



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:53 AM UTC

PDB ID : 1HCY / pdb_00001hcy
Title : CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PAN-
ULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION
Authors : Volbeda, A.; Hol, W.G.J.
Deposited on : 1991-05-15
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

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>.

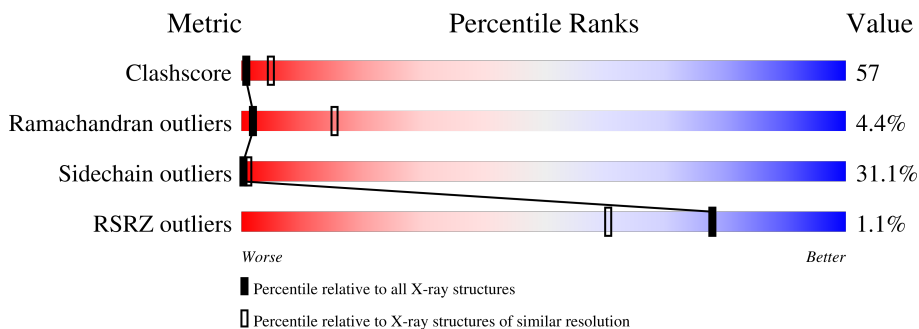
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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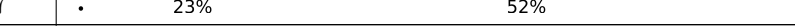
X-RAY DIFFRACTION

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	657	
1	B	657	
1	C	657	
1	D	657	
1	E	657	
1	F	657	
2	G	2	

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	1	X	-	-	-
2	NAG	H	1	X	-	-	-
2	NAG	I	1	X	-	-	-
2	NAG	J	1	X	-	-	-
2	NAG	K	1	X	-	-	-
2	NAG	L	1	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	B	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	C	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	D	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	E	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	F	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	conflict	UNP P04254
A	163	PRO	GLN	conflict	UNP P04254
A	458	ASN	LYS	conflict	UNP P04254
A	514	SER	LYS	conflict	UNP P04254
B	32	ASP	GLU	conflict	UNP P04254
B	163	PRO	GLN	conflict	UNP P04254
B	458	ASN	LYS	conflict	UNP P04254
B	514	SER	LYS	conflict	UNP P04254
C	32	ASP	GLU	conflict	UNP P04254
C	163	PRO	GLN	conflict	UNP P04254
C	458	ASN	LYS	conflict	UNP P04254
C	514	SER	LYS	conflict	UNP P04254
D	32	ASP	GLU	conflict	UNP P04254
D	163	PRO	GLN	conflict	UNP P04254
D	458	ASN	LYS	conflict	UNP P04254
D	514	SER	LYS	conflict	UNP P04254
E	32	ASP	GLU	conflict	UNP P04254

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	conflict	UNP P04254
E	458	ASN	LYS	conflict	UNP P04254
E	514	SER	LYS	conflict	UNP P04254
F	32	ASP	GLU	conflict	UNP P04254
F	163	PRO	GLN	conflict	UNP P04254
F	458	ASN	LYS	conflict	UNP P04254
F	514	SER	LYS	conflict	UNP P04254

- 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				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cu	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	4	Total	O	0	0
			4	4		

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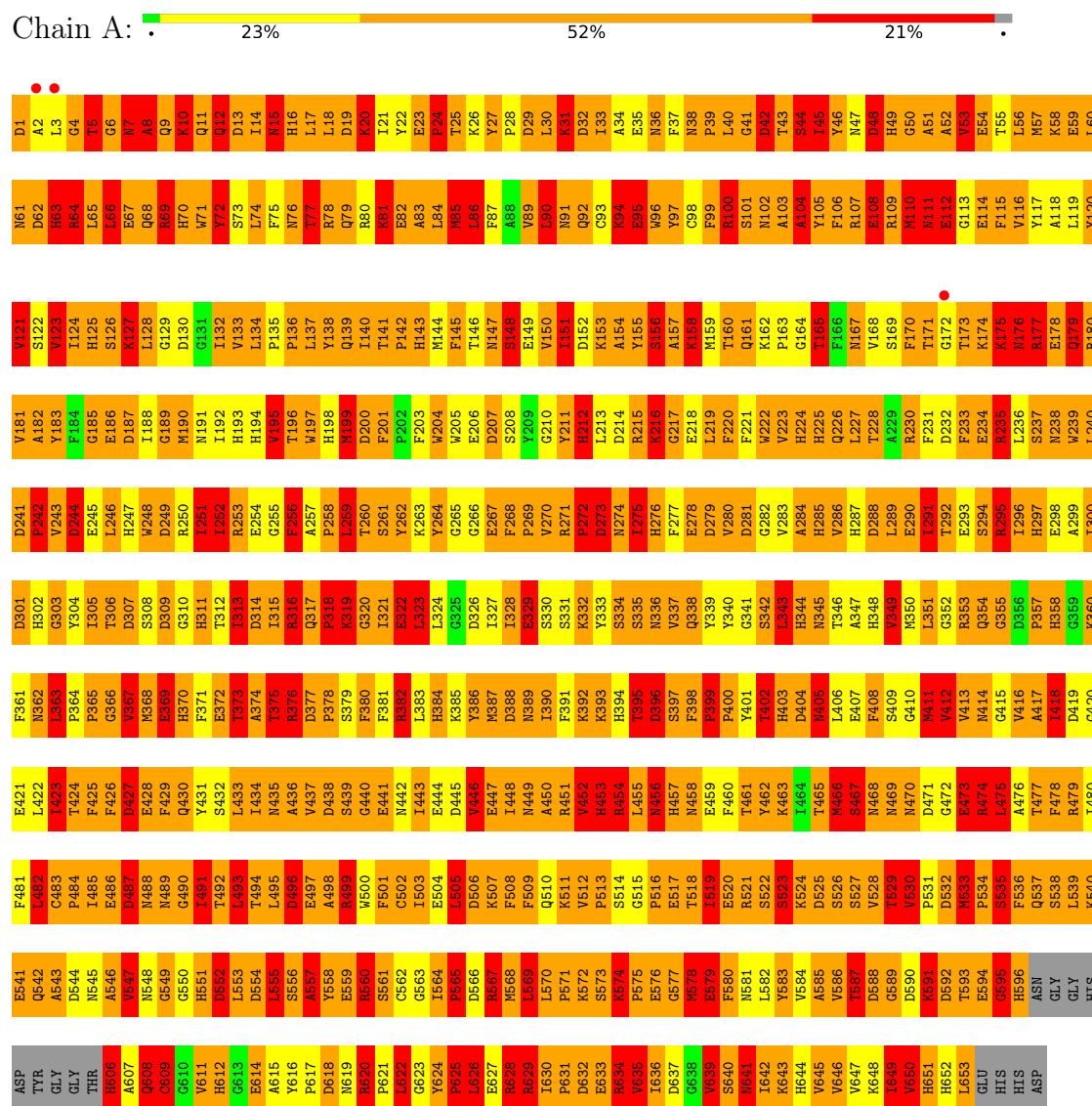
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		
4	F	1	Total	O	0	0
			1	1		

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ARTHROPODAN HEMOCYANIN



• Molecule 1: ARTHROPODAN HEMOCYANIN







E541	Q542	A543	D544	N545	A546	Y547	N548	Q549	G550	H551	D552	L553	D554	L555	S556	A557	L558	N559	R560	S561	L562	G563	O564	P565	D566	R567	M568	L569	L570	P571	K572	S573	K574	P575	E576	G577	K578	E579	F580	N581	L582	K583	Y584	A585	V586	T587	D588	G589	D590	K591	D592	T593	E594	L595	H596	ASN	GLY	HIS
ASP	TYR	GLY	GLY	THR	H606	A607	Q608	C609	G610	H611	H612	G613	E614	A615	S616	P617	D618	N619	R620	P621	L622	G623	Y624	P625	L626	E627	R628	R629	I630	L631	D632	E633	R634	V635	I636	D637	G638	V639	S640	N641	I642	K643	H644	V645	V646	V647	D648	I649	V650	H651	H652	L653	GLU	HIS	HIS	ASP		

