



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 12:36 AM BST

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.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

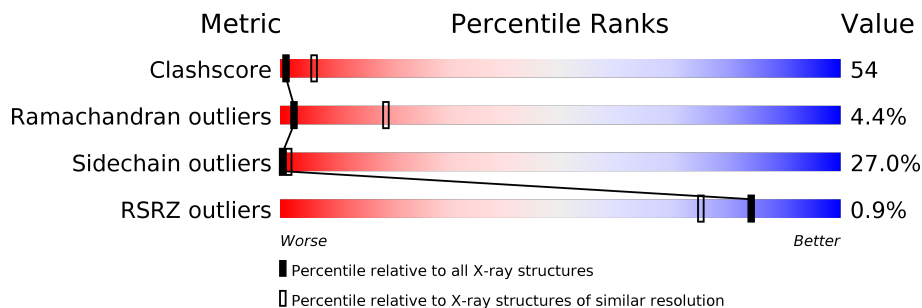
1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	 6% 29% 47% 16% .
1	B	657	 6% 29% 46% 16% .
1	C	657	 6% 30% 47% 16% .
1	D	657	 6% 29% 47% 16% .
1	E	657	 6% 28% 47% 16% .
1	F	657	 6% 30% 46% 15% .
2	G	2	 100%

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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	H	2	-	-	-	X
2	NAG	I	1	X	-	-	-
2	NAG	I	2	-	-	-	X
2	NAG	J	1	X	-	-	-
2	NAG	J	2	-	-	-	X
2	NAG	K	1	X	-	-	-
2	NAG	K	2	-	-	-	X
2	NAG	L	1	X	-	-	-
2	NAG	L	2	-	-	-	X

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	644	5239	3322	904	992	21	0	0	0
1	B	644	5239	3322	904	992	21	0	0	0
1	C	644	5239	3322	904	992	21	0	0	0
1	D	644	5239	3322	904	992	21	0	0	0
1	E	644	5239	3322	904	992	21	0	0	0
1	F	644	5239	3322	904	992	21	0	0	0

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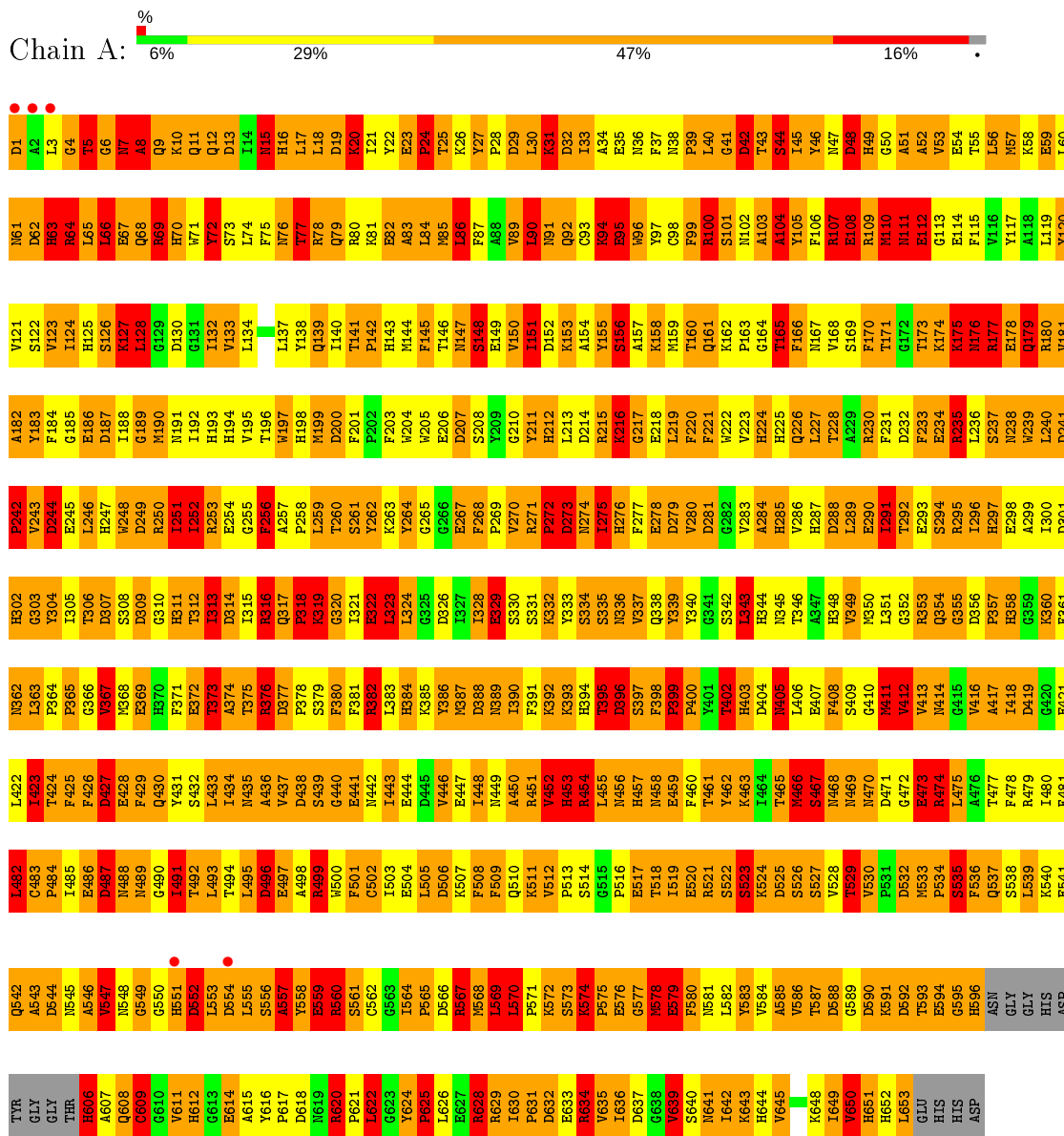
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total O 2 2	0	0
4	E	3	Total O 3 3	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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



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H302	N862	L422	L482	Q542	Tyr
G303	L363	L423	C483	A543	GLY
Y304	L63	L424	P484	D544	GLY
I305	P365	F425	I485	N545	THR
F306	F426	F427	E486	A546	
D307	V367	D427	D487	V547	H606
S308	K368	E428	M488	N548	AG07
D309	E369	F429	M489	G549	Q608
G310	H370	Q430	G490	G550	C609
H311	F371	Y431	I491	H511	G610
T312	E372	S432	T492	D512	N611
I313	K373	L433	L493	D513	H612
D314	A374	L434	T494	D514	G613
I315	T375	M435	L495	L555	E614
R316	R376	A436	D496	L556	A615
Q317	D377	V437	E497	S557	R616
R318	F378	D438	A498	E558	P617
K319	S379	S439	R499	N559	D618
G320	F380	G440	W500	R560	N619
I321	F381	E441	F501	S561	R620
E322	R382	M442	C502	C562	P621
L323	L383	I443	F503	G563	L622
L324	H384	E444	E504	E564	G623
K325	K385	D445	L505	P565	M624
D326	Y386	V446	D506	D566	P625
I327	K387	E447	K507	R567	L626
E328	D388	I448	F508	R568	E627
E329	N389	N449	F509	R569	R628
S330	I390	A450	Q510	L570	L629
S331	F391	R451	K511	P631	L630
K332	K392	V452	V512	K572	P631
Y333	K393	E453	P513	S573	D632
S334	H394	R454	S514	R574	E633
S335	T395	L455	G515	P575	R634
N336	D396	M456	P516	E576	V635
V337	S397	H457	E517	G577	L636
Q338	F398	N458	T518	N578	D637
Y339	F399	E459	I519	E579	G638
Y340	P400	F460	E520	F580	R639
G341	Y401	T461	R521	N581	S640
S342	F402	Y462	S522	L582	N641
L343	H403	K463	S523	Y583	L642
H344	D404	L464	K524	V584	R643
N345	M405	T465	D525	A585	H644
T346	L406	M466	S526	N586	V645
A347	E407	S467	S527	T587	R646
H348	F408	N468	F528	D688	L649
V349	S409	N469	T529	G589	V650
M350	G410	N470	V530	D590	H651
L351	M411	D471	P531	K591	M652
G352	V412	G472	D532	D592	L653
R353	V413	E473	M533	T593	L653
Q354	M414	R474	P534	E594	GLU
G355	G415	L475	S535	G595	HIS
D356	V416	A476	F536	H596	HIS
P357	A417	T477	O537	ASN	ASP
H358	I418	F478	S538	GLY	ASP
G359	D419	R479	L539	GLY	ASP
K360	G420	I480	K540	HIS	ASP
F361	E421	F481	E541	ASP	ASP

