



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:23 PM UTC

PDB ID : 7D76 / pdb_00007d76
EMDB ID : EMD-30602
Title : Cryo-EM structure of the beclomethasone-bound adhesion receptor GPR97-Go complex
Authors : Ping, Y.; Mao, C.; Xiao, P.; Zhao, R.; Jiang, Y.; Yang, Z.; An, W.; Shen, D.; Yang, F.; Zhang, H.; Qu, C.; Shen, Q.; Tian, C.; Li, Z.; Li, S.; Wang, G.; Tao, X.; Wen, X.; Zhong, Y.; Yang, J.; Yi, F.; Yu, X.; Xu, E.; Zhang, Y.; Sun, J.
Deposited on : 2020-10-03
Resolution : 3.10 Å(reported)
Based on initial model : 6G79

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

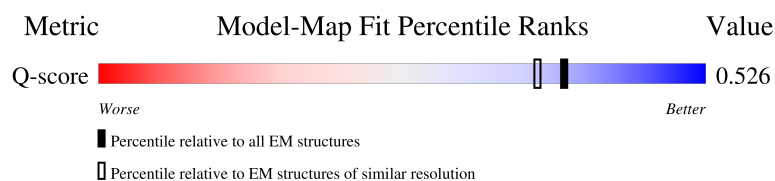
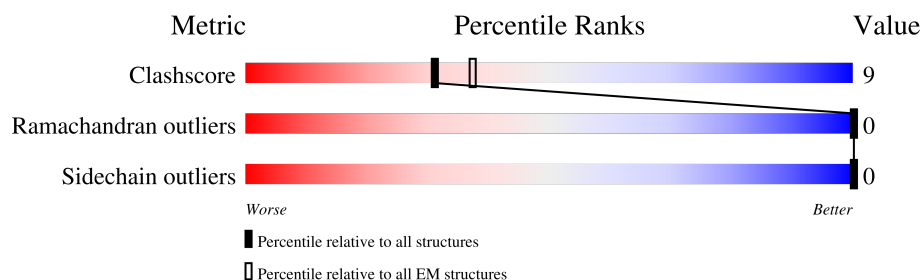
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

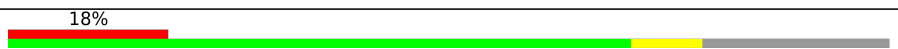
The reported resolution of this entry is 3.10 Å.

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	14724 (2.60 - 3.60)

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	226	
2	B	346	
3	G	71	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	R	561	39%9%53%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7015 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 Guanine nucleotide-binding protein G(o) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	215	Total	C	N	O	S	0	0
			1707	1085	287	324	11		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	341	HIS	-	expression tag	UNP P62873
B	342	HIS	-	expression tag	UNP P62873
B	343	HIS	-	expression tag	UNP P62873
B	344	HIS	-	expression tag	UNP P62873
B	345	HIS	-	expression tag	UNP P62873
B	346	HIS	-	expression tag	UNP P62873

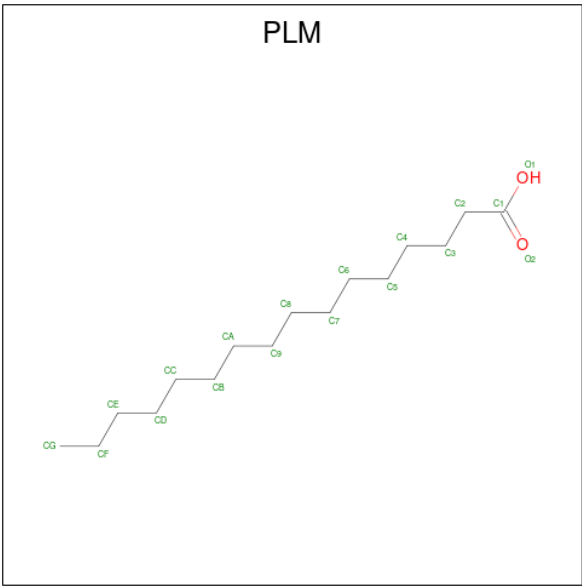
- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 4 is a protein called Adhesion G protein-coupled receptor G3; GPR97.

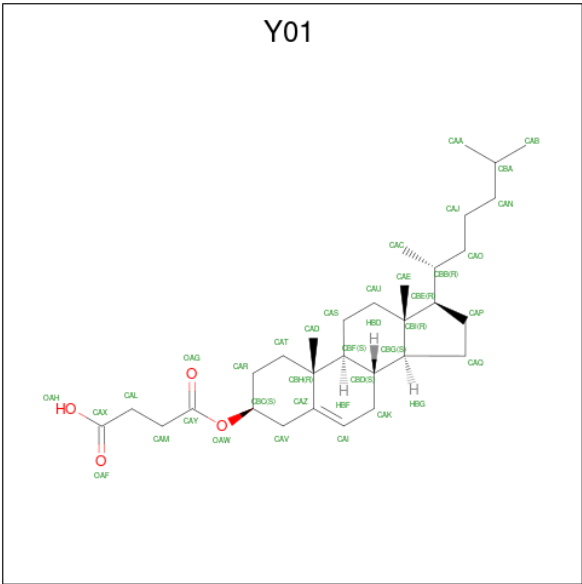
Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	265	Total	C	N	O	S	1	0
			2107	1408	344	344	11		

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



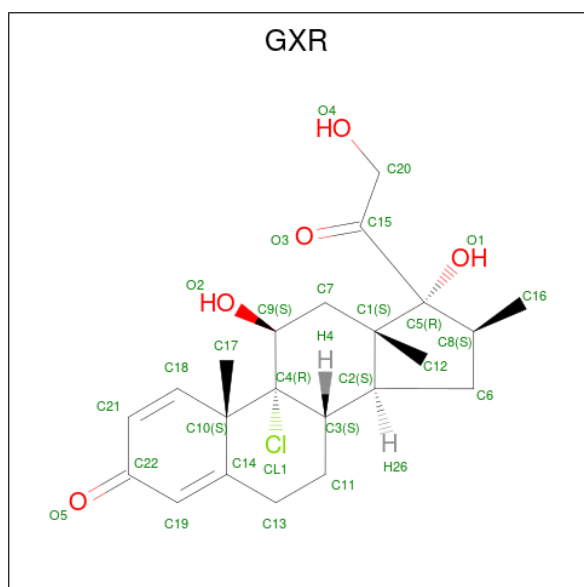
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			17	16	1	
5	R	1	Total	C	O	0
			18	16	2	
5	R	1	Total	C	O	0
			18	16	2	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	O	0
			35	31	4	

- Molecule 7 is (8 {S},9 {R},10 {S},11 {S},13 {S},14 {S},16 {S},17 {R})-9-chloranyl-10,13,16-trimethyl-11,17-bis(oxidanyl)-17-(2-oxidanylethanoyl)-6,7,8,11,12,14,15,16-octahydrocyclopenta[a]phenanthren-3-one (CCD ID: GXR) (formula: $C_{22}H_{29}ClO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	Cl	O	0
			28	22	1	5	

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
8	R	1	Total	C	O	0
			28	27	1	
8	R	1	Total	C	O	0
			28	27	1	

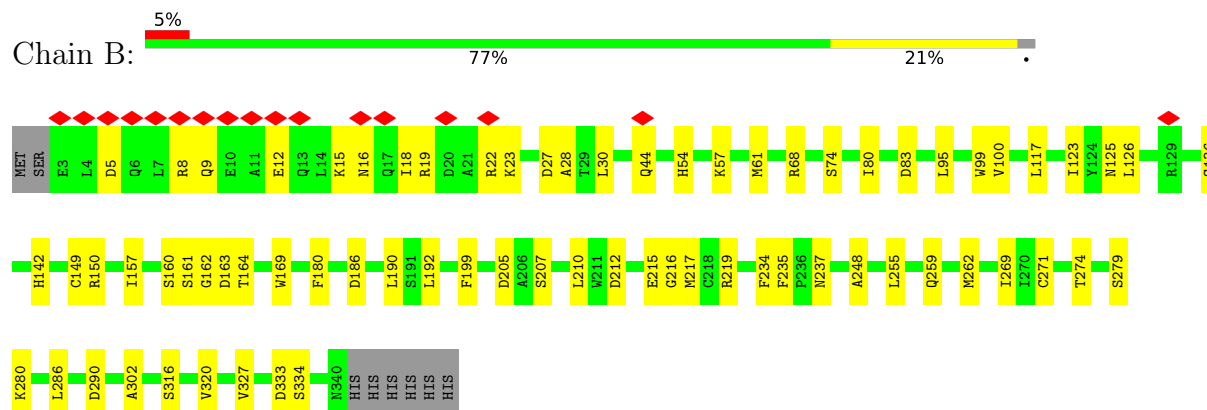
3 Residue-property plots

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.

