



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 07:17 am BST

PDB ID : 7O7M
EMDB ID : EMD-12748
Title : (h-alpha2M)4 native II
Authors : Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.
Deposited on : 2021-04-13
Resolution : 6.60 Å(reported)

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<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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

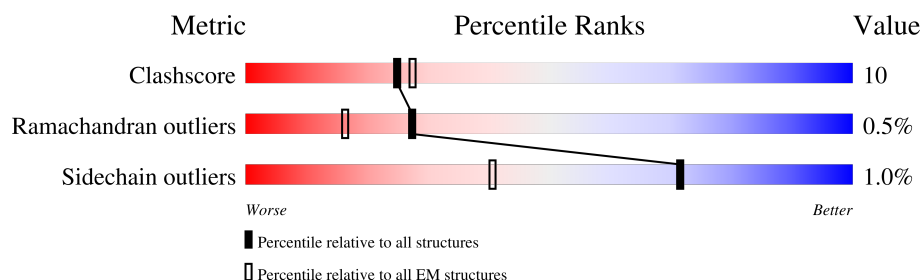
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



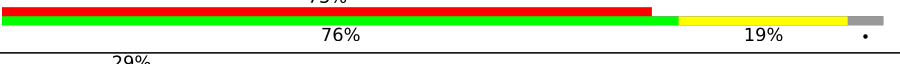

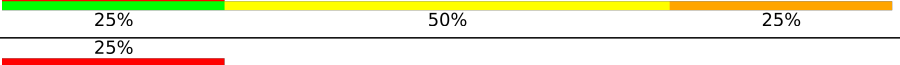
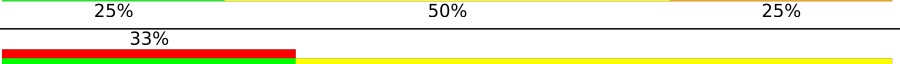
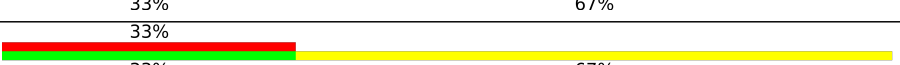
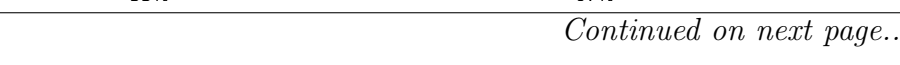
The reported resolution of this entry is 6.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1474	
1	B	1474	
1	C	1474	
1	D	1474	
2	E	4	
2	H	4	
3	F	3	
3	I	3	

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Mol	Chain	Length	Quality of chain
4	G	2	100%
			50%50%
4	J	2	100%
			50%50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 44614 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 Alpha-2-macroglobulin.

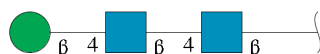
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	B	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	C	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	D	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	4	Total	C	N	O	0	0
			50	28	2	20		
2	H	4	Total	C	N	O	0	0
			50	28	2	20		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

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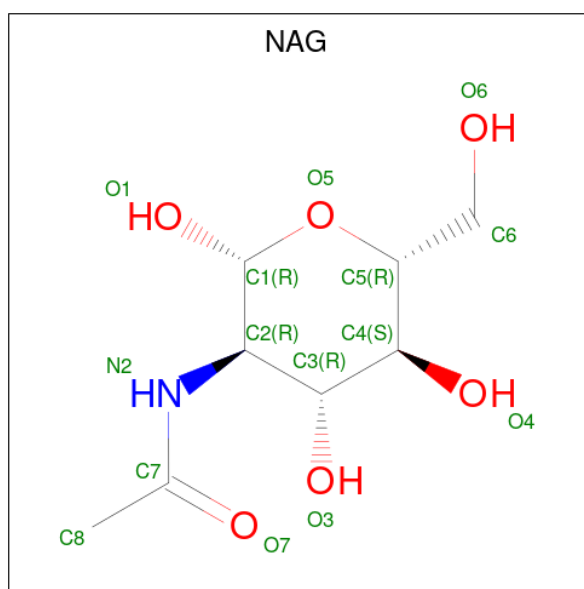
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

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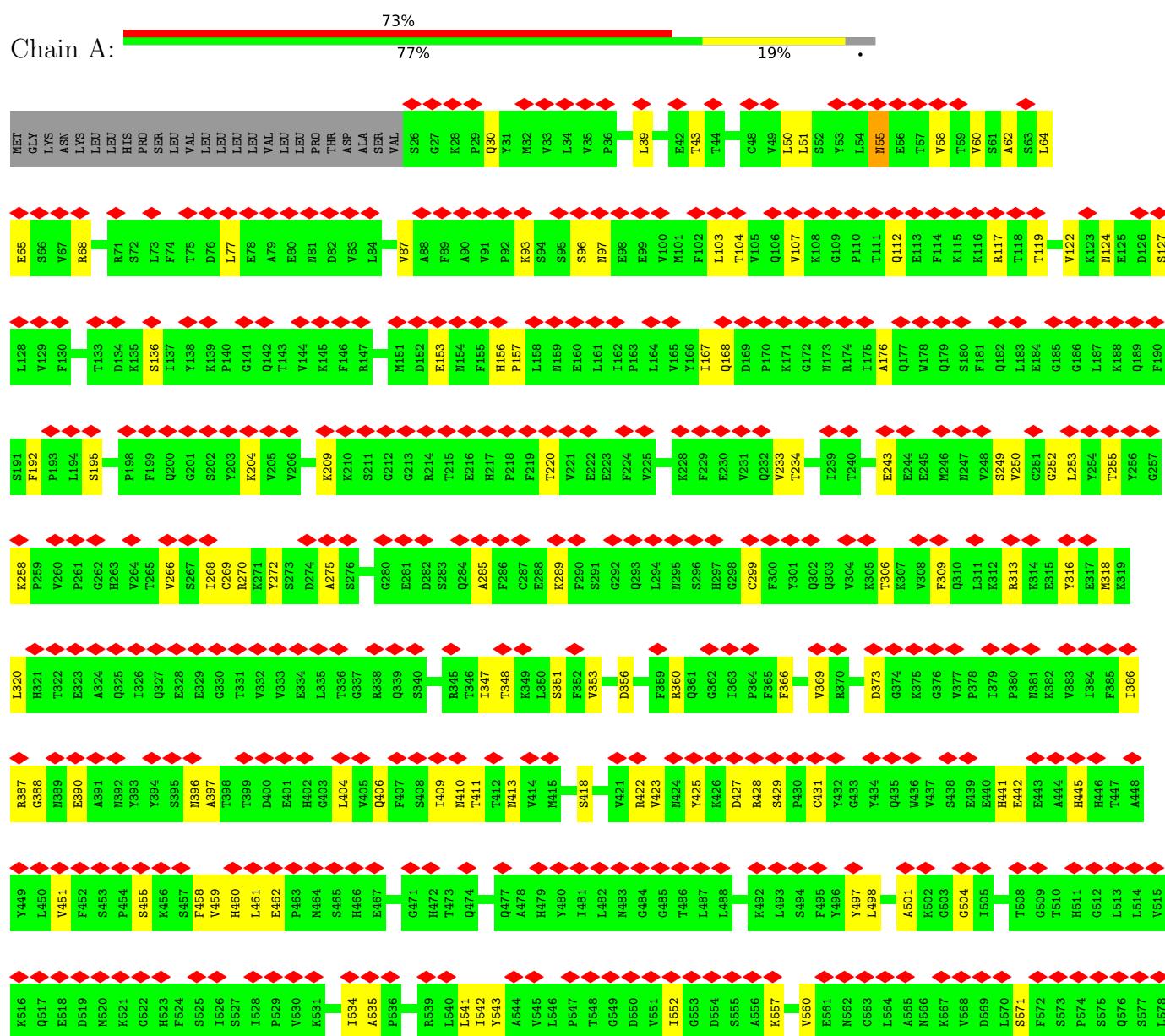
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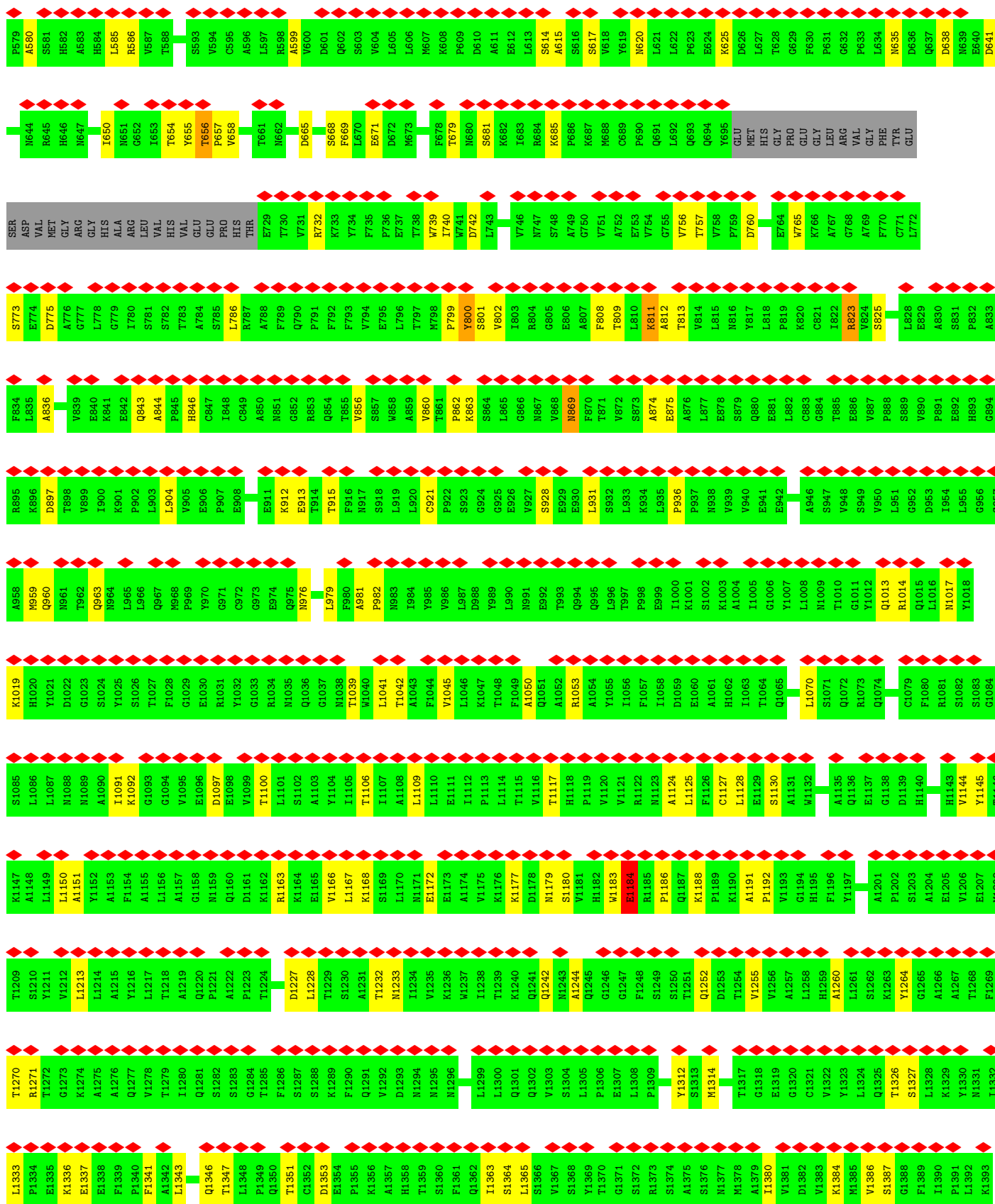
Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	

