



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:16 PM EDT

PDB ID : 3CU7 / pdb_00003cu7
Title : Human Complement Component 5
Authors : Fredslund, F.; Andersen, G.R.
Deposited on : 2008-04-16
Resolution : 3.10 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 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

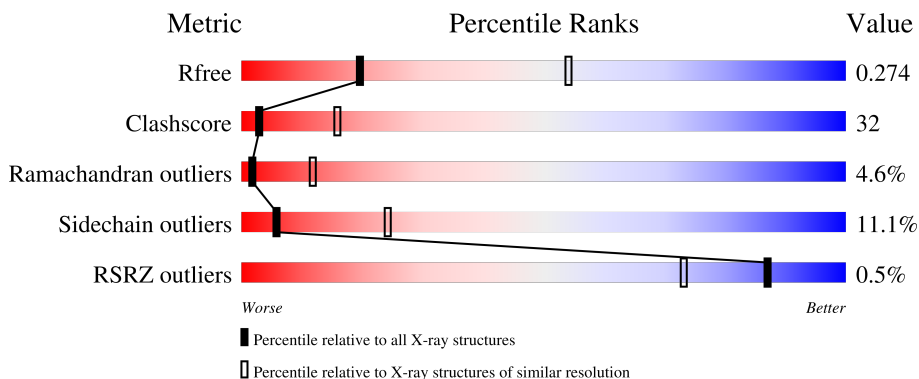
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1676	
1	B	1676	
2	C	2	
2	D	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24655 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1625	12861	8239	2111	2458	53	0	0	0
1	B	1481	11701	7493	1930	2232	46	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ILE	VAL	SEE REMARK 999	UNP P01031
B	802	ILE	VAL	SEE REMARK 999	UNP P01031

- 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cd	0	0
			5	5		
4	B	4	Total	Cd	0	0
			4	4		

