



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:32 PM BST

PDB ID : 5NIT
Title : Glucose oxidase mutant A2
Authors : Hoffmann, K.
Deposited on : 2017-03-27
Resolution : 1.87 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

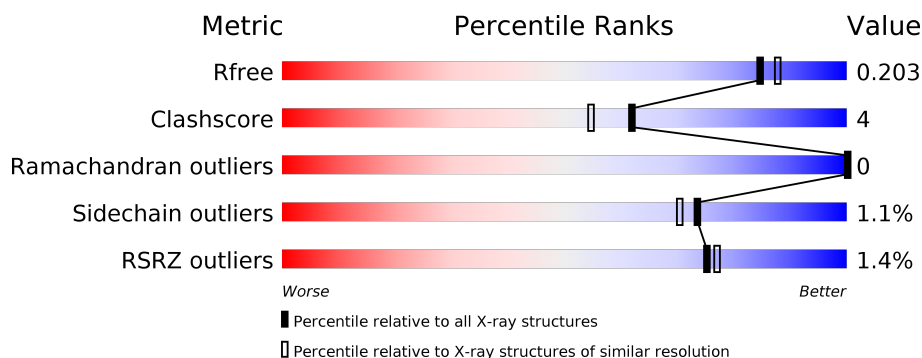
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	581	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 10%, yellow 20%, green 91%, green 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">91%</div> <div style="position: absolute; bottom: -10px; right: 0;">9%</div> </div> </div>
2	B	4	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, yellow 50%, orange 50%, orange 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">50%</div> <div style="position: absolute; bottom: -10px; right: 0;">50%</div> </div> </div>

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
6	DIO	A	615	-	-	X	-
6	DIO	A	617	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5170 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.

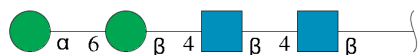
- Molecule 1 is a protein called Glucose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	10	0
			4473	2823	761	874	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	VAL	THR	engineered mutation	UNP P13006
A	94	VAL	ILE	engineered mutation	UNP P13006
A	162	THR	ALA	engineered mutation	UNP P13006
A	537	LYS	ARG	engineered mutation	UNP P13006
A	556	VAL	MET	engineered mutation	UNP P13006

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



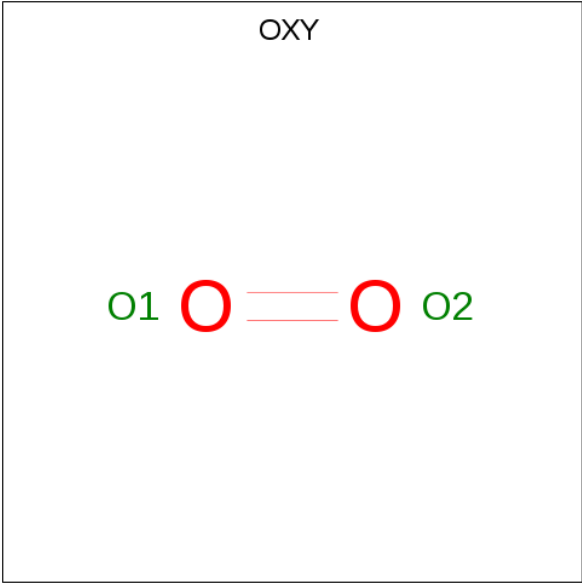
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



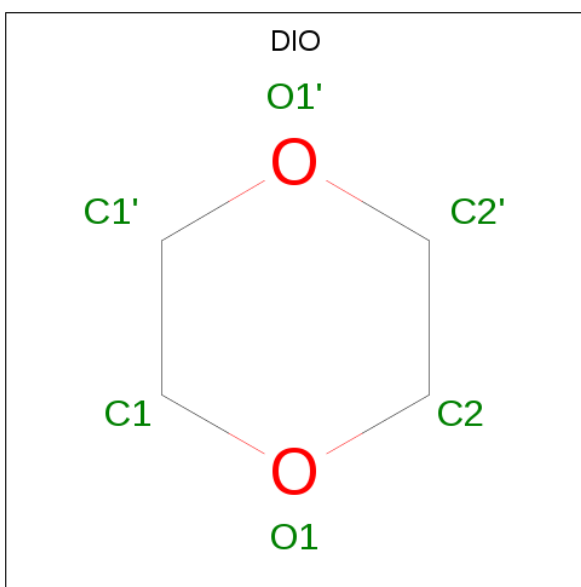
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



