



wwPDB EM Validation Summary Report ⓘ

May 18, 2025 – 08:18 PM EDT

PDB ID : 6N7K / pdb_00006n7k
EMDB ID : EMD-0358
Title : Cryo-EM structure of tetrameric Ptch1 in complex with ShhNp (form II)
Authors : Yan, N.; Gong, X.; Qian, H.W.
Deposited on : 2018-11-27
Resolution : 6.50 Å(reported)

This is a wwPDB EM Validation Summary 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

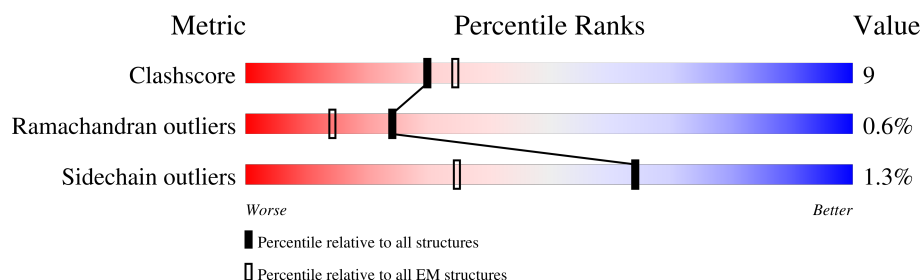
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1349	<div> <div>35%</div> <div>59%</div> <div>14%</div> <div>27%</div> </div>
1	B	1349	<div> <div>37%</div> <div>62%</div> <div>11%</div> <div>27%</div> </div>
1	D	1349	<div> <div>62%</div> <div>60%</div> <div>13%</div> <div>27%</div> </div>
1	E	1349	<div> <div>55%</div> <div>61%</div> <div>12%</div> <div>27%</div> </div>
2	C	174	<div> <div>20%</div> <div>70%</div> <div>28%</div> </div>
2	F	174	<div> <div>60%</div> <div>70%</div> <div>28%</div> </div>
3	G	2	<div> <div>100%</div> </div>
3	H	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	2	100% 
3	J	2	100% 

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	1808	-	-	X	-
5	CLR	B	1508	-	-	X	-
5	CLR	D	1808	-	-	X	-
5	CLR	E	1508	-	-	X	-
8	PLM	C	205	-	-	X	-
8	PLM	F	205	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 34484 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 Protein patched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	991	Total	C	N	O	S	0	0
			7807	5091	1282	1392	42		
1	B	988	Total	C	N	O	S	0	0
			7708	5029	1267	1372	40		
1	D	991	Total	C	N	O	S	0	0
			7807	5091	1282	1392	42		
1	E	988	Total	C	N	O	S	0	0
			7708	5029	1267	1372	40		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q13635
A	-19	ALA	-	expression tag	UNP Q13635
A	-18	ASP	-	expression tag	UNP Q13635
A	-17	TYR	-	expression tag	UNP Q13635
A	-16	LYS	-	expression tag	UNP Q13635
A	-15	ASP	-	expression tag	UNP Q13635
A	-14	ASP	-	expression tag	UNP Q13635
A	-13	ASP	-	expression tag	UNP Q13635
A	-12	ASP	-	expression tag	UNP Q13635
A	-11	LYS	-	expression tag	UNP Q13635
A	-10	SER	-	expression tag	UNP Q13635
A	-9	GLY	-	expression tag	UNP Q13635
A	-8	PRO	-	expression tag	UNP Q13635
A	-7	ASP	-	expression tag	UNP Q13635
A	-6	GLU	-	expression tag	UNP Q13635
A	-5	VAL	-	expression tag	UNP Q13635
A	-4	ASP	-	expression tag	UNP Q13635
A	-3	ALA	-	expression tag	UNP Q13635
A	-2	SER	-	expression tag	UNP Q13635
A	-1	GLY	-	expression tag	UNP Q13635
A	0	ARG	-	expression tag	UNP Q13635
A	1306	LEU	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1307	GLU	-	expression tag	UNP Q13635
A	1308	GLY	-	expression tag	UNP Q13635
A	1309	SER	-	expression tag	UNP Q13635
A	1310	ASP	-	expression tag	UNP Q13635
A	1311	GLU	-	expression tag	UNP Q13635
A	1312	VAL	-	expression tag	UNP Q13635
A	1313	ASP	-	expression tag	UNP Q13635
A	1314	ALA	-	expression tag	UNP Q13635
A	1315	VAL	-	expression tag	UNP Q13635
A	1316	GLU	-	expression tag	UNP Q13635
A	1317	GLY	-	expression tag	UNP Q13635
A	1318	SER	-	expression tag	UNP Q13635
A	1319	HIS	-	expression tag	UNP Q13635
A	1320	HIS	-	expression tag	UNP Q13635
A	1321	HIS	-	expression tag	UNP Q13635
A	1322	HIS	-	expression tag	UNP Q13635
A	1323	HIS	-	expression tag	UNP Q13635
A	1324	HIS	-	expression tag	UNP Q13635
A	1325	HIS	-	expression tag	UNP Q13635
A	1326	HIS	-	expression tag	UNP Q13635
A	1327	HIS	-	expression tag	UNP Q13635
A	1328	HIS	-	expression tag	UNP Q13635
B	-20	MET	-	initiating methionine	UNP Q13635
B	-19	ALA	-	expression tag	UNP Q13635
B	-18	ASP	-	expression tag	UNP Q13635
B	-17	TYR	-	expression tag	UNP Q13635
B	-16	LYS	-	expression tag	UNP Q13635
B	-15	ASP	-	expression tag	UNP Q13635
B	-14	ASP	-	expression tag	UNP Q13635
B	-13	ASP	-	expression tag	UNP Q13635
B	-12	ASP	-	expression tag	UNP Q13635
B	-11	LYS	-	expression tag	UNP Q13635
B	-10	SER	-	expression tag	UNP Q13635
B	-9	GLY	-	expression tag	UNP Q13635
B	-8	PRO	-	expression tag	UNP Q13635
B	-7	ASP	-	expression tag	UNP Q13635
B	-6	GLU	-	expression tag	UNP Q13635
B	-5	VAL	-	expression tag	UNP Q13635
B	-4	ASP	-	expression tag	UNP Q13635
B	-3	ALA	-	expression tag	UNP Q13635
B	-2	SER	-	expression tag	UNP Q13635
B	-1	GLY	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP Q13635
B	1306	LEU	-	expression tag	UNP Q13635
B	1307	GLU	-	expression tag	UNP Q13635
B	1308	GLY	-	expression tag	UNP Q13635
B	1309	SER	-	expression tag	UNP Q13635
B	1310	ASP	-	expression tag	UNP Q13635
B	1311	GLU	-	expression tag	UNP Q13635
B	1312	VAL	-	expression tag	UNP Q13635
B	1313	ASP	-	expression tag	UNP Q13635
B	1314	ALA	-	expression tag	UNP Q13635
B	1315	VAL	-	expression tag	UNP Q13635
B	1316	GLU	-	expression tag	UNP Q13635
B	1317	GLY	-	expression tag	UNP Q13635
B	1318	SER	-	expression tag	UNP Q13635
B	1319	HIS	-	expression tag	UNP Q13635
B	1320	HIS	-	expression tag	UNP Q13635
B	1321	HIS	-	expression tag	UNP Q13635
B	1322	HIS	-	expression tag	UNP Q13635
B	1323	HIS	-	expression tag	UNP Q13635
B	1324	HIS	-	expression tag	UNP Q13635
B	1325	HIS	-	expression tag	UNP Q13635
B	1326	HIS	-	expression tag	UNP Q13635
B	1327	HIS	-	expression tag	UNP Q13635
B	1328	HIS	-	expression tag	UNP Q13635
D	-20	MET	-	initiating methionine	UNP Q13635
D	-19	ALA	-	expression tag	UNP Q13635
D	-18	ASP	-	expression tag	UNP Q13635
D	-17	TYR	-	expression tag	UNP Q13635
D	-16	LYS	-	expression tag	UNP Q13635
D	-15	ASP	-	expression tag	UNP Q13635
D	-14	ASP	-	expression tag	UNP Q13635
D	-13	ASP	-	expression tag	UNP Q13635
D	-12	ASP	-	expression tag	UNP Q13635
D	-11	LYS	-	expression tag	UNP Q13635
D	-10	SER	-	expression tag	UNP Q13635
D	-9	GLY	-	expression tag	UNP Q13635
D	-8	PRO	-	expression tag	UNP Q13635
D	-7	ASP	-	expression tag	UNP Q13635
D	-6	GLU	-	expression tag	UNP Q13635
D	-5	VAL	-	expression tag	UNP Q13635
D	-4	ASP	-	expression tag	UNP Q13635
D	-3	ALA	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q13635
D	-1	GLY	-	expression tag	UNP Q13635
D	0	ARG	-	expression tag	UNP Q13635
D	1306	LEU	-	expression tag	UNP Q13635
D	1307	GLU	-	expression tag	UNP Q13635
D	1308	GLY	-	expression tag	UNP Q13635
D	1309	SER	-	expression tag	UNP Q13635
D	1310	ASP	-	expression tag	UNP Q13635
D	1311	GLU	-	expression tag	UNP Q13635
D	1312	VAL	-	expression tag	UNP Q13635
D	1313	ASP	-	expression tag	UNP Q13635
D	1314	ALA	-	expression tag	UNP Q13635
D	1315	VAL	-	expression tag	UNP Q13635
D	1316	GLU	-	expression tag	UNP Q13635
D	1317	GLY	-	expression tag	UNP Q13635
D	1318	SER	-	expression tag	UNP Q13635
D	1319	HIS	-	expression tag	UNP Q13635
D	1320	HIS	-	expression tag	UNP Q13635
D	1321	HIS	-	expression tag	UNP Q13635
D	1322	HIS	-	expression tag	UNP Q13635
D	1323	HIS	-	expression tag	UNP Q13635
D	1324	HIS	-	expression tag	UNP Q13635
D	1325	HIS	-	expression tag	UNP Q13635
D	1326	HIS	-	expression tag	UNP Q13635
D	1327	HIS	-	expression tag	UNP Q13635
D	1328	HIS	-	expression tag	UNP Q13635
E	-20	MET	-	initiating methionine	UNP Q13635
E	-19	ALA	-	expression tag	UNP Q13635
E	-18	ASP	-	expression tag	UNP Q13635
E	-17	TYR	-	expression tag	UNP Q13635
E	-16	LYS	-	expression tag	UNP Q13635
E	-15	ASP	-	expression tag	UNP Q13635
E	-14	ASP	-	expression tag	UNP Q13635
E	-13	ASP	-	expression tag	UNP Q13635
E	-12	ASP	-	expression tag	UNP Q13635
E	-11	LYS	-	expression tag	UNP Q13635
E	-10	SER	-	expression tag	UNP Q13635
E	-9	GLY	-	expression tag	UNP Q13635
E	-8	PRO	-	expression tag	UNP Q13635
E	-7	ASP	-	expression tag	UNP Q13635
E	-6	GLU	-	expression tag	UNP Q13635
E	-5	VAL	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	ASP	-	expression tag	UNP Q13635
E	-3	ALA	-	expression tag	UNP Q13635
E	-2	SER	-	expression tag	UNP Q13635
E	-1	GLY	-	expression tag	UNP Q13635
E	0	ARG	-	expression tag	UNP Q13635
E	1306	LEU	-	expression tag	UNP Q13635
E	1307	GLU	-	expression tag	UNP Q13635
E	1308	GLY	-	expression tag	UNP Q13635
E	1309	SER	-	expression tag	UNP Q13635
E	1310	ASP	-	expression tag	UNP Q13635
E	1311	GLU	-	expression tag	UNP Q13635
E	1312	VAL	-	expression tag	UNP Q13635
E	1313	ASP	-	expression tag	UNP Q13635
E	1314	ALA	-	expression tag	UNP Q13635
E	1315	VAL	-	expression tag	UNP Q13635
E	1316	GLU	-	expression tag	UNP Q13635
E	1317	GLY	-	expression tag	UNP Q13635
E	1318	SER	-	expression tag	UNP Q13635
E	1319	HIS	-	expression tag	UNP Q13635
E	1320	HIS	-	expression tag	UNP Q13635
E	1321	HIS	-	expression tag	UNP Q13635
E	1322	HIS	-	expression tag	UNP Q13635
E	1323	HIS	-	expression tag	UNP Q13635
E	1324	HIS	-	expression tag	UNP Q13635
E	1325	HIS	-	expression tag	UNP Q13635
E	1326	HIS	-	expression tag	UNP Q13635
E	1327	HIS	-	expression tag	UNP Q13635
E	1328	HIS	-	expression tag	UNP Q13635

- Molecule 2 is a protein called Sonic hedgehog protein.

