



wwPDB EM Validation Summary Report i

Nov 6, 2022 – 04:18 PM EST

PDB ID : 6N7K
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 i 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](#) ①) were used in the production of this report:

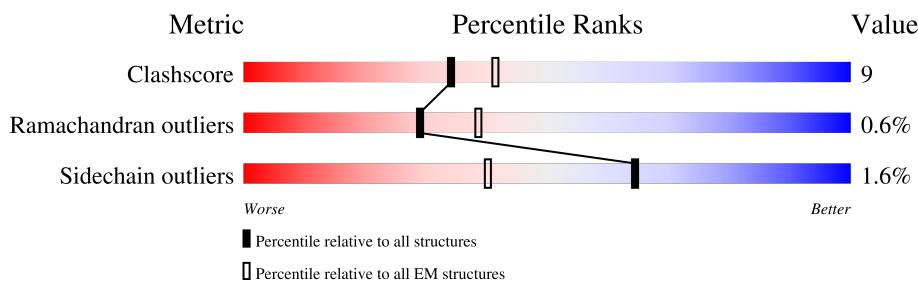
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

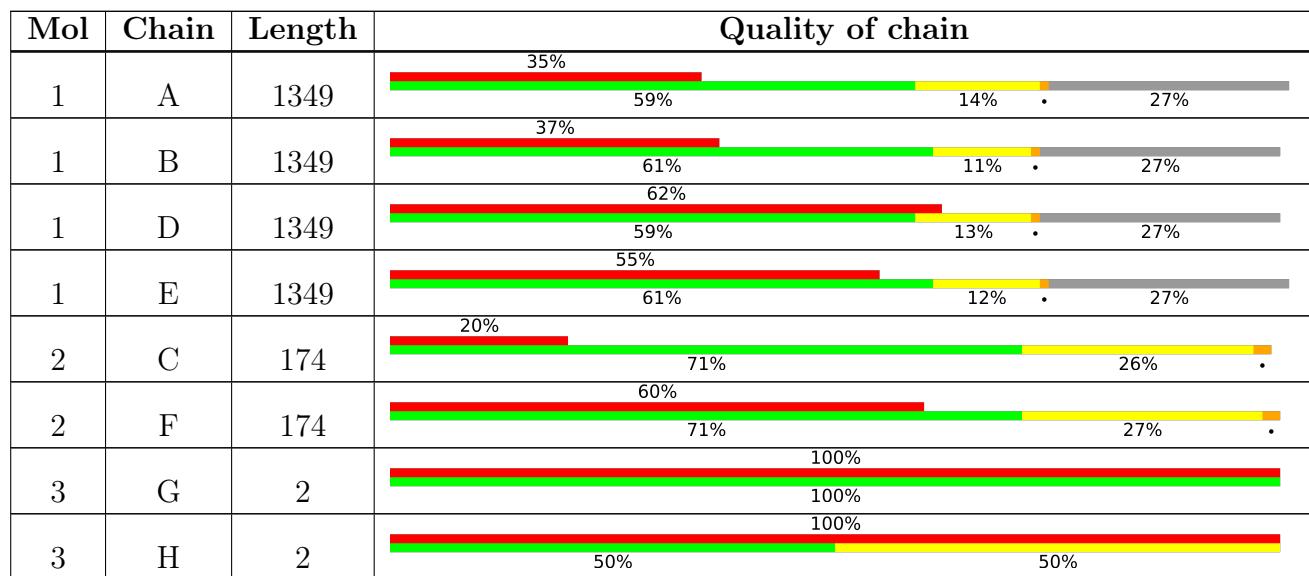
The reported resolution of this entry is 6.50 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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.



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Mol	Chain	Length	Quality of chain		
			100%	100%	100%
3	I	2			
3	J	2	50%		50%

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 7807	N 5091	O 1282	S 1392	42	0
1	B	988	Total	C 7708	N 5029	O 1267	S 1372	40	0
1	D	991	Total	C 7807	N 5091	O 1282	S 1392	42	0
1	E	988	Total	C 7708	N 5029	O 1267	S 1372	40	0

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		

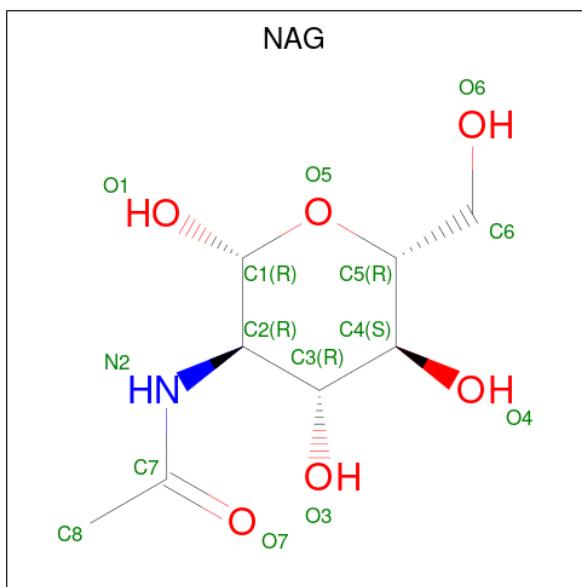
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	174	Total	C	N	O	S	0	0
			1371	853	253	259	6		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aacetamido-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 (three-letter code: NAG) (formula: C₈H₁₅NO₆).



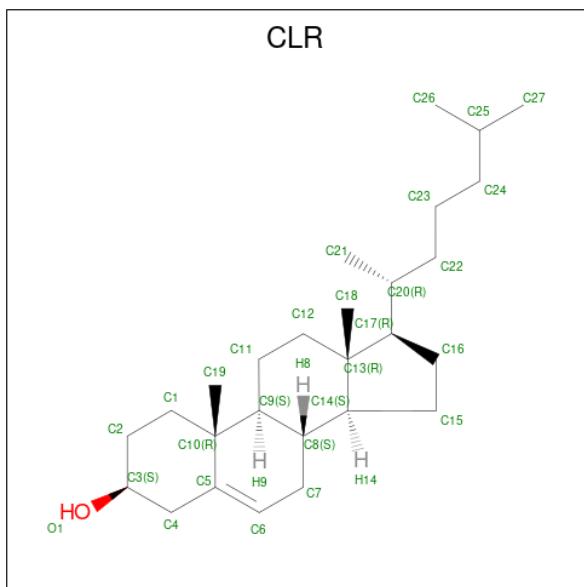
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	
4	A	1	Total	C	N	O	0
			70	40	5	25	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			70	40	5	25	
4	B	1	Total	C	N	O	0
			70	40	5	25	
4	B	1	Total	C	N	O	0
			70	40	5	25	
4	B	1	Total	C	N	O	0
			70	40	5	25	
4	B	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	E	1	Total	C	N	O	0
			70	40	5	25	
4	E	1	Total	C	N	O	0
			70	40	5	25	
4	E	1	Total	C	N	O	0
			70	40	5	25	
4	E	1	Total	C	N	O	0
			70	40	5	25	
4	E	1	Total	C	N	O	0
			70	40	5	25	

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			84	81	3	
5	A	1	Total	C	O	0
			84	81	3	
5	A	1	Total	C	O	0
			84	81	3	
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
			84	81	3	
5	D	1	Total	C	O	0
			84	81	3	
5	D	1	Total	C	O	0
			84	81	3	
5	E	1	Total	C	O	0
			28	27	1	
5	F	1	Total	C	O	0
			28	27	1	

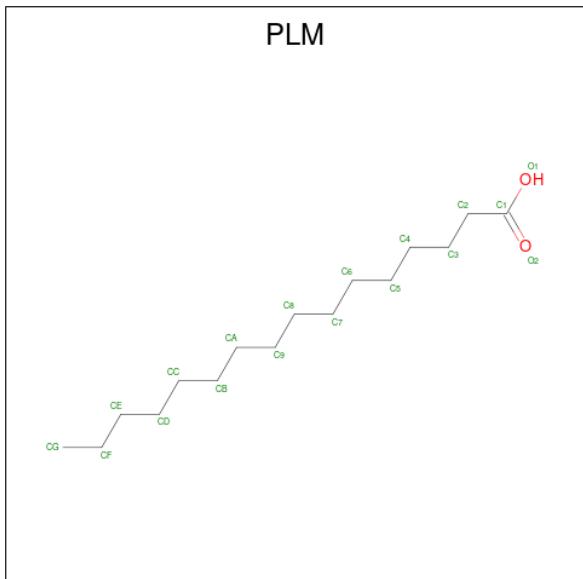
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: 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 (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