• Molecule 1: ARTHROPODAN HEMOCYANIN



D1	N61	L121	E242	H302	N862	L422	L482	Q542	D1
A2	D62	S122	V243	G303	L363	L423	C483	A543	A2
L3	R63	V123	D244	Y304	L63	L424	P484	D544	L3
G4	R64	I124	E245	I305	P365	F425	I485	N545	G4
T5	L65	H125	L246	F306	F426	F427	E486	A546	T5
G6	L66	D126	D247	D307	V367	D427	D487	V547	G6
R7	R67	K127	K248	S308	K368	E428	M488	N548	R7
A8	Q68	L128	D249	D309	E369	F429	M489	G549	A8
Q9	R69	G129	R250	G310	H370	Q430	G490	G550	Q9
K10	H70	N130	I251	H311	F371	Y431	I491	H511	K10
Q11	W71	G131	T252	T312	E372	S432	T492	D512	Q11
Q12	Y72	L132	E253	I313	K373	L433	L493	D513	Q12
D13	S73	H133	E254	D314	A374	L434	T494	D514	D13
L14	L74	V134	G255	I315	T375	M435	L495	L555	L14
N15	F75	L134	F256	R316	R376	A436	D496	S556	N15
R16	N76	L137	A257	Q317	D377	V437	E497	S557	R16
L17	T77	H138	P258	F318	F378	D438	A498	E558	L17
R18	R78	Q139	L259	K319	S379	S439	R499	N559	R18
D19	Q79	I140	T260	G320	F380	G440	W500	R560	D19
R20	R80	T141	S261	I321	F381	E441	F501	S561	R20
L21	R81	P202	Y262	E322	R382	M442	C502	C562	L21
Y22	E82	F203	K263	L323	L383	I443	F503	G563	Y22
E23	E83	W204	Y264	L324	H384	E444	E504	E564	E23
P24	L84	V205	G265	G325	K385	D445	L505	P565	P24
T25	M85	T146	G266	D326	Y386	V446	D506	D566	T25
R26	L86	D207	E267	I327	K387	E447	K507	R567	R26
Y27	F87	S148	F268	E328	D388	I448	F508	R568	Y27
R28	A88	Y209	P269	E329	N389	N449	F509	R569	R28
L29	V89	G210	V270	S330	I390	A450	Q510	L570	L29
L30	L90	I151	R271	S331	F391	R451	K511	P631	L30
K31	N91	D152	P272	K332	K392	V452	V512	K572	K31
D32	Q92	K153	D273	Y333	K393	E453	P513	S573	D32
L33	C93	D154	N274	S334	H394	R454	S514	R574	L33
A34	R94	Y155	I275	S335	T395	L455	G515	P575	A34
E35	E95	K216	R276	N336	D396	M456	P516	E576	E35
N36	W96	G217	F277	V337	S397	H457	E517	G577	N36
F37	Y97	K158	E278	Q338	F398	N458	T518	N578	F37
N38	C98	M159	D279	Y339	F399	E459	I519	E579	N38
P39	F99	T160	V280	Y340	P400	F460	E520	F580	P39
L40	R100	Q161	D281	G341	Y401	T461	R521	N581	L40
G41	S101	K162	G282	S342	F402	Y462	S522	L582	G41
D42	M102	V223	V283	L343	H403	K463	S523	Y583	D42
T43	A103	H224	A284	H344	D404	L464	K524	V584	T43
R44	M104	H225	H285	N345	M405	T465	D525	A585	R44
I45	Y105	Q226	V286	T346	L406	M466	S526	N586	I45
Y46	F106	L227	H287	A347	E407	S467	S527	T587	Y46
N47	R107	V168	D288	H348	F408	N468	F528	D688	N47
D48	E108	A229	L289	V349	S409	N469	T529	G589	D48
H49	R109	R230	E290	M350	G410	N470	V530	D590	H49
G50	M110	F231	L291	L351	M411	D471	P531	K591	G50
A51	M111	D232	T292	G352	V412	G472	D532	D592	A51
A52	F233	E293	E294	R353	V413	E473	M533	T593	A52
V53	K174	S294	R295	Q354	M414	R474	P534	E594	V53
E54	K175	R295	L296	G355	G415	L475	L475	G595	E54
T55	M176	L296	H297	D356	V416	A476	F536	H596	T55
L56	R177	S297	E298	P357	A417	T477	O537	ASN	L56
M57	E178	M298	E299	H358	A417	F478	S538	GLY	M57
K58	Q179	W299	A299	I359	D419	R479	L539	GLY	K58
E59	R180	L240	I300	K360	G420	I480	K540	HIS	E59
L60	Y120	V181	D301	F361	E421	F481	E541	ASP	L60

TYR	GLY	GLY	THR	H606	Q608	G609	V610	H611	H612	G613	E614	A615	Y616	P617	D618	N619	R620	F621	L622	G623	Y624	P625	L626	E627	R628	R629	I630	P631	D632	E633	R634	V635	I636	D637	G638	R639	S640	M641	I642	K643	H644	V645	K648	I649	V650	H651	H652	L653	GLU	HIS	HIS	HIS	ASP
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● Molecule 1: ARTHROPODAN HEMOCYANIN



D1	A2	L3	G4	T5	L66	G6	H7	Q8	R9	K10	H11	Q11	Q12	H13	L14	H15	H16	L17	L18	D19	R20	L21	Y22	E23	L24	H25	T26	L27	H28	F29	L30	L31	Q32	L33	C34	R35	A36	E37	N38	Y39	F37	L38	F39	L40	S101	N102	K103	H104	S105	L106	F107	M108	R109	H110	M111	A51	A52	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120
H61	D62	H63	R64	L65	L66	E67	Q68	R69	H70	H71	Y72	H73	S74	L74	F75	H76	H77	R78	Q79	R80	R81	L21	Y22	E23	L84	H85	T86	L87	H88	F89	L90	L91	Q92	L93	C94	R95	A96	E97	N98	Y97	F97	L98	F99	L100	S101	N102	K103	H104	S105	L106	F107	M108	R109	H110	M111	A51	A52	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120
V121	S122	H123	F124	E125	H126	K127	L128	H129	M130	H131	L132	H133	L134	L137	Y138	H139	R140	Q141	D142	F201	F202	L43	H43	E43	M44	F45	L46	H47	S148	E149	L150	H151	L152	K153	L154	Y155	E156	A157	K158	H159	L160	Q161	K162	P163	G164	H225	F166	M167	V168	S169	F170	H171	G172	T173	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120			
A182	Y183	F184	E185	H186	L187	H188	H189	M190	H191	L192	H193	H194	V195	H196	H197	H198	P199	Q200	D201	F202	F201	L43	H43	E43	M44	F45	L46	H47	S148	E149	L150	H151	L152	K153	L154	Y155	E156	A157	K158	H159	L160	Q161	K162	P163	G164	H225	F166	M167	V168	S169	F170	H171	G172	T173	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120			
P242	V243	D244	F245	G246	H247	H248	D249	H250	M191	L192	H193	H194	G255	F256	H197	P258	M199	D260	S261	F202	F201	L43	H43	E43	M44	F45	L46	H47	S148	E149	L150	H151	L152	K153	L154	Y155	E156	A157	K158	H159	L160	Q161	K162	P163	G164	H225	F166	M167	V168	S169	F170	H171	G172	T173	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120			
H302	G303	Y304	L305	T306	H307	S308	G309	D310	H311	L312	H313	H314	L315	R316	H317	P318	R319	G320	S321	E322	L323	Y324	H325	G326	H327	L328	H329	E330	L331	H332	Y333	S334	L335	H336	E337	V337	Q338	H339	Y340	G341	S342	H343	H344	H345	H285	V286	H287	L227	D228	L229	R230	E231	D232	T292	E293	S294	R295	L296	H297	E298	A299	L300	D301	F361			
N362	L363	P364	P365	F366	V367	K368	E369	H370	F371	E372	T373	D374	T375	R376	H377	P378	S379	G380	F381	E382	L383	H384	K385	G386	H387	L388	H389	E390	L391	H392	K393	K394	H395	D396	S397	F397	H398	P399	P400	Y401	G402	H403	D404	H405	L406	F407	F408	S409	G410	H411	V412	H413	M414	G415	H416	L417	V418	A419	L420	H421	F481						
L422	E423	F424	F425	F426	H427	E428	F429	Q430	Y431	L432	L433	L434	L435	A436	H437	D438	S439	G440	E441	M442	I443	I444	E445	V446	E447	L448	H449	M450	Q451	H452	H453	H454	L455	M456	H457	H458	E459	F460	T461	Y462	K463	D464	T465	M466	F467	M468	H469	M470	G471	D472	G473	E474	R475	L476	H477	F478	R479	L480	G481	F481							
L482	C483	P484	L485	E486	D487	M488	M489	G490	L491	E492	L493	L494	L495	D496	E497	R498	R499	H500	F501	C502	I503	E504	P505	D506	K507	F508	H509	Q510	L511	H512	V513	H514	G515	E516	T517	H518	L519	E520	H521	S522	S523	K524	D525	S526	S527	H528	T529	H530	V531	D532	M533	P534	S535	L536	H537	S538	L539	E541									
Q542	A543	D544	N545	A546	H547	M548	G549	H550	H551	D552	L553	D554	L555	S556	A557	E558	R559	R560	S561	C562	G563	E564	P565	D566	E567	M568	L569	I570	L571	H572	H573	H574	P575	E576	G577	H578	E579	F580	M581	L582	Y583	V584	A585	V586	H587	D588	G589	D590	K591	D592	H593	E594	G595	H596	ASN	GLY	GLY	HIS	ASP								