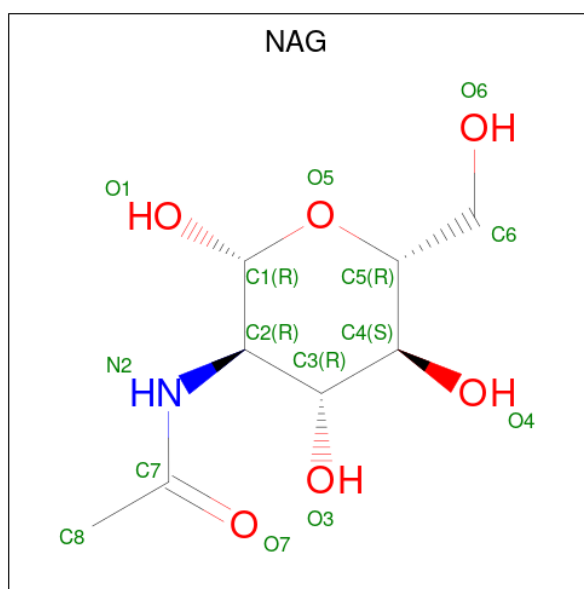
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	174	Total	C	N	O	S	0	0
			1371	853	253	259	6		
2	F	174	Total	C	N	O	S	0	0
			1371	853	253	259	6		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



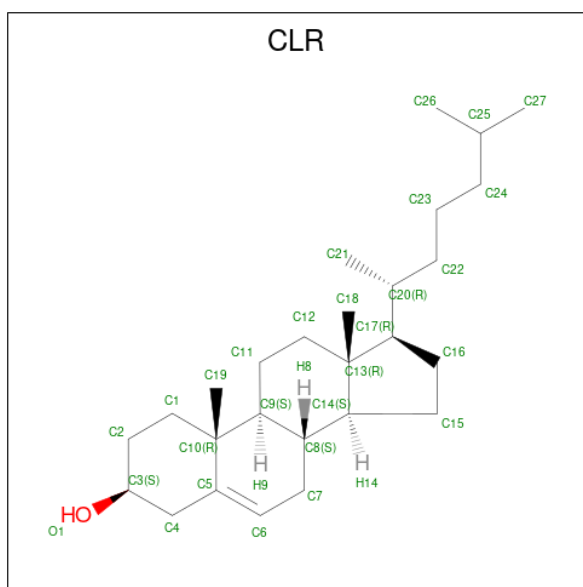
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	
5	D	1	Total	C	O	0
			28	27	1	
5	D	1	Total	C	O	0
			28	27	1	
5	D	1	Total	C	O	0
			28	27	1	
5	E	1	Total	C	O	0
			28	27	1	
5	F	1	Total	C	O	0
			28	27	1	

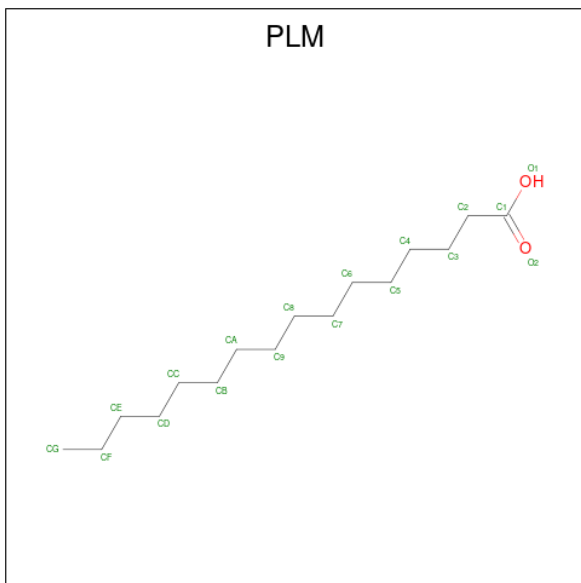
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Zn	0
			1	1	
6	F	1	Total	Zn	0
			1	1	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	C	2	Total 2	Ca 2	0
7	F	2	Total 2	Ca 2	0

- Molecule 8 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).

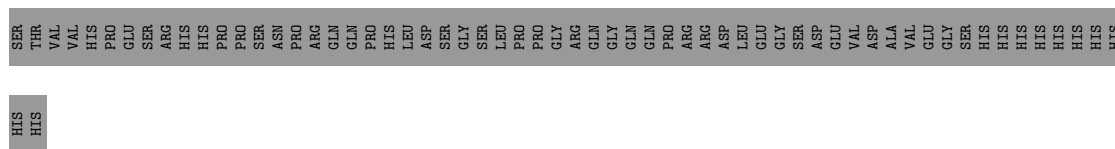


Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total 17	C 16	O 1	0
8	F	1	Total 17	C 16	O 1	0

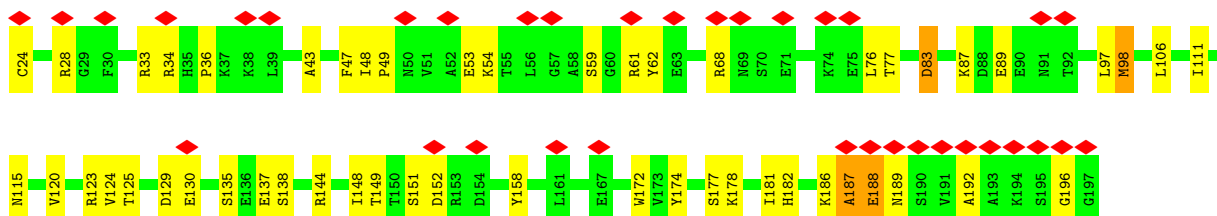


ARG	ARG	ALA	ALA	PRO	ASP	ARG	ASP	TYR	LEU	HIS	ARG	PRO	SER	TYR	CYS	ASP	ALA	ALA	PHE	LEU	GLN	GLN	ILE	SER	LYS	GLY	LYS	ALA	THR	GLY	R73	K74	A75	F76	L77	W78	L79	R80	F83	Q84	R85	L86	L87	C92	Y93	I94	Q95	K96	N97	C98	G99	K100	F101	L102	V103															
V104	G105	L106	L107	I108	F109	G110	A111	F112	A113	V114	G115	L116	K117	A118	A119	N120	A121	E122	T123	N124	V125	E126	E127	L128	V130	E131	V132	G133	G134	R135	V136	S137	R138	E139	L140	N141	Y142	I147	G148	E149	G214	S277	A151	M152	F153	G99	N154	P155	Q156	L157	M158	I159	Q160	T161	P162	K163	E164	E165	G166											
A167	N168	V169	L170	T171	T172	E173	A174	L175	L176	Q177	H178	L179	D180	S181	A182	L183	Q184	A185	S186	R187	M192	Y193	Q196	N197	K198	L199	E200	H201	L202	C203	Y204	K205	S206	G207	E208	L209	I210	T211	E212	T213	G214	Y215	M216	D217	T220	E221	Y224	P225	C226	L227	I228	I229	P162	K163	E164	E165	G166													
D233	C234	F235	W236	E237	G238	A239	K240	L241	Q242	S243	G244	T245	A246	Y247	L248	L249	G250	K251	P252	P253	L254	R255	W256	T257	N258	F259	L262	E263	F264	L265	E266	E267	L268	K269	K270	I271	W272	Y273	Q274	V275	D276	S277	W278	E279	E280	M281	L282	N283	K284	A285	E286	V287	G288	G290	Y291	M292	D293													
R294	P295	C296	L297	M298	P299	A300	D301	P302	D303	C304	P305	A306	T307	A308	P309	N310	K311	N312	S313	T314	K315	P316	L317	D318	M319	A320	L321	V322	L323	N324	G325	G326	G329	K333	W337	Q338	E339	E340	L341	T342	V343	G344	G345	T346	V347	K348	N349	S350	T351	G352	K353	L354	V355	S356																
A357	H358	A359	L360	Q361	T362	M363	F364	Q365	L366	M367	T368	Q371	M372	Y373	E374	H375	F376	K377	G378	Y379	E380	Y381	W382	S383	H384	I385	N386	W387	D390	L395	L396	E397	A398	W399	Q400	R401	T402	Y403	V404	E405	V406	V407	H408	Q409	S410	V411	A412	Q413	N414	S415	T416	L420	S421	F422	T423															
T424	T425	T426	L427	D428	D429	L430	L431	K432	S433	F434	S435	D436	V437	S438	V439	I440	R441	V442	A443	S444	G445	V446	L447	L448	M449	L450	A451	V452	A453	C454	L455	T456	M457	L458	R459	W460	D461	C462	S463	K464	S465	Q466	Q467	A468	V469	G470	L471	A472	G473	V474	L475	L476	V477	A478	L479	S480	V481	A482	A483											
G484	L485	G486	L487	C488	S489	L490	L491	S492	G493	S494	F495	N496	A497	A498	T499	T500	Q501	W502	L503	P504	F505	L506	A507	L508	G509	V510	G511	V512	D513	D514	V515	F516	L517	L518	A519	H520	A521	F522	S523	E524	T525	G526	O527	N528	K529	R530	T531	F532	F533	E534	D535	R536	T537	G538	F539	C540	L541	R542	R543											
T544	G545	A546	S547	V548	A549	L550	T551	S552	I553	S554	N555	V556	T557	A558	F559	F560	M561	A562	A563	L564	I565	P566	T567	P568	A569	L570	R571	A572	F573	S574	L575	Q576	A577	A578	V579	W580	V581	V582	F583	N584	F585	A586	M587	W588	L589	L590	T591	F592	P593	A594	I595	L596	S597	M598	D599	L600	Y601	R602	R603											
E604	D605	R606	ARG	LEU	ASP	PRO	HIS	THR	PHE	CYS	THR	SER	PRO	ALA	CYS	VAL	SER	ARG	ARG	VAL	ILE	GLN	VAL	GLU	PRO	GLN	ALA	THR	THR	THR	ASP	HIS	ASP	ASN	LEU	SER	GLN	TYR	SER	PRO	PRO	GLU	PRO	PRO	PRO	PRO	TYR	SER	SER	SER	HIS	ASP	LEU	ALA	HIS	GLU	THR	GLN	PHE	THR	ASP	ILE	THR	NET	GLN	SER	HIS	THR	VAL	GLN
LEU	ARG	THR	GLU	PRO	THR	ASP	PRO	HIS	THR	VAL	THR	THR	THR	ALA	ALA	GLU	PRO	ARG	ARG	VAL	ILE	GLN	SER	VAL	GLU	PRO	GLN	ALA	THR	THR	THR	ASP	HIS	ASP	ASN	LEU	SER	CYS	GLN	TYR	SER	PRO	PRO	GLU	PRO	PRO	PRO	PRO	TYR	SER	SER	SER	HIS	ASP	LEU	ALA	HIS	GLU	THR	GLN	PHE	THR	ASP	ILE	THR	NET	GLN			
GLU	PRO	PRO	PRO	THR	K729	W730	T731	L732	S733	S734	F735	A736	E737	K738	H739	Y740	A741	P742	F743	L744	L745	L746	K747	P747	K748	A749	K750	V751	P752	V753	I754	F755	H756	F757	L758	G759	L760	L761	G762	L763	S764	L765	M766	G767	E768	T769	R770	V771	R772	D773	G774	L775	M776	L777	T778	D779	I780	V781	P782	R783										
E784	T785	R786	E787	W788	D789	F790	T791	A792	A793	K796	Y797	F798	S799	H799	F900	Y901	N902	I905	V906	T907	Q908	K909	A910	D911	Y912	P913	N914	I915	Q916	H917	L918	R924	S827	N828	V829	K830	Y831	V832	M833	L834	E835	E836	T837	R838	Q839	L840	P841	K842	M843	W844	L845	W851	D857	A858	Y920															
F859	D860	S861	D862	W863	E864	T865	G866	K867	I868	M869	N871	N872	Y873	K874	N875	G876	S877	D878	V881	L882	A883	Y884	K885	L886	L887	V888	Q889	T890	G891	H892	S892	R893	D894	K895	P896	I897	V899	K900	Q901	L902	T903	K904	Q905	R906	L907	V908	D909	A910	D911	M911	W912	L913	I914	N915	P916	S917	Y920													