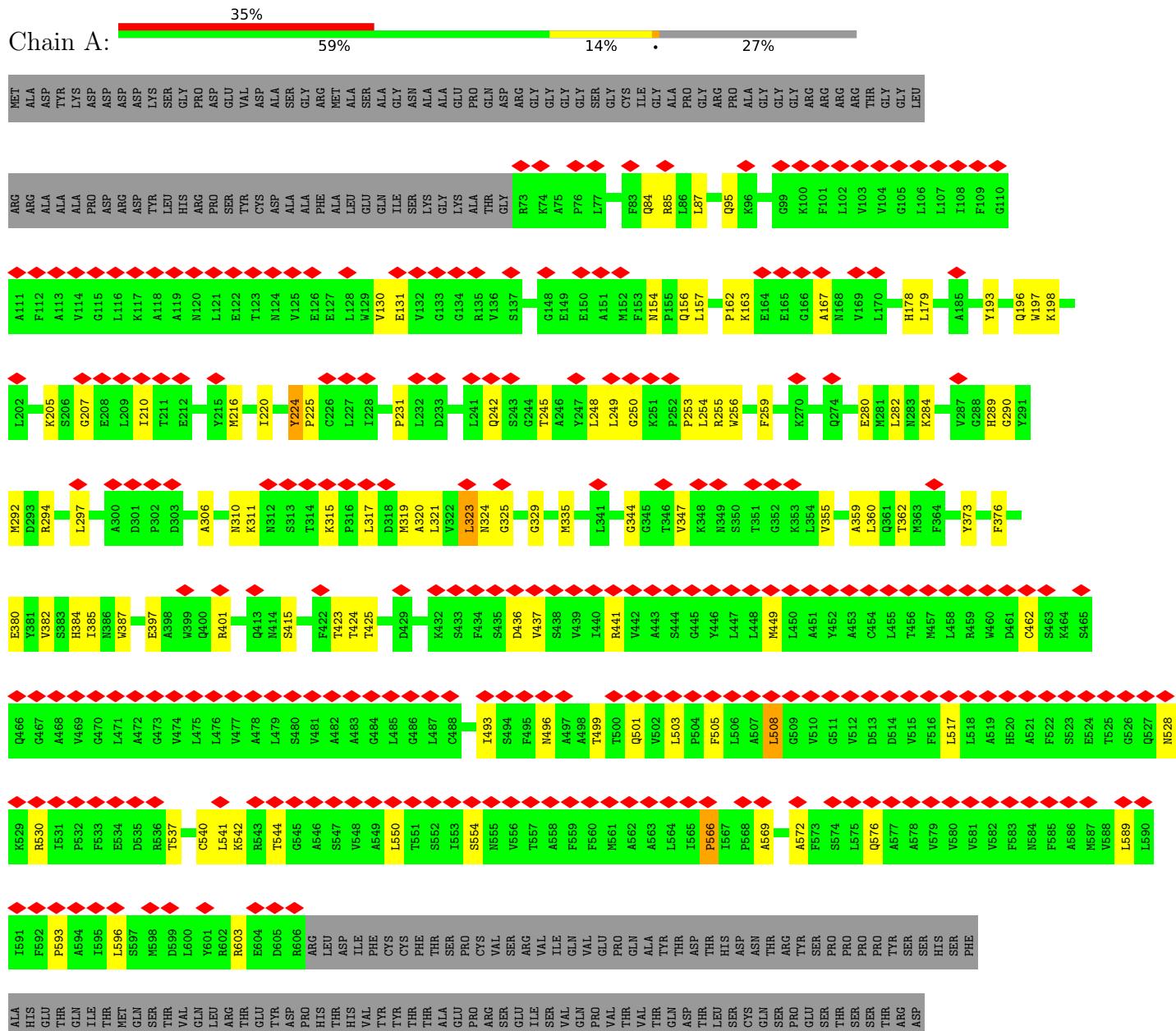


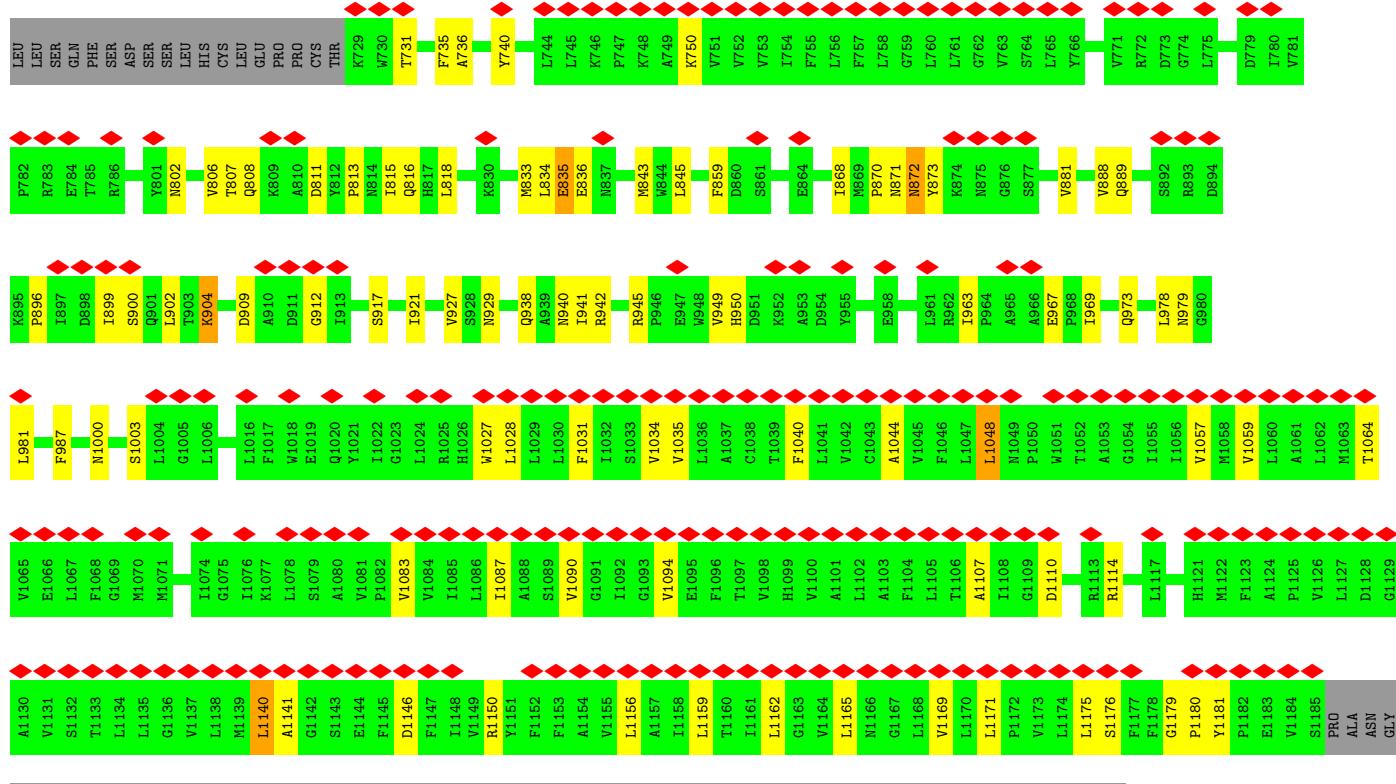
Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total 17	C 16	O 1	0
8	F	1	Total 17	C 16	O 1	0

3 Residue-property plots ⓘ

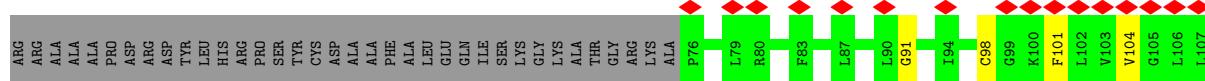
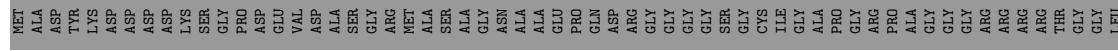
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

