Full wwPDB X-ray Structure Validation 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)

The following versions of software and data (see references ⓘ) were used in the production of this report:

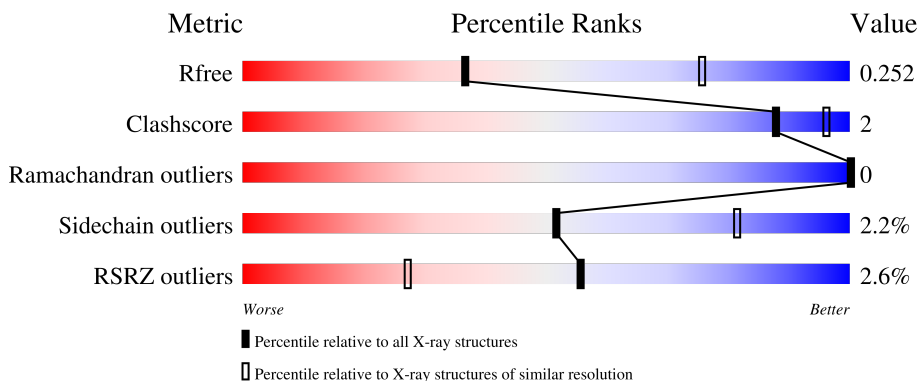|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	Percentile Ranks	Value
Rfree		0.252
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		2.6%

Worse — *Better*

▮ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution

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 <=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	4% 86% 5% 9%
2	D	816	.% 89% 7% ·
2	E	816	3% 51% · 45%

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Mol	Chain	Length	Quality of chain
2	F	816	2% 87% 8% 6%
3	G	8	62% 25% 12%
4	H	7	71% 14% 14%

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 ⓘ

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

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

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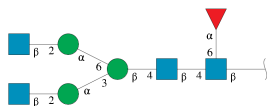
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	8	Total 195	C 56	H 96	N 4	O 39	18	0	0

- 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.
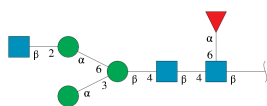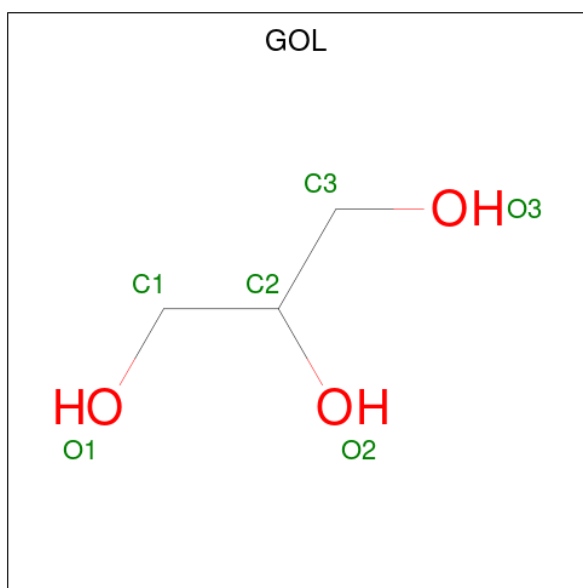

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	7	Total 167	C 48	H 82	N 3	O 34	15	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
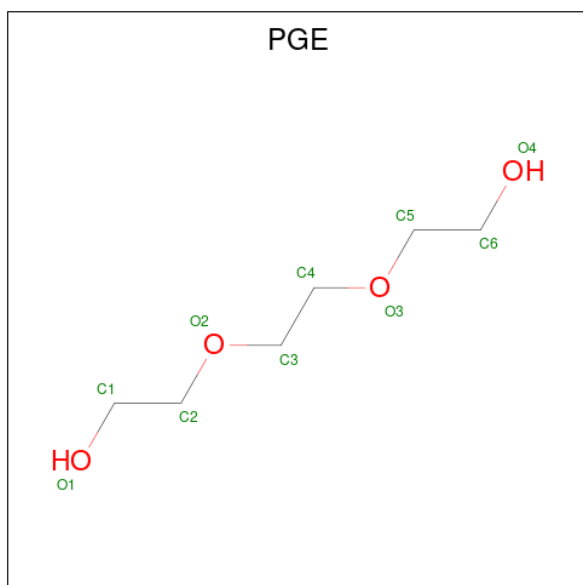
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total 24	C 6	H 14	O 4	1	0
6	D	1	Total 24	C 6	H 14	O 4	1	0
6	D	1	Total 24	C 6	H 14	O 4	1	0
6	F	1	Total 16	C 4	H 9	O 3	1	0
6	F	1	Total 24	C 6	H 14	O 4	1	0

