

wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 07:41 AM EDT

PDB ID : 6SOZ

Title : Glycosylated Trypanosoma brucei transferrin receptor in complex with human

transferrin

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Deposited on : 2019-08-30

Resolution : 3.42 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.37.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

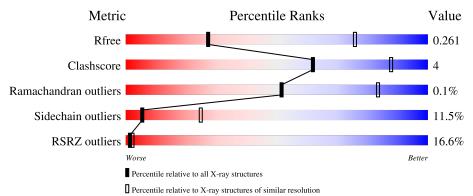
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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 $(\# \mathrm{Entries})$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range(Å)}) \end{aligned}$		
R_{free}	130704	1486 (3.50-3.34)		
Clashscore	141614	1572 (3.50-3.34)		
Ramachandran outliers	138981	1534 (3.50-3.34)		
Sidechain outliers	138945	1535 (3.50-3.34)		
RSRZ outliers	127900	1395 (3.50-3.34)		

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 <=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						
			5%						
1	A	399	6	1%	18%	•	19%		
			9%						
2	В	338		69%		24%	• 5%		
			25%						
3	С	677		83%			12% • •		
4	D	3		67%		33%)		
4	E	3	33%	33%		33%			

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Mol	Chain	Length	Quality of chain
5	F	2	100%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10211 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 ESAG6, subunit of heterodimeric transferrin receptor.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	323	Total	С	N	О	S	0	0	0
1	11	020	2500	1554	443	492	11			

• Molecule 2 is a protein called ESAG7, subunit of heterodimeric transferrin receptor.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	320	Total 2490	C 1561	N 433	O 484	S 12	0	0	0

• Molecule 3 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	651	Total 5058	C 3181	N 878	O 955	S 44	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	VAL	ILE	conflict	UNP P02787

• Molecule 4 is an oligosaccharide called 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
4	D	3	Total C N O 39 22 2 15	0	0	0
4	E	3	Total C N O 39 22 2 15	0	0	0

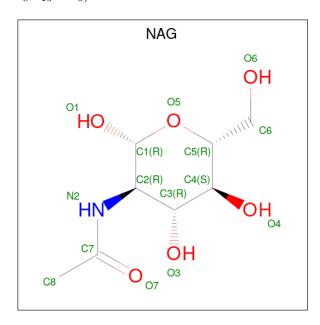


• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

 \bullet Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



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

• Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).



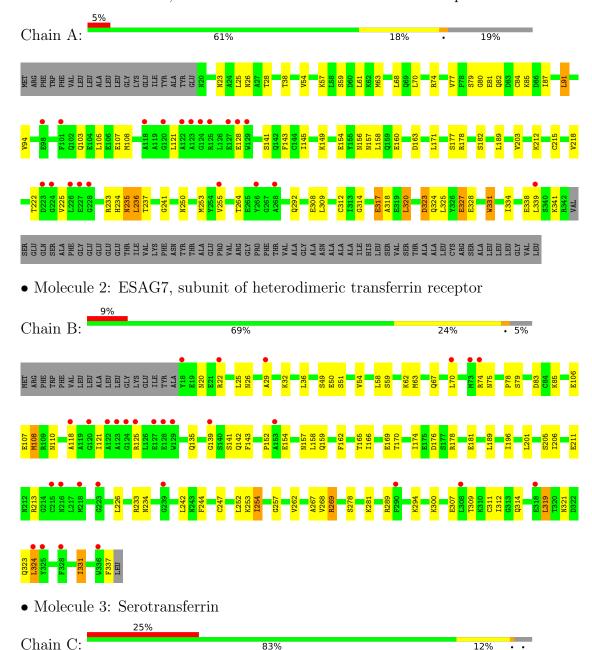
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	Total Fe 1 1	1	0