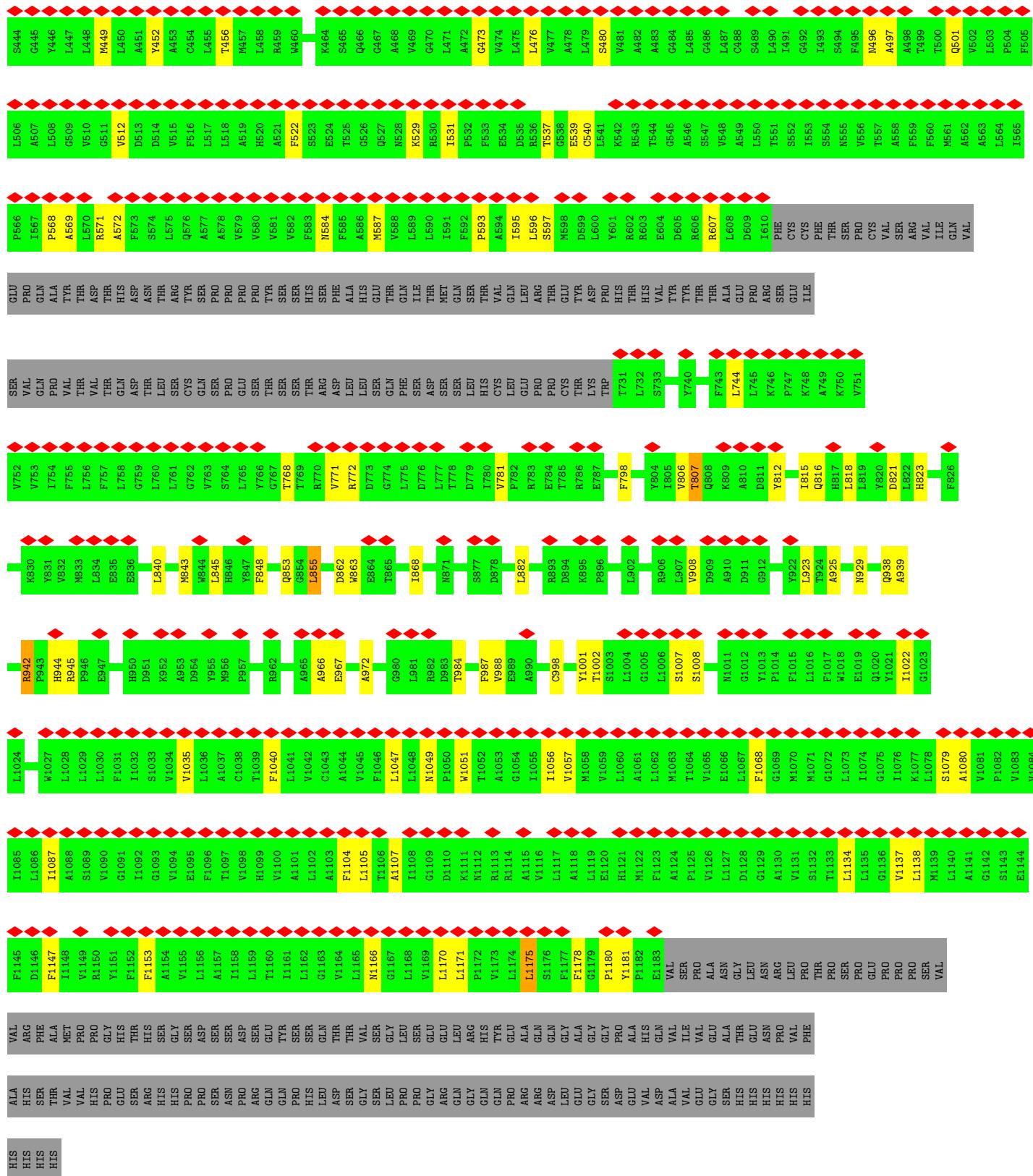
- Molecule 1: Protein patched homolog 1





- Molecule 1: Protein patched homolog 1

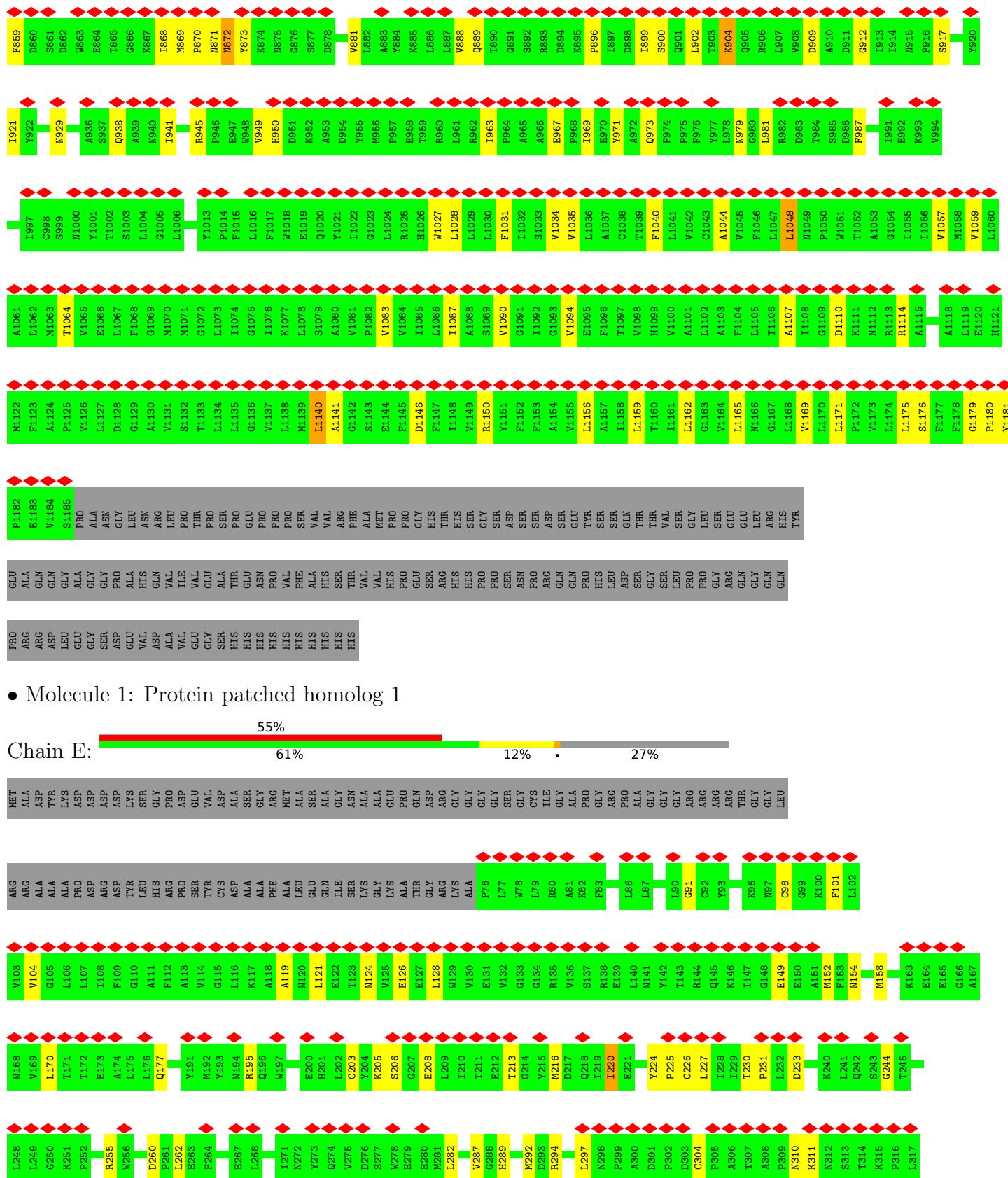




- Molecule 1: Protein patched homolog 1



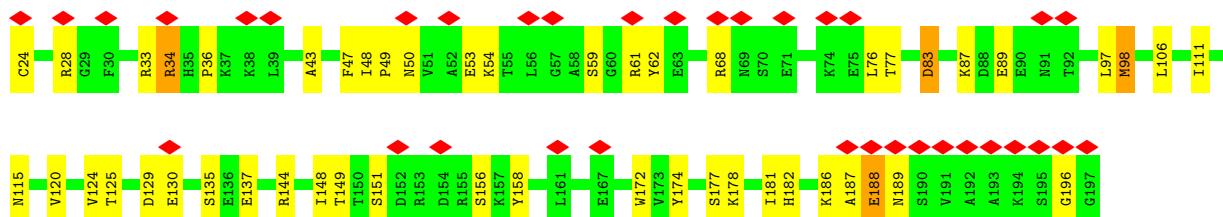
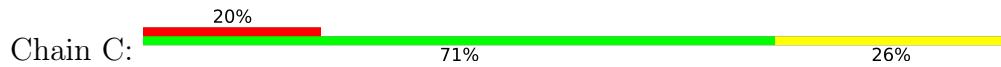
LEU	E604	T544	G484	D233	V104	ARG
GLU	GS45	A357	P295	C234	N168	ARG
PRO	D605	T424	H358	F235	I105	ALA
PRO	R606	K729	A546	T426	V169	ASP
CYS	T731	ILE	A549	L427	L106	TYR
THR	Y740	PHE	L550	L428	L107	LYS
TYR	K741	CYS	T551	D429	T171	ASP
ASP	A742	VAL	S552	N296	T108	ASP
ASP	K743	TYR	S553	P299	F109	ARG
THR	T744	THR	S554	F300	E173	ASP
PRO	A745	GLN	T555	A300	G110	ASP
THR	A746	ALA	F495	D301	A174	TYR
ALA	A747	CYS	S496	F304	A111	LYS
ALA	A748	VAL	S556	P305	T174	SER
GLU	A749	TYR	K492	P302	F112	GLY
PRO	K750	TYR	A493	P303	F113	ALA
SER	S557	VAL	S494	S243	F114	ASP
PRO	T751	VAL	S495	P305	G115	GLU
THR	A752	TYR	S496	C244	H178	VAL
ALA	A753	VAL	A306	C245	L179	VAL
GLU	A754	PRO	A307	A246	L116	ASP
VAL	H759	ARG	H371	A247	F117	ASP
VAL	Y740	VAL	H372	A248	L177	ALA
VAL	K741	ILE	S438	A249	S177	ALA
VAL	K742	SER	S439	A250	A118	GLY
VAL	F743	VAL	S440	A251	A119	ARG
VAL	L744	GLN	A441	M92	M120	TYR
VAL	L745	PRO	V442	M93	N120	LYS
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VAL	P747	THR	S443	P252	E122	ALA
VAL	K748	ASP	V378	P253	S187	SER
VAL	A749	GLN	Y379	R187	A182	PHE
VAL	K750	ASP	E374	N310	A119	ALA
VAL	L751	VAL	H375	L249	M120	ALA
VAL	L752	SER	H376	N310	N120	ALA
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VAL	L754	GLN	V502	G250	L121	SER
VAL	K755	PRO	A562	H377	G117	GLU
VAL	A756	GLN	A563	S313	S186	GLN
VAL	L757	VAL	A564	S314	T123	ALA
VAL	K758	TYR	A565	P309	T123	GLY
VAL	A759	ASP	F505	P309	T124	ALA
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VAL	L761	ASP	P506	P310	T125	ALA
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VAL	L772	VAL	A575	P310	T125	ALA
VAL	K773	ASP	A576	P310	T125	ALA
VAL	A774	VAL	A577	P310	T125	ALA
VAL	K775	SER	A578	P310	T125	ALA
VAL	L776	ASP	A579	P310	T125	ALA
VAL	F777	THR	A580	P310	T125	ALA
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VAL	K779	SER	A582	P310	T125	ALA
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VAL	L782	ALA	A585	P310	T125	ALA
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VAL	A784	ASP	A587	P310	T125	ALA
VAL	K785	THR	A588	P310	T125	ALA
VAL	L786	SER	A589	P310	T125	ALA
VAL	K787	ASP	A590	P310	T125	ALA
VAL	A788	ILE	A591	P310	T125	ALA
VAL	K789	ASP	A592	P310	T125	ALA
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VAL	K791	ASP	A594	P310	T125	ALA
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VAL	A796	ASP	A599	P310	T125	ALA
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VAL	A800	ILE	A603	P310	T125	ALA
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VAL	A812	ILE	A615	P310	T125	ALA
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VAL	A888	ILE	A691	P310	T125	ALA
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VAL	A890	VAL	A693	P310	T125	ALA
VAL	K891	ASP	A694	P310	T125	ALA
VAL	A892	ILE	A695	P310	T125	ALA
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VAL	K915	ASP	A718	P310	T125	ALA
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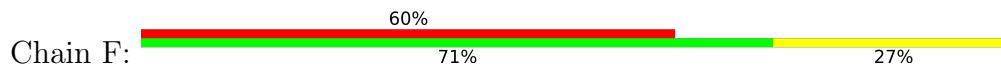
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THR	V773	W401	Q402	R403	D320	M321	A322	L325	G469	Q529	M569	H470	M530	K531	B532	G472	I533	H411	F476	G475	H328	C329	H330	G331	L332	H412	F477	G476	H338	C339	H339	G340	L341
ARG	V774	W402	Q403	R404	D321	M322	A323	L326	G470	Q530	M570	H471	M531	K532	B533	G473	I534	H412	F477	G476	H329	C330	H331	G332	L333	H413	F478	G477	H340	C341	H342	G343	L344
PHE	V775	W403	Q404	R405	D322	M323	A324	L327	G471	Q531	M571	H472	M532	K533	B534	G474	I535	H413	F478	G477	H330	C331	H332	G333	L334	H414	F479	G478	H341	C342	H343	G344	L345
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LEU	V777	W405	Q406	R407	D324	M325	A326	L329	G473	Q533	M573	H474	M534	K535	B536	G476	I537	H415	F479	G478	H332	C333	H334	G335	L335	H416	F481	G480	H343	C344	H345	G346	L347
VAL	V778	W406	Q407	R408	D325	M326	A327	L330	G474	Q534	M574	H475	M535	K536	B537	G477	I538	H416	F479	G478	H333	C334	H335	G336	L336	H417	F482	G481	H344	C345	H346	G347	L348
ILEU	V779	W407	Q408	R409	D326	M327	A328	L331	G475	Q535	M575	H476	M536	K537	B538	G478	I539	H417	F479	G478	H334	C335	H336	G337	L337	H418	F483	G482	H345	C346	H347	G348	L349
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LEU	V786	W414	Q415	R416	D333	M334	A335	L338	G482	Q542	M582	H483	M543	K544	B543	G479	I544	H425	F480	G479	H341	C342	H343	G343	L343	H426	F490	G489	H353	C354	H355	G356	L357
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LEU	V801	W429	Q430	R431	D348	M349	A350	L353	G497	Q557	M597	H498	M558	K559	B558	G479	I559	H440	F480	G479	H356	C357	H358	G358	L358	H441	F499	G498	H371	C372	H372	G372	L372
LEU	V802	W430	Q431	R432	D349	M350	A351	L354	G498	Q558	M598	H499	M559	K560	B559	G479	I560	H441	F480	G479	H357	C358	H359	G359	L359	H442	F499	G498	H372	C373	H373	G373	L373
LEU	V803	W431	Q432	R433	D350	M351	A352	L355	G499	Q559	M599	H500	M560	K561	B560	G479	I561	H442	F480	G479	H358	C359	H360	G360	L360	H443	F499	G498	H373	C374	H374	G374	L374
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LEU	V807	W435	Q436	R437	D354	M355	A356	L359	G503	Q563	M603	H504	M564	K565	B564	G479	I565	H446	F480	G479	H362	C363	H364	G364	L364	H447	F499	G498	H377	C378	H378	G378	L378
LEU	V808	W436	Q437	R438	D355	M356	A357	L360	G504	Q564	M604	H505	M565	K566	B565	G479	I566	H447	F480	G479	H363	C364	H365	G365	L365	H448	F499	G498	H378	C379	H379	G379	L379
LEU	V809	W437	Q438	R439	D356	M357	A358	L361	G505	Q565	M605	H506	M566	K567	B566	G479	I567	H448	F480	G479	H364	C365	H366	G366	L366	H449	F499	G498	H379	C380	H380	G380	L380
LEU	V810	W438	Q439	R440	D357	M358	A359	L362	G506	Q566	M606	H507	M567	K568	B567	G479	I568	H449	F480	G479	H365	C366	H367	G367	L367	H450	F499	G498	H380	C381	H381	G381	L381
LEU	V811	W439	Q440	R441	D358	M359	A360	L363	G507	Q567	M607	H508	M568	K569	B568	G479	I569	H451	F480	G479	H366	C367	H368	G368	L368	H452	F499	G498	H382	C383	H383	G383	L383
LEU	V812	W440	Q441	R442	D359	M360	A361	L364	G508	Q568	M608	H509	M569	K570	B569	G479	I570	H453	F480	G479	H367	C368	H369	G369	L369	H454	F499	G498	H384	C385	H385	G385	L385
LEU	V813	W441	Q442	R443	D360	M361	A362	L365	G509	Q569	M609	H510	M570	K571	B570	G479	I571	H455	F480	G479	H368	C369	H369	G369	L369								

HIS

- 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 (i)

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 (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/8000	0.71	6/10883 (0.1%)
1	B	0.48	0/7897	0.70	5/10749 (0.0%)
1	D	0.45	0/8000	0.71	6/10883 (0.1%)
1	E	0.48	0/7897	0.70	5/10749 (0.0%)
2	C	0.56	1/1401 (0.1%)	0.76	3/1886 (0.2%)
2	F	0.56	1/1401 (0.1%)	0.76	4/1886 (0.2%)
All	All	0.47	2/34596 (0.0%)	0.71	29/47036 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	98	MET	C-N	8.19	1.52	1.34
2	F	98	MET	C-N	8.16	1.52	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	83	ASP	O-C-N	-7.34	110.96	122.70
2	C	83	ASP	O-C-N	-7.33	110.97	122.70
1	B	297	LEU	CA-CB-CG	7.03	131.48	115.30
1	E	297	LEU	CA-CB-CG	6.99	131.39	115.30
1	A	323	LEU	CA-CB-CG	6.33	129.86	115.30

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7807	0	7828	111	0
1	B	7708	0	7664	120	0
1	D	7807	0	7828	110	0
1	E	7708	0	7664	123	0
2	C	1371	0	1329	37	0
2	F	1371	0	1329	35	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	615	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 615 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%)	22 63
1	B	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	41 76
1	D	987/1349 (73%)	858 (87%)	122 (12%)	7 (1%)	22 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	41 76
2	C	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	13 50
2	F	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	13 50
All	All	4286/5744 (75%)	3733 (87%)	529 (12%)	24 (1%)	29 66

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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	832/1147 (72%)	820 (99%)	12 (1%)	67 80
1	B	808/1147 (70%)	795 (98%)	13 (2%)	62 79
1	D	832/1147 (72%)	820 (99%)	12 (1%)	67 80
1	E	808/1147 (70%)	795 (98%)	13 (2%)	62 79
2	C	142/144 (99%)	138 (97%)	4 (3%)	43 65
2	F	142/144 (99%)	138 (97%)	4 (3%)	43 65
All	All	3564/4876 (73%)	3506 (98%)	58 (2%)	64 79

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	188	GLU
2	F	50	ASN
1	D	550	LEU
2	F	34	ARG

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Mol	Chain	Res	Type
1	E	584	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	496	ASN
1	E	156	GLN
2	F	107	ASN
1	D	576	GLN
1	D	929	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

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	3,1	14,14,15	0.24	0	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	H	1	3,1	14,14,15	0.43	0	17,19,21	0.66	0
3	NAG	H	2	3	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.25	0	17,19,21	0.57	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	J	1	3,1	14,14,15	0.43	0	17,19,21	0.65	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	0.25	0	17,19,21	0.69	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	3,1	-	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	3,1	-	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	3,1	-	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	3,1	-	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($^{\circ}$)	Ideal($^{\circ}$)
3	H	2	NAG	C1-O5-C5	2.53	115.62	112.19
3	J	2	NAG	C1-O5-C5	2.52	115.60	112.19

There are no chirality outliers.

