



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 05:20 PM EDT

PDB ID : 1HCY
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

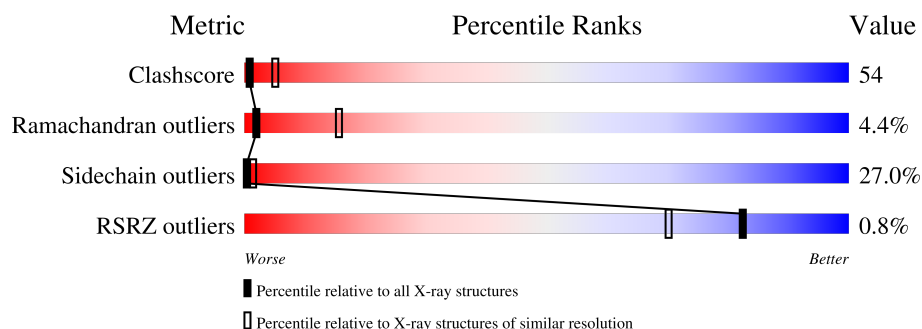
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (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 (three-letter code: 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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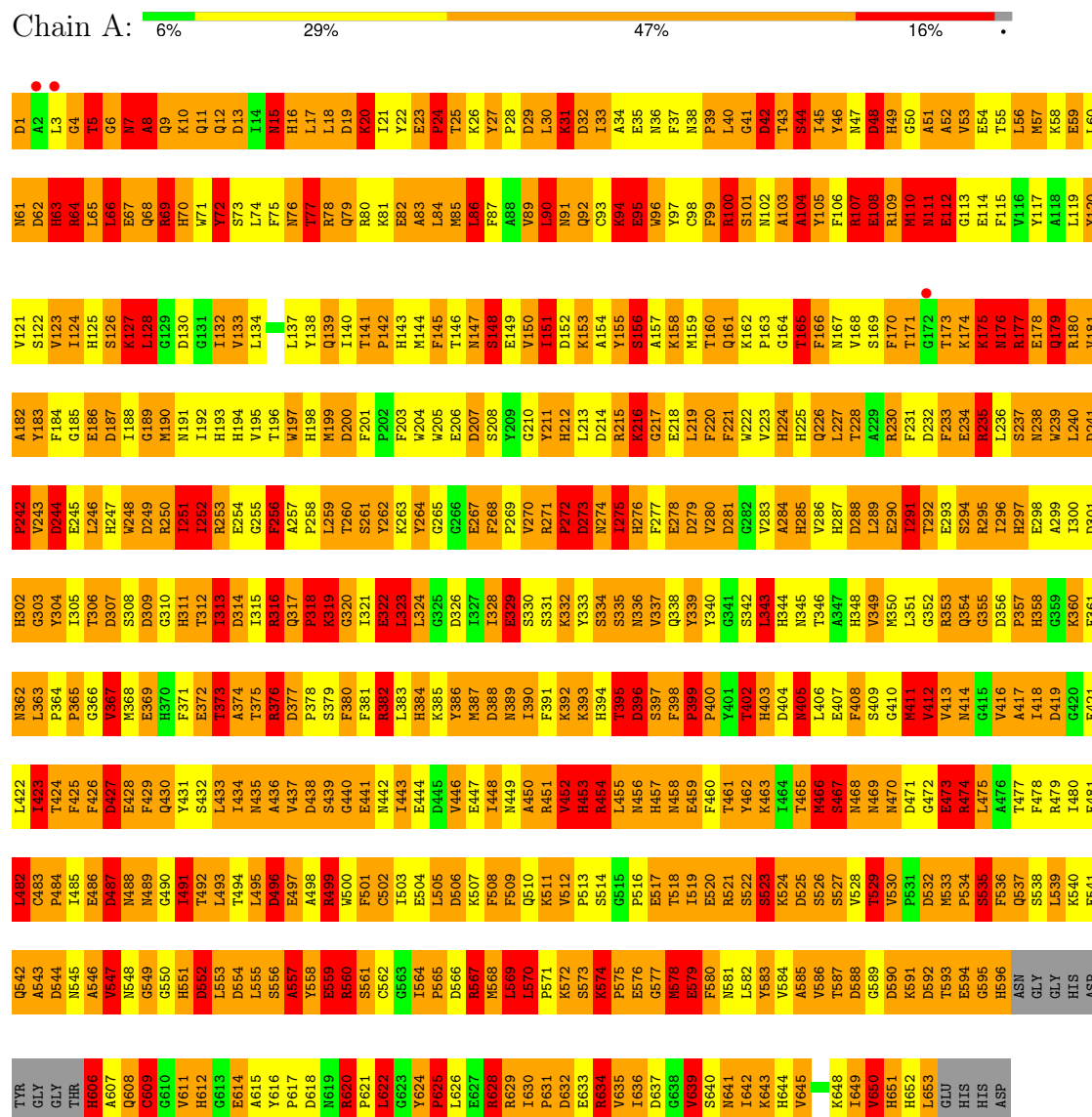
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		
4	F	1	Total	O	0	0
			1	1		

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



D1	A2	L3	G4	T5	G6	A7	A8	Q9	W10	Q11	Q12	Q13	T14	R15	H16	L17	L18	D19	R20	I21	Y22	E23	L24	P25	T26	K26	Y27	P28	D29	L30	N31	D32	I33	E34	N36	F37	N38	P39	L40	G41	D42	N43	T44	S44	I45	Y46	N47	D48	R49	G50	A51	A52	V53	E54	T55	F56	M57	K58	L59	L60		
N61	D62	H63	H64	L65	L66	E67	Q68	R69	H70	W71	Y72	S73	L74	F75	N76	T77	R78	Q79	R80	R81	E82	A83	L84	M85	L86	F87	A88	V89	L90	N91	Q92	C93	R94	E95	W96	Y97	C98	P99	R100	S101	N102	A103	I104	Y105	F106	E107	R108	M109	M110	N111	E112	G113	K114	T115	F116	Y117	A118	R119	L119	S120		
V121	S122	V123	I124	H125	S126	K127	L128	G129	H130	G131	I132	V133	L134		L137	Y138	Q139	T140	T141	P142	H143	M144	F145	T146	N147	S148	E149	G150	I151	D152	K153	A154	Y155	K156	G157	K158	M159	T160	Q161	K162	P163	G164	T165	F166	N167	V168	S169	R170	T171	G172	T173	K174	K175	L176	R177	E178	Q179	R180	L180	V181		
A182	Y183	F184	G185	E186	D187	I188	G189	M190	I191	I192	H193	V194	V195	T196	W197	H198	M199	D200	F201	P202	F203	W204	W205	E206	D207	S208	P209	G210	Y211	H212	L213	R214	K215	H216	G217	E218	L219	F220	W220	D221	W222	V223	H224	H225	Q226	L227	T228	L229	A229	R230	F231	D232	F233	E234	R235	L236	H237	N238	W239	L240	D241	
P242	V243	D244	E245	L246	H247	Q248	D249	R250	I251	I252	R253	E254	G255	P256	A257	P258	L259	T260	S261	Y262	K263	W264	G265	G266	E267	F268	P269	G270	R271	H272	L273	N274	H275	F277	E278	D279	W280	D281	G282	V283	A284	H285	V286	H287	D288	L289	E290	I291	T292	R293	Q294	R295	L296	H297	E298	A299	I300	D301				
H302	G303	Y304	I305	T306	D307	S308	D309	G310	T312	T313	R313	D314	I315	R316	D317	P318	K319	G320	I321	E322	L323	Y324	G325	G326	I327	I328	E329	S330	S331	K332	Y333	S334	S335	V337	Q338	Y339	G340	G341	L342	L343	H344	N345	T346	A347	H348	V349	S409	G410	M411	V412	V413	Q414	G415	L416	A417	I418	H358	E298	A299	G359	L360	D361
N362	L363	P364	P365	G366	V367	K368	E369	H370	F371	E372	K373	A374	T375	R376	D377	S378	S379	G380	F381	R382	L383	H384	K385	Y386	M387	D388	N389	I390	F391	K392	K393	H394	T395	D396	S397	F398	E399	P400	Y401	T402	H403	D404	M405	L406	F407	N408	S409	N470	D471	G472	E473	R474	L475	G476	F477	F478	R479	I480	F481			
L422	I423	A428	F429	E430	D431	E432	E433	Q434	Q435	W436	L437	L438	N439	A440	V441	D442	S443	G444	E445	N446	L447	E448	D449	D450	V451	E452	F453	A454	N455	L456	H457	L458	G459	M460	N461	E462	F463	A464	L465	L466	D467	M468	S469	T470	L471	G472	H473	L474	L475	G476	F477	F478	R479	I480	F481							
L482	C483	P484	I485	E486	D487	N488	G489	G490	I491	T492	L493	L494	N495	D496	E497	A498	R499	W500	F501	C502	I503	E504	L505	D506	K507	F508	F509	Q510	K511	V512	P513	S514	G515	E517	T518	I519	E520	R521	S522	S523	K524	D525	S526	S527	V528	T529	F530	P531	D532	M533	P534	S535	F536	Q537	S538	L539	K540	E541				
Q542	A543	D544	N545	E546	V547	N548	G549	G550	H551	D552	L553	E554	L555	S556	F557	D558	E559	R560	S561	C562	G563	H564	P565	D566	R567	M568	L569	L570	P571	K572	S573	P575	E576	G577	K578	E579	F580	N581	L582	Y583	V584	A585	V586	T587	D588	G589	H590	K591	D592	T593	E594	G595	H596	ASN	GLY	GLY	HIS	ASP				
TYR	GLY	GLY	THR	H606	A607	Q608	E609	G610	V611	H612	G613	E614	A615	V616	F617	N618	Y619	R620	P621	L622	G623	Y624	P625	L626	E627	R628	R629	L630	P631	D632	E633	R634	V635	L636	D637	G638	S640	N641	T642	K643	H644	V645		R648	T649	V650	H651	H652	L653	HIS	HIS	E54										

