



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 8, 2024 – 01:10 pm BST

PDB ID : 8Q5U
Title : Endoglycosidase S2 in complex with IgG1 Fc
Authors : Sudol, A.S.L.; Tews, I.; Crispin, M.
Deposited on : 2023-08-09
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

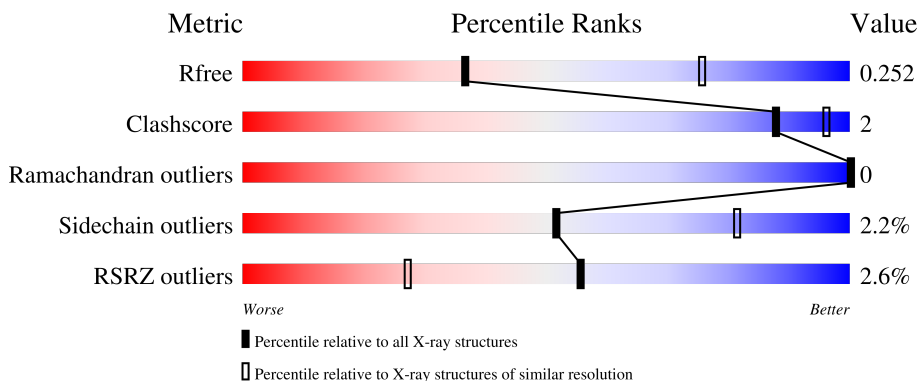
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	227	 88% 8%
1	B	227	 88% 9%
1	C	227	 86% 5% 9%
2	D	816	 89% 7%
2	E	816	 51% 45%

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Mol	Chain	Length	Quality of chain
2	F	816	
3	G	8	
4	H	7	

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	PGE	D	903	-	-	-	X
6	PGE	F	901	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 41611 atoms, of which 20443 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 Uncharacterized protein DKFZp686C11235.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	208	Total 3267	C 1049	H 1620	N 276	O 315	S 7	62	0	0
1	C	206	Total 3187	C 1025	H 1580	N 271	O 304	S 7	66	0	0
1	B	207	Total 3224	C 1029	H 1606	N 275	O 307	S 7	62	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	CYS	LEU	engineered mutation	UNP Q6MZV7
A	382	ALA	GLU	engineered mutation	UNP Q6MZV7
C	234	CYS	LEU	engineered mutation	UNP Q6MZV7
C	382	ALA	GLU	engineered mutation	UNP Q6MZV7
B	234	CYS	LEU	engineered mutation	UNP Q6MZV7
B	382	ALA	GLU	engineered mutation	UNP Q6MZV7

- Molecule 2 is a protein called Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	D	788	Total 12398	C 3936	H 6137	N 1069	O 1241	S 15	183	0	0
2	E	447	Total 6793	C 2166	H 3346	N 585	O 687	S 9	133	0	0
2	F	769	Total 11928	C 3801	H 5879	N 1029	O 1204	S 15	192	0	0

There are 36 discrepancies between the modelled and reference sequences:

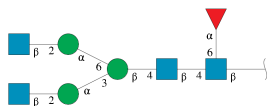
Chain	Residue	Modelled	Actual	Comment	Reference
D	37	MET	-	initiating methionine	UNP A0A8H2N1T2
D	184	ALA	ASP	engineered mutation	UNP A0A8H2N1T2

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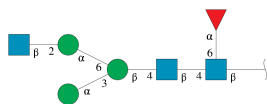
Chain	Residue	Modelled	Actual	Comment	Reference
D	186	LEU	GLU	engineered mutation	UNP A0A8H2N1T2
D	844	LEU	-	expression tag	UNP A0A8H2N1T2
D	845	LEU	-	expression tag	UNP A0A8H2N1T2
D	846	GLU	-	expression tag	UNP A0A8H2N1T2
D	847	HIS	-	expression tag	UNP A0A8H2N1T2
D	848	HIS	-	expression tag	UNP A0A8H2N1T2
D	849	HIS	-	expression tag	UNP A0A8H2N1T2
D	850	HIS	-	expression tag	UNP A0A8H2N1T2
D	851	HIS	-	expression tag	UNP A0A8H2N1T2
D	852	HIS	-	expression tag	UNP A0A8H2N1T2
E	37	MET	-	initiating methionine	UNP A0A8H2N1T2
E	184	ALA	ASP	engineered mutation	UNP A0A8H2N1T2
E	186	LEU	GLU	engineered mutation	UNP A0A8H2N1T2
E	844	LEU	-	expression tag	UNP A0A8H2N1T2
E	845	LEU	-	expression tag	UNP A0A8H2N1T2
E	846	GLU	-	expression tag	UNP A0A8H2N1T2
E	847	HIS	-	expression tag	UNP A0A8H2N1T2
E	848	HIS	-	expression tag	UNP A0A8H2N1T2
E	849	HIS	-	expression tag	UNP A0A8H2N1T2
E	850	HIS	-	expression tag	UNP A0A8H2N1T2
E	851	HIS	-	expression tag	UNP A0A8H2N1T2
E	852	HIS	-	expression tag	UNP A0A8H2N1T2
F	37	MET	-	initiating methionine	UNP A0A8H2N1T2
F	184	ALA	ASP	engineered mutation	UNP A0A8H2N1T2
F	186	LEU	GLU	engineered mutation	UNP A0A8H2N1T2
F	844	LEU	-	expression tag	UNP A0A8H2N1T2
F	845	LEU	-	expression tag	UNP A0A8H2N1T2
F	846	GLU	-	expression tag	UNP A0A8H2N1T2
F	847	HIS	-	expression tag	UNP A0A8H2N1T2
F	848	HIS	-	expression tag	UNP A0A8H2N1T2
F	849	HIS	-	expression tag	UNP A0A8H2N1T2
F	850	HIS	-	expression tag	UNP A0A8H2N1T2
F	851	HIS	-	expression tag	UNP A0A8H2N1T2
F	852	HIS	-	expression tag	UNP A0A8H2N1T2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



