Full wwPDB X-ray Structure Validation Report

Aug 21, 2020 – 06:45 AM BST

PDB ID	:	2YL9
Title	:	INHIBITION OF THE PNEUMOCOCCAL VIRULENCE FACTOR STRH AND MOLECULAR INSIGHTS INTO N-GLYCAN RECOGNITION AND HYDROLYSIS
Authors	:	Pluvinage, B.; Higgins, M.A.; Abbott, D.W.; Robb, C.; Dalia, A.B.; Deng, L.; Weiser, J.N.; Parsons, T.B.; Fairbanks, A.J.; Vocadlo, D.J.; Boraston, A.B.
Deposited on	:	2011-06-01
Resolution	:	2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

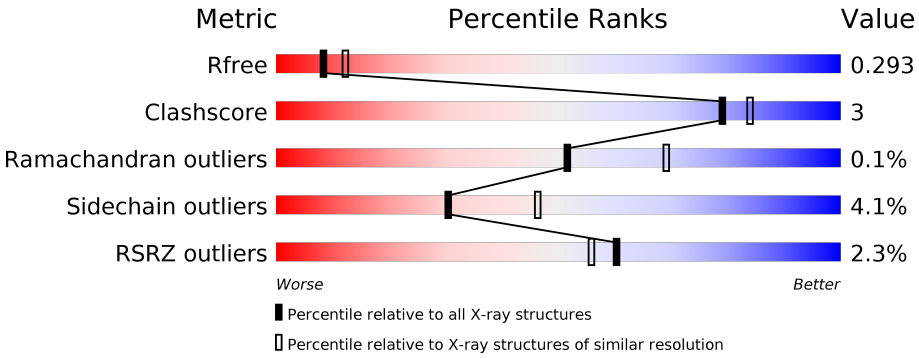
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	457	80% 9% • 10%
1	B	457	2% 79% 9% • 11%
1	C	457	2% 79% 9% • 10%
1	D	457	4% 82% 6% • 10%
2	E	4	50% 50%
2	F	4	25% 75%

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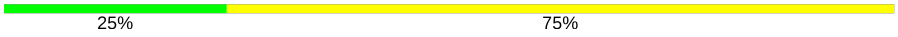
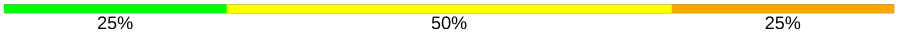
Mol	Chain	Length	Quality of chain
2	G	4	
2	H	4	

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
2	NAG	E	1	-	-	-	X
2	NAG	F	1	-	-	-	X
2	NAG	G	1	-	-	-	X
2	NAG	H	1	-	-	-	X
2	MAN	H	3	-	-	-	X
3	EDO	A	1109	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14260 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 BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	8	0	0
			3269	2096	532	629	12			
1	B	409	Total	C	N	O	S	17	0	0
			3258	2089	530	627	12			
1	C	410	Total	C	N	O	S	19	1	0
			3271	2097	533	629	12			
1	D	411	Total	C	N	O	S	36	0	0
			3269	2096	532	629	12			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	606	MET	-	expression tag	UNP P49610
A	607	GLY	-	expression tag	UNP P49610
A	608	SER	-	expression tag	UNP P49610
A	609	SER	-	expression tag	UNP P49610
A	610	HIS	-	expression tag	UNP P49610
A	611	HIS	-	expression tag	UNP P49610
A	612	HIS	-	expression tag	UNP P49610
A	613	HIS	-	expression tag	UNP P49610
A	614	HIS	-	expression tag	UNP P49610
A	615	HIS	-	expression tag	UNP P49610
A	616	SER	-	expression tag	UNP P49610
A	617	SER	-	expression tag	UNP P49610
A	618	GLY	-	expression tag	UNP P49610
A	619	LEU	-	expression tag	UNP P49610
A	620	VAL	-	expression tag	UNP P49610
A	621	PRO	-	expression tag	UNP P49610
A	622	ARG	-	expression tag	UNP P49610
A	623	GLY	-	expression tag	UNP P49610
A	624	SER	-	expression tag	UNP P49610
A	625	HIS	-	expression tag	UNP P49610
A	626	MET	-	expression tag	UNP P49610

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Chain	Residue	Modelled	Actual	Comment	Reference
A	805	GLN	GLU	engineered mutation	UNP P49610
B	606	MET	-	expression tag	UNP P49610
B	607	GLY	-	expression tag	UNP P49610
B	608	SER	-	expression tag	UNP P49610
B	609	SER	-	expression tag	UNP P49610
B	610	HIS	-	expression tag	UNP P49610
B	611	HIS	-	expression tag	UNP P49610
B	612	HIS	-	expression tag	UNP P49610
B	613	HIS	-	expression tag	UNP P49610
B	614	HIS	-	expression tag	UNP P49610
B	615	HIS	-	expression tag	UNP P49610
B	616	SER	-	expression tag	UNP P49610
B	617	SER	-	expression tag	UNP P49610
B	618	GLY	-	expression tag	UNP P49610
B	619	LEU	-	expression tag	UNP P49610
B	620	VAL	-	expression tag	UNP P49610
B	621	PRO	-	expression tag	UNP P49610
B	622	ARG	-	expression tag	UNP P49610
B	623	GLY	-	expression tag	UNP P49610
B	624	SER	-	expression tag	UNP P49610
B	625	HIS	-	expression tag	UNP P49610
B	626	MET	-	expression tag	UNP P49610
B	805	GLN	GLU	engineered mutation	UNP P49610
C	606	MET	-	expression tag	UNP P49610
C	607	GLY	-	expression tag	UNP P49610
C	608	SER	-	expression tag	UNP P49610
C	609	SER	-	expression tag	UNP P49610
C	610	HIS	-	expression tag	UNP P49610
C	611	HIS	-	expression tag	UNP P49610
C	612	HIS	-	expression tag	UNP P49610
C	613	HIS	-	expression tag	UNP P49610
C	614	HIS	-	expression tag	UNP P49610
C	615	HIS	-	expression tag	UNP P49610
C	616	SER	-	expression tag	UNP P49610
C	617	SER	-	expression tag	UNP P49610
C	618	GLY	-	expression tag	UNP P49610
C	619	LEU	-	expression tag	UNP P49610
C	620	VAL	-	expression tag	UNP P49610
C	621	PRO	-	expression tag	UNP P49610
C	622	ARG	-	expression tag	UNP P49610
C	623	GLY	-	expression tag	UNP P49610
C	624	SER	-	expression tag	UNP P49610

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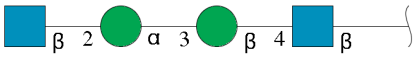
Chain	Residue	Modelled	Actual	Comment	Reference
C	625	HIS	-	expression tag	UNP P49610
C	626	MET	-	expression tag	UNP P49610
C	805	GLN	GLU	engineered mutation	UNP P49610
D	606	MET	-	expression tag	UNP P49610
D	607	GLY	-	expression tag	UNP P49610
D	608	SER	-	expression tag	UNP P49610
D	609	SER	-	expression tag	UNP P49610
D	610	HIS	-	expression tag	UNP P49610
D	611	HIS	-	expression tag	UNP P49610
D	612	HIS	-	expression tag	UNP P49610
D	613	HIS	-	expression tag	UNP P49610
D	614	HIS	-	expression tag	UNP P49610
D	615	HIS	-	expression tag	UNP P49610
D	616	SER	-	expression tag	UNP P49610
D	617	SER	-	expression tag	UNP P49610
D	618	GLY	-	expression tag	UNP P49610
D	619	LEU	-	expression tag	UNP P49610
D	620	VAL	-	expression tag	UNP P49610
D	621	PRO	-	expression tag	UNP P49610
D	622	ARG	-	expression tag	UNP P49610
D	623	GLY	-	expression tag	UNP P49610
D	624	SER	-	expression tag	UNP P49610
D	625	HIS	-	expression tag	UNP P49610
D	626	MET	-	expression tag	UNP P49610
D	805	GLN	GLU	engineered mutation	UNP P49610

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	F	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	G	4	Total	C	N	O	0	0	0
			51	28	2	21			

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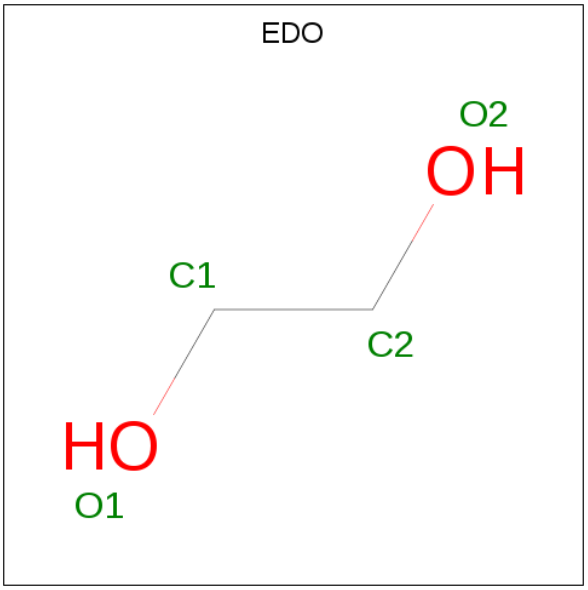
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	4	Total C N O 51 28 2 21	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