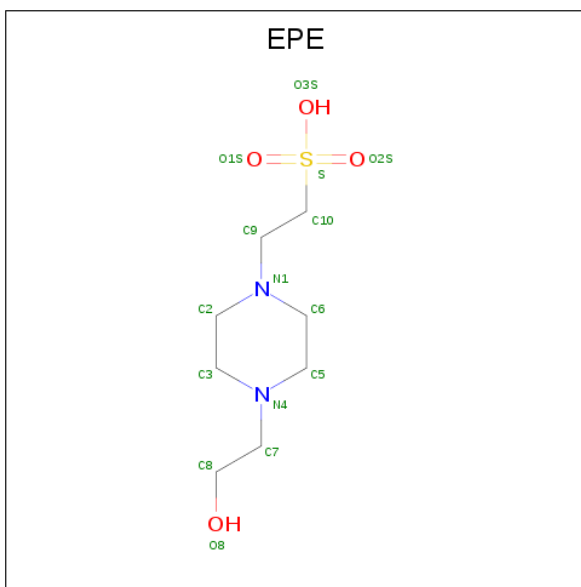
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

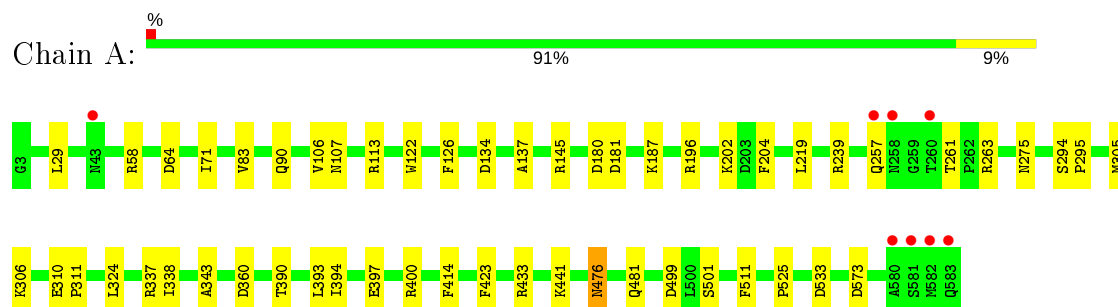
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	427	Total	O	0	0
			427	427		

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: Glucose oxidase



- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.66 Å 128.66 Å 77.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	111.42 – 1.87 45.27 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.5 (111.42-1.87) 99.4 (45.27-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.87 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.165 , 0.204 0.168 , 0.203	Depositor DCC
R_{free} test set	3243 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5170	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, NAG, OXY, BMA, EPE, FAD, 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	0.98	2/4611 (0.0%)	0.97	16/6291 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ARG	C-N	-7.56	1.16	1.34
1	A	122	TRP	CE3-CZ3	5.12	1.47	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	196	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	400	ARG	O-C-N	-7.33	110.97	122.70
1	A	145	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	337	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	196	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	360	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	204	PHE	CB-CG-CD1	5.67	124.77	120.80
1	A	58	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	533	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	64	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	573	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	181	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	134	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	433	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	499	ASP	CB-CG-OD1	5.08	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4473	0	4282	36	0
2	B	50	0	43	2	0
3	A	53	0	31	4	0
4	A	2	0	0	0	0
5	A	42	0	39	0	0
6	A	108	0	144	18	2
7	A	15	0	18	0	0
8	A	427	0	0	12	1
All	All	5170	0	4557	41	3

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 4.

All (41) 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:511:PHE:O	6:A:617:DIO:H1'2	1.85	0.76
1:A:107:ASN:HB2	3:A:601:FAD:C5X	2.16	0.75
1:A:187:LYS:NZ	8:A:707:HOH:O	2.28	0.66
1:A:275:ASN:O	8:A:702:HOH:O	2.13	0.65
1:A:107:ASN:HB2	3:A:601:FAD:N5	2.12	0.65
1:A:441:LYS:NZ	8:A:708:HOH:O	2.33	0.62
1:A:263:ARG:CZ	8:A:712:HOH:O	2.48	0.60
1:A:90:GLN:HE21	6:A:617:DIO:H22	1.67	0.59
1:A:390:THR:HG23	6:A:615:DIO:H11	1.88	0.55
1:A:343:ALA:HA	6:A:620:DIO:H1'1	1.91	0.51
2:B:1:NAG:H62	2:B:2:NAG:H82	1.92	0.51
1:A:397:GLU:HB3	6:A:621:DIO:H1'2	1.93	0.51
1:A:202[A]:LYS:NZ	8:A:701:HOH:O	2.11	0.50
1:A:294:SER:N	1:A:295:PRO:HD2	2.27	0.49
1:A:239:ARG:O	8:A:705:HOH:O	2.20	0.49
1:A:305[A]:MET:HE1	1:A:324:LEU:HD21	1.95	0.49
1:A:126:PHE:O	1:A:525:PRO:HD3	2.11	0.49
1:A:263:ARG:NE	8:A:712:HOH:O	2.46	0.48
1:A:393:LEU:HD23	6:A:615:DIO:C1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:PHE:O	6:A:617:DIO:C1'	2.59	0.47
1:A:393:LEU:HD23	6:A:615:DIO:H12	1.96	0.47
1:A:83:VAL:HA	6:A:616:DIO:H1'1	1.96	0.47
1:A:137:ALA:HA	6:A:610:DIO:H11	1.96	0.46
1:A:71:ILE:HG21	1:A:106:VAL:HG12	1.97	0.46
1:A:180:ASP:CB	6:A:622:DIO:H21	2.45	0.46
1:A:476:ASN:HD22	1:A:481:GLN:HG2	1.82	0.45
6:A:616:DIO:H22	8:A:945:HOH:O	2.16	0.45
1:A:306:LYS:NZ	8:A:703:HOH:O	2.14	0.45
1:A:107:ASN:CB	3:A:601:FAD:C5X	2.93	0.44
1:A:310:GLU:HB3	1:A:311:PRO:HD3	2.00	0.43
1:A:107:ASN:HB2	3:A:601:FAD:C4X	2.47	0.43
1:A:338:ILE:HD11	6:A:620:DIO:H12	2.00	0.43
2:B:2:NAG:H3	2:B:2:NAG:H83	2.01	0.42
1:A:113:ARG:HD3	6:A:610:DIO:H12	2.02	0.42
1:A:414:PHE:O	1:A:423:PHE:HA	2.20	0.42
1:A:394:ILE:HG23	6:A:621:DIO:H22	2.02	0.42
1:A:29:LEU:HD23	1:A:29:LEU:C	2.41	0.41
1:A:263:ARG:NH2	8:A:712:HOH:O	2.51	0.41
1:A:90:GLN:NE2	6:A:617:DIO:H22	2.34	0.41
6:A:615:DIO:H12	8:A:981:HOH:O	2.21	0.40
6:A:615:DIO:C1	8:A:981:HOH:O	2.69	0.40