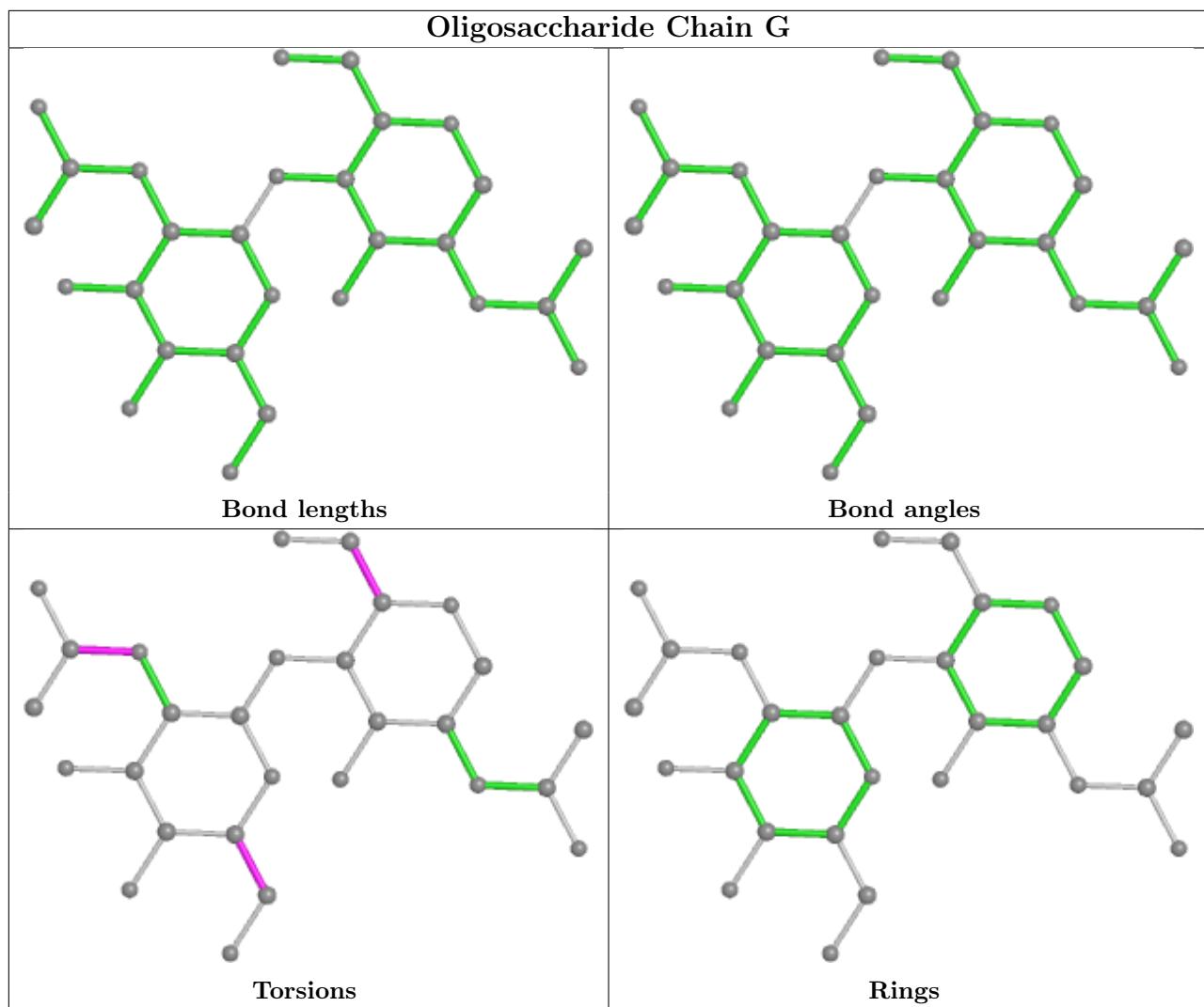
5 of 14 torsion outliers are listed below:

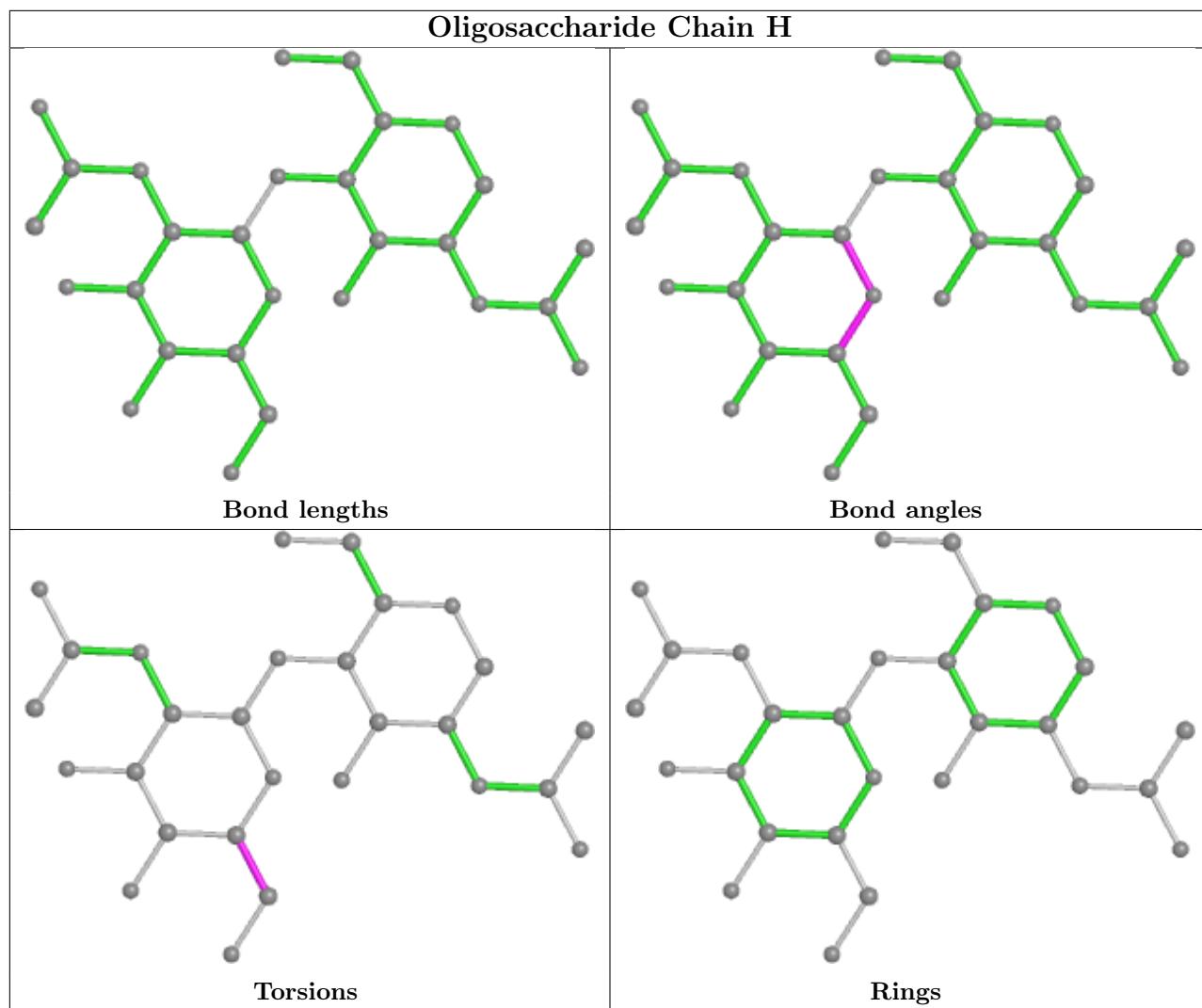
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

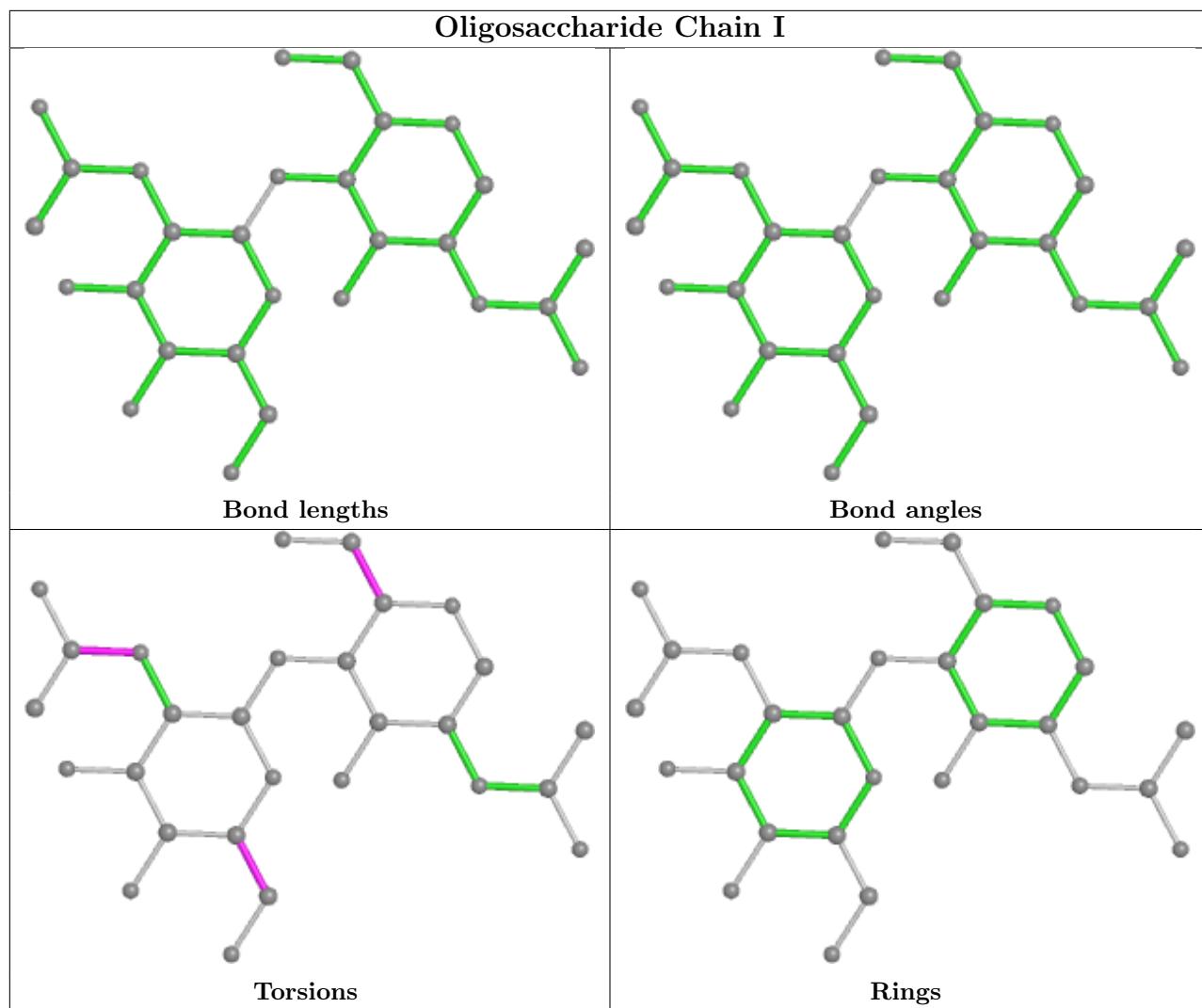
There are no ring outliers.

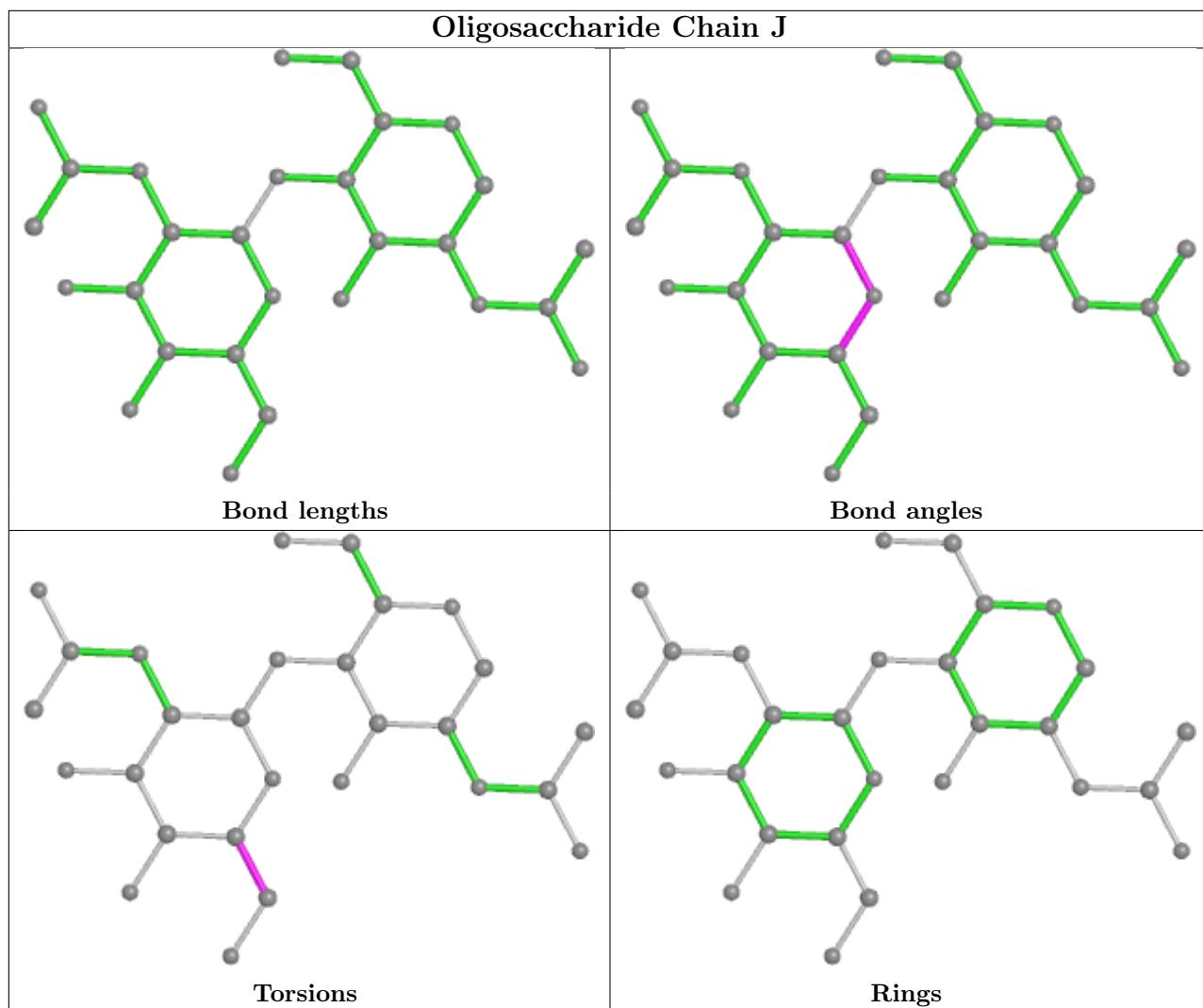
No monomer is involved in short contacts.