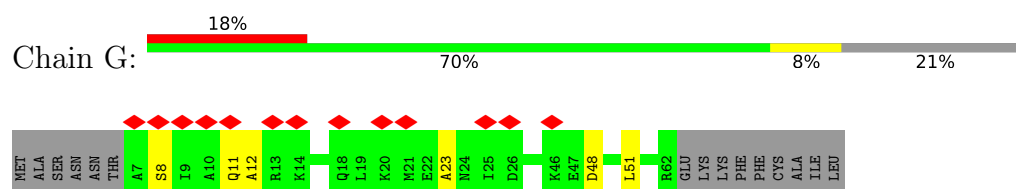
- Molecule 1: Guanine nucleotide-binding protein G(o) subunit alpha



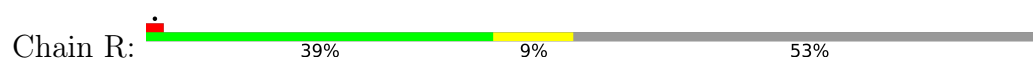
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: Adhesion G protein-coupled receptor G3; GPR97



K471	N472	R473	V476	L479	L492	A493	I494	F495	T496	S501	L508	L512	C519	T522	L526	P527	SER	GLN	SER	THR	THR	VAL	SER	SER	SER	THR	ALA	LEU	ASP	GLN	ALA	HIS	SER	ALA	SER	ALA	SER	GLN	GLU										
R341	F346	H346	Y347	L350	F353	L358	E359	A360	F371	H377	L380	K381	L382	S383	W387	F390	V394	Y403	I408	R409	D410	R411	E412	N413	S416	L419	R423	E424	G425	T426	T427	N428	A430	T434	T457	S461	E468	R469	G470										
SER	SER	GLU	GLY	CYS	SER	THR	GLU	VAL	ARG	PRO	GLU	GLY	THR	VAL	CYS	CYS	ASP	ALA	LEU	LEU	LEU	ARG	PRO	THR	LEU	ASP	GLN	S263	Q273	A305	H309	G314	S315	L316	N320	L324	Y325	N326	V327	G328	K332	D335	C338						
GLY	LEU	GLY	ASP	GLY	SER	SER	VAL	GLN	LEU	ASN	ARG	VAL	THR	LEU	GLY	VAL	PHE	THR	ILE	SER	PRO	GLN	ARG	THR	VAL	PRO	PRO	ASN	MET	ALA	VAL	THR	ILE	SER	VAL	PHE	TRP	ASP	VAL	THR	LYS	THR	GLY	THR	THR	GLY	ASP	ARG	LEU
PHE	SER	LEU	GLY	PRO	SER	GLN	VAL	MET	LYS	ASP	GLY	GLN	PRO	PRO	GLN	VAL	THR	ARG	LEU	PRO	LYS	ALA	GLU	THR	VAL	ASN	PRO	THR	ARG	LEU	ALA	VAL	THR	ILE	LEU	VAL	ASP	GLY	ASN	MET	THR	TYR	ASN	GLN	ASP	LEU	TYR		
ASP	LEU	TYR	LYS	ASP	ASP	ALA	LYS	LEU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	ASN	LEU	TYR	GLU	TYR	ALA	PHE	GLN	HIS	GLY	MET	GLY	THR	GLN	THR	GLY	VAL	LYS	LEU	CYS	THR	ASN	GLN	ASN	MET	TYR	ASN	GLN	ASP	ALA			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166116	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	49310	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.352	Depositor
Minimum map value	-0.236	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	194.68802, 194.68802, 194.68802	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: Y01, GXR, CLR, PLM

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	0.30	1/1736 (0.1%)	0.38	0/2336
2	B	0.22	0/2647	0.40	0/3589
3	G	0.14	0/435	0.32	0/587
4	R	0.22	0/2166	0.42	0/2941
All	All	0.24	1/6984 (0.0%)	0.40	0/9453

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	ASN	C-N	8.73	1.45	1.33

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	1707	0	1699	33	0
2	B	2600	0	2505	42	0
3	G	429	0	441	4	0
4	R	2107	0	2158	37	0
5	A	17	0	31	2	0
5	R	36	0	62	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	35	0	49	2	0
7	R	28	0	0	0	0
8	R	56	0	92	14	0
All	All	7015	0	7037	124	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 9.