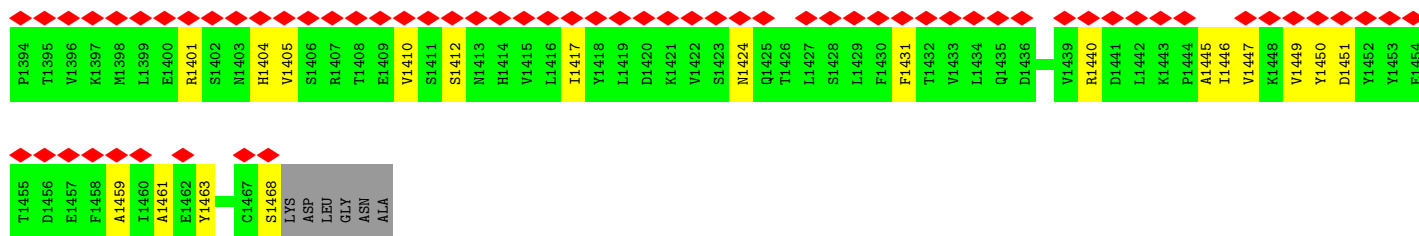
3 Residue-property plots

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.

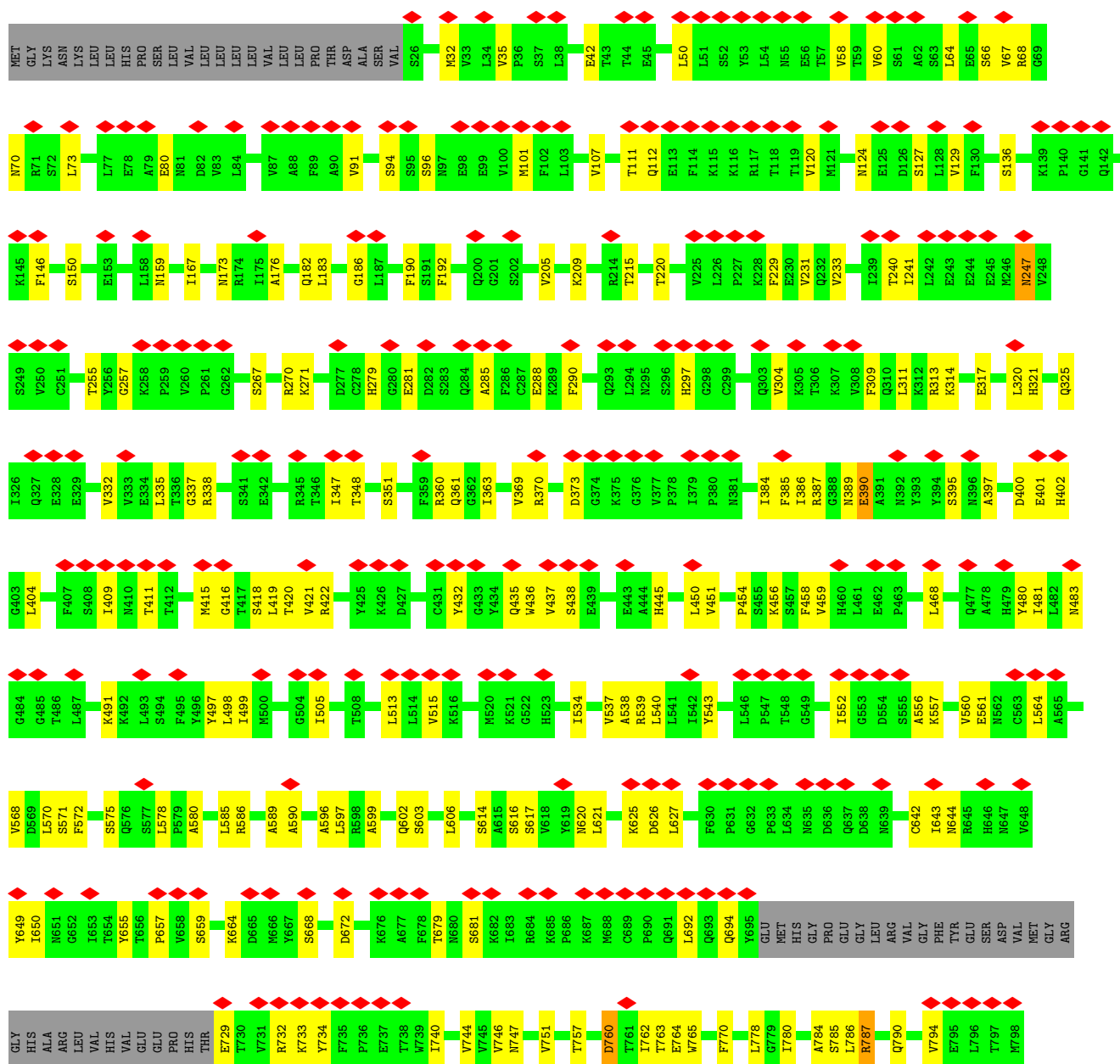
• Molecule 1: Alpha-2-macroglobulin



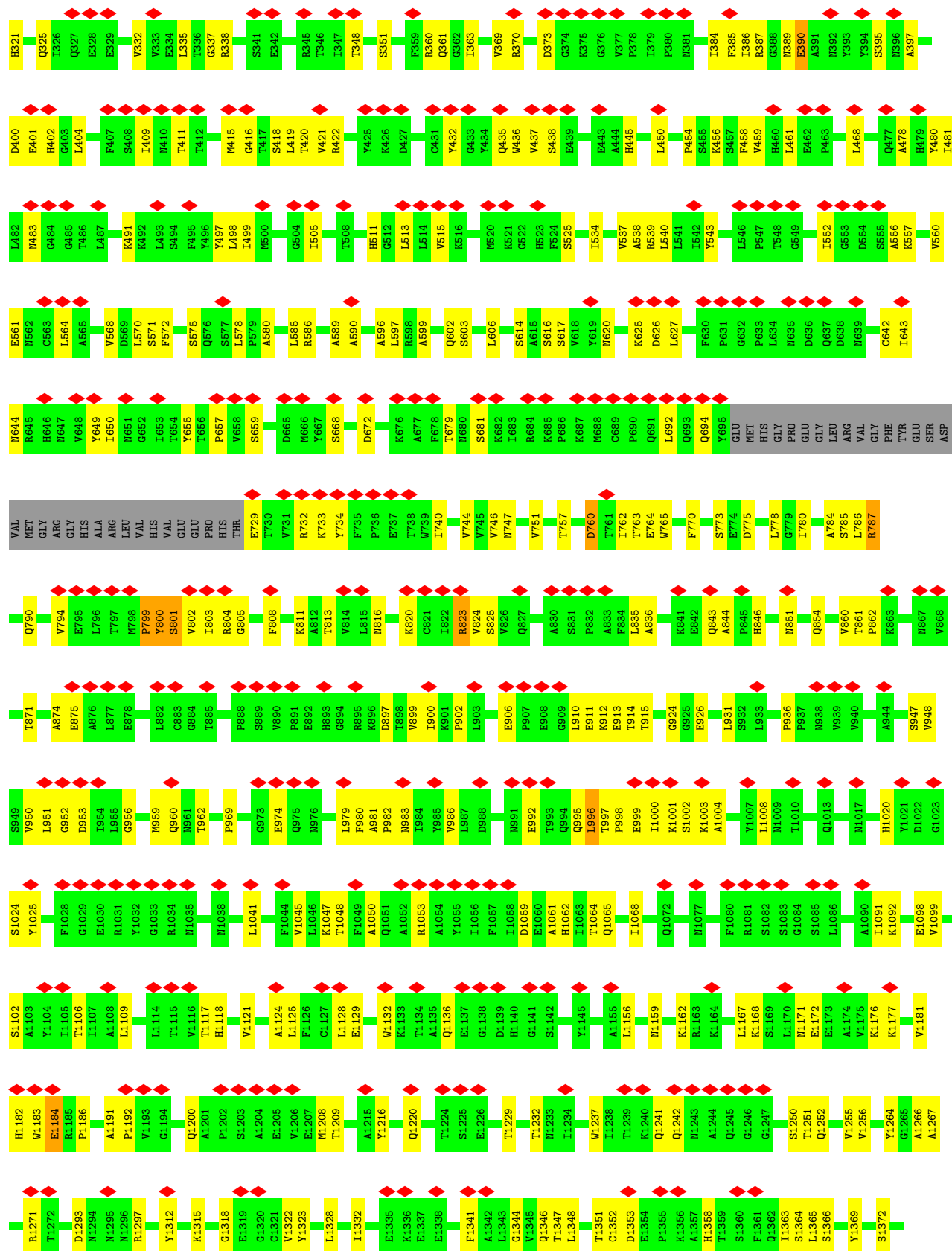


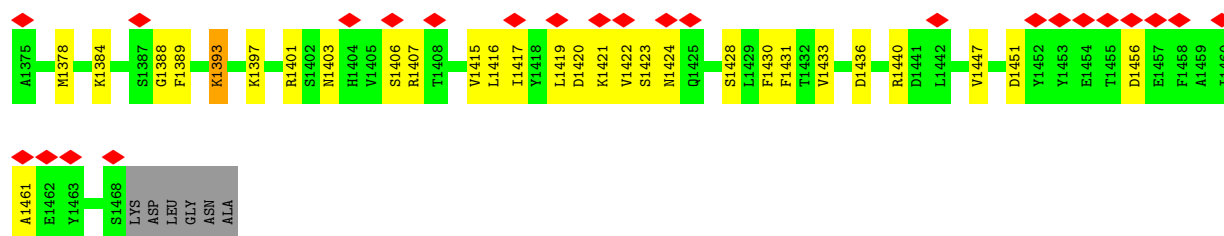


• Molecule 1: Alpha-2-macroglobulin



F190	F191	F192	F193	F194	F195	P198	F199	Q200	G201	S202	Y203	K204	V205	V206	K209	K210	S211	G212	G213	R214	T215	E216	H217	P218	F219	T220	V221	E222	E223	F224	V225	K228	F229	E230	V231	Q232	V233	T234	I239	T240	E243	E244	E245	M246	N247	V248	S249	C250	G251	G252	L253	Y254	T255	Y256						
G257	K258	P259	V260	P261	G262	H263	V264	T265	V266	S267	E268	C269	R270	K271	Y272	S273	D274	A275	S276	G280	E281	D282	S283	Q284	A285	F286	Q287	L288	K289	F290	S291	G292	Q293	L294	N295	S296	H297	G298	C299	F300	Y301	Q302	Q303	V304	T306	K307	V308	F309	Q310	L311	K312	R313	E315	Y316	E317	N318				
K319	L320	H321	T322	E323	Q325	I326	Q327	E328	E329	G330	T331	V332	V333	E334	L335	T336	G337	R338	Q339	S340	R345	T346	T347	T348	K349	L350	S351	F352	V353	D356	F359	R360	N295	Q361	G362	I363	P364	F365	F366	V369	R370	D373	G374	K375	G376	F377	P378	I379	P380	N381	K382	V383	I384	F385						
I386	R387	C388	N389	E390	A391	N392	Y393	Y394	S395	N396	T398	T399	D400	E401	H402	G403	L404	Y405	Q406	F407	S408	I409	N410	T411	T412	N413	V414	S351	F352	S418	V421	R422	V423	N424	Y425	K426	D427	R428	S429	P430	C431	Y432	G433	Y434	Q435	H436	V437	S438	E439	E440	H441	E442	E443	A444	H445	H446	T447			
A448	Y449	L450	V451	F452	A453	P454	S455	K456	S457	F458	V459	H460	L461	E462	P463	M464	S465	H466	E467	G471	H472	T473	Q474	Q477	A478	H479	Y480	I481	L482	N483	G484	G485	T486	L487	L488	K492	L493	S494	F495	Y496	Y497	L498	A501	K502	G503	G504	I505	T508	G509	T510	H511	G512	L513	L514						
V515	K516	Q517	E518	D519	M520	K521	G522	H523	F524	S525	I526	S527	L528	P529	V530	K531	I534	A535	P536	R539	L540	L541	I542	Y543	A544	V545	L546	P547	T548	G549	D550	G551	I552	G553	D554	S555	A556	K557	V560	E561	N562	C563	L564	A565	N566	K567	V568	D569	L570	S571	F572	S573	P574	S575	Q576	S577				
L578	P579	A580	S581	H582	H584	L585	R586	V587	T588	S593	V594	C595	A596	L597	R598	A599	D601	Q602	S603	V604	L605	L606	H607	K608	P609	D610	A611	E612	L613	S614	A615	S616	S617	V618	V619	N620	L621	L622	P623	E624	K625	D626	L627	T628	G629	F630	P631	G632	P633	L634	N635	D636	Q637	D638	N639	E640				
D641	N644	R645	H646	H647	L650	N651	G652	L653	T654	V655	T656	P657	V658	T661	N662	D665	S668	F669	L670	E671	D672	H673	F678	T679	N680	S681	K682	L683	R684	K685	P686	K687	C688	C689	P690	Q691	L692	Q693	Q694	V695	GLU	MET	HIS	GLY	PRO	GLU	GLY	LEU	ARG	VAL	PHE	TYR								
GLU	SER	ASP	VAL	MET	ARG	HIS	ALA	ARG	LEU	VAL	HIS	VAL	GLU	PRO	HIS	THR	E729	F730	W731	R732	K733	Y734	F735	P736	E737	T738	W739	I740	W741	D742	S681	L743	V746	N747	S748	G750	V751	E752	E753	W754	G755	W756	T757	W758	F759	D760	E764	W765	K766	A767	G768	A769	F770	C771						
L772	S773	E774	A775	G777	L778	G779	W780	S781	T782	T783	W784	S785	L786	R787	A788	F789	Q790	P791	F792	F793	W794	E795	L796	T797	W798	F799	Y800	S801	V802	T803	R804	G805	E806	A807	F808	T809	L810	A812	T813	W814	L815	N816	Y817	L818	P819	R820	C821	R823	W824	S825	L828	E829	A830	S831	P832					
A833	P834	L835	A836	W839	E840	K841	E842	Q843	A844	P845	H846	C847	I848	C849	A850	N851	G852	R853	Q854	T855	V856	S857	W858	A859	V860	T861	P862	K863	S864	L865	G866	N867	V868	N869	F870	T871	W872	S873	K874	E875	A876	L877	E878	S879	Q880	E881	L882	C883	Q884	T885	E886	V887	P888	S889	W890	P891	E892	H893		
G894	R895	K896	D897	T898	V899	I900	K901	P902	L903	L904	V905	E906	P907	E908	E911	K912	E913	T914	T915	F916	N917	P918	L919	L920	C921	P922	S923	G924	G925	E926	V927	S928	E929	E930	L931	S932	L933	K934	L935	P936	P937	N938	V939	P940	E941	G942	A946	S947	V948	S949	G1011	Y1012	Q1013	R1014	G952	L953	I954	L955	G956	
S957	A958	N959	Q960	N961	T962	Q963	N964	L965	L966	Q967	N968	P969	Y970	G971	C972	G973	E974	Q975	N976	L979	F980	A981	P982	N983	L984	Y985	V986	L987	D988	Y989	L990	N991	E992	T993	Q994	Q995	L996	T997	P998	E999	I1000	K1001	S1002	K1003	A1004	T1005	L1006	Y1007	L1008	N1009	T1010	G1011	Y1012	Q1013	R1014	G952	L953	I954	L955	G956





- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



- Molecule 4: 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, C2	Depositor
Number of particles used	30618	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 ($e^-/\text{\AA}^2$)	39.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	47775	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (\AA)	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.047, 1.047, 1.047	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: BMA, NAG, MAN

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	0/11249	0.61	4/15286 (0.0%)
1	B	0.33	0/11248	0.62	3/15283 (0.0%)
1	C	0.32	0/11249	0.61	4/15286 (0.0%)
1	D	0.33	0/11248	0.62	3/15283 (0.0%)
All	All	0.33	0/44994	0.62	14/61138 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	801	SER	N-CA-C	-6.57	93.27	111.00
1	D	801	SER	N-CA-C	-6.57	93.27	111.00
1	A	55	ASN	CB-CA-C	6.51	123.43	110.40
1	C	55	ASN	CB-CA-C	6.51	123.43	110.40
1	B	760	ASP	CB-CG-OD1	5.91	123.62	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11004	0	10891	186	0
1	B	11004	0	10888	271	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	11004	0	10891	193	0
1	D	11004	0	10888	267	0
2	E	50	0	43	3	0
2	H	50	0	43	3	0
3	F	39	0	34	1	0
3	I	39	0	34	1	0
4	G	28	0	25	3	0
4	J	28	0	25	3	0
5	A	112	0	104	5	0
5	B	70	0	65	6	0
5	C	112	0	104	5	0
5	D	70	0	65	6	0
All	All	44614	0	44100	915	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 10.

The worst 5 of 915 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:55:ASN:HD22	5:C:2001:NAG:C1	1.06	1.57
1:A:55:ASN:HD22	5:A:2001:NAG:C1	1.06	1.55
1:B:1424:ASN:ND2	4:G:1:NAG:C1	1.70	1.52
1:D:1424:ASN:ND2	4:J:1:NAG:C1	1.70	1.51
1:B:247:ASN:HD21	5:B:2003:NAG:C1	1.27	1.45

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	1406/1474 (95%)	1190 (85%)	209 (15%)	7 (0%)	25	64
1	B	1404/1474 (95%)	1163 (83%)	233 (17%)	8 (1%)	22	60
1	C	1406/1474 (95%)	1190 (85%)	209 (15%)	7 (0%)	25	64
1	D	1404/1474 (95%)	1163 (83%)	233 (17%)	8 (1%)	22	60
All	All	5620/5896 (95%)	4706 (84%)	884 (16%)	30 (0%)	27	64

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	800	TYR
1	A	1184	GLU
1	B	1184	GLU
1	C	800	TYR
1	C	1184	GLU

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	1236/1290 (96%)	1220 (99%)	16 (1%)	65	77
1	B	1236/1290 (96%)	1227 (99%)	9 (1%)	81	87
1	C	1236/1290 (96%)	1220 (99%)	16 (1%)	65	77
1	D	1236/1290 (96%)	1227 (99%)	9 (1%)	81	87
All	All	4944/5160 (96%)	4894 (99%)	50 (1%)	71	82

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	ARG
1	C	863	LYS
1	D	1397	LYS
1	C	396	ASN
1	C	732	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1425	GLN
1	C	182	GLN
1	D	435	GLN
1	C	112	GLN
1	C	474	GLN

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 ⓘ

18 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	E	1	2	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	1.07	1 (5%)
2	BMA	E	3	2	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
2	MAN	E	4	2	11,11,12	0.23	0	15,15,17	0.58	0
3	NAG	F	1	1,3	14,14,15	0.33	0	17,19,21	0.84	0
3	NAG	F	2	3	14,14,15	0.29	0	17,19,21	0.73	0
3	BMA	F	3	3	11,11,12	0.23	0	15,15,17	0.63	0
4	NAG	G	1	4	14,14,15	0.63	0	17,19,21	1.66	4 (23%)
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
2	NAG	H	1	2	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.39	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	H	3	2	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
2	MAN	H	4	2	11,11,12	0.23	0	15,15,17	0.58	0
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.84	0
3	NAG	I	2	3	14,14,15	0.29	0	17,19,21	0.73	0
3	BMA	I	3	3	11,11,12	0.23	0	15,15,17	0.63	0
4	NAG	J	1	4	14,14,15	0.63	0	17,19,21	1.66	4 (23%)
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.83	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	E	1	2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
2	NAG	H	1	2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	MAN	H	4	2	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	O5-C1-C2	-4.00	104.98	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	O5-C1-C2	-4.00	104.98	111.29
2	E	2	NAG	C1-O5-C5	3.42	116.83	112.19
2	H	2	NAG	C1-O5-C5	3.42	116.83	112.19
4	G	1	NAG	O4-C4-C3	3.32	118.03	110.35

