



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 04:59 AM JST

PDB ID : 5AW9 / pdb_00005aw9
Title : Kinetics by X-ray crystallography: native E2.MgF42-.2K+ crystal for Rb+ bound crystals
Authors : Ogawa, H.; Cornelius, F.; Hirata, A.; Toyoshima, C.
Deposited on : 2015-07-01
Resolution : 2.80 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

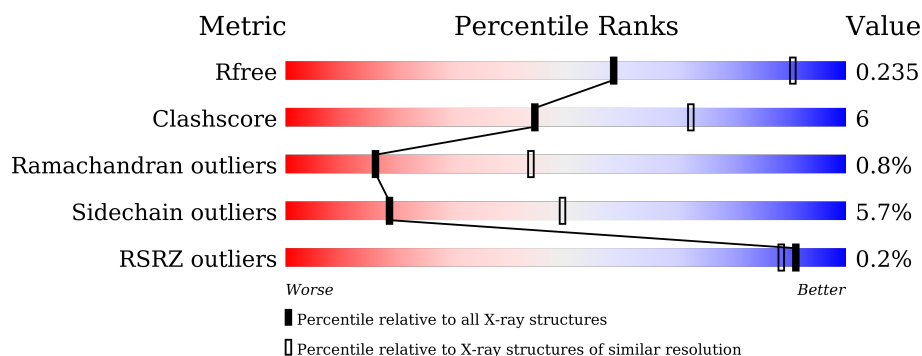
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1028	
2	B	305	
3	G	74	
4	C	2	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10362 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 Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	992	Total	C	N	O	S	0	0	0
			7675	4886	1290	1453	46			

- Molecule 2 is a protein called Na⁺,K⁺-ATPase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	268	Total	C	N	O	S	0	0	0
			2174	1409	358	396	11			

- Molecule 3 is a protein called Phospholemman-like protein.

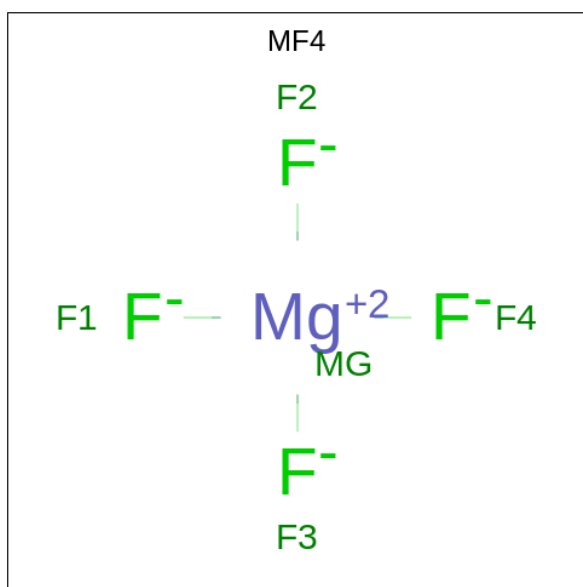
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	39	Total	C	N	O	S	0	0	0
			305	200	50	54	1			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is TETRAFLUOROMAGNESATE(2-) (CCD ID: MF4) (formula: F₄Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	F	Mg	0	0
			5	4	1		

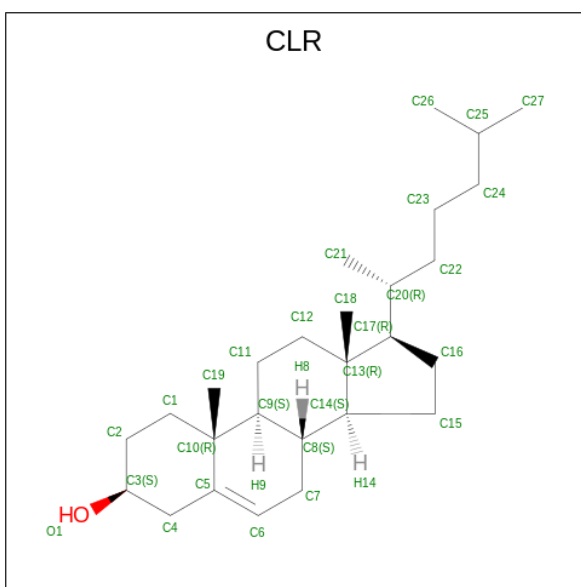
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