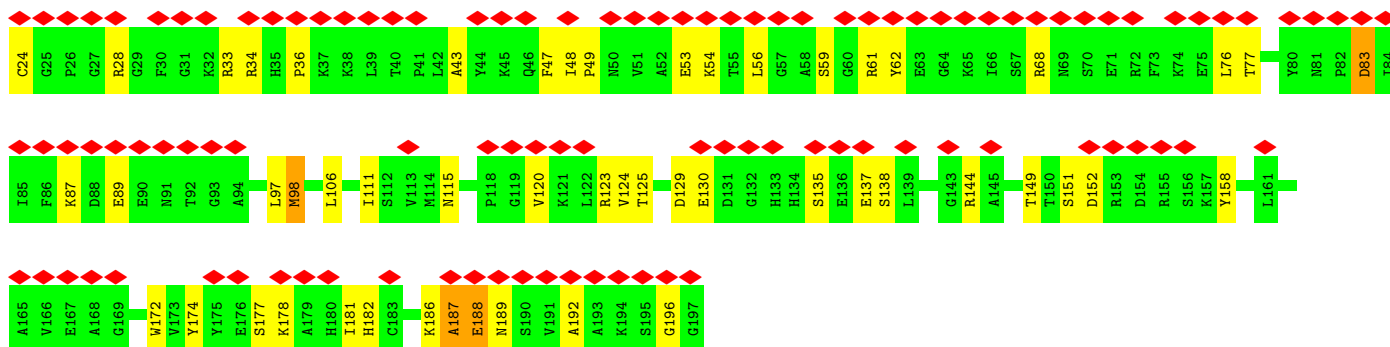
PHE	F1147	I1087	W1027	R962	I897	E836	R772	THR	HIS	V588	N528	A468	W399
ALA	I1148	A1088	L1028	T963	D898	M837	D773	ARG	SER	L589	K529	V469	Q400
MET	V1149	S1089	L1029	P964	I899	L840	G774	ASP	PHE	L590	R530	G470	R401
PRO	R1150	V1090	L1030	A965	Q901	L841	L775	LEU	HIS	I591	I531	L471	H408
GLY	G1091	G1091	F1031	A966	L902	K842	L776	SER	GLU	P593	P532	A472	Q409
HIS	F1152	I1092	I1032	E967	T903	M843	L777	GLN	THR	A594	F533	G473	S410
THR	F1153	G1093	S1033	P968	K904	M844	L778	PHE	GLN	P594	E534	V474	V411
HIS	A1154	V1094	V1034	P969	Q905	L845	L779	SER	ILE	A595	D535	L475	A412
GLY	V1155	E1095	V1035	E970	R906	M846	L780	ASP	THR	L596	R536	L476	Q413
ASP	L1156	F1096	L1036	Y971	R906	M847	L781	SER	MET	L597	T537	V477	M414
SER	A1157	T1097	A1037	A972	L907	F848	F782	LEU	SER	M598	G538	A478	S415
SER	I1158	V1098	Q973	Q973	V908	R849	R783	HIS	THR	D599	E539	L479	L420
ASP	L1159	F974	D850	E784	D909	R850	R783	CYS	VAL	L500	C540	S480	S421
SER	T1160	V1100	A910	M851	A910	W851	T785	LEU	GLN	Y601	L541	V481	F422
THR	I1161	A1101	D911	L852	D911	L852	R786	PRO	THR	R602	K542	V482	T423
SER	L1162	L1102	G912	Q853	G912	Q853	E787	PRO	ARG	R603	R543	A482	T424
GLY	G1163	C1043	I913	Q854	I913	Q854	F788	CYS	GLU	E604	T544	A483	T425
THR	F1164	A1044	I914	L855	I914	L855	F789	THR	TYR	D605	G545	G484	T426
THR	L1165	V1045	N915	Q856	N915	Q856	F790	LYS	ASP	R606	A546	L485	T427
VAL	M1166	F1046	P916	D857	P916	D857	F791	TRP	PRO	R607	S547	G486	T428
SER	G1167	L1047	S917	A858	S917	A858	F795	THR	HIS	L608	V548	C488	D429
GLY	L1168	L1048	A918	F859	A918	F859	K796	THR	VAL	D609	L550	S489	I430
LEU	V1169	N1049	F919	D860	F919	D860	F797	THR	THR	I610	T551	L490	L431
GLY	L1170	P1050	Y920	S861	Y920	S861	F798	THR	THR	PHE	S552	I491	K432
LEU	L1171	W1051	I921	D862	I921	D862	F798	THR	ALA	CYS	I553	G492	S433
ARG	P1172	T1052	Y922	W863	Y922	W863	F798	THR	GLU	THR	S554	I493	F434
THR	V1173	A1053	L923	E864	L923	E864	M803	THR	PRO	PHE	R555	S494	S435
HIS	L1174	G1054	A925	T865	A925	T865	I805	THR	ARG	SER	V556	F495	D436
GLY	L1175	I1055	N929	G866	N929	G866	W806	THR	SER	CYS	T557	M496	V437
GLN	S1176	I1056	I868	G867	I868	G867	K867	THR	ILE	VAL	A558	A497	S438
GLY	F1177	V1057	W869	S877	W869	S877	Q808	SER	SER	SER	F559	A498	V439
GLY	G1178	M1058	P870	D878	P870	D878	K809	VAL	VAL	ARG	F560	T499	I440
GLY	P1179	V1059	M871	D879	M871	D879	A810	GLN	PRO	GLN	M561	T500	R441
PRO	Y1181	A1061	N872	S877	N872	S877	W811	VAL	VAL	VAL	A562	Q501	V442
ALA	P1182	S1003	N873	K874	N873	K874	F813	VAL	VAL	GLU	A563	V502	A443
HIS	E1183	L1004	Q838	M875	Q838	M875	W814	THR	THR	PRO	L564	L503	S444
GLN	VAL	G1005	A939	G876	A939	G876	I815	ASP	ASP	ALA	I565	P504	G445
ILE	VAL	L1006	R942	S877	R942	S877	Q816	THR	THR	TYR	P566	F505	Y446
VAL	PRO	S1007	P943	S877	P943	S877	L817	LEU	SER	THR	I567	L506	L447
GLY	ALA	S1008	H944	D878	H944	D878	L818	SER	ASP	ASP	P568	A507	L448
THR	GLY	P1010	R945	D879	R945	D879	L819	GLN	ASP	ASP	A569	L508	M449
LEU	ASN	N1011	P946	G880	N1011	G880	W820	THR	ASN	ASP	L570	G509	L450
ASN	ARG	G1012	E947	W881	G1012	W881	L822	THR	THR	THR	A571	V510	A451
ARG	VAL	Y1013	W948	L882	Y1013	L882	R823	ARG	ARG	ARG	A572	G511	Y452
VAL	THR	P1014	V949	A883	P1014	A883	R824	THR	THR	THR	F573	V512	A453
ALA	THR	F1015	H950	K884	F1015	K884	S825	SER	SER	PRO	S574	D513	C454
PRO	PRO	L1016	D951	L886	L1016	L886	F826	PRO	PRO	PRO	L575	D514	L455
SER	SER	K952	K952	L887	K952	L887	S827	PRO	PRO	PRO	Q576	V515	T456
PRO	PRO	A953	A953	V888	A953	V888	S827	THR	THR	THR	A577	F516	M457
GLY	GLY	W1018	D954	V888	W1018	D954	W829	SER	SER	SER	A578	L517	L458
PRO	PRO	E1019	Y955	Q889	E1019	Y955	K830	THR	THR	THR	V579	L518	M458
PRO	PRO	Q1020	M956	T890	Q1020	M956	R831	SER	SER	SER	V580	A519	R459
VAL	VAL	Y1021	P957	G891	Y1021	P957	F832	THR	THR	THR	V581	H520	C462
ARG	ARG	I1022	E958	S892	I1022	E958	M833	SER	SER	SER	V582	A521	S463
		G1023	T959	R893	G1023	T959	L834	THR	THR	THR	F583	F522	K464
		L1024	R960	D894	L1024	R960	E835	SER	SER	SER	N584	S523	S465
		R1025	L961	K895	R1025	L961	P896	THR	THR	THR	F585	E524	Q466
		H1026			H1026			SER	SER	SER	A586	T525	G467
											M587	G526	Q527



- Molecule 2: Sonic hedgehog protein



- Molecule 2: Sonic hedgehog protein



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, PLM, CA, NAG, ZN

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	0.39	0/8000	0.70	0/10883
1	B	0.41	0/7897	0.70	2/10749 (0.0%)
1	D	0.38	0/8000	0.70	0/10883
1	E	0.41	0/7897	0.70	2/10749 (0.0%)
2	C	0.66	2/1401 (0.1%)	0.93	13/1886 (0.7%)
2	F	0.66	2/1401 (0.1%)	0.93	13/1886 (0.7%)
All	All	0.42	4/34596 (0.0%)	0.72	30/47036 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
1	D	0	7
1	E	0	6
2	C	0	1
2	F	0	1
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	98	MET	C-N	13.72	1.52	1.33
2	F	98	MET	C-N	13.67	1.52	1.33
2	F	123	ARG	C-N	11.99	1.45	1.33
2	C	123	ARG	C-N	11.93	1.45	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	83	ASP	CA-C-N	10.39	136.50	123.10
2	C	83	ASP	C-N-CA	10.39	136.50	123.10
2	F	83	ASP	CA-C-N	10.37	136.48	123.10
2	F	83	ASP	C-N-CA	10.37	136.48	123.10
2	F	83	ASP	O-C-N	-9.28	110.96	122.19

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	VAL	Peptide
1	A	224	TYR	Peptide
1	A	317	LEU	Peptide
1	A	835	GLU	Peptide
1	A	836	GLU	Peptide

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	7807	0	7828	113	0
1	B	7708	0	7664	120	0
1	D	7807	0	7828	112	0
1	E	7708	0	7664	122	0
2	C	1371	0	1329	37	0
2	F	1371	0	1329	36	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
4	A	70	0	65	0	0
4	B	70	0	65	1	0
4	D	70	0	65	1	0
4	E	70	0	65	1	0
5	A	84	0	138	35	0
5	B	28	0	46	30	0
5	C	28	0	45	19	0
5	D	84	0	138	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	46	33	0
5	F	28	0	45	19	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	C	2	0	0	0	0
7	F	2	0	0	0	0
8	C	17	0	31	16	0
8	F	17	0	31	16	0
All	All	34484	0	34522	616	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.

The worst 5 of 616 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1147:PHE:HE2	8:C:205:PLM:CG	1.16	1.54
1:A:220:ILE:CD1	5:A:1808:CLR:C6	1.84	1.53
1:E:1147:PHE:HE2	8:F:205:PLM:CG	1.16	1.53
1:D:220:ILE:CD1	5:D:1808:CLR:C6	1.84	1.52
1:B:1147:PHE:CE2	8:C:205:PLM:CG	1.93	1.50

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	987/1349 (73%)	857 (87%)	123 (12%)	7 (1%)	19	57
1	B	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	37	73
1	D	987/1349 (73%)	858 (87%)	122 (12%)	7 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	37	73
2	C	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	11	44
2	F	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	11	44
All	All	4286/5744 (75%)	3733 (87%)	529 (12%)	24 (1%)	24	60

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	939	ALA
2	C	188	GLU
1	E	939	ALA
2	F	188	GLU
1	A	424	THR

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	832/1147 (72%)	825 (99%)	7 (1%)	79	85
1	B	808/1147 (70%)	793 (98%)	15 (2%)	52	69
1	D	832/1147 (72%)	825 (99%)	7 (1%)	79	85
1	E	808/1147 (70%)	793 (98%)	15 (2%)	52	69
2	C	142/144 (99%)	140 (99%)	2 (1%)	62	75
2	F	142/144 (99%)	140 (99%)	2 (1%)	62	75
All	All	3564/4876 (73%)	3516 (99%)	48 (1%)	64	77

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	450	LEU
1	E	287	VAL
1	D	550	LEU
1	E	159	ILE

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Mol	Chain	Res	Type
1	E	354	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	929	ASN
1	E	1049	ASN
1	B	853	GLN
1	B	846	HIS
2	F	35	HIS

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 ⓘ

8 monosaccharides 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	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.25	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.56	0
3	NAG	H	1	1,3	14,14,15	0.45	0	17,19,21	0.67	0
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.55	0
3	NAG	J	1	1,3	14,14,15	0.46	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.71	1 (5%)

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
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C1-O5-C5	2.57	115.62	112.19
3	J	2	NAG	C1-O5-C5	2.55	115.60	112.19

There are no chirality outliers.

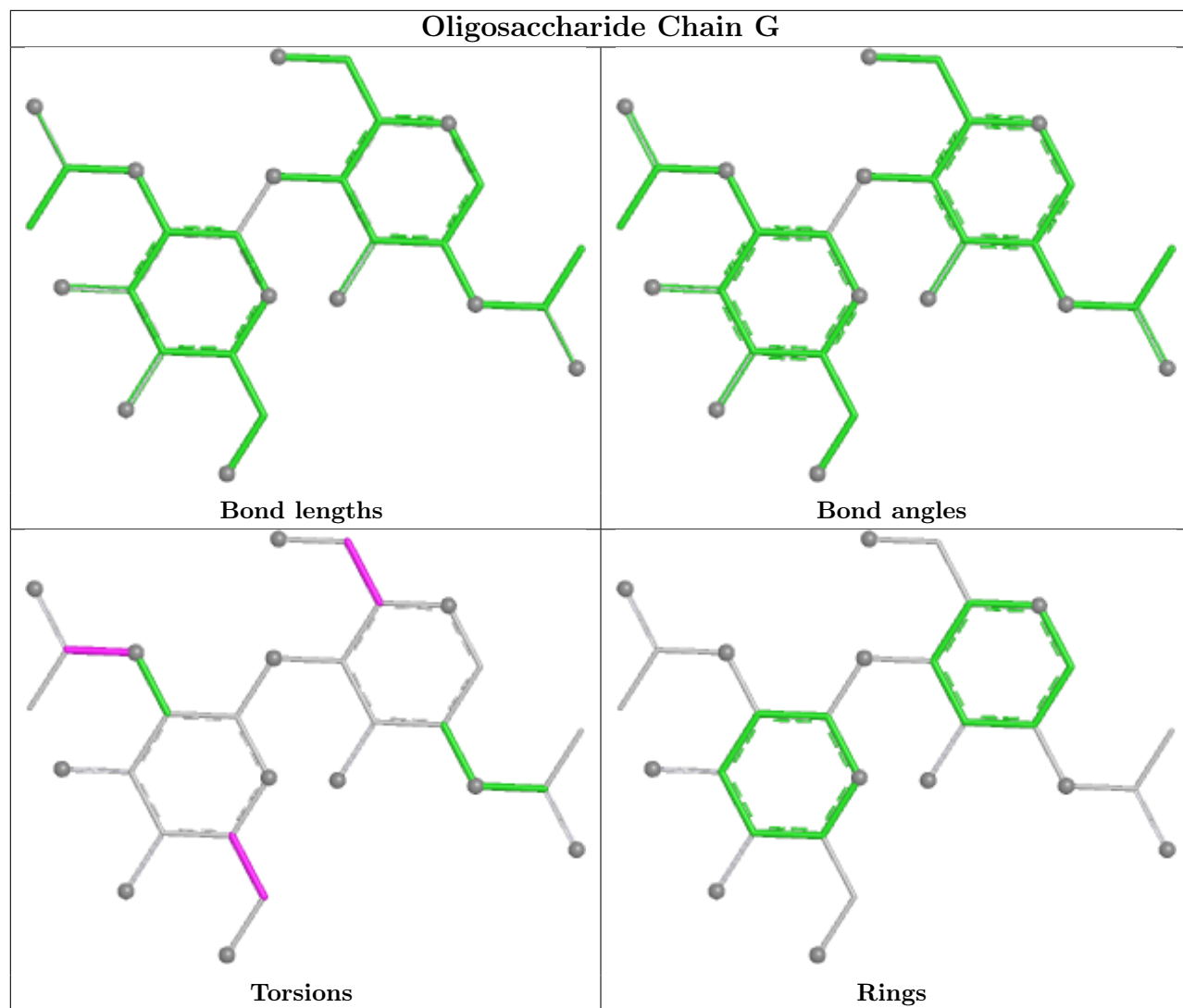
5 of 14 torsion outliers are listed below:

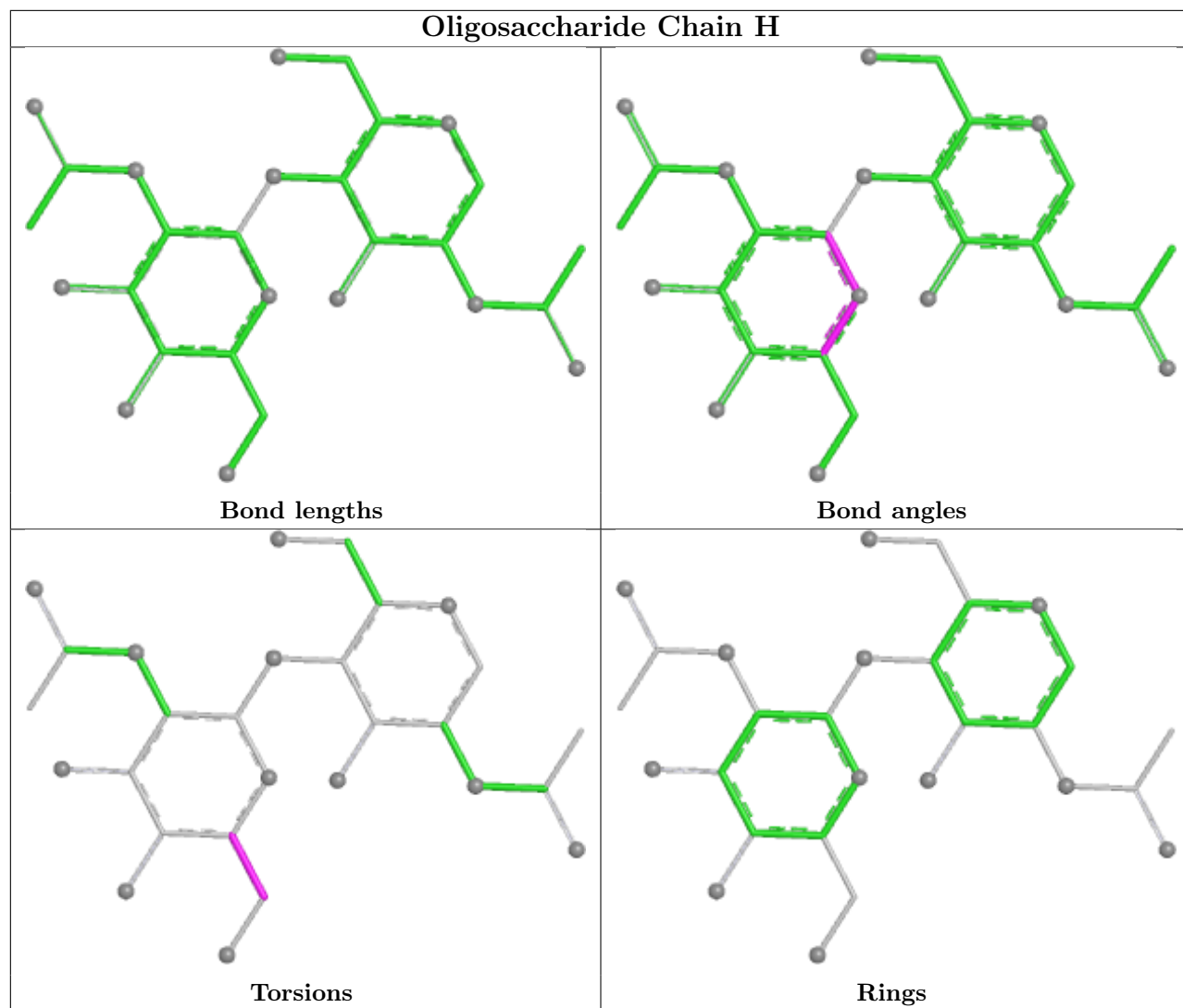
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

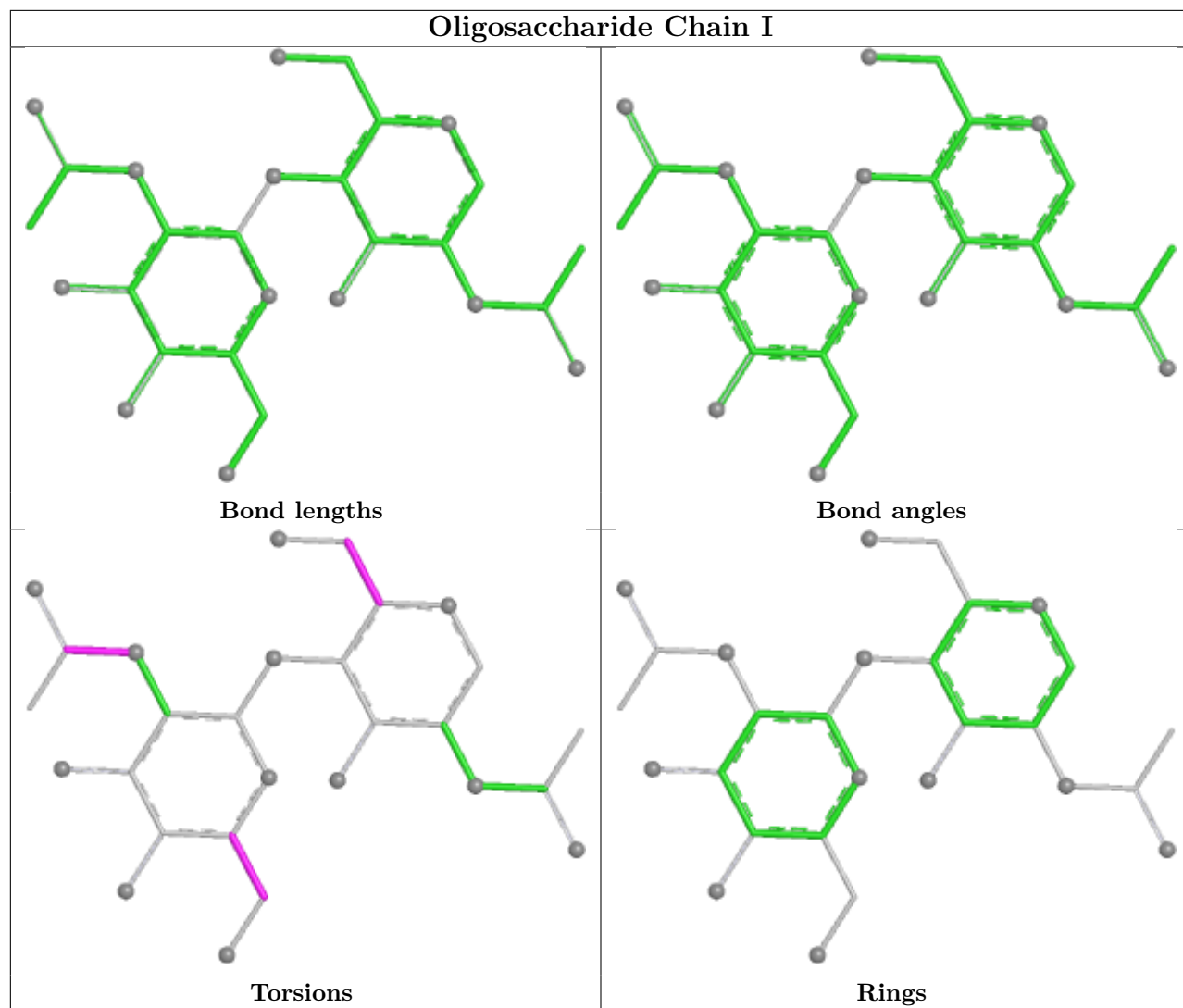
There are no ring outliers.

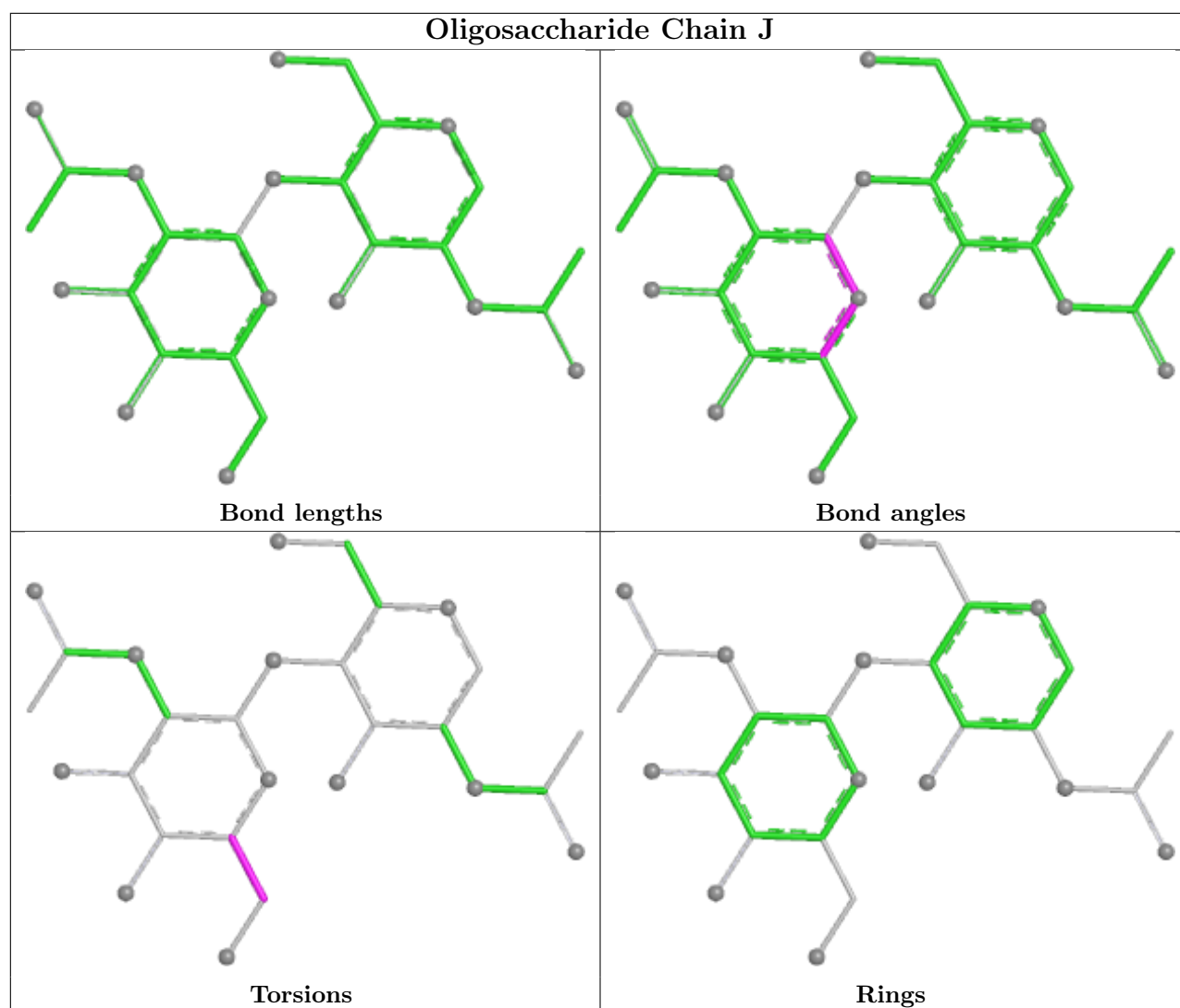
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 for Mogul analysis.

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	$\# Z > 2$
4	NAG	A	1803	1	14,14,15	0.79	1 (7%)	17,19,21	1.28	2 (11%)
5	CLR	B	1508	-	31,31,31	0.90	2 (6%)	48,48,48	1.58	9 (18%)
8	PLM	F	205	2	15,16,17	0.32	0	14,15,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1503	1	14,14,15	0.92	1 (7%)	17,19,21	1.40	3 (17%)
5	CLR	A	1809	-	31,31,31	0.72	0	48,48,48	1.56	9 (18%)
4	NAG	B	1504	1	14,14,15	0.75	1 (7%)	17,19,21	0.77	1 (5%)
5	CLR	D	1808	-	31,31,31	1.03	2 (6%)	48,48,48	1.67	8 (16%)
4	NAG	B	1502	1	14,14,15	0.55	0	17,19,21	0.39	0
4	NAG	E	1505	1	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	A	1802	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	D	1804	1	14,14,15	0.22	0	17,19,21	0.59	0
4	NAG	B	1501	1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
4	NAG	D	1807	1	14,14,15	0.40	0	17,19,21	0.42	0
5	CLR	F	201	2	31,31,31	1.02	1 (3%)	48,48,48	1.97	8 (16%)
4	NAG	B	1505	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	E	1503	1	14,14,15	0.95	1 (7%)	17,19,21	1.40	3 (17%)
5	CLR	C	201	2	31,31,31	1.02	1 (3%)	48,48,48	1.98	9 (18%)
4	NAG	E	1502	1	14,14,15	0.54	0	17,19,21	0.39	0
4	NAG	E	1501	1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
4	NAG	A	1807	1	14,14,15	0.40	0	17,19,21	0.42	0
5	CLR	D	1810	-	31,31,31	0.68	0	48,48,48	1.27	6 (12%)
5	CLR	E	1508	-	31,31,31	0.90	2 (6%)	48,48,48	1.58	9 (18%)
4	NAG	A	1804	1	14,14,15	0.22	0	17,19,21	0.59	0
8	PLM	C	205	2	15,16,17	0.32	0	14,15,17	0.66	0
4	NAG	D	1803	1	14,14,15	0.78	1 (7%)	17,19,21	1.28	2 (11%)
4	NAG	A	1801	1	14,14,15	0.87	1 (7%)	17,19,21	2.39	4 (23%)
5	CLR	A	1810	-	31,31,31	0.67	0	48,48,48	1.27	6 (12%)
5	CLR	D	1809	-	31,31,31	0.73	0	48,48,48	1.56	9 (18%)
4	NAG	D	1802	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	D	1801	1	14,14,15	0.88	1 (7%)	17,19,21	2.39	4 (23%)
5	CLR	A	1808	-	31,31,31	1.04	2 (6%)	48,48,48	1.67	8 (16%)
4	NAG	E	1504	1	14,14,15	0.75	0	17,19,21	0.77	1 (5%)

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
4	NAG	A	1803	1	-	4/6/23/26	0/1/1/1
5	CLR	B	1508	-	-	4/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PLM	F	205	2	-	7/14/14/15	-
4	NAG	B	1503	1	-	2/6/23/26	0/1/1/1
5	CLR	A	1809	-	-	2/10/68/68	0/4/4/4
4	NAG	B	1504	1	-	4/6/23/26	0/1/1/1
5	CLR	D	1808	-	-	9/10/68/68	0/4/4/4
4	NAG	B	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1505	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1802	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1804	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1807	1	-	3/6/23/26	0/1/1/1
5	CLR	F	201	2	-	3/10/68/68	0/4/4/4
4	NAG	B	1505	1	-	4/6/23/26	0/1/1/1
4	NAG	E	1503	1	-	2/6/23/26	0/1/1/1
5	CLR	C	201	2	-	3/10/68/68	0/4/4/4
4	NAG	E	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1807	1	-	3/6/23/26	0/1/1/1
5	CLR	D	1810	-	-	6/10/68/68	0/4/4/4
5	CLR	E	1508	-	-	4/10/68/68	0/4/4/4
4	NAG	A	1804	1	-	1/6/23/26	0/1/1/1
8	PLM	C	205	2	-	7/14/14/15	-
4	NAG	D	1803	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1801	1	-	6/6/23/26	0/1/1/1
5	CLR	A	1810	-	-	6/10/68/68	0/4/4/4
5	CLR	D	1809	-	-	2/10/68/68	0/4/4/4
4	NAG	D	1802	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1801	1	-	6/6/23/26	0/1/1/1
5	CLR	A	1808	-	-	9/10/68/68	0/4/4/4
4	NAG	E	1504	1	-	4/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	CLR	C13-C14	-2.79	1.49	1.55
5	F	201	CLR	C13-C14	-2.77	1.49	1.55
4	D	1801	NAG	C1-C2	2.65	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	NAG	C1-C2	2.63	1.55	1.52
5	A	1808	CLR	C13-C14	-2.61	1.50	1.55

