



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:41 PM UTC

PDB ID : 4PPH / pdb_00004pph
Title : Crystal structure of conglutin gamma, a unique basic 7S globulin from lupine seeds
Authors : Czubinski, J.; Barciszewski, J.; Gilski, M.; Lampart-Szczapa, E.; Jaskolski, M.
Deposited on : 2014-02-27
Resolution : 2.01 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

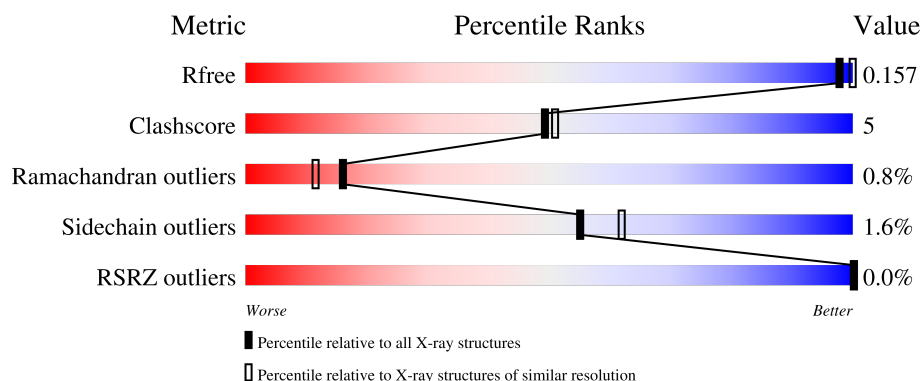
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	417	
1	B	417	
1	C	417	
1	D	417	
1	E	417	

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Mol	Chain	Length	Quality of chain
1	F	417	83% 10% • 6%
2	G	3	33% 67%
3	H	2	50% 50%

2 Entry composition [i](#)

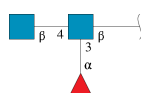
There are 6 unique types of molecules in this entry. The entry contains 19098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Conglutin gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	25	2	0
			2996	1887	529	563	17			
1	B	391	Total	C	N	O	S	26	7	0
			3020	1905	533	565	17			
1	C	392	Total	C	N	O	S	33	3	0
			3017	1900	534	566	17			
1	D	392	Total	C	N	O	S	30	2	0
			3017	1900	534	567	16			
1	E	391	Total	C	N	O	S	47	4	0
			3007	1895	530	565	17			
1	F	392	Total	C	N	O	S	46	3	0
			3011	1897	532	565	17			

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



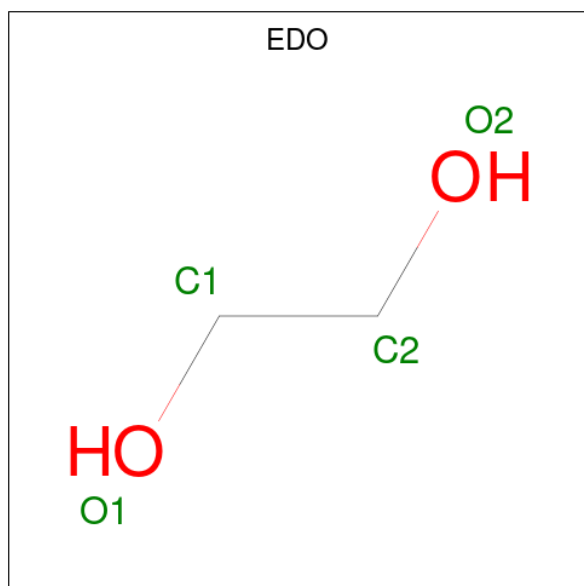
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



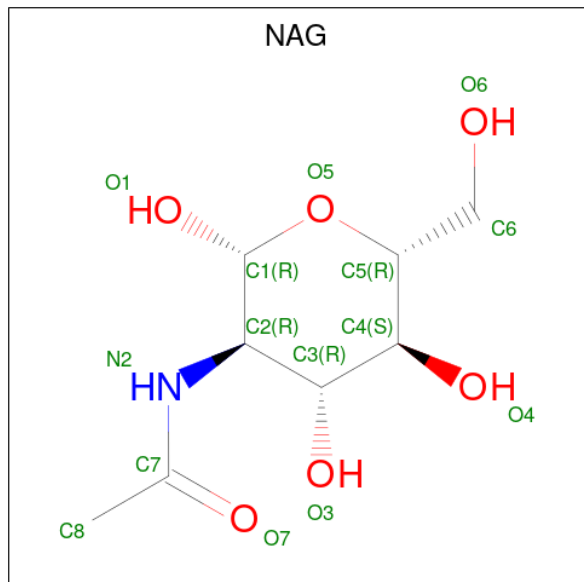
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

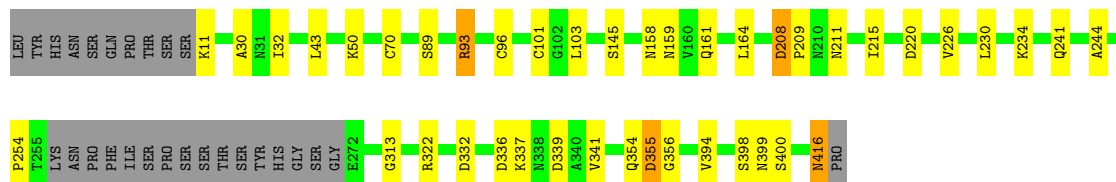
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	143	Total	O	0	0
			143	143		
6	B	146	Total	O	0	0
			146	146		
6	C	128	Total	O	0	0
			128	128		
6	D	124	Total	O	0	0
			124	124		
6	E	102	Total	O	0	0
			102	102		
6	F	151	Total	O	0	0
			151	151		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