All (3) 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)
8:A:822:HOH:O	8:A:1102:HOH:O[6_765]	1.21	0.99
6:A:615:DIO:O1'	6:A:615:DIO:O1'[6_764]	1.24	0.96
6:A:615:DIO:C1'	6:A:615:DIO:O1'[6_764]	1.85	0.35

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	589/581 (101%)	569 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	472/467 (101%)	467 (99%)	5 (1%)	73	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	LEU
1	A	257	GLN
1	A	261	THR
1	A	476	ASN
1	A	501	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	398	ASN
1	A	407	ASN
1	A	457	ASN
1	A	476	ASN
1	A	514	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 ⓘ

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	B	1	1,2	14,14,15	0.85	0	17,19,21	1.74	4 (23%)
2	NAG	B	2	2	14,14,15	1.00	0	17,19,21	1.80	5 (29%)
2	BMA	B	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.67	6 (40%)
2	MAN	B	4	2	11,11,12	0.62	0	15,15,17	2.24	4 (26%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C2-C3	2.72	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	C1-O5-C5	6.46	120.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O7-C7-C8	-4.61	113.49	122.06
2	B	1	NAG	C1-O5-C5	3.97	117.57	112.19
2	B	1	NAG	O5-C1-C2	-3.58	105.63	111.29
2	B	2	NAG	C2-N2-C7	3.37	127.69	122.90
2	B	3	BMA	O3-C3-C2	3.33	116.38	109.99
2	B	4	MAN	O4-C4-C3	-3.24	102.85	110.35
2	B	2	NAG	C8-C7-N2	2.74	120.73	116.10
2	B	3	BMA	O2-C2-C3	2.71	115.57	110.14
2	B	4	MAN	C6-C5-C4	2.49	118.84	113.00
2	B	1	NAG	O4-C4-C5	-2.27	103.65	109.30
2	B	2	NAG	C1-C2-N2	2.16	114.17	110.49
2	B	3	BMA	C2-C3-C4	-2.12	107.23	110.89
2	B	3	BMA	O3-C3-C4	2.11	115.23	110.35
2	B	3	BMA	O2-C2-C1	-2.10	104.86	109.15
2	B	2	NAG	O7-C7-N2	2.06	125.74	121.95
2	B	3	BMA	O5-C5-C6	2.04	110.40	107.20
2	B	4	MAN	O2-C2-C1	2.03	113.31	109.15
2	B	1	NAG	C8-C7-N2	2.03	119.53	116.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

