.47
1:A:290:ASP:HB3	1:A:294:GLU:H	1.79	0.47
1:C:183:ARG:NH2	1:C:184:TYR:OH	2.48	0.47
1:A:235:LEU:O	1:A:238:LEU:HG	2.15	0.47
1:C:236:ARG:O	1:C:239:ARG:HB3	2.15	0.47
1:C:307:LEU:HD23	1:C:307:LEU:HA	1.76	0.46
1:B:265:TRP:NE1	3:B:701:A1E7E:O1	2.46	0.46
2:D:201:PHE:O	2:D:204:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HD2	1:A:242:ARG:HA	1.73	0.46
1:B:110:LEU:HD11	1:B:176:TRP:HE1	1.81	0.46
1:C:232:LEU:HG	1:C:233:GLN:OE1	2.15	0.46
1:B:236:ARG:NH2	1:B:237:MET:HE1	2.31	0.46
1:B:316:THR:HG22	1:B:341:VAL:HG13	1.98	0.46
1:B:117:ARG:CZ	1:B:125:TYR:HB3	2.46	0.46
2:D:174:VAL:HG22	2:D:202:LEU:HD11	1.97	0.46
1:A:112:TYR:O	1:A:116:GLU:HG2	2.16	0.46
1:C:194:ALA:HA	1:C:199:CYS:SG	2.55	0.46
1:A:284:LYS:O	1:A:287:PRO:HD2	2.16	0.46
1:C:284:LYS:HG2	1:C:285:ASP:N	2.31	0.46
2:D:231:LEU:HB3	2:D:235:TRP:CZ2	2.51	0.46
1:A:131:LEU:O	1:A:134:LEU:HD12	2.16	0.46
1:C:134:LEU:HD12	1:C:135:GLY:N	2.32	0.45
1:C:163:ALA:HA	1:C:166:ILE:HG22	1.99	0.45
1:B:236:ARG:HH21	1:B:237:MET:HE1	1.81	0.45
1:C:140:ALA:O	1:C:230:ARG:NH2	2.32	0.45
1:B:160:GLU:O	1:B:164:ILE:HG13	2.16	0.45
1:C:153:GLY:O	1:C:157:LEU:HG	2.17	0.45
1:B:133:VAL:HB	1:B:237:MET:SD	2.56	0.45
1:B:275:SER:O	1:B:279:VAL:HG13	2.16	0.45
1:C:160:GLU:O	1:C:164:ILE:HG13	2.16	0.45
2:D:76:LEU:HD12	2:D:77:GLN:N	2.31	0.45
2:D:156:TRP:HA	2:D:159:ARG:HE	1.82	0.45
1:C:162:PHE:HA	1:C:165:PHE:HD2	1.82	0.45
2:D:209:ARG:NH1	2:D:209:ARG:HB3	2.31	0.45
1:A:234:ILE:HG22	2:D:243:ILE:HD12	1.99	0.45
4:D:1202:9PE:H2DA	4:D:1202:9PE:H2G	1.71	0.45
1:A:356:ALA:O	1:A:359:VAL:HG12	2.17	0.45
1:A:144:THR:O	1:A:146:LYS:NZ	2.38	0.44
1:A:185:LYS:HG2	1:A:186:GLY:N	2.32	0.44
1:B:147:GLU:H	1:B:147:GLU:CD	2.25	0.44
1:C:110:LEU:HD11	1:C:176:TRP:NE1	2.32	0.44
2:D:203:GLN:HA	2:D:206:ARG:HB3	1.99	0.44
1:A:331:LEU:O	1:A:335:THR:HG23	2.17	0.44
2:D:206:ARG:HH21	2:D:209:ARG:HB2	1.82	0.44
1:B:331:LEU:O	1:B:335:THR:HG23	2.17	0.44
2:D:250:TYR:OH	2:D:254:LYS:NZ	2.32	0.44
1:C:174:ARG:O	1:C:178:ALA:HB2	2.17	0.44
1:A:194:ALA:O	1:A:200:MET:HE2	2.17	0.44
1:B:284:LYS:O	1:B:287:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:O	1:C:238:LEU:HG	2.17	0.44
1:B:192:LYS:HA	1:B:192:LYS:HD3	1.88	0.44
1:C:269:PHE:CD1	1:C:269:PHE:C	2.95	0.44
4:D:1202:9PE:H2CA	4:D:1202:9PE:H29	1.86	0.44
1:B:110:LEU:HD23	1:B:111:ILE:HG13	2.00	0.43
1:B:163:ALA:HB1	1:B:167:PHE:CZ	2.53	0.43
1:B:137:LEU:HD23	1:B:138:ILE:HD13	2.01	0.43
1:B:280:TYR:CD2	1:B:281:LEU:HD23	2.53	0.43
1:C:131:LEU:HA	1:C:134:LEU:HG	2.00	0.43
1:B:175:ILE:HD12	1:B:193:PHE:HD2	1.83	0.43
1:B:174:ARG:O	1:B:178:ALA:HB2	2.18	0.43
1:B:198:LEU:HA	1:B:201:LEU:HG	2.01	0.43
1:B:162:PHE:HA	1:B:165:PHE:HD2	1.84	0.43
2:D:210:MET:HE2	2:D:210:MET:HA	2.00	0.43
1:A:158:LEU:O	1:A:161:THR:OG1	2.25	0.43
1:C:260:GLU:HG2	2:D:916:PHE:HD2	1.84	0.43
1:C:110:LEU:HD11	1:C:176:TRP:HE1	1.84	0.43
2:D:98:VAL:O	2:D:102:VAL:HG22	2.19	0.43
1:A:233:GLN:HA	1:A:236:ARG:NE	2.21	0.43
2:D:230:GLU:N	2:D:230:GLU:OE1	2.51	0.43
1:A:357:LEU:HD11	1:B:360:GLN:HG3	2.00	0.43
1:B:125:TYR:O	1:B:129:VAL:HG12	2.19	0.43
2:D:156:TRP:O	2:D:160:LEU:HG	2.18	0.43
1:A:149:GLU:OE1	1:A:149:GLU:N	2.50	0.42
1:A:263:THR:HG22	1:B:246:THR:HG22	2.01	0.42
1:B:110:LEU:HD11	1:B:176:TRP:NE1	2.34	0.42
2:D:177:ALA:O	2:D:181:VAL:HG12	2.18	0.42
1:C:159:LEU:HA	1:C:162:PHE:HD2	1.84	0.42
1:A:192:LYS:O	1:A:195:ARG:HB3	2.18	0.42
1:B:351:LEU:O	1:B:355:LEU:HG	2.20	0.42
2:D:172:ILE:O	2:D:176:ILE:HG12	2.20	0.42
1:A:142:LEU:HA	1:A:145:PHE:HE2	1.85	0.42
1:A:203:ILE:HD12	1:A:206:LEU:HD21	2.00	0.42
1:A:346:LEU:HA	1:A:346:LEU:HD12	1.80	0.42
1:C:263:THR:OG1	2:D:216:THR:HG22	2.19	0.42
2:D:79:PHE:CD2	2:D:80:LEU:HD23	2.55	0.42
1:C:159:LEU:HA	1:C:162:PHE:CD2	2.54	0.42
1:C:167:PHE:HA	1:C:170:GLU:CD	2.45	0.42
2:D:211:ASP:OD1	2:D:211:ASP:C	2.62	0.42
2:D:251:LEU:HD23	2:D:251:LEU:HA	1.84	0.42
2:D:287:TRP:CE3	2:D:287:TRP:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:OE2	1:B:294:GLU:HA	2.19	0.42
2:D:166:PRO:O	2:D:170:ILE:HG13	2.19	0.42
2:D:286:THR:OG1	2:D:287:TRP:N	2.53	0.42
1:A:323:THR:HA	1:A:324:PRO:HD3	1.95	0.41
1:C:110:LEU:HD23	1:C:111:ILE:HG13	2.01	0.41
1:C:239:ARG:O	1:C:239:ARG:NH1	2.36	0.41
2:D:127:ILE:O	2:D:131:VAL:HG23	2.20	0.41
2:D:199:LEU:HG	2:D:203:GLN:HE22	1.85	0.41
2:D:281:ASP:OD1	2:D:282:LYS:N	2.52	0.41
1:C:240:MET:SD	1:C:240:MET:N	2.93	0.41
2:D:74:ARG:H	2:D:74:ARG:HG2	1.72	0.41
2:D:87:PRO:HB2	2:D:92:PHE:HE1	1.84	0.41
2:D:128:LEU:O	2:D:132:THR:HG22	2.19	0.41
2:D:286:THR:O	2:D:290:ARG:HG3	2.20	0.41
1:C:125:TYR:O	1:C:129:VAL:HG12	2.20	0.41
2:D:243:ILE:HG13	2:D:244:LEU:N	2.33	0.41
2:D:918:LEU:HD23	2:D:918:LEU:HA	1.87	0.41
1:A:110:LEU:HD11	1:A:176:TRP:HE1	1.85	0.41
1:A:196:LYS:HD2	1:A:197:PRO:CD	2.49	0.41
1:A:285:ASP:OD1	1:A:285:ASP:C	2.63	0.41
1:B:142:LEU:HA	1:B:145:PHE:CD2	2.54	0.41
1:B:200:MET:O	1:B:203:ILE:HG12	2.20	0.41
1:B:277:PHE:HE1	1:B:281:LEU:HD11	1.85	0.41
1:C:350:ILE:HG13	2:D:913:GLY:HA2	2.02	0.41
2:D:144:ILE:HD13	2:D:144:ILE:HA	1.88	0.41
1:A:310:GLY:O	1:A:314:LEU:HB2	2.20	0.41
1:B:125:TYR:O	1:B:128:LEU:HG	2.21	0.41
1:B:154:ASP:OD1	1:B:155:TRP:HD1	2.04	0.41
1:C:130:PHE:CE1	1:C:134:LEU:HD23	2.56	0.41
1:C:133:VAL:HG12	1:C:237:MET:HE1	2.03	0.41
1:C:167:PHE:O	1:C:170:GLU:HG2	2.21	0.41
1:C:265:TRP:NE1	3:C:701:A1E7E:O1	2.42	0.41
1:C:290:ASP:HB3	1:C:294:GLU:N	2.35	0.41
1:C:331:LEU:O	1:C:335:THR:HG23	2.21	0.41
2:D:912:LEU:O	2:D:916:PHE:CD1	2.74	0.41
1:A:275:SER:OG	1:A:336:PHE:HB3	2.20	0.41
1:A:179:GLY:HA2	1:A:184:TYR:HB2	2.04	0.40
1:A:359:VAL:HG11	2:D:227:HIS:CD2	2.55	0.40
1:B:229:LEU:HB3	1:B:230:ARG:H	1.76	0.40
1:C:118:PRO:HA	1:C:242:ARG:HH21	1.86	0.40
1:C:196:LYS:O	1:C:197:PRO:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:ILE:O	2:D:208:ILE:HG13	2.21	0.40
2:D:912:LEU:O	2:D:916:PHE:HD1	2.04	0.40
2:D:912:LEU:HD23	2:D:912:LEU:HA	1.90	0.40
1:A:277:PHE:CE1	1:B:230:ARG:HB2	2.55	0.40
2:D:136:PHE:HA	2:D:139:GLU:OE2	2.21	0.40
2:D:150:CYS:O	2:D:153:TYR:N	2.53	0.40
1:A:139:LEU:HA	1:A:142:LEU:HB3	2.04	0.40
1:C:192:LYS:O	1:C:195:ARG:HG2	2.22	0.40
1:A:197:PRO:CA	1:A:200:MET:HE3	2.48	0.40
1:B:257:HIS:O	1:B:261:LEU:HG	2.21	0.40
1:B:362:GLN:O	1:B:365:GLN:HB3	2.22	0.40
1:C:298:GLU:CD	1:C:300:PHE:H	2.28	0.40
2:D:86:ARG:HH21	2:D:212:ARG:HH22	1.68	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	235/620 (38%)	213 (91%)	22 (9%)	0	100	100
1	B	235/620 (38%)	212 (90%)	22 (9%)	1 (0%)	30	65
1	C	235/620 (38%)	215 (92%)	20 (8%)	0	100	100
2	D	243/753 (32%)	227 (93%)	16 (7%)	0	100	100
All	All	948/2613 (36%)	867 (92%)	80 (8%)	1 (0%)	49	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	MET

