



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:45 AM BST

PDB ID : 4N8D
Title : DPP4 complexed with syn-7aa
Authors : Ostermann, N.; Zink, F.; Kroemer, M.
Deposited on : 2013-10-17
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
buster-report : 1.1.7 (2018)
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

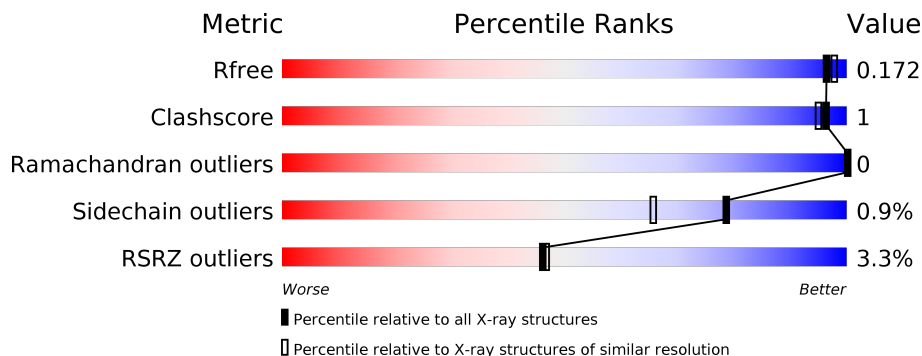
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	740	 2% 95%
1	B	740	 4% 96%
2	C	5	 40% 60%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14344 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	6015	3859	990	1140	26	0	8	0
1	B	733	6062	3889	999	1148	26	0	8	0

There are 26 discrepancies between the modelled and reference sequences:

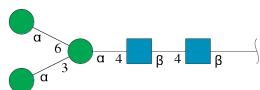
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	ILE	SER	conflict	UNP P27487
A	767	ALA	-	expression tag	UNP P27487
A	768	ALA	-	expression tag	UNP P27487
A	769	ALA	-	expression tag	UNP P27487
A	770	SER	-	expression tag	UNP P27487
A	771	TRP	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	PRO	-	expression tag	UNP P27487
A	775	GLN	-	expression tag	UNP P27487
A	776	PHE	-	expression tag	UNP P27487
A	777	GLU	-	expression tag	UNP P27487
A	778	LYS	-	expression tag	UNP P27487
B	437	ILE	SER	conflict	UNP P27487
B	767	ALA	-	expression tag	UNP P27487
B	768	ALA	-	expression tag	UNP P27487
B	769	ALA	-	expression tag	UNP P27487
B	770	SER	-	expression tag	UNP P27487
B	771	TRP	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	PRO	-	expression tag	UNP P27487
B	775	GLN	-	expression tag	UNP P27487
B	776	PHE	-	expression tag	UNP P27487
B	777	GLU	-	expression tag	UNP P27487

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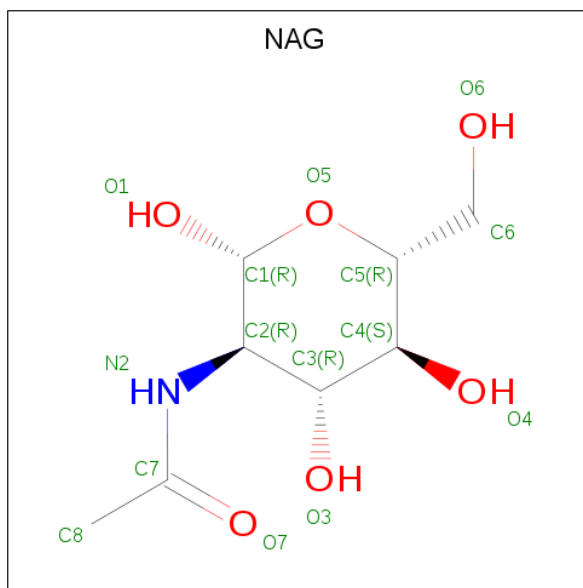
Chain	Residue	Modelled	Actual	Comment	Reference
B	778	LYS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-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	5	61	34	2	25	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



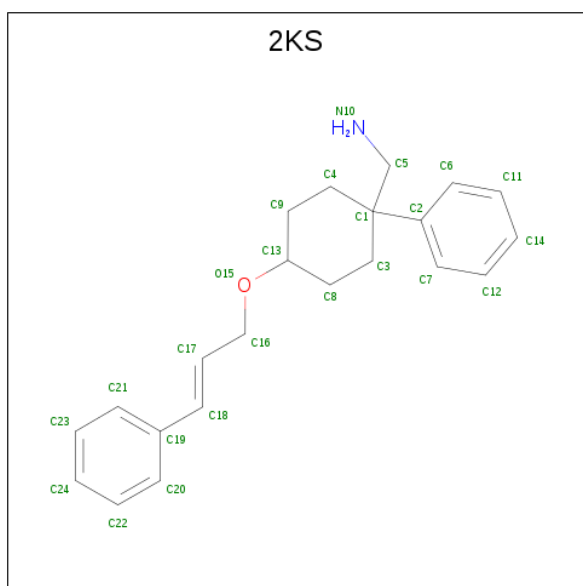
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5	4 1		
4	A	1	Total	O S	0	0
			5	4 1		
4	A	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1-(cis-1-phenyl-4-(((2E)-3-phenylprop-2-en-1-yl)oxy)cyclohexyl)methanamine (three-letter code: 2KS) (formula: C₂₂H₂₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			24	22	1	1		
5	B	1	Total	C	N	O	0	0
			24	22	1	1		