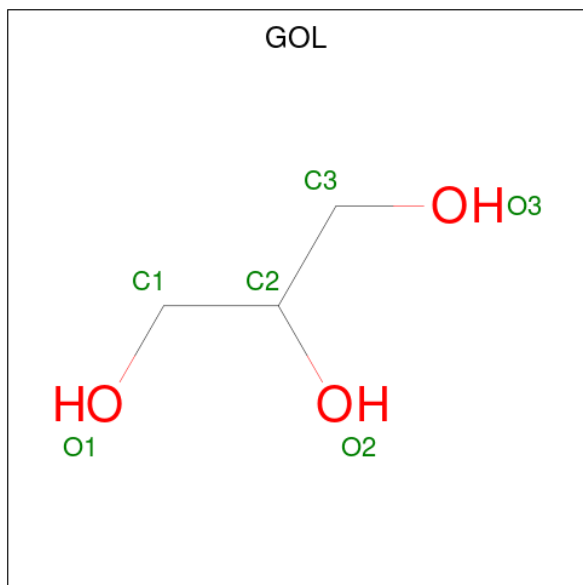
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
3	G	8	195	56	96	4	39	18	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
4	H	7	167	48	82	3	34	15	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



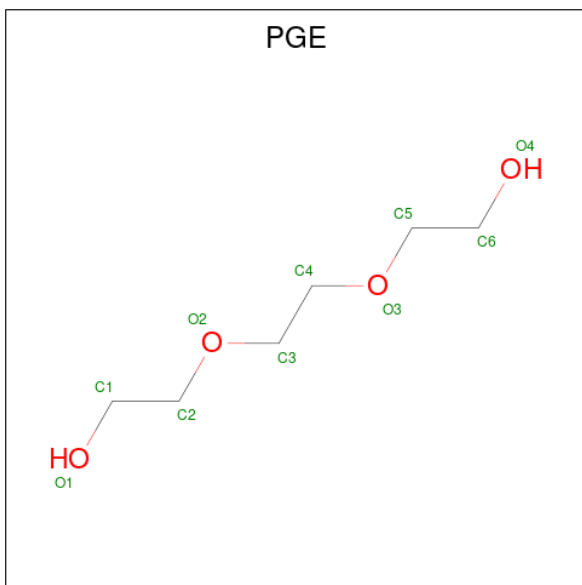
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	14	3	8	3	2	0
5	D	1	14	3	8	3	2	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	2	0
			14	3	8	3		
5	B	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	1	0
			24	6	14	4		
6	D	1	Total	C	H	O	1	0
			24	6	14	4		
6	D	1	Total	C	H	O	1	0
			24	6	14	4		
6	F	1	Total	C	H	O	1	0
			16	4	9	3		
6	F	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	Ca	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total	O	0	0
			43	43		
8	D	105	Total	O	0	0
			105	105		
8	C	1	Total	O	0	0
			1	1		
8	E	19	Total	O	0	0
			19	19		
8	F	51	Total	O	0	0
			51	51		
8	B	62	Total	O	0	0
			62	62		

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.

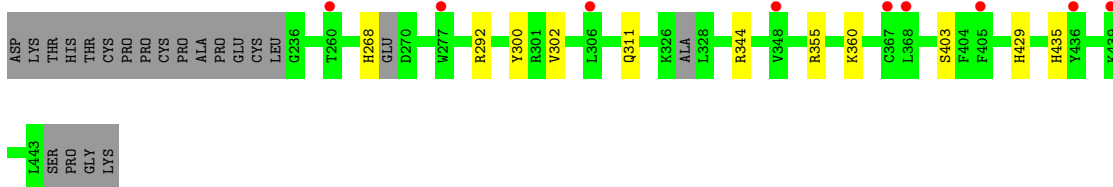
- Molecule 1: Uncharacterized protein DKFZp686C11235

Chain A: 




- Molecule 1: Uncharacterized protein DKFZp686C11235

Chain C: 




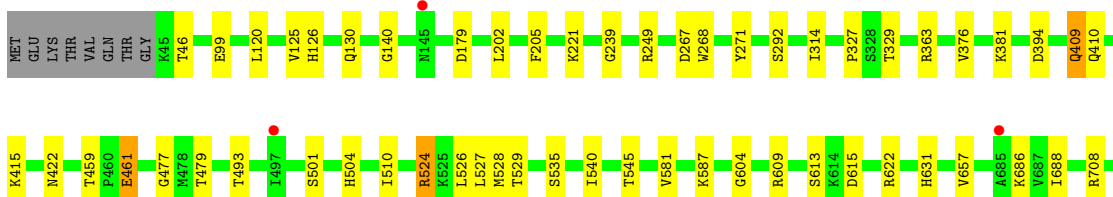
- Molecule 1: Uncharacterized protein DKFZp686C11235