P1240	G1151	V991	T916	T844	H773	V694	P619	V542	D468	V307	L224	M149
G1243	I1152	G996	W917	T844	L774	W695	L620	Y543	W469	K308	F227	D150
T1244	F1081	L0000	Y922	W846	W775	K697	E621	F645	H473	E309	I231	D151
R1246	L1085	L1001	K925	W847	E776	D701	Q625	V544	L477	L310	E232	K153
M1247	G1087	H1002	T936	W848	L779	G702	F626	G548	W478	Y313	P233	A155
L1248	Q1088	L1003	L927	W849	W780	W703	G635	E549	W479	S314	F237	K156
E1249	V1089	A1008	R928	T850	F781	G704	G636	E490	E499	E316	Y240	R157
T1250	M1090	K852	W929	W851	R782	W706	A636	T551	N398	D317	Y240	E158
T1251	K1091	K783	R783	W852	R782	W706	G637	T551	N319	E158	K241	V160
A1252	M1092	K784	K784	W853	R783	W706	G638	T551	N319	E158	N242	V160
Y1253	M1093	R854	R785	W854	R784	W706	G639	S556	N483	E158	F243	L161
A1254	M1094	R855	R786	W855	R785	W706	L640	W560	I484	N320	F243	L161
L1255	Q1095	R856	Q787	W856	R786	W706	M641	W560	I485	K321	F243	T162
L1256	V1015	W857	W788	W857	R787	D708	M642	W561	T487	Y322	T249	D165
T1257	V1016	F789	W789	W858	R788	I718	M643	L561	L404	L323	T249	P166
L1258	P1017	R936	A789	W859	R789	G721	A643	N562	L404	L323	I250	P166
S1259	F1019	E937	L790	W860	L790	W729	M644	N563	T411	Y324	K251	W171
L1260	Y1020	S938	T795	W861	T795	W729	V645	E564	R412	V327	A952	D172
M1261	M1021	S940	T796	W862	T796	E730	F646	E565	R412	V328	R253	M173
N1262	F1022	T867	W797	W863	W797	F728	L651	Q570	D414	V329	N257	M173
K1263	Y942	W868	E798	W864	E798	T729	T652	D494	D415	I330	K258	M174
D1264	T943	R868	T799	W865	T799	W729	F653	K495	G416	E331	V259	E175
N1265	L944	R871	I802	W866	I802	E730	L654	I496	V417	S332	V259	E176
Y1266	VAL	W871	G883	W867	G883	C732	T655	I497	A418	T333	T261	D178
V1267	ILE	W872	I804	W868	I804	C732	T656	I498	H498	F336	I267	H179
M1268	ASP	W873	S805	W869	S805	W733	M656	D578	Y499	P351	G270	K189
P1269	HIS	W874	N806	W870	N806	W733	M657	A579	L504	N355	I271	I190
Y1193	GLN	W875	T807	W871	T807	A579	M658	A579	L504	L342	R272	P191
S1196	GLY	W876	G808	W872	G808	W733	M659	A579	L504	I342	E273	S192
K1200	THR	W877	R809	W873	R809	L738	D660	D660	K508	Y347	V265	M193
L1201	LYS	W878	C810	W874	C810	R738	D661	S583	I509	S350	Y266	P194
H1202	SER	W879	W811	W875	W811	R738	S584	P584	I509	P351	I267	R196
P1203	ARG	W880	T814	W876	T814	I742	G663	Q585	T514	N355	L267	K189
Q1204	ARG	W881	R818	W877	R818	S743	G664	Q586	A521	L431	I271	I190
F1205	THR	W882	R819	W878	R819	HIS	G665	Q587	S522	P443	R272	P191
R1206	THR	W883	F820	W879	F820	LYS	G666	Q588	S522	N446	E273	S192
S1207	THR	W884	R821	W880	R821	ASP	G667	Q589	S522	N446	D274	M193
W1208	THR	W885	R822	W881	R822	MET	G668	S589	A521	N446	D274	P194
S1210	THR	W886	R823	W882	R823	GLN	G669	S589	S522	N446	D274	P194
K1213	THR	W887	R824	W883	R824	L752	G670	S589	S522	N446	D274	P194
D1289	THR	W888	R825	W884	R825	H753	ARG	S589	S522	N446	D274	P194
T1287	THR	W889	R826	W885	R826	THR	ARG	S589	S522	N446	D274	P194
Q1288	THR	W890	R827	W886	R827	THR	ARG	S589	S522	N446	D274	P194
I1294	THR	W891	R828	W887	R828	THR	ARG	S589	S522	N446	D274	P194
L1291	THR	W892	R829	W888	R829	THR	ARG	S589	S522	N446	D274	P194
M1292	THR	W893	R830	W889	R830	THR	ARG	S589	S522	N446	D274	P194
I1293	THR	W894	R831	W890	R831	THR	ARG	S589	S522	N446	D274	P194
Y1295	THR	W895	R832	W891	R832	THR	ARG	S589	S522	N446	D274	P194
G1283	THR	W896	R833	W892	R833	THR	ARG	S589	S522	N446	D274	P194
F1284	THR	W897	R834	W893	R834	THR	ARG	S589	S522	N446	D274	P194
Y1285	THR	W898	R835	W894	R835	THR	ARG	S589	S522	N446	D274	P194
S1286	THR	W899	R836	W895	R836	THR	ARG	S589	S522	N446	D274	P194
T1287	THR	W900	R837	W896	R837	THR	ARG	S589	S522	N446	D274	P194
Q1288	THR	W901	R838	W897	R838	THR	ARG	S589	S522	N446	D274	P194
D1289	THR	W902	R839	W898	R839	THR	ARG	S589	S522	N446	D274	P194
T1290	THR	W903	R840	W899	R840	THR	ARG	S589	S522	N446	D274	P194
I1291	THR	W904	R841	W900	R841	THR	ARG	S589	S522	N446	D274	P194
M1292	THR	W905	R842	W901	R842	THR	ARG	S589	S522	N446	D274	P194
N1293	THR	W906	R843	W902	R843	THR	ARG	S589	S522	N446	D274	P194
I1294	THR	W907	R844	W903	R844	THR	ARG	S589	S522	N446	D274	P194
G1295	THR	W908	R845	W904	R845	THR	ARG	S589	S522	N446	D274	P194
L1295	THR	W909	R846	W905	R846	THR	ARG	S589	S522	N446	D274	P194
G1296	THR	W910	R847	W906	R847	THR	ARG	S589	S522	N446	D274	P194
L1297	THR	W911	R848	W907	R848	THR	ARG	S589	S522	N446	D274	P194
T1298	THR	W912	R849	W908	R849	THR	ARG	S589	S522	N446	D274	P194
E1299	THR	W913	R850	W909	R850	THR	ARG	S589	S522	N446	D274	P194
Y1300	THR	W914	R851	W910	R851	THR	ARG	S589	S522	N446	D274	P194
D1236	THR	W915	R852	W911	R852	THR	ARG	S589	S522	N446	D274	P194
K206	K206	K206	K206	K206	K206	K206	K206	K206	K206	K206	K206	K206
E207	E207	E207	E207	E207	E207	E207	E207	E207	E207	E207	E207	E207
D208	D208	D208	D208	D208	D208	D208	D208	D208	D208	D208	D208	D208
F209	F209	F209	F209	F209	F209	F209	F209	F209	F209	F209	F209	F209
S210	S210	S210	S210	S210	S210	S210	S210	S210	S210	S210	S210	S210
T211	T211	T211	T211	T211	T211	T211	T211	T211	T211	T211	T211	T211
M289	M289	M289	M289	M289	M289	M289	M289	M289	M289	M289	M289	M289
T214	T214	T214	T214	T214	T214	T214	T214	T214	T214	T214	T214	T214
A215	A215	A215	A215	A215	A215	A215	A215	A215	A215	A215	A215	A215
Y216	Y216	Y216	Y216	Y216	Y216	Y216	Y216	Y216	Y216	Y216	Y216	Y216
I293	I293	I293	I293	I293	I293	I293	I293	I293	I293	I293	I293	I293
V219	V219	V219	V219	V219	V219	V219	V219	V219	V219	V219	V219	V219
K220	K220	K220	K220	K220	K220	K220	K220	K220	K220	K220	K220	K220
E221	E221	E221	E221	E221	E221	E221	E221	E221	E221	E221	E221	E221
Y222	Y222	Y222	Y222	Y222	Y222	Y222	Y222	Y222	Y222	Y222	Y222	Y222
V299	V299	V299	V299	V299	V299	V299	V299	V299	V299	V299	V299	V299
L379	L379	L379	L379	L379	L379	L379	L379	L379	L379	L379	L379	L379

