



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:26 PM UTC

PDB ID : 8QSL / pdb_00008qsl
EMDB ID : EMD-18635
Title : Cryo-EM structure of human SLC15A4 dimer in outward open state in LMNG
Authors : Rehan, S.; Matsuoka, R.; Jazayeri, A.; Duerr, K.L.
Deposited on : 2023-10-10
Resolution : 2.81 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.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)
Validation Pipeline (wwPDB-VP) : 2.49

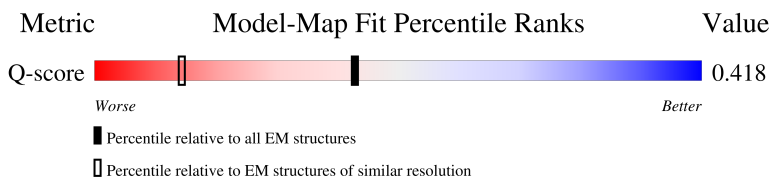
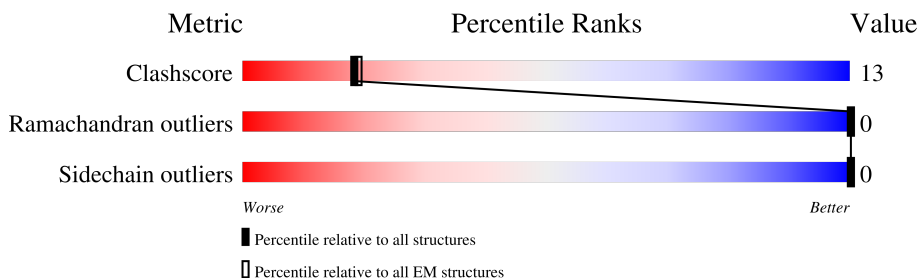
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

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	577	
1	C	577	

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.

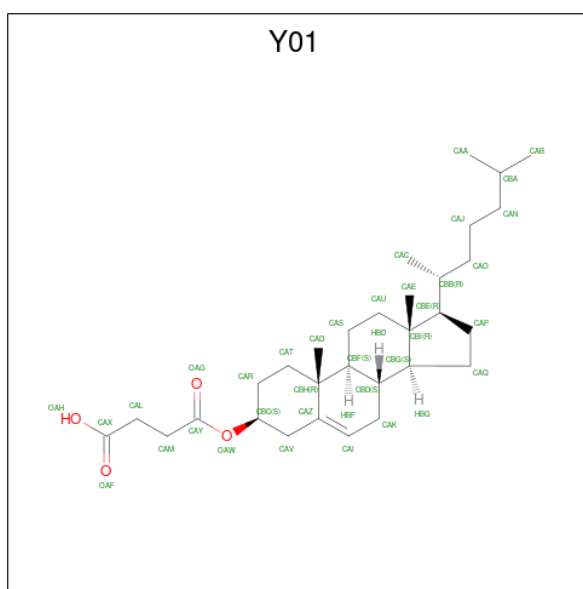
- Molecule 1 is a protein called Solute carrier family 15 member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	523	Total 3978	C 2617	N 654	O 683	S 24	0	0
1	C	523	Total 3978	C 2617	N 654	O 683	S 24	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ALA	LEU	engineered mutation	UNP Q8N697
A	15	ALA	LEU	engineered mutation	UNP Q8N697
C	14	ALA	LEU	engineered mutation	UNP Q8N697
C	15	ALA	LEU	engineered mutation	UNP Q8N697

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



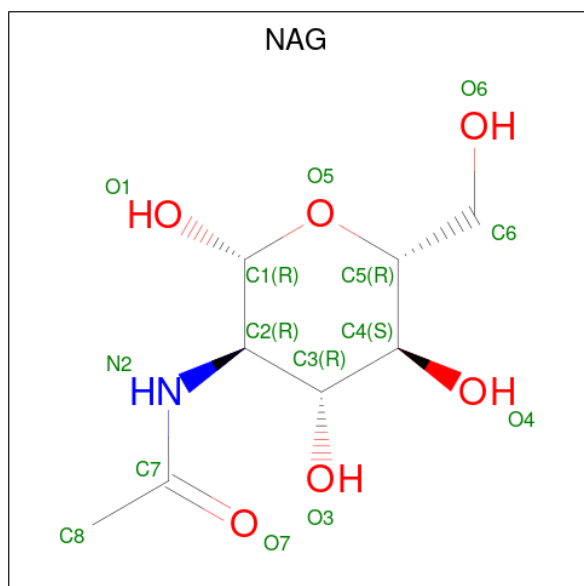
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	

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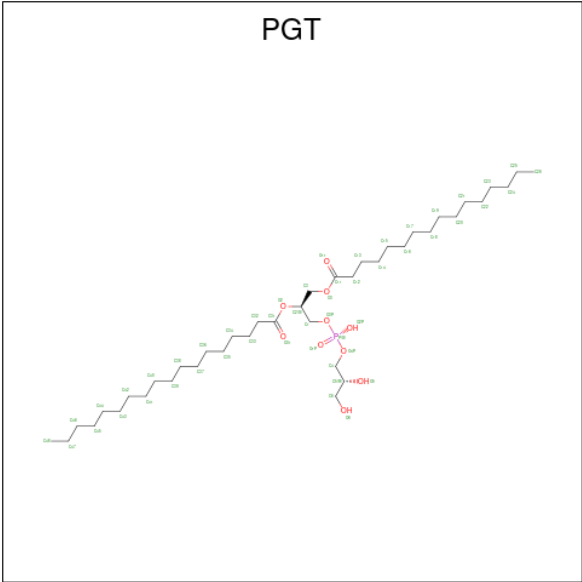
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	

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



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

- Molecule 4 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).

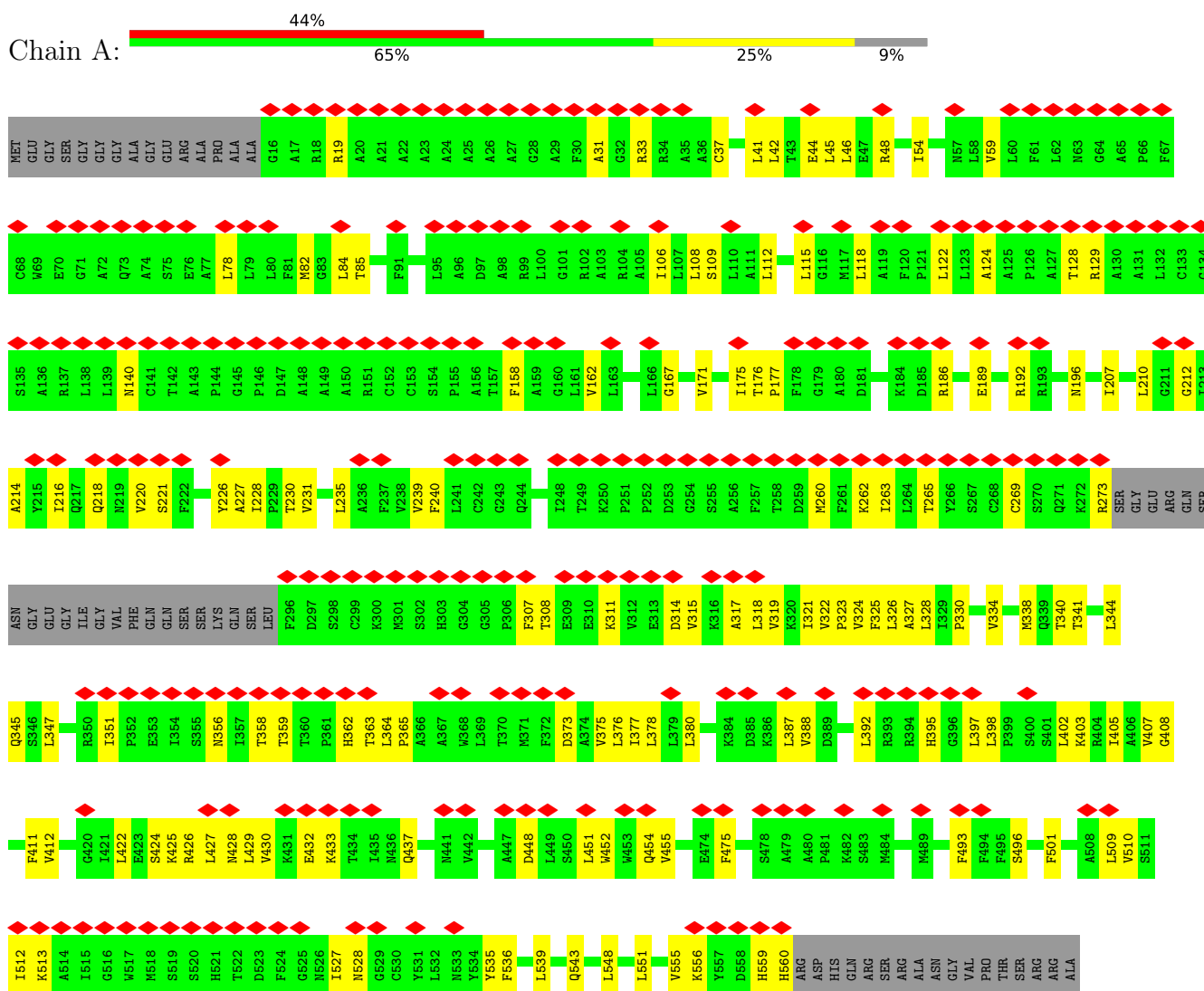


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			51	40	10	1	
4	C	1	Total	C	O	P	0
			51	40	10	1	

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: Solute carrier family 15 member 4



• Molecule 1: Solute carrier family 15 member 4



V510	S511	I512	K513	A514	I515	G516	W517	W518	S519	S520	H521	T522	D523	F524	G525	W526	I527	W528	G529	C530	Y531	L532	W533	Y534	Y535	F536	L539	Q543	L548	L549	F550	L551	V555	K556	Y557	D558	H559	H560	ARG	ASP	HIS	GLN	ARG	SER	ARG	ALA	ASN	GLY	VAL	PRO	THR	SER	ARG	ARG	ALA		
G420	L421	L422	E423	S424	K425	R426	L427	N428	L429	V430	K431	E432	K433	T434	L435	N436	Q437	N441	V442	A447	D448	L449	S450	L451	W452	W453	Q454	V455	P456	Q457	I461	E474	F475	S478	A479	A480	P481	K482	S483	W484	I488	W489	F493	F494	F495	S496	F501	A508	L509								
R350	I351	P352	E353	I354	S355	N356	L357	T358	T359	T360	P361	H362	T363	L364	P365	A366	A367	W368	L369	T370	M371	F372	D373	A374	V375	L376	I377	L378	L379	L380	K384	D385	K386	L387	V388	D389	L392	R393	R394	H395	G396	L397	L398	P399	S400	S401	L402	K403	R404	I405	A406	V407	G408	M409	F410	F411	V412
I1E	GLY	VAL	PHE	GLN	GLN	SER	SER	LYS	GLN	SER	LEU	F296	D297	S298	C299	K300	M301	S302	H303	G304	G305	P306	F307	T308	E309	E310	K311	V312	E313	D314	V315	K316	A317	L318	I321	V322	P323	V324	F325	L326	A327	L328	I329	P330	V334	M338	Q339	T340	T341	L344	Q345	S346	L347	H348	L349		
Q217	Q218	N219	V220	S221	F222	Y226	A227	T230	V231	L235	A236	F237	V238	V239	F240	L241	C242	G243	Q244	I248	T249	K250	P251	P252	D253	G254	S255	A256	F257	T258	D259	M260	F261	K262	T263	L264	T265	Y266	S267	C268	C269	S270	Q271	K272	R273	SER	GLY	GLN	ARG	GLN	SER	ASN	GLY	GLY			
R137	L138	L139	N140	C141	T142	A143	P144	G145	P146	D147	A148	A149	A150	R151	C152	C153	S154	P155	A156	T157	F158	A159	G160	L161	V162	L163	L166	V171	I175	T176	P177	F178	G179	A180	D181	K184	D185	R186	E189	R192	R193	N196	I207	L210	G211	G212	I213	A214	Y215	I216							
E70	G71	A72	Q73	A74	S75	E76	A77	L78	L79	L80	F81	M82	G83	L84	T85	F91	L95	A96	D97	A98	R99	L100	G101	R102	A103	R104	A105	I106	L107	L108	S109	L110	A111	L112	L115	G116	M117	L118	A119	F120	P121	L122	L123	A124	A125	P126	A127	T128	R129	A130	A131	L132	C133	G134	S135	A136	
MET	GLU	GLY	SER	GLY	GLY	ALA	GLU	ARG	ALA	PRO	ALA	ALA	G16	A17	R18	R19	A20	A21	A22	A23	A24	A25	A26	A27	G28	A29	F30	A31	G32	R33	R34	A35	A36	C37	L41	L42	T43	E44	L45	E47	R48	N57	L58	V59	L60	F61	L62	N63	G64	A65	P66	F67	C68	W69			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	438976	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.593	Depositor
Minimum map value	-0.332	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.207	Depositor
Map size (Å)	250.79999, 250.79999, 250.79999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NAG, PGT

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	0.17	0/4079	0.36	0/5549
1	C	0.17	0/4079	0.37	0/5549
All	All	0.17	0/8158	0.37	0/11098