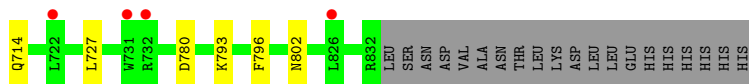
Chain B: 



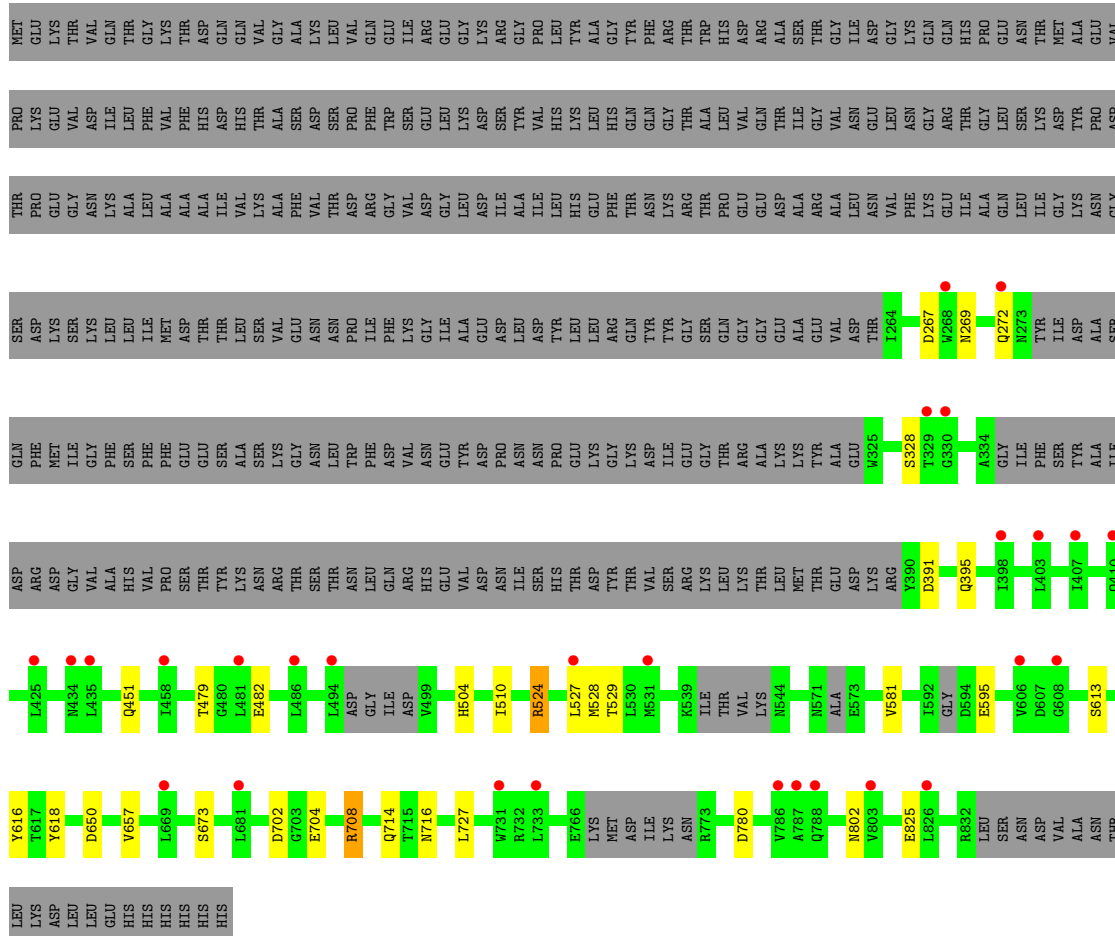
- Molecule 2: Endo-beta-N-acetylglucosaminidase

Chain D: 

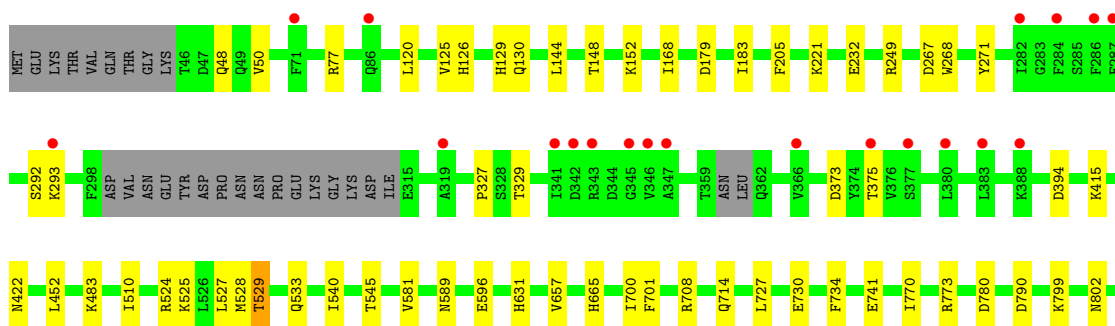
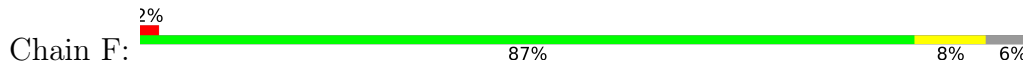