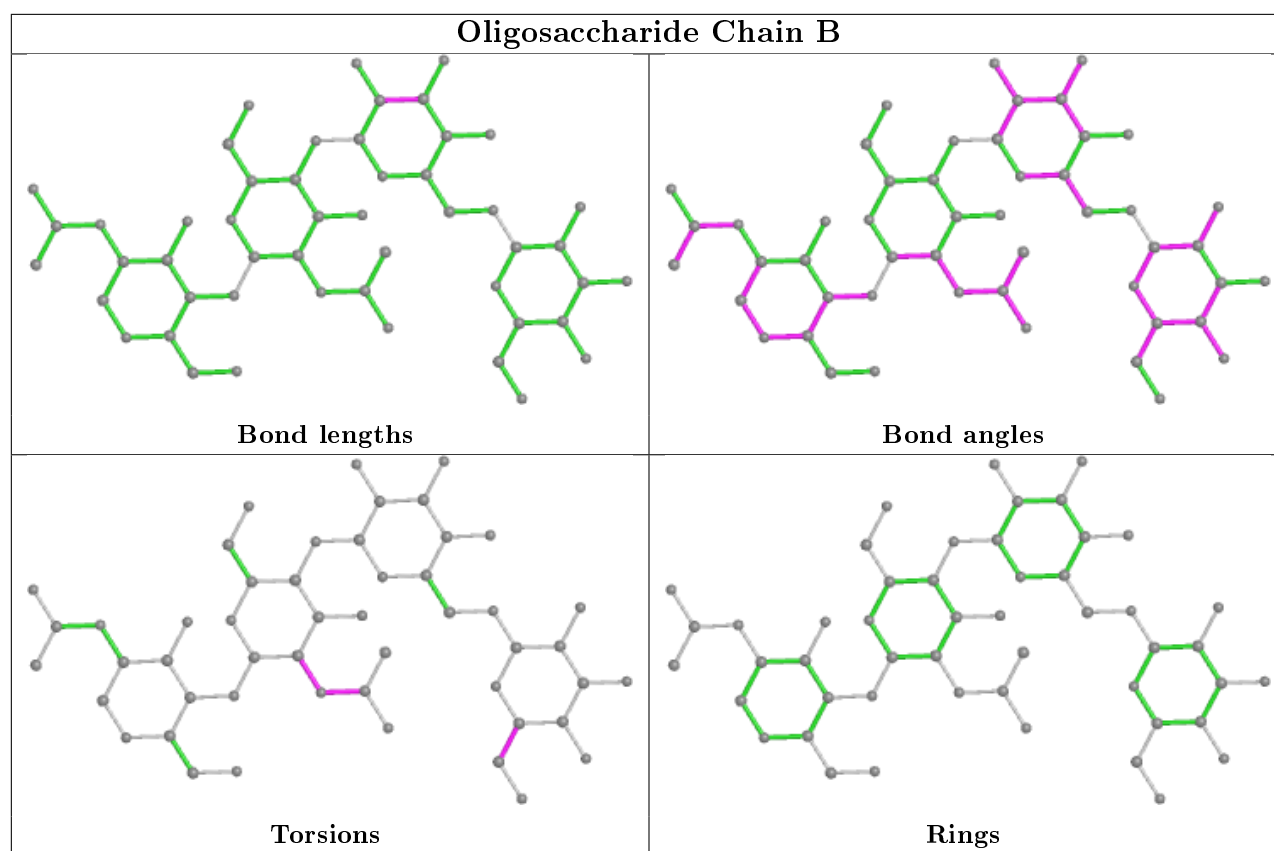
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0
2	B	1	NAG	1	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](#)

