



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:29 AM UTC

PDB ID : 7A5O / pdb_00007a5o
EMDB ID : EMD-10517
Title : Human MUC2 AAs 21-1397
Authors : Javitt, G.; Khmelnsky, L.; Albert, L.; Elad, N.; Ilani, T.; Diskin, R.; Fass, D.
Deposited on : 2020-08-21
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

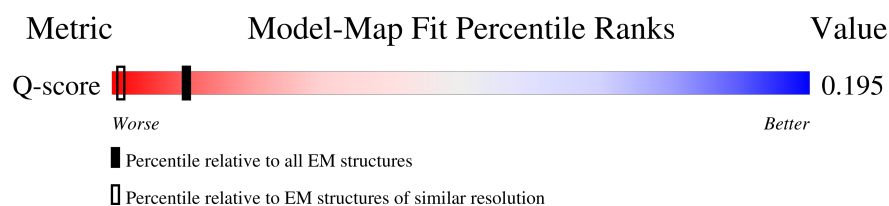
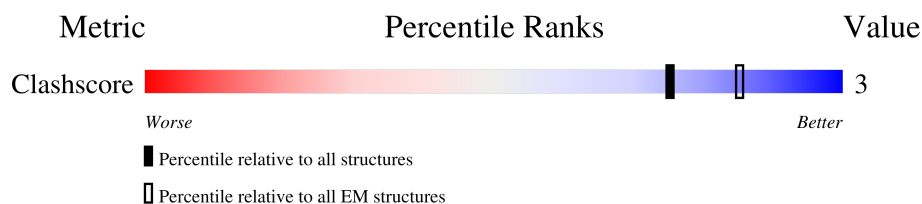
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

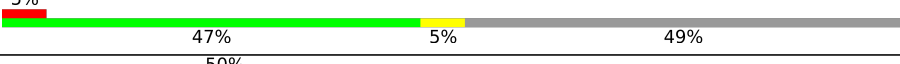
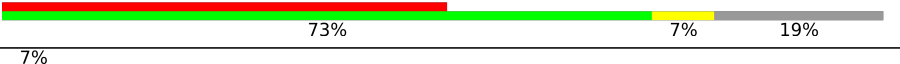
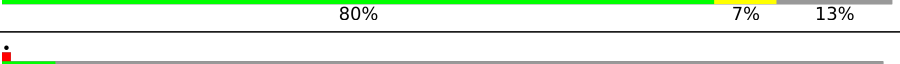
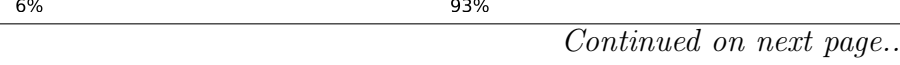
The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	13114 (2.45 - 3.45)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1383	
1	B	1383	
1	C	1383	
1	D	1383	
1	E	1383	
1	F	1383	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	1383	
1	H	1383	
1	I	1383	
1	J	1383	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55254 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 Mucin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1205	Total	C	N	O	S	4	0
			9125	5668	1579	1760	118		
1	B	708	Total	C	N	O	S	3	0
			5276	3278	918	1013	67		
1	C	1115	Total	C	N	O	S	4	0
			8429	5239	1459	1622	109		
1	D	497	Total	C	N	O	S	1	0
			3849	2390	661	747	51		
1	E	1205	Total	C	N	O	S	4	0
			9125	5668	1579	1760	118		
1	F	90	Total	C	N	O	S	0	0
			696	429	120	138	9		
1	G	1115	Total	C	N	O	S	4	0
			8429	5239	1459	1622	109		
1	H	497	Total	C	N	O	S	1	0
			3849	2390	661	747	51		
1	I	708	Total	C	N	O	S	3	0
			5276	3278	918	1013	67		
1	J	90	Total	C	N	O	S	0	0
			696	429	120	138	9		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1325	THR	PRO	conflict	UNP Q02817
A	1398	HIS	-	expression tag	UNP Q02817
A	1399	HIS	-	expression tag	UNP Q02817
A	1400	HIS	-	expression tag	UNP Q02817
A	1401	HIS	-	expression tag	UNP Q02817
A	1402	HIS	-	expression tag	UNP Q02817
A	1403	HIS	-	expression tag	UNP Q02817
B	1325	THR	PRO	conflict	UNP Q02817
B	1398	HIS	-	expression tag	UNP Q02817
B	1399	HIS	-	expression tag	UNP Q02817

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1400	HIS	-	expression tag	UNP Q02817
B	1401	HIS	-	expression tag	UNP Q02817
B	1402	HIS	-	expression tag	UNP Q02817
B	1403	HIS	-	expression tag	UNP Q02817
C	1325	THR	PRO	conflict	UNP Q02817
C	1398	HIS	-	expression tag	UNP Q02817
C	1399	HIS	-	expression tag	UNP Q02817
C	1400	HIS	-	expression tag	UNP Q02817
C	1401	HIS	-	expression tag	UNP Q02817
C	1402	HIS	-	expression tag	UNP Q02817
C	1403	HIS	-	expression tag	UNP Q02817
D	1325	THR	PRO	conflict	UNP Q02817
D	1398	HIS	-	expression tag	UNP Q02817
D	1399	HIS	-	expression tag	UNP Q02817
D	1400	HIS	-	expression tag	UNP Q02817
D	1401	HIS	-	expression tag	UNP Q02817
D	1402	HIS	-	expression tag	UNP Q02817
D	1403	HIS	-	expression tag	UNP Q02817
E	1325	THR	PRO	conflict	UNP Q02817
E	1398	HIS	-	expression tag	UNP Q02817
E	1399	HIS	-	expression tag	UNP Q02817
E	1400	HIS	-	expression tag	UNP Q02817
E	1401	HIS	-	expression tag	UNP Q02817
E	1402	HIS	-	expression tag	UNP Q02817
E	1403	HIS	-	expression tag	UNP Q02817
F	1325	THR	PRO	conflict	UNP Q02817
F	1398	HIS	-	expression tag	UNP Q02817
F	1399	HIS	-	expression tag	UNP Q02817
F	1400	HIS	-	expression tag	UNP Q02817
F	1401	HIS	-	expression tag	UNP Q02817
F	1402	HIS	-	expression tag	UNP Q02817
F	1403	HIS	-	expression tag	UNP Q02817
G	1325	THR	PRO	conflict	UNP Q02817
G	1398	HIS	-	expression tag	UNP Q02817
G	1399	HIS	-	expression tag	UNP Q02817
G	1400	HIS	-	expression tag	UNP Q02817
G	1401	HIS	-	expression tag	UNP Q02817
G	1402	HIS	-	expression tag	UNP Q02817
G	1403	HIS	-	expression tag	UNP Q02817
H	1325	THR	PRO	conflict	UNP Q02817
H	1398	HIS	-	expression tag	UNP Q02817
H	1399	HIS	-	expression tag	UNP Q02817

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	1400	HIS	-	expression tag	UNP Q02817
H	1401	HIS	-	expression tag	UNP Q02817
H	1402	HIS	-	expression tag	UNP Q02817
H	1403	HIS	-	expression tag	UNP Q02817
I	1325	THR	PRO	conflict	UNP Q02817
I	1398	HIS	-	expression tag	UNP Q02817
I	1399	HIS	-	expression tag	UNP Q02817
I	1400	HIS	-	expression tag	UNP Q02817
I	1401	HIS	-	expression tag	UNP Q02817
I	1402	HIS	-	expression tag	UNP Q02817
I	1403	HIS	-	expression tag	UNP Q02817
J	1325	THR	PRO	conflict	UNP Q02817
J	1398	HIS	-	expression tag	UNP Q02817
J	1399	HIS	-	expression tag	UNP Q02817
J	1400	HIS	-	expression tag	UNP Q02817
J	1401	HIS	-	expression tag	UNP Q02817
J	1402	HIS	-	expression tag	UNP Q02817
J	1403	HIS	-	expression tag	UNP Q02817

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

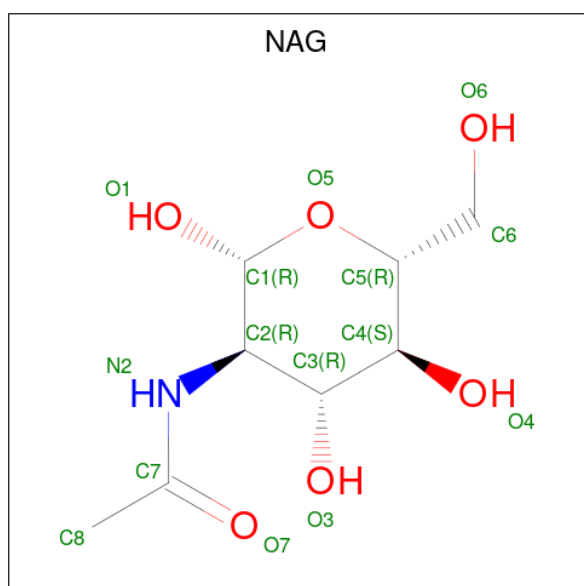


Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	5	Total	Ca	0
			5	5	
3	B	2	Total	Ca	0
			2	2	
3	C	3	Total	Ca	0
			3	3	
3	D	3	Total	Ca	0
			3	3	
3	E	5	Total	Ca	0
			5	5	
3	F	2	Total	Ca	0
			2	2	
3	G	3	Total	Ca	0
			3	3	
3	H	3	Total	Ca	0
			3	3	
3	I	2	Total	Ca	0
			2	2	
3	J	2	Total	Ca	0
			2	2	

- 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	

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	23	Total	O	0
			23	23	
5	B	10	Total	O	0
			10	10	
5	C	22	Total	O	0
			22	22	
5	D	13	Total	O	0
			13	13	
5	E	23	Total	O	0
			23	23	
5	F	1	Total	O	0
			1	1	
5	G	22	Total	O	0
			22	22	
5	H	13	Total	O	0
			13	13	

Continued on next page...

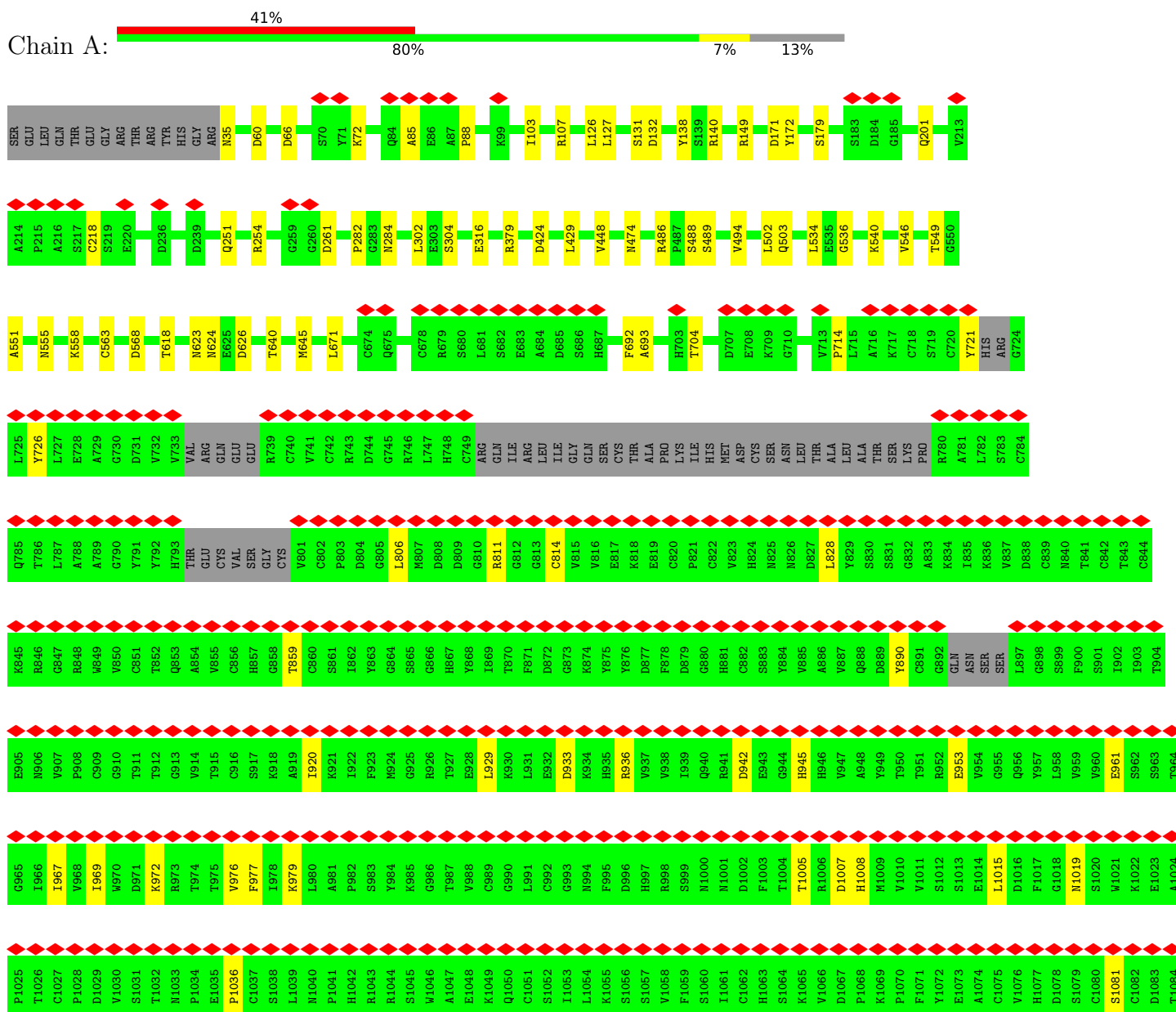
Continued from previous page...

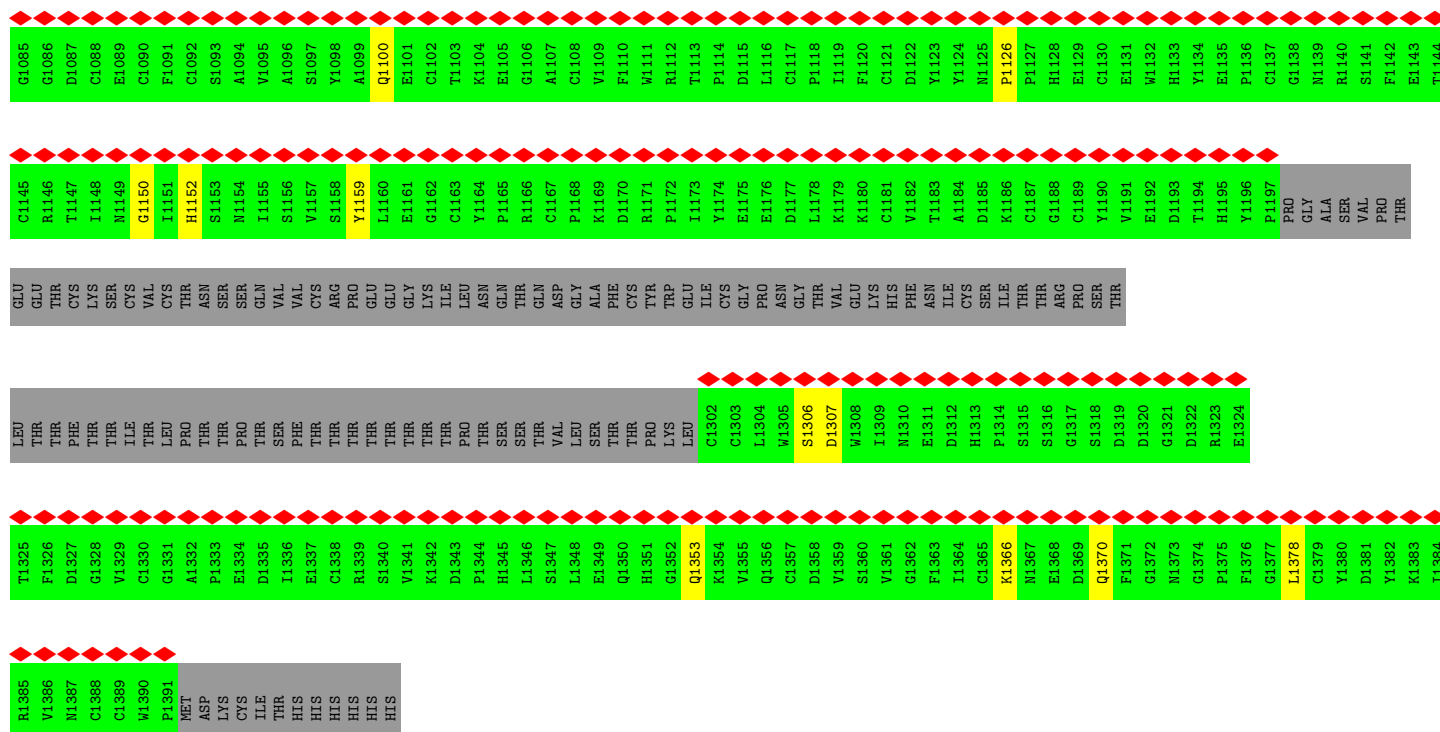
Mol	Chain	Residues	Atoms		AltConf
5	I	10	Total	O	0
			10	10	
5	J	1	Total	O	0
			1	1	