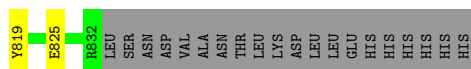


• Molecule 2: Endo-beta-N-acetylglucosaminidase

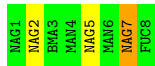


• Molecule 2: Endo-beta-N-acetylglucosaminidase





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	228.78Å 228.78Å 161.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 3.00 49.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.91-3.00) 93.7 (49.91-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.216 , 0.252 0.221 , 0.252	Depositor DCC
R_{free} test set	4385 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	41611	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: NAG, BMA, GOL, FUC, MAN, PGE, CA

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	0.30	0/1693	0.55	0/2309
1	B	0.30	0/1660	0.54	0/2262
1	C	0.30	0/1650	0.54	0/2249
2	D	0.28	0/6379	0.53	0/8619
2	E	0.28	0/3500	0.52	0/4732
2	F	0.28	0/6161	0.51	0/8334
All	All	0.28	0/21043	0.53	0/28505

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	4
2	E	0	1
2	F	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	363	ARG	Sidechain
2	D	524	ARG	Sidechain
2	D	609	ARG	Sidechain
2	D	622	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	524	ARG	Sidechain

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	1647	1620	1603	6	0
1	B	1618	1606	1581	6	0
1	C	1607	1580	1548	6	0
2	D	6261	6137	6102	29	0
2	E	3447	3346	3262	13	0
2	F	6049	5879	5814	24	0
3	G	99	96	85	1	0
4	H	85	82	73	1	0
5	A	6	8	8	1	0
5	B	12	16	16	0	0
5	D	6	8	8	0	0
6	D	30	42	42	4	0
6	F	17	23	23	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	A	43	0	0	2	0
8	B	62	0	0	2	0
8	C	1	0	0	0	0
8	D	105	0	0	1	0
8	E	19	0	0	1	0
8	F	51	0	0	2	0
All	All	21168	20443	20165	83	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 2.

The worst 5 of 83 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:F:144:LEU:HD11	2:F:183:ILE:HD13	1.67	0.76
2:F:452:LEU:O	8:F:1001:HOH:O	2.11	0.68
2:E:595:GLU:HG3	2:E:618:TYR:CD2	2.29	0.68
2:F:148:THR:HA	2:F:152:LYS:HE2	1.75	0.68
1:A:295:GLN:HG2	8:A:635:HOH:O	1.95	0.67

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	206/227 (91%)	203 (98%)	3 (2%)	0	100	100
1	B	203/227 (89%)	201 (99%)	2 (1%)	0	100	100
1	C	200/227 (88%)	196 (98%)	4 (2%)	0	100	100
2	D	786/816 (96%)	756 (96%)	30 (4%)	0	100	100
2	E	431/816 (53%)	411 (95%)	20 (5%)	0	100	100
2	F	763/816 (94%)	732 (96%)	31 (4%)	0	100	100
All	All	2589/3129 (83%)	2499 (96%)	90 (4%)	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	190/209 (91%)	188 (99%)	2 (1%)	73	90
1	B	185/209 (88%)	183 (99%)	2 (1%)	73	90
1	C	181/209 (87%)	180 (99%)	1 (1%)	86	95
2	D	678/712 (95%)	666 (98%)	12 (2%)	59	85
2	E	360/712 (51%)	349 (97%)	11 (3%)	40	75
2	F	645/712 (91%)	624 (97%)	21 (3%)	38	73
All	All	2239/2763 (81%)	2190 (98%)	49 (2%)	52	81

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	205	PHE
2	F	528	MET
2	F	232	GLU
2	F	293	LYS
2	F	589	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

15 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
3	NAG	G	1	3,1	14,14,15	0.59	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.51	0	17,19,21	1.33	1 (5%)
3	BMA	G	3	3	11,11,12	0.64	0	15,15,17	0.94	0
3	MAN	G	4	3	11,11,12	0.43	0	15,15,17	0.64	0
3	NAG	G	5	3	14,14,15	0.41	0	17,19,21	0.89	1 (5%)
3	MAN	G	6	3	11,11,12	0.53	0	15,15,17	0.70	0
3	NAG	G	7	3	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
3	FUC	G	8	3	10,10,11	0.46	0	14,14,16	0.45	0
4	NAG	H	1	4,1	14,14,15	0.51	0	17,19,21	0.44	0
4	NAG	H	2	4	14,14,15	0.42	0	17,19,21	1.04	1 (5%)
4	BMA	H	3	4	11,11,12	0.39	0	15,15,17	0.55	0
4	MAN	H	4	4	11,11,12	0.38	0	15,15,17	0.68	0
4	NAG	H	5	4	14,14,15	0.55	0	17,19,21	0.59	0
4	MAN	H	6	4	11,11,12	0.43	0	15,15,17	0.59	0
4	FUC	H	7	4	10,10,11	0.44	0	14,14,16	0.61	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	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	NAG	G	5	3	-	1/6/23/26	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	0/1/1/1
3	NAG	G	7	3	-	2/6/23/26	0/1/1/1
3	FUC	G	8	3	-	-	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	NAG	H	5	4	-	1/6/23/26	0/1/1/1
4	MAN	H	6	4	-	1/2/19/22	0/1/1/1
4	FUC	H	7	4	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	O5-C1-C2	4.60	118.56	111.29
4	H	2	NAG	O5-C1-C2	3.28	116.46	111.29
3	G	7	NAG	O5-C1-C2	2.29	114.91	111.29
3	G	5	NAG	O5-C1-C2	2.06	114.54	111.29