● Molecule 1: ARTHROPODAN HEMOCYANIN



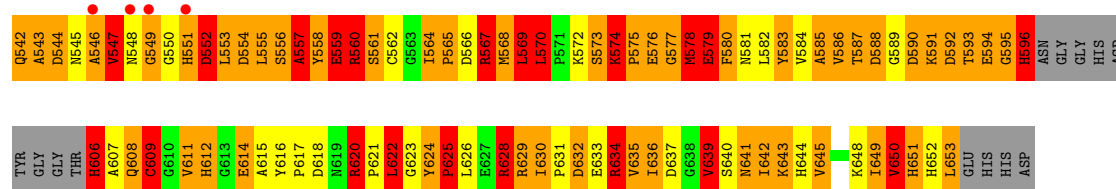
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A182	Y183	F184	G185	E186	D187	I188	G189	M190	I191	I192	H193	V194	V195	T196	W197	H198	M199	D200	F201	P202	F203	W204	W205	E206	D207	S208	P209	G210	Y211	H212	L213	D214	R215	K216	G217	E218	L219	F220	W221	W222	V223	H224	H225	Q226	L227	T228	L229	A229	R230	F231	D232	F233	E234	R235	L236	H237	N238	W239	L240	D241
V121	S122	V123	I124	H125	S126	K127	L128	G129	H130	G131	I132	V133	L134		L137	Y138	Q139	T140	T141	P142	H143	M144	F145	T146	N147	S148	E149	G150	I151	D152	K153	A154	Y155	K156	G157	K158	M159	T160	Q161	K162	P163	G164	T165	F166	N167	V168	S169	R170	T171	G172	T173	K174	K175	L176	R177	E178	Q179	R180	L181	
M61	D62	H63	H64	L65	L66	E67	Q68	R69	H70	W71	Y72	S73	L74	F75	N76	T77	R78	Q79	R80	R81	E82	A83	L84	M85	L86	F87	A88	V89	L90	N91	Q92	C93	R94	E95	W96	Y97	C98	P99	R100	S101	N102	A103	I104	Y105	F106	E107	R108	M109	M110	N111	E112	G113	K114	T115	F116	Y117	A118	R119	L120	
D1	A2	L3	G4	T5	G6	A7	A8	Q9	W10	Q11	Q12	Q13	T14	R15	H16	L17	L18	D19	R20	I21	Y22	E23	L24	P25	T26	K26	Y27	P28	D29	L30	N31	D32	I33	E34	N36	F37	N38	P39	L40	G41	D42	N43	T44	S44	I45	Y46	N47	D48	R49	G50	A51	A52	V53	E54	T55	F56	M57	K58	L59	L60

TYR	Q542	L482	L422	N362	H302
	A543	C483	I423	L363	G303
GLY	D544	P484	T424	P364	Y304
THR	N545	I485	F425	G366	I306
	A546	E486	F426	G366	T306
A607	V547	D487	D427	V667	D307
Q608	N548	M488	E428	M368	S308
	G549	N489	F429	E369	D309
G610	G550	G490	Q430	H370	G310
H611	H551	L491	Y431	F371	H311
H612	D552	T492	S432	E372	T312
G613	L553	L493	L433	T373	T313
E614	D554	T494	A374	A374	D314
A615	L555	L495	M435	T375	T315
Y616	S556	D496	A436	R376	R316
P617	A557	E497	V437	D377	Q317
D618	Y558	A498	D438	P378	P318
N619	E559	R499	S439	S379	K319
R620	R560	W500	G440	F380	G320
P621	S561	F501	E441	F381	I321
L622	C562	C502	M442	R382	E322
G623	G563	I503	I443	L383	L323
Y624	T564	E504	E444	H384	L324
P625	P565	L505	D445	K385	G325
L626	D566	D506	V446	Y386	D326
E627	R567	K507	E447	M387	I327
R628	M568	F508	I448	D388	L328
P629	L569	F509	N449	N389	E329
L630	L570	Q510	A450	I390	S330
P631	P571	K511	R451	F391	S331
D632	K572	V512	V452	K392	K332
E633	S573	P513	H453	K393	Y333
R634	K574	G514	R454	H394	S334
V635	P575	G515	L455	T395	S335
I636	E576	P516	M456	D396	N336
D637	G577	B517	H457	S397	V337
G638	R578	T518	N458	F398	Q338
V639	E579	I519	E459	P399	Y339
S640	F580	B520	F460	P400	Y340
N641	N581	R521	T461	Y401	G341
I642	L582	S522	Y462	T402	S342
K643	Y583	S523	K463	H403	L343
H644	V584	K524	T464	D404	H344
V645	A585	D525	T465	M405	N345
L646	V586	S526	M466	L406	T346
I649	T587	S527	S467	E407	A347
V650	D588	V528	N468	F408	H348
H651	G589	T529	N469	S409	V349
	D590	V530	M470	G410	M350
K648	K591	P531	D471	M411	L351
H652	D592	D532	G472	V412	G352
L653	H593	M533	E473	V413	R353
GLU	T593	P534	R474	M414	Q354
HIS	E594	P534	E474	M414	G354
HIS	G595	S535	L475	G415	G355
ASP	H596	V536	A476	V416	D356
GLY	ASN	Q537	T477	A417	P357
	GLY	S538	F478	I418	H358
GLY	GLY	L539	R479	D419	G359
	HIS	HIS	I480	F420	K360
ASP	ASP	E541	F481	G421	P361