3 Residue-property plots

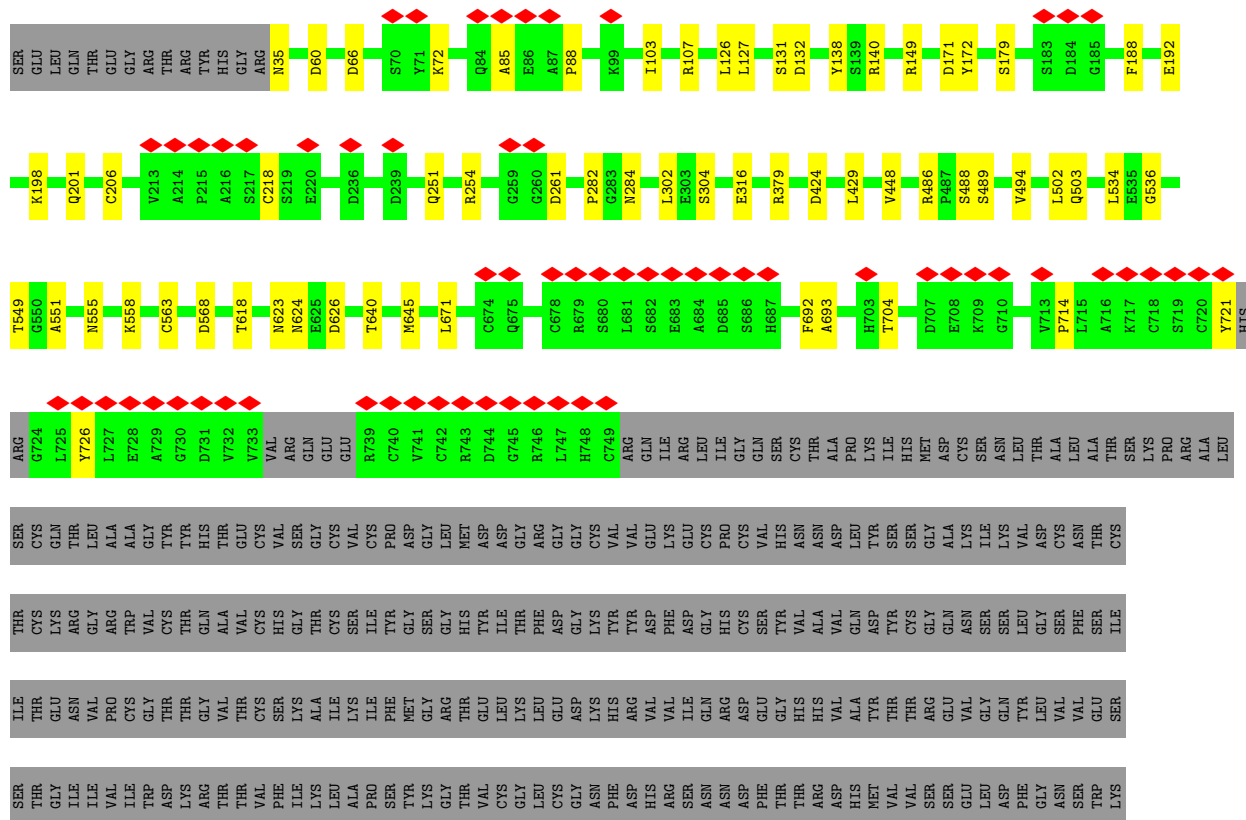
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

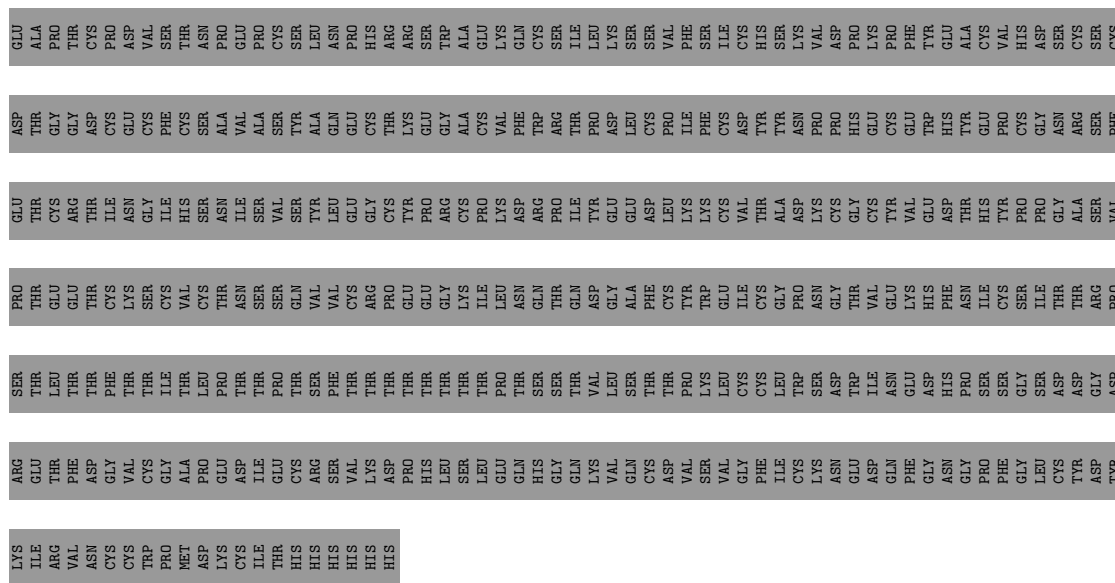
• Molecule 1: Mucin-2



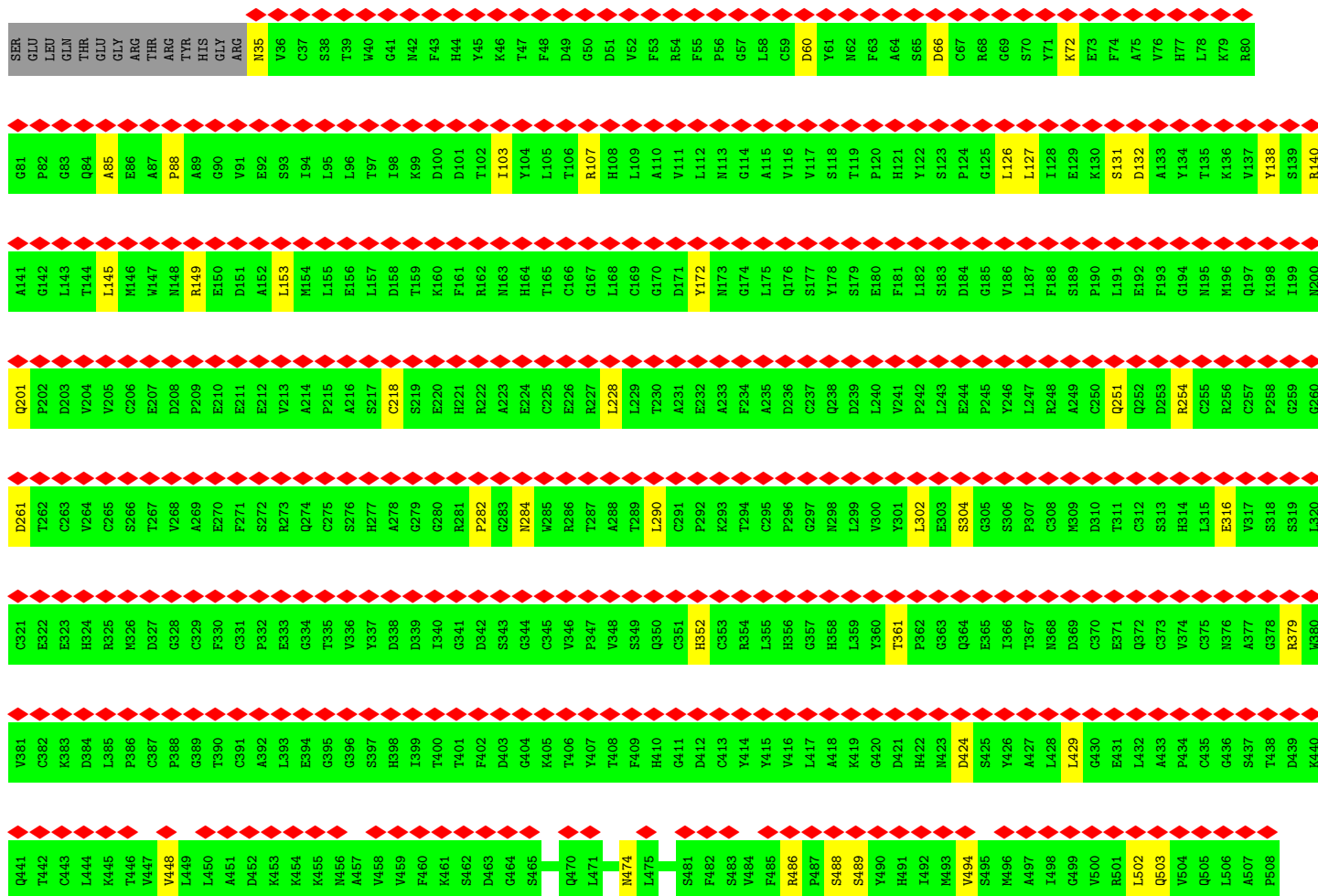
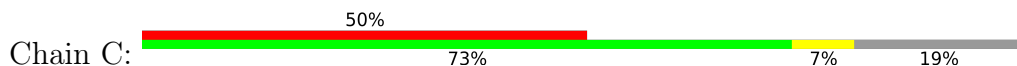


