



Full wwPDB EM Validation Report ⓘ

Jul 23, 2026 – 05:21 AM JST

PDB ID : 23SO / pdb_000023so
EMDB ID : EMD-69218
Title : Cryo-EM structure of the cebranopadol-mu opioid receptor-Gi complex
Authors : Lai, Y.; Huang, X.; Shen, S.; Hu, W.; Xu, H.E.; Wang, Y.
Deposited on : 2026-02-16
Resolution : 2.95 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:

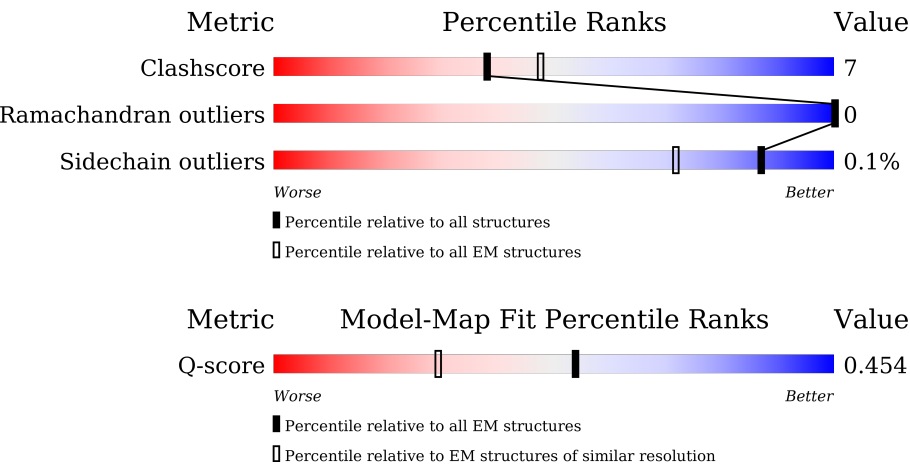
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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	13114 (2.45 - 3.45)

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	B	345	12% 78% 19% .
2	C	68	37% 75% 7% 18%
3	A	354	7% 53% 10% 36%
3	F	354	5% 95%

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Mol	Chain	Length	Quality of chain
4	M	400	 60% 12% 28%
4	R	400	 59% 13% 28%
5	E	247	 27% 81% 13% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11705 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(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	336	2578	1590	462	505	21	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 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		
2	C	56	436	274	77	82	3	0	0

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	18	138	87	22	28	1	0	0
3	A	225	1816	1154	300	349	13	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	203	ALA	GLY	engineered mutation	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
F	326	SER	ALA	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

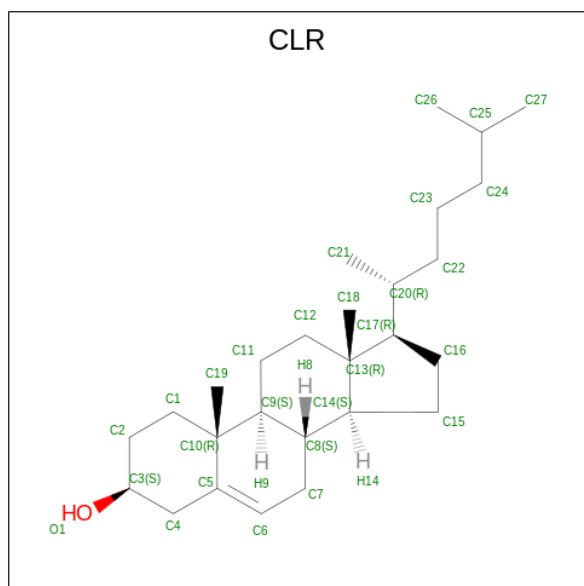
- Molecule 4 is a protein called Mu-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	288	Total	C	N	O	S	0	0
			2315	1536	369	384	26		
4	R	287	Total	C	N	O	S	0	0
			2309	1533	368	383	25		

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	231	Total	C	N	O	S	0	0
			1777	1128	294	345	10		

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



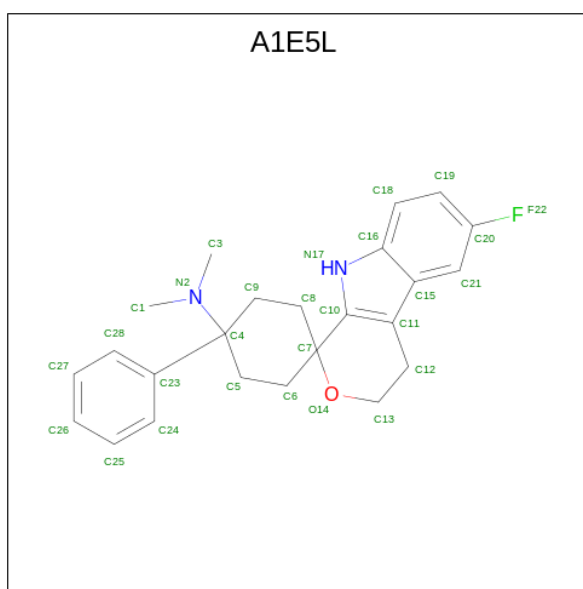
Mol	Chain	Residues	Atoms			AltConf
6	M	1	Total	C	O	0
			28	27	1	
6	M	1	Total	C	O	0
			28	27	1	

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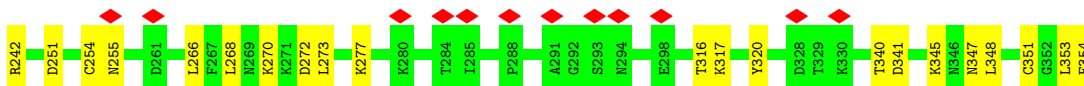
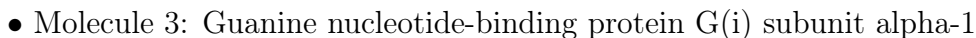
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Mol	Chain	Residues	Atoms			AltConf
6	M	1	Total	C	O	0
			28	27	1	
6	M	1	Total	C	O	0
			28	27	1	
6	M	1	Total	C	O	0
			28	27	1	
6	R	1	Total	C	O	0
			28	27	1	
6	R	1	Total	C	O	0
			28	27	1	
6	R	1	Total	C	O	0
			28	27	1	
6	R	1	Total	C	O	0
			28	27	1	
6	R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

- Molecule 7 is Cebranopadol (CCD ID: A1E5L) (formula: $C_{24}H_{27}FN_2O$) (labeled as "Ligand of Interest" by depositor).

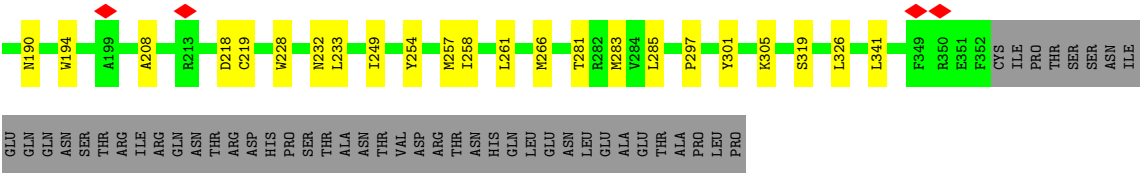


Mol	Chain	Residues	Atoms					AltConf
7	M	1	Total	C	F	N	O	0
			28	24	1	2	1	
7	R	1	Total	C	F	N	O	0
			28	24	1	2	1	

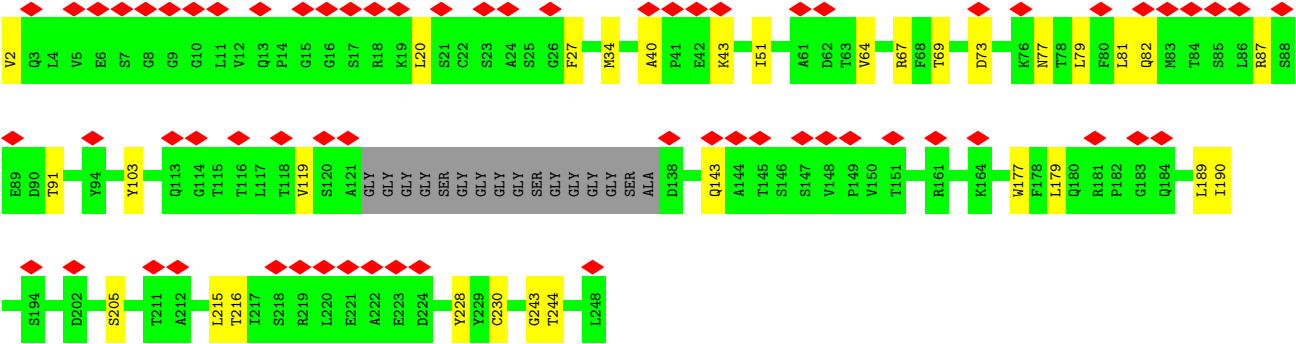
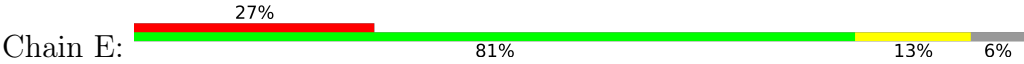


NET	ASP	SER	SER	SER	ALA	ALA	PRO	THR	ASN	ALA	SER	ASN	CYS	THR	ASP	ALA	ALA	TYR	SER	SER	CYS	SER	PRO	PRO	ALA	PRO	SER	PRO	GLY	SER	TRP	VAL	ASN	LEU	SER	HIS	LEU	ASP	GLY	ASN	LEU	SER	ASP	CYS	GLY	PRO	ASN	THR	ASP	LEU	GLY	GLY	ASP	SER	LEU	CYS	PRO
THR	GLY	SER	PRO	PRO	S66	S67	T68	T69	A70	I71	T72	I73	M74	C81	A97	K100	L112	T122	L123	S127	V128	M132	G133	T134	M135	P136	V145	D149	I150	Y151	T155	A170	V171	R181	K187	M194	I195	L196	A199	I200	Y212	E213															
I236	C237	V238	F241	A242	I249	M257	R260	E272	N276	R279	M283	V295	T296	P297	Y301	T309	E312	T313	T314	W320	L324	N330	N334	P335	V336	F340	L341	R350	E351	F352	C353	ILE	PRO	THR	SER	SER	ASN	ILE	GLU	ILE																	

[illegible]



● Molecule 5: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	3.526	Depositor
Minimum map value	-2.118	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	296.64, 296.64, 296.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82400006, 0.82400006, 0.82400006	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: A1E5L, 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	B	0.12	0/2625	0.37	0/3559
2	C	0.08	0/442	0.24	0/595
3	A	0.15	0/1846	0.35	0/2476
3	F	0.05	0/138	0.15	0/184
4	M	0.28	0/2374	0.56	0/3233
4	R	0.28	0/2368	0.52	0/3225
5	E	0.39	0/1821	0.68	0/2468
All	All	0.25	0/11614	0.50	0/15740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2578	0	2477	43	0
2	C	436	0	450	6	0
3	A	1816	0	1805	24	0
3	F	138	0	140	1	0
4	M	2315	0	2405	37	0
4	R	2309	0	2400	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1777	0	1714	20	0
6	M	140	0	230	24	0
6	R	140	0	230	25	0
7	M	28	0	0	0	0
7	R	28	0	0	0	0
All	All	11705	0	11851	175	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 7.