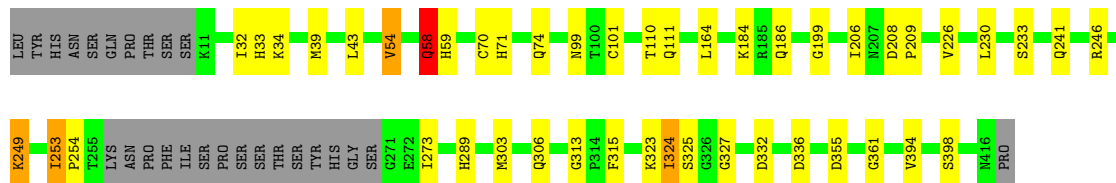
- Molecule 1: Conglutin gamma

Chain A: 



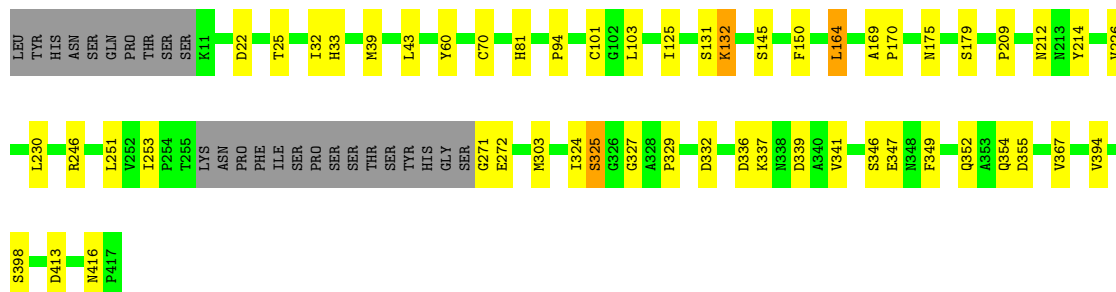
- Molecule 1: Conglutin gamma

Chain B: 



- Molecule 1: Conglutin gamma

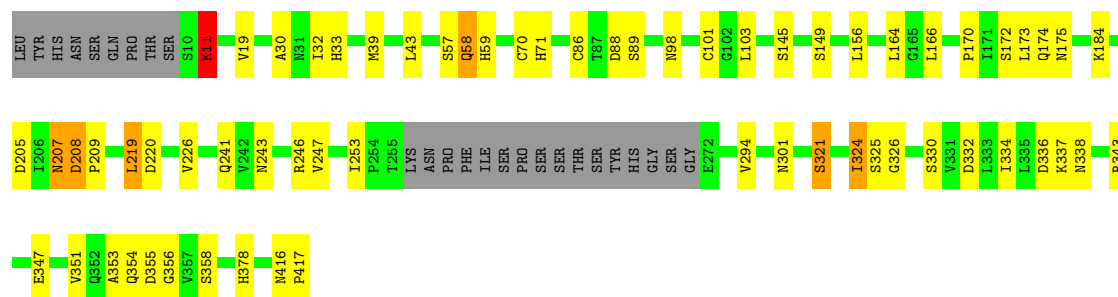
Chain C: 



- Molecule 1: Conglutin gamma

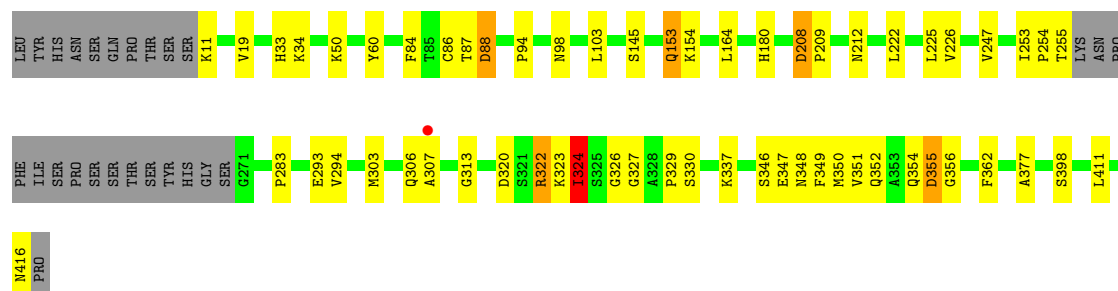
Chain D: 





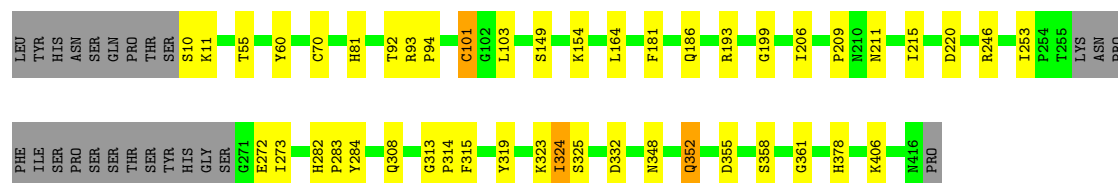
• Molecule 1: Conglutin gamma

Chain E: 80% 13% • 6%



• Molecule 1: Conglutin gamma

Chain F: 83% 10% • 6%



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

Chain G: 33% 67%



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

Chain H: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	121.99Å 121.99Å 188.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.76 – 2.01 43.76 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.76-2.01) 99.6 (43.76-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.145 , 0.174 0.143 , 0.157	Depositor DCC
R_{free} test set	999 reflections (0.44%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.098 for -h,-k,l 0.107 for h,-h-k,-l 0.248 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19098	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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, EDO, FUC