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

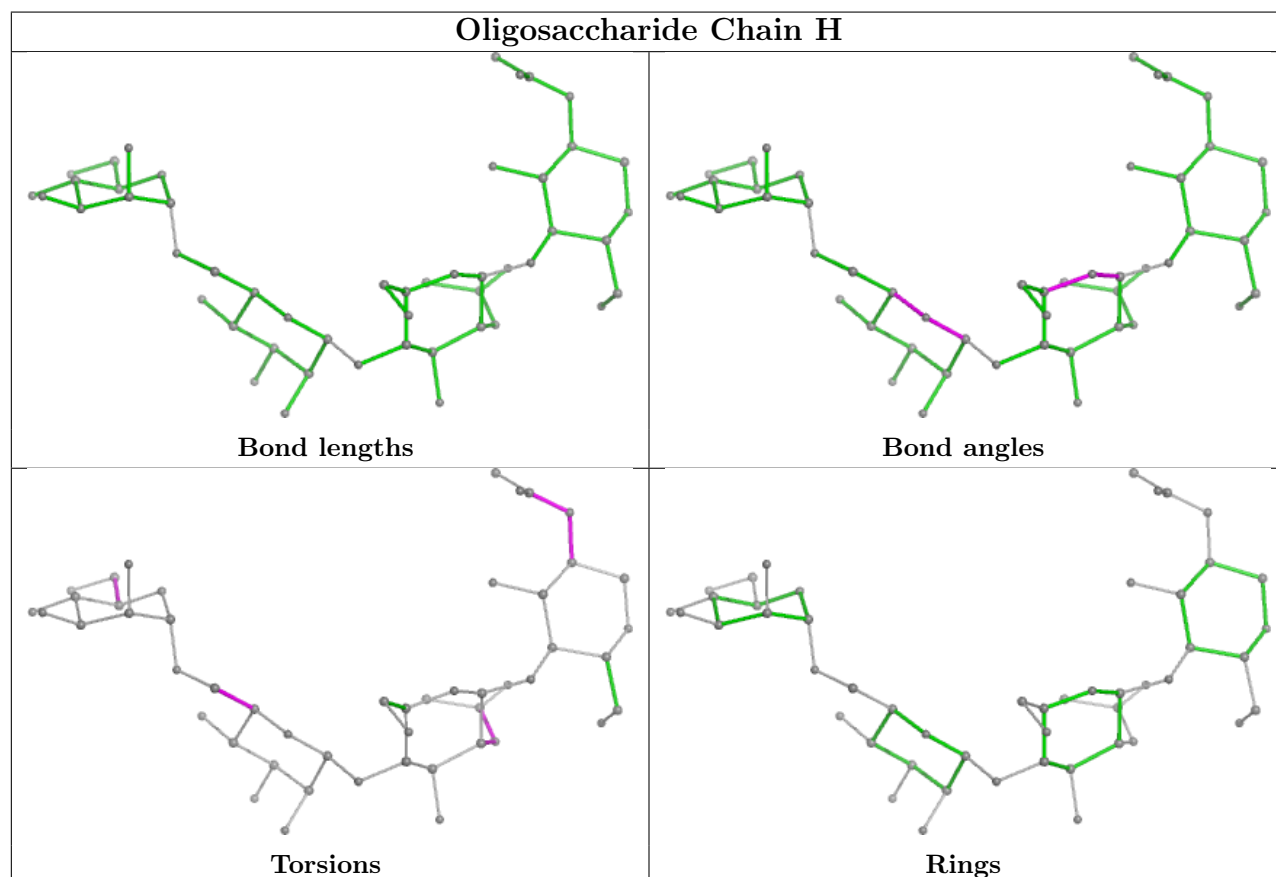
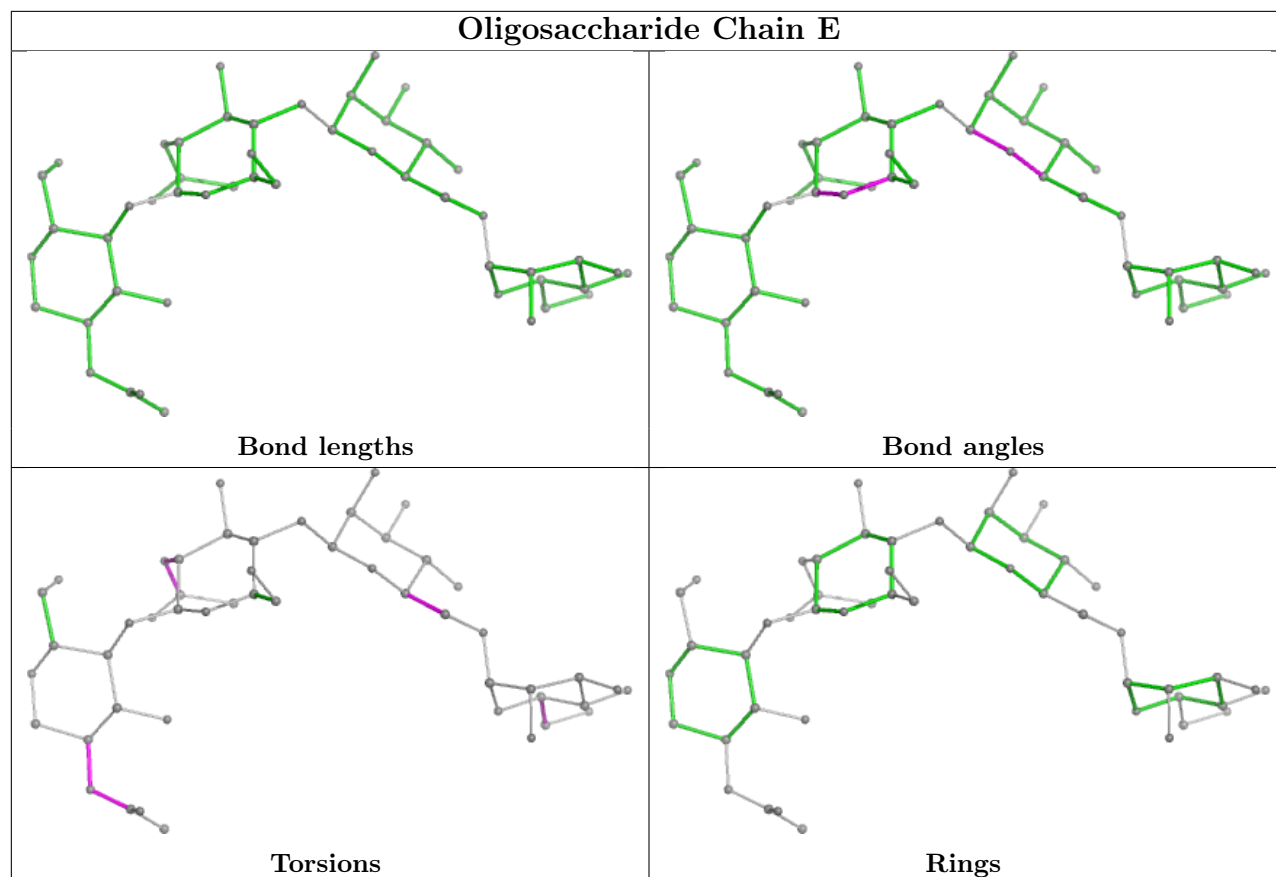
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

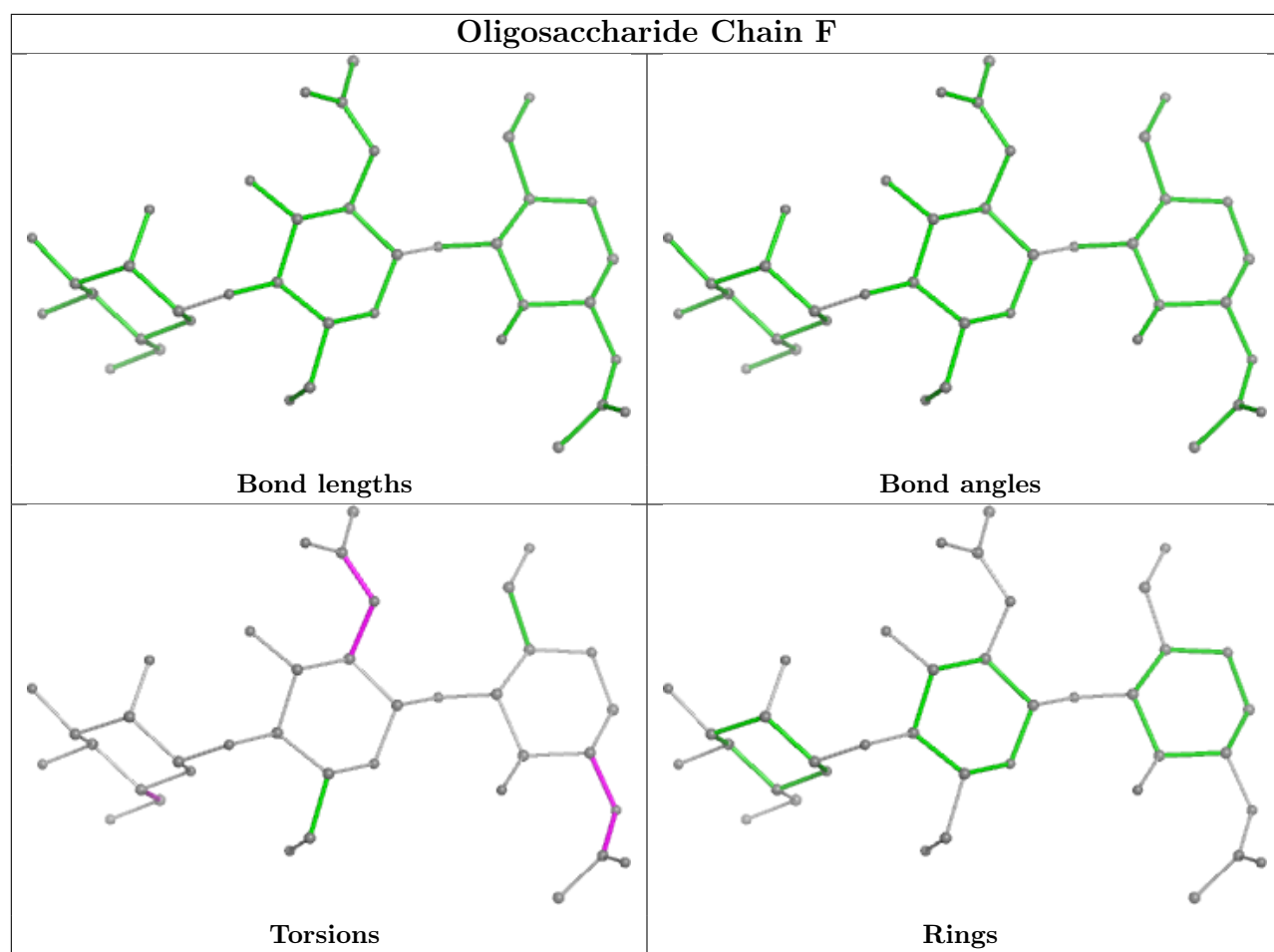
There are no ring outliers.