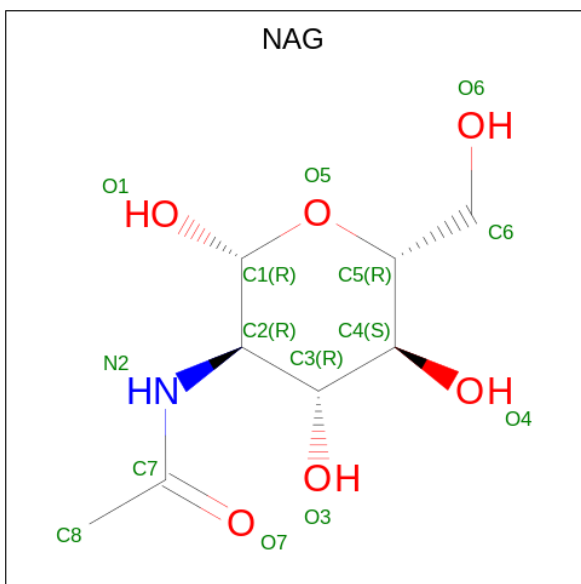
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	K	0	0
			3	3		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	129	Total 129	O 129	0	0

- Molecule 1: Na, K-ATPase alpha subunit

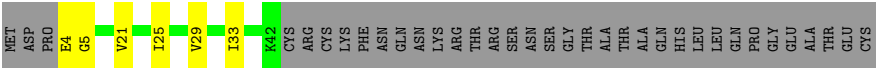
Y929	K727	L530	L361	T239	P87	MET
D933	A728	K531	E365	S246		GLY
L934		M534	E365	S246	I90	LYS
I935	V741			T247		GLY
I936			W392	N248	C93	THR
	A746	F571		C249		ALA
	D747		T417	V250	L96	SER
R940	N748	P576	W418	E251		ASP
I944	I758	T580	R423	G252	L103	THR
		T581	I424	T253		LYS
L968	E763		A425	A254	I106	GLU
		G587	A426	R255		P80
T974	R766	L588	L427		L110	ALA
L983	L780	M589	A431	T260		ALA
K984		I592		R264	T121	THR
	N783	M593	Q434		E122	SER
Y987	I784	P594		N267	D123	GLU
	R785	P596	W440			ASN
Y994		R596		I270	D128	ALA
	T806		R445		Y131	THR
I997		V599		S275		LYS
	M816		S454			LYS
G1014	V817	V616		I284	L136	LYS
	P818	T617	L457			GLY
Q1019	A819	G618		F291	V140	LYS
	I820	D619	C463	I294	S160	LYS
	S821	H620		T295		ASP
Y1023	L822	P621	R471	T296	V165	LYS
						ILE
	M832	V631	P475		L170	LYS
	K833	G632		F301		ASP
		L633	V478		D174	LYS
	V845	L670	M483	V304		ARG
I846				S305	L190	
E847		T675			V191	L32
R848		E876	M486	T308	E192	
		V677	E494	L309		D42
	V854	L678		L318	D202	
			K497		I263	L46
F866		L682	S496	F323	R204	
S868			S499	L394	I205	L51
Y869		R692			I206	H52
	F870		R502	I327		
V871		P695	Y503		H209	T57
I872		Q696				D58
			W506	T339	K212	L59
	K886			L344	V213	T60
			L515	T345	E223	R61
	R889	V702	D516			L63
			R517	M351	T226	T64
						M65
Q905		V712	L522	K384	P229	A66
		A713	L523	N355	E230	
S921			M524	C356	F231	L72
S925		V719			P236	N78
I926		V726	E528	K359		