All (124) 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)
8:R:605:CLR:H222	8:R:605:CLR:H273	1.43	0.98
8:R:605:CLR:H211	8:R:606:CLR:H151	1.48	0.94
8:R:605:CLR:H212	8:R:606:CLR:H72	1.57	0.86
8:R:605:CLR:H222	8:R:605:CLR:C27	2.10	0.81
4:R:457:ILE:HG13	4:R:476:VAL:HG21	1.63	0.79
5:A:401:PLM:H52	4:R:479:LEU:HD11	1.68	0.75
8:R:605:CLR:H212	8:R:606:CLR:C7	2.17	0.73
1:A:341:ASP:OD1	4:R:472:ASN:ND2	2.23	0.71
8:R:605:CLR:C21	8:R:606:CLR:H151	2.20	0.70
1:A:187:GLU:OE2	1:A:198:ARG:NH1	2.26	0.69
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.77	0.67
1:A:324:THR:HG22	1:A:326:ALA:H	1.58	0.67
4:R:338:CYS:HA	4:R:341:ARG:HB2	1.75	0.67
2:B:16:ASN:HD22	2:B:19:ARG:HH12	1.44	0.66
1:A:55:ILE:HA	1:A:188:THR:HG22	1.78	0.66
2:B:271:CYS:HB3	2:B:290:ASP:HB2	1.75	0.66
1:A:252:ASP:O	1:A:256:ASN:ND2	2.27	0.65
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.80	0.63
4:R:358:LEU:HD22	4:R:382:LEU:HD22	1.81	0.63
2:B:161:SER:OG	2:B:163:ASP:OD1	2.17	0.63
1:A:318:GLU:OE1	4:R:471:LYS:NZ	2.32	0.63
2:B:162:GLY:HA2	2:B:186:ASP:HB2	1.79	0.62
2:B:149:CYS:O	2:B:150:ARG:NH1	2.34	0.60
2:B:248:ALA:HB1	2:B:269:ILE:HG22	1.84	0.60
3:G:48:ASP:HB3	3:G:51:LEU:HB3	1.84	0.59
2:B:215:GLU:HB3	2:B:217:MET:HG2	1.84	0.58
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.84	0.58
1:A:348:LEU:O	1:A:353:LEU:HB2	2.05	0.57
2:B:22:ARG:O	2:B:259:GLN:NE2	2.37	0.56
4:R:383:SER:HG	4:R:387:TRP:CD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ILE:HD11	3:G:23:ALA:HA	1.88	0.56
3:G:8:SER:HB2	3:G:11:GLN:HE21	1.71	0.56
1:A:189:HIS:ND1	1:A:189:HIS:O	2.39	0.55
2:B:5:ASP:O	2:B:9:GLN:HG2	2.07	0.55
4:R:316:LEU:O	4:R:320:ASN:ND2	2.34	0.54
4:R:430:ALA:O	4:R:434:THR:OG1	2.22	0.53
2:B:30:LEU:HD23	2:B:262:MET:HE3	1.90	0.53
4:R:353:PHE:HZ	4:R:494:ILE:HD11	1.73	0.53
1:A:255:CYS:O	1:A:317:LYS:NZ	2.42	0.53
1:A:38:LEU:HD21	1:A:46:LYS:HB2	1.89	0.52
1:A:44:SER:HA	1:A:227:ASP:HB2	1.91	0.52
4:R:508:LEU:HD23	4:R:512:LEU:HD23	1.90	0.52
1:A:40:GLY:O	1:A:46:LYS:NZ	2.27	0.52
2:B:279:SER:OG	2:B:280:LYS:N	2.42	0.51
5:A:401:PLM:H82	4:R:360:ALA:HA	1.92	0.51
4:R:314:GLY:HA3	5:R:602:PLM:H72	1.92	0.51
2:B:12:GLU:HA	2:B:15:LYS:HE2	1.92	0.51
4:R:394:VAL:HG11	8:R:606:CLR:H261	1.93	0.51
2:B:68:ARG:NH2	2:B:83:ASP:OD2	2.43	0.51
2:B:142:HIS:CD2	2:B:169:TRP:HZ2	2.29	0.51
1:A:343:ILE:HD12	4:R:371:PHE:HE1	1.76	0.50
1:A:344:ILE:HG21	4:R:457:ILE:HD11	1.93	0.50
1:A:349:ARG:HD2	1:A:354:TYR:CZ	2.48	0.49
1:A:349:ARG:CD	1:A:354:TYR:CE2	2.95	0.48
4:R:519:CYS:HA	4:R:522:THR:HG22	1.94	0.48
1:A:49:ILE:HG23	1:A:50:VAL:HG23	1.95	0.48
4:R:326:ASN:HD21	4:R:345:PHE:HB2	1.79	0.48
4:R:353:PHE:CZ	4:R:494:ILE:HD11	2.49	0.47
2:B:234:PHE:HE1	2:B:255:LEU:HD11	1.80	0.47
1:A:257:ASN:OD1	1:A:258:LYS:N	2.46	0.47
2:B:99:TRP:HB3	2:B:117:LEU:HD12	1.96	0.47
8:R:605:CLR:C21	8:R:606:CLR:H72	2.35	0.47
1:A:349:ARG:HD2	1:A:354:TYR:CE2	2.49	0.47
2:B:333:ASP:O	2:B:334:SER:OG	2.31	0.47
4:R:461:SER:OG	4:R:473:ARG:NH1	2.45	0.46
4:R:383:SER:HG	4:R:387:TRP:HD1	1.62	0.46
4:R:273:GLN:HA	4:R:324:LEU:HD21	1.98	0.46
4:R:492:LEU:O	4:R:496:THR:OG1	2.30	0.46
1:A:55:ILE:HG23	1:A:56:ILE:H	1.80	0.46
2:B:262:MET:SD	2:B:302:ALA:HB2	2.56	0.46
2:B:212:ASP:HB2	2:B:219:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:305:ALA:O	4:R:309[A]:HIS:ND1	2.49	0.46
2:B:123:ILE:O	2:B:136:SER:OG	2.27	0.45
2:B:192:LEU:HD23	2:B:199:PHE:HB3	1.96	0.45
4:R:338:CYS:CA	4:R:341:ARG:HB2	2.44	0.45
2:B:274:THR:HG21	2:B:316:SER:HA	1.97	0.45
4:R:350:LEU:HB2	4:R:390:PRO:HB3	1.99	0.45
4:R:427:THR:O	4:R:428:MET:HE2	2.17	0.45
2:B:164:THR:HA	2:B:186:ASP:HA	1.98	0.45
4:R:347:TYR:HB2	4:R:394:VAL:HG21	1.98	0.45
1:A:53:MET:HA	1:A:190:PHE:HB3	1.98	0.45
4:R:408:ILE:O	4:R:416:SER:OG	2.34	0.45
1:A:301:ALA:HB1	1:A:323:MET:HE1	1.98	0.44
2:B:205:ASP:OD2	2:B:207:SER:OG	2.31	0.44
8:R:605:CLR:H273	8:R:605:CLR:C22	2.24	0.44
2:B:54:HIS:CE1	2:B:80:ILE:HD12	2.53	0.44
1:A:39:LEU:HD13	1:A:254:ILE:HG13	1.99	0.43
4:R:423:ARG:O	4:R:428:MET:HE1	2.18	0.43
2:B:23:LYS:HE3	2:B:23:LYS:HB2	1.67	0.43
1:A:339:VAL:O	1:A:343:ILE:HG13	2.18	0.43
2:B:286:LEU:HD22	2:B:327:VAL:HG11	1.99	0.43
1:A:321:CYS:SG	1:A:322:HIS:N	2.92	0.42
2:B:8:ARG:HH22	3:G:12:ALA:HB1	1.84	0.42
2:B:44:GLN:O	2:B:44:GLN:HG2	2.19	0.42
2:B:180:PHE:CE1	2:B:216:GLY:HA2	2.54	0.42
4:R:403:TYR:O	4:R:423:ARG:HD3	2.19	0.42
4:R:411:ARG:NH1	4:R:411:ARG:O	2.53	0.42
1:A:291:TYR:HB2	1:A:303:TYR:CE2	2.54	0.42
6:R:601:Y01:HAE1	6:R:601:Y01:HAS2	1.80	0.42
2:B:57:LYS:O	2:B:74:SER:OG	2.20	0.42
2:B:150:ARG:HA	2:B:150:ARG:HD3	1.85	0.42
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.89	0.41
2:B:27:ASP:OD2	2:B:28:ALA:N	2.54	0.41
2:B:125:ASN:OD1	2:B:126:LEU:N	2.53	0.41
8:R:606:CLR:H183	8:R:606:CLR:H20	1.79	0.41
2:B:149:CYS:HB2	2:B:157:ILE:HD11	2.01	0.41
4:R:326:ASN:HB3	4:R:419:LEU:HD11	2.01	0.41
1:A:221:ALA:HB2	1:A:342:ILE:HD13	2.02	0.41
4:R:377:HIS:HB3	4:R:380:LEU:HB3	2.03	0.41
4:R:526:LEU:HD23	4:R:526:LEU:HA	1.92	0.41
8:R:606:CLR:H162	8:R:606:CLR:H221	1.62	0.41
2:B:61:MET:HE2	2:B:61:MET:HB2	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:492:LEU:HD23	4:R:492:LEU:HA	1.91	0.41
1:A:41:ALA:O	1:A:44:SER:OG	2.31	0.41
1:A:324:THR:HG22	1:A:326:ALA:N	2.32	0.41
1:A:343:ILE:HD12	4:R:371:PHE:CE1	2.55	0.41
2:B:235:PHE:HD2	2:B:237:ASN:OD1	2.04	0.41
6:R:601:Y01:HBB	6:R:601:Y01:HAE2	1.54	0.41
8:R:606:CLR:H232	8:R:606:CLR:C16	2.50	0.40
1:A:51:LYS:HD3	1:A:51:LYS:HA	1.72	0.40
2:B:160:SER:HB3	2:B:190:LEU:HD23	2.02	0.40
8:R:605:CLR:H212	8:R:606:CLR:H71	1.99	0.40
1:A:209:ARG:O	1:A:213:ILE:HB	2.21	0.40
8:R:605:CLR:H111	8:R:606:CLR:H6	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/226 (93%)	200 (95%)	11 (5%)	0	100	100
2	B	336/346 (97%)	320 (95%)	16 (5%)	0	100	100
3	G	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
4	R	264/561 (47%)	252 (96%)	12 (4%)	0	100	100
All	All	865/1204 (72%)	824 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/194 (97%)	188 (100%)	0	100	100
2	B	281/289 (97%)	281 (100%)	0	100	100
3	G	45/58 (78%)	45 (100%)	0	100	100
4	R	221/483 (46%)	221 (100%)	0	100	100
All	All	735/1024 (72%)	735 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	214	HIS
1	A	270	ASN
1	A	295	ASN
1	A	307	GLN
1	A	333	GLN
2	B	16	ASN
2	B	119	ASN
2	B	311	HIS
3	G	11	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
5	PLM	A	401	1	15,16,17	0.32	0	14,15,17	0.66	0
6	Y01	R	601	-	38,38,38	4.02	17 (44%)	57,57,57	1.84	12 (21%)
5	PLM	R	603	-	17,17,17	0.55	0	17,17,17	0.74	0
8	CLR	R	605	-	31,31,31	0.60	0	48,48,48	1.52	8 (16%)
5	PLM	R	602	-	17,17,17	0.55	0	17,17,17	0.75	0
8	CLR	R	606	-	31,31,31	0.61	0	48,48,48	1.54	8 (16%)
7	GXR	R	604	-	28,31,31	1.25	4 (14%)	43,53,53	2.40	13 (30%)

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	PLM	A	401	1	-	6/14/14/15	-
6	Y01	R	601	-	-	8/19/77/77	0/4/4/4
5	PLM	R	603	-	-	7/15/15/15	-
8	CLR	R	605	-	-	5/10/68/68	0/4/4/4
5	PLM	R	602	-	-	5/15/15/15	-
8	CLR	R	606	-	-	4/10/68/68	0/4/4/4
7	GXR	R	604	-	-	6/8/84/84	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	Y01	CAU-CAS	-11.34	1.30	1.53
6	R	601	Y01	CAS-CBF	-10.22	1.36	1.53
6	R	601	Y01	CBI-CBE	-9.31	1.37	1.55
6	R	601	Y01	CBH-CBF	8.49	1.69	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	Y01	CBH-CAZ	-5.40	1.42	1.52
6	R	601	Y01	CBI-CBG	4.93	1.64	1.55
6	R	601	Y01	CAQ-CBG	-4.70	1.44	1.54
6	R	601	Y01	CAU-CBI	4.43	1.61	1.54
6	R	601	Y01	CAQ-CAP	4.36	1.65	1.54
6	R	601	Y01	CBD-CBF	-4.09	1.45	1.53
6	R	601	Y01	CAP-CBE	3.66	1.61	1.54
6	R	601	Y01	OAW-CBC	-3.38	1.38	1.46
7	R	604	GXR	C5-C15	3.15	1.57	1.53
6	R	601	Y01	OAW-CAY	3.02	1.42	1.34
6	R	601	Y01	CAK-CAI	2.78	1.55	1.50
6	R	601	Y01	CBD-CBG	2.57	1.58	1.53
7	R	604	GXR	C1-C2	-2.53	1.50	1.54
6	R	601	Y01	CBB-CBE	2.38	1.58	1.54
7	R	604	GXR	C5-C1	2.30	1.59	1.56
7	R	604	GXR	C4-CL1	2.29	1.87	1.79
6	R	601	Y01	CAM-CAY	2.09	1.56	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	604	GXR	C20-C15-C5	7.68	124.11	117.63
6	R	601	Y01	CBI-CBG-CBD	-6.10	105.76	114.41
6	R	601	Y01	CBI-CBE-CBB	-6.01	110.22	119.50
7	R	604	GXR	C1-C5-C15	5.83	120.48	112.86
7	R	604	GXR	C10-C18-C21	-5.23	120.41	124.37
8	R	606	CLR	C13-C17-C20	-4.90	111.93	119.50
8	R	605	CLR	C13-C17-C20	-4.90	111.94	119.50
7	R	604	GXR	C18-C10-C14	-4.84	109.50	112.33
8	R	606	CLR	C13-C14-C8	-4.32	108.28	114.41
8	R	605	CLR	C13-C14-C8	-4.22	108.42	114.41
6	R	601	Y01	OAW-CAY-CAM	3.95	120.03	111.48
7	R	604	GXR	C21-C22-C19	-3.63	113.44	117.12
6	R	601	Y01	CAS-CBF-CBH	-3.59	108.66	113.08
7	R	604	GXR	C10-C14-C19	-3.52	119.63	122.15
7	R	604	GXR	O3-C15-C5	-3.38	118.78	122.78
6	R	601	Y01	CAP-CAQ-CBG	-3.07	99.14	105.14
6	R	601	Y01	CAS-CAU-CBI	-2.82	107.98	112.74
8	R	605	CLR	C11-C12-C13	-2.77	108.07	112.74
8	R	606	CLR	C8-C7-C6	-2.76	108.94	112.76
8	R	605	CLR	C8-C7-C6	-2.70	109.02	112.76
8	R	606	CLR	C11-C12-C13	-2.70	108.18	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	604	GXR	O1-C5-C15	-2.53	101.75	107.25
7	R	604	GXR	C12-C1-C2	-2.52	106.86	111.72
7	R	604	GXR	C18-C21-C22	-2.51	119.37	121.49
6	R	601	Y01	CBG-CBI-CBE	2.49	102.96	100.10
8	R	606	CLR	C11-C9-C10	-2.46	110.06	113.08
8	R	606	CLR	C17-C13-C14	2.45	102.91	100.10
8	R	605	CLR	C11-C9-C10	-2.43	110.09	113.08
7	R	604	GXR	C5-C1-C2	2.37	101.48	99.35
8	R	605	CLR	C10-C9-C8	-2.30	109.35	112.71
8	R	605	CLR	C17-C13-C14	2.30	102.74	100.10
6	R	601	Y01	CAU-CAS-CBF	2.29	117.03	113.14
6	R	601	Y01	CBH-CBF-CBD	-2.28	109.38	112.71
8	R	606	CLR	C23-C22-C20	-2.25	108.78	115.08
7	R	604	GXR	C4-C10-C14	2.25	109.18	106.89
6	R	601	Y01	CAC-CBB-CBE	-2.24	109.53	112.88
6	R	601	Y01	CAD-CBH-CBF	-2.16	109.24	111.66
8	R	606	CLR	C10-C9-C8	-2.16	109.56	112.71
7	R	604	GXR	O1-C5-C8	-2.10	104.62	110.84
6	R	601	Y01	CBF-CBD-CBG	-2.09	106.36	109.09
8	R	605	CLR	C23-C22-C20	-2.06	109.30	115.08