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	0.69	0/3073	0.93	5/4180 (0.1%)
1	B	0.71	0/3117	0.93	6/4239 (0.1%)
1	C	0.69	0/3096	0.94	4/4212 (0.1%)
1	D	0.70	0/3092	1.01	14/4207 (0.3%)
1	E	0.73	0/3092	1.03	11/4205 (0.3%)
1	F	0.72	0/3093	0.97	7/4207 (0.2%)
All	All	0.71	0/18563	0.97	47/25250 (0.2%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	SER	N-CA-C	10.45	122.75	111.36
1	D	57	SER	N-CA-C	8.70	121.56	109.29
1	E	348	ASN	N-CA-C	-7.70	102.89	111.28
1	C	339	ASP	N-CA-C	-7.69	103.87	113.18
1	B	253	ILE	N-CA-C	7.64	115.78	107.60
1	E	11	LYS	CA-C-N	7.02	126.94	119.85
1	E	11	LYS	C-N-CA	7.02	126.94	119.85
1	F	253	ILE	CA-C-N	6.78	126.76	119.78
1	F	253	ILE	C-N-CA	6.78	126.76	119.78
1	D	208	ASP	CA-C-N	6.76	127.03	119.32
1	D	208	ASP	C-N-CA	6.76	127.03	119.32
1	F	325	SER	N-CA-C	-6.54	103.86	112.24
1	D	324	ILE	N-CA-C	6.43	119.20	112.83
1	F	199	GLY	N-CA-C	-6.31	104.11	112.81
1	A	208	ASP	CA-C-N	6.28	126.76	119.47
1	A	208	ASP	C-N-CA	6.28	126.76	119.47
1	A	313	GLY	CA-C-N	6.27	127.41	120.45
1	A	313	GLY	C-N-CA	6.27	127.41	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	SER	CB-CA-C	-6.17	106.69	114.40
1	D	11	LYS	CA-C-N	6.07	126.04	120.03
1	D	11	LYS	C-N-CA	6.07	126.04	120.03
1	D	253	ILE	CA-C-N	6.05	125.81	119.76
1	D	253	ILE	C-N-CA	6.05	125.81	119.76
1	E	208	ASP	CA-C-N	5.99	126.42	119.47
1	E	208	ASP	C-N-CA	5.99	126.42	119.47
1	D	207	ASN	CA-C-N	-5.99	115.06	122.42
1	D	207	ASN	C-N-CA	-5.99	115.06	122.42
1	B	289	HIS	N-CA-C	5.89	118.17	111.11
1	E	87	THR	N-CA-C	-5.77	104.91	112.41
1	C	272	GLU	N-CA-C	-5.76	100.58	109.52
1	D	219	LEU	N-CA-C	5.75	117.54	111.28
1	F	93	ARG	N-CA-C	-5.71	102.99	108.07
1	D	347	GLU	N-CA-C	-5.71	106.27	113.18
1	E	313	GLY	CA-C-N	5.68	126.75	120.45
1	E	313	GLY	C-N-CA	5.68	126.75	120.45
1	A	93	ARG	N-CA-C	-5.60	103.09	108.07
1	B	199	GLY	N-CA-C	-5.59	105.10	112.81
1	B	58	GLN	N-CA-C	5.56	122.65	110.80
1	C	416	ASN	N-CA-C	5.52	117.03	110.07
1	F	149	SER	N-CA-C	5.46	117.23	111.28
1	E	253	ILE	CA-C-N	5.30	125.06	119.76
1	E	253	ILE	C-N-CA	5.30	125.06	119.76
1	B	313	GLY	CA-C-N	5.21	126.23	120.45
1	B	313	GLY	C-N-CA	5.21	126.23	120.45
1	C	347	GLU	N-CA-C	-5.15	106.95	113.18
1	F	55	THR	N-CA-C	-5.12	101.41	109.25
1	E	347	GLU	N-CA-C	-5.05	107.11	114.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	2921	30	0
1	B	3020	0	2953	31	0
1	C	3017	0	2937	39	0
1	D	3017	0	2939	40	0
1	E	3007	0	2936	37	0
1	F	3011	0	2935	24	0
2	G	38	0	34	0	0
3	H	28	0	25	1	0
4	A	24	0	36	5	0
4	B	20	0	30	0	0
4	C	20	0	30	3	0
4	D	36	0	54	7	0
4	E	4	0	6	1	0
4	F	24	0	36	3	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	A	143	0	0	0	0
6	B	146	0	0	1	0
6	C	128	0	0	4	0
6	D	124	0	0	2	0
6	E	102	0	0	2	0
6	F	151	0	0	2	0
All	All	19098	0	17911	192	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 5.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:H	1:A:416:ASN:HD22	1.20	0.84
1:E:50:LYS:H	4:E:501:EDO:H11	1.43	0.84
1:E:60:TYR:HB3	1:E:94:PRO:HG2	1.66	0.77
1:C:125:ILE:HA	4:C:506:EDO:H22	1.67	0.76
1:C:352:GLN:NE2	1:C:354:GLN:O	2.20	0.75
1:E:86:CYS:H	1:E:98:ASN:ND2	1.84	0.74
1:E:86:CYS:H	1:E:98:ASN:HD22	1.35	0.74
1:E:84:PHE:HE2	1:E:86:CYS:HB2	1.53	0.73
1:A:399:ASN:HB3	4:A:506:EDO:H21	1.71	0.72
1:C:325:SER:O	1:C:327:GLY:HA2	1.90	0.72
1:C:246:ARG:NH1	1:C:332:ASP:OD2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:LEU:HD23	1:D:145:SER:HB2	1.75	0.69
1:A:416:ASN:HD22	1:A:416:ASN:N	1.92	0.68
1:E:346:SER:HA	1:E:349:PHE:CE2	2.29	0.68
1:C:170:PRO:O	1:C:175[B]:ASN:ND2	2.27	0.67
1:E:84:PHE:CE2	1:E:86:CYS:HB2	2.29	0.67
1:A:103:LEU:HD23	1:A:145:SER:HB2	1.77	0.67
1:A:70:CYS:HA	1:A:101[B]:CYS:SG	2.36	0.66
1:F:284:TYR:H	4:F:504:EDO:H22	1.60	0.65
1:D:209:PRO:HB3	1:D:219:LEU:HD21	1.79	0.65
1:F:220:ASP:HB2	6:F:743:HOH:O	1.97	0.65
1:B:323:LYS:O	1:B:325:SER:N	2.30	0.64
1:B:186:GLN:HE22	1:B:206:ILE:HG12	1.62	0.64
1:C:32:ILE:HG13	1:C:43:LEU:HD12	1.79	0.64
1:B:74:GLN:HG3	4:C:502:EDO:H21	1.79	0.64