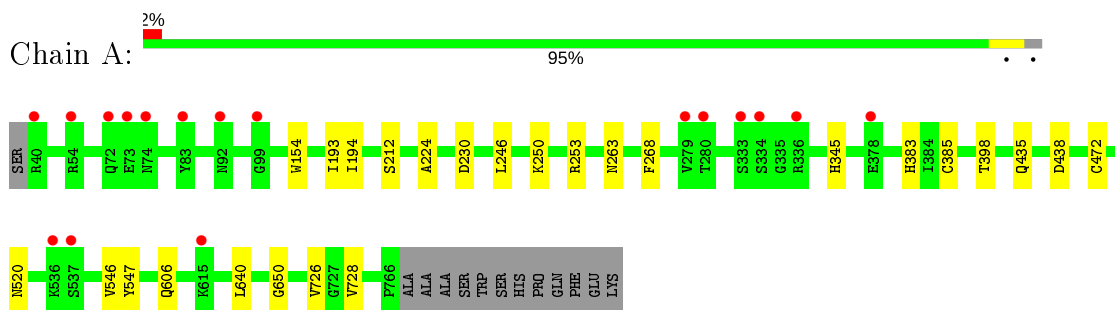
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1040	Total	O	0	0
			1040	1040		
6	B	920	Total	O	0	0
			920	920		

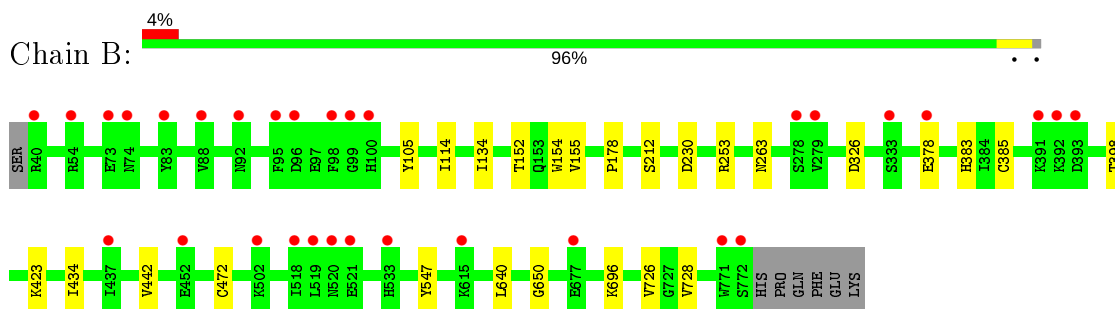
3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.31Å 121.92Å 190.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.16 – 1.65 24.15 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.16-1.65) 99.8 (24.15-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 1.65Å)	Xtrriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.155 , 0.170 0.156 , 0.172	Depositor DCC
R_{free} test set	4879 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14344	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: 2KS, NAG, SO4, MAN

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	0.54	0/6187	0.63	0/8415
1	B	0.50	0/6237	0.61	0/8483
All	All	0.52	0/12424	0.62	0/16898

There are no bond length outliers.

There are no bond angle outliers.

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	6015	0	5723	14	0
1	B	6062	0	5763	12	0
2	C	61	0	52	0	0
3	A	84	0	78	2	0
3	B	84	0	78	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	24	0	27	0	0
5	B	24	0	27	0	0
6	A	1040	0	0	1	0
6	B	920	0	0	0	0
All	All	14344	0	11748	24	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 1.