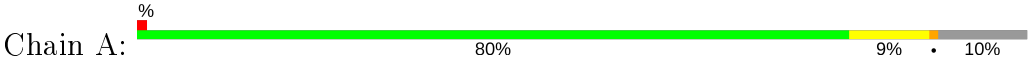
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	208	Total O 214 214	0	6
4	B	196	Total O 197 197	0	1
4	C	206	Total O 207 207	0	1
4	D	187	Total O 190 190	0	3

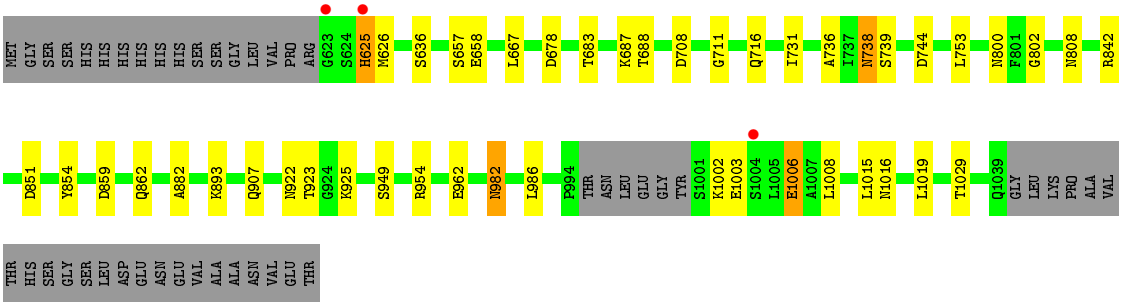
3 Residue-property plots (i)

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: BETA-N-ACETYLHEXOSAMINIDASE

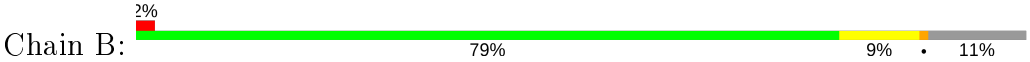
Chain A:

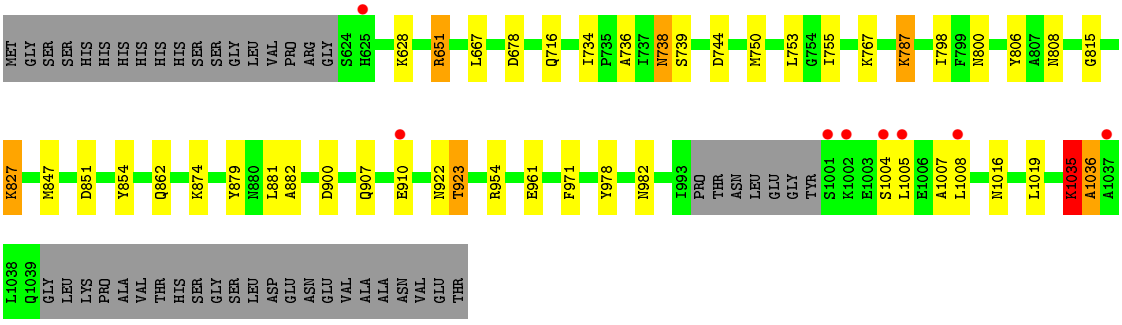




- Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

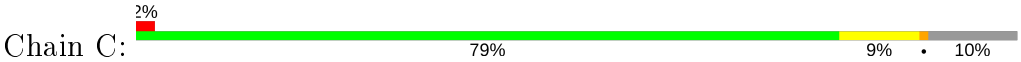
Chain B:

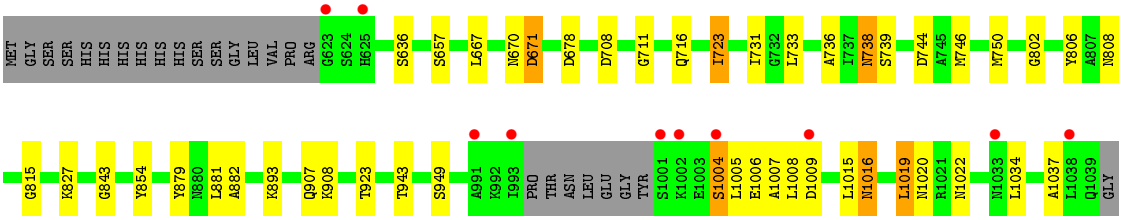




- Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

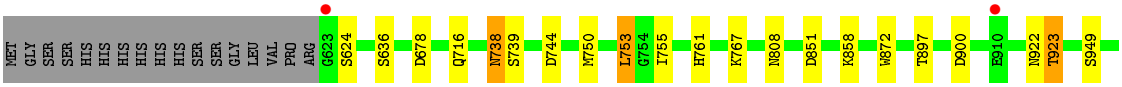
Chain C:

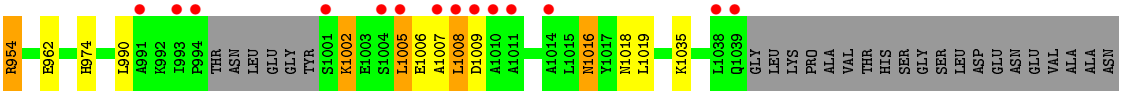




• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain D:





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

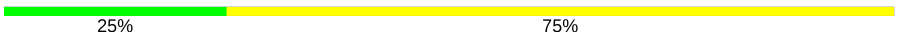
Chain E:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

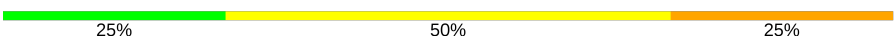
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.27Å 115.89Å 132.35Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	40.74 – 2.65 40.74 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.74-2.65) 95.5 (40.74-2.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.229 , 0.298 0.228 , 0.293	Depositor DCC
R_{free} test set	2822 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 27.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14260	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5886e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: BMA, EDO, 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	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.70	2/3342 (0.1%)	0.58	3/4513 (0.1%)
1	B	0.77	5/3330 (0.2%)	0.76	10/4496 (0.2%)
1	C	0.62	6/3343 (0.2%)	0.72	12/4512 (0.3%)
1	D	1.07	10/3342 (0.3%)	1.19	10/4513 (0.2%)
All	All	0.81	23/13357 (0.2%)	0.85	35/18034 (0.2%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1002	LYS	CE-NZ	-33.42	0.65	1.49
1	D	1009	ASP	CG-OD1	32.43	2.00	1.25
1	D	1009	ASP	CG-OD2	-30.59	0.55	1.25
1	B	767	LYS	CE-NZ	-27.92	0.79	1.49
1	D	767	LYS	CE-NZ	-26.48	0.82	1.49
1	B	787	LYS	CE-NZ	21.35	2.02	1.49
1	C	908	LYS	CD-CE	-17.35	1.07	1.51
1	C	827	LYS	CD-CE	-15.92	1.11	1.51
1	B	1004	SER	CA-CB	13.53	1.73	1.52
1	D	1035	LYS	CB-CG	-13.44	1.16	1.52
1	D	1006	GLU	CB-CG	-13.36	1.26	1.52
1	C	1006	GLU	CB-CG	-13.22	1.27	1.52
1	A	1006	GLU	CB-CG	-11.27	1.30	1.52
1	B	1005	LEU	CA-CB	-10.67	1.29	1.53
1	D	1005	LEU	CA-CB	-9.93	1.30	1.53
1	D	1008	LEU	CB-CG	-9.86	1.24	1.52
1	D	1002	LYS	CA-CB	-8.70	1.34	1.53
1	C	1008	LEU	CB-CG	-8.43	1.28	1.52
1	C	1037	ALA	CA-CB	-8.30	1.35	1.52
1	D	1007	ALA	CA-CB	-7.87	1.35	1.52
1	B	1035	LYS	CG-CD	-6.85	1.29	1.52
1	C	1005	LEU	CA-CB	-5.78	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	990	LEU	CB-CG	-5.42	1.36	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1009	ASP	CB-CG-OD2	54.85	167.67	118.30
1	D	1009	ASP	CB-CG-OD1	-41.39	81.05	118.30
1	B	1007	ALA	N-CA-CB	24.16	143.92	110.10
1	B	787	LYS	CD-CE-NZ	-20.73	64.01	111.70
1	C	1005	LEU	N-CA-CB	17.23	144.87	110.40
1	A	1002	LYS	CD-CE-NZ	16.37	149.34	111.70
1	C	1007	ALA	N-CA-CB	15.64	131.99	110.10
1	C	1006	GLU	CA-CB-CG	15.39	147.26	113.40
1	B	1035	LYS	CB-CG-CD	13.83	147.55	111.60
1	A	1008	LEU	CD1-CG-CD2	-12.66	72.52	110.50
1	D	1005	LEU	N-CA-CB	12.63	135.67	110.40
1	D	1002	LYS	N-CA-CB	12.61	133.30	110.60
1	A	1008	LEU	CB-CG-CD2	11.62	130.75	111.00
1	C	827	LYS	CG-CD-CE	10.54	143.54	111.90
1	D	1009	ASP	OD1-CG-OD2	-9.95	104.40	123.30
1	C	1005	LEU	CB-CA-C	-9.83	91.53	110.20
1	B	767	LYS	CD-CE-NZ	9.78	134.20	111.70
1	C	1004	SER	CB-CA-C	-8.87	93.25	110.10
1	B	1035	LYS	CG-CD-CE	8.06	136.09	111.90
1	D	1007	ALA	N-CA-CB	7.67	120.84	110.10
1	C	1005	LEU	CA-CB-CG	7.49	132.52	115.30
1	B	1008	LEU	CA-CB-CG	7.38	132.27	115.30
1	B	1005	LEU	N-CA-CB	7.22	124.85	110.40
1	D	1002	LYS	CA-CB-CG	7.11	129.03	113.40
1	C	1008	LEU	CA-CB-CG	7.07	131.57	115.30
1	B	1036	ALA	N-CA-CB	7.05	119.98	110.10
1	B	1004	SER	N-CA-CB	-6.45	100.82	110.50
1	D	1008	LEU	CB-CG-CD1	-6.25	100.37	111.00
1	C	827	LYS	CD-CE-NZ	-6.14	97.57	111.70
1	D	1008	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	C	1006	GLU	CB-CG-CD	-6.04	97.89	114.20
1	D	1035	LYS	CA-CB-CG	5.84	126.24	113.40
1	C	908	LYS	CG-CD-CE	5.32	127.87	111.90
1	C	1037	ALA	N-CA-CB	5.32	117.54	110.10
1	B	1007	ALA	CB-CA-C	-5.10	102.44	110.10