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1801	NAG	C2-N2-C7	8.40	134.16	122.90
4	A	1801	NAG	C2-N2-C7	8.38	134.14	122.90
5	F	201	CLR	C13-C17-C20	-5.65	110.77	119.50
5	C	201	CLR	C13-C17-C20	-5.64	110.78	119.50
5	C	201	CLR	C13-C14-C8	-5.61	106.44	114.41

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

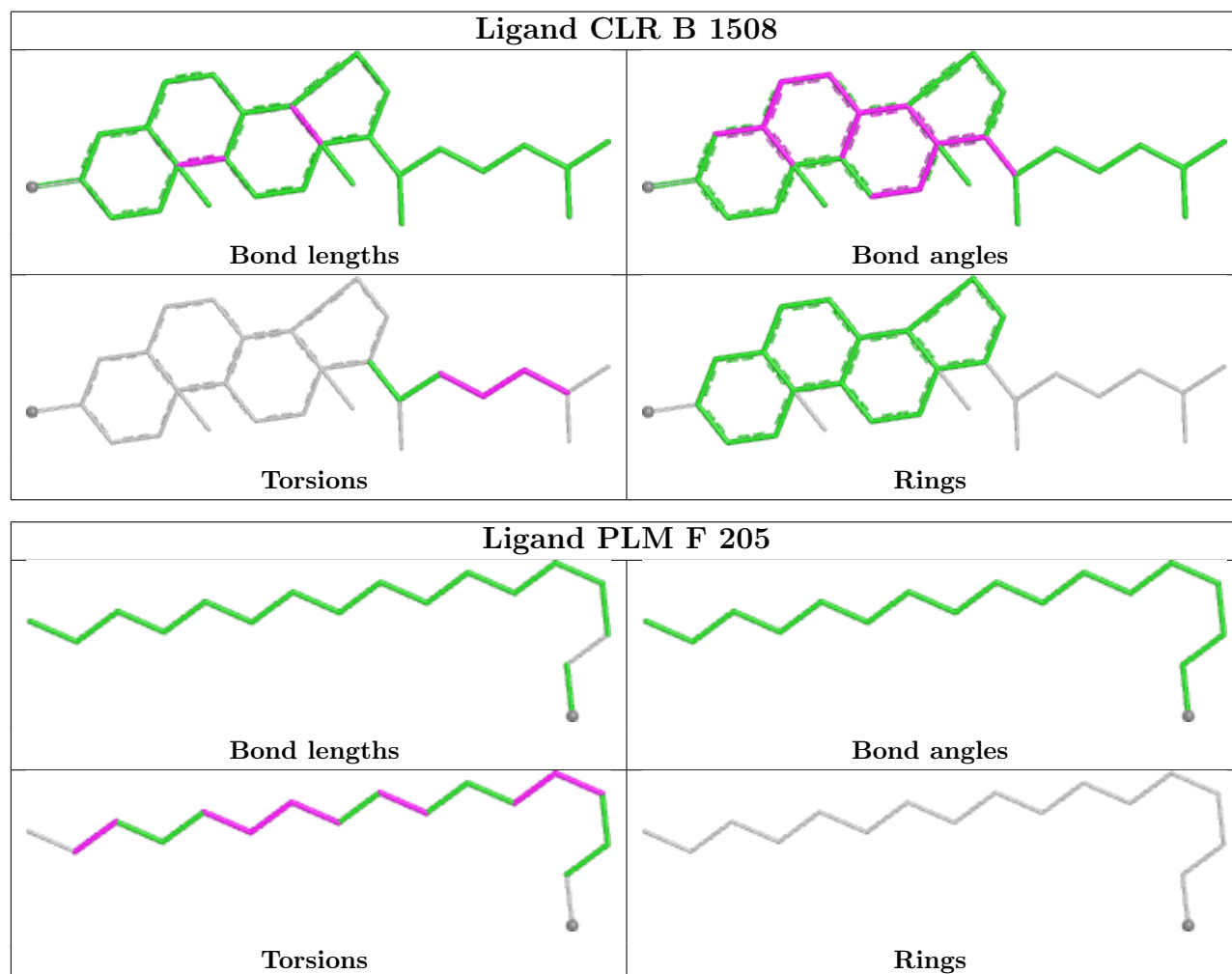
Mol	Chain	Res	Type	Atoms
5	C	201	CLR	C17-C20-C22-C23
5	F	201	CLR	C17-C20-C22-C23
5	A	1810	CLR	C13-C17-C20-C21
5	D	1810	CLR	C13-C17-C20-C21
5	C	201	CLR	C22-C23-C24-C25

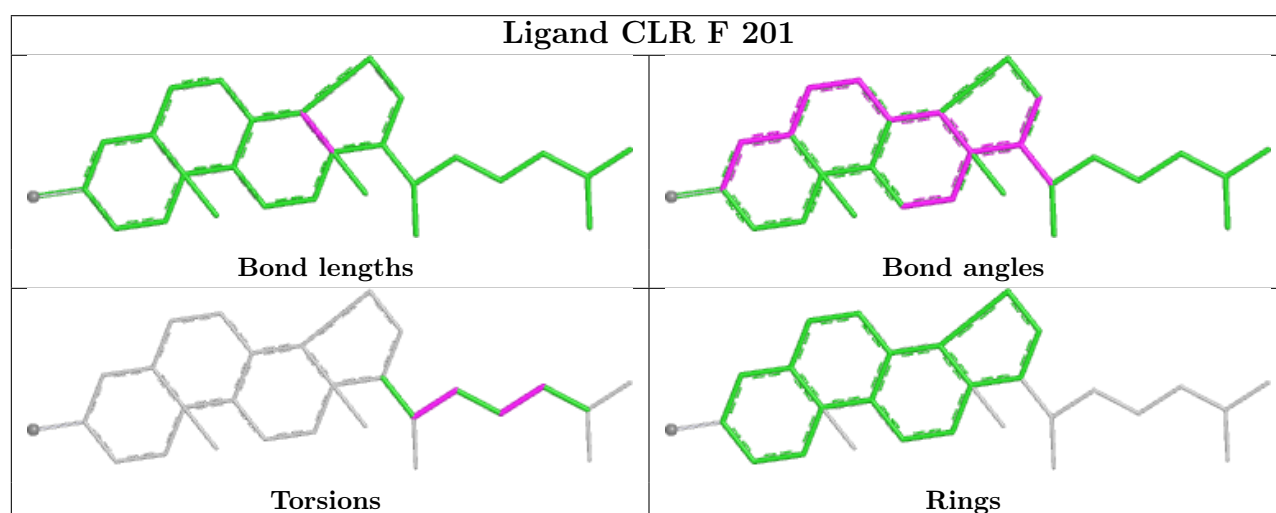
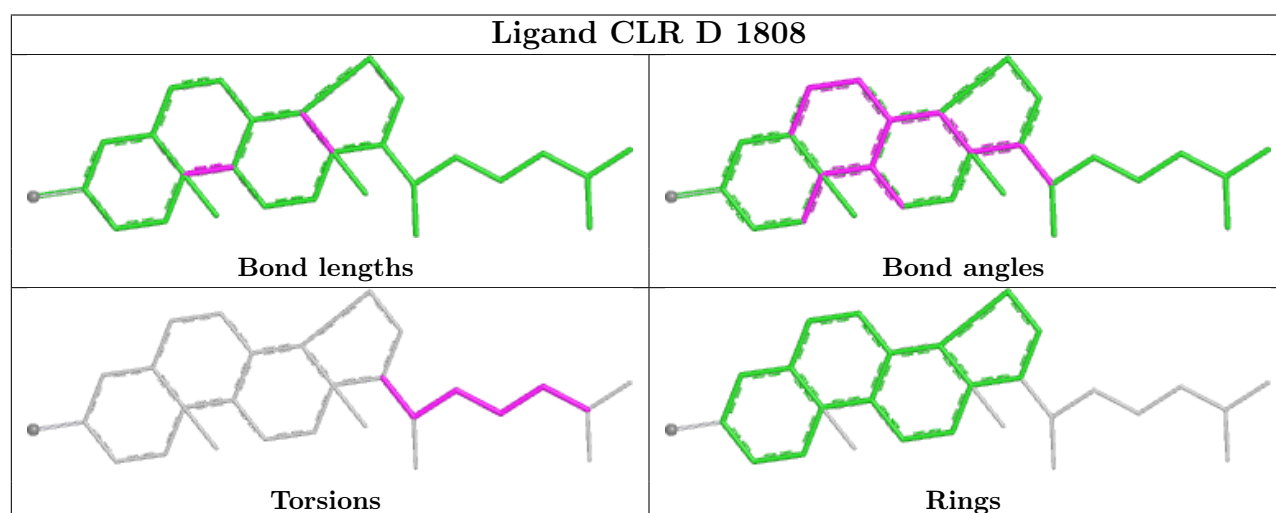
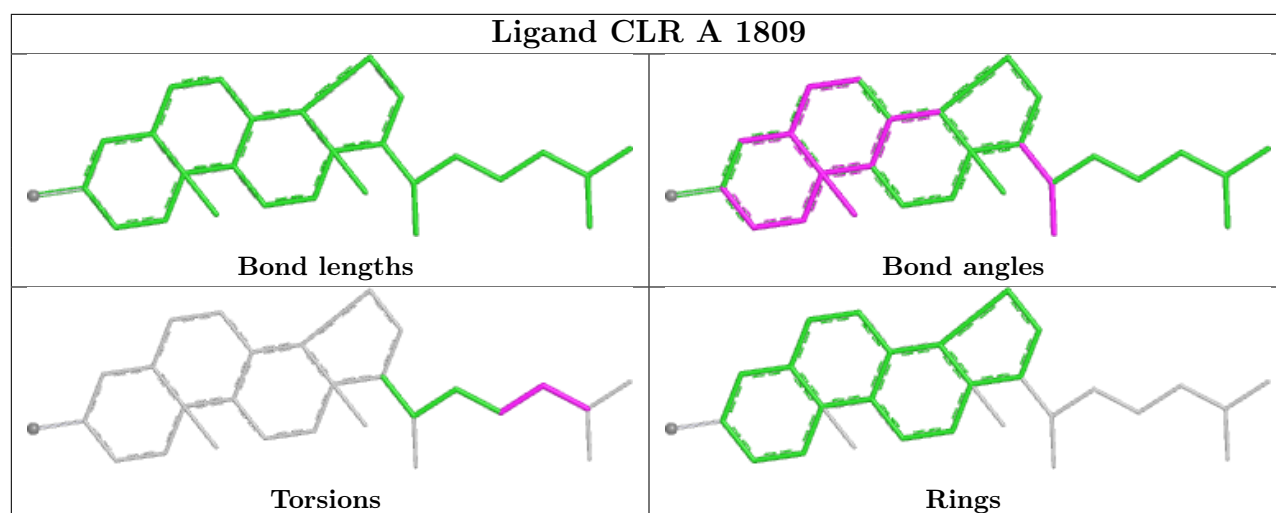
There are no ring outliers.

15 monomers are involved in 206 short contacts:

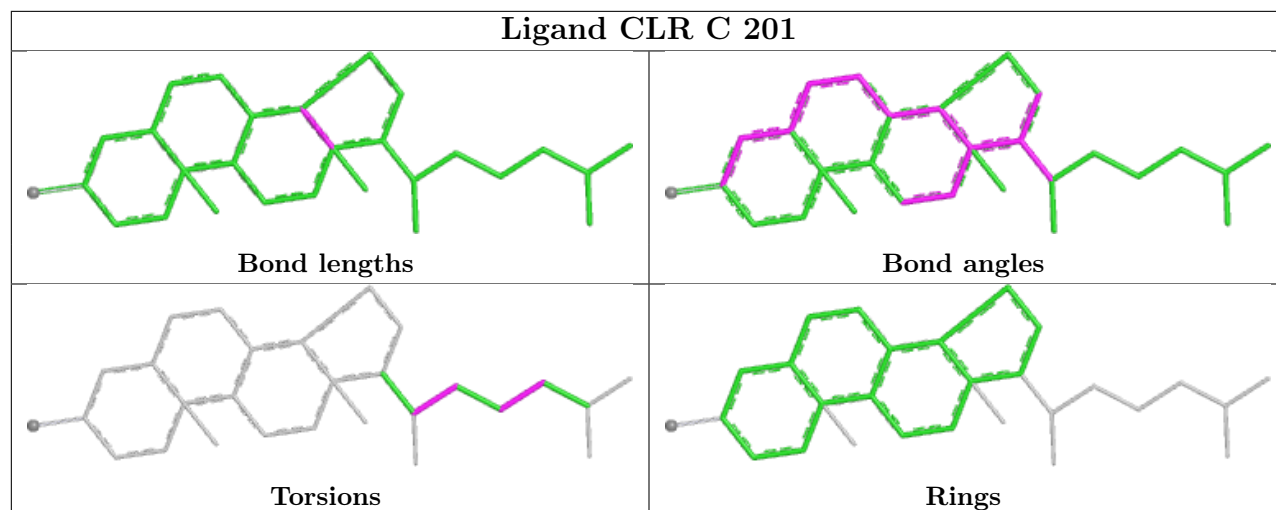
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1508	CLR	30	0
8	F	205	PLM	16	0
5	A	1809	CLR	1	0
5	D	1808	CLR	30	0
4	D	1804	NAG	1	0
4	B	1501	NAG	1	0
5	F	201	CLR	19	0
5	C	201	CLR	19	0
4	E	1501	NAG	1	0
5	D	1810	CLR	3	0
5	E	1508	CLR	33	0
8	C	205	PLM	16	0
5	A	1810	CLR	3	0
5	D	1809	CLR	2	0
5	A	1808	CLR	31	0

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.