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

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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total O 43 43		0	0
8	D	105	Total O 105 105		0	0
8	C	1	Total O 1 1		0	0
8	E	19	Total O 19 19		0	0
8	F	51	Total O 51 51		0	0
8	B	62	Total O 62 62		0	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: Uncharacterized protein DKFZp686C11235

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• Molecule 1: Uncharacterized protein DKFZp686C11235

• Molecule 2: Endo-beta-N-acetylglucosaminidase

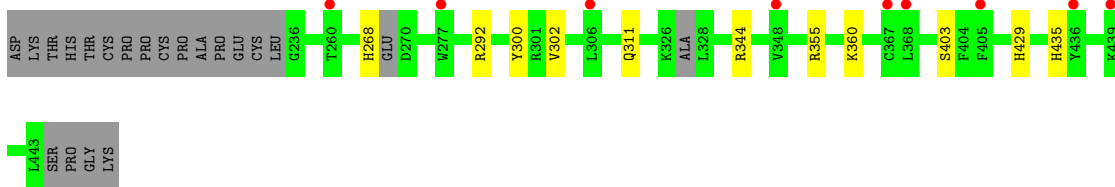Q714 L722 L727 W731 R732 D780 K793 F796 N802 L826 R832 LEU SER ASN ASP VAL ALA ASN THR LEU LYS ASP LEU LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: Endo-beta-N-acetylglucosaminidase

Chain E:

3%

51%	•	45%

MET GLU LYS THR VAL GLN THR GLY LYS THR ASP GLN GLN VAL GLY ALA LYS LEU VAL GLN GLU ILE ARG GLU GLY LYS ARG PRO LEU THR ALA GLY TYR PHE ARG THR TRP HIS ASP ARG ALA SER THR GLY ILE ASP GLY LYS GLN HIS PRO GLU ASN THR MET ALA GLU VAL

PRO LYS GLU VAL ASP ILE LEU PHE VAL PHE HIS ASP ASN THR ALA SER ASP SER PRO PHE TRP SER GLU LEU LYS ASP SER VAL VAL HIS LEU LEU GLN GLN THR ALA LEU VAL GLN THR ILE GLY VAL ASN GLU LEU ASN GLY ARG THR GLY LEU SER LYS ASP TYR PRO ASP

THR PRO GLU ASN LYS LEU ALA ALA ALA ILE VAL LYS ALA PHE VAL THR ASP ARG GLY VAL ASP GLY LEU ASP ILE ALA ILE LEU GLU HIS GLY PHE THR ASN LYS ARG THR PRO GLU GLU ASP ALA ALA ALA LEU ASN VAL PHE LYS GLU LEU ASN GLY ARG THR GLY LEU LYS ASN GLY

SER ASP LYS SER LYS LEU LEU LEU MET ASP THR THR LEU SER VAL GLU ASN ASN PRO ILE PHE LYS ILE ALA GLU ASP LEU ASP TYR LEU LEU ARG GLN TYR TYR GLY SER GLN GLY GLU GLU ALA GLU ASP VAL ASP THR I264 ASP D267 W268 N269 GLY Q272 N273 TYR ILE ASP ALA SER

GLN PHE MET ILE GLY PHE SER PHE PHE GLU GLU SER ALA SER LYS GLY ASN LEU TRP PHE ASP VAL ASN GLU HIS GLU ASN ILE GLY VAL GLY THR TYR LEU ARG GLN TYR TYR GLY SER GLN GLY GLU GLU ALA GLU GLU W325 ALA LYS LYS TYR ALA GLU S328 T329 G330 A334 GLY ILE PHE SER TYR ALA ILE

ASP ARG ASP GLY VAL ALA HIS VAL PRO SER THR TYR LYS ASN ARG THR SER ASN LEU GLN ARG GLU HIS ASP VAL ASP ASN ILE SER HIS THR ASP TYR THR VAL SER ARG ARG LEU LYS THR LEU MET THR GLU ASP LYS ARG Y390 D391 GLN Q395 ILE I398 L403 I407 Q410

L425 N434 L435 Q451 I458 T479 G480 L481 E482 L486 L494 ASP GLY ILE ASP V499 H504 I510 R524 L527 M528 T529 L530 M531 K539 ILE THR VAL LYS N544 N571 ALA E573 V581 I592 GLY D594 E595 V606 D607 G608 S613

