



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:56 AM UTC

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

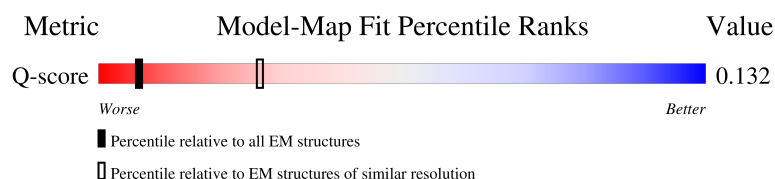
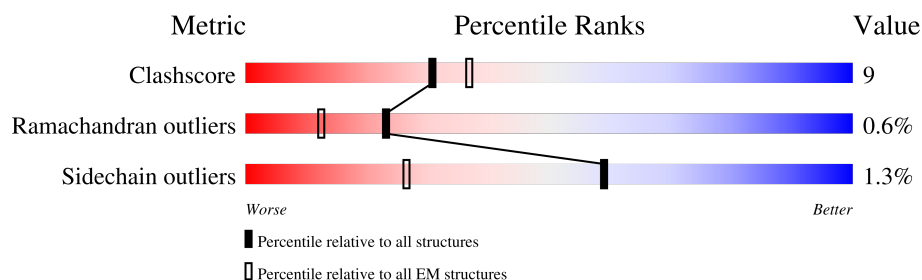
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	556 (6.00 - 7.00)

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	35% 59% 14% 27%
1	B	1349	37% 62% 11% 27%
1	D	1349	62% 60% 13% 27%
1	E	1349	55% 61% 12% 27%

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Mol	Chain	Length	Quality of chain
2	C	174	
2	F	174	
3	G	2	
3	H	2	
3	I	2	
3	J	2	

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.

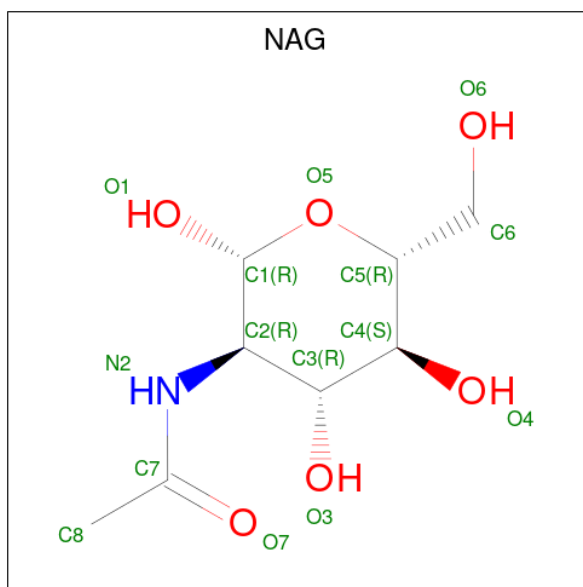
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	174	Total	C	N	O	S	0	0
			1371	853	253	259	6		
2	F	174	Total	C	N	O	S	0	0
			1371	853	253	259	6		

- 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: $C_8H_{15}NO_6$).



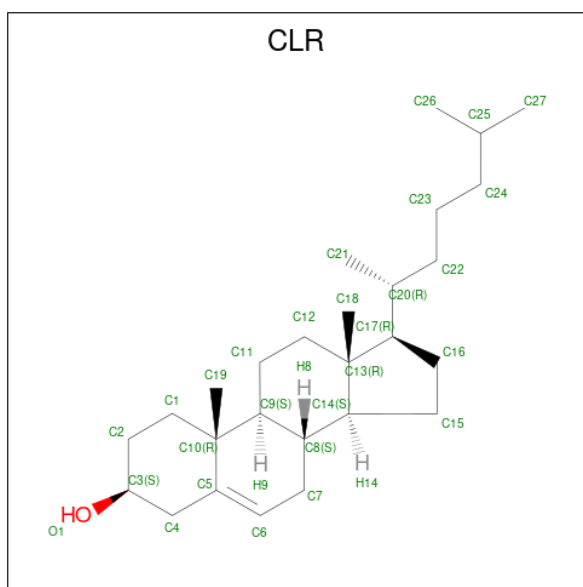
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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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	

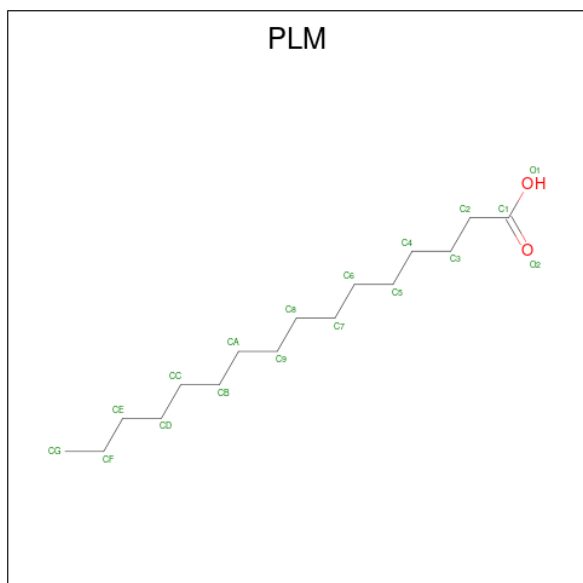
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

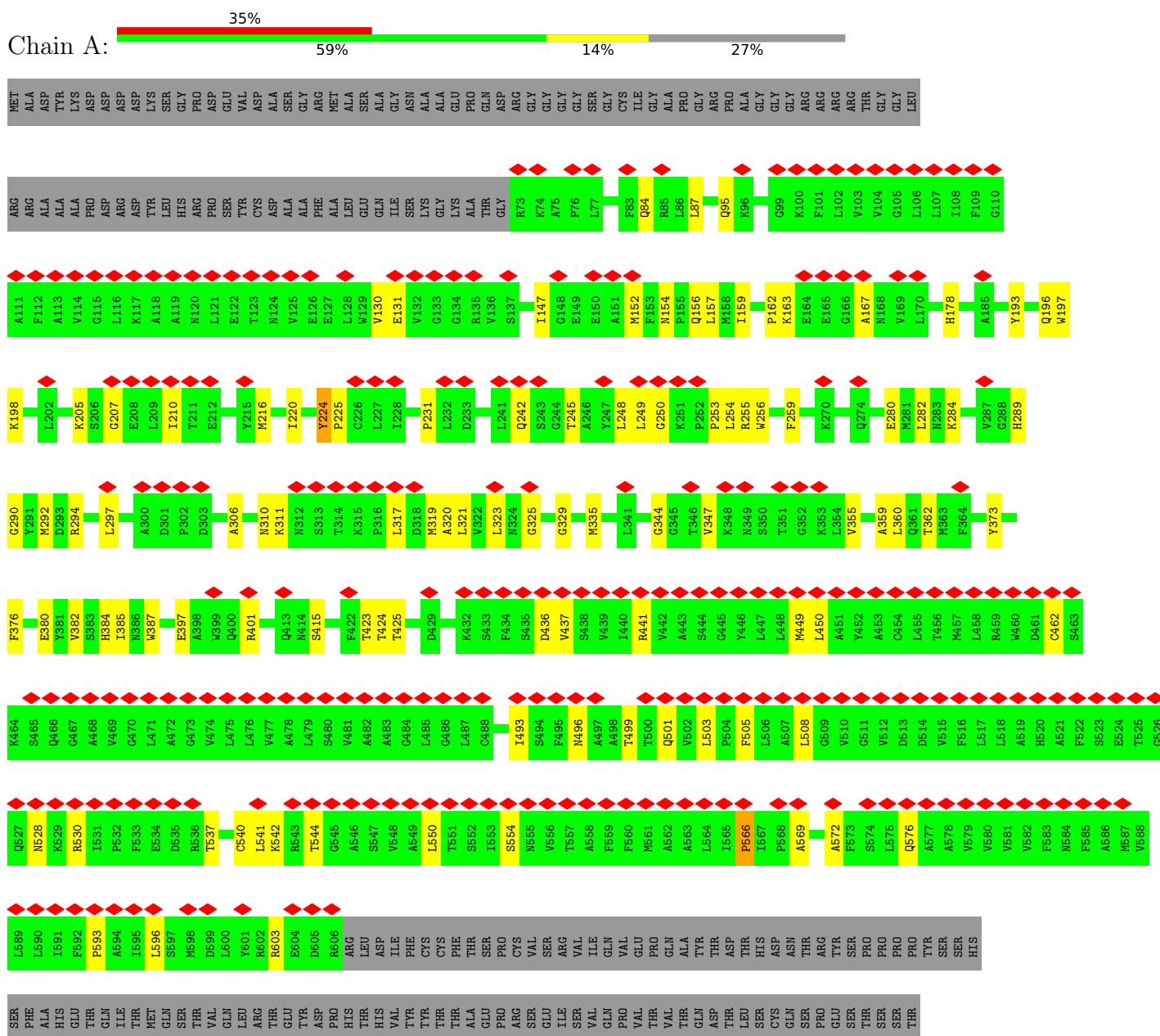


Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total 17	C 16	O 1	0
8	F	1	Total 17	C 16	O 1	0

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.

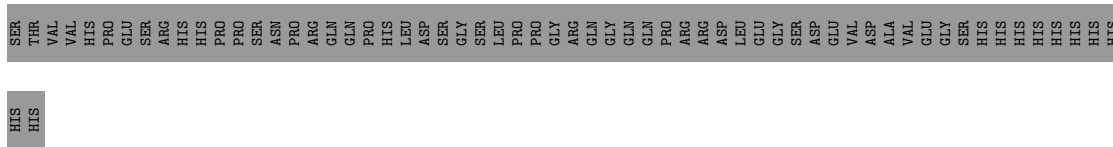
- Molecule 1: Protein patched homolog 1



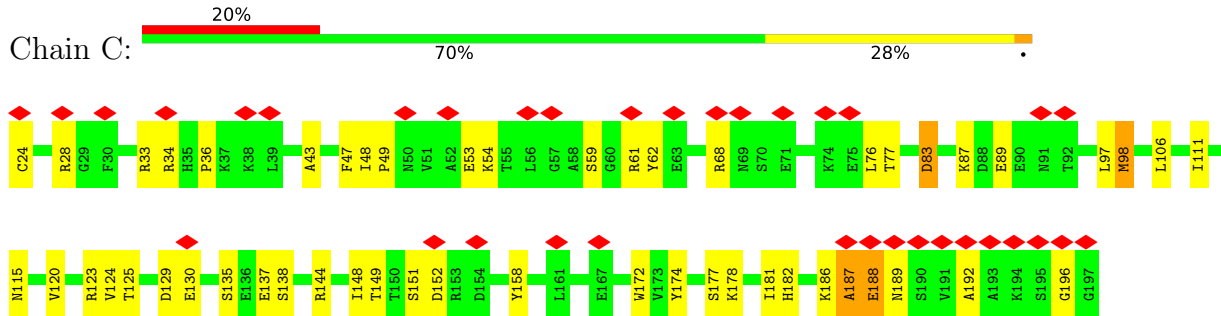


ARG	ARG	ALA	ALA	PRO	ASP	ARG	ASP	TYR	LEU	HIS	ARG	PRO	SER	TYR	CYS	ASP	ALA	ALA	PHE	LEU	GLU	GLN	ILE	SER	LYS	GLY	LYS	ALA	THR	GLY	R73	R74	A75	P76	L77	W78	L79	R80	F83	Q84	R85	L86	L87	C92	Y93	I94	Q95	K96	N97	C98	G99	K100	F101	L102	V103													
V104	G105	L106	L107	I108	F109	G110	A111	F112	A113	V114	G115	L116	K117	A118	A119	N120	A121	E122	T123	N124	V125	E126	E127	L128	W129	V130	E131	V132	H201	G133	L202	C203	Y204	K205	S206	G207	E208	L209	I210	T211	E212	T213	G214	Y215	M216	D217	I147	G148	E149	E150	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	G133	L202	C203	Y204	K205	S206	G207	E208	L209	I210	T211	E212	T213	G214	Y215	M216	D217	I220	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	Y272	N273	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	I395	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	Y446	L447	L448	M449	L450	A451	Y452	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	L493	S494	F495	N496	A497	A498	T499	T500	Q501	Y502	L503	P504	F505	L506	A507	L508	G509	V510	G511	V512	D513	D514	V515	F516	L517	L518	A519	H520	A521	F522	S523	E524	T525	G526	Q527	N528	K529	R530	T531	F532	F533	E534	D535	R536	T537	G538	F539	C540	L541	K542	R543									
T544	G545	A546	S547	V548	A549	L550	T551	S552	T553	S554	N555	V556	T557	A558	F559	F560	M561	A562	A563	L564	T565	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	T595	L596	S597	M598	D599	L600	Y601	R602	R603									
E604	D605	R606	ARG	LEU	ASP	PRO	HIS	THR	PHE	CYS	THR	SER	PRO	CYS	VAL	SER	ARG	ARG	VAL	ILE	GLN	VAL	GLU	PRO	GLN	ALA	THR	TYR	THR	THR	ASP	HIS	ASP	ASN	LEU	THR	ARG	GLN	TYR	SER	PRO	PRO	GLU	PRO	PRO	PRO	TYR	SER	SER	HIS	ASP	LEU	ALA	HIS	GLU	THR	THR	VAL	GLN									
LEU	ARG	PRO	GLU	THR	TYR	ASP	PRO	HIS	THR	VAL	THR	THR	THR	ALA	ALA	GLU	PRO	ARG	ARG	VAL	ILE	GLN	SER	VAL	GLN	PRO	GLN	ALA	THR	TYR	THR	THR	ASP	HIS	ASP	ASN	LEU	THR	ARG	GLN	TYR	SER	PRO	PRO	GLU	PRO	PRO	PRO	TYR	SER	SER	HIS	ASP	LEU	ALA	HIS	GLU	THR	THR	VAL	GLN							
GLU	PRO	PRO	PRO	THR	K729	W730	T731	L732	S733	S734	F735	A736	E737	K738	H739	Y740	A741	P742	F743	L744	L745	L746	P747	K748	A749	P750	V751	P752	V753	I754	F755	L756	F757	L758	G759	L760	N761	G762	V763	S764	L765	Y766	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	R824	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	M912	W913	I914	N915	P916	S917	Y920												

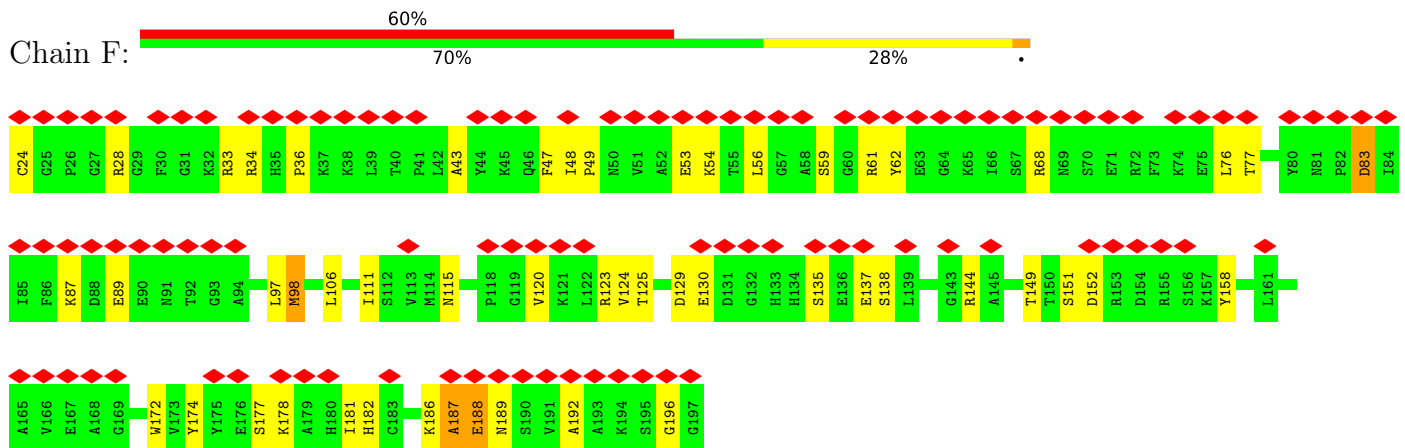
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GLY	F1151	G1091	L1030	A965	Q901	K842	L775	LEU	I591	R530	L471	H408	GLY	R1150	V1090	L1030	L1029	A965	S900	L776	L776	LEU	I592	L472	H409	GLY	R1151	V1091	L1031	L1030	A966	Q902	K843	R838	THR	V591	R531	L473	GLY	Q401	Q400	
HIS	F1152	G1092	F1032	A966	L902	K844	L777	GLN	I593	P532	G473	H410	HIS	F1153	G1093	L1033	L1032	A967	S903	L778	L777	GLN	P533	G474	H411	HIS	F1154	G1094	L1034	L1033	P968	Q903	K845	R839	THR	V592	L474	GLY	Q402	Q401		
THR	F1153	G1093	S1033	P968	T903	K844	L778	THR	P594	A594	V474	H412	THR	F1154	G1094	V1034	L1034	P969	K904	T779	L779	THR	E534	V475	H413	THR	F1155	G1095	V1035	L1035	E970	Q905	L845	R840	THR	V593	L475	GLY	Q403	Q402		
GLY	V1155	V1094	V1036	E970	Q906	K846	T780	SER	I595	L595	V476	A412	GLY	V1156	V1095	L1036	L1036	E971	K906	T781	L781	MET	L476	V477	H414	GLY	V1157	F1096	L1037	L1036	E972	Q907	K847	R841	ASP	V594	L477	GLY	Q404	Q403		
ASP	V1156	F1096	L1036	E971	R906	K847	T781	LEU	S597	S597	V477	Q413	ASP	V1157	F1097	A1037	L1037	A972	R907	T782	L782	SER	V478	V478	H415	ASP	V1158	I1098	C1038	C1038	Q973	V908	F848	R842	SER	V595	L478	GLY	Q405	Q404		
SER	A1157	T1097	A1037	Q973	L907	F848	F782	HIS	M598	G538	A478	S415	SER	A1158	I1098	C1038	C1038	Q974	V909	F783	R783	THR	A479	S416	SER	A1159	L1100	V1099	T1039	F974	D909	R849	R843	ASP	V596	L479	GLY	Q406	Q405			
GLY	T1100	V1100	F1040	F975	D909	R849	R783	VAL	D599	C540	L479	L420	GLY	T1101	V1101	D850	L850	F974	D910	R784	E784	GLN	L480	S417	GLY	T1102	L1102	V1102	C1043	F975	D911	R850	R844	ASP	V597	L480	GLY	Q407	Q406			
THR	T1101	A1101	L1041	N979	D911	R851	T785	THR	Y601	K542	V480	L421	THR	T1102	L1102	L851	L851	F976	A910	T786	R786	THR	V481	S418	THR	T1103	L1103	C1043	L1043	Q980	D912	R852	R845	THR	V598	L481	GLY	Q408	Q407			
SER	L1102	L1102	C1043	Q980	G912	Q853	T786	GLY	Y602	R543	A482	F422	SER	L1103	L1103	Q853	Q853	F977	A911	T787	R787	GLY	V482	S419	SER	L1104	L1104	C1044	L1044	Q981	G913	Q854	R846	THR	V599	L482	GLY	Q409	Q408			
GLN	F1103	A1103	A1044	R982	I914	Q854	T787	THR	Y603	T544	A483	T423	GLN	F1104	L1104	L854	L854	F978	A912	T788	R788	THR	V483	S420	GLN	F1105	L1105	L1045	L1045	Q982	I915	Q855	R847	THR	V600	L483	GLY	Q410	Q409			
THR	V1104	L1105	V1045	D983	N915	Q855	T788	THR	Y604	L545	A484	T424	THR	L1105	L1105	L855	L855	F979	A913	T789	R789	THR	V484	S421	THR	L1106	L1106	F1046	L1046	Q983	D916	Q856	R848	SER	V601	L484	GLY	Q411	Q410			
VAL	L1105	T1106	F1046	D983	N916	Q856	T789	THR	Y605	L546	A485	T425	VAL	L1106	L1106	L856	L856	F980	A914	T790	R790	THR	V485	S422	SER	L1107	L1107	L1047	L1047	Q984	D917	Q857	R849	SER	V602	L485	GLY	Q412	Q411			
SER	G1107	A1107	L1047	Q984	S917	D857	T790	THR	Y606	S547	A486	T426	SER	G1108	L1108	L857	L857	F981	A915	T791	R791	THR	V486	S423	GLY	L1108	L1108	L1048	L1048	Q985	D918	Q858	R850	GLY	V603	L486	GLY	Q413	Q412			
GLY	L1108	L1108	L1048	Q985	S918	D858	T791	ALA	Y607	V548	A487	T427	GLY	L1109	L1109	L858	L858	F982	A916	T792	R792	ALA	V487	S424	GLY	L1110	L1110	L1049	L1049	Q986	D919	Q859	R851	GLY	V604	L487	GLY	Q414	Q413			
LEU	L1111	K1111	T1052	Q986	S919	D859	T792	THR	Y608	L549	A488	T428	LEU	L1112	L1112	L859	L859	F983	A917	T793	R793	THR	V488	S425	GLY	L1113	L1113	L1050	L1050	Q987	D920	Q860	R852	GLY	V605	L488	GLY	Q415	Q414			
ARG	P1172	R1112	A1053	Q986	S920	D860	T793	THR	Y609	L550	A489	T429	ARG	P1173	R1113	L1051	L1051	F984	A918	T794	R794	THR	V489	S426	GLY	L1114	L1114	L1051	L1051	Q988	D921	Q861	R853	GLY	V606	L489	GLY	Q416	Q415			
THR	V1173	R1113	A1053	Q987	S921	D861	T794	THR	Y610	T551	A490	T430	THR	V1174	R1114	L1052	L1052	F985	A919	T795	R795	THR	V490	S427	GLY	L1115	L1115	L1052	L1052	Q989	D922	Q862	R854	GLY	V607	L490	GLY	Q417	Q416			
ALA	L1175	R1115	L1055	Q988	S922	D862	T795	THR	Y611	S552	A491	T431	ALA	L1176	R1116	L1053	L1053	F986	A920	T796	R796	THR	V491	S428	GLY	L1116	L1116	L1053	L1053	Q990	D923	Q863	R855	GLY	V608	L491	GLY	Q418	Q417			
GLN	S1176	R1117	L1056	Q989	S923	D863	T796	THR	Y612	S553	A492	T432	GLN	S1177	R1117	L1054	L1054	F987	A921	T797	R797	THR	V492	S429	GLY	L1117	L1117	L1054	L1054	Q991	D924	Q864	R856	GLY	V609	L492	GLY	Q419	Q418			
GLY	F1177	R1118	L1057	Q990	S924	D864	T797	THR	Y613	S554	A493	T433	GLY	F1178	R1118	L1055	L1055	F988	A922	T798	R798	THR	V493	S430	GLY	L1118	L1118	L1055	L1055	Q992	D925	Q865	R857	GLY	V610	L493	GLY	Q420	Q419			
GLY	G1179	R1119	L1060	Q991	S925	D865	T798	THR	Y614	S555	A494	T434	GLY	G1180	R1120	L1056	L1056	F989	A923	T799	R799	THR	V494	S431	GLY	L1119	L1119	L1056	L1056	Q993	D926	Q866	R858	GLY	V611	L494	GLY	Q421	Q420			
PRO	P1180	R1121	L1061	Q992	S926	D866	T799	THR	Y615	S556	A495	T435	PRO	P1181	R1121	L1057	L1057	F990	A924	T800	R800	THR	V495	S432	GLY	L1120	L1120	L1057	L1057	Q994	D927	Q867	R859	GLY	V612	L495	GLY	Q422	Q421			
ALA	Y1181	R1122	L1062	Q993	S927	D867	T800	THR	Y616	S557	A496	T436	ALA	Y1182	R1122	L1058	L1058	F991	A925	T801	R801	THR	V496	S433	GLY	L1121	L1121	L1058	L1058	Q995	D928	Q868	R860	GLY	V613	L496	GLY	Q423	Q422			
HIS	P1182	R1123	L1063	Q994	S928	D868	T801	THR	Y617	S558	A497	T437	HIS	P1183	R1123	L1059	L1059	F992	A926	T802	R802	THR	V497	S434	GLY	L1122	L1122	L1059	L1059	Q996	D929	Q869	R861	GLY	V614	L497	GLY	Q424	Q423			
GLN	E1183	R1124	L1064	Q995	S929	D869	T802	THR	Y618	S559	A498	T438	GLN	E1184	R1124	L1060	L1060	F993	A927	T803	R803	THR	V498	S435	GLY	L1123	L1123	L1060	L1060	Q997	D930	Q870	R862	GLY	V615	L498	GLY	Q425	Q424			
VAL	VAL	R1125	L1065	Q996	S930	D870	T803	THR	Y619	S560	A499	T439	VAL	VAL	R1125	L1061	L1061	F994	A928	T804	R804	THR	V499	S436	GLY	L1124	L1124	L1061	L1061	Q998	D931	Q871	R863	GLY	V616	L499	GLY	Q426	Q425			
VAL	VAL	R1126	L1066	Q997	S931	D871	T804	THR	Y620	S561	A500	T440	VAL	VAL	R1126	L1062	L1062	F995	A929	T805	R805	THR	V500	S437	GLY	L1125	L1125	L1062	L1062	Q999	D932	Q872	R864	GLY	V617	L500	GLY	Q427	Q426			
GLY	VAL	R1127	L1067	Q998	S932	D872	T805	THR	Y621	S562	A501	T441	GLY	VAL	R1127	L1063	L1063	F996	A930	T806	R806	THR	V501	S438	GLY	L1126	L1126	L1063	L1063	Q1000	D933	Q873	R865	GLY	V618	L501	GLY	Q428	Q427			
GLY	VAL	R1128	L1068	Q999	S933	D873	T806	THR	Y622	S563	A502	T442	GLY	VAL	R1128	L1064	L1064	F997	A931	T807	R807	THR	V502	S439	GLY	L1127	L1127	L1064	L1064	Q1001	D934	Q874	R866	GLY	V619	L502	GLY	Q429	Q428			
ASN	VAL	R1129	L1069	Q1000	S934	D874	T807	THR	Y623	S564	A503	T443	ASN	VAL	R1129	L1065	L1065	F998	A932	T808	R808	THR	V503	S440	GLY	L1128	L1128	L1065	L1065	Q1002	D935	Q875	R867	GLY	V620	L503	GLY	Q430	Q429			
ASN	VAL	R1130	L1070	Q1001	S935	D875	T808	THR	Y624	S565	A504	T444	ASN	VAL	R1130	L1066	L1066	F999	A933	T809	R809	THR	V504	S441	GLY	L1129	L1129	L1066	L1066	Q1003	D936	Q876	R868	GLY	V621	L504	GLY	Q431	Q430			
VAL	VAL	R1131	L1071	Q1002	S936	D876	T809	THR	Y625	S566	A505	T445	VAL	VAL	R1131	L1067	L1067	F1000	A934	T810	R810	THR	V505	S442	GLY	L1130	L1130	L1067	L1067	Q1004	D937	Q877	R869	GLY	V622	L505	GLY	Q432	Q431			
PHE	VAL	R1132	L1072	Q1003	S937	D877	T810	THR	Y626	S567	A506	T446	PHE	VAL	R1132	L1068	L1068	F1001	A935	T811	R811	THR	V506	S443	GLY	L1131	L1131	L1068	L1068	Q1005	D938	Q878	R870	GLY	V623	L506	GLY	Q433	Q432			
ALA	VAL	R1133	L1073	Q1004	S938	D878	T811	THR	Y627	S568	A507	T447	ALA	VAL	R1133	L1069	L1069	F1002	A936	T812	R812	THR	V507	S444	GLY	L1132	L1132	L1069	L1069	Q1006	D939	Q879	R871	GLY	V624	L507	GLY	Q434	Q433			
THR	THR	R1134	L1074	Q1005	S939	D879	T812	THR	Y628	S569	A508	T448	THR	THR	R1134	L1070	L1070	F1003	A937	T813	R813	THR	V508	S445	GLY	L1133	L1133	L1070	L1070	Q1007	D940	Q880	R872	GLY	V625	L508	GLY	Q435	Q434			
PRO	PRO	R1135	L1075	Q1006	S940	D880	T813	THR	Y629	S570	A509	T449	PRO	PRO	R1135	L1071	L1071	F1004	A938	T814	R814	THR	V509	S446	GLY	L1134	L1134	L1071	L1071	Q1008	D941	Q881	R873	GLY	V626	L509	GLY	Q436	Q435			
GLY	GLY	R1136	L1076																																							