All (175) 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)
4:R:88:ASN:HD21	4:R:116:ASP:HB2	1.41	0.84
4:R:233:LEU:HD22	6:R:503:CLR:H12	1.61	0.82
4:R:137:PHE:HB3	4:R:141:LEU:HD23	1.62	0.80
4:R:233:LEU:CD2	6:R:503:CLR:H12	2.17	0.74
1:B:271:CYS:HB2	1:B:290:ASP:HB2	1.70	0.73
5:E:40:ALA:HB3	5:E:43:LYS:HB2	1.72	0.69
5:E:20:LEU:HD12	5:E:81:LEU:HD23	1.73	0.69
4:M:122:THR:HB	4:M:145:VAL:HG13	1.75	0.69
4:R:232:ASN:ND2	6:R:504:CLR:H9	2.09	0.67
4:M:112:LEU:HD21	4:M:334:ASN:HB3	1.77	0.67
4:M:134:THR:HG23	4:M:136:PRO:HD3	1.77	0.67
1:B:294:CYS:HB3	1:B:308:LEU:HB2	1.77	0.65
4:R:283:MET:HE1	4:R:341:LEU:HD12	1.79	0.65
4:R:233:LEU:HD21	6:R:503:CLR:H112	1.79	0.64
4:M:81:CYS:HB2	4:M:123:LEU:HD23	1.79	0.63
4:M:320:TRP:O	4:M:324:ILE:HD12	1.98	0.63
1:B:42:ARG:NH1	1:B:304:ARG:O	2.32	0.62
3:A:251:ASP:OD1	3:A:255:ASN:ND2	2.32	0.62
4:M:74:MET:SD	4:M:127:SER:OG	2.56	0.62
3:A:270:LYS:HD2	3:A:273:LEU:HD12	1.80	0.62
4:M:249:ILE:HG12	6:M:501:CLR:H41	1.81	0.62
5:E:205:SER:OG	5:E:216:THR:OG1	2.17	0.62
4:R:74:MET:HE2	4:R:131:LEU:HD13	1.82	0.61
3:A:185:VAL:HB	3:A:200:ASP:HB3	1.83	0.61
4:R:99:THR:HG22	4:R:101:MET:H	1.66	0.61
1:B:161:SER:OG	1:B:163:ASP:OD1	2.18	0.60
4:R:232:ASN:HD22	6:R:504:CLR:H14	1.66	0.60
4:M:200:ILE:HA	6:M:504:CLR:H71	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASN:ND2	2:C:59:ASN:HD21	2.00	0.59
1:B:331:SER:OG	1:B:333:ASP:OD1	2.19	0.59
4:M:249:ILE:HG12	6:M:501:CLR:H6	1.85	0.59
1:B:156:GLN:HB3	1:B:168:LEU:HD11	1.85	0.58
4:R:249:ILE:HG12	6:R:505:CLR:H6	1.85	0.58
4:M:170:ALA:HB2	4:M:181:ARG:HD2	1.86	0.58
3:A:33:GLU:HG2	3:A:195:HIS:HB2	1.85	0.58
4:R:297:PRO:HB3	6:R:502:CLR:H222	1.84	0.57
1:B:212:ASP:HB3	1:B:215:GLU:HB2	1.85	0.57
4:R:88:ASN:ND2	4:R:113:ALA:O	2.39	0.56
4:M:295:TRP:CD1	4:M:330:ASN:HD22	2.23	0.56
4:R:257:MET:HE2	4:R:261:LEU:HD11	1.87	0.56
4:R:74:MET:SD	4:R:127:SER:OG	2.64	0.55
1:B:75:GLN:O	1:B:98:SER:OG	2.24	0.55
5:E:69:THR:HB	5:E:82:GLN:HB3	1.87	0.55
5:E:179:LEU:HD13	5:E:228:TYR:CE1	2.42	0.55
6:M:504:CLR:H273	6:R:503:CLR:H212	1.89	0.54
4:R:228:TRP:CE3	6:R:504:CLR:H72	2.43	0.54
4:R:232:ASN:HD22	6:R:504:CLR:H9	1.72	0.54
1:B:30:LEU:HD23	1:B:262:MET:HB2	1.90	0.54
4:R:93:TYR:OH	4:R:97:ARG:NH2	2.40	0.54
1:B:46:ARG:NH1	2:C:63:GLU:OE2	2.41	0.53
4:R:228:TRP:CZ3	6:R:504:CLR:H152	2.43	0.53
6:M:505:CLR:H9	6:R:505:CLR:H152	1.91	0.53
1:B:81:ILE:HB	1:B:91:HIS:HB2	1.90	0.53
4:M:283:MET:HE1	4:M:341:LEU:HD13	1.91	0.52
6:M:505:CLR:H21	6:R:505:CLR:H72	1.90	0.52
4:R:232:ASN:ND2	6:R:504:CLR:H14	2.24	0.52
4:M:194:TRP:CD1	6:M:502:CLR:H181	2.45	0.52
1:B:266:HIS:ND1	1:B:268:ASN:OD1	2.41	0.52
5:E:179:LEU:HB2	5:E:189:LEU:HD11	1.91	0.51
4:R:281:THR:O	4:R:285:LEU:HG	2.11	0.51
4:R:181:ARG:NH1	3:A:351:CYS:SG	2.70	0.51
4:M:249:ILE:CG1	6:M:501:CLR:H41	2.40	0.50
1:B:146:LEU:HA	1:B:161:SER:HA	1.92	0.50
4:M:187:LYS:HE3	6:M:502:CLR:H22	1.92	0.50
3:A:348:LEU:HB3	3:A:354:PHE:HB2	1.94	0.50
1:B:279:SER:HA	1:B:320:VAL:HG11	1.92	0.50
4:R:233:LEU:HD22	6:R:503:CLR:C1	2.37	0.50
3:A:266:LEU:N	3:A:320:TYR:O	2.34	0.50
6:M:501:CLR:H242	6:R:504:CLR:H193	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:170:ALA:HB1	3:A:347:ASN:HB3	1.94	0.50
5:E:143:GLN:HG3	5:E:243:GLY:H	1.76	0.50
4:M:171:VAL:HG12	4:M:260:ARG:HD3	1.93	0.49
1:B:210:LEU:HD22	1:B:255:LEU:HD22	1.93	0.49
4:M:171:VAL:HG21	4:M:257:MET:HG3	1.95	0.49
1:B:187:VAL:HA	1:B:203:ALA:HA	1.94	0.49
1:B:256:ARG:HB3	2:C:28:ILE:HG12	1.95	0.49
1:B:68:ARG:HD3	5:E:103:TYR:CZ	2.48	0.49
4:M:237:CYS:HB3	6:M:504:CLR:H112	1.95	0.48
4:R:190:ASN:O	4:R:194:TRP:HD1	1.96	0.48
5:E:73:ASP:O	5:E:77:ASN:N	2.46	0.48
1:B:89:LYS:NZ	3:A:20:ASP:OD1	2.44	0.48
4:M:237:CYS:CB	6:M:504:CLR:H112	2.44	0.48
4:M:320:TRP:CE2	4:M:324:ILE:HD11	2.48	0.48
5:E:67:ARG:HD3	5:E:87:ARG:HH22	1.78	0.48
1:B:160:SER:HB3	1:B:190:LEU:HD23	1.96	0.47
1:B:11:ALA:HB2	2:C:16:VAL:HG22	1.97	0.47
1:B:284:LEU:HD12	1:B:297:TRP:O	2.15	0.47
4:M:301:TYR:CE1	6:M:503:CLR:H191	2.50	0.47
4:M:149:ASP:OD1	4:M:150:TYR:N	2.48	0.47
3:A:22:ASN:O	3:A:25:GLU:HG2	2.15	0.46
4:R:174:PRO:HG2	3:A:340:THR:HG23	1.98	0.46
4:M:297:PRO:HA	6:M:503:CLR:H222	1.97	0.46
3:A:227:LEU:HD21	3:A:268:LEU:HD13	1.96	0.46
1:B:245:SER:OG	1:B:246:ASP:N	2.49	0.46
5:E:34:MET:HB2	5:E:51:ILE:HG22	1.97	0.46
1:B:145:TYR:O	1:B:162:GLY:N	2.48	0.46
4:R:120:THR:HG23	4:R:123:LEU:HD12	1.98	0.46
4:R:266:MET:HE1	3:A:341:ASP:HB3	1.98	0.46
3:A:33:GLU:OE1	3:A:197:LYS:NZ	2.41	0.46
1:B:121:CYS:HB3	1:B:139:LEU:HB2	1.98	0.45
4:M:196:LEU:HD21	6:M:504:CLR:H272	1.98	0.45
3:A:9:ASP:O	3:A:13:VAL:HG23	2.16	0.45
1:B:202:GLY:HA3	1:B:229:ILE:HG21	1.99	0.45
1:B:316:SER:H	1:B:331:SER:HA	1.82	0.45
4:R:297:PRO:HG3	4:R:326:LEU:HD23	1.99	0.45
3:A:228:SER:O	3:A:277:LYS:NZ	2.46	0.45
5:E:143:GLN:NE2	5:E:230:CYS:SG	2.90	0.45
1:B:38:ASP:OD1	1:B:38:ASP:N	2.49	0.45
4:M:241:PHE:CD2	6:M:504:CLR:H20	2.52	0.45
4:R:171:VAL:HG21	4:R:257:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:254:TYR:O	4:R:258:ILE:HG12	2.17	0.45
4:M:236:ILE:CD1	6:M:505:CLR:H112	2.47	0.45
6:M:504:CLR:H222	6:M:504:CLR:C18	2.47	0.45
1:B:124:TYR:CE2	1:B:135:VAL:HG22	2.51	0.45
3:A:272:ASP:OD1	3:A:273:LEU:N	2.50	0.45
1:B:254:ASP:HB3	1:B:257:ALA:HB3	1.98	0.44
4:R:151:TYR:O	4:R:155:THR:HG23	2.17	0.44
6:R:505:CLR:H221	6:R:505:CLR:H162	1.50	0.44
1:B:51:LEU:HB3	1:B:82:TRP:CZ3	2.52	0.44
1:B:286:LEU:HG	1:B:296:VAL:HG13	2.00	0.44
4:M:236:ILE:HD11	6:M:505:CLR:H112	1.98	0.44
4:M:301:TYR:CD1	6:M:503:CLR:H8	2.53	0.44
5:E:143:GLN:OE1	5:E:244:THR:OG1	2.35	0.44
4:R:228:TRP:HE3	6:R:504:CLR:H151	1.82	0.44
4:R:135:TRP:CE2	4:R:137:PHE:HB2	2.52	0.44
5:E:91:THR:HB	5:E:119:VAL:HG22	2.00	0.44
1:B:114:CYS:SG	1:B:122:SER:HB2	2.58	0.43
4:R:301:TYR:CE2	4:R:305:LYS:HD2	2.53	0.43
4:M:69:THR:O	4:M:73:ILE:HG12	2.18	0.43
3:A:254:CYS:O	3:A:317:LYS:NZ	2.50	0.43
4:R:228:TRP:HE3	6:R:504:CLR:H72	1.83	0.43
4:M:336:VAL:HA	4:M:340:PHE:HB2	2.00	0.43
4:R:152:ASN:HA	4:R:155:THR:OG1	2.19	0.43
1:B:88:ASN:HB2	3:A:16:SER:HB2	2.00	0.43
4:M:276:ASN:OD1	4:M:279:ARG:NH1	2.52	0.43
4:R:228:TRP:CE3	6:R:504:CLR:C15	3.02	0.43
4:R:228:TRP:HE3	6:R:504:CLR:C15	2.32	0.43
5:E:34:MET:HG3	5:E:79:LEU:HD13	2.00	0.43
1:B:104:ALA:HB3	1:B:113:ALA:HB3	2.01	0.43
1:B:316:SER:HB3	1:B:332:TRP:CD1	2.53	0.43
4:R:75:ALA:O	4:R:79:ILE:HG12	2.19	0.43
4:R:301:TYR:CD1	6:R:502:CLR:H8	2.53	0.43
5:E:177:TRP:HB2	5:E:190:ILE:HB	2.01	0.43
1:B:49:ARG:HH22	2:C:62:ARG:N	2.16	0.42
1:B:297:TRP:CD1	1:B:304:ARG:HA	2.54	0.42
4:M:151:TYR:O	4:M:155:THR:HG23	2.19	0.42
3:A:35:LYS:HG2	3:A:197:LYS:HE2	2.01	0.42
4:M:128:VAL:O	4:M:132:MET:HG2	2.20	0.42
6:M:504:CLR:H222	6:M:504:CLR:H183	2.02	0.42
4:R:101:MET:SD	6:R:501:CLR:H41	2.59	0.42
5:E:64:VAL:HG12	5:E:67:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:114:LEU:O	4:R:118:LEU:HG	2.19	0.42
4:R:125:PHE:HE2	4:R:141:LEU:HD21	1.85	0.41
3:A:316:THR:O	3:A:345:LYS:NZ	2.53	0.41
4:R:146:ILE:HD12	4:R:208:ALA:HB1	2.02	0.41
5:E:69:THR:O	5:E:81:LEU:HD12	2.20	0.41
5:E:205:SER:O	5:E:215:LEU:HD12	2.20	0.41
1:B:170:ASP:HB3	1:B:173:THR:HB	2.03	0.41
1:B:340:ASN:HD22	2:C:59:ASN:HD21	1.68	0.41
4:R:95:ILE:HA	4:R:99:THR:HB	2.02	0.41
4:R:228:TRP:HZ3	6:R:504:CLR:H152	1.83	0.41
3:F:347:ASN:HB3	4:M:170:ALA:HB1	2.01	0.41
6:M:503:CLR:H211	6:M:503:CLR:H231	1.81	0.41
4:R:319:SER:OG	6:R:502:CLR:H72	2.21	0.41
4:R:257:MET:HE1	3:A:353:LEU:HD22	2.03	0.41
4:M:238:VAL:O	4:M:242:ALA:HB3	2.21	0.40
4:R:218:ASP:OD1	4:R:219:CYS:N	2.54	0.40
3:A:188:HIS:ND1	3:A:197:LYS:HG2	2.36	0.40
1:B:82:TRP:CH2	1:B:89:LYS:HE3	2.55	0.40
6:M:501:CLR:H162	6:M:501:CLR:H222	1.77	0.40
1:B:48:ARG:HE	1:B:340:ASN:HB3	1.86	0.40
4:M:132:MET:HE3	4:M:134:THR:O	2.22	0.40
5:E:2:VAL:HG22	5:E:27:PHE:HB3	2.04	0.40
4:M:301:TYR:HE1	6:M:503:CLR:H191	1.86	0.40
3:A:229:ASP:HB3	3:A:242:ARG:HG3	2.02	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	B	334/345 (97%)	328 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	54/68 (79%)	54 (100%)	0	0	100	100
3	A	221/354 (62%)	220 (100%)	1 (0%)	0	100	100
3	F	16/354 (4%)	16 (100%)	0	0	100	100
4	M	286/400 (72%)	282 (99%)	4 (1%)	0	100	100
4	R	285/400 (71%)	280 (98%)	5 (2%)	0	100	100
5	E	227/247 (92%)	221 (97%)	6 (3%)	0	100	100
All	All	1423/2168 (66%)	1401 (98%)	22 (2%)	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	B	278/287 (97%)	278 (100%)	0	100	100
2	C	46/56 (82%)	46 (100%)	0	100	100
3	A	201/306 (66%)	201 (100%)	0	100	100
3	F	16/306 (5%)	16 (100%)	0	100	100
4	M	262/359 (73%)	261 (100%)	1 (0%)	84	92
4	R	261/359 (73%)	261 (100%)	0	100	100
5	E	195/198 (98%)	195 (100%)	0	100	100
All	All	1259/1871 (67%)	1258 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	214	GLN