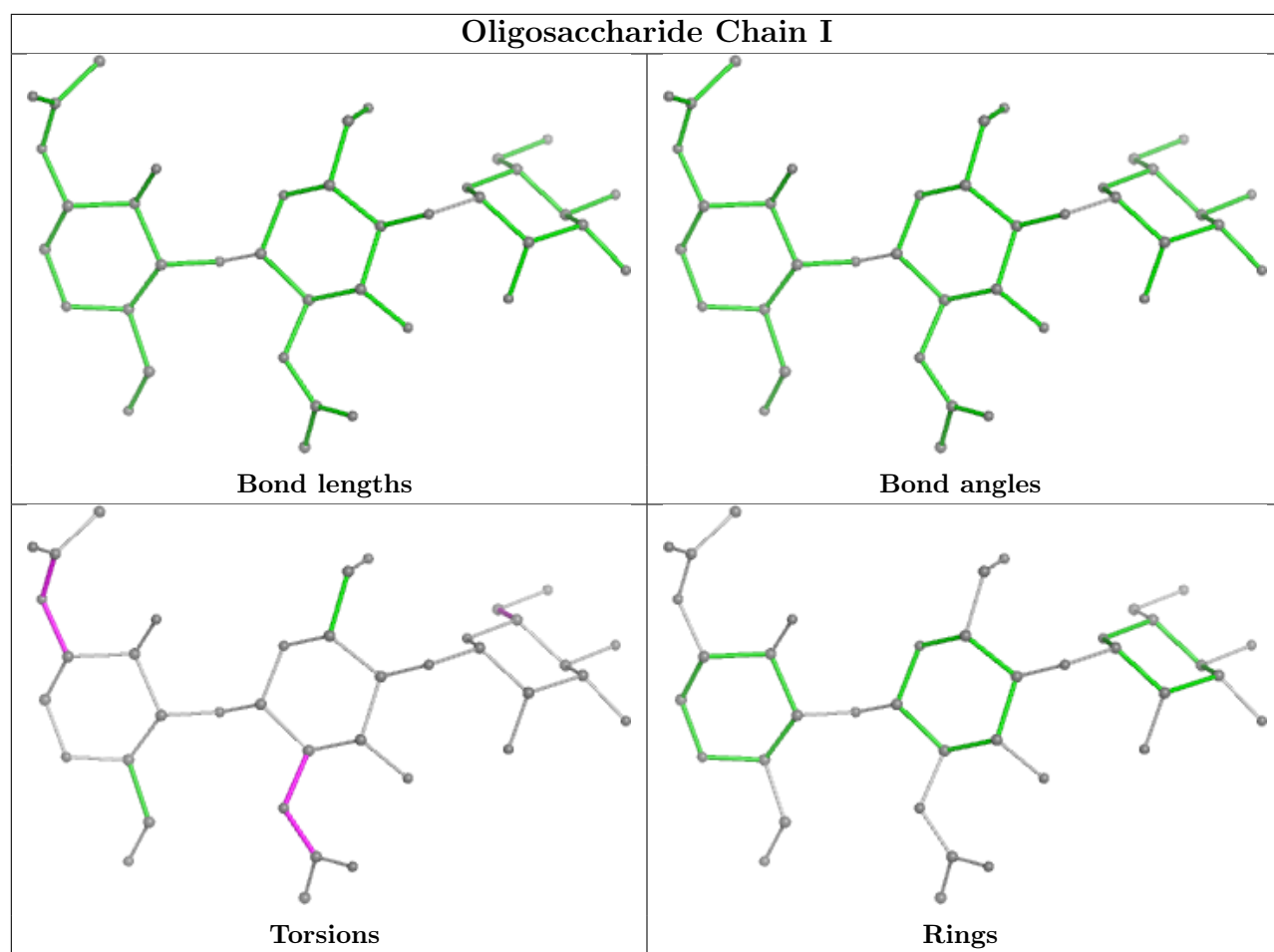
10 monomers are involved in 14 short contacts:

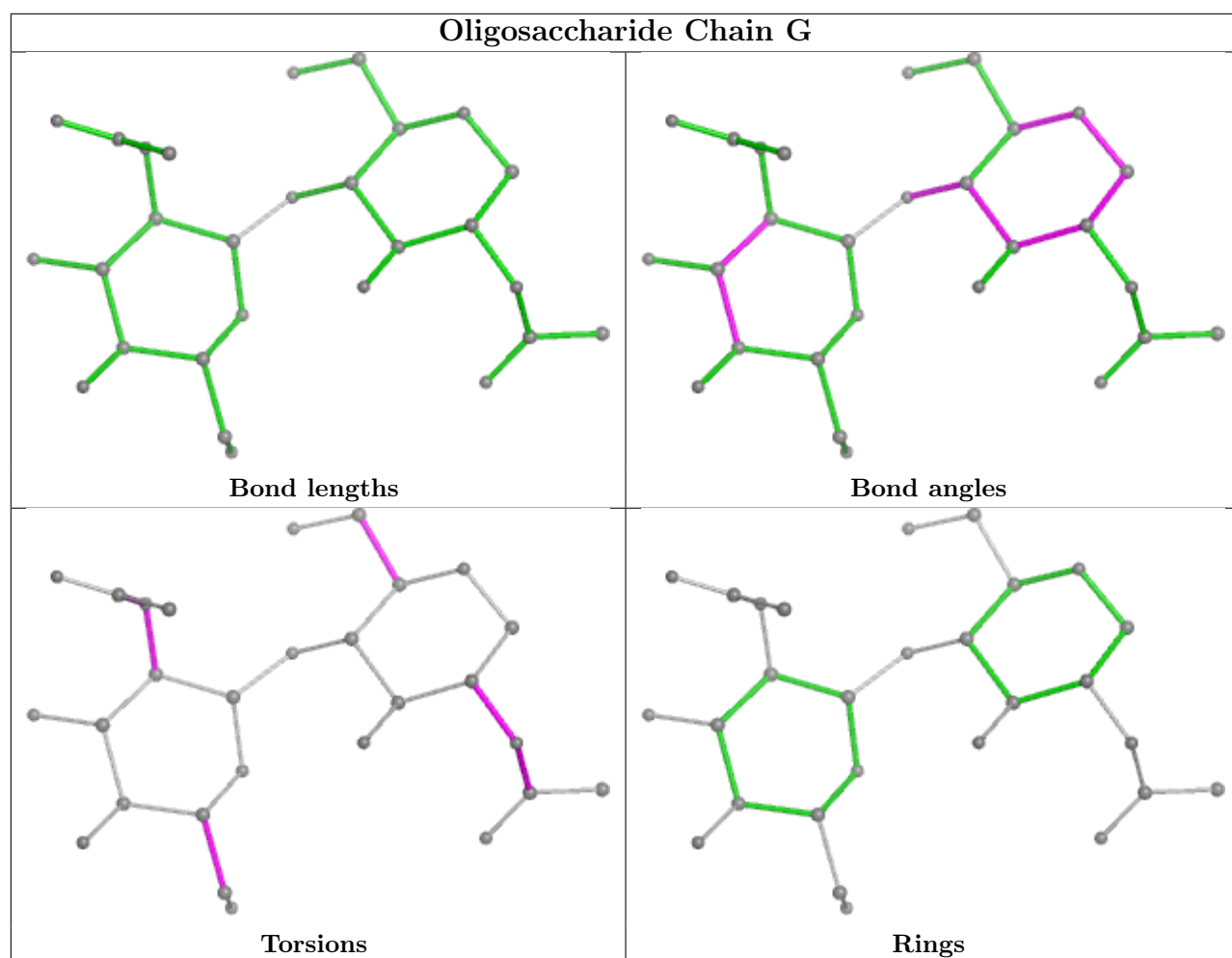
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	1	0
3	F	1	NAG	1	0
4	G	1	NAG	3	0
4	J	1	NAG	3	0
2	E	1	NAG	1	0
2	H	2	NAG	2	0
3	I	1	NAG	1	0
2	H	1	NAG	1	0
2	E	2	NAG	2	0
3	F	2	NAG	1	0