TYR	GLY	GLY	THR	H606	Q608	G609	V610	H611	H612	G613	E614	A615	Y616	P617	D618	N619	R620	F621	L622	G623	Y624	P625	L626	E627	R628	R629	I630	P631	D632	E633	R634	V635	I636	D637	G638	R639	S640	M641	I642	K643	H644	V645	K648	I649	V650	H651	H652	L653	GLU	HIS	HIS	HIS	ASP
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● Molecule 1: ARTHROPODAN HEMOCYANIN



D1	A2	L3	G4	T5	L66	G6	H7	Q8	R9	K10	H11	Q11	Q12	H13	L14	H15	H16	L17	L18	D19	R20	L21	Y22	E23	L24	H25	T26	L27	H28	F29	L30	L31	Q32	L33	C34	R35	A36	E37	N38	Y39	F37	L38	F39	L40	S101	N102	K103	H104	S105	L106	F107	M108	R109	H110	M111	A51	A52	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120
H61	D62	H63	R64	L65	L66	E67	Q68	R69	H70	H71	Y72	H73	S74	L74	F75	H76	H77	R78	Q79	R80	R81	L21	Y22	E23	L84	H85	T86	L87	H88	F89	L90	L91	Q92	L93	C94	R95	A96	E97	N98	Y97	F97	L98	F99	L100	S101	N102	K103	H104	S105	L106	F107	M108	R109	H110	M111	A51	A52	G113	E114	T55	F115	L116	H57	H58	E59	L119	Y120

V121	Y182	P242	H202	N862	L422	L482	Q542	TVR
S122	Y183	V243	G303	L363	I423	C483	A643	GLY
I124	F184	D244	Y304	P364	T424	P484	D644	GLY
H126	G185	E245	I305	P365	F425	T485	N545	THR
S127	E186	L246	T306	G366	F426	F486	A546	H606
L128	H187	H247	D307	G367	D427	D487	V547	A607
G129	I188	V248	S308	N368	F428	M488	N548	Q808
D130	G189	D249	D309	E369	F429	M489	G549	C809
G131	M190	M190	G310	H370	Q430	G490	G550	G610
H133	N191	I251	H311	F371	Y431	T491	H511	H612
V133	I192	L252	T312	E372	S432	T492	L513	G613
L134	H193	H193	D313	T373	L433	L493	L553	G614
L137	H194	E254	I314	A374	I434	T494	D554	A615
L138	V195	G255	I315	T375	M435	L495	L555	A616
L139	T196	F256	R316	R376	A436	D496	S556	Y616
L140	W197	A257	Q317	D377	F437	E497	A557	P617
Q139	Y198	P258	R318	P378	D438	A498	W558	N618
I140	M199	L259	K319	S379	S439	R499	Y559	N619
T141	D200	T260	G320	F380	G440	H500	R560	R620
P142	T201	S261	I321	F381	E441	F501	S561	P621
H143	P202	Y262	E322	R382	M442	G502	C562	L622
M144	F203	K263	L323	H383	I443	T503	S563	G623
F145	W204	Y264	L324	H384	E444	E504	S564	Y624
T146	W205	G265	G325	K385	D445	L505	P565	P625
M147	E206	G266	D326	Y386	V446	D506	D566	L626
S148	D207	E267	S327	M387	E447	K507	R567	E627
E149	S208	F268	I328	D388	I448	F508	M568	R628
V150	G210	P269	E329	N389	M449	F509	L569	R629
I151	V211	R271	S330	I390	A450	Q510	L570	I630
D152	H212	K272	S331	H391	R451	K511	P571	P631
K153	L213	P273	K332	K392	V452	V512	K572	D632
A154	D214	D274	S333	K393	R453	P513	S573	E633
S155	R215	K275	S334	H394	R454	S514	R574	R634
A156	K216	H276	S335	T395	L455	G515	P575	V635
A157	G217	F277	N336	D396	M456	P516	E576	I636
K158	E218	E278	V337	F397	H457	E517	G577	D637
M159	L219	D279	Q338	F398	M458	T518	N578	G638
Q161	F220	V280	Y340	P400	F460	E520	E579	V639
K162	W221	D281	G341	Y401	T461	R521	N581	S640
G164	H223	G282	L343	H403	Y462	S522	L582	I642
T165	H224	A284	H344	D404	K463	S523	Y583	K643
F166	H225	H285	N345	M405	T464	D524	V584	H644
M167	Q226	V286	T346	L406	T465	S525	A585	V645
V168	L227	H287	A347	L407	S467	S527	V587	K648
S169	A229	D288	H348	F408	M468	V528	D588	I649
F170	R230	L289	V349	S409	M469	T529	G589	V650
T171	F231	E290	M350	G410	M470	V530	D590	H651
G172	D232	I291	L351	M411	D471	P531	K591	H652
T173	F233	T292	G352	V412	G472	D532	D592	L653
K174	E234	E293	R353	V413	E473	M533	T593	GLU
K175	R235	S294	Q354	M414	R474	P534	E594	HIS
M176	L236	R295	G355	G415	L475	S535	G595	HIS
E178	W237	I296	D356	V416	A476	F536	H596	ASP
Q179	M238	H297	R357	A417	T477	Q537	ASN	GLY
R180	W239	E298	H358	I418	F478	S538	GLY	GLY
V181	L240	A299	G359	D419	R479	L539	HIS	HIS
	D241	I300	K360	G420	T480	K540	ASP	ASP
		F361	E421					

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

- 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 – 3.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 75.6 (8.00-3.16)	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 , 41.1	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	19
1	B	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	19
1	C	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	19
1	D	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	2	19
1	F	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	2	19
All	All	3840/3942 (97%)	3140 (82%)	532 (14%)	168 (4%)	2	19

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 [i](#)

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	C	474	ARG
1	D	259	LEU
1	F	375	THR
1	C	529	THR
1	D	53	VAL

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

Mol	Chain	Res	Type
1	C	453	HIS
1	D	225	HIS
1	F	338	GLN
1	C	469	ASN
1	D	15	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1,2	14,14,15	18.09	3 (21%)	17,19,21	10.94	12 (70%)
2	NAG	G	2	2	14,14,15	21.54	4 (28%)	17,19,21	10.95	7 (41%)
2	NAG	H	1	1,2	14,14,15	18.09	3 (21%)	17,19,21	10.94	12 (70%)
2	NAG	H	2	2	14,14,15	21.55	4 (28%)	17,19,21	10.95	7 (41%)
2	NAG	I	1	1,2	14,14,15	18.09	3 (21%)	17,19,21	10.94	12 (70%)
2	NAG	I	2	2	14,14,15	21.55	4 (28%)	17,19,21	10.96	7 (41%)
2	NAG	J	1	1,2	14,14,15	18.09	3 (21%)	17,19,21	10.94	12 (70%)
2	NAG	J	2	2	14,14,15	21.55	4 (28%)	17,19,21	10.95	7 (41%)
2	NAG	K	1	1,2	14,14,15	18.09	4 (28%)	17,19,21	10.94	12 (70%)
2	NAG	K	2	2	14,14,15	21.55	4 (28%)	17,19,21	10.95	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	1	1,2	14,14,15	18.10	3 (21%)	17,19,21	10.94	12 (70%)
2	NAG	L	2	2	14,14,15	21.54	4 (28%)	17,19,21	10.95	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	1,2	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	1,2	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	1,2	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	1,2	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	1,2	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	1,2	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	78.92	3.14	1.50
2	H	2	NAG	C8-C7	78.89	3.14	1.50
2	J	2	NAG	C8-C7	78.89	3.14	1.50
2	K	2	NAG	C8-C7	78.88	3.14	1.50
2	G	2	NAG	C8-C7	78.88	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	-38.27	51.30	116.10
2	J	2	NAG	C8-C7-N2	-38.26	51.33	116.10
2	G	2	NAG	C8-C7-N2	-38.25	51.33	116.10
2	L	2	NAG	C8-C7-N2	-38.25	51.34	116.10
2	K	2	NAG	C8-C7-N2	-38.25	51.34	116.10