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	601	Y01	CAO-CBB-CBE-CAP
6	R	601	Y01	CAO-CBB-CBE-CBI
6	R	601	Y01	CAC-CBB-CBE-CBI
6	R	601	Y01	OAG-CAY-OAW-CBC
6	R	601	Y01	CAM-CAY-OAW-CBC
7	R	604	GXR	C20-C15-C5-C1
7	R	604	GXR	O3-C15-C5-C1
7	R	604	GXR	C20-C15-C5-O1
7	R	604	GXR	O3-C15-C5-O1
7	R	604	GXR	C5-C15-C20-O4
7	R	604	GXR	O3-C15-C20-O4
6	R	601	Y01	CAC-CBB-CBE-CAP
8	R	606	CLR	C13-C17-C20-C22
6	R	601	Y01	CAJ-CAO-CBB-CAC
8	R	606	CLR	C13-C17-C20-C21
8	R	605	CLR	C21-C20-C22-C23
5	A	401	PLM	C7-C8-C9-CA

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Mol	Chain	Res	Type	Atoms
5	R	602	PLM	C5-C6-C7-C8
5	A	401	PLM	C9-CA-CB-CC
8	R	606	CLR	C16-C17-C20-C21
5	R	603	PLM	CA-CB-CC-CD
5	R	603	PLM	CB-CC-CD-CE
5	R	602	PLM	C7-C8-C9-CA
5	A	401	PLM	C5-C6-C7-C8
5	A	401	PLM	CB-CC-CD-CE
8	R	606	CLR	C16-C17-C20-C22
5	R	602	PLM	C2-C3-C4-C5
5	R	602	PLM	C4-C5-C6-C7
5	R	603	PLM	C5-C6-C7-C8
5	R	603	PLM	C3-C4-C5-C6
6	R	601	Y01	CAJ-CAO-CBB-CBE
5	A	401	PLM	CC-CD-CE-CF
5	R	602	PLM	C3-C4-C5-C6
8	R	605	CLR	C13-C17-C20-C21
8	R	605	CLR	C13-C17-C20-C22
5	A	401	PLM	C3-C4-C5-C6
5	R	603	PLM	C6-C7-C8-C9
5	R	603	PLM	O1-C1-C2-C3
5	R	603	PLM	O2-C1-C2-C3
8	R	605	CLR	C22-C23-C24-C25
8	R	605	CLR	C17-C20-C22-C23

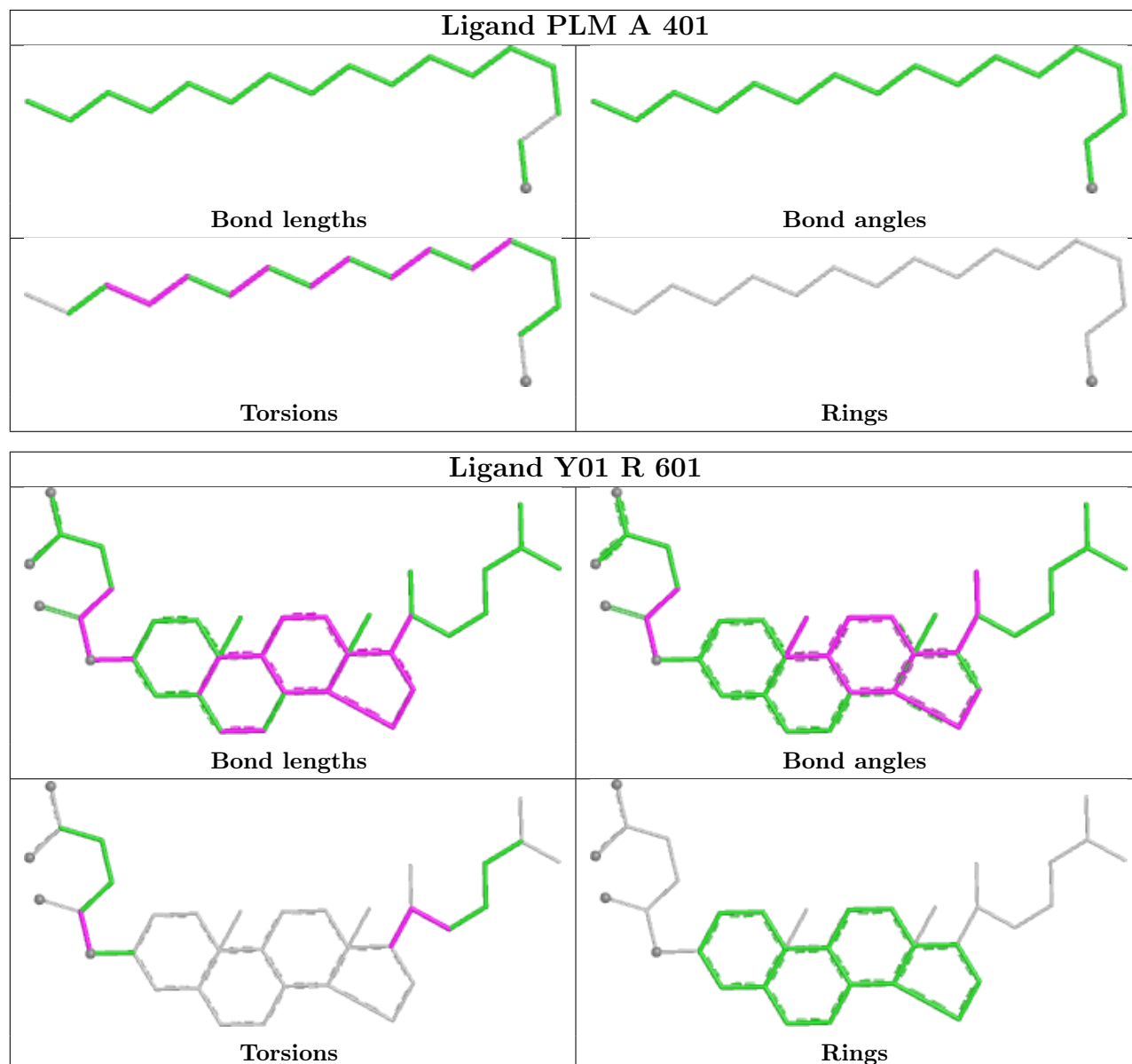
There are no ring outliers.