Y616 T617 Y618 D650 V657 L569 S673 L681 D702 G703 E704 R708 Q714 T715 N716 L727 W731 R732 L733 E766 LYS MET ASP ILE LYS ASN R773 D780 V786 A787 Q788 N802 V803 E825 L826 R832 LEU SER ASN ASP VAL ALA ASN THR

LEU LYS ASP LEU LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: Endo-beta-N-acetylglucosaminidase

Chain F:

2%

87%	8%	6%

MET GLU LYS THR VAL GLN THR GLY LYS T46 D47 Q48 Q49 V50 F71 R77 Q86 L120 V125 H126 H129 Q130 L144 T148 K152 I168 D179 I183 F205 K221 E232 R249 D267 W268 Y271 I282 G283 F284 S285 F286 F287

S292 K293 F298 ASP VAL ASN GLU TYR ASP PRO ASN ASN PRO GLU LYS GLY LYS ASP ILE E315 A319 P327 S328 T329 I341 D342 R343 D344 G345 V346 A347 T359 ASN LEU Q362 V366 D373 Y374 T375 V376 S377 L380 L383 K388 D394 K415

N422 L452 K483 I510 R524 K525 L526 L527 M528 T529 Q533 I540 T545 V581 N589 E596 H631 V657 H665 I700 F701 R708 Q714 L727 E730 F734 E741 I770 R773 D780 D790 K799 N802

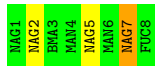Y819 E825 R832 LEU SER ASN ASP VAL ALA ASN THR LEU LYS ASP LEU LEU GLU HIS HIS HIS HIS HIS HIS

• 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

Chain G:

62%	25%	12%

NAG1 NAG2 BMA3 MAN4 NAG5 MAN6 NAG7 FUC8

• 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

Chain H:

71%	14%	14%

NAG1 NAG2 BMA3 MAN4 NAG5 MAN6 FUC7

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.52 (at 3.01Å)	Xtriage
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	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

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.

All (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
2	F	524	ARG	Sidechain

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	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.