1:A:89:SER:HB2	1:A:93:ARG:CZ	2.28	0.63
1:A:354:GLN:HB3	1:A:355:ASP:OD1	2.03	0.59
1:B:246:ARG:NH1	1:B:332:ASP:OD2	2.34	0.59
1:B:99:ASN:HD21	1:C:271:GLY:HA3	1.69	0.58
1:D:88:ASP:OD1	1:D:89:SER:N	2.34	0.58
1:D:246:ARG:NH1	1:D:332:ASP:OD2	2.36	0.57
1:F:246:ARG:NH1	1:F:332:ASP:OD2	2.36	0.57
1:E:355:ASP:OD1	1:E:356:GLY:N	2.30	0.57
1:C:70:CYS:HA	1:C:101[B]:CYS:SG	2.45	0.57
1:E:254:PRO:O	1:E:255:THR:OG1	2.22	0.57
1:B:32:ILE:HG13	1:B:43:LEU:HD12	1.87	0.56
1:C:332:ASP:HB3	1:C:341:VAL:CG1	2.36	0.55
1:B:43:LEU:HD21	1:B:54[B]:VAL:HG12	1.87	0.55
1:B:324:ILE:O	1:B:327:GLY:N	2.39	0.54
1:A:93:ARG:HG2	1:A:96:CYS:HB3	1.90	0.54
1:B:246:ARG:HD3	6:B:701:HOH:O	2.07	0.53
1:F:11:LYS:HE3	1:F:181:PHE:O	2.08	0.53
1:F:272:GLU:OE1	1:F:273:ILE:N	2.40	0.53
1:F:186:GLN:HE22	1:F:206:ILE:HG12	1.73	0.53
1:F:308:GLN:HG2	1:F:319:TYR:CE2	2.43	0.53
1:C:332:ASP:HB3	1:C:341:VAL:HG13	1.90	0.53
1:F:60:TYR:HB3	1:F:94:PRO:HG2	1.90	0.53
1:C:246:ARG:HH21	4:D:508:EDO:H12	1.74	0.53
1:A:32:ILE:HG13	1:A:43:LEU:HD12	1.90	0.53
1:B:70:CYS:HA	1:B:101[B]:CYS:SG	2.49	0.53
1:A:416:ASN:H	1:A:416:ASN:ND2	1.98	0.53
1:D:32:ILE:HG13	1:D:43:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:HB3	1:A:336:ASP:HB2	1.92	0.52
1:C:81:HIS:HD2	6:C:683:HOH:O	1.91	0.52
1:D:170:PRO:O	1:D:175[B]:ASN:ND2	2.44	0.51
1:C:103:LEU:HD23	1:C:145:SER:HB2	1.91	0.51
1:F:282:HIS:HB2	4:F:504:EDO:H21	1.93	0.51
1:E:180:HIS:HD2	6:E:671:HOH:O	1.94	0.50
1:E:324:ILE:O	1:E:326:GLY:N	2.41	0.50
1:E:324:ILE:C	1:E:326:GLY:H	2.20	0.50
1:E:346:SER:O	1:E:350:MET:HG2	2.12	0.50
1:C:169:ALA:O	1:C:175[A]:ASN:ND2	2.42	0.50
1:D:378[A]:HIS:HD2	4:D:505:EDO:H11	1.77	0.50
1:C:336:ASP:N	6:C:714:HOH:O	2.44	0.49
1:D:30:ALA:HA	4:D:502:EDO:H21	1.94	0.49
1:C:251:LEU:HD21	4:D:508:EDO:H11	1.93	0.49
1:E:283:PRO:HA	1:E:377:ALA:HB3	1.95	0.49
1:D:416:ASN:HD22	1:D:417:PRO:HD2	1.77	0.49
1:A:337:LYS:CB	1:A:339:ASP:OD2	2.60	0.49
1:C:253:ILE:HD11	1:D:294:VAL:HG11	1.94	0.49
1:F:315:PHE:CE1	1:F:361:GLY:HA2	2.48	0.49
1:A:11:LYS:HD3	1:F:11:LYS:HD3	1.95	0.48
1:E:153:GLN:HG2	1:E:154:LYS:HD2	1.95	0.48
1:E:293:GLU:HG3	1:E:294:VAL:N	2.28	0.48
1:D:184:LYS:NZ	6:D:621:HOH:O	2.46	0.48
1:E:153:GLN:HG2	1:E:154:LYS:CD	2.43	0.48
1:D:247:VAL:HA	1:D:330:SER:O	2.13	0.48
1:D:416:ASN:ND2	1:D:417:PRO:HD2	2.28	0.48
1:A:50:LYS:HB2	4:A:509:EDO:H12	1.94	0.48
1:A:244:ALA:HA	1:A:254:PRO:HD3	1.95	0.48
1:D:241:GLN:HB3	1:D:336:ASP:HB2	1.95	0.48
1:C:303:MET:SD	1:C:329:PRO:HD3	2.54	0.48
1:F:406:LYS:NZ	6:F:743:HOH:O	2.46	0.48
1:B:71:HIS:HD2	6:C:691:HOH:O	1.97	0.47
1:E:307:ALA:O	1:E:320:ASP:N	2.46	0.47
1:D:354:GLN:HB3	1:D:355:ASP:OD1	2.13	0.47
1:F:209:PRO:HA	1:F:215:ILE:HD11	1.95	0.47
1:F:272:GLU:CD	1:F:273:ILE:H	2.22	0.47
1:B:241:GLN:HB3	1:B:336:ASP:HB2	1.97	0.47
1:B:226:VAL:HG23	1:B:398:SER:HB3	1.95	0.47
1:B:315:PHE:CE1	1:B:361:GLY:HA2	2.50	0.47
1:C:336:ASP:HB3	4:C:504:EDO:H22	1.96	0.47
1:D:58:GLN:HG3	1:D:59:HIS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:GLN:NE2	1:F:206:ILE:HG12	2.29	0.47
1:A:337:LYS:HB3	1:A:339:ASP:OD2	2.14	0.47
1:C:253:ILE:HD12	1:D:294:VAL:HG21	1.97	0.47
1:A:355:ASP:CG	1:A:356:GLY:H	2.23	0.46
1:D:324:ILE:C	1:D:326:GLY:H	2.21	0.46
1:D:325:SER:O	1:D:325:SER:OG	2.33	0.46
1:D:174:GLN:NE2	1:D:175[A]:ASN:OD1	2.48	0.46
1:A:30:ALA:HA	4:A:507:EDO:H12	1.97	0.46
1:C:209:PRO:HA	1:C:212:ASN:HB2	1.97	0.46
1:A:332:ASP:HB3	1:A:341:VAL:HG13	1.96	0.46
1:D:70:CYS:HA	1:D:101:CYS:SG	2.55	0.46
1:D:205:ASP:OD1	1:D:207:ASN:OD1	2.34	0.46
1:B:99:ASN:ND2	1:C:271:GLY:HA3	2.30	0.46
1:D:220:ASP:N	1:D:220:ASP:OD1	2.49	0.46
1:D:351:VAL:O	1:D:358:SER:HA	2.16	0.46
1:C:251:LEU:HD22	1:D:294:VAL:HG13	1.97	0.46
1:A:226:VAL:HG23	1:A:398:SER:HB3	1.98	0.45
1:A:400:SER:H	4:A:506:EDO:H21	1.81	0.45
1:D:19:VAL:HG12	1:D:30:ALA:HB2	1.97	0.45
1:E:153:GLN:HE21	1:E:154:LYS:HD3	1.80	0.45
1:B:303:MET:HE3	1:B:324:ILE:HD12	1.98	0.45
1:D:172:SER:OG	1:D:175[A]:ASN:OD1	2.35	0.45