4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.26Å 144.26Å 241.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.29 – 3.10 29.29 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.29-3.10) 97.4 (29.29-3.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.11Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.236 , 0.281 0.231 , 0.274	Depositor DCC
R_{free} test set	5010 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 135.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.008 for -h,-k,l 0.468 for h,-h-k,-l 0.009 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24655	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CD, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/13137	0.79	15/17820 (0.1%)
1	B	0.32	0/11954	0.78	12/16219 (0.1%)
All	All	0.32	0/25091	0.78	27/34039 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	LEU	CA-C-N	8.98	129.03	119.78
1	A	1003	LEU	C-N-CA	8.98	129.03	119.78
1	B	1003	LEU	CA-C-N	8.92	128.97	119.78
1	B	1003	LEU	C-N-CA	8.92	128.97	119.78
1	B	934	VAL	N-CA-C	7.85	117.60	106.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12861	0	12817	846	0
1	B	11701	0	11669	752	0
2	C	28	0	25	2	0
2	D	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
All	All	24655	0	24562	1587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

The worst 5 of 1587 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:A:1538:GLU:HG2	1:A:1539:LEU:HG	1.31	1.12
1:A:253:ARG:HH22	1:A:257:ASN:HA	1.13	1.11
1:B:253:ARG:HH22	1:B:257:ASN:HA	1.12	1.10
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	1.30	1.08
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	1.31	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1615/1676 (96%)	1282 (79%)	257 (16%)	76 (5%)	2	11
1	B	1471/1676 (88%)	1191 (81%)	214 (14%)	66 (4%)	2	12
All	All	3086/3352 (92%)	2473 (80%)	471 (15%)	142 (5%)	2	12

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	A	261	THR
1	A	308	LYS
1	A	336	PHE
1	A	490	SER

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	1441/1484 (97%)	1282 (89%)	159 (11%)	6	24
1	B	1314/1484 (88%)	1168 (89%)	146 (11%)	6	24
All	All	2755/2968 (93%)	2450 (89%)	305 (11%)	6	24

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	814	THR
1	B	1363	THR
1	B	894	HIS
1	B	1067	SER
1	B	1502	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	656	ASN
1	B	1130	GLN
1	B	706	ASN
1	B	1029	ASN
1	B	1221	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](#)

4 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	C	1	2,1	14,14,15	0.51	0	17,19,21	0.73	0
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.50	0	17,19,21	0.73	0
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	0.82	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	2.26	115.22	112.19
2	D	2	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