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	1807	1	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	A	1801	1	14,14,15	0.82	1 (7%)	17,19,21	2.25	3 (17%)
4	NAG	B	1501	1	14,14,15	0.70	1 (7%)	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1505	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	D	1807	1	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	E	1501	1	14,14,15	0.70	1 (7%)	17,19,21	0.68	0
4	NAG	B	1504	1	14,14,15	0.74	1 (7%)	17,19,21	0.75	1 (5%)
4	NAG	A	1804	1	14,14,15	0.22	0	17,19,21	0.57	0
5	CLR	E	1508	-	31,31,31	0.87	2 (6%)	48,48,48	1.52	9 (18%)
4	NAG	E	1503	1	14,14,15	0.96	1 (7%)	17,19,21	1.34	3 (17%)
4	NAG	A	1802	1	14,14,15	0.23	0	17,19,21	0.55	0
8	PLM	C	205	2	16,16,17	0.35	0	15,15,17	0.74	0
4	NAG	B	1505	1	14,14,15	0.24	0	17,19,21	0.46	0
5	CLR	A	1809	-	31,31,31	0.70	0	48,48,48	1.51	9 (18%)
5	CLR	D	1810	-	31,31,31	0.66	0	48,48,48	1.24	5 (10%)
5	CLR	F	201	2	31,31,31	0.98	1 (3%)	48,48,48	1.91	8 (16%)
5	CLR	D	1809	-	31,31,31	0.70	0	48,48,48	1.51	9 (18%)
4	NAG	D	1803	1	14,14,15	0.81	1 (7%)	17,19,21	1.23	1 (5%)
8	PLM	F	205	2	16,16,17	0.34	0	15,15,17	0.74	0
5	CLR	B	1508	-	31,31,31	0.87	2 (6%)	48,48,48	1.53	9 (18%)
4	NAG	B	1502	1	14,14,15	0.52	0	17,19,21	0.38	0
4	NAG	E	1504	1	14,14,15	0.74	1 (7%)	17,19,21	0.75	1 (5%)
5	CLR	A	1808	-	31,31,31	1.00	2 (6%)	48,48,48	1.61	8 (16%)
4	NAG	D	1802	1	14,14,15	0.24	0	17,19,21	0.55	0
5	CLR	D	1808	-	31,31,31	1.00	2 (6%)	48,48,48	1.61	8 (16%)
5	CLR	C	201	2	31,31,31	0.99	1 (3%)	48,48,48	1.91	8 (16%)
4	NAG	D	1804	1	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	B	1503	1	14,14,15	0.93	1 (7%)	17,19,21	1.34	3 (17%)
5	CLR	A	1810	-	31,31,31	0.65	0	48,48,48	1.24	5 (10%)
4	NAG	E	1502	1	14,14,15	0.50	0	17,19,21	0.38	0
4	NAG	D	1801	1	14,14,15	0.82	1 (7%)	17,19,21	2.25	4 (23%)
4	NAG	A	1803	1	14,14,15	0.82	1 (7%)	17,19,21	1.22	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	1807	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1801	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1505	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1807	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1504	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1804	1	-	1/6/23/26	0/1/1/1
5	CLR	E	1508	-	-	4/10/68/68	0/4/4/4
4	NAG	E	1503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1802	1	-	1/6/23/26	0/1/1/1
8	PLM	C	205	2	-	7/13/14/15	-
4	NAG	B	1505	1	-	4/6/23/26	0/1/1/1
5	CLR	A	1809	-	-	2/10/68/68	0/4/4/4
5	CLR	D	1810	-	-	6/10/68/68	0/4/4/4
5	CLR	F	201	2	-	3/10/68/68	0/4/4/4
5	CLR	D	1809	-	-	2/10/68/68	0/4/4/4
4	NAG	D	1803	1	-	3/6/23/26	0/1/1/1
8	PLM	F	205	2	-	7/13/14/15	-
5	CLR	B	1508	-	-	4/10/68/68	0/4/4/4
4	NAG	B	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1504	1	-	4/6/23/26	0/1/1/1
5	CLR	A	1808	-	-	9/10/68/68	0/4/4/4
4	NAG	D	1802	1	-	1/6/23/26	0/1/1/1
5	CLR	D	1808	-	-	9/10/68/68	0/4/4/4
5	CLR	C	201	2	-	3/10/68/68	0/4/4/4
4	NAG	D	1804	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1503	1	-	2/6/23/26	0/1/1/1
5	CLR	A	1810	-	-	6/10/68/68	0/4/4/4
4	NAG	E	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1801	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1803	1	-	3/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1503	NAG	O5-C1	-2.75	1.39	1.43
4	A	1803	NAG	O5-C1	-2.73	1.39	1.43
4	D	1803	NAG	O5-C1	-2.71	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	CLR	C13-C14	-2.70	1.49	1.55
4	B	1503	NAG	O5-C1	-2.68	1.39	1.43

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	1801	NAG	C2-N2-C7	7.90	134.16	122.90
4	A	1801	NAG	C2-N2-C7	7.89	134.14	122.90
5	F	201	CLR	C13-C17-C20	-5.56	110.77	119.49
5	C	201	CLR	C13-C17-C20	-5.56	110.78	119.49
5	C	201	CLR	C13-C14-C8	-5.36	106.44	114.38

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

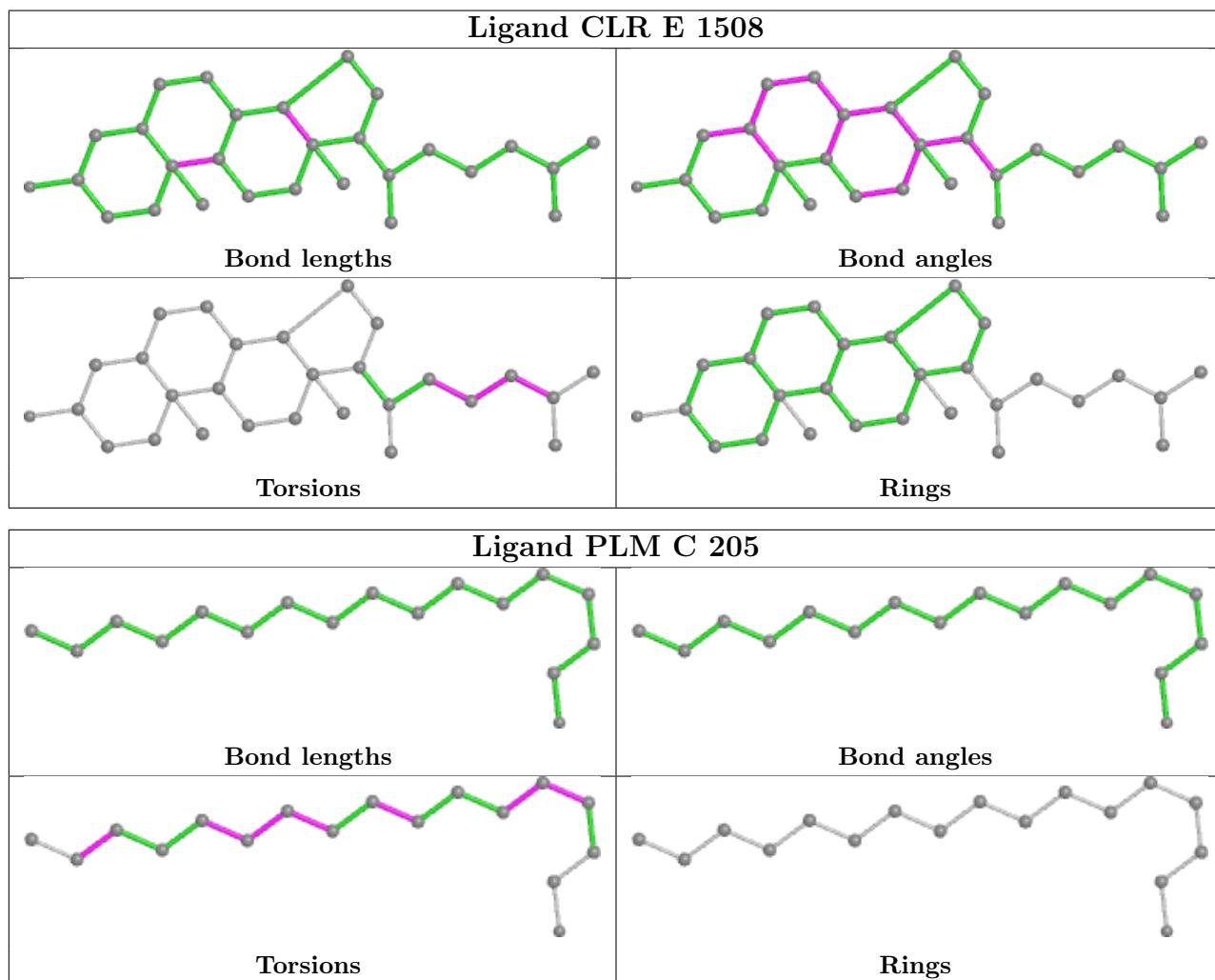
Mol	Chain	Res	Type	Atoms
5	C	201	CLR	C17-C20-C22-C23
5	F	201	CLR	C17-C20-C22-C23
5	A	1810	CLR	C13-C17-C20-C21
5	D	1810	CLR	C13-C17-C20-C21
5	C	201	CLR	C22-C23-C24-C25

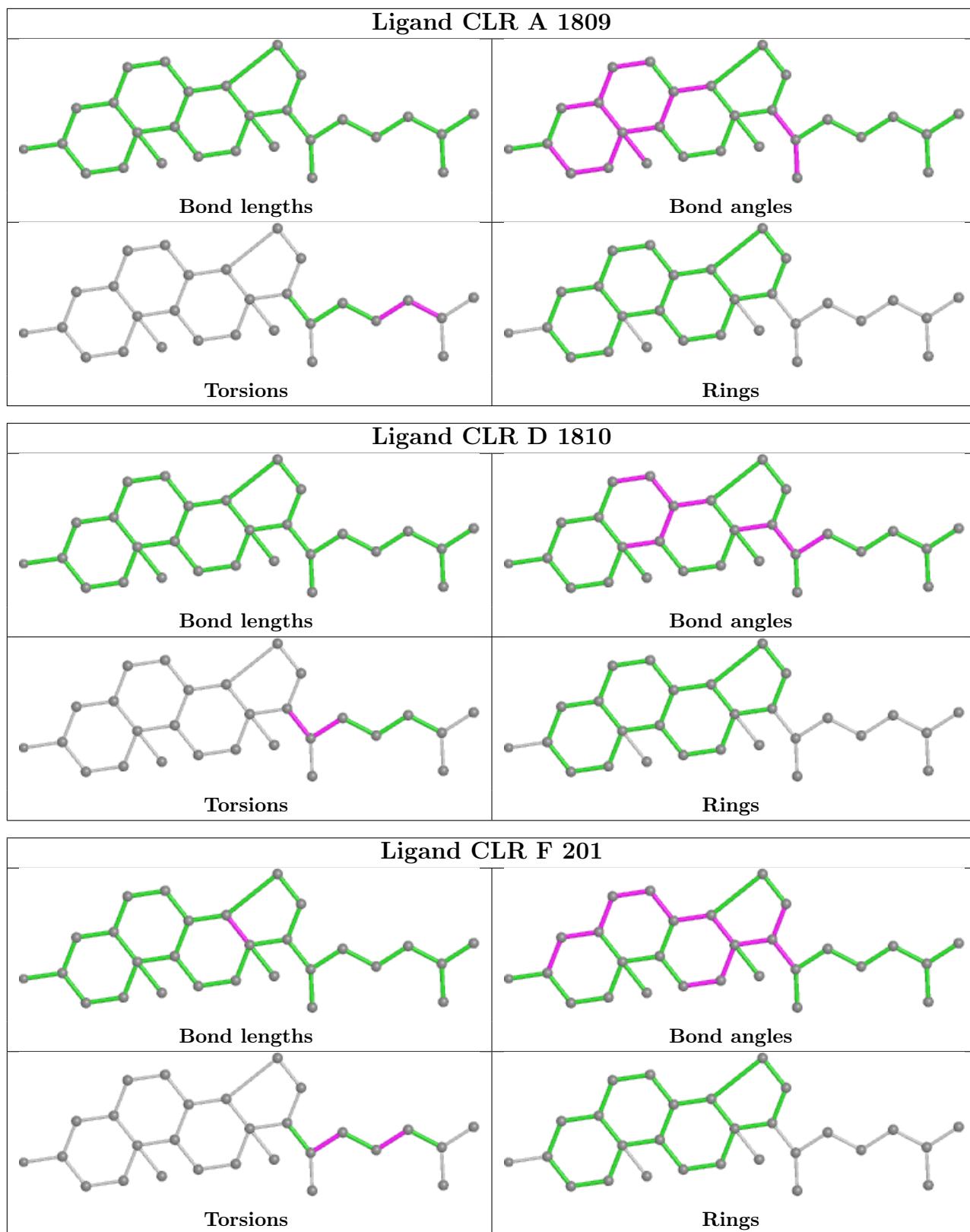
There are no ring outliers.