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

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	3978	0	4062	105	0
1	C	3978	0	4062	107	0
2	A	210	0	294	11	0
2	C	210	0	294	10	0
3	A	14	0	13	1	0
3	C	14	0	13	1	0
4	A	51	0	78	1	0
4	C	51	0	78	1	0
All	All	8506	0	8894	227	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 13.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLN:O	1:C:218:GLN:NE2	2.04	0.90
1:A:227:ALA:O	1:A:230:THR:OG1	1.97	0.83
1:C:227:ALA:O	1:C:230:THR:OG1	1.97	0.81
1:C:425:LYS:NZ	2:C:602:Y01:OAG	2.13	0.81
1:C:433:LYS:NZ	1:C:448:ASP:OD2	2.17	0.78
1:A:425:LYS:NZ	2:A:602:Y01:OAG	2.17	0.77
1:A:433:LYS:NZ	1:A:448:ASP:OD2	2.18	0.76
1:A:218:GLN:O	1:A:218:GLN:NE2	2.19	0.76
1:C:124:ALA:O	1:C:129:ARG:NH2	2.19	0.75
1:A:124:ALA:O	1:A:129:ARG:NH2	2.20	0.74
1:A:403:LYS:O	1:A:407:VAL:HG23	1.89	0.72
1:C:403:LYS:O	1:C:407:VAL:HG23	1.88	0.72
2:C:605:Y01:HAC1	2:C:605:Y01:HAE2	1.74	0.70
2:A:605:Y01:HAC1	2:A:605:Y01:HAE2	1.74	0.69
1:C:347:LEU:O	1:C:437:GLN:NE2	2.26	0.68
2:C:601:Y01:HAA2	2:C:601:Y01:HAC3	1.75	0.68
2:A:601:Y01:HAC3	2:A:601:Y01:HAA2	1.75	0.68
1:A:556:LYS:O	1:A:560:HIS:ND1	2.26	0.68
1:A:108:LEU:HD13	1:A:112:LEU:HD23	1.77	0.67
1:C:321:ILE:HG22	1:C:325:PHE:CE2	2.31	0.66
1:C:19:ARG:NH1	1:C:395:HIS:O	2.30	0.65
1:A:265:THR:O	1:A:269:CYS:N	2.30	0.65
1:C:556:LYS:O	1:C:560:HIS:ND1	2.24	0.65
1:A:207:ILE:HD12	1:A:378:LEU:HD12	1.79	0.64
1:A:260:MET:SD	1:A:260:MET:N	2.70	0.64
1:A:19:ARG:NH1	1:A:395:HIS:O	2.31	0.64
1:C:207:ILE:HD12	1:C:378:LEU:HD12	1.80	0.63
1:A:262:LYS:O	1:A:265:THR:OG1	2.15	0.63
1:A:317:ALA:O	1:A:321:ILE:HG13	1.98	0.62
1:A:347:LEU:O	1:A:437:GLN:NE2	2.32	0.62
1:C:265:THR:O	1:C:269:CYS:N	2.31	0.62
1:C:122:LEU:O	1:C:128:THR:OG1	2.18	0.61
1:C:260:MET:SD	1:C:260:MET:N	2.73	0.61
1:A:140:ASN:OD1	3:A:604:NAG:N2	2.34	0.61
1:C:262:LYS:O	1:C:265:THR:OG1	2.16	0.61
1:A:356:ASN:OD1	1:A:356:ASN:O	2.19	0.61
1:C:140:ASN:OD1	3:C:604:NAG:N2	2.34	0.61
1:C:31:ALA:O	1:C:33:ARG:N	2.33	0.60
1:A:269:CYS:O	1:A:273:ARG:N	2.35	0.60
1:C:219:ASN:ND2	1:C:363:THR:OG1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:HG22	1:A:325:PHE:CE2	2.37	0.59
1:C:338:MET:HE1	1:C:412:VAL:HG12	1.84	0.59
1:C:356:ASN:OD1	1:C:356:ASN:O	2.19	0.59
1:C:269:CYS:O	1:C:273:ARG:N	2.36	0.59
1:A:338:MET:HE1	1:A:412:VAL:HG12	1.84	0.58
1:A:122:LEU:O	1:A:128:THR:OG1	2.20	0.58
1:A:493:PHE:O	1:A:496:SER:OG	2.20	0.57
1:C:493:PHE:O	1:C:496:SER:OG	2.20	0.57
1:A:358:THR:O	1:A:359:THR:OG1	2.21	0.57
1:A:31:ALA:O	1:A:33:ARG:N	2.33	0.57
1:C:218:GLN:HE21	1:C:218:GLN:C	2.06	0.57
1:C:338:MET:HE1	1:C:412:VAL:CG1	2.36	0.56
1:A:338:MET:HE1	1:A:412:VAL:CG1	2.36	0.56
1:C:317:ALA:O	1:C:321:ILE:HG13	2.05	0.56
1:C:253:ASP:OD1	1:C:253:ASP:O	2.23	0.56
1:C:434:THR:C	1:C:435:ILE:HD13	2.30	0.56
4:A:608:PGT:O1P	4:A:608:PGT:O6	2.24	0.56
1:A:422:LEU:HD12	1:A:422:LEU:O	2.06	0.55
1:C:422:LEU:O	1:C:422:LEU:HD12	2.06	0.55
1:A:231:VAL:O	1:A:235:LEU:HG	2.07	0.55
1:C:376:LEU:O	1:C:380:LEU:HD23	2.08	0.54
2:A:601:Y01:HAD3	2:A:602:Y01:CAE	2.38	0.54
1:C:82:MET:O	1:C:85:THR:OG1	2.22	0.54
1:C:358:THR:O	1:C:359:THR:OG1	2.22	0.54
2:C:607:Y01:HAC1	2:C:607:Y01:HAE2	1.89	0.54
1:A:452:TRP:O	1:A:455:VAL:HG23	2.08	0.54
1:C:231:VAL:O	1:C:235:LEU:HG	2.08	0.54
1:C:310:GLU:OE1	1:C:310:GLU:N	2.35	0.54
2:C:601:Y01:HAD3	2:C:602:Y01:CAE	2.38	0.54
1:A:376:LEU:O	1:A:380:LEU:HD23	2.07	0.53
1:A:426:ARG:NH2	1:A:527:ILE:HD12	2.23	0.53
2:A:607:Y01:HAC1	2:A:607:Y01:HAE2	1.89	0.53
1:C:157:THR:O	1:C:161:LEU:HD23	2.09	0.53
1:A:82:MET:O	1:A:85:THR:OG1	2.21	0.53
1:A:373:ASP:OD1	1:A:377:ILE:HD11	2.09	0.53
1:C:452:TRP:O	1:C:455:VAL:HG23	2.10	0.52
1:C:348:HIS:CE1	1:C:527:ILE:HG22	2.45	0.52
1:A:210:LEU:O	1:A:214:ALA:HB3	2.09	0.52
1:C:102:ARG:O	1:C:106:ILE:HG12	2.10	0.52
1:A:59:VAL:HG23	1:A:78:LEU:HD12	1.91	0.52
1:C:59:VAL:HG23	1:C:78:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:SER:OG	1:C:171:VAL:HG13	2.11	0.51
1:C:212:GLY:O	1:C:216:ILE:HG13	2.10	0.51
1:C:340:THR:O	1:C:344:LEU:HD12	2.10	0.51
1:A:408:GLY:O	1:A:412:VAL:HG23	2.11	0.51
1:A:212:GLY:O	1:A:216:ILE:HG13	2.10	0.50
1:C:408:GLY:O	1:C:412:VAL:HG23	2.11	0.50
1:A:318:LEU:O	1:A:322:VAL:HG23	2.12	0.50
1:C:210:LEU:O	1:C:214:ALA:HB3	2.12	0.49
1:A:340:THR:O	1:A:344:LEU:HD12	2.12	0.49
1:C:115:LEU:HD12	1:C:115:LEU:O	2.12	0.49
1:A:42:LEU:O	1:A:46:LEU:HD23	2.13	0.49
1:A:109:SER:OG	1:A:171:VAL:HG13	2.13	0.49
1:C:362:HIS:O	1:C:363:THR:OG1	2.28	0.49
1:A:362:HIS:O	1:A:363:THR:OG1	2.28	0.49
1:C:432:GLU:OE1	1:C:432:GLU:N	2.40	0.49
1:C:344:LEU:HD12	1:C:344:LEU:H	1.78	0.49
1:C:373:ASP:OD1	1:C:377:ILE:HD11	2.12	0.48
1:A:122:LEU:HD22	1:A:122:LEU:H	1.79	0.48
1:C:42:LEU:O	1:C:46:LEU:HD23	2.13	0.48
1:C:424:SER:O	1:C:428:ASN:OD1	2.32	0.48
1:A:118:LEU:O	1:A:122:LEU:CD2	2.62	0.48
1:C:318:LEU:O	1:C:322:VAL:HG23	2.14	0.48
1:A:402:LEU:HA	1:A:405:ILE:HD12	1.95	0.48
2:A:603:Y01:HAU2	2:A:603:Y01:HAC1	1.96	0.48
1:C:362:HIS:C	1:C:363:THR:HG1	2.21	0.48
1:C:501:PHE:HB3	2:C:606:Y01:HAE1	1.96	0.48
1:C:78:LEU:HD23	1:C:78:LEU:O	2.14	0.48
2:C:603:Y01:HAC1	2:C:603:Y01:HAU2	1.96	0.47
1:A:427:LEU:O	1:A:430:VAL:HG22	2.15	0.47
1:A:115:LEU:HD12	1:A:115:LEU:O	2.15	0.47
1:A:424:SER:O	1:A:428:ASN:OD1	2.33	0.47
1:C:175:ILE:HG23	1:C:176:THR:N	2.30	0.47
1:C:207:ILE:HD11	1:C:375:VAL:HA	1.97	0.47
1:A:501:PHE:HB3	2:A:606:Y01:HAE1	1.96	0.46
1:A:78:LEU:HD23	1:A:78:LEU:O	2.15	0.46
1:A:451:LEU:O	1:A:451:LEU:HD12	2.15	0.46
1:C:402:LEU:HA	1:C:405:ILE:HD12	1.97	0.46
1:C:451:LEU:O	1:C:451:LEU:HD12	2.15	0.46
1:A:207:ILE:HD11	1:A:375:VAL:HA	1.98	0.46
1:A:323:PRO:HA	1:A:326:LEU:HD12	1.98	0.46
1:C:311:LYS:HA	1:C:314:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD12	1:A:344:LEU:H	1.81	0.45
1:C:535:TYR:CE1	1:C:539:LEU:HD11	2.51	0.45
1:A:54:ILE:HD13	1:A:226:TYR:HE1	1.81	0.45
1:C:334:VAL:HG11	1:C:543:GLN:HE21	1.82	0.45
1:C:323:PRO:HA	1:C:326:LEU:HD12	1.97	0.45
1:A:175:ILE:HG23	1:A:176:THR:N	2.31	0.45
1:C:307:PHE:O	1:C:308:THR:C	2.59	0.45
1:A:189:GLU:OE1	1:A:189:GLU:N	2.33	0.45
1:C:108:LEU:O	1:C:112:LEU:HD23	2.17	0.45
1:C:192:ARG:O	1:C:196:ASN:OD1	2.34	0.45
1:C:260:MET:HE3	1:C:260:MET:HA	1.99	0.45
1:A:513:LYS:O	1:A:513:LYS:HD3	2.17	0.45
1:A:535:TYR:CE1	1:A:539:LEU:HD11	2.52	0.44
1:A:351:ILE:HD12	1:A:351:ILE:HA	1.89	0.44
1:C:310:GLU:O	1:C:314:ASP:OD2	2.35	0.44
1:C:364:LEU:C	1:C:364:LEU:HD23	2.43	0.44
1:A:307:PHE:O	1:A:308:THR:C	2.59	0.44
1:C:536:PHE:HA	1:C:539:LEU:HD12	1.99	0.44
1:A:311:LYS:HA	1:A:314:ASP:OD2	2.18	0.44
1:A:548:LEU:HD11	2:C:601:Y01:HAB1	1.99	0.44
1:C:551:LEU:O	1:C:555:VAL:HG23	2.18	0.44
1:A:176:THR:OG1	1:A:177:PRO:HD3	2.17	0.44
2:A:601:Y01:HAB1	1:C:548:LEU:HD11	1.99	0.44
1:C:364:LEU:HD23	1:C:365:PRO:O	2.17	0.44
1:C:513:LYS:O	1:C:513:LYS:HD3	2.18	0.44
1:A:551:LEU:O	1:A:555:VAL:HG23	2.18	0.44
1:C:509:LEU:HD23	1:C:510:VAL:N	2.33	0.44
1:A:334:VAL:HG11	1:A:543:GLN:HE21	1.83	0.44
1:C:324:VAL:HG11	1:C:475:PHE:CE2	2.53	0.44
1:C:488:ILE:N	1:C:488:ILE:HD13	2.33	0.44
1:A:528:ASN:C	1:A:528:ASN:OD1	2.60	0.43
1:C:327:ALA:O	1:C:330:PRO:HD2	2.18	0.43
1:C:220:VAL:HG12	1:C:221:SER:N	2.33	0.43
1:C:189:GLU:OE1	1:C:189:GLU:N	2.33	0.43
1:A:327:ALA:O	1:A:330:PRO:HD2	2.18	0.43
1:A:220:VAL:HG12	1:A:221:SER:N	2.32	0.43
1:A:536:PHE:HA	1:A:539:LEU:HD12	2.01	0.43
4:C:608:PGT:O1P	4:C:608:PGT:O6	2.31	0.43
1:A:559:HIS:ND1	1:A:559:HIS:C	2.76	0.43
1:C:186:ARG:HD3	1:C:186:ARG:N	2.34	0.43
1:A:106:ILE:HG21	1:A:240:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HD12	1:A:228:ILE:HD12	2.01	0.43
1:C:345:GLN:OE1	1:C:454:GLN:NE2	2.52	0.43
1:C:427:LEU:O	1:C:430:VAL:HG22	2.19	0.43
1:A:37:CYS:O	1:A:41:LEU:HD13	2.19	0.43
1:C:509:LEU:O	1:C:512:ILE:HD12	2.18	0.43
2:C:601:Y01:HAD3	2:C:602:Y01:HAE2	2.01	0.43
1:C:535:TYR:CD1	1:C:539:LEU:HD11	2.54	0.43
1:A:186:ARG:HD3	1:A:186:ARG:N	2.34	0.43
1:A:509:LEU:HD23	1:A:510:VAL:N	2.34	0.43
1:C:457:GLN:O	1:C:461:ILE:HG12	2.19	0.43
2:A:601:Y01:HAD3	2:A:602:Y01:HAE2	2.01	0.42
1:C:44:GLU:OE1	1:C:48:ARG:HG2	2.19	0.42
1:C:176:THR:OG1	1:C:177:PRO:HD3	2.18	0.42
1:C:392:LEU:CD2	1:C:397:LEU:HD12	2.50	0.42
1:A:535:TYR:CD1	1:A:539:LEU:HD11	2.54	0.42
1:A:167:GLY:O	1:A:171:VAL:HG13	2.19	0.42
1:A:324:VAL:HG11	1:A:475:PHE:CE2	2.53	0.42
1:A:235:LEU:O	1:A:239:VAL:HG13	2.19	0.42
1:C:235:LEU:O	1:C:239:VAL:HG13	2.20	0.42
1:A:432:GLU:H	1:A:432:GLU:CD	2.26	0.42
1:C:193:ARG:HA	1:C:196:ASN:OD1	2.20	0.42
1:C:351:ILE:HD13	1:C:437:GLN:OE1	2.20	0.42
1:C:37:CYS:O	1:C:41:LEU:HD13	2.19	0.42
1:C:409:MET:HE1	1:C:550:PHE:CG	2.55	0.42
1:A:45:LEU:C	1:A:45:LEU:HD23	2.45	0.42
1:A:509:LEU:O	1:A:512:ILE:HD12	2.19	0.41
1:C:171:VAL:O	1:C:175:ILE:HG22	2.20	0.41
1:C:432:GLU:H	1:C:432:GLU:CD	2.28	0.41
1:A:84:LEU:HD12	1:A:84:LEU:O	2.20	0.41
1:A:392:LEU:CD2	1:A:397:LEU:HD12	2.49	0.41
1:A:398:LEU:HD11	2:A:603:Y01:HAD3	2.01	0.41
1:A:407:VAL:HG12	1:A:411:PHE:CE2	2.56	0.41
1:C:84:LEU:HD12	1:C:84:LEU:O	2.20	0.41
1:C:407:VAL:HG12	1:C:411:PHE:CE2	2.55	0.41
1:A:263:ILE:HG21	1:A:311:LYS:HG2	2.03	0.41
1:A:322:VAL:HB	1:A:323:PRO:HD3	2.03	0.41
1:A:429:LEU:O	1:A:432:GLU:OE1	2.39	0.41
2:A:601:Y01:HAU2	2:A:601:Y01:HAC1	2.02	0.41
1:C:122:LEU:H	1:C:122:LEU:HD22	1.85	0.41
1:A:345:GLN:OE1	1:A:454:GLN:NE2	2.52	0.41
1:C:115:LEU:HD12	1:C:115:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:O	1:A:196:ASN:OD1	2.38	0.41
1:C:325:PHE:HA	1:C:328:LEU:HD12	2.03	0.41
1:A:115:LEU:HD12	1:A:115:LEU:C	2.46	0.41
1:A:158:PHE:O	1:A:162:VAL:HG12	2.21	0.41
1:A:387:LEU:HD23	1:A:388:VAL:N	2.36	0.41
1:C:318:LEU:HD23	1:C:322:VAL:HG23	2.03	0.41
1:C:334:VAL:HG11	1:C:543:GLN:NE2	2.36	0.41
1:C:387:LEU:HD23	1:C:388:VAL:N	2.36	0.41
1:A:171:VAL:O	1:A:175:ILE:HG22	2.20	0.41
1:C:398:LEU:HD11	2:C:603:Y01:HAD3	2.02	0.41
1:A:44:GLU:OE1	1:A:48:ARG:HG2	2.20	0.40
1:A:341:THR:HA	1:A:344:LEU:CD1	2.51	0.40
1:A:364:LEU:HD23	1:A:364:LEU:C	2.46	0.40
1:A:315:VAL:O	1:A:319:VAL:HG23	2.21	0.40
1:C:324:VAL:HG11	1:C:475:PHE:HE2	1.86	0.40
1:C:341:THR:HA	1:C:344:LEU:HD13	2.03	0.40
1:A:227:ALA:O	1:A:231:VAL:HG23	2.21	0.40
1:A:325:PHE:HA	1:A:328:LEU:HD12	2.02	0.40
1:A:432:GLU:CD	1:A:432:GLU:N	2.79	0.40
1:A:513:LYS:HA	1:A:513:LYS:HE2	2.04	0.40
1:A:364:LEU:HD23	1:A:365:PRO:O	2.22	0.40
1:A:422:LEU:HD12	1:A:422:LEU:C	2.47	0.40
1:C:227:ALA:O	1:C:231:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/577 (90%)	476 (92%)	43 (8%)	0	100	100
1	C	519/577 (90%)	472 (91%)	47 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1038/1154 (90%)	948 (91%)	90 (9%)	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	410/448 (92%)	410 (100%)	0	100	100
1	C	410/448 (92%)	410 (100%)	0	100	100
All	All	820/896 (92%)	820 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	A	437	GLN
1	C	174	ASN
1	C	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