● Molecule 1: ARTHROPODAN HEMOCYANIN



D1	A2	L3	G4	T5	G6	N7	A8	Q9	K10	G11	Q12	S13	D14	I15	N16	D17	L18	D19	K20	I21	Y22	E23	P24	T25	K26	Y27	P28	D29	L30	N31	D32	I33	A34	E35	N36	F37	N38	P39	L40	G41	D42	K43	H44	V45	Y46	N47	D48	G49	G50	A51	A52	V53	E54	T55	F56	M57	K58	E59	L60
N61	D62	H63	R64	G65	L66	E67	Q68	R69	H70	W71	Y72	S73	D74	I75	F76	N77	T78	R79	K80	L81	P82	H83	A84	L85	M86	L87	F88	R89	D90	L91	N92	Q93	C94	K95	E96	W97	C98	F99	R100	L101	N102	A103	A104	Y105	F106	R107	E108	R109	M110	M111	E112	G113	E114	F115	V116	Y117	A118	L119	Y120
H121	S122	I123	I124	H125	S126	K127	L128	D129	H130	G131	I132	I133	L134	P135	N136	W137	H138	H139	Q140	T141	P142	H143	W144	F145	T146	M147	S148	E149	G150	G151	H152	L153	D154	K155	A156	Y157	C158	M159	T160	F161	N162	K163	A164	G165	T166	F167	S168	A169	F170	T171	G172	K173	E174	F175	M176	R177	E178	Q179	R180
V181	A182	F183	G184	H185	E186	D187	I188	D189	M190	N191	I192	H193	H194	V195	N196	W197	H198	M199	D200	F201	P202	H203	W204	W205	E206	D207	S208	V209	G210	G211	H212	L213	D214	A215	R216	G217	E218	L219	F220	F221	G222	G223	G224	H225	Q226	L227	V228	A229	R230	F231	D232	F233	K234	R235	L236	S237	N238	W239	L240
D241	P242	V243	D244	E245	L246	H247	W248	D249	G250	H251	L252	R253	E254	G255	F256	A257	P258	L259	T260	S261	Y262	K263	W264	G265	G266	E267	F268	P269	G270	R271	P272	D273	N274	L275	H276	F277	E278	D279	V280	D281	G282	V283	A284	H285	V286	H287	D288	L289	E290	L291	E292	E293	S294	R295	L296	H297	E298	A299	I300
D301	H302	G303	Y304	T305	T306	D307	S308	D309	G310	H311	T312	L313	D314	I315	R316	Q317	P318	K319	G320	I321	E322	L323	L324	G325	D326	I327	L328	N329	S330	S331	K332	Y333	S334	N335	V336	V337	Q338	Y339	Y340	G341	S342	L343	H344	N345	T346	A347	H348	S349	M350	L351	G352	K353	Q354	G355	D356	P357	H358	G359	K360
F361	N362	L363	P364	G365	G366	V367	M368	E369	H370	F371	E372	T373	A374	T375	R376	D377	P378	S379	F380	F381	L382	L383	H384	K385	Y386	K387	D388	N389	I390	S391	K392	K393	H394	T395	D396	S397	F398	P399	P400	Y401	T402	H403	D404	M405	L406	E407	F408	S409	G410	M411	V412	V413	N414	G415	V416	A417	L418	G419	G420
E421	L422	L423	T424	F425	F426	D427	E428	N429	G430	Y431	S432	L433	L434	N435	A436	V437	D438	S439	G440	E441	M442	L443	E444	D445	V446	E447	L448	N449	A450	A451	V452	H453	R454	L455	N456	H457	N458	E459	F460	T461	Y462	K463	L464	T465	M466	S467	N468	N469	M470	D471	G472	E473	R474	L475	A476	T477	F478	R479	L480
F481	L482	C483	P484	L485	E486	D487	N488	N489	G490	L491	T492	L493	T494	L495	D496	E497	A498	R499	W500	F501	C502	L503	E504	L505	D506	F507	L508	F509	Q510	K511	V512	P513	S514	G515	P516	E517	T518	L519	E520	R521	S522	K523	K524	D525	S526	S527	V528	T529	V530	P531	D532	M533	P534	G535	S536	Q537	S538	L539	K540
E541	Q542	A543	D544	N545	A546	Y547	N548	Q549	G550	H551	D552	L553	D554	L555	S556	A557	L558	N559	R560	S561	L562	G563	O564	P565	D566	R567	M568	L569	L570	P571	K572	S573	K574	P575	E576	G577	K578	E579	F580	N581	L582	K583	Y584	A585	V586	T587	D588	G589	D590	K591	D592	T593	E594	L595	H596	ASN	GLY	HIS	ASP
ASP	TYR	GLY	GLY	THR	H606	A607	Q608	C609	G610	H611	H612	G613	E614	A615	S616	P617	D618	N619	R620	P621	L622	G623	Y624	P625	L626	E627	R628	R629	I630	L631	D632	E633	R634	V635	I636	D637	G638	V639	S640	N641	I642	K643	H644	V645	V646	V647	D648	I649	V650	H651	H652	L653	GLU	HIS	HIS	ASP			

● Molecule 1: ARTHROPODAN HEMOCYANIN



D1	A2	L3	G4	T5	G6	N7	A8	Q9	K10	G11	Q12	D13	I14	N15	H16	L17	L18	D19	K20	I21	Y22	E23	P24	T25	K26	Y27	P28	D29	L30	N31	D32	I33	A34	E35	N36	F37	N38	P39	L40	G41	D42	K43	H44	V45	Y46	N47	D48	G49	G50	A51	A52	V53	E54	T55	F56	M57	K58	E59	L60
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N61	D62	H63	R64	L65	L66	E67	Q68	R69	H70	W71	Y72	S73	L74	F75	N76	T77	R78	Q79	R80	K81	E82	A83	L84	M85	L86	F87	A88	V89	L90	N91	Q92	C93	K94	E95	W96	Y97	C98	F99	R100	S101	N102	A103	A104	Y105	F106	E107	E108	R109	M110	M111	E112	G113	E114	F115	M116	Y117	A118	L119	Q120		
V121	S122	Y123	I124	H125	S126	K127	L128	G129	M130	D131	G132	V133	L134	P135	T136	L137	Y138	Q139	I140	T141	P142	H143	M144	F145	T146	M147	S148	E149	V150	I151	D152	K153	A154	Y155	S156	A157	K158	M159	T160	Q161	K162	P163	G164	T165	F166	V167	S168	Y169	S169	F170	T171	G172	T173	K174	R235	K175	M176	A177	E178	Q179	Y120
V181	A182	F183	G184	G185	E186	D187	I188	G189	M190	N191	I192	H193	H194	V195	T196	Y197	H198	R199	D200	T201	P202	F203	W204	W205	E206	D207	S208	Y209	G210	Y211	H212	L213	D214	R215	K216	H217	E218	L219	F220	F221	W222	V223	H224	H225	Q226	L227	T228	A229	R230	F231	D232	F233	E234	R235	L236	S237	W238	A239	L240		
D241	P242	V243	F244	E245	L246	H247	W248	D249	R250	I251	R252	L253	E254	G255	F256	A257	H258	L259	T260	S261	Y262	K263	Y264	G265	G266	E267	F268	P269	V270	R271	P272	D273	N274	L275	H276	F277	E278	D279	V280	D281	G282	V283	A284	H285	V286	H287	L288	E289	E290	L291	G292	E293	S294	R295	L296	H297	E298	A299	I300		
D301	H302	G303	Y304	T305	L306	D307	S308	D309	G310	H311	T312	L313	D314	I315	R316	Q317	P318	K319	G320	S321	E322	K323	L324	G325	D326	I327	F328	N329	E330	S331	K332	Y333	S334	S335	N336	V337	Q338	Y339	Y340	G341	S342	L343	H344	N345	T346	A347	H348	Y349	K350	L351	G352	R353	Q354	G355	L356	P357	H358	G359	K360		
F361	N362	L363	P364	P365	G366	D367	K368	E369	H370	F371	E372	T373	A374	T375	R376	D377	P378	S379	F380	F381	R382	L383	H384	K385	Y386	K387	L388	N389	L390	F391	K392	K393	H394	T395	D396	S397	F398	P399	P400	Y401	T402	H403	D404	N405	L406	E407	N408	S409	C410	M411	V412	V413	N414	C415	V416	A417	T418	D419	G420		
E421	L422	T423	T424	F425	E426	D427	E428	F429	Q430	Y431	S432	L433	I434	N435	A436	V437	D438	S439	G440	E441	R442	L443	E444	D445	V446	E447	L448	N449	Q450	A451	V452	H453	R454	L455	N456	H457	N458	E459	F460	T461	Y462	K463	L464	T465	N466	S467	N468	T529	V530	P531	D532	M533	E534	H535	L475	A476	T477	F478	R479	I480	
F481	L482	C483	P484	E485	E486	D487	N488	M489	G490	H491	T492	L493	T494	L495	D496	S497	A498	R499	W500	F501	C502	L503	E504	L505	D506	K507	F508	L509	Q510	K511	V512	P513	S514	G515	P516	E517	T518	L519	E520	R521	S522	S523	K524	D525	S526	S527	V528	T529	V530	P531	D532	M533	E534	H535	L475	A476	T477	F478	R479	I480	
E541	Q542	A543	D544	N545	E546	V547	N548	G549	G550	H551	D552	L553	D554	L555	S556	A557	Y558	E559	R560	S561	C562	G563	Y624	P625	D626	E627	R628	L629	L630	P631	D632	E633	R634	I636	E637	G638	V639	F640	N581	L582	K643	V584	A585	V586	T587	K648	G589	D590	K591	D592	T593	E594	H595	H596	ASN	GLY	GLY	HIS			
ASP	TYR	GLY	GLY	THR	H606	A607	Q608	G609	G610	G611	H612	G613	E614	A615	V616	P617	D618	N619	R620	P621	L622	G623	Y624	P625	D626	E627	R628	L629	L630	P631	D632	E633	R634	I636	E637	G638	V639	F640	N581	L582	K643	V584	A585	V586	T587	K648	G589	D590	K591	D592	T593	E594	H595	H596	ASN	GLY	GLY	HIS	ASP		