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	196/533 (37%)	195 (100%)	1 (0%)	81	82
1	B	196/533 (37%)	196 (100%)	0	100	100
1	C	196/533 (37%)	195 (100%)	1 (0%)	81	82
2	D	206/635 (32%)	203 (98%)	3 (2%)	57	71
All	All	794/2234 (36%)	789 (99%)	5 (1%)	76	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	ASP
1	C	273	ILE
2	D	100	LEU
2	D	101	LEU
2	D	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	362	GLN
2	D	259	HIS

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](#)

6 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
5	YJ0	D	1203	-	90,90,90	0.26	0	136,138,138	0.77	5 (3%)
3	A1E7E	C	701	-	26,28,28	3.28	10 (38%)	33,40,40	7.31	6 (18%)
4	9PE	D	1202	-	39,39,39	0.98	4 (10%)	42,44,44	0.96	2 (4%)
3	A1E7E	B	701	-	26,28,28	3.27	10 (38%)	33,40,40	7.31	6 (18%)
3	A1E7E	D	1201	-	26,28,28	3.27	9 (34%)	33,40,40	7.31	5 (15%)
3	A1E7E	A	701	-	26,28,28	3.27	9 (34%)	33,40,40	7.31	8 (24%)

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
5	YJ0	D	1203	-	10/10/33/34	12/32/200/200	1/10/10/10
3	A1E7E	C	701	-	-	8/14/17/17	0/4/4/4
4	9PE	D	1202	-	-	21/43/43/43	-
3	A1E7E	B	701	-	-	7/14/17/17	0/4/4/4
3	A1E7E	D	1201	-	-	8/14/17/17	0/4/4/4
3	A1E7E	A	701	-	-	7/14/17/17	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	A1E7E	C19-C20	12.28	1.54	1.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	A1E7E	C19-C20	12.27	1.54	1.18
3	D	1201	A1E7E	C19-C20	12.27	1.54	1.18
3	A	701	A1E7E	C19-C20	12.27	1.54	1.18
3	A	701	A1E7E	C18-C19	6.45	1.55	1.47
3	C	701	A1E7E	C18-C19	6.40	1.55	1.47
3	B	701	A1E7E	C18-C19	6.36	1.55	1.47
3	D	1201	A1E7E	C18-C19	6.35	1.55	1.47
3	C	701	A1E7E	C7-N1	5.07	1.46	1.37
3	B	701	A1E7E	C7-N1	5.05	1.46	1.37
3	A	701	A1E7E	C7-N1	5.01	1.46	1.37
3	D	1201	A1E7E	C7-N1	5.00	1.46	1.37
3	C	701	A1E7E	C15-C14	-3.28	1.39	1.50
3	B	701	A1E7E	C15-C14	-3.28	1.39	1.50
3	D	1201	A1E7E	C15-C14	-3.27	1.39	1.50
3	B	701	A1E7E	C16-C14	-3.25	1.39	1.50
3	C	701	A1E7E	C16-C14	-3.25	1.39	1.50
3	D	1201	A1E7E	C16-C14	-3.25	1.39	1.50
3	A	701	A1E7E	C16-C14	-3.25	1.39	1.50
3	A	701	A1E7E	C15-C14	-3.24	1.39	1.50
3	C	701	A1E7E	C8-N1	2.84	1.47	1.39
3	A	701	A1E7E	C8-N1	2.82	1.46	1.39
3	B	701	A1E7E	C8-N1	2.78	1.46	1.39
3	D	1201	A1E7E	C8-N1	2.75	1.46	1.39
3	D	1201	A1E7E	C16-C15	-2.50	1.39	1.48
4	D	1202	9PE	O21-C2	-2.49	1.40	1.46
3	C	701	A1E7E	C16-C15	-2.48	1.39	1.48
3	A	701	A1E7E	C16-C15	-2.47	1.39	1.48
4	D	1202	9PE	O31-C31	2.46	1.40	1.33
3	B	701	A1E7E	C16-C15	-2.45	1.39	1.48
4	D	1202	9PE	O21-C21	2.22	1.40	1.34
3	B	701	A1E7E	C17-C13	2.21	1.43	1.40
3	A	701	A1E7E	O1-C7	-2.17	1.18	1.23
3	D	1201	A1E7E	C17-C13	2.14	1.43	1.40
3	C	701	A1E7E	C17-C13	2.12	1.43	1.40
4	D	1202	9PE	O31-C3	-2.11	1.40	1.45
3	C	701	A1E7E	O1-C7	-2.11	1.19	1.23
3	A	701	A1E7E	C17-C13	2.08	1.43	1.40
3	D	1201	A1E7E	O1-C7	-2.08	1.19	1.23
3	C	701	A1E7E	C6-C7	2.07	1.54	1.50
3	B	701	A1E7E	O1-C7	-2.05	1.19	1.23
3	B	701	A1E7E	C6-C7	2.03	1.54	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1201	A1E7E	C18-C19-C20	-38.96	112.30	177.67
3	C	701	A1E7E	C18-C19-C20	-38.94	112.34	177.67
3	B	701	A1E7E	C18-C19-C20	-38.90	112.41	177.67
3	A	701	A1E7E	C18-C19-C20	-38.86	112.47	177.67
3	C	701	A1E7E	C16-C14-C13	10.01	150.22	120.68
3	A	701	A1E7E	C16-C14-C13	10.00	150.19	120.68
3	D	1201	A1E7E	C16-C14-C13	9.97	150.11	120.68
3	B	701	A1E7E	C16-C14-C13	9.97	150.09	120.68
3	D	1201	A1E7E	C15-C14-C13	9.89	149.85	120.68
3	B	701	A1E7E	C15-C14-C13	9.86	149.77	120.68
3	A	701	A1E7E	C15-C14-C13	9.84	149.73	120.68
3	C	701	A1E7E	C15-C14-C13	9.83	149.69	120.68
4	D	1202	9PE	O21-C21-C22	3.91	119.93	111.50
5	D	1203	YJ0	C20-C15-C16	3.76	118.37	112.73
3	B	701	A1E7E	C17-N3-N2	-3.19	110.35	111.72
3	A	701	A1E7E	C17-N3-N2	-3.07	110.40	111.72
3	D	1201	A1E7E	C17-N3-N2	-3.02	110.42	111.72
3	C	701	A1E7E	C17-N3-N2	-2.91	110.47	111.72
3	A	701	A1E7E	C6-C7-N1	2.77	120.38	116.24
4	D	1202	9PE	O31-C31-C32	2.59	120.02	111.91
3	B	701	A1E7E	N1-C8-N2	2.39	128.16	123.58
3	A	701	A1E7E	N1-C8-N2	2.33	128.03	123.58
5	D	1203	YJ0	C15-C20-C19	2.27	113.22	109.65
3	B	701	A1E7E	C12-C13-C17	2.20	120.38	117.62
5	D	1203	YJ0	C13-C12-C11	2.17	110.64	107.27
3	C	701	A1E7E	C12-C13-C17	2.17	120.33	117.62
5	D	1203	YJ0	C5-C6-C7	-2.16	99.86	103.37
3	D	1201	A1E7E	C6-C7-N1	2.14	119.43	116.24
3	C	701	A1E7E	C6-C7-N1	2.11	119.39	116.24
3	A	701	A1E7E	C12-C13-C17	2.04	120.18	117.62
5	D	1203	YJ0	C12-C11-C16	2.03	117.39	114.38
3	A	701	A1E7E	C18-N3-C17	-2.02	126.81	129.19

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	1203	YJ0	C57
5	D	1203	YJ0	C11
5	D	1203	YJ0	C16
5	D	1203	YJ0	C59
5	D	1203	YJ0	C5
5	D	1203	YJ0	C6
5	D	1203	YJ0	C12

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Mol	Chain	Res	Type	Atom
5	D	1203	YJ0	C64
5	D	1203	YJ0	C56
5	D	1203	YJ0	C32