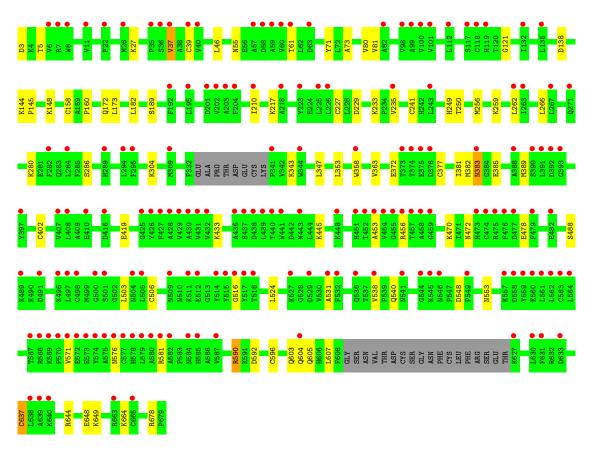
3 Residue-property plots (i)

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: ESAG6, subunit of heterodimeric transferrin receptor







 \bullet Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 67% 33%

NAG1 NAG2 MAN3

 $\bullet \ \, Molecule \ 4: \ alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose$

Chain E: 33% 33% 33%

NAG1 NAG2 MAN3

 \bullet Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	128.18Å 117.87Å 134.55Å	Depositor
a, b, c, α , β , γ	90.00° 111.45° 90.00°	Depositor
Resolution (Å)	39.59 - 3.42	Depositor
Resolution (A)	38.76 - 3.42	EDS
% Data completeness	99.0 (39.59-3.42)	Depositor
(in resolution range)	99.0 (38.76-3.42)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.62 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D.	0.211 , 0.241	Depositor
R, R_{free}	0.230 , 0.261	DCC
R_{free} test set	1239 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	154.2	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 171.5	EDS
L-test for twinning ²	$ < L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms $(Å^2)$	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: FE, NAG, 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 C	Chain	Bond lengths		Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.52	0/2535	0.78	2/3414~(0.1%)	
2	В	0.54	0/2526	0.82	5/3403~(0.1%)	
3	С	0.47	0/5172	0.67	0/6986	
All	All	0.50	0/10233	0.73	7/13803~(0.1%)	

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	110	ASN	CB-CG-ND2	9.24	138.88	116.70
2	В	110	ASN	OD1-CG-ND2	-6.49	106.97	121.90
2	В	26	ASN	CB-CG-ND2	5.62	130.18	116.70
1	A	79	SER	N-CA-C	-5.39	96.45	111.00
2	В	26	ASN	OD1-CG-ND2	-5.34	109.62	121.90

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	2500	0	2470	37	0
2	В	2490	0	2467	37	0
3	С	5058	0	4902	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	39	0	34	2	0
4	Е	39	0	34	1	0
5	F	28	0	25	4	0
6	A	28	0	26	4	0
6	В	28	0	26	1	0
7	С	1	0	0	0	0
All	All	10211	0	9984	89	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 4.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\r{A}}) \end{array}$
1:A:233:ARG:HG3	2:B:139:GLY:H	1.47	0.77
2:B:74:ARG:HH21	2:B:331:ILE:HD11	1.50	0.77
1:A:154:GLU:H	1:A:157:ASN:HD22	1.34	0.76
1:A:94:VAL:HG21	1:A:309:LEU:HD21	1.69	0.74
2:B:233:ARG:HA	6:B:404:NAG:H62	1.68	0.74

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	Perce	ntiles
1	A	321/399 (80%)	306 (95%)	15 (5%)	0	100	100
2	В	318/338 (94%)	297 (93%)	21 (7%)	0	100	100
3	С	645/677 (95%)	609 (94%)	35 (5%)	1 (0%)	47	80
All	All	1284/1414 (91%)	1212 (94%)	71 (6%)	1 (0%)	51	83



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	363	VAL

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	ain Analysed Rotameric Outliers		Percentiles		
1	A	268/327~(82%)	229 (85%)	39 (15%)	3	16
2	В	268/283 (95%)	229 (85%)	39 (15%)	3	16
3	С	547/570 (96%)	500 (91%)	47 (9%)	10	38
All	All	1083/1180 (92%)	958 (88%)	125 (12%)	5	25