16 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
2	Y01	C	601	-	38,38,38	0.57	0	57,57,57	0.57	0
2	Y01	C	605	-	38,38,38	0.55	0	57,57,57	0.87	1 (1%)
4	PGT	A	608	-	50,50,50	0.50	0	53,56,56	0.45	0
2	Y01	A	607	-	38,38,38	0.56	0	57,57,57	0.67	0
2	Y01	A	605	-	38,38,38	0.55	0	57,57,57	0.90	1 (1%)
2	Y01	A	603	-	38,38,38	0.60	0	57,57,57	1.16	4 (7%)
2	Y01	A	606	-	38,38,38	0.55	0	57,57,57	0.59	0
2	Y01	A	601	-	38,38,38	0.57	0	57,57,57	0.55	0
2	Y01	C	602	-	38,38,38	0.56	0	57,57,57	0.83	2 (3%)
2	Y01	C	607	-	38,38,38	0.56	0	57,57,57	0.67	0
3	NAG	C	604	1	14,14,15	0.77	0	17,19,21	0.86	0
2	Y01	C	603	-	38,38,38	0.61	0	57,57,57	1.16	4 (7%)
4	PGT	C	608	-	50,50,50	0.50	0	53,56,56	0.45	0
2	Y01	C	606	-	38,38,38	0.55	0	57,57,57	0.59	0
3	NAG	A	604	1	14,14,15	0.77	0	17,19,21	0.86	0
2	Y01	A	602	-	38,38,38	0.57	0	57,57,57	0.79	1 (1%)

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	Y01	C	601	-	-	4/19/77/77	0/4/4/4
2	Y01	C	605	-	-	7/19/77/77	0/4/4/4
4	PGT	A	608	-	-	25/55/55/55	-
2	Y01	A	607	-	-	8/19/77/77	0/4/4/4
2	Y01	A	605	-	-	7/19/77/77	0/4/4/4
2	Y01	A	603	-	-	4/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	A	606	-	-	8/19/77/77	0/4/4/4
2	Y01	A	601	-	-	4/19/77/77	0/4/4/4
2	Y01	C	602	-	-	8/19/77/77	0/4/4/4
2	Y01	C	607	-	-	8/19/77/77	0/4/4/4
3	NAG	C	604	1	-	0/6/23/26	0/1/1/1
2	Y01	C	603	-	-	4/19/77/77	0/4/4/4
4	PGT	C	608	-	-	25/55/55/55	-
2	Y01	C	606	-	-	8/19/77/77	0/4/4/4
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	Y01	A	602	-	-	7/19/77/77	0/4/4/4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	Y01	CAR-CBC-CAV	4.27	116.90	110.97
2	C	603	Y01	CAR-CBC-CAV	4.25	116.88	110.97
2	C	603	Y01	CBC-CAV-CAZ	4.04	117.42	111.45
2	A	603	Y01	CBC-CAV-CAZ	4.03	117.40	111.45
2	C	603	Y01	CAT-CBH-CAZ	-2.98	103.61	108.74
2	A	603	Y01	CAT-CBH-CAZ	-2.97	103.63	108.74
2	A	605	Y01	CAK-CBD-CBF	2.49	112.59	109.72
2	C	602	Y01	CAR-CBC-CAV	-2.40	107.64	110.97
2	C	605	Y01	CAK-CBD-CBF	2.28	112.36	109.72
2	A	602	Y01	CAR-CBC-CAV	-2.07	108.09	110.97
2	A	603	Y01	CAT-CBH-CBF	2.06	111.47	108.74
2	C	603	Y01	CAT-CBH-CBF	2.05	111.45	108.74
2	C	602	Y01	OAW-CBC-CAV	2.01	112.19	108.04

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	Y01	CAM-CAY-OAW-CBC
2	A	607	Y01	OAG-CAY-OAW-CBC
2	C	603	Y01	CAM-CAY-OAW-CBC
2	C	607	Y01	OAG-CAY-OAW-CBC
4	A	608	PGT	C1-O3P-P-O4P
4	A	608	PGT	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
4	C	608	PGT	C1-O3P-P-O4P
4	C	608	PGT	C4-O4P-P-O3P
2	A	602	Y01	CAV-CBC-OAW-CAY
2	A	603	Y01	OAG-CAY-OAW-CBC
2	C	603	Y01	OAG-CAY-OAW-CBC
2	A	607	Y01	CAM-CAY-OAW-CBC
2	C	607	Y01	CAM-CAY-OAW-CBC
2	C	602	Y01	CAR-CBC-OAW-CAY
2	A	602	Y01	CAM-CAY-OAW-CBC
2	C	602	Y01	CAM-CAY-OAW-CBC
2	A	605	Y01	CAJ-CAO-CBB-CAC
2	A	606	Y01	CAJ-CAO-CBB-CAC
2	C	605	Y01	CAJ-CAO-CBB-CAC
4	A	608	PGT	C5-C4-O4P-P
4	C	608	PGT	C5-C4-O4P-P
2	C	606	Y01	CAJ-CAO-CBB-CAC
2	A	606	Y01	CAJ-CAO-CBB-CBE
2	C	606	Y01	CAJ-CAO-CBB-CBE
2	A	602	Y01	CAJ-CAO-CBB-CBE
2	A	605	Y01	CAJ-CAO-CBB-CBE
2	C	602	Y01	CAJ-CAO-CBB-CBE
2	C	605	Y01	CAJ-CAO-CBB-CBE
2	C	602	Y01	OAG-CAY-OAW-CBC
2	A	602	Y01	OAG-CAY-OAW-CBC
2	A	602	Y01	CAJ-CAO-CBB-CAC
2	C	602	Y01	CAJ-CAO-CBB-CAC
2	A	601	Y01	CAO-CAJ-CAN-CBA
2	A	606	Y01	CAN-CAJ-CAO-CBB
2	C	601	Y01	CAO-CAJ-CAN-CBA
2	C	606	Y01	CAN-CAJ-CAO-CBB
2	A	605	Y01	CAX-CAL-CAM-CAY
2	A	607	Y01	CAJ-CAO-CBB-CBE
2	C	607	Y01	CAJ-CAO-CBB-CBE
2	C	605	Y01	CAX-CAL-CAM-CAY
4	A	608	PGT	C4-C5-C6-O6
4	C	608	PGT	C4-C5-C6-O6
2	A	606	Y01	CAM-CAY-OAW-CBC
2	C	606	Y01	CAM-CAY-OAW-CBC
2	A	605	Y01	CAJ-CAN-CBA-CAA
2	C	605	Y01	CAJ-CAN-CBA-CAA
2	C	602	Y01	CAV-CBC-OAW-CAY
4	A	608	PGT	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
4	C	608	PGT	C13-C14-C15-C16
2	A	605	Y01	CAJ-CAN-CBA-CAB
2	C	605	Y01	CAJ-CAN-CBA-CAB
4	C	608	PGT	C16-C17-C18-C19
4	A	608	PGT	C16-C17-C18-C19
4	A	608	PGT	C33-C34-C35-C36
4	A	608	PGT	C42-C43-C44-C45
4	C	608	PGT	C42-C43-C44-C45
4	C	608	PGT	C33-C34-C35-C36
2	A	607	Y01	CAJ-CAO-CBB-CAC
2	C	607	Y01	CAJ-CAO-CBB-CAC
4	A	608	PGT	C32-C31-O2-C2
4	C	608	PGT	C32-C31-O2-C2
2	A	606	Y01	OAG-CAY-OAW-CBC
2	C	606	Y01	OAG-CAY-OAW-CBC
4	A	608	PGT	C20-C21-C22-C23
4	C	608	PGT	C20-C21-C22-C23
4	A	608	PGT	O31-C31-O2-C2
4	C	608	PGT	O31-C31-O2-C2
4	C	608	PGT	C35-C36-C37-C38
4	A	608	PGT	C35-C36-C37-C38
4	A	608	PGT	C31-C32-C33-C34
4	C	608	PGT	C31-C32-C33-C34
4	A	608	PGT	O5-C5-C6-O6
4	C	608	PGT	O5-C5-C6-O6
2	A	602	Y01	CAR-CBC-OAW-CAY
4	A	608	PGT	O3P-C1-C2-O2
2	A	606	Y01	CAO-CAJ-CAN-CBA
2	C	606	Y01	CAO-CAJ-CAN-CBA
4	A	608	PGT	C1-C2-C3-O3
4	C	608	PGT	C1-C2-C3-O3
4	A	608	PGT	C1-O3P-P-O1P
4	A	608	PGT	C4-O4P-P-O1P
4	C	608	PGT	C1-O3P-P-O1P
4	C	608	PGT	C4-O4P-P-O1P
2	C	601	Y01	CAL-CAM-CAY-OAW
2	A	601	Y01	CAL-CAM-CAY-OAW
2	C	602	Y01	CAO-CAJ-CAN-CBA
2	A	602	Y01	CAO-CAJ-CAN-CBA
4	A	608	PGT	C2-C1-O3P-P
2	A	601	Y01	CAM-CAL-CAX-OAF
2	C	601	Y01	CAM-CAL-CAX-OAF

Continued on next page...

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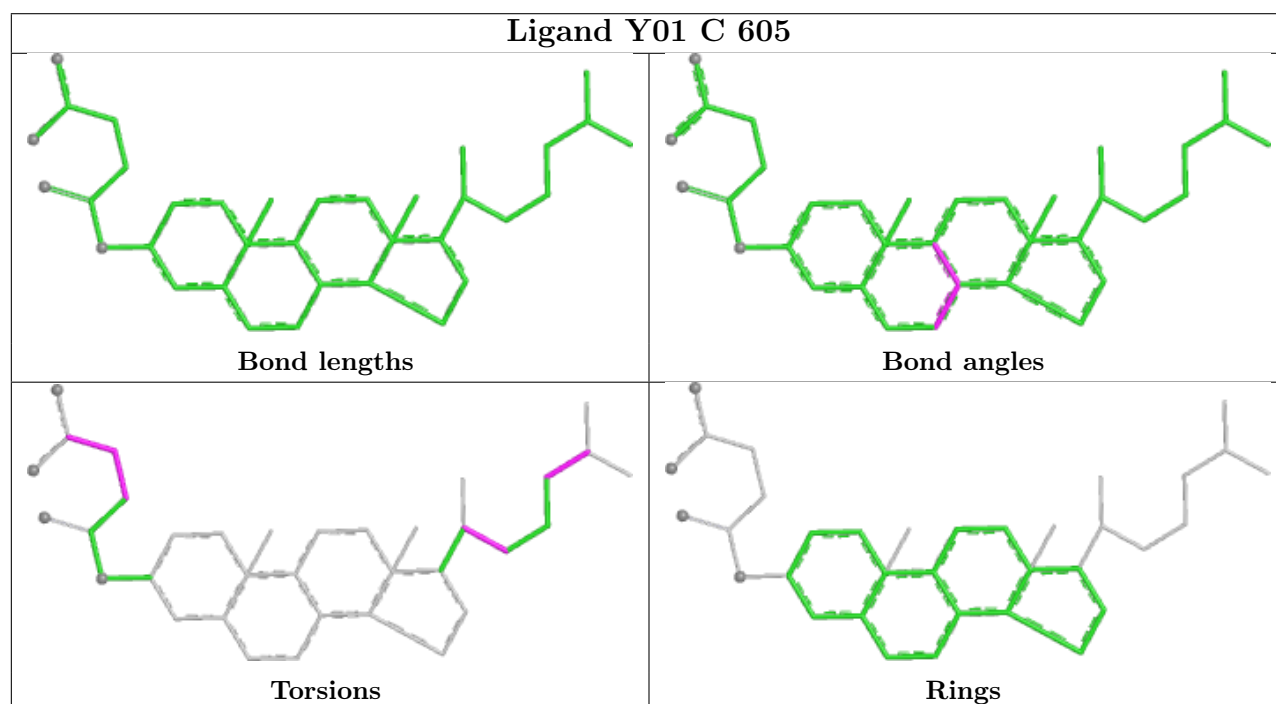
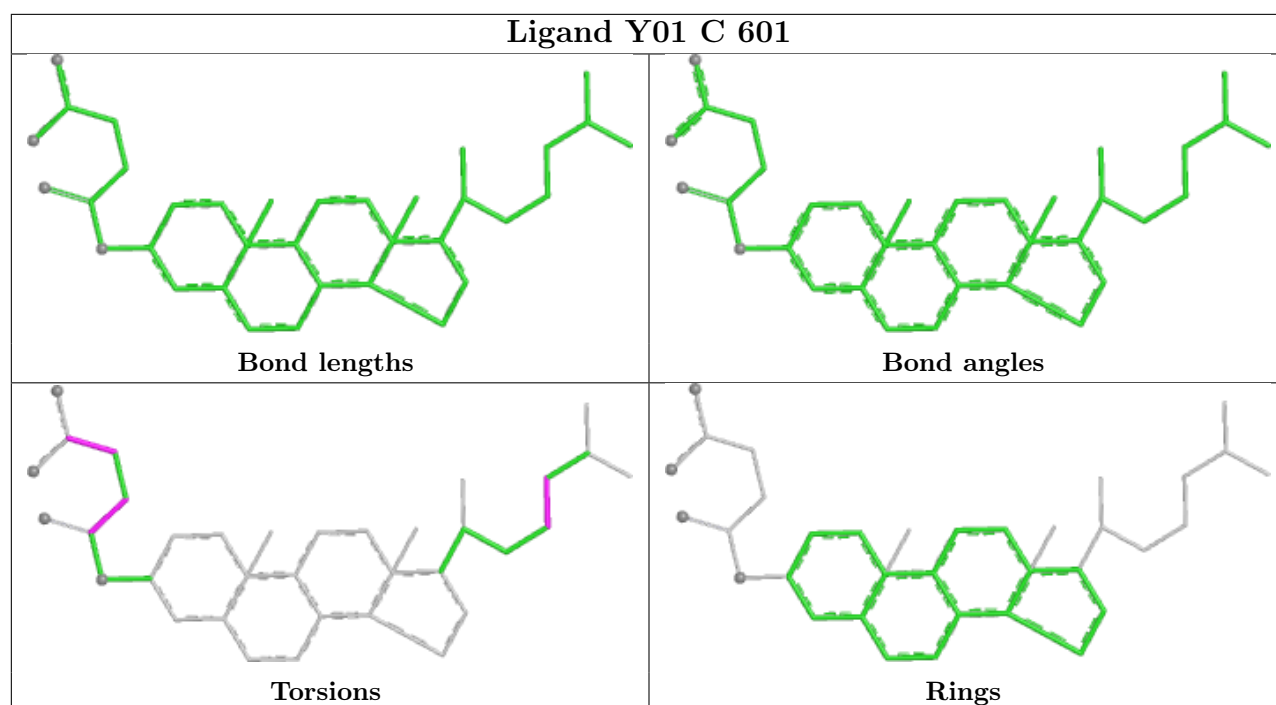
Mol	Chain	Res	Type	Atoms
2	A	603	Y01	CAJ-CAN-CBA-CAB
2	C	603	Y01	CAJ-CAN-CBA-CAB
2	C	601	Y01	CAM-CAL-CAX-OAH
4	C	608	PGT	O3P-C1-C2-O2
2	A	607	Y01	CAM-CAL-CAX-OAF
2	A	601	Y01	CAM-CAL-CAX-OAH
2	C	607	Y01	CAM-CAL-CAX-OAH
2	A	607	Y01	CAM-CAL-CAX-OAH
2	A	606	Y01	CAM-CAL-CAX-OAF
2	C	606	Y01	CAM-CAL-CAX-OAF
2	C	607	Y01	CAM-CAL-CAX-OAF
2	C	607	Y01	CAC-CBB-CBE-CBI
4	C	608	PGT	C2-C1-O3P-P
2	A	606	Y01	CAM-CAL-CAX-OAH
2	C	606	Y01	CAM-CAL-CAX-OAH
2	A	607	Y01	CAC-CBB-CBE-CBI
4	A	608	PGT	O3P-C1-C2-C3
2	A	607	Y01	CAO-CBB-CBE-CAP
2	C	607	Y01	CAO-CBB-CBE-CAP
4	A	608	PGT	O4P-C4-C5-O5
4	C	608	PGT	O2-C31-C32-C33
4	C	608	PGT	O3P-C1-C2-C3
4	A	608	PGT	O2-C31-C32-C33
2	C	605	Y01	CAM-CAL-CAX-OAF
2	A	605	Y01	CAM-CAL-CAX-OAF
4	A	608	PGT	C15-C16-C17-C18
2	C	605	Y01	CAM-CAL-CAX-OAH
4	C	608	PGT	C15-C16-C17-C18
2	A	605	Y01	CAM-CAL-CAX-OAH
2	C	603	Y01	CAJ-CAN-CBA-CAA
4	A	608	PGT	O31-C31-C32-C33
4	C	608	PGT	O31-C31-C32-C33
4	C	608	PGT	O4P-C4-C5-O5
2	A	603	Y01	CAJ-CAN-CBA-CAA
2	C	602	Y01	CAM-CAL-CAX-OAH
4	C	608	PGT	C41-C42-C43-C44
4	A	608	PGT	C41-C42-C43-C44

