



## Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 06:55 AM JST

PDB ID : 7VAB  
EMDB ID : EMD-31836  
Title : Cryo-EM structure of the non-acylated tirzepatide (LY3298176)-bound human GIPR-Gs complex  
Authors : Zhao, F.H.; Zhou, Q.T.; Cong, Z.T.; Hang, K.N.; Zou, X.Y.; Zhang, C.; Chen, Y.; Dai, A.T.; Liang, A.Y.; Ming, Q.Q.; Wang, M.; Chen, L.N.; Xu, P.Y.; Chang, R.L.; Feng, W.B.; Xia, T.; Zhang, Y.; Wu, B.L.; Yang, D.H.; Zhao, L.H.; Xu, H.E.; Wang, M.W.  
Deposited on : 2021-08-28  
Resolution : 3.20 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>.

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

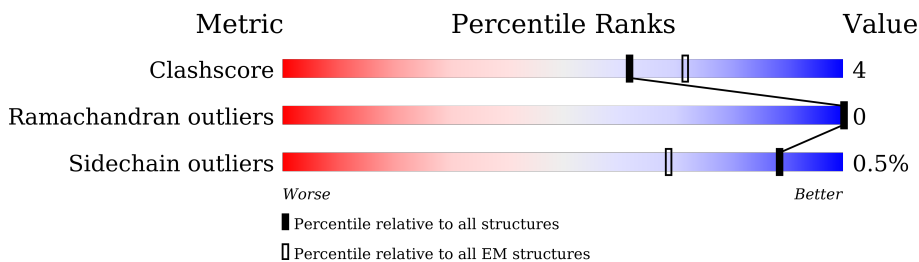
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	R	573	
2	P	39	
3	A	361	
4	B	371	
5	G	64	
6	N	140	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8772 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 Gastric inhibitory polypeptide receptor,Gastric inhibitory polypeptide receptor,Gastric inhibitory polypeptide receptor,human glucose-dependent insulinotropic polypeptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	288	2399	1579	423	387	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	345	PHE	THR	engineered mutation	UNP P48546

- Molecule 2 is a protein called Non-acylated\_tirzepatide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	P	27	220	147	32	41	0	0

- Molecule 3 is a protein called mini-Gs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	235	1950	1232	350	360	8	0	0

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	341	2616	1612	470	513	21	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

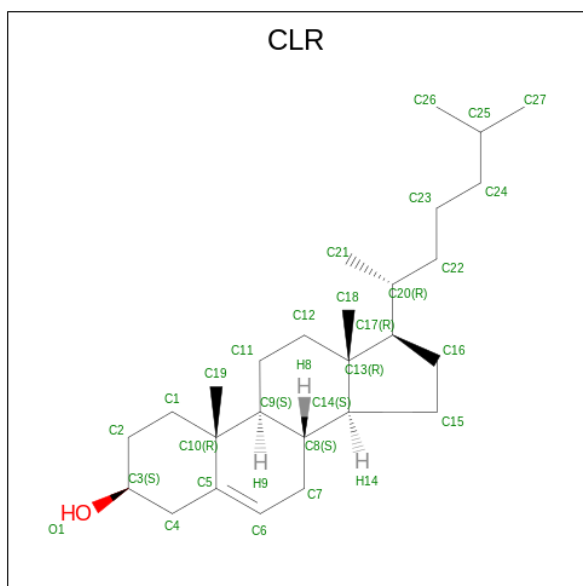
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	57	436	273	77	83	3	0	0

- Molecule 6 is a protein called Nonobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	129	983	611	173	193	6	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).

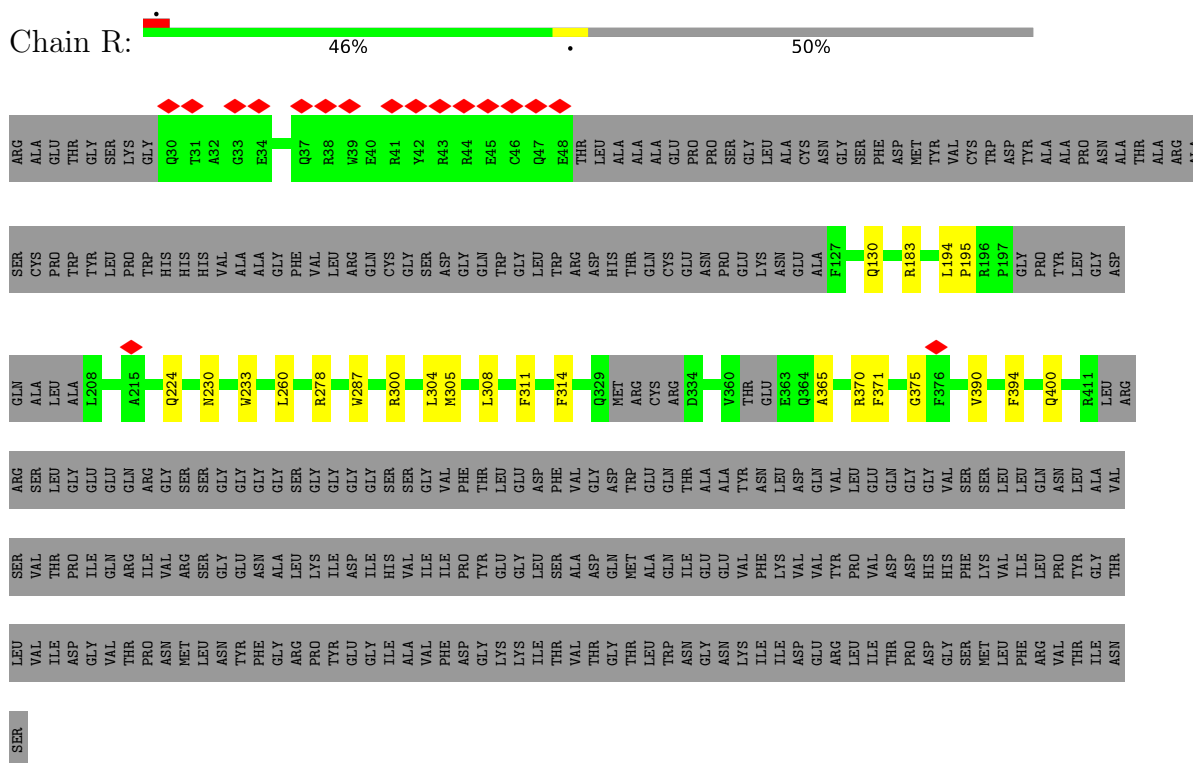


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	R	1	168	162	6	0
7	R	1	168	162	6	0
7	R	1	168	162	6	0
7	R	1	168	162	6	0
7	R	1	168	162	6	0
7	R	1	168	162	6	0

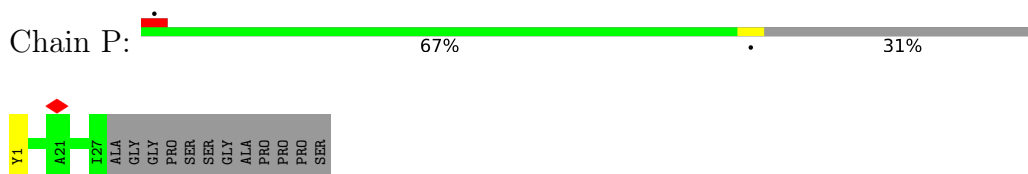
### 3 Residue-property plots [i](#)