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

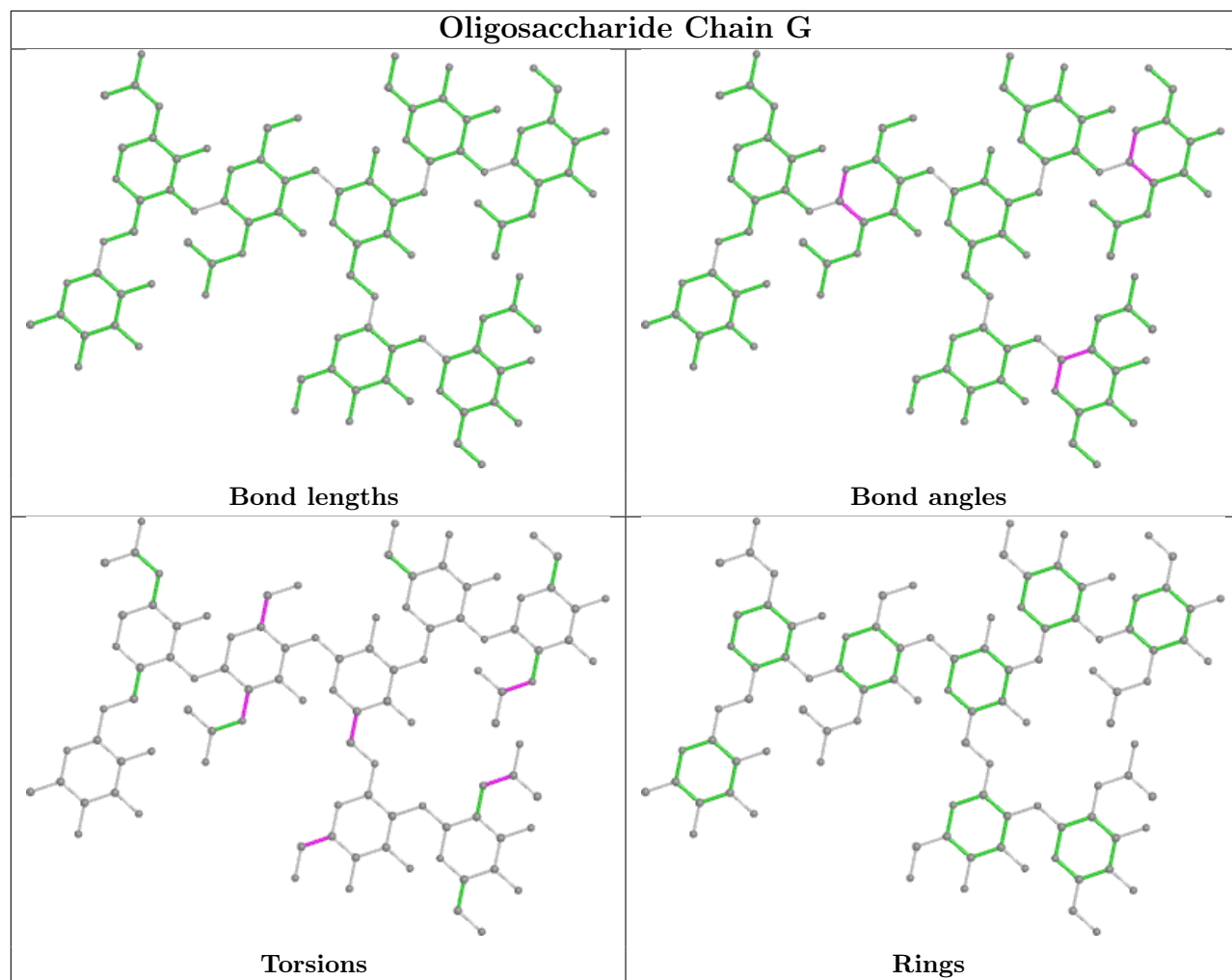
Mol	Chain	Res	Type	Atoms
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	G	6	MAN	O5-C5-C6-O6
3	G	6	MAN	C4-C5-C6-O6
3	G	7	NAG	C8-C7-N2-C2