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	174	ILE
3	С	488	SER
2	В	307	GLU
3	С	478	GLU
3	С	590	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	323	GLN
3	С	383	ASN
3	С	605	GLN
3	С	584	ASN
2	В	135	GLN

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)

8 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	Trno	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Mol Type Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NAG	D	1	1,4	14,14,15	0.36	0	17,19,21	0.71	0
4	NAG	D	2	4	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
4	MAN	D	3	4	11,11,12	0.39	0	15,15,17	1.11	1 (6%)
4	NAG	Е	1	1,4	14,14,15	0.38	0	17,19,21	0.97	1 (5%)
4	NAG	Е	2	4	14,14,15	0.33	0	17,19,21	0.72	0
4	MAN	E	3	4	11,11,12	0.50	0	15,15,17	1.13	2 (13%)
5	NAG	F	1	5,2	14,14,15	0.42	0	17,19,21	1.36	2 (11%)
5	NAG	F	2	5	14,14,15	0.53	0	17,19,21	1.78	4 (23%)

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	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	MAN	D	3	4	-	1/2/19/22	0/1/1/1
4	NAG	Ε	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	MAN	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1



There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}({}^o)$	$\operatorname{Ideal}({}^{o})$
5	F	2	NAG	C1-O5-C5	5.49	119.63	112.19
5	F	1	NAG	C1-O5-C5	-4.14	106.59	112.19
4	D	3	MAN	C1-O5-C5	3.45	116.87	112.19
4	D	2	NAG	O5-C1-C2	-3.44	105.86	111.29
4	Е	3	MAN	C1-O5-C5	3.39	116.79	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	2	NAG	O5-C5-C6-O6
4	Е	3	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	Е	2	NAG	C4-C5-C6-O6
4	Е	1	NAG	O5-C5-C6-O6

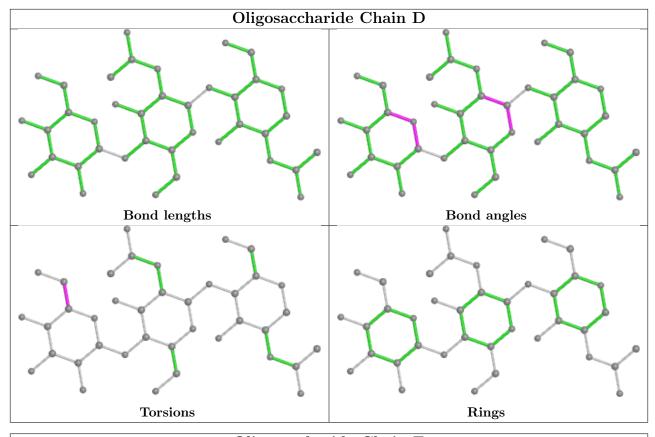
There are no ring outliers.

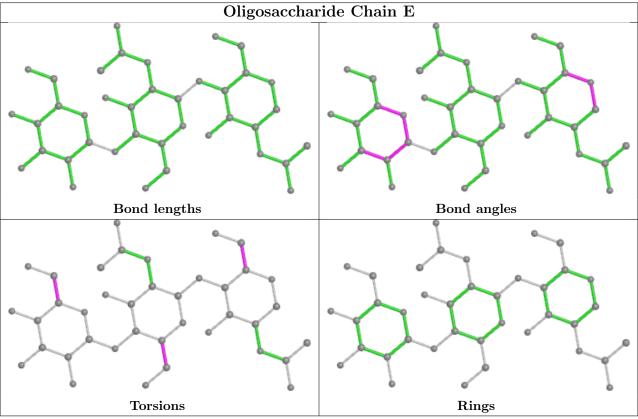
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
5	F	1	NAG	4	0
4	D	2	NAG	1	0
5	F	2	NAG	2	0
4	Е	1	NAG	1	0