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

- Molecule 1: Gastric inhibitory polypeptide receptor, Gastric inhibitory polypeptide receptor, Gastric inhibitory polypeptide receptor, human glucose-dependent insulinotropic polypeptide receptor

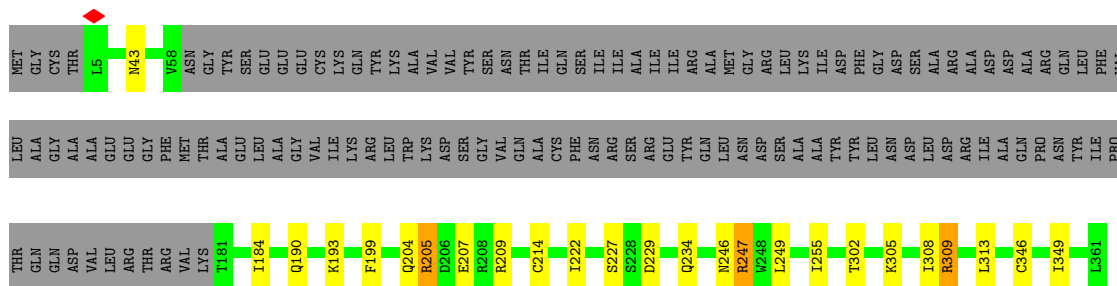


- Molecule 2: Non-acylated\_tirzepatide

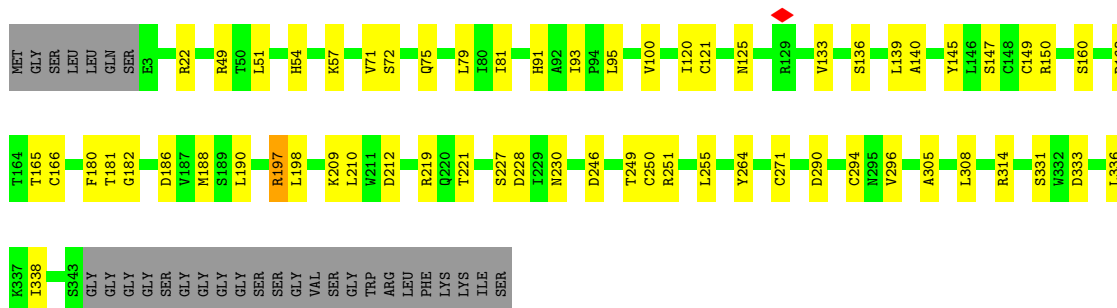
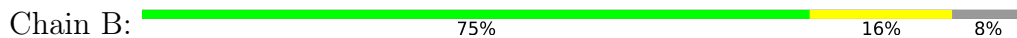


- Molecule 3: mini-Gs

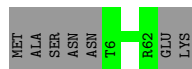
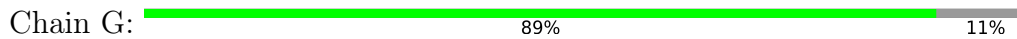




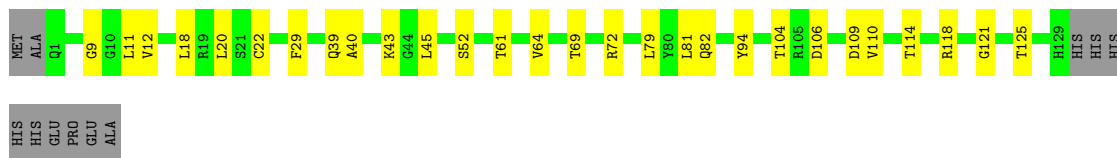
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



• Molecule 6: Nonobody-35



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1251553	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.414	Depositor
Minimum map value	-4.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.243	Depositor
Map size (Å)	274.176, 274.176, 274.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.071, 1.071, 1.071	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: AIB, CLR

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	R	0.27	0/2456	0.44	0/3328
2	P	0.24	0/213	0.35	0/288
3	A	0.25	0/1989	0.45	0/2677
4	B	0.26	0/2663	0.52	0/3610
5	G	0.23	0/442	0.39	0/597
6	N	0.26	0/1004	0.53	1/1360 (0.1%)
All	All	0.26	0/8767	0.47	1/11860 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	12	VAL	C-N-CA	5.66	135.85	121.70

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	R	2399	0	2470	13	0
2	P	220	0	219	1	0
3	A	1950	0	1925	17	0
4	B	2616	0	2518	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	436	0	448	0	0
6	N	983	0	945	17	0
7	R	168	0	276	5	0
All	All	8772	0	8801	79	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 4.