● Molecule 1: ARTHROPODAN HEMOCYANIN

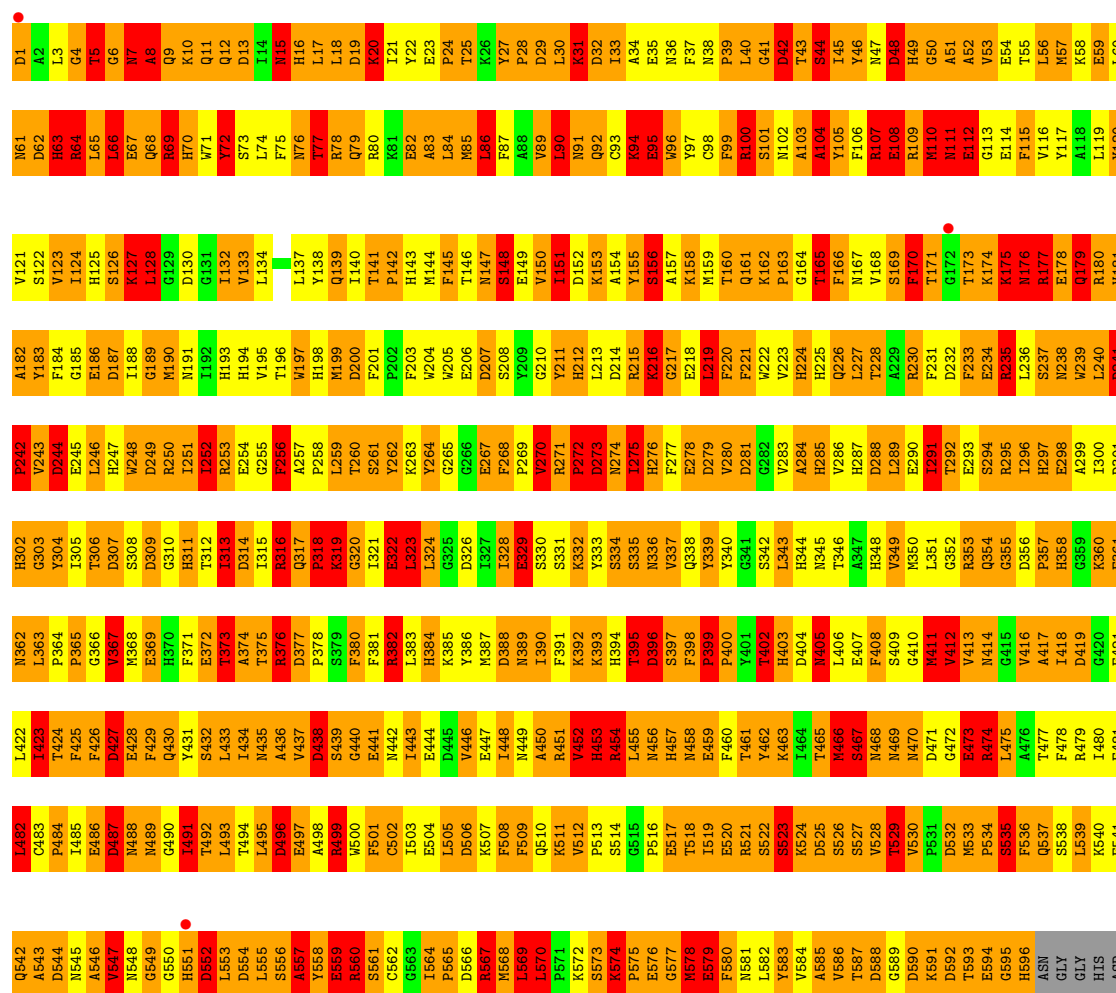


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N362	L363	P364	P365	G366	V367	M368	E369	H370	F371	E372	T373	A374	T375	R376	D377	P378	S379	F380	G381	R382	L383	H384	K385	Y386	M387	D388	N389	L390	F391	K392	K393	H394	T395	D396	S397	F398	P399	P400	G401	T402	H403	D404	M405	L406	E407	F408	S409	G410	M411	V412	V413	A414	G415	V416	A417	L418	D419	G420	E421			
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P242	V243	D244	L245	L246	H247	N248	D249	R250	L251	L252	R253	E254	G255	F256	P257	P258	L259	T260	S261	Y262	K263	Y264	G265	G266	E267	P268	F269	V270	R271	K272	L273	N274	H275	F276	D277	D278	V279	L280	D281	G282	L283	A284	H285	V286	H287	L288	L289	E290	L291	T292	E293	Q294	R295	L296	H297	E298	A299	L300	D301			
A182	Y183	F184	G185	E186	D187	L188	G189	M190	N191	L192	H193	H194	V195	L196	Y197	H198	M199	D200	F201	F202	F203	A204	G205	E206	D207	S208	Y209	G210	L211	Y212	L213	L214	R215	K216	L217	E218	L219	M159	F99	F220	F221	L222	L223	H224	L225	Q226	T227	L228	L229	A229	F170	T231	D232	F233	E234	R235	L236	S237	N238	W239	L240	D241
V121	S122	V123	L124	H125	L126	K127	L128	G129	H130	G131	L132	V133	L134	L137	Q138	Q139	V140	T141	T142	F143	H144	F145	F146	H147	S148	E149	V150	V151	L152	K153	A154	S155	L156	A157	K158	L159	T160	Q161	K162	P163	G164	T165	F166	M167	V168	S169	F169	T171	G172	T173	K174	R175	N176	R177	E178	Q179	L180	V181				
N61	D62	H63	R64	L65	L66	E67	Q68	R69	H70	H71	Y72	S73	L74	F75	N76	T77	R78	O79	R80	K81	E82	A83	L84	P85	L86	F87	A88	V89	L90	N91	Q92	C93	K94	E95	Y96	Y97	C98	F99	R100	S101	N102	A103	A104	Y105	F106	R107	E108	R109	M110	N111	E112	A52	G50	L55	V116	Y117	M57	K58	E59	L60		
D1	A2	L3	G4	T5	G6	N7	A8	Q9	H10	K10	Q11	D12	D13	T14	N15	H16	L17	L18	R20	Y21	D22	E23	E24	P25	K26	Y27	P28	D29	L30	D31	R32	L33	A34	E35	N36	F37	N38	P39	L40	G41	D42	T43	S44	Y45	L46	N47	D48	H49	G50	A51	A52	V53	E54	L55	L56	M57	K58	E59	L60			



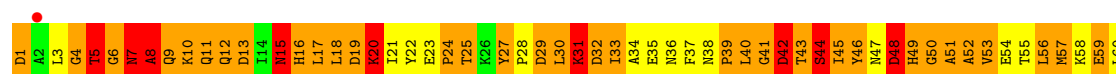
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E: 6% 28% 47% 16%



• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain F: 6% 30% 46% 15%



Q542	L482	L422	N362	H302	P242	A182	V121	N61
A543	C483	L423	L363	G303	V243	A183	S122	D62
D544	P484	T424	P364	Y304	D244	F184	V123	H63
N545	L485	F425	P365	T306	E245	G184	I124	R64
A546	E486	F426	G366	T306	L246	E186	H125	L65
V547	D487	D427	V367	D307	H247	D187	S126	L66
N548	N488	E428	M368	S308	W248	I188	K127	E67
C609	N489	F429	E369	D309	D249	L128	L128	Q68
G550	C490	Q430	H370	G310	R250	M190	G129	R69
V611	H551	T491	F371	H311	I251	N191	D130	H70
D552	T492	S432	E372	T312	T252	I192	G131	W71
L553	L493	L433	T373	L313	R253	H193	I132	Y72
E614	T494	L434	A374	D314	E254	H194	L133	S73
A615	L495	N435	T375	I315	G255	V195	L134	F74
V616	D496	A436	R376	R316	F256	T196	L135	L75
P617	E497	V437	P377	Q317	A257	W197	L137	N76
D618	A498	D438	D378	P318	P258	H198	Y138	T77
V619	R499	S439	S379	K319	L259	M199	Q139	R78
R620	W500	E440	F380	G320	T260	D201	T140	Q79
P621	F501	E441	F381	I321	S261	F201	T141	R80
L622	C502	N442	R382	E322	Y262	P202	P142	K81
G623	I503	L443	L383	L323	K263	F203	H143	E82
Y624	E504	E444	H384	L324	Y264	W204	M144	A83
P625	L505	D445	K385	G325	G265	W205	F145	L84
L626	D506	V446	Y386	D326	G266	E206	T146	M85
E627	K507	E447	M387	I327	F267	D207	N147	L86
R628	F508	L448	D388	I328	F268	S208	S148	F87
R629	F509	N449	N389	E329	P269	Y209	E149	A88
I630	Q510	A450	I390	S330	W270	G210	V150	V89
P631	K511	R451	F391	S331	R271	Y211	T151	L90
D632	V512	V452	K392	K332	P272	H212	D152	N91
E633	P513	R453	K393	Y333	D273	L213	K153	Q92
R634	S514	R454	H394	S334	N274	D214	A154	C93
V635	G515	L455	T395	S335	I275	R215	Y155	K94
I636	P516	M456	D396	N336	H276	K216	S156	E95
D637	E517	H457	S397	V337	F277	G217	A157	N96
G638	T518	N458	F398	Q338	E278	E218	K158	Y97
R639	T519	E459	P399	Y339	D279	L219	M159	C98
S640	E520	P460	P400	Y340	V280	F220	T160	F99
N641	R521	T461	Y401	G341	D281	F221	Q161	R100
I642	S522	Y462	T402	S342	G282	W222	K162	S101
K643	S523	K463	H403	L343	V283	V223	P163	M102
H644	K524	T464	D404	H344	A284	H224	G164	A103
V645	D525	T465	N405	N345	H285	H225	T165	A104
K648	S526	M466	L406	T346	V286	Q226	F166	Y105
I649	V526	S467	E407	A347	H287	L227	N167	F106
V650	T528	N468	F408	H348	D288	T228	V168	R107
D589	G589	N469	S409	V349	L289	A229	S169	E108
H651	D590	T470	G410	M350	E290	R230	F170	R109
H652	P531	D471	M411	L351	I291	F231	T171	M110
L653	D532	G472	V412	G352	T292	D232	G172	N111
GLU	T593	E473	V413	R353	E293	F233	T173	E112
HIS	P534	R474	N414	Q354	S294	E234	K174	G113
HIS	S535	L475	G415	G355	R295	R235	K175	E114
ASP	F536	A476	V416	D356	I296	L236	N176	F115
	Q537	T477	A417	P357	H297	S237	R177	V116
	S538	F478	I418	H358	E298	W238	E178	Y117
	L539	R479	D419	G359	A299	Q179	Q179	A118
	K540	T480	H180	K360	I300	L240	R180	L119
	E541	F481	E201	F361	R201	S201	V181	C94