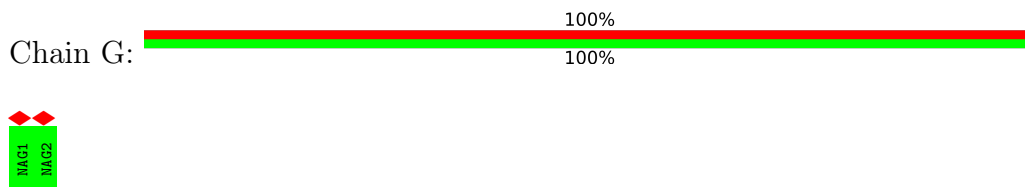
- Molecule 2: Sonic hedgehog protein



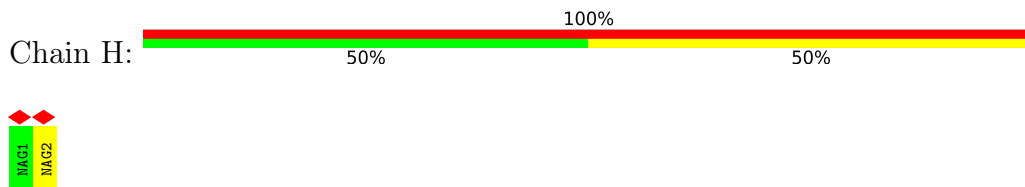
- Molecule 2: Sonic hedgehog protein



- 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 ($\text{\AA}$)	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 ($\text{\AA}$)	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: 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	0.39	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

All (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
2	C	83	ASP	O-C-N	-9.27	110.97	122.19
2	C	196	GLY	N-CA-C	8.94	126.84	115.21
2	F	196	GLY	N-CA-C	8.89	126.77	115.21
2	F	192	ALA	N-CA-C	8.34	122.22	108.96
2	C	192	ALA	N-CA-C	8.32	122.19	108.96
2	F	187	ALA	N-CA-C	7.05	121.11	112.23
2	C	187	ALA	N-CA-C	7.01	121.07	112.23
1	B	216	MET	N-CA-C	-6.74	103.94	111.28
1	E	216	MET	N-CA-C	-6.71	103.96	111.28
2	F	138	SER	O-C-N	6.22	130.38	123.16
2	C	138	SER	O-C-N	6.20	130.35	123.16
2	F	138	SER	CA-C-N	-6.06	109.17	121.18
2	F	138	SER	C-N-CA	-6.06	109.17	121.18
2	C	138	SER	CA-C-N	-6.05	109.21	121.18
2	C	138	SER	C-N-CA	-6.05	109.21	121.18
1	B	384	HIS	N-CA-C	-5.36	107.75	114.56
1	E	384	HIS	N-CA-C	-5.35	107.77	114.56
2	C	196	GLY	CA-C-N	-5.20	112.33	121.70
2	C	196	GLY	C-N-CA	-5.20	112.33	121.70
2	F	196	GLY	CA-C-N	-5.20	112.34	121.70
2	F	196	GLY	C-N-CA	-5.20	112.34	121.70
2	C	123	ARG	CA-C-N	5.08	129.22	122.01
2	C	123	ARG	C-N-CA	5.08	129.22	122.01
2	F	123	ARG	CA-C-N	5.05	129.19	122.01
2	F	123	ARG	C-N-CA	5.05	129.19	122.01

There are no chirality outliers.

All (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
1	A	870	PRO	Peptide
1	A	912	GLY	Peptide
1	B	1107	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	B	327	CYS	Peptide
1	B	357	ALA	Peptide
1	B	385	ILE	Peptide
1	B	938	GLN	Peptide
1	B	942	ARG	Peptide
2	C	83	ASP	Mainchain
1	D	130	VAL	Peptide
1	D	224	TYR	Peptide
1	D	317	LEU	Peptide
1	D	835	GLU	Peptide
1	D	836	GLU	Peptide
1	D	870	PRO	Peptide
1	D	912	GLY	Peptide
1	E	1107	ALA	Peptide
1	E	327	CYS	Peptide
1	E	357	ALA	Peptide
1	E	385	ILE	Peptide
1	E	938	GLN	Peptide
1	E	942	ARG	Peptide
2	F	83	ASP	Mainchain