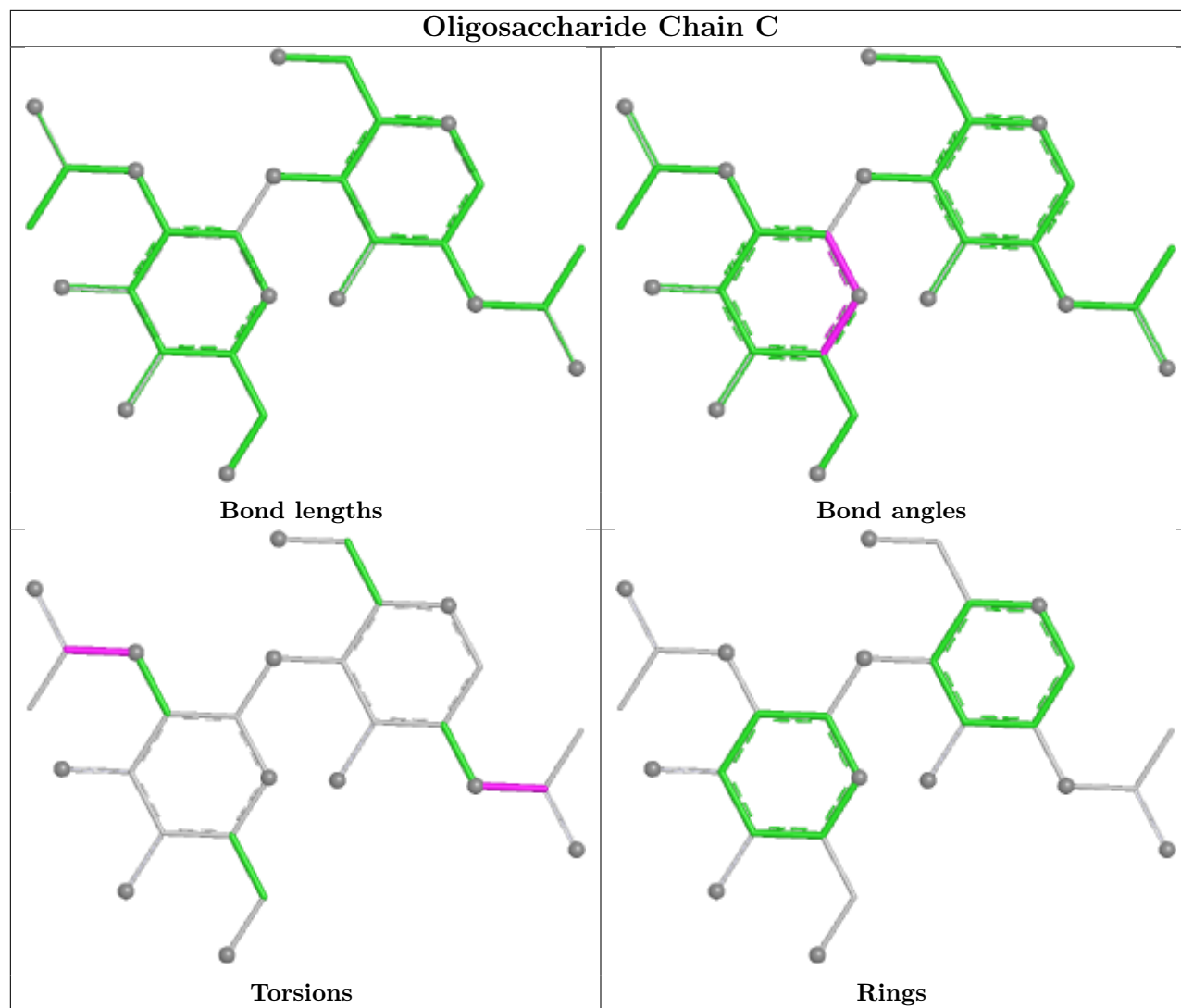
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2