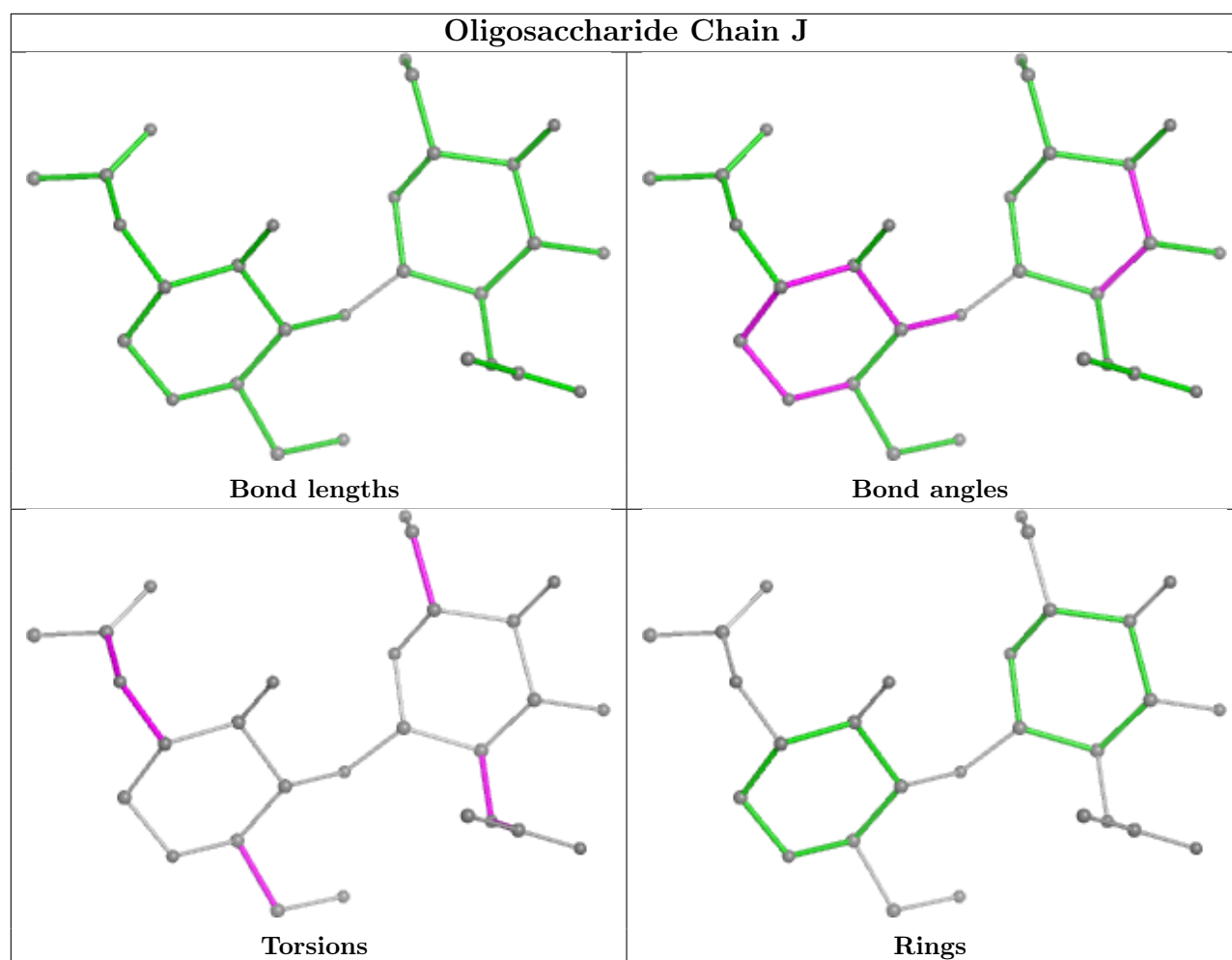
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	2004	-	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
5	NAG	A	2001	-	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	C	2002	-	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	A	2002	-	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	A	2005	1	14,14,15	0.36	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	2005	1	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
5	NAG	C	2003	1	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
5	NAG	C	2008	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	B	2002	-	14,14,15	0.27	0	17,19,21	0.79	0
5	NAG	C	2004	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	A	2004	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	C	2006	1	14,14,15	0.33	0	17,19,21	0.84	0
5	NAG	D	2004	-	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
5	NAG	A	2008	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	B	2003	-	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	D	2001	1	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	B	2001	1	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	D	2005	1	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	D	2002	-	14,14,15	0.27	0	17,19,21	0.79	0
5	NAG	A	2003	1	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
5	NAG	C	2001	-	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	B	2005	1	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	D	2003	-	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	A	2006	1	14,14,15	0.33	0	17,19,21	0.84	0
5	NAG	A	2007	1	14,14,15	0.30	0	17,19,21	0.67	0
5	NAG	C	2007	1	14,14,15	0.30	0	17,19,21	0.67	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
5	NAG	B	2004	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2001	-	-	1/6/23/26	0/1/1/1
5	NAG	C	2002	-	-	3/6/23/26	0/1/1/1
5	NAG	A	2002	-	-	3/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2008	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2002	-	-	4/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2004	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2003	-	-	4/6/23/26	0/1/1/1
5	NAG	D	2001	1	-	1/6/23/26	0/1/1/1
5	NAG	B	2001	1	-	1/6/23/26	0/1/1/1
5	NAG	D	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2002	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2001	-	-	1/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2003	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2007	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2007	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	NAG	C1-O5-C5	3.89	117.47	112.19
5	C	2001	NAG	C1-O5-C5	3.89	117.47	112.19
5	B	2001	NAG	C1-O5-C5	3.84	117.40	112.19
5	D	2001	NAG	C1-O5-C5	3.84	117.40	112.19
5	B	2004	NAG	O5-C5-C6	2.48	111.10	107.20

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2002	NAG	C3-C2-N2-C7
5	A	2002	NAG	C8-C7-N2-C2
5	A	2002	NAG	O7-C7-N2-C2
5	A	2004	NAG	C8-C7-N2-C2
5	A	2004	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2004	NAG	1	0
5	A	2001	NAG	5	0
5	D	2004	NAG	1	0
5	B	2003	NAG	4	0
5	D	2005	NAG	1	0
5	C	2001	NAG	5	0
5	B	2005	NAG	1	0
5	D	2003	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	629:GLY	C	630:PHE	N	5.14
1	D	629:GLY	C	630:PHE	N	5.14

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12748. These allow visual inspection of the internal detail of the map and identification of artifacts.

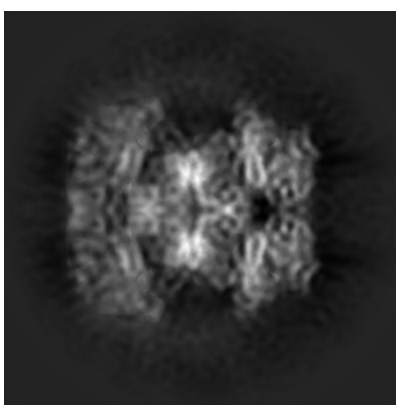
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

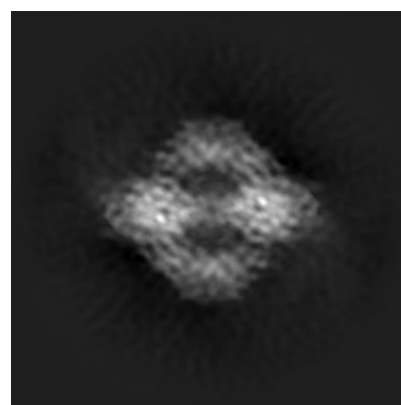
6.1.1 Primary map



X



Y

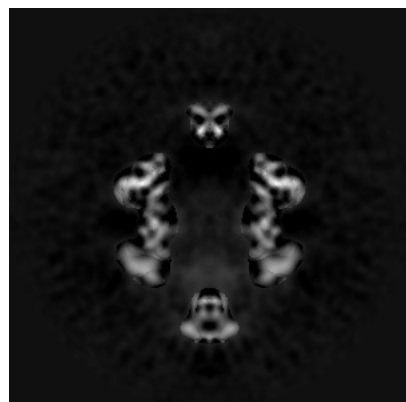


Z

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

6.2 Central slices [i](#)

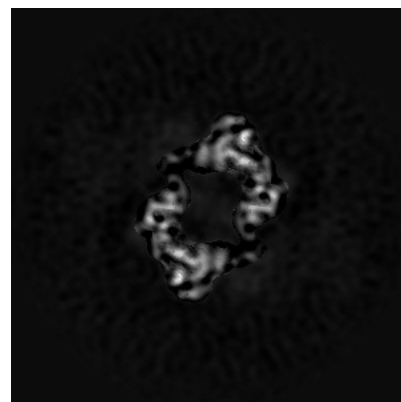
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

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: 130



Y Index: 160



Z Index: 195

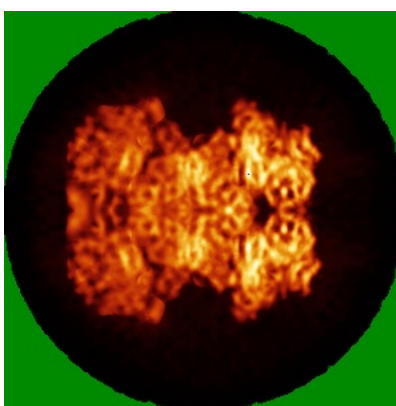
The images above show the largest variance slices of the map in three orthogonal directions.