- Molecule 2: Na⁺,K⁺-ATPase beta subunit

LEU	ASP	ASP	THR	TYR	G169	A171	K174	P175	C176		N182	Y188	K193	N194	E200	E201		N207	Q208	Y209		P212	L213		A217	LYS	ARG	GLU	GLU	ASP	R223	I226	G227		F232		L242		R251		L261	A262	I263		N267	L268	T269	Q270	N271		C278			
ALA	ALA	GLY	LVS	SER	LVS	THR	GLY	GLY	TRP	LVS	PHE	LEU	TRP	ASP	SER	GLU	LVS	LVS	GLU	F25	R28		W33		I52		L58		V73	A74	P75		H80		M106	H107	K108	L109	M110	D111		S122	P123		I135		D139		L157	K158	N159	C160	SER	GLY



- Molecule 3: Phospholemman-like protein



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.97Å 50.67Å 163.07Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.9 (15.00-2.80) 92.9 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.217 , 0.265 0.221 , 0.235	Depositor DCC
R_{free} test set	2063 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10362	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: K, MG, CLR, NAG, MF4

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	0.61	0/7825	1.02	3/10616 (0.0%)
2	B	0.61	0/2229	0.95	4/3002 (0.1%)
3	G	0.64	0/309	1.04	0/419
All	All	0.61	0/10363	1.01	7/14037 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASP	N-CA-C	7.61	119.59	108.86
2	B	174	LYS	CA-C-N	6.59	126.97	119.92
2	B	174	LYS	C-N-CA	6.59	126.97	119.92
2	B	74	ALA	CA-C-N	-5.72	114.48	120.38
2	B	74	ALA	C-N-CA	-5.72	114.48	120.38

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	7675	0	7699	96	0
2	B	2174	0	2146	28	0
3	G	305	0	318	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	25	0	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	A	3	0	0	0	0
8	B	28	0	46	0	0
9	B	14	0	13	0	0
10	A	129	0	0	3	0
All	All	10362	0	10247	123	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 6.

The worst 5 of 123 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)
2:B:74:ALA:HB3	2:B:75:PRO:HD3	1.69	0.75
1:A:677:VAL:HG21	10:A:2222:HOH:O	1.89	0.73
1:A:935:ILE:HG23	1:A:944:ILE:HD12	1.72	0.71
1:A:425:ALA:HB2	1:A:589:MET:HE1	1.70	0.71
1:A:61:ARG:HH11	1:A:61:ARG:HB3	1.55	0.70

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	990/1028 (96%)	942 (95%)	42 (4%)	6 (1%)	21 51
2	B	262/305 (86%)	227 (87%)	32 (12%)	3 (1%)	11 36
3	G	37/74 (50%)	32 (86%)	4 (11%)	1 (3%)	4 15
All	All	1289/1407 (92%)	1201 (93%)	78 (6%)	10 (1%)	16 44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	74	ALA
1	A	524	ASN
2	B	201	GLU
1	A	121	THR
1	A	128	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	840/869 (97%)	792 (94%)	48 (6%)	18	49
2	B	234/266 (88%)	220 (94%)	14 (6%)	17	47
3	G	32/62 (52%)	31 (97%)	1 (3%)	35	70
All	All	1106/1197 (92%)	1043 (94%)	63 (6%)	18	49

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	530	LEU
2	B	194	ASN
1	A	719	VAL
2	B	176	CYS
2	B	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	207	ASN
2	B	284	ASN
2	B	271	ASN
1	A	754	ASN
2	B	194	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 ⓘ

2 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
4	NAG	C	1	4,2	14,14,15	0.58	0	17,19,21	1.60	1 (5%)
4	NAG	C	2	4	14,14,15	0.85	1 (7%)	17,19,21	1.98	3 (17%)

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
4	NAG	C	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2	NAG	C1-C2	2.21	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	5.75	119.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	C2-N2-C7	5.30	130.45	122.90
4	C	2	NAG	C1-O5-C5	4.23	117.93	112.19
4	C	2	NAG	C1-C2-N2	2.30	114.42	110.49

There are no chirality outliers.