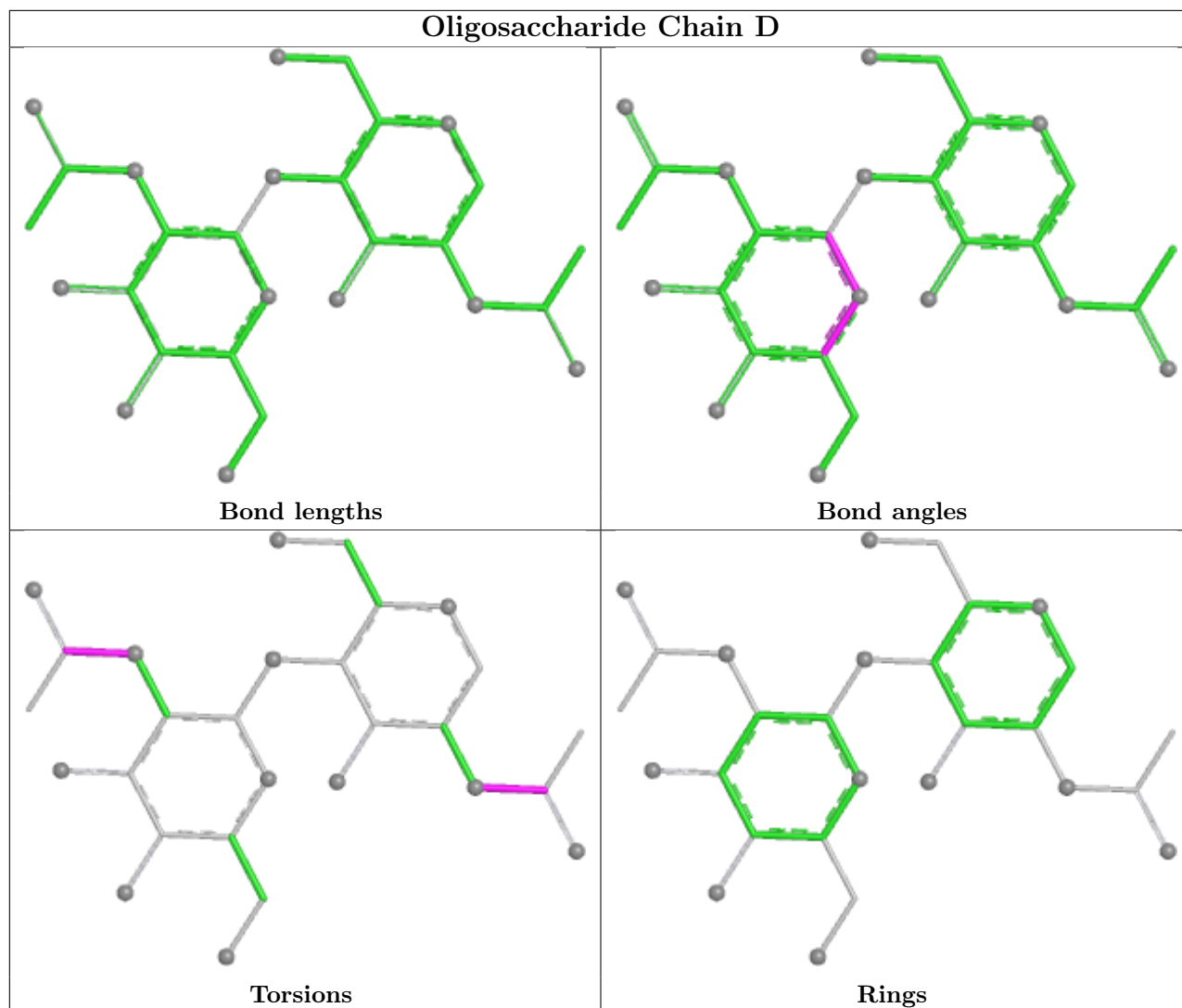
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	C	1	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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	2003	1	14,14,15	0.58	0	17,19,21	0.93	1 (5%)
3	NAG	B	2003	1	14,14,15	0.61	0	17,19,21	1.09	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	NAG	O5-C1-C2	2.73	115.52	111.29
3	A	2003	NAG	O5-C1-C2	2.10	114.54	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	B	2003	NAG	C8-C7-N2-C2
3	B	2003	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	1625/1676 (96%)	-0.31	10 (0%) 85 70	73, 136, 224, 290	0
1	B	1481/1676 (88%)	-0.37	4 (0%) 90 80	75, 131, 205, 267	0
All	All	3106/3352 (92%)	-0.34	14 (0%) 87 73	73, 133, 215, 290	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1655	SER	4.0
1	B	77	ASN	2.6
1	A	1643	THR	2.6
1	A	81	ASN	2.4
1	B	62	LYS	2.4