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:E:1147:PHE:CE2	8:F:205:PLM:CG	1.93	1.48
1:D:220:ILE:CD1	5:D:1808:CLR:H6	0.96	1.43
1:A:220:ILE:CD1	5:A:1808:CLR:H6	0.96	1.41
1:E:216:MET:SD	5:F:201:CLR:H41	1.65	1.35
1:B:216:MET:SD	5:C:201:CLR:H41	1.65	1.34
1:A:220:ILE:HD13	5:A:1808:CLR:C6	1.53	1.29
1:B:1147:PHE:CZ	8:C:205:PLM:HG2	1.73	1.24
1:D:220:ILE:HD13	5:D:1808:CLR:C6	1.53	1.23
1:E:1147:PHE:CZ	8:F:205:PLM:HG2	1.73	1.20
1:E:216:MET:SD	5:F:201:CLR:C4	2.29	1.19
1:B:216:MET:SD	5:C:201:CLR:C4	2.29	1.18
1:B:1147:PHE:HE2	8:C:205:PLM:HG1	0.99	1.15
1:E:121:LEU:HD12	5:E:1508:CLR:H192	1.16	1.14
1:E:1147:PHE:CE2	8:F:205:PLM:HG2	1.71	1.10
1:E:1147:PHE:HE2	8:F:205:PLM:HG1	0.99	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD12	5:B:1508:CLR:H192	1.16	1.08
1:A:220:ILE:HD11	5:A:1808:CLR:H6	1.09	1.07
1:B:1147:PHE:CE2	8:C:205:PLM:HG2	1.71	1.07
1:E:437:VAL:HG11	5:E:1508:CLR:H121	1.09	1.06
1:B:437:VAL:HG11	5:B:1508:CLR:H121	1.09	1.05
5:D:1808:CLR:H162	5:D:1808:CLR:H231	1.39	1.04
1:D:220:ILE:HD11	5:D:1808:CLR:H6	1.09	1.04
5:A:1808:CLR:H162	5:A:1808:CLR:H231	1.39	1.03
8:F:205:PLM:HC2	8:F:205:PLM:H81	1.39	1.03
1:E:121:LEU:HD12	5:E:1508:CLR:C19	1.89	1.02
8:C:205:PLM:H81	8:C:205:PLM:HC2	1.39	1.02
1:B:121:LEU:HD12	5:B:1508:CLR:C19	1.89	1.01
1:E:152:MET:SD	2:F:28:ARG:NH1	2.33	1.01
1:B:152:MET:SD	2:C:28:ARG:NH1	2.33	1.01
1:A:220:ILE:HD11	5:A:1808:CLR:C6	1.66	1.00
1:E:437:VAL:HG11	5:E:1508:CLR:C12	1.94	0.97
1:B:437:VAL:HG11	5:B:1508:CLR:C12	1.94	0.96
1:D:220:ILE:HD11	5:D:1808:CLR:C6	1.66	0.96
1:B:1147:PHE:CE2	8:C:205:PLM:HG1	1.82	0.95
1:E:1147:PHE:HE2	8:F:205:PLM:HG3	1.33	0.94
2:F:187:ALA:O	2:F:189:ASN:N	2.01	0.93
2:F:76:LEU:HD23	2:F:97:LEU:HB3	1.50	0.92
2:C:187:ALA:O	2:C:189:ASN:N	2.01	0.92
1:B:1147:PHE:CE2	8:C:205:PLM:HG3	2.02	0.92
1:E:216:MET:SD	5:F:201:CLR:H6	2.10	0.92
5:B:1508:CLR:H273	5:B:1508:CLR:H221	1.50	0.91
2:C:76:LEU:HD23	2:C:97:LEU:HB3	1.50	0.91
1:E:437:VAL:CG1	5:E:1508:CLR:H121	2.01	0.91
1:B:216:MET:SD	5:C:201:CLR:H6	2.10	0.91
1:E:1147:PHE:CE2	8:F:205:PLM:HG1	1.82	0.90
5:E:1508:CLR:H211	5:E:1508:CLR:H242	1.54	0.90
5:E:1508:CLR:H221	5:E:1508:CLR:H273	1.50	0.90
1:B:437:VAL:CG1	5:B:1508:CLR:H121	2.01	0.89
5:B:1508:CLR:H242	5:B:1508:CLR:H211	1.54	0.88
1:B:119:ALA:HB1	5:B:1508:CLR:H72	1.55	0.88
1:E:119:ALA:HB1	5:E:1508:CLR:H72	1.55	0.87
1:E:1147:PHE:CE2	8:F:205:PLM:HG3	2.02	0.87
1:B:1147:PHE:HE2	8:C:205:PLM:HG3	1.32	0.84
5:A:1808:CLR:H221	5:A:1808:CLR:H181	1.59	0.83
1:E:282:LEU:HD21	5:F:201:CLR:C21	2.09	0.83
5:E:1508:CLR:H213	5:E:1508:CLR:C27	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1508:CLR:H213	5:B:1508:CLR:C27	2.09	0.82
5:D:1808:CLR:H181	5:D:1808:CLR:H221	1.59	0.82
8:C:205:PLM:HC2	8:C:205:PLM:C8	2.03	0.81
1:A:249:LEU:HD12	2:C:135:SER:HB2	1.63	0.81
1:B:282:LEU:HD21	5:C:201:CLR:C21	2.09	0.81
1:A:1171:LEU:O	1:A:1175:LEU:HB2	1.80	0.81
1:D:1171:LEU:O	1:D:1175:LEU:HB2	1.81	0.81
1:B:1147:PHE:HZ	8:C:205:PLM:HG2	1.45	0.81
5:E:1508:CLR:H221	5:E:1508:CLR:H262	1.64	0.80
5:A:1808:CLR:H162	5:A:1808:CLR:C23	2.02	0.80
5:A:1808:CLR:C25	5:A:1808:CLR:H213	2.12	0.80
1:D:249:LEU:HD12	2:F:135:SER:HB2	1.63	0.79
5:D:1808:CLR:H162	5:D:1808:CLR:C23	2.02	0.79
5:B:1508:CLR:H221	5:B:1508:CLR:H262	1.64	0.79
1:B:121:LEU:CD1	5:B:1508:CLR:H192	2.08	0.79
1:B:216:MET:SD	5:C:201:CLR:C6	2.70	0.79
1:E:149:GLU:OE1	2:F:28:ARG:NH1	2.16	0.79
1:E:216:MET:SD	5:F:201:CLR:C6	2.70	0.79
5:D:1808:CLR:C25	5:D:1808:CLR:H213	2.12	0.79
1:B:149:GLU:OE1	2:C:28:ARG:NH1	2.16	0.77
5:C:201:CLR:H183	5:C:201:CLR:H212	1.67	0.76
1:E:121:LEU:CD1	5:E:1508:CLR:H192	2.08	0.75
5:F:201:CLR:H183	5:F:201:CLR:H212	1.67	0.75
8:F:205:PLM:HC2	8:F:205:PLM:C8	2.03	0.74
5:A:1808:CLR:H213	5:A:1808:CLR:H25	1.70	0.74
1:B:220:ILE:HG13	5:C:201:CLR:H152	1.70	0.73
1:E:220:ILE:HG13	5:F:201:CLR:H152	1.70	0.73
5:A:1808:CLR:H231	5:A:1808:CLR:C16	2.18	0.73
5:D:1808:CLR:H213	5:D:1808:CLR:H25	1.70	0.73
5:E:1508:CLR:H262	5:E:1508:CLR:C22	2.17	0.72
1:A:1028:LEU:HD12	1:A:1083:VAL:HG22	1.72	0.72
1:D:1028:LEU:HD12	1:D:1083:VAL:HG22	1.72	0.72
1:A:220:ILE:CD1	5:A:1808:CLR:C7	2.67	0.72
1:A:220:ILE:HD12	5:A:1808:CLR:C6	2.15	0.71
5:B:1508:CLR:H262	5:B:1508:CLR:C22	2.17	0.71
5:B:1508:CLR:H273	5:B:1508:CLR:C22	2.20	0.71
1:A:220:ILE:HD13	5:A:1808:CLR:H6	0.71	0.71
1:D:220:ILE:HD13	5:D:1808:CLR:H6	0.71	0.71
5:B:1508:CLR:H273	5:B:1508:CLR:H213	1.72	0.70
5:E:1508:CLR:H273	5:E:1508:CLR:C22	2.20	0.70
1:D:220:ILE:CD1	5:D:1808:CLR:C7	2.67	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1808:CLR:H231	5:D:1808:CLR:C16	2.18	0.69
5:D:1808:CLR:H221	5:D:1808:CLR:C18	2.23	0.69
1:B:216:MET:HE2	1:B:216:MET:CA	2.23	0.69
5:E:1508:CLR:H273	5:E:1508:CLR:H213	1.72	0.69
1:B:216:MET:HE2	1:B:216:MET:HA	1.75	0.69
5:A:1808:CLR:H221	5:A:1808:CLR:C18	2.23	0.68
1:D:220:ILE:HD12	5:D:1808:CLR:C6	2.15	0.68
5:A:1808:CLR:H213	5:A:1808:CLR:H272	1.76	0.68
1:B:154:ASN:ND2	2:C:28:ARG:HG2	2.08	0.68
1:E:216:MET:CA	1:E:216:MET:HE2	2.23	0.68
5:E:1508:CLR:H242	5:E:1508:CLR:C21	2.24	0.68
5:B:1508:CLR:H242	5:B:1508:CLR:C21	2.24	0.68
1:E:1147:PHE:HZ	8:F:205:PLM:HG2	1.45	0.68
1:D:335:MET:SD	5:D:1808:CLR:H211	2.34	0.68
1:E:216:MET:SD	5:F:201:CLR:C5	2.81	0.68
1:E:282:LEU:HD21	5:F:201:CLR:H212	1.75	0.67
1:A:335:MET:SD	5:A:1808:CLR:H211	2.34	0.67
1:E:434:PHE:HZ	8:F:205:PLM:HG3	1.60	0.67
1:E:154:ASN:ND2	2:F:28:ARG:HG2	2.08	0.67
1:B:434:PHE:HZ	8:C:205:PLM:HG3	1.60	0.67
1:B:216:MET:SD	5:C:201:CLR:C5	2.82	0.67
1:B:282:LEU:HD21	5:C:201:CLR:H212	1.75	0.67
5:D:1808:CLR:H213	5:D:1808:CLR:H272	1.76	0.67
1:E:216:MET:HE2	1:E:216:MET:HA	1.75	0.66
5:D:1808:CLR:H213	5:D:1808:CLR:C27	2.26	0.66
2:C:187:ALA:C	2:C:189:ASN:N	2.54	0.66
1:B:154:ASN:HD22	2:C:28:ARG:HG2	1.60	0.65
5:E:1508:CLR:H213	5:E:1508:CLR:H272	1.77	0.65
1:B:496:ASN:HD21	1:B:572:ALA:HB3	1.61	0.65
5:A:1808:CLR:H213	5:A:1808:CLR:C27	2.26	0.65
1:D:248:LEU:HD23	1:D:250:GLY:H	1.62	0.65
2:C:144:ARG:HH21	2:C:186:LYS:HA	1.62	0.65
1:E:496:ASN:HD21	1:E:572:ALA:HB3	1.61	0.65
5:B:1508:CLR:H213	5:B:1508:CLR:H272	1.78	0.65
1:E:154:ASN:HD22	2:F:28:ARG:HG2	1.60	0.64
2:F:187:ALA:C	2:F:189:ASN:N	2.54	0.64
2:F:144:ARG:HH21	2:F:186:LYS:HA	1.62	0.64
1:A:248:LEU:HD23	1:A:250:GLY:H	1.62	0.64
1:B:121:LEU:CD1	5:B:1508:CLR:C19	2.73	0.63
1:B:988:VAL:HG13	1:B:1022:ILE:HG22	1.81	0.63
1:D:1114:ARG:HH22	1:D:1181:TYR:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:ALA:O	1:D:740:TYR:HB2	1.99	0.63
1:A:736:ALA:O	1:A:740:TYR:HB2	1.99	0.62
1:E:945:ARG:NH1	1:E:967:GLU:O	2.32	0.62
1:D:873:TYR:HB2	1:D:881:VAL:HG22	1.82	0.62
1:D:282:LEU:HD21	5:D:1808:CLR:H192	1.82	0.62
1:B:945:ARG:NH1	1:B:967:GLU:O	2.32	0.62
1:E:988:VAL:HG13	1:E:1022:ILE:HG22	1.81	0.62
1:A:1114:ARG:HH22	1:A:1181:TYR:HA	1.64	0.61
1:B:128:LEU:HB2	1:B:569:ALA:HB2	1.82	0.61
1:D:210:ILE:HD11	1:D:949:VAL:HG21	1.83	0.61
1:B:119:ALA:CB	5:B:1508:CLR:H72	2.30	0.61
1:B:342:ILE:HD12	1:B:343:VAL:HG23	1.82	0.61
1:E:342:ILE:HD12	1:E:343:VAL:HG23	1.82	0.61
5:F:201:CLR:C16	5:F:201:CLR:H232	2.31	0.61
1:E:121:LEU:CD1	5:E:1508:CLR:C19	2.73	0.60
5:C:201:CLR:C16	5:C:201:CLR:H232	2.31	0.60
1:A:210:ILE:HD11	1:A:949:VAL:HG21	1.82	0.60
1:A:290:GLY:O	1:A:294:ARG:NH1	2.34	0.60
1:E:128:LEU:HB2	1:E:569:ALA:HB2	1.82	0.60
1:A:873:TYR:HB2	1:A:881:VAL:HG22	1.82	0.60
1:E:434:PHE:CZ	8:F:205:PLM:HG3	2.37	0.60
1:B:434:PHE:CZ	8:C:205:PLM:HG3	2.37	0.60
1:D:290:GLY:O	1:D:294:ARG:NH1	2.33	0.60
1:A:282:LEU:HD21	5:A:1808:CLR:H192	1.82	0.59
1:E:1104:PHE:HE2	1:E:1180:PRO:HD2	1.67	0.59
1:E:925:ALA:O	1:E:929:ASN:HB2	2.02	0.59
1:B:289:HIS:HB3	1:B:292:MET:HB2	1.85	0.59
5:F:201:CLR:H232	5:F:201:CLR:H161	1.85	0.59
1:B:1104:PHE:HE2	1:B:1180:PRO:HD2	1.67	0.59
1:B:862:ASP:HB3	1:B:868:ILE:HG12	1.86	0.58
1:B:925:ALA:O	1:B:929:ASN:HB2	2.03	0.58
1:D:205:LYS:HD2	1:D:224:TYR:HD2	1.68	0.58
1:E:289:HIS:HB3	1:E:292:MET:HB2	1.85	0.58
1:E:476:LEU:HD11	1:E:595:ILE:HD12	1.85	0.58
5:A:1808:CLR:H25	5:A:1808:CLR:C21	2.33	0.58
5:B:1508:CLR:H221	5:B:1508:CLR:C27	2.17	0.58
1:D:833:MET:HB2	1:D:979:ASN:HB2	1.86	0.58
1:E:119:ALA:CB	5:E:1508:CLR:H72	2.30	0.58
1:E:203:CYS:O	2:F:33:ARG:NH2	2.37	0.58
1:D:306:ALA:HA	1:D:311:LYS:HD3	1.86	0.58
5:E:1508:CLR:H221	5:E:1508:CLR:C27	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HD11	1:B:595:ILE:HD12	1.85	0.58
1:B:203:CYS:O	2:C:33:ARG:NH2	2.37	0.58
5:D:1808:CLR:H25	5:D:1808:CLR:C21	2.33	0.58
5:C:201:CLR:H232	5:C:201:CLR:H161	1.85	0.57
1:E:1049:ASN:HD22	1:E:1105:LEU:HD21	1.69	0.57
1:A:306:ALA:HA	1:A:311:LYS:HD3	1.86	0.57
1:E:855:LEU:HD11	1:E:882:LEU:HD22	1.86	0.57
2:F:158:TYR:HB3	2:F:181:ILE:HD11	1.86	0.57
1:A:833:MET:HB2	1:A:979:ASN:HB2	1.86	0.57
1:E:862:ASP:HB3	1:E:868:ILE:HG12	1.86	0.57
1:A:1107:ALA:HB3	1:A:1114:ARG:HG3	1.87	0.57
1:D:566:PRO:HD2	1:D:1027:TRP:HH2	1.70	0.57
1:B:216:MET:SD	5:C:201:CLR:H42	2.39	0.57
1:A:449:MET:HG2	1:A:508:LEU:HD21	1.86	0.57
1:D:1107:ALA:HB3	1:D:1114:ARG:HG3	1.87	0.57
1:A:205:LYS:HD2	1:A:224:TYR:HD2	1.68	0.57
2:C:158:TYR:HB3	2:C:181:ILE:HD11	1.86	0.57
1:B:326:GLY:O	1:B:336:HIS:NE2	2.37	0.57
1:B:855:LEU:HD11	1:B:882:LEU:HD22	1.86	0.57
1:D:593:PRO:HA	1:D:596:LEU:HG	1.87	0.56
1:A:593:PRO:HA	1:A:596:LEU:HG	1.87	0.56
1:A:806:VAL:HG23	1:A:973:GLN:HB3	1.87	0.56
1:B:98:CYS:SG	1:B:597:SER:OG	2.61	0.56
1:D:449:MET:HG2	1:D:508:LEU:HD21	1.86	0.56
1:B:1049:ASN:HD22	1:B:1105:LEU:HD21	1.69	0.56
1:D:806:VAL:HG23	1:D:973:GLN:HB3	1.87	0.56
1:E:326:GLY:O	1:E:336:HIS:NE2	2.37	0.56
1:B:1051:TRP:HH2	1:B:1178:PHE:HB3	1.71	0.56
1:D:929:ASN:HD21	1:D:950:HIS:H	1.54	0.56
1:A:929:ASN:HD21	1:A:950:HIS:H	1.53	0.56
1:E:205:LYS:HA	1:E:226:CYS:HA	1.88	0.56
1:B:821:ASP:OD2	1:B:1001:TYR:OH	2.24	0.56
1:A:566:PRO:HD2	1:A:1027:TRP:HH2	1.70	0.56
5:B:1508:CLR:H221	5:B:1508:CLR:C26	2.26	0.55
2:C:120:VAL:HG13	2:C:151:SER:HB3	1.88	0.55
1:D:373:TYR:HA	1:D:387:TRP:HE1	1.72	0.55
1:E:1147:PHE:CZ	8:F:205:PLM:CG	2.50	0.55
1:D:294:ARG:NH2	1:D:329:GLY:O	2.40	0.55
1:D:220:ILE:HD12	5:D:1808:CLR:C7	2.37	0.55
1:E:821:ASP:OD2	1:E:1001:TYR:OH	2.24	0.55
2:F:120:VAL:HG13	2:F:151:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:MET:SD	5:F:201:CLR:H42	2.39	0.55
2:C:62:TYR:CE2	2:C:137:GLU:HG2	2.42	0.55
5:D:1808:CLR:C21	5:D:1808:CLR:C24	2.85	0.55
1:E:425:THR:O	1:E:429:ASP:N	2.38	0.55
1:E:1051:TRP:HH2	1:E:1178:PHE:HB3	1.71	0.55
1:A:294:ARG:NH2	1:A:329:GLY:O	2.40	0.54
1:B:205:LYS:HA	1:B:226:CYS:HA	1.88	0.54
1:B:101:PHE:HA	1:B:104:VAL:HG12	1.89	0.54
1:E:101:PHE:HA	1:E:104:VAL:HG12	1.89	0.54
1:E:529:LYS:NZ	1:E:531:ILE:O	2.41	0.54
1:A:436:ASP:O	1:A:501:GLN:NE2	2.39	0.54
5:A:1808:CLR:C25	5:A:1808:CLR:C21	2.85	0.54
5:E:1508:CLR:C21	5:E:1508:CLR:C24	2.85	0.54
1:A:373:TYR:HA	1:A:387:TRP:HE1	1.72	0.54
5:B:1508:CLR:H273	5:B:1508:CLR:C21	2.37	0.54
2:F:62:TYR:CE2	2:F:137:GLU:HG2	2.42	0.54
5:A:1808:CLR:C21	5:A:1808:CLR:C24	2.85	0.54
1:B:425:THR:O	1:B:429:ASP:N	2.38	0.54
5:E:1508:CLR:H221	5:E:1508:CLR:C26	2.26	0.54
1:D:436:ASP:O	1:D:501:GLN:NE2	2.39	0.54
5:C:201:CLR:C16	5:C:201:CLR:C23	2.85	0.54
1:D:813:PRO:O	1:D:816:GLN:NE2	2.41	0.54
1:A:220:ILE:HD12	5:A:1808:CLR:C7	2.37	0.53
1:B:213:THR:HG22	1:B:216:MET:HB2	1.91	0.53
1:A:84:GLN:HB3	1:A:542:LYS:HD2	1.90	0.53
1:A:868:ILE:HG22	1:A:872:ASN:HB2	1.90	0.53
1:B:195:ARG:O	1:B:381:TYR:OH	2.24	0.53
1:A:813:PRO:O	1:A:816:GLN:NE2	2.42	0.53
1:A:540:CYS:SG	1:A:541:LEU:N	2.82	0.53
2:C:53:GLU:OE2	2:C:54:LYS:NZ	2.32	0.53
1:D:84:GLN:HB3	1:D:542:LYS:HD2	1.90	0.53
1:D:131:GLU:HA	1:D:566:PRO:HB2	1.90	0.53
1:D:868:ILE:HG22	1:D:872:ASN:HB2	1.90	0.53
1:A:131:GLU:HA	1:A:566:PRO:HB2	1.90	0.53
1:B:529:LYS:NZ	1:B:531:ILE:O	2.41	0.53
1:E:195:ARG:O	1:E:381:TYR:OH	2.24	0.53
1:E:807:THR:HG23	1:E:972:ALA:HB3	1.91	0.53
5:F:201:CLR:C16	5:F:201:CLR:C23	2.85	0.53
1:B:807:THR:HG23	1:B:972:ALA:HB3	1.91	0.52
1:E:522:PHE:HD1	1:E:540:CYS:HB2	1.74	0.52
1:A:540:CYS:O	1:A:544:THR:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:945:ARG:NH2	1:D:967:GLU:O	2.43	0.52
5:E:1508:CLR:H273	5:E:1508:CLR:C21	2.37	0.52
1:E:1002:THR:HG22	1:E:1007:SER:HA	1.91	0.52
1:B:522:PHE:HD1	1:B:540:CYS:HB2	1.74	0.52
1:A:156:GLN:HG3	1:A:423:THR:HB	1.92	0.52
2:C:68:ARG:HD2	2:C:130:GLU:OE1	2.09	0.52
5:F:201:CLR:C21	5:F:201:CLR:H183	2.34	0.52
1:A:528:ASN:ND2	1:A:530:ARG:O	2.43	0.52
5:B:1508:CLR:C27	5:B:1508:CLR:C21	2.86	0.52
1:D:335:MET:SD	5:D:1808:CLR:C21	2.98	0.52
1:E:213:THR:HG22	1:E:216:MET:HB2	1.90	0.52
5:E:1508:CLR:C27	5:E:1508:CLR:C21	2.85	0.52
1:A:462:CYS:O	1:A:603:ARG:NH1	2.41	0.52
1:A:1040:PHE:HB2	1:A:1057:VAL:HG21	1.92	0.52
1:D:540:CYS:SG	1:D:541:LEU:N	2.82	0.52
1:E:119:ALA:HB1	5:E:1508:CLR:C7	2.36	0.52
2:F:68:ARG:HD2	2:F:130:GLU:OE1	2.09	0.52
1:B:437:VAL:HG11	5:B:1508:CLR:H212	1.92	0.52
1:B:1002:THR:HG22	1:B:1007:SER:HA	1.91	0.52
5:B:1508:CLR:C21	5:B:1508:CLR:C24	2.85	0.52
1:D:528:ASN:ND2	1:D:530:ARG:O	2.43	0.52
1:A:731:THR:O	1:A:735:PHE:CB	2.59	0.51
1:D:156:GLN:HG3	1:D:423:THR:HB	1.92	0.51
1:D:1040:PHE:HB2	1:D:1057:VAL:HG21	1.92	0.51
1:B:1040:PHE:HB2	1:B:1057:VAL:HG21	1.91	0.51
1:D:245:THR:H	1:D:255:ARG:HG3	1.75	0.51
1:E:1040:PHE:HB2	1:E:1057:VAL:HG21	1.91	0.51
1:A:245:THR:H	1:A:255:ARG:HG3	1.75	0.51
1:B:812:TYR:O	1:B:816:GLN:NE2	2.44	0.51
1:E:437:VAL:HG11	5:E:1508:CLR:H212	1.92	0.51
1:A:335:MET:SD	5:A:1808:CLR:C21	2.98	0.51
1:A:380:GLU:HB3	2:C:43:ALA:HB3	1.93	0.51
1:D:163:LYS:NZ	1:D:415:SER:O	2.41	0.51
1:E:812:TYR:O	1:E:816:GLN:NE2	2.44	0.51
1:D:731:THR:O	1:D:735:PHE:CB	2.59	0.51
1:A:945:ARG:NH2	1:A:967:GLU:O	2.43	0.51
1:A:162:PRO:HB3	1:A:167:ALA:HB3	1.93	0.51
1:A:750:LYS:NZ	1:A:1176:SER:OG	2.44	0.51
1:D:750:LYS:NZ	1:D:1176:SER:OG	2.44	0.51
1:D:811:ASP:H	1:D:815:ILE:HD12	1.76	0.51
1:B:942:ARG:HA	1:B:944:HIS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:PRO:HB3	1:D:167:ALA:HB3	1.93	0.50
2:F:59:SER:O	2:F:144:ARG:NH2	2.45	0.50
1:A:225:PRO:O	1:A:242:GLN:NE2	2.34	0.50
1:A:815:ILE:HG23	1:A:818:LEU:HD12	1.94	0.50
1:E:942:ARG:HA	1:E:944:HIS:H	1.76	0.50
1:A:1165:LEU:O	1:A:1169:VAL:HB	2.12	0.50
1:B:119:ALA:HB1	5:B:1508:CLR:C7	2.36	0.50
5:D:1808:CLR:C25	5:D:1808:CLR:C21	2.85	0.50
1:A:921:ILE:HG23	1:A:963:ILE:HG21	1.94	0.50
1:D:921:ILE:HG23	1:D:963:ILE:HG21	1.93	0.50
1:A:499:THR:O	1:A:503:LEU:HB3	2.11	0.50
1:A:811:ASP:H	1:A:815:ILE:HD12	1.76	0.50
1:D:1165:LEU:O	1:D:1169:VAL:HB	2.12	0.50
1:D:462:CYS:O	1:D:603:ARG:NH1	2.41	0.50
1:D:540:CYS:O	1:D:544:THR:N	2.39	0.50
1:D:815:ILE:HG23	1:D:818:LEU:HD12	1.94	0.50
1:E:91:GLY:O	1:E:537:THR:OG1	2.30	0.50
1:E:430:ILE:HG12	1:E:781:VAL:HG12	1.94	0.50
1:A:154:ASN:O	1:A:156:GLN:NE2	2.39	0.50
1:D:207:GLY:O	1:D:224:TYR:OH	2.26	0.50
1:D:280:GLU:HG3	1:D:284:LYS:HE3	1.93	0.50
1:D:380:GLU:HB3	2:F:43:ALA:HB3	1.92	0.50
1:B:126:GLU:OE1	2:C:28:ARG:NH2	2.45	0.50
1:D:95:GLN:NE2	1:D:537:THR:OG1	2.45	0.50
1:D:154:ASN:O	1:D:156:GLN:NE2	2.39	0.50
1:D:499:THR:O	1:D:503:LEU:HB3	2.11	0.49
5:D:1808:CLR:C18	5:D:1808:CLR:C22	2.87	0.49
1:D:245:THR:HG22	1:D:255:ARG:HD2	1.94	0.49
1:E:126:GLU:OE1	2:F:28:ARG:NH2	2.45	0.49
1:B:819:LEU:HB3	1:B:843:MET:HE1	1.94	0.49
1:B:1147:PHE:CZ	8:C:205:PLM:CG	2.50	0.49
1:E:819:LEU:HB3	1:E:843:MET:HE1	1.94	0.49
1:A:1059:VAL:HG21	1:A:1171:LEU:HD21	1.94	0.49
2:F:54:LYS:O	2:F:61:ARG:NH1	2.45	0.49
1:A:95:GLN:NE2	1:A:537:THR:OG1	2.45	0.49
1:A:245:THR:HG22	1:A:255:ARG:HD2	1.94	0.49
2:C:54:LYS:O	2:C:61:ARG:NH1	2.46	0.49
2:C:59:SER:O	2:C:144:ARG:NH2	2.45	0.49
2:C:77:THR:HG22	2:C:98:MET:O	2.12	0.49
5:E:1508:CLR:H121	5:E:1508:CLR:H212	1.95	0.49
1:B:984:THR:HA	1:B:987:PHE:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1059:VAL:HG21	1:D:1171:LEU:HD21	1.94	0.49
1:E:208:GLU:HG3	2:F:34:ARG:HG2	1.94	0.49
1:E:984:THR:HA	1:E:987:PHE:HD2	1.78	0.49
1:B:91:GLY:O	1:B:537:THR:OG1	2.30	0.49
2:F:77:THR:HG22	2:F:98:MET:O	2.12	0.49
1:A:280:GLU:HG3	1:A:284:LYS:HE3	1.93	0.49
1:A:941:ILE:HG23	1:A:969:ILE:HG23	1.95	0.49
5:B:1508:CLR:H121	5:B:1508:CLR:H212	1.95	0.49
1:D:1044:ALA:O	1:D:1048:LEU:N	2.46	0.49
1:B:430:ILE:HG12	1:B:781:VAL:HG12	1.94	0.49
1:A:1035:VAL:HG21	1:A:1087:ILE:HG23	1.95	0.48
1:B:208:GLU:HG3	2:C:34:ARG:HG2	1.94	0.48
1:D:1035:VAL:HG21	1:D:1087:ILE:HG23	1.95	0.48
1:B:815:ILE:HG23	1:B:818:LEU:HD23	1.94	0.48
5:F:201:CLR:C27	5:F:201:CLR:H222	2.42	0.48
1:E:294:ARG:NH2	1:E:329:GLY:O	2.32	0.48
1:E:437:VAL:HG21	5:E:1508:CLR:C12	2.43	0.48
1:A:1146:ASP:O	1:A:1150:ARG:HB2	2.14	0.48
1:B:437:VAL:HG21	5:B:1508:CLR:C12	2.43	0.48
2:C:111:ILE:O	2:C:115:ASN:ND2	2.47	0.48
1:E:480:SER:HB3	1:E:587:MET:HG3	1.95	0.48
1:E:815:ILE:HG23	1:E:818:LEU:HD23	1.94	0.48
1:E:568:PRO:HA	1:E:571:ARG:HB3	1.95	0.48
1:A:1044:ALA:O	1:A:1048:LEU:N	2.46	0.48
1:B:480:SER:HB3	1:B:587:MET:HG3	1.95	0.48
1:E:1104:PHE:CG	1:E:1175:LEU:HD21	2.48	0.48
1:D:889:GLN:NE2	1:D:896:PRO:O	2.47	0.48
1:D:1146:ASP:O	1:D:1150:ARG:HB2	2.14	0.48
1:A:889:GLN:NE2	1:A:896:PRO:O	2.47	0.48
1:B:260:ASP:HB3	1:B:292:MET:HG3	1.96	0.48
1:B:1104:PHE:CG	1:B:1175:LEU:HD21	2.48	0.48
5:B:1508:CLR:C27	5:B:1508:CLR:C22	2.88	0.48
1:B:823:HIS:CE1	1:B:840:LEU:HB2	2.49	0.48
1:B:1171:LEU:O	1:B:1175:LEU:HB3	2.14	0.48
5:D:1810:CLR:H162	5:D:1810:CLR:H221	1.59	0.48
2:F:53:GLU:HB3	2:F:172:TRP:CD2	2.49	0.48
1:B:216:MET:HA	1:B:216:MET:CE	2.40	0.47
2:F:111:ILE:O	2:F:115:ASN:ND2	2.47	0.47
1:E:1171:LEU:O	1:E:1175:LEU:HB3	2.14	0.47
2:F:87:LYS:HE2	2:F:89:GLU:HB3	1.96	0.47
1:A:320:ALA:HA	1:A:323:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:TYR:H	1:D:197:TRP:HZ3	1.63	0.47
1:A:496:ASN:HD21	1:A:572:ALA:HB3	1.79	0.47
5:A:1808:CLR:C18	5:A:1808:CLR:C22	2.87	0.47
1:E:128:LEU:CD1	8:F:205:PLM:HB2	2.45	0.47
1:E:531:ILE:HG21	1:E:539:GLU:HG3	1.97	0.47
1:B:128:LEU:CD1	8:C:205:PLM:HB2	2.45	0.47
1:B:452:TYR:O	1:B:456:THR:OG1	2.29	0.47
1:D:941:ILE:HG23	1:D:969:ILE:HG23	1.95	0.47
1:B:1079:SER:OG	1:B:1080:ALA:N	2.48	0.47
1:D:320:ALA:HA	1:D:323:LEU:HG	1.96	0.47
1:D:505:PHE:HD2	1:D:1140:LEU:HD23	1.79	0.47
1:E:1166:ASN:HA	1:E:1170:LEU:HB3	1.97	0.47
1:A:889:GLN:HE22	1:A:896:PRO:HB2	1.79	0.47
1:B:497:ALA:O	1:B:501:GLN:NE2	2.48	0.47
1:B:568:PRO:HA	1:B:571:ARG:HB3	1.95	0.47
1:B:1166:ASN:HA	1:B:1170:LEU:HB3	1.97	0.47
1:D:347:VAL:HG13	1:D:355:VAL:HB	1.96	0.47
1:A:505:PHE:HD2	1:A:1140:LEU:HD23	1.79	0.47
1:B:170:LEU:HD23	1:B:357:ALA:HB2	1.97	0.47
1:B:853:GLN:HE21	1:B:908:VAL:HG11	1.80	0.47
2:C:87:LYS:HE2	2:C:89:GLU:HB3	1.96	0.47
1:D:889:GLN:HE22	1:D:896:PRO:HB2	1.79	0.47
1:E:823:HIS:CE1	1:E:840:LEU:HB2	2.49	0.47
1:E:1079:SER:OG	1:E:1080:ALA:N	2.48	0.47
5:E:1508:CLR:C27	5:E:1508:CLR:C22	2.88	0.47
1:A:207:GLY:O	1:A:224:TYR:OH	2.26	0.47
2:C:174:TYR:HB3	2:C:182:HIS:HB3	1.97	0.47
1:D:496:ASN:HD21	1:D:572:ALA:HB3	1.79	0.47
1:E:98:CYS:SG	1:E:597:SER:OG	2.61	0.47
1:A:297:LEU:H	1:A:310:ASN:HD22	1.63	0.46
1:D:1064:THR:HG21	1:D:1090:VAL:HG22	1.97	0.46
1:B:531:ILE:HG21	1:B:539:GLU:HG3	1.97	0.46
1:A:384:HIS:CD2	1:A:385:ILE:HG23	2.51	0.46
2:C:53:GLU:HB3	2:C:172:TRP:CD2	2.49	0.46
1:E:260:ASP:HB3	1:E:292:MET:HG3	1.96	0.46
1:A:163:LYS:NZ	1:A:415:SER:O	2.40	0.46
1:A:193:TYR:H	1:A:197:TRP:HZ3	1.63	0.46
1:A:1064:THR:HG21	1:A:1090:VAL:HG22	1.97	0.46
5:C:201:CLR:C27	5:C:201:CLR:H222	2.42	0.46
1:E:170:LEU:HD23	1:E:357:ALA:HB2	1.97	0.46
2:F:174:TYR:HB3	2:F:182:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:LEU:CD2	5:F:201:CLR:C21	2.89	0.46
1:D:297:LEU:H	1:D:310:ASN:HD22	1.63	0.46
1:E:244:GLY:HA3	1:E:255:ARG:HA	1.98	0.46
1:A:256:TRP:HH2	5:A:1808:CLR:H112	1.80	0.46
1:D:344:GLY:N	1:D:359:ALA:O	2.48	0.46
1:B:1137:VAL:HG12	1:B:1153:PHE:HD1	1.81	0.46
2:C:47:PHE:HB3	2:C:174:TYR:HD1	1.81	0.46
1:E:1137:VAL:HG12	1:E:1153:PHE:HD1	1.81	0.46
2:F:47:PHE:HB3	2:F:174:TYR:HD1	1.81	0.46
1:A:347:VAL:HG13	1:A:355:VAL:HB	1.96	0.45
5:C:201:CLR:H8	5:C:201:CLR:H182	1.62	0.45
1:E:1056:ILE:HD13	1:E:1056:ILE:HA	1.84	0.45
1:D:225:PRO:O	1:D:242:GLN:NE2	2.34	0.45
2:F:48:ILE:HG13	2:F:49:PRO:HD3	1.98	0.45
1:B:244:GLY:HA3	1:B:255:ARG:HA	1.98	0.45
1:D:256:TRP:HH2	5:D:1808:CLR:H112	1.80	0.45
1:D:1000:ASN:O	1:D:1003:SER:OG	2.28	0.45
1:E:497:ALA:O	1:E:501:GLN:NE2	2.48	0.45
1:A:493:ILE:HG22	1:A:576:GLN:HE21	1.81	0.45
1:A:1110:ASP:N	1:A:1110:ASP:OD1	2.49	0.45
1:B:149:GLU:CD	2:C:28:ARG:HH12	2.25	0.45
2:C:48:ILE:HG13	2:C:49:PRO:HD3	1.98	0.45
5:C:201:CLR:C21	5:C:201:CLR:H183	2.34	0.45
1:D:493:ILE:HG22	1:D:576:GLN:HE21	1.81	0.45
1:D:384:HIS:CD2	1:D:385:ILE:HG23	2.51	0.45
5:D:1809:CLR:H193	5:D:1809:CLR:H111	1.84	0.45
5:D:1810:CLR:H183	5:D:1810:CLR:H20	1.83	0.45
1:E:216:MET:HA	1:E:216:MET:CE	2.40	0.45
1:B:768:THR:HG22	1:B:1068:PHE:HD2	1.83	0.45
1:D:1110:ASP:OD1	1:D:1110:ASP:N	2.49	0.44
1:A:259:PHE:CE2	5:A:1808:CLR:H21	2.53	0.44
1:A:437:VAL:HG11	5:A:1810:CLR:H151	1.99	0.44
1:D:147:ILE:HG12	1:D:152:MET:HE1	1.99	0.44
1:D:196:GLN:OE1	1:D:198:LYS:NZ	2.50	0.44
1:D:437:VAL:HG11	5:D:1810:CLR:H151	1.99	0.44
1:A:1031:PHE:HA	1:A:1034:VAL:HG12	1.99	0.44
1:B:282:LEU:CD2	5:C:201:CLR:C21	2.89	0.44
1:D:259:PHE:CE2	5:D:1808:CLR:H21	2.53	0.44
1:E:853:GLN:HE21	1:E:908:VAL:HG11	1.80	0.44
1:A:344:GLY:N	1:A:359:ALA:O	2.48	0.44
1:A:909:ASP:N	1:A:909:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:938:GLN:O	1:D:973:GLN:NE2	2.51	0.44
1:E:768:THR:HG22	1:E:1068:PHE:HD2	1.83	0.44
2:F:106:LEU:HD21	2:F:124:VAL:HG21	1.99	0.44
1:A:196:GLN:OE1	1:A:198:LYS:NZ	2.50	0.44
1:A:938:GLN:O	1:A:973:GLN:NE2	2.51	0.44
1:B:427:LEU:HD22	2:C:24:CYS:SG	2.58	0.44
5:D:1808:CLR:H193	5:D:1808:CLR:H111	1.79	0.44
1:A:496:ASN:ND2	1:A:569:ALA:O	2.51	0.44
1:D:1031:PHE:HA	1:D:1034:VAL:HG12	2.00	0.44
1:B:437:VAL:CG1	5:B:1508:CLR:H212	2.48	0.44
1:A:147:ILE:HG12	1:A:152:MET:HE1	2.00	0.43
5:A:1808:CLR:H8	5:A:1808:CLR:H182	1.68	0.43
1:D:1162:LEU:HD13	1:D:1165:LEU:HD21	2.00	0.43
5:B:1508:CLR:H273	5:B:1508:CLR:C20	2.48	0.43
1:D:441:ARG:NH2	1:D:1141:ALA:O	2.51	0.43
1:D:496:ASN:ND2	1:D:569:ALA:O	2.51	0.43
5:E:1508:CLR:H273	5:E:1508:CLR:C20	2.48	0.43
1:A:441:ARG:NH2	1:A:1141:ALA:O	2.51	0.43
1:A:900:SER:O	1:A:904:LYS:NZ	2.52	0.43
1:A:1162:LEU:HD13	1:A:1165:LEU:HD21	2.00	0.43
5:A:1808:CLR:C16	5:A:1808:CLR:H272	2.48	0.43
2:C:106:LEU:HD21	2:C:124:VAL:HG21	1.99	0.43
1:E:149:GLU:CD	2:F:28:ARG:HH12	2.25	0.43
1:E:427:LEU:HD22	2:F:24:CYS:SG	2.58	0.43
1:E:449:MET:HE1	1:E:1132:SER:HB2	2.01	0.43
1:E:230:THR:OG1	1:E:233:ASP:N	2.52	0.43
5:F:201:CLR:H182	5:F:201:CLR:H8	1.62	0.43
1:D:178:HIS:NE2	1:D:362:THR:OG1	2.48	0.43
1:D:872:ASN:ND2	4:D:1804:NAG:O7	2.51	0.43
5:D:1808:CLR:C16	5:D:1808:CLR:H272	2.48	0.43
1:A:981:LEU:HB3	1:A:987:PHE:CE1	2.54	0.43
1:B:449:MET:HE1	1:B:1132:SER:HB2	2.01	0.43
1:D:319:MET:HB3	1:D:321:LEU:HG	2.00	0.43
1:D:900:SER:O	1:D:904:LYS:NZ	2.52	0.43
1:E:437:VAL:CG1	5:E:1508:CLR:H212	2.48	0.43
1:D:1156:LEU:HD13	1:D:1159:LEU:HD13	2.01	0.43
1:E:1130:ALA:O	1:E:1133:THR:OG1	2.31	0.43
5:F:201:CLR:H111	5:F:201:CLR:H193	1.72	0.43
5:A:1810:CLR:H221	5:A:1810:CLR:H162	1.58	0.43
1:B:294:ARG:NH2	1:B:329:GLY:O	2.32	0.43
1:D:981:LEU:HB3	1:D:987:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1179:GLY:HA2	1:D:1180:PRO:HD3	1.88	0.43
1:E:361:GLN:HB2	1:E:798:PHE:CE2	2.54	0.43
1:E:945:ARG:HA	1:E:945:ARG:HD3	1.85	0.43
1:E:1047:LEU:HD23	1:E:1105:LEU:HD22	2.00	0.43
1:A:1156:LEU:HD13	1:A:1159:LEU:HD13	2.01	0.43
5:A:1810:CLR:H183	5:A:1810:CLR:H20	1.83	0.43
1:B:848:PHE:HE1	1:B:923:LEU:HA	1.84	0.43
4:B:1501:NAG:N2	4:B:1501:NAG:O4	2.52	0.43
1:E:412:ALA:O	1:E:415:SER:OG	2.34	0.43
1:A:397:GLU:OE2	1:A:401:ARG:NH2	2.39	0.42
1:B:361:GLN:HB2	1:B:798:PHE:CE2	2.54	0.42
8:C:205:PLM:H91	8:C:205:PLM:H62	1.57	0.42
1:A:216:MET:HE2	1:A:216:MET:HB3	1.90	0.42
1:A:859:PHE:HZ	1:A:902:LEU:HD11	1.84	0.42
1:D:376:PHE:HB3	1:D:382:VAL:HG21	2.01	0.42
2:F:125:THR:CG2	2:F:149:THR:HG23	2.49	0.42
2:F:177:SER:OG	2:F:178:LYS:N	2.52	0.42
2:C:125:THR:CG2	2:C:149:THR:HG23	2.50	0.42
5:F:201:CLR:H222	5:F:201:CLR:H25	1.57	0.42
5:A:1808:CLR:H213	5:A:1808:CLR:C24	2.49	0.42
1:B:230:THR:OG1	1:B:233:ASP:N	2.52	0.42
1:A:376:PHE:HB3	1:A:382:VAL:HG21	2.01	0.42
5:A:1808:CLR:H231	5:A:1808:CLR:H272	1.59	0.42
1:B:771:VAL:O	1:B:772:ARG:NE	2.52	0.42
1:E:771:VAL:O	1:E:772:ARG:NE	2.52	0.42
1:B:945:ARG:HA	1:B:945:ARG:HD3	1.85	0.42
1:D:909:ASP:OD1	1:D:909:ASP:N	2.50	0.42
1:A:959:THR:OG1	2:C:152:ASP:OD1	2.37	0.42
1:B:593:PRO:HA	1:B:596:LEU:HB2	2.02	0.42
1:B:945:ARG:HH11	1:B:966:ALA:HB1	1.85	0.42
1:D:554:SER:HB2	1:D:1094:VAL:HG21	2.02	0.42
2:F:68:ARG:CG	2:F:130:GLU:OE1	2.68	0.42
1:A:319:MET:HB3	1:A:321:LEU:HG	2.01	0.42
1:A:1000:ASN:O	1:A:1003:SER:OG	2.28	0.42
1:B:206:SER:HB3	1:B:227:LEU:HD12	2.02	0.42
1:B:216:MET:CA	1:B:216:MET:CE	2.95	0.42
1:D:157:LEU:H	1:D:157:LEU:HG	1.67	0.42
1:E:473:GLY:HA2	1:E:476:LEU:HD12	2.01	0.42
4:E:1501:NAG:O4	4:E:1501:NAG:N2	2.52	0.42
1:A:554:SER:HB2	1:A:1094:VAL:HG21	2.02	0.42
2:C:68:ARG:CG	2:C:130:GLU:OE1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:LEU:HA	1:D:544:THR:HG21	2.02	0.42
1:E:231:PRO:HG3	1:E:342:ILE:HD13	2.01	0.42
1:B:210:ILE:H	1:B:210:ILE:HG13	1.56	0.42
1:B:843:MET:H	1:B:843:MET:HG2	1.72	0.42
1:D:1146:ASP:O	1:D:1150:ARG:CB	2.68	0.42
1:E:437:VAL:HG11	5:E:1508:CLR:C11	2.50	0.42
2:F:76:LEU:HD23	2:F:97:LEU:CB	2.37	0.42
2:C:177:SER:OG	2:C:178:LYS:N	2.52	0.41
1:D:959:THR:OG1	2:F:152:ASP:OD1	2.37	0.41
1:E:304:CYS:HB2	1:E:311:LYS:HD3	2.02	0.41
1:E:593:PRO:HA	1:E:596:LEU:HB2	2.01	0.41
1:E:1134:LEU:O	1:E:1138:LEU:HB2	2.20	0.41
1:A:1179:GLY:HA2	1:A:1180:PRO:HD3	1.89	0.41
1:B:1056:ILE:HD13	1:B:1056:ILE:HA	1.84	0.41
5:C:201:CLR:H222	5:C:201:CLR:H25	1.57	0.41
5:C:201:CLR:H222	5:C:201:CLR:H272	2.02	0.41
5:D:1809:CLR:H191	5:D:1809:CLR:H8	1.85	0.41
1:B:231:PRO:HG3	1:B:342:ILE:HD13	2.01	0.41
1:B:473:GLY:HA2	1:B:476:LEU:HD12	2.01	0.41
1:B:1134:LEU:O	1:B:1138:LEU:HB2	2.20	0.41
1:E:945:ARG:HH11	1:E:966:ALA:HB1	1.85	0.41
5:D:1808:CLR:H231	5:D:1808:CLR:H272	1.59	0.41
1:B:863:TRP:HA	1:B:868:ILE:HD11	2.03	0.41
1:B:1047:LEU:HD23	1:B:1105:LEU:HD22	2.00	0.41
1:A:1146:ASP:O	1:A:1150:ARG:CB	2.68	0.41
5:E:1508:CLR:H211	5:E:1508:CLR:C24	2.29	0.41
2:F:56:LEU:HD13	2:F:56:LEU:HA	1.88	0.41
1:A:231:PRO:HG2	1:A:360:LEU:HD13	2.03	0.41
1:A:423:THR:O	1:A:425:THR:N	2.54	0.41
1:A:927:VAL:HG11	1:A:945:ARG:HB2	2.03	0.41
8:F:205:PLM:H91	8:F:205:PLM:H62	1.57	0.41
1:A:940:ASN:HD22	1:A:942:ARG:HH12	1.69	0.41
5:A:1809:CLR:H8	5:A:1809:CLR:H191	1.85	0.41
2:C:124:VAL:HG22	2:C:148:ILE:HG22	2.03	0.41
1:E:224:TYR:HA	1:E:225:PRO:HD3	1.89	0.41
1:E:848:PHE:HE1	1:E:923:LEU:HA	1.84	0.41
1:A:978:LEU:HD23	1:A:978:LEU:HA	1.86	0.41
1:B:124:ASN:HB3	1:B:127:GLU:OE1	2.22	0.41
1:D:807:THR:OG1	1:D:808:GLN:N	2.55	0.41
1:D:843:MET:HG2	1:D:845:LEU:H	1.85	0.41
1:E:206:SER:HB3	1:E:227:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:486:GLY:O	1:E:489:SER:OG	2.39	0.41
1:A:178:HIS:NE2	1:A:362:THR:OG1	2.48	0.40
1:A:807:THR:OG1	1:A:808:GLN:N	2.55	0.40
1:A:843:MET:HG2	1:A:845:LEU:H	1.85	0.40
1:D:859:PHE:HZ	1:D:902:LEU:HD11	1.84	0.40
1:E:863:TRP:HA	1:E:868:ILE:HD11	2.03	0.40
1:A:289:HIS:CD2	1:A:292:MET:HB2	2.57	0.40
1:D:869:MET:SD	1:D:902:LEU:HG	2.62	0.40
1:A:888:VAL:HG13	1:A:899:ILE:HA	2.02	0.40
1:B:304:CYS:HB2	1:B:311:LYS:HD3	2.02	0.40
2:C:76:LEU:HD23	2:C:97:LEU:CB	2.37	0.40
1:D:147:ILE:HD11	1:D:971:TYR:CZ	2.56	0.40
1:D:570:LEU:HD23	1:D:570:LEU:HA	1.94	0.40
1:D:888:VAL:HG13	1:D:899:ILE:HA	2.02	0.40
1:E:231:PRO:HG2	1:E:360:LEU:HD23	2.03	0.40
1:B:371:GLN:NE2	2:C:33:ARG:H	2.19	0.40
1:B:1035:VAL:HG21	1:B:1087:ILE:HG23	2.04	0.40
1:D:827:SER:HB3	1:D:840:LEU:HD11	2.04	0.40
1:E:158:MET:HB3	1:E:362:THR:HG23	2.03	0.40
1:E:371:GLN:NE2	2:F:33:ARG:H	2.19	0.40
1:E:957:PRO:HA	1:E:960:ARG:HB3	2.03	0.40
5:E:1508:CLR:H8	5:E:1508:CLR:H182	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	987/1349 (73%)	857 (87%)	123 (12%)	7 (1%)	18	56
1	B	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	36	72
1	D	987/1349 (73%)	858 (87%)	122 (12%)	7 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	36	72
2	C	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	10	44
2	F	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	10	44
All	All	4286/5744 (75%)	3733 (87%)	529 (12%)	24 (1%)	23	59