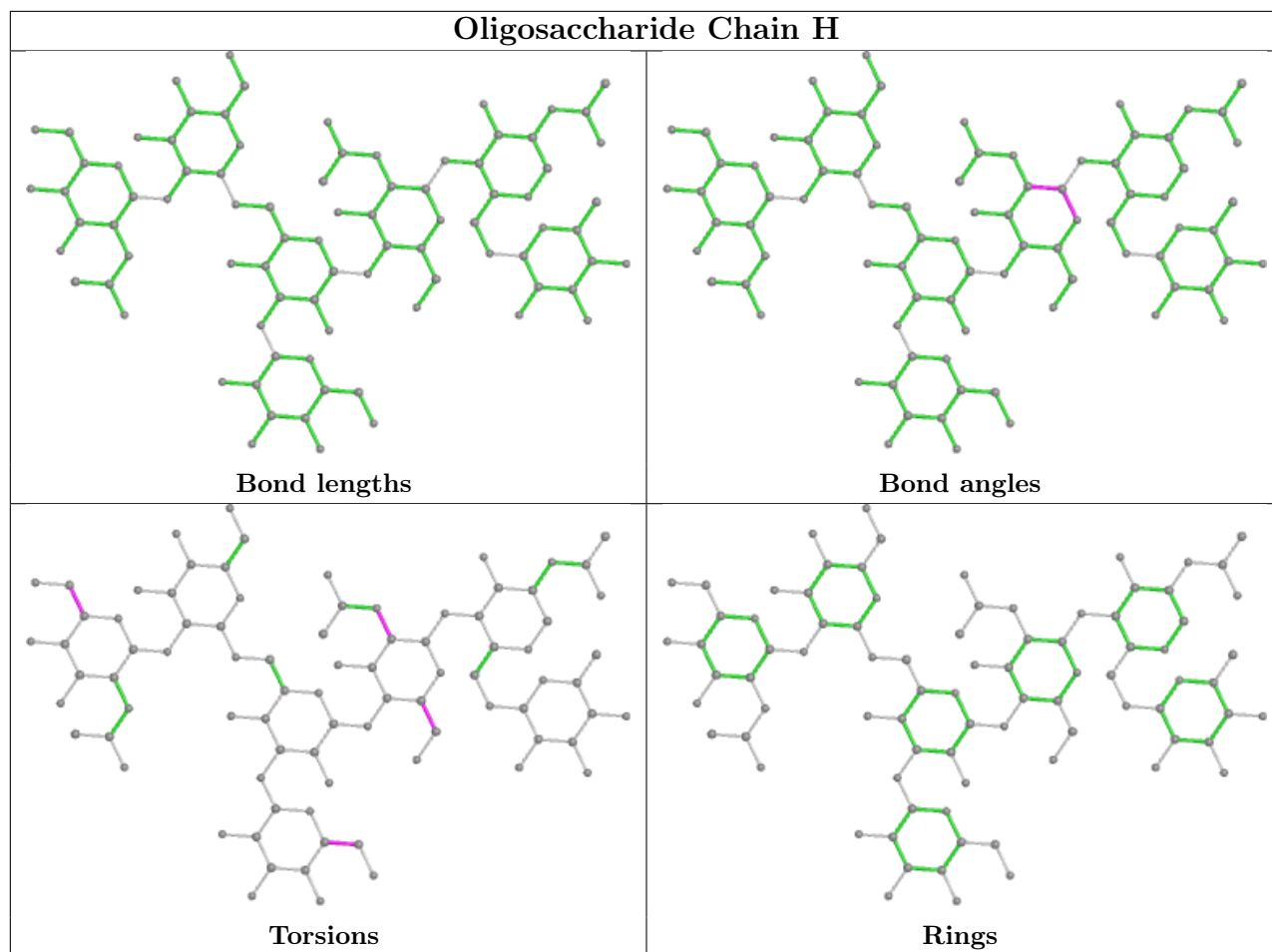
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
3	G	7	NAG	1	0
4	H	2	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
5	GOL	B	502	-	5,5,5	0.10	0	5,5,5	0.29	0
6	PGE	D	902	-	9,9,9	0.20	0	8,8,8	0.12	0
6	PGE	F	901	-	6,6,9	0.23	0	5,5,8	0.25	0
5	GOL	D	904	-	5,5,5	0.10	0	5,5,5	0.28	0
6	PGE	F	902	-	9,9,9	0.25	0	8,8,8	0.11	0
5	GOL	B	501	-	5,5,5	0.10	0	5,5,5	0.36	0
6	PGE	D	901	-	9,9,9	0.21	0	8,8,8	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	501	-	5,5,5	0.09	0	5,5,5	0.30	0
6	PGE	D	903	-	9,9,9	0.22	0	8,8,8	0.17	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
5	GOL	B	502	-	-	4/4/4/4	-
6	PGE	D	902	-	-	3/7/7/7	-
6	PGE	F	901	-	-	1/4/4/7	-
5	GOL	D	904	-	-	0/4/4/4	-
6	PGE	F	902	-	-	4/7/7/7	-
5	GOL	B	501	-	-	2/4/4/4	-
6	PGE	D	901	-	-	6/7/7/7	-
5	GOL	A	501	-	-	0/4/4/4	-
6	PGE	D	903	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GOL	C1-C2-C3-O3
5	B	502	GOL	C1-C2-C3-O3
5	B	502	GOL	O2-C2-C3-O3
6	D	901	PGE	O1-C1-C2-O2
6	F	902	PGE	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	901	PGE	4	0
5	A	501	GOL	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, 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	208/227 (91%)	0.12	1 (0%) 91 75	61, 85, 125, 152	0
1	B	207/227 (91%)	0.28	3 (1%) 75 49	59, 86, 146, 175	0
1	C	206/227 (90%)	0.41	9 (4%) 34 13	94, 119, 160, 183	0
2	D	788/816 (96%)	0.22	7 (0%) 84 63	57, 91, 120, 153	0
2	E	447/816 (54%)	0.28	28 (6%) 20 6	83, 134, 159, 166	0
2	F	769/816 (94%)	0.18	20 (2%) 56 27	84, 107, 140, 157	0
All	All	2625/3129 (83%)	0.23	68 (2%) 56 27	57, 104, 149, 183	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	277	TRP	4.9
2	F	346	VAL	4.8
2	E	435	LEU	4.7
2	D	826	LEU	4.3
2	E	330	GLY	4.1