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	3269	0	3197	20	0
1	B	3258	0	3187	22	0
1	C	3271	0	3202	18	0
1	D	3269	0	3197	17	0
2	E	51	0	45	0	0
2	F	51	0	45	0	0
2	G	51	0	45	0	0
2	H	51	0	45	1	0
3	A	61	0	90	1	0
3	B	32	0	48	0	0
3	C	28	0	42	0	0
3	D	60	0	90	2	0
4	A	214	0	0	0	0
4	B	197	0	0	0	0
4	C	207	0	0	1	0
4	D	190	0	0	0	0
All	All	14260	0	13233	75	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 3.

All (75) 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:B:678:ASP:H	1:B:716:GLN:HE21	1.41	0.66
1:A:683:THR:HG23	1:A:688:THR:HG22	1.77	0.65
1:D:1016:ASN:HD22	1:D:1018:ASN:H	1.46	0.61
1:C:678:ASP:H	1:C:716:GLN:NE2	2.00	0.60
1:A:625:HIS:CD2	1:A:626:MET:HG3	2.37	0.58
1:A:658:GLU:HG3	1:A:982:ASN:OD1	2.03	0.58
1:A:922:ASN:HA	1:A:925:LYS:HB2	1.85	0.57
1:B:678:ASP:H	1:B:716:GLN:NE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:ASN:HD22	1:D:739:SER:H	1.52	0.55
1:D:738:ASN:HD22	1:D:739:SER:N	2.04	0.55
1:C:657:SER:HA	1:C:731:ILE:HD11	1.88	0.55
1:C:738:ASN:HD22	1:C:739:SER:H	1.53	0.55
1:A:625:HIS:HD2	1:A:626:MET:HG3	1.71	0.54
1:B:854:TYR:O	1:B:882:ALA:HB2	2.08	0.54
1:C:738:ASN:ND2	1:C:802:GLY:HA3	2.24	0.53
1:C:667:LEU:HA	1:C:736:ALA:HB3	1.92	0.51
1:B:667:LEU:HA	1:B:736:ALA:HB3	1.92	0.50
1:A:986:LEU:HD11	1:A:1015:LEU:HD22	1.94	0.50
1:B:738:ASN:HD22	1:B:739:SER:H	1.58	0.50
1:D:750:MET:HA	1:D:753:LEU:HB2	1.94	0.50
1:D:761:HIS:N	3:D:1107:EDO:H22	2.26	0.49
1:A:842:ARG:HA	3:A:1108:EDO:H11	1.94	0.49
1:A:859:ASP:HB2	1:A:862:GLN:HE22	1.78	0.49
1:A:738:ASN:HD22	1:A:739:SER:H	1.60	0.48
1:B:806:TYR:O	1:B:815:GLY:HA3	2.14	0.48
1:B:923:THR:HG23	1:B:971:PHE:HA	1.96	0.48
1:D:761:HIS:H	3:D:1107:EDO:H22	1.79	0.48
1:A:657:SER:HA	1:A:731:ILE:HD11	1.95	0.47
1:C:636:SER:HB3	1:C:949:SER:HA	1.96	0.47
1:C:746:MET:O	1:C:750:MET:HG2	2.15	0.47
1:A:859:ASP:HB2	1:A:862:GLN:NE2	2.29	0.47
1:D:962:GLU:CD	1:D:962:GLU:H	2.17	0.47
1:A:962:GLU:CD	1:A:962:GLU:H	2.18	0.46
1:B:651:ARG:NH1	1:B:961:GLU:OE1	2.48	0.46
1:D:1016:ASN:ND2	1:D:1018:ASN:H	2.13	0.46
1:B:738:ASN:HD22	1:B:739:SER:N	2.13	0.46
1:C:1016:ASN:HB3	1:C:1019:LEU:HD22	1.98	0.46
1:C:723:ILE:HG22	1:C:733:LEU:HD22	1.98	0.46
1:B:734:ILE:HG23	1:B:798:ILE:HB	1.97	0.45
1:B:628:LYS:HG3	1:B:978:TYR:CE2	2.51	0.45
1:B:827:LYS:HE3	1:B:827:LYS:HA	1.98	0.45
1:A:636:SER:HB3	1:A:949:SER:HA	1.99	0.45
1:C:854:TYR:O	1:C:882:ALA:HB2	2.16	0.44
1:A:736:ALA:HA	1:A:800:ASN:O	2.18	0.43
1:B:651:ARG:CD	1:D:962:GLU:HG2	2.48	0.43
1:C:708:ASP:HB3	1:C:711:GLY:O	2.17	0.43
1:B:734:ILE:HD12	1:B:798:ILE:HD12	2.00	0.43
1:A:678:ASP:H	1:A:716:GLN:NE2	2.17	0.43
1:C:1015:LEU:HD21	1:C:1034:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:872:TRP:HA	1:D:897:THR:O	2.19	0.43
2:H:1:NAG:H3	2:H:1:NAG:H83	2.01	0.43
1:B:800:ASN:HA	1:B:847:MET:O	2.18	0.43
1:B:907:GLN:HE22	1:B:954:ARG:HH12	1.66	0.42
1:C:806:TYR:O	1:C:815:GLY:HA3	2.18	0.42
1:D:900:ASP:HB3	1:D:922:ASN:HB3	2.01	0.42
1:A:854:TYR:O	1:A:882:ALA:HB2	2.19	0.42
1:A:708:ASP:HB3	1:A:711:GLY:O	2.19	0.41
1:D:750:MET:HB2	1:D:755:ILE:HD12	2.02	0.41
1:C:879:TYR:CE2	1:C:881:LEU:HD21	2.56	0.41
1:B:750:MET:HB3	1:B:755:ILE:HB	2.03	0.41
1:B:900:ASP:HB3	1:B:922:ASN:HB3	2.02	0.41
1:B:651:ARG:NE	1:D:962:GLU:HG2	2.36	0.41
1:D:678:ASP:H	1:D:716:GLN:NE2	2.18	0.41
1:D:636:SER:HB3	1:D:949:SER:HA	2.01	0.41
1:B:874:LYS:NZ	1:C:843:GLY:O	2.49	0.41
1:D:923:THR:HG22	1:D:974:HIS:CD2	2.56	0.41
1:A:667:LEU:HA	1:A:736:ALA:HB3	2.01	0.41
1:B:1035:LYS:HG3	1:B:1036:ALA:N	2.36	0.41
1:C:893[A]:LYS:HG2	4:C:1219:HOH:O	2.20	0.41
1:D:954:ARG:HB2	1:D:954:ARG:HE	1.50	0.41
1:B:879:TYR:CE2	1:B:881:LEU:HD21	2.55	0.41
1:A:738:ASN:ND2	1:A:802:GLY:HA3	2.36	0.40
1:C:670:ASN:O	1:C:671:ASP:HB2	2.22	0.40
1:A:738:ASN:HD22	1:A:739:SER:N	2.18	0.40
1:C:1020:ASN:OD1	1:C:1022:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/457 (89%)	390 (96%)	17 (4%)	0	100	100
1	B	405/457 (89%)	391 (96%)	14 (4%)	0	100	100
1	C	407/457 (89%)	387 (95%)	19 (5%)	1 (0%)	47	64
1	D	407/457 (89%)	389 (96%)	17 (4%)	1 (0%)	47	64
All	All	1626/1828 (89%)	1557 (96%)	67 (4%)	2 (0%)	51	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	624	SER
1	C	671	ASP

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	338/376 (90%)	321 (95%)	17 (5%)	24	38
1	B	337/376 (90%)	322 (96%)	15 (4%)	27	42
1	C	338/376 (90%)	327 (97%)	11 (3%)	38	54
1	D	338/376 (90%)	325 (96%)	13 (4%)	33	49
All	All	1351/1504 (90%)	1295 (96%)	56 (4%)	30	46