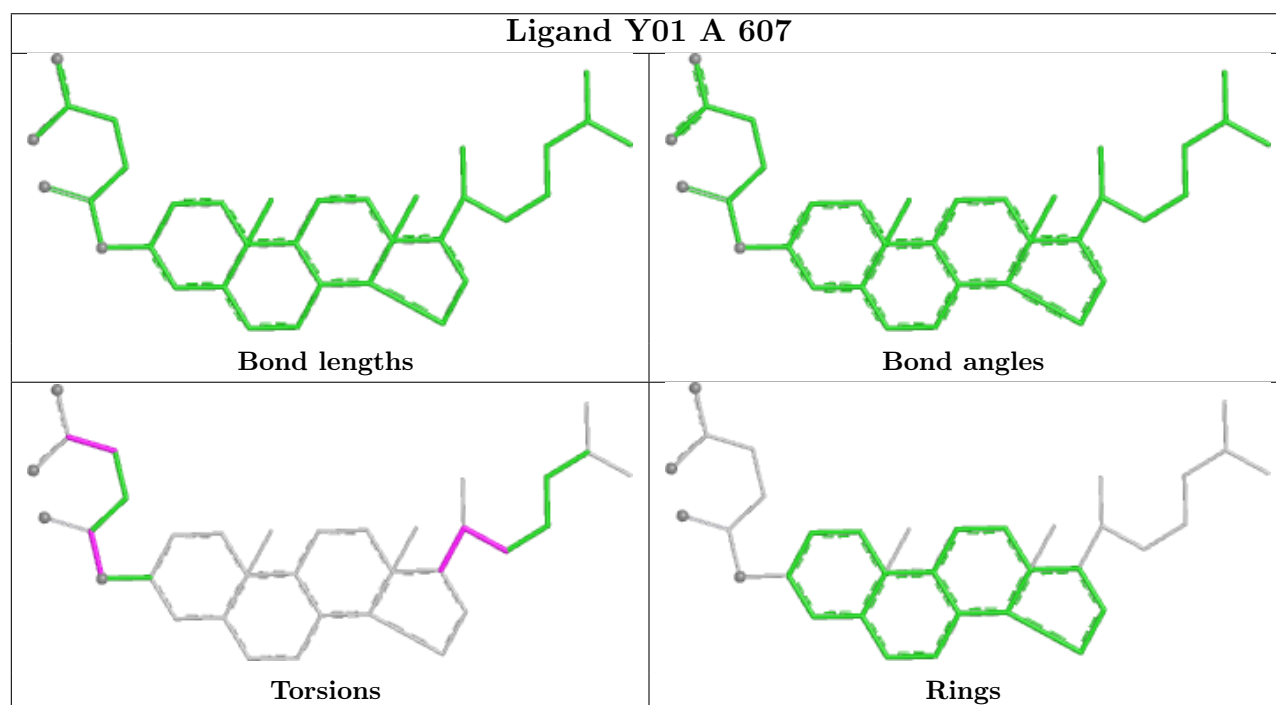
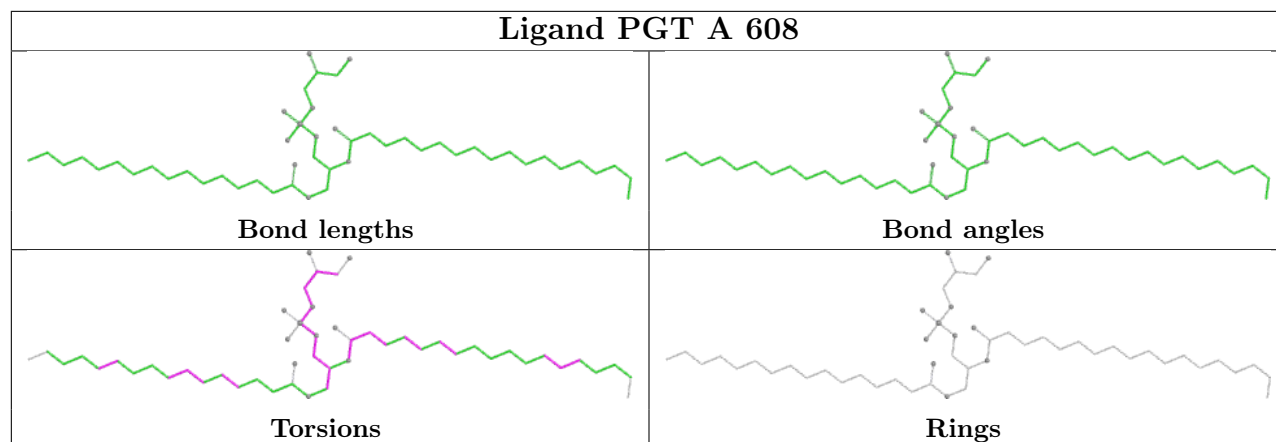
There are no ring outliers.

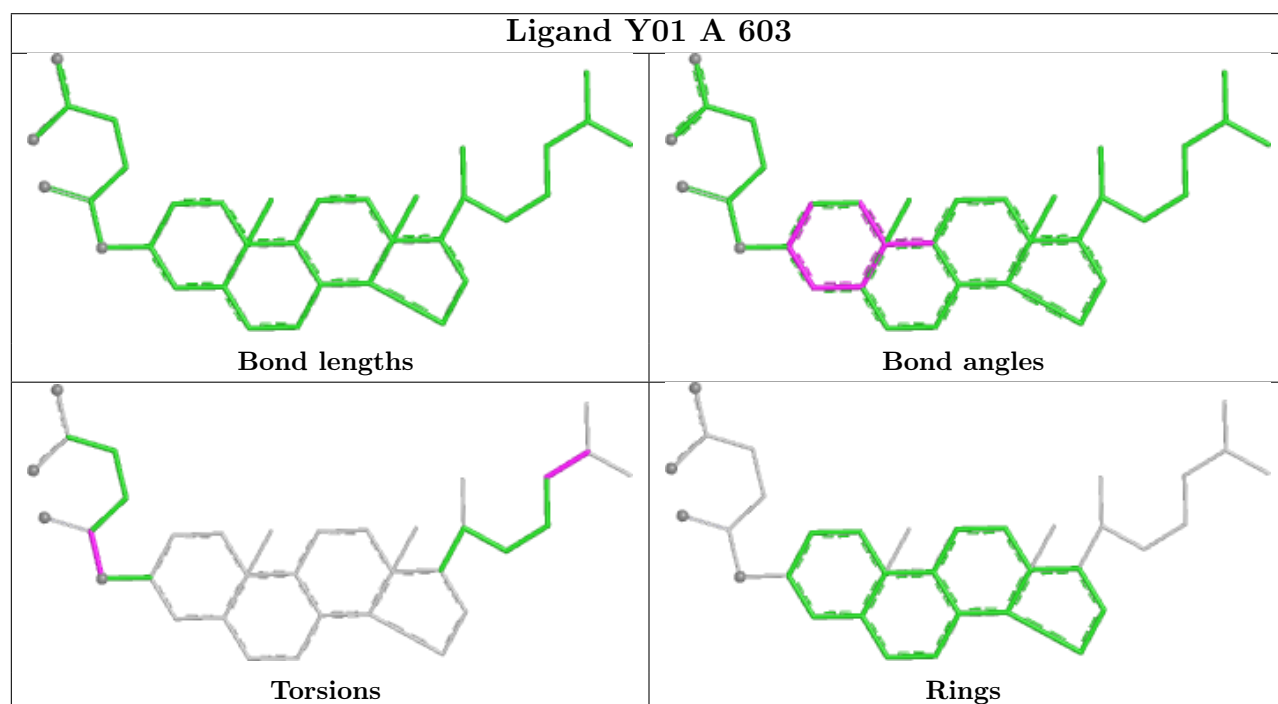
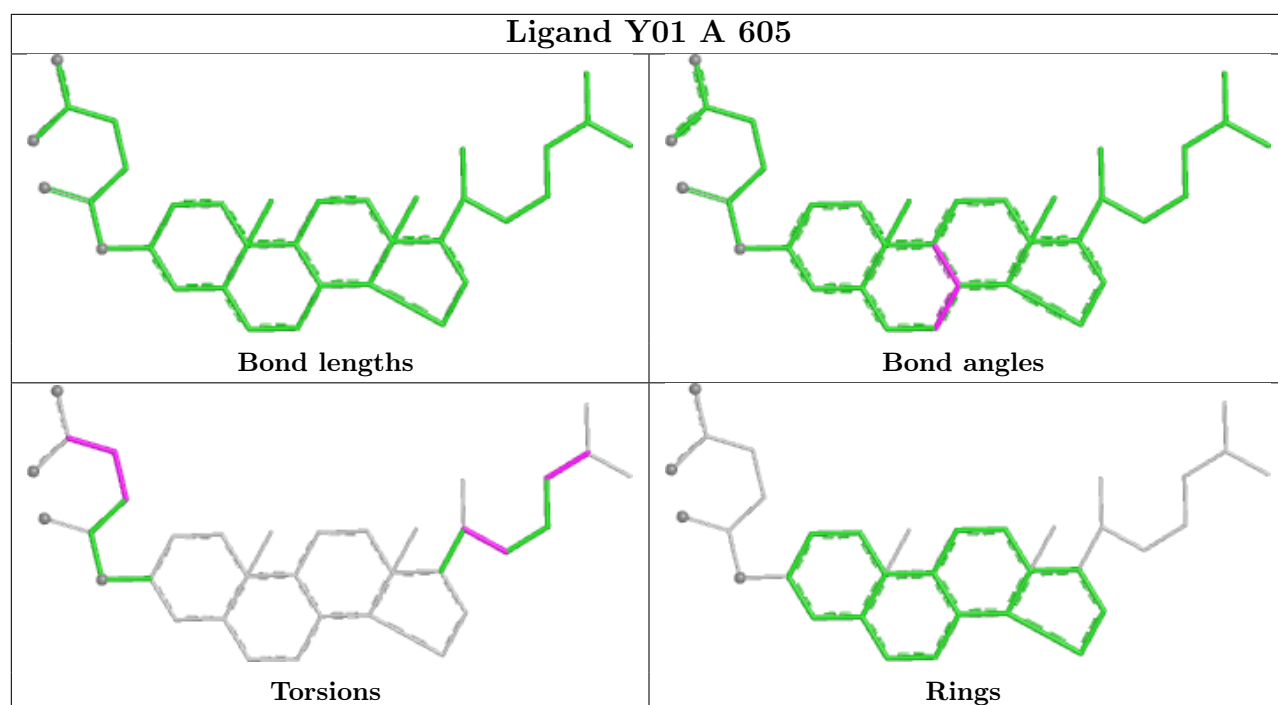
16 monomers are involved in 25 short contacts:

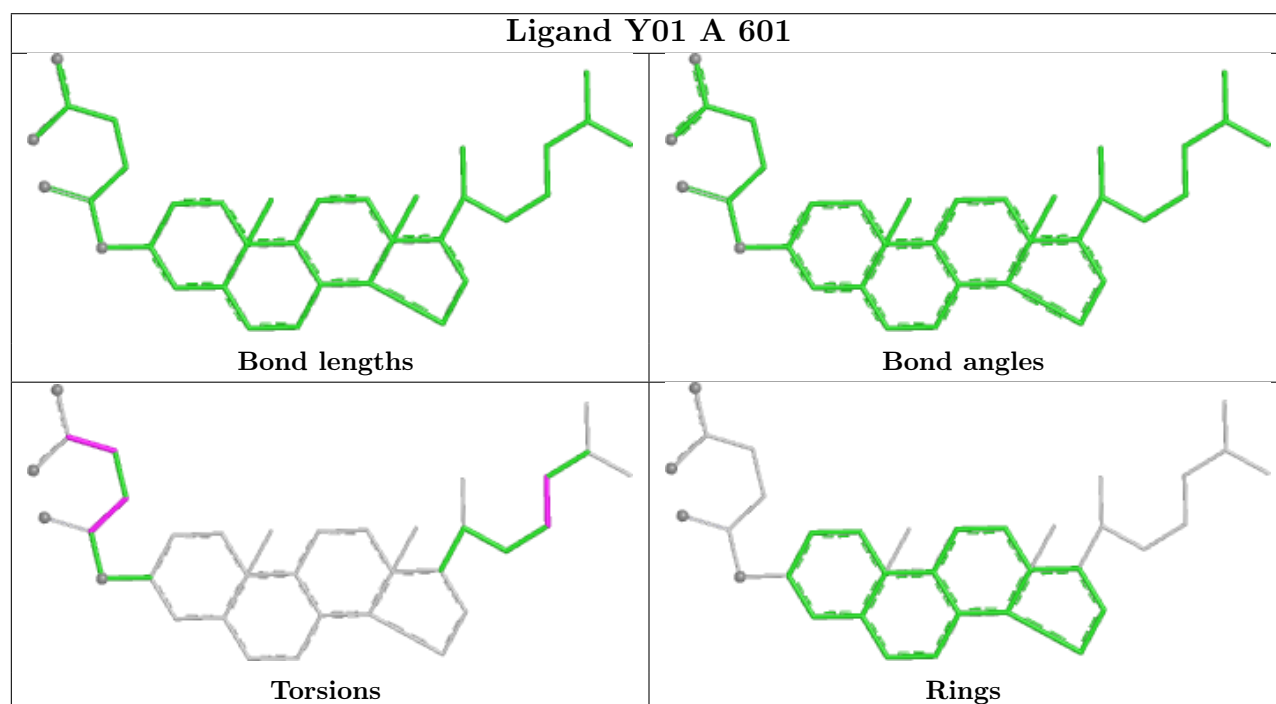
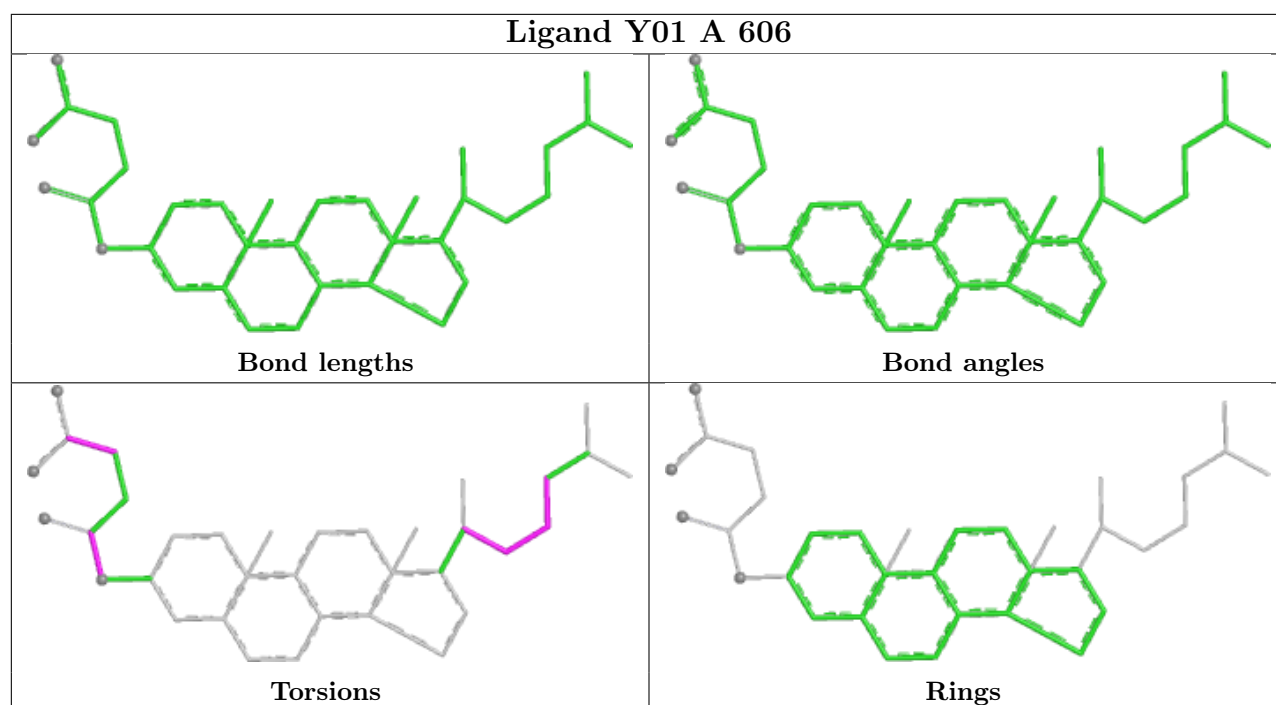
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	Y01	4	0
2	C	605	Y01	1	0
4	A	608	PGT	1	0
2	A	607	Y01	1	0
2	A	605	Y01	1	0
2	A	603	Y01	2	0
2	A	606	Y01	1	0
2	A	601	Y01	5	0
2	C	602	Y01	3	0
2	C	607	Y01	1	0
3	C	604	NAG	1	0
2	C	603	Y01	2	0
4	C	608	PGT	1	0
2	C	606	Y01	1	0
3	A	604	NAG	1	0
2	A	602	Y01	3	0

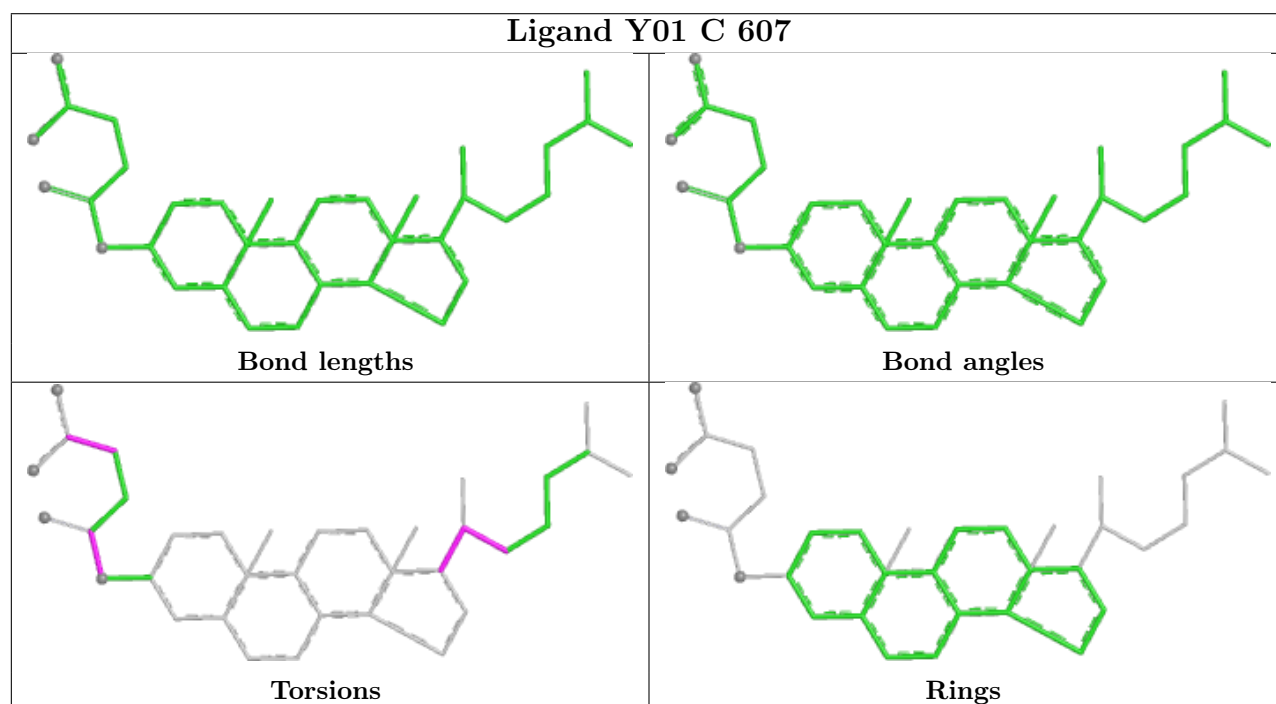
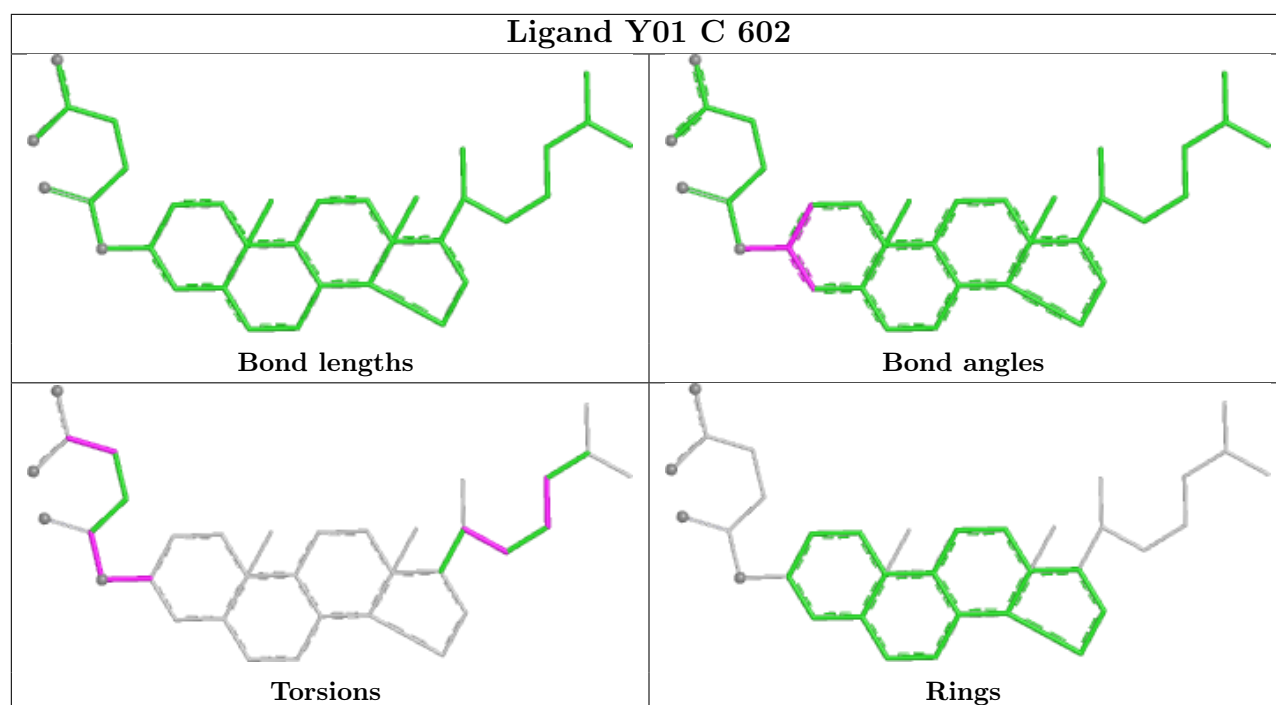
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