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	A1E7E	C9-C8-N1-C7
3	B	701	A1E7E	N2-C8-N1-C7
3	C	701	A1E7E	C9-C8-N1-C7
3	C	701	A1E7E	N2-C8-N1-C7
3	C	701	A1E7E	C17-C13-C14-C16
3	D	1201	A1E7E	C9-C8-N1-C7
4	D	1202	9PE	C1-O11-P-O12
4	D	1202	9PE	C1-O11-P-O13
4	D	1202	9PE	C1-O11-P-O14
5	D	1203	YJ0	C29-C28-C53-O54
5	D	1203	YJ0	C28-C53-O54-C55
3	D	1201	A1E7E	C5-C6-C7-O1
3	D	1201	A1E7E	C3-C6-C7-O1
3	C	701	A1E7E	C5-C6-C7-O1
3	C	701	A1E7E	C3-C6-C7-N1
3	C	701	A1E7E	C3-C6-C7-O1
3	D	1201	A1E7E	C5-C6-C7-N1
4	D	1202	9PE	O32-C31-O31-C3
3	B	701	A1E7E	C5-C6-C7-O1
3	C	701	A1E7E	C5-C6-C7-N1
3	D	1201	A1E7E	C3-C6-C7-N1
3	B	701	A1E7E	C5-C6-C7-N1
3	B	701	A1E7E	C3-C6-C7-N1
3	B	701	A1E7E	C3-C6-C7-O1
4	D	1202	9PE	C32-C31-O31-C3
4	D	1202	9PE	C2B-C2C-C2D-C2E
3	A	701	A1E7E	C5-C6-C7-N1
3	A	701	A1E7E	C5-C6-C7-O1
4	D	1202	9PE	C31-C32-C33-C34
4	D	1202	9PE	C21-C22-C23-C24
3	A	701	A1E7E	C3-C6-C7-N1
3	A	701	A1E7E	C3-C6-C7-O1
4	D	1202	9PE	C2D-C2E-C2F-C2G
4	D	1202	9PE	C29-C2A-C2B-C2C
4	D	1202	9PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	D	1202	9PE	C28-C29-C2A-C2B
5	D	1203	YJ0	C26-C27-C28-C53
5	D	1203	YJ0	O1-C9-O39-C34
5	D	1203	YJ0	O60-C59-C61-O62
5	D	1203	YJ0	C25-C9-O39-C34
4	D	1202	9PE	C2F-C2G-C2H-C2I
5	D	1203	YJ0	O36-C35-C37-O38
5	D	1203	YJ0	O1-C38-C39-O2
4	D	1202	9PE	C2C-C2D-C2E-C2F
4	D	1202	9PE	C32-C33-C34-C35
5	D	1203	YJ0	C27-C28-C53-O54
4	D	1202	9PE	C11-O13-P-O14
3	C	701	A1E7E	C12-C13-C14-C16
5	D	1203	YJ0	C57-C58-O63-C64
3	D	1201	A1E7E	N2-C8-N1-C7
3	A	701	A1E7E	C17-C13-C14-C15
3	A	701	A1E7E	C17-C13-C14-C16
3	B	701	A1E7E	C17-C13-C14-C15
3	D	1201	A1E7E	C17-C13-C14-C15
3	D	1201	A1E7E	C17-C13-C14-C16
5	D	1203	YJ0	C59-C58-O63-C64
4	D	1202	9PE	C33-C34-C35-C36
4	D	1202	9PE	C23-C24-C25-C26
4	D	1202	9PE	C24-C25-C26-C27
5	D	1203	YJ0	C24-C23-O25-C26
4	D	1202	9PE	O21-C21-C22-C23
3	A	701	A1E7E	N2-C8-N1-C7
4	D	1202	9PE	O22-C21-C22-C23

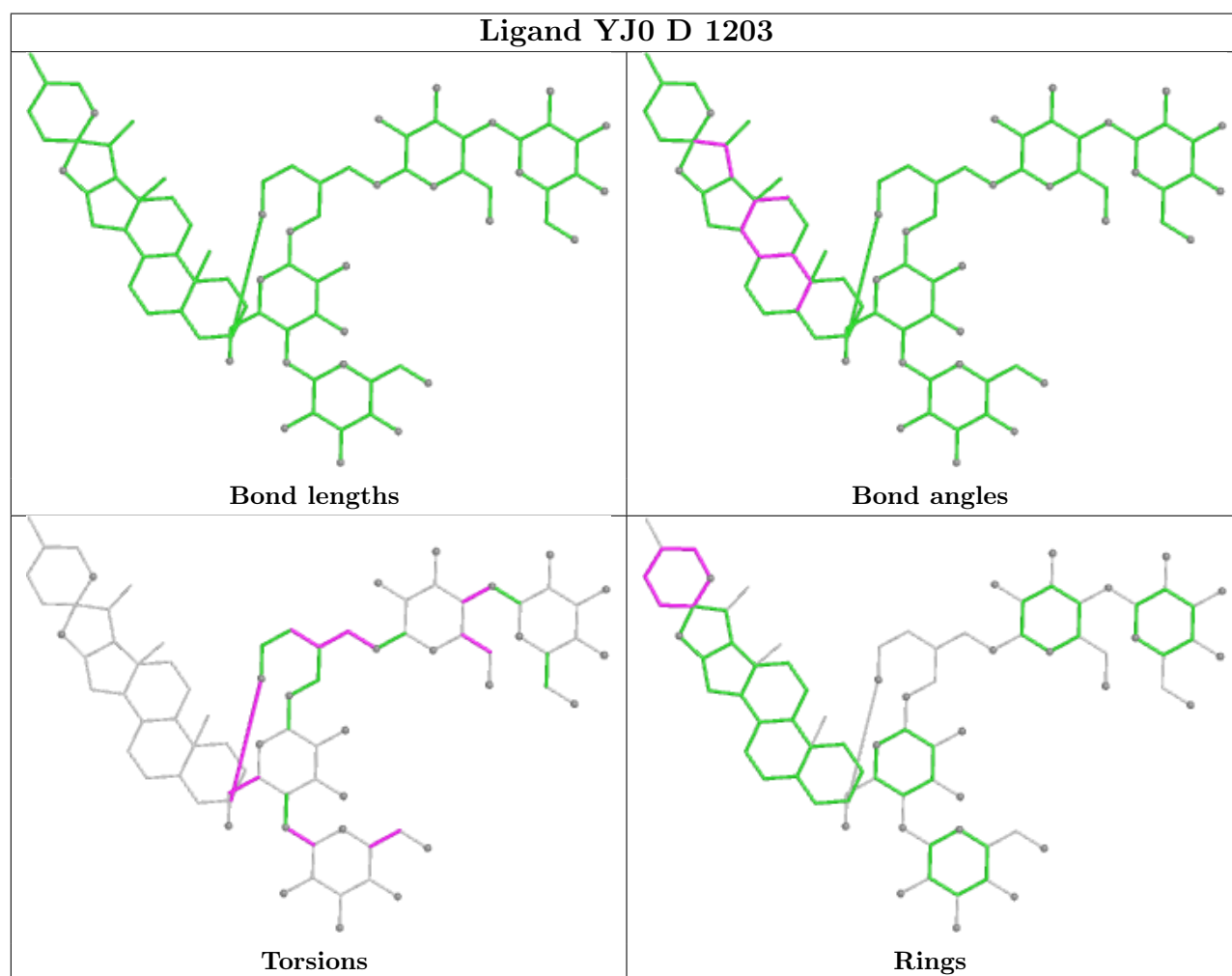
All (1) ring outliers are listed below:

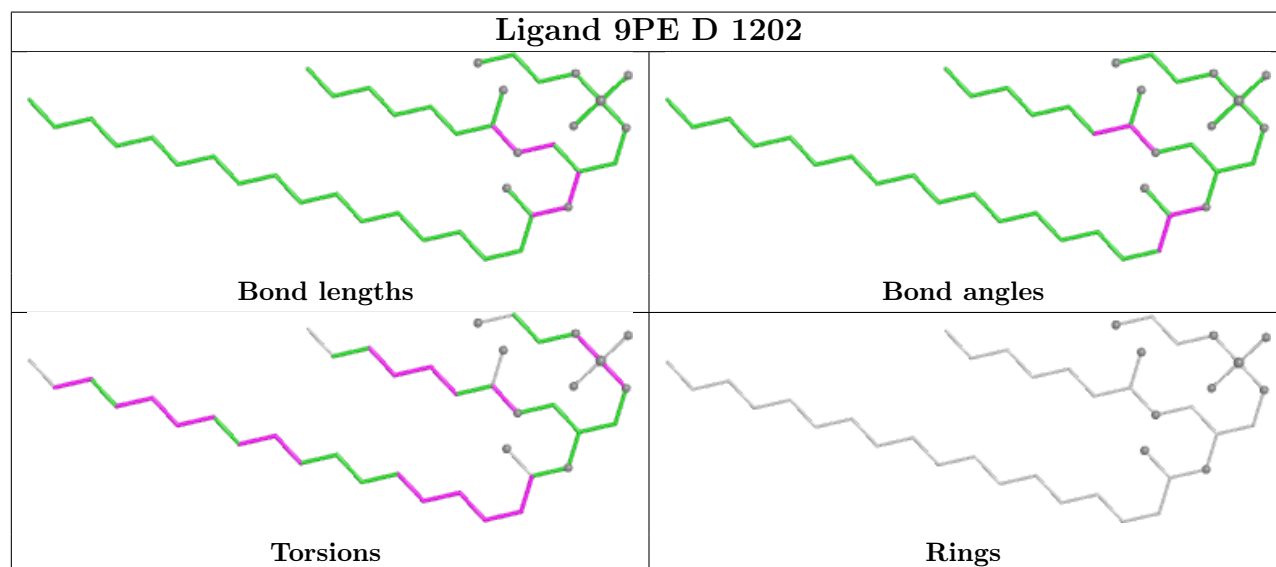
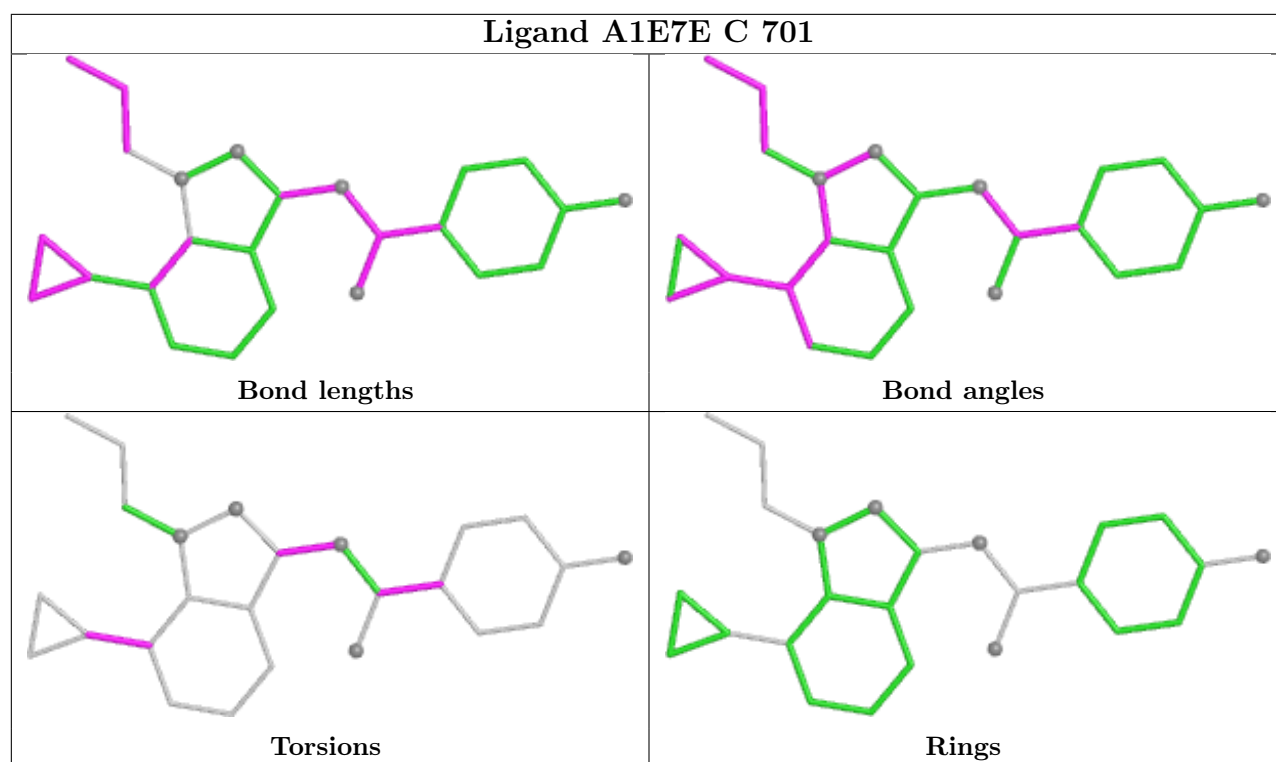
Mol	Chain	Res	Type	Atoms
5	D	1203	YJ0	C2-C3-C4-C5-C81-O80