5 of 6 chirality outliers are listed below:

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

5 of 30 torsion outliers are listed below:

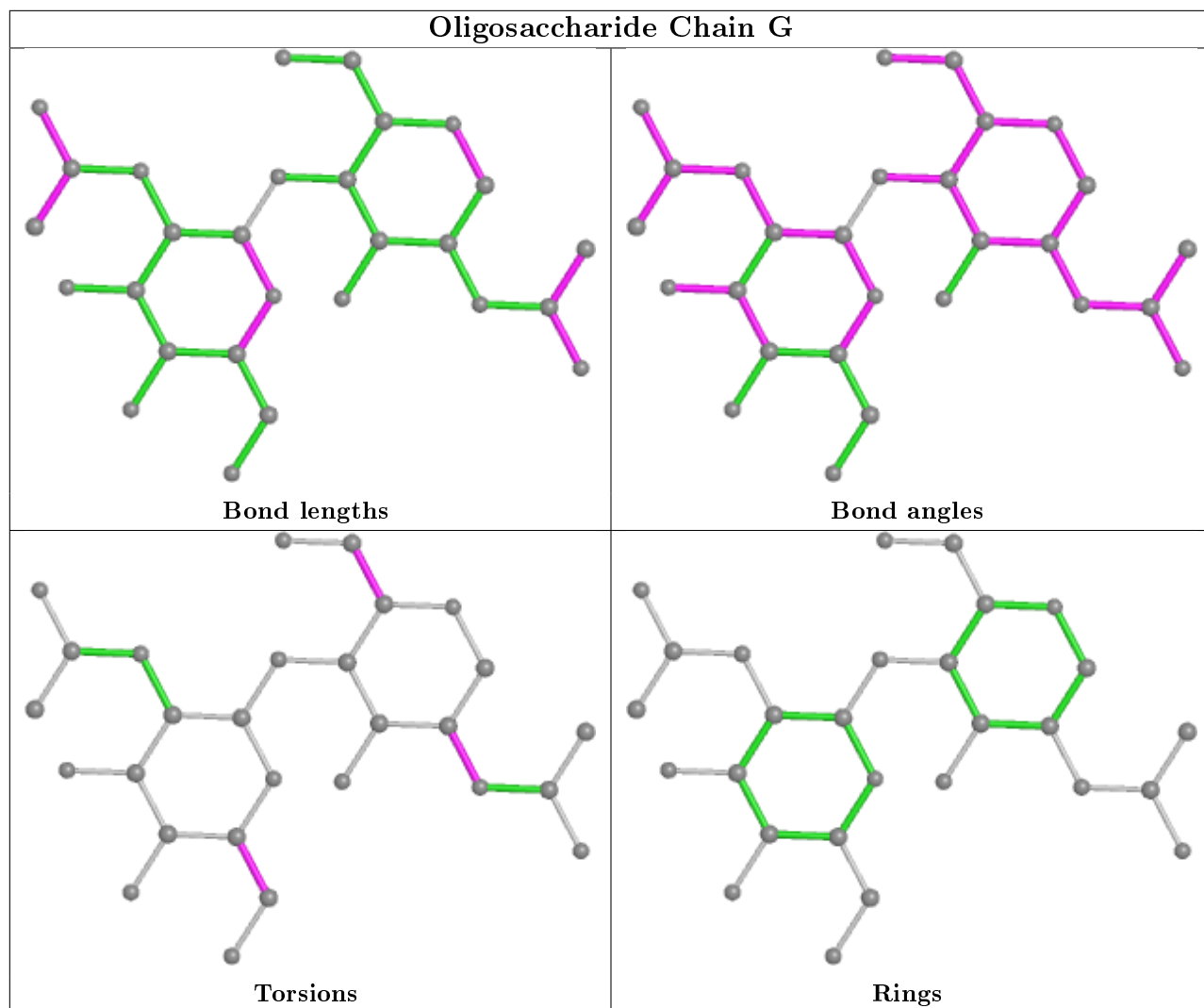
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

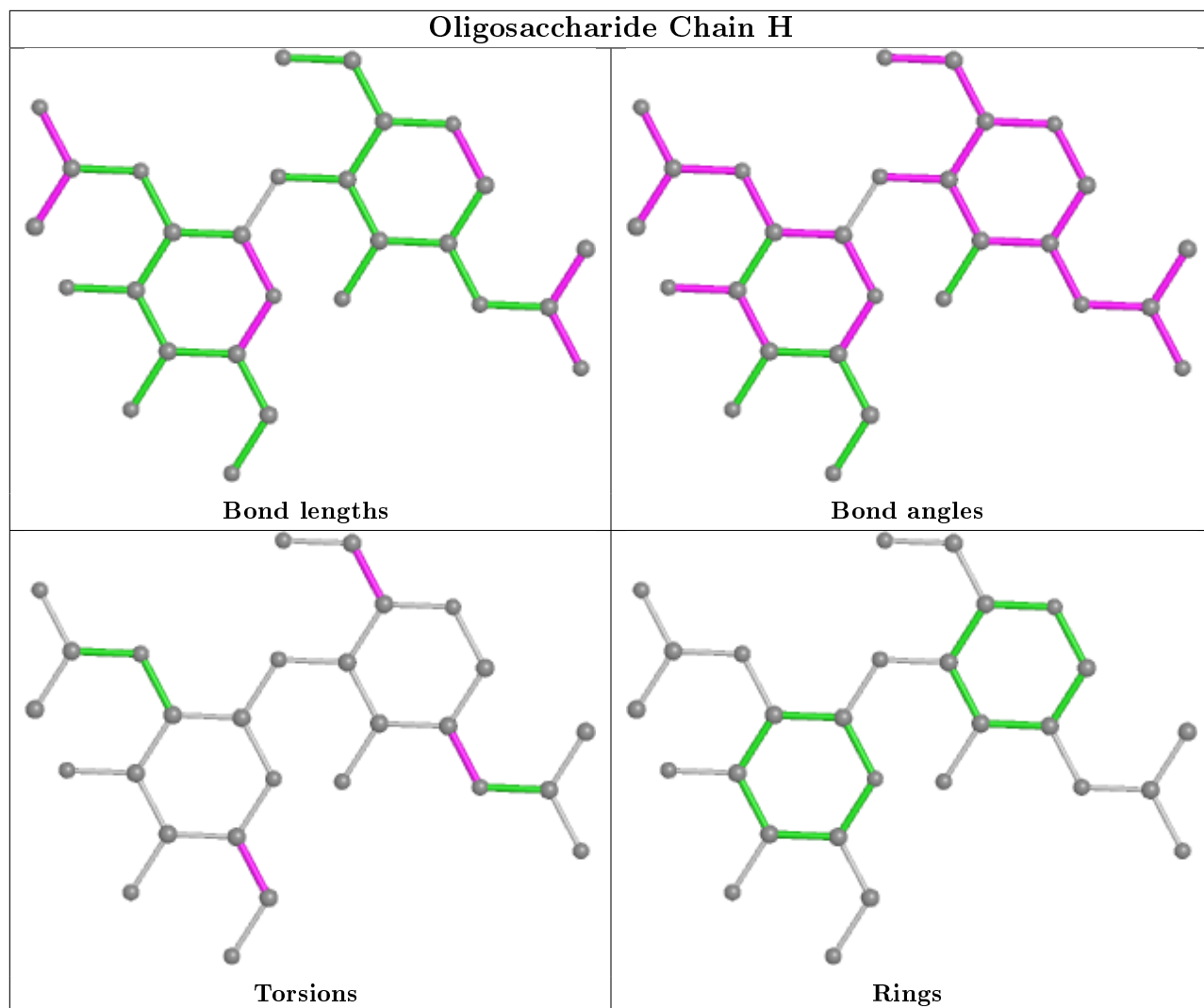
There are no ring outliers.