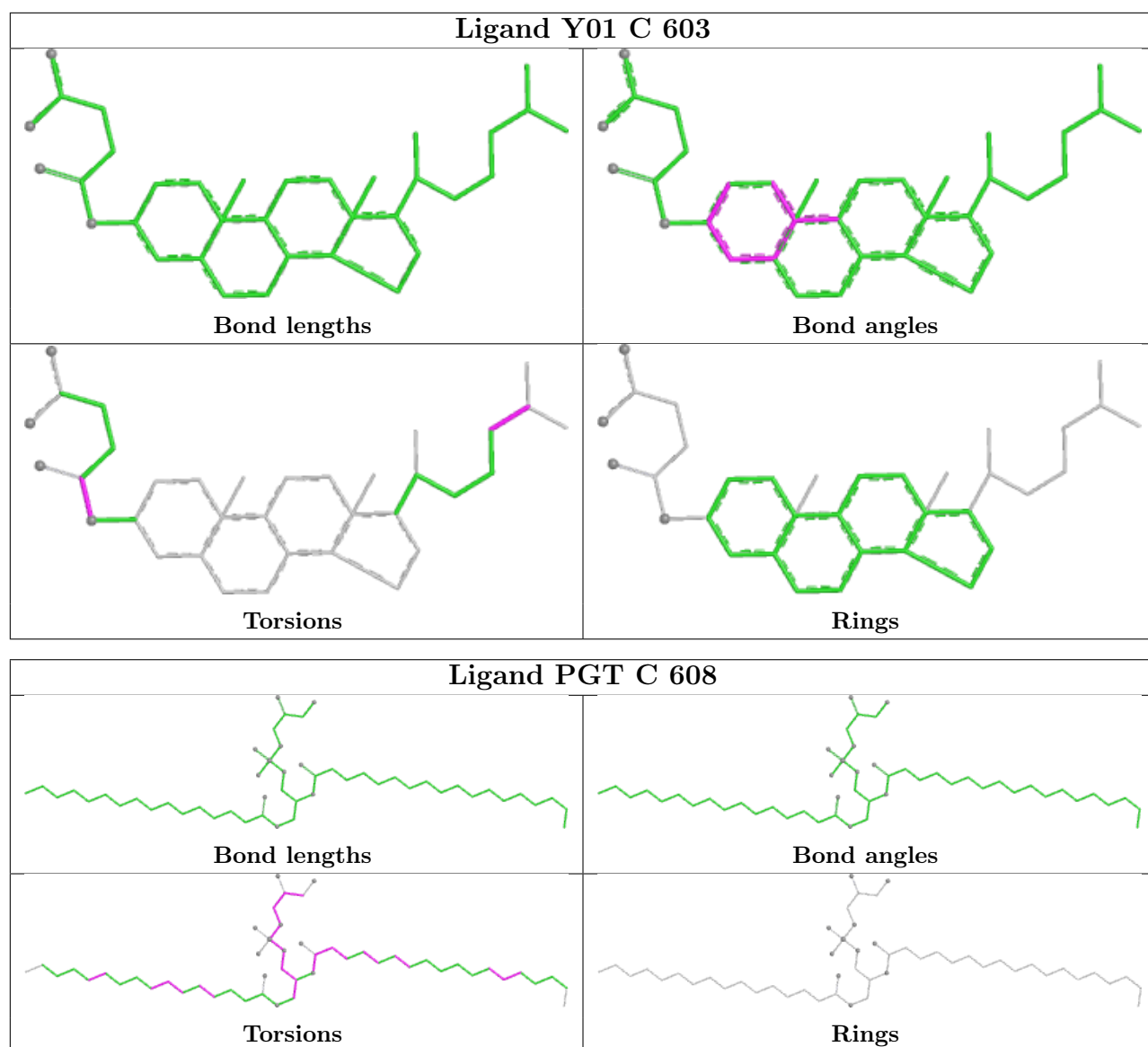


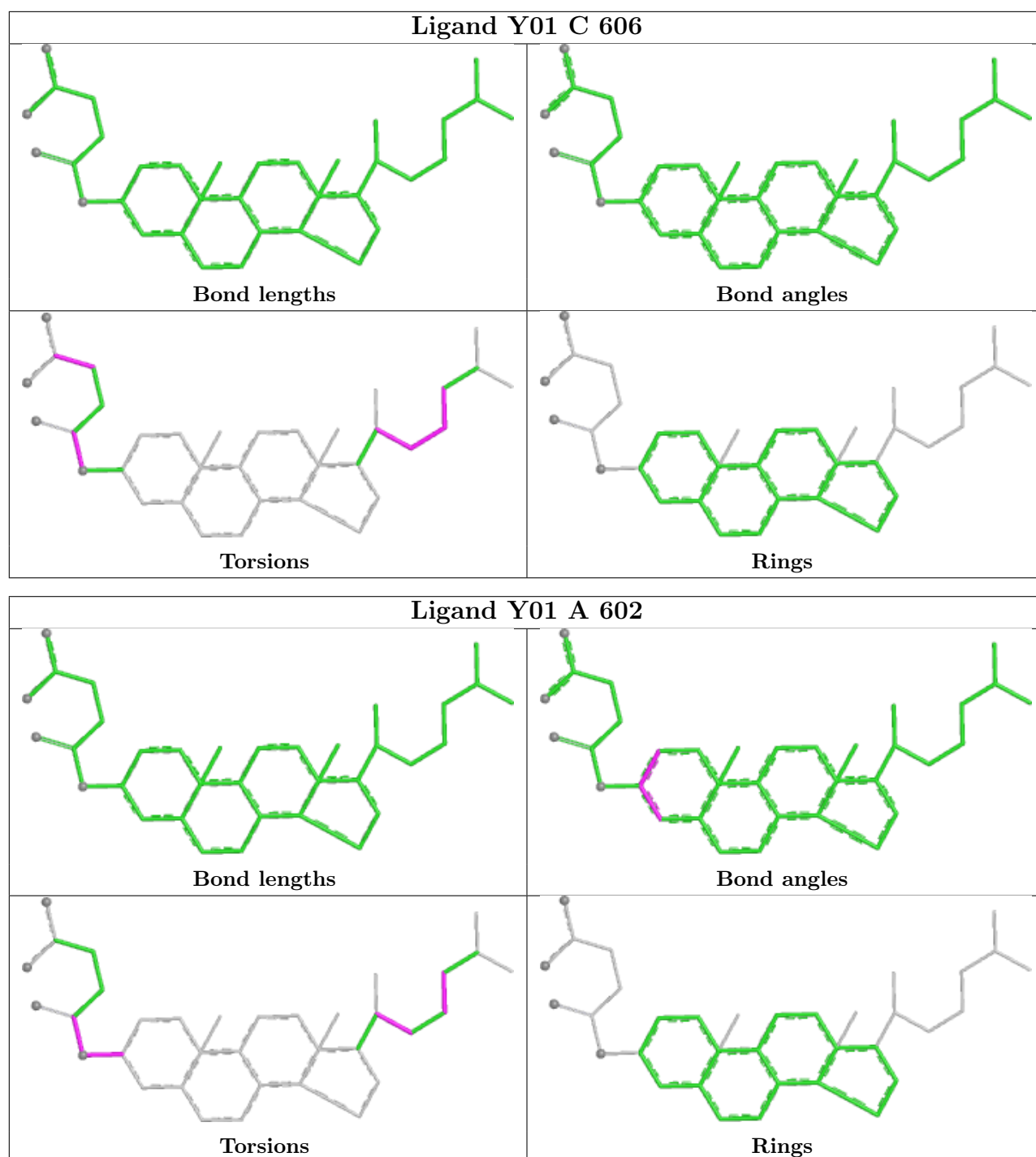












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

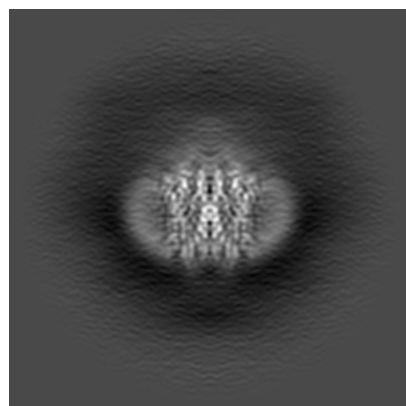
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18635. These allow visual inspection of the internal detail of the map and identification of artifacts.

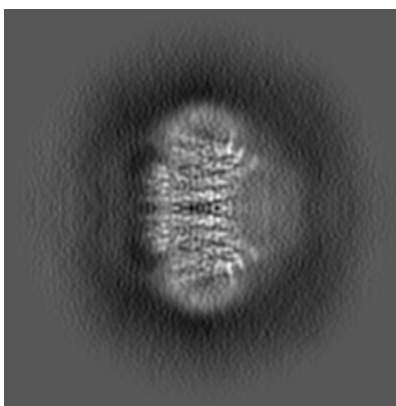
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

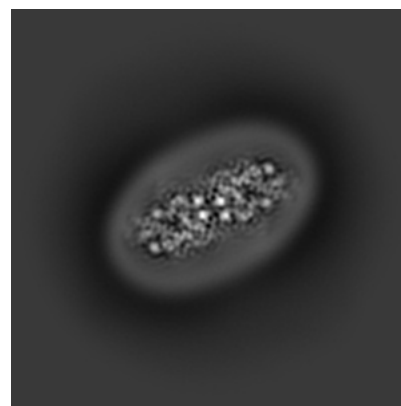
6.1.1 Primary map



X

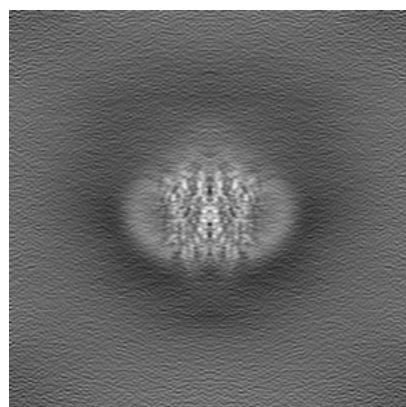


Y

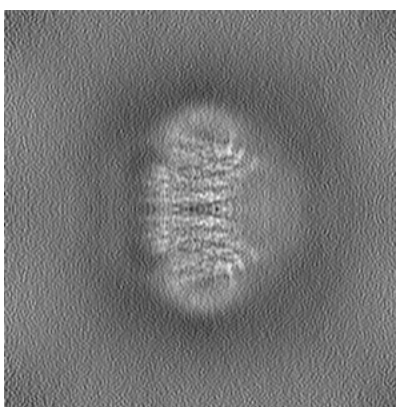


Z

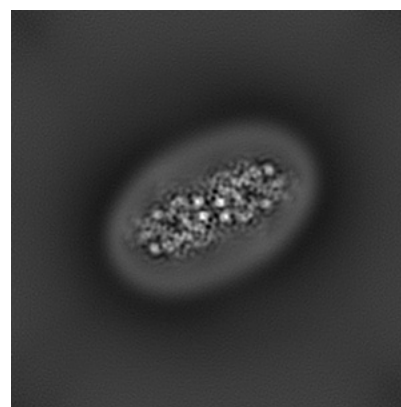
6.1.2 Raw map



X



Y

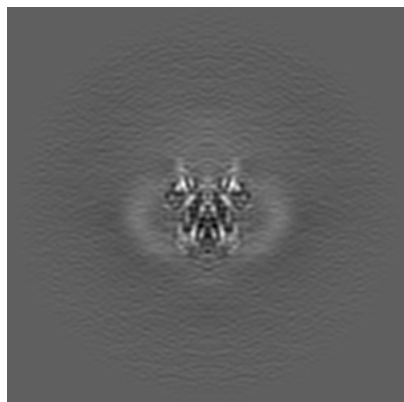


Z

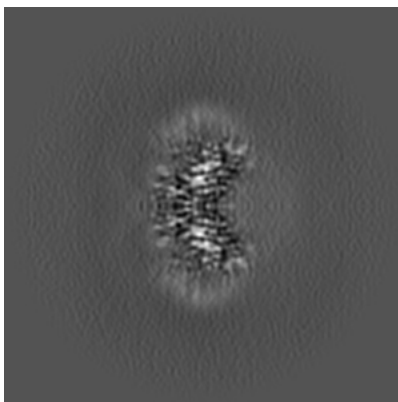
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

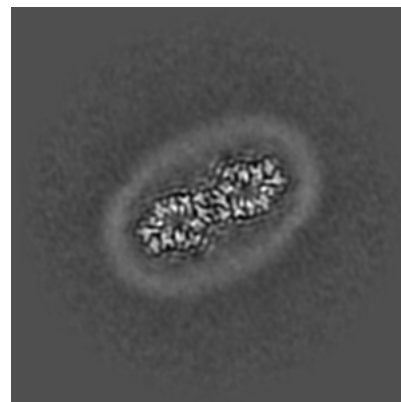
6.2.1 Primary map



X Index: 120

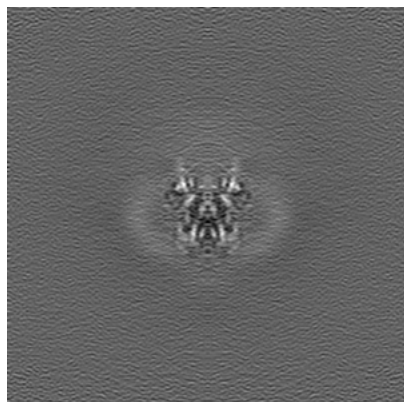


Y Index: 120

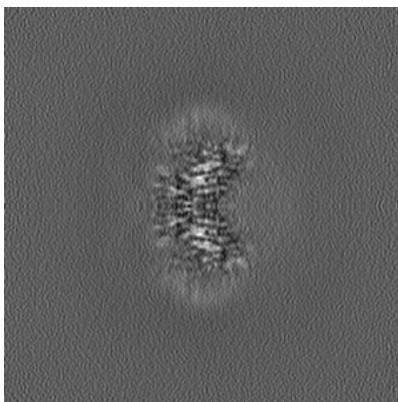


Z Index: 120

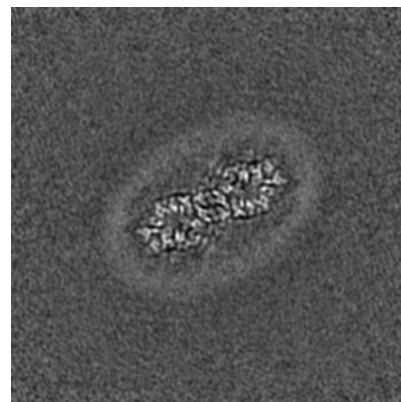
6.2.2 Raw map



X Index: 120



Y Index: 120

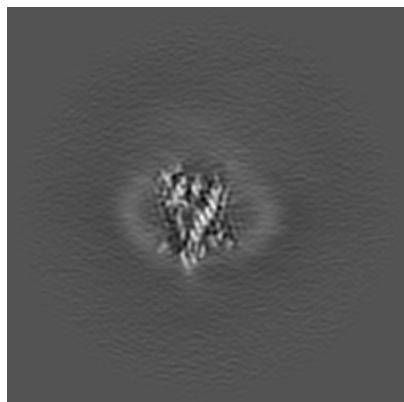


Z Index: 120

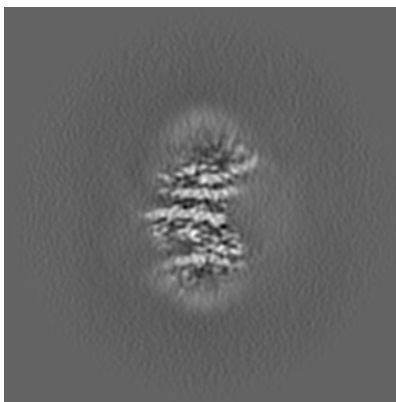
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

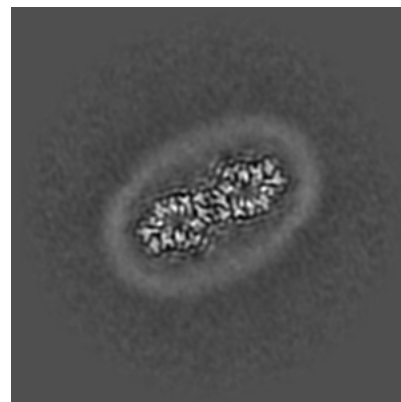
6.3.1 Primary map



X Index: 104

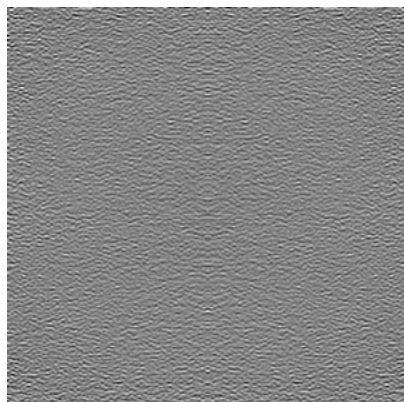


Y Index: 116

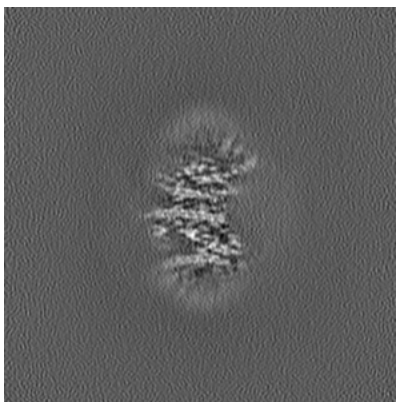


Z Index: 120

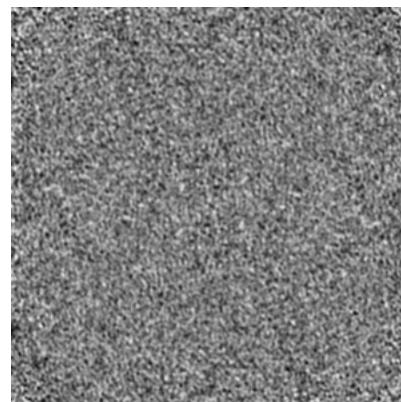
6.3.2 Raw map



X Index: 0



Y Index: 117

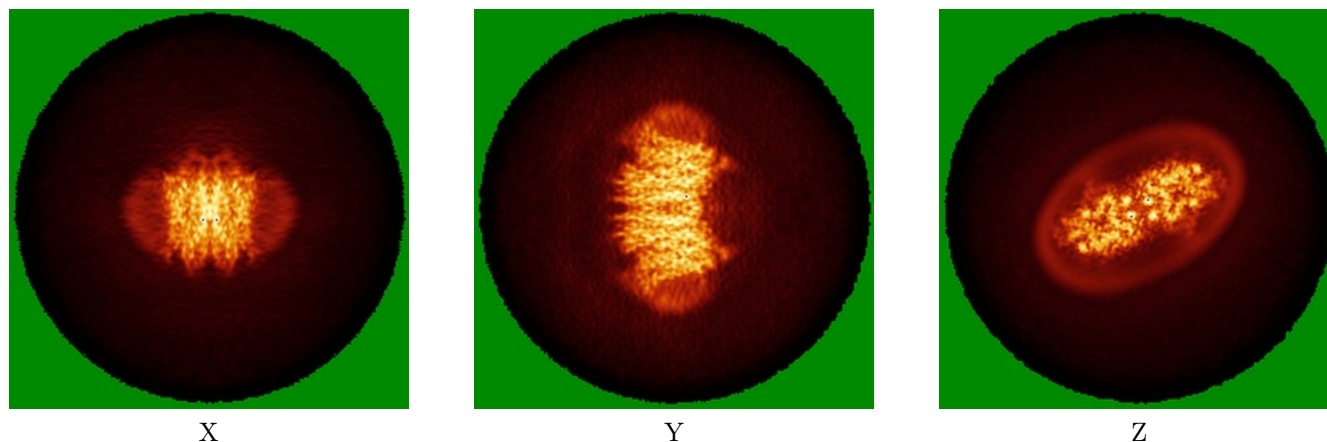


Z Index: 0

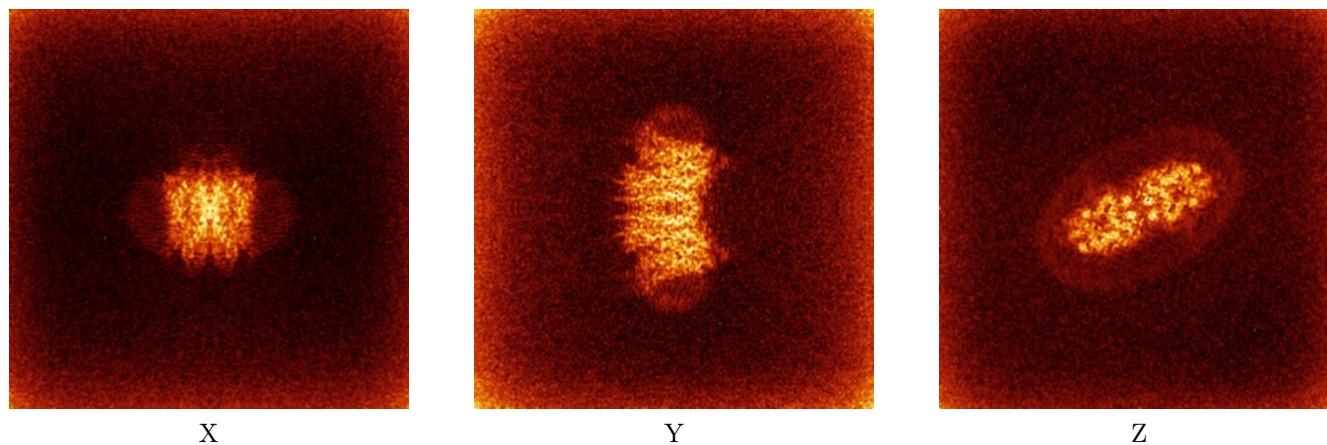
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