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

Mol	Chain	Res	Type
1	B	225	HIS
1	B	340	ASN
4	M	173	HIS
4	M	190	ASN
4	M	330	ASN
4	R	88	ASN
4	R	190	ASN
4	R	232	ASN
3	A	322	HIS
5	E	180	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
6	CLR	M	502	-	31,31,31	0.34	0	48,48,48	0.56	0
6	CLR	R	505	-	31,31,31	0.29	0	48,48,48	0.73	1 (2%)
6	CLR	R	504	-	31,31,31	0.34	0	48,48,48	0.87	2 (4%)
6	CLR	M	501	-	31,31,31	0.28	0	48,48,48	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLR	R	501	-	31,31,31	0.33	0	48,48,48	0.69	1 (2%)
6	CLR	M	504	-	31,31,31	0.33	0	48,48,48	0.93	2 (4%)
6	CLR	R	503	-	31,31,31	0.34	0	48,48,48	0.60	0
6	CLR	M	503	-	31,31,31	0.30	0	48,48,48	0.42	0
6	CLR	R	502	-	31,31,31	0.30	0	48,48,48	0.45	0
7	A1E5L	R	506	-	29,32,32	2.85	17 (58%)	36,49,49	2.47	11 (30%)
6	CLR	M	505	-	31,31,31	0.32	0	48,48,48	0.90	1 (2%)
7	A1E5L	M	506	-	29,32,32	2.85	15 (51%)	36,49,49	2.46	10 (27%)

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
6	CLR	M	502	-	-	8/10/68/68	0/4/4/4
6	CLR	R	505	-	-	10/10/68/68	0/4/4/4
6	CLR	R	504	-	-	4/10/68/68	0/4/4/4
6	CLR	M	501	-	-	6/10/68/68	0/4/4/4
6	CLR	R	501	-	-	5/10/68/68	0/4/4/4
6	CLR	M	504	-	-	6/10/68/68	0/4/4/4
6	CLR	R	503	-	-	9/10/68/68	0/4/4/4
6	CLR	M	503	-	-	10/10/68/68	0/4/4/4
6	CLR	R	502	-	-	8/10/68/68	0/4/4/4
7	A1E5L	R	506	-	-	1/12/39/39	0/5/5/5
6	CLR	M	505	-	-	5/10/68/68	0/4/4/4
7	A1E5L	M	506	-	-	0/12/39/39	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	506	A1E5L	C4-C23	6.73	1.61	1.52
7	R	506	A1E5L	C4-C23	6.42	1.60	1.52
7	M	506	A1E5L	C15-C11	5.49	1.54	1.44
7	R	506	A1E5L	C15-C11	5.43	1.54	1.44
7	M	506	A1E5L	C6-C7	4.57	1.59	1.53
7	R	506	A1E5L	C6-C7	4.28	1.58	1.53
7	M	506	A1E5L	C8-C7	4.03	1.58	1.53
7	M	506	A1E5L	C9-C4	3.92	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	506	A1E5L	C8-C7	3.90	1.58	1.53
7	R	506	A1E5L	C5-C4	3.85	1.57	1.54
7	R	506	A1E5L	C9-C4	3.84	1.57	1.54
7	R	506	A1E5L	C10-C11	3.77	1.43	1.36
7	M	506	A1E5L	C10-C11	3.72	1.43	1.36
7	R	506	A1E5L	C28-C23	3.48	1.44	1.39
7	M	506	A1E5L	C28-C23	3.46	1.44	1.39
7	M	506	A1E5L	C21-C15	3.31	1.45	1.39
7	R	506	A1E5L	C21-C15	3.30	1.45	1.39
7	R	506	A1E5L	C19-C20	3.28	1.43	1.37
7	M	506	A1E5L	C19-C20	3.25	1.43	1.37
7	M	506	A1E5L	C5-C4	2.97	1.57	1.54
7	M	506	A1E5L	C15-C16	2.78	1.45	1.41
7	R	506	A1E5L	C15-C16	2.72	1.44	1.41
7	R	506	A1E5L	C1-N2	2.62	1.51	1.46
7	M	506	A1E5L	C25-C24	2.48	1.44	1.38
7	M	506	A1E5L	C1-N2	2.44	1.50	1.46
7	M	506	A1E5L	C18-C16	2.40	1.43	1.39
7	R	506	A1E5L	C25-C24	2.38	1.43	1.38
7	R	506	A1E5L	C18-C16	2.37	1.43	1.39
7	M	506	A1E5L	C21-C20	2.18	1.41	1.37
7	R	506	A1E5L	C21-C20	2.17	1.41	1.37
7	R	506	A1E5L	C12-C11	2.14	1.52	1.50
7	R	506	A1E5L	C3-N2	2.04	1.50	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	506	A1E5L	C12-C11-C10	-6.95	114.02	122.56
7	R	506	A1E5L	C12-C11-C10	-6.67	114.37	122.56
7	R	506	A1E5L	C21-C15-C16	-5.70	113.95	119.42
7	M	506	A1E5L	C21-C15-C16	-5.63	114.02	119.42
7	M	506	A1E5L	C16-N17-C10	5.22	116.53	109.08
7	R	506	A1E5L	C16-N17-C10	5.20	116.51	109.08
7	M	506	A1E5L	C21-C15-C11	4.79	140.96	132.93
7	R	506	A1E5L	C21-C15-C11	4.77	140.91	132.93
7	M	506	A1E5L	C12-C11-C15	4.33	139.06	130.59
7	R	506	A1E5L	C12-C11-C15	4.19	138.80	130.59
7	M	506	A1E5L	C11-C10-N17	-3.76	105.60	109.90
7	R	506	A1E5L	C11-C10-N17	-3.74	105.62	109.90
7	R	506	A1E5L	C8-C7-C6	-2.96	106.50	109.73
7	R	506	A1E5L	C5-C6-C7	2.78	115.55	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	504	CLR	C17-C13-C14	-2.77	96.79	100.07
7	R	506	A1E5L	C18-C16-C15	2.68	124.88	122.19
7	M	506	A1E5L	C8-C7-C6	-2.67	106.81	109.73
7	M	506	A1E5L	C18-C16-C15	2.59	124.80	122.19
6	M	505	CLR	C16-C17-C13	-2.58	100.73	103.84
6	R	504	CLR	C1-C2-C3	2.55	113.74	110.47
6	R	505	CLR	C1-C2-C3	2.38	113.52	110.47
7	M	506	A1E5L	C9-C8-C7	2.36	115.04	112.19
6	M	504	CLR	C13-C17-C20	2.27	123.05	119.49
7	M	506	A1E5L	C5-C6-C7	2.27	114.93	112.19
6	R	501	CLR	C2-C3-C4	-2.19	107.30	110.31
7	R	506	A1E5L	C28-C23-C4	2.05	124.36	120.96
7	R	506	A1E5L	C15-C16-N17	-2.03	105.90	108.22
6	R	504	CLR	C9-C10-C5	-2.02	106.48	109.65

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	501	CLR	C13-C17-C20-C21
6	M	501	CLR	C13-C17-C20-C22
6	M	501	CLR	C16-C17-C20-C22
6	R	503	CLR	C13-C17-C20-C21
6	R	503	CLR	C16-C17-C20-C22
6	R	505	CLR	C13-C17-C20-C21
6	R	505	CLR	C13-C17-C20-C22
6	R	505	CLR	C16-C17-C20-C22
6	M	501	CLR	C16-C17-C20-C21
6	R	503	CLR	C16-C17-C20-C21
6	R	505	CLR	C16-C17-C20-C21
6	R	503	CLR	C13-C17-C20-C22
6	M	503	CLR	C21-C20-C22-C23
6	M	505	CLR	C21-C20-C22-C23
6	R	503	CLR	C21-C20-C22-C23
6	R	505	CLR	C21-C20-C22-C23
6	M	502	CLR	C13-C17-C20-C22
6	R	501	CLR	C13-C17-C20-C22
6	R	501	CLR	C13-C17-C20-C21
6	M	502	CLR	C16-C17-C20-C21
6	R	501	CLR	C16-C17-C20-C21
6	M	503	CLR	C17-C20-C22-C23
6	R	501	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
6	M	502	CLR	C17-C20-C22-C23
6	R	505	CLR	C17-C20-C22-C23
6	M	504	CLR	C16-C17-C20-C21
6	M	502	CLR	C13-C17-C20-C21
6	R	503	CLR	C17-C20-C22-C23
6	M	504	CLR	C13-C17-C20-C22
6	R	503	CLR	C22-C23-C24-C25
6	M	505	CLR	C17-C20-C22-C23
6	R	503	CLR	C20-C22-C23-C24
6	R	504	CLR	C20-C22-C23-C24
6	M	502	CLR	C16-C17-C20-C22
6	M	504	CLR	C13-C17-C20-C21
6	R	504	CLR	C22-C23-C24-C25
6	M	502	CLR	C21-C20-C22-C23
6	M	504	CLR	C20-C22-C23-C24
6	R	505	CLR	C20-C22-C23-C24
6	M	501	CLR	C22-C23-C24-C25
6	R	504	CLR	C23-C24-C25-C27
6	M	503	CLR	C23-C24-C25-C26
6	M	503	CLR	C23-C24-C25-C27
6	R	502	CLR	C21-C20-C22-C23
6	M	503	CLR	C13-C17-C20-C22
6	R	504	CLR	C23-C24-C25-C26
6	M	503	CLR	C22-C23-C24-C25
6	R	501	CLR	C22-C23-C24-C25
6	M	503	CLR	C13-C17-C20-C21
6	R	502	CLR	C22-C23-C24-C25
6	M	503	CLR	C16-C17-C20-C21
6	M	503	CLR	C20-C22-C23-C24
6	M	503	CLR	C16-C17-C20-C22
6	R	505	CLR	C23-C24-C25-C27
6	R	502	CLR	C13-C17-C20-C21
6	R	502	CLR	C13-C17-C20-C22
6	R	505	CLR	C23-C24-C25-C26
6	R	502	CLR	C16-C17-C20-C21
6	M	505	CLR	C23-C24-C25-C27
6	R	502	CLR	C16-C17-C20-C22
6	R	502	CLR	C23-C24-C25-C26
6	R	505	CLR	C22-C23-C24-C25
6	M	505	CLR	C23-C24-C25-C26
6	M	504	CLR	C23-C24-C25-C27
6	M	504	CLR	C23-C24-C25-C26