All (24) 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:253:ARG:HH21	1:B:253:ARG:HH21	1.20	0.89
1:B:434[A]:ILE:HG22	1:B:442:VAL:HG22	1.67	0.76
1:A:520:ASN:HD22	3:A:811:NAG:H83	1.63	0.63
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.88	0.55
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.90	0.53
1:A:546[B]:VAL:HG12	1:A:606:GLN:OE1	2.10	0.51
1:A:435:GLN:HE21	1:A:438:ASP:HB3	1.77	0.49
1:B:378:GLU:CD	1:B:378:GLU:H	2.15	0.49
1:A:345:HIS:HD2	6:A:955:HOH:O	1.95	0.49
1:A:383:HIS:HD2	1:A:398:THR:OG1	1.97	0.47
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.51	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.98	0.45
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.98	0.45
1:A:253:ARG:NH2	1:B:253:ARG:HH21	2.02	0.45
1:B:383:HIS:HD2	1:B:398:THR:OG1	2.00	0.44
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.44
1:A:193[B]:ILE:HG22	1:A:194:ILE:HG12	2.00	0.43
1:B:152:THR:HG21	1:B:155:VAL:HG22	2.01	0.43
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.55	0.42
1:B:154:TRP:CE2	1:B:212[B]:SER:HB3	2.54	0.42
1:B:696:LYS:HG2	1:B:728:VAL:HG22	2.02	0.42
1:B:134:ILE:HD13	1:B:178:PRO:HB3	2.03	0.41
1:A:520:ASN:ND2	3:A:811:NAG:H83	2.31	0.41
1:A:246:LEU:HD21	1:A:250:LYS:HG3	2.03	0.40

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	733/740 (99%)	711 (97%)	22 (3%)	0	100	100
1	B	739/740 (100%)	719 (97%)	20 (3%)	0	100	100
All	All	1472/1480 (100%)	1430 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	660/662 (100%)	655 (99%)	5 (1%)	81	70
1	B	663/662 (100%)	656 (99%)	7 (1%)	73	57
All	All	1323/1324 (100%)	1311 (99%)	12 (1%)	78	66

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	ASP
1	A	263	ASN
1	A	385	CYS
1	A	472	CYS
1	A	547	TYR
1	B	230	ASP
1	B	263	ASN
1	B	326	ASP
1	B	385	CYS
1	B	423	LYS
1	B	472	CYS
1	B	547	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	263	ASN
1	A	345	HIS
1	A	363	HIS
1	A	383	HIS
1	A	435	GLN
1	A	572	ASN
1	B	263	ASN
1	B	344	GLN
1	B	363	HIS
1	B	383	HIS
1	B	388	GLN
1	B	435	GLN
1	B	572	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](#)

5 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	1,2	14,14,15	0.34	0	17,19,21	0.51	0
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	0.99	2 (11%)
2	MAN	C	3	2	11,11,12	0.39	0	15,15,17	1.64	3 (20%)
2	MAN	C	4	2	11,11,12	0.33	0	15,15,17	0.76	1 (6%)
2	MAN	C	5	2	11,11,12	0.36	0	15,15,17	0.75	0

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	1/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	MAN	C1-O5-C5	4.71	118.57	112.19
2	C	3	MAN	O2-C2-C1	-2.94	103.14	109.15
2	C	4	MAN	C1-O5-C5	2.80	115.99	112.19
2	C	2	NAG	O4-C4-C5	-2.80	102.35	109.30
2	C	2	NAG	O5-C1-C2	-2.48	107.37	111.29
2	C	3	MAN	C1-C2-C3	2.17	112.33	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