24 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
6	DIO	A	618	-	6,6,6	0.63	0	6,6,6	1.50	1 (16%)
5	NAG	A	609	1	14,14,15	1.13	2 (14%)	17,19,21	1.68	3 (17%)
7	EPE	A	628	-	15,15,15	1.26	1 (6%)	18,20,20	2.67	9 (50%)
6	DIO	A	615	-	6,6,6	0.58	0	6,6,6	0.80	0
5	NAG	A	608	1	14,14,15	0.83	0	17,19,21	1.71	4 (23%)
6	DIO	A	614	-	6,6,6	0.60	0	6,6,6	1.76	2 (33%)
6	DIO	A	623	-	6,6,6	0.48	0	6,6,6	0.43	0
6	DIO	A	613	-	6,6,6	0.73	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	607	1	14,14,15	1.49	2 (14%)	17,19,21	1.81	6 (35%)
4	OXY	A	602	-	1,1,1	0.06	0	-		
6	DIO	A	610	-	6,6,6	0.55	0	6,6,6	0.74	0
6	DIO	A	620	-	6,6,6	0.61	0	6,6,6	0.56	0
6	DIO	A	625	-	6,6,6	0.49	0	6,6,6	0.88	0
6	DIO	A	621	-	6,6,6	0.50	0	6,6,6	0.80	0
3	FAD	A	601	-	51,58,58	1.73	8 (15%)	60,89,89	2.30	15 (25%)
6	DIO	A	627	-	6,6,6	0.52	0	6,6,6	0.66	0
6	DIO	A	626	-	6,6,6	0.64	0	6,6,6	1.25	1 (16%)
6	DIO	A	616	-	6,6,6	0.49	0	6,6,6	0.65	0
6	DIO	A	612	-	6,6,6	0.62	0	6,6,6	0.75	0
6	DIO	A	624	-	6,6,6	0.54	0	6,6,6	1.17	0
6	DIO	A	611	-	6,6,6	0.74	0	6,6,6	0.97	0
6	DIO	A	619	-	6,6,6	0.38	0	6,6,6	1.50	1 (16%)
6	DIO	A	622	-	6,6,6	0.57	0	6,6,6	0.46	0
6	DIO	A	617	-	6,6,6	0.63	0	6,6,6	0.81	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
6	DIO	A	618	-	-	-	0/1/1/1
5	NAG	A	609	1	-	0/6/23/26	0/1/1/1
7	EPE	A	628	-	-	4/9/19/19	0/1/1/1
6	DIO	A	615	-	-	-	0/1/1/1
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1
6	DIO	A	614	-	-	-	0/1/1/1
6	DIO	A	623	-	-	-	0/1/1/1
6	DIO	A	613	-	-	-	0/1/1/1
5	NAG	A	607	1	-	0/6/23/26	0/1/1/1
6	DIO	A	622	-	-	-	0/1/1/1
6	DIO	A	610	-	-	-	0/1/1/1
6	DIO	A	620	-	-	-	0/1/1/1
6	DIO	A	625	-	-	-	0/1/1/1
6	DIO	A	621	-	-	-	0/1/1/1
3	FAD	A	601	-	-	3/30/50/50	0/6/6/6
6	DIO	A	627	-	-	-	0/1/1/1
6	DIO	A	626	-	-	-	0/1/1/1
6	DIO	A	616	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DIO	A	612	-	-	-	0/1/1/1
6	DIO	A	624	-	-	-	0/1/1/1
6	DIO	A	611	-	-	-	0/1/1/1
6	DIO	A	619	-	-	-	0/1/1/1
6	DIO	A	617	-	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C4X-C10	7.57	1.46	1.38
3	A	601	FAD	C9A-N10	4.47	1.44	1.38
3	A	601	FAD	C4-C4X	4.05	1.48	1.41
7	A	628	EPE	C10-S	-3.97	1.71	1.77
3	A	601	FAD	C1'-N10	-3.90	1.44	1.48
5	A	607	NAG	O5-C1	3.51	1.49	1.43
5	A	607	NAG	C1-C2	3.38	1.57	1.52
3	A	601	FAD	C9A-C5X	3.22	1.49	1.42
5	A	609	NAG	O5-C1	-3.17	1.38	1.43
3	A	601	FAD	C4X-N5	2.54	1.37	1.33
3	A	601	FAD	C8-C7	2.21	1.46	1.40
5	A	609	NAG	O7-C7	2.12	1.28	1.23
3	A	601	FAD	C5'-C4'	2.05	1.54	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C4-N3-C2	9.91	123.51	115.14
7	A	628	EPE	O2S-S-C10	5.98	114.11	106.92
3	A	601	FAD	C4X-N5-C5X	5.52	122.29	116.77
7	A	628	EPE	C5-N4-C3	4.73	119.48	108.83
3	A	601	FAD	C4X-C4-N3	-4.40	117.41	123.43
5	A	609	NAG	C1-C2-N2	-4.38	103.01	110.49
3	A	601	FAD	O4B-C1B-C2B	-4.30	100.65	106.93
7	A	628	EPE	C3-C2-N1	-3.95	102.55	110.64
5	A	608	NAG	C1-O5-C5	3.88	117.45	112.19
3	A	601	FAD	C4-C4X-N5	3.81	122.95	118.60
7	A	628	EPE	C5-C6-N1	-3.80	102.84	110.64
5	A	607	NAG	O4-C4-C5	-3.59	100.38	109.30
3	A	601	FAD	N3A-C2A-N1A	-3.48	123.23	128.68
3	A	601	FAD	C4-C4X-C10	-3.42	117.69	119.95
3	A	601	FAD	C1'-N10-C9A	3.37	120.94	118.29
6	A	614	DIO	C2'-O1'-C1'	3.20	120.57	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	O2P-P-O1P	3.15	127.80	112.24
5	A	607	NAG	O5-C1-C2	-2.97	106.60	111.29
6	A	618	DIO	C2-O1-C1	2.94	119.72	109.89
7	A	628	EPE	O1S-S-C10	2.94	110.45	106.92
3	A	601	FAD	O2B-C2B-C3B	2.89	121.18	111.82
5	A	607	NAG	O5-C5-C6	2.84	111.66	107.20
3	A	601	FAD	C5'-C4'-C3'	-2.79	106.81	112.20
3	A	601	FAD	C10-C4X-N5	-2.76	119.35	121.26
5	A	608	NAG	C1-C2-N2	-2.72	105.85	110.49
3	A	601	FAD	C2A-N1A-C6A	2.65	123.29	118.75
5	A	607	NAG	C8-C7-N2	2.62	120.53	116.10
5	A	608	NAG	C4-C3-C2	2.55	114.75	111.02
7	A	628	EPE	O3S-S-O2S	-2.50	105.16	111.27
6	A	619	DIO	C2-O1-C1	2.50	118.25	109.89
6	A	626	DIO	C2'-O1'-C1'	2.48	118.16	109.89
5	A	609	NAG	O5-C1-C2	-2.44	107.44	111.29
5	A	607	NAG	C1-C2-N2	2.43	114.64	110.49
6	A	614	DIO	C2-O1-C1	2.41	117.95	109.89
5	A	609	NAG	C2-N2-C7	-2.40	119.48	122.90
3	A	601	FAD	C1B-N9A-C4A	-2.40	122.43	126.64
5	A	608	NAG	C6-C5-C4	-2.36	107.48	113.00
7	A	628	EPE	C8-C7-N4	-2.21	105.45	113.40
5	A	607	NAG	O7-C7-N2	-2.14	118.02	121.95
3	A	601	FAD	O2A-PA-O1A	2.13	122.75	112.24
7	A	628	EPE	O3S-S-O1S	2.10	116.42	111.27
7	A	628	EPE	C9-N1-C2	2.07	116.53	111.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