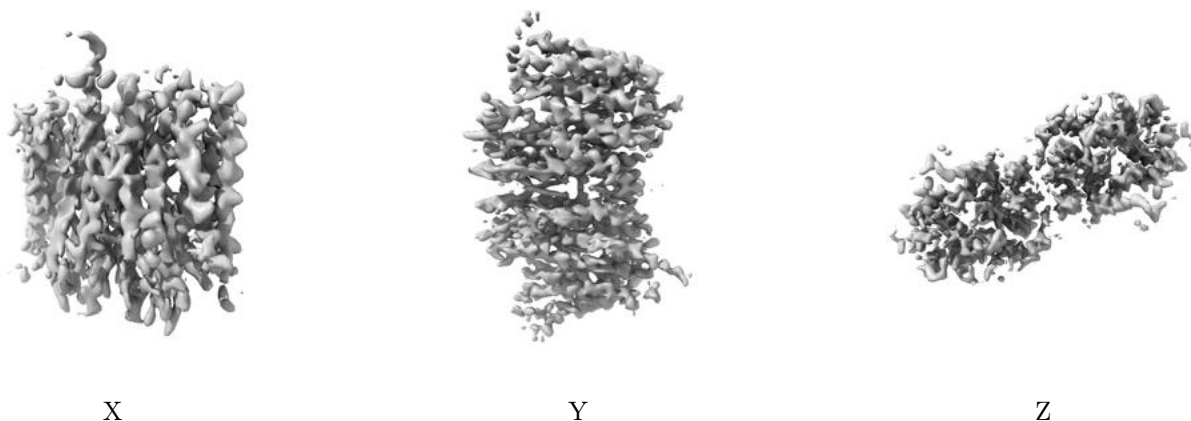
6.4.2 Raw map



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.

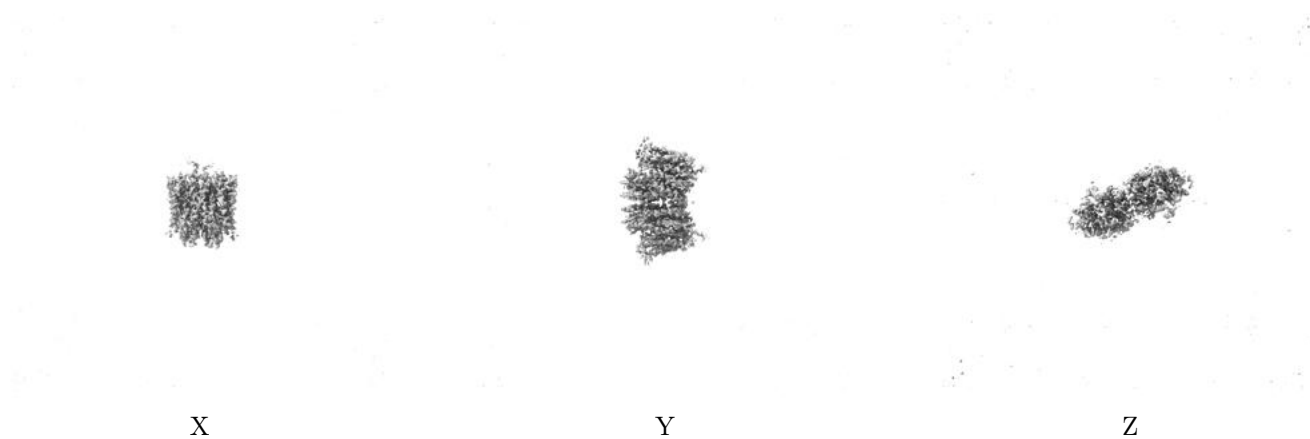
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.207. 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.

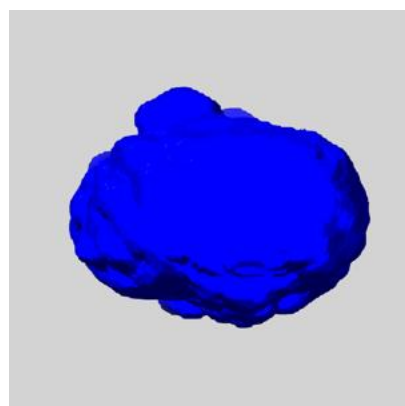
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

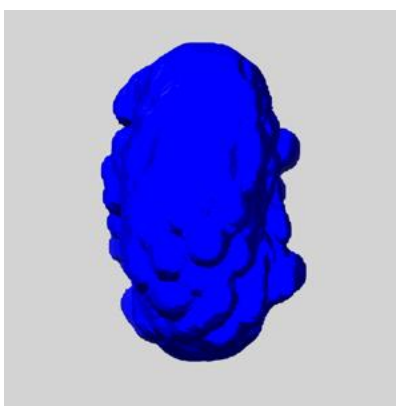
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

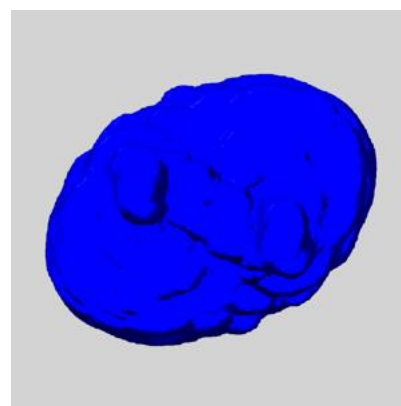
6.6.1 emd_18635_msk_1.map [i](#)



X



Y

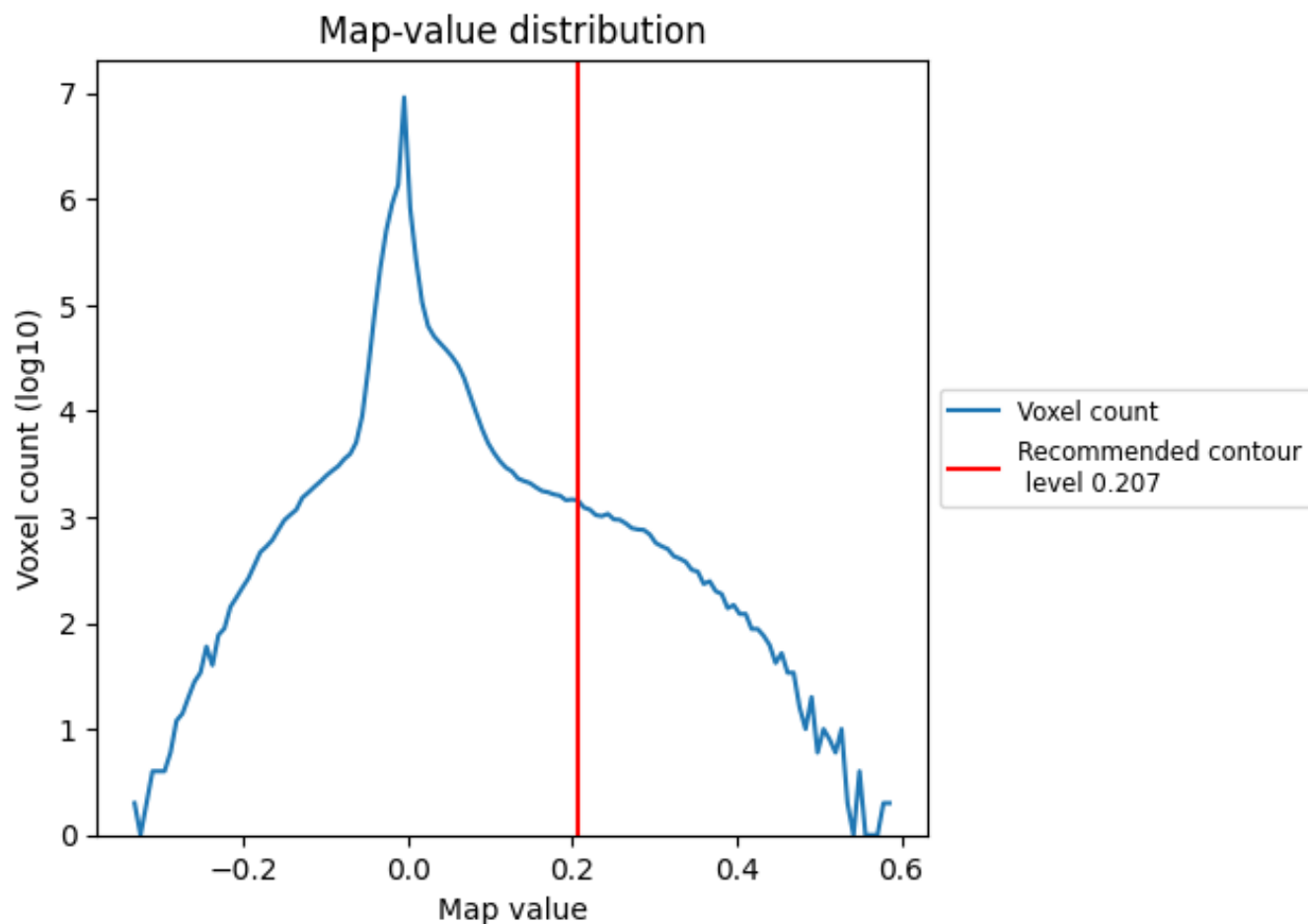


Z

7 Map analysis [i](#)

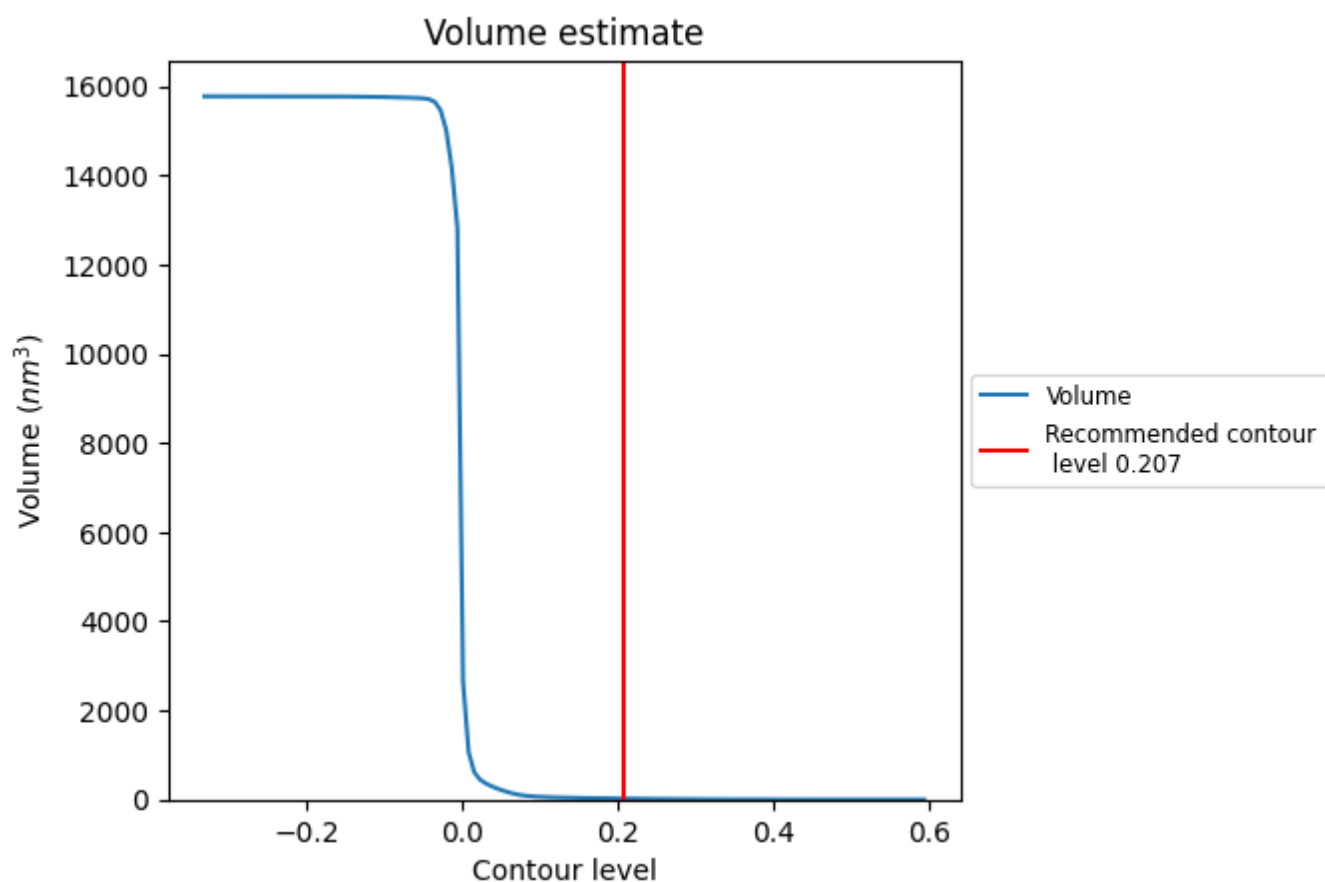
This section contains the results of statistical analysis of the map.

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.