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

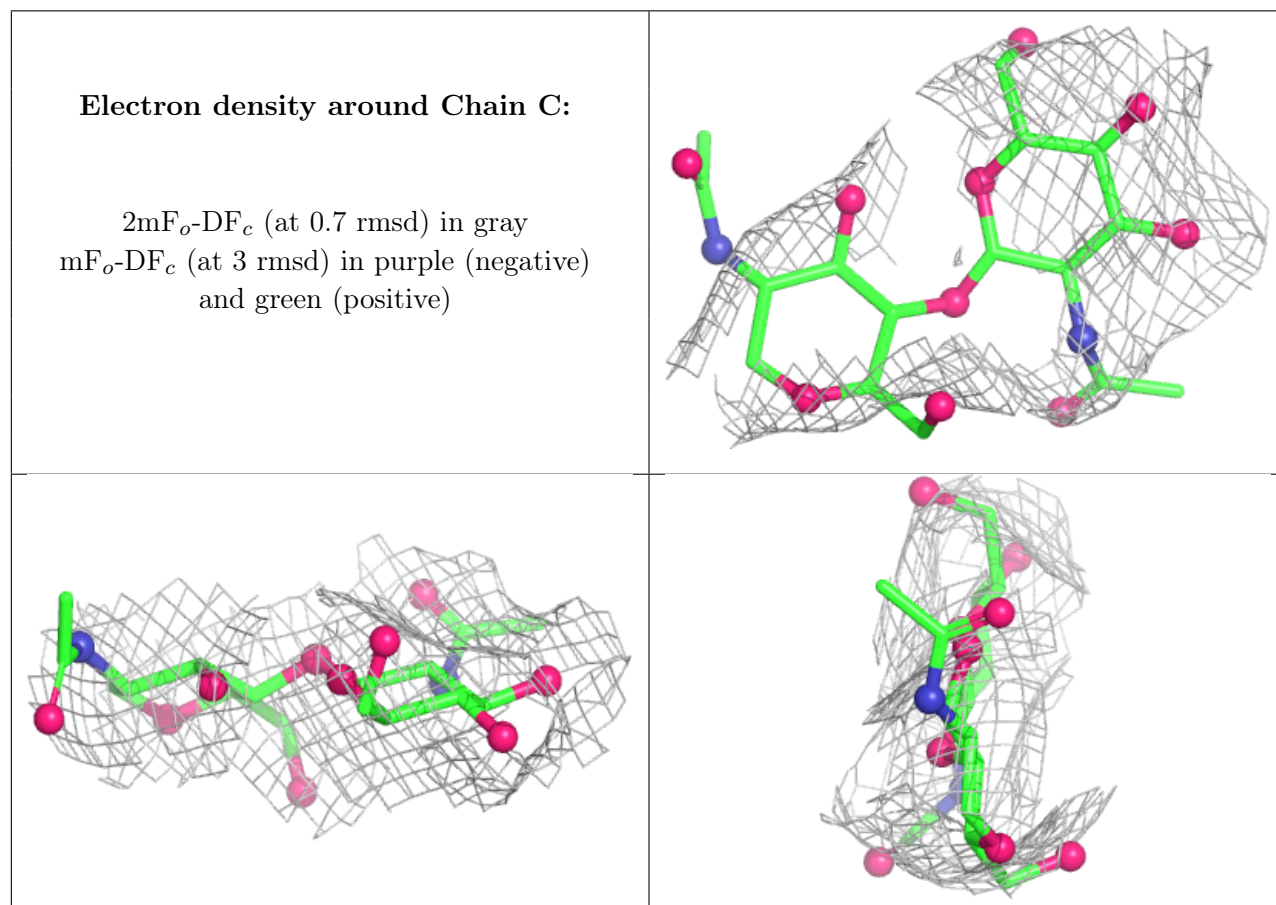
There are no non-standard protein/DNA/RNA residues in this entry.