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	625	HIS
1	A	687	LYS
1	A	738	ASN
1	A	744	ASP
1	A	753	LEU
1	A	808	ASN
1	A	851	ASP
1	A	893	LYS
1	A	907	GLN

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Mol	Chain	Res	Type
1	A	923	THR
1	A	954	ARG
1	A	982	ASN
1	A	1003	GLU
1	A	1006	GLU
1	A	1016	ASN
1	A	1019	LEU
1	A	1029	THR
1	B	651	ARG
1	B	738	ASN
1	B	744	ASP
1	B	753	LEU
1	B	787	LYS
1	B	808	ASN
1	B	827	LYS
1	B	851	ASP
1	B	862	GLN
1	B	910	GLU
1	B	923	THR
1	B	982	ASN
1	B	1016	ASN
1	B	1019	LEU
1	B	1035	LYS
1	C	723	ILE
1	C	738	ASN
1	C	744	ASP
1	C	808	ASN
1	C	907	GLN
1	C	923	THR
1	C	943	THR
1	C	1004	SER
1	C	1009	ASP
1	C	1016	ASN
1	C	1019	LEU
1	D	738	ASN
1	D	744	ASP
1	D	753	LEU
1	D	808	ASN
1	D	851	ASP
1	D	858	LYS
1	D	923	THR
1	D	954	ARG

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Mol	Chain	Res	Type
1	D	1002	LYS
1	D	1005	LEU
1	D	1008	LEU
1	D	1016	ASN
1	D	1019	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	625	HIS
1	A	632	ASN
1	A	670	ASN
1	A	710	ASN
1	A	716	GLN
1	A	738	ASN
1	A	808	ASN
1	A	907	GLN
1	A	922	ASN
1	A	929	ASN
1	A	975	ASN
1	A	982	ASN
1	A	1016	ASN
1	A	1033	ASN
1	B	670	ASN
1	B	716	GLN
1	B	738	ASN
1	B	761	HIS
1	B	808	ASN
1	B	814	GLN
1	B	907	GLN
1	B	922	ASN
1	B	929	ASN
1	B	975	ASN
1	B	982	ASN
1	B	1016	ASN
1	B	1033	ASN
1	C	632	ASN
1	C	670	ASN
1	C	716	GLN
1	C	738	ASN
1	C	814	GLN
1	C	907	GLN

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Mol	Chain	Res	Type
1	C	922	ASN
1	C	975	ASN
1	C	982	ASN
1	C	1016	ASN
1	D	670	ASN
1	D	716	GLN
1	D	738	ASN
1	D	757	ASN
1	D	808	ASN
1	D	907	GLN
1	D	929	ASN
1	D	974	HIS
1	D	975	ASN
1	D	982	ASN
1	D	1016	ASN
1	D	1033	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

16 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	E	1	2	15,15,15	0.41	0	21,21,21	0.65	0
2	BMA	E	2	2	11,11,12	0.69	0	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	E	3	2	11,11,12	0.60	0	15,15,17	0.84	0
2	NAG	E	4	2	14,14,15	0.67	1 (7%)	17,19,21	2.22	6 (35%)
2	NAG	F	1	2	15,15,15	0.44	0	21,21,21	0.80	0
2	BMA	F	2	2	11,11,12	0.67	0	15,15,17	0.84	1 (6%)
2	MAN	F	3	2	11,11,12	0.62	0	15,15,17	0.92	1 (6%)
2	NAG	F	4	2	14,14,15	0.66	1 (7%)	17,19,21	2.19	6 (35%)
2	NAG	G	1	2	15,15,15	0.48	0	21,21,21	1.07	1 (4%)
2	BMA	G	2	2	11,11,12	0.66	0	15,15,17	0.85	0
2	MAN	G	3	2	11,11,12	0.57	0	15,15,17	1.06	1 (6%)
2	NAG	G	4	2	14,14,15	0.67	1 (7%)	17,19,21	2.30	4 (23%)
2	NAG	H	1	2	15,15,15	0.65	0	21,21,21	1.53	5 (23%)
2	BMA	H	2	2	11,11,12	0.71	0	15,15,17	0.92	2 (13%)
2	MAN	H	3	2	11,11,12	0.61	0	15,15,17	0.90	0
2	NAG	H	4	2	14,14,15	0.50	0	17,19,21	1.63	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
2	NAG	E	1	2	-	0/6/26/26	0/1/1/1
2	BMA	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	4	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2	-	2/6/26/26	0/1/1/1
2	BMA	F	2	2	-	0/2/19/22	0/1/1/1
2	MAN	F	3	2	-	2/2/19/22	0/1/1/1
2	NAG	F	4	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	2	-	4/6/26/26	0/1/1/1
2	BMA	G	2	2	-	0/2/19/22	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	4	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	2	-	3/6/26/26	0/1/1/1
2	BMA	H	2	2	-	0/2/19/22	0/1/1/1
2	MAN	H	3	2	-	2/2/19/22	0/1/1/1
2	NAG	H	4	2	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	NAG	C1-C2	2.11	1.55	1.52
2	F	4	NAG	C1-C2	2.08	1.55	1.52
2	E	4	NAG	C1-C2	2.07	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	4	NAG	C1-O5-C5	6.78	121.37	112.19
2	E	4	NAG	C1-O5-C5	5.69	119.90	112.19
2	F	4	NAG	C1-O5-C5	5.62	119.81	112.19
2	H	4	NAG	C1-O5-C5	5.16	119.19	112.19
2	F	4	NAG	C2-N2-C7	3.95	128.53	122.90
2	G	4	NAG	O5-C1-C2	3.78	117.25	111.29
2	E	4	NAG	C2-N2-C7	3.58	128.01	122.90
2	G	4	NAG	C2-N2-C7	3.57	127.99	122.90
2	E	4	NAG	O5-C1-C2	3.54	116.88	111.29
2	H	1	NAG	C2-N2-C7	3.48	131.65	123.18
2	F	4	NAG	C1-C2-N2	3.31	116.15	110.49
2	H	1	NAG	C8-C7-N2	3.27	121.63	116.10
2	E	4	NAG	C1-C2-N2	3.00	115.61	110.49
2	G	1	NAG	C4-C3-C2	2.85	114.51	110.34
2	F	4	NAG	O5-C1-C2	2.63	115.44	111.29
2	G	4	NAG	C1-C2-N2	2.45	114.67	110.49
2	H	1	NAG	O5-C1-C2	2.42	111.95	109.52
2	H	1	NAG	O7-C7-C8	-2.39	117.61	122.06
2	E	4	NAG	C3-C4-C5	-2.38	106.00	110.24
2	G	3	MAN	C1-O5-C5	2.36	115.39	112.19
2	E	2	BMA	C1-C2-C3	2.34	112.55	109.67
2	H	4	NAG	C2-N2-C7	2.33	126.22	122.90
2	H	2	BMA	C1-C2-C3	2.30	112.50	109.67
2	E	4	NAG	O5-C5-C6	2.20	110.66	107.20
2	F	4	NAG	O5-C5-C6	2.19	110.64	107.20
2	F	4	NAG	C3-C4-C5	-2.15	106.41	110.24
2	H	1	NAG	C1-C2-C3	2.12	113.43	110.54
2	F	2	BMA	C1-C2-C3	2.11	112.26	109.67
2	F	3	MAN	C1-O5-C5	2.06	114.98	112.19
2	H	2	BMA	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	H	3	MAN	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	3	MAN	O5-C5-C6-O6
2	F	3	MAN	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	4	NAG	C8-C7-N2-C2
2	H	4	NAG	O7-C7-N2-C2
2	G	4	NAG	O5-C5-C6-O6
2	G	4	NAG	C4-C5-C6-O6
2	E	4	NAG	O5-C5-C6-O6
2	E	4	NAG	C4-C5-C6-O6
2	F	4	NAG	C4-C5-C6-O6
2	H	4	NAG	O5-C5-C6-O6
2	F	3	MAN	O5-C5-C6-O6
2	F	4	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C3-C2-N2-C7
2	E	4	NAG	C3-C2-N2-C7
2	F	4	NAG	C3-C2-N2-C7
2	G	4	NAG	C3-C2-N2-C7

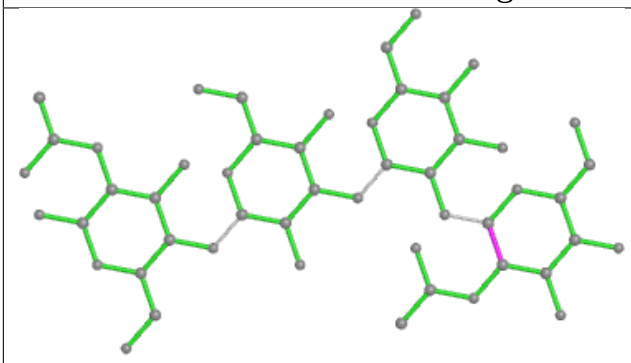
There are no ring outliers.