All (79) 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)
3:A:205:ARG:HD3	3:A:207:GLU:H	1.59	0.67
4:B:71:VAL:HG22	4:B:81:ILE:HG12	1.77	0.67
4:B:271:CYS:HB3	4:B:290:ASP:HB3	1.79	0.64
4:B:166:CYS:HB2	4:B:180:PHE:HB2	1.83	0.59
6:N:29:PHE:O	6:N:72:ARG:NH2	2.37	0.57
3:A:209:ARG:NH1	6:N:109:ASP:OD2	2.36	0.57
3:A:234:GLN:HG2	6:N:61:THR:HG23	1.88	0.56
3:A:246:ASN:HB3	3:A:249:LEU:HB2	1.87	0.56
1:R:371:PHE:O	1:R:375:GLY:N	2.39	0.55
1:R:130:GLN:HG3	1:R:371:PHE:HZ	1.71	0.55
3:A:43:ASN:ND2	3:A:229:ASP:OD2	2.39	0.55
4:B:294:CYS:HB2	4:B:308:LEU:HB2	1.88	0.55
4:B:79:LEU:HB3	4:B:93:ILE:HB	1.89	0.55
4:B:230:ASN:ND2	4:B:246:ASP:OD1	2.39	0.54
1:R:300:ARG:HH11	1:R:304:LEU:HD21	1.72	0.54
3:A:184:ILE:HD11	3:A:199:PHE:HB3	1.89	0.54
4:B:93:ILE:HG12	4:B:133:VAL:HG21	1.89	0.54
4:B:160:SER:HB2	4:B:190:LEU:HD23	1.90	0.54
4:B:331:SER:OG	4:B:333:ASP:OD1	2.27	0.53
4:B:51:LEU:HB2	4:B:336:LEU:HB2	1.90	0.52
6:N:22:CYS:HB3	6:N:79:LEU:HB3	1.92	0.52
4:B:75:GLN:NE2	4:B:100:VAL:O	2.42	0.52
1:R:394:PHE:O	1:R:400:GLN:NE2	2.38	0.51
4:B:182:GLY:O	4:B:209:LYS:NZ	2.43	0.51
6:N:52:SER:O	6:N:72:ARG:NH1	2.44	0.51
3:A:190:GLN:HE21	3:A:193:LYS:HA	1.75	0.51
1:R:183:ARG:HD3	1:R:230:ASN:HD22	1.76	0.51
4:B:95:LEU:HD13	4:B:100:VAL:HG21	1.92	0.51
4:B:49:ARG:HB2	4:B:338:ILE:HD12	1.93	0.51
4:B:210:LEU:HD22	4:B:255:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:214:CYS:HA	4:B:57:LYS:HZ1	1.76	0.50
1:R:224:GLN:NE2	2:P:1:TYR:OH	2.45	0.50
6:N:110:VAL:O	6:N:118:ARG:NH2	2.45	0.50
6:N:9:GLY:HA2	6:N:18:LEU:HD21	1.94	0.50
3:A:227:SER:HB2	3:A:308:ILE:HD13	1.94	0.50
1:R:278:ARG:HH11	1:R:287:TRP:HA	1.76	0.49
6:N:94:TYR:O	6:N:121:GLY:HA2	2.13	0.48
6:N:61:THR:HB	6:N:64:VAL:HG22	1.96	0.48
1:R:390:VAL:HA	1:R:394:PHE:HD2	1.78	0.48
3:A:205:ARG:NH1	4:B:186:ASP:OD1	2.47	0.47
1:R:233:TRP:HH2	1:R:260:LEU:HD23	1.78	0.47
4:B:81:ILE:HD12	4:B:91:HIS:HB2	1.96	0.47
3:A:204:GLN:HE22	4:B:145:TYR:HB3	1.80	0.47
4:B:22:ARG:NH2	4:B:221:THR:O	2.48	0.47
4:B:296:VAL:O	4:B:305:ALA:N	2.49	0.46
1:R:311:PHE:O	1:R:314:PHE:HB3	2.15	0.46
3:A:302:THR:HA	3:A:305:LYS:HG2	1.98	0.46
4:B:149:CYS:O	4:B:150:ARG:NE	2.48	0.46
4:B:54:HIS:NE2	4:B:72:SER:OG	2.40	0.46
6:N:104:THR:OG1	6:N:106:ASP:OD1	2.31	0.46
1:R:365:ALA:O	1:R:370:ARG:NE	2.49	0.46
7:R:602:CLR:H183	7:R:602:CLR:H20	1.88	0.46
4:B:165:THR:HG22	4:B:181:THR:HG22	1.98	0.45
6:N:20:LEU:HD12	6:N:81:LEU:HD23	1.98	0.45
7:R:601:CLR:H183	7:R:601:CLR:H20	1.89	0.45
6:N:40:ALA:HB3	6:N:43:LYS:HB2	1.99	0.45
3:A:205:ARG:HH21	6:N:114:THR:HB	1.82	0.45
4:B:212:ASP:OD2	4:B:219:ARG:NH2	2.50	0.45
7:R:601:CLR:H222	7:R:601:CLR:H162	1.80	0.45
4:B:197:ARG:HD3	4:B:198:LEU:HG	1.97	0.45
6:N:39:GLN:HB2	6:N:45:LEU:HD23	1.98	0.44
6:N:69:THR:HB	6:N:82:GLN:HB3	2.00	0.44
3:A:222:ILE:HG13	3:A:255:ILE:HB	2.00	0.44
4:B:121:CYS:HB3	4:B:139:LEU:HB2	2.00	0.43
7:R:604:CLR:H222	7:R:604:CLR:H162	1.83	0.43
7:R:606:CLR:H222	7:R:606:CLR:H162	1.73	0.43
4:B:227:SER:OG	4:B:228:ASP:N	2.51	0.43
1:R:194:LEU:HD12	1:R:195:PRO:HD2	2.00	0.43
6:N:11:LEU:HD23	6:N:125:THR:HB	2.00	0.43
3:A:346:CYS:HA	3:A:349:ILE:HD12	2.01	0.43
4:B:249:THR:OG1	4:B:251:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:120:ILE:HG12	4:B:140:ALA:HB2	2.02	0.42
3:A:309:ARG:HE	3:A:313:LEU:HD11	1.85	0.41
4:B:250:CYS:HB2	4:B:264:TYR:HB2	2.02	0.41
3:A:247:ARG:NH2	6:N:106:ASP:OD2	2.53	0.41
1:R:305:MET:O	1:R:308:LEU:HB3	2.22	0.40
4:B:125:ASN:HB2	4:B:136:SER:HB2	2.03	0.40
4:B:147:SER:OG	4:B:188:MET:O	2.31	0.40
4:B:163:ASP:OD1	4:B:165:THR:OG1	2.37	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	R	278/573 (48%)	277 (100%)	1 (0%)	0	100	100
2	P	23/39 (59%)	23 (100%)	0	0	100	100
3	A	231/361 (64%)	226 (98%)	5 (2%)	0	100	100
4	B	339/371 (91%)	331 (98%)	8 (2%)	0	100	100
5	G	55/64 (86%)	55 (100%)	0	0	100	100
6	N	127/140 (91%)	121 (95%)	6 (5%)	0	100	100
All	All	1053/1548 (68%)	1033 (98%)	20 (2%)	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	R	254/483 (53%)	254 (100%)	0	100	100
2	P	22/29 (76%)	22 (100%)	0	100	100
3	A	212/315 (67%)	209 (99%)	3 (1%)	67	86
4	B	283/302 (94%)	281 (99%)	2 (1%)	84	94
5	G	46/52 (88%)	46 (100%)	0	100	100
6	N	107/116 (92%)	107 (100%)	0	100	100
All	All	924/1297 (71%)	919 (100%)	5 (0%)	89	95

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

Mol	Chain	Res	Type
3	A	205	ARG
3	A	247	ARG
3	A	309	ARG
4	B	197	ARG
4	B	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	173	HIS
1	R	224	GLN
1	R	230	ASN
3	A	190	GLN
3	A	197	HIS
3	A	204	GLN
3	A	329	HIS
4	B	88	ASN
4	B	266	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AIB	P	2	2	1,5,6	1.25	0	2,7,9	1.23	0
2	AIB	P	13	2	1,5,6	1.41	0	2,7,9	1.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AIB	P	2	2	-	0/2/3/6	-
2	AIB	P	13	2	-	0/2/3/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z  > 2$
7	CLR	R	603	-	31,31,31	0.61	0	48,48,48	1.27	6 (12%)
7	CLR	R	601	-	31,31,31	0.59	0	48,48,48	1.37	6 (12%)
7	CLR	R	606	-	31,31,31	0.59	0	48,48,48	1.31	5 (10%)
7	CLR	R	605	-	31,31,31	0.60	0	48,48,48	1.36	6 (12%)
7	CLR	R	604	-	31,31,31	0.60	0	48,48,48	1.44	8 (16%)
7	CLR	R	602	-	31,31,31	0.59	0	48,48,48	1.39	6 (12%)

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
7	CLR	R	603	-	-	4/10/68/68	0/4/4/4
7	CLR	R	601	-	-	4/10/68/68	0/4/4/4
7	CLR	R	606	-	-	4/10/68/68	0/4/4/4
7	CLR	R	605	-	-	4/10/68/68	0/4/4/4
7	CLR	R	604	-	-	4/10/68/68	0/4/4/4
7	CLR	R	602	-	-	4/10/68/68	0/4/4/4