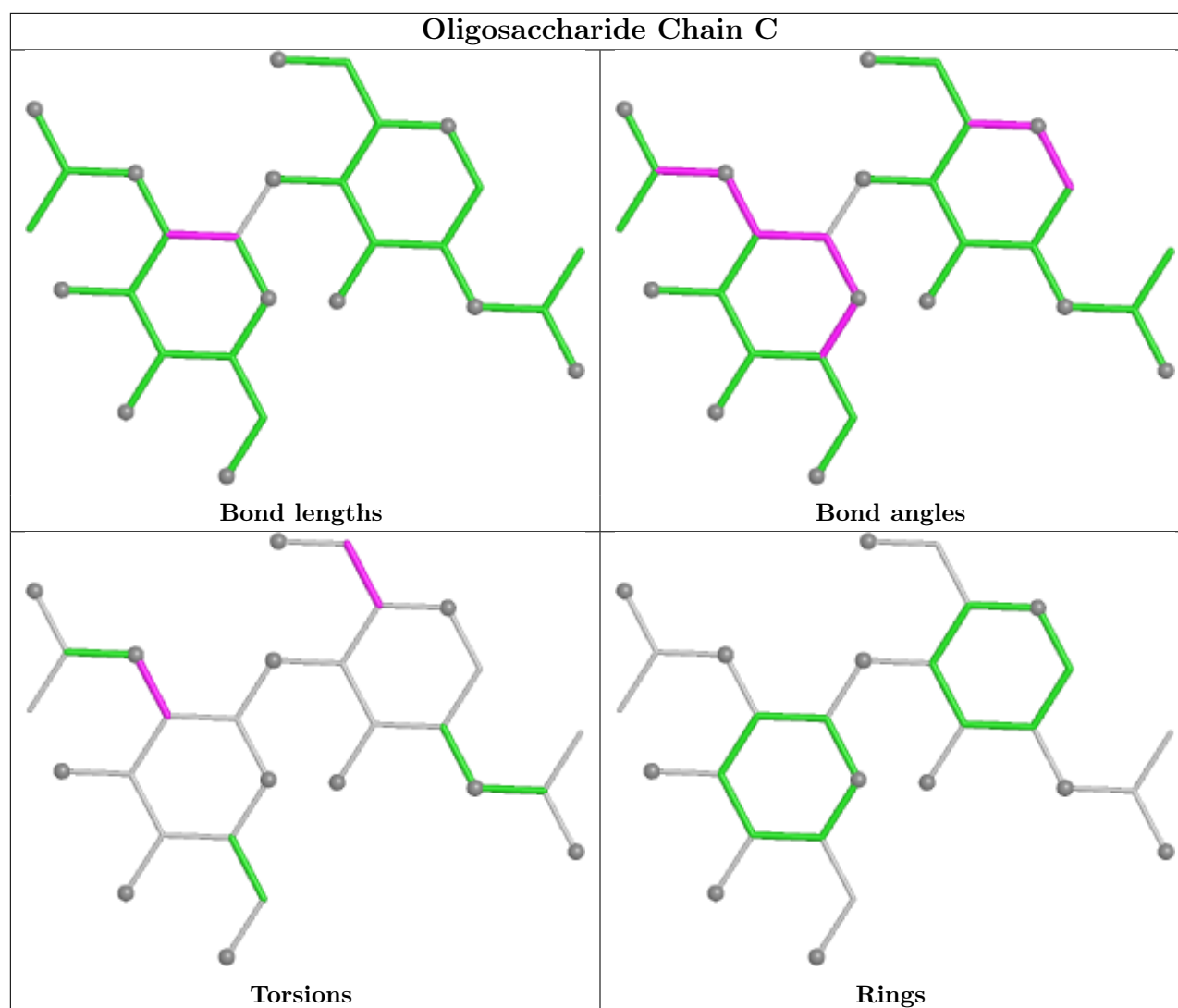
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
8	CLR	B	3001	-	31,31,31	0.80	0	48,48,48	1.46	9 (18%)
5	MF4	A	2001	1	0,4,4	-	-	-		
9	NAG	B	4021	2	14,14,15	0.77	0	17,19,21	1.14	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
8	CLR	B	3001	-	-	2/10/68/68	0/4/4/4
9	NAG	B	4021	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3001	CLR	C1-C2-C3	4.29	115.98	110.47
8	B	3001	CLR	C4-C5-C10	3.81	121.48	116.42
8	B	3001	CLR	C4-C5-C6	-3.11	116.13	120.61
8	B	3001	CLR	C16-C17-C13	2.69	107.08	103.84
9	B	4021	NAG	C1-O5-C5	2.57	115.68	112.19

There are no chirality outliers.