All (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
1	B	389	GLU
1	D	424	THR
1	E	389	GLU
1	A	834	LEU
1	A	835	GLU
1	A	917	SER
1	D	834	LEU
1	D	835	GLU
1	D	917	SER
1	A	325	GLY
1	B	1181	TYR
1	D	325	GLY
1	E	1181	TYR
1	A	253	PRO
1	D	253	PRO
1	A	566	PRO
2	C	36	PRO
1	D	566	PRO
2	F	36	PRO

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%)	73	80
1	B	808/1147 (70%)	793 (98%)	15 (2%)	50	67
1	D	832/1147 (72%)	825 (99%)	7 (1%)	73	80
1	E	808/1147 (70%)	793 (98%)	15 (2%)	50	67
2	C	142/144 (99%)	140 (99%)	2 (1%)	59	72
2	F	142/144 (99%)	140 (99%)	2 (1%)	59	72
All	All	3564/4876 (73%)	3516 (99%)	48 (1%)	59	74

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	A	157	LEU
1	A	159	ILE
1	A	254	LEU
1	A	450	LEU
1	A	550	LEU
1	A	1048	LEU
1	B	94	ILE
1	B	159	ILE
1	B	210	ILE
1	B	220	ILE
1	B	287	VAL
1	B	297	LEU
1	B	354	LEU
1	B	362	THR
1	B	431	LEU
1	B	785	THR
1	B	806	VAL
1	B	807	THR
1	B	845	LEU
1	B	868	ILE
1	B	1171	LEU
2	C	129	ASP
2	C	188	GLU
1	D	87	LEU
1	D	157	LEU
1	D	159	ILE
1	D	254	LEU
1	D	450	LEU
1	D	550	LEU

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Mol	Chain	Res	Type
1	D	1048	LEU
1	E	94	ILE
1	E	159	ILE
1	E	210	ILE
1	E	220	ILE
1	E	287	VAL
1	E	297	LEU
1	E	354	LEU
1	E	362	THR
1	E	431	LEU
1	E	785	THR
1	E	806	VAL
1	E	807	THR
1	E	845	LEU
1	E	868	ILE
1	E	1171	LEU
2	F	129	ASP
2	F	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	310	ASN
1	A	324	ASN
1	A	358	HIS
1	A	408	HIS
1	A	496	ASN
1	A	576	GLN
1	A	584	ASN
1	A	816	GLN
1	A	828	ASN
1	A	871	ASN
1	A	872	ASN
1	A	889	GLN
1	A	901	GLN
1	A	929	ASN
1	B	124	ASN
1	B	154	ASN
1	B	178	HIS
1	B	218	GLN
1	B	371	GLN

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Mol	Chain	Res	Type
1	B	496	ASN
1	B	584	ASN
1	B	817	HIS
1	B	846	HIS
1	B	853	GLN
1	B	929	ASN
1	B	938	GLN
1	B	1049	ASN
2	C	35	HIS
2	C	50	ASN
2	C	79	ASN
2	C	107	ASN
2	C	189	ASN
1	D	95	GLN
1	D	310	ASN
1	D	324	ASN
1	D	408	HIS
1	D	496	ASN
1	D	576	GLN
1	D	584	ASN
1	D	828	ASN
1	D	871	ASN
1	D	872	ASN
1	D	889	GLN
1	D	901	GLN
1	D	929	ASN
1	E	124	ASN
1	E	154	ASN
1	E	178	HIS
1	E	218	GLN
1	E	408	HIS
1	E	409	GLN
1	E	496	ASN
1	E	584	ASN
1	E	817	HIS
1	E	846	HIS
1	E	853	GLN
1	E	929	ASN
1	E	938	GLN
1	E	1049	ASN
2	F	35	HIS
2	F	50	ASN

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Mol	Chain	Res	Type
2	F	79	ASN
2	F	107	ASN
2	F	189	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
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.