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	604	CLR	C13-C17-C20	-4.39	112.62	119.49
7	R	602	CLR	C13-C17-C20	-4.12	113.03	119.49
7	R	601	CLR	C13-C17-C20	-3.92	113.34	119.49
7	R	605	CLR	C13-C17-C20	-3.80	113.54	119.49
7	R	606	CLR	C19-C10-C9	-3.01	108.09	111.68
7	R	606	CLR	C13-C17-C20	-2.89	114.96	119.49
7	R	605	CLR	C21-C20-C17	-2.78	108.66	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	604	CLR	C21-C20-C17	-2.73	108.74	112.92
7	R	604	CLR	C19-C10-C9	-2.67	108.49	111.68
7	R	603	CLR	C19-C10-C9	-2.64	108.53	111.68
7	R	603	CLR	C13-C17-C20	-2.64	115.35	119.49
7	R	605	CLR	C19-C10-C9	-2.58	108.60	111.68
7	R	602	CLR	C19-C10-C9	-2.58	108.60	111.68
7	R	602	CLR	C21-C20-C17	-2.57	108.98	112.92
7	R	603	CLR	C7-C8-C14	-2.52	107.25	110.91
7	R	601	CLR	C19-C10-C9	-2.50	108.70	111.68
7	R	601	CLR	C21-C20-C17	-2.47	109.14	112.92
7	R	605	CLR	C7-C8-C14	-2.46	107.34	110.91
7	R	601	CLR	C13-C14-C8	-2.39	110.84	114.38
7	R	604	CLR	C7-C8-C14	-2.39	107.45	110.91
7	R	602	CLR	C13-C14-C8	-2.37	110.86	114.38
7	R	603	CLR	C21-C20-C22	-2.34	106.69	110.36
7	R	601	CLR	C7-C8-C14	-2.34	107.51	110.91
7	R	602	CLR	C7-C8-C14	-2.27	107.61	110.91
7	R	604	CLR	C13-C14-C8	-2.26	111.04	114.38
7	R	604	CLR	C3-C4-C5	-2.18	108.33	112.03
7	R	606	CLR	C9-C10-C5	2.17	113.05	109.65
7	R	605	CLR	C13-C14-C8	-2.11	111.25	114.38
7	R	605	CLR	C3-C4-C5	-2.11	108.45	112.03
7	R	602	CLR	C3-C4-C5	-2.08	108.50	112.03
7	R	601	CLR	C4-C5-C6	-2.08	117.61	120.61
7	R	606	CLR	C13-C14-C8	-2.02	111.39	114.38
7	R	603	CLR	C4-C5-C10	2.02	119.10	116.42
7	R	606	CLR	C4-C5-C10	2.00	119.08	116.42
7	R	604	CLR	C4-C5-C10	2.00	119.08	116.42
7	R	603	CLR	C3-C4-C5	-2.00	108.63	112.03
7	R	604	CLR	C4-C5-C6	-2.00	117.72	120.61

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	602	CLR	C13-C17-C20-C21
7	R	604	CLR	C13-C17-C20-C21
7	R	604	CLR	C16-C17-C20-C21
7	R	601	CLR	C13-C17-C20-C21
7	R	605	CLR	C13-C17-C20-C21
7	R	601	CLR	C16-C17-C20-C21
7	R	602	CLR	C16-C17-C20-C21

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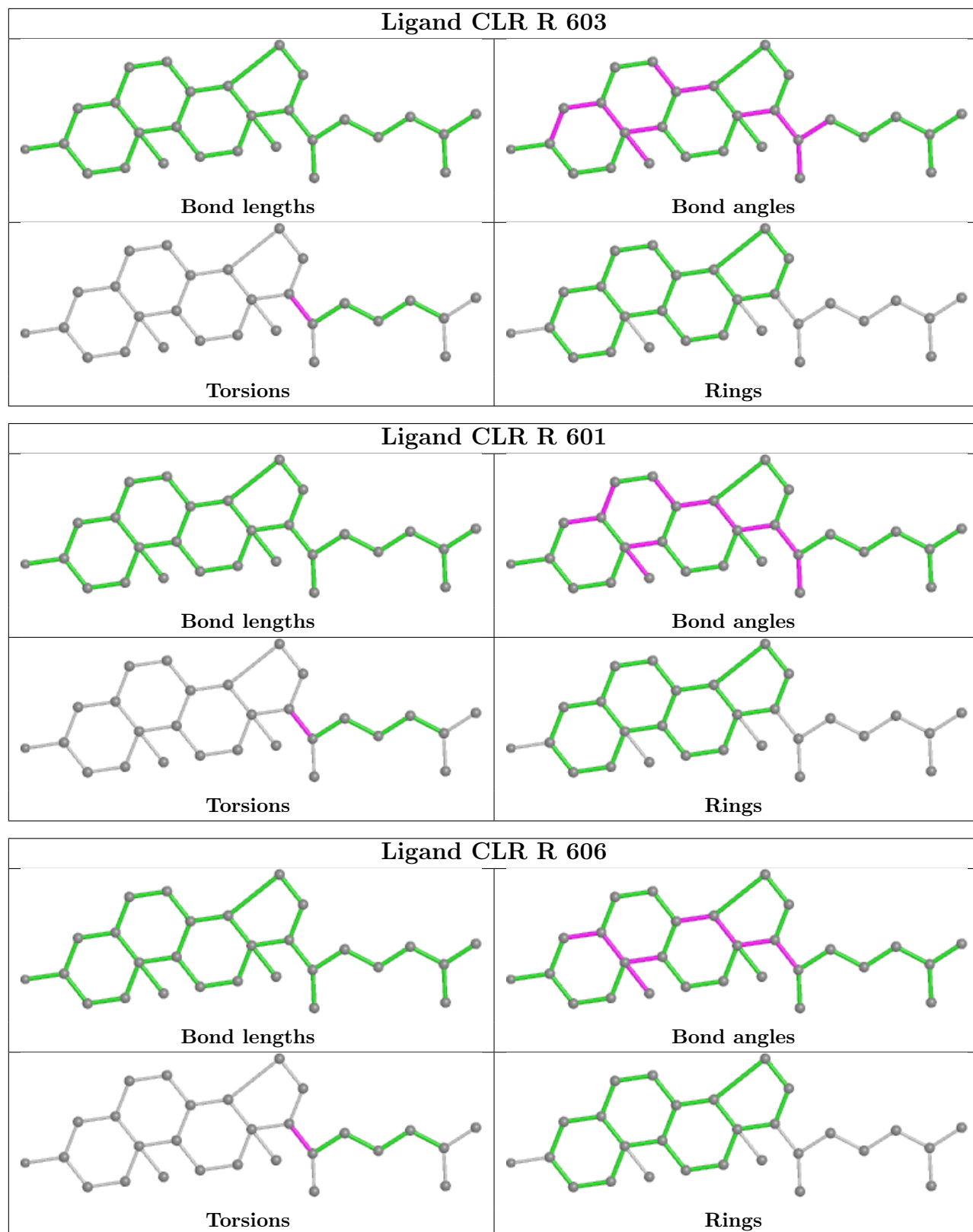
Mol	Chain	Res	Type	Atoms
7	R	605	CLR	C16-C17-C20-C21
7	R	604	CLR	C16-C17-C20-C22
7	R	601	CLR	C13-C17-C20-C22
7	R	602	CLR	C13-C17-C20-C22
7	R	604	CLR	C13-C17-C20-C22
7	R	605	CLR	C13-C17-C20-C22
7	R	601	CLR	C16-C17-C20-C22
7	R	602	CLR	C16-C17-C20-C22
7	R	605	CLR	C16-C17-C20-C22
7	R	606	CLR	C13-C17-C20-C21
7	R	603	CLR	C13-C17-C20-C21
7	R	606	CLR	C13-C17-C20-C22
7	R	606	CLR	C16-C17-C20-C21
7	R	603	CLR	C16-C17-C20-C21
7	R	606	CLR	C16-C17-C20-C22
7	R	603	CLR	C13-C17-C20-C22
7	R	603	CLR	C16-C17-C20-C22