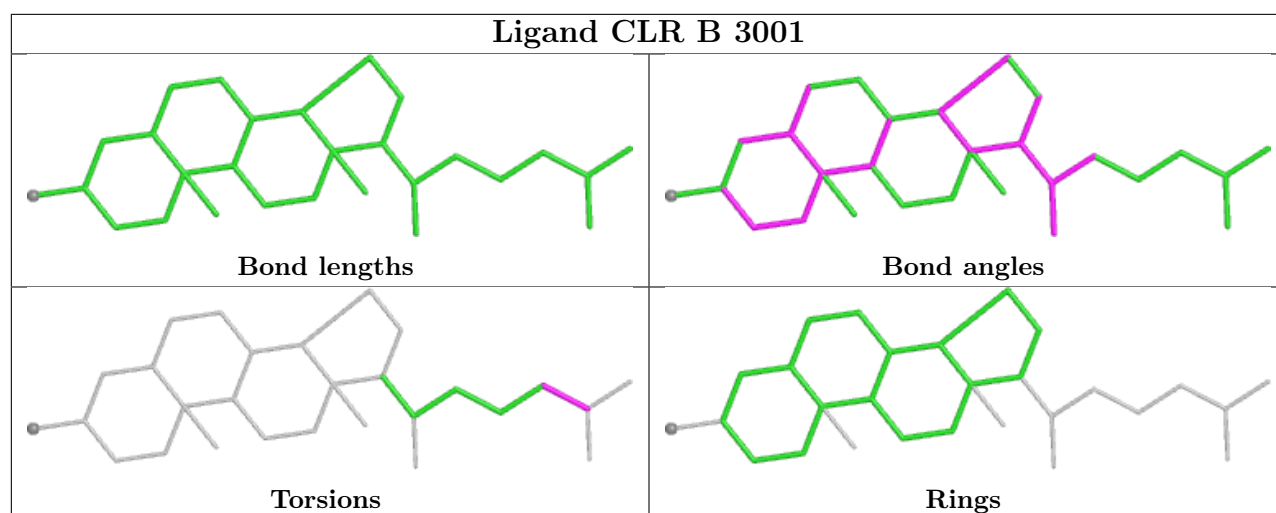
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	3001	CLR	C23-C24-C25-C26
8	B	3001	CLR	C23-C24-C25-C27

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	992/1028 (96%)	-0.56	2 (0%) 91 88	46, 77, 133, 193	0
2	B	268/305 (87%)	-0.10	1 (0%) 88 84	63, 123, 159, 173	0
3	G	39/74 (52%)	-0.51	0 100 100	63, 75, 136, 153	0
All	All	1299/1407 (92%)	-0.46	3 (0%) 91 88	46, 84, 149, 193	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	268	LEU	2.9
1	A	231	PHE	2.6
1	A	1023	TYR	2.1