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

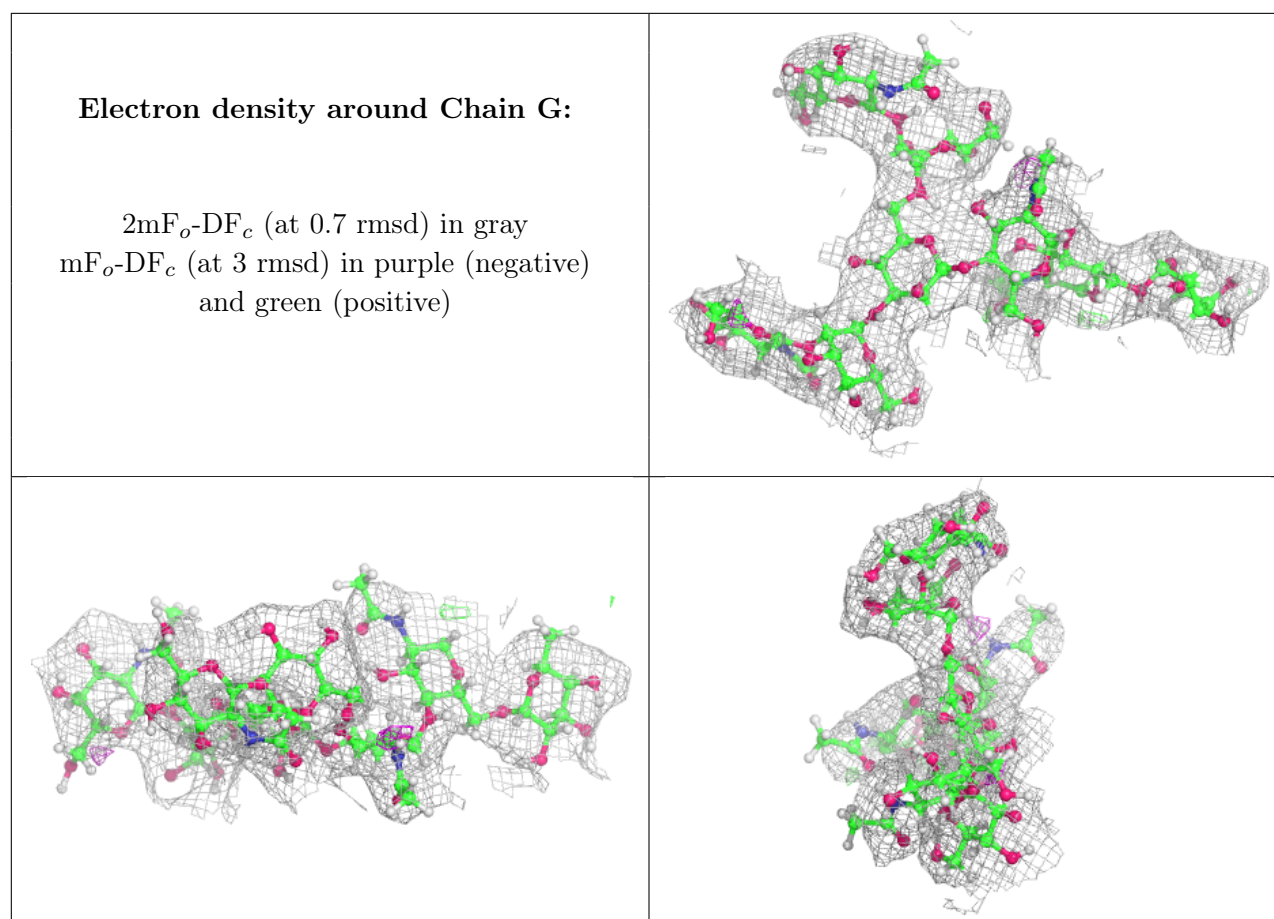
There are no non-standard protein/DNA/RNA residues in this entry.