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

Chain G:  100%

MAC1
MAC2

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

Chain H:  100%

MAC1
MAC2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%MAG1
MAG2

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

Chain K:  100%MAG1
MAG2

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

Chain L:  100%MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 8.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 71.9 (8.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CORELS, PROLSQ	Depositor
R, R_{free}	0.221 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 38.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.095 for -h-l,k,h 0.095 for l,k,-h-l 0.105 for h,-k,-h-l 0.097 for -h-l,-k,l 0.104 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	31790	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	2.16	163/5385 (3.0%)	4.71	1837/7301 (25.2%)
1	B	2.16	164/5385 (3.0%)	4.71	1833/7301 (25.1%)
1	C	2.16	163/5385 (3.0%)	4.71	1832/7301 (25.1%)
1	D	2.16	162/5385 (3.0%)	4.71	1834/7301 (25.1%)
1	E	2.16	163/5385 (3.0%)	4.71	1831/7301 (25.1%)
1	F	2.16	162/5385 (3.0%)	4.71	1836/7301 (25.1%)
All	All	2.16	977/32310 (3.0%)	4.71	11003/43806 (25.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
All	All	0	42

The worst 5 of 977 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	ASP	N-CA	11.35	1.60	1.46
1	C	273	ASP	N-CA	11.34	1.60	1.46
1	A	273	ASP	N-CA	11.33	1.60	1.46
1	D	273	ASP	N-CA	11.33	1.60	1.46
1	B	273	ASP	N-CA	11.33	1.60	1.46

The worst 5 of 11003 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	390	ILE	N-CA-C	-25.99	89.46	111.81
1	B	390	ILE	N-CA-C	-25.99	89.46	111.81
1	D	390	ILE	N-CA-C	-25.98	89.46	111.81
1	F	390	ILE	N-CA-C	-25.98	89.47	111.81
1	A	390	ILE	N-CA-C	-25.97	89.47	111.81

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	177	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	499	ARG	Sidechain

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	5239	0	4950	600	1
1	B	5239	0	4950	587	0
1	C	5239	0	4950	591	0
1	D	5239	0	4950	610	0
1	E	5239	0	4950	589	1
1	F	5239	0	4950	572	0
2	G	28	0	25	6	0
2	H	28	0	25	6	0
2	I	28	0	25	6	0
2	J	28	0	25	6	0
2	K	28	0	25	6	0
2	L	28	0	25	6	0
3	A	2	0	0	0	0
4	A	176	0	0	32	0
4	B	4	0	0	1	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	1	0
4	F	1	0	0	0	0
All	All	31790	0	29850	3505	1

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 57.

The worst 5 of 3505 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HG22	1:B:141:THR:HG23	1.20	1.18
1:A:140:ILE:HG22	1:A:141:THR:HG23	1.20	1.17
1:F:140:ILE:HG22	1:F:141:THR:HG23	1.20	1.17
1:E:140:ILE:HG22	1:E:141:THR:HG23	1.20	1.15
1:D:140:ILE:HG22	1:D:141:THR:HG23	1.20	1.15

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:OD2	1:E:547:VAL:O[1_556]	1.86	0.34

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 X-ray entries followed by that with respect to entries of similar resolution.

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	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	2	15
1	B	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
1	C	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
1	D	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	2	15
1	F	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	15
All	All	3840/3942 (97%)	3140 (82%)	532 (14%)	168 (4%)	2	15

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	147	ASN
1	A	176	ASN
1	A	473	GLU
1	A	552	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	B	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	C	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	D	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	E	570/580 (98%)	393 (69%)	177 (31%)	0	1
1	F	570/580 (98%)	393 (69%)	177 (31%)	0	1
All	All	3420/3480 (98%)	2358 (69%)	1062 (31%)	0	1

5 of 1062 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	165	THR
1	F	281	ASP
1	F	158	LYS
1	F	586	VAL
1	C	140	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	GLN
1	F	394	HIS
1	E	453	HIS
1	F	36	ASN
1	F	606	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	G	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	G	2	2	14,14,15	21.58	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	H	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	H	2	2	14,14,15	21.59	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	I	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	I	2	2	14,14,15	21.59	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	J	1	2,1	14,14,15	18.11	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	J	2	2	14,14,15	21.59	4 (28%)	17,19,21	11.25	7 (41%)
2	NAG	K	1	2,1	14,14,15	18.11	4 (28%)	17,19,21	11.29	12 (70%)
2	NAG	K	2	2	14,14,15	21.58	4 (28%)	17,19,21	11.25	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	1	2,1	14,14,15	18.12	3 (21%)	17,19,21	11.29	12 (70%)
2	NAG	L	2	2	14,14,15	21.57	4 (28%)	17,19,21	11.25	7 (41%)

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	G	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C8-C7	79.03	3.14	1.50
2	H	2	NAG	C8-C7	79.01	3.14	1.50
2	J	2	NAG	C8-C7	79.00	3.14	1.50
2	K	2	NAG	C8-C7	78.99	3.14	1.50
2	G	2	NAG	C8-C7	78.99	3.14	1.50

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C8-C7-N2	-39.08	51.30	116.12
2	J	2	NAG	C8-C7-N2	-39.07	51.33	116.12
2	G	2	NAG	C8-C7-N2	-39.07	51.33	116.12
2	L	2	NAG	C8-C7-N2	-39.06	51.34	116.12
2	K	2	NAG	C8-C7-N2	-39.06	51.34	116.12

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	H	1	NAG	C1
2	I	1	NAG	C1
2	J	1	NAG	C1
2	K	1	NAG	C1

5 of 30 torsion outliers are listed below:

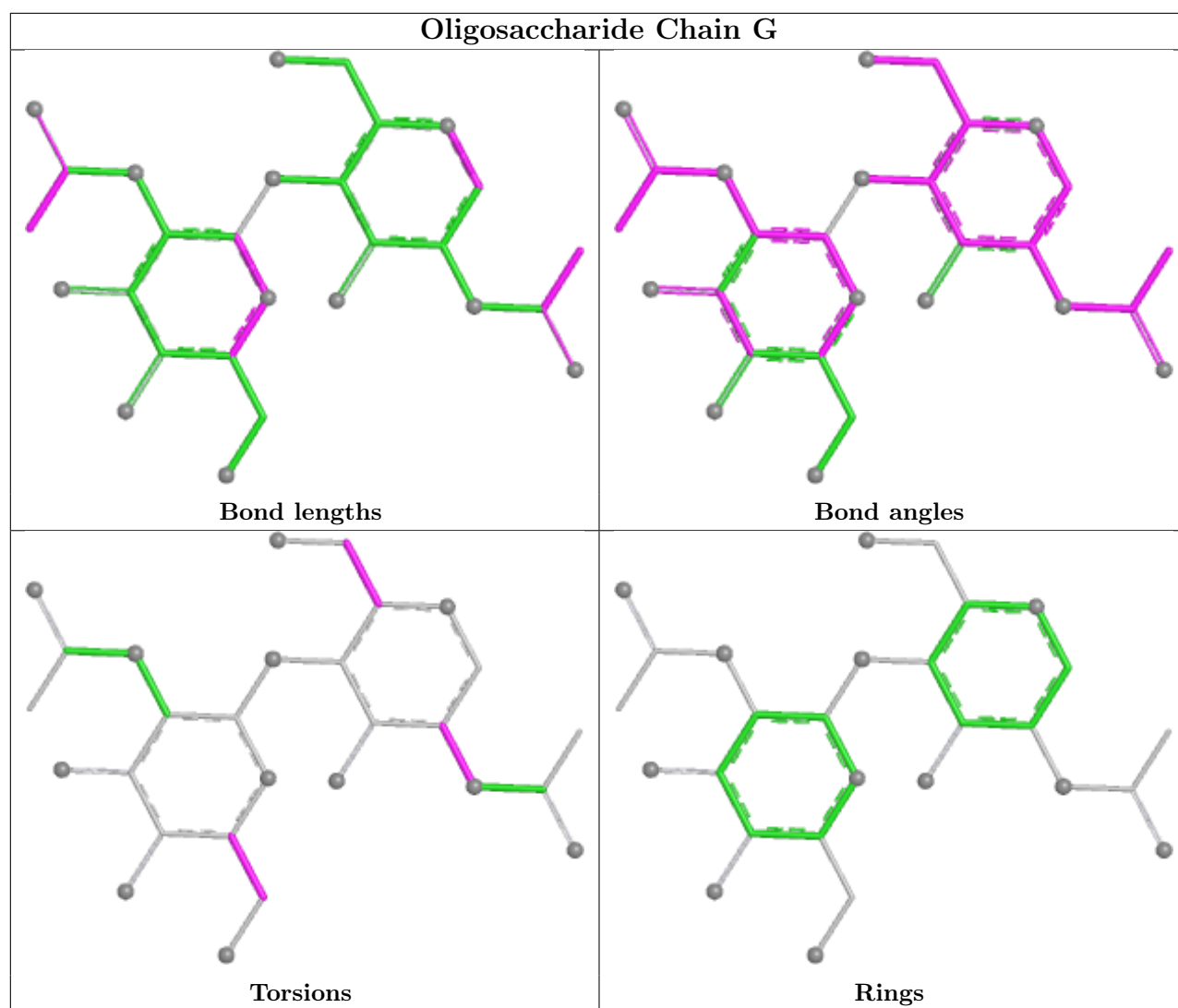
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6

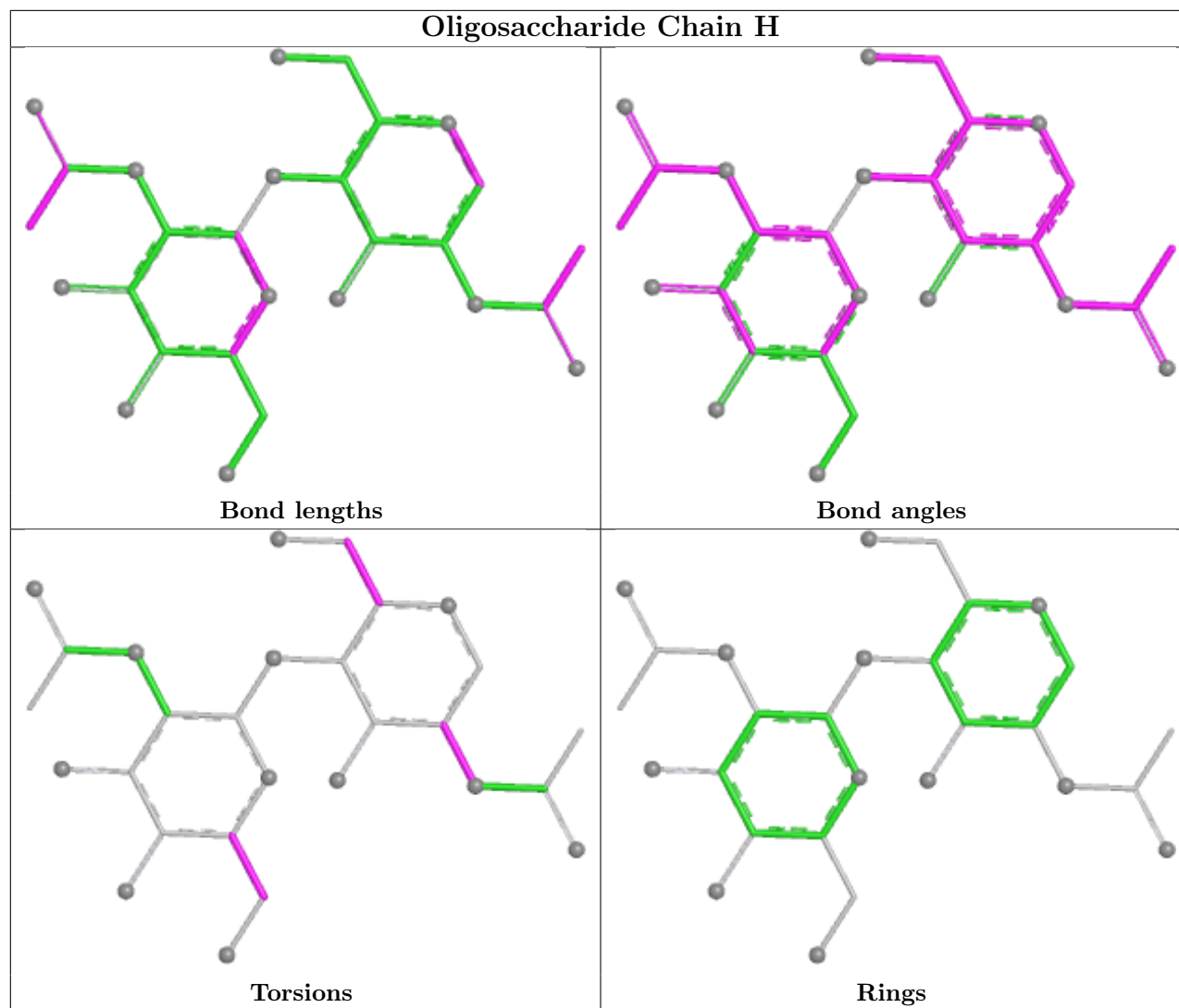
There are no ring outliers.