5 monomers are involved in 7 short contacts:

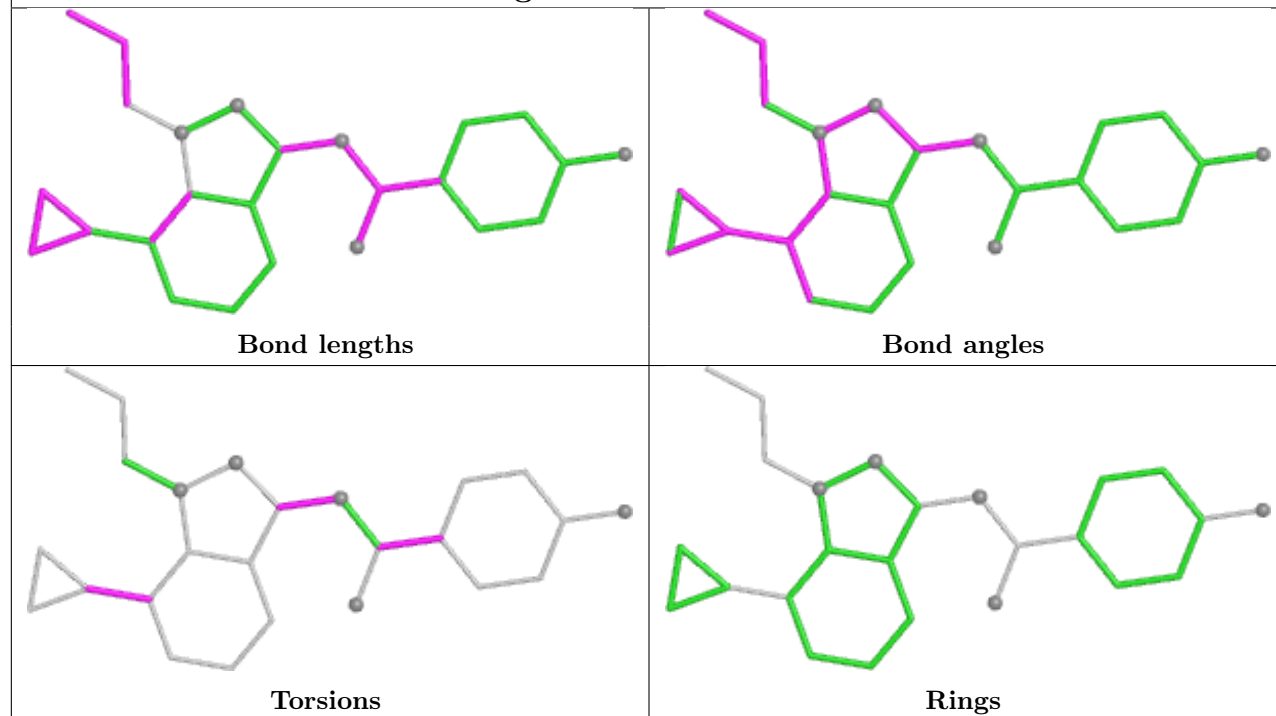
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1203	YJ0	2	0
3	C	701	A1E7E	1	0
4	D	1202	9PE	2	0
3	B	701	A1E7E	1	0
3	A	701	A1E7E	1	0

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.

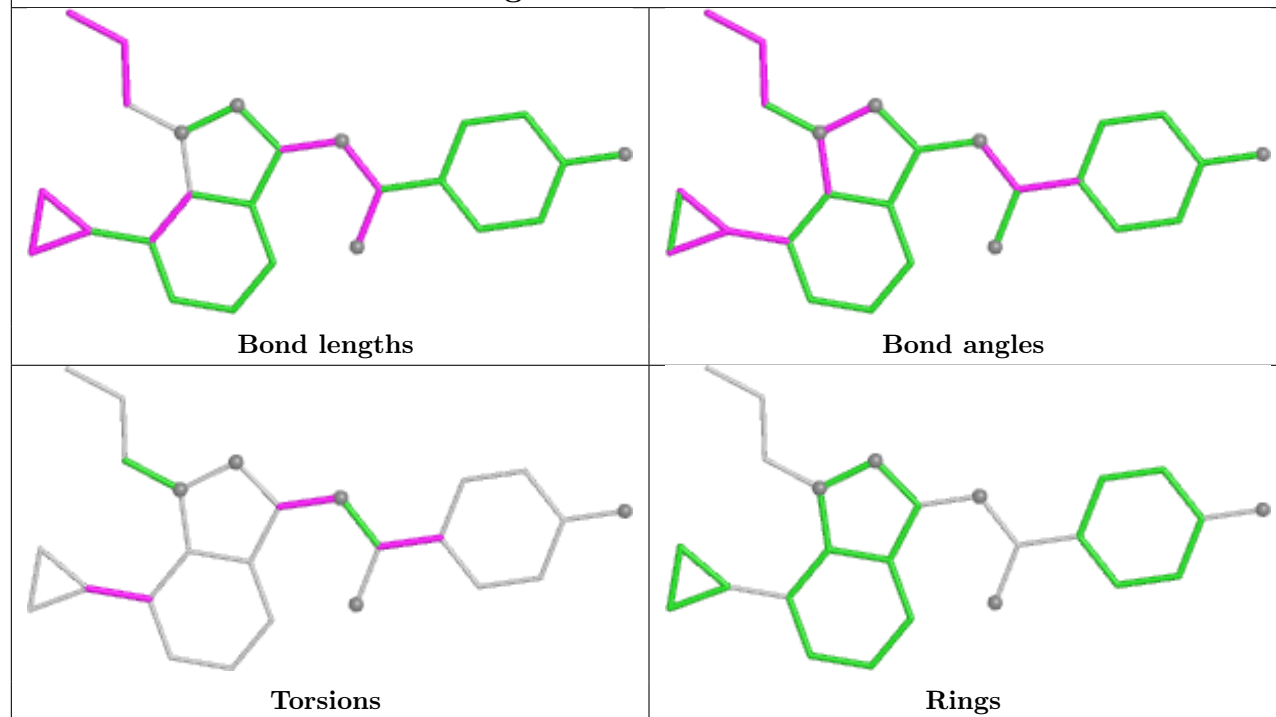


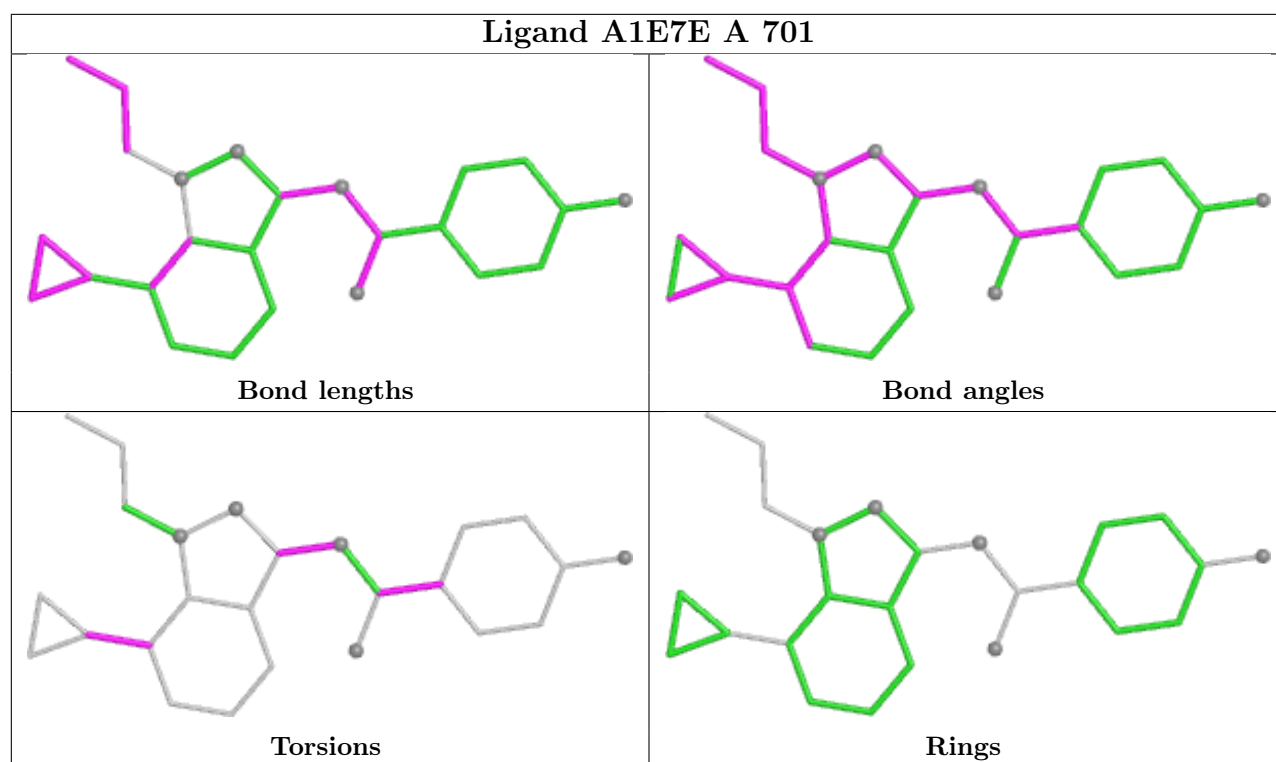


Ligand A1E7E B 701



Ligand A1E7E D 1201





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.