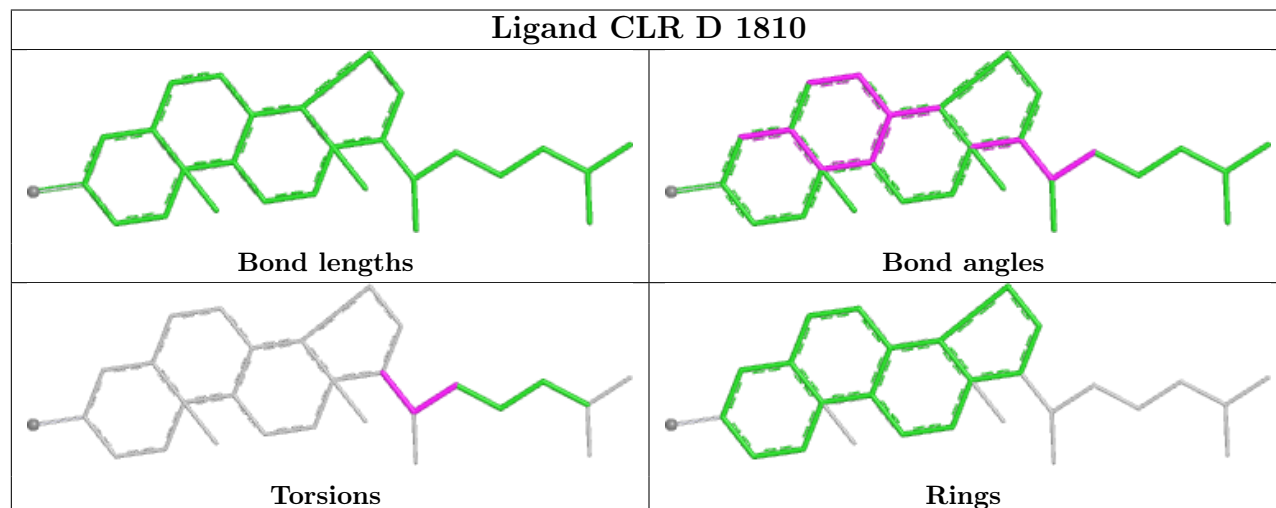




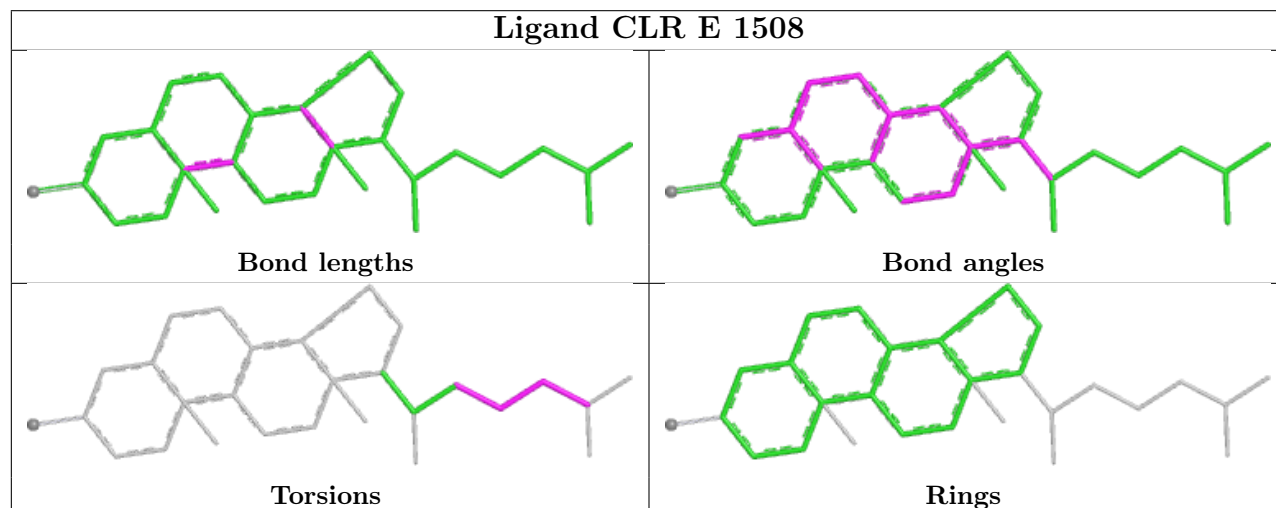
Ligand CLR C 201

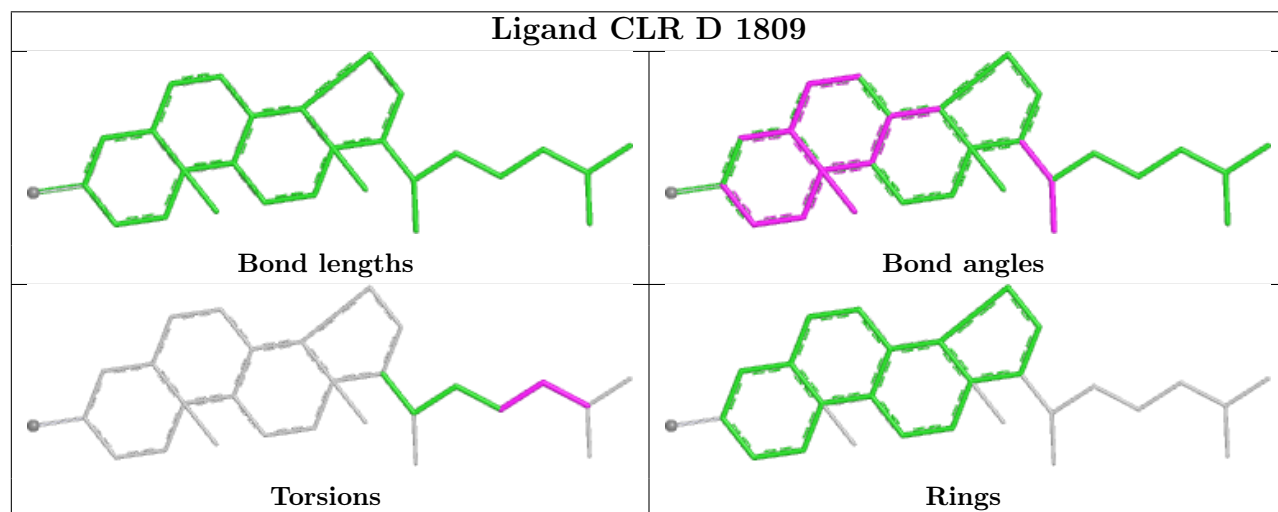
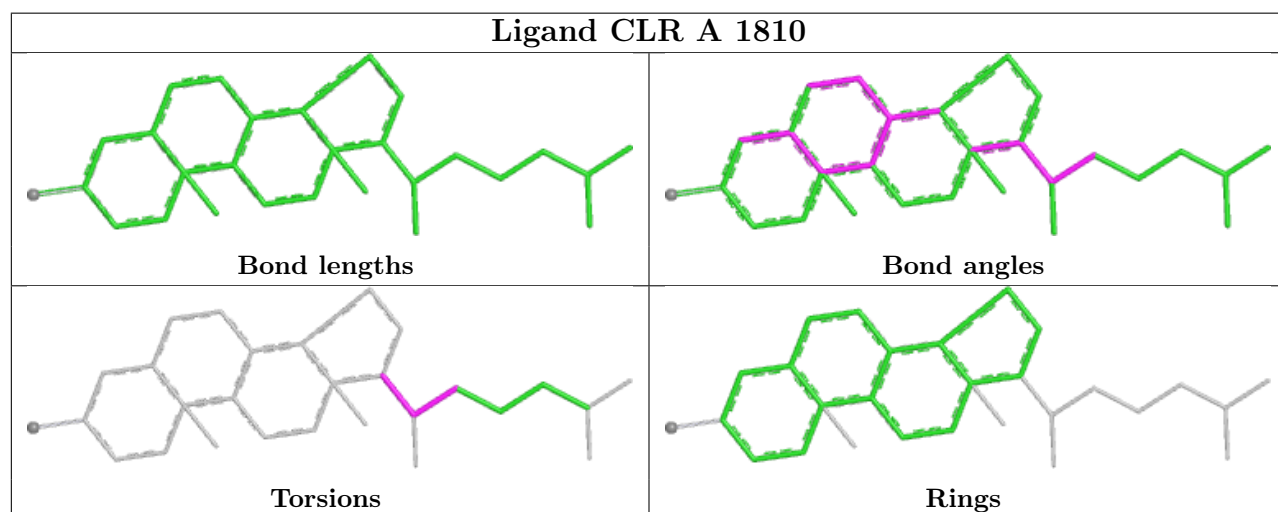
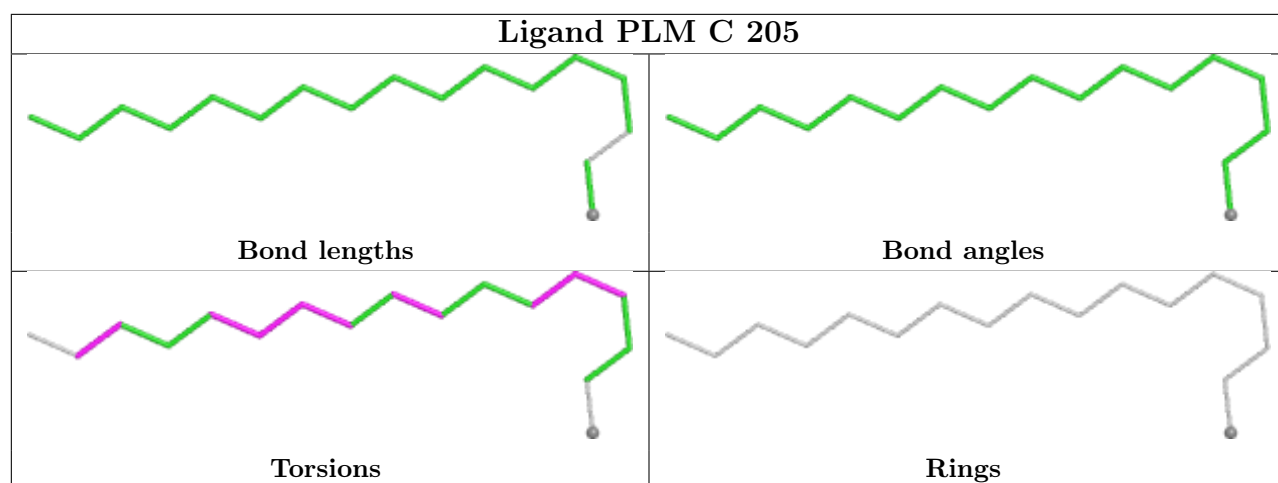


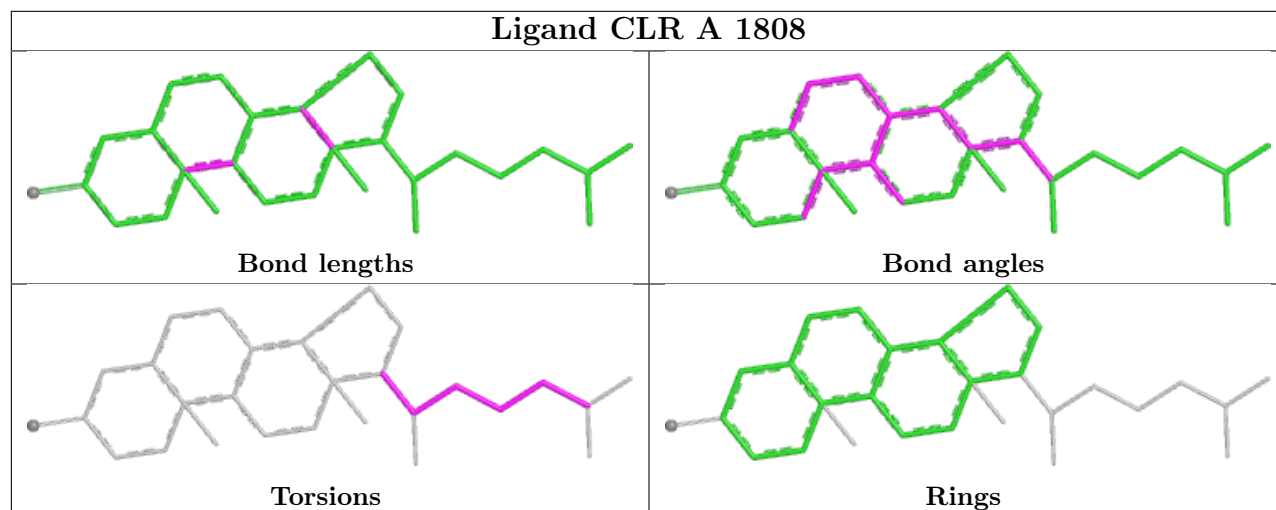
Ligand CLR D 1810



Ligand CLR E 1508







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.

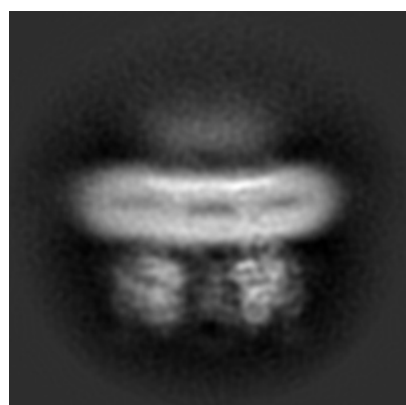
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0358. These allow visual inspection of the internal detail of the map and identification of artifacts.