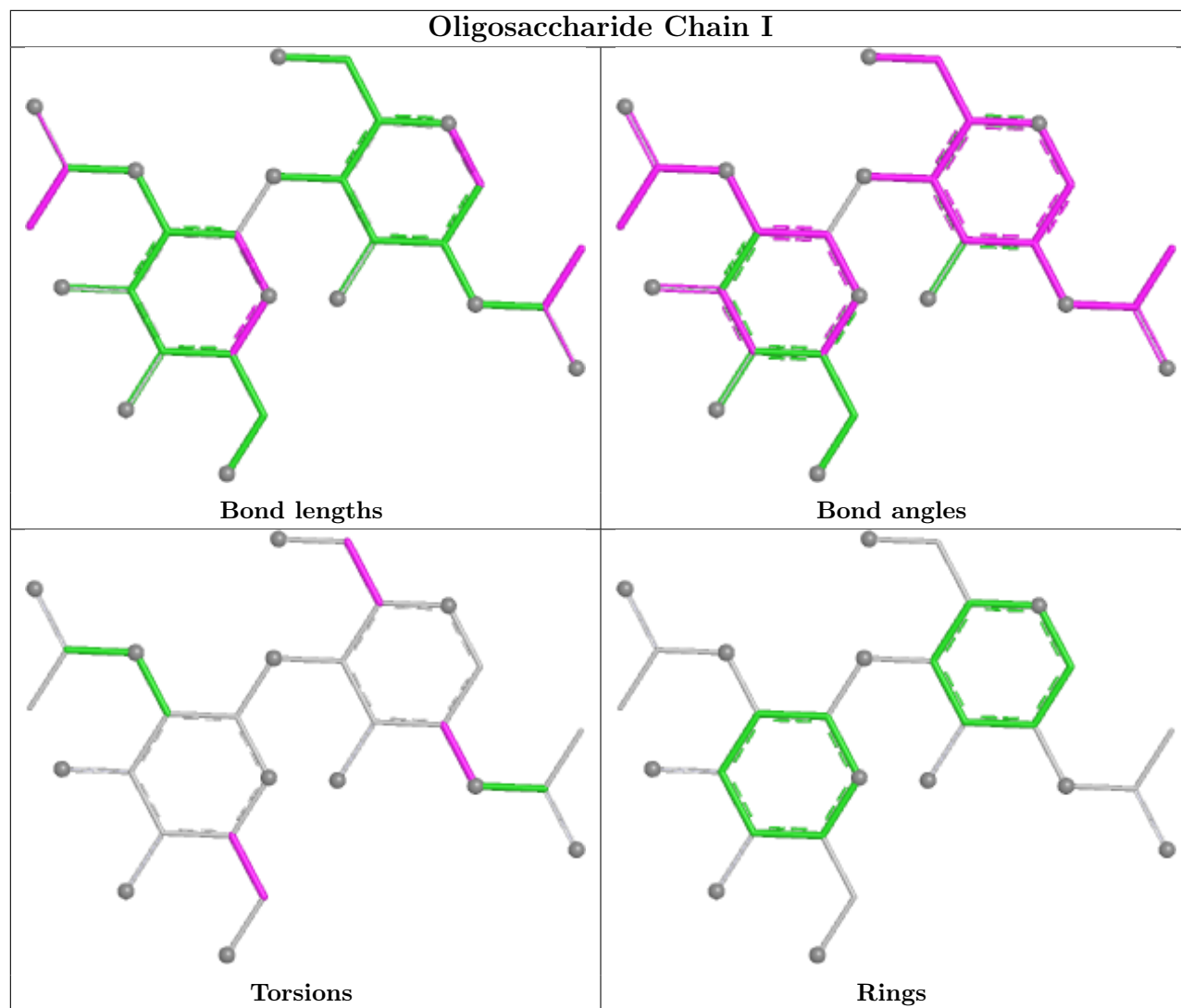
12 monomers are involved in 36 short contacts:

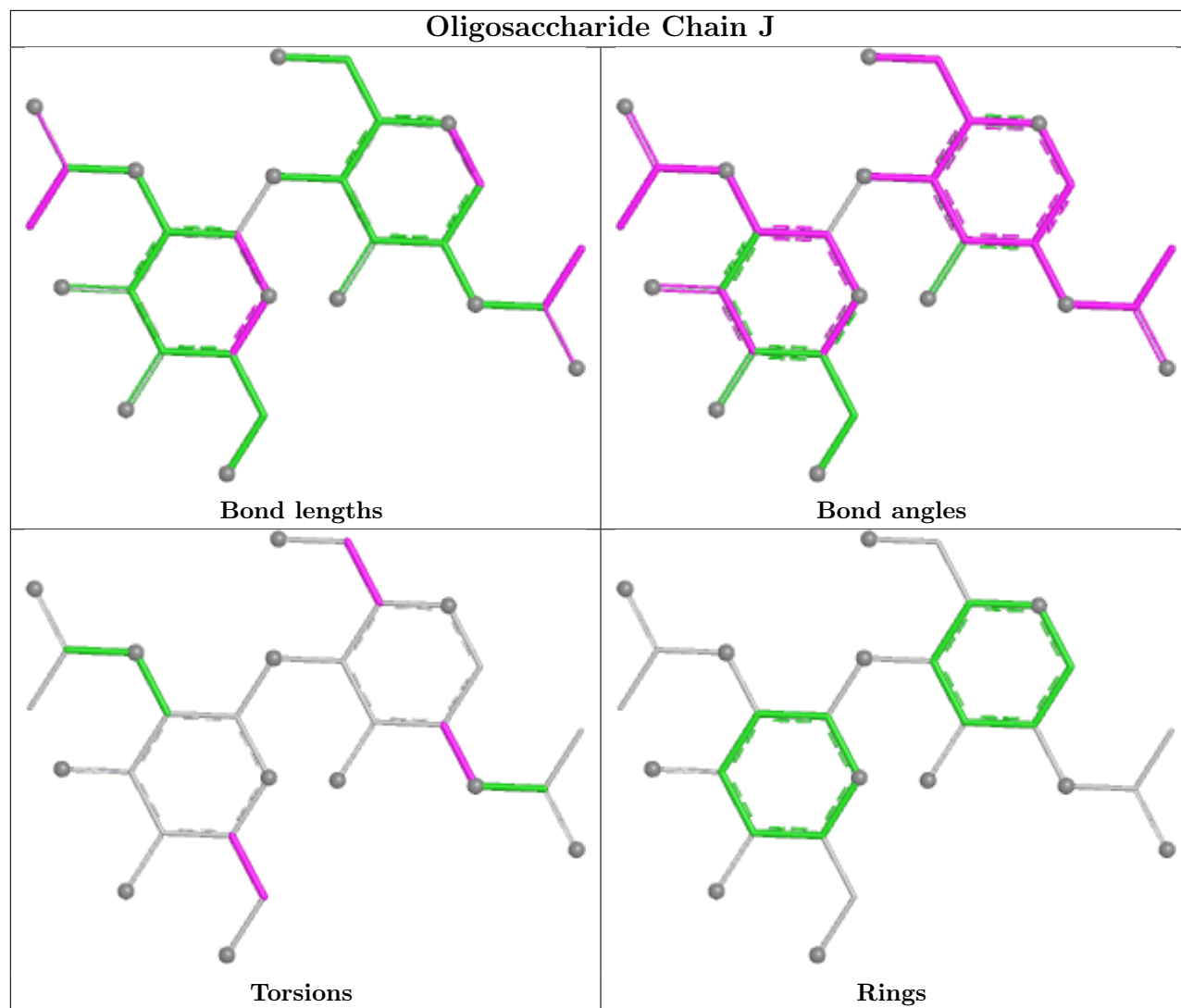
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	4	0
2	H	1	NAG	4	0
2	H	2	NAG	2	0
2	J	2	NAG	2	0
2	G	1	NAG	4	0
2	L	2	NAG	2	0
2	I	1	NAG	4	0
2	G	2	NAG	2	0
2	I	2	NAG	2	0
2	K	2	NAG	2	0
2	L	1	NAG	4	0
2	K	1	NAG	4	0