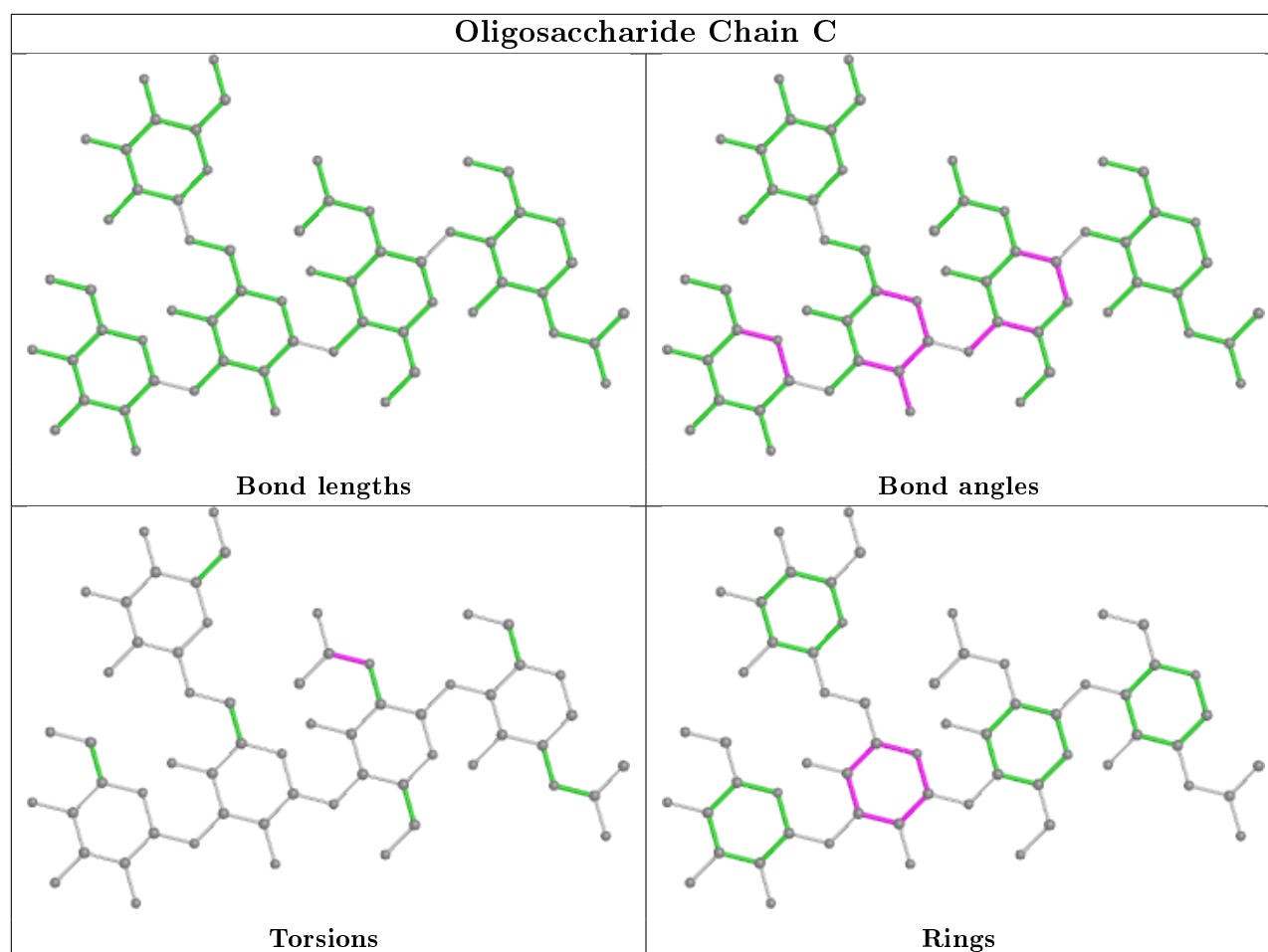
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5

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](#)

20 ligands 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$
3	NAG	A	806	1	14,14,15	0.28	0	17,19,21	0.47	0
3	NAG	B	806	1	14,14,15	0.27	0	17,19,21	0.83	1 (5%)
4	SO4	A	813	-	4,4,4	0.11	0	6,6,6	0.13	0
4	SO4	A	814	-	4,4,4	0.19	0	6,6,6	0.12	0
3	NAG	A	811	1	14,14,15	0.40	0	17,19,21	0.53	0
3	NAG	A	809	1	14,14,15	0.29	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	807	-	4,4,4	0.23	0	6,6,6	0.32	0
3	NAG	A	810	1	14,14,15	0.28	0	17,19,21	1.37	3 (17%)
3	NAG	B	805	1	14,14,15	0.31	0	17,19,21	0.55	0
5	2KS	B	810	-	26,26,26	1.53	4 (15%)	30,34,34	1.09	2 (6%)
3	NAG	B	801	1	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
4	SO4	A	812	-	4,4,4	0.17	0	6,6,6	0.16	0
5	2KS	A	815	-	26,26,26	1.43	3 (11%)	30,34,34	0.92	1 (3%)
3	NAG	A	807	1	14,14,15	0.25	0	17,19,21	0.49	0
4	SO4	B	809	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	B	808	-	4,4,4	0.17	0	6,6,6	0.06	0
3	NAG	A	808	1	14,14,15	0.32	0	17,19,21	0.63	0
3	NAG	B	804	1	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	B	803	1	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	B	802	1	14,14,15	0.33	0	17,19,21	0.60	0

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	806	1	-	0/6/23/26	0/1/1/1
3	NAG	B	806	1	-	0/6/23/26	0/1/1/1
3	NAG	A	811	1	-	2/6/23/26	0/1/1/1
3	NAG	A	809	1	-	0/6/23/26	0/1/1/1
3	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NAG	B	805	1	-	0/6/23/26	0/1/1/1
5	2KS	B	810	-	-	2/16/28/28	0/3/3/3
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
5	2KS	A	815	-	-	2/16/28/28	0/3/3/3
3	NAG	A	807	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
3	NAG	B	804	1	-	0/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	810	2KS	C9-C13	2.75	1.58	1.51
5	B	810	2KS	C1-C2	2.68	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	815	2KS	C7-C2	2.67	1.43	1.39
5	B	810	2KS	C7-C2	2.32	1.43	1.39
5	A	815	2KS	C9-C13	2.31	1.57	1.51
5	B	810	2KS	C8-C13	2.24	1.57	1.51
5	A	815	2KS	C8-C13	2.13	1.56	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	810	NAG	O5-C1-C2	-3.73	105.40	111.29
3	A	810	NAG	C1-O5-C5	3.27	116.62	112.19
3	B	806	NAG	C1-O5-C5	2.95	116.19	112.19
5	B	810	2KS	C4-C9-C13	2.70	114.94	110.33
3	B	801	NAG	C1-O5-C5	2.66	115.80	112.19
5	B	810	2KS	C11-C6-C2	2.29	123.16	120.76
5	A	815	2KS	C4-C9-C13	2.07	113.86	110.33
3	A	810	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	811	NAG	C8-C7-N2-C2
3	A	811	NAG	O7-C7-N2-C2
5	A	815	2KS	C17-C18-C19-C20
5	A	815	2KS	C17-C18-C19-C21
5	B	810	2KS	C17-C18-C19-C20
5	B	810	2KS	C17-C18-C19-C21