1 monomer is involved in 1 short contact:

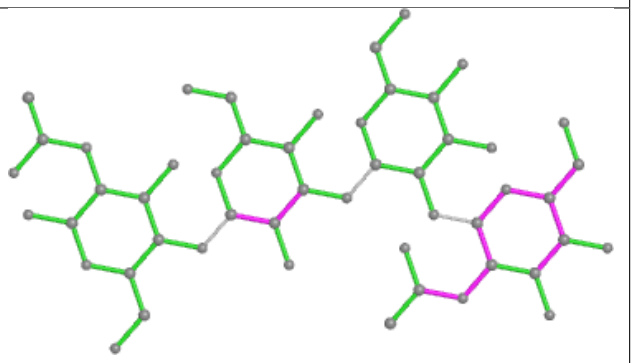
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0

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

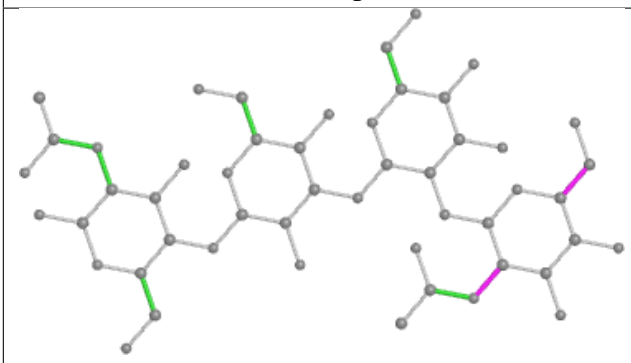
Oligosaccharide Chain E



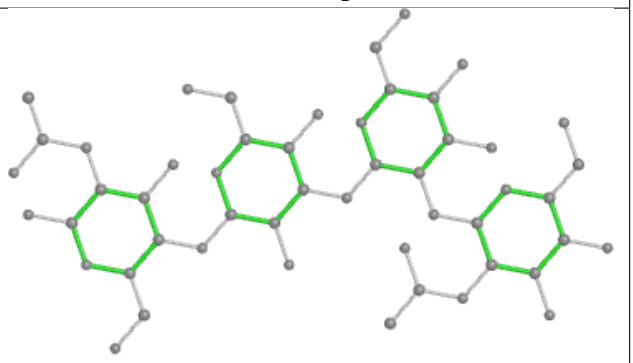
Bond lengths



Bond angles

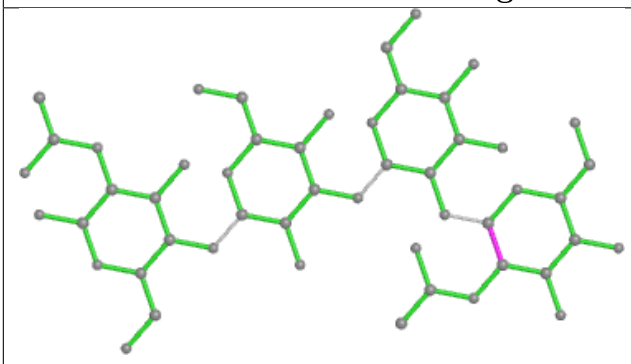


Torsions

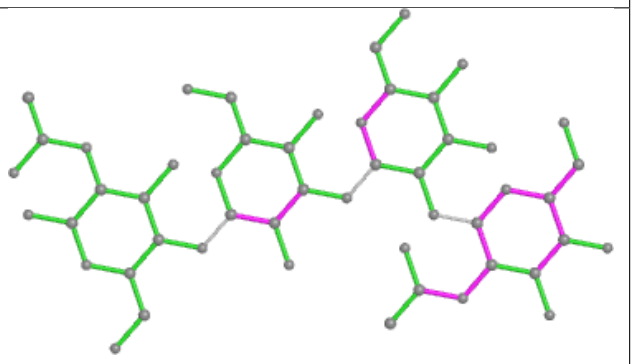


Rings

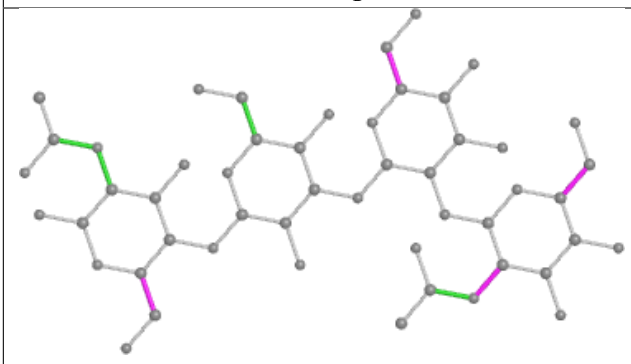
Oligosaccharide Chain F



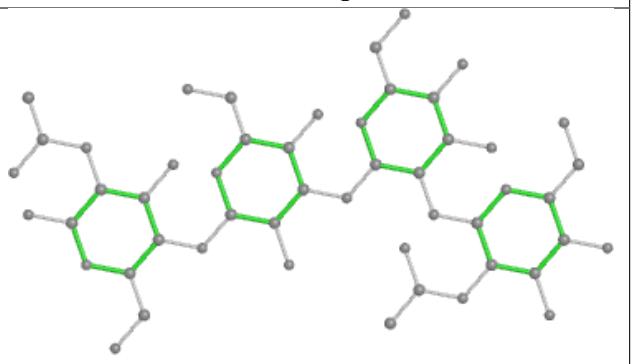
Bond lengths



Bond angles

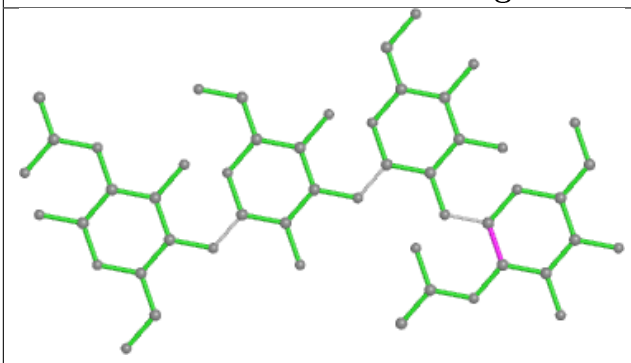


Torsions

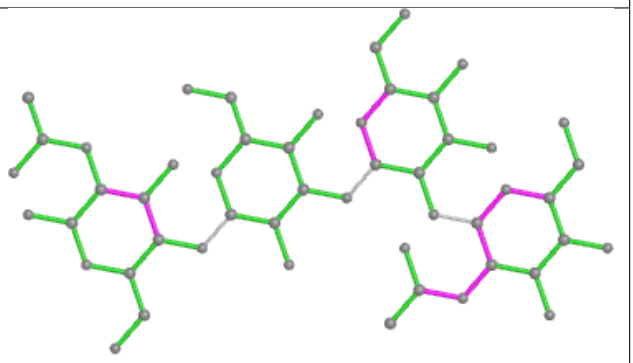


Rings

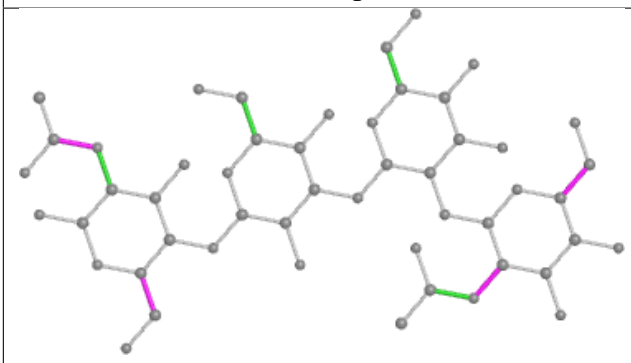
Oligosaccharide Chain G



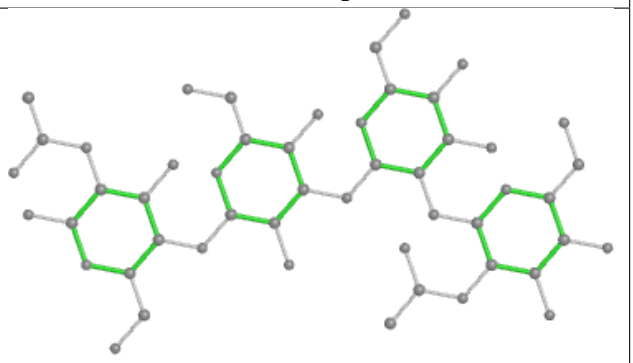
Bond lengths



Bond angles

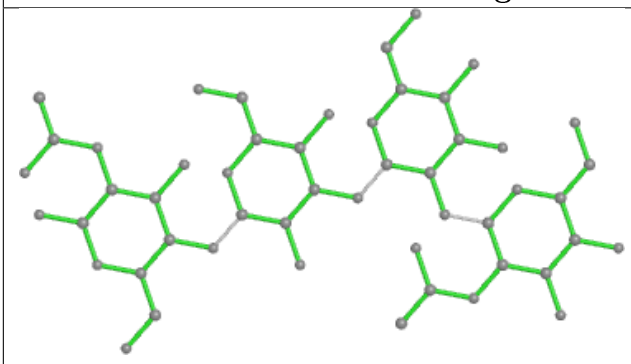


Torsions

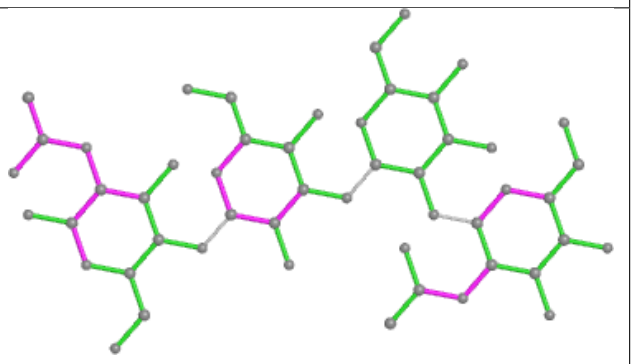


Rings

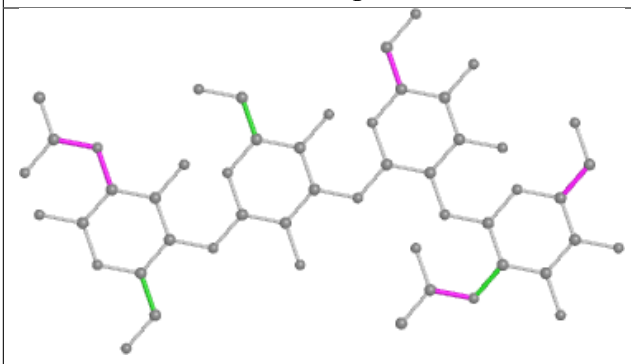
Oligosaccharide Chain H



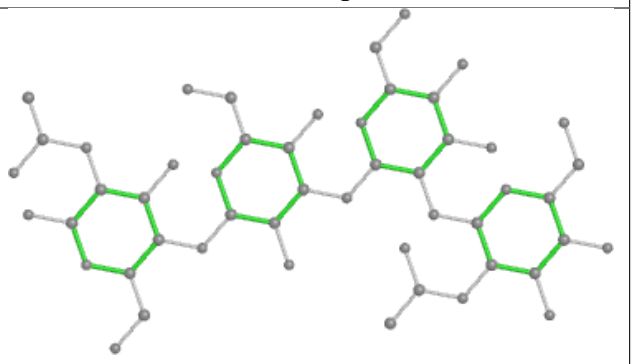
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 1 is modelled with single atom - leaving 45 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	$\#\|Z\| > 2$
3	EDO	A	1107	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	A	1119	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	A	1114	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	D	1117	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	A	1115	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	C	1106	-	3,3,3	0.50	0	2,2,2	0.23	0
3	EDO	D	1116	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	B	1111	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	D	1115	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	1113	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	C	1109	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	1117	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	C	1107	-	3,3,3	0.48	0	2,2,2	0.26	0
3	EDO	D	1110	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	B	1107	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	A	1111	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	A	1118	-	3,3,3	0.48	0	2,2,2	0.26	0
3	EDO	D	1106	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	B	1112	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	C	1105	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	D	1108	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	D	1109	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	A	1120	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	D	1112	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	A	1110	-	3,3,3	0.47	0	2,2,2	0.07	0
3	EDO	B	1108	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	A	1108	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EDO	B	1109	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	C	1111	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	D	1113	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	D	1118	-	3,3,3	0.46	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	D	1101	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	A	1116	-	3,3,3	0.49	0	2,2,2	0.30	0
3	EDO	B	1106	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	A	1109	-	3,3,3	0.51	0	2,2,2	0.07	0
3	EDO	D	1114	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	D	1111	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	C	1110	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	C	1108	-	3,3,3	0.48	0	2,2,2	0.31	0
3	EDO	B	1110	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	A	1106	-	3,3,3	0.49	0	2,2,2	0.28	0
3	EDO	B	1105	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EDO	A	1105	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	D	1119	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	D	1107	-	3,3,3	0.45	0	2,2,2	0.28	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	EDO	A	1107	-	-	1/1/1/1	-
3	EDO	A	1119	-	-	1/1/1/1	-