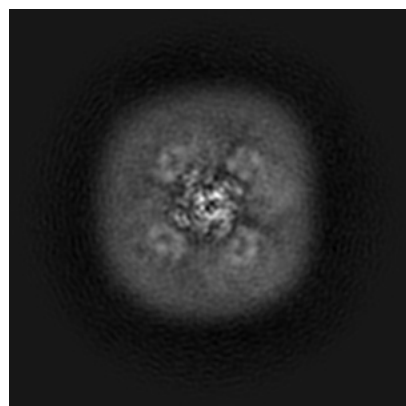
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69854. These allow visual inspection of the internal detail of the map and identification of artifacts.

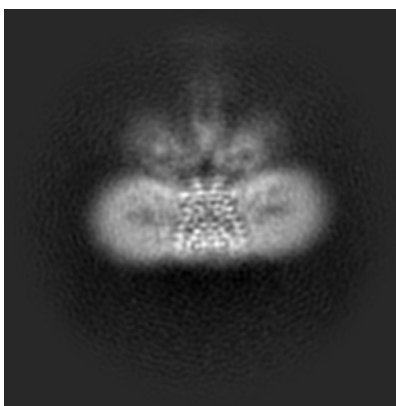
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

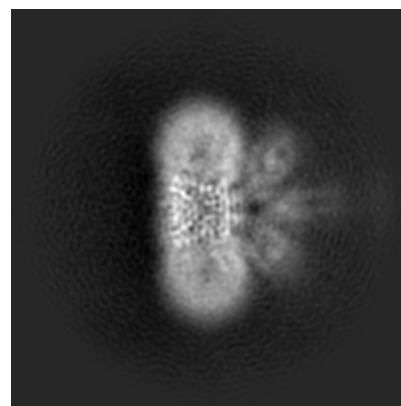
6.1.1 Primary map



X

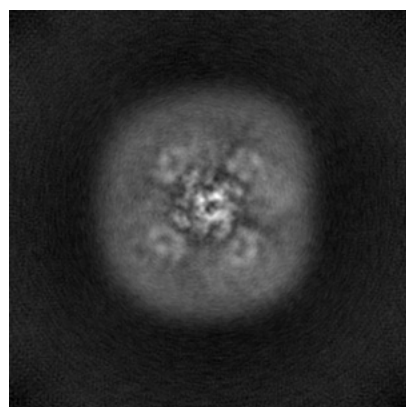


Y

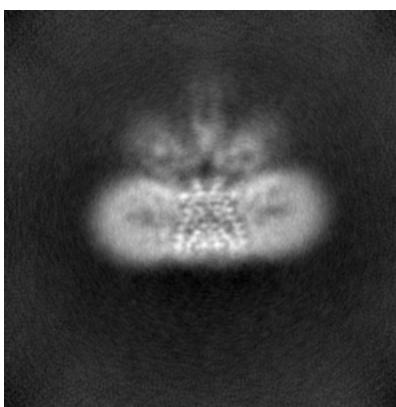


Z

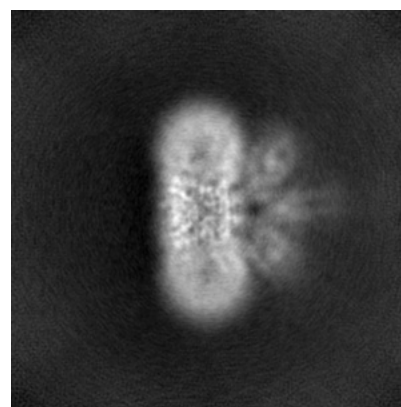
6.1.2 Raw map



X



Y

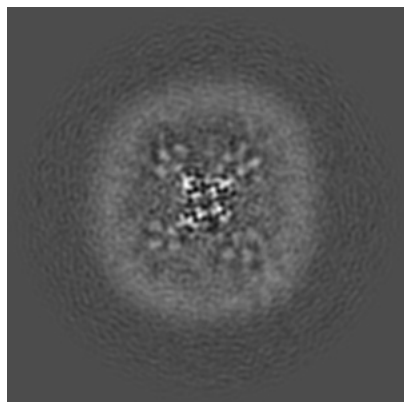


Z

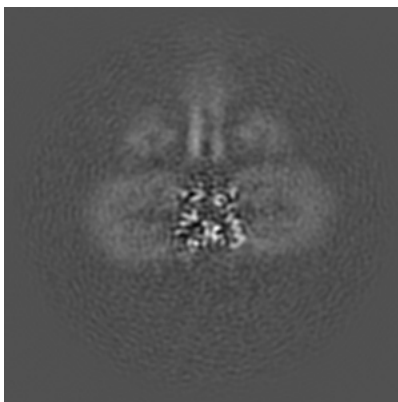
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

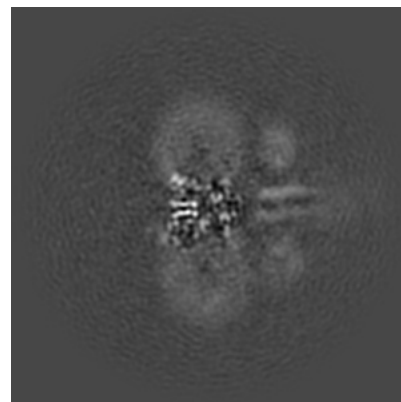
6.2.1 Primary map



X Index: 120

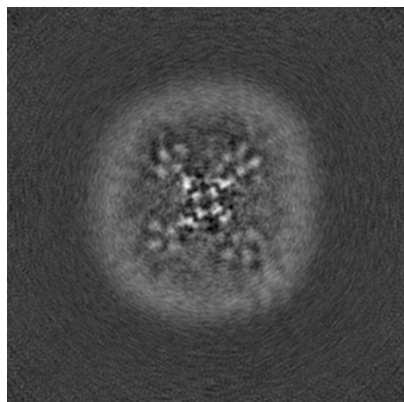


Y Index: 120

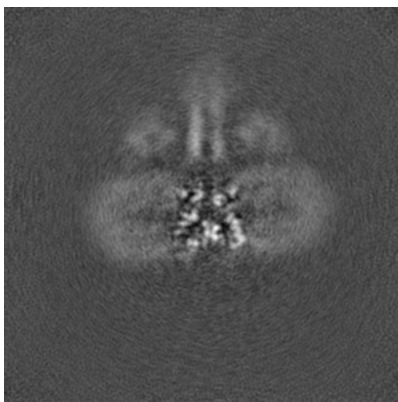


Z Index: 120

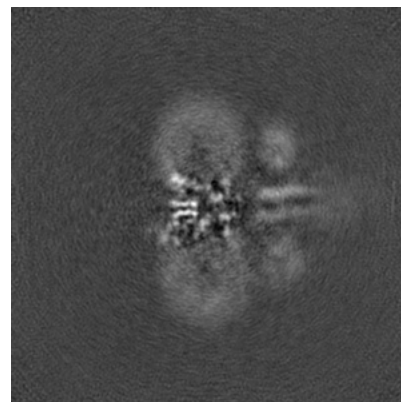
6.2.2 Raw map



X Index: 120



Y Index: 120

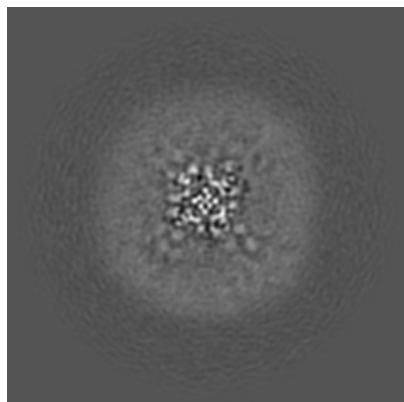


Z Index: 120

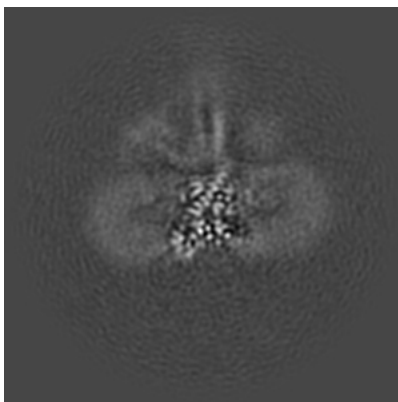
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