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

Chain G:

100%

NAG1
NAG2

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

Chain H:

100%

NAG1
NAG2

- 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 [i](#)

5.1 Standard geometry [i](#)

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	1.67	39/5385 (0.7%)	3.87	1158/7301 (15.9%)
1	B	1.67	40/5385 (0.7%)	3.87	1154/7301 (15.8%)
1	C	1.67	38/5385 (0.7%)	3.87	1154/7301 (15.8%)
1	D	1.67	38/5385 (0.7%)	3.87	1151/7301 (15.8%)
1	E	1.67	39/5385 (0.7%)	3.87	1156/7301 (15.8%)
1	F	1.67	39/5385 (0.7%)	3.87	1154/7301 (15.8%)
All	All	1.67	233/32310 (0.7%)	3.87	6927/43806 (15.8%)

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 233 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	GLY	N-CA	9.44	1.60	1.46
1	D	217	GLY	N-CA	9.44	1.60	1.46
1	C	217	GLY	N-CA	9.42	1.60	1.46
1	B	217	GLY	N-CA	9.42	1.60	1.46
1	A	217	GLY	N-CA	9.41	1.60	1.46

The worst 5 of 6927 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	628	ARG	NE-CZ-NH2	-45.56	97.52	120.30
1	E	628	ARG	NE-CZ-NH2	-45.53	97.54	120.30
1	C	628	ARG	NE-CZ-NH2	-45.49	97.56	120.30
1	D	628	ARG	NE-CZ-NH2	-45.48	97.56	120.30
1	A	628	ARG	NE-CZ-NH2	-45.47	97.56	120.30

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 [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	5239	0	4942	566	1
1	B	5239	0	4942	549	0
1	C	5239	0	4942	561	0
1	D	5239	0	4942	580	0
1	E	5239	0	4942	558	1
1	F	5239	0	4943	539	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	31	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	29803	3312	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 54.

The worst 5 of 3312 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%)	416 (73%)	154 (27%)	0	1
1	B	570/580 (98%)	416 (73%)	154 (27%)	0	1
1	C	570/580 (98%)	416 (73%)	154 (27%)	0	1
1	D	570/580 (98%)	416 (73%)	154 (27%)	0	1
1	E	570/580 (98%)	416 (73%)	154 (27%)	0	1
1	F	570/580 (98%)	416 (73%)	154 (27%)	0	1
All	All	3420/3480 (98%)	2496 (73%)	924 (27%)	0	1

5 of 924 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	15	ASN
1	F	502	CYS
1	D	482	LEU
1	F	467	SER
1	F	151	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	36	ASN
1	F	92	GLN
1	F	469	ASN
1	C	47	ASN
1	C	36	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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:

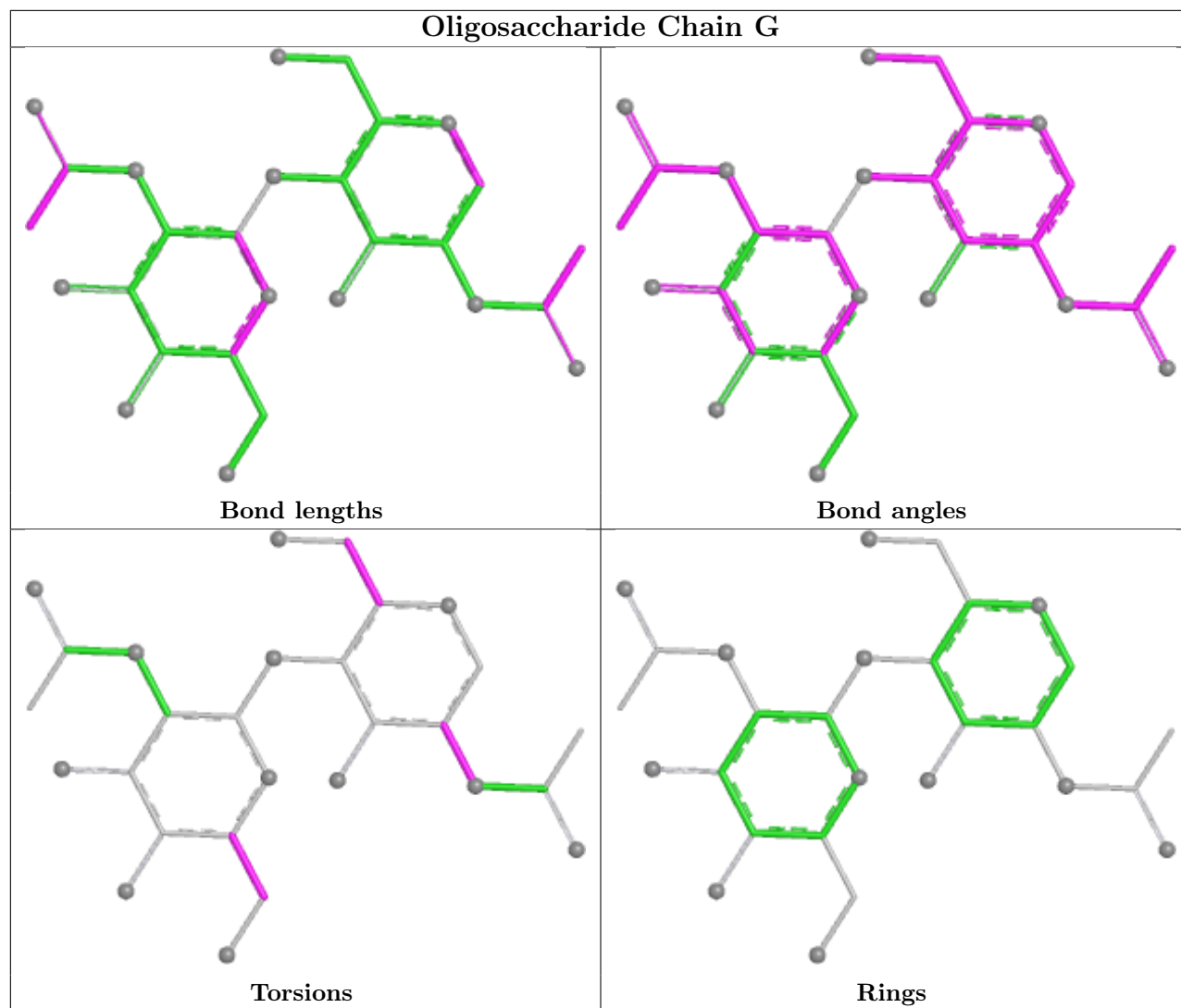
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6

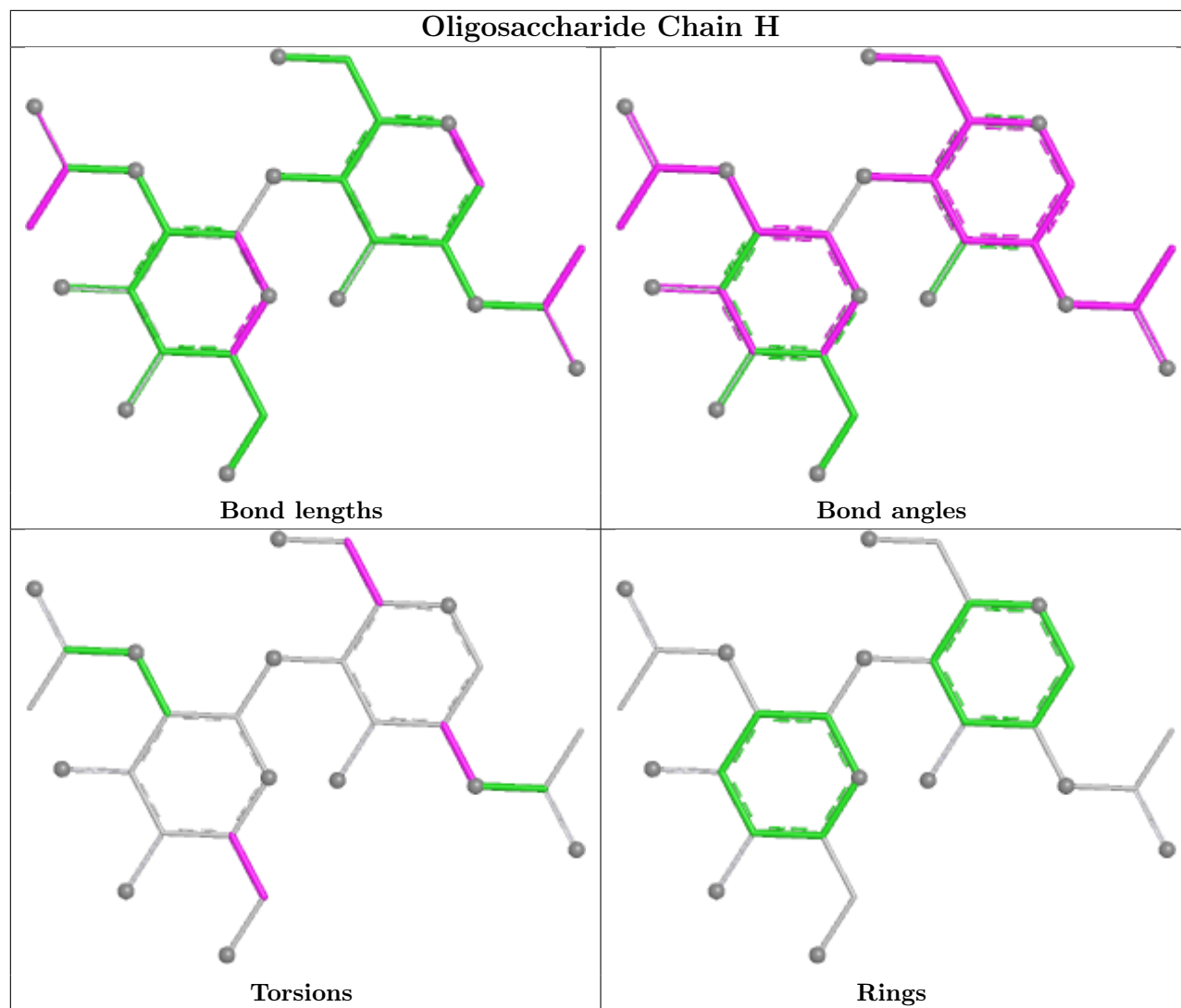
There are no ring outliers.