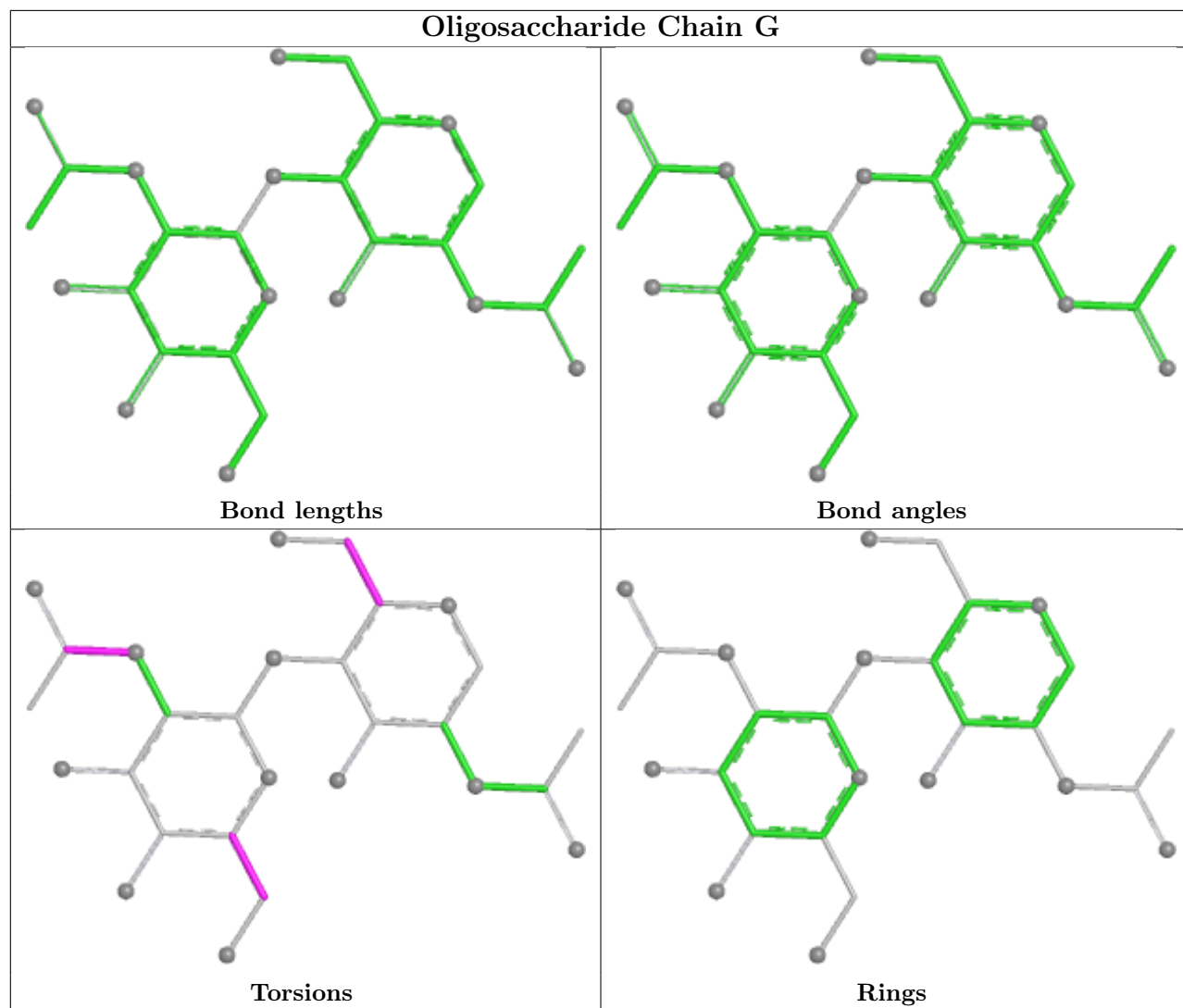
All (14) torsion outliers are listed below:

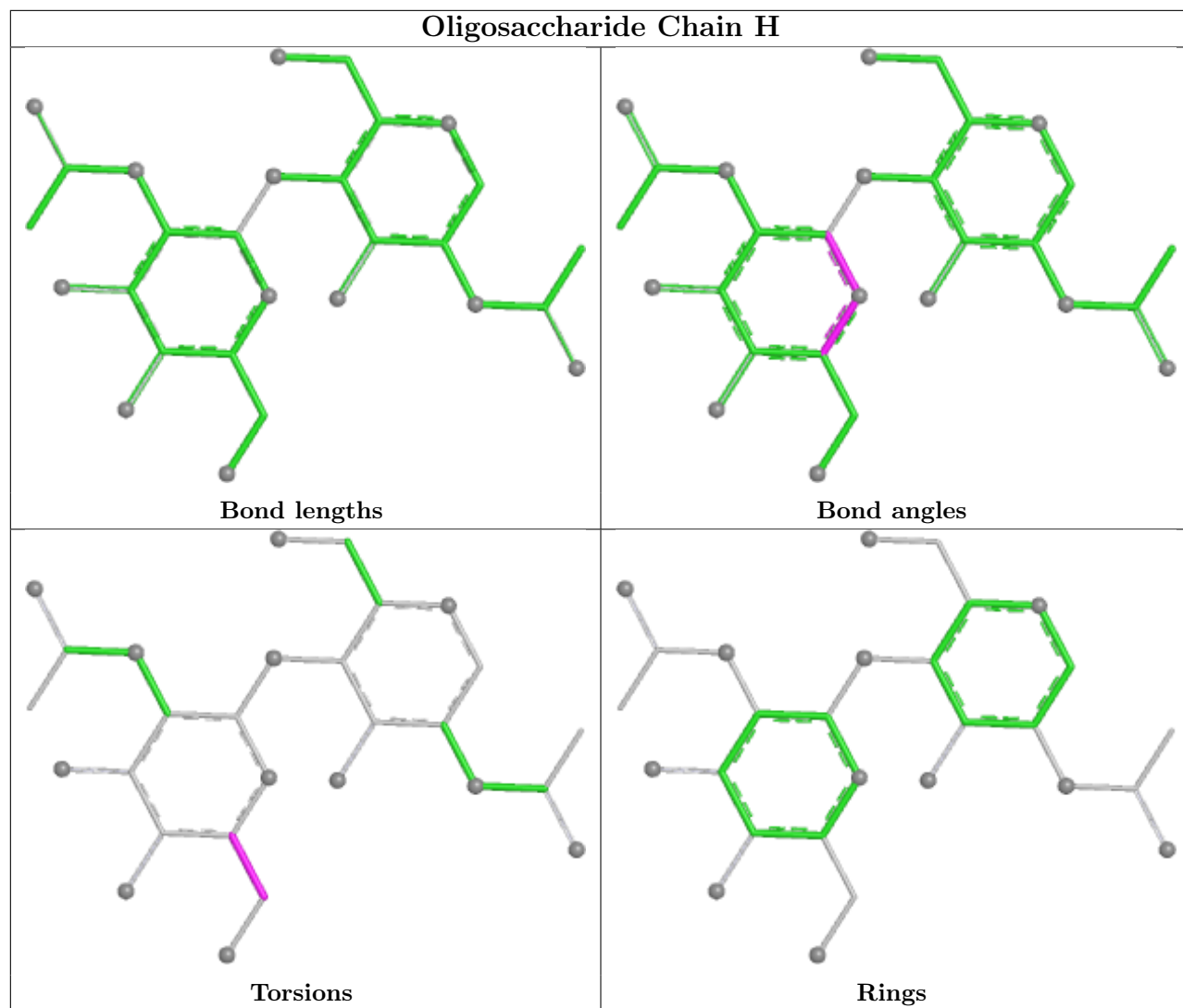
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

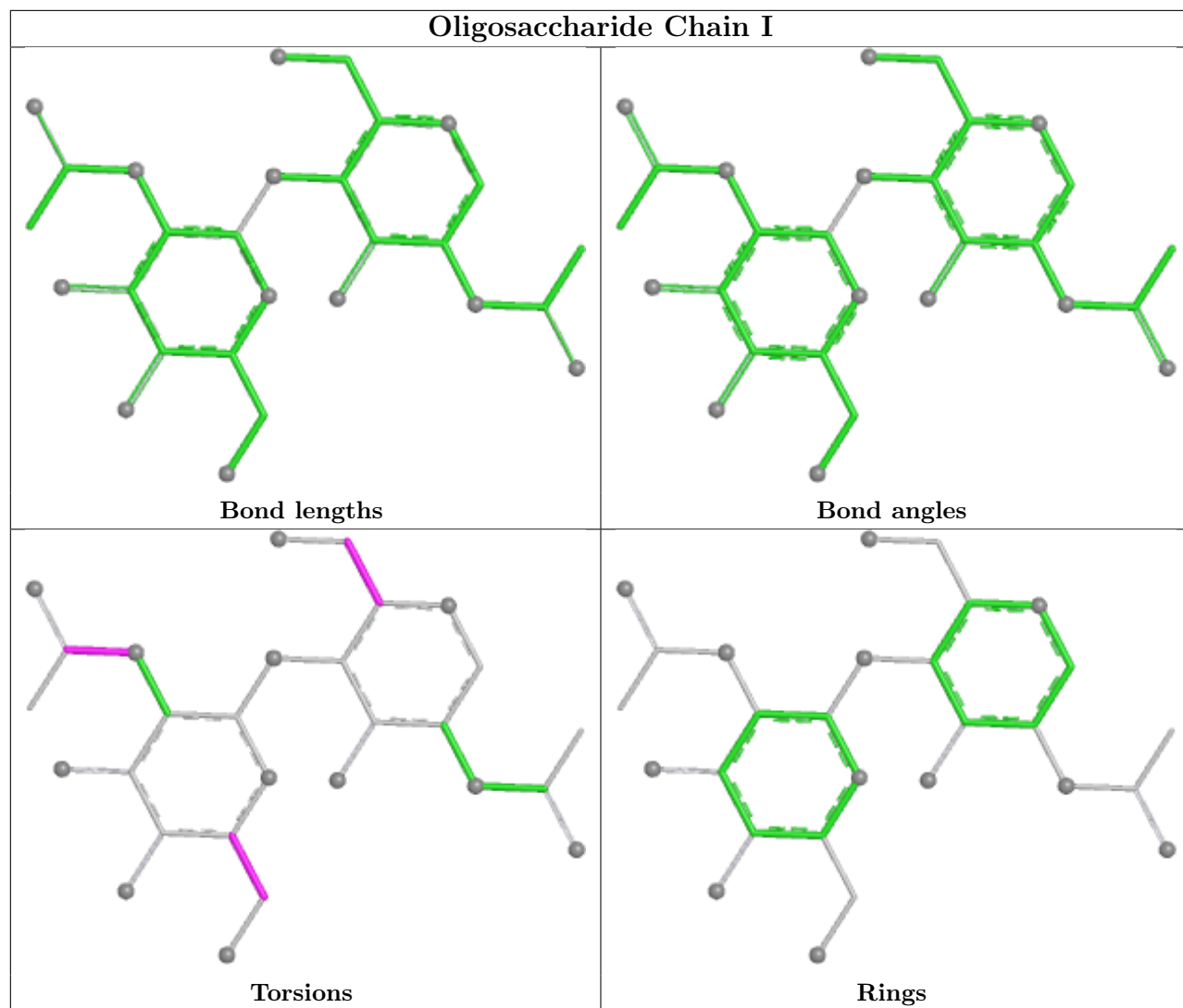
There are no ring outliers.

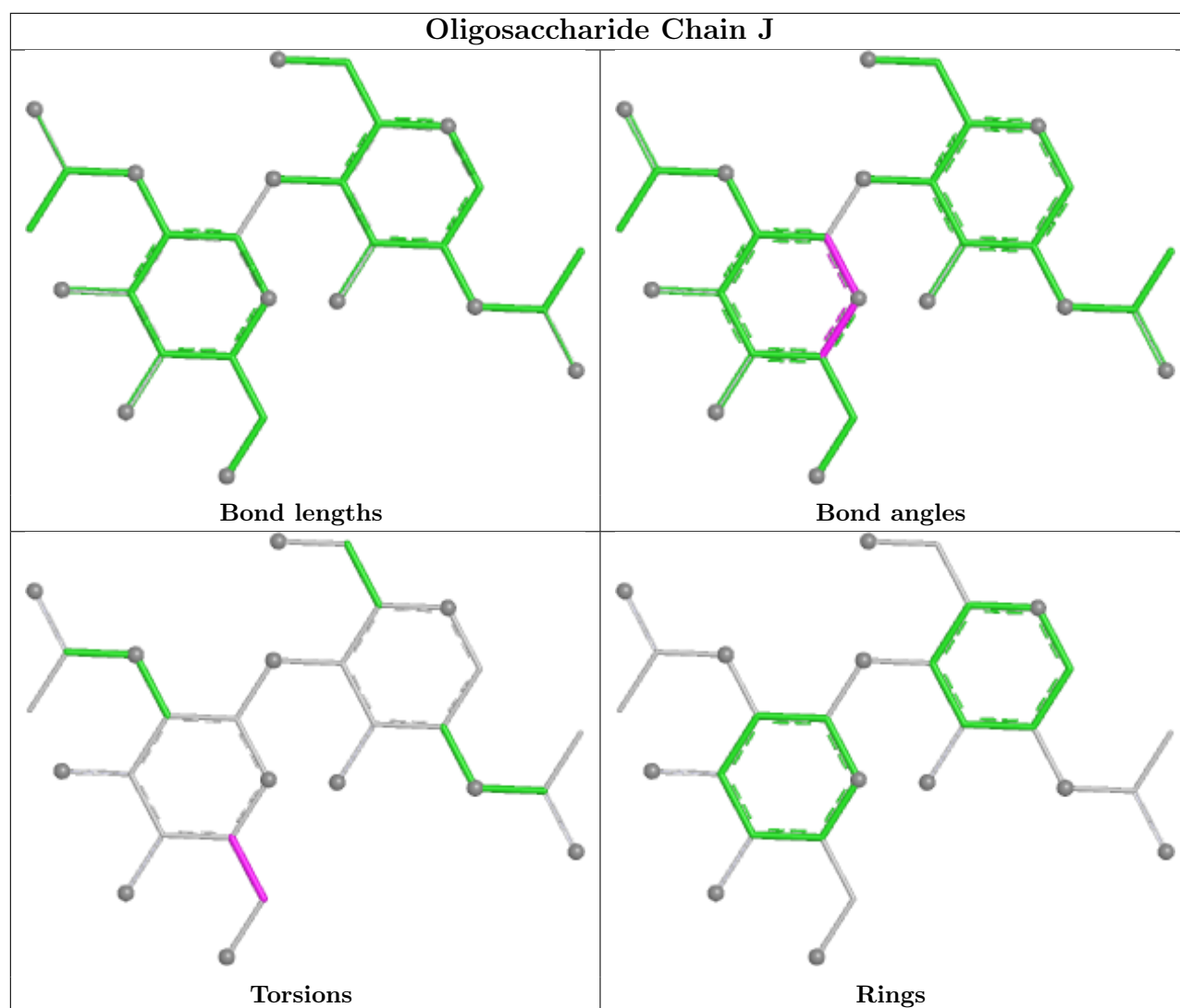
No monomer is involved in short contacts.

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	B	1504	1	14,14,15	0.75	1 (7%)	17,19,21	0.77	1 (5%)
5	CLR	A	1808	-	31,31,31	1.04	2 (6%)	48,48,48	1.67	8 (16%)
4	NAG	E	1502	1	14,14,15	0.54	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PLM	C	205	2	15,16,17	0.32	0	14,15,17	0.66	0
4	NAG	B	1502	1	14,14,15	0.55	0	17,19,21	0.39	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	A	1802	1	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	E	1505	1	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	D	1804	1	14,14,15	0.22	0	17,19,21	0.59	0
4	NAG	D	1801	1	14,14,15	0.88	1 (7%)	17,19,21	2.39	4 (23%)
4	NAG	A	1807	1	14,14,15	0.40	0	17,19,21	0.42	0
4	NAG	D	1802	1	14,14,15	0.24	0	17,19,21	0.57	0
5	CLR	A	1809	-	31,31,31	0.72	0	48,48,48	1.56	9 (18%)
5	CLR	D	1810	-	31,31,31	0.68	0	48,48,48	1.27	6 (12%)
5	CLR	C	201	2	31,31,31	1.02	1 (3%)	48,48,48	1.98	9 (18%)
4	NAG	B	1503	1	14,14,15	0.92	1 (7%)	17,19,21	1.40	3 (17%)
5	CLR	B	1508	-	31,31,31	0.90	2 (6%)	48,48,48	1.58	9 (18%)
4	NAG	D	1807	1	14,14,15	0.40	0	17,19,21	0.42	0
4	NAG	E	1501	1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
4	NAG	B	1501	1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
4	NAG	A	1803	1	14,14,15	0.79	1 (7%)	17,19,21	1.28	2 (11%)
5	CLR	D	1808	-	31,31,31	1.03	2 (6%)	48,48,48	1.67	8 (16%)
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%)
8	PLM	F	205	2	15,16,17	0.32	0	14,15,17	0.66	0
4	NAG	E	1503	1	14,14,15	0.95	1 (7%)	17,19,21	1.40	3 (17%)
5	CLR	E	1508	-	31,31,31	0.90	2 (6%)	48,48,48	1.58	9 (18%)
4	NAG	D	1803	1	14,14,15	0.78	1 (7%)	17,19,21	1.28	2 (11%)
4	NAG	A	1804	1	14,14,15	0.22	0	17,19,21	0.59	0
4	NAG	E	1504	1	14,14,15	0.75	0	17,19,21	0.77	1 (5%)
4	NAG	A	1801	1	14,14,15	0.87	1 (7%)	17,19,21	2.39	4 (23%)

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	B	1504	1	-	4/6/23/26	0/1/1/1
5	CLR	A	1808	-	-	9/10/68/68	0/4/4/4

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

All (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
4	E	1503	NAG	O5-C1	-2.60	1.39	1.43
5	D	1808	CLR	C13-C14	-2.58	1.50	1.55
4	A	1803	NAG	O5-C1	-2.58	1.39	1.43
4	D	1803	NAG	O5-C1	-2.56	1.39	1.43
5	D	1808	CLR	C10-C9	-2.55	1.52	1.56
4	B	1503	NAG	O5-C1	-2.53	1.39	1.43
5	A	1808	CLR	C10-C9	-2.50	1.52	1.56
5	E	1508	CLR	C10-C9	-2.29	1.52	1.56
5	B	1508	CLR	C10-C9	-2.24	1.52	1.56
5	E	1508	CLR	C13-C14	-2.11	1.51	1.55
4	B	1501	NAG	O5-C1	2.11	1.47	1.43
4	E	1501	NAG	O5-C1	2.10	1.47	1.43
5	B	1508	CLR	C13-C14	-2.10	1.51	1.55
4	B	1504	NAG	O5-C1	2.05	1.47	1.43