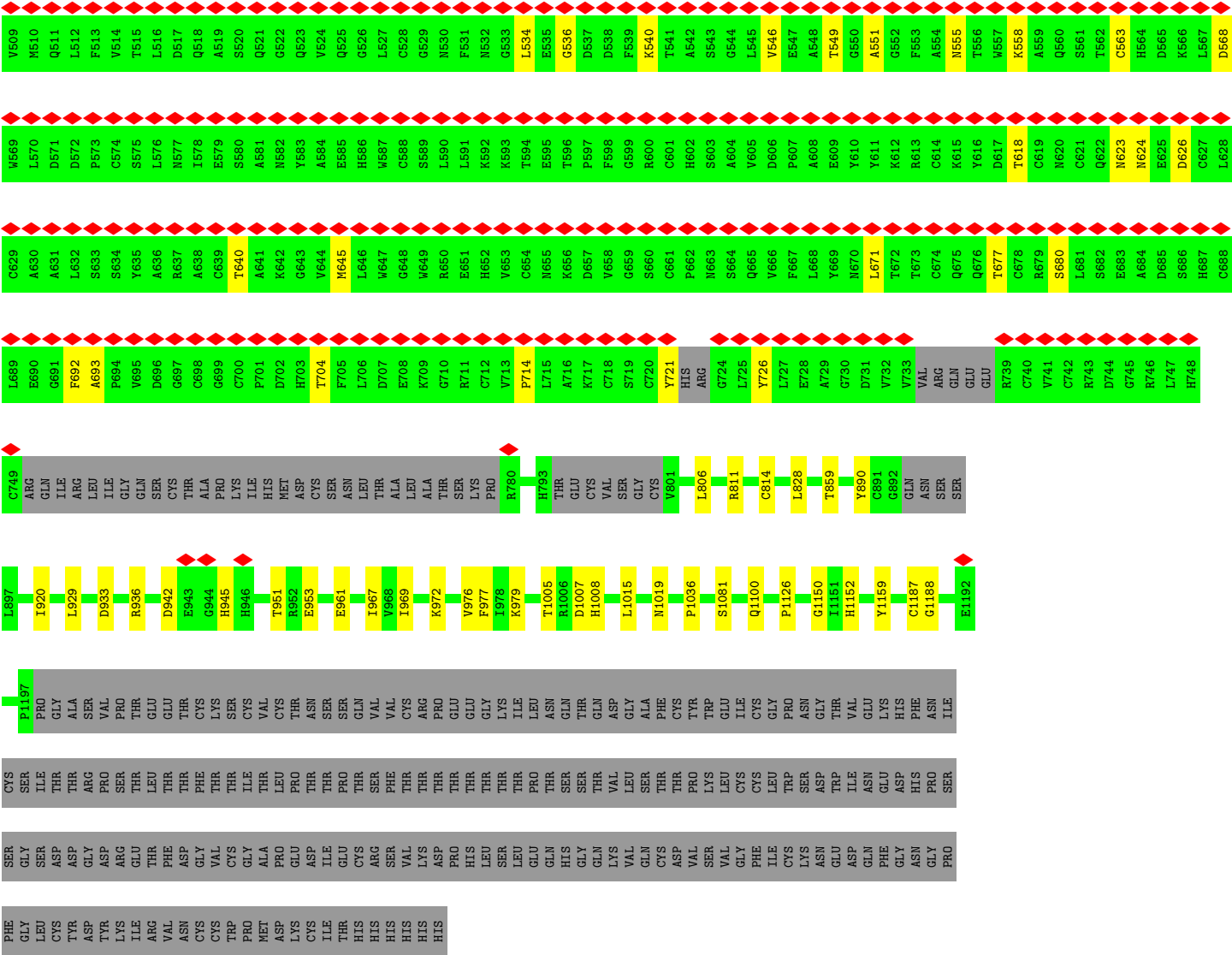
• Molecule 1: Mucin-2



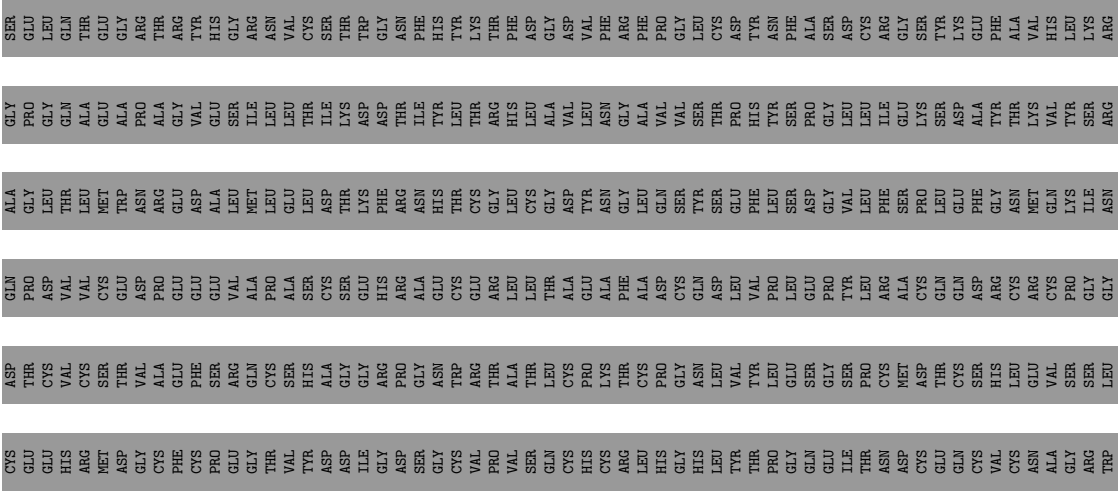


- Molecule 1: Mucin-2





● Molecule 1: Mucin-2



K921	S861	V801	V741	L681	C621	S561	R501	Q441	V381	C321	D261	Q201	A141
I922	I862	C802	C742	S682	Q622	T562	L502	T442	C382	E322	T262	P202	G142
F923	Y863	P803	R743	E683	N623	C563	Q503	L444	K383	E323	C263	D203	L143
M924	G864	D804	D744	A684	N624	H564	W504	L444	D384	H324	V264	V204	T144
G925	S865	G805	G745	D685	E625	D564	Q505	K445	L385	R325	C265	V205	L145
R926	C866	L806	R746	S686	D626	K566	L506	T446	P386	M326	S266	C206	M146
T927	H867	M807	L747	H687	C627	L567	A507	Y447	C387	D327	T267	E207	W147
F928	L868	D808	H748	C688	L628	D568	P508	V448	P388	G328	V268	D208	M148
L929	I869	D809	C749	L689	C629	W569	V509	L449	G389	C329	A269	P209	R149
K930	T870	G810	ARG	E690	A630	L570	M510	L450	T390	F330	E270	E210	E150
L931	F871	R811	GLN	G691	A631	D571	Q511	A451	C391	C331	F271	E211	D151
E932	D872	G812	ILE	F692	L632	D572	L512	D452	A392	P332	S272	E212	A152
D933	ARG	LEU	ARG	A693	S633	P573	F513	K453	L393	E333	R273	V213	L155
K934	G874	C814	ILE	P694	S634	C574	W514	K454	E394	G334	Q274	A214	M154
H935	Y875	V815	GLY	V695	Y635	S575	T515	K455	G395	T335	C275	P215	L155
R936	Y876	V816	SER	D696	A636	L576	L516	M456	G396	V336	S276	A216	E156
V937	D877	E817	CYS	D697	R637	N577	D517	A457	S397	Y337	H277	S217	L157
V938	F878	K818	THR	C698	A638	L578	Q518	V458	H398	D338	A278	C218	D158
I939	D879	E819	ALA	G699	C639	E579	A519	V459	I399	D339	G279	S219	T159
C940	G880	C820	LYS	C700	T640	S580	S520	F460	T400	I340	G280	E220	K160
R941	H881	P821	ILE	P701	A641	A581	Q521	D462	T401	G341	G281	H221	F161
D942	C882	C822	MET	D702	K642	N582	Q522	S462	F402	D342	P282	R222	R162
E943	S883	V823	ASP	H703	G643	Y583	Q523	D463	D403	S343	G283	A223	N163
G944	Y884	H824	CYS	T704	V644	A584	W524	G464	G404	C344	N284	E224	H164
H945	V885	N825	SER	F705	N645	E585	Q525	S465	K405	C345	W285	C225	T165
H946	A886	N826	ASN	L706	L646	H586	Q526	V466	T406	V346	R286	E226	C166
V947	D887	D827	THR	D707	W647	W587	L527	L467	Y407	P347	T287	R227	G167
A948	Q888	L828	ALA	E708	G648	C588	C528	L468	T408	V348	A288	L228	L168
Y949	D889	Y829	LEU	K709	W649	S589	G529	N469	F409	S349	T289	L229	C169
T950	Y890	S830	ALA	G710	R650	L590	N530	Q470	H410	Q350	L290	T230	G170
T951	C891	S831	THR	R711	E651	L591	F531	L471	G411	C351	C291	A231	D171
R952	G892	Q832	LYS	C712	H652	K592	N532	Q472	D412	H352	P292	E232	Y172
E953	GLN	A833	PRO	V713	V653	K593	G533	V473	C413	C353	K293	A233	N173
V954	ASN	K334	R780	P714	C654	T594	L534	M474	Y414	R354	T294	F234	G174
G955	SER	I835	L782	L715	N655	E595	E535	L475	Y415	L355	C295	A235	L175
Q956	SER	K336	L782	A716	K656	T596	Q536	P476	V416	H356	P296	D236	L176
Y957	L897	V837	S783	R717	D657	P597	D537	H477	L417	G357	G297	C237	Q176
L958	S999	D838	C784	C718	V658	F598	D538	V478	A418	H358	N298	Q238	Y178
V959	F900	C839	Q785	S719	G659	G599	F539	T479	K419	L299	L299	D239	S179
V960	S901	N840	T786	C720	R660	G600	K540	A480	D420	Y360	V300	L240	E180
E961	I902	T841	L787	Y721	S660	C601	Y541	S481	D421	T361	Y301	V241	F181
S962	I903	C842	A788	HIS	C661	H602	A542	S481	H422	P362	L302	P242	L182
G963	T904	T843	R789	ARG	P662	H602	A542	F482	H422	P362	L302	P242	L182
V964	S963	C844	G790	G724	N663	S603	S543	S483	M423	G363	E303	P242	L182
G965	E905	C844	Y791	L725	S664	A604	G544	V484	D424	Q364	S304	E244	S184
G966	N906	K845	Y792	L726	Q665	A604	G544	V484	D424	Q364	S304	E244	S184
I967	V907	R846	H793	Y726	V666	D606	V546	F485	S425	E365	G305	P245	G185
V968	P908	G847	THR	L727	V666	D606	V546	R486	Y426	I366	G306	Y246	V186
I969	P908	G847	THR	L727	V667	P607	E547	P487	Y426	I366	G306	Y246	V186
V969	C909	R848	GLU	E728	F667	P607	E547	P487	Y426	I366	G306	Y246	V186
I970	C909	R848	CYS	A729	L668	A608	A548	S488	A427	T367	S306	Y246	V186
K971	G910	W849	CYS	A729	L668	A608	A548	S488	A427	T367	S306	Y246	V186
D972	VAL	V850	VAL	G730	N670	E609	T549	S489	L428	N368	P307	L247	V186
R973	T911	S851	SER	D731	N670	E609	T549	S489	L428	N368	P307	L247	V186
K974	T912	C851	GLY	T732	L671	Y611	G550	Y490	G430	C370	D310	C250	P190
L975	G913	T852	CYS	V733	T672	K612	A551	H491	E431	E371	T311	Q251	L191
V976	R973	Q853	ARG	VAL	T672	K612	G552	L492	L432	Q372	C312	Q252	E192
T977	S915	A854	GLN	ARG	C674	C614	F553	M493	A433	C373	S313	Q252	E192
F978	T915	A854	GLN	ARG	C674	C614	F553	M493	A433	C373	S313	Q252	E192
V979	C916	V855	GLU	GLN	C674	C614	A554	V494	P434	V374	H314	R254	G194
I979	S917	C956	GLU	GLN	Q675	K615	N555	S495	C435	C375	L315	C255	N195
K979	S917	C956	GLU	GLN	Q675	K615	N555	S495	C435	C375	L315	C255	N195
L980	K918	H857	THR	R739	T677	D617	T556	M496	G436	N376	E316	C255	N195
V980	A919	G858	R739	C740	T678	T618	K558	A497	T438	G378	S318	P258	K198
I981	I920	T859	C740	C740	C678	C619	A559	G499	V440	R379	S319	G259	I980



[illegible]

Chain G: 81% 73% 7% 19%

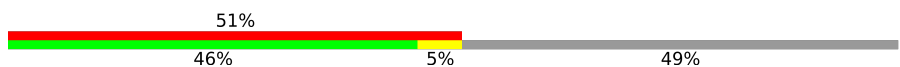


D261	C321	V381	Q441	R501	S561	C621	L681	V741	W801	S861	K921	A981
T262	E322	C382	T442	L502	T562	Q622	S682	C742	C802	I862	I922	P982
C263	E323	K383	C443	Q503	C563	N623	E683	R743	P803	Y863	F923	S983
V264	H324	D384	L444	V504	H644	N624	A684	D744	D804	G864	H924	Y984
C265	H325	L385	K445	Q505	D565	E625	D685	G745	S805	S865	K925	K985
S266	M326	P386	T446	L506	K566	D626	S686	R746	L806	G866	H926	G986
T267	D327	C387	V447	A507	L567	C627	H687	L747	M807	H867	T927	T987
V268	G328	P388	V448	P508	D568	L628	C688	H748	D808	Y868	E928	V988
A269	C329	G389	L449	V509	W569	C629	L689	C749	D809	I869	L929	C989
E270	F330	T390	L450	M510	L570	A630	E690	ARG	G810	T870	K930	G990
F271	C331	C391	A451	Q511	D571	A631	G691	TLE	R811	F871	L931	L991
S272	P332	A392	D452	L512	D572	L632	F692	ARG	G812	D872	E932	C992
R273	E333	L393	K453	F513	P573	S633	A693	LEU	S813	G873	D933	G993
Q274	G334	E394	K454	V514	C574	S634	P694	TLE	C814	K874	K934	N994
C275	T335	G395	K455	T515	S575	Y635	V695	GLY	W815	Y875	H935	F995
S276	V336	G396	M456	L516	L576	A636	D696	SER	V816	Y876	R936	D996
H277	Y337	S397	A457	D517	N577	R637	G697	CYS	E817	D877	V937	H997
A278	D338	H398	L458	Q518	I578	A638	C698	THR	K818	F878	V938	V998
G279	D339	I399	V459	A519	E579	C639	G699	ALA	E819	D879	I939	S999
G280	I340	T400	F460	S520	S580	T640	C700	LYS	C820	G880	Q940	N1000
R281	G341	T401	K461	Q521	A581	A641	P701	TLE	P821	H881	R941	N1001
G283	D342	F402	S462	G522	N582	K642	D702	HIS	C822	C882	D942	D1002
N284	S343	D403	D463	Q523	Y583	G643	H703	ASP	W823	S883	E943	F1003
W285	G344	G404	G464	V524	A584	V644	T704	CYS	H824	Y884	Q944	T1004
R286	C345	K405	S465	Q525	E585	M645	F705	ASN	N825	Y885	H945	T1005
T287	V346	T406	V466	G526	H586	L646	L706	LEU	N826	A886	H946	R1006
A288	P347	Y407	L467	L527	W587	W647	D707	THR	D827	Y887	V947	D1007
T289	V348	T408	L468	C528	C588	G648	E708	ALA	L828	Q888	A948	H1008
F409	S349	F409	M469	G529	S589	W649	K709	ALA	Y829	D889	Y949	M1009
H410	Q350	H410	Q470	N530	L590	R650	G710	SER	S830	Y890	T950	V1010
C351	G351	G411	L471	F531	L591	E651	R711	LYS	S831	C891	T951	V1011
P292	H352	D412	Q472	N532	K592	H652	C712	PRO	G832	GLN	R952	S1012
K293	C353	C413	V473	G533	K593	V653	V713	PRO	A833	ASN	E953	S1013
T294	R354	Y414	M474	L534	T594	C654	P714	A781	K834	SER	V954	E1014
C295	L355	Y415	L475	E535	E595	M655	L715	L782	I835	SER	G955	L1015
P296	H356	V416	P476	G536	T596	K656	A716	S783	K836	L897	Q956	D1016
G297	G357	L417	H477	D537	P597	D657	K717	C784	R837	G898	Y957	F1017
N298	H358	A418	V478	D538	F598	V658	C718	Q785	D838	S899	L958	G1018
L299	L359	K419	T479	F539	G599	G659	S719	T786	C839	F900	V959	N1019
V300	Y360	G420	A480	K540	R600	S660	C720	L787	N840	S901	V960	S1020
Y301	T361	D421	S481	T541	C601	C661	Y721	A788	T841	I902	E961	M1021
L302	P362	H422	F482	A542	H602	P662	HIS	A789	C842	R903	S962	K1022
E303	G363	M423	S483	S543	S603	M663	ARG	G790	T843	T904	S963	E1023
S304	Q364	D424	V484	G544	A604	S664	G724	Y791	C844	E905	T964	A1024
G305	E365	S425	F485	L545	V605	Q665	Y726	Y792	K845	R906	G965	P1025
S306	I366	Y426	R486	V546	D606	V666	L727	H793	R846	V907	I966	T1026
P307	T367	A427	P487	E547	P607	F667	E728	THR	G847	F908	P967	C1027
C308	N368	L428	S488	A548	A608	L668	C728	GLU	R848	C909	V968	P1028
M309	D369	L429	S489	T549	E609	Y669	A729	CYS	W849	G910	I969	D1029
D310	C370	G430	Y490	G550	Y610	Y670	G730	VAL	V850	T911	N970	V1030
T311	E371	E431	H491	A551	Y611	L671	D731	GLY	C851	C912	D971	S1031
C312	Q372	L432	I492	G552	K612	T672	V732	CYS	T852	G913	T972	T1032
S313	C373	A433	M493	F553	R613	G673	VAL	ARG	K853	V914	R973	P1033
H314	V374	P434	V494	N555	C614	C674	GLN	GLN	A854	T915	T974	N1034
L315	C375	C435	S495	T556	K615	Q675	GLU	GLU	W855	C916	T975	E1035
E316	N376	G436	M496	T557	Y616	Q676	GLU	GLU	C856	S917	Y976	P1036
V317	A377	S437	A497	W557	D617	T677	R739	THR	H857	G918	F977	C1037
S318	G378	T438	I498	K558	T618	C678	C740	CYS	C858	A919	T978	S1038
S319	R379	D439	G499	A559	C619	R679	C740		T859	N920	K979	L1039
L320	W380	K440	V500	Q560	N620	S680			C860		L980	N1040



HIS
HIS
HIS

Chain I:





- 

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  100% 50% 50%



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

Chain O:  100% 50% 50%



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

Chain P:  100% 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	178136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.714	Depositor
Minimum map value	-1.867	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/9358	0.58	0/12718
1	B	0.29	0/5406	0.57	0/7355
1	C	0.32	0/8643	0.59	0/11748
1	D	0.35	0/3952	0.60	0/5363
1	E	0.32	0/9358	0.58	0/12718
1	F	0.22	0/715	0.46	0/970
1	G	0.32	0/8643	0.60	0/11748
1	H	0.35	0/3952	0.61	0/5363
1	I	0.29	0/5406	0.57	0/7355
1	J	0.22	0/715	0.46	0/970
All	All	0.32	0/56148	0.59	0/76308