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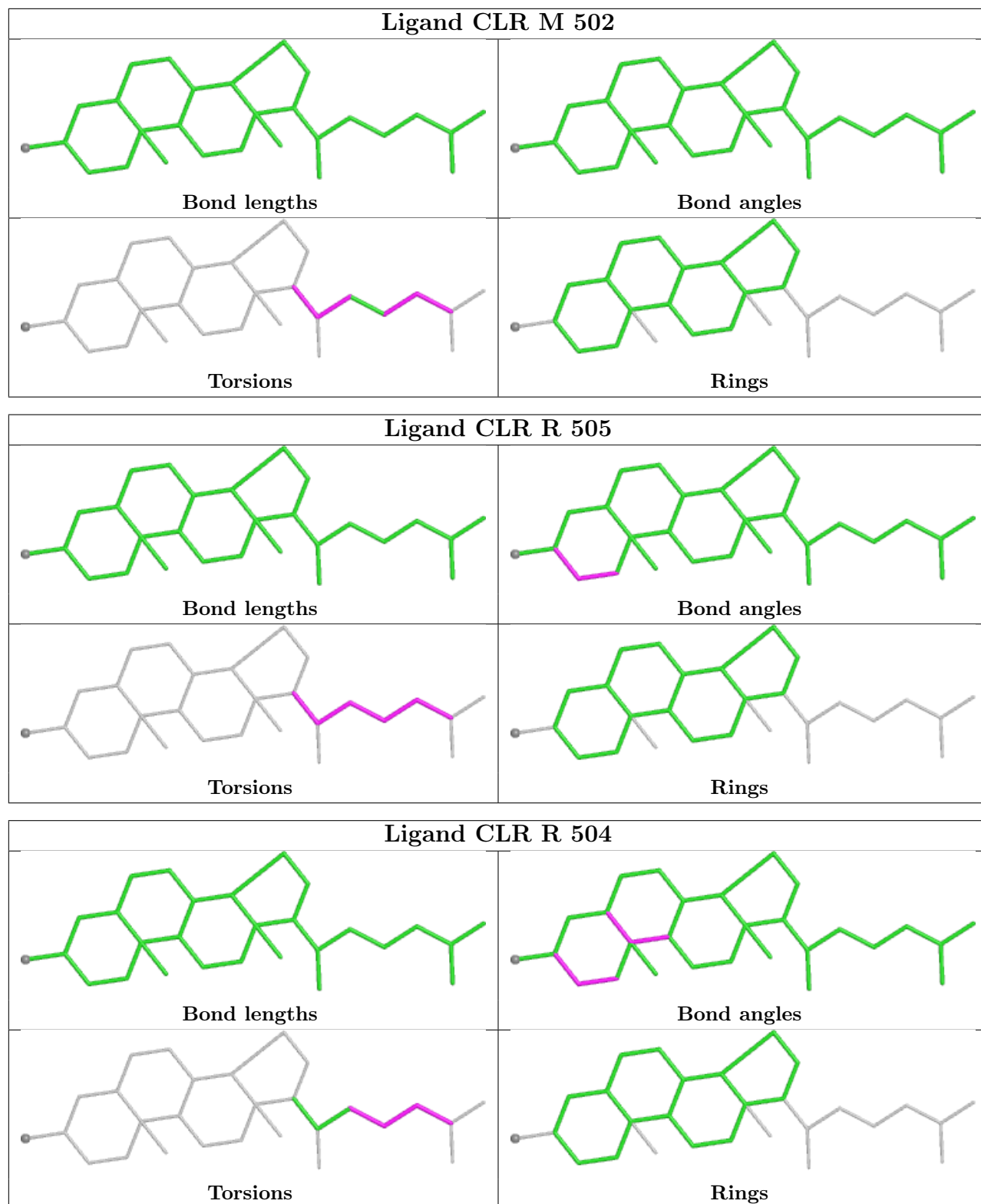
Mol	Chain	Res	Type	Atoms
6	M	502	CLR	C23-C24-C25-C26
6	M	505	CLR	C20-C22-C23-C24
7	R	506	A1E5L	C24-C23-C4-N2
6	R	502	CLR	C23-C24-C25-C27
6	R	503	CLR	C23-C24-C25-C27
6	M	501	CLR	C20-C22-C23-C24
6	M	502	CLR	C22-C23-C24-C25

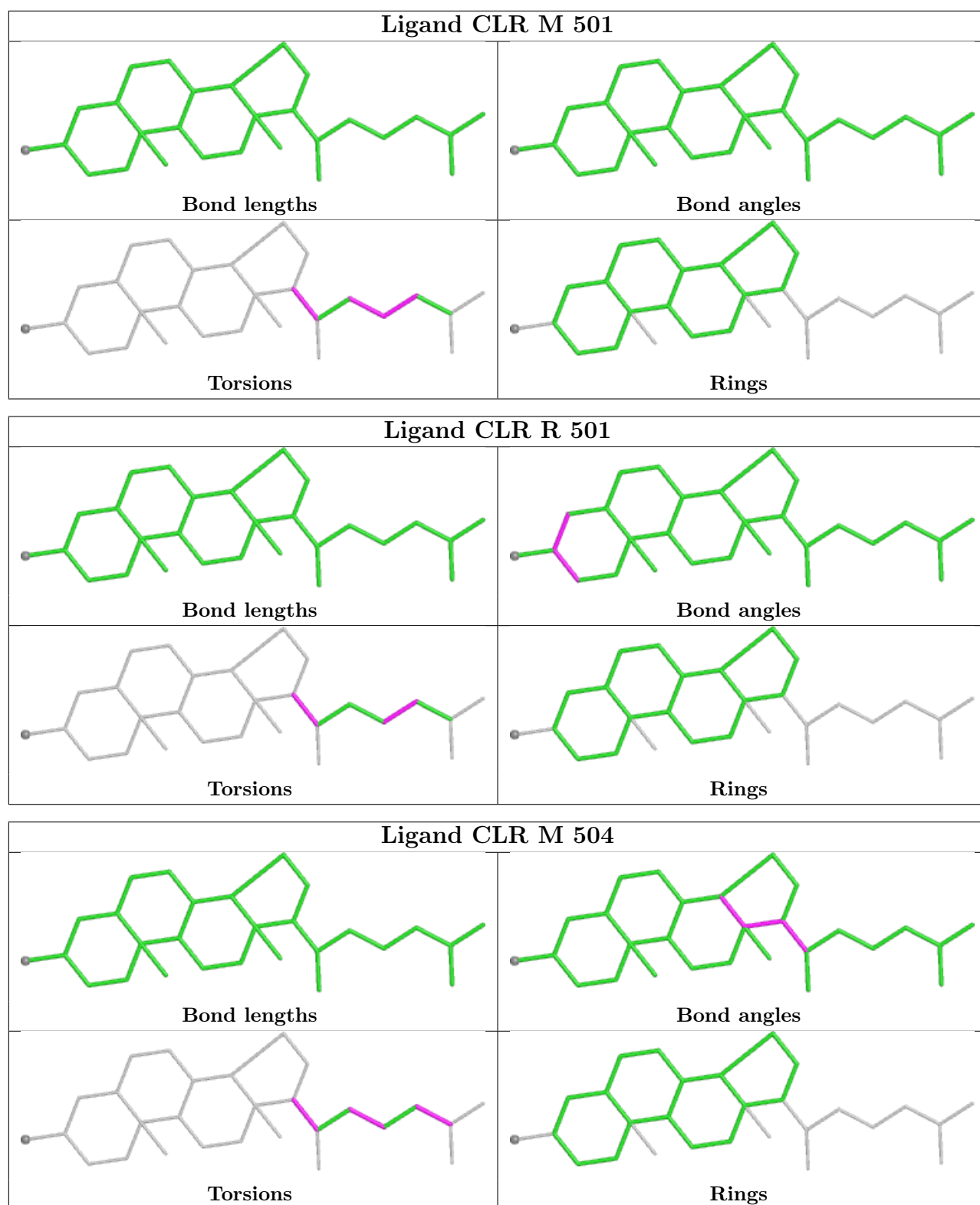
There are no ring outliers.

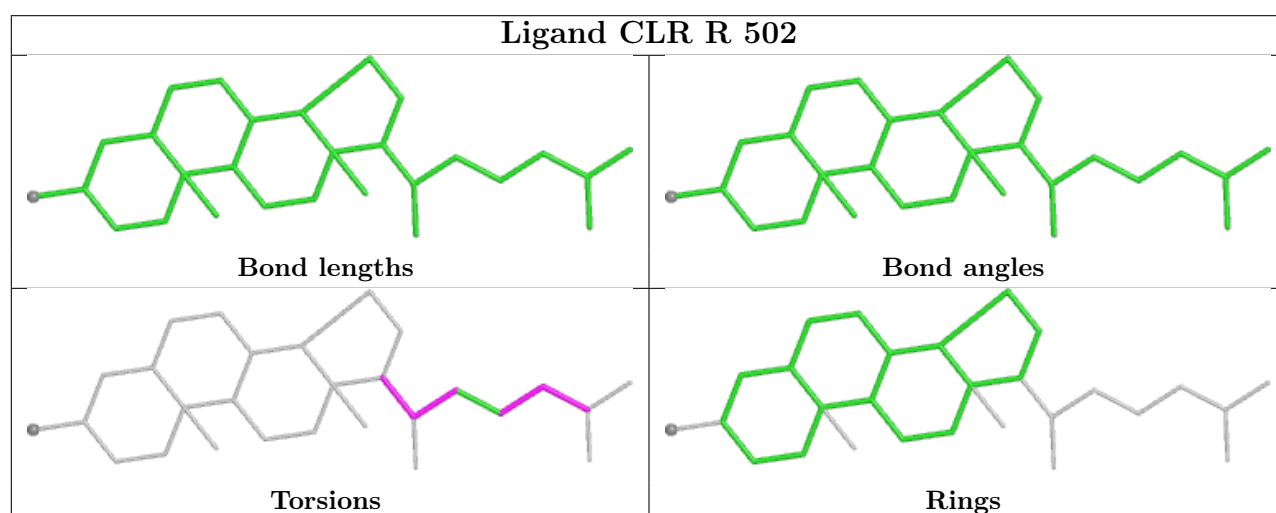
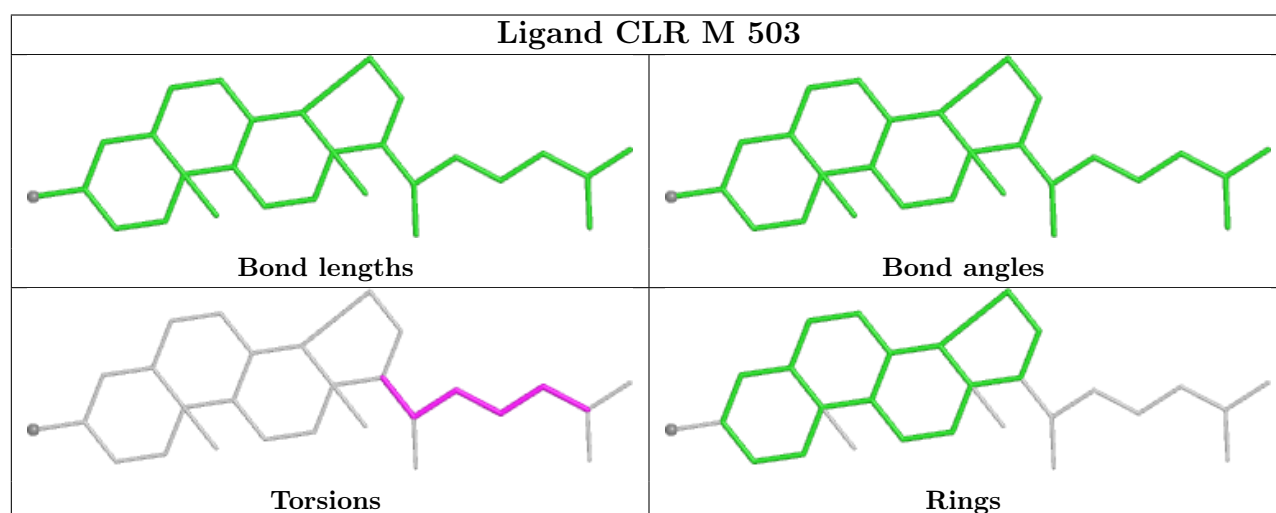
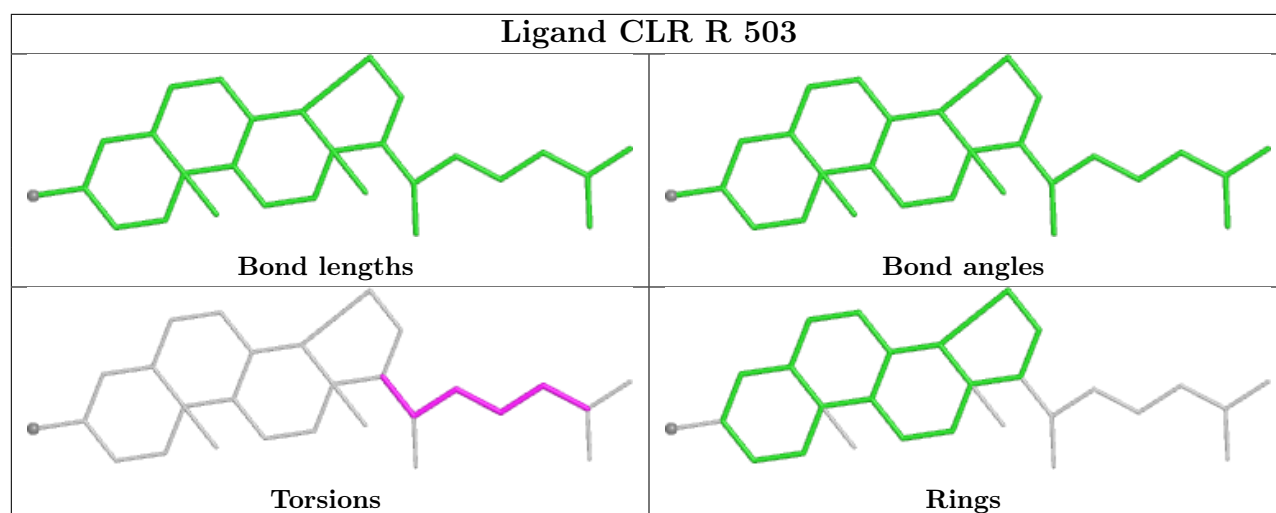
10 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	502	CLR	2	0
6	R	505	CLR	4	0
6	R	504	CLR	12	0
6	M	501	CLR	5	0
6	R	501	CLR	1	0
6	M	504	CLR	8	0
6	R	503	CLR	5	0
6	M	503	CLR	5	0
6	R	502	CLR	3	0
6	M	505	CLR	4	0