All (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
5	F	201	CLR	C13-C14-C8	-5.60	106.46	114.41
5	C	201	CLR	C8-C7-C6	-4.94	105.92	112.76
5	F	201	CLR	C8-C7-C6	-4.90	105.98	112.76
5	E	1508	CLR	C13-C17-C20	-4.79	112.09	119.50
5	B	1508	CLR	C13-C17-C20	-4.76	112.14	119.50
5	D	1808	CLR	C13-C14-C8	-4.72	107.72	114.41
5	A	1808	CLR	C13-C14-C8	-4.70	107.75	114.41
5	C	201	CLR	C3-C4-C5	-4.59	104.75	112.05
5	F	201	CLR	C3-C4-C5	-4.57	104.77	112.05
5	A	1809	CLR	C10-C9-C8	-4.50	106.14	112.71
5	D	1809	CLR	C10-C9-C8	-4.49	106.16	112.71
5	D	1808	CLR	C13-C17-C20	-4.44	112.64	119.50
5	A	1808	CLR	C13-C17-C20	-4.42	112.68	119.50
5	B	1508	CLR	C13-C14-C8	-4.05	108.66	114.41
5	E	1508	CLR	C13-C14-C8	-4.04	108.67	114.41
4	B	1503	NAG	C2-N2-C7	3.92	128.16	122.90
4	E	1503	NAG	C2-N2-C7	3.92	128.15	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	NAG	C1-C2-N2	3.81	116.44	110.43
4	D	1801	NAG	C1-C2-N2	3.79	116.40	110.43
5	F	201	CLR	C17-C13-C14	3.69	104.33	100.10
5	C	201	CLR	C17-C13-C14	3.66	104.30	100.10
4	D	1803	NAG	C2-N2-C7	3.47	127.56	122.90
4	A	1803	NAG	C2-N2-C7	3.46	127.54	122.90
5	A	1808	CLR	C17-C13-C14	3.12	103.68	100.10
5	B	1508	CLR	C7-C8-C9	3.10	113.30	109.72
5	E	1508	CLR	C7-C8-C9	3.07	113.27	109.72
5	D	1808	CLR	C11-C9-C10	-3.06	109.32	113.08
5	D	1808	CLR	C17-C13-C14	3.05	103.60	100.10
5	A	1808	CLR	C11-C9-C10	-3.04	109.33	113.08
5	D	1809	CLR	C1-C10-C9	2.92	112.60	108.74
5	A	1809	CLR	C1-C10-C9	2.91	112.59	108.74
5	A	1810	CLR	C13-C17-C20	-2.87	115.06	119.50
5	D	1809	CLR	C14-C8-C9	2.85	112.81	109.09
5	A	1809	CLR	C14-C8-C9	2.84	112.79	109.09
5	D	1810	CLR	C13-C17-C20	-2.81	115.16	119.50
5	D	1808	CLR	C1-C10-C9	2.80	112.44	108.74
5	B	1508	CLR	C14-C8-C9	-2.79	105.44	109.09
5	A	1808	CLR	C1-C10-C9	2.79	112.43	108.74
5	E	1508	CLR	C14-C8-C9	-2.76	105.48	109.09
5	D	1809	CLR	C21-C20-C17	2.74	117.00	112.88
5	A	1809	CLR	C21-C20-C17	2.73	116.98	112.88
5	D	1809	CLR	C19-C10-C9	-2.72	108.61	111.66
5	A	1809	CLR	C19-C10-C9	-2.72	108.61	111.66
5	E	1508	CLR	C4-C5-C10	2.70	119.88	116.42
5	B	1508	CLR	C4-C5-C10	2.69	119.87	116.42
5	B	1508	CLR	C17-C13-C14	2.66	103.16	100.10
5	E	1508	CLR	C17-C13-C14	2.65	103.14	100.10
5	D	1808	CLR	C7-C6-C5	-2.62	120.60	125.02
5	A	1808	CLR	C7-C6-C5	-2.59	120.66	125.02
5	A	1810	CLR	C8-C7-C6	-2.50	109.30	112.76
5	D	1810	CLR	C8-C7-C6	-2.46	109.35	112.76
5	A	1809	CLR	C1-C2-C3	2.46	113.73	110.48
5	D	1809	CLR	C1-C2-C3	2.44	113.72	110.48
5	E	1508	CLR	C11-C12-C13	-2.44	108.62	112.74
5	B	1508	CLR	C11-C12-C13	-2.44	108.63	112.74
4	E	1503	NAG	C4-C3-C2	2.42	114.56	111.02
4	B	1503	NAG	C4-C3-C2	2.41	114.54	111.02
5	A	1810	CLR	C14-C8-C9	2.39	112.21	109.09
5	D	1810	CLR	C14-C8-C9	2.39	112.20	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1508	CLR	C7-C6-C5	-2.38	121.01	125.02
5	D	1810	CLR	C22-C20-C17	2.36	115.23	110.33
4	E	1503	NAG	C1-C2-N2	2.36	114.14	110.43
5	B	1508	CLR	C7-C6-C5	-2.36	121.04	125.02
5	A	1810	CLR	C22-C20-C17	2.35	115.19	110.33
4	B	1503	NAG	C1-C2-N2	2.33	114.11	110.43
5	D	1810	CLR	C10-C9-C8	-2.33	109.32	112.71
4	B	1504	NAG	C1-O5-C5	2.29	115.26	112.19
4	E	1504	NAG	C1-O5-C5	2.29	115.26	112.19
5	A	1810	CLR	C10-C9-C8	-2.29	109.37	112.71
5	A	1809	CLR	C7-C6-C5	-2.28	121.17	125.02
5	D	1809	CLR	C7-C6-C5	-2.27	121.18	125.02
5	C	201	CLR	C4-C5-C6	-2.27	117.49	120.57
5	D	1809	CLR	C4-C5-C10	2.23	119.28	116.42
5	A	1809	CLR	C4-C5-C10	2.22	119.27	116.42
5	F	201	CLR	C4-C5-C6	-2.21	117.57	120.57
4	A	1803	NAG	C1-C2-N2	2.20	113.90	110.43
4	D	1803	NAG	C1-C2-N2	2.19	113.88	110.43
5	A	1808	CLR	C7-C8-C9	2.16	112.21	109.72
5	D	1809	CLR	C1-C10-C5	-2.15	105.04	108.74
4	A	1801	NAG	C8-C7-N2	2.14	119.67	116.12
5	B	1508	CLR	C10-C5-C6	-2.14	119.80	122.93
5	A	1809	CLR	C1-C10-C5	-2.14	105.05	108.74
5	C	201	CLR	C16-C17-C13	2.14	106.35	103.84
5	D	1808	CLR	C7-C8-C9	2.14	112.19	109.72
4	D	1801	NAG	C8-C7-N2	2.13	119.66	116.12
5	A	1808	CLR	C10-C9-C8	-2.13	109.60	112.71
5	D	1808	CLR	C10-C9-C8	-2.13	109.60	112.71
5	E	1508	CLR	C10-C5-C6	-2.13	119.83	122.93
5	C	201	CLR	C11-C12-C13	-2.08	109.22	112.74
5	F	201	CLR	C16-C17-C13	2.08	106.29	103.84
5	F	201	CLR	C11-C12-C13	-2.06	109.27	112.74
4	D	1801	NAG	C1-O5-C5	2.03	114.91	112.19
5	A	1810	CLR	C4-C5-C10	2.03	119.02	116.42
5	C	201	CLR	C7-C6-C5	-2.03	121.60	125.02
4	A	1801	NAG	C1-O5-C5	2.02	114.89	112.19
5	D	1810	CLR	C4-C5-C10	2.01	119.00	116.42

There are no chirality outliers.

All (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
5	F	201	CLR	C22-C23-C24-C25
5	A	1810	CLR	C16-C17-C20-C21
5	D	1810	CLR	C16-C17-C20-C21
5	A	1810	CLR	C13-C17-C20-C22
5	D	1810	CLR	C13-C17-C20-C22
4	A	1801	NAG	C4-C5-C6-O6
4	D	1801	NAG	C4-C5-C6-O6
4	B	1505	NAG	O5-C5-C6-O6
4	E	1505	NAG	O5-C5-C6-O6
5	A	1810	CLR	C16-C17-C20-C22
5	D	1810	CLR	C16-C17-C20-C22
4	B	1505	NAG	C4-C5-C6-O6
4	E	1505	NAG	C4-C5-C6-O6
4	A	1803	NAG	O5-C5-C6-O6
4	D	1803	NAG	O5-C5-C6-O6
4	E	1504	NAG	C4-C5-C6-O6
4	A	1801	NAG	O5-C5-C6-O6
4	D	1801	NAG	O5-C5-C6-O6
4	B	1504	NAG	C4-C5-C6-O6
5	A	1810	CLR	C17-C20-C22-C23
5	D	1810	CLR	C17-C20-C22-C23
8	C	205	PLM	C6-C7-C8-C9
8	F	205	PLM	C6-C7-C8-C9
4	A	1803	NAG	C4-C5-C6-O6
4	D	1803	NAG	C4-C5-C6-O6
5	A	1810	CLR	C21-C20-C22-C23
5	D	1810	CLR	C21-C20-C22-C23
5	A	1808	CLR	C22-C23-C24-C25
5	D	1808	CLR	C22-C23-C24-C25
4	A	1801	NAG	C8-C7-N2-C2
4	A	1801	NAG	O7-C7-N2-C2
4	B	1504	NAG	C8-C7-N2-C2
4	B	1504	NAG	O7-C7-N2-C2
4	B	1505	NAG	C8-C7-N2-C2
4	B	1505	NAG	O7-C7-N2-C2
4	D	1801	NAG	C8-C7-N2-C2
4	D	1801	NAG	O7-C7-N2-C2
4	E	1504	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	E	1504	NAG	O7-C7-N2-C2
4	E	1505	NAG	C8-C7-N2-C2
4	E	1505	NAG	O7-C7-N2-C2
5	A	1808	CLR	C13-C17-C20-C21
5	D	1808	CLR	C13-C17-C20-C21
5	A	1808	CLR	C13-C17-C20-C22
5	D	1808	CLR	C13-C17-C20-C22
4	A	1807	NAG	O5-C5-C6-O6
4	D	1807	NAG	O5-C5-C6-O6
8	C	205	PLM	C9-CA-CB-CC
8	F	205	PLM	C9-CA-CB-CC
4	B	1504	NAG	O5-C5-C6-O6
4	E	1504	NAG	O5-C5-C6-O6
5	A	1808	CLR	C16-C17-C20-C21
5	D	1808	CLR	C16-C17-C20-C21
8	C	205	PLM	C2-C3-C4-C5
8	F	205	PLM	C2-C3-C4-C5
8	C	205	PLM	CA-CB-CC-CD
8	F	205	PLM	CA-CB-CC-CD
5	C	201	CLR	C21-C20-C22-C23
5	F	201	CLR	C21-C20-C22-C23
8	C	205	PLM	CD-CE-CF-CG
8	F	205	PLM	CD-CE-CF-CG
5	A	1808	CLR	C23-C24-C25-C26
5	D	1808	CLR	C23-C24-C25-C26
4	A	1802	NAG	O5-C5-C6-O6
4	D	1802	NAG	O5-C5-C6-O6
5	A	1808	CLR	C17-C20-C22-C23
5	D	1808	CLR	C17-C20-C22-C23
4	A	1804	NAG	O5-C5-C6-O6
4	D	1804	NAG	O5-C5-C6-O6
8	C	205	PLM	C3-C4-C5-C6
8	F	205	PLM	C3-C4-C5-C6
4	A	1803	NAG	C1-C2-N2-C7
4	B	1503	NAG	C1-C2-N2-C7
4	D	1803	NAG	C1-C2-N2-C7
4	E	1503	NAG	C1-C2-N2-C7
5	A	1808	CLR	C23-C24-C25-C27
5	D	1808	CLR	C23-C24-C25-C27
5	B	1508	CLR	C22-C23-C24-C25
5	E	1508	CLR	C22-C23-C24-C25
4	A	1801	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	1803	NAG	C3-C2-N2-C7
4	D	1801	NAG	C3-C2-N2-C7
4	D	1803	NAG	C3-C2-N2-C7
5	A	1808	CLR	C16-C17-C20-C22
5	D	1808	CLR	C16-C17-C20-C22
8	C	205	PLM	C8-C9-CA-CB
8	F	205	PLM	C8-C9-CA-CB
5	E	1508	CLR	C23-C24-C25-C26
5	B	1508	CLR	C23-C24-C25-C26
5	A	1809	CLR	C22-C23-C24-C25
5	D	1809	CLR	C22-C23-C24-C25
5	B	1508	CLR	C20-C22-C23-C24
5	E	1508	CLR	C20-C22-C23-C24
5	B	1508	CLR	C23-C24-C25-C27
5	E	1508	CLR	C23-C24-C25-C27
5	A	1808	CLR	C20-C22-C23-C24
5	D	1808	CLR	C20-C22-C23-C24
4	A	1801	NAG	C1-C2-N2-C7
4	A	1807	NAG	C1-C2-N2-C7
4	D	1801	NAG	C1-C2-N2-C7
4	D	1807	NAG	C1-C2-N2-C7
4	B	1503	NAG	C3-C2-N2-C7
4	E	1503	NAG	C3-C2-N2-C7
4	B	1501	NAG	O5-C5-C6-O6
4	E	1501	NAG	O5-C5-C6-O6
4	A	1807	NAG	C4-C5-C6-O6
4	D	1807	NAG	C4-C5-C6-O6
5	A	1809	CLR	C23-C24-C25-C27
5	D	1809	CLR	C23-C24-C25-C27

There are no ring outliers.

15 monomers are involved in 206 short contacts:

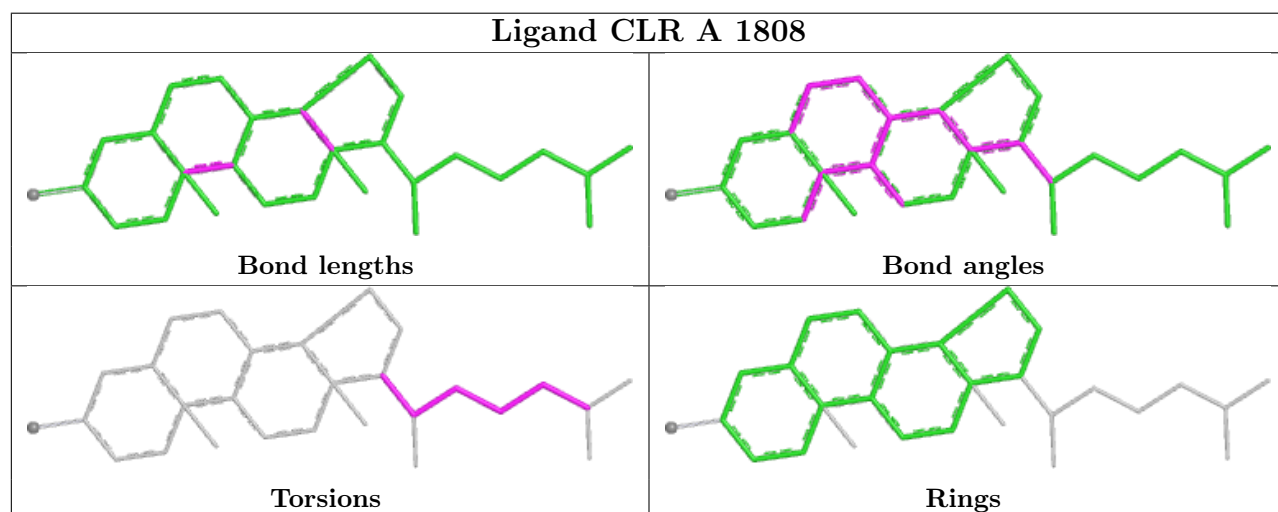
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1808	CLR	31	0
8	C	205	PLM	16	0
5	F	201	CLR	19	0
4	D	1804	NAG	1	0
5	A	1809	CLR	1	0
5	D	1810	CLR	3	0
5	C	201	CLR	19	0
5	B	1508	CLR	30	0

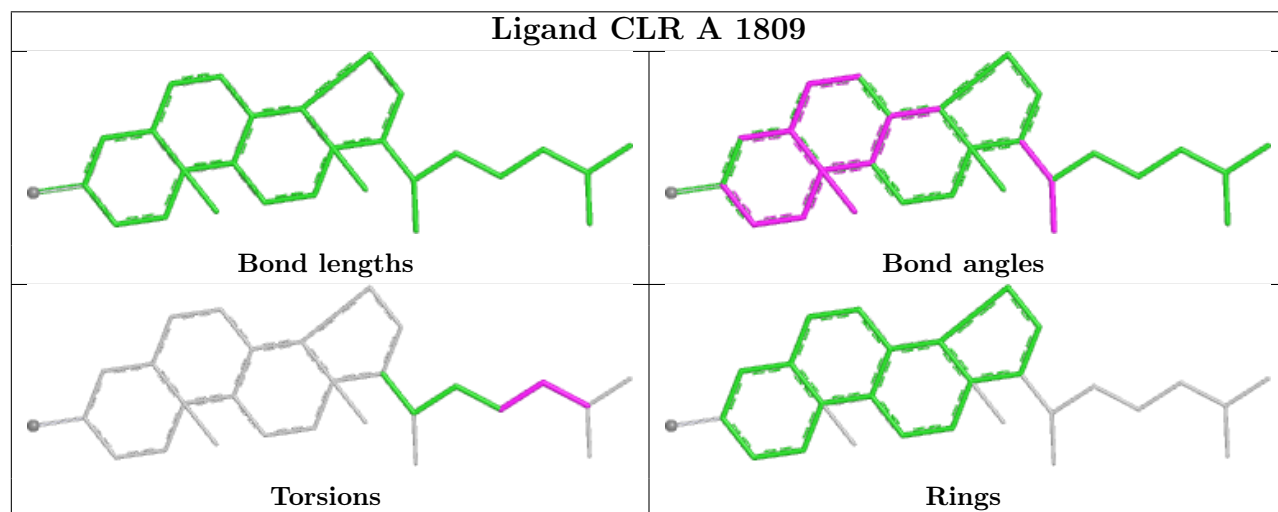
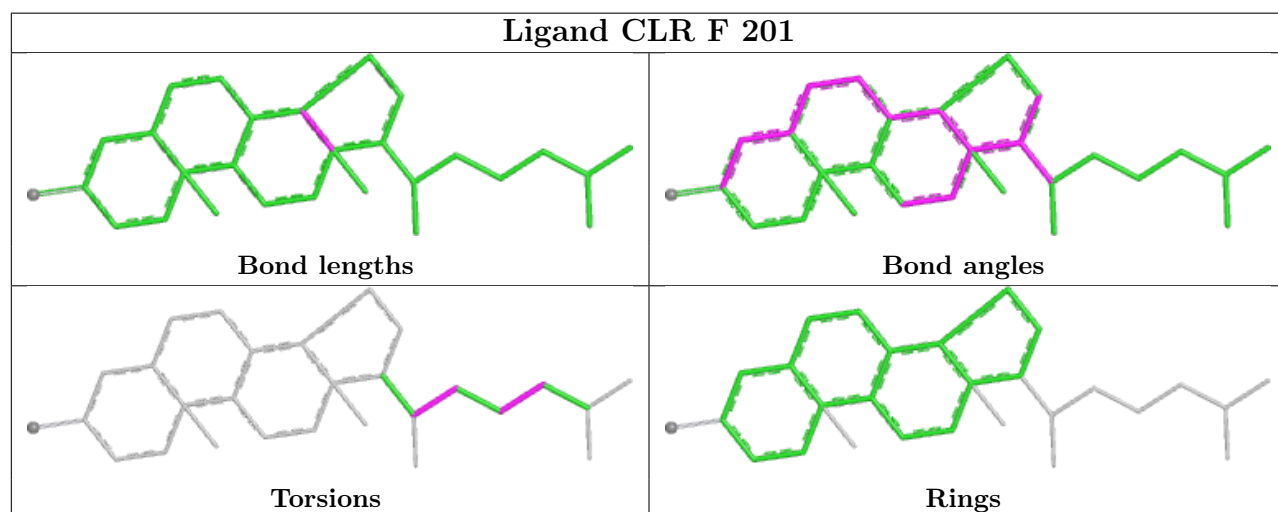
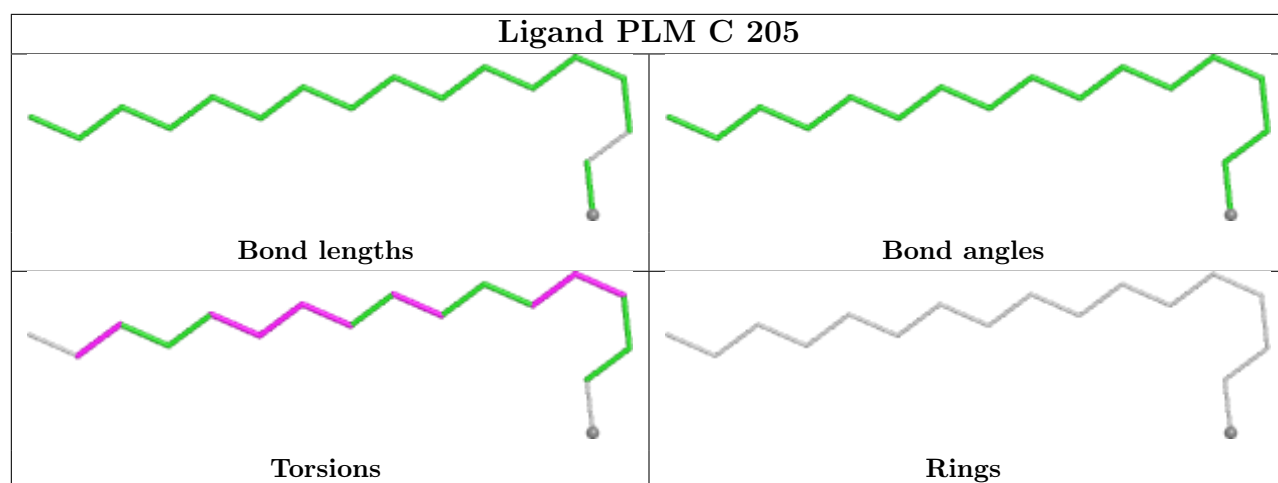
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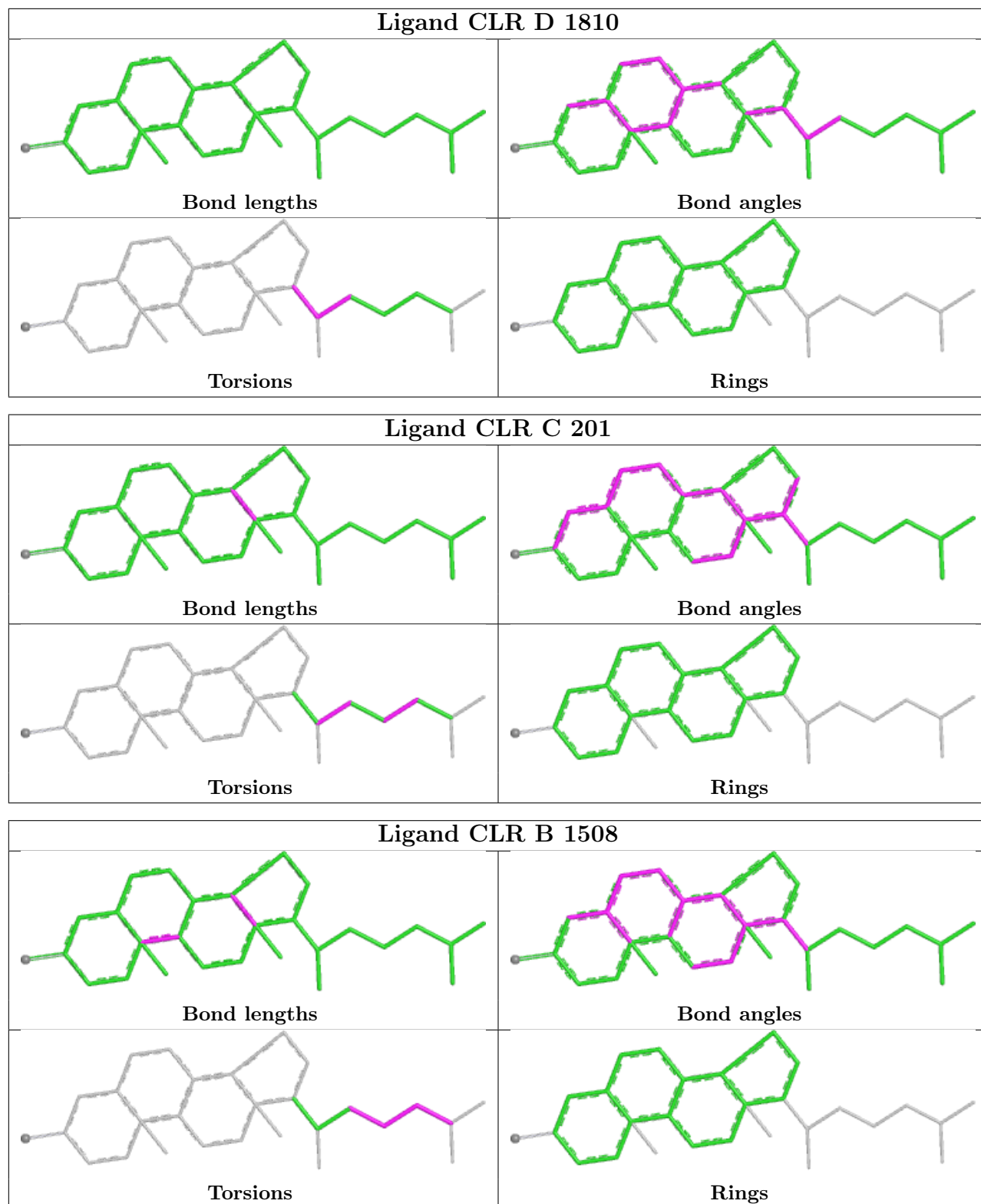
Continued from previous page...