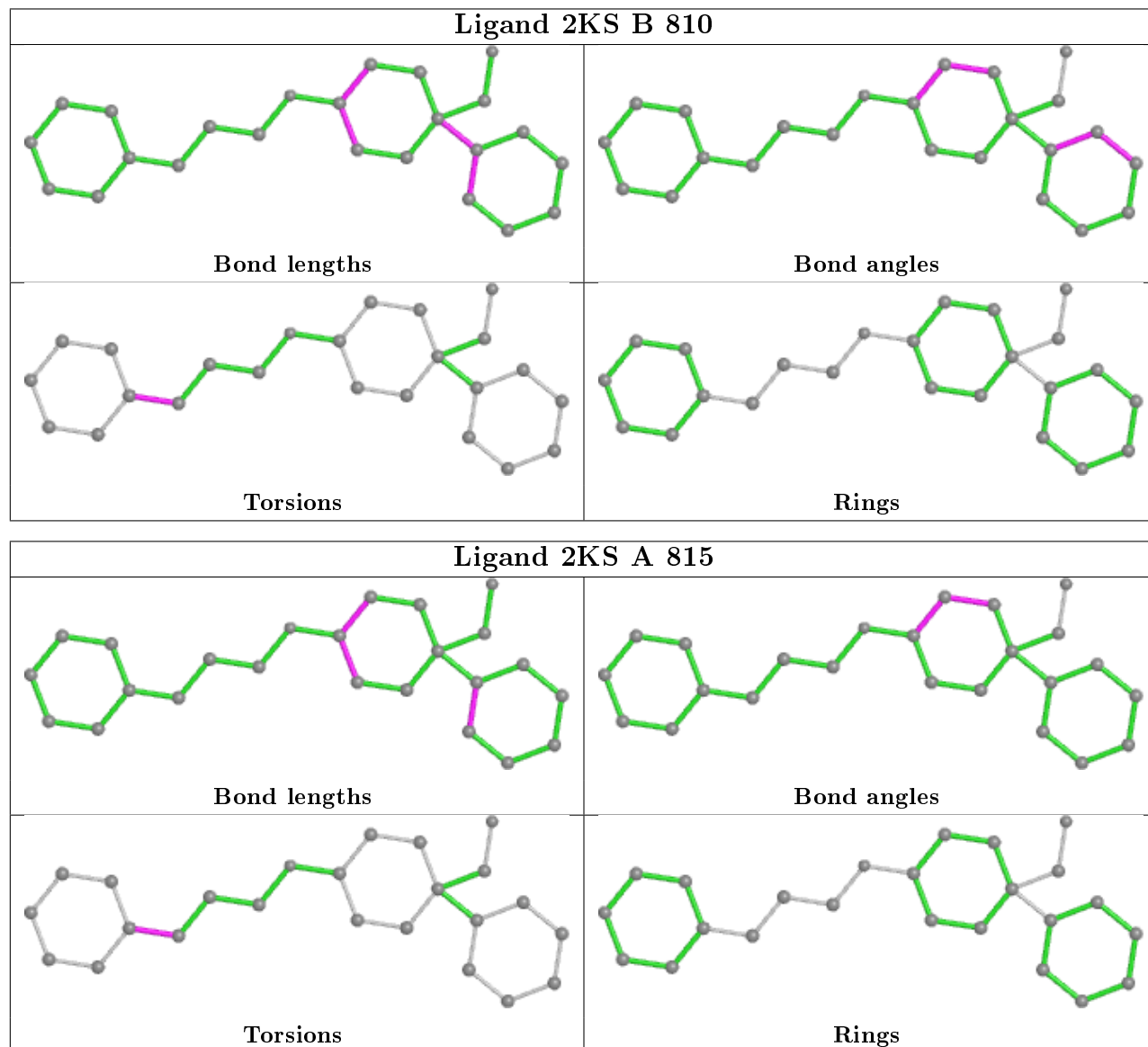
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	811	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 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