All (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
1:B:443:LEU:O	8:B:601:HOH:O	2.14	0.66
2:F:665:HIS:ND1	8:F:1002:HOH:O	2.32	0.60
2:D:587:LYS:HE2	6:D:901:PGE:H4	1.84	0.59
1:A:256:THR:OG1	8:A:601:HOH:O	2.15	0.59
2:F:529:THR:O	2:F:533:GLN:HG2	2.02	0.58
2:D:540:ILE:HG23	2:D:545:THR:HG21	1.86	0.57
2:E:702:ASP:O	2:E:825:GLU:OE2	2.25	0.55
2:F:373:ASP:OD2	2:F:375:THR:OG1	2.25	0.54
2:F:540:ILE:HG23	2:F:545:THR:HG21	1.90	0.54
2:D:524:ARG:O	2:D:528:MET:HG2	2.08	0.53
4:H:1:NAG:O3	4:H:2:NAG:H2	2.09	0.53
1:C:311:GLN:OE1	2:F:819:TYR:HA	2.10	0.52
2:D:510:ILE:HD11	2:D:527:LEU:HD13	1.93	0.51
2:D:604:GLY:O	8:D:1001:HOH:O	2.18	0.51
2:F:394:ASP:OD1	2:F:415:LYS:NZ	2.43	0.51
2:D:99:GLU:O	2:D:381:LYS:HG3	2.09	0.51
1:B:355:ARG:NH2	8:B:604:HOH:O	2.36	0.51
2:D:329:THR:HB	2:D:422:ASN:ND2	2.25	0.51
2:E:595:GLU:HG3	2:E:618:TYR:CE2	2.45	0.51
2:D:394:ASP:OD1	2:D:415:LYS:NZ	2.44	0.50
2:E:524:ARG:O	2:E:528:MET:HG2	2.11	0.50
2:D:409:GLN:HG3	2:D:410:GLN:HG3	1.93	0.50
2:D:459:THR:OG1	2:D:461:GLU:HG2	2.11	0.49
2:F:329:THR:HB	2:F:422:ASN:ND2	2.27	0.49
1:C:355:ARG:H	1:C:355:ARG:CD	2.24	0.49
2:F:510:ILE:HD11	2:F:527:LEU:HD13	1.95	0.49
2:F:179:ASP:O	2:F:221:LYS:HA	2.13	0.48
1:A:267:SER:OG	1:A:270:ASP:OD1	2.32	0.48
2:D:179:ASP:O	2:D:221:LYS:HA	2.14	0.48
2:D:126:HIS:O	2:D:130:GLN:HG2	2.14	0.48
2:D:581:VAL:HG21	2:D:657:VAL:HG21	1.96	0.48
2:E:510:ILE:HD11	2:E:527:LEU:HD13	1.96	0.48
2:F:581:VAL:HG21	2:F:657:VAL:HG21	1.96	0.48
2:E:581:VAL:HG21	2:E:657:VAL:HG21	1.95	0.47
2:F:734:PHE:CD2	2:F:825:GLU:HB3	2.50	0.47
2:F:144:LEU:CD2	2:F:168:ILE:HD13	2.45	0.46
2:D:314:ILE:HG22	2:D:376:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.98	0.46
2:D:140:GLY:HA3	3:G:7:NAG:H81	1.98	0.46
2:E:650:ASP:OD2	2:E:673:SER:OG	2.22	0.46
2:D:535:SER:HB3	2:D:540:ILE:HD11	1.98	0.45
2:F:126:HIS:O	2:F:130:GLN:HG3	2.16	0.45
2:D:268:TRP:CD1	2:D:327:PRO:HB3	2.52	0.45
2:E:269:ASN:O	2:E:272:GLN:HG2	2.17	0.45
1:B:355:ARG:NE	1:B:355:ARG:H	2.14	0.45
2:F:700:ILE:HG13	2:F:701:PHE:CE2	2.52	0.44
2:F:734:PHE:HD2	2:F:825:GLU:HB3	1.83	0.44
2:D:477:GLY:HA2	2:D:501:SER:HB2	1.99	0.44
2:E:613:SER:OG	2:E:616:TYR:HB2	2.18	0.44
2:F:268:TRP:CD1	2:F:327:PRO:HB3	2.53	0.44
2:D:686:LYS:HD2	2:D:688:ILE:HG22	2.00	0.44
1:C:344:ARG:NH1	1:C:403:SER:HB3	2.33	0.44
2:D:120:LEU:O	2:D:125:VAL:HG23	2.19	0.43
2:F:727:LEU:HD11	2:F:802:ASN:HB3	2.00	0.43
2:D:793:LYS:HE3	2:D:796:PHE:CD2	2.54	0.43
1:A:278:TYR:HB2	1:A:320:LYS:HB3	2.01	0.43
2:D:479:THR:O	2:D:504:HIS:ND1	2.47	0.43
2:E:727:LEU:HD11	2:E:802:ASN:HB3	2.01	0.43
1:B:429:HIS:O	1:B:435:HIS:HA	2.19	0.42
2:F:120:LEU:O	2:F:125:VAL:HG23	2.19	0.42
2:E:716:ASN:OD1	8:E:1001:HOH:O	2.21	0.42
1:A:433:HIS:HA	5:A:501:GOL:H32	2.01	0.42
2:E:708:ARG:NH1	1:B:253:ILE:O	2.53	0.42
2:D:267:ASP:HB3	2:D:271:TYR:CE2	2.55	0.42
2:F:267:ASP:HB3	2:F:271:TYR:CE2	2.55	0.42
2:D:727:LEU:HD11	2:D:802:ASN:HB3	2.01	0.41
2:D:493:THR:HG22	6:D:901:PGE:H52	2.03	0.41
2:D:587:LYS:HE2	6:D:901:PGE:H5	2.02	0.41
1:C:429:HIS:O	1:C:435:HIS:HA	2.21	0.41
1:C:268:HIS:CD2	1:C:300:TYR:HH	2.38	0.41
1:C:292:ARG:CG	1:C:302:VAL:HG22	2.51	0.41
2:D:202:LEU:HD11	2:D:239:GLY:HA3	2.02	0.41
2:D:613:SER:OG	2:D:615:ASP:OD1	2.36	0.41
2:E:479:THR:O	2:E:504:HIS:ND1	2.45	0.41
1:A:429:HIS:O	1:A:435:HIS:HA	2.21	0.40
2:D:587:LYS:HE2	6:D:901:PGE:C4	2.50	0.40
2:F:50:VAL:HG11	2:F:129:HIS:HB3	2.02	0.40
2:F:770:ILE:HD13	2:F:773:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

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	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 ⓘ

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

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PROTEIN DATA BANK

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2239/2763 (81%)	2190 (98%)	49 (2%)	52 81