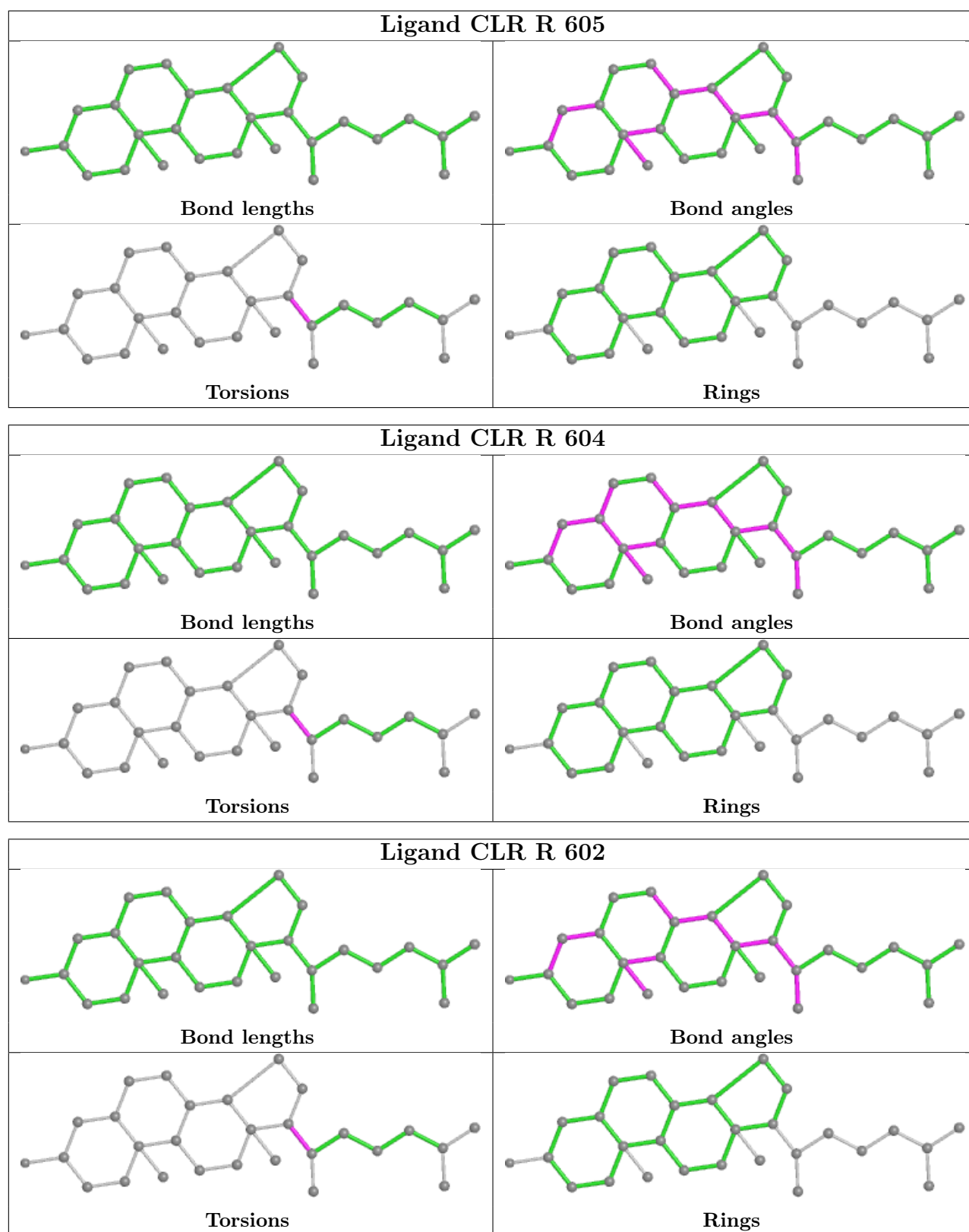
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	601	CLR	2	0
7	R	606	CLR	1	0
7	R	604	CLR	1	0
7	R	602	CLR	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.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

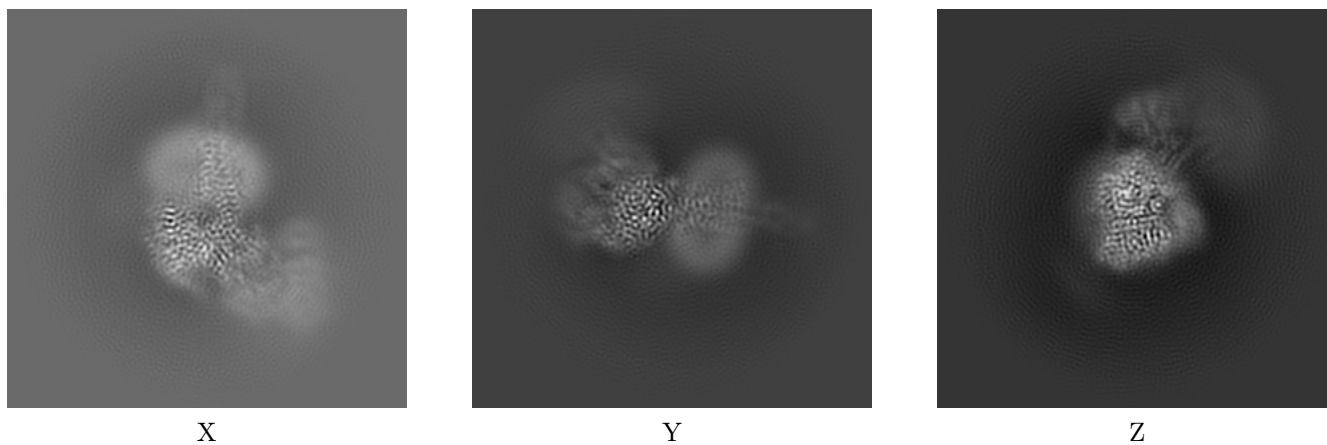
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31836. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

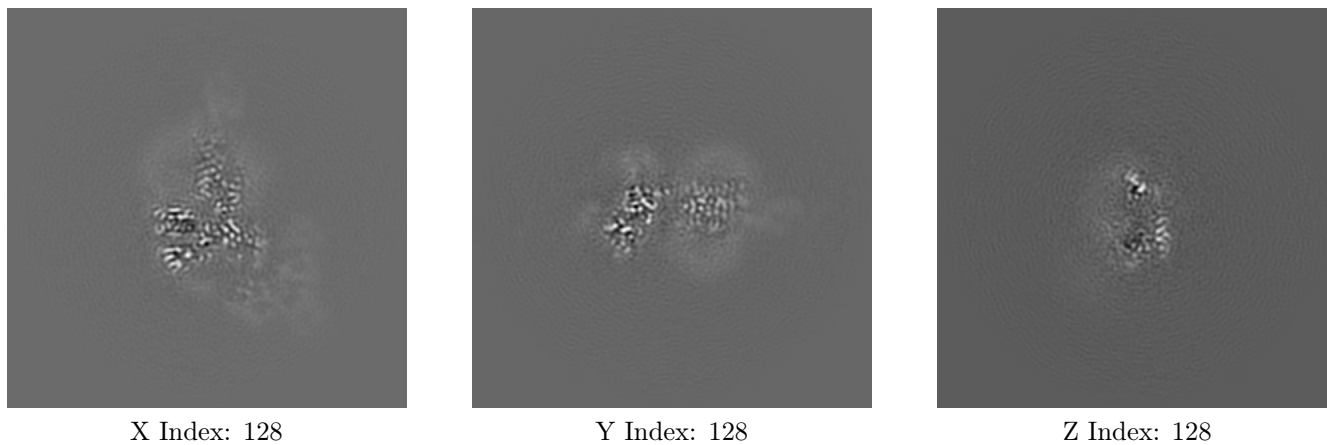
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