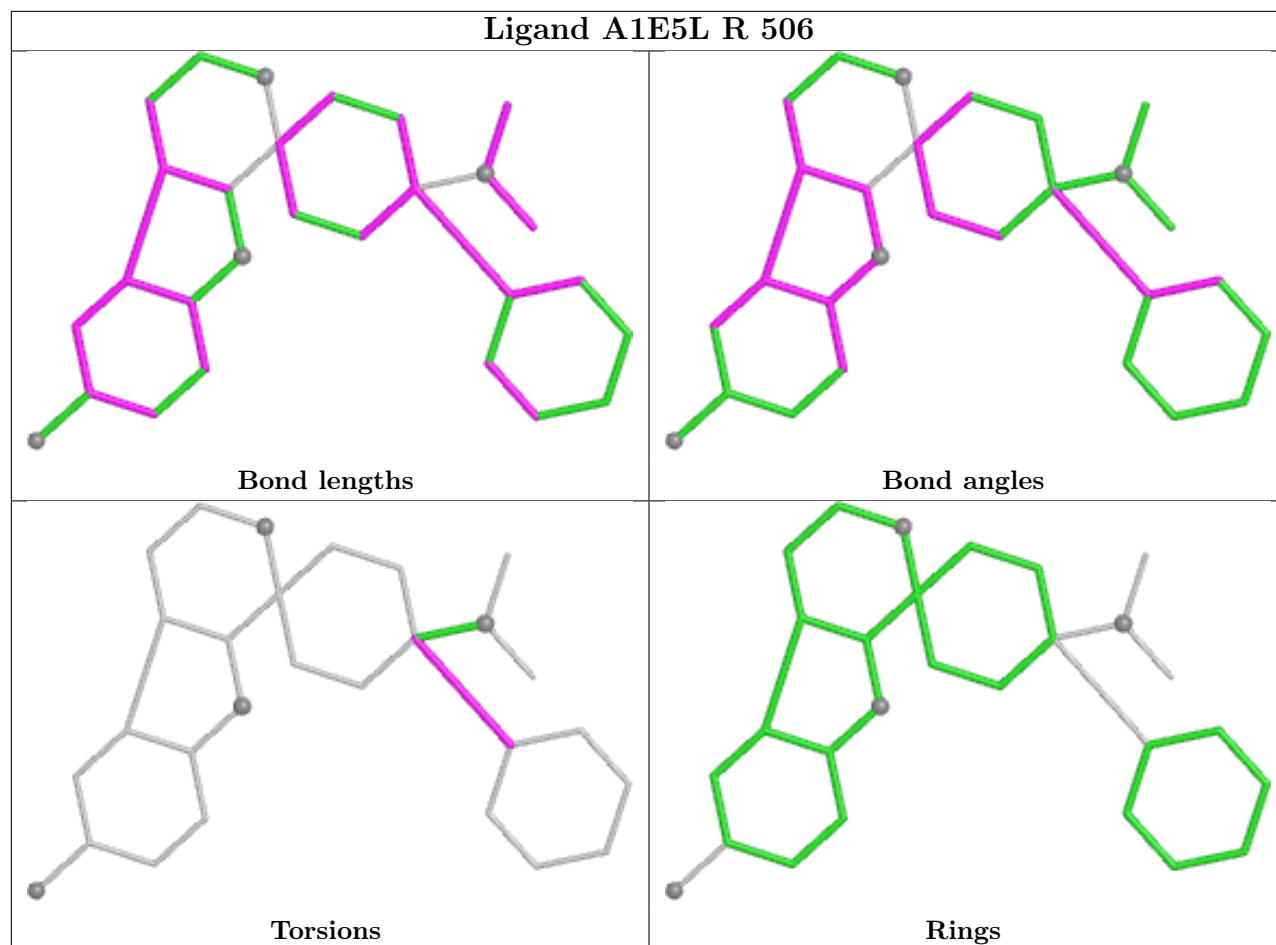
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



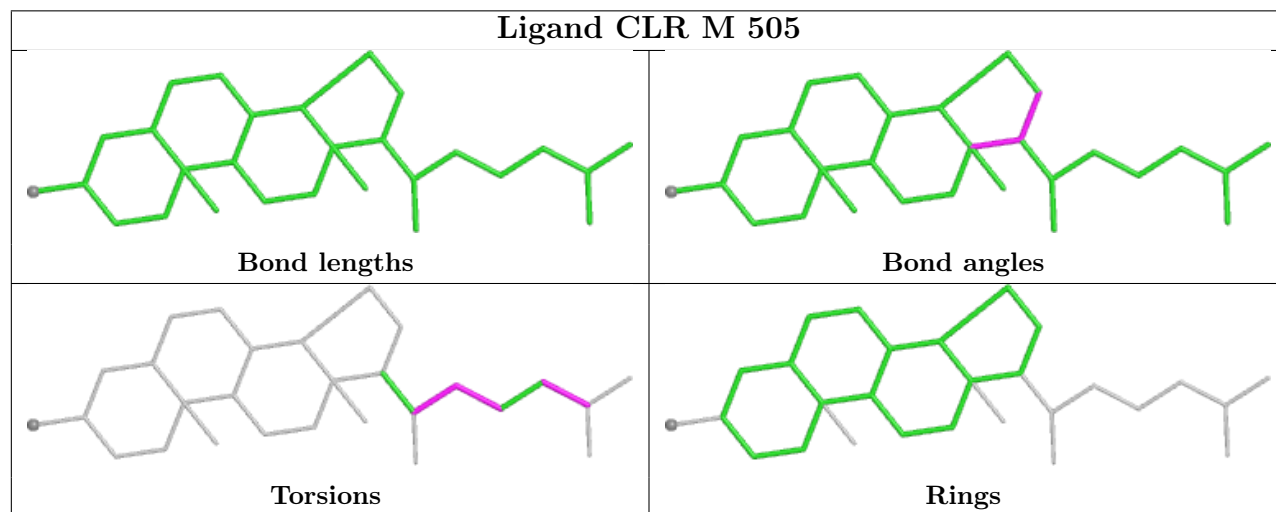


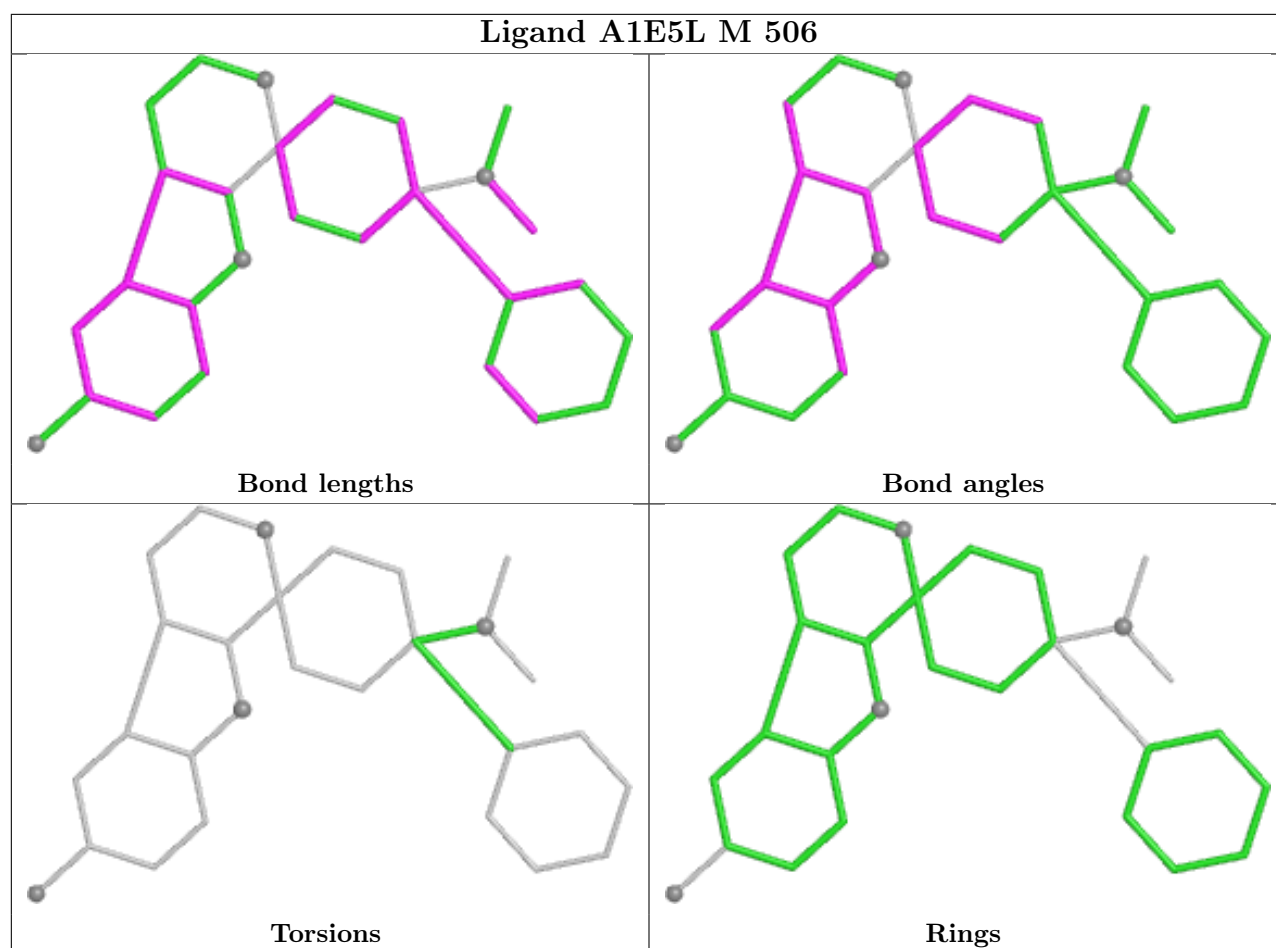


Ligand A1E5L R 506



Ligand CLR M 505





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.

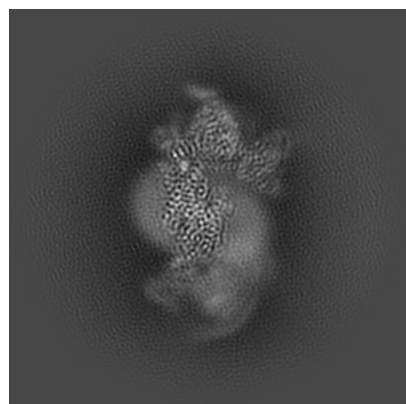
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69218. These allow visual inspection of the internal detail of the map and identification of artifacts.

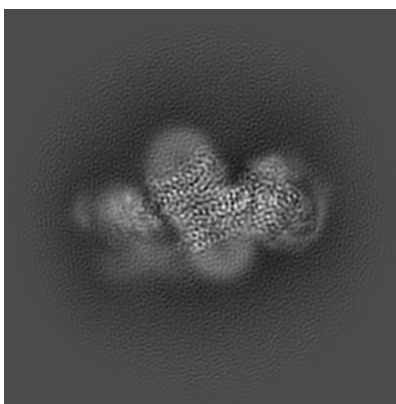
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

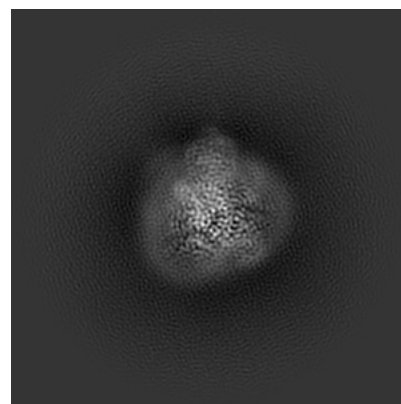
6.1.1 Primary map



X

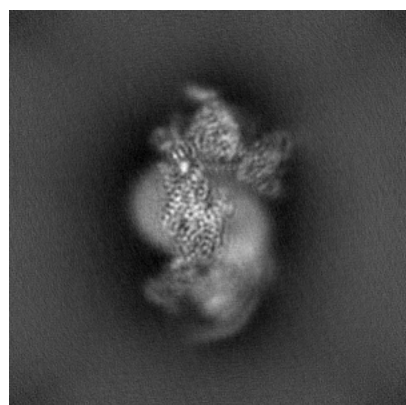


Y

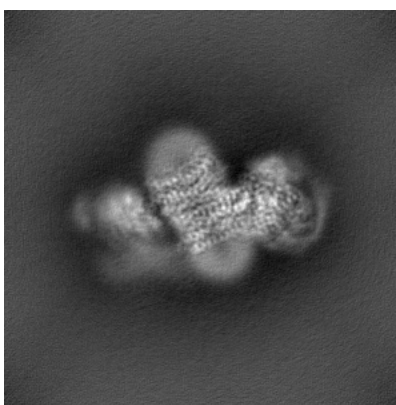


Z

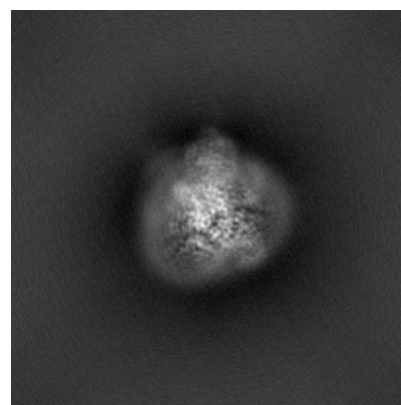
6.1.2 Raw map



X



Y

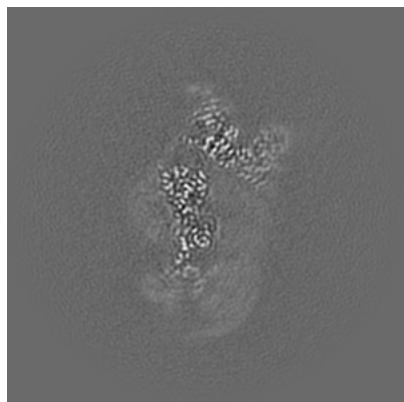


Z

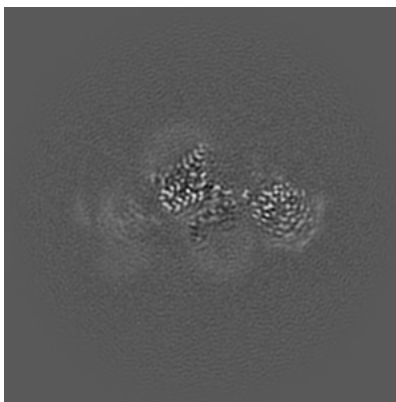
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