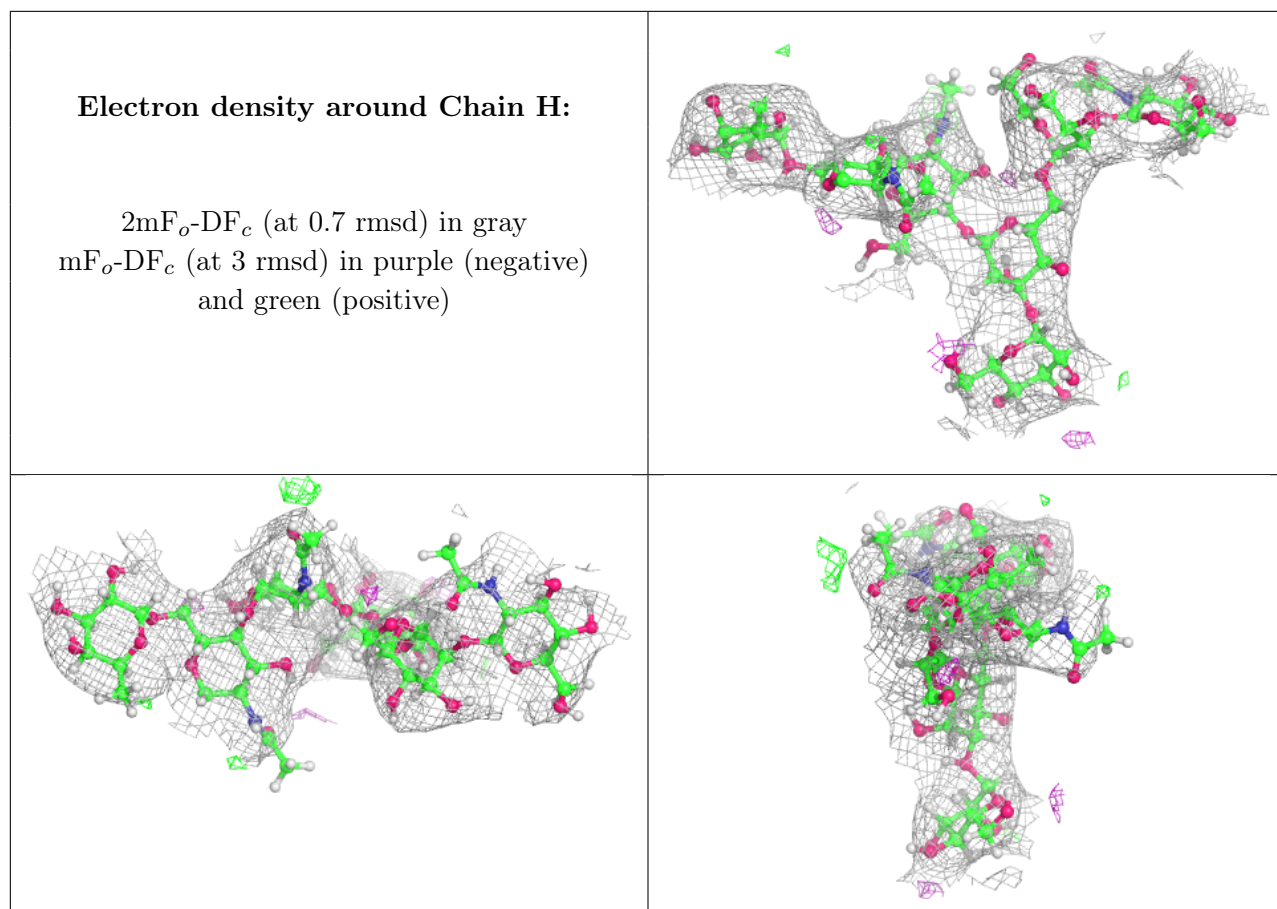
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
4	MAN	H	6	11/12	0.82	0.19	69,123,129,130	3
4	NAG	H	5	14/15	0.86	0.27	69,144,147,153	3
4	NAG	H	2	14/15	0.88	0.22	69,128,134,138	2
4	MAN	H	4	11/12	0.90	0.19	69,124,128,137	2
3	NAG	G	7	14/15	0.91	0.27	69,91,95,97	3
4	NAG	H	1	14/15	0.91	0.19	69,118,127,127	1
4	BMA	H	3	11/12	0.92	0.15	69,123,127,129	1
3	NAG	G	5	14/15	0.92	0.30	69,88,92,95	3
3	MAN	G	6	11/12	0.93	0.19	69,85,88,88	2
4	FUC	H	7	10/11	0.93	0.15	69,106,109,110	3
3	NAG	G	1	14/15	0.95	0.22	63,72,90,96	1
3	NAG	G	2	14/15	0.96	0.27	65,71,76,80	2
3	BMA	G	3	11/12	0.97	0.20	69,71,73,75	2
3	FUC	G	8	10/11	0.97	0.21	69,74,74,77	3
3	MAN	G	4	11/12	0.97	0.24	69,71,74,81	2

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
6	PGE	D	903	10/10	0.51	1.23	69,142,148,150	1
6	PGE	F	902	10/10	0.65	0.34	69,125,132,133	1
6	PGE	F	901	7/10	0.67	0.52	69,104,108,109	1
5	GOL	D	904	6/6	0.76	0.37	69,105,108,110	2
5	GOL	A	501	6/6	0.77	0.33	69,96,100,100	2
5	GOL	B	502	6/6	0.79	0.31	69,112,116,116	2
7	CA	D	905	1/1	0.80	0.18	135,135,135,135	0
6	PGE	D	901	10/10	0.82	0.48	69,105,110,111	1
5	GOL	B	501	6/6	0.85	0.36	69,104,107,109	2
6	PGE	D	902	10/10	0.85	0.52	69,116,118,119	1
7	CA	F	903	1/1	0.90	0.13	123,123,123,123	0
7	CA	E	901	1/1	0.96	0.19	124,124,124,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.