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

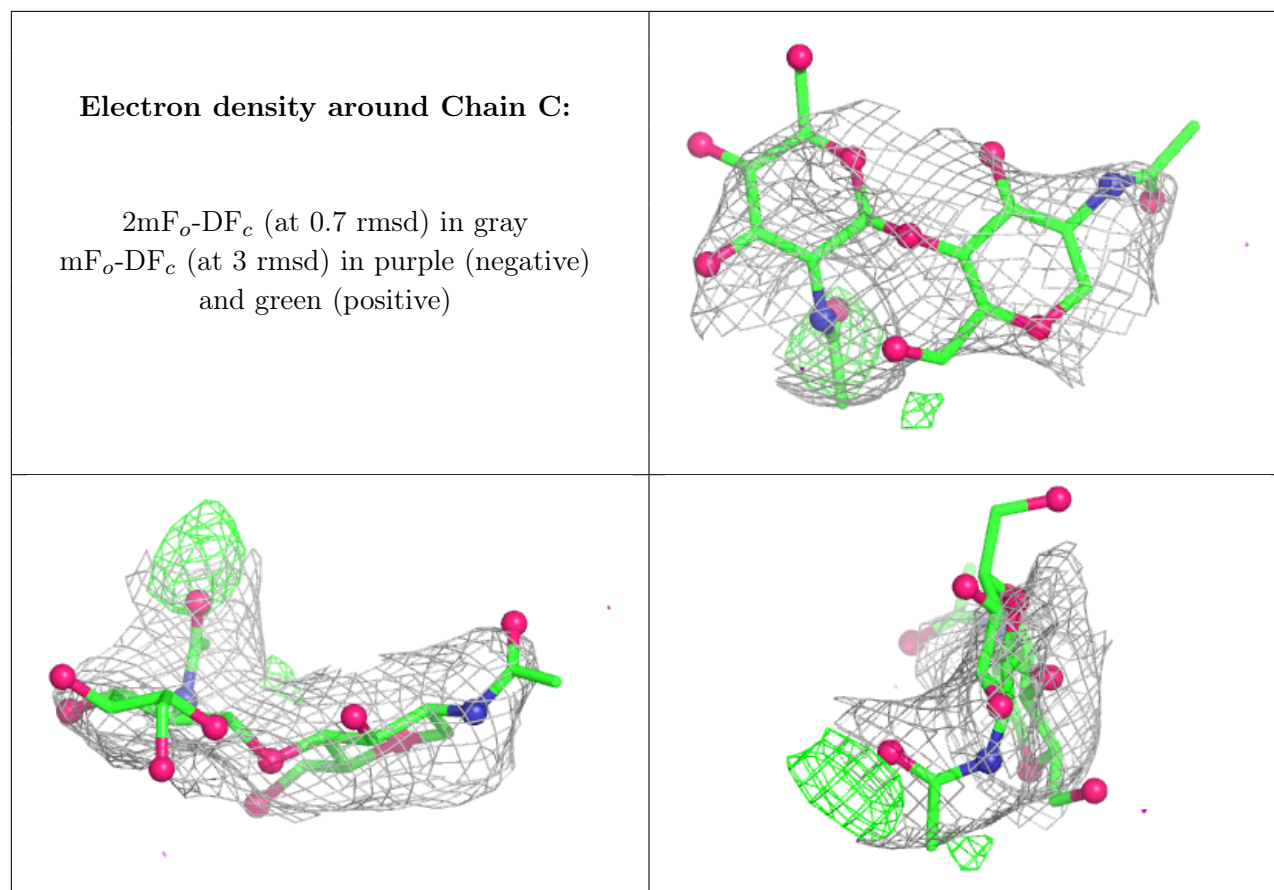
There are no non-standard protein/DNA/RNA residues in this entry.

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
4	NAG	C	1	14/15	-	-	122,139,146,150	0
4	NAG	C	2	14/15	-	-	121,153,160,161	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](#)

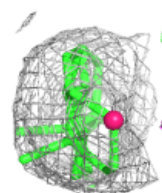
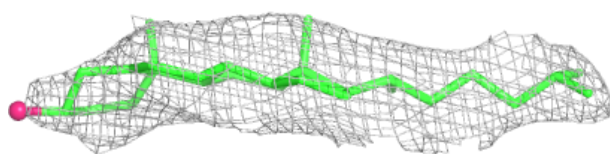
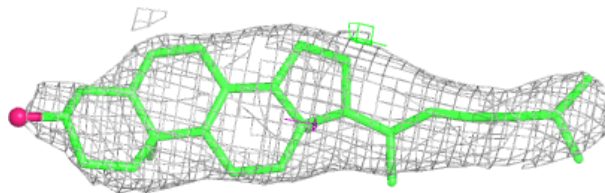
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	B	4021	14/15	0.75	0.07	133,144,149,157	0
8	CLR	B	3001	28/28	0.89	0.09	105,113,128,129	0
5	MF4	A	2001	5/5	0.97	0.07	48,48,50,55	0
7	K	A	2005	1/1	0.97	0.06	69,69,69,69	0
7	K	A	2003	1/1	0.98	0.03	70,70,70,70	0
7	K	A	2004	1/1	0.99	0.03	76,76,76,76	0
6	MG	A	2002	1/1	1.00	0.02	53,53,53,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLR B 3001:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.