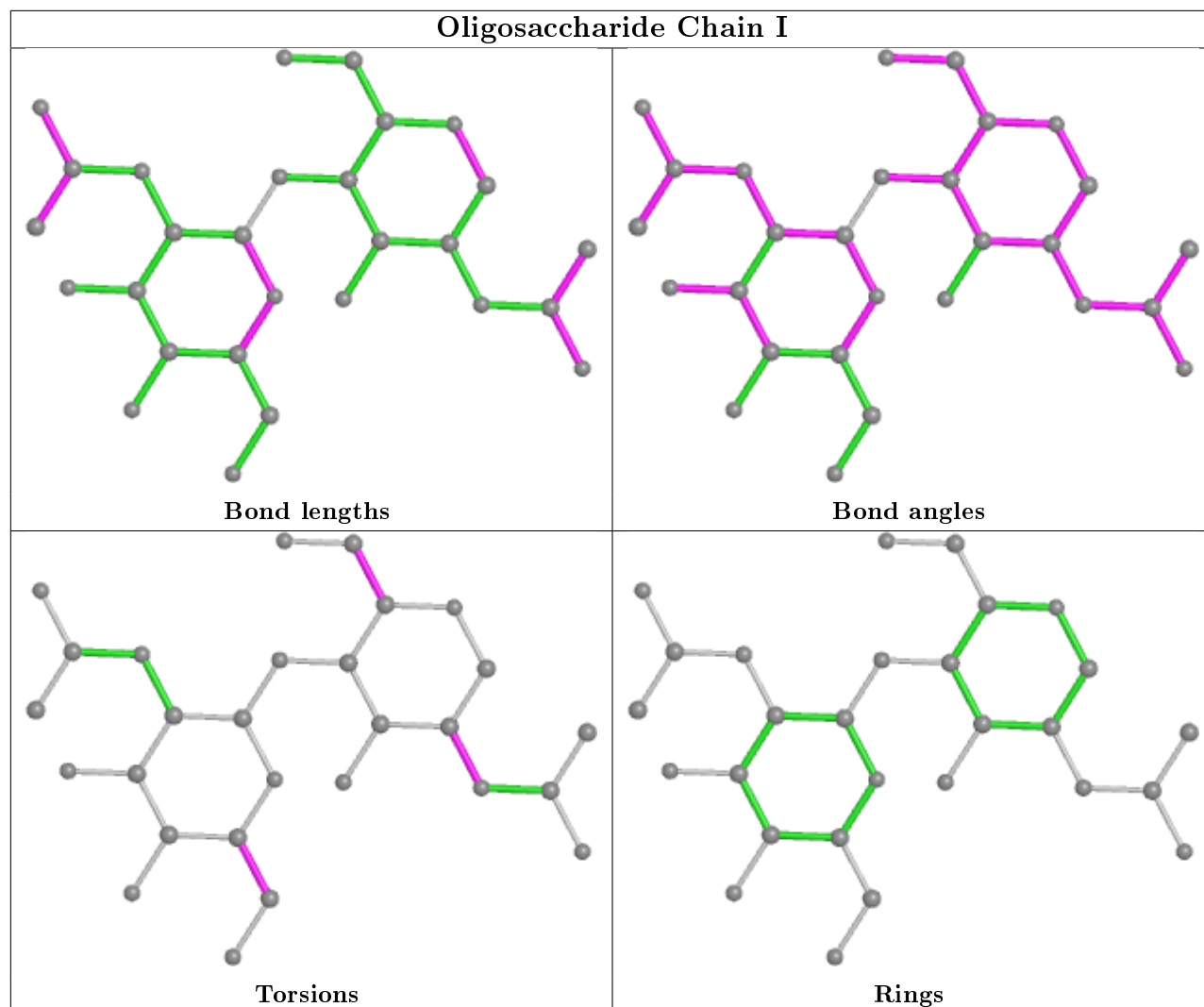
12 monomers are involved in 36 short contacts:

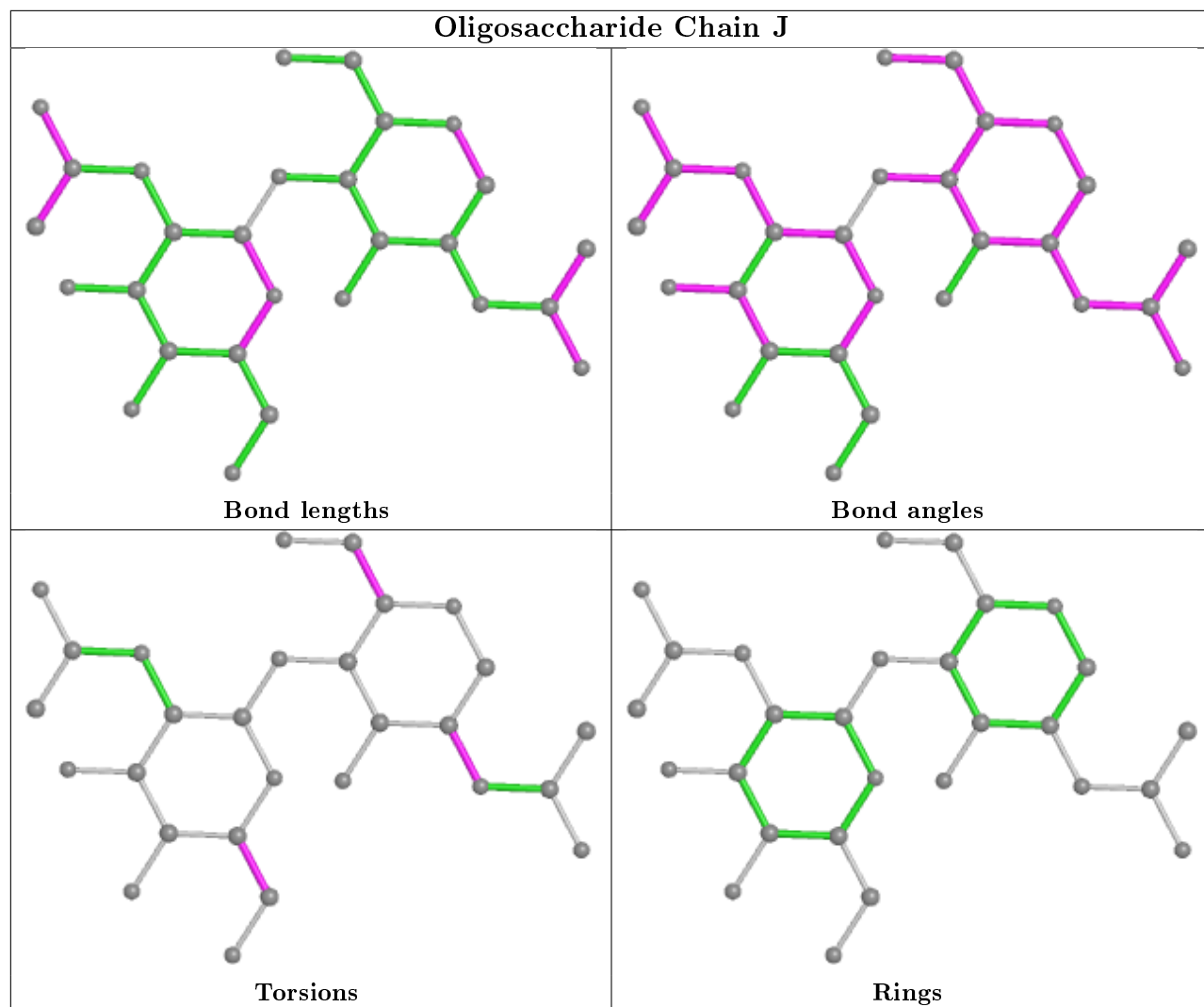
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	NAG	2	0
2	G	1	NAG	4	0
2	H	1	NAG	4	0
2	L	1	NAG	4	0
2	L	2	NAG	2	0
2	I	2	NAG	2	0
2	K	1	NAG	4	0
2	G	2	NAG	2	0
2	I	1	NAG	4	0
2	J	1	NAG	4	0
2	K	2	NAG	2	0
2	H	2	NAG	2	0