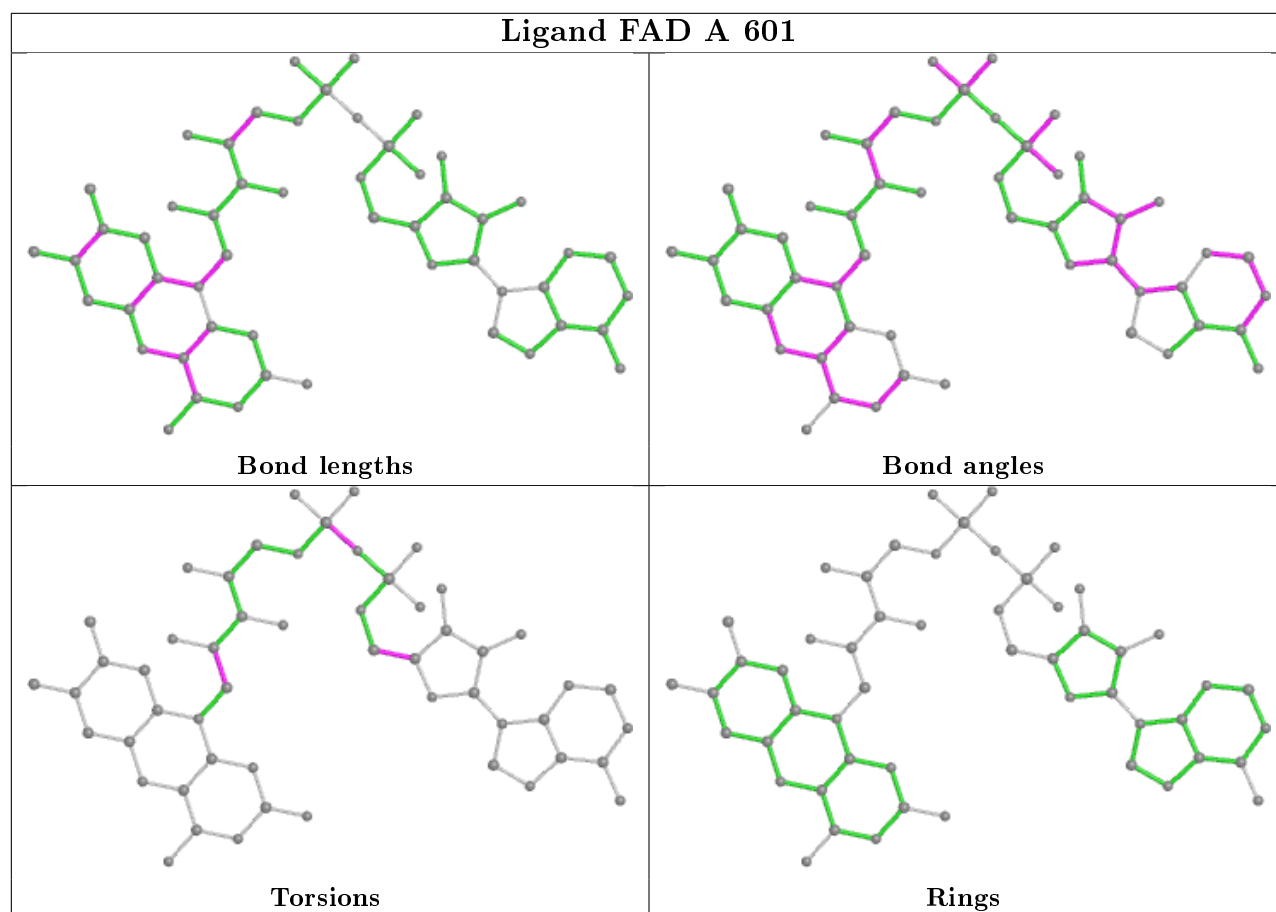
Mol	Chain	Res	Type	Atoms
3	A	601	FAD	N10-C1'-C2'-O2'
3	A	601	FAD	PA-O3P-P-O5'
7	A	628	EPE	C8-C7-N4-C3
7	A	628	EPE	C8-C7-N4-C5
7	A	628	EPE	C9-C10-S-O3S
7	A	628	EPE	N4-C7-C8-O8
3	A	601	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	615	DIO	5	2
6	A	610	DIO	2	0
6	A	620	DIO	2	0
6	A	621	DIO	2	0
3	A	601	FAD	4	0
6	A	616	DIO	2	0
6	A	622	DIO	1	0
6	A	617	DIO	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	400:ARG	C	401:ASP	N	1.16