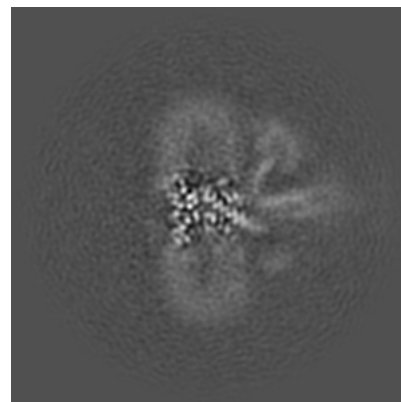
6.3.1 Primary map



X Index: 102

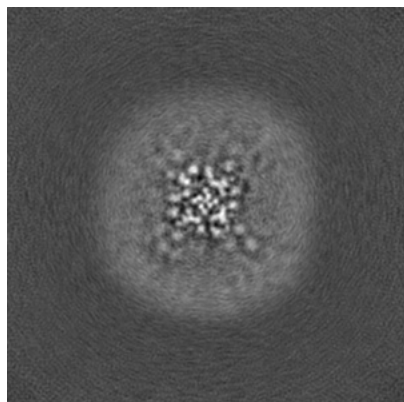


Y Index: 124

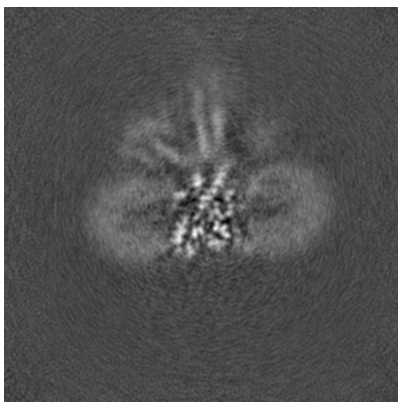


Z Index: 127

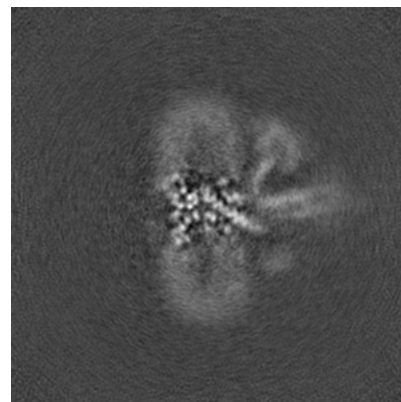
6.3.2 Raw map



X Index: 102



Y Index: 126

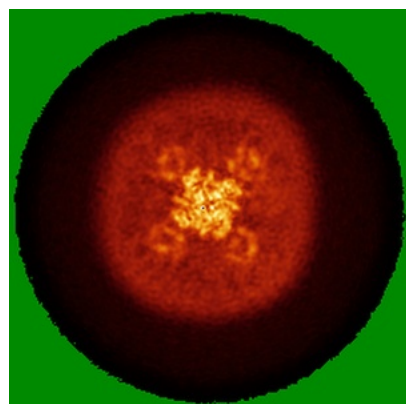


Z Index: 127

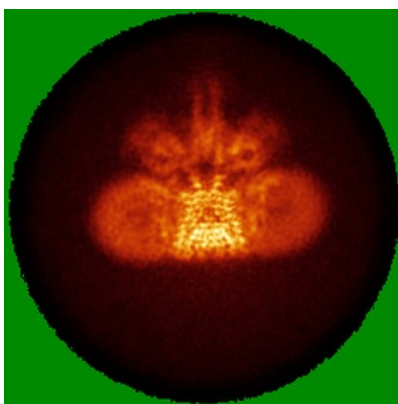
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

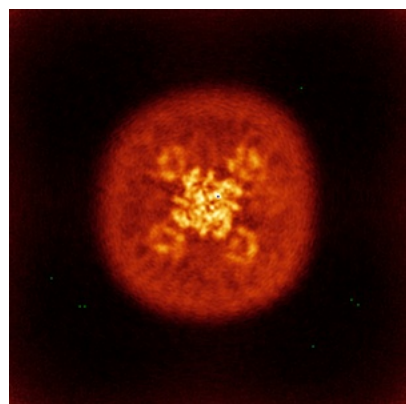


Y

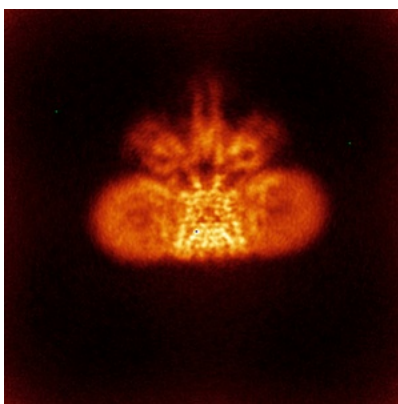


Z

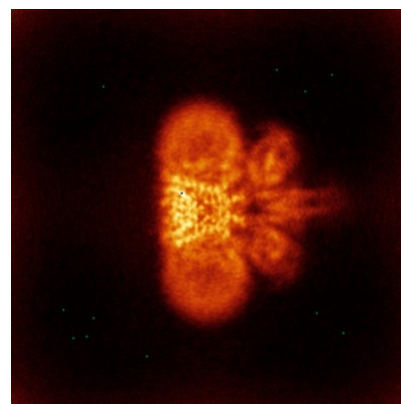
6.4.2 Raw map



X



Y

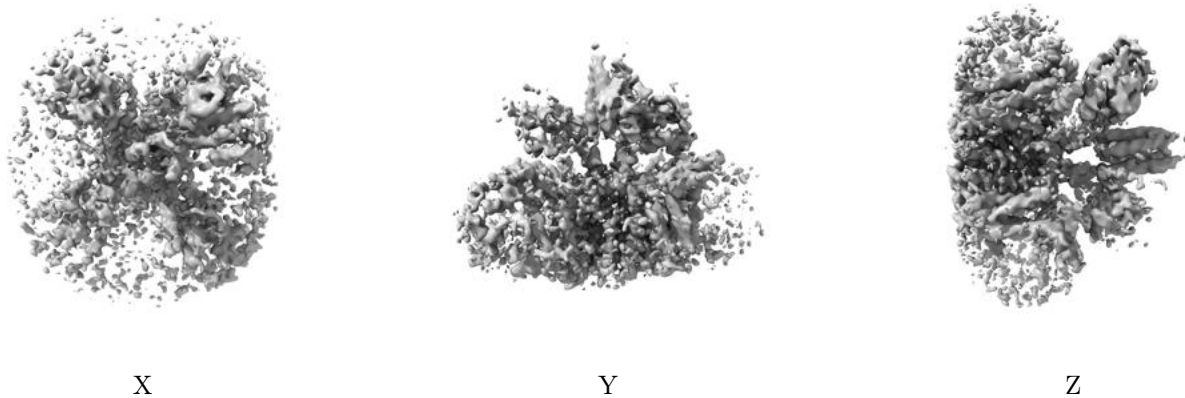


Z

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.

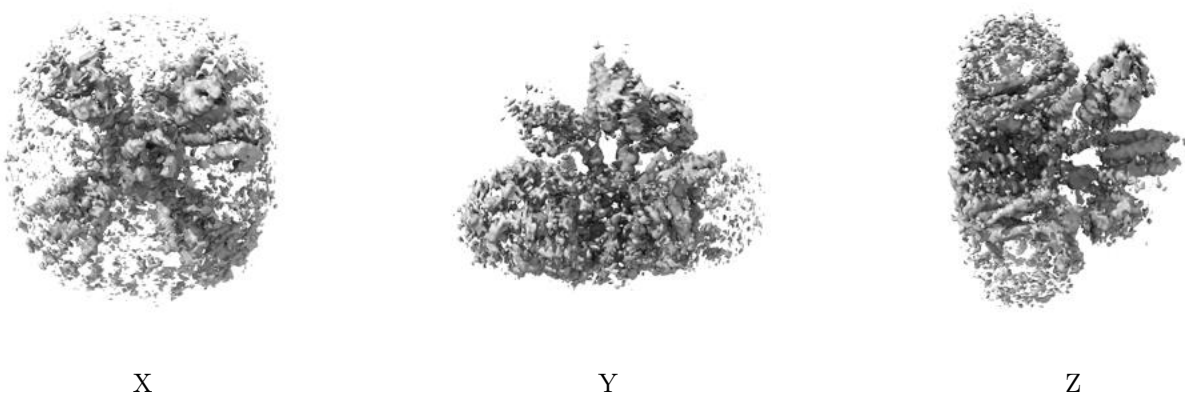
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.371. 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.

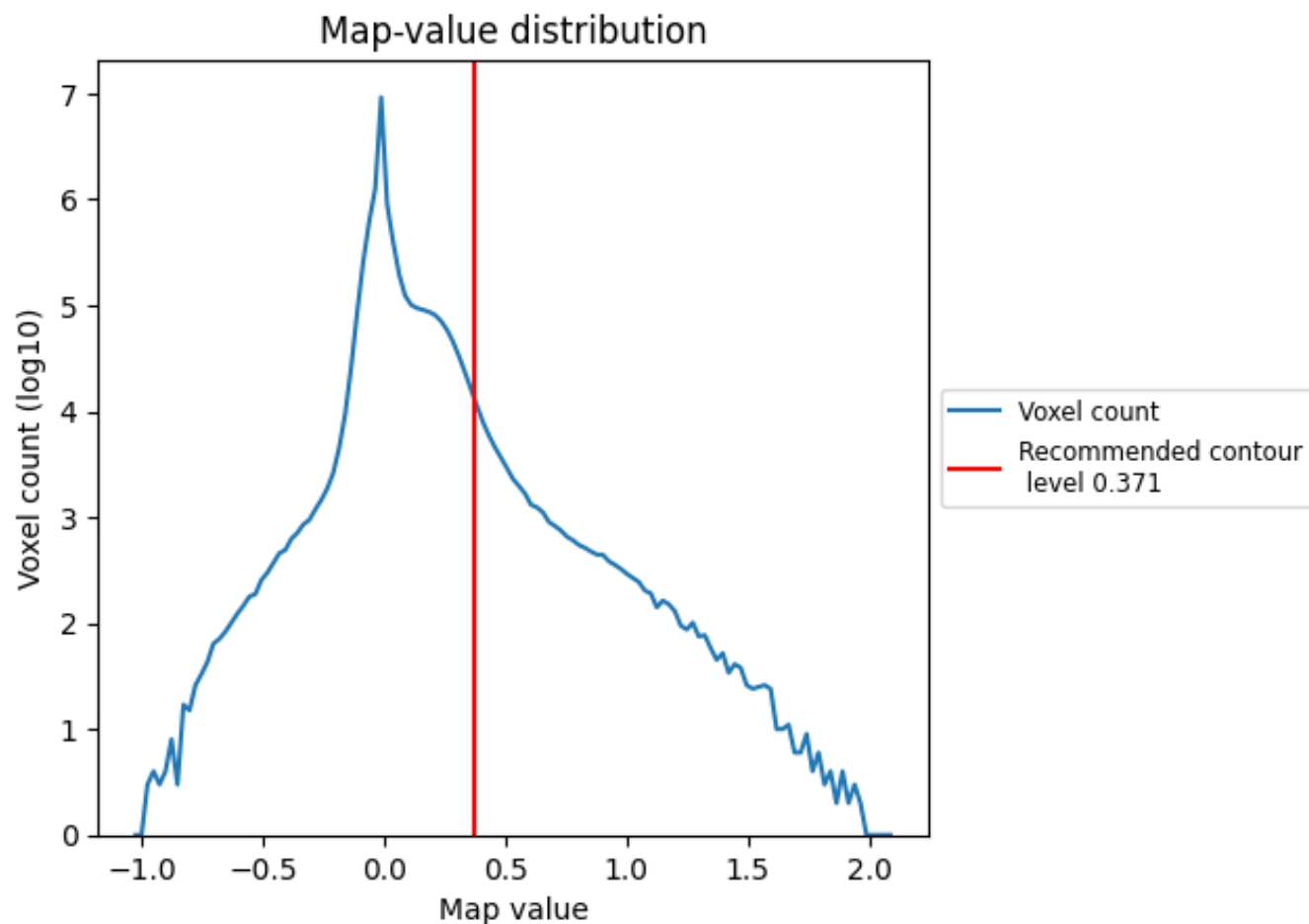
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