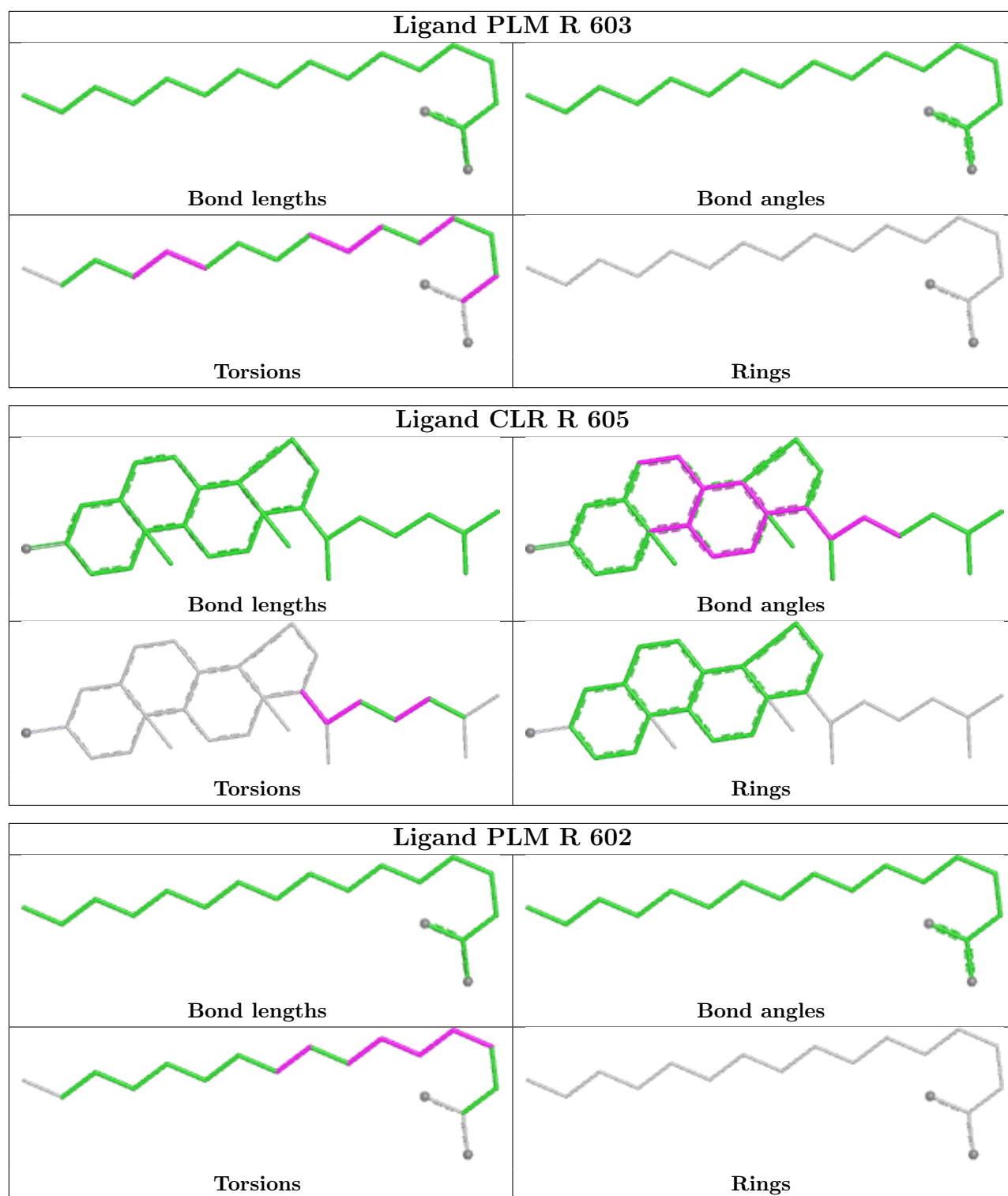
5 monomers are involved in 19 short contacts:

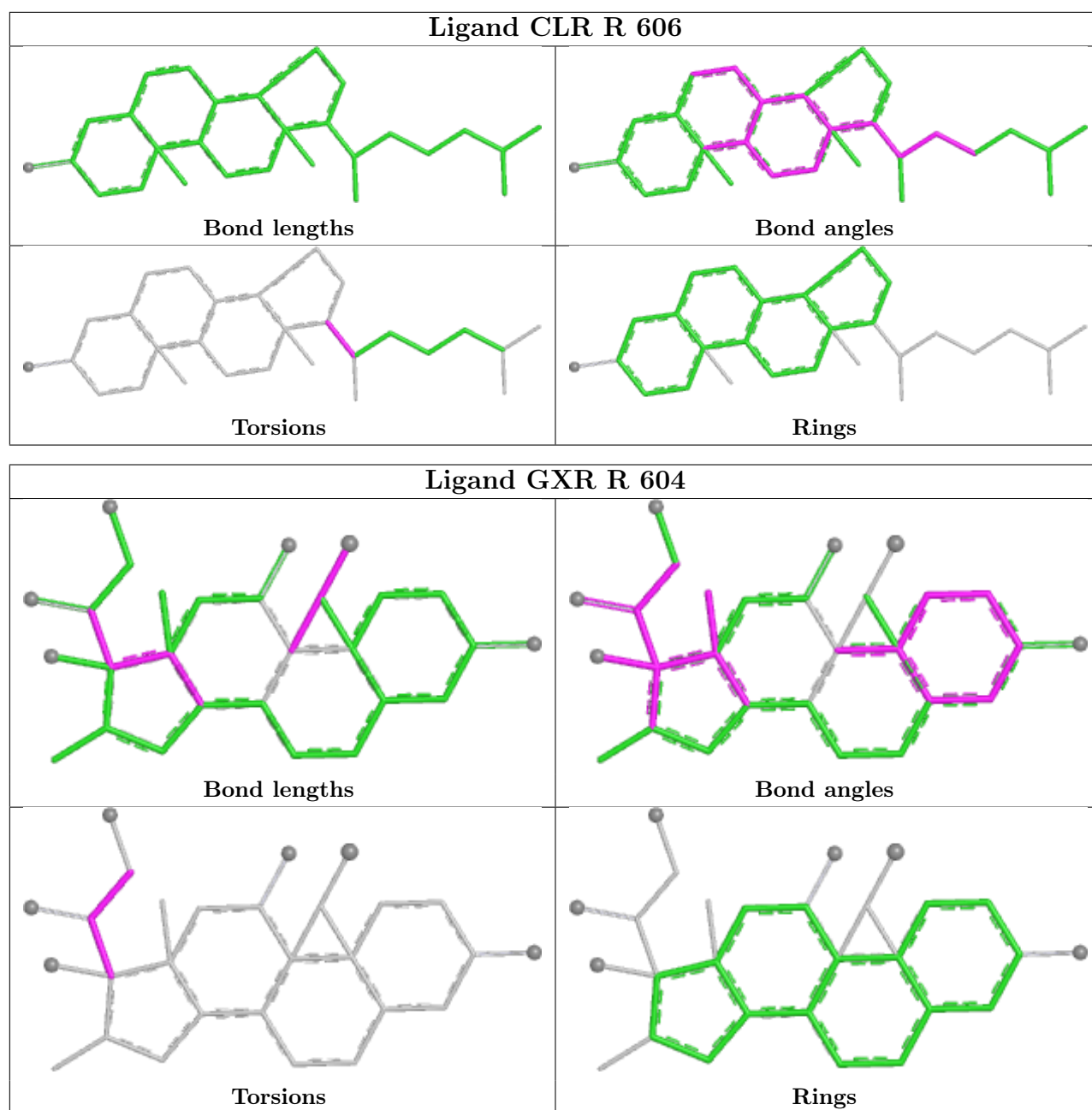
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	PLM	2	0
6	R	601	Y01	2	0
8	R	605	CLR	10	0
5	R	602	PLM	1	0
8	R	606	CLR	11	0

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.

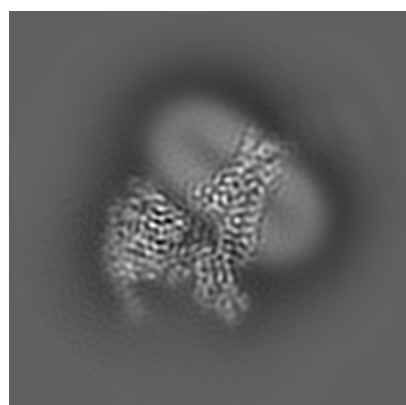
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30602. These allow visual inspection of the internal detail of the map and identification of artifacts.

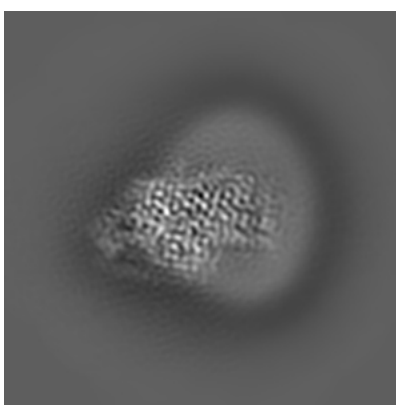
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

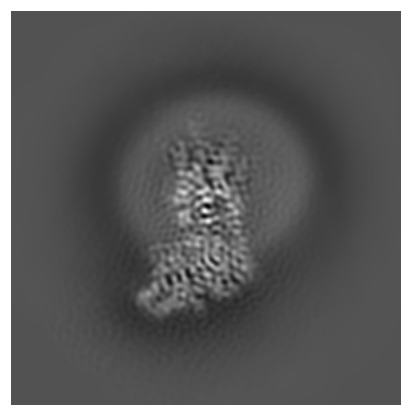
6.1.1 Primary map



X



Y

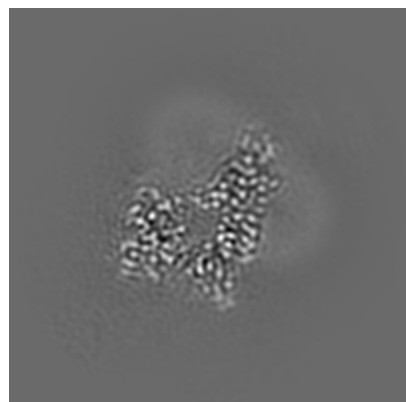


Z

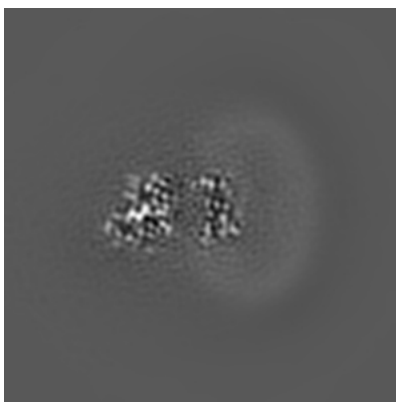
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