1:E:247:VAL:HA	1:E:330:SER:O	2.17	0.45
1:B:249:LYS:HB3	1:B:249:LYS:HE2	1.71	0.45
1:B:323:LYS:C	1:B:325:SER:H	2.23	0.45
1:E:153:GLN:O	1:E:154:LYS:HD2	2.16	0.45
1:C:337:LYS:HA	1:C:337:LYS:HD3	1.66	0.44
1:A:400:SER:H	4:A:506:EDO:C2	2.30	0.44
1:C:33:HIS:HA	1:C:39:MET:O	2.17	0.44
1:C:230:LEU:HD13	1:C:394:VAL:CG2	2.47	0.44
1:E:226:VAL:HG23	1:E:398:SER:HB3	2.00	0.44
1:E:86:CYS:SG	1:E:88:ASP:HB3	2.56	0.44
1:A:234:LYS:HG2	1:F:81:HIS:CG	2.53	0.44
1:B:99:ASN:OD1	1:C:271:GLY:HA3	2.18	0.44
1:E:324:ILE:HA	1:E:324:ILE:HD13	1.61	0.44
1:F:348:ASN:O	1:F:378[B]:HIS:CD2	2.71	0.44
1:B:184:LYS:HZ3	1:B:186:GLN:HB2	1.82	0.44
1:C:346:SER:HA	1:C:349:PHE:CE2	2.53	0.44
1:C:60:TYR:HB3	1:C:94:PRO:HG2	1.99	0.44
1:C:22:ASP:OD2	1:C:25:THR:HG23	2.18	0.43
1:A:234:LYS:HE3	1:F:81:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:HG23	1:C:398:SER:HB3	2.00	0.43
1:B:58:GLN:HB2	1:B:59:HIS:H	1.47	0.43
1:E:209:PRO:O	1:E:212:ASN:HB2	2.19	0.43
1:C:150:PHE:CD1	1:C:150:PHE:C	2.96	0.43
1:D:156:LEU:O	4:D:506:EDO:H21	2.19	0.43
1:F:103:LEU:HD12	1:F:103:LEU:HA	1.85	0.43
1:B:233:SER:HA	1:B:273:ILE:HD13	2.00	0.43
1:B:208:ASP:HA	1:B:209:PRO:HD2	1.82	0.43
1:C:132:LYS:HE3	1:C:132:LYS:HB3	1.55	0.43
1:E:346:SER:HA	1:E:349:PHE:CZ	2.54	0.43
1:C:355:ASP:OD1	1:C:355:ASP:N	2.50	0.42
1:D:332:ASP:CG	1:D:343:ARG:HG2	2.43	0.42
1:A:158:ASN:O	1:A:159:ASN:HB2	2.18	0.42
1:E:222:LEU:HA	1:E:225:LEU:HG	2.01	0.42
1:D:88:ASP:CG	1:D:89:SER:H	2.26	0.42
1:D:301:ASN:ND2	4:D:508:EDO:H21	2.34	0.42
1:E:352:GLN:C	1:E:354:GLN:H	2.28	0.42
1:D:166:LEU:HD21	1:D:173:LEU:HD23	2.01	0.42
1:D:226:VAL:HG21	4:D:509:EDO:H21	2.02	0.42
1:F:352:GLN:HE21	1:F:358:SER:HB2	1.84	0.42
1:B:34:LYS:HE2	1:B:34:LYS:HB3	1.71	0.42
1:D:243:ASN:N	1:D:334:ILE:O	2.49	0.42
1:B:230:LEU:HD13	1:B:394:VAL:CG2	2.50	0.42
1:E:411:LEU:HD23	1:E:411:LEU:HA	1.96	0.42
1:C:32:ILE:HD11	1:C:164:LEU:HD22	2.02	0.42
1:C:131:SER:HA	1:C:214:TYR:HA	2.00	0.42
1:E:34:LYS:HB3	1:E:34:LYS:HE2	1.79	0.42
1:A:211:ASN:O	1:A:215:ILE:HG13	2.20	0.41
1:B:253:ILE:HA	1:B:254:PRO:HD3	1.89	0.41
1:C:179:SER:HB3	6:C:723:HOH:O	2.20	0.41
1:E:303:MET:SD	1:E:329:PRO:HD3	2.60	0.41
1:F:283:PRO:HD2	4:F:504:EDO:H21	2.01	0.41
1:A:230:LEU:HD13	1:A:394:VAL:CG2	2.50	0.41
1:C:324:ILE:O	1:C:325:SER:OG	2.34	0.41
1:F:92:THR:HG22	3:H:1:NAG:H81	2.02	0.41
1:D:86:CYS:N	1:D:98:ASN:OD1	2.43	0.41
1:D:71:HIS:HA	6:D:671:HOH:O	2.20	0.41
1:B:184:LYS:NZ	1:B:186:GLN:HB2	2.35	0.41
1:C:132:LYS:HD2	1:C:413:ASP:OD2	2.21	0.41
1:E:352:GLN:HG3	1:E:354:GLN:O	2.20	0.41
1:A:220:ASP:OD1	1:A:220:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASP:HA	1:D:209:PRO:HD2	1.71	0.41
1:D:321:SER:HG	1:D:356:GLY:C	2.28	0.41
1:E:208:ASP:HA	1:E:209:PRO:HD2	1.71	0.41
1:B:33:HIS:HA	1:B:39:MET:O	2.21	0.41
1:E:349:PHE:HB2	1:E:362:PHE:CE1	2.56	0.41
1:B:110:THR:O	1:B:111:GLN:HB2	2.20	0.41
1:F:70:CYS:HA	1:F:101[A]:CYS:SG	2.60	0.41
1:B:324:ILE:O	1:B:325:SER:C	2.64	0.41
1:E:103:LEU:HD23	1:E:145:SER:HB2	2.02	0.41
1:A:208:ASP:HA	1:A:209:PRO:HD2	1.72	0.40
1:B:303:MET:CE	1:B:324:ILE:HD12	2.52	0.40
1:F:313:GLY:HA3	1:F:314:PRO:HD2	1.99	0.40
1:A:89:SER:HB2	1:A:93:ARG:NH1	2.37	0.40
1:D:33:HIS:HA	1:D:39:MET:O	2.21	0.40
1:D:166:LEU:HD23	1:D:173:LEU:HB3	2.04	0.40
1:E:19[B]:VAL:HG23	6:E:607:HOH:O	2.22	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	388/417 (93%)	374 (96%)	13 (3%)	1 (0%)	36	35
1	B	394/417 (94%)	378 (96%)	13 (3%)	3 (1%)	16	11
1	C	391/417 (94%)	378 (97%)	12 (3%)	1 (0%)	36	35
1	D	390/417 (94%)	373 (96%)	13 (3%)	4 (1%)	12	8
1	E	391/417 (94%)	374 (96%)	11 (3%)	6 (2%)	8	4
1	F	391/417 (94%)	372 (95%)	16 (4%)	3 (1%)	16	11
All	All	2345/2502 (94%)	2249 (96%)	78 (3%)	18 (1%)	16	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ASP
1	B	58	GLN
1	D	58	GLN
1	D	338	ASN
1	E	88	ASP
1	E	324	ILE
1	F	323	LYS
1	F	355	ASP
1	B	324	ILE
1	C	325	SER
1	D	11	LYS
1	E	322	ARG
1	E	355	ASP
1	E	323	LYS
1	B	355	ASP
1	D	353	ALA
1	F	324	ILE
1	E	327	GLY