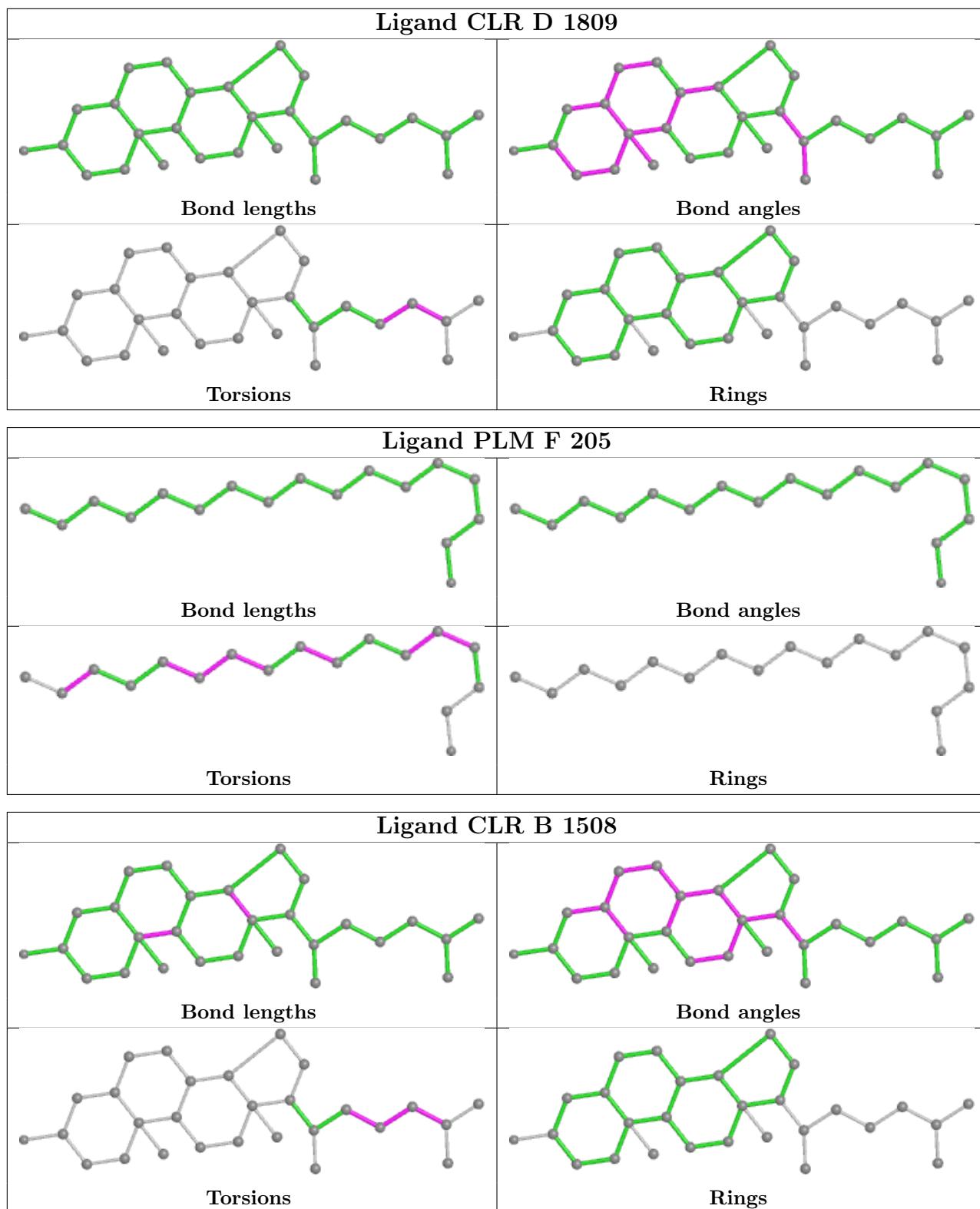
15 monomers are involved in 206 short contacts:

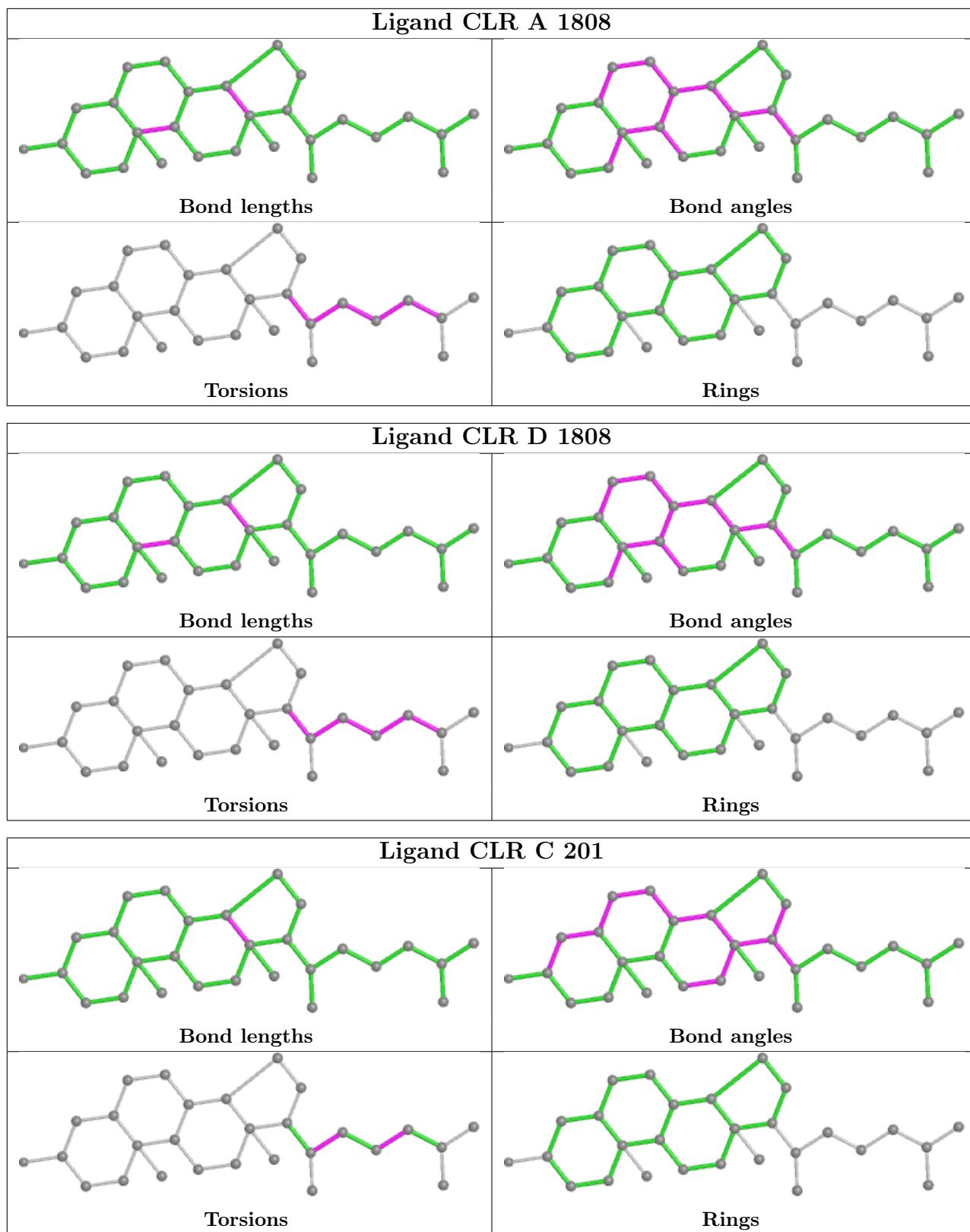
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1501	NAG	1	0
4	E	1501	NAG	1	0
5	E	1508	CLR	33	0
8	C	205	PLM	16	0
5	A	1809	CLR	1	0
5	D	1810	CLR	3	0
5	F	201	CLR	19	0
5	D	1809	CLR	2	0
8	F	205	PLM	16	0
5	B	1508	CLR	30	0
5	A	1808	CLR	31	0
5	D	1808	CLR	30	0
5	C	201	CLR	19	0
4	D	1804	NAG	1	0
5	A	1810	CLR	3	0

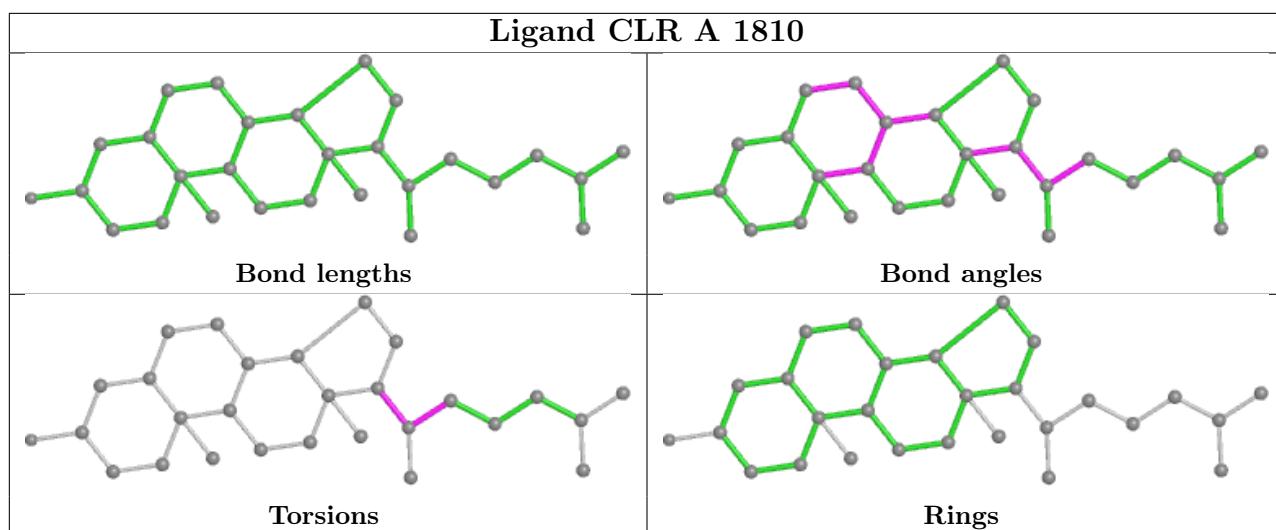
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

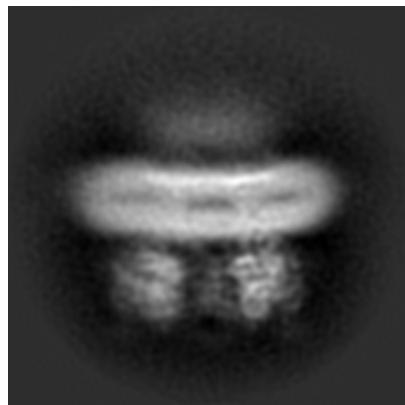
6 Map visualisation (i)

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

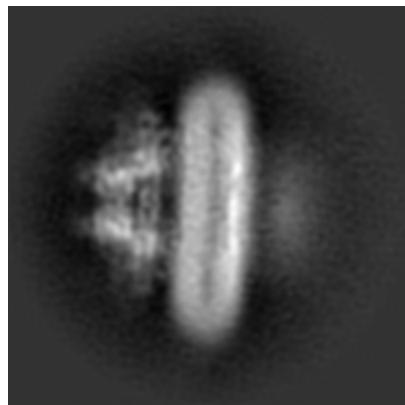
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