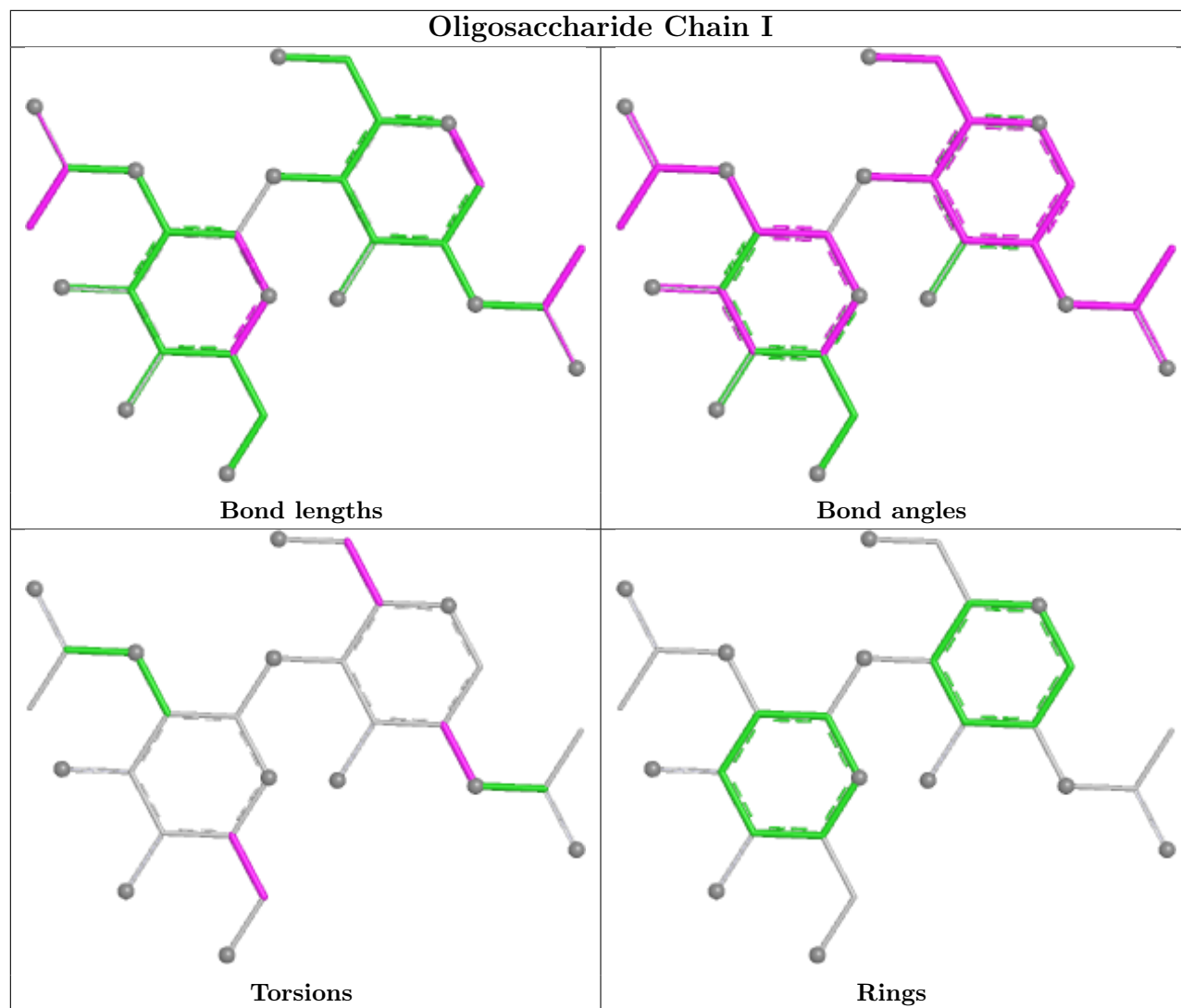
12 monomers are involved in 36 short contacts:

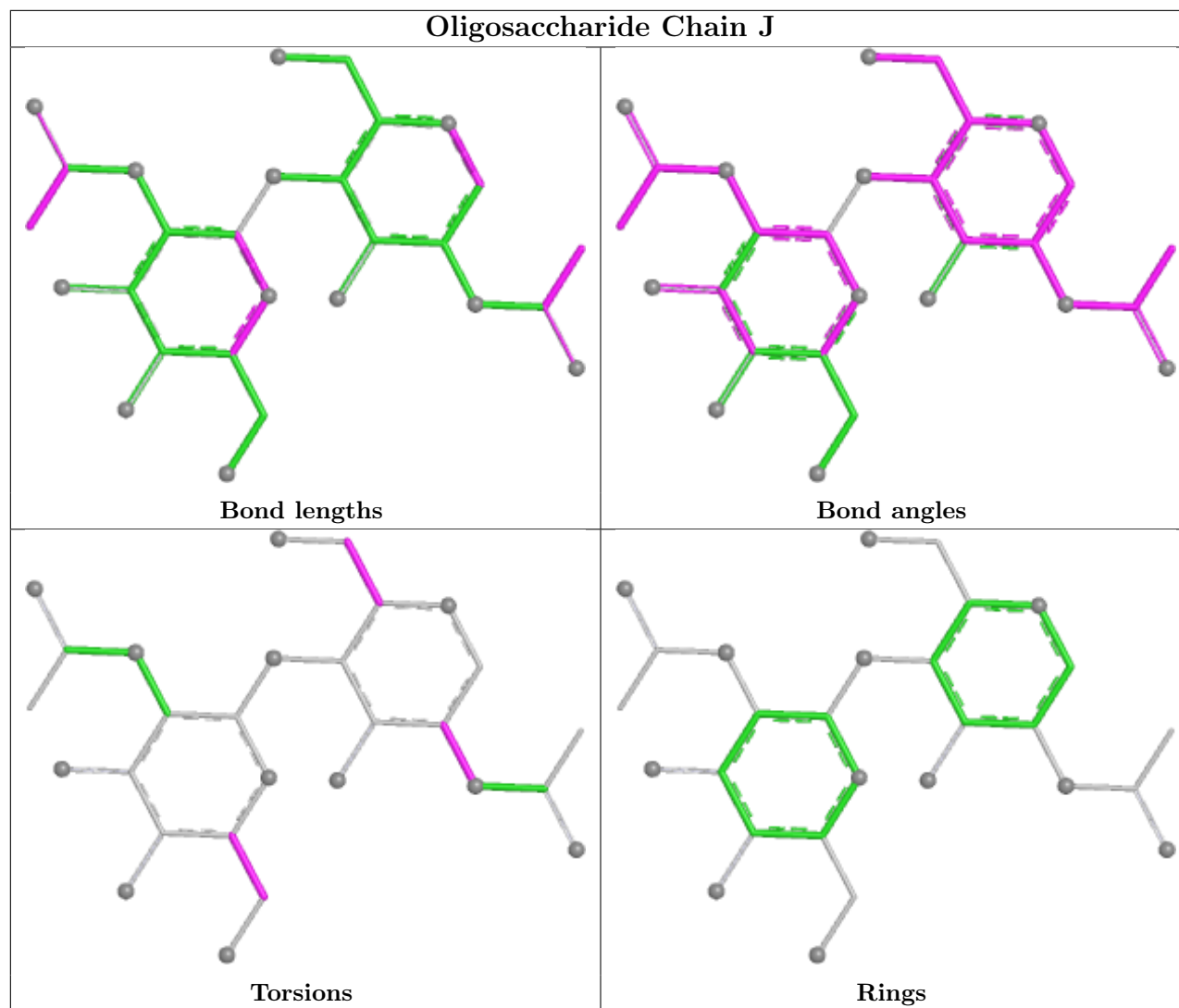
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	2	0
2	L	2	NAG	2	0
2	K	1	NAG	4	0
2	K	2	NAG	2	0
2	J	1	NAG	4	0
2	G	2	NAG	2	0
2	I	1	NAG	4	0
2	H	1	NAG	4	0
2	I	2	NAG	2	0
2	J	2	NAG	2	0
2	G	1	NAG	4	0
2	L	1	NAG	4	0