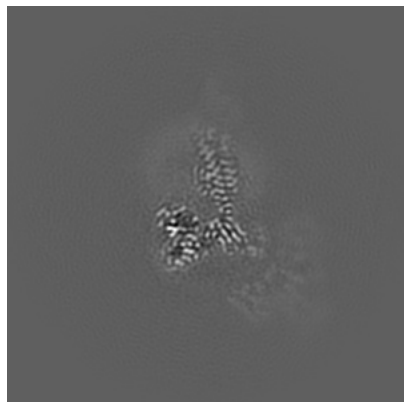
#### 6.2.1 Primary map



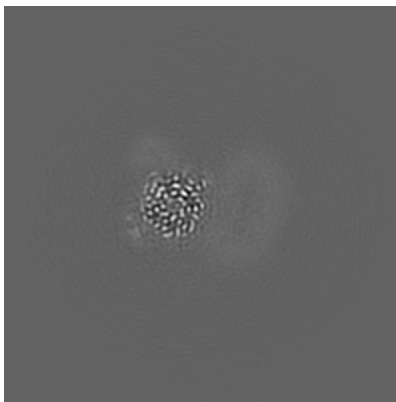
The images above show central slices of the map in three orthogonal directions.

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

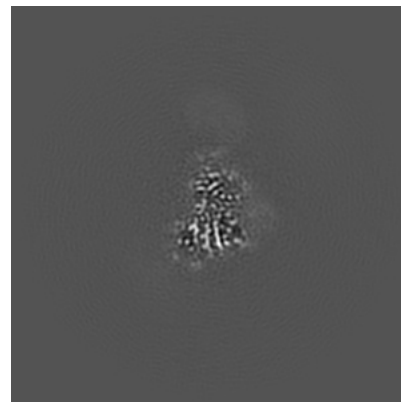
### 6.3.1 Primary map



X Index: 132



Y Index: 108



Z Index: 113

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

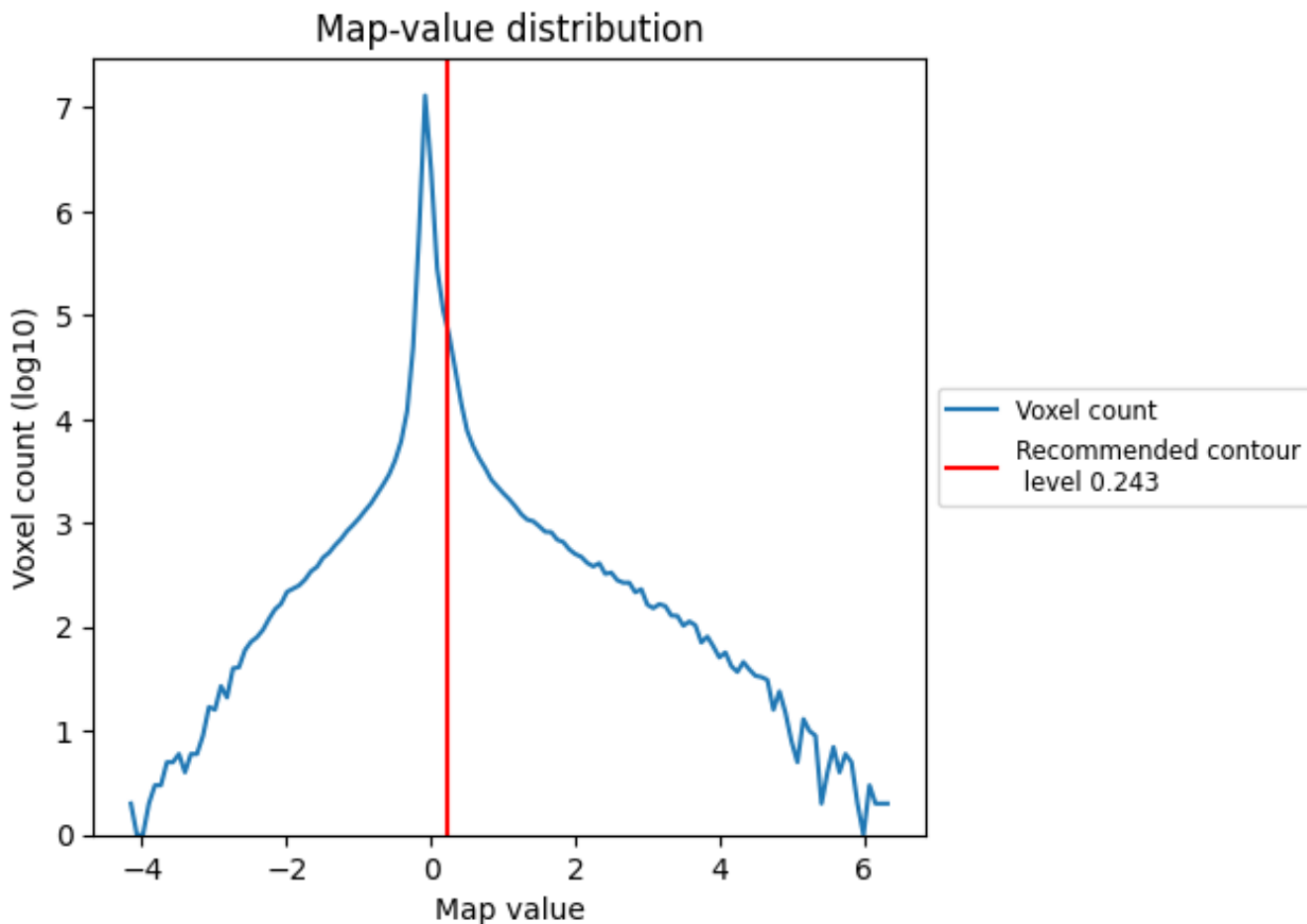
## 6.5 Mask visualisation

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.