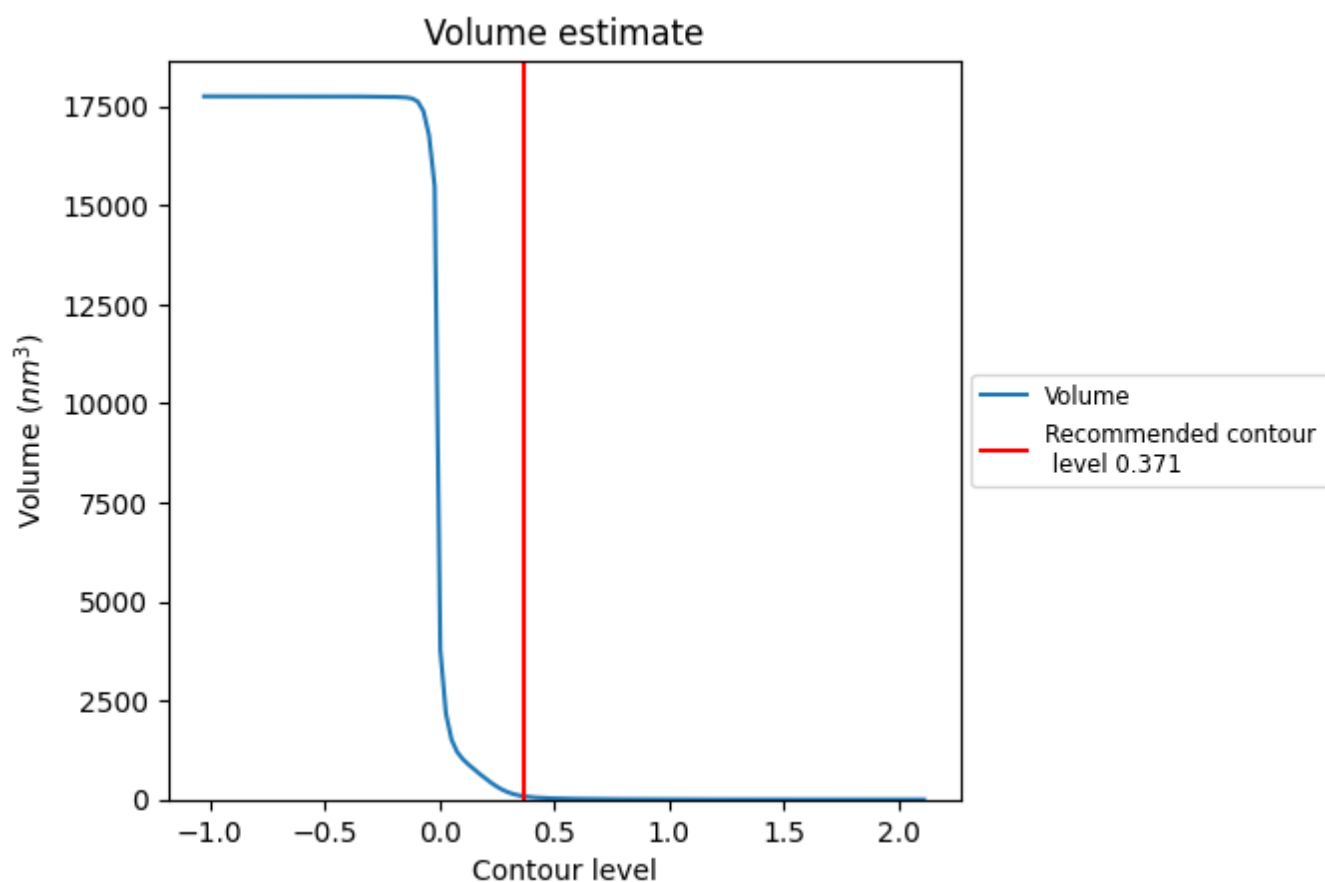
This section contains the results of statistical analysis of the map.

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.

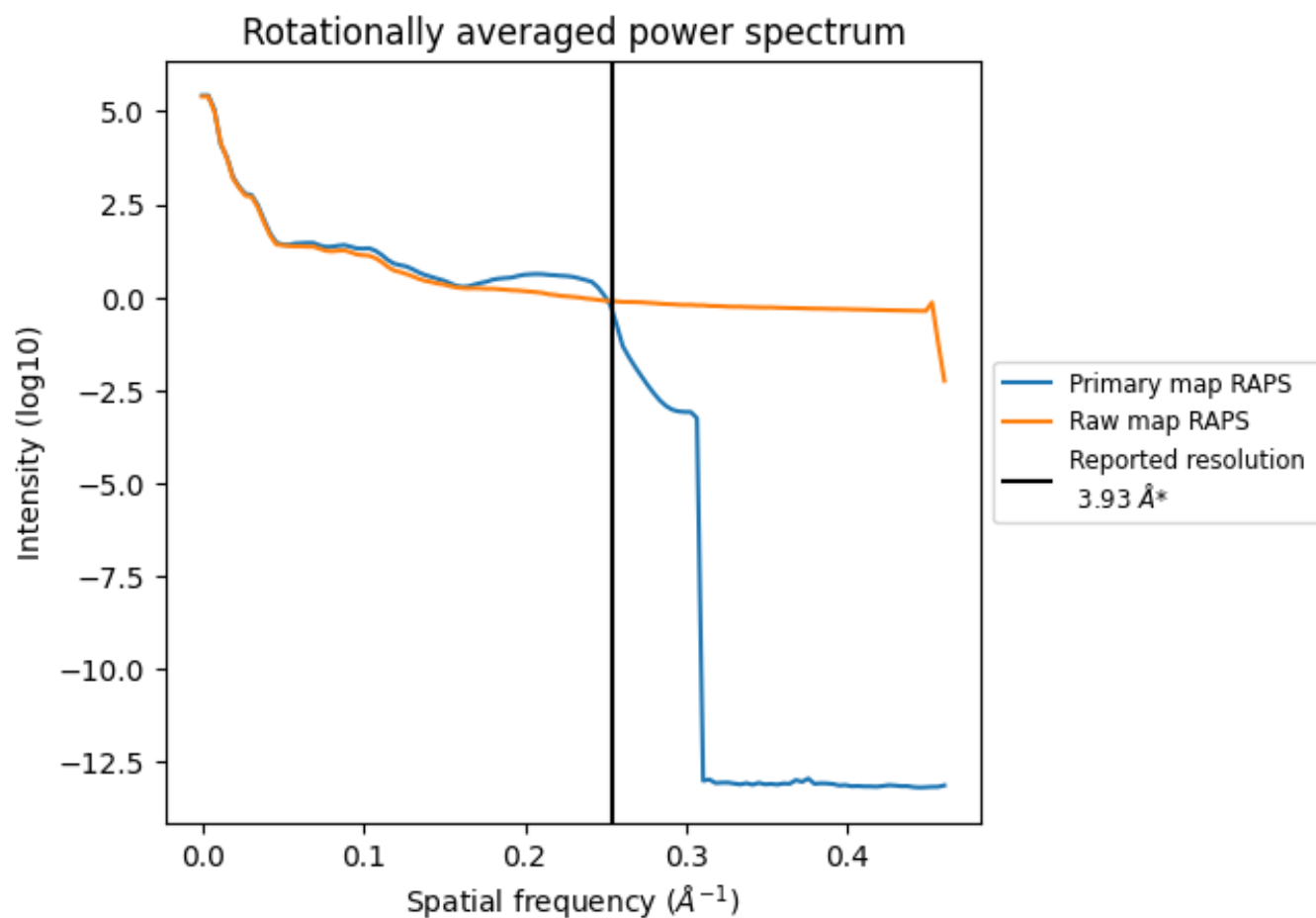
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm³; this corresponds to an approximate mass of 73 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 ⓘ

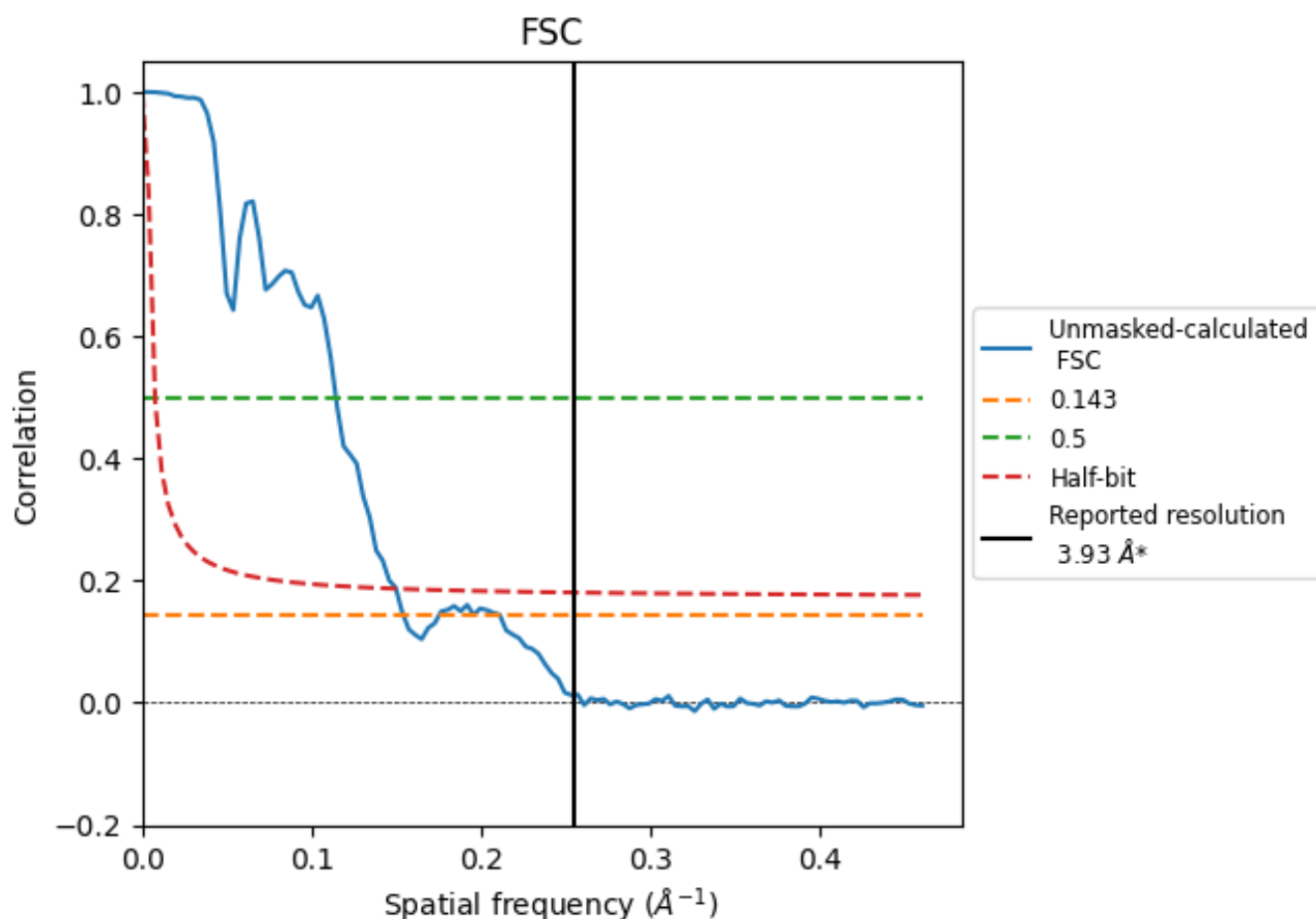


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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 0.254 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