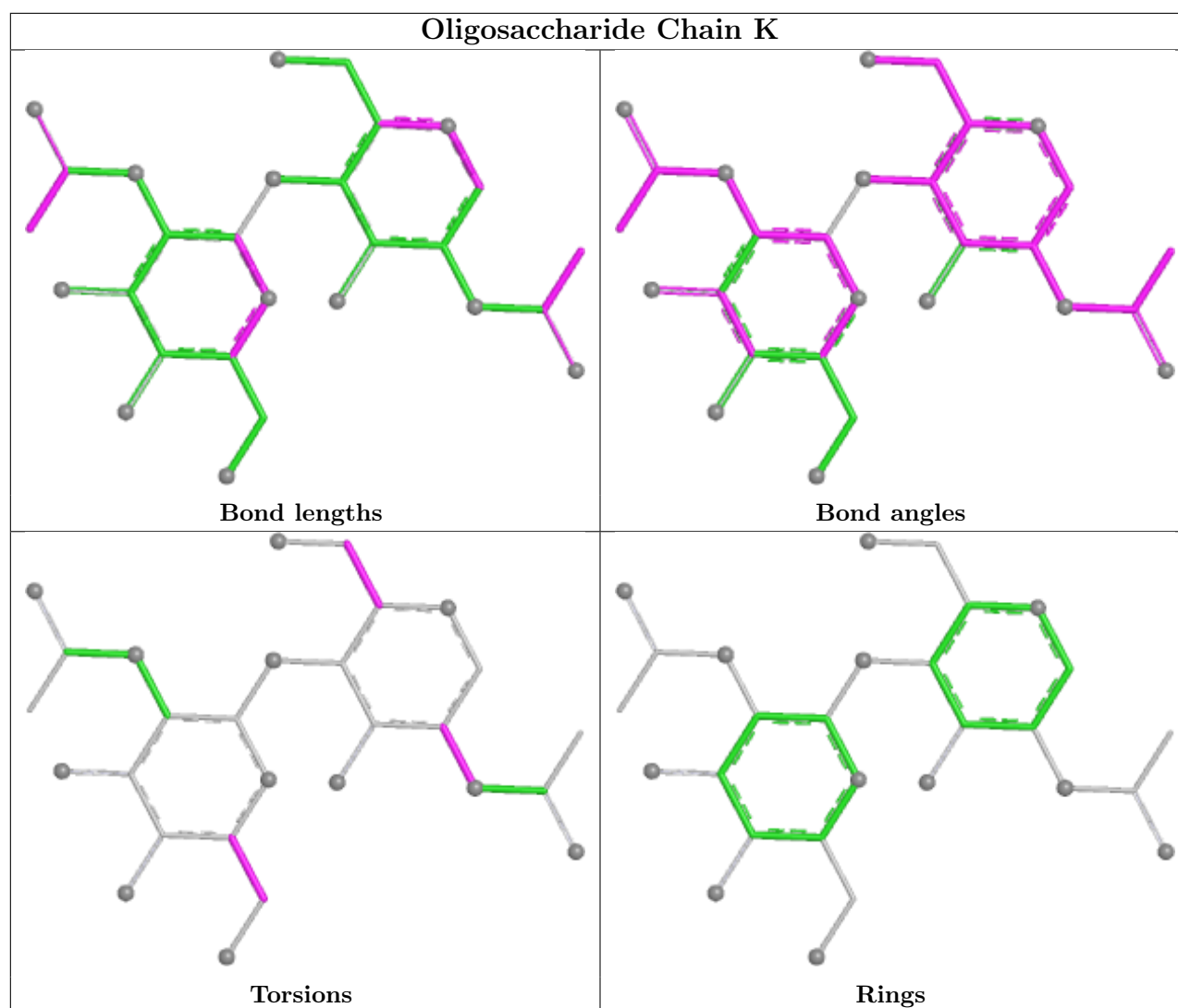
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

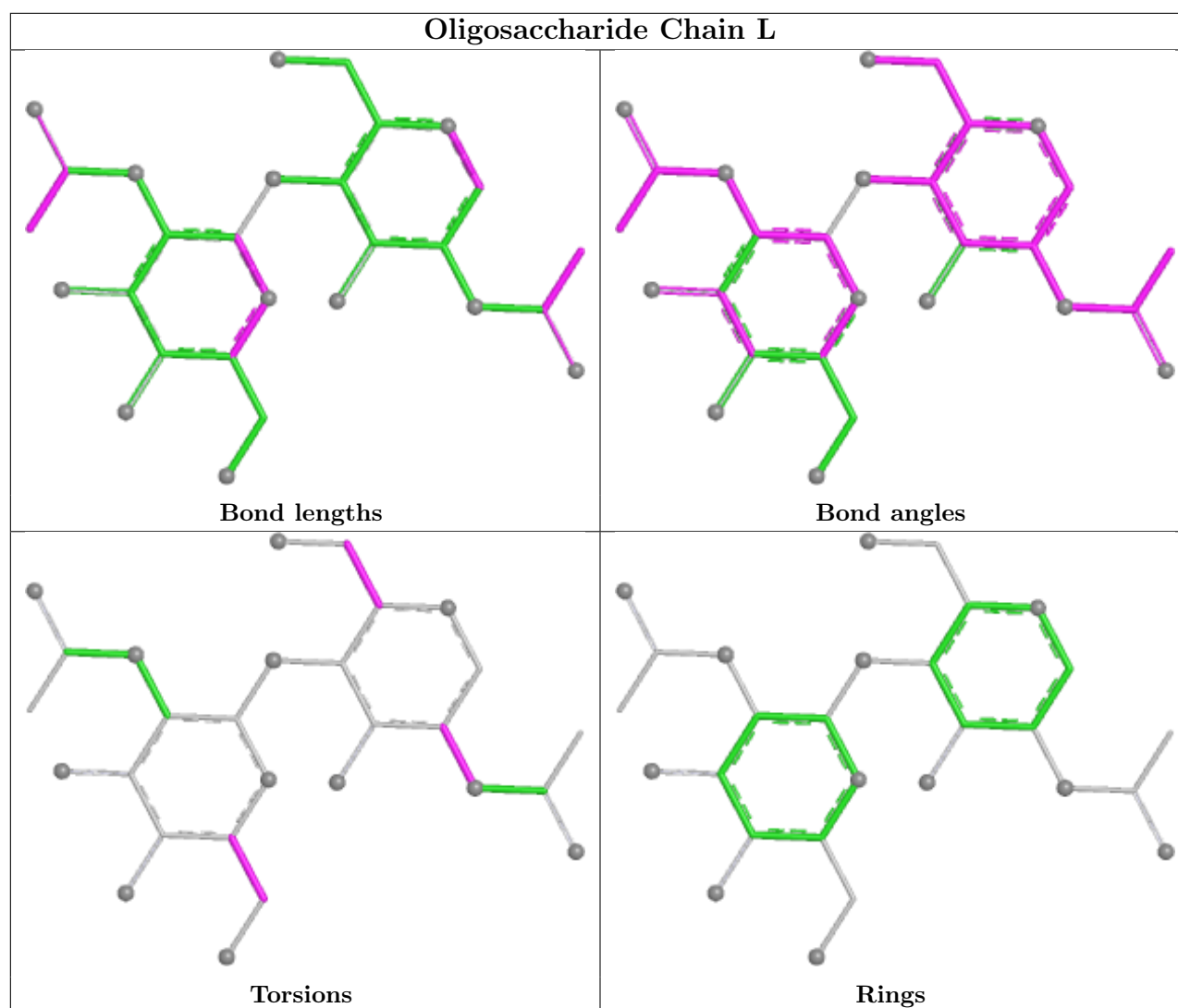












5.6 Ligand geometry [i](#)

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%)	-0.48	3 (0%) 87 78	2, 11, 53, 85	0
1	B	644/657 (98%)	-0.38	4 (0%) 85 76	2, 11, 53, 85	0
1	C	644/657 (98%)	-0.32	8 (1%) 76 61	2, 11, 53, 85	0
1	D	644/657 (98%)	-0.34	7 (1%) 77 63	2, 11, 53, 85	0
1	E	644/657 (98%)	-0.38	3 (0%) 87 78	2, 11, 53, 85	0
1	F	644/657 (98%)	-0.38	6 (0%) 81 68	2, 11, 53, 85	0
All	All	3864/3942 (98%)	-0.38	31 (0%) 82 70	2, 11, 54, 85	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	548	ASN	4.6
1	A	3	LEU	3.9
1	F	2	ALA	3.8
1	C	1	ASP	3.8
1	C	640	SER	3.7