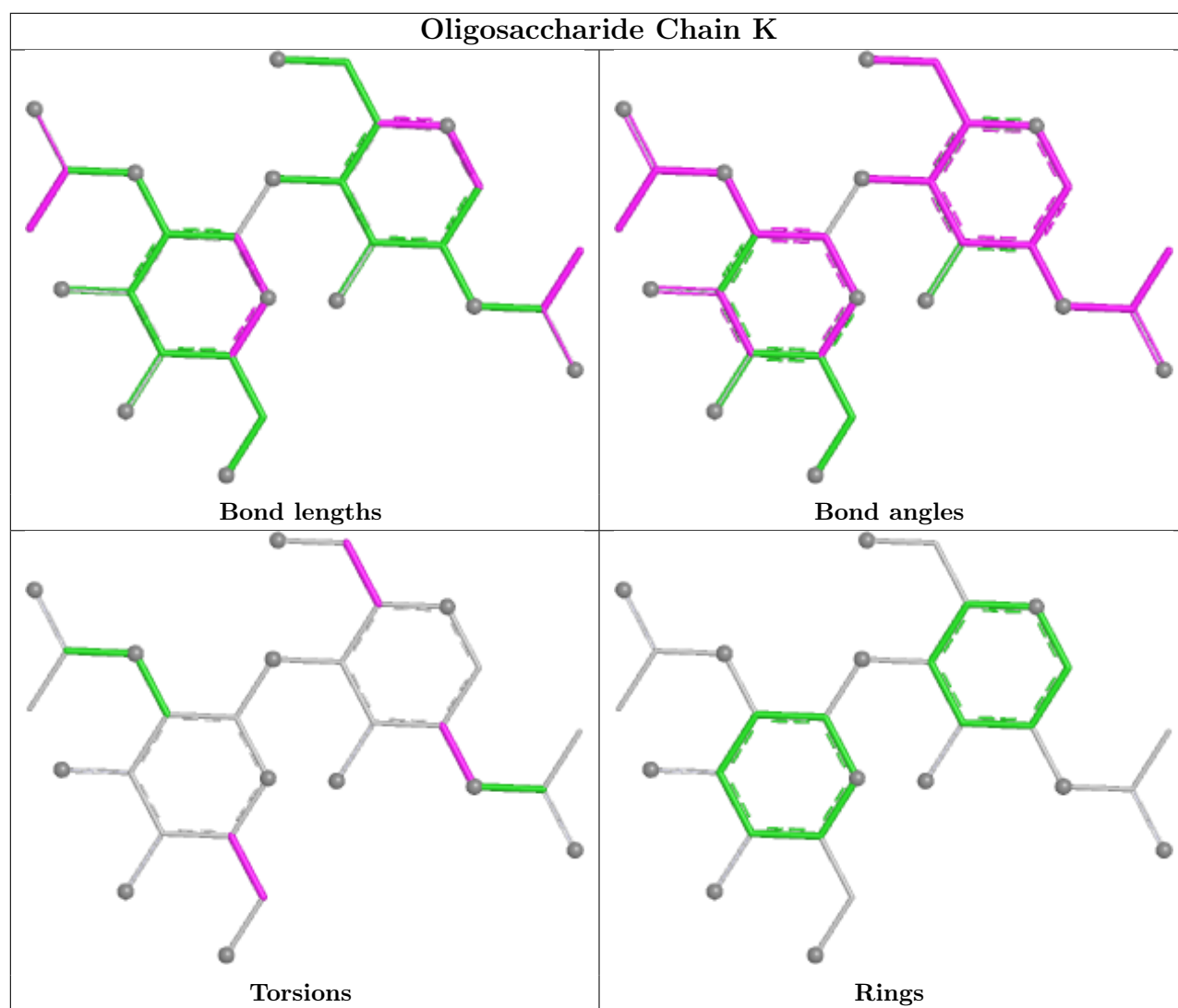
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

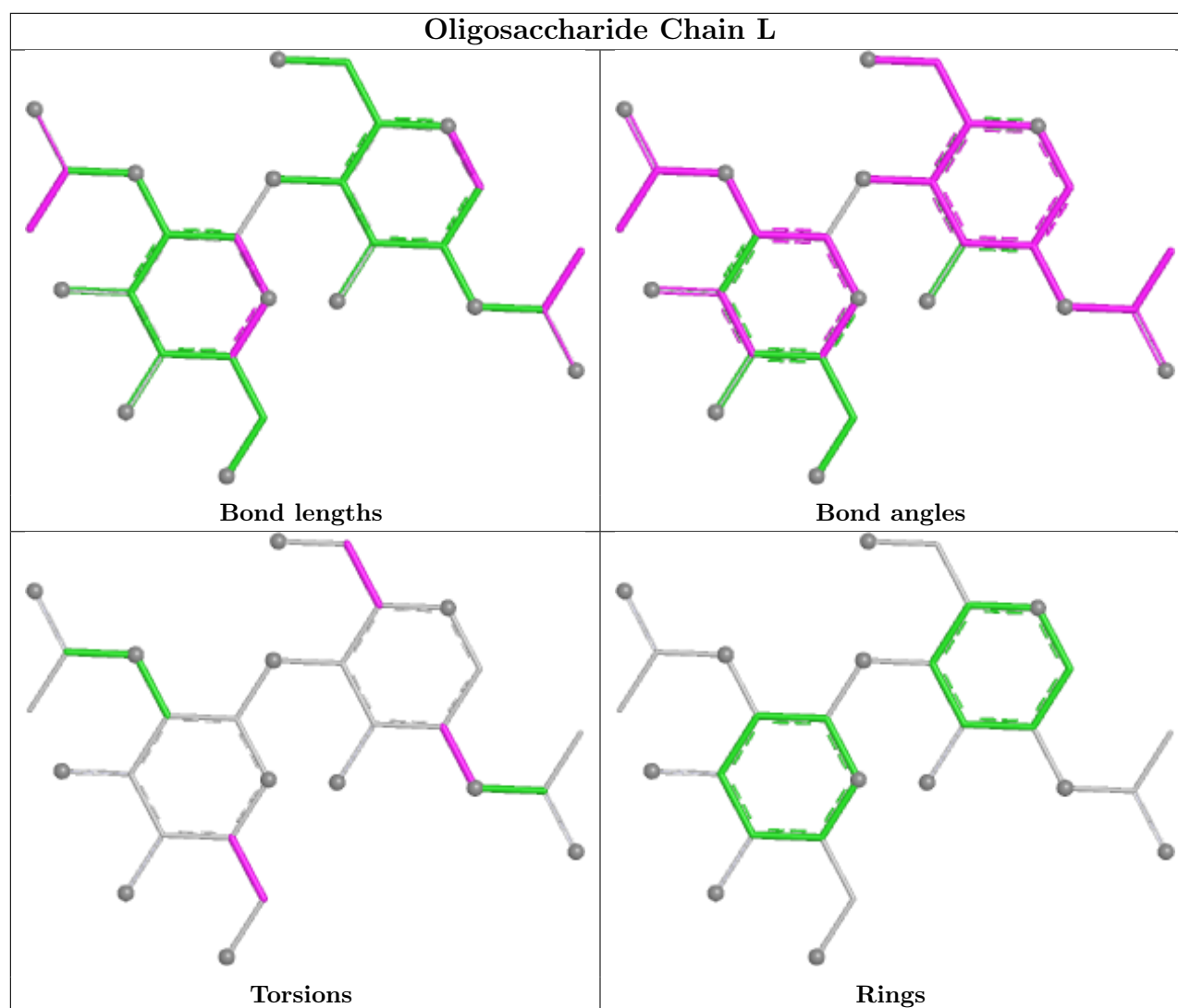












5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	644/657 (98%)	-0.33	3 (0%) 87 76	2, 11, 53, 85	0
1	B	644/657 (98%)	-0.23	7 (1%) 78 61	2, 11, 53, 85	0
1	C	644/657 (98%)	-0.17	8 (1%) 76 58	2, 11, 53, 85	0
1	D	644/657 (98%)	-0.19	10 (1%) 70 51	2, 11, 53, 85	0
1	E	644/657 (98%)	-0.23	5 (0%) 82 67	2, 11, 53, 85	0
1	F	644/657 (98%)	-0.23	9 (1%) 73 54	2, 11, 53, 85	0
All	All	3864/3942 (98%)	-0.23	42 (1%) 78 61	2, 11, 54, 85	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	548	ASN	4.7
1	A	3	LEU	4.0
1	C	1	ASP	4.0
1	F	2	ALA	4.0
1	C	640	SER	3.9