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	581/581 (100%)	-0.40	8 (1%) 75 77	13, 18, 29, 74	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	MET	5.3
1	A	583	GLN	5.2
1	A	258	ASN	5.1
1	A	260	THR	3.0
1	A	581[A]	SER	2.9
1	A	257	GLN	2.7
1	A	43	ASN	2.3
1	A	580	ALA	2.0

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

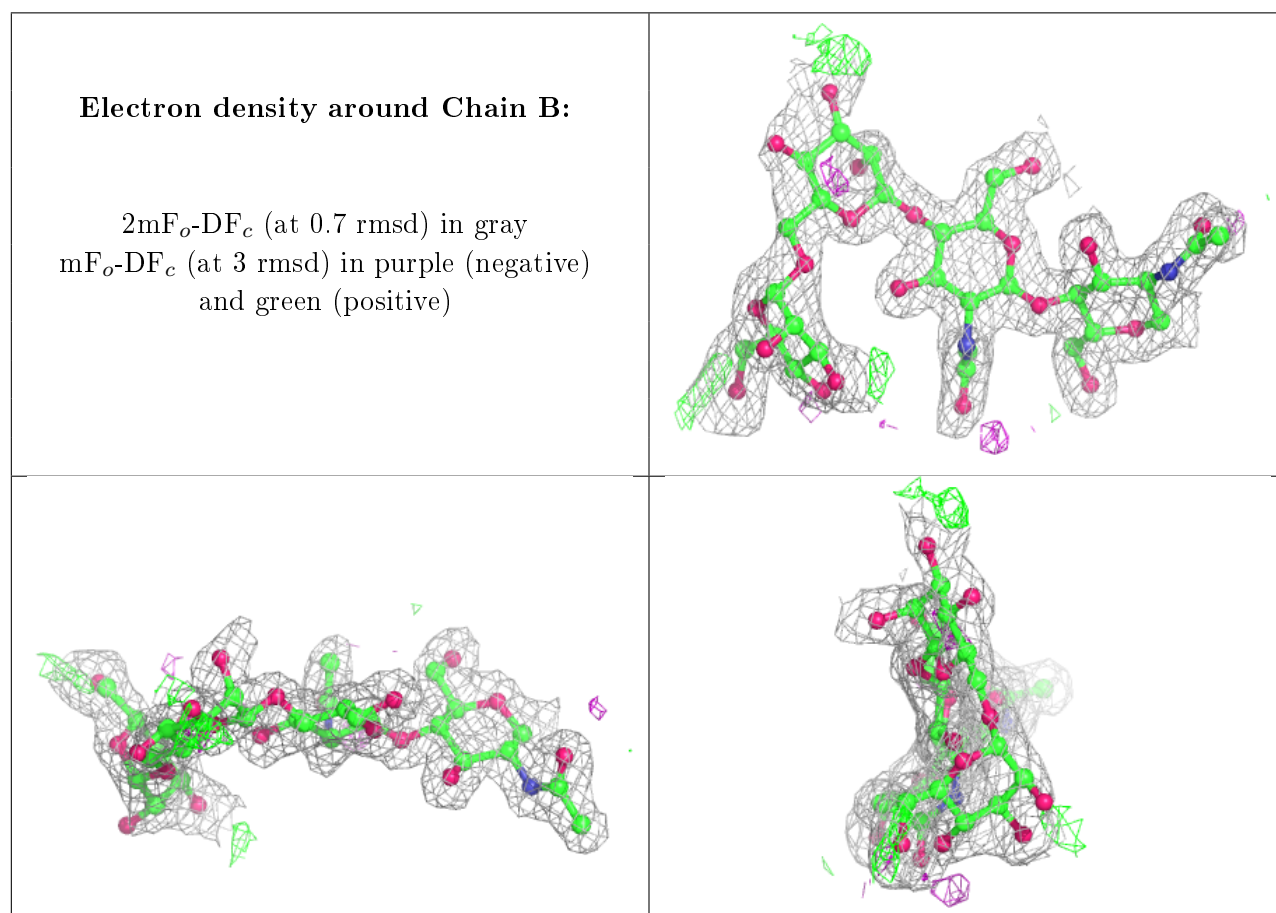
There are no non-standard protein/DNA/RNA residues in this entry.

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	BMA	B	3	11/12	0.78	0.33	39,46,54,55	0
2	MAN	B	4	11/12	0.78	0.23	47,49,52,58	0
2	NAG	B	2	14/15	0.94	0.17	25,27,33,34	0
2	NAG	B	1	14/15	0.98	0.11	20,21,22,24	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.