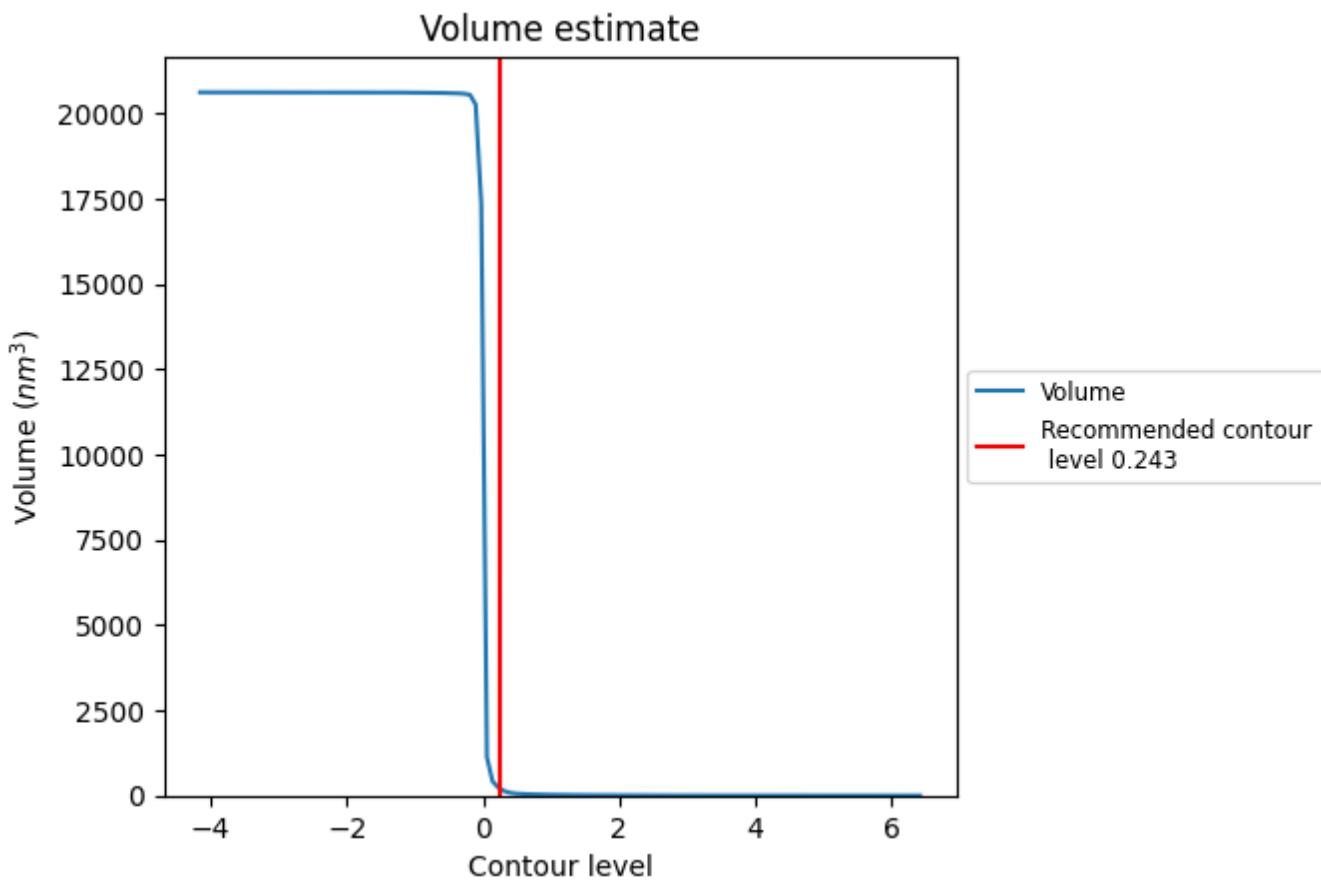
### 7.1 Map-value distribution [i](#)



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.



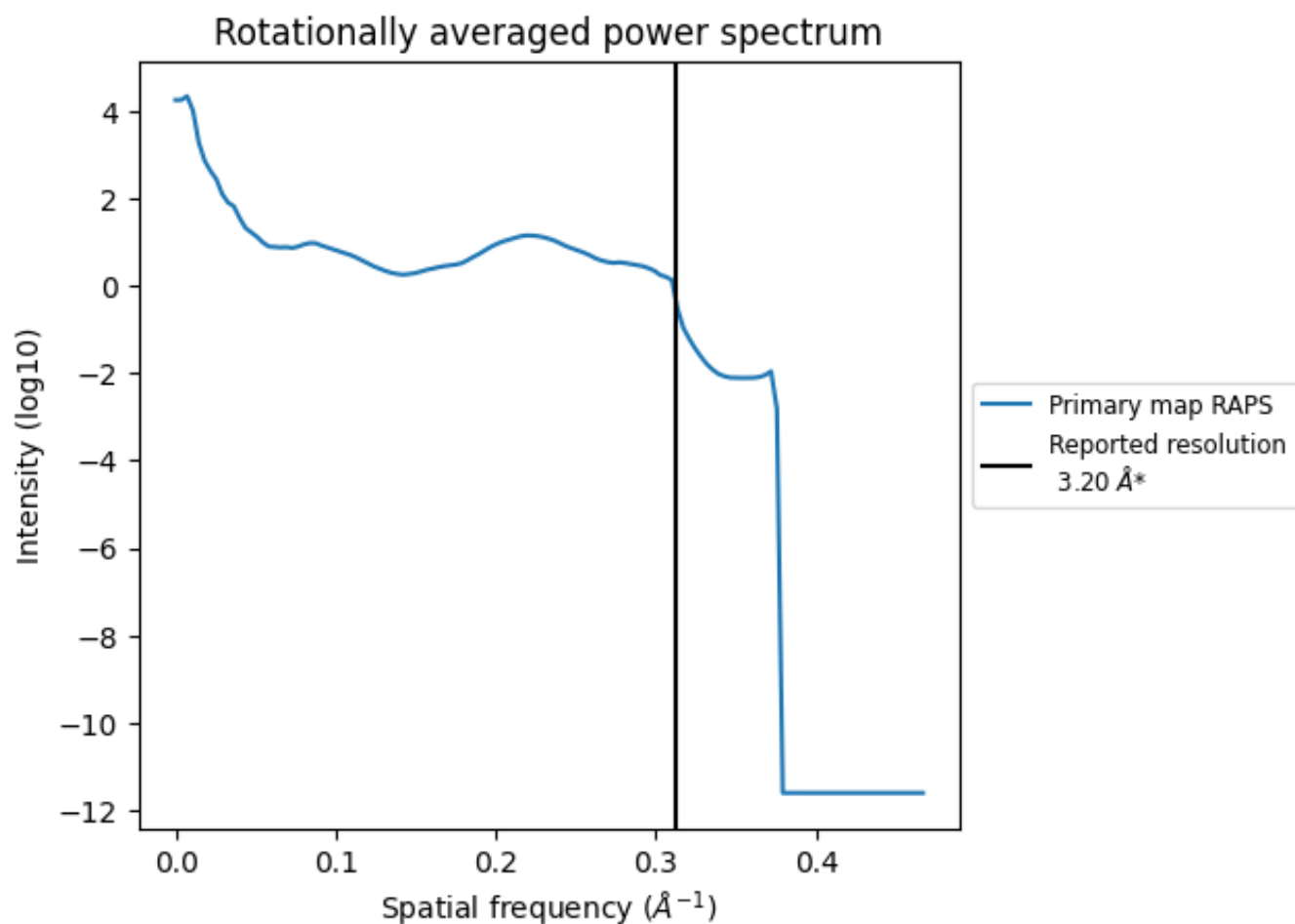
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm<sup>3</sup>; this corresponds to an approximate mass of 191 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.312 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