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

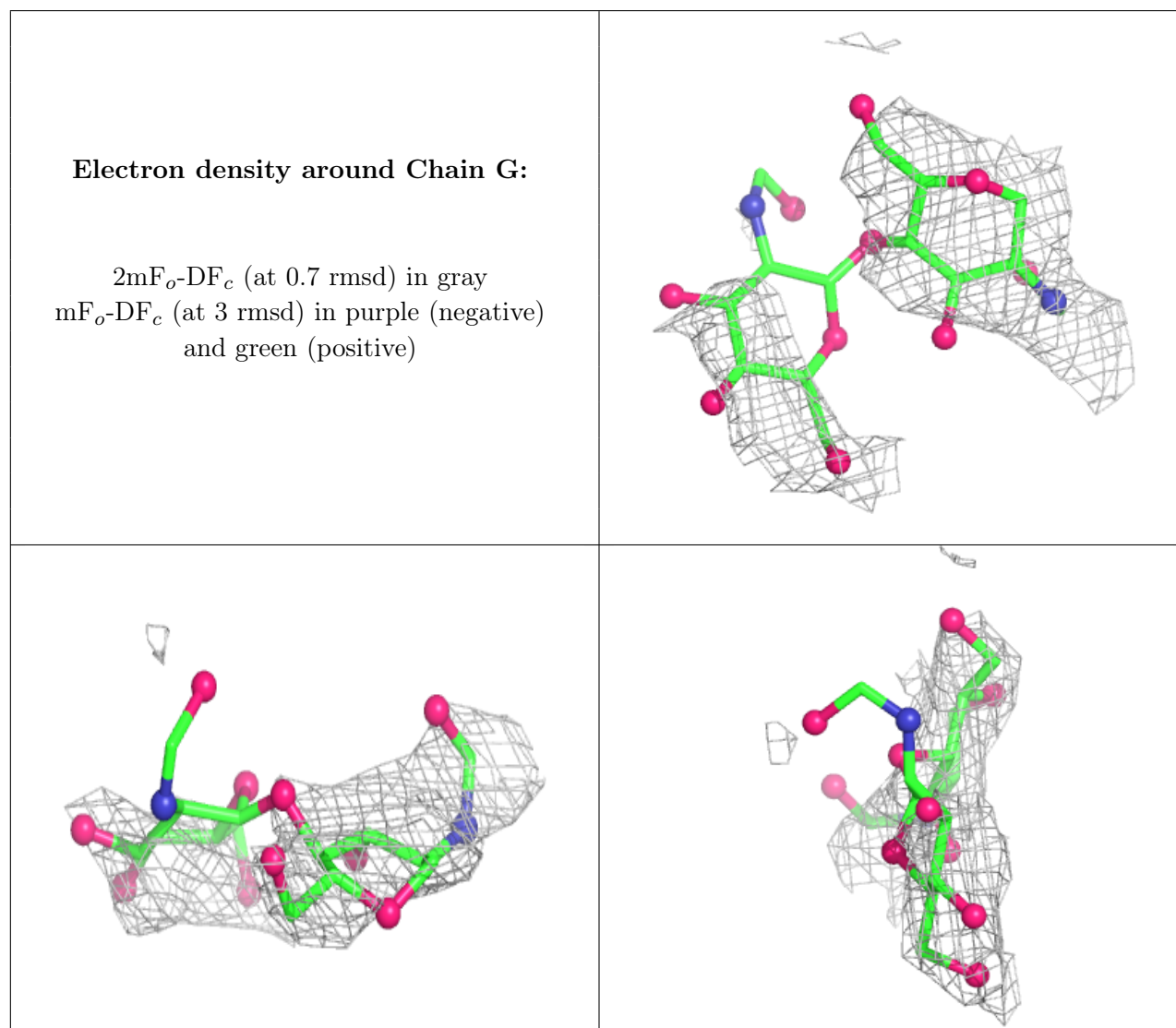
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

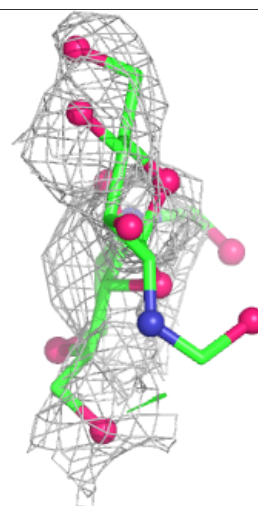
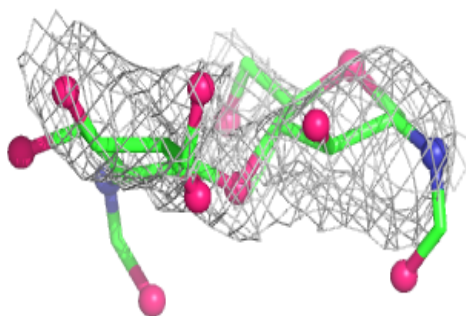
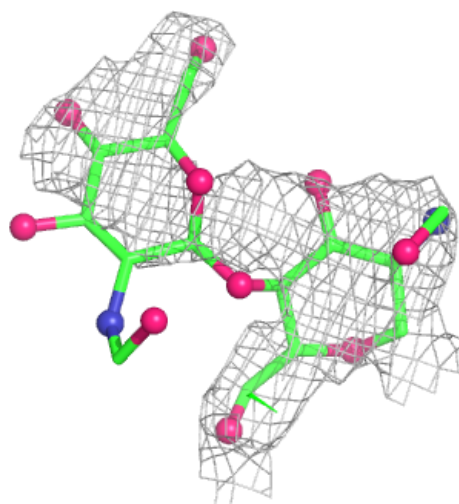
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	J	2	14/15	0.47	0.20	73,82,87,89	0
2	NAG	L	2	14/15	0.60	0.18	73,82,87,89	0
2	NAG	J	1	14/15	0.63	0.18	52,57,68,70	0
2	NAG	I	2	14/15	0.65	0.23	73,82,87,89	0
2	NAG	G	2	14/15	0.66	0.15	73,82,87,89	0
2	NAG	H	2	14/15	0.66	0.18	73,82,87,89	0
2	NAG	K	2	14/15	0.68	0.18	73,82,87,89	0
2	NAG	H	1	14/15	0.71	0.13	52,57,68,70	0
2	NAG	L	1	14/15	0.77	0.13	52,57,68,70	0
2	NAG	K	1	14/15	0.78	0.15	52,57,68,70	0
2	NAG	G	1	14/15	0.78	0.12	52,57,68,70	0
2	NAG	I	1	14/15	0.80	0.12	52,57,68,70	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



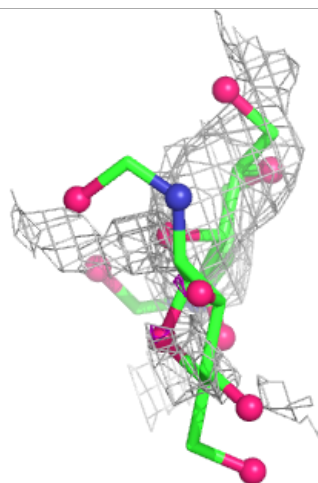
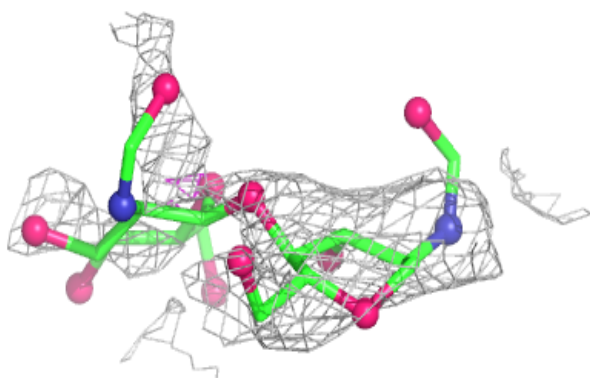
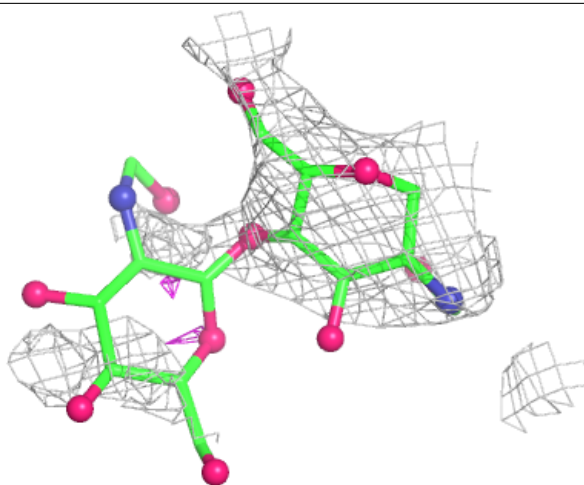
Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