3	EDO	A	1114	-	-	0/1/1/1	-
3	EDO	D	1117	-	-	1/1/1/1	-
3	EDO	A	1115	-	-	0/1/1/1	-
3	EDO	C	1106	-	-	1/1/1/1	-
3	EDO	D	1116	-	-	1/1/1/1	-
3	EDO	B	1111	-	-	0/1/1/1	-
3	EDO	D	1115	-	-	1/1/1/1	-
3	EDO	A	1113	-	-	1/1/1/1	-
3	EDO	C	1109	-	-	1/1/1/1	-
3	EDO	A	1117	-	-	1/1/1/1	-
3	EDO	C	1107	-	-	1/1/1/1	-
3	EDO	D	1110	-	-	1/1/1/1	-
3	EDO	B	1107	-	-	1/1/1/1	-
3	EDO	A	1111	-	-	1/1/1/1	-
3	EDO	A	1118	-	-	0/1/1/1	-
3	EDO	D	1106	-	-	1/1/1/1	-
3	EDO	B	1112	-	-	0/1/1/1	-
3	EDO	C	1105	-	-	1/1/1/1	-
3	EDO	D	1108	-	-	1/1/1/1	-
3	EDO	D	1109	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1120	-	-	0/1/1/1	-
3	EDO	D	1112	-	-	0/1/1/1	-
3	EDO	A	1110	-	-	1/1/1/1	-
3	EDO	B	1108	-	-	1/1/1/1	-
3	EDO	A	1108	-	-	0/1/1/1	-
3	EDO	B	1109	-	-	1/1/1/1	-
3	EDO	C	1111	-	-	1/1/1/1	-
3	EDO	D	1113	-	-	1/1/1/1	-
3	EDO	D	1118	-	-	1/1/1/1	-
3	EDO	D	1101	-	-	1/1/1/1	-
3	EDO	A	1116	-	-	0/1/1/1	-
3	EDO	B	1106	-	-	1/1/1/1	-
3	EDO	A	1109	-	-	0/1/1/1	-
3	EDO	D	1114	-	-	1/1/1/1	-
3	EDO	D	1111	-	-	1/1/1/1	-
3	EDO	C	1110	-	-	1/1/1/1	-
3	EDO	C	1108	-	-	1/1/1/1	-
3	EDO	B	1110	-	-	1/1/1/1	-
3	EDO	A	1106	-	-	1/1/1/1	-
3	EDO	B	1105	-	-	1/1/1/1	-
3	EDO	A	1105	-	-	0/1/1/1	-
3	EDO	D	1119	-	-	0/1/1/1	-
3	EDO	D	1107	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1106	EDO	O1-C1-C2-O2
3	C	1109	EDO	O1-C1-C2-O2
3	D	1116	EDO	O1-C1-C2-O2
3	D	1115	EDO	O1-C1-C2-O2
3	D	1110	EDO	O1-C1-C2-O2
3	B	1107	EDO	O1-C1-C2-O2
3	D	1108	EDO	O1-C1-C2-O2
3	D	1113	EDO	O1-C1-C2-O2
3	A	1110	EDO	O1-C1-C2-O2
3	B	1109	EDO	O1-C1-C2-O2
3	C	1111	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	1106	EDO	O1-C1-C2-O2
3	D	1111	EDO	O1-C1-C2-O2
3	C	1110	EDO	O1-C1-C2-O2
3	B	1110	EDO	O1-C1-C2-O2
3	A	1107	EDO	O1-C1-C2-O2
3	C	1107	EDO	O1-C1-C2-O2
3	A	1111	EDO	O1-C1-C2-O2
3	C	1105	EDO	O1-C1-C2-O2
3	C	1108	EDO	O1-C1-C2-O2
3	D	1117	EDO	O1-C1-C2-O2
3	D	1106	EDO	O1-C1-C2-O2
3	D	1107	EDO	O1-C1-C2-O2
3	D	1118	EDO	O1-C1-C2-O2
3	D	1101	EDO	O1-C1-C2-O2
3	A	1117	EDO	O1-C1-C2-O2
3	A	1106	EDO	O1-C1-C2-O2
3	A	1113	EDO	O1-C1-C2-O2
3	A	1119	EDO	O1-C1-C2-O2
3	D	1114	EDO	O1-C1-C2-O2
3	B	1108	EDO	O1-C1-C2-O2
3	D	1109	EDO	O1-C1-C2-O2
3	B	1105	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1108	EDO	1	0
3	D	1107	EDO	2	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, 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>2			OWAB(Å^2)	Q<0.9
1	A	411/457 (89%)	-0.22	3 (0%)	87	87	5, 14, 33, 46	11 (2%)
1	B	409/457 (89%)	-0.21	8 (1%)	65	60	3, 13, 37, 55	16 (3%)
1	C	410/457 (89%)	-0.21	10 (2%)	59	54	4, 12, 37, 51	16 (3%)
1	D	411/457 (89%)	-0.14	16 (3%)	39	35	4, 14, 42, 55	18 (4%)
All	All	1641/1828 (89%)	-0.20	37 (2%)	60	56	3, 13, 37, 55	61 (3%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1004	SER	5.3
1	D	1004	SER	5.2
1	D	991	ALA	4.8
1	D	623	GLY	3.6
1	D	994	PRO	3.6
1	D	1007	ALA	3.5
1	A	623	GLY	3.5
1	A	625	HIS	3.4
1	C	623	GLY	3.3
1	D	993	ILE	3.3
1	D	1038	LEU	3.2
1	A	1004	SER	3.2
1	C	625	HIS	3.1
1	C	1001	SER	2.9
1	D	1005	LEU	2.9
1	B	1001	SER	2.8
1	C	1002	LYS	2.8
1	C	991	ALA	2.6
1	D	1014	ALA	2.6
1	B	910	GLU	2.6
1	D	1039	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1008	LEU	2.5
1	B	1037	ALA	2.5
1	C	1004	SER	2.5
1	C	993	ILE	2.4
1	D	1010	ALA	2.4
1	C	1009	ASP	2.3
1	D	1008	LEU	2.3
1	D	1011	ALA	2.2
1	D	1001	SER	2.2
1	D	1009	ASP	2.2
1	B	1005	LEU	2.2
1	B	1002	LYS	2.1
1	C	1033	ASN	2.1
1	C	1038	LEU	2.1
1	D	910	GLU	2.1
1	B	625	HIS	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, 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	B-factors(Å^2)	Q<0.9
2	NAG	H	1	15/15	0.51	0.56	61,63,63,63	0
2	NAG	G	1	15/15	0.51	0.61	65,67,68,68	0
2	NAG	E	1	15/15	0.55	0.42	62,63,63,63	0
2	NAG	F	1	15/15	0.59	0.52	56,58,58,58	0
2	BMA	G	2	11/12	0.75	0.37	61,64,64,64	0
2	BMA	E	2	11/12	0.75	0.32	60,61,62,62	0
2	BMA	H	2	11/12	0.76	0.32	58,60,60,60	0
2	MAN	H	3	11/12	0.77	0.45	55,57,57,57	0
2	MAN	F	3	11/12	0.79	0.40	49,51,52,52	0
2	NAG	H	4	14/15	0.80	0.26	52,53,53,54	0
2	BMA	F	2	11/12	0.80	0.24	53,55,55,55	0
2	NAG	E	4	14/15	0.82	0.28	55,56,56,57	0