6.1 Protein, DNA and RNA chains

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	727/740 (98%)	-0.22	17 (2%) 60 61	12, 21, 43, 69	0
1	B	733/740 (99%)	-0.14	31 (4%) 36 35	13, 25, 51, 71	0
All	All	1460/1480 (98%)	-0.18	48 (3%) 46 47	12, 23, 48, 71	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	6.7
1	A	74	ASN	6.2
1	B	615	LYS	5.8
1	B	279	VAL	5.2
1	B	74	ASN	4.9
1	B	437	ILE	4.6
1	A	73	GLU	4.5
1	B	96	ASP	4.5
1	B	772	SER	4.3
1	B	73	GLU	4.2
1	B	98	PHE	4.1
1	A	92	ASN	4.1
1	B	771	TRP	3.8
1	B	521	GLU	3.7
1	A	40	ARG	3.7
1	A	72	GLN	3.7
1	B	40	ARG	3.5
1	B	278	SER	3.3
1	A	83	TYR	3.2
1	B	393	ASP	3.1
1	B	99	GLY	3.1
1	A	333	SER	3.1
1	B	88	VAL	3.0
1	A	336	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	537	SER	2.9
1	B	333	SER	2.9
1	B	520	ASN	2.9
1	B	83	TYR	2.6
1	B	519	LEU	2.6
1	B	92	ASN	2.6
1	B	452	GLU	2.6
1	B	677	GLU	2.5
1	A	54	ARG	2.5
1	A	615	LYS	2.5
1	B	391	LYS	2.5
1	A	378	GLU	2.4
1	A	334	SER	2.4
1	B	100	HIS	2.4
1	B	378	GLU	2.3
1	B	95	PHE	2.3
1	A	536	LYS	2.3
1	A	99	GLY	2.2
1	B	533	HIS	2.2
1	B	502	LYS	2.1
1	A	280	THR	2.1
1	B	518	ILE	2.1
1	B	54	ARG	2.1
1	B	392	LYS	2.0

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.

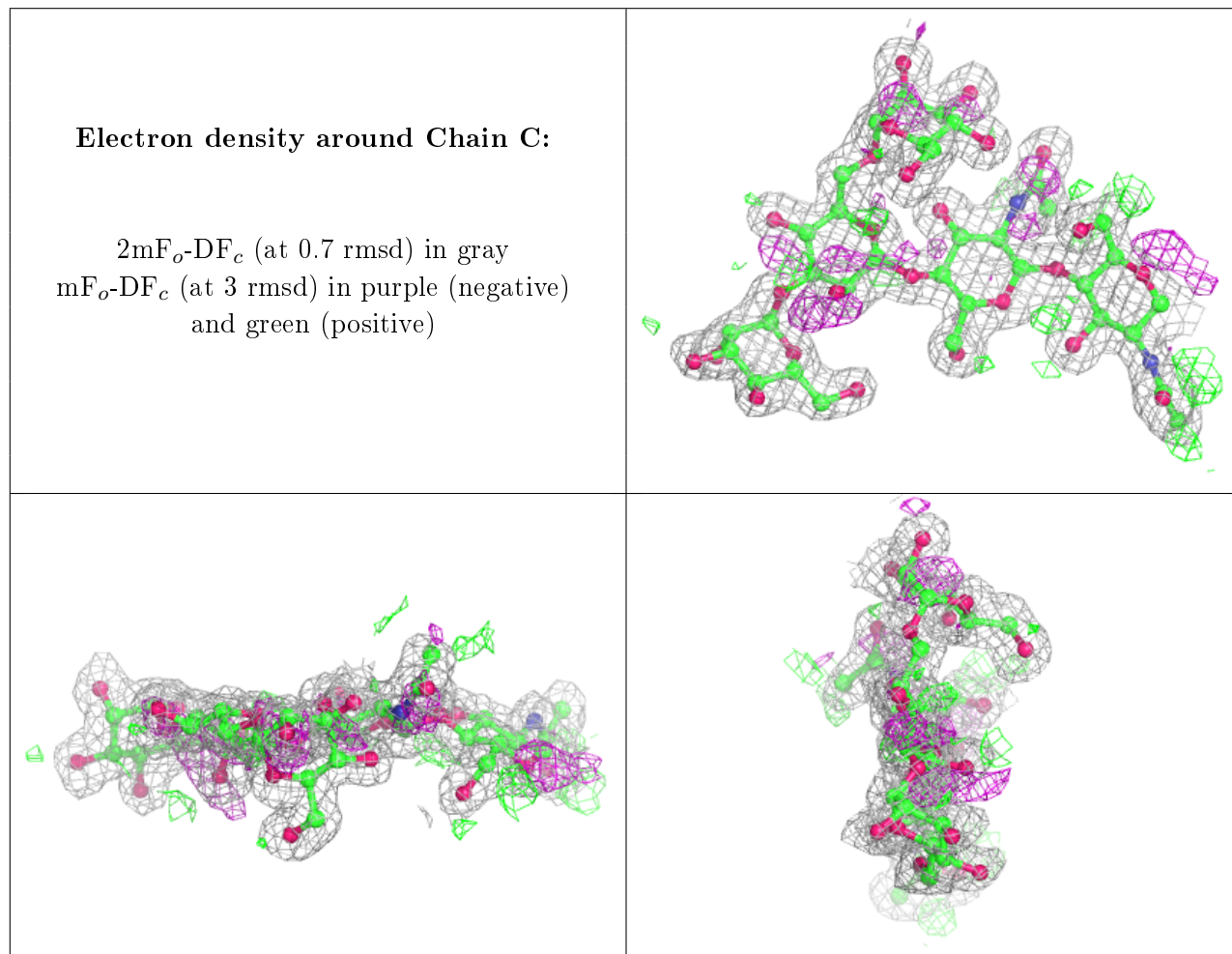
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	3	11/12	0.80	0.20	30,34,40,41	0
2	NAG	C	2	14/15	0.85	0.16	30,35,39,41	0
2	MAN	C	5	11/12	0.86	0.16	27,30,33,38	0
2	NAG	C	1	14/15	0.89	0.15	28,31,33,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	C	4	11/12	0.92	0.26	43,47,49,51	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.