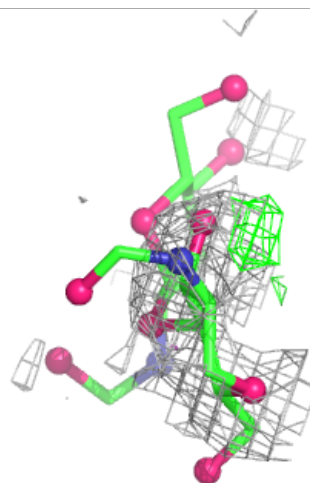
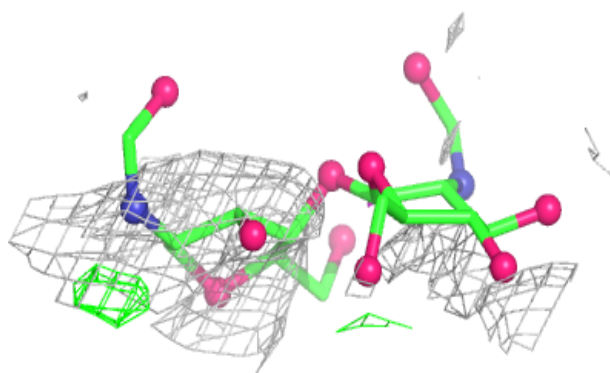
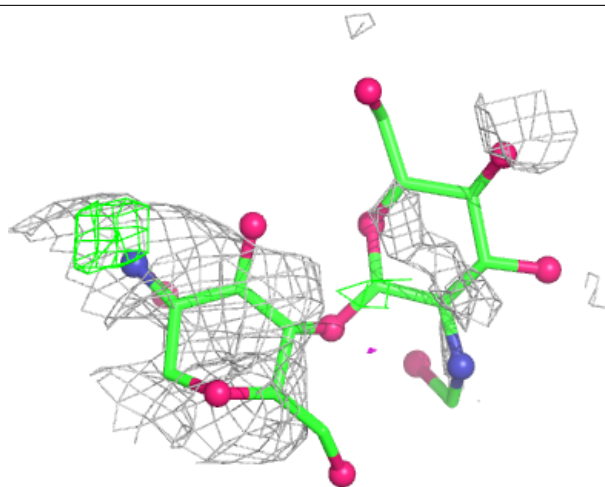
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



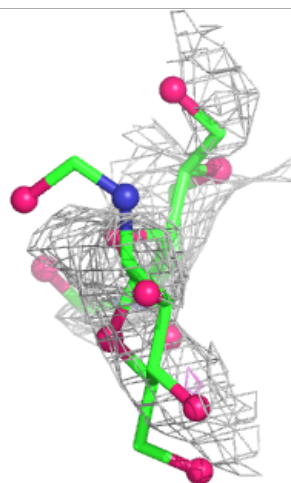
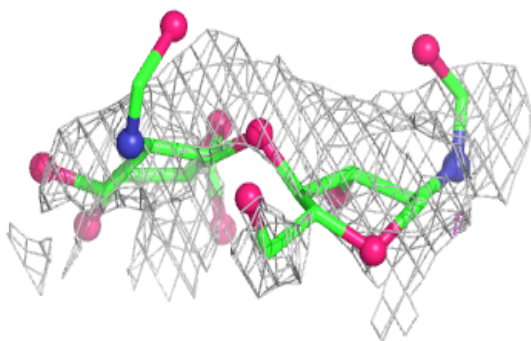
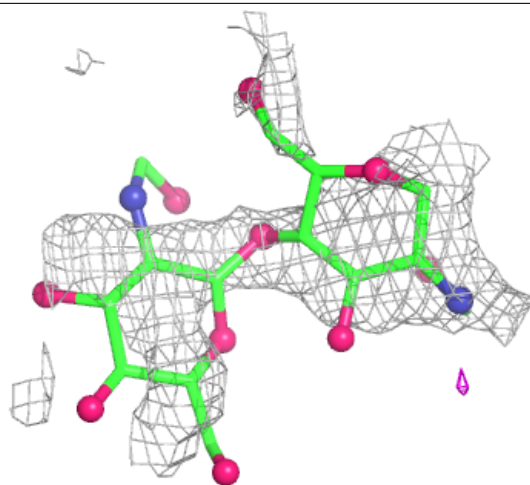
Electron density around Chain J:

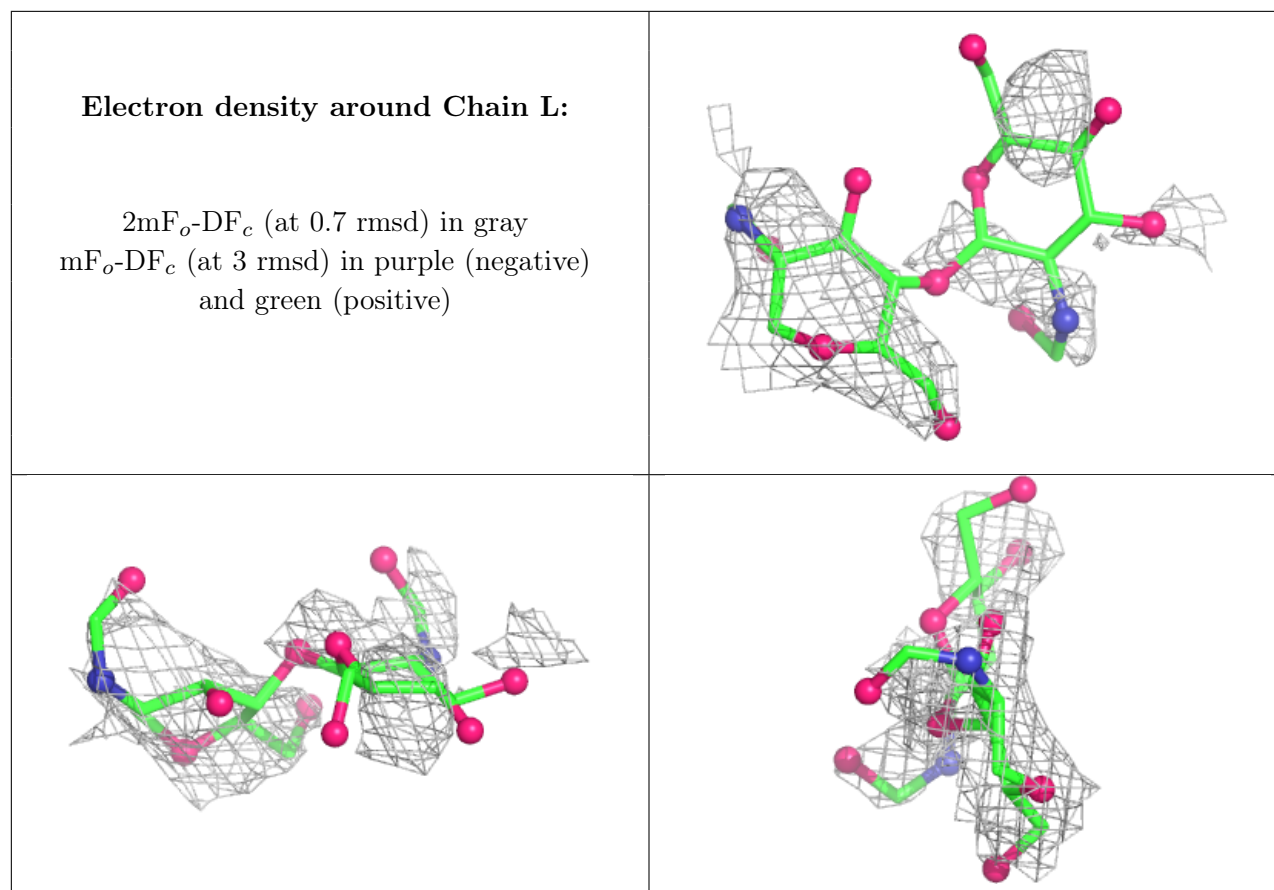
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	A	666	1/1	0.96	0.03	10,10,10,10	0
3	CU	A	665	1/1	0.98	0.03	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.