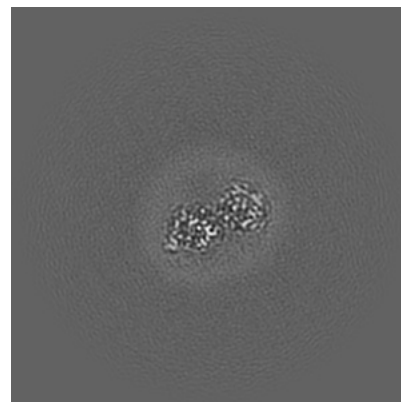
6.2.1 Primary map



X Index: 180

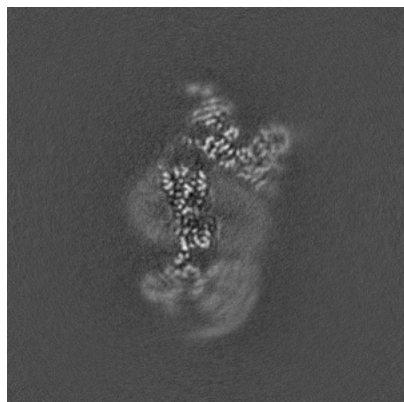


Y Index: 180

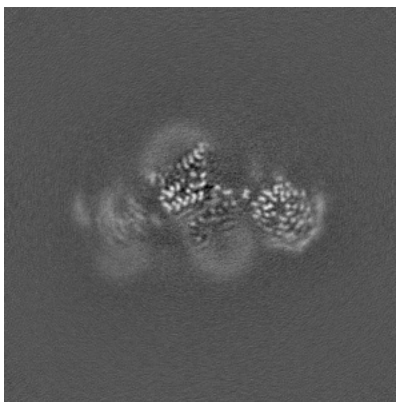


Z Index: 180

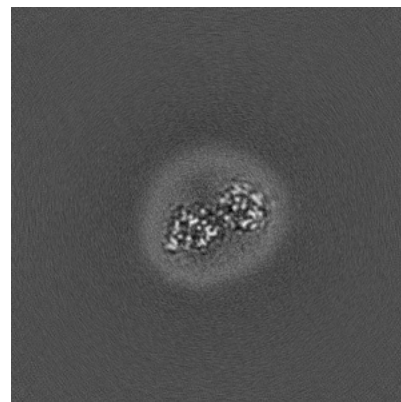
6.2.2 Raw map



X Index: 180



Y Index: 180

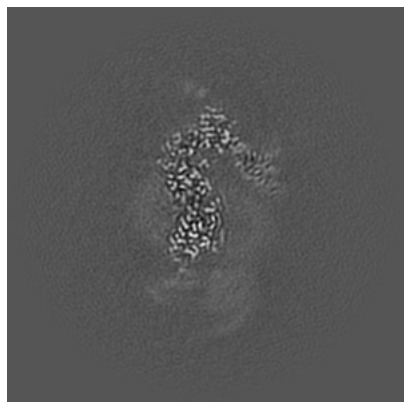


Z Index: 180

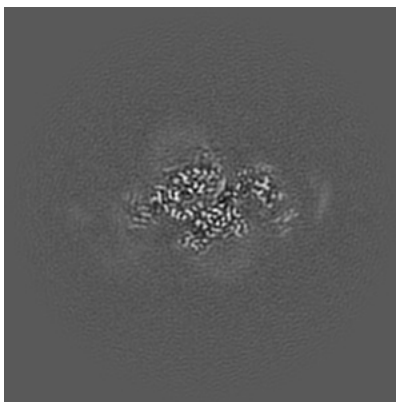
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

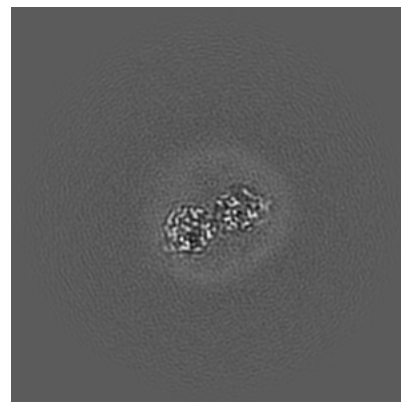
6.3.1 Primary map



X Index: 192

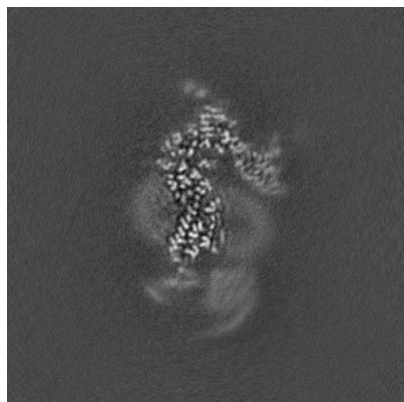


Y Index: 165

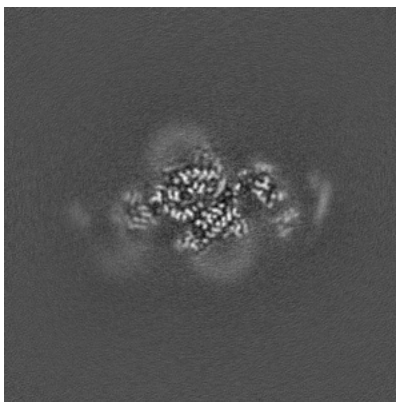


Z Index: 173

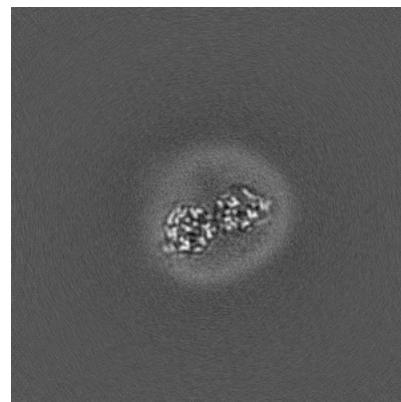
6.3.2 Raw map



X Index: 192



Y Index: 165

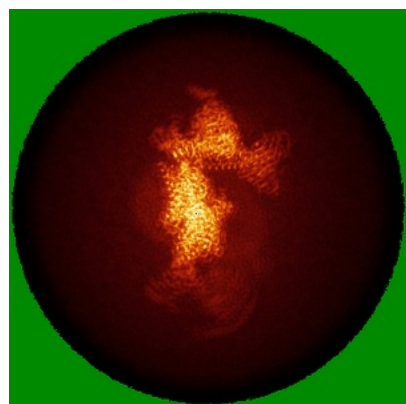


Z Index: 173

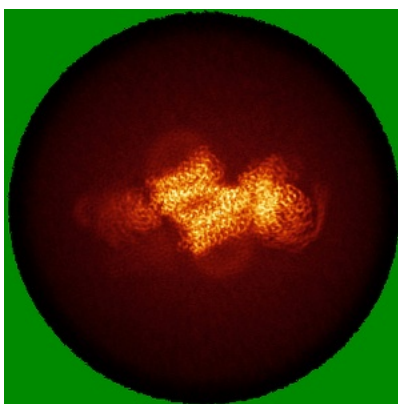
The images above show the largest variance slices of the map in three orthogonal directions.

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

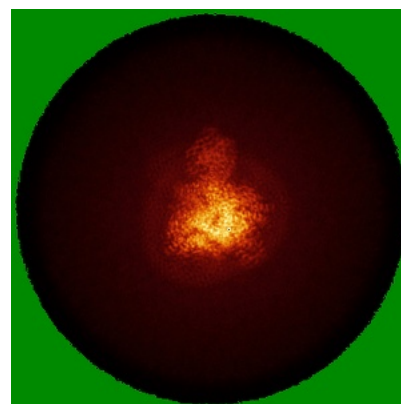
6.4.1 Primary map



X

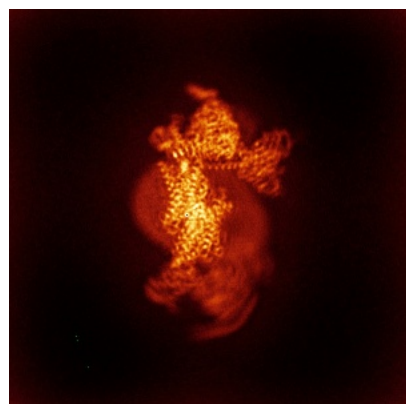


Y

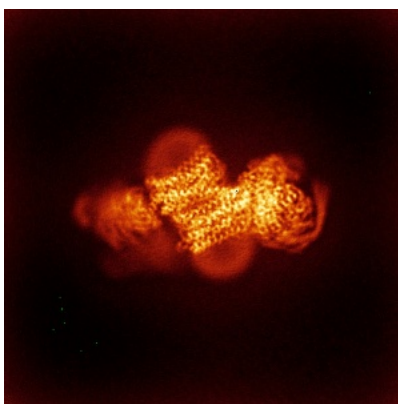


Z

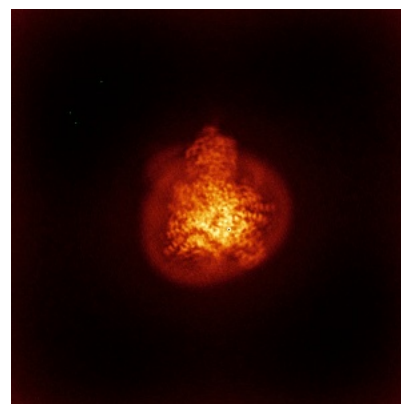
6.4.2 Raw map



X



Y

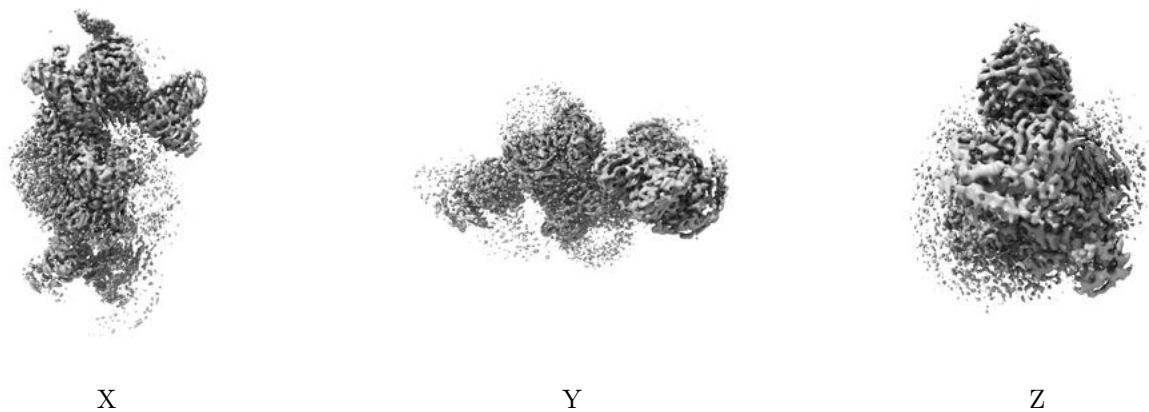


Z

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.