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	2
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	2
1	G	0	2
1	H	0	1
1	I	0	1
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1126	PRO	Peptide
1	A	424	ASP	Peptide
1	B	424	ASP	Peptide
1	C	1126	PRO	Peptide
1	C	424	ASP	Peptide
1	D	1126	PRO	Peptide
1	E	1126	PRO	Peptide
1	E	424	ASP	Peptide
1	G	1126	PRO	Peptide
1	G	424	ASP	Peptide
1	H	1126	PRO	Peptide
1	I	424	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9125	0	8366	60	0
1	B	5276	0	4839	34	0
1	C	8429	0	7755	62	0
1	D	3849	0	3527	20	0
1	E	9125	0	8366	62	0
1	F	696	0	611	2	0
1	G	8429	0	7755	61	0
1	H	3849	0	3527	19	0
1	I	5276	0	4839	35	0
1	J	696	0	611	3	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	E	28	0	26	0	0
4	G	28	0	26	0	0
4	I	28	0	26	0	0
5	A	23	0	0	0	0
5	B	10	0	0	0	0
5	C	22	0	0	0	0
5	D	13	0	0	0	0
5	E	23	0	0	0	0
5	F	1	0	0	0	0
5	G	22	0	0	0	0
5	H	13	0	0	0	0
5	I	10	0	0	0	0
5	J	1	0	0	0	0
All	All	55254	0	50502	324	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 3.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ASN:N	1:C:172:TYR:HH	1.66	0.93
1:G:35:ASN:N	1:G:172:TYR:HH	1.66	0.92
1:E:474:ASN:ND2	1:G:474:ASN:ND2	2.18	0.91
1:A:474:ASN:ND2	1:C:474:ASN:ND2	2.18	0.91
1:A:35:ASN:N	1:A:172:TYR:HH	1.71	0.89
1:E:35:ASN:N	1:E:172:TYR:HH	1.71	0.88
1:I:35:ASN:N	1:I:172:TYR:HH	1.73	0.87
1:B:35:ASN:N	1:B:172:TYR:HH	1.74	0.86
1:A:474:ASN:CG	1:C:474:ASN:HD21	1.86	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:474:ASN:HD21	1:G:474:ASN:CG	1.86	0.82
1:E:474:ASN:HD21	1:G:474:ASN:ND2	1.78	0.80
1:A:474:ASN:ND2	1:C:474:ASN:HD21	1.77	0.78
1:E:60:ASP:OD2	1:E:201:GLN:NE2	2.21	0.73
1:B:60:ASP:OD2	1:B:201:GLN:NE2	2.22	0.72
1:A:60:ASP:OD2	1:A:201:GLN:NE2	2.21	0.72
1:C:60:ASP:OD2	1:C:201:GLN:NE2	2.21	0.72
1:I:60:ASP:OD2	1:I:201:GLN:NE2	2.22	0.72
1:G:60:ASP:OD2	1:G:201:GLN:NE2	2.22	0.71
1:E:474:ASN:CG	1:G:474:ASN:ND2	2.50	0.70
1:A:474:ASN:ND2	1:C:474:ASN:CG	2.50	0.70
1:A:474:ASN:CG	1:C:474:ASN:ND2	2.51	0.69
1:E:474:ASN:CG	1:G:474:ASN:HD21	2.04	0.66
1:A:474:ASN:HD21	1:C:474:ASN:CG	2.05	0.65
1:E:474:ASN:ND2	1:G:474:ASN:CG	2.50	0.65
1:G:618:THR:O	1:G:624:ASN:ND2	2.33	0.62
1:B:618:THR:O	1:B:624:ASN:ND2	2.33	0.62
1:C:618:THR:O	1:C:624:ASN:ND2	2.33	0.62
1:I:618:THR:O	1:I:624:ASN:ND2	2.33	0.61
1:A:618:THR:O	1:A:624:ASN:ND2	2.33	0.61
1:E:618:THR:O	1:E:624:ASN:ND2	2.33	0.61
1:E:474:ASN:ND2	1:G:474:ASN:HD21	1.97	0.60
1:A:474:ASN:HD21	1:C:474:ASN:ND2	1.98	0.60
1:G:640:THR:HG22	1:G:645:MET:HA	1.85	0.59
1:B:640:THR:HG22	1:B:645:MET:HA	1.85	0.59
1:A:640:THR:HG22	1:A:645:MET:HA	1.85	0.59
1:E:640:THR:HG22	1:E:645:MET:HA	1.85	0.59
1:C:640:THR:HG22	1:C:645:MET:HA	1.85	0.57
1:I:640:THR:HG22	1:I:645:MET:HA	1.85	0.57
1:I:623:ASN:ND2	1:I:626:ASP:OD2	2.38	0.57
1:A:623:ASN:ND2	1:A:626:ASP:OD2	2.38	0.57
1:E:623:ASN:ND2	1:E:626:ASP:OD2	2.38	0.57
1:G:623:ASN:ND2	1:G:626:ASP:OD2	2.38	0.57
1:B:623:ASN:ND2	1:B:626:ASP:OD2	2.38	0.56
1:A:929:LEU:HD22	1:A:936:ARG:HD3	1.88	0.56
1:C:218:CYS:O	1:C:251:GLN:NE2	2.39	0.56
1:D:929:LEU:HD22	1:D:936:ARG:HD3	1.88	0.56
1:C:623:ASN:ND2	1:C:626:ASP:OD2	2.38	0.56
1:C:929:LEU:HD22	1:C:936:ARG:HD3	1.88	0.55
1:H:929:LEU:HD22	1:H:936:ARG:HD3	1.88	0.55
1:B:218:CYS:O	1:B:251:GLN:NE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:CYS:O	1:E:251:GLN:NE2	2.39	0.55
1:A:558:LYS:HD2	1:A:563:CYS:HB2	1.89	0.55
1:G:558:LYS:HD2	1:G:563:CYS:HB2	1.89	0.55
1:A:218:CYS:O	1:A:251:GLN:NE2	2.39	0.55
1:B:254:ARG:NH1	1:B:261:ASP:OD1	2.40	0.55
1:C:254:ARG:NH1	1:C:261:ASP:OD1	2.40	0.55
1:I:218:CYS:O	1:I:251:GLN:NE2	2.40	0.55
1:I:254:ARG:NH1	1:I:261:ASP:OD1	2.40	0.55
1:E:929:LEU:HD22	1:E:936:ARG:HD3	1.88	0.55
1:G:929:LEU:HD22	1:G:936:ARG:HD3	1.88	0.54
1:G:218:CYS:O	1:G:251:GLN:NE2	2.40	0.54
1:H:1353:GLN:NE2	1:H:1378:LEU:O	2.41	0.54
1:E:558:LYS:HD2	1:E:563:CYS:HB2	1.89	0.54
1:E:1353:GLN:NE2	1:E:1378:LEU:O	2.41	0.54
1:G:254:ARG:NH1	1:G:261:ASP:OD1	2.40	0.54
1:I:558:LYS:HD2	1:I:563:CYS:HB2	1.89	0.54
1:D:1353:GLN:NE2	1:D:1378:LEU:O	2.41	0.54
1:E:254:ARG:NH1	1:E:261:ASP:OD1	2.40	0.54
1:J:1353:GLN:NE2	1:J:1378:LEU:O	2.41	0.54
1:C:558:LYS:HD2	1:C:563:CYS:HB2	1.89	0.54
1:A:1353:GLN:NE2	1:A:1378:LEU:O	2.41	0.54
1:I:551:ALA:O	1:I:555:ASN:ND2	2.41	0.54
1:A:254:ARG:NH1	1:A:261:ASP:OD1	2.40	0.53
1:B:558:LYS:HD2	1:B:563:CYS:HB2	1.89	0.53
1:F:1353:GLN:NE2	1:F:1378:LEU:O	2.41	0.53
1:A:551:ALA:O	1:A:555:ASN:ND2	2.41	0.53
1:B:704:THR:HA	1:B:714:PRO:HA	1.90	0.53
1:E:551:ALA:O	1:E:555:ASN:ND2	2.41	0.53
1:B:551:ALA:O	1:B:555:ASN:ND2	2.41	0.53
1:C:551:ALA:O	1:C:555:ASN:ND2	2.41	0.53
1:E:103:ILE:HD11	1:E:126:LEU:HD21	1.91	0.53
1:G:551:ALA:O	1:G:555:ASN:ND2	2.41	0.53
1:E:721:TYR:HA	1:E:726:TYR:HA	1.91	0.53
1:B:103:ILE:HD11	1:B:126:LEU:HD21	1.91	0.52
1:E:704:THR:HA	1:E:714:PRO:HA	1.91	0.52
1:I:721:TYR:HA	1:I:726:TYR:HA	1.91	0.52
1:A:704:THR:HA	1:A:714:PRO:HA	1.91	0.52
1:C:704:THR:HA	1:C:714:PRO:HA	1.91	0.52
1:G:103:ILE:HD11	1:G:126:LEU:HD21	1.91	0.52
1:G:704:THR:HA	1:G:714:PRO:HA	1.91	0.52
1:E:811:ARG:HH21	1:E:828:LEU:HG	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:704:THR:HA	1:I:714:PRO:HA	1.91	0.52
1:A:140:ARG:NH1	1:C:933:ASP:OD2	2.43	0.52
1:A:721:TYR:HA	1:A:726:TYR:HA	1.91	0.52
1:I:103:ILE:HD11	1:I:126:LEU:HD21	1.91	0.52
1:A:811:ARG:HH21	1:A:828:LEU:HG	1.75	0.52
1:A:933:ASP:OD2	1:C:140:ARG:NH1	2.43	0.52
1:A:1366:LYS:O	1:A:1370:GLN:NE2	2.43	0.52
1:B:107[A]:ARG:HD2	1:B:149:ARG:HB3	1.92	0.52
1:C:103:ILE:HD11	1:C:126:LEU:HD21	1.91	0.52
1:C:721:TYR:HA	1:C:726:TYR:HA	1.91	0.52
1:H:811:ARG:HH21	1:H:828:LEU:HG	1.75	0.52
1:H:933:ASP:OD2	1:I:140:ARG:NH1	2.43	0.52
1:I:107[A]:ARG:HD2	1:I:149:ARG:HB3	1.92	0.52
1:A:107[A]:ARG:HD2	1:A:149:ARG:HB3	1.92	0.51
1:D:1366:LYS:O	1:D:1370:GLN:NE2	2.43	0.51
1:A:103:ILE:HD11	1:A:126:LEU:HD21	1.91	0.51
1:B:721:TYR:HA	1:B:726:TYR:HA	1.91	0.51
1:E:1366:LYS:O	1:E:1370:GLN:NE2	2.43	0.51
1:D:811:ARG:HH21	1:D:828:LEU:HG	1.75	0.51
1:B:140:ARG:NH1	1:D:933:ASP:OD2	2.43	0.51
1:E:107[A]:ARG:HD2	1:E:149:ARG:HB3	1.92	0.51
1:E:1015:LEU:O	1:E:1019:ASN:ND2	2.44	0.51
1:G:1015:LEU:O	1:G:1019:ASN:ND2	2.44	0.51
1:D:1015:LEU:O	1:D:1019:ASN:ND2	2.44	0.51
1:E:933:ASP:OD2	1:G:140:ARG:NH1	2.43	0.51
1:G:721:TYR:HA	1:G:726:TYR:HA	1.91	0.51
1:H:1015:LEU:O	1:H:1019:ASN:ND2	2.44	0.51
1:G:107[A]:ARG:HD2	1:G:149:ARG:HB3	1.92	0.50
1:C:107[A]:ARG:HD2	1:C:149:ARG:HB3	1.92	0.50
1:E:140:ARG:NH1	1:G:933:ASP:OD2	2.43	0.50
1:C:811:ARG:HH21	1:C:828:LEU:HG	1.75	0.50
1:C:1015:LEU:O	1:C:1019:ASN:ND2	2.44	0.50
1:D:859:THR:OG1	1:D:979:LYS:NZ	2.44	0.50
1:A:474:ASN:ND2	1:C:474:ASN:OD1	2.45	0.50
1:A:1015:LEU:O	1:A:1019:ASN:ND2	2.44	0.50
1:G:811:ARG:HH21	1:G:828:LEU:HG	1.75	0.50
1:A:379:ARG:HE	1:C:1008:HIS:CD2	2.31	0.49
1:D:942:ASP:OD2	1:D:945:HIS:HB3	2.13	0.49
1:D:1036:PRO:HB3	1:D:1081:SER:HB3	1.95	0.48
1:E:379:ARG:HE	1:G:1008:HIS:CD2	2.31	0.48
1:E:1008:HIS:CD2	1:G:379:ARG:HE	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:486:ARG:HE	1:G:489:SER:HA	1.78	0.48
1:B:379:ARG:HE	1:D:1008:HIS:CD2	2.31	0.48
1:B:486:ARG:HE	1:B:489:SER:HA	1.78	0.48
1:E:942:ASP:OD2	1:E:945:HIS:HB3	2.13	0.48
1:H:1036:PRO:HB3	1:H:1081:SER:HB3	1.95	0.48
1:F:1366:LYS:O	1:F:1370:GLN:NE2	2.46	0.48
1:G:942:ASP:OD2	1:G:945:HIS:HB3	2.13	0.48
1:H:942:ASP:OD2	1:H:945:HIS:HB3	2.13	0.48
1:H:1366:LYS:O	1:H:1370:GLN:NE2	2.46	0.48
1:C:486:ARG:HE	1:C:489:SER:HA	1.78	0.48
1:C:1036:PRO:HB3	1:C:1081:SER:HB3	1.95	0.48
1:E:486:ARG:HE	1:E:489:SER:HA	1.78	0.48
1:I:486:ARG:HE	1:I:489:SER:HA	1.79	0.48
1:A:942:ASP:OD2	1:A:945:HIS:HB3	2.13	0.48
1:C:942:ASP:OD2	1:C:945:HIS:HB3	2.13	0.48
1:J:1366:LYS:O	1:J:1370:GLN:NE2	2.46	0.48
1:A:1008:HIS:CD2	1:C:379:ARG:HE	2.31	0.48
1:A:1036:PRO:HB3	1:A:1081:SER:HB3	1.95	0.48
1:C:284:ASN:HD21	1:C:302:LEU:HA	1.79	0.48
1:E:859:THR:OG1	1:E:979:LYS:NZ	2.44	0.48
1:H:1008:HIS:CD2	1:I:379:ARG:HE	2.31	0.48
1:I:85:ALA:HB3	1:I:88:PRO:HD2	1.96	0.47
1:A:486:ARG:HE	1:A:489:SER:HA	1.79	0.47
1:E:284:ASN:HD21	1:E:302:LEU:HA	1.79	0.47
1:G:859:THR:OG1	1:G:979:LYS:NZ	2.44	0.47
1:A:859:THR:OG1	1:A:979:LYS:NZ	2.44	0.47
1:A:284:ASN:HD21	1:A:302:LEU:HA	1.79	0.47
1:D:1150:GLY:O	1:D:1152:HIS:ND1	2.47	0.47
1:G:1036:PRO:HB3	1:G:1081:SER:HB3	1.95	0.47
1:E:1036:PRO:HB3	1:E:1081:SER:HB3	1.95	0.47
1:B:284:ASN:HD21	1:B:302:LEU:HA	1.79	0.47
1:G:85:ALA:HB3	1:G:88:PRO:HD2	1.96	0.47
1:G:284:ASN:HD21	1:G:302:LEU:HA	1.79	0.47
1:H:859:THR:OG1	1:H:979:LYS:NZ	2.44	0.47
1:E:961:GLU:HG3	1:E:967:ILE:HG12	1.97	0.47
1:B:85:ALA:HB3	1:B:88:PRO:HD2	1.96	0.47
1:C:961:GLU:HG3	1:C:967:ILE:HG12	1.97	0.47
1:G:503:GLN:HE21	1:G:692:PHE:HD1	1.63	0.47
1:G:961:GLU:HG3	1:G:967:ILE:HG12	1.97	0.47
1:D:806:LEU:HB3	1:D:814:CYS:HB3	1.97	0.46
1:D:961:GLU:HG3	1:D:967:ILE:HG12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:LEU:HB3	1:E:814:CYS:HB3	1.97	0.46
1:A:961:GLU:HG3	1:A:967:ILE:HG12	1.97	0.46
1:E:85:ALA:HB3	1:E:88:PRO:HD2	1.96	0.46
1:H:961:GLU:HG3	1:H:967:ILE:HG12	1.97	0.46
1:I:284:ASN:HD21	1:I:302:LEU:HA	1.79	0.46
1:E:127:LEU:HD23	1:E:138:TYR:HD2	1.80	0.46
1:A:806:LEU:HB3	1:A:814:CYS:HB3	1.97	0.46
1:B:503:GLN:HE21	1:B:692:PHE:HD1	1.63	0.46
1:E:474:ASN:OD1	1:G:474:ASN:ND2	2.45	0.46
1:C:127:LEU:HD23	1:C:138:TYR:HD2	1.81	0.46
1:A:85:ALA:HB3	1:A:88:PRO:HD2	1.96	0.46
1:C:806:LEU:HB3	1:C:814:CYS:HB3	1.97	0.46
1:A:503:GLN:HE21	1:A:692:PHE:HD1	1.64	0.46
1:C:85:ALA:HB3	1:C:88:PRO:HD2	1.96	0.46
1:I:503:GLN:HE21	1:I:692:PHE:HD1	1.63	0.46
1:G:806:LEU:HB3	1:G:814:CYS:HB3	1.97	0.46
1:I:127:LEU:HD23	1:I:138:TYR:HD2	1.80	0.46
1:B:127:LEU:HD23	1:B:138:TYR:HD2	1.80	0.46
1:H:806:LEU:HB3	1:H:814:CYS:HB3	1.97	0.46
1:C:1150:GLY:O	1:C:1152:HIS:ND1	2.48	0.45
1:E:503:GLN:HE21	1:E:692:PHE:HD1	1.64	0.45
1:A:282:PRO:HD2	1:A:304:SER:HB2	1.99	0.45
1:C:503:GLN:HE21	1:C:692:PHE:HD1	1.64	0.45
1:A:1150:GLY:O	1:A:1152:HIS:ND1	2.48	0.45
1:C:859:THR:OG1	1:C:979:LYS:NZ	2.44	0.45
1:G:127:LEU:HD23	1:G:138:TYR:HD2	1.80	0.45
1:C:953:GLU:OE2	1:C:972:LYS:NZ	2.43	0.45
1:A:127:LEU:HD23	1:A:138:TYR:HD2	1.80	0.45
1:B:488:SER:HB2	1:B:671:LEU:HD22	1.99	0.45
1:I:282:PRO:HD2	1:I:304:SER:HB2	1.99	0.45
1:G:282:PRO:HD2	1:G:304:SER:HB2	1.99	0.45
1:I:488:SER:HB2	1:I:671:LEU:HD22	1.99	0.45
1:G:1150:GLY:O	1:G:1152:HIS:ND1	2.48	0.44
1:H:1150:GLY:O	1:H:1152:HIS:ND1	2.47	0.44
1:D:1005:THR:OG1	1:D:1007:ASP:OD1	2.35	0.44
1:E:282:PRO:HD2	1:E:304:SER:HB2	1.99	0.44
1:C:282:PRO:HD2	1:C:304:SER:HB2	1.99	0.44
1:G:488:SER:HB2	1:G:671:LEU:HD22	1.99	0.44
1:E:488:SER:HB2	1:E:671:LEU:HD22	1.99	0.44
1:C:488:SER:HB2	1:C:671:LEU:HD22	1.99	0.43
1:C:549:THR:HB	1:C:568:ASP:OD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:920:ILE:HD11	1:C:976:VAL:HG21	2.00	0.43
1:B:282:PRO:HD2	1:B:304:SER:HB2	1.99	0.43
1:A:488:SER:HB2	1:A:671:LEU:HD22	1.99	0.43
1:A:1306:SER:OG	1:A:1307:ASP:N	2.52	0.43
1:D:1306:SER:OG	1:D:1307:ASP:N	2.52	0.43
1:G:920:ILE:HD11	1:G:976:VAL:HG21	2.00	0.43
1:H:920:ILE:HD11	1:H:976:VAL:HG21	2.00	0.43
1:B:131:SER:OG	1:B:132:ASP:N	2.52	0.43
1:A:131:SER:OG	1:A:132:ASP:N	2.52	0.43
1:A:1005:THR:OG1	1:A:1007:ASP:OD1	2.35	0.43
1:E:131:SER:OG	1:E:132:ASP:N	2.52	0.43
1:E:316:GLU:OE2	1:G:890:TYR:HB3	2.19	0.43
1:I:429:LEU:HB2	1:I:448:VAL:HB	2.01	0.43
1:D:920:ILE:HD11	1:D:976:VAL:HG21	2.00	0.43
1:E:503:GLN:HE22	1:E:693:ALA:H	1.67	0.43
1:G:549:THR:HB	1:G:568:ASP:OD2	2.18	0.43
1:A:503:GLN:HE22	1:A:693:ALA:H	1.67	0.43
1:A:890:TYR:HB3	1:C:316:GLU:OE2	2.19	0.43
1:B:549:THR:HB	1:B:568:ASP:OD2	2.18	0.43
1:E:920:ILE:HD11	1:E:976:VAL:HG21	2.00	0.43
1:A:494:VAL:HB	1:A:502:LEU:HB2	2.01	0.42
1:B:316:GLU:OE2	1:D:890:TYR:HB3	2.19	0.42
1:C:503:GLN:HE22	1:C:693:ALA:H	1.67	0.42
1:E:890:TYR:HB3	1:G:316:GLU:OE2	2.19	0.42
1:I:677:THR:O	1:I:680:SER:OG	2.34	0.42
1:A:429:LEU:HB2	1:A:448:VAL:HB	2.01	0.42
1:A:549:THR:HB	1:A:568:ASP:OD2	2.18	0.42
1:C:494:VAL:HB	1:C:502:LEU:HB2	2.01	0.42
1:G:503:GLN:HE22	1:G:693:ALA:H	1.68	0.42
1:C:131:SER:OG	1:C:132:ASP:N	2.52	0.42
1:G:131:SER:OG	1:G:132:ASP:N	2.52	0.42
1:H:1306:SER:OG	1:H:1307:ASP:N	2.52	0.42
1:B:35:ASN:N	1:B:172:TYR:OH	2.46	0.42
1:E:549:THR:HB	1:E:568:ASP:OD2	2.18	0.42
1:H:1100:GLN:HE21	1:H:1159:TYR:HE2	1.68	0.42
1:I:534:LEU:HG	1:I:536:GLY:H	1.85	0.42
1:G:429:LEU:HB2	1:G:448:VAL:HB	2.01	0.42
1:G:534:LEU:HG	1:G:536:GLY:H	1.85	0.42
1:J:1306:SER:OG	1:J:1307:ASP:N	2.52	0.42
1:A:316:GLU:OE2	1:C:890:TYR:HB3	2.19	0.42
1:A:534:LEU:HG	1:A:536:GLY:H	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:LEU:HB2	1:C:448:VAL:HB	2.01	0.42
1:E:429:LEU:HB2	1:E:448:VAL:HB	2.01	0.42
1:E:534:LEU:HG	1:E:536:GLY:H	1.85	0.42
1:E:1306:SER:OG	1:E:1307:ASP:N	2.52	0.42
1:A:920:ILE:HD11	1:A:976:VAL:HG21	2.00	0.42
1:E:494:VAL:HB	1:E:502:LEU:HB2	2.02	0.42
1:A:66:ASP:HB3	1:A:72:LYS:HG3	2.02	0.42
1:B:494:VAL:HB	1:B:502:LEU:HB2	2.01	0.42
1:G:66:ASP:HB3	1:G:72:LYS:HG3	2.02	0.42
1:G:494:VAL:HB	1:G:502:LEU:HB2	2.01	0.42
1:I:494:VAL:HB	1:I:502:LEU:HB2	2.01	0.42
1:I:503:GLN:HE22	1:I:693:ALA:H	1.67	0.42
1:B:503:GLN:HE22	1:B:693:ALA:H	1.67	0.42
1:E:66:ASP:HB3	1:E:72:LYS:HG3	2.02	0.42
1:H:890:TYR:HB3	1:I:316:GLU:OE2	2.19	0.42
1:A:171:ASP:OD2	1:A:179:SER:OG	2.38	0.42
1:B:429:LEU:HB2	1:B:448:VAL:HB	2.01	0.42
1:C:540:LYS:HA	1:C:546:VAL:HA	2.02	0.42
1:I:549:THR:HB	1:I:568:ASP:OD2	2.18	0.42
1:I:131:SER:OG	1:I:132:ASP:N	2.52	0.41
1:C:677:THR:O	1:C:680:SER:OG	2.35	0.41
1:E:1005:THR:OG1	1:E:1007:ASP:OD1	2.35	0.41
1:B:534:LEU:HG	1:B:536:GLY:H	1.85	0.41
1:C:534:LEU:HG	1:C:536:GLY:H	1.85	0.41
1:G:540:LYS:HA	1:G:546:VAL:HA	2.02	0.41
1:I:66:ASP:HB3	1:I:72:LYS:HG3	2.02	0.41
1:I:540:LYS:HA	1:I:546:VAL:HA	2.02	0.41
1:C:1100:GLN:HE21	1:C:1159:TYR:HE2	1.68	0.41
1:A:540:LYS:HA	1:A:546:VAL:HA	2.02	0.41
1:B:66:ASP:HB3	1:B:72:LYS:HG3	2.02	0.41
1:C:66:ASP:HB3	1:C:72:LYS:HG3	2.02	0.41
1:E:1150:GLY:O	1:E:1152:HIS:ND1	2.47	0.41
1:I:35:ASN:HB3	1:I:36:VAL:H	1.72	0.41
1:E:1100:GLN:HE21	1:E:1159:TYR:HE2	1.68	0.41
1:G:677:THR:O	1:G:680:SER:OG	2.34	0.41
1:G:936:ARG:HH21	1:G:951:THR:HB	1.86	0.41
1:G:1005:THR:OG1	1:G:1007:ASP:OD1	2.35	0.41
1:G:1187:CYS:SG	1:G:1188:GLY:N	2.94	0.41
1:A:1100:GLN:HE21	1:A:1159:TYR:HE2	1.68	0.41
1:B:171:ASP:OD2	1:B:179:SER:OG	2.38	0.41
1:D:1100:GLN:HE21	1:D:1159:TYR:HE2	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:LYS:NZ	1:G:206:CYS:O	2.52	0.41
1:A:953:GLU:OE2	1:A:972:LYS:NZ	2.43	0.41
1:C:969:ILE:HB	1:C:977:PHE:HB2	2.03	0.41
1:D:969:ILE:HB	1:D:977:PHE:HB2	2.03	0.41
1:E:516:LEU:HD11	1:E:524:VAL:HG11	2.03	0.41
1:H:936:ARG:HH21	1:H:951:THR:HB	1.86	0.41
1:A:969:ILE:HB	1:A:977:PHE:HB2	2.03	0.40
1:D:1187:CYS:SG	1:D:1188:GLY:N	2.94	0.40
1:E:936:ARG:HH21	1:E:951:THR:HB	1.86	0.40
1:E:1187:CYS:SG	1:E:1188:GLY:N	2.94	0.40
1:G:171:ASP:OD2	1:G:179:SER:OG	2.38	0.40
1:I:67:CYS:HB2	1:I:166:CYS:HB3	1.99	0.40
1:I:171:ASP:OD2	1:I:179:SER:OG	2.38	0.40
1:C:145:LEU:HD11	1:C:153:LEU:HD11	2.03	0.40
1:C:1187:CYS:SG	1:C:1188:GLY:N	2.94	0.40
1:G:1100:GLN:HE21	1:G:1159:TYR:HE2	1.68	0.40
1:B:198:LYS:NZ	1:B:206:CYS:O	2.52	0.40
1:C:228:LEU:HD11	1:C:290:LEU:HD21	2.04	0.40
1:E:540:LYS:HA	1:E:546:VAL:HA	2.02	0.40
1:G:969:ILE:HB	1:G:977:PHE:HB2	2.03	0.40
1:H:1187:CYS:SG	1:H:1188:GLY:N	2.94	0.40
1:C:936:ARG:HH21	1:C:951:THR:HB	1.86	0.40
1:E:52:VAL:O	1:E:248:ARG:NH2	2.55	0.40
1:E:969:ILE:HB	1:E:977:PHE:HB2	2.03	0.40
1:B:188:PHE:HA	1:B:192:GLU:OE2	2.22	0.40
1:C:352:HIS:HD2	1:C:361:THR:HA	1.87	0.40
1:C:1005:THR:OG1	1:C:1007:ASP:OD1	2.35	0.40
1:G:352:HIS:HD2	1:G:361:THR:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