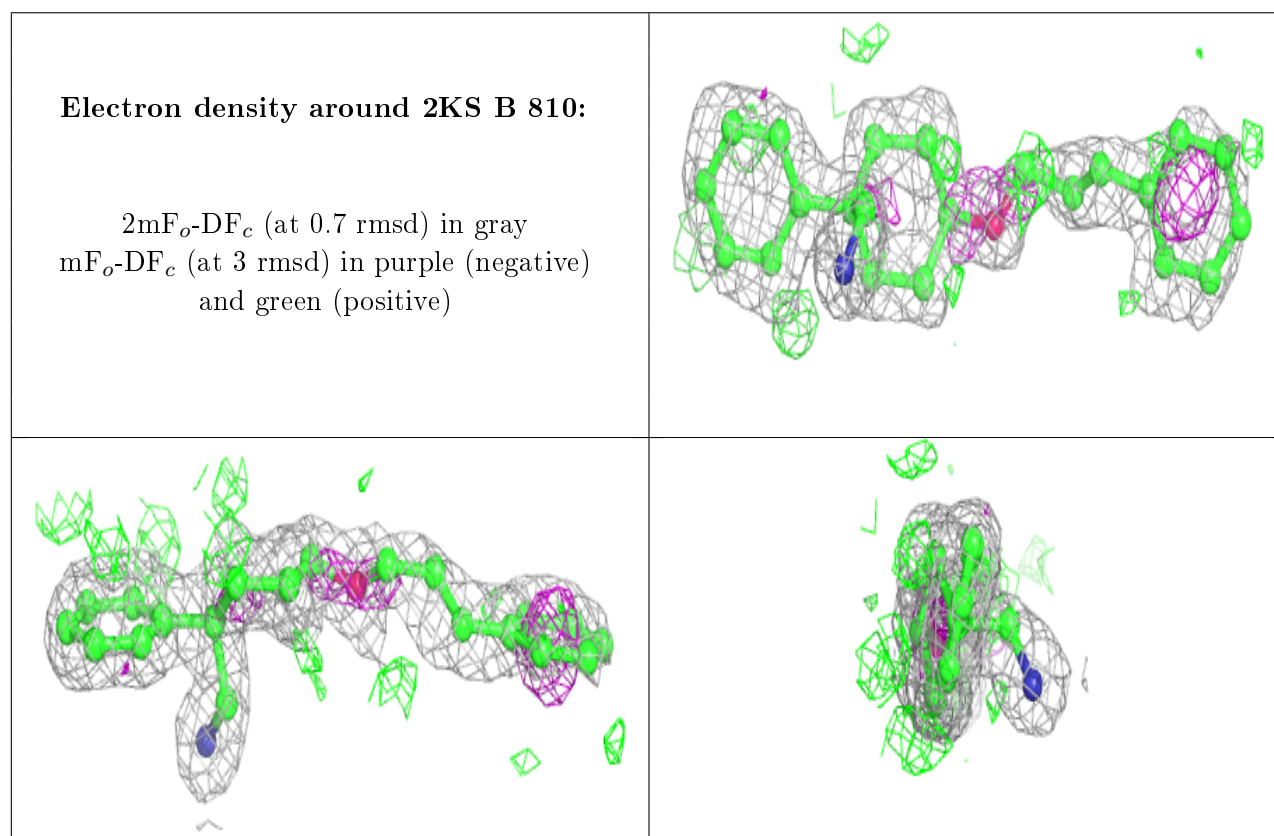
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	809	5/5	0.70	0.35	91,92,92,93	0
3	NAG	B	801	14/15	0.77	0.24	45,54,62,66	0
3	NAG	B	803	14/15	0.77	0.25	33,41,51,53	0