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

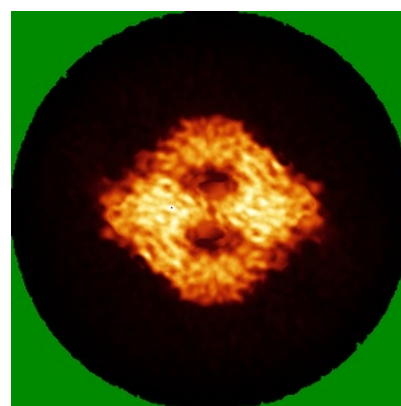
6.4.1 Primary map



X



Y

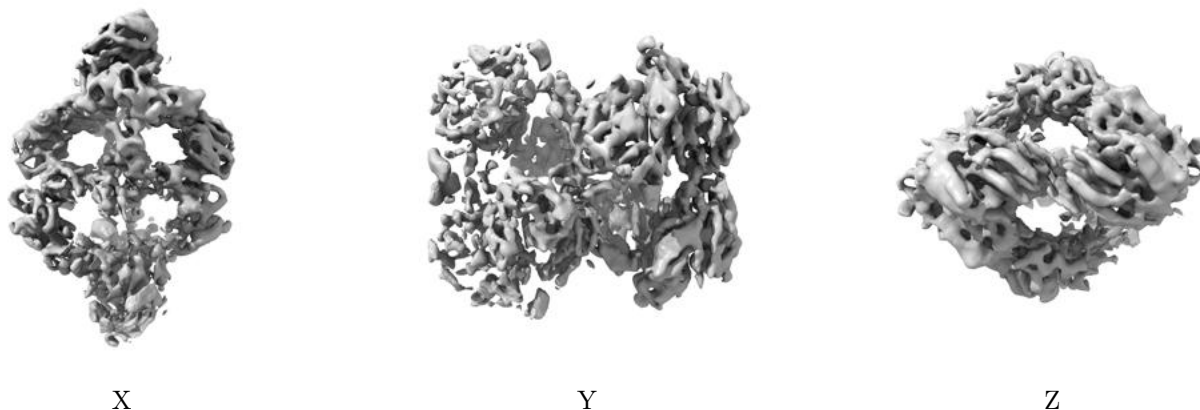


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

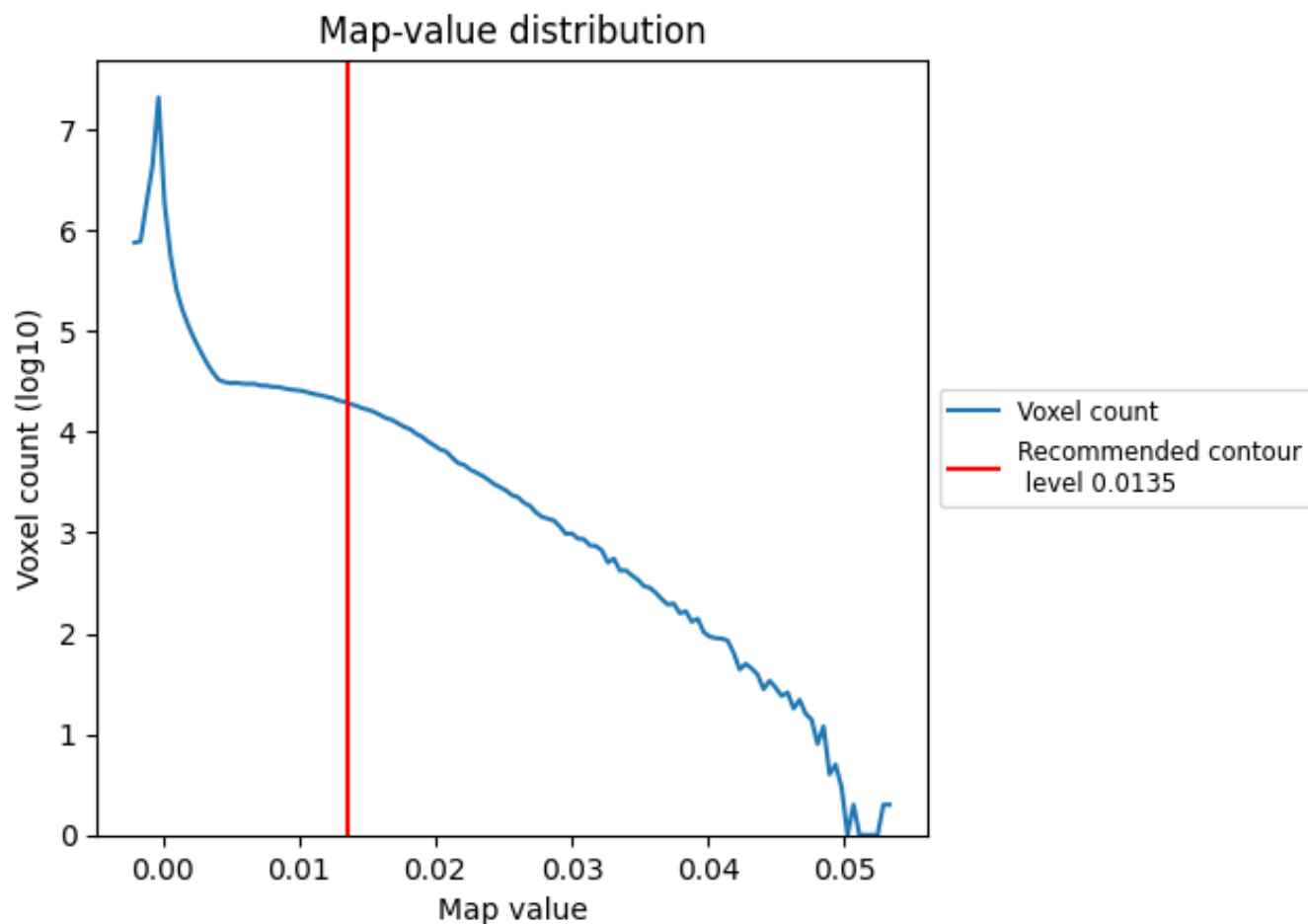
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

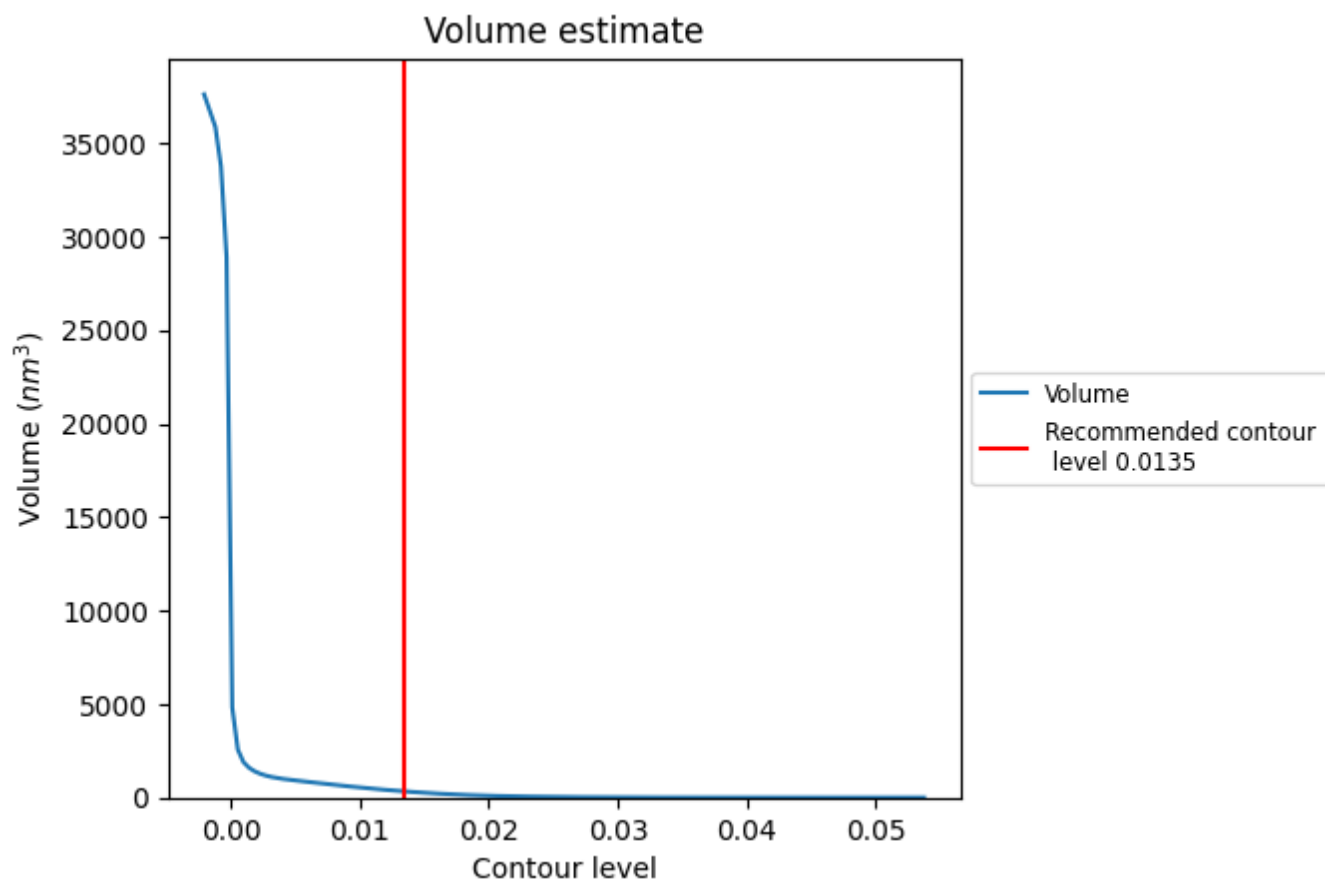
This section contains the results of statistical analysis of the map.

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.

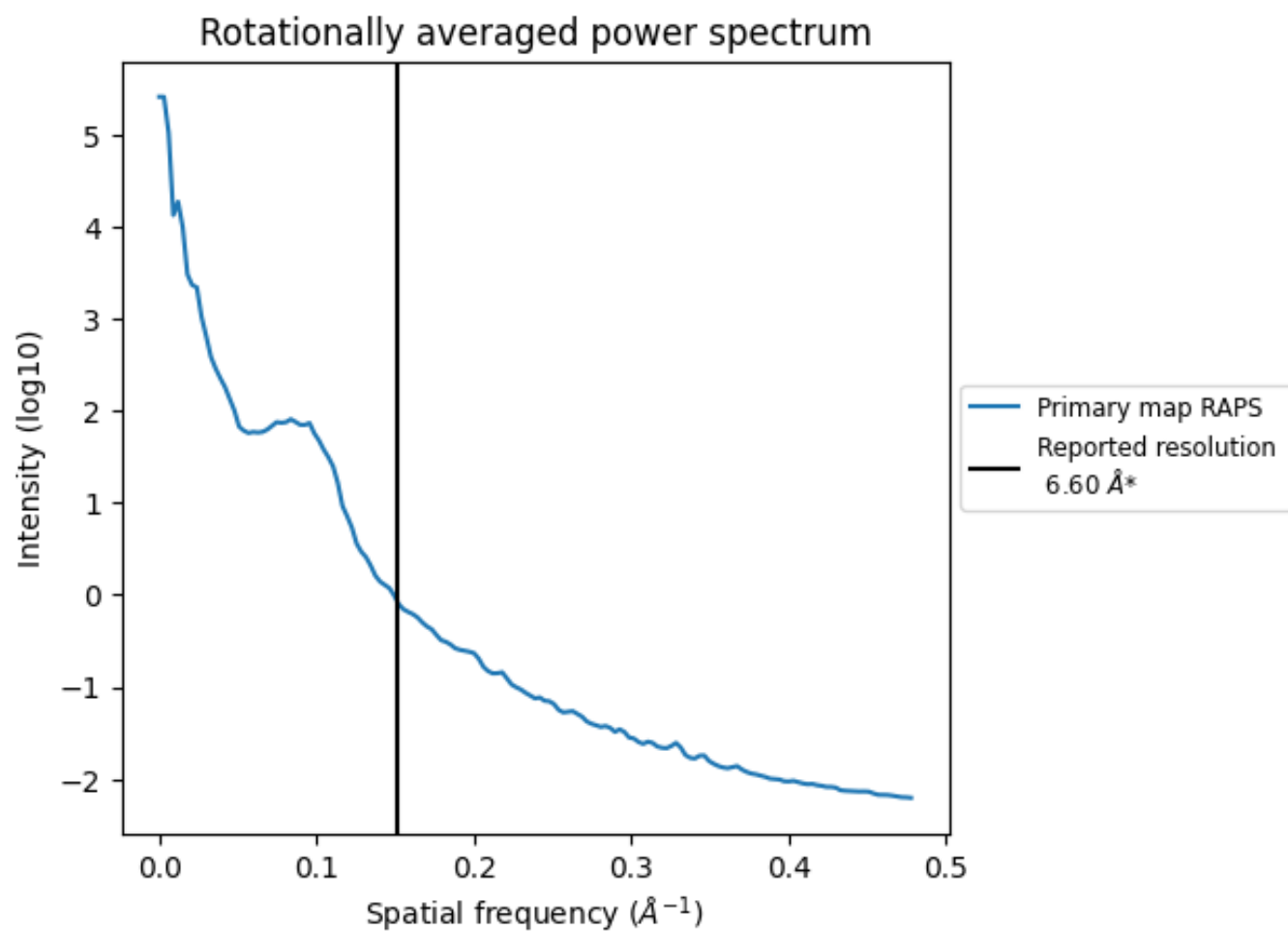
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm^3 ; this corresponds to an approximate mass of 297 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 0.152 Å⁻¹