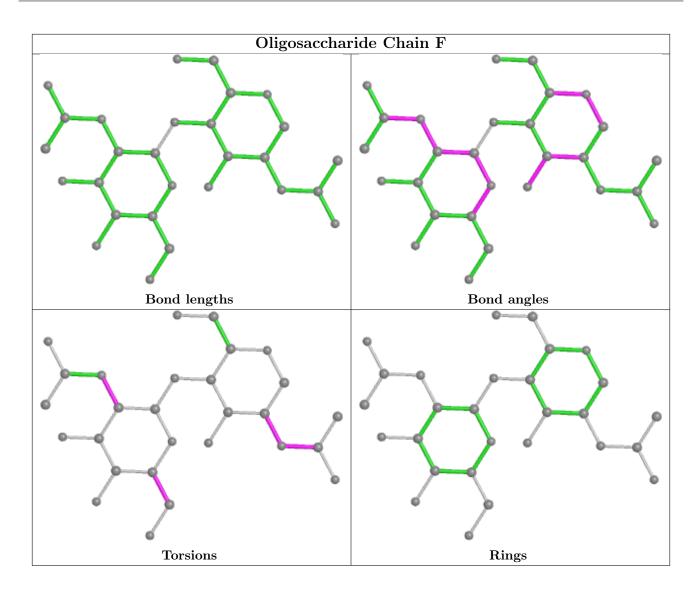
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	Bo	Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
6	NAG	В	401	2	14,14,15	0.49	0	17,19,21	1.99	3 (17%)	
6	NAG	A	405	1	14,14,15	0.31	0	17,19,21	1.49	4 (23%)	
6	NAG	A	401	1	14,14,15	0.35	0	17,19,21	1.32	3 (17%)	



	Mol Type		Chain	Res	Link	Bond lengths			Bond angles		
	MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	6	NAG	В	404	2	14,14,15	0.42	0	17,19,21	1.05	2 (11%)

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	NAG	В	401	2	-	5/6/23/26	0/1/1/1
6	NAG	A	405	1	-	4/6/23/26	0/1/1/1
6	NAG	A	401	1	-	5/6/23/26	0/1/1/1
6	NAG	В	404	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
6	В	401	NAG	C1-O5-C5	6.51	121.01	112.19
6	A	405	NAG	C1-O5-C5	3.36	116.74	112.19
6	В	401	NAG	C1-C2-N2	3.24	116.02	110.49
6	A	401	NAG	C1-C2-N2	3.14	115.86	110.49
6	В	404	NAG	C1-C2-N2	-3.05	105.28	110.49

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	401	NAG	C1-C2-N2-C7
6	В	404	NAG	C1-C2-N2-C7
6	A	405	NAG	C8-C7-N2-C2
6	A	405	NAG	O7-C7-N2-C2
6	В	401	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	405	NAG	2	0
6	A	401	NAG	2	0
6	В	404	NAG	1	0



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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	323/399~(80%)	0.33	20 (6%) 20 22	132, 192, 240, 256	0
2	В	320/338 (94%)	0.47	29 (9%) 9 12	123, 183, 234, 256	0
3	С	651/677 (96%)	1.23	166 (25%) 0 0	158, 240, 292, 296	0
All	All	1294/1414 (91%)	0.82	215 (16%) 1 2	123, 216, 288, 296	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	580	ALA	12.5
3	С	517	TYR	9.1
3	С	498	CYS	8.6
3	С	579	LEU	8.5
3	С	452	THR	8.4

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, 95^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
4	MAN	D	3	11/12	0.50	0.27	264,266,268,268	0
5	NAG	F	2	14/15	0.68	0.35	202,213,226,229	0
5	NAG	F	1	14/15	0.86	0.25	168,174,180,191	0