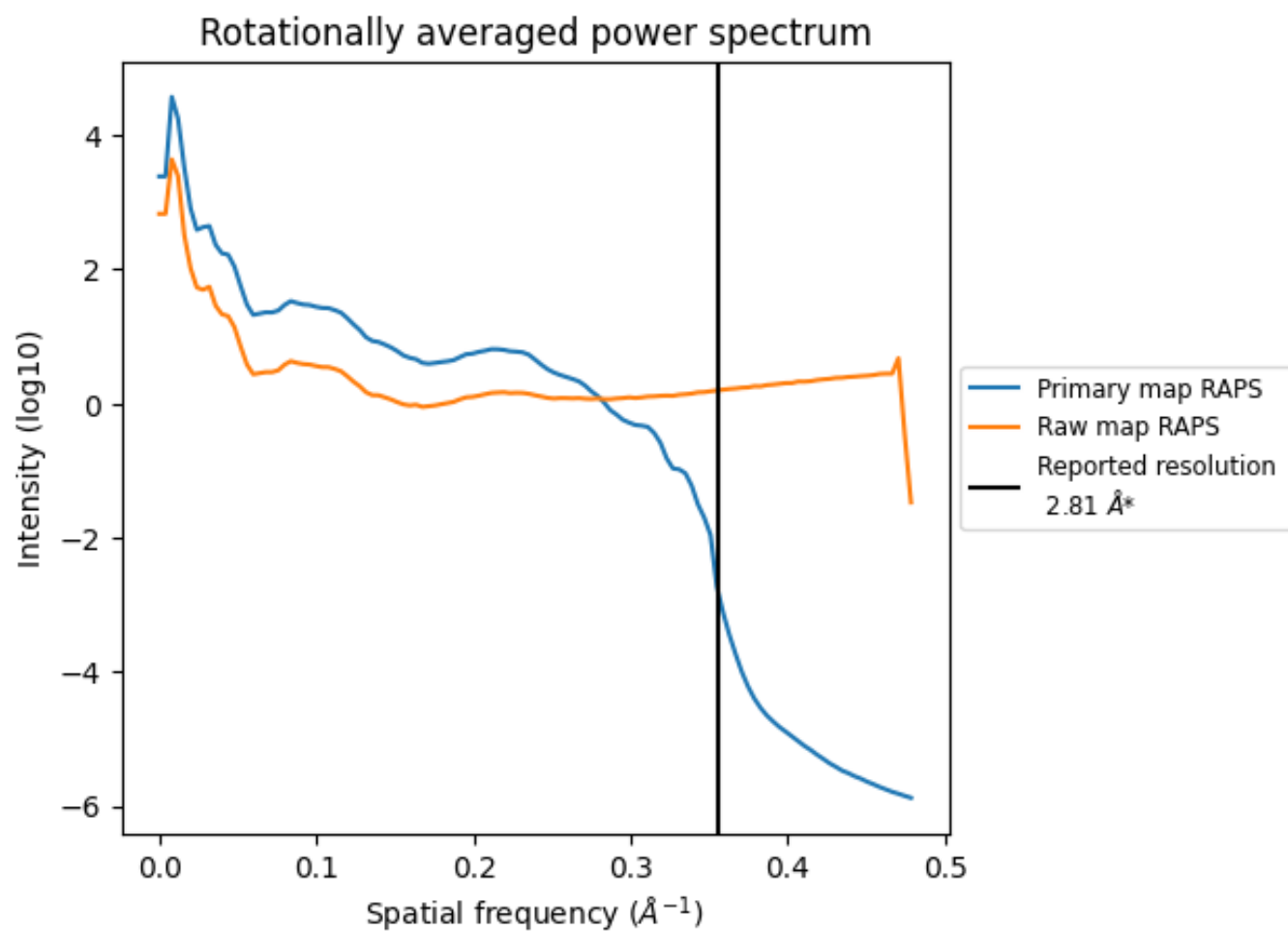
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21 nm^3 ; this corresponds to an approximate mass of 19 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 ⓘ

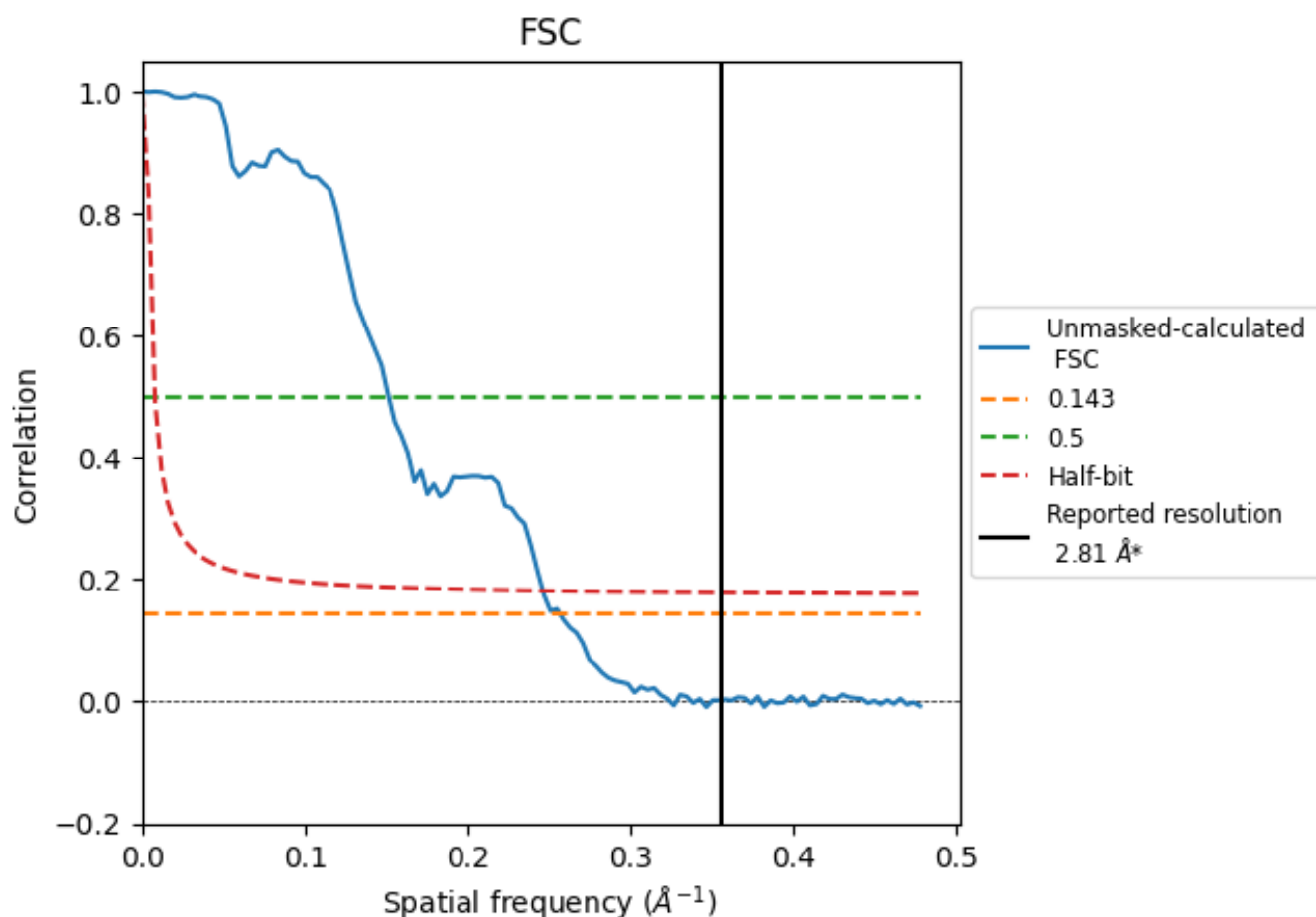


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

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 0.356 Å⁻¹

8.2 Resolution estimates [i](#)

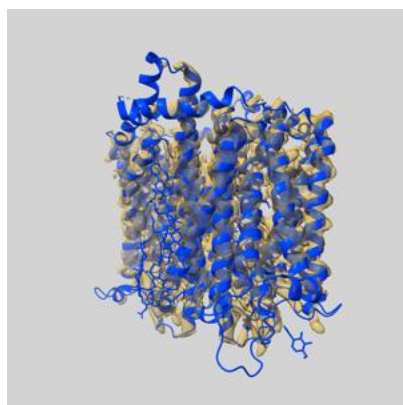
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.59	4.06

*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 3.89 differs from the reported value 2.81 by more than 10 %

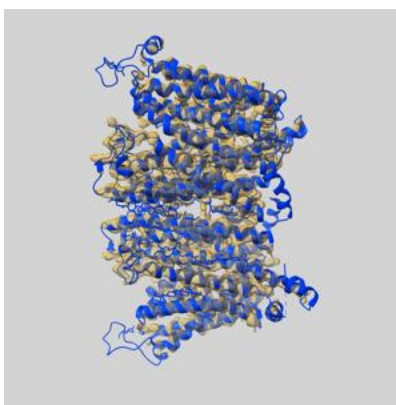
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18635 and PDB model 8QSL. Per-residue inclusion information can be found in section [3](#) on page [6](#).

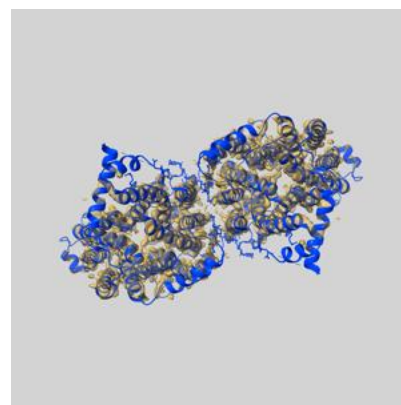
9.1 Map-model overlay [i](#)



X



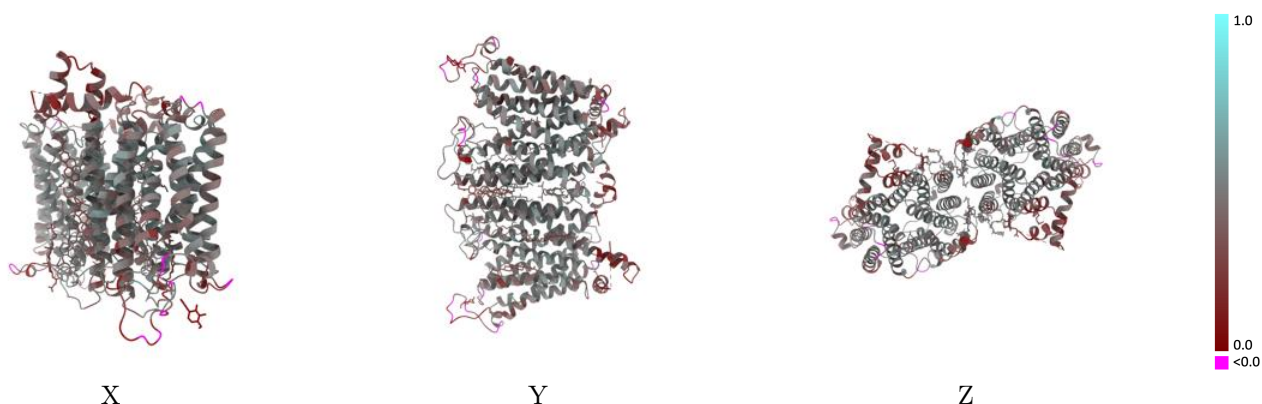
Y



Z

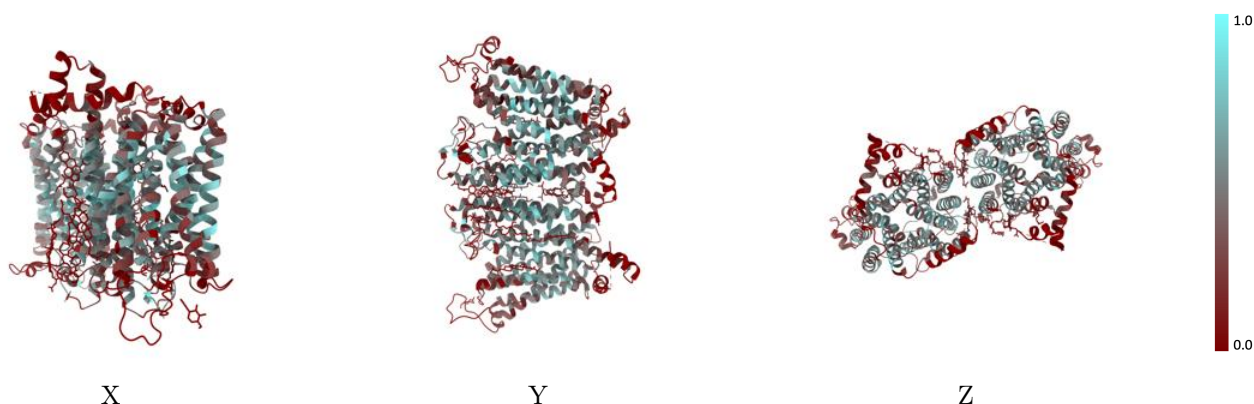
The images above show the 3D surface view of the map at the recommended contour level 0.207 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



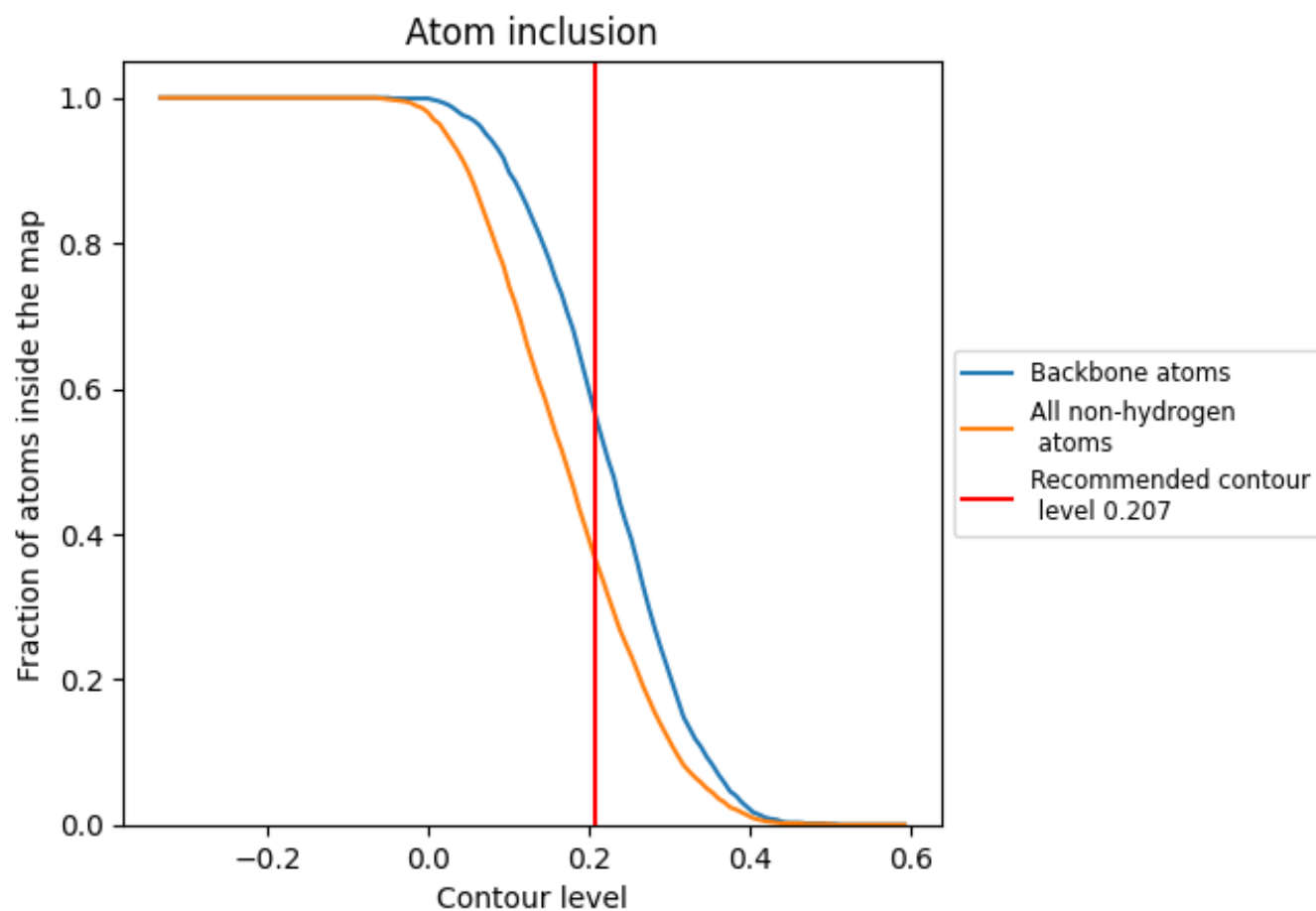
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.207).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 37% 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 (0.207) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3700	0.4180
A	0.3710	0.4180
C	0.3700	0.4170