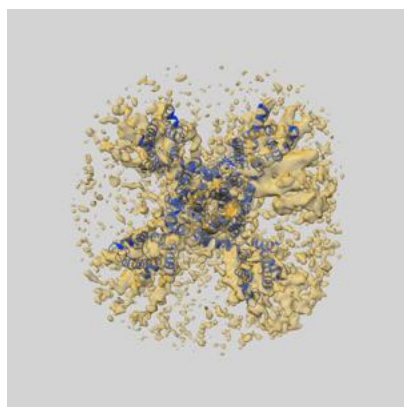
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.49	8.76	6.68

*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 6.49 differs from the reported value 3.93 by more than 10 %

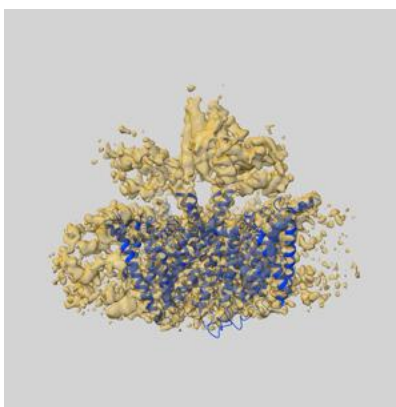
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69854 and PDB model 24VW. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

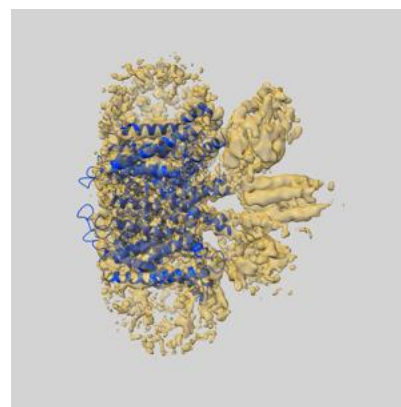
9.1 Map-model overlay [i](#)



X



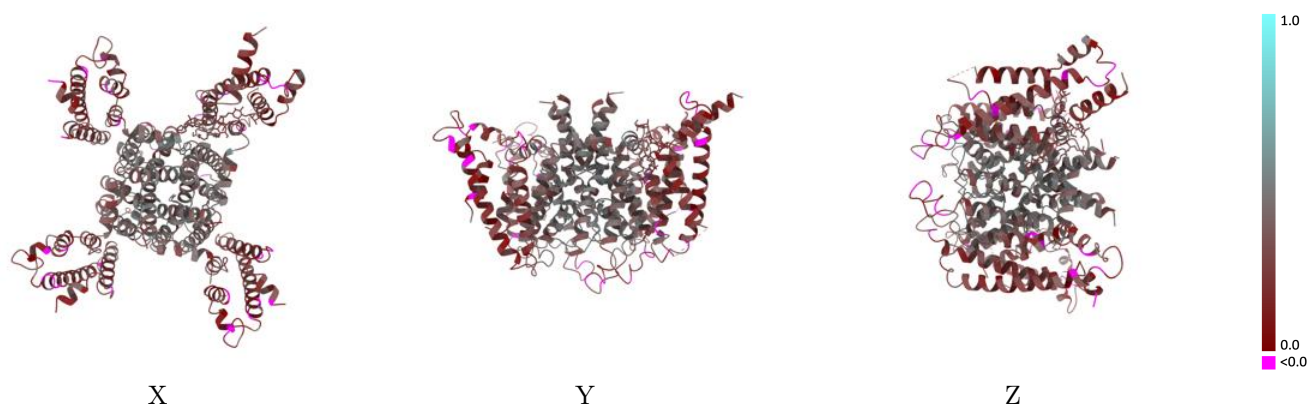
Y



Z

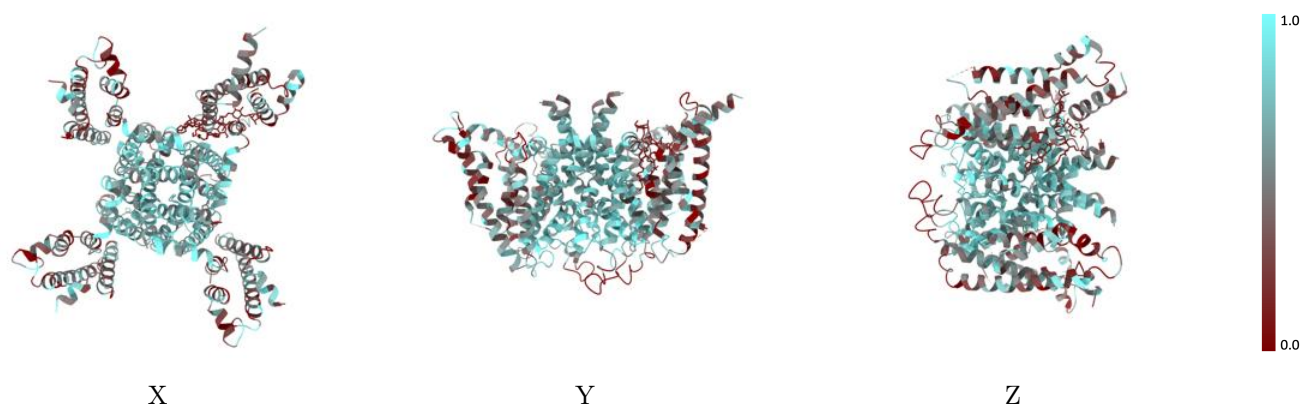
The images above show the 3D surface view of the map at the recommended contour level 0.371 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



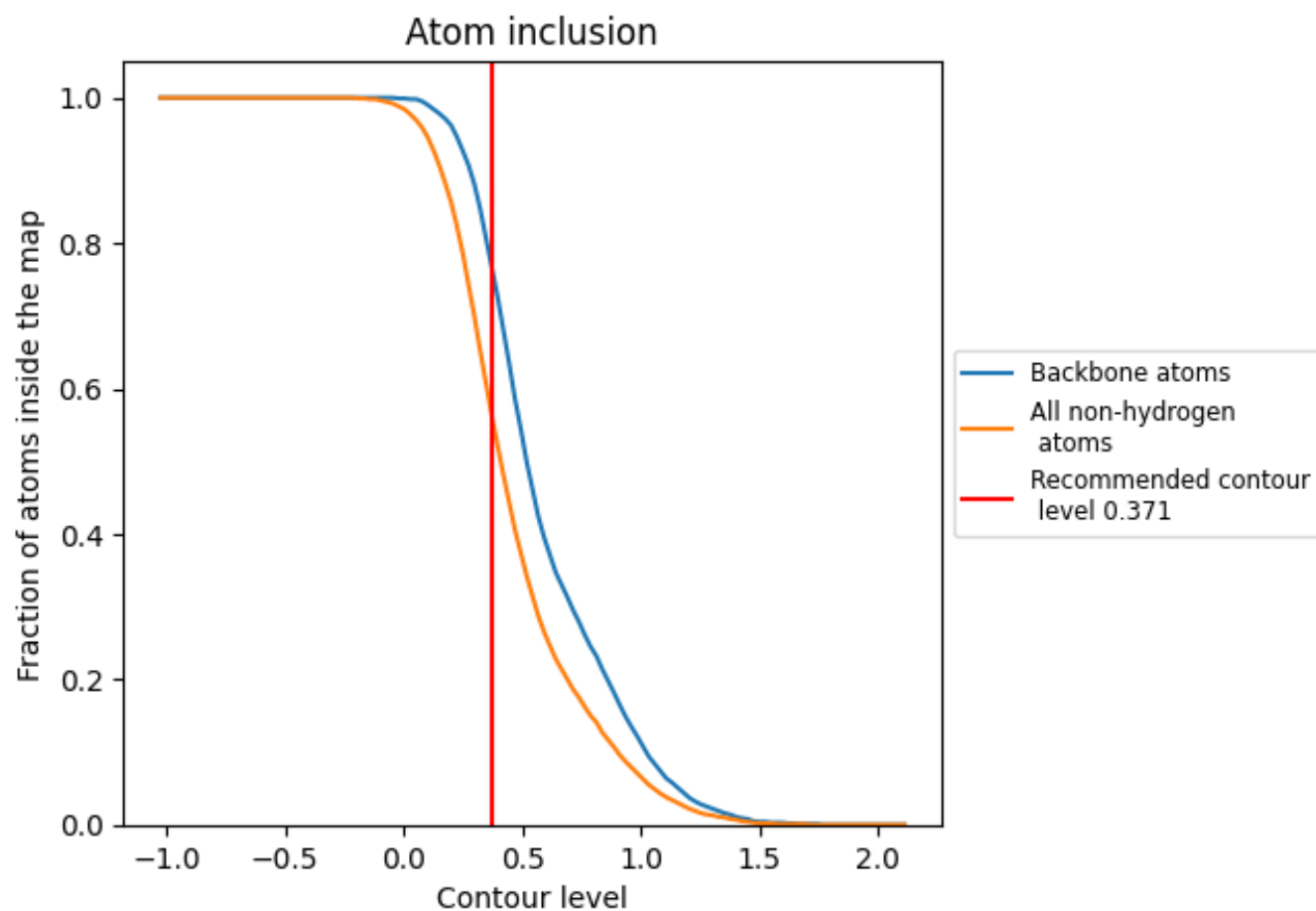
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.371).

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 56% 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 (0.371) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.3020
A	0.5750	0.2900
B	0.5710	0.3000
C	0.5590	0.3090
D	0.5530	0.3090