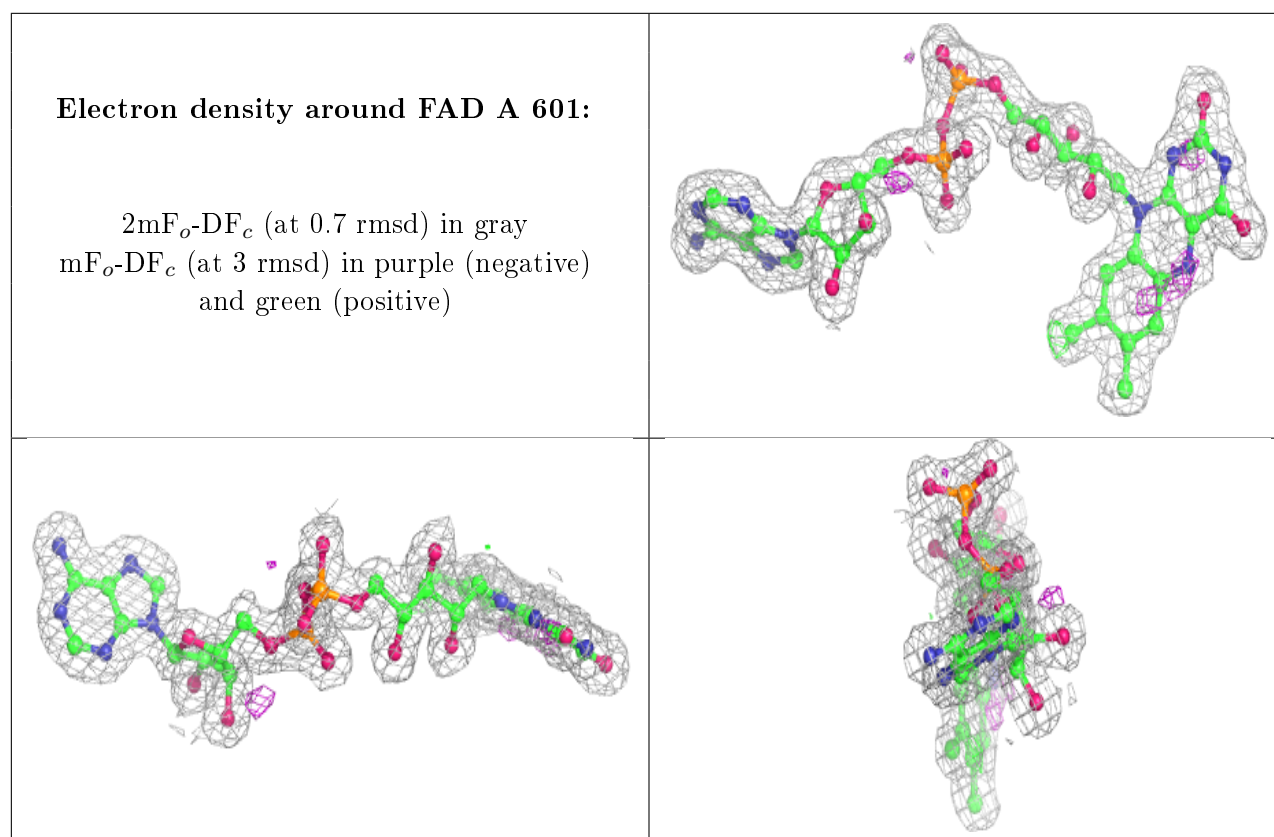
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EPE	A	628	15/15	0.74	0.31	43,47,58,63	0
6	DIO	A	616	6/6	0.77	0.18	38,43,44,46	0
6	DIO	A	620	6/6	0.84	0.35	49,50,53,56	0
6	DIO	A	615	6/6	0.85	0.34	48,57,62,65	0
6	DIO	A	626	6/6	0.85	0.14	52,52,54,55	0
6	DIO	A	623	6/6	0.85	0.23	43,43,45,45	6
6	DIO	A	613	6/6	0.87	0.12	43,45,49,50	0
6	DIO	A	627	6/6	0.88	0.21	52,54,57,57	0
6	DIO	A	614	6/6	0.88	0.20	42,43,43,44	0
6	DIO	A	625	6/6	0.88	0.17	50,52,53,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	609	14/15	0.90	0.10	30,34,42,48	0
5	NAG	A	608	14/15	0.90	0.18	30,35,38,41	0
6	DIO	A	624	6/6	0.90	0.14	44,47,47,48	0
6	DIO	A	619	6/6	0.90	0.10	28,29,31,31	0
6	DIO	A	622	6/6	0.92	0.10	39,40,41,43	0
6	DIO	A	612	6/6	0.93	0.09	31,33,35,36	0
6	DIO	A	610	6/6	0.93	0.10	31,32,32,33	0
6	DIO	A	617	6/6	0.93	0.14	36,38,39,40	0
6	DIO	A	611	6/6	0.94	0.12	25,28,31,33	0
6	DIO	A	621	6/6	0.94	0.09	37,38,38,40	0
5	NAG	A	607	14/15	0.94	0.11	15,18,25,25	0
6	DIO	A	618	6/6	0.94	0.10	35,37,39,39	0
3	FAD	A	601	53/53	0.97	0.08	12,14,18,19	0
4	OXY	A	602	2/2	0.99	0.09	23,23,23,23	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.