12 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	$\# Z > 2$
2	NAG	K	1	2,1	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	K	2	2	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.32	0	17,19,21	0.48	0
2	NAG	L	2	2	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.33	0	17,19,21	0.49	0
2	NAG	M	2	2	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.32	0	17,19,21	0.48	0
2	NAG	N	2	2	14,14,15	0.29	0	17,19,21	0.60	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	O	2	2	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
2	NAG	P	1	2,1	14,14,15	0.34	0	17,19,21	0.49	0
2	NAG	P	2	2	14,14,15	0.29	0	17,19,21	0.61	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
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	NAG	C1-O5-C5	2.07	114.95	112.19
2	K	2	NAG	C1-O5-C5	2.06	114.95	112.19
2	L	2	NAG	C1-O5-C5	2.06	114.94	112.19
2	M	2	NAG	C1-O5-C5	2.04	114.92	112.19
2	O	2	NAG	C1-O5-C5	2.04	114.92	112.19
2	N	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6

Continued on next page...

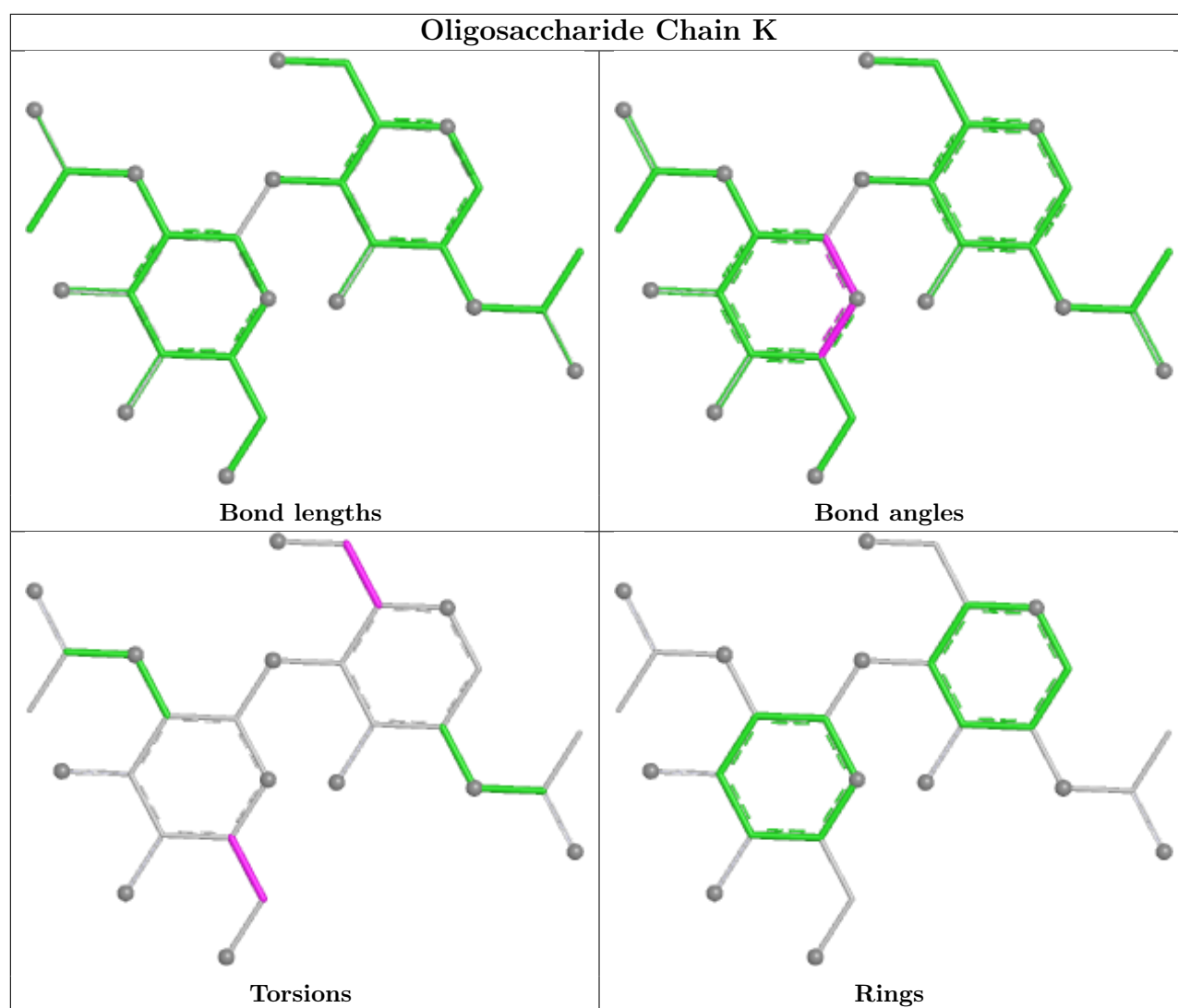
Continued from previous page...

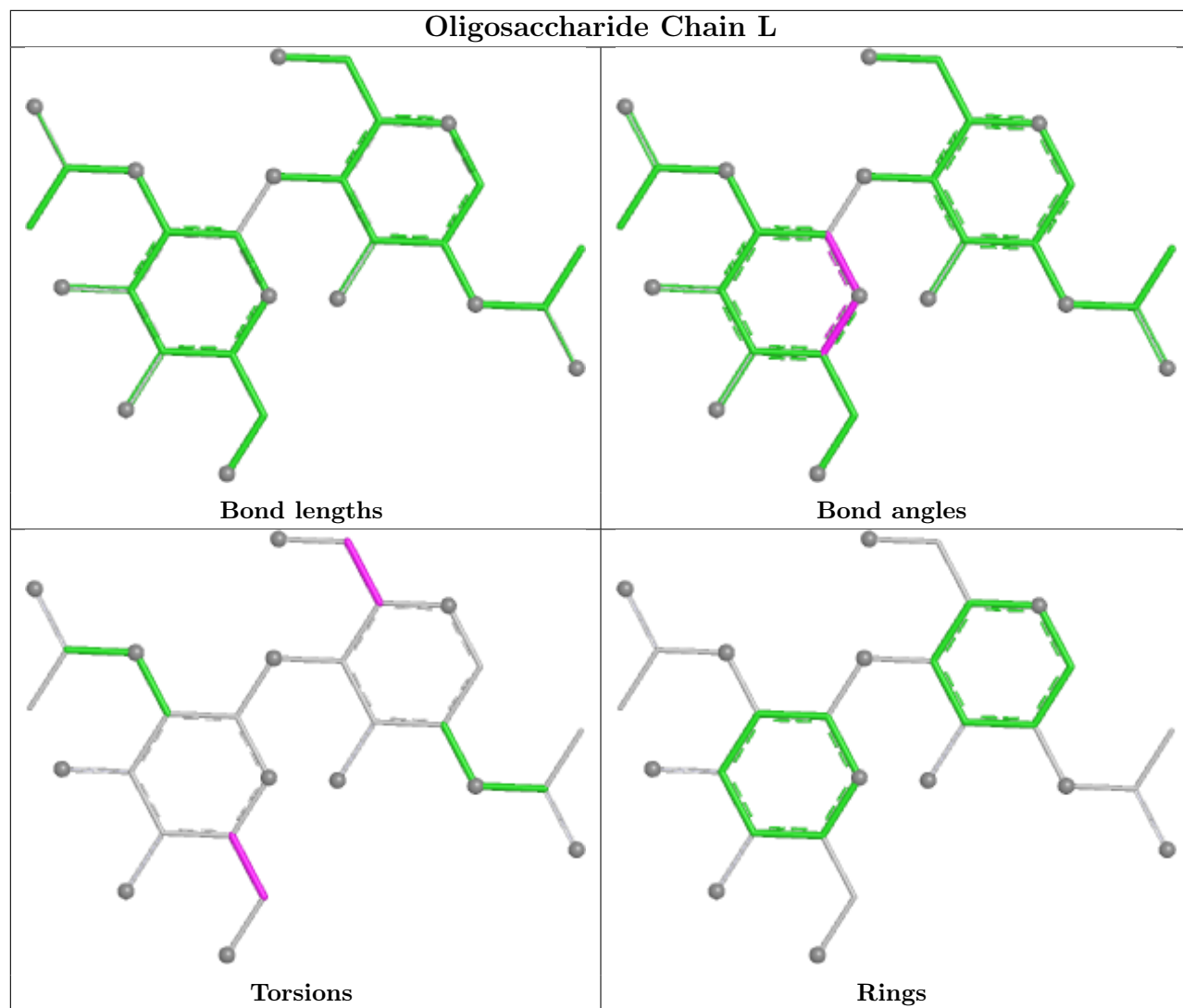
Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6