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	THR
1	A	295	GLN
2	D	46	THR
2	D	205	PHE
2	D	249	ARG
2	D	292	SER
2	D	409	GLN
2	D	461	GLU
2	D	526	LEU
2	D	529	THR
2	D	631	HIS
2	D	708	ARG
2	D	714	GLN
2	D	780	ASP
1	C	360	LYS
2	E	267	ASP
2	E	328	SER
2	E	391	ASP
2	E	395	GLN
2	E	451	GLN
2	E	482	GLU
2	E	529	THR
2	E	704	GLU
2	E	708	ARG
2	E	714	GLN
2	E	780	ASP
2	F	48	GLN
2	F	77	ARG
2	F	205	PHE
2	F	232	GLU
2	F	249	ARG
2	F	292	SER
2	F	293	LYS
2	F	483	LYS
2	F	525	LYS
2	F	528	MET
2	F	529	THR

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Mol	Chain	Res	Type
2	F	589	ASN
2	F	596	GLU
2	F	631	HIS
2	F	708	ARG
2	F	714	GLN
2	F	730	GLU
2	F	741	GLU
2	F	780	ASP
2	F	790	ASP
2	F	799	LYS
1	B	340	LYS
1	B	355	ARG

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

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 ⓘ

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

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles			
					Counts	RMSZ	#|Z| > 2		Counts	RMSZ	#|Z| > 2	
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(^{o})	Ideal(^{o})
3	G	2	NAG	O5-C1-C2	4.60	118.56	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

All (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
3	G	7	NAG	O7-C7-N2-C2
3	G	2	NAG	O5-C5-C6-O6
3	G	5	NAG	C8-C7-N2-C2
4	H	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C4-C5-C6-O6
4	H	5	NAG	C4-C5-C6-O6
4	H	6	MAN	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
3	G	3	BMA	O5-C5-C6-O6

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.