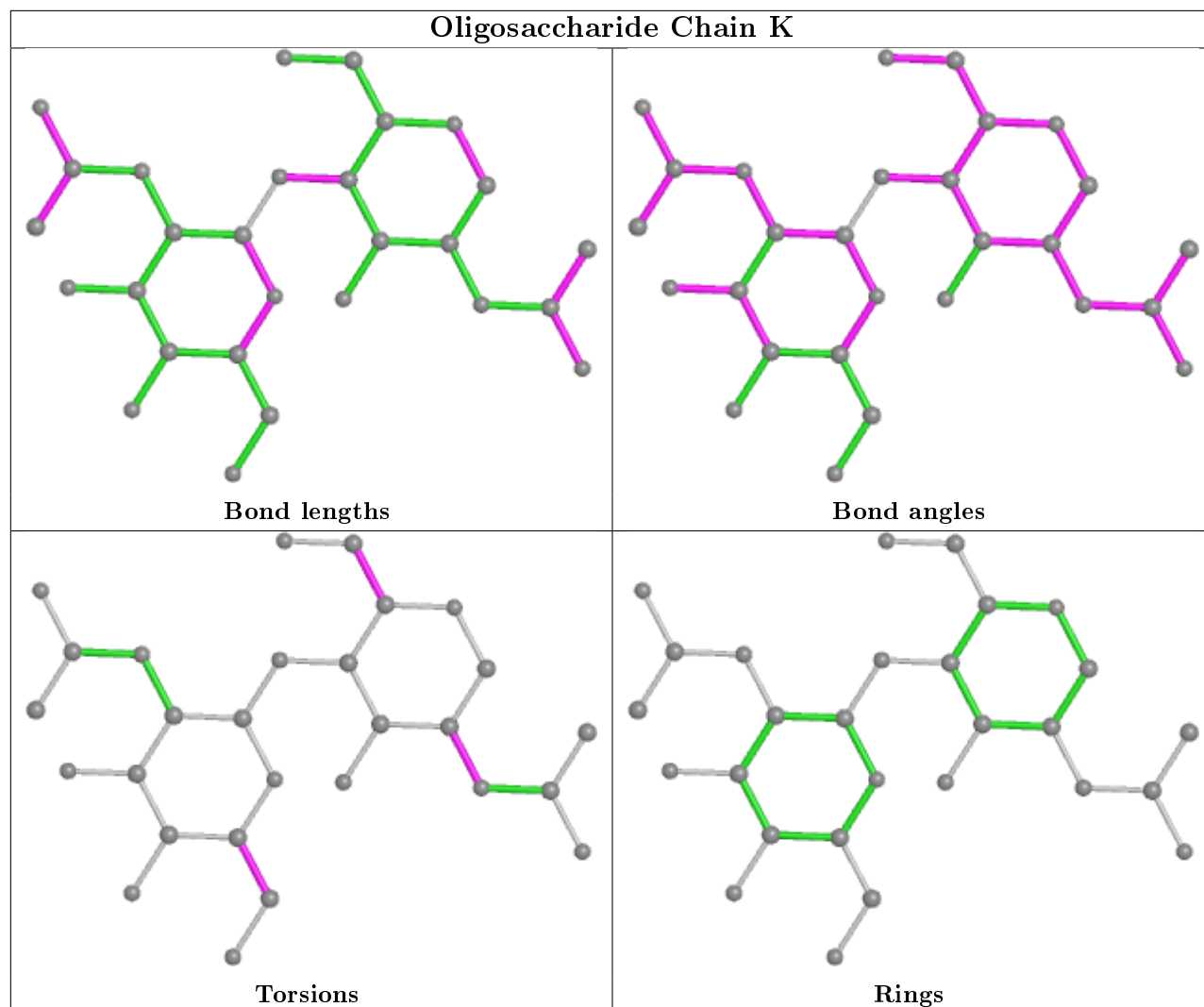
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

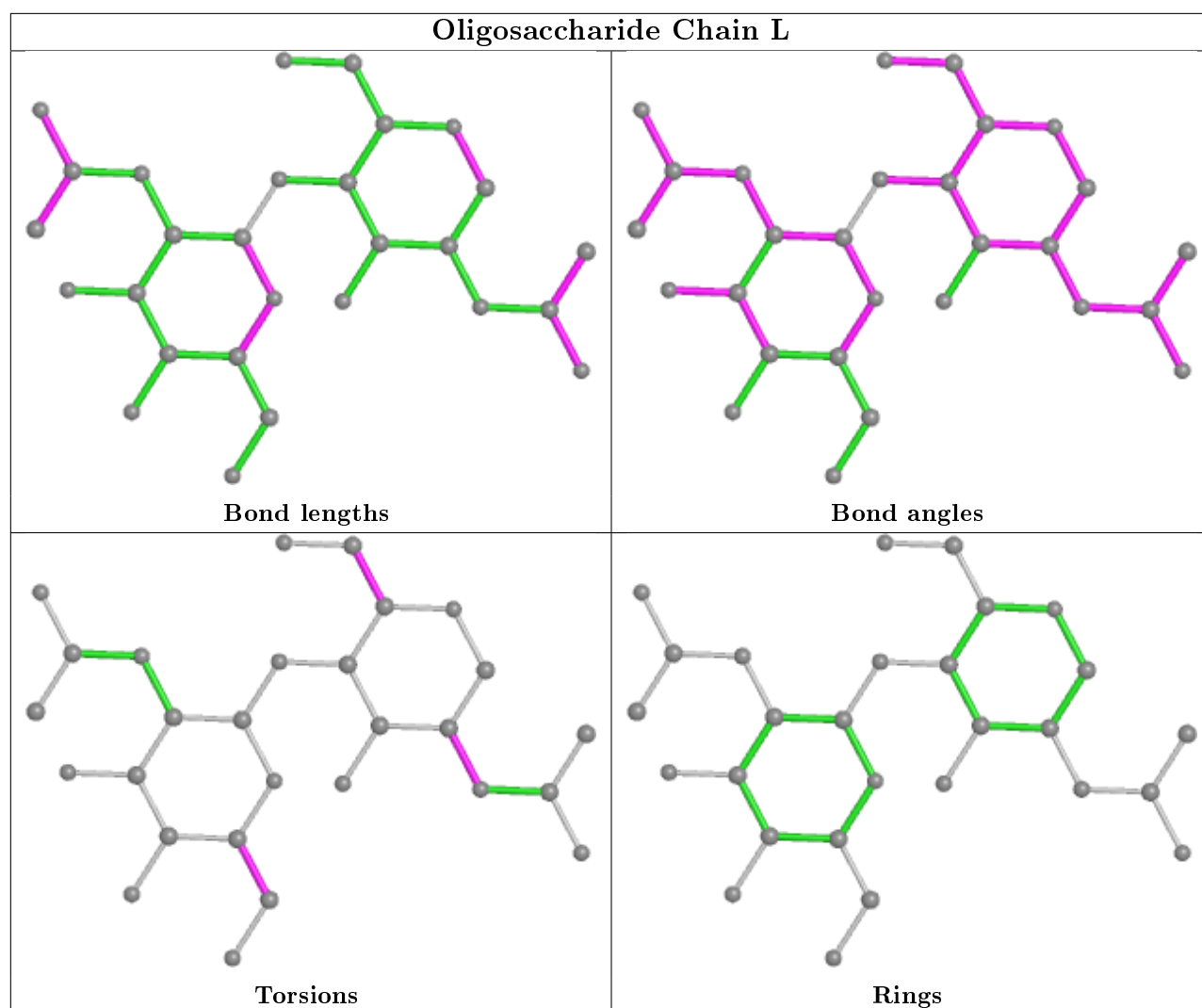












5.6 Ligand geometry [i](#)

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%)	-0.63	5 (0%) 86 78	2, 11, 53, 85	0
1	B	644/657 (98%)	-0.58	4 (0%) 89 83	2, 11, 53, 85	0
1	C	644/657 (98%)	-0.57	6 (0%) 84 75	2, 11, 53, 85	0
1	D	644/657 (98%)	-0.55	8 (1%) 79 67	2, 11, 53, 85	0
1	E	644/657 (98%)	-0.55	6 (0%) 84 75	2, 11, 53, 85	0
1	F	644/657 (98%)	-0.50	7 (1%) 80 69	2, 11, 53, 85	0
All	All	3864/3942 (98%)	-0.56	36 (0%) 84 75	2, 11, 54, 85	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	5.8
1	B	2	ALA	4.3
1	A	3	LEU	4.2
1	F	2	ALA	4.1
1	D	4	GLY	4.0