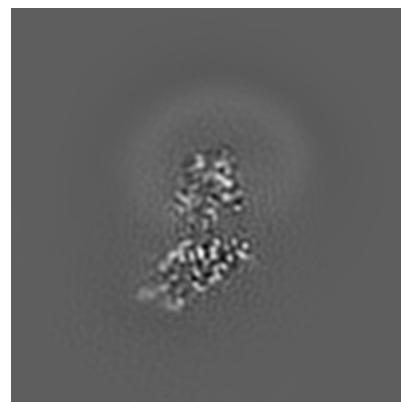
6.2.1 Primary map



X Index: 96



Y Index: 96

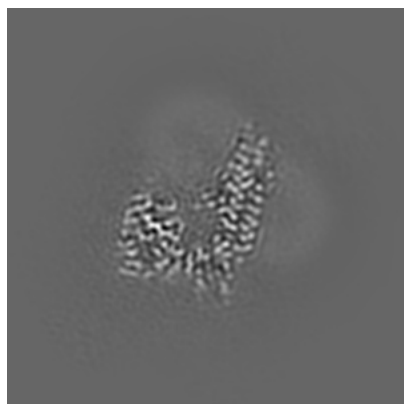


Z Index: 96

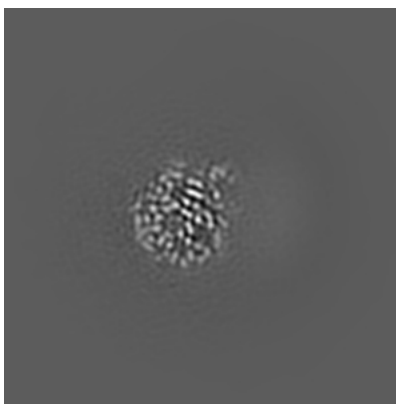
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

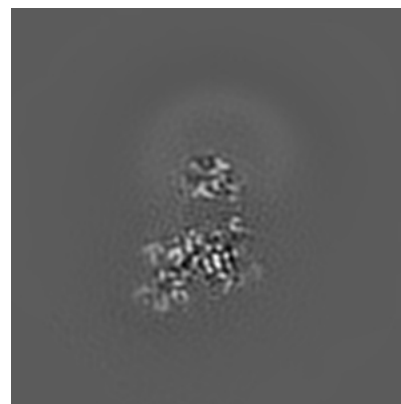
6.3.1 Primary map



X Index: 98



Y Index: 69

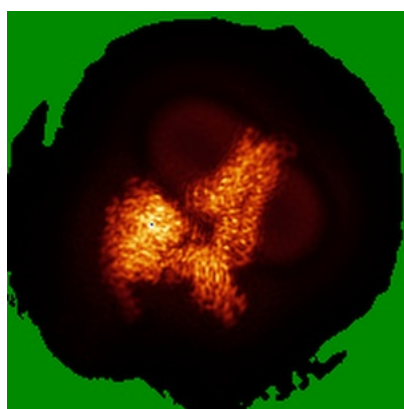


Z Index: 87

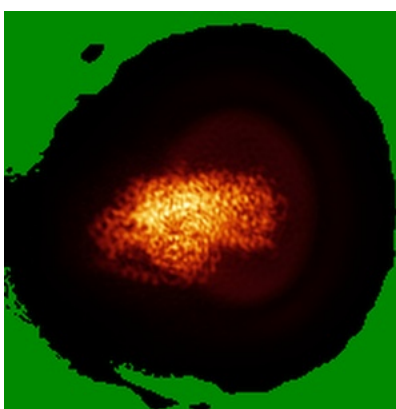
The images above show the largest variance slices of the map in three orthogonal directions.

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

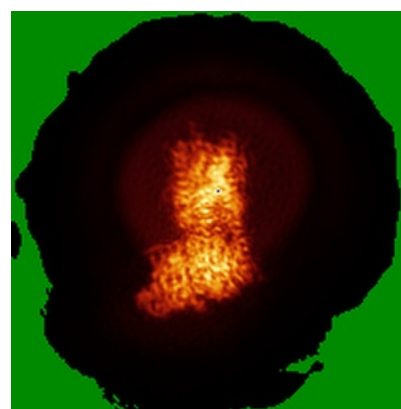
6.4.1 Primary map



X



Y



Z

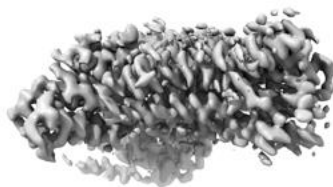
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

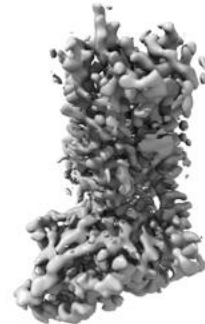
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

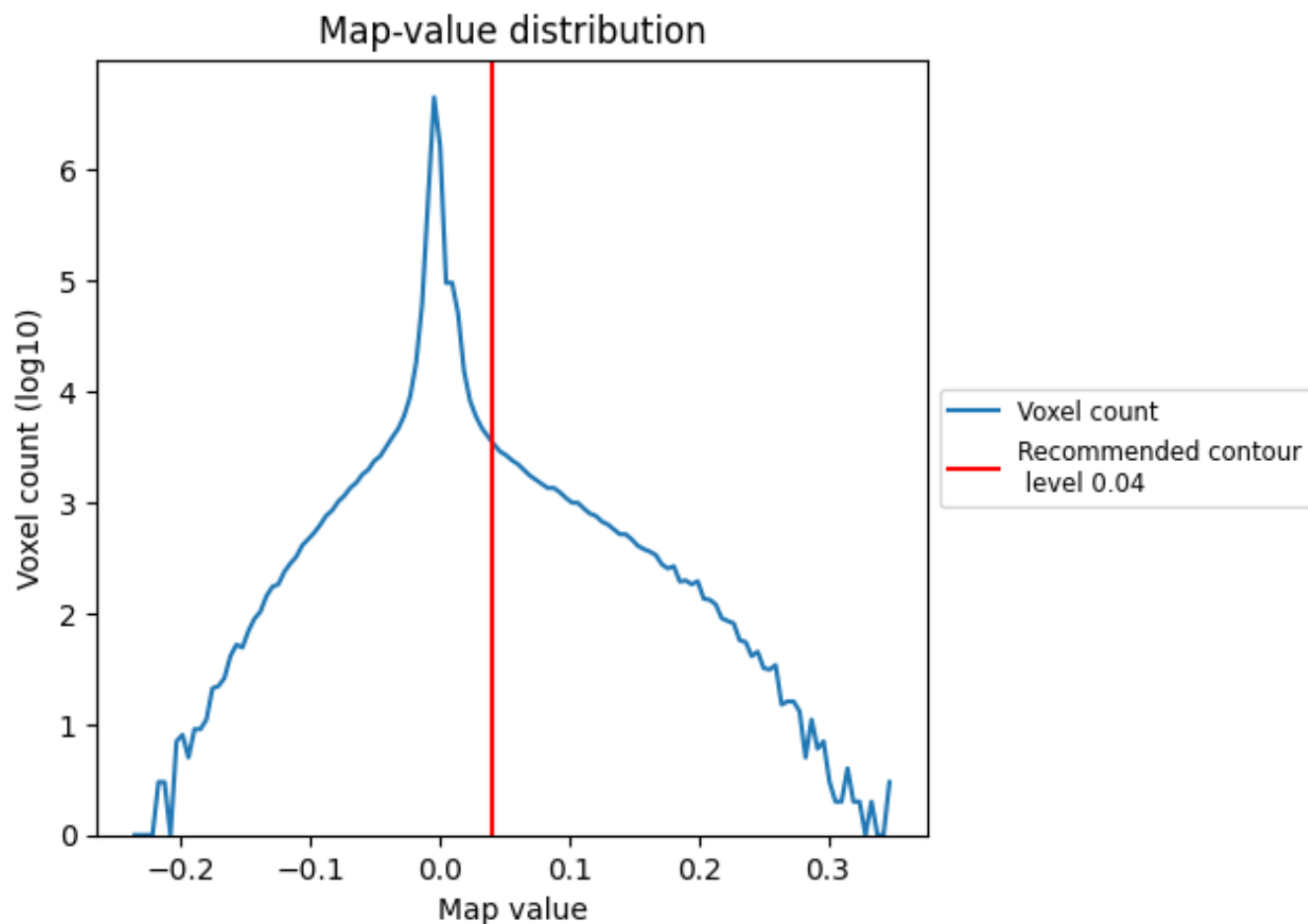
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