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
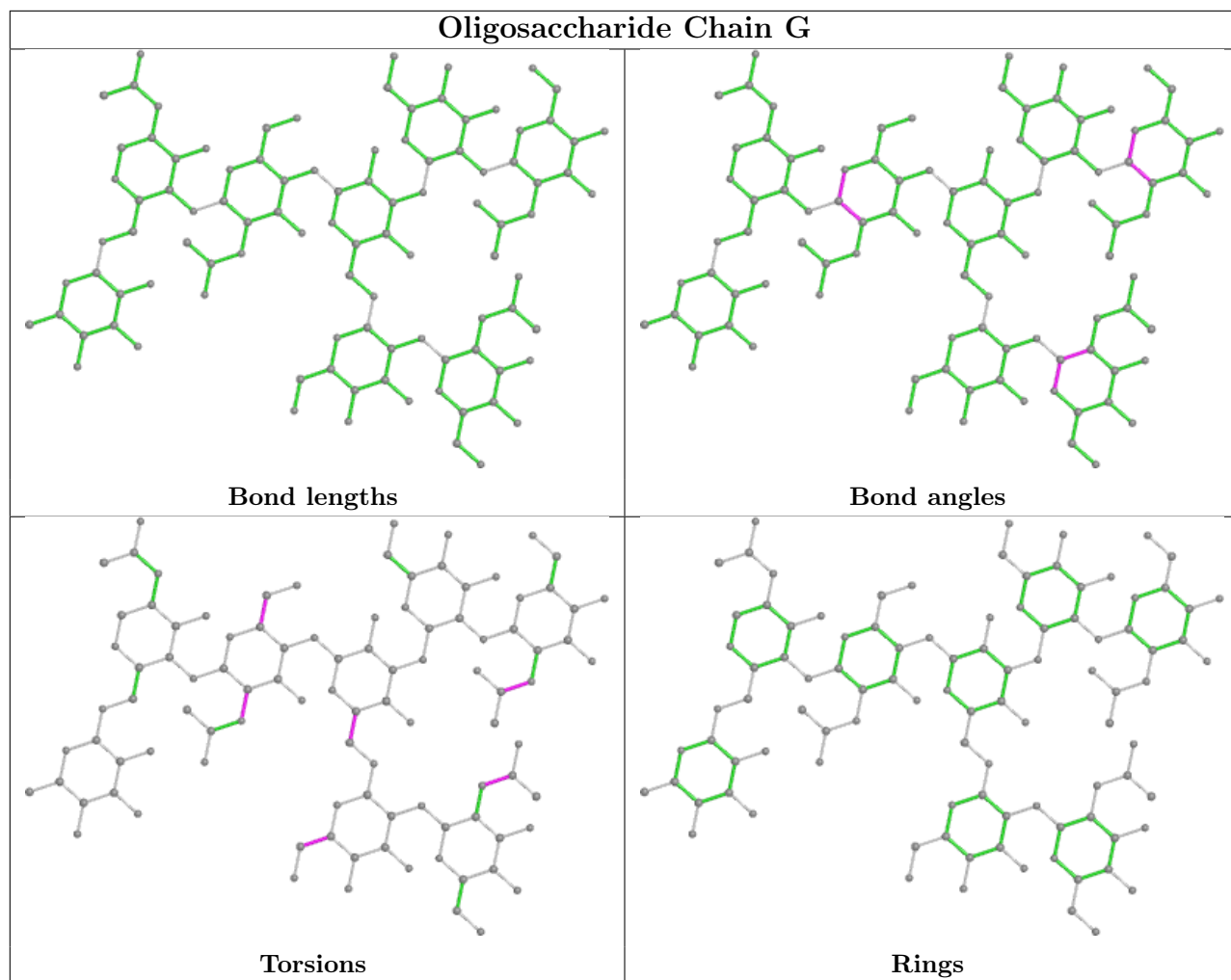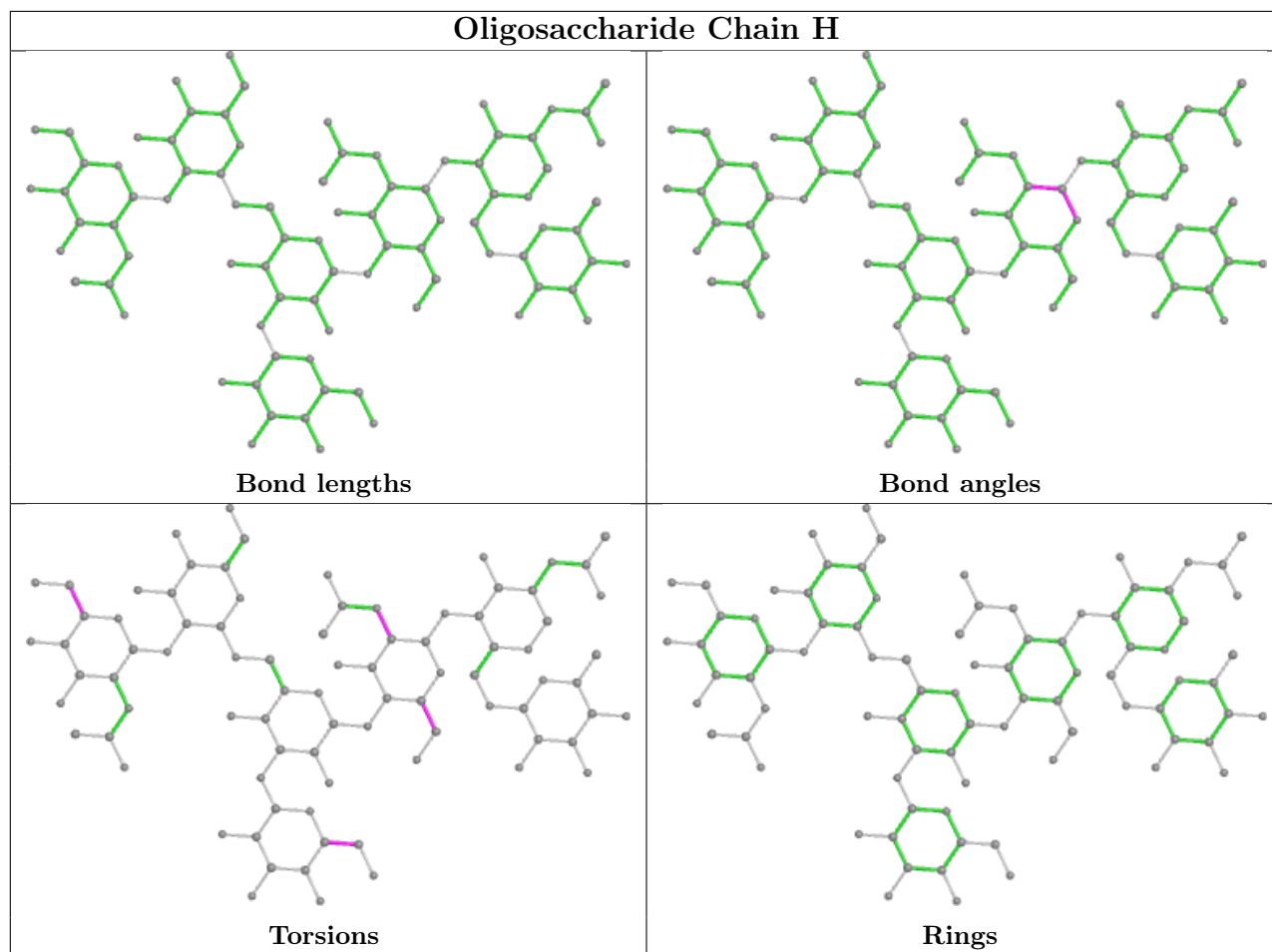
5.6 Ligand geometry ⓘ

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.