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	339/362 (94%)	335 (99%)	4 (1%)	63	70
1	B	344/362 (95%)	338 (98%)	6 (2%)	53	60
1	C	341/362 (94%)	338 (99%)	3 (1%)	70	78
1	D	341/362 (94%)	337 (99%)	4 (1%)	63	70
1	E	341/362 (94%)	333 (98%)	8 (2%)	44	49
1	F	341/362 (94%)	332 (97%)	9 (3%)	40	44
All	All	2047/2172 (94%)	2013 (98%)	34 (2%)	55	60

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	164	LEU
1	A	322	ARG
1	A	416	ASN
1	B	54[A]	VAL
1	B	54[B]	VAL
1	B	58	GLN
1	B	164	LEU
1	B	249	LYS
1	B	306	GLN
1	C	132	LYS
1	C	164	LEU
1	C	367	VAL
1	D	11	LYS
1	D	149	SER
1	D	164	LEU
1	D	337	LYS
1	E	153	GLN
1	E	164	LEU
1	E	306	GLN
1	E	322	ARG
1	E	324	ILE
1	E	337	LYS
1	E	351	VAL
1	E	416	ASN
1	F	10	SER
1	F	101[A]	CYS
1	F	101[B]	CYS
1	F	154	LYS
1	F	164	LEU
1	F	193	ARG
1	F	211	ASN
1	F	324	ILE
1	F	352	GLN