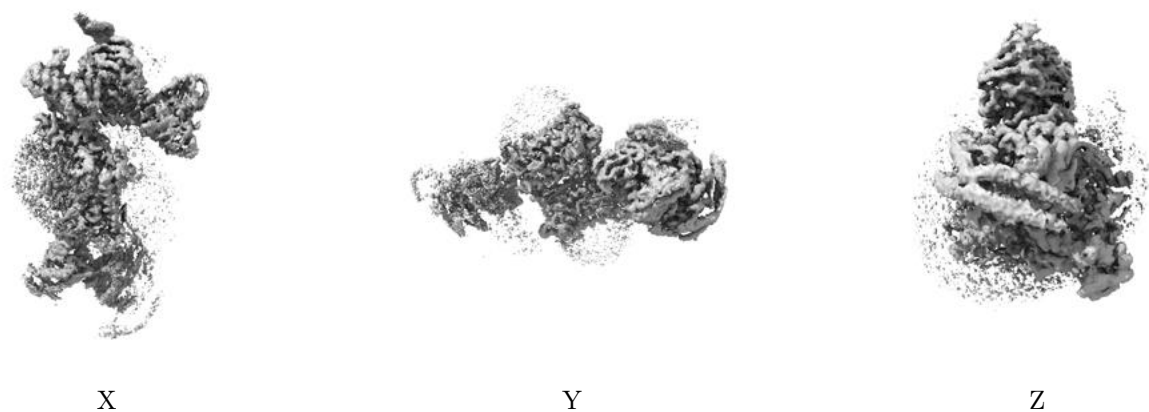
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

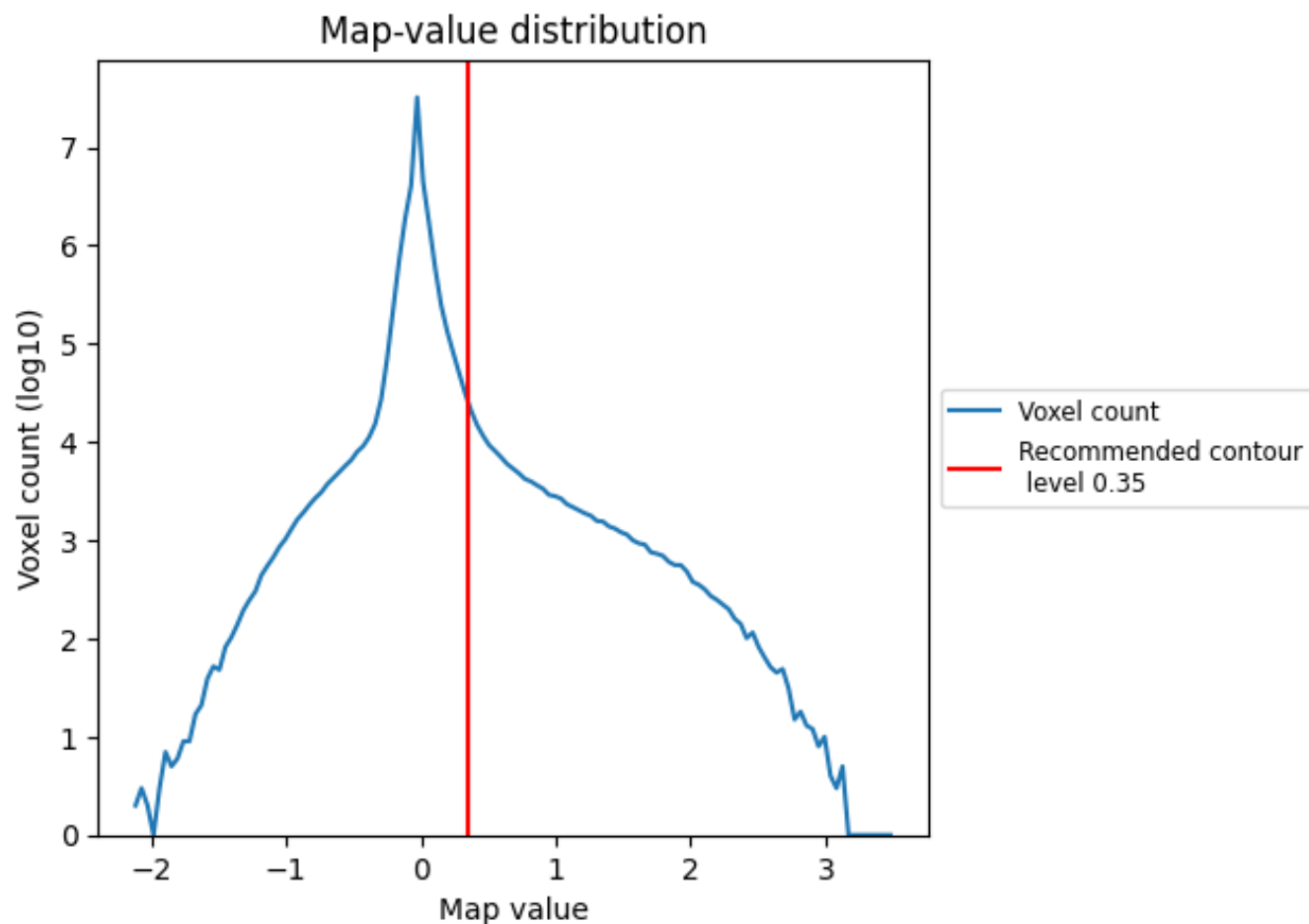
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

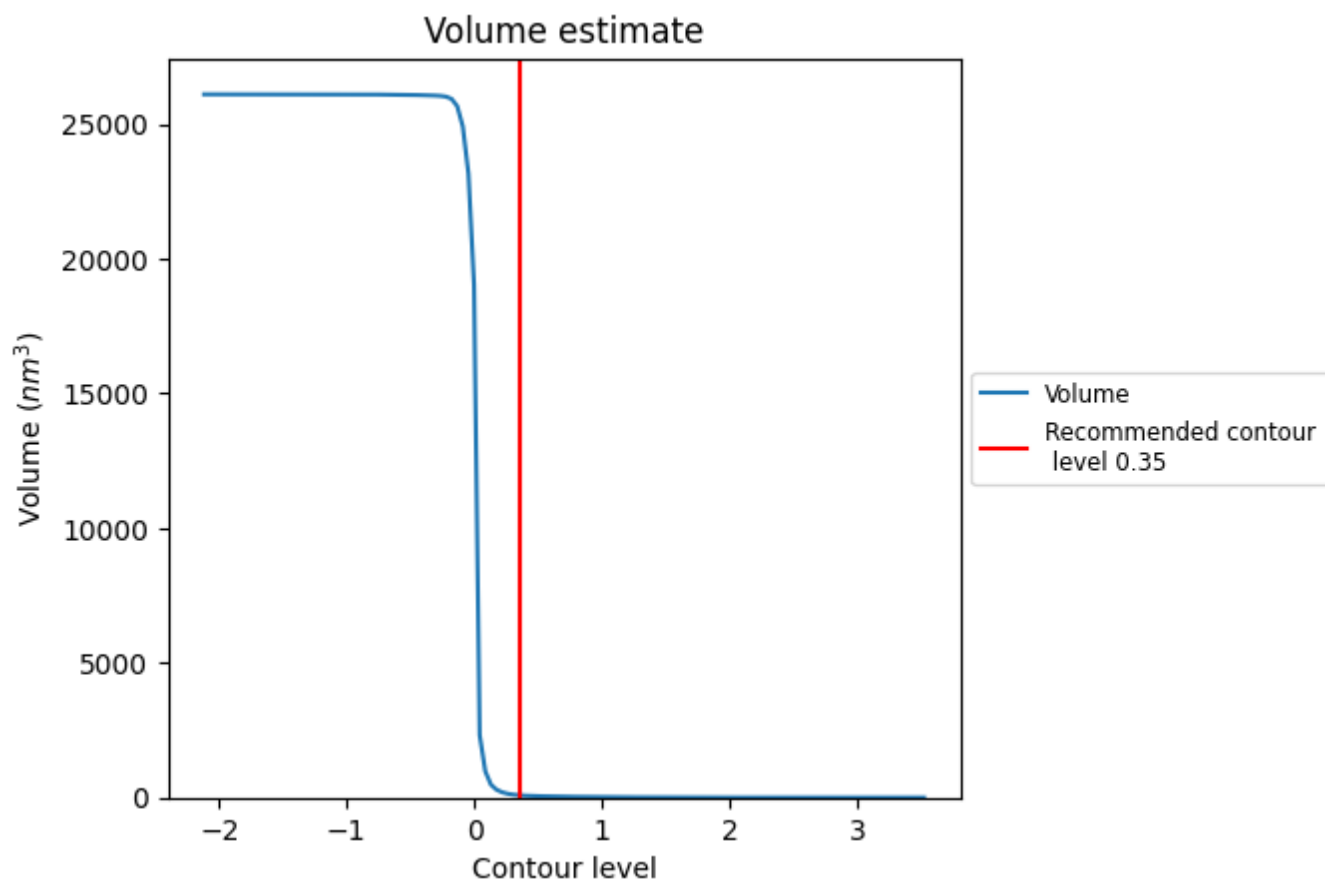
This section contains the results of statistical analysis of the map.

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.

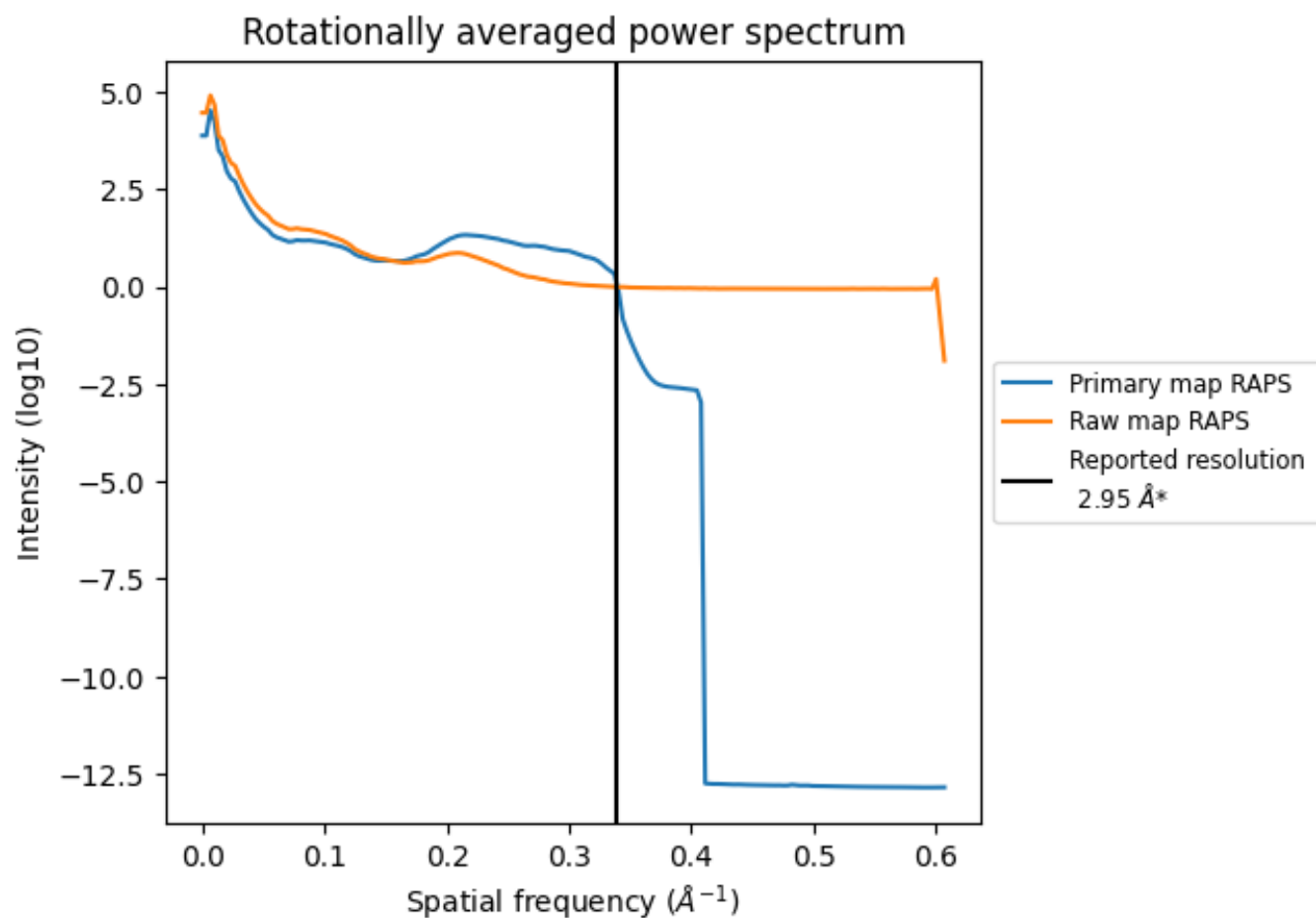
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm^3 ; this corresponds to an approximate mass of 77 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 ⓘ