All (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
6	D	901	PGE	O2-C3-C4-O3
6	D	903	PGE	O3-C5-C6-O4
6	D	903	PGE	O2-C3-C4-O3
5	B	501	GOL	O2-C2-C3-O3
6	F	902	PGE	O2-C3-C4-O3
6	D	903	PGE	O1-C1-C2-O2
6	F	902	PGE	O3-C5-C6-O4
6	D	902	PGE	O3-C5-C6-O4
6	D	901	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
6	D	903	PGE	C4-C3-O2-C2
6	D	903	PGE	C3-C4-O3-C5
5	B	502	GOL	O1-C1-C2-O2
6	F	902	PGE	C6-C5-O3-C4
6	F	901	PGE	O1-C1-C2-O2
6	D	901	PGE	O3-C5-C6-O4
6	D	901	PGE	C1-C2-O2-C3
6	D	902	PGE	C1-C2-O2-C3
6	D	901	PGE	C3-C4-O3-C5
5	B	502	GOL	O1-C1-C2-C3
6	D	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 ⓘ

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	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

All (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
2	F	341	ILE	3.8
1	C	348	VAL	3.5
2	E	403	LEU	3.5
2	F	345	GLY	3.5
2	E	398	ILE	3.4
2	F	284	PHE	3.4
2	F	319	ALA	3.3
2	F	286	PHE	3.3
2	E	458	ILE	3.2
2	E	329	THR	3.0
2	D	722	LEU	2.9
2	E	826	LEU	2.9
2	E	788	GLN	2.9
2	E	787	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	527	LEU	2.8
1	C	367	CYS	2.8
2	F	377	SER	2.8
2	F	347	ALA	2.8
2	E	407	ILE	2.7
1	C	368	LEU	2.7
2	E	486	LEU	2.7
2	F	71	PHE	2.6
2	E	733	LEU	2.6
2	F	366	VAL	2.6
2	E	268	TRP	2.6
2	E	410	GLN	2.6
2	F	287	PHE	2.5
2	D	731	TRP	2.5
1	C	260	THR	2.5
2	E	531	MET	2.5
2	D	145	ASN	2.4
2	F	388	LYS	2.4
2	E	606	VAL	2.4
2	E	434	ASN	2.4
2	E	681	LEU	2.4
2	D	685	ALA	2.4
2	E	481	LEU	2.4
2	E	669	LEU	2.4
2	F	375	THR	2.3
1	B	297	ASN	2.3
1	B	299	THR	2.3
2	E	272	GLN	2.3
2	D	732	ARG	2.3
1	C	306	LEU	2.3
2	F	293	LYS	2.2
2	E	494	LEU	2.2
1	A	288	LYS	2.2
2	E	786	VAL	2.2
2	E	803	VAL	2.2
2	F	343	ARG	2.2
2	E	608	GLY	2.2
2	F	380	LEU	2.2
2	F	383	LEU	2.2
2	F	342	ASP	2.1
1	C	405	PHE	2.1
2	D	497	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	271	PRO	2.1
2	E	425	LEU	2.1
1	C	436	TYR	2.1
1	C	439	LYS	2.1
2	F	282	ILE	2.1
2	E	731	TRP	2.0
2	F	86	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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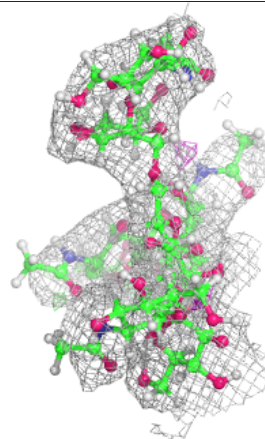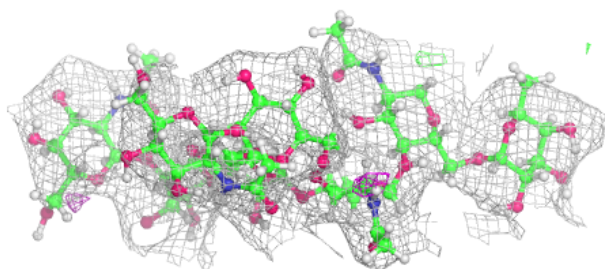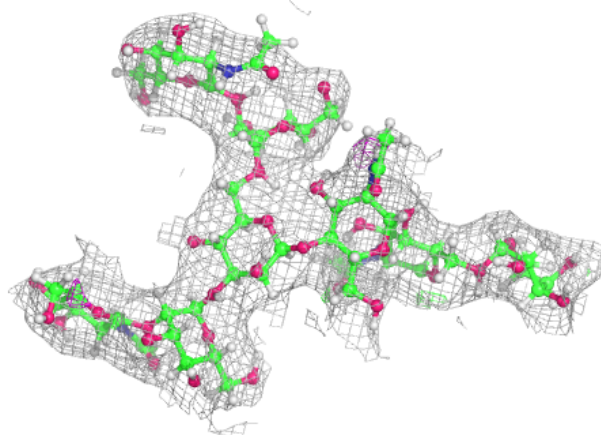
6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	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.