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	71	HIS
1	A	198	ASN
1	A	241	GLN
1	A	243	ASN

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Mol	Chain	Res	Type
1	A	338	ASN
1	A	416	ASN
1	B	40	GLN
1	B	71	HIS
1	B	81	HIS
1	B	111	GLN
1	B	158	ASN
1	B	180	HIS
1	B	207	ASN
1	B	212	ASN
1	B	248	ASN
1	B	416	ASN
1	C	81	HIS
1	C	158	ASN
1	C	159	ASN
1	C	212	ASN
1	C	235	GLN
1	D	20	GLN
1	D	40	GLN
1	D	111	GLN
1	D	186	GLN
1	D	207	ASN
1	D	216	HIS
1	D	297	GLN
1	D	348	ASN
1	D	416	ASN
1	E	71	HIS
1	E	81	HIS
1	E	98	ASN
1	E	153	GLN
1	E	161	GLN
1	E	180	HIS
1	E	198	ASN
1	E	213	ASN
1	E	352	GLN
1	E	354	GLN
1	E	368	HIS
1	F	20	GLN
1	F	40	GLN
1	F	71	HIS
1	F	211	ASN
1	F	235	GLN

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Mol	Chain	Res	Type
1	F	241	GLN
1	F	352	GLN

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 ⓘ

5 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	G	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	0.65	0
2	FUC	G	2	2	10,10,11	1.25	1 (10%)	14,14,16	0.95	0
2	NAG	G	3	2	14,14,15	0.50	0	17,19,21	0.58	0
3	NAG	H	1	3,1	14,14,15	0.92	1 (7%)	17,19,21	0.62	0
3	NAG	H	2	3	14,14,15	0.66	0	17,19,21	0.43	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
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	2.88	1.48	1.43
3	H	1	NAG	O5-C1	-2.85	1.38	1.43
2	G	2	FUC	C4-C5	2.57	1.58	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

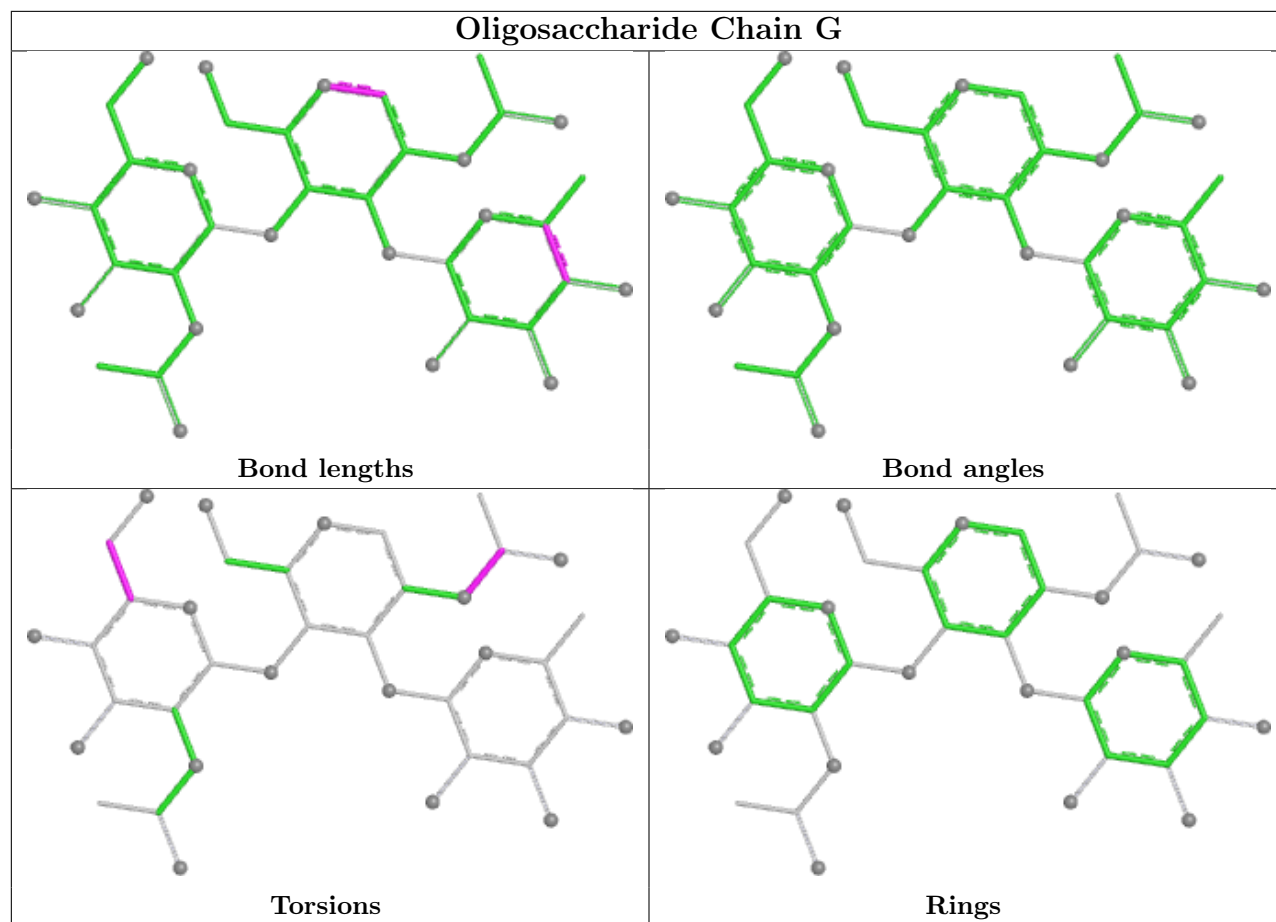
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	G	3	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	3	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6