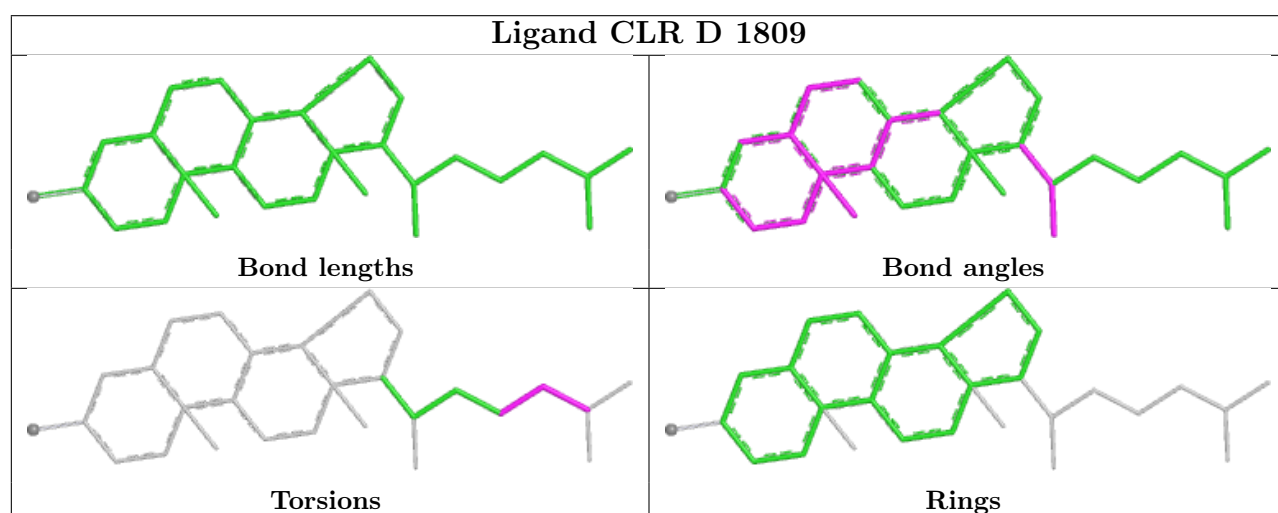
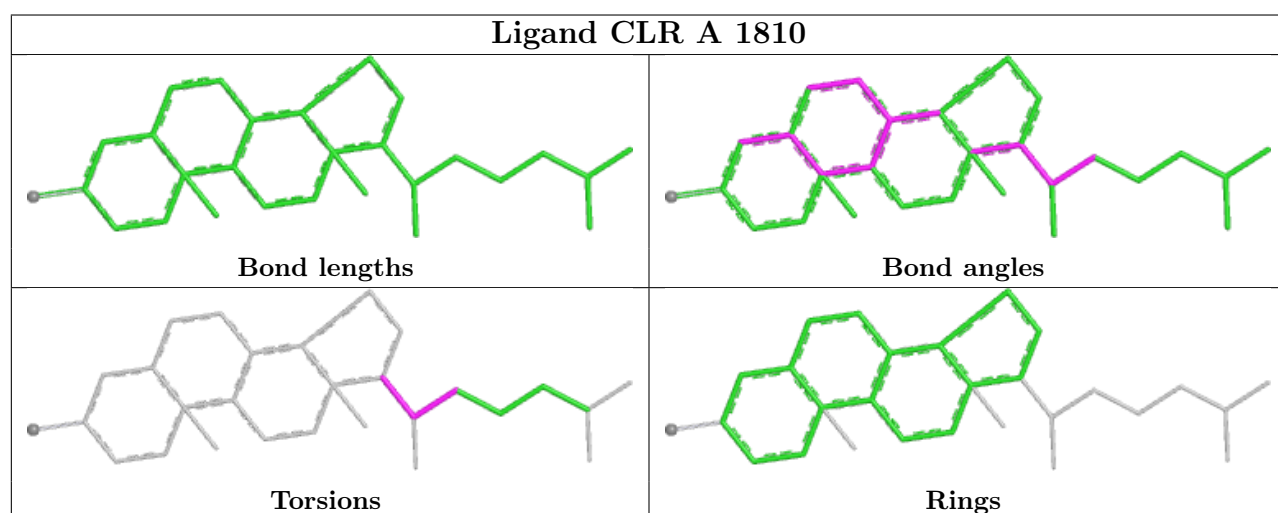
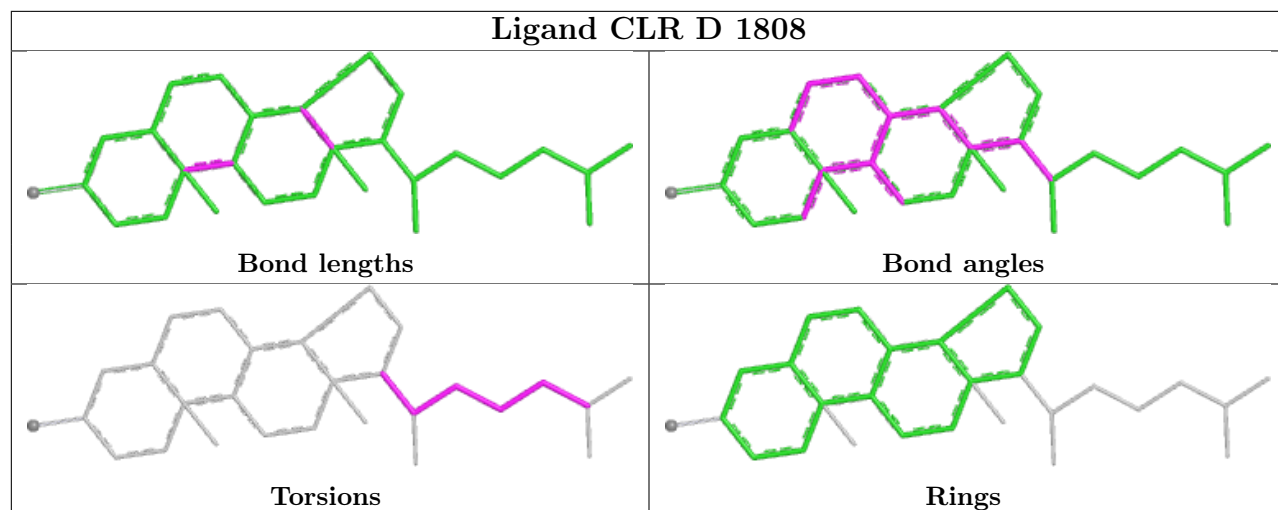
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1501	NAG	1	0
4	B	1501	NAG	1	0
5	D	1808	CLR	30	0
5	A	1810	CLR	3	0
5	D	1809	CLR	2	0
8	F	205	PLM	16	0
5	E	1508	CLR	33	0

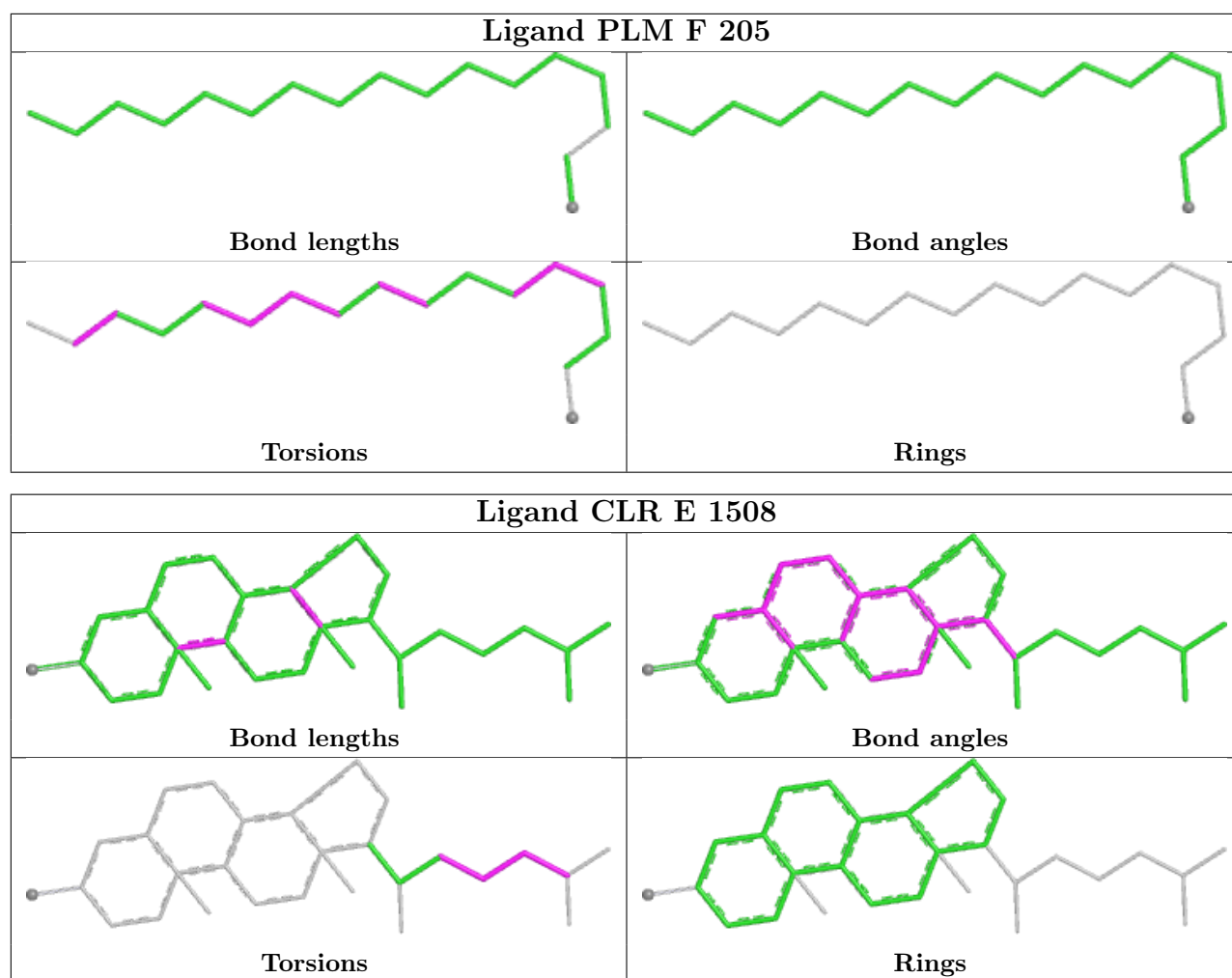
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

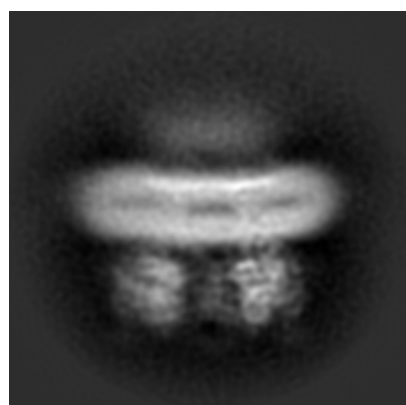
6 Map visualisation [i](#)

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.

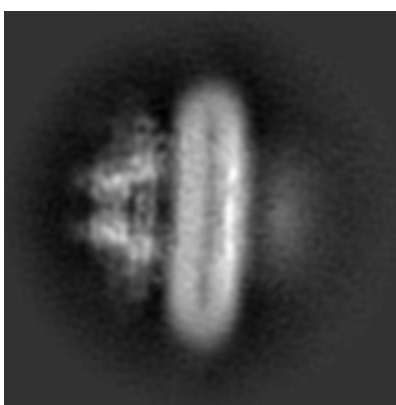
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

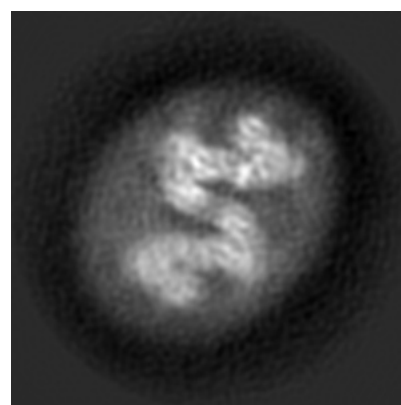
6.1.1 Primary map



X



Y

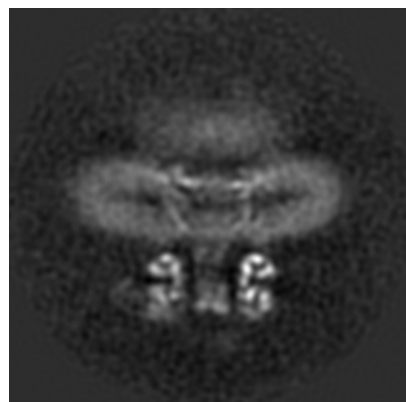


Z

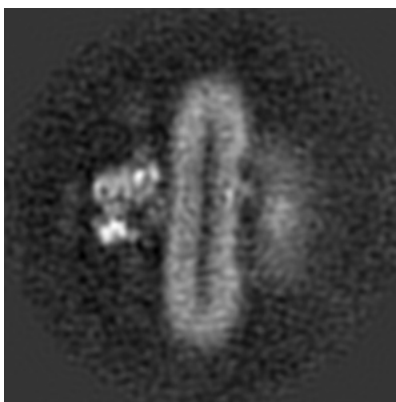
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

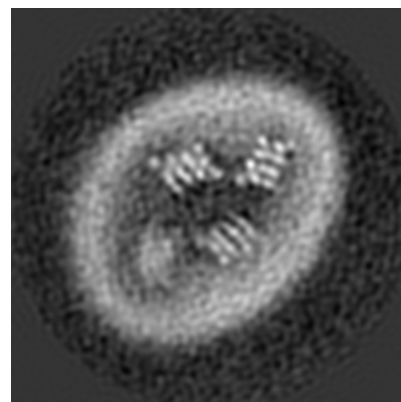
6.2.1 Primary map



X Index: 140



Y Index: 140

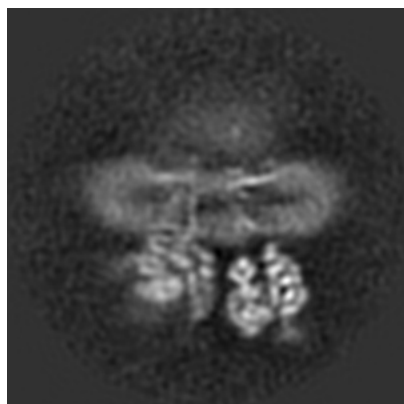


Z Index: 140

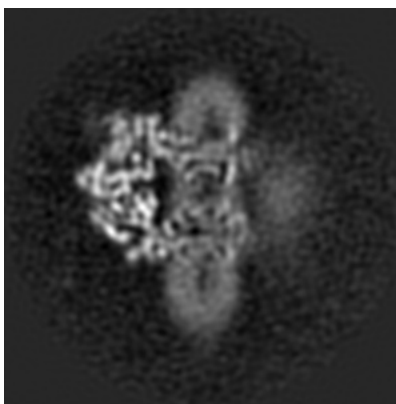
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

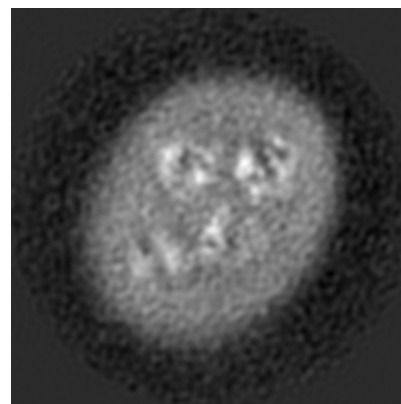
6.3.1 Primary map



X Index: 163



Y Index: 167



Z Index: 158

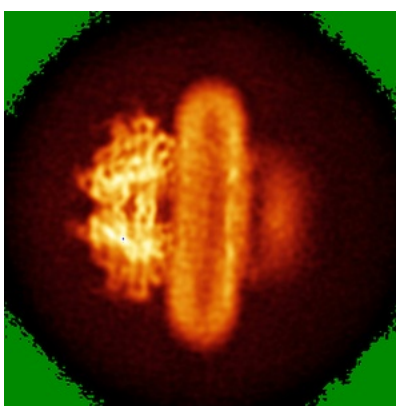
The images above show the largest variance slices of the map in three orthogonal directions.

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

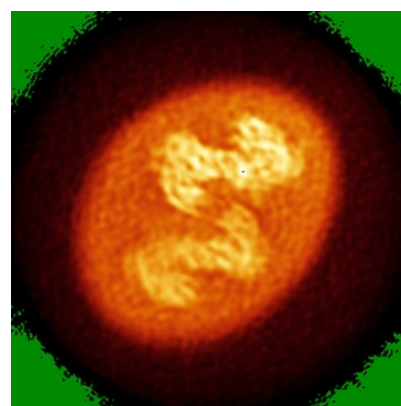
6.4.1 Primary map



X



Y

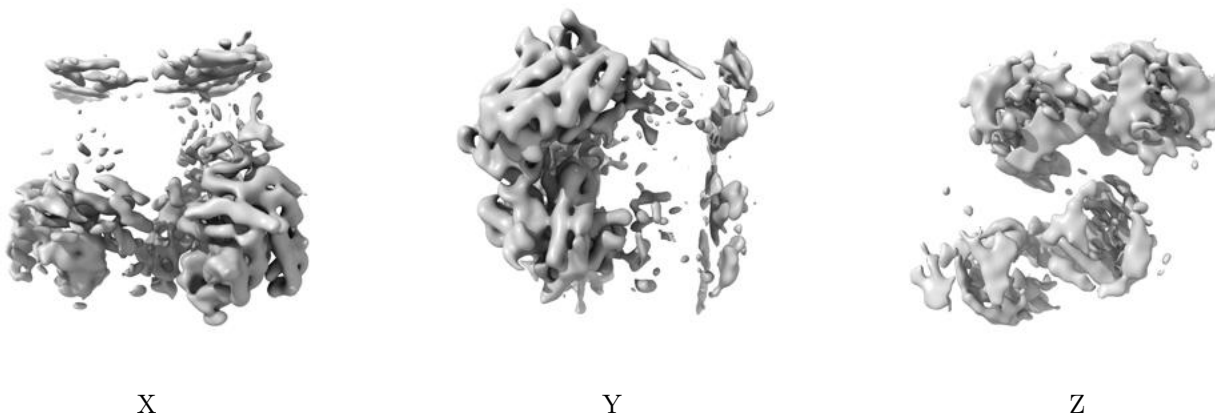


Z

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.