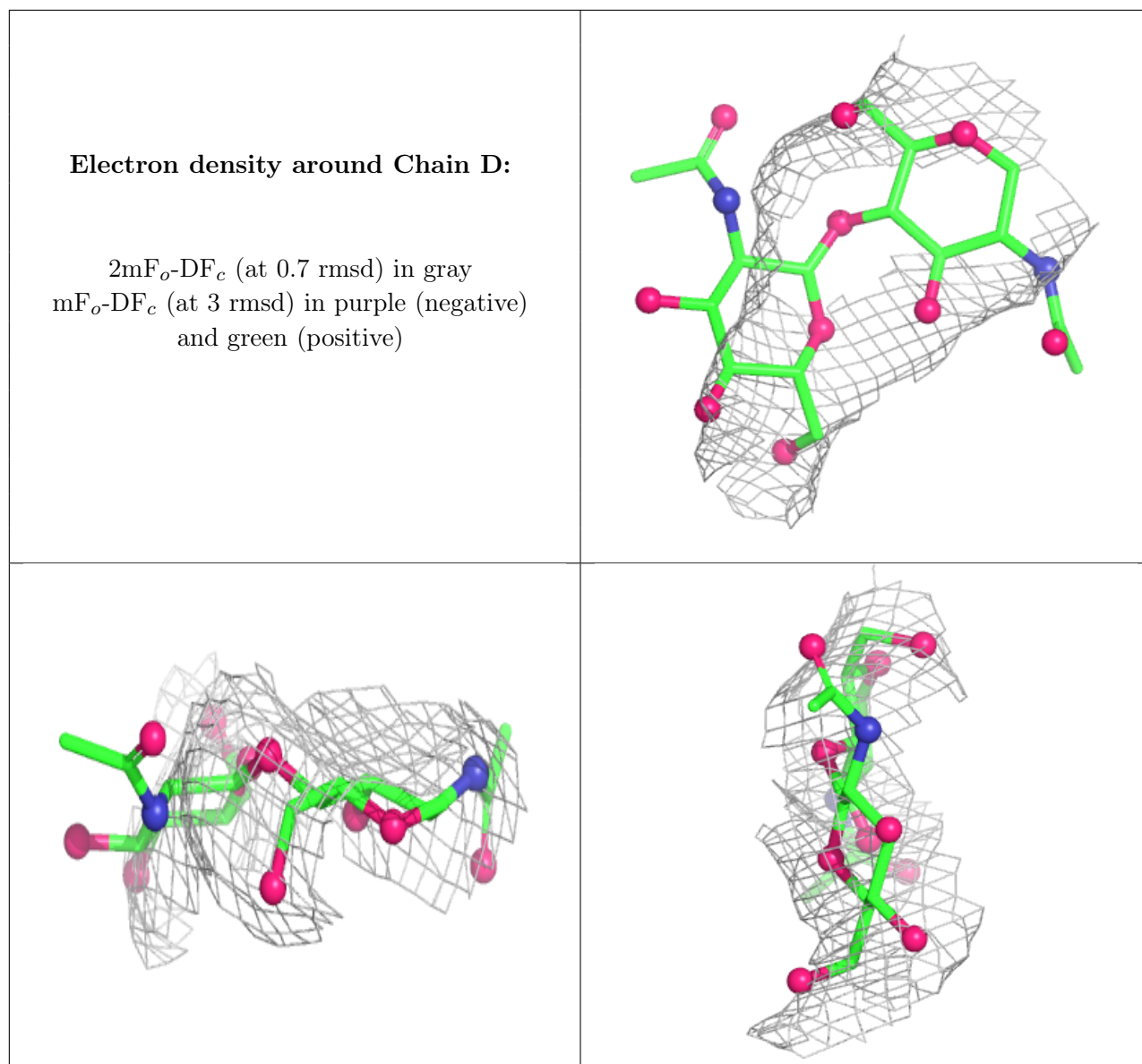
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.90	0.09	249,258,261,262	0
2	NAG	D	2	14/15	0.93	0.09	251,259,262,262	0
2	NAG	C	1	14/15	0.96	0.11	257,259,270,271	0
2	NAG	D	1	14/15	0.97	0.09	263,269,274,275	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.





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	NAG	B	2003	14/15	0.93	0.09	246,252,259,262	0
3	NAG	A	2003	14/15	0.94	0.07	215,223,233,237	0
4	CD	A	2008	1/1	0.96	0.06	282,282,282,282	0
4	CD	A	2007	1/1	0.97	0.04	184,184,184,184	0
4	CD	A	2004	1/1	0.98	0.05	123,123,123,123	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CD	B	2005	1/1	0.98	0.03	181,181,181,181	0
4	CD	B	2007	1/1	0.98	0.04	264,264,264,264	0
4	CD	B	2004	1/1	0.99	0.04	239,239,239,239	0
4	CD	A	2005	1/1	0.99	0.03	243,243,243,243	0
4	CD	B	2006	1/1	0.99	0.05	183,183,183,183	0
4	CD	A	2006	1/1	0.99	0.02	189,189,189,189	0

6.5 Other polymers [i](#)

There are no such residues in this entry.