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

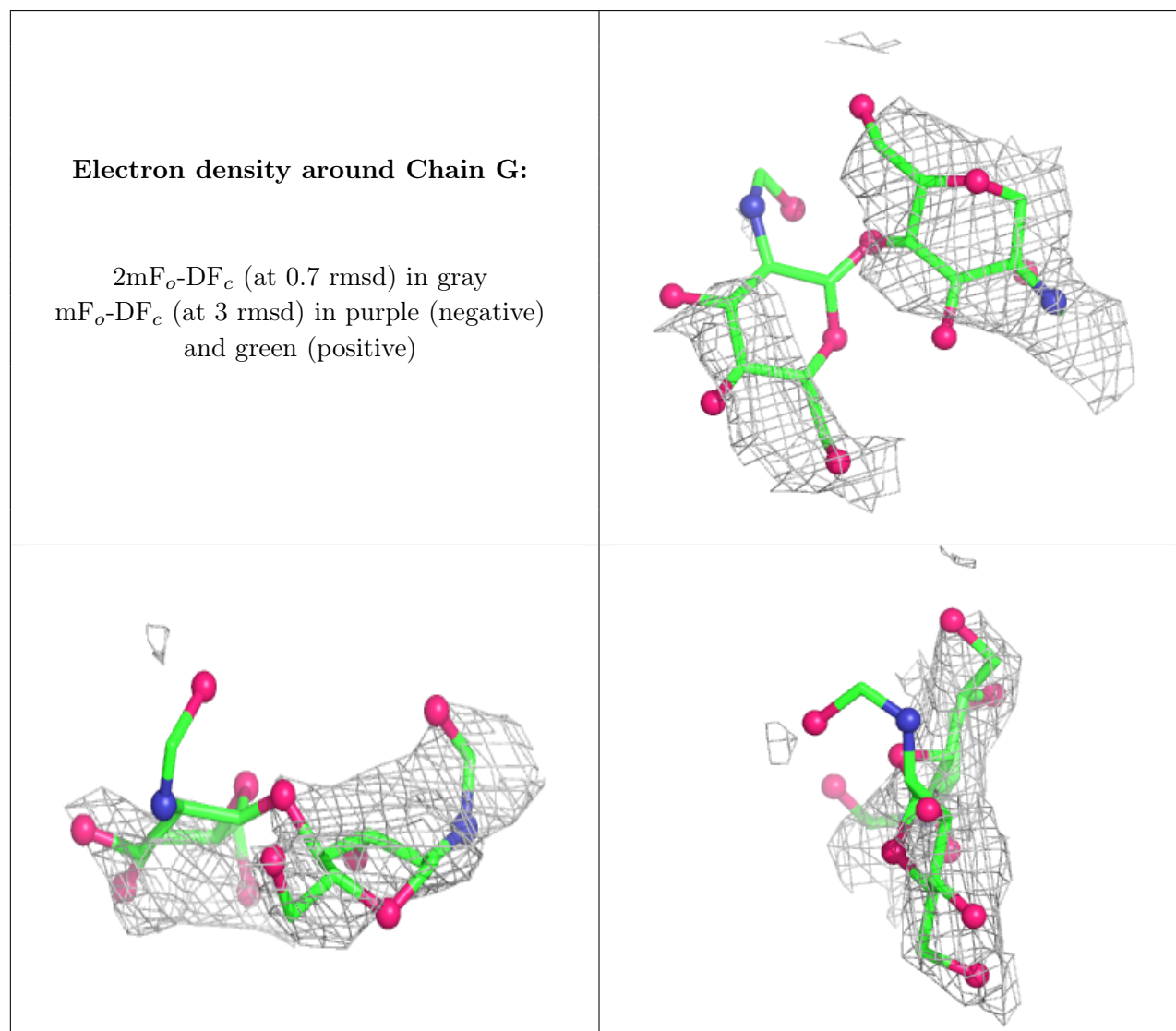
There are no non-standard protein/DNA/RNA residues in this entry.

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.

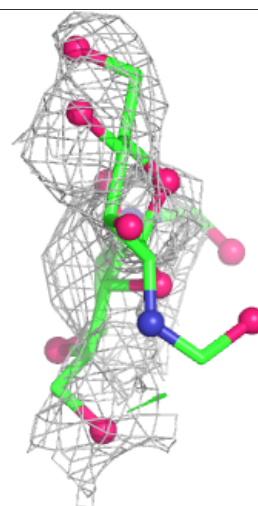
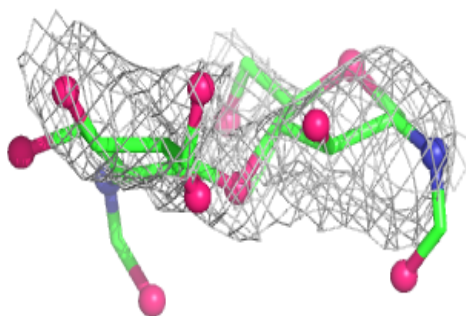
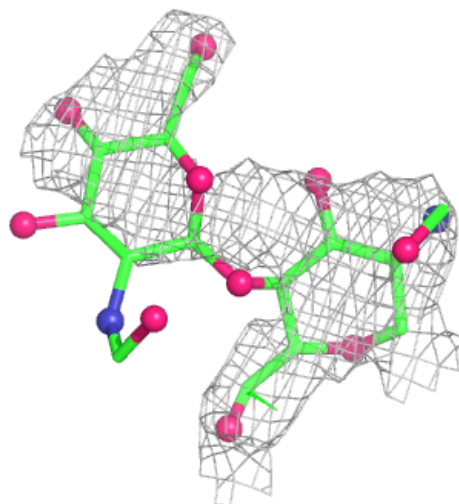
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	J	2	14/15	0.47	0.20	73,82,87,89	0
2	NAG	L	2	14/15	0.60	0.18	73,82,87,89	0
2	NAG	J	1	14/15	0.63	0.18	52,57,68,70	0
2	NAG	I	2	14/15	0.65	0.23	73,82,87,89	0
2	NAG	G	2	14/15	0.66	0.15	73,82,87,89	0
2	NAG	H	2	14/15	0.66	0.18	73,82,87,89	0
2	NAG	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.



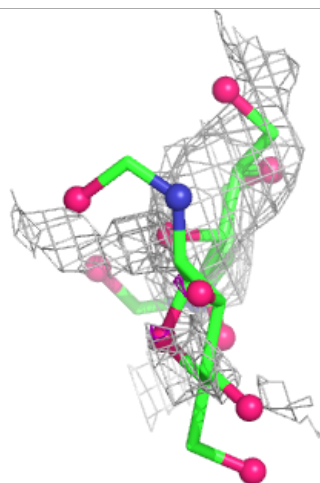
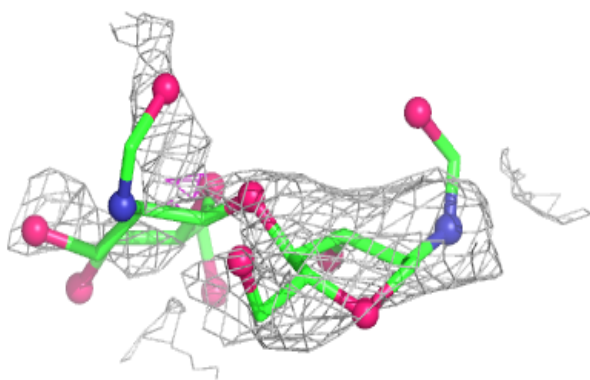
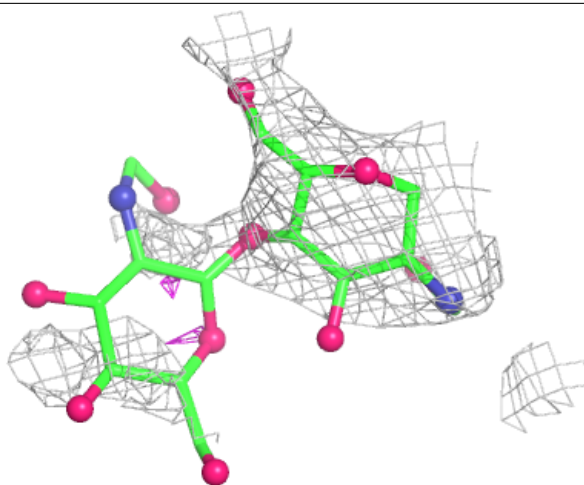
Electron density around Chain H:

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



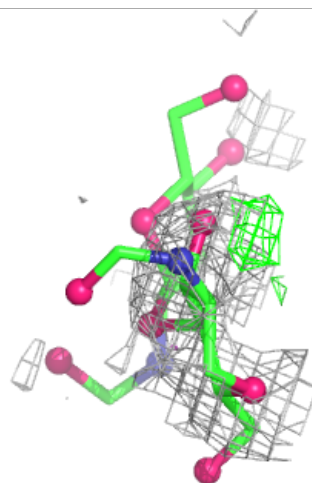
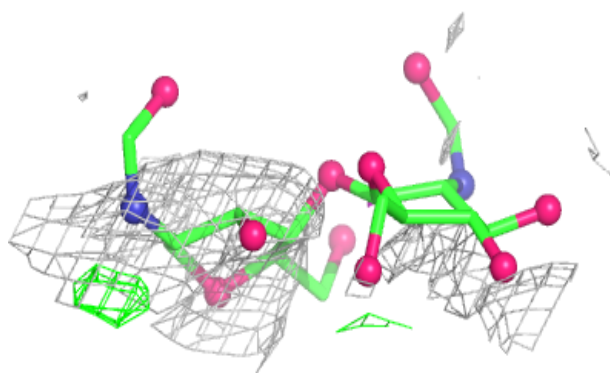
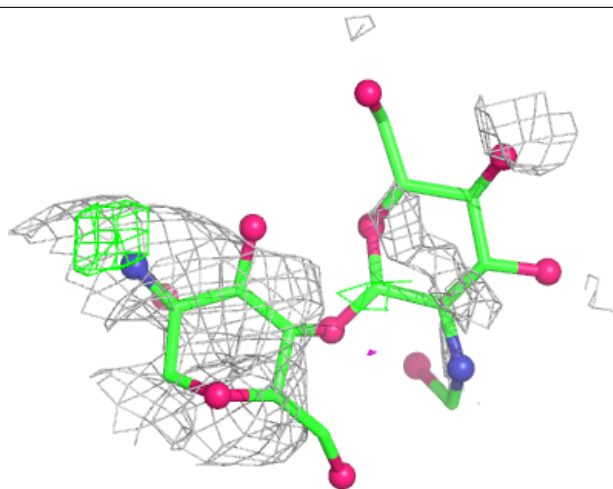
Electron density around Chain I:

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



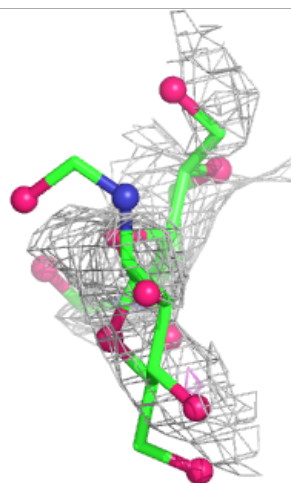
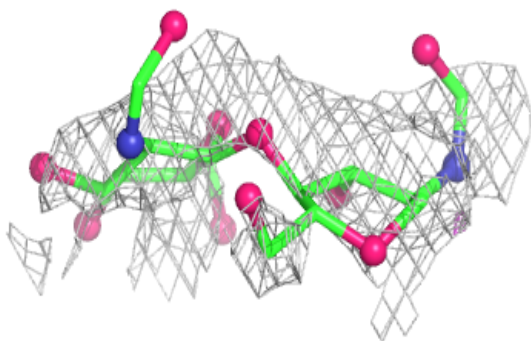
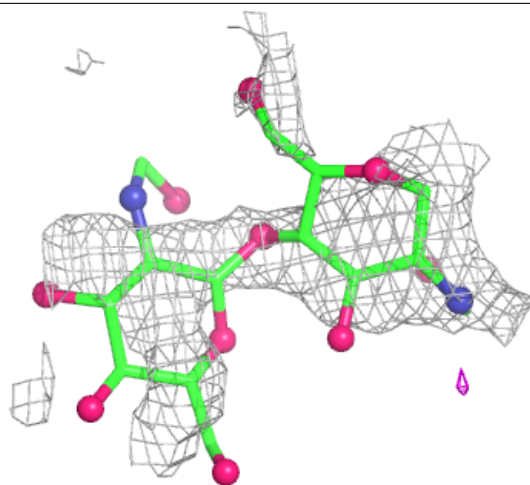
Electron density around Chain J:

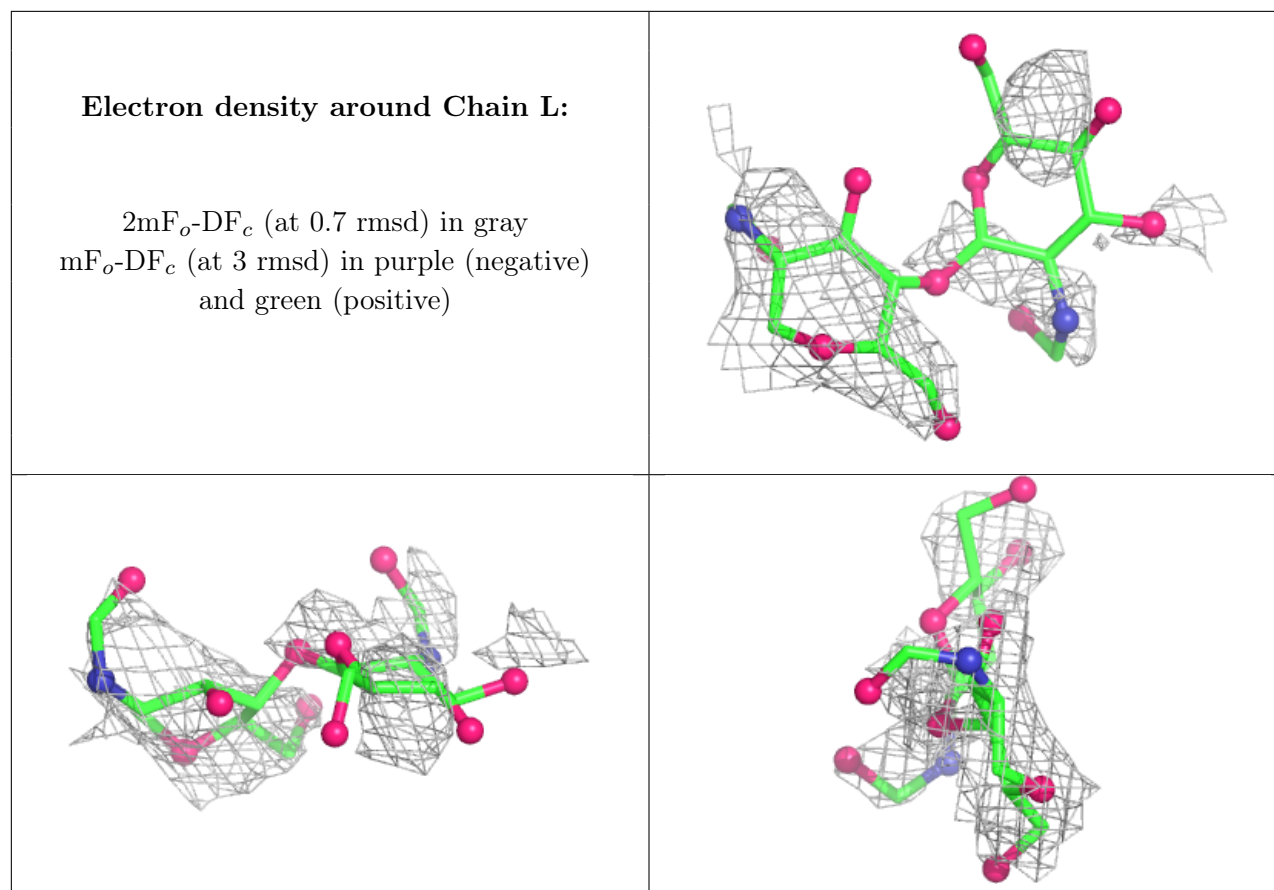
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\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	0.04	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.