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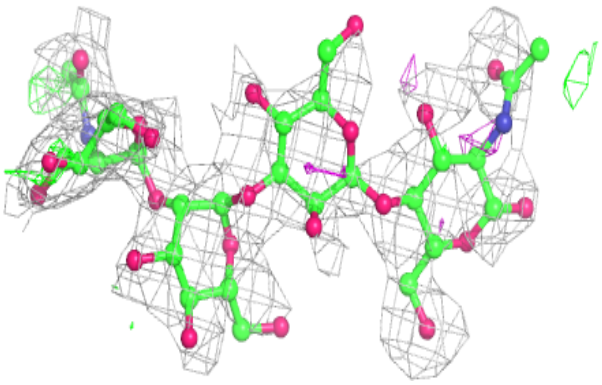
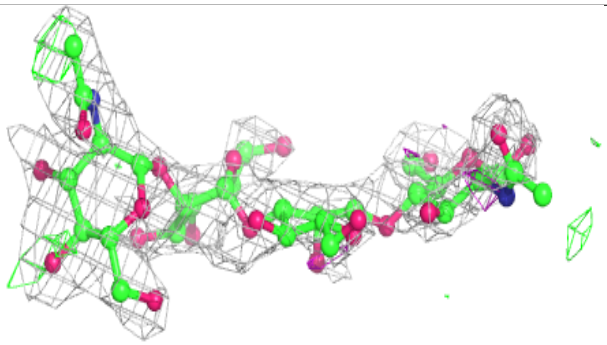
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	E	3	11/12	0.84	0.27	58,59,60,60	0
2	MAN	G	3	11/12	0.85	0.31	57,59,60,60	0
2	NAG	F	4	14/15	0.87	0.31	45,46,46,47	0
2	NAG	G	4	14/15	0.89	0.24	53,54,55,55	0

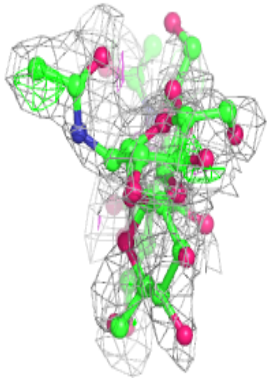
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