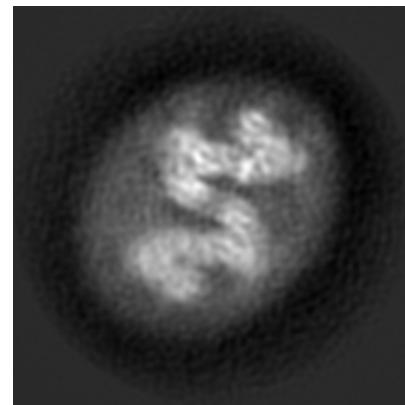
6.1.1 Primary map



X



Y

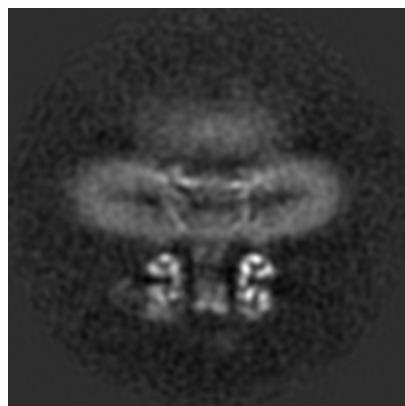


Z

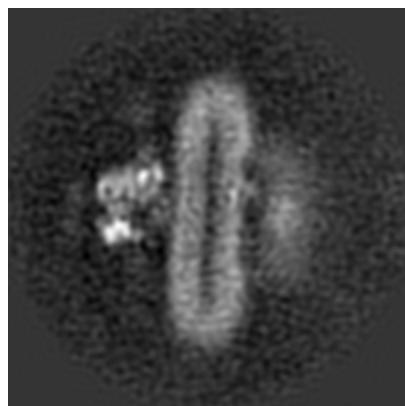
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

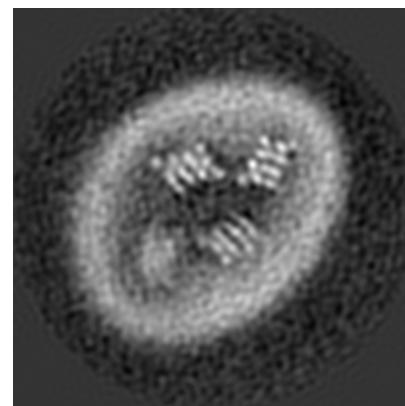
6.2.1 Primary map



X Index: 140



Y Index: 140

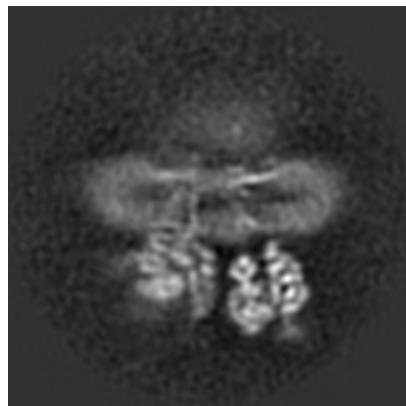


Z Index: 140

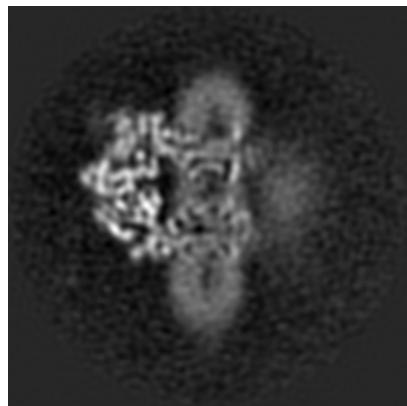
The images above show central slices of the map in three orthogonal directions.

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

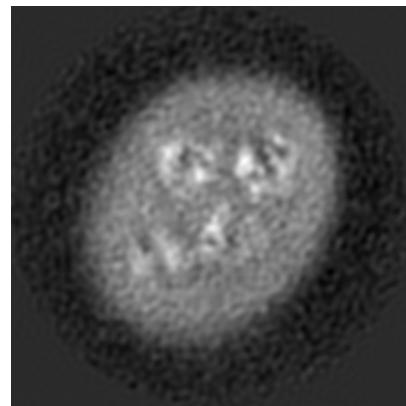
6.3.1 Primary map



X Index: 163



Y Index: 167

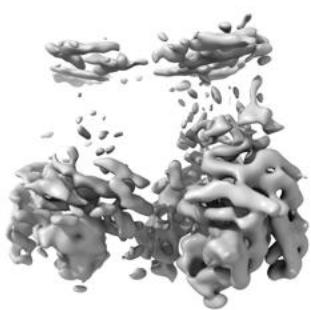


Z Index: 158

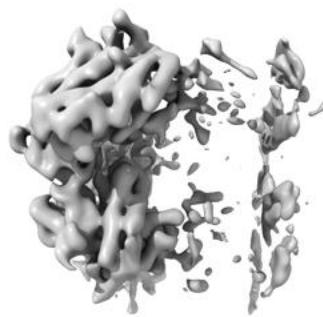
The images above show the largest variance slices of the map in three orthogonal directions.

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

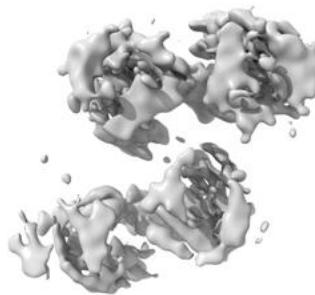
6.4.1 Primary map



X



Y



Z

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

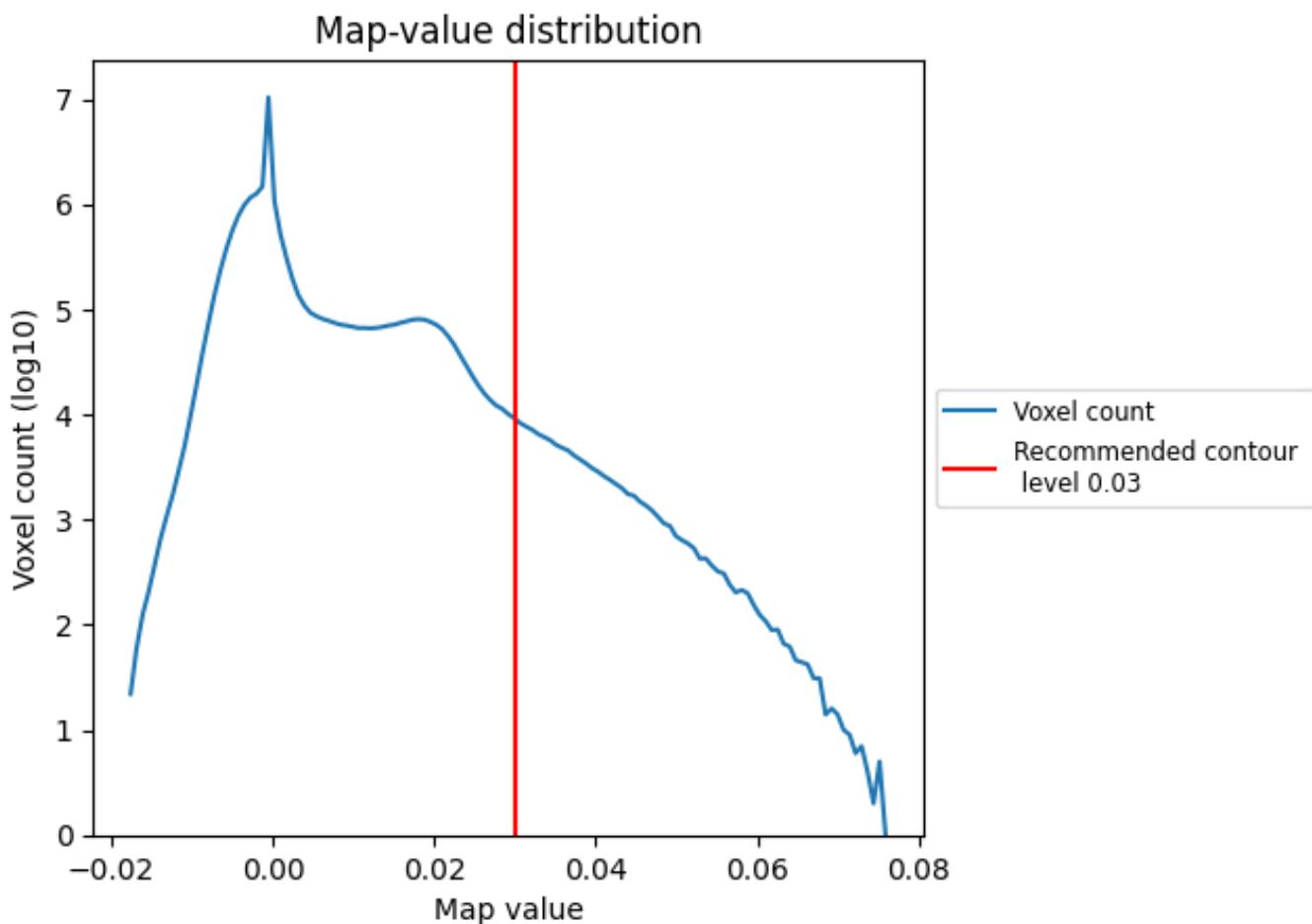
6.5 Mask visualisation

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

7 Map analysis (i)

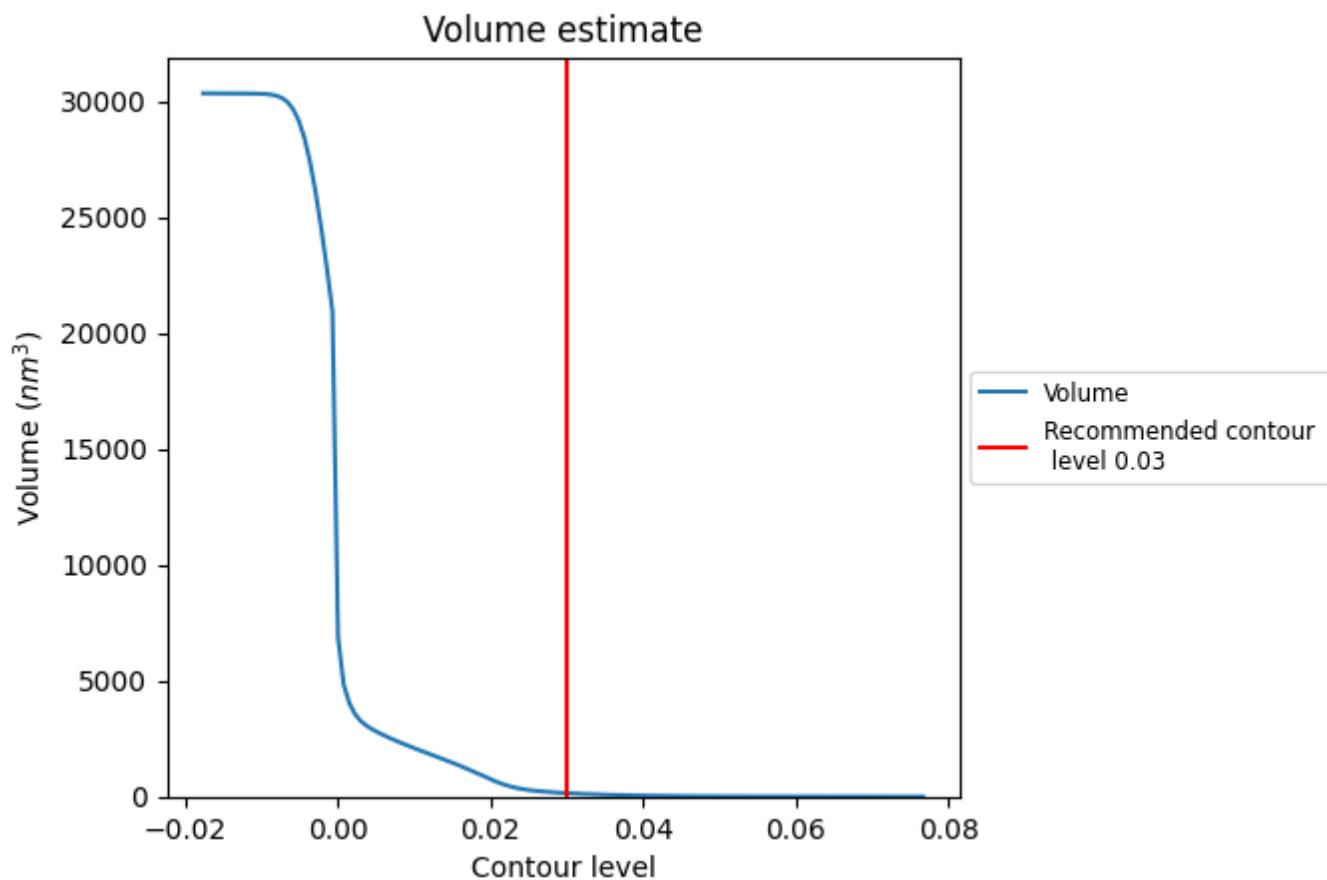
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