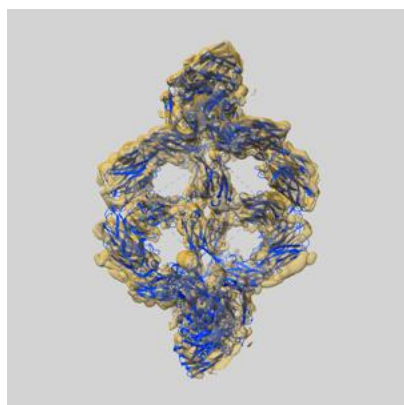
8 Fourier-Shell correlation

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

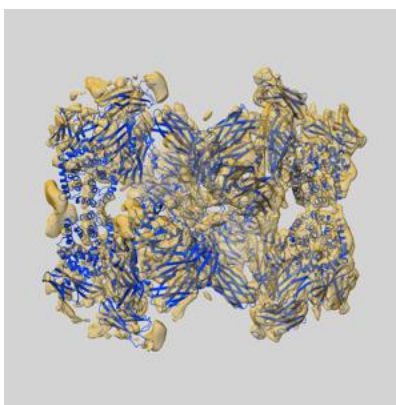
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12748 and PDB model 7O7M. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

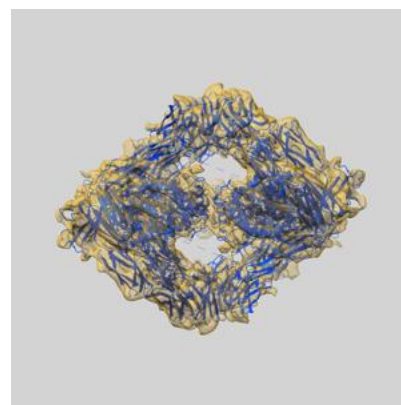
9.1 Map-model overlay [i](#)



X



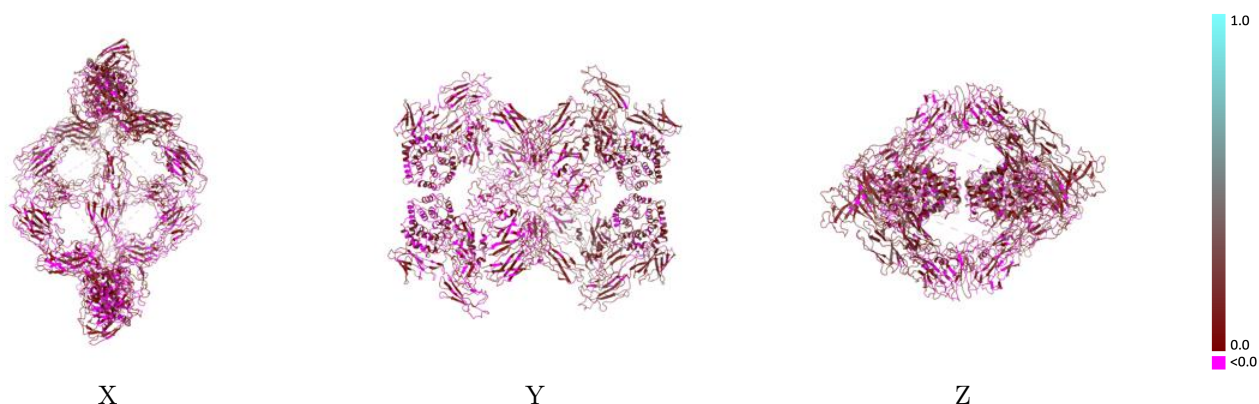
Y



Z

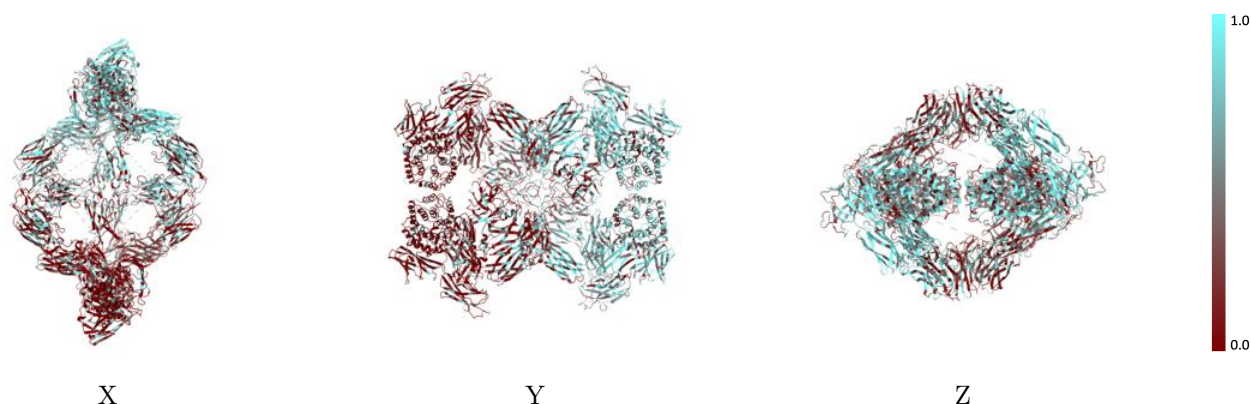
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



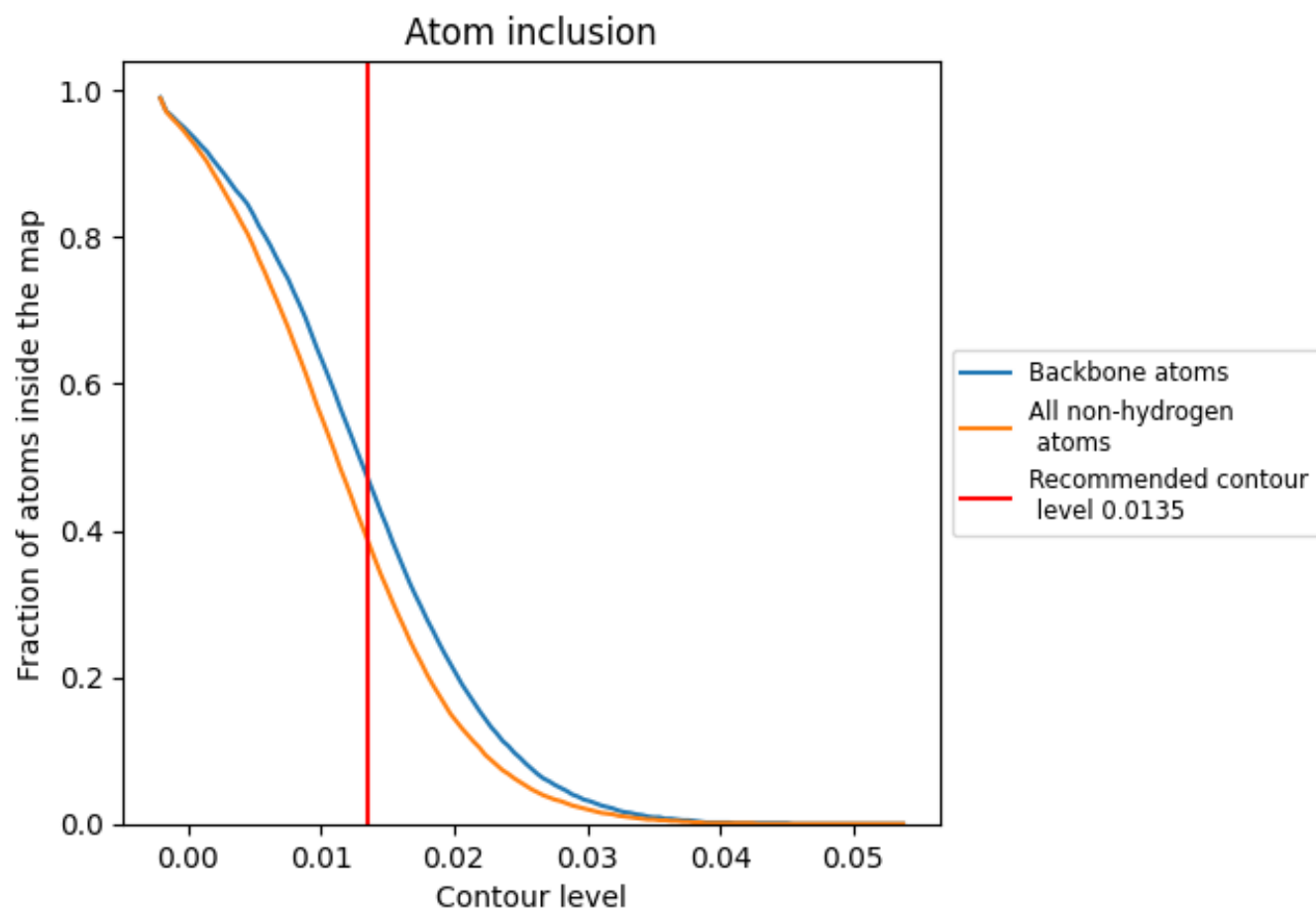
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).























9.4 Atom inclusion ⓘ



At the recommended contour level, 47% of all backbone atoms, 39% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3870	 0.0970
A	 0.2130	 0.0550
B	 0.5610	 0.1380
C	 0.2130	 0.0530
D	 0.5610	 0.1390
E	 0.5800	 0.2000
F	 0.3850	 0.2290
G	 0.1430	 0.2210
H	 0.5800	 0.2060
I	 0.3850	 0.2110
J	 0.1430	 0.2120