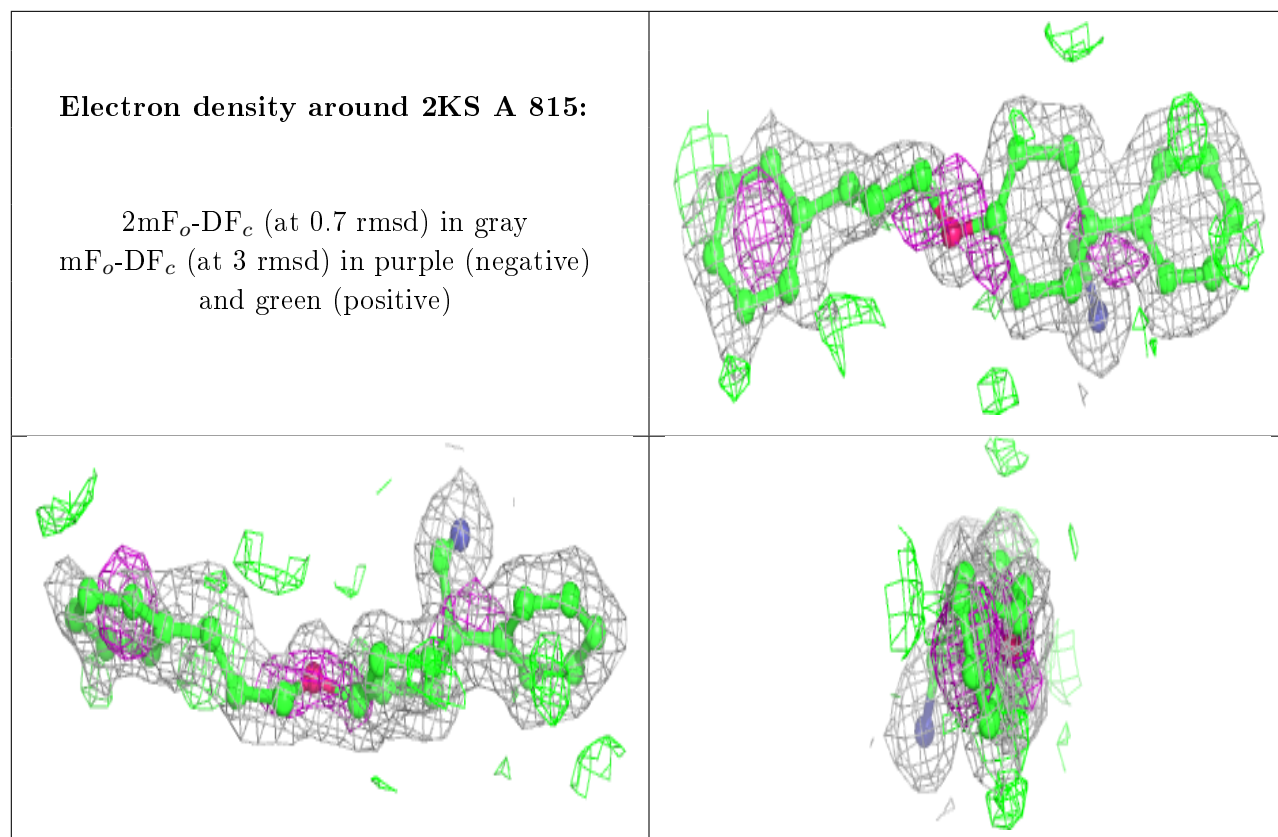
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	2KS	B	810	24/24	0.78	0.21	19,29,53,54	0
4	SO4	A	814	5/5	0.78	0.36	72,76,76,78	0
5	2KS	A	815	24/24	0.80	0.19	16,23,47,48	0
3	NAG	A	807	14/15	0.84	0.26	30,42,57,58	0
3	NAG	B	806	14/15	0.86	0.26	33,39,49,50	0
3	NAG	A	806	14/15	0.86	0.23	33,39,44,45	0
3	NAG	B	802	14/15	0.86	0.25	35,38,45,49	0
3	NAG	A	810	14/15	0.87	0.21	23,32,40,41	0
3	NAG	A	809	14/15	0.87	0.17	37,43,48,49	0
3	NAG	A	811	14/15	0.89	0.16	21,29,37,41	0
4	SO4	B	807	5/5	0.89	0.23	52,59,59,61	0
4	SO4	B	808	5/5	0.90	0.19	87,87,89,89	0
3	NAG	B	805	14/15	0.92	0.19	33,41,44,46	0
4	SO4	A	812	5/5	0.94	0.18	60,61,62,63	0
3	NAG	B	804	14/15	0.94	0.13	24,31,36,36	0
3	NAG	A	808	14/15	0.95	0.14	24,31,37,37	0
4	SO4	A	813	5/5	0.99	0.21	46,46,48,48	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.