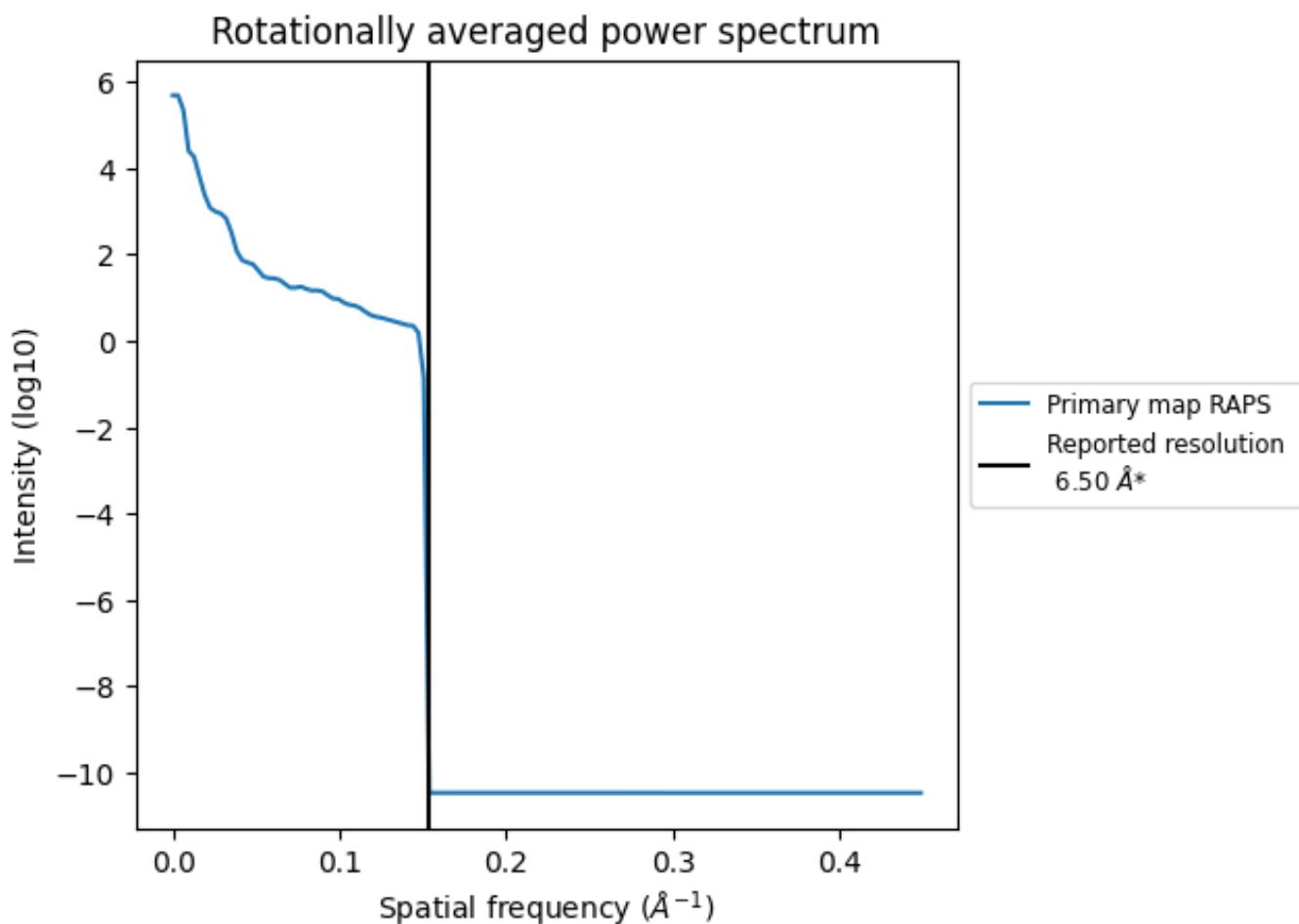
7.2 Volume estimate (i)



The volume at the recommended contour level is 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.154 \AA^{-1}

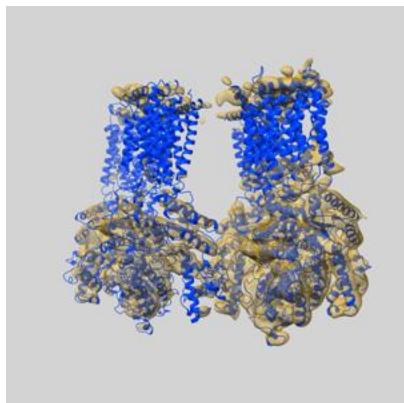
8 Fourier-Shell correlation

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

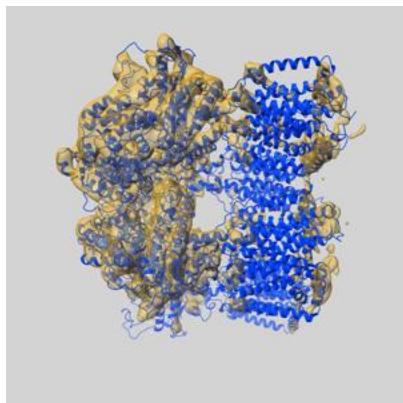
9 Map-model fit (i)

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.

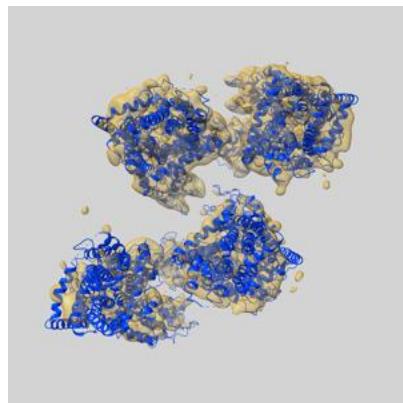
9.1 Map-model overlay (i)



X



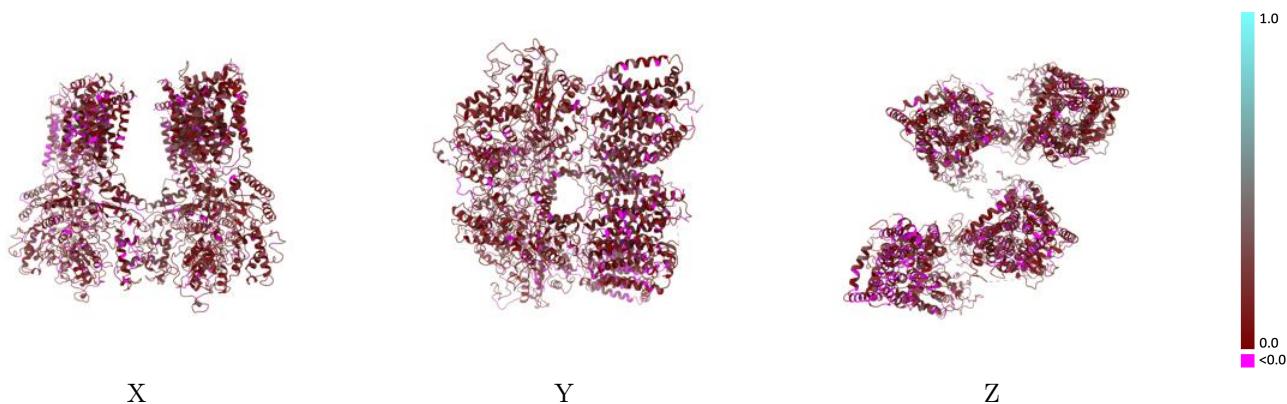
Y



Z

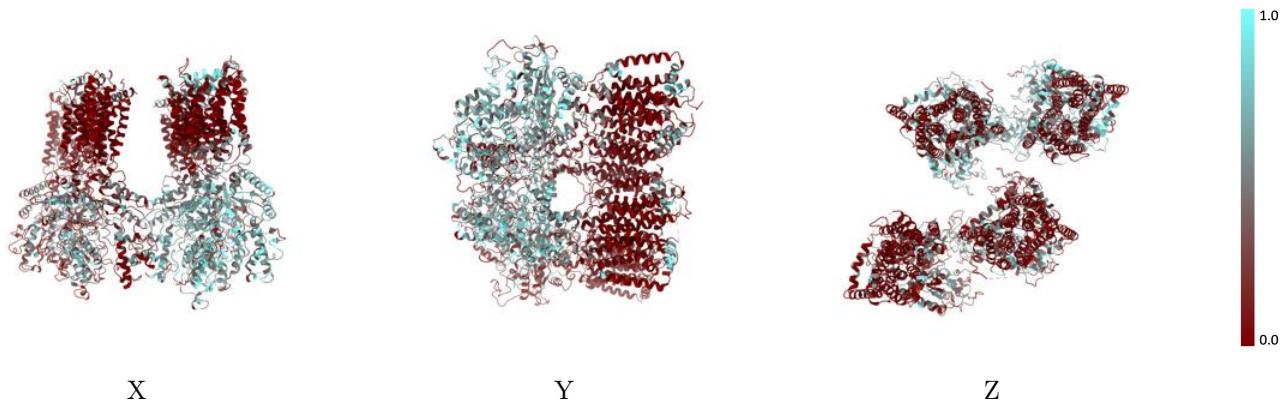
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



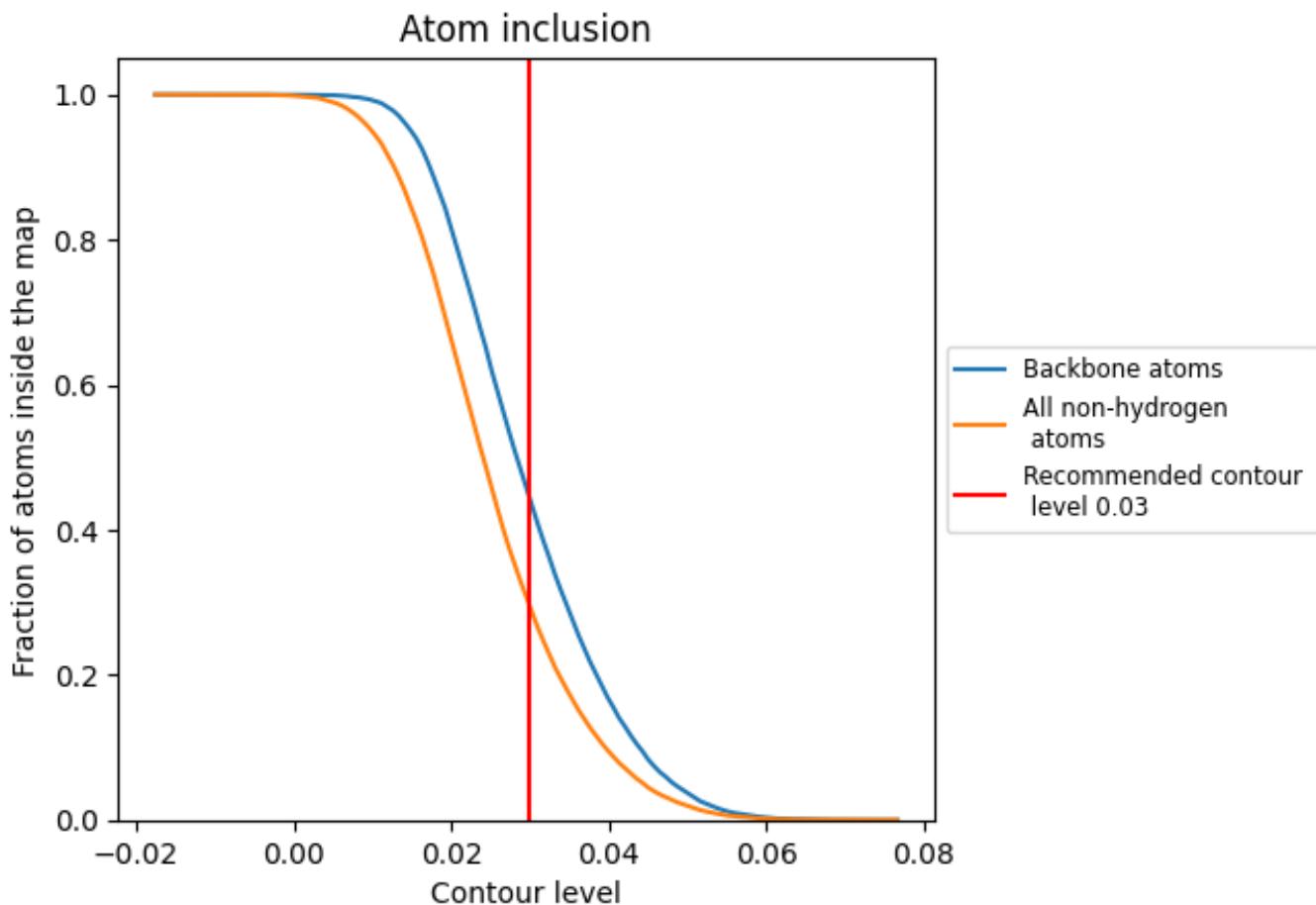
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.2933	0.1320
A	0.3888	0.1540
B	0.3820	0.1470
C	0.5958	0.1560
D	0.1444	0.1000
E	0.2041	0.1230
F	0.3203	0.1380
G	0.0000	0.1940
H	0.0000	0.2760
I	0.0000	0.1120
J	0.0000	0.0750