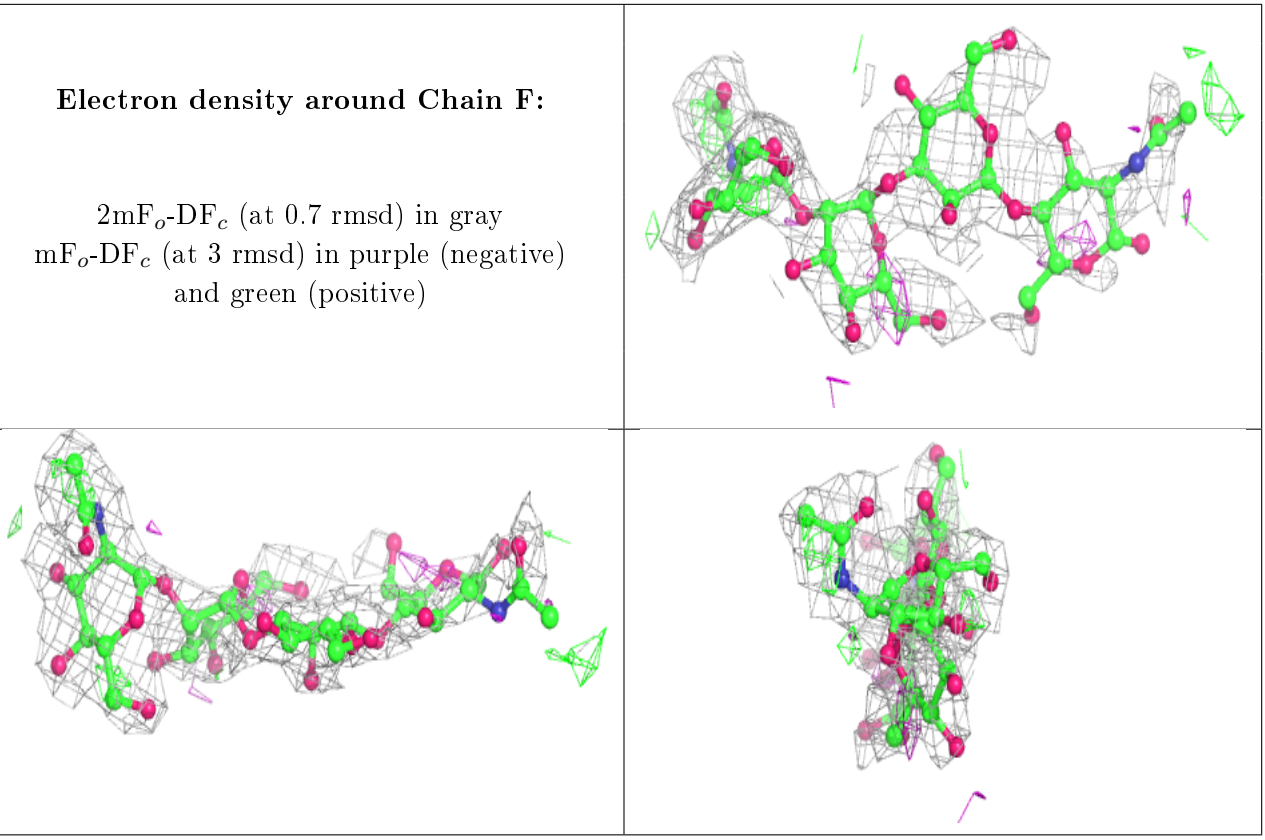






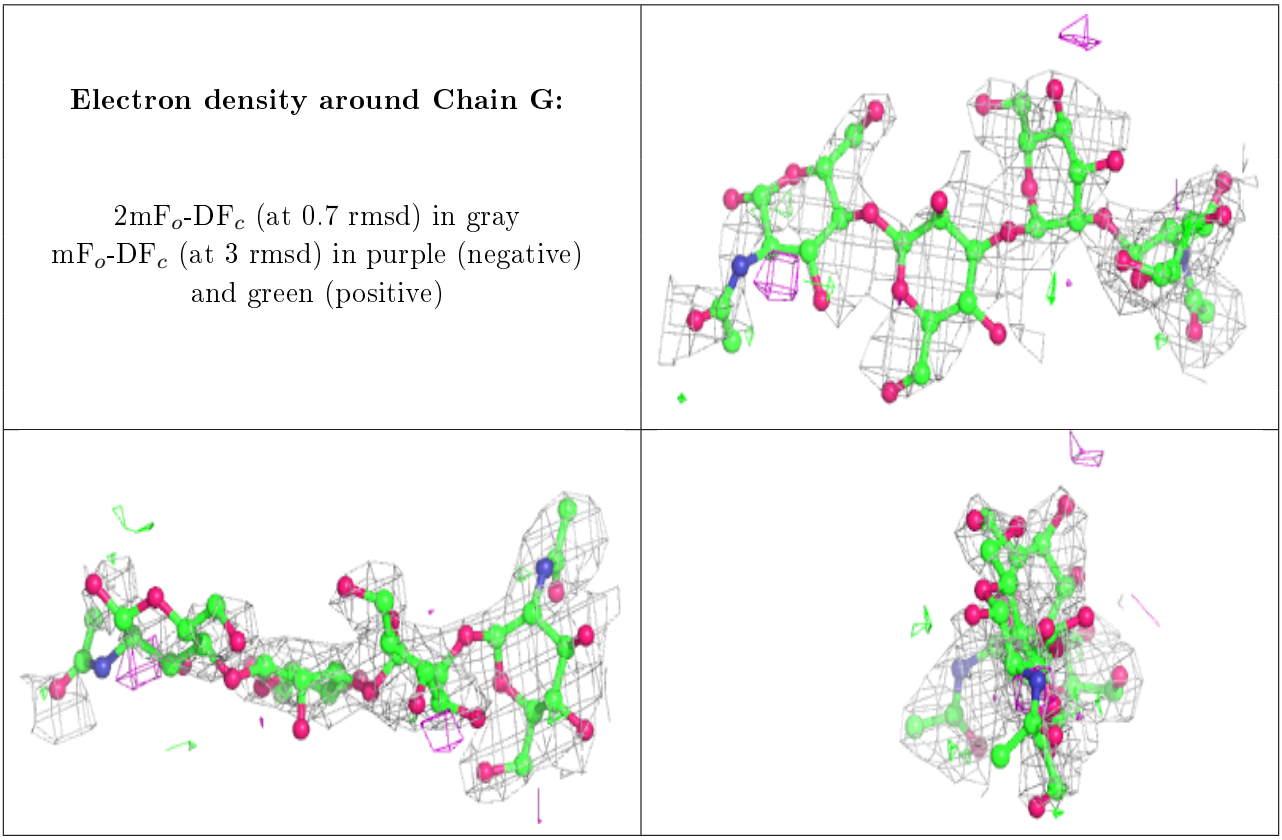
Electron density around Chain F:

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



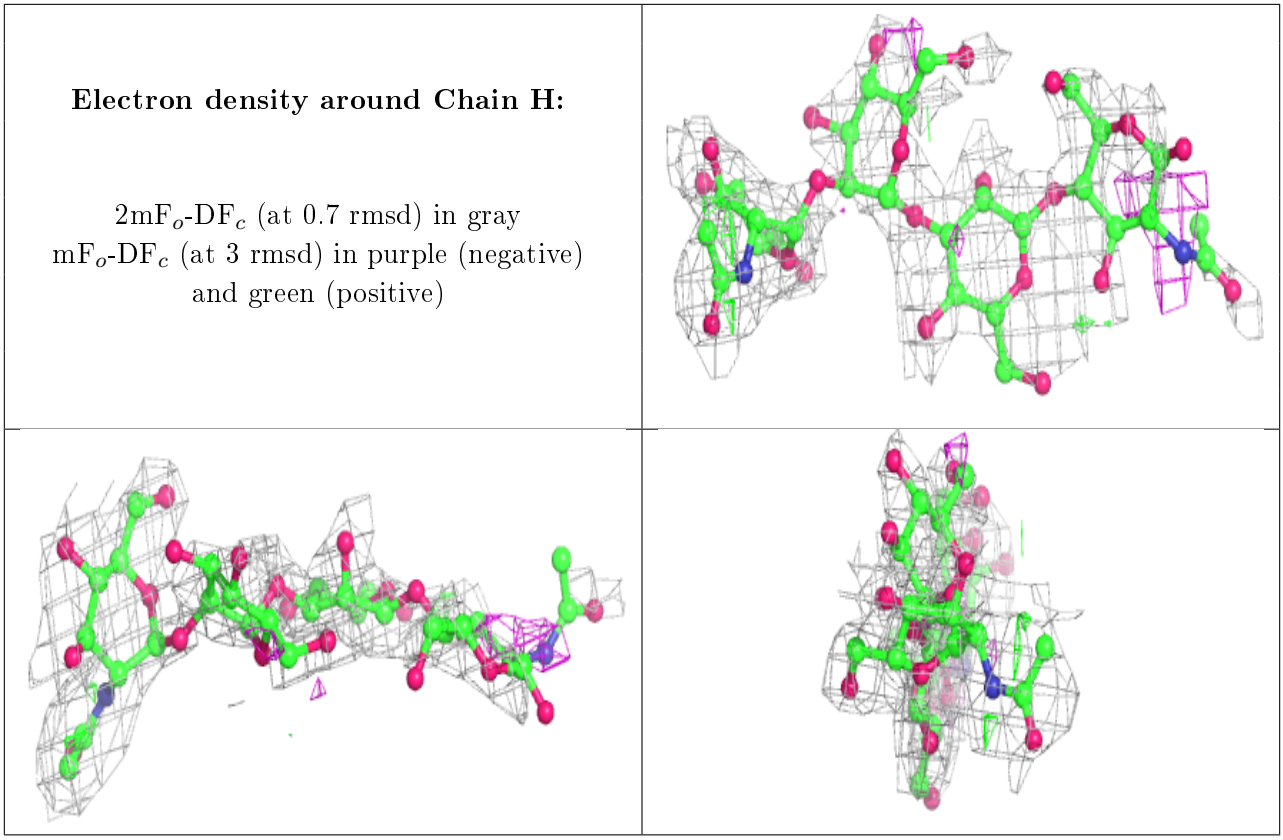
Electron density around Chain G:

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



Electron density around Chain H:

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



6.4 Ligands

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	B-factors(Å^2)	Q<0.9
3	EDO	A	1109	4/4	0.62	0.47	38,39,39,39	0
3	EDO	C	1109	4/4	0.71	0.21	51,52,52,52	0
3	EDO	A	1118	4/4	0.72	0.34	56,57,57,57	0
3	EDO	C	1105	4/4	0.74	0.30	51,52,52,52	0
3	EDO	B	1105	4/4	0.74	0.35	23,24,24,24	0
3	EDO	A	1110	4/4	0.75	0.34	34,34,34,34	0
3	EDO	D	1119	4/4	0.75	0.30	45,46,46,46	0
3	EDO	D	1107	4/4	0.77	0.27	27,27,27,27	0
3	EDO	D	1108	4/4	0.78	0.33	31,31,32,32	0
3	EDO	D	1106	4/4	0.78	0.37	31,32,32,32	0
3	EDO	A	1111	4/4	0.78	0.31	50,50,50,50	0
3	EDO	C	1110	4/4	0.79	0.36	27,28,28,28	0
3	EDO	A	1114	4/4	0.79	0.24	55,55,55,55	0
3	EDO	A	1108	4/4	0.79	0.31	26,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	1120	4/4	0.80	0.26	32,32,32,32	0
3	EDO	D	1101	4/4	0.80	0.22	50,50,50,50	0
3	EDO	C	1107	4/4	0.81	0.32	30,30,30,31	0
3	EDO	D	1116	4/4	0.81	0.32	31,31,31,31	0
3	EDO	C	1106	4/4	0.81	0.26	21,22,22,22	0
3	EDO	C	1111	4/4	0.81	0.29	47,47,47,47	0
3	EDO	D	1109	4/4	0.81	0.33	38,38,38,39	0
3	EDO	D	1111	4/4	0.82	0.22	31,31,31,31	0
3	EDO	A	1113	4/4	0.83	0.35	47,47,47,47	0
3	EDO	D	1114	4/4	0.83	0.32	44,45,45,45	0
3	EDO	B	1109	4/4	0.85	0.33	52,53,53,53	0
3	EDO	B	1112	4/4	0.85	0.15	41,42,42,42	0
3	EDO	A	1115	4/4	0.86	0.13	32,32,32,32	0
3	EDO	A	1119	4/4	0.86	0.17	41,41,41,41	0
3	EDO	A	1112	1/4	0.86	0.25	22,22,22,22	0
3	EDO	D	1113	4/4	0.86	0.22	41,42,42,42	0
3	EDO	A	1106	4/4	0.86	0.26	29,30,30,30	0
3	EDO	B	1107	4/4	0.86	0.23	39,39,39,39	0
3	EDO	A	1116	4/4	0.86	0.23	37,38,38,38	0
3	EDO	B	1108	4/4	0.87	0.18	25,25,25,25	0
3	EDO	D	1118	4/4	0.87	0.25	38,38,38,38	0
3	EDO	A	1105	4/4	0.87	0.25	31,31,31,31	0
3	EDO	C	1108	4/4	0.87	0.21	27,27,28,28	0
3	EDO	A	1117	4/4	0.88	0.28	43,43,43,43	0
3	EDO	B	1106	4/4	0.90	0.24	15,15,15,15	0
3	EDO	A	1107	4/4	0.90	0.20	24,24,24,24	0
3	EDO	B	1111	4/4	0.91	0.21	40,40,40,41	0
3	EDO	D	1110	4/4	0.91	0.20	24,25,25,25	0
3	EDO	D	1117	4/4	0.92	0.15	34,34,34,34	0
3	EDO	B	1110	4/4	0.92	0.23	25,26,26,26	0
3	EDO	D	1115	4/4	0.92	0.19	49,49,49,49	0
3	EDO	D	1112	4/4	0.95	0.14	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.