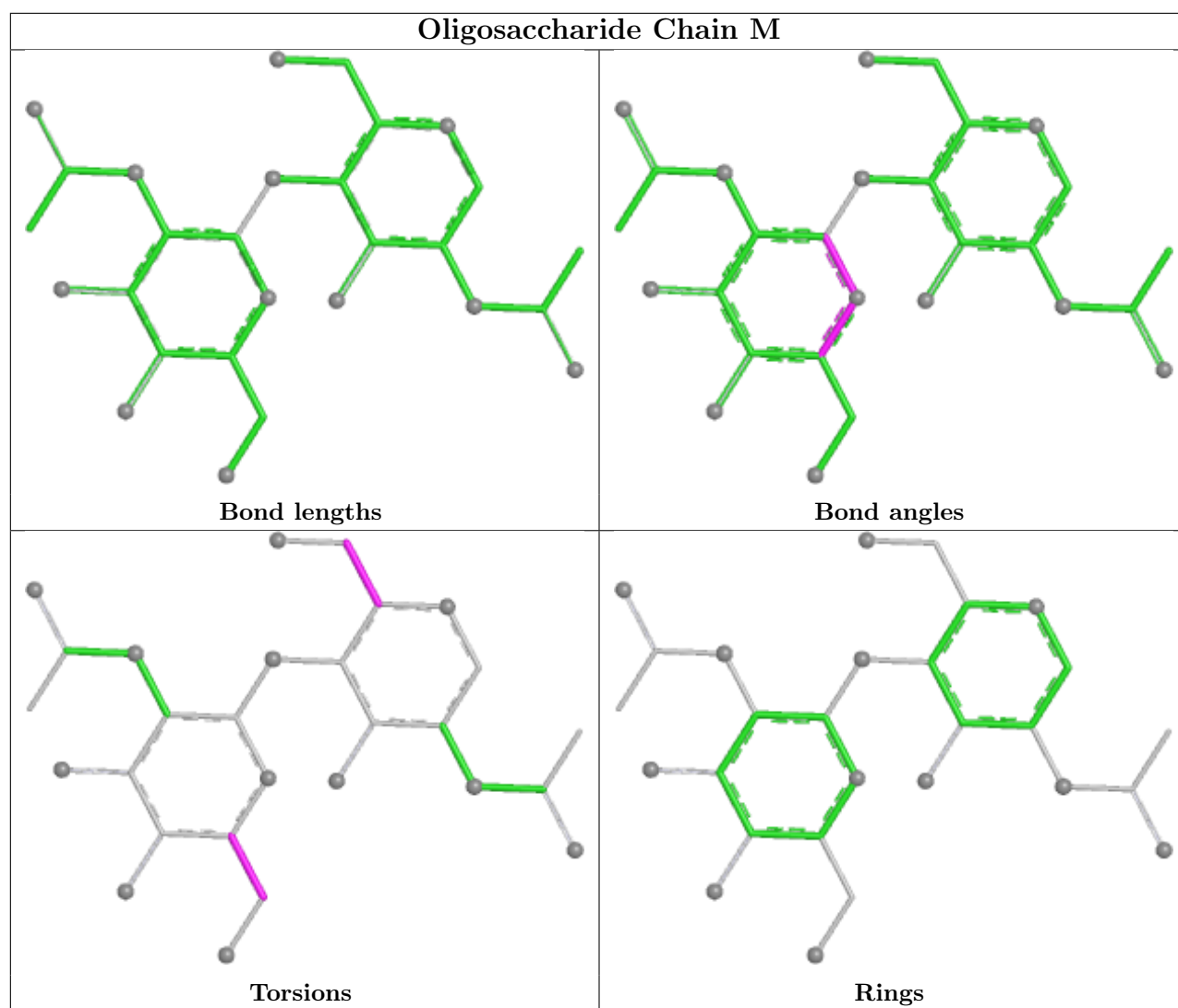
There are no ring outliers.

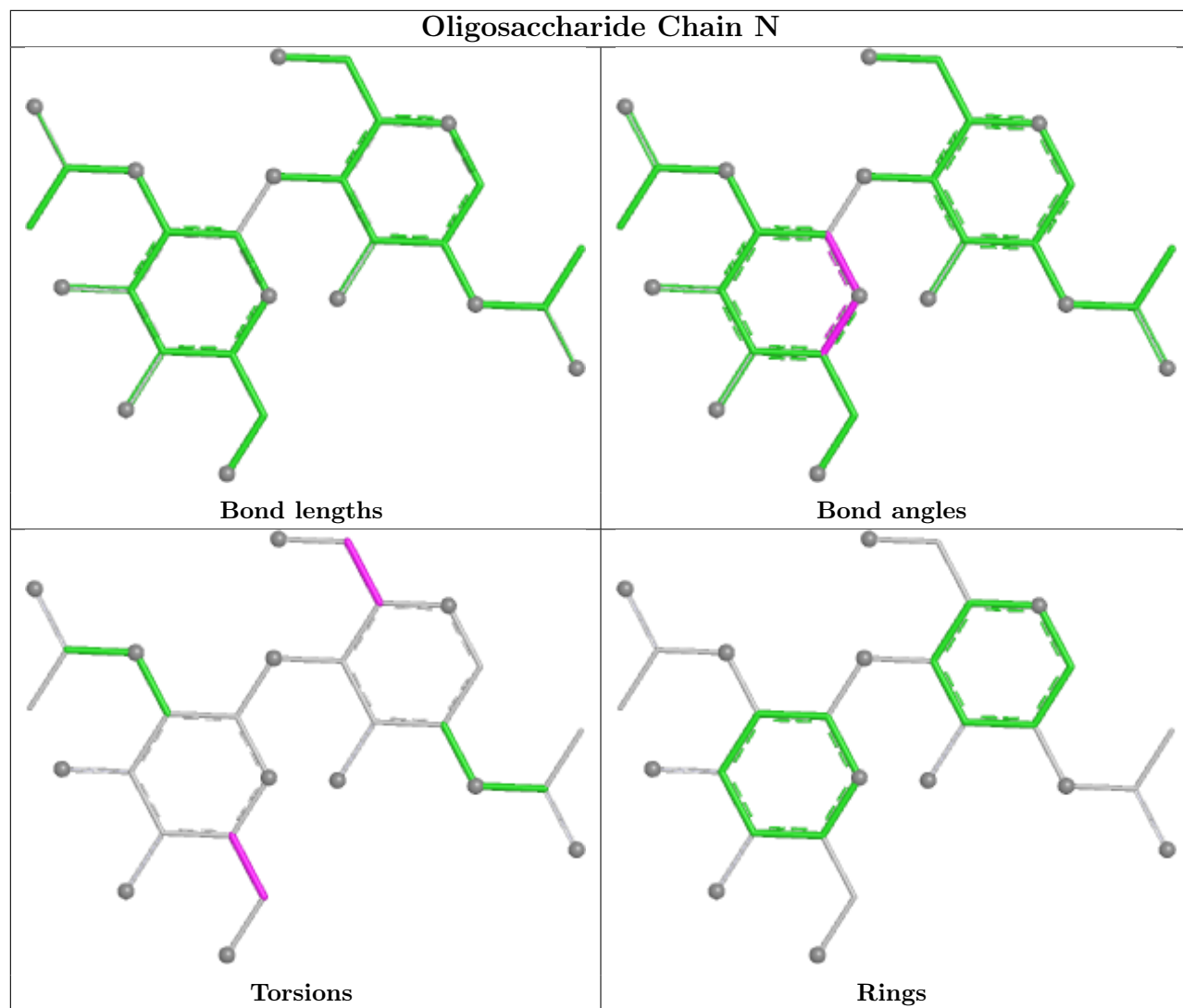
No monomer is involved in short contacts.

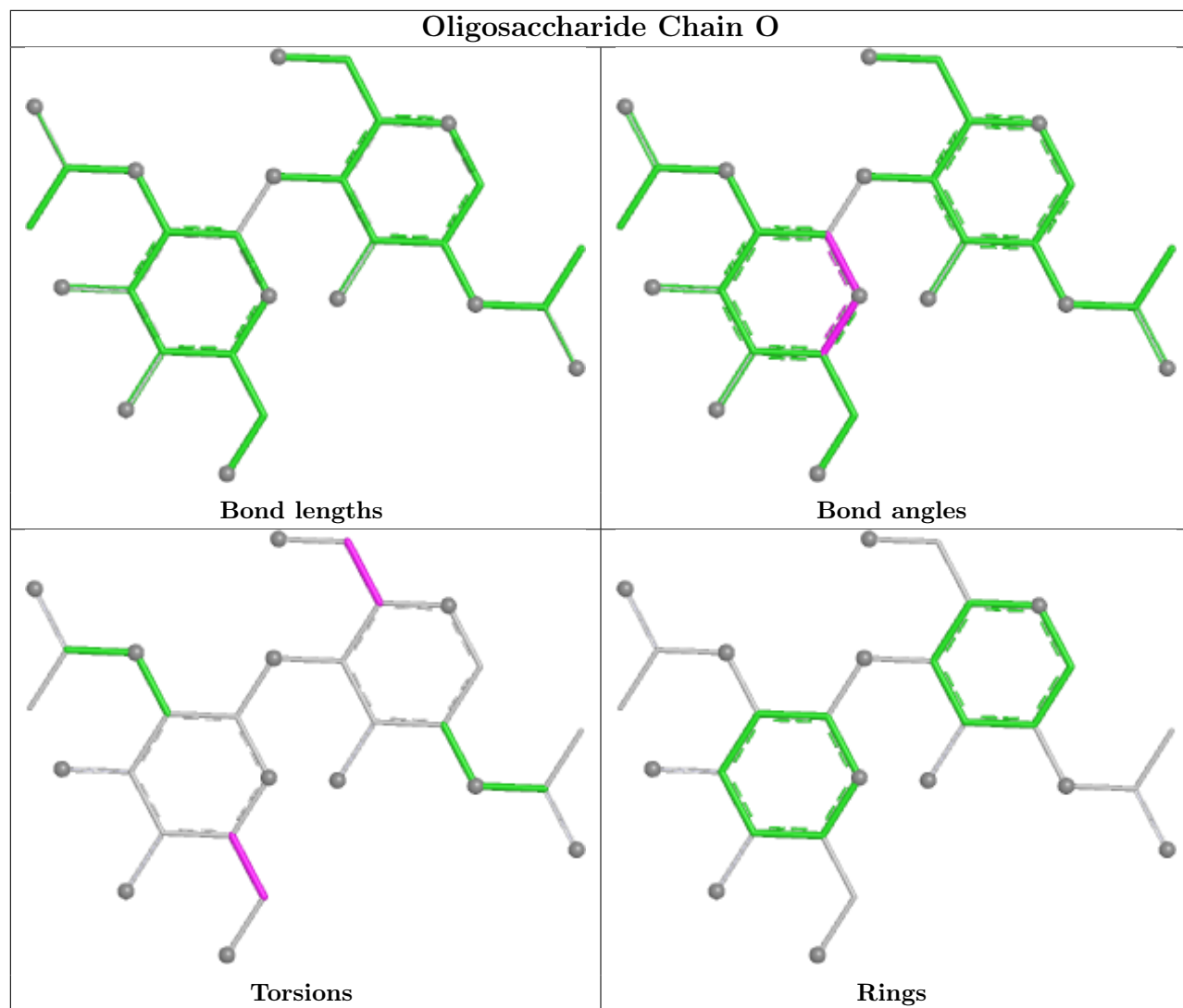
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

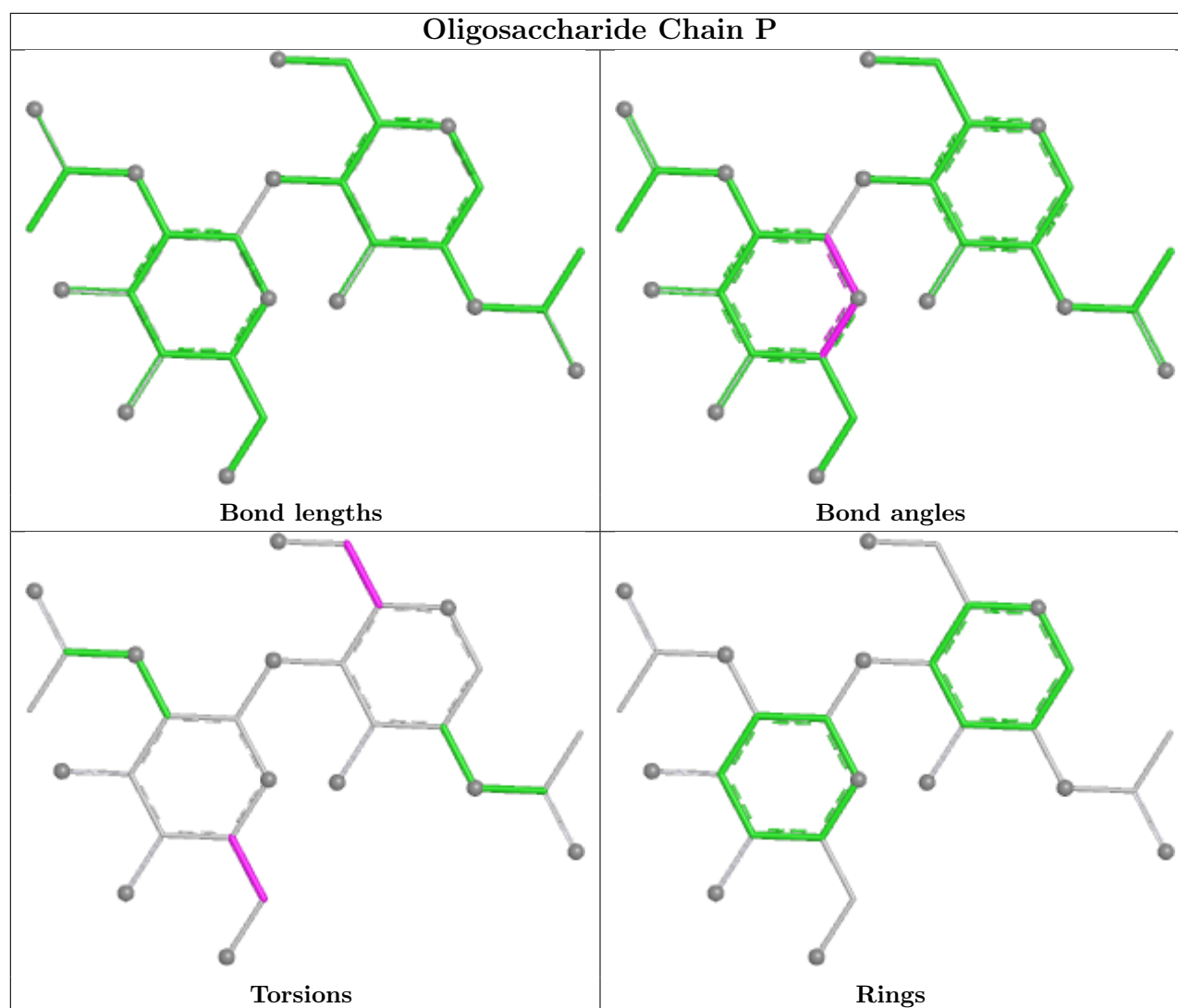












5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 30 are monoatomic - leaving 12 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	G	2004	1	14,14,15	1.31	2 (14%)	17,19,21	1.28	1 (5%)
4	NAG	B	2003	1	14,14,15	1.31	2 (14%)	17,19,21	1.28	1 (5%)
4	NAG	A	1506	1	14,14,15	1.32	2 (14%)	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	2007	1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	B	2004	1	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	C	2005	1	14,14,15	0.36	0	17,19,21	0.51	0
4	NAG	I	2003	1	14,14,15	1.32	2 (14%)	17,19,21	1.27	1 (5%)
4	NAG	E	2006	1	14,14,15	1.33	2 (14%)	17,19,21	1.28	1 (5%)
4	NAG	A	1507	1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	C	2004	1	14,14,15	1.32	2 (14%)	17,19,21	1.29	1 (5%)
4	NAG	G	2005	1	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	I	2004	1	14,14,15	0.34	0	17,19,21	0.52	0