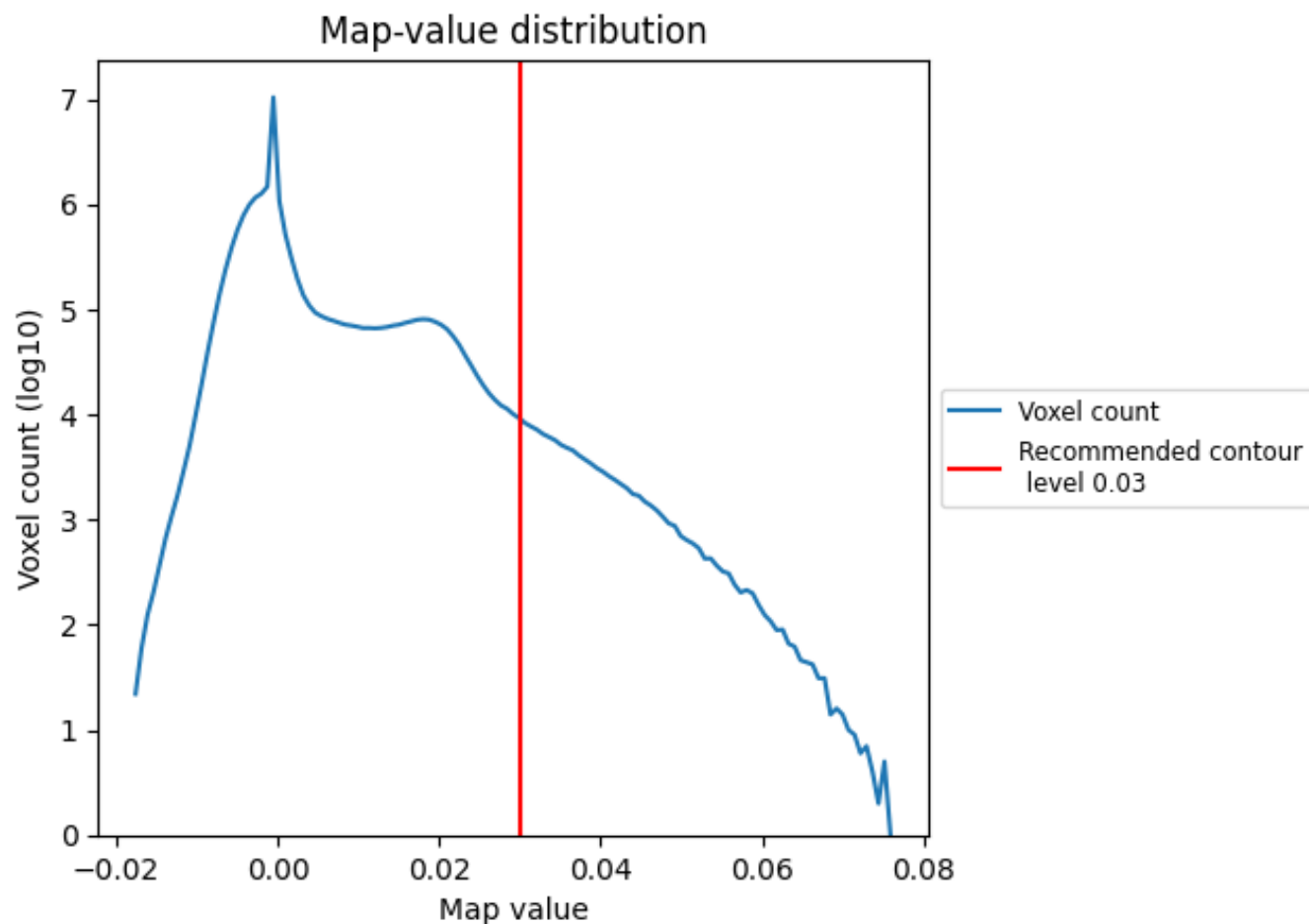
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

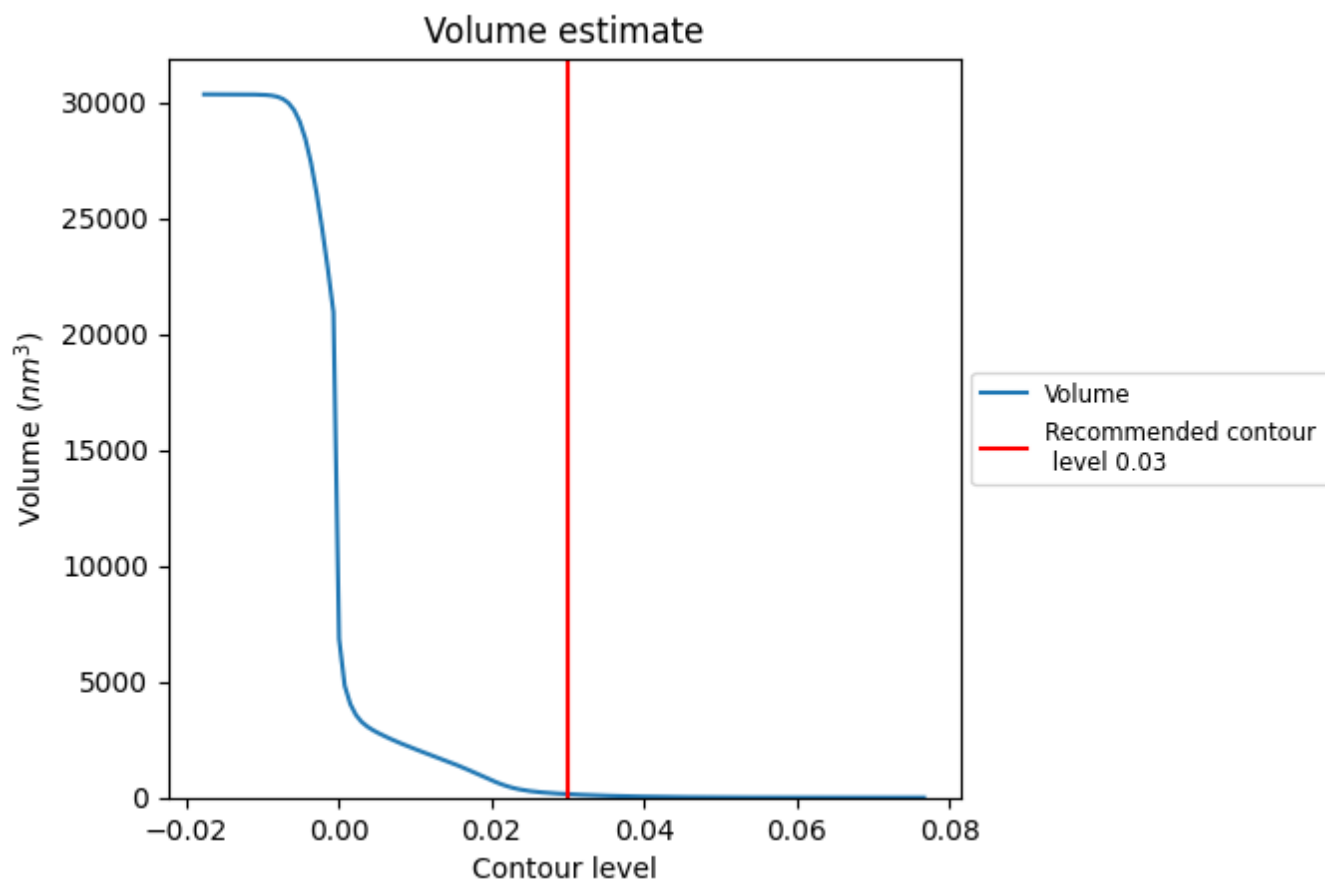
This section contains the results of statistical analysis of the map.

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.

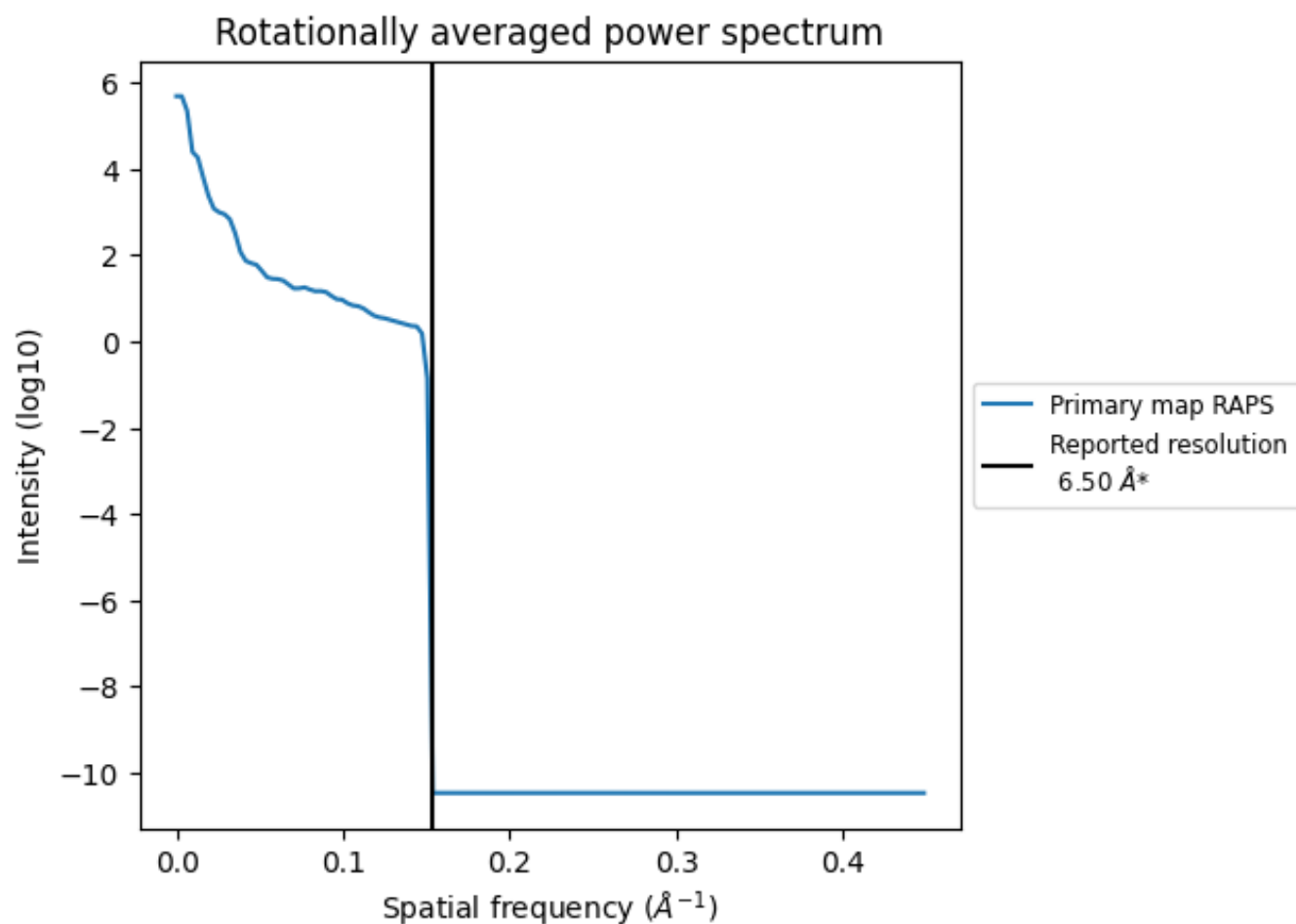
7.2 Volume estimate [i](#)



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 Å⁻¹

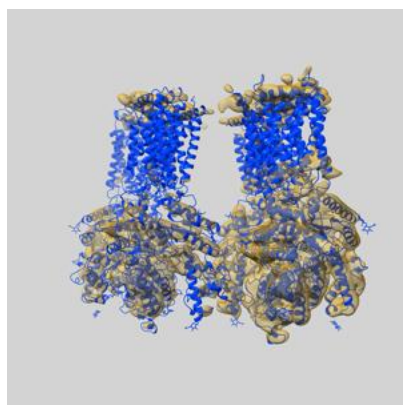
8 Fourier-Shell correlation ⓘ

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

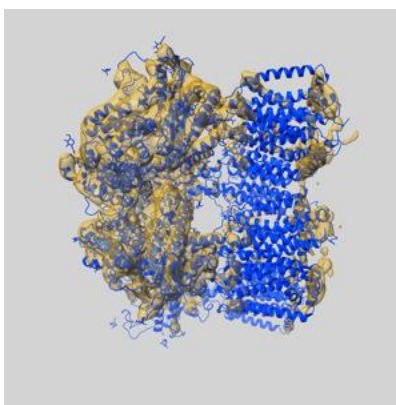
9 Map-model fit [i](#)

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](#).

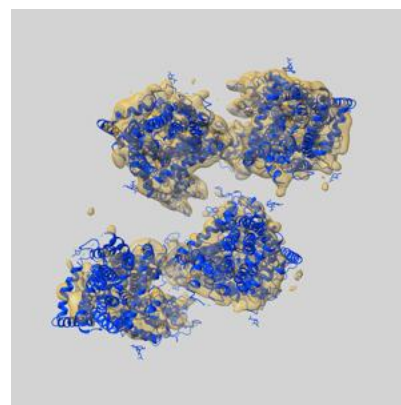
9.1 Map-model overlay [i](#)



X



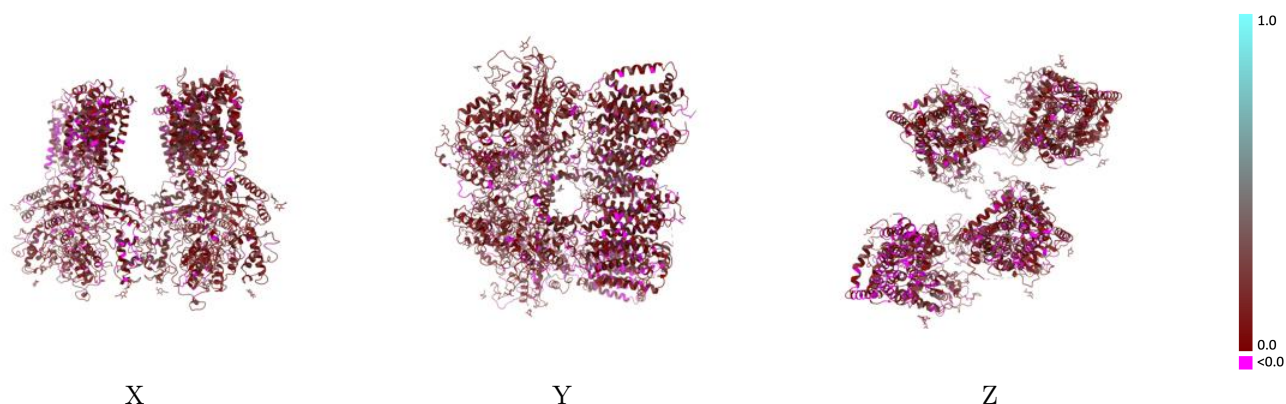
Y



Z

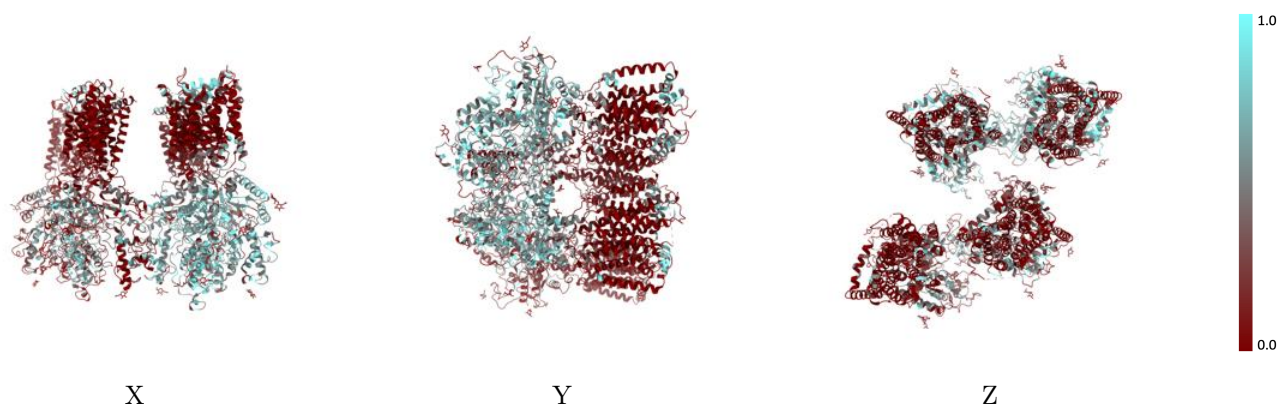
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



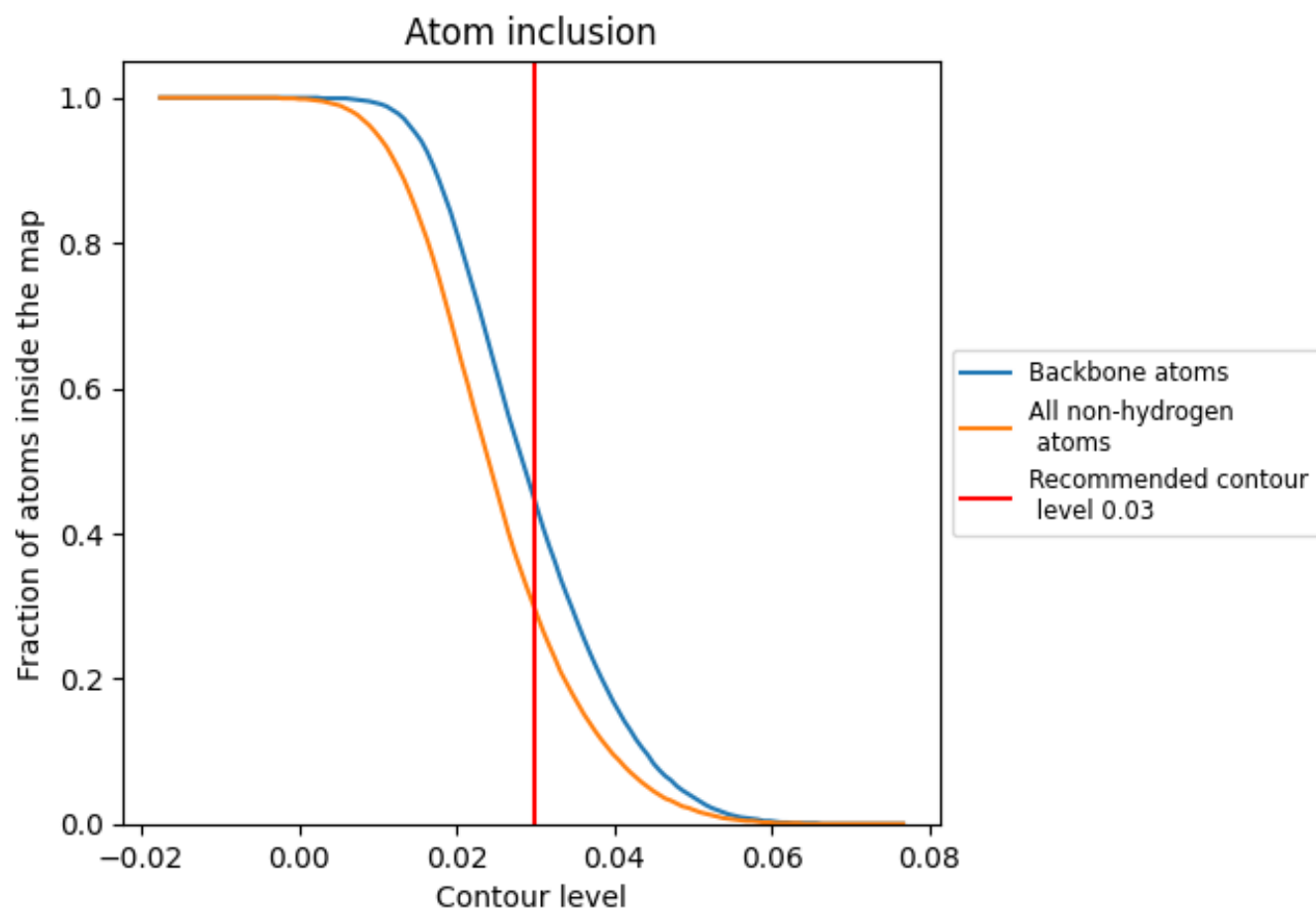
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.2930	0.1320
A	0.3890	0.1540
B	0.3820	0.1470
C	0.5960	0.1560
D	0.1440	0.1000
E	0.2040	0.1230
F	0.3200	0.1380
G	0.0000	0.1940
H	0.0000	0.2760
I	0.0000	0.1120
J	0.0000	0.0750

1.0
0.0
<0.0