Electron density around Chain G:

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

Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
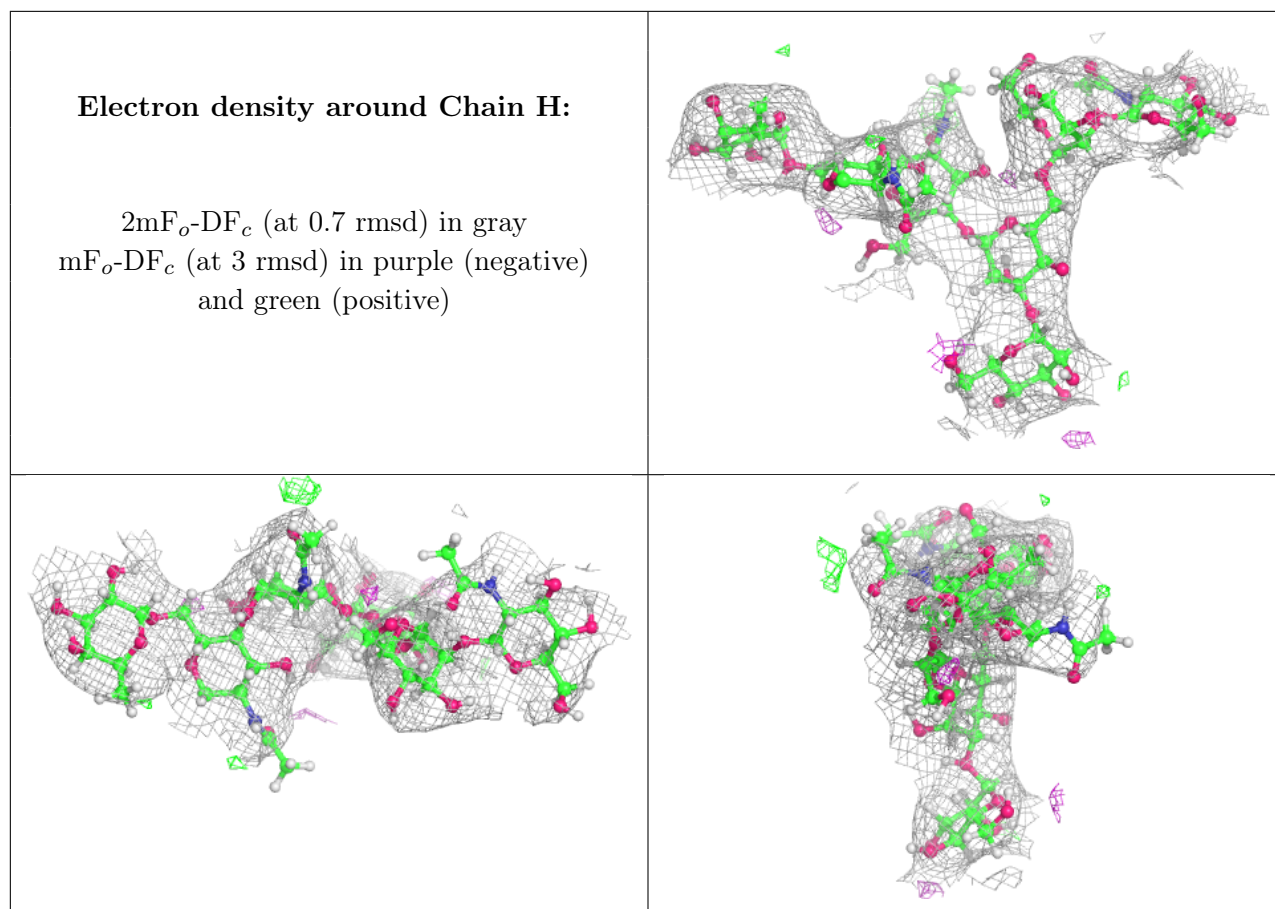
6.4 Ligands (i)

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.