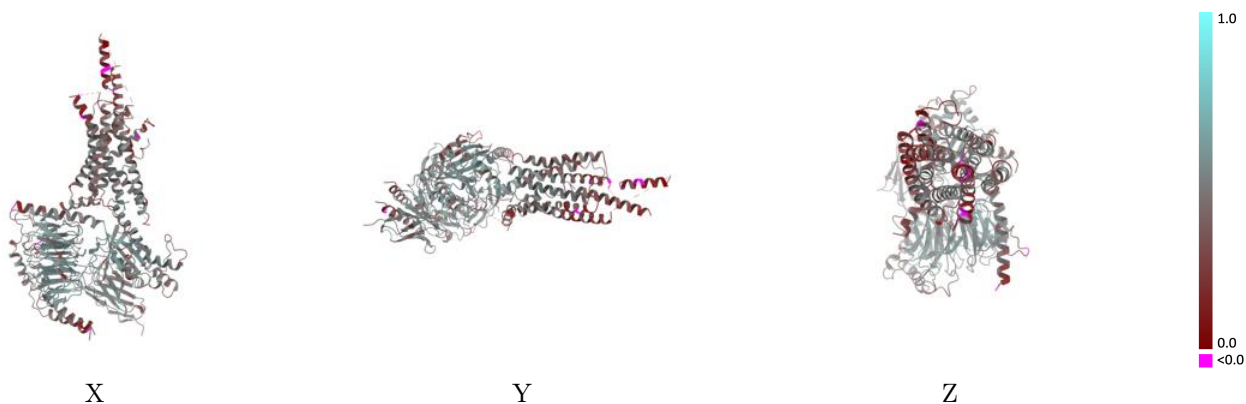
This section contains information regarding the fit between EMDB map EMD-31836 and PDB model 7VAB. Per-residue inclusion information can be found in section 3 on page 6.

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



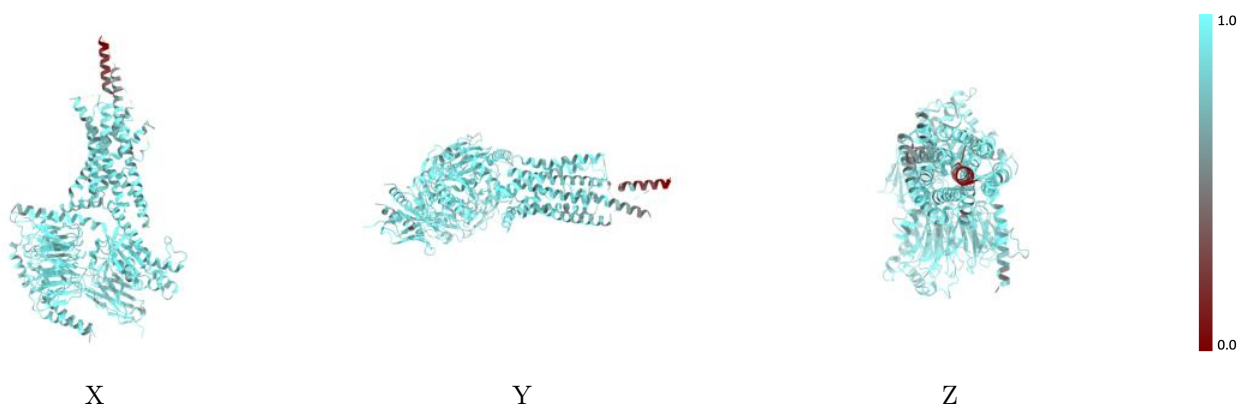
The images above show the 3D surface view of the map at the recommended contour level 0.243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



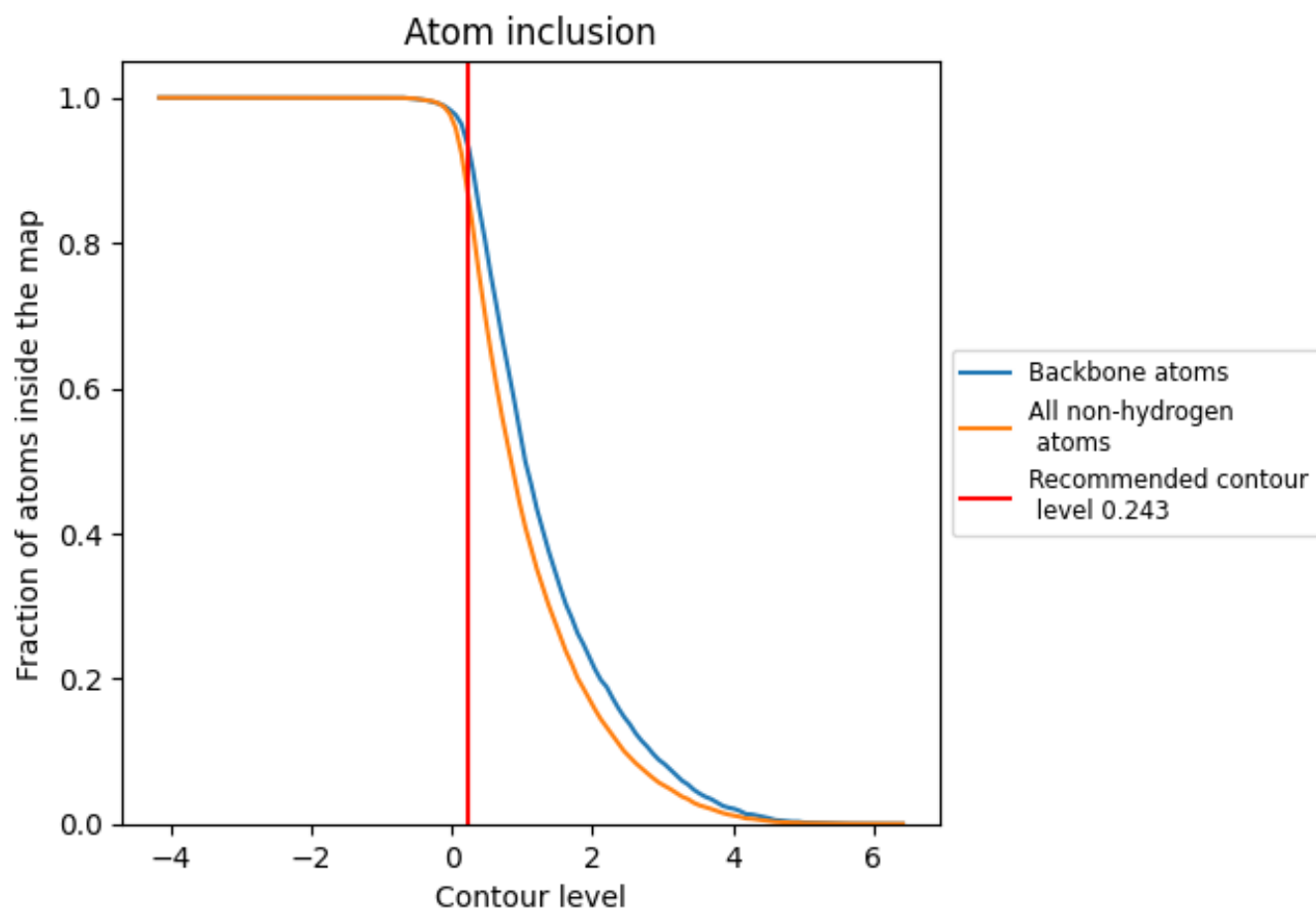
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.243).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8615	 0.4370
A	 0.8882	 0.4760
B	 0.9073	 0.4920
G	 0.8555	 0.4100
N	 0.9010	 0.4800
P	 0.6774	 0.2990
R	 0.7961	 0.3520