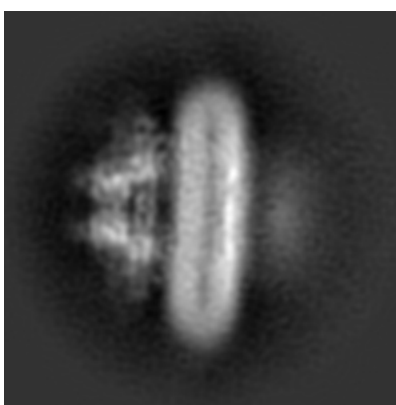
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

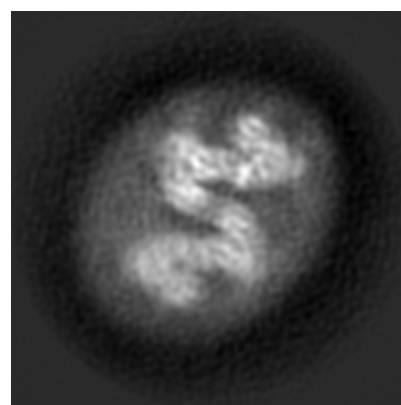
6.1.1 Primary map



X



Y

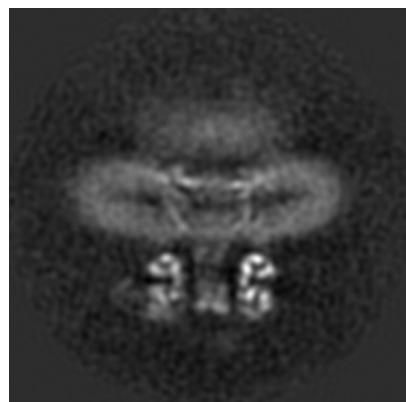


Z

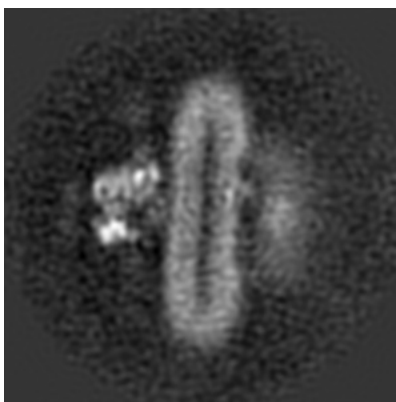
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

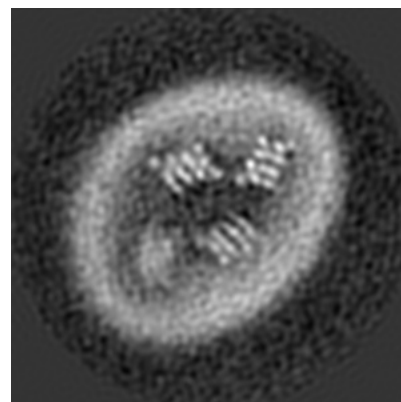
6.2.1 Primary map



X Index: 140



Y Index: 140

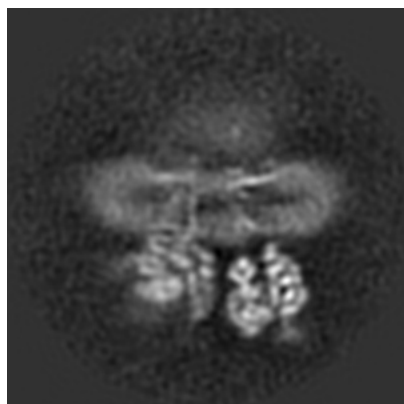


Z Index: 140

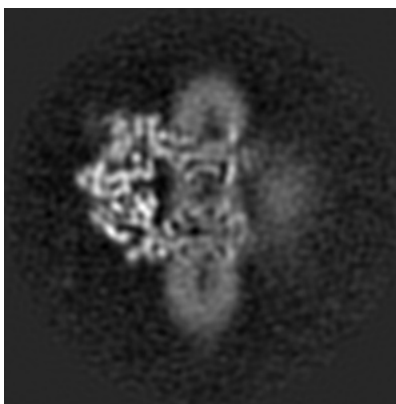
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

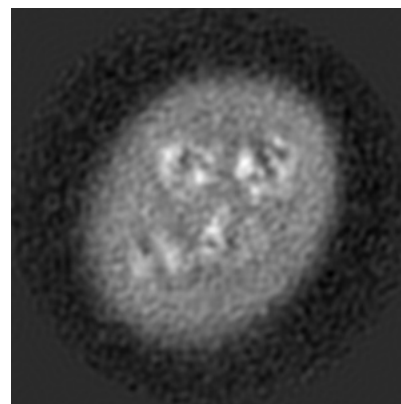
6.3.1 Primary map



X Index: 163



Y Index: 167



Z Index: 158

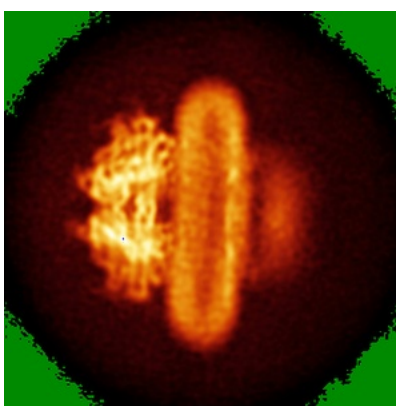
The images above show the largest variance slices of the map in three orthogonal directions.

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

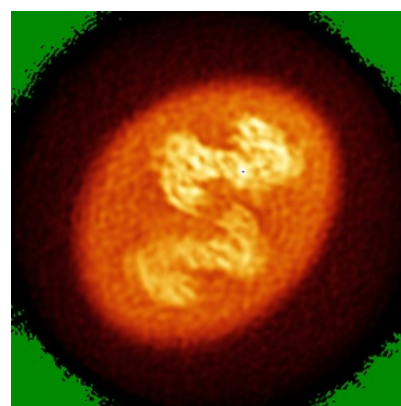
6.4.1 Primary map



X



Y

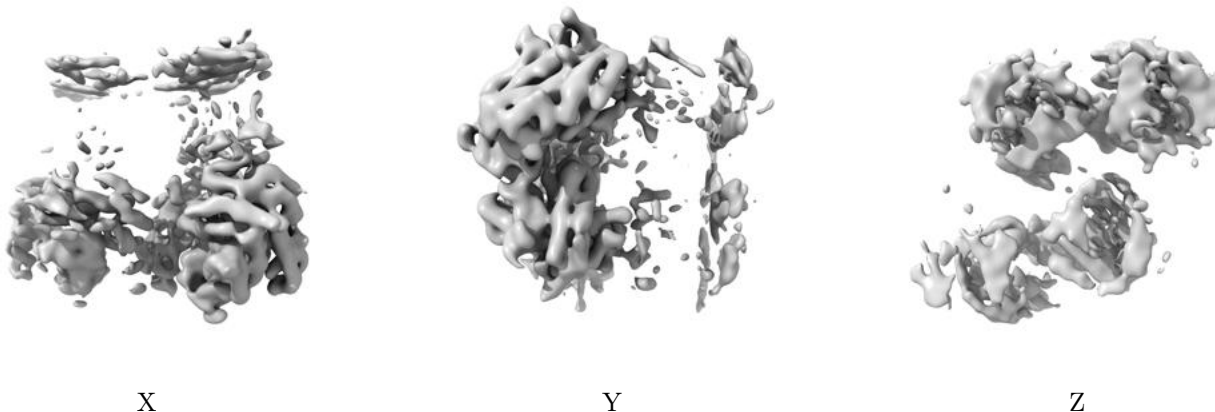


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

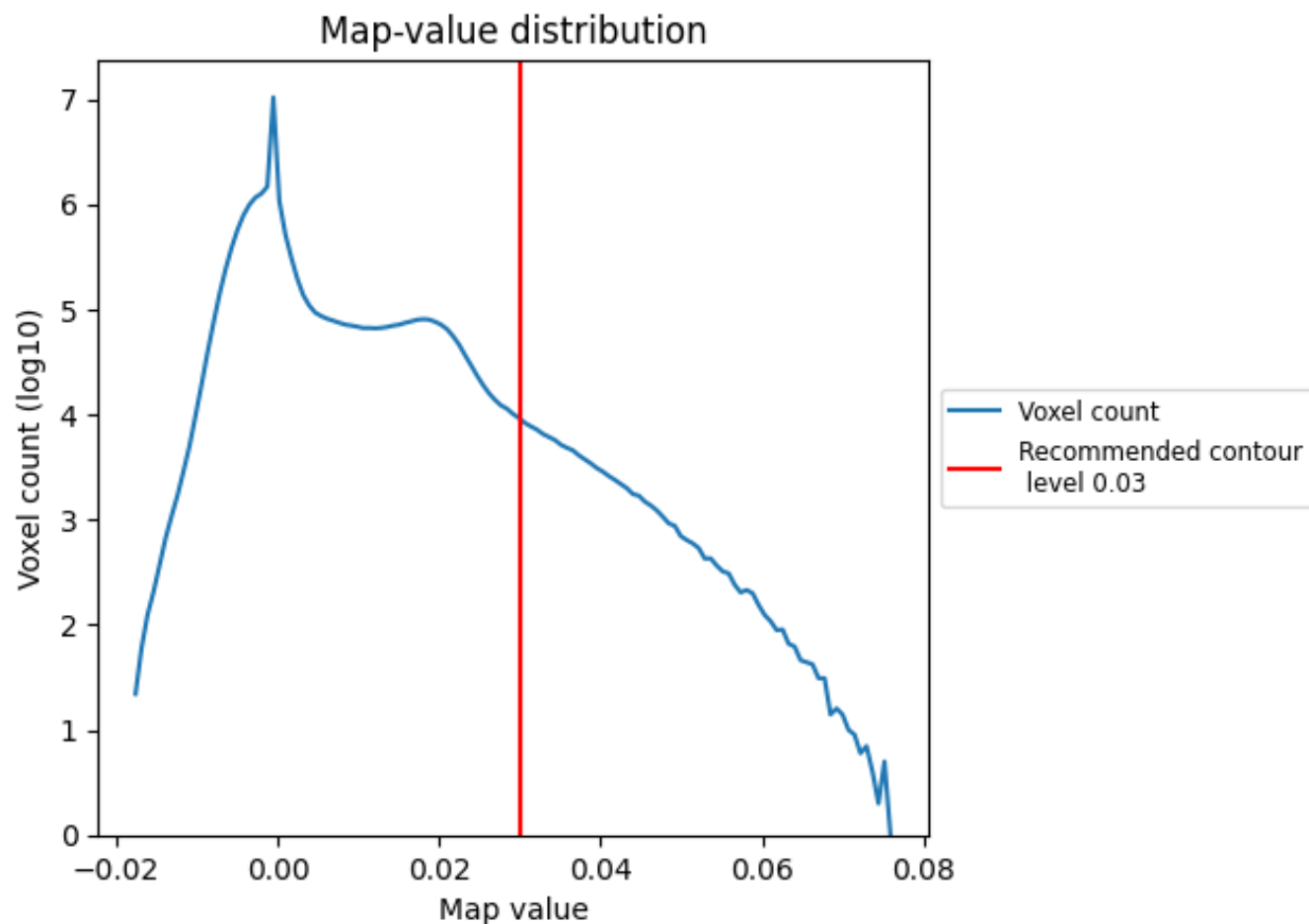
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

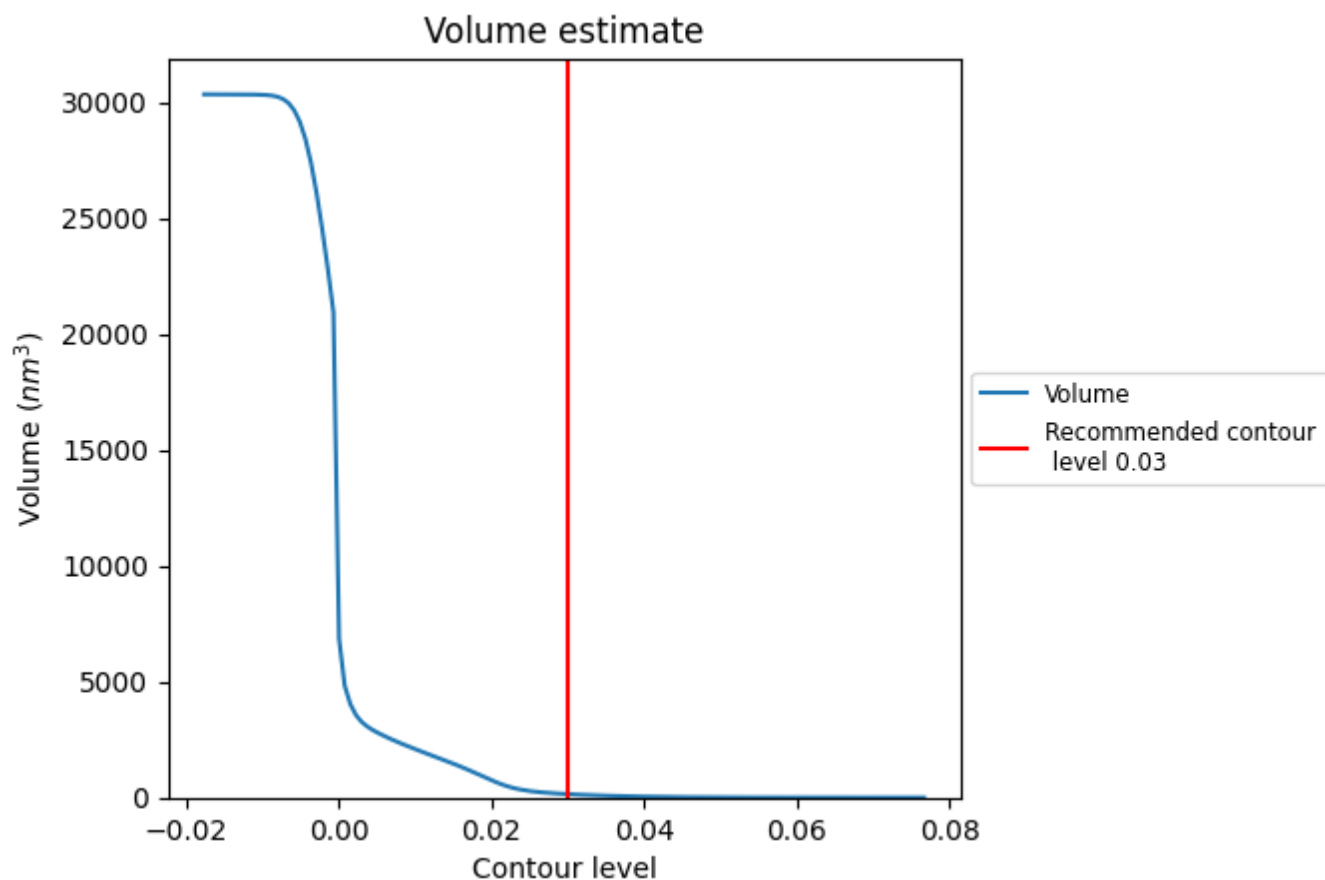
This section contains the results of statistical analysis of the map.