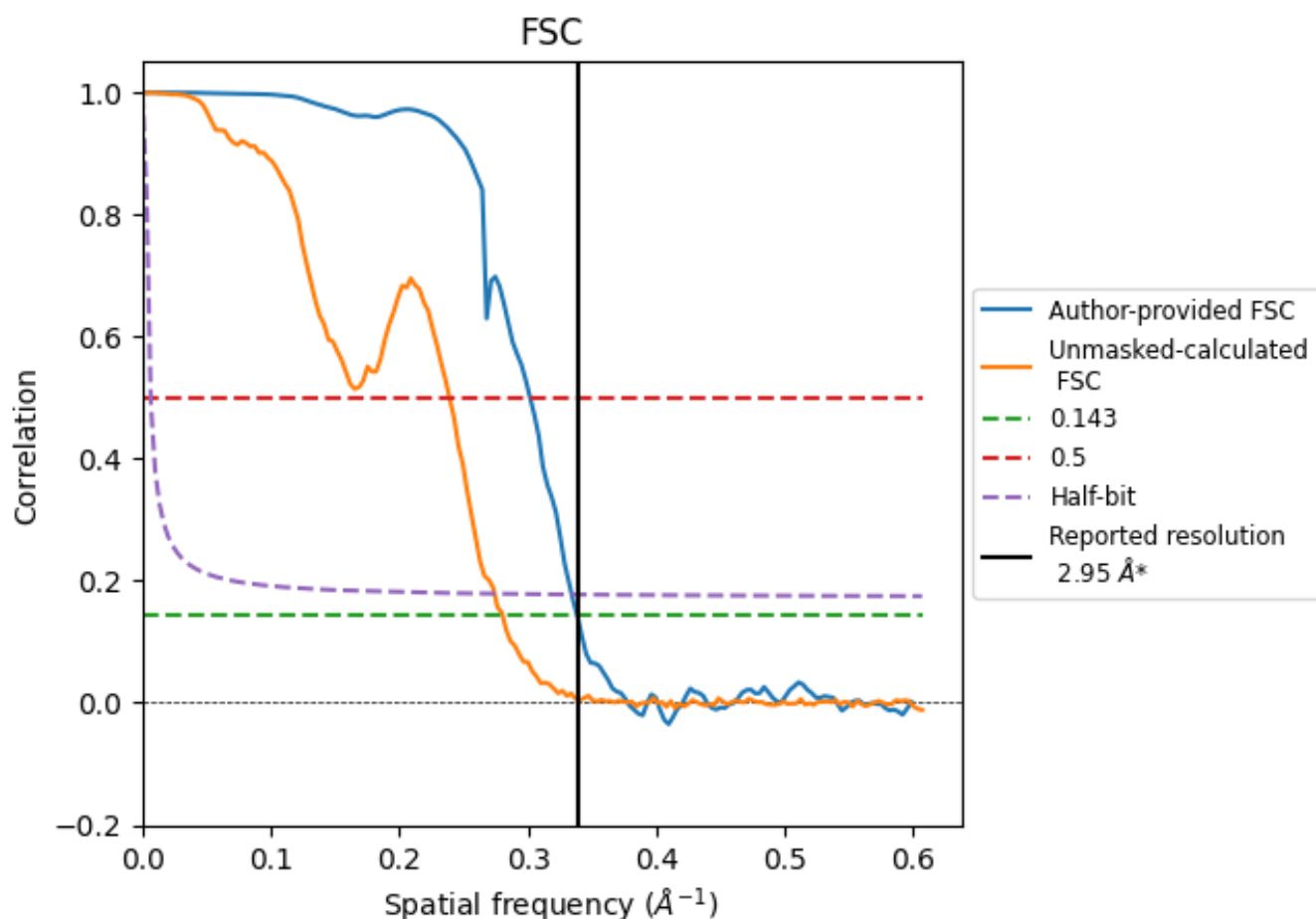


*Reported resolution corresponds to spatial frequency of 0.339 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.339 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

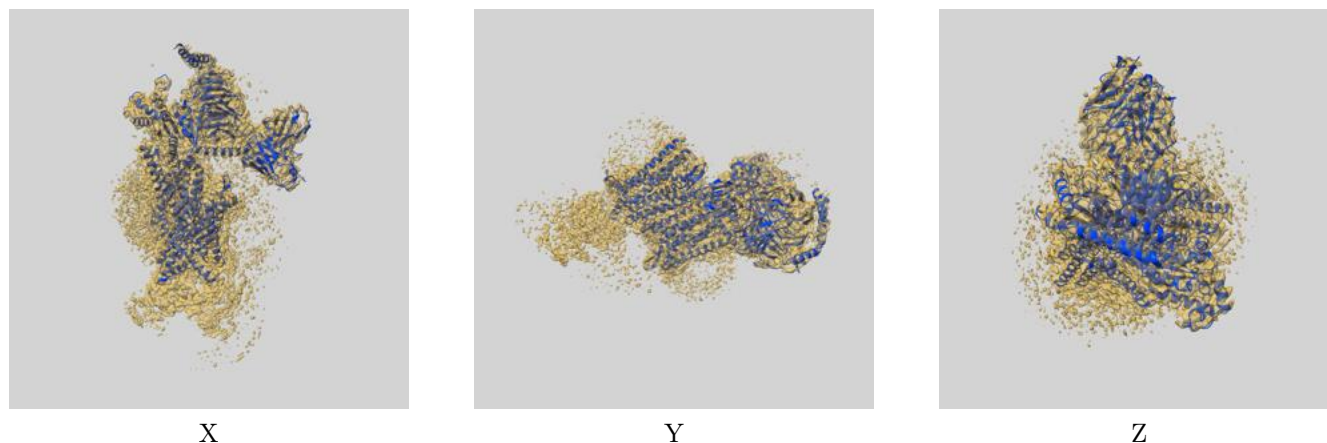
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.31	2.99
Unmasked-calculated*	3.57	4.18	3.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

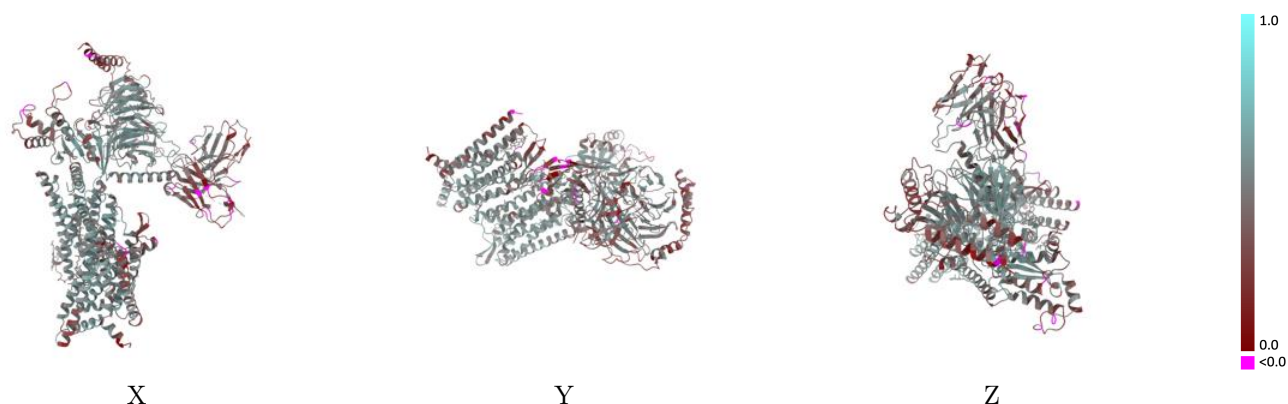
This section contains information regarding the fit between EMDB map EMD-69218 and PDB model 23SO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



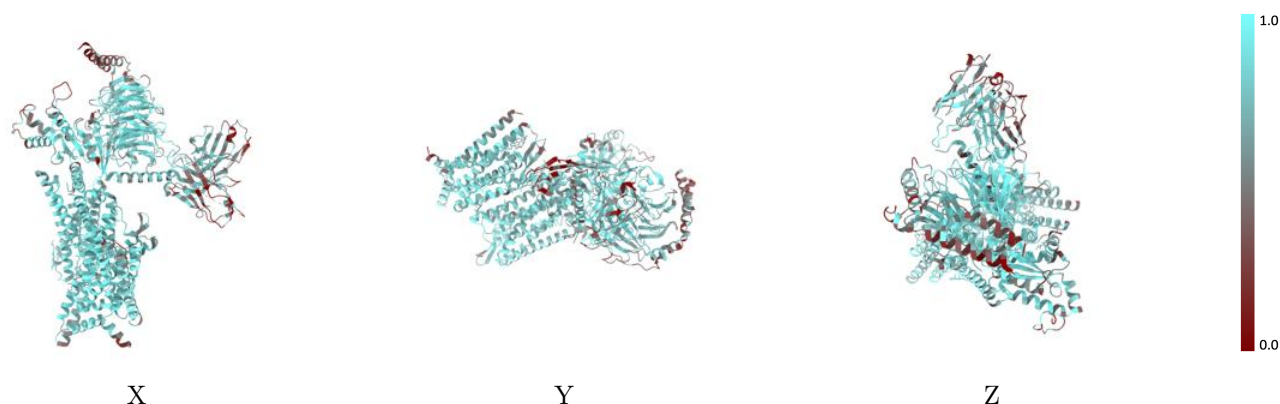
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



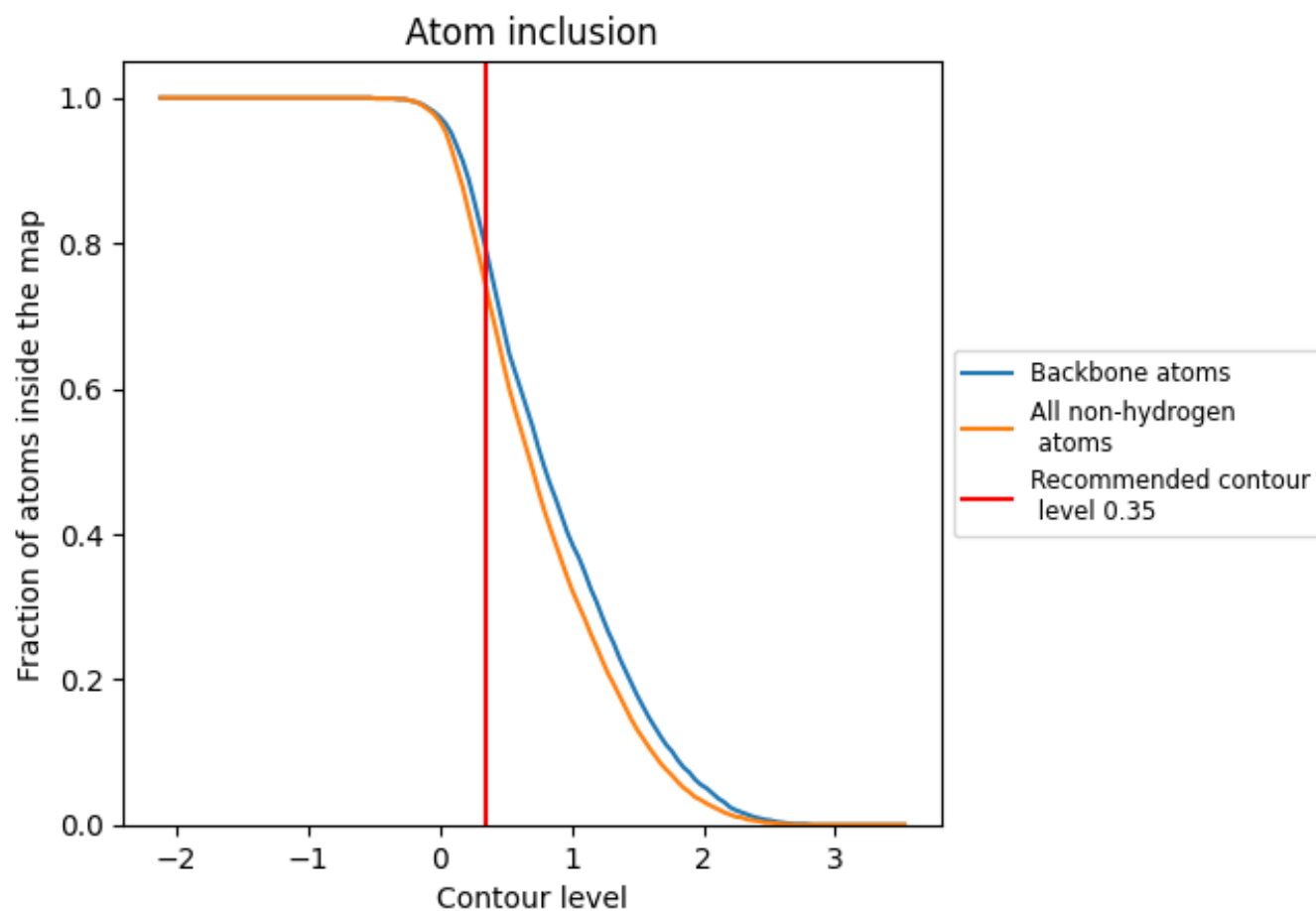
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.4540
A	0.7270	0.4540
B	0.7470	0.4650
C	0.4550	0.2860
E	0.5810	0.3590
F	0.8190	0.5230
M	0.7950	0.4680
R	0.8480	0.5230

1.0

0.0

<0.0