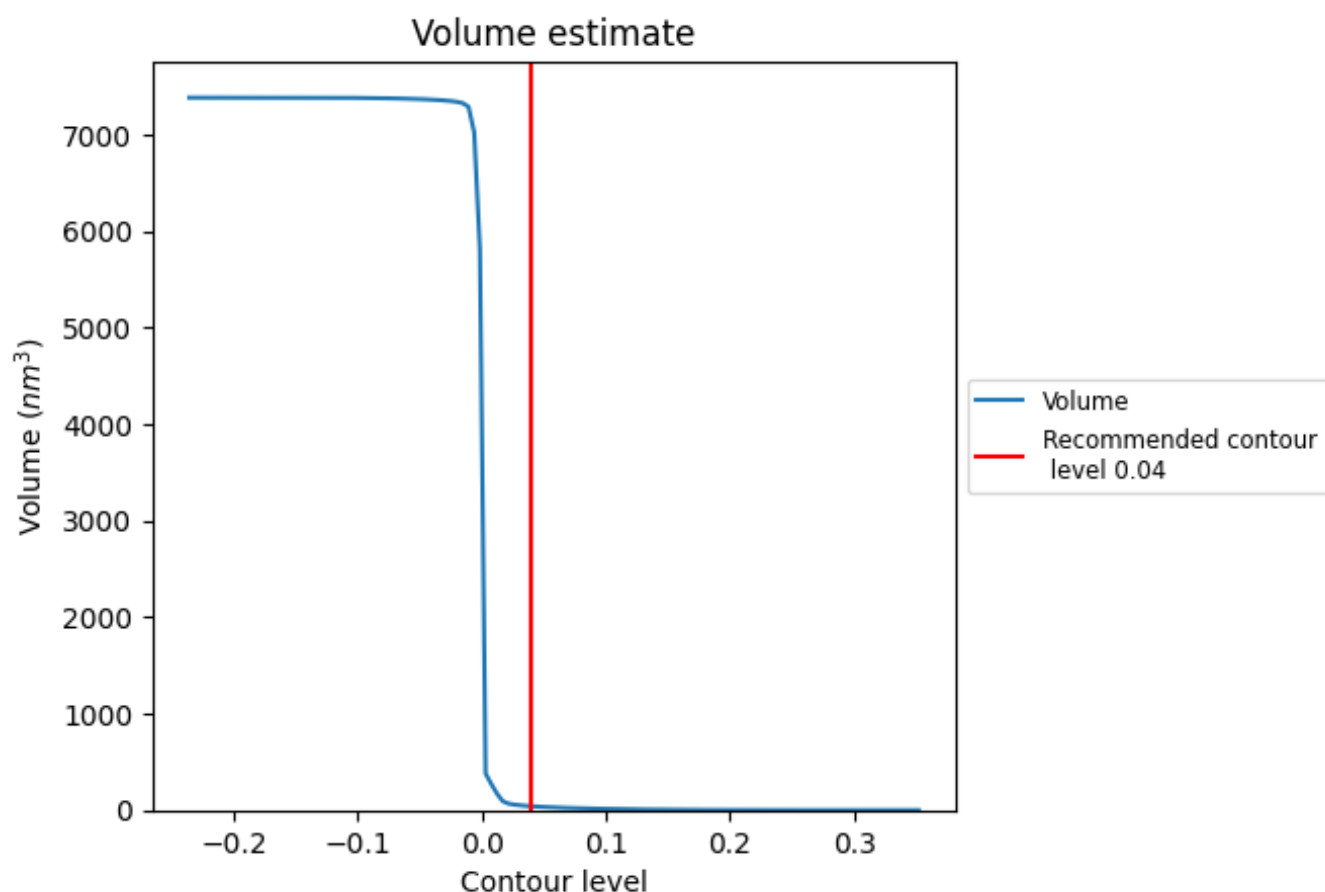
This section contains the results of statistical analysis of the map.

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.

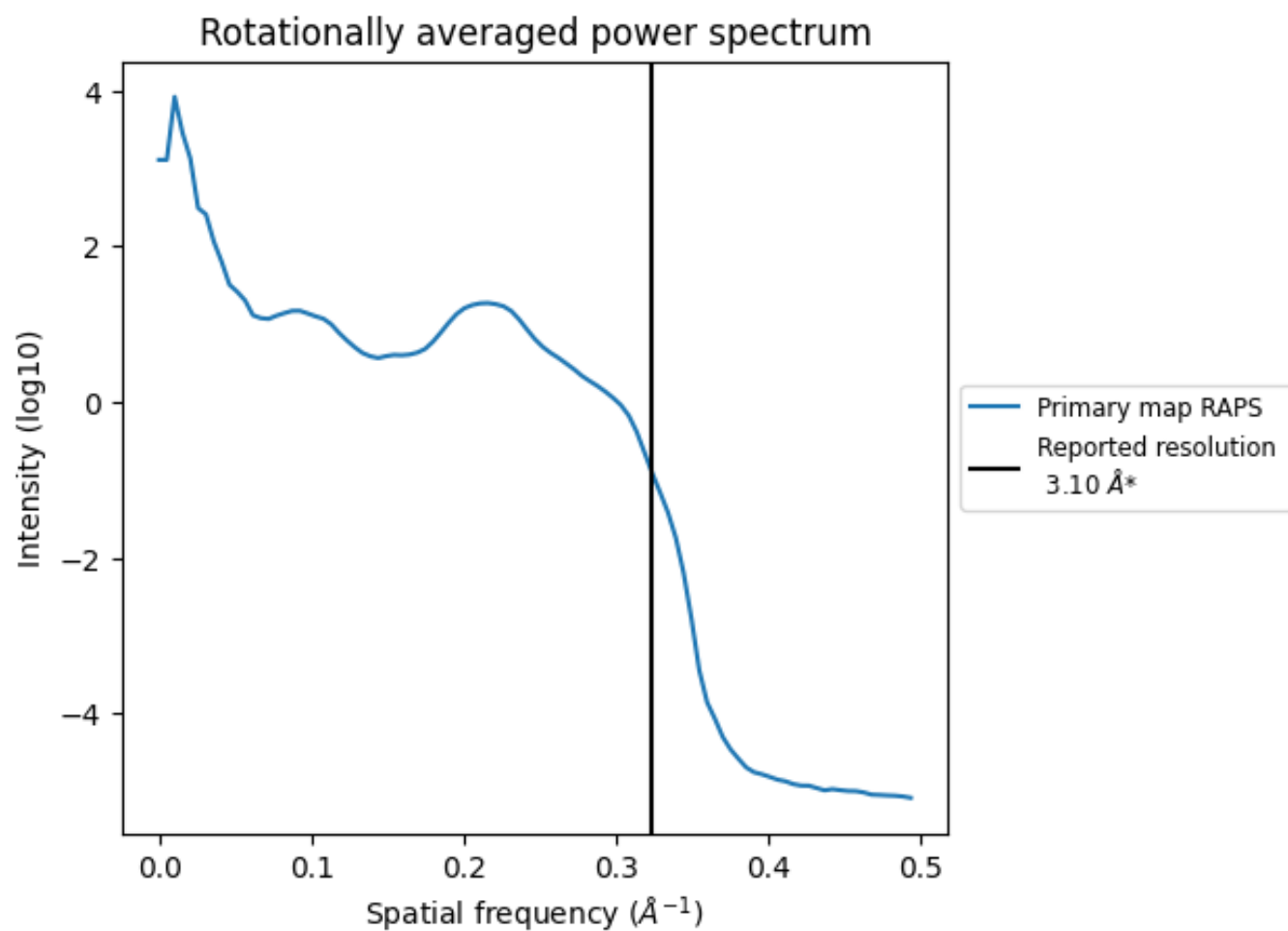
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm^3 ; this corresponds to an approximate mass of 36 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 ⓘ