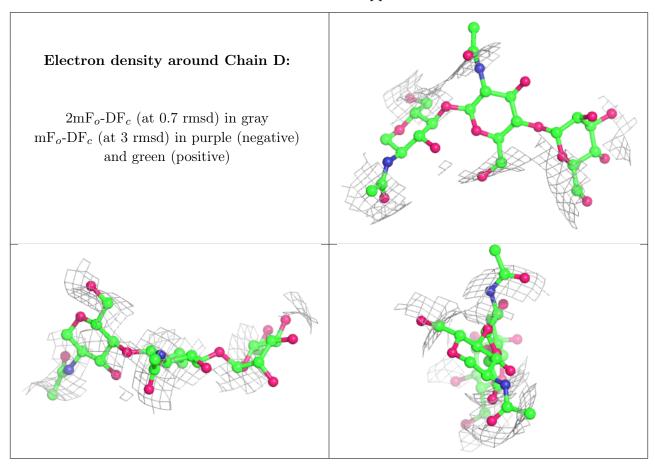
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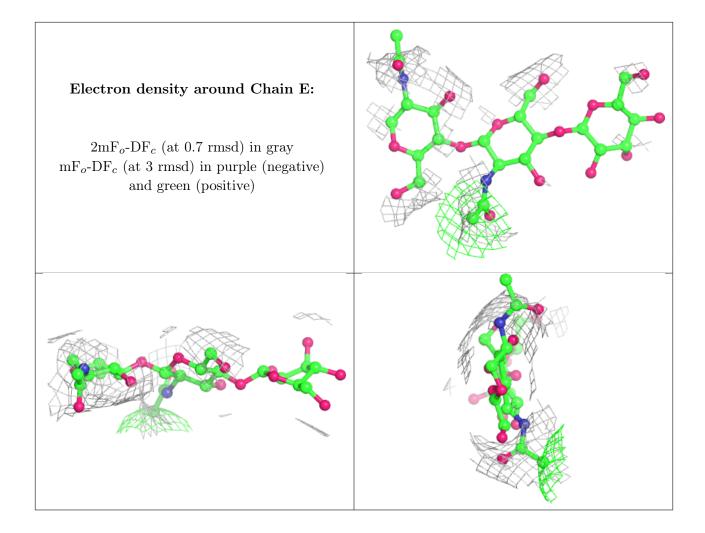
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	NAG	D	2	14/15	0.88	0.17	248,252,256,260	0
4	MAN	Е	3	11/12	0.88	0.13	239,240,242,242	0
4	NAG	Е	2	14/15	0.89	0.12	231,235,238,240	0
4	NAG	D	1	14/15	0.89	0.14	198,211,222,235	0
4	NAG	Е	1	14/15	0.93	0.17	210,222,224,229	0

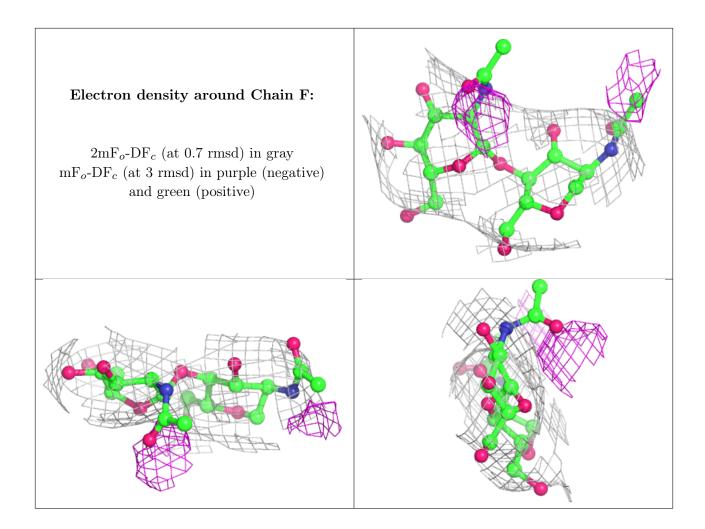
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.











6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.