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	G	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1506	1	-	2/6/23/26	0/1/1/1
4	NAG	E	2007	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
4	NAG	I	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	E	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1507	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	G	2005	1	-	4/6/23/26	0/1/1/1
4	NAG	I	2004	1	-	4/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2003	NAG	O5-C1	4.23	1.50	1.43
4	A	1506	NAG	O5-C1	4.23	1.50	1.43
4	E	2006	NAG	O5-C1	4.22	1.50	1.43
4	B	2003	NAG	O5-C1	4.22	1.50	1.43
4	C	2004	NAG	O5-C1	4.20	1.50	1.43
4	G	2004	NAG	O5-C1	4.20	1.50	1.43
4	E	2006	NAG	C1-C2	2.52	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2004	NAG	C1-C2	2.48	1.55	1.52
4	A	1506	NAG	C1-C2	2.46	1.55	1.52
4	I	2003	NAG	C1-C2	2.40	1.55	1.52
4	B	2003	NAG	C1-C2	2.39	1.55	1.52
4	G	2004	NAG	C1-C2	2.37	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2004	NAG	C1-O5-C5	5.10	119.02	112.19
4	A	1506	NAG	C1-O5-C5	5.09	119.00	112.19
4	G	2004	NAG	C1-O5-C5	5.08	119.00	112.19
4	E	2006	NAG	C1-O5-C5	5.06	118.97	112.19
4	B	2003	NAG	C1-O5-C5	5.06	118.97	112.19
4	I	2003	NAG	C1-O5-C5	5.04	118.94	112.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1507	NAG	O5-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6
4	E	2007	NAG	O5-C5-C6-O6
4	G	2005	NAG	O5-C5-C6-O6
4	I	2004	NAG	O5-C5-C6-O6
4	B	2004	NAG	C4-C5-C6-O6
4	G	2005	NAG	C4-C5-C6-O6
4	I	2004	NAG	C4-C5-C6-O6
4	A	1506	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	E	2006	NAG	O5-C5-C6-O6
4	I	2003	NAG	O5-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	G	2004	NAG	O5-C5-C6-O6
4	A	1507	NAG	C4-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	E	2007	NAG	C4-C5-C6-O6
4	A	1507	NAG	C8-C7-N2-C2
4	A	1507	NAG	O7-C7-N2-C2
4	B	2004	NAG	C8-C7-N2-C2
4	B	2004	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	2005	NAG	C8-C7-N2-C2
4	C	2005	NAG	O7-C7-N2-C2
4	E	2007	NAG	C8-C7-N2-C2
4	E	2007	NAG	O7-C7-N2-C2
4	G	2005	NAG	C8-C7-N2-C2
4	G	2005	NAG	O7-C7-N2-C2
4	I	2004	NAG	C8-C7-N2-C2
4	I	2004	NAG	O7-C7-N2-C2
4	A	1506	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	E	2006	NAG	C4-C5-C6-O6
4	I	2003	NAG	C4-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	G	2004	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

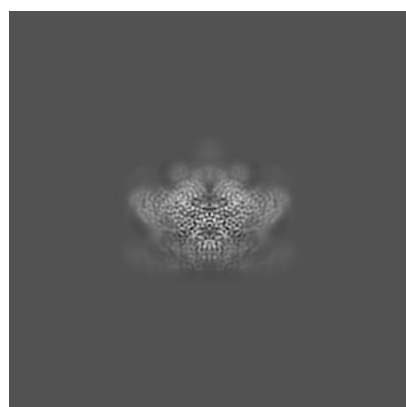
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10517. These allow visual inspection of the internal detail of the map and identification of artifacts.

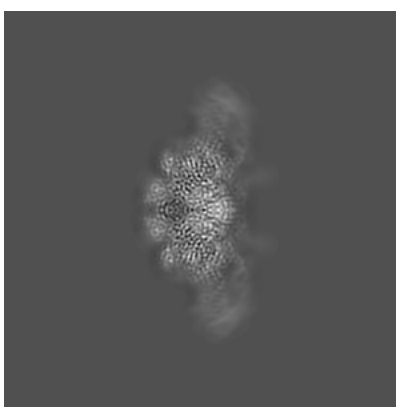
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

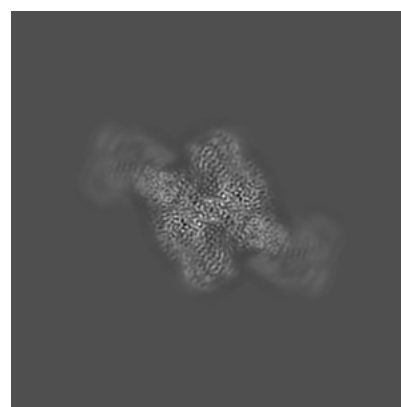
6.1.1 Primary map



X



Y



Z

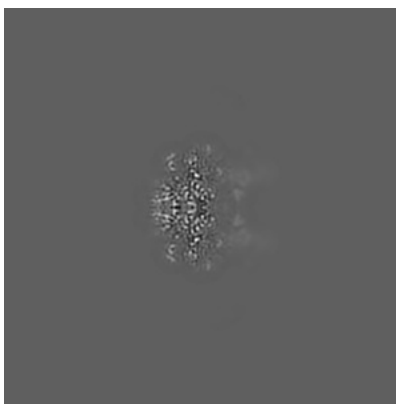
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

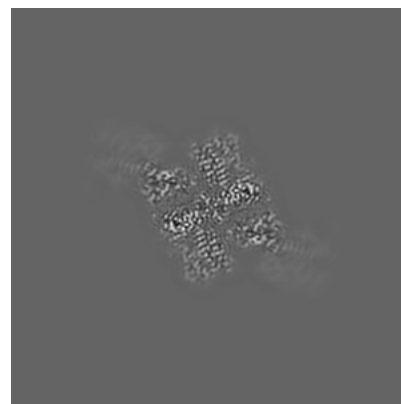
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

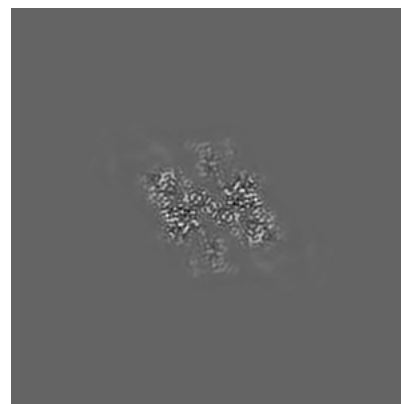
6.3.1 Primary map



X Index: 200



Y Index: 212

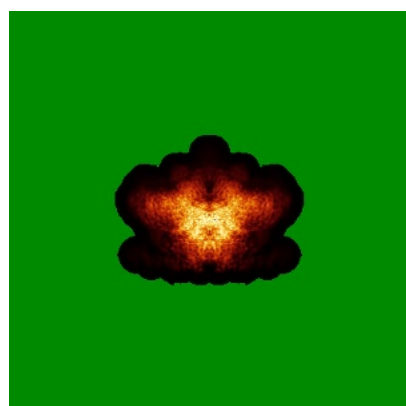


Z Index: 189

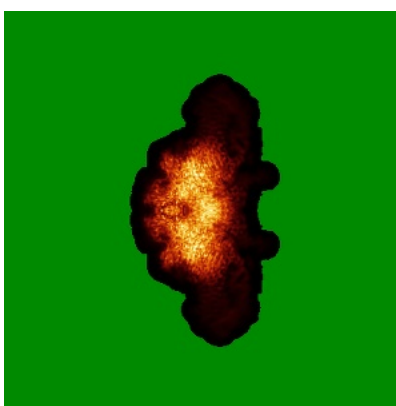
The images above show the largest variance slices of the map in three orthogonal directions.

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

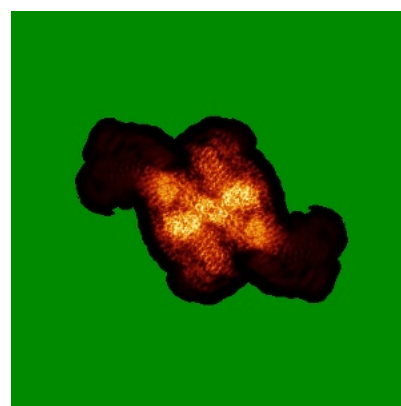
6.4.1 Primary map



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 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

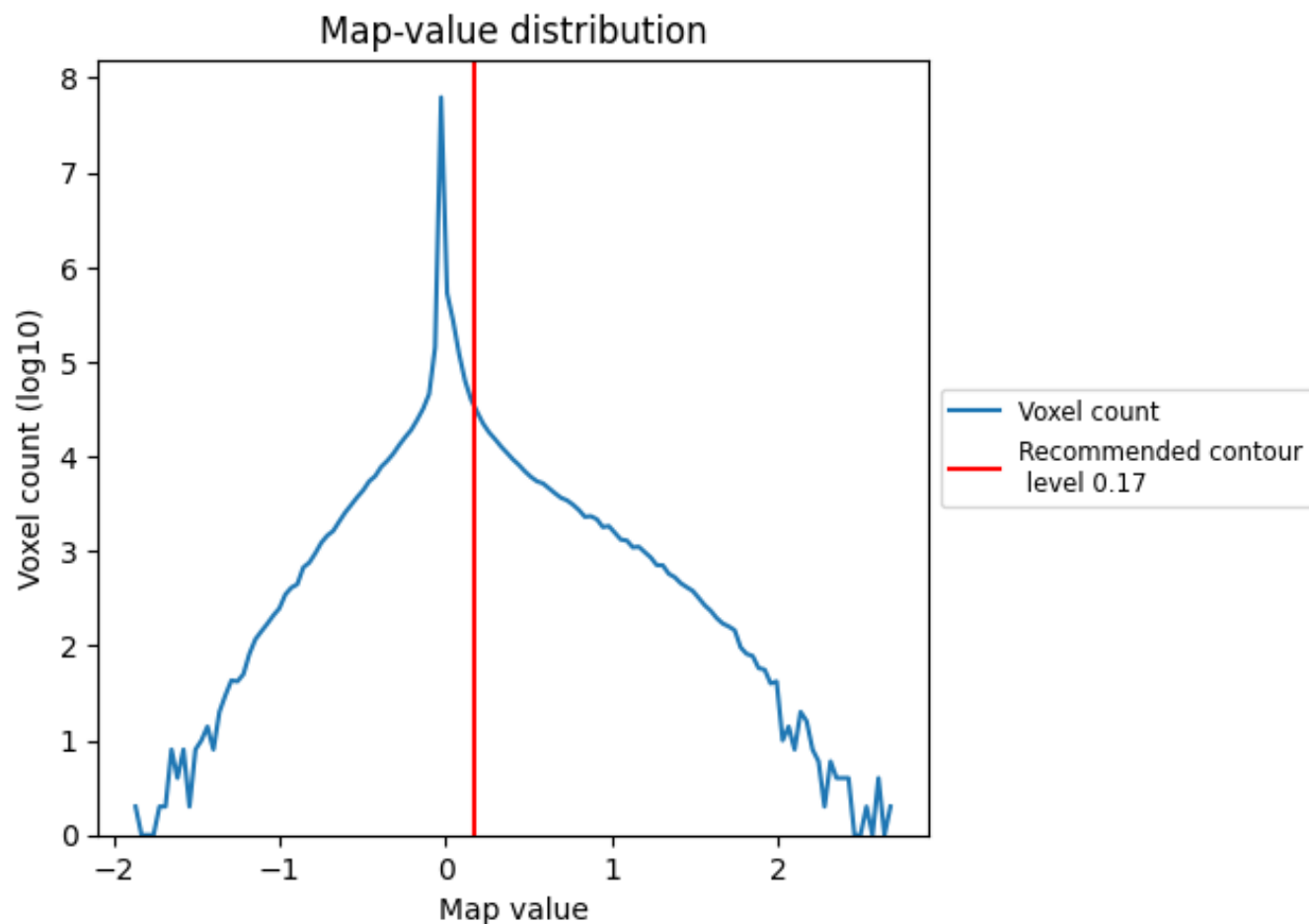
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

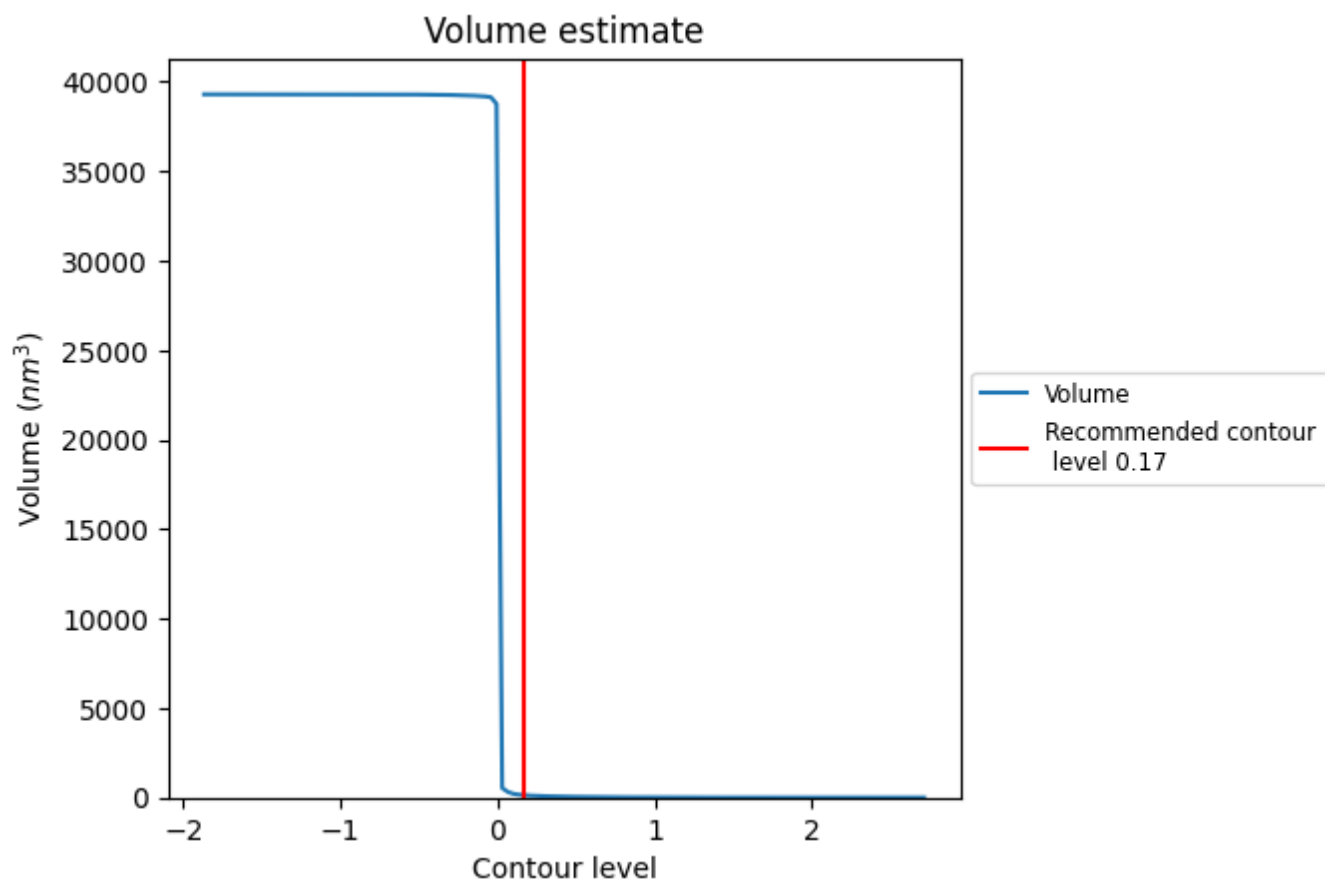
This section contains the results of statistical analysis of the map.

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.