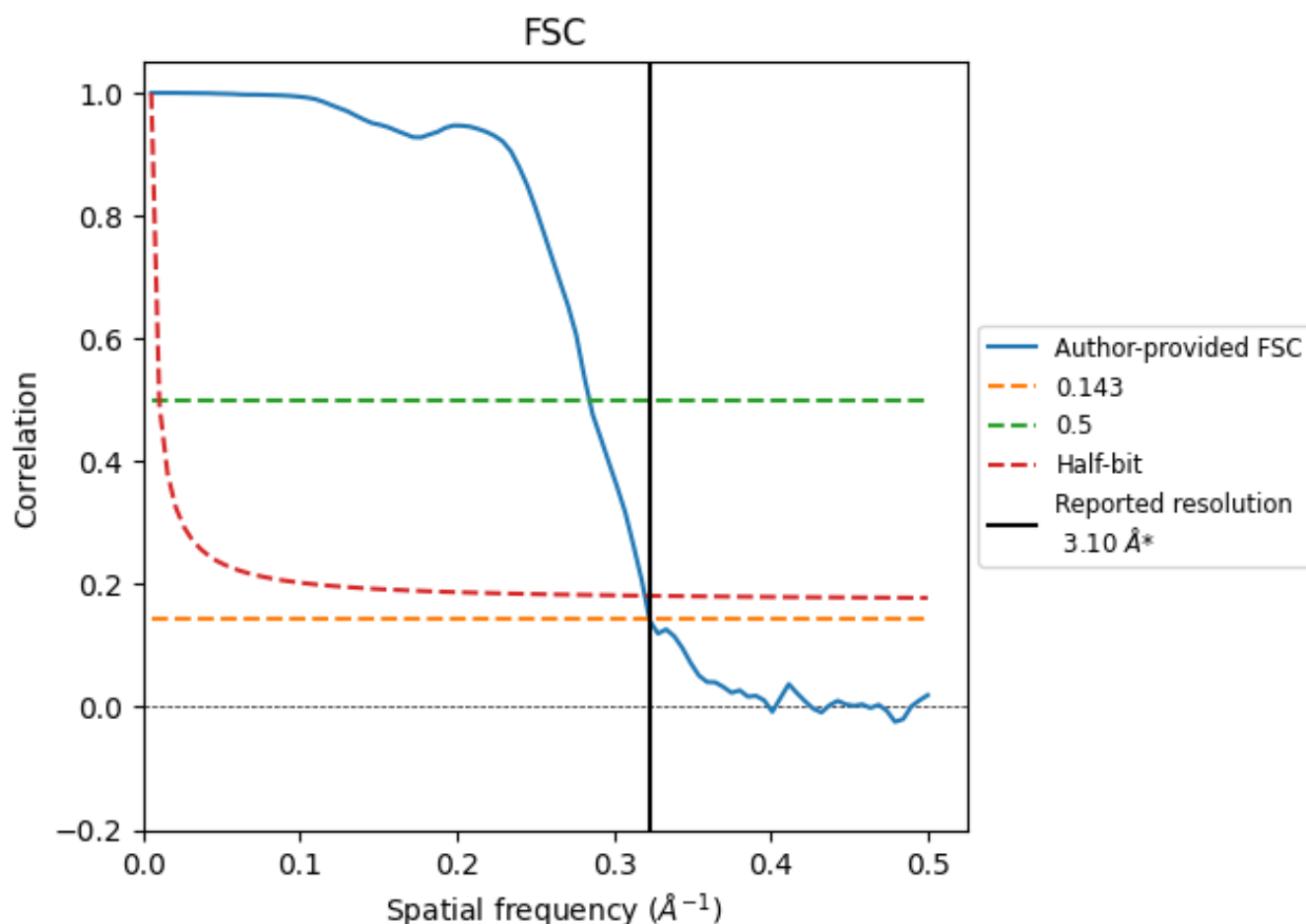


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

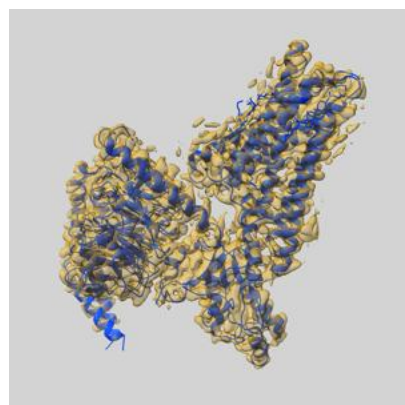
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.52	3.13
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

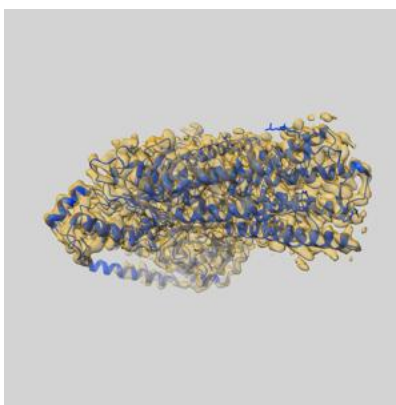
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30602 and PDB model 7D76. Per-residue inclusion information can be found in section [3](#) on page [8](#).

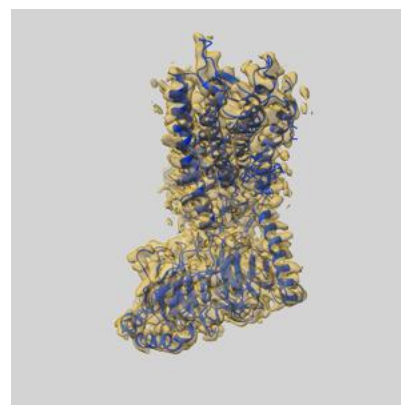
9.1 Map-model overlay [i](#)



X



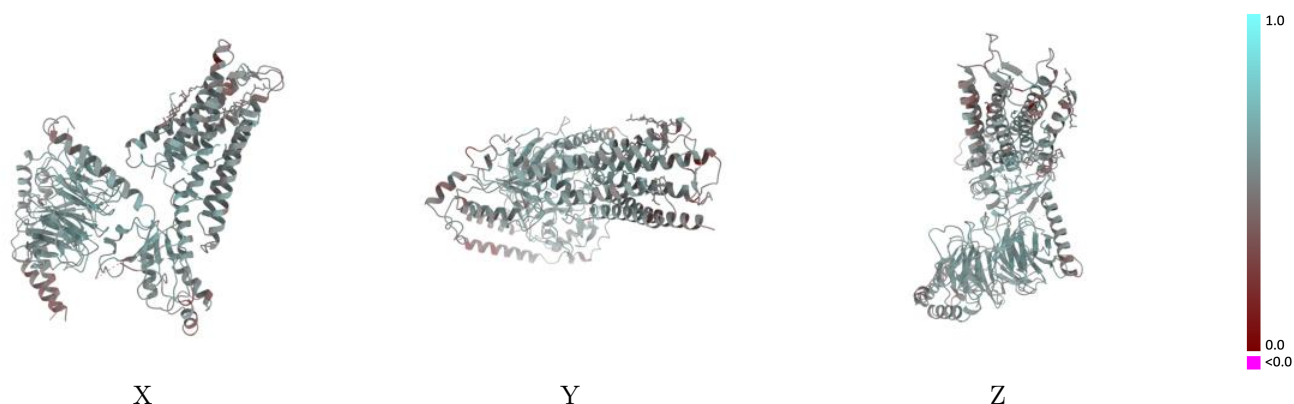
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)



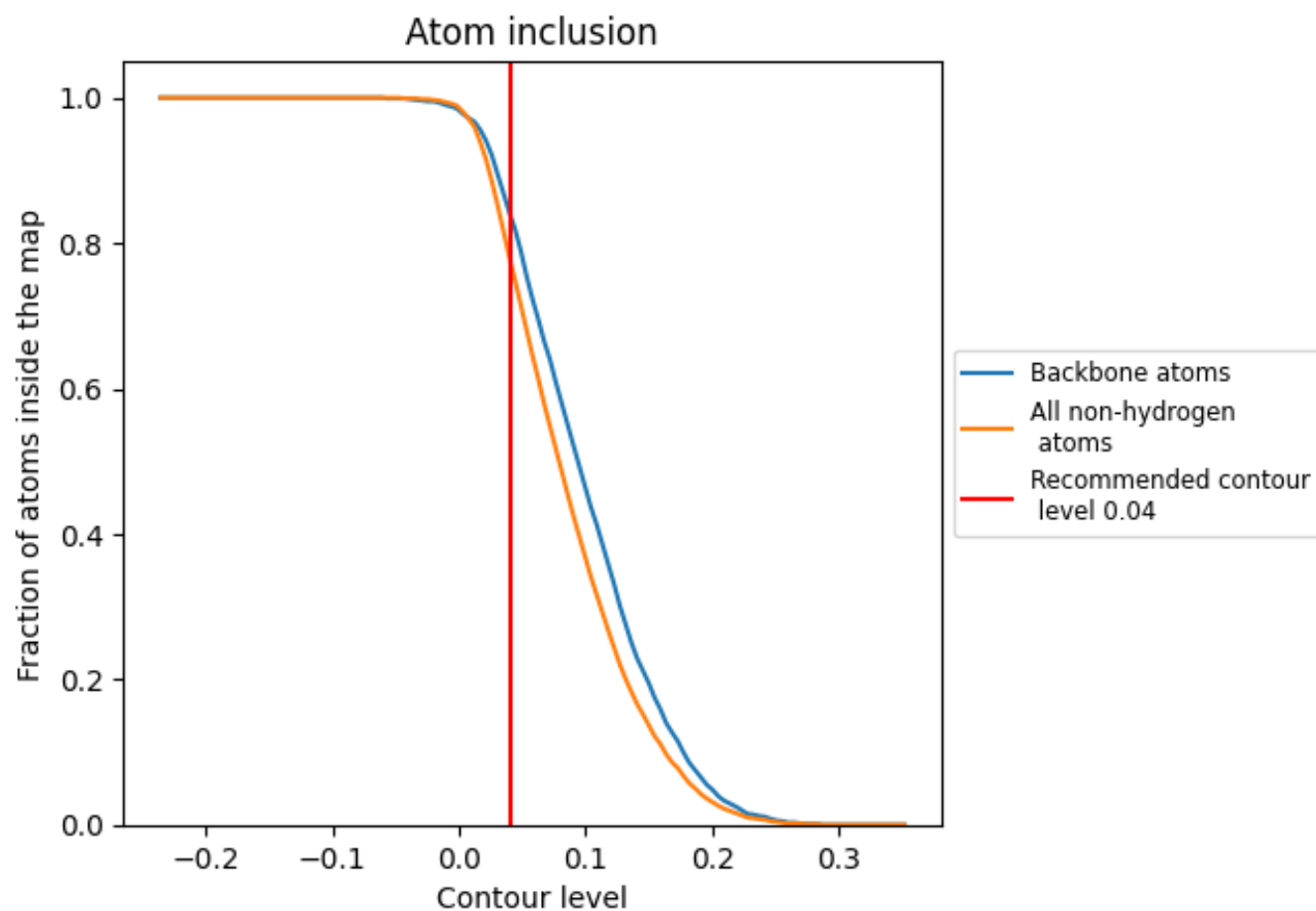
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.5260
A	0.7980	0.5240
B	0.8150	0.5500
G	0.5500	0.4800
R	0.7660	0.5080