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

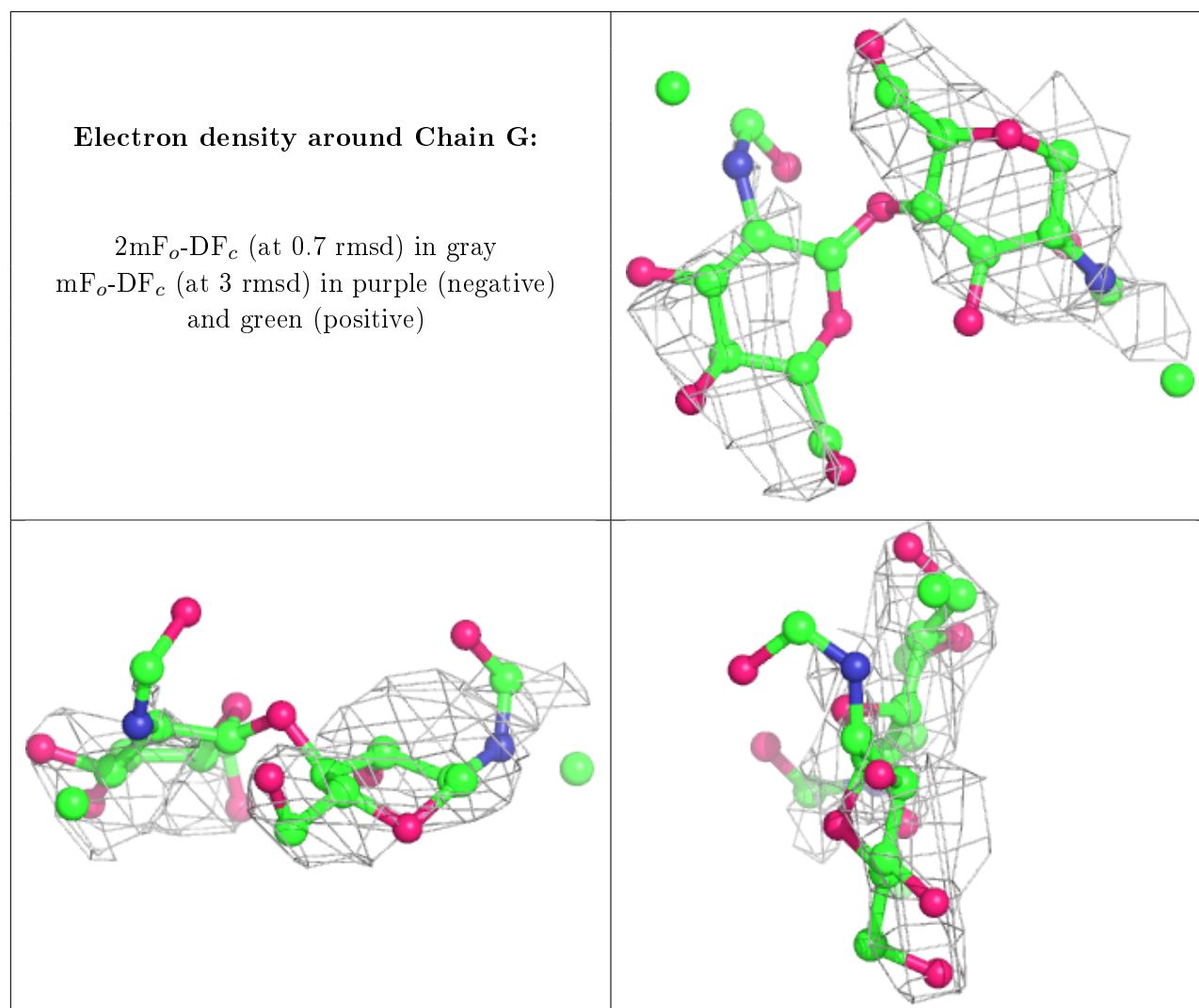
There are no non-standard protein/DNA/RNA residues in this entry.

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.

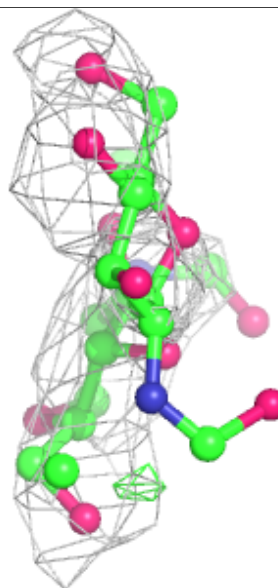
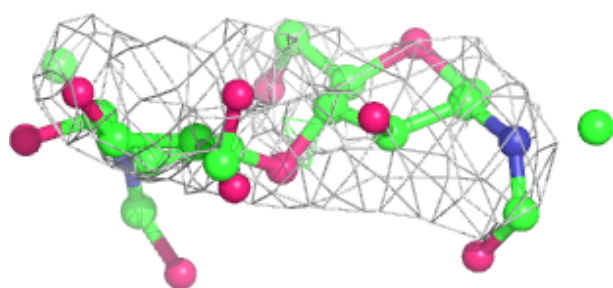
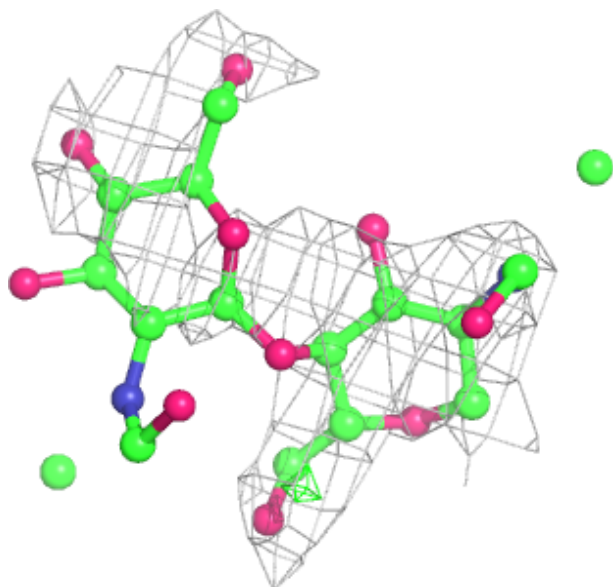
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	I	2	14/15	0.46	0.68	73,82,87,89	0
2	NAG	J	2	14/15	0.48	0.56	73,82,87,89	0
2	NAG	L	2	14/15	0.68	0.47	73,82,87,89	0
2	NAG	H	2	14/15	0.70	0.42	73,82,87,89	0
2	NAG	K	2	14/15	0.71	0.48	73,82,87,89	0
2	NAG	J	1	14/15	0.75	0.36	52,57,68,70	0
2	NAG	G	2	14/15	0.77	0.39	73,82,87,89	0
2	NAG	K	1	14/15	0.78	0.37	52,57,68,70	0
2	NAG	H	1	14/15	0.79	0.33	52,57,68,70	0
2	NAG	I	1	14/15	0.81	0.32	52,57,68,70	0
2	NAG	G	1	14/15	0.81	0.34	52,57,68,70	0
2	NAG	L	1	14/15	0.82	0.33	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.



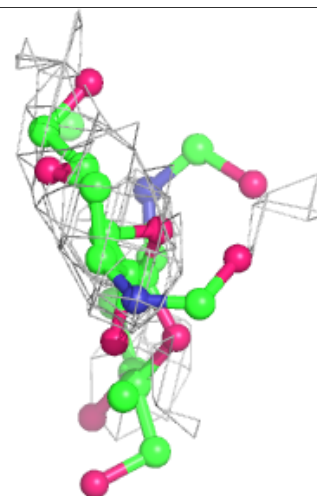
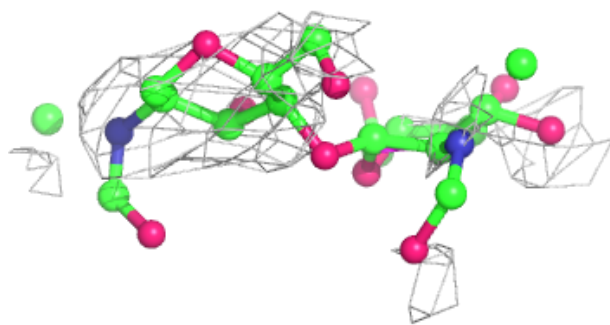
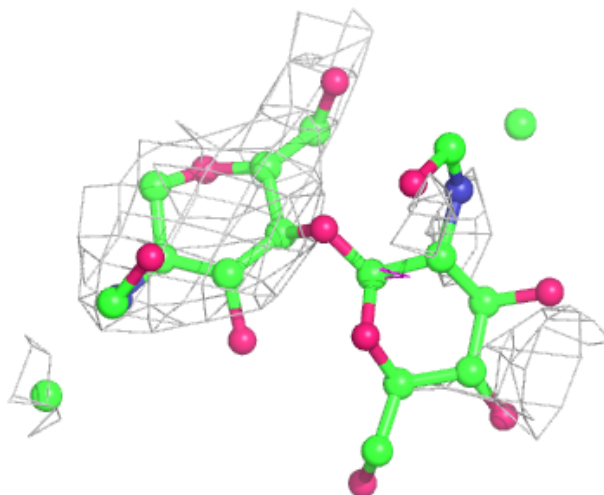
Electron density around Chain H:

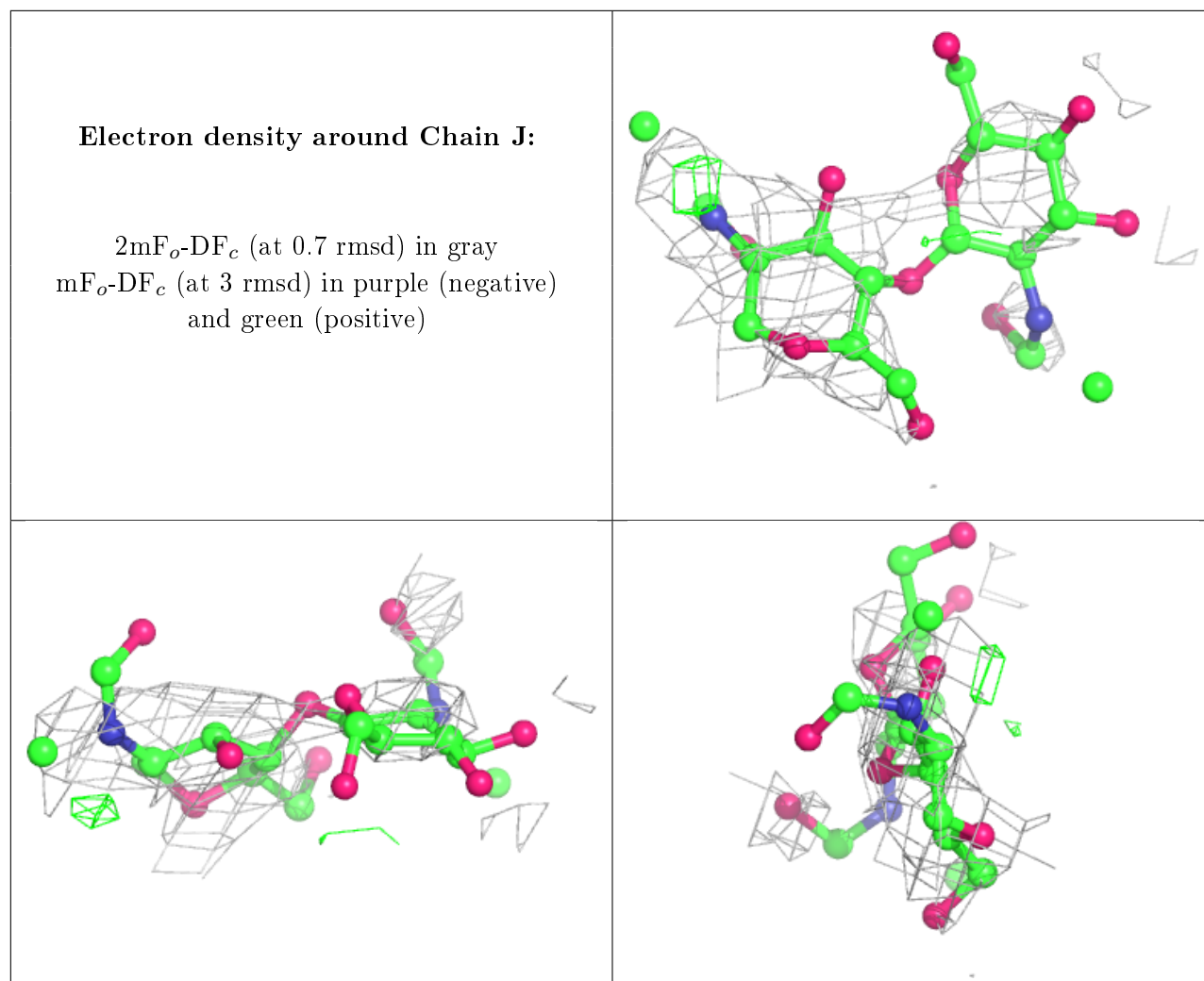
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

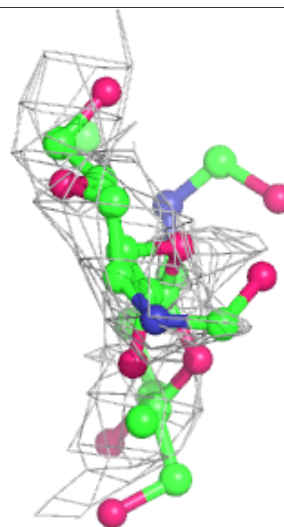
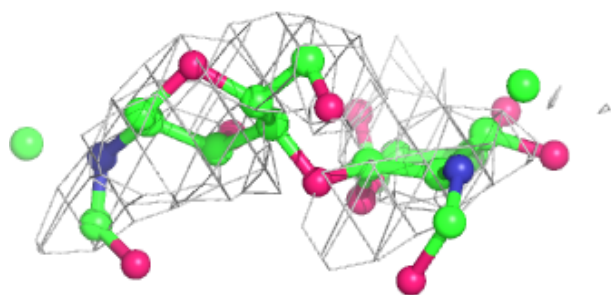
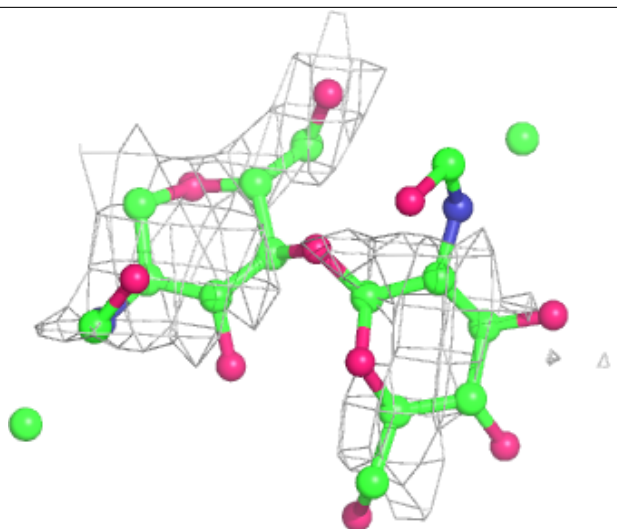
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

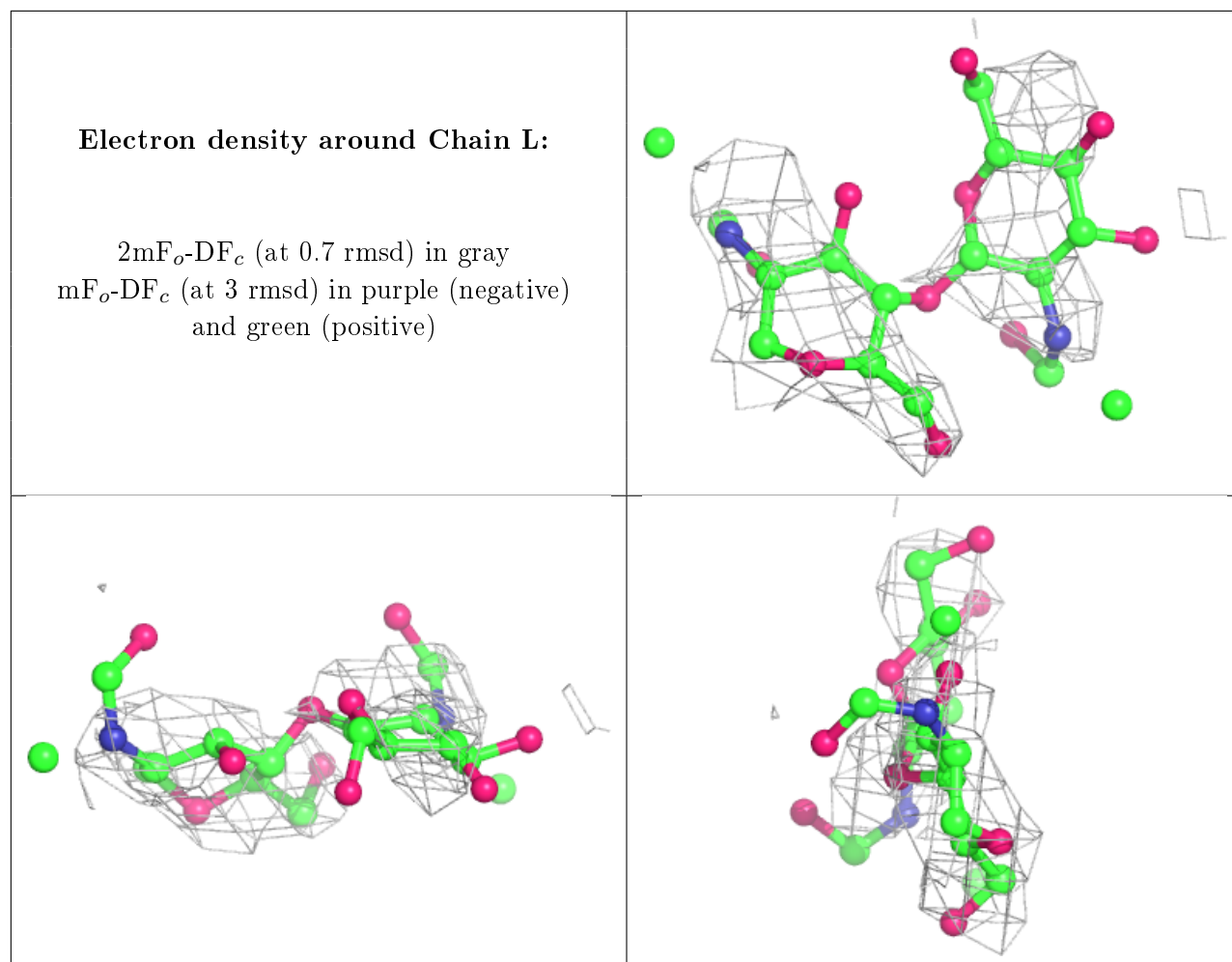




Electron density around Chain K:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
3	CU	A	666	1/1	0.97	0.05	10,10,10,10	0
3	CU	A	665	1/1	0.98	0.06	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.