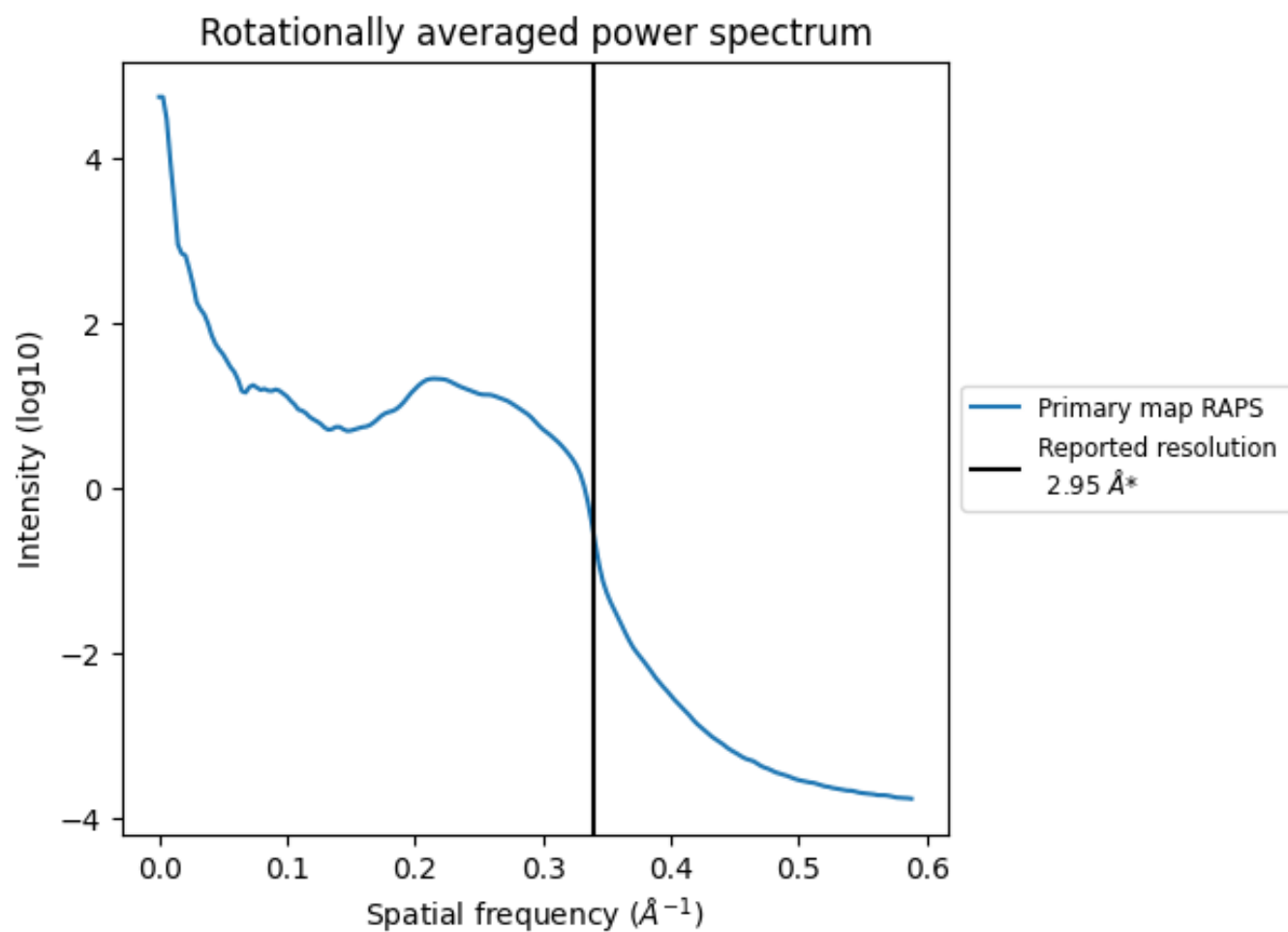
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm^3 ; this corresponds to an approximate mass of 120 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

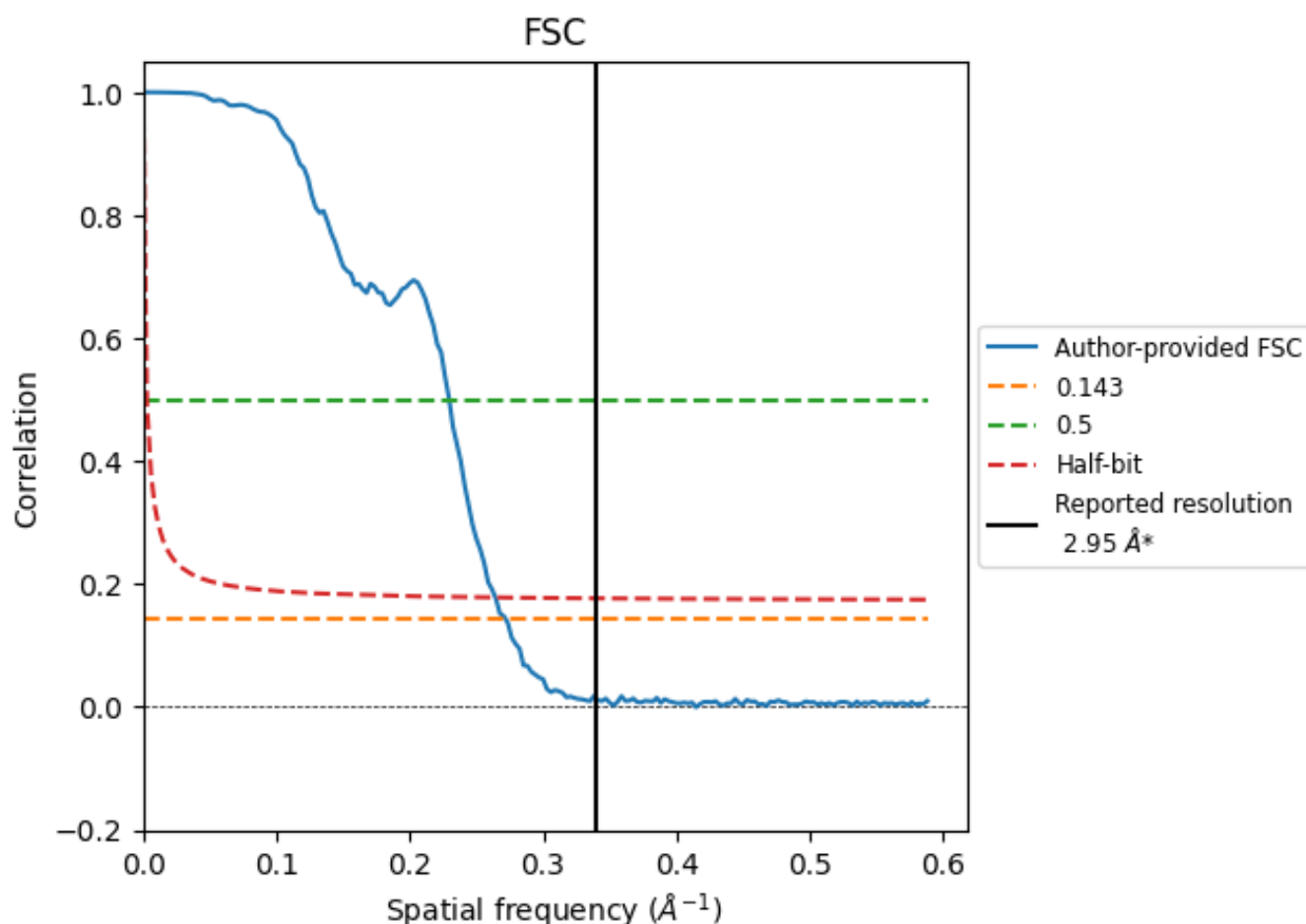


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

8.2 Resolution estimates [i](#)

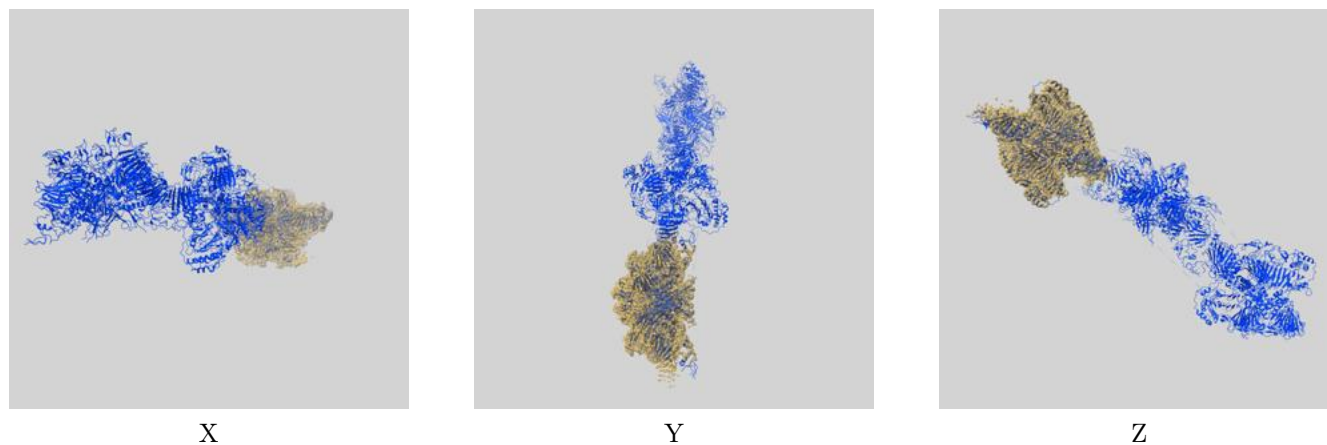
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	3.68	4.36	3.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

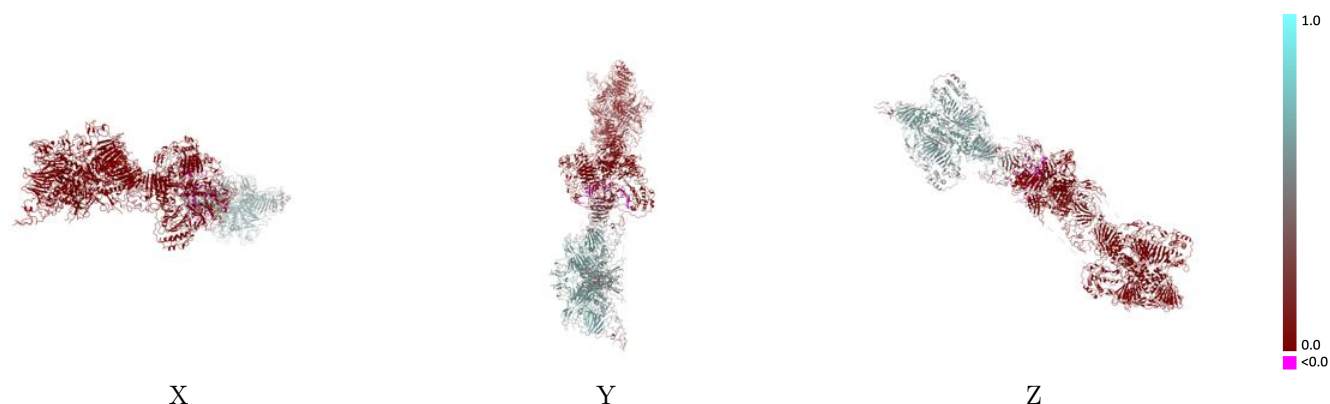
This section contains information regarding the fit between EMDB map EMD-10517 and PDB model 7A5O. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



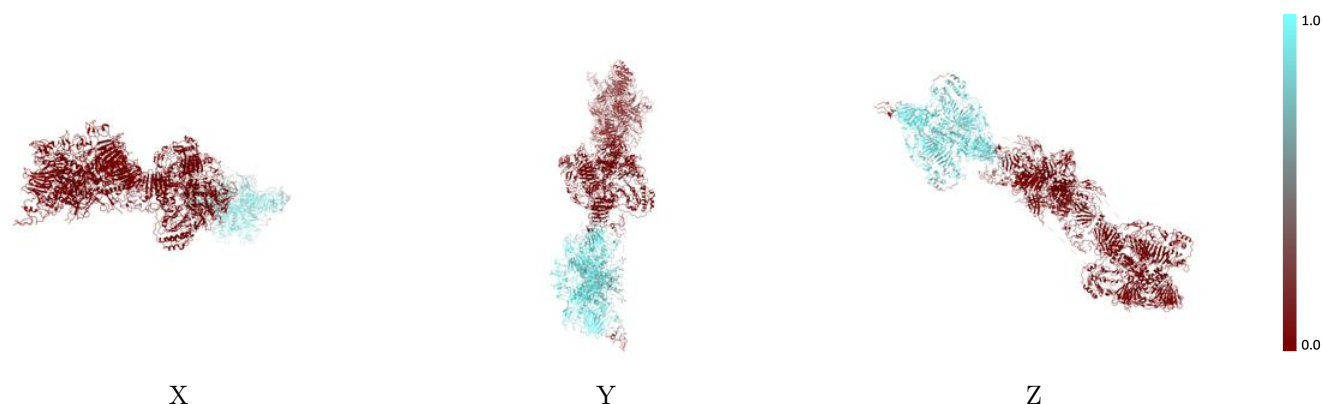
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



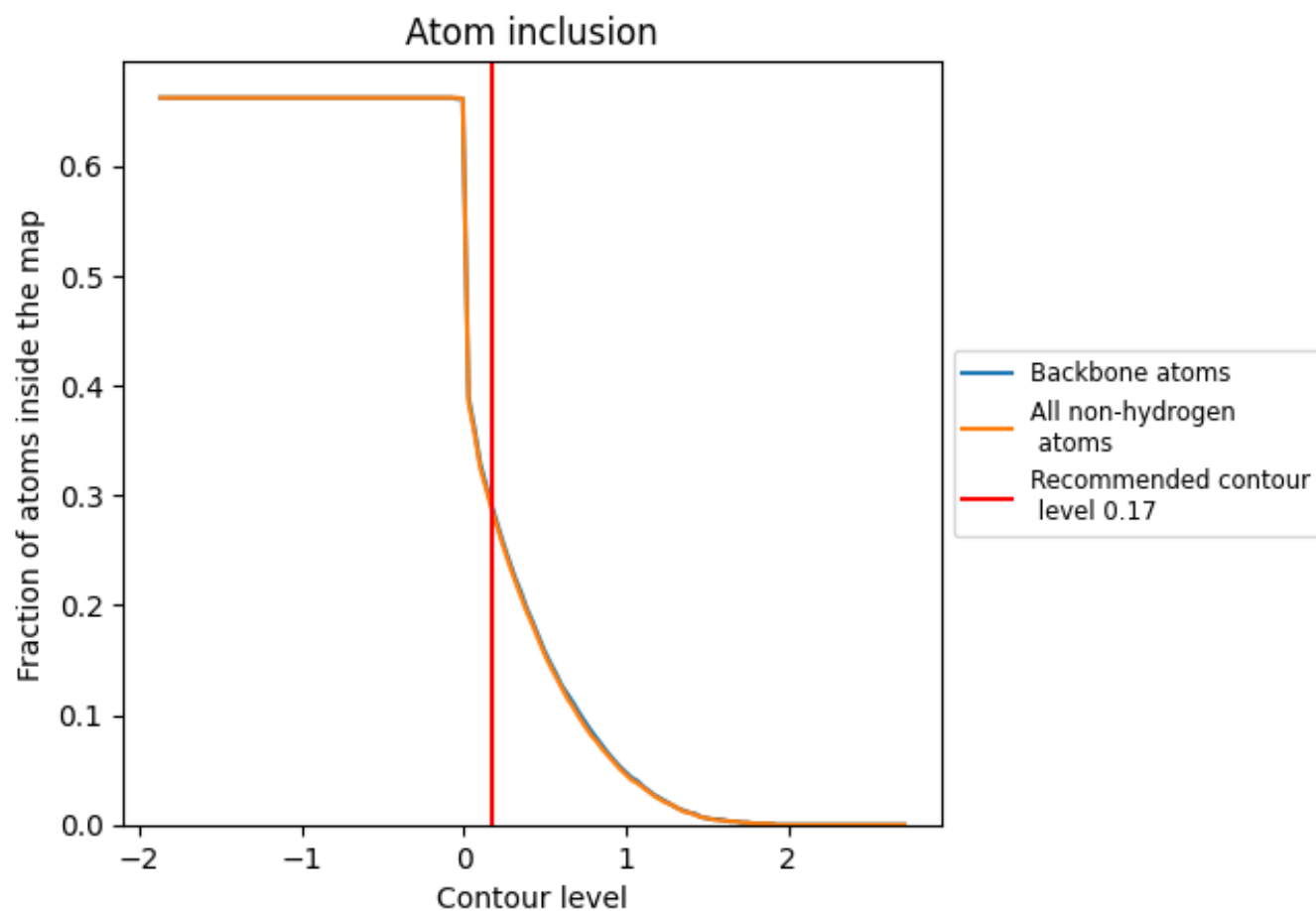
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 29% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2880	0.1950
A	0.4810	0.3130
B	0.8300	0.5300
C	0.3600	0.2920
D	0.7620	0.4810
E	0.0600	0.0390
F	0.7890	0.5130
G	0.0000	-0.0020
H	0.0000	0.0010
I	0.0000	0.0000
J	0.0000	0.0000
K	0.0000	0.0000
L	0.8210	0.5480
M	0.8210	0.5460
N	0.0000	0.0000
O	0.0000	0.0000
P	0.0000	0.0000

1.0

0.0

<0.0