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.

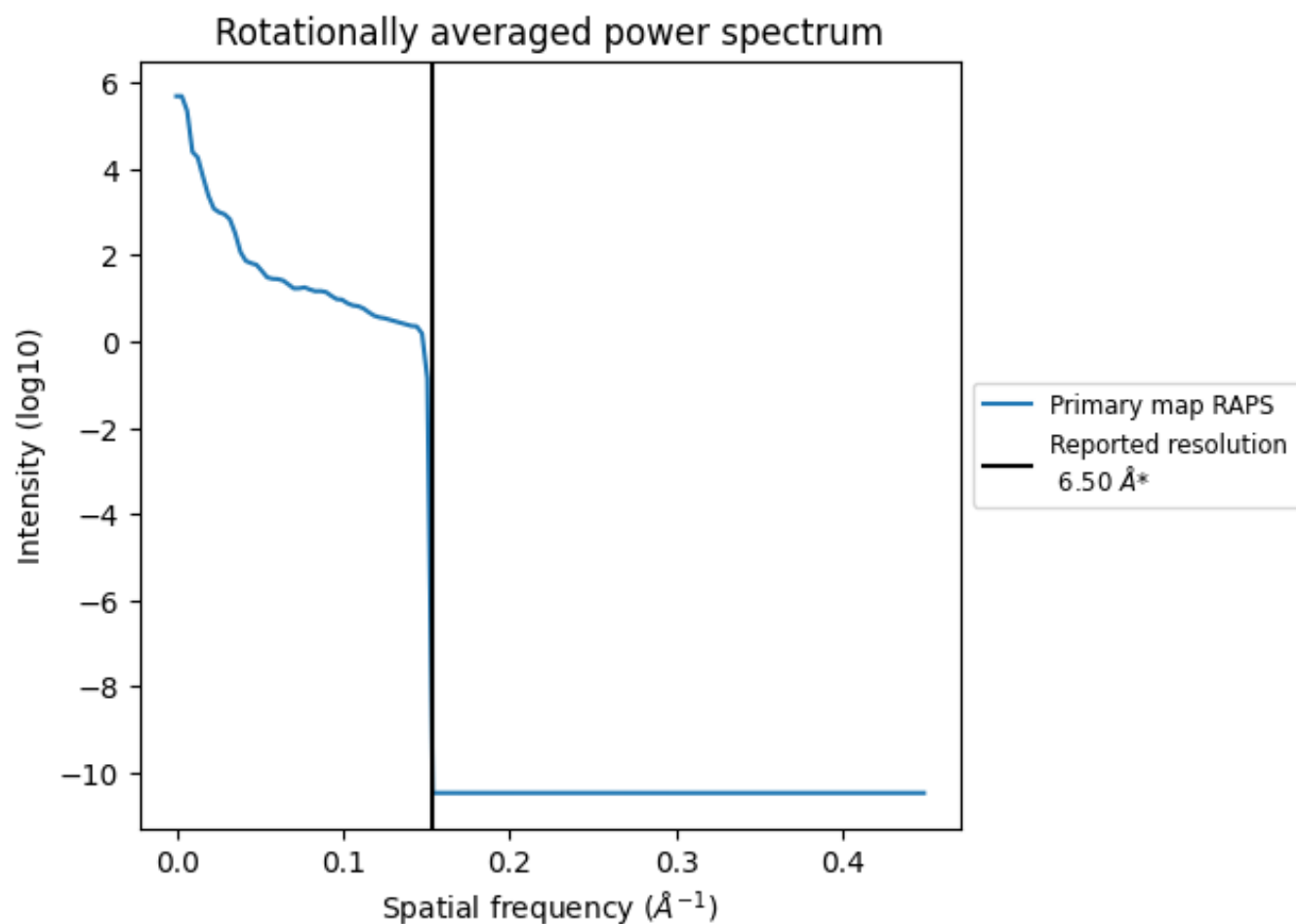
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 134 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 0.154 \AA^{-1}

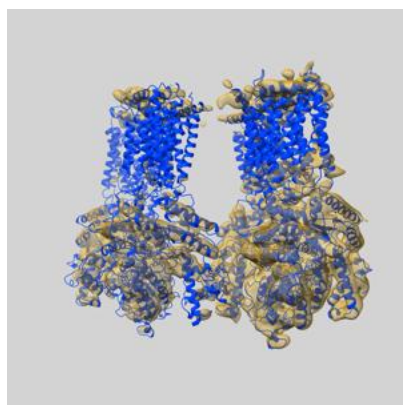
8 Fourier-Shell correlation

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

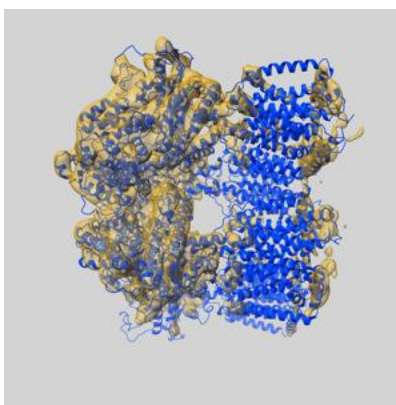
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0358 and PDB model 6N7K. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

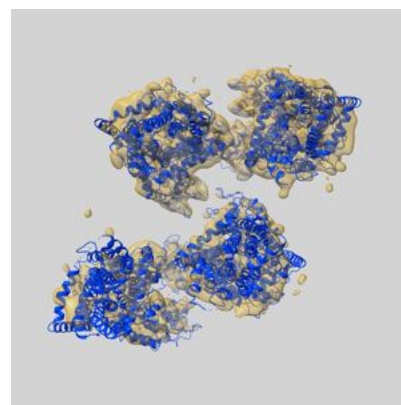
9.1 Map-model overlay [i](#)



X



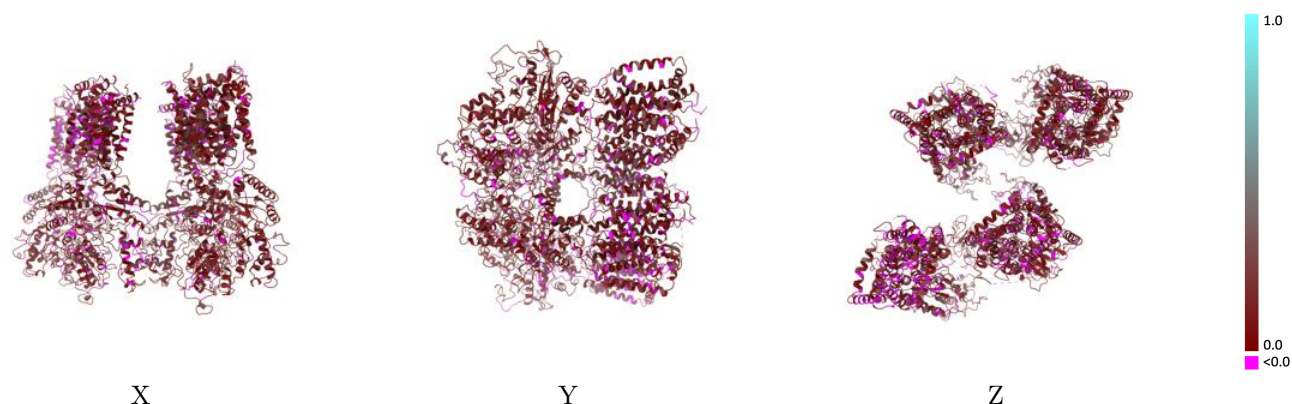
Y



Z

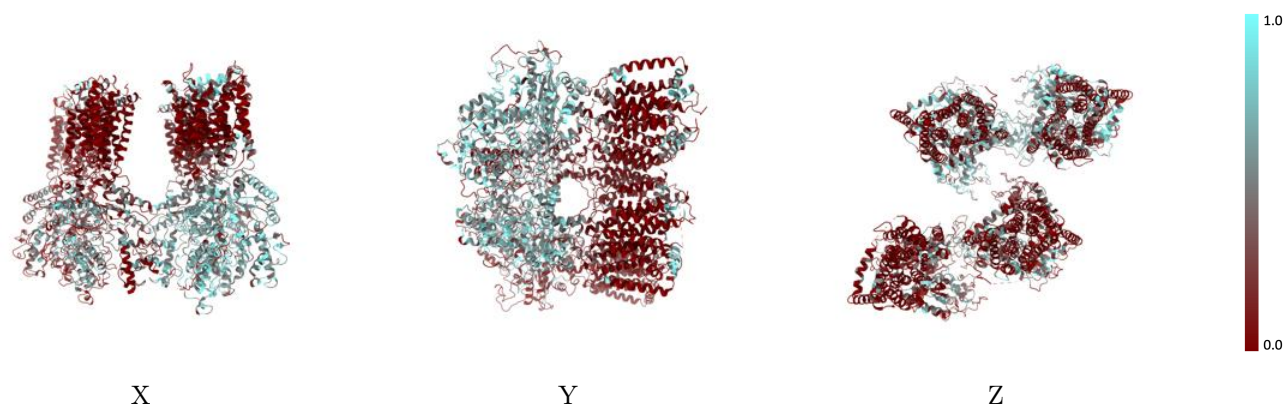
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



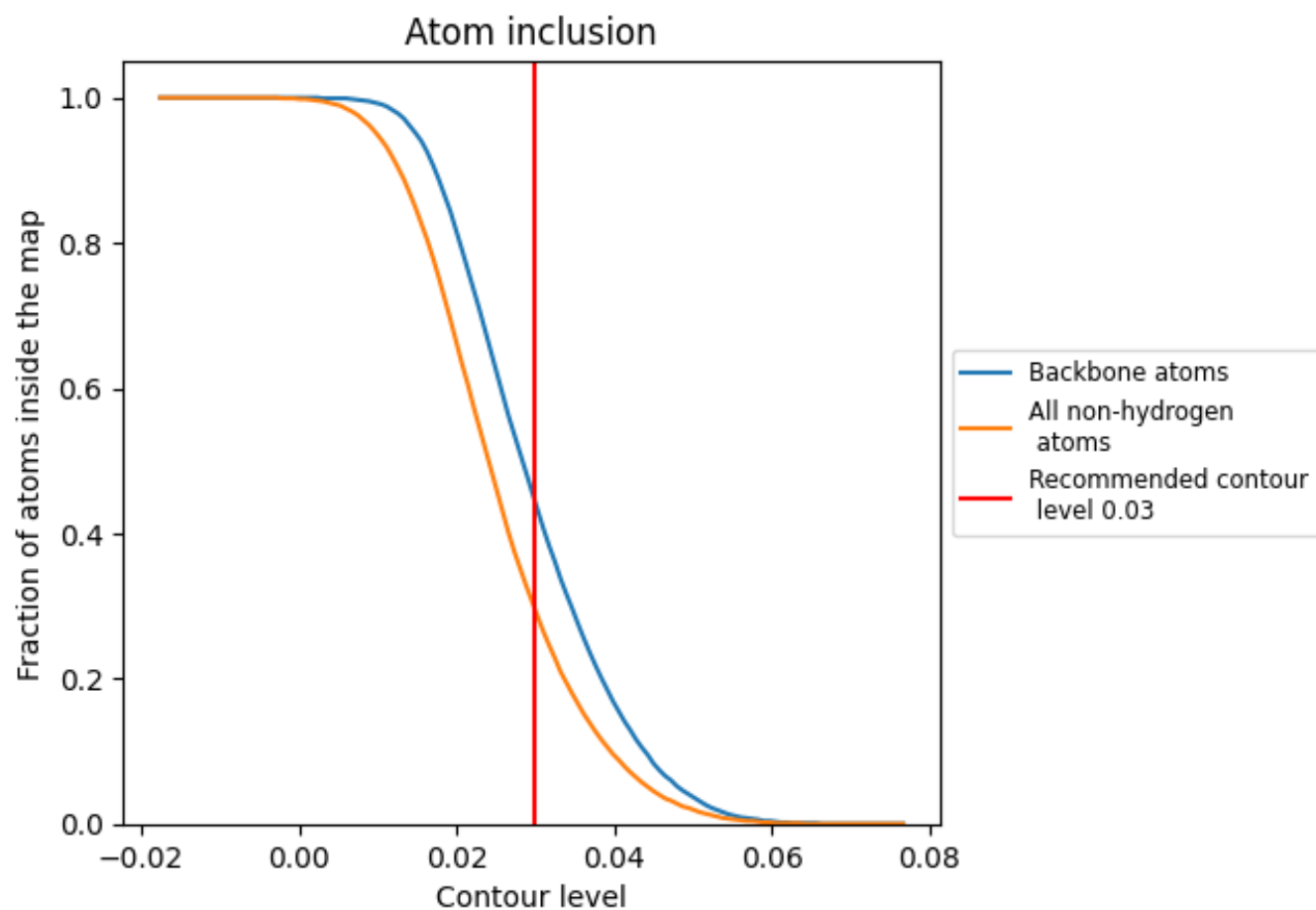
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 29% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2930	<div></div> 0.1320
A	<div></div> 0.3890	<div></div> 0.1540
B	<div></div> 0.3820	<div></div> 0.1470
C	<div></div> 0.5960	<div></div> 0.1560
D	<div></div> 0.1440	<div></div> 0.1000
E	<div></div> 0.2040	<div></div> 0.1230
F	<div></div> 0.3200	<div></div> 0.1380
G	<div></div> 0.0000	<div></div> 0.1940
H	<div></div> 0.0000	<div></div> 0.2760
I	<div></div> 0.0000	<div></div> 0.1120
J	<div></div> 0.0000	<div></div> 0.0750

1.0
0.0
<0.0