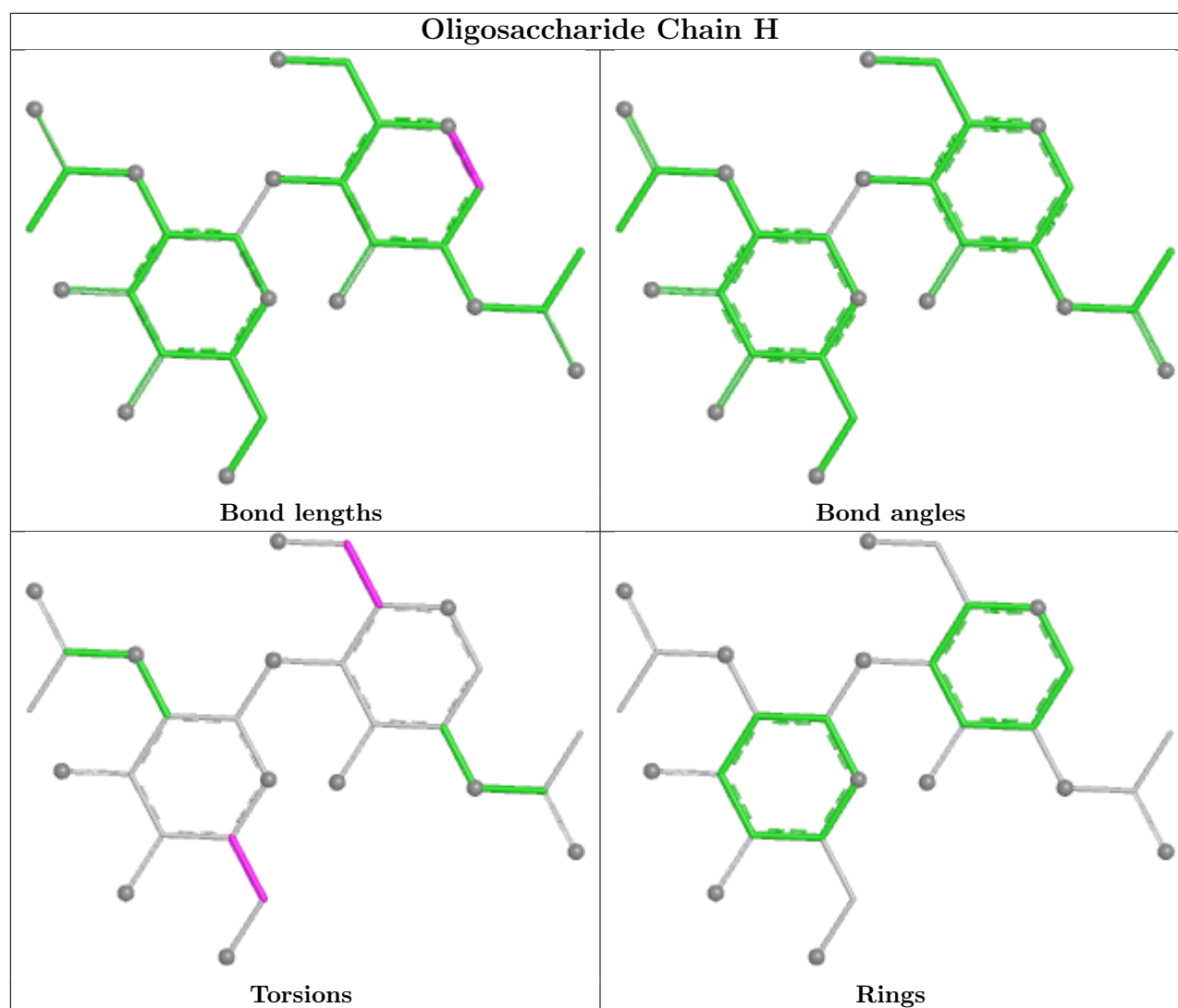
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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.





5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	D	503	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	F	506	-	3,3,3	0.35	0	2,2,2	0.27	0
4	EDO	C	506	-	3,3,3	0.56	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	505	-	3,3,3	0.48	0	2,2,2	0.26	0
4	EDO	D	506	-	3,3,3	0.43	0	2,2,2	0.11	0
4	EDO	F	507	-	3,3,3	0.49	0	2,2,2	0.11	0
4	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.22	0
4	EDO	A	504	-	3,3,3	0.52	0	2,2,2	0.14	0
4	EDO	A	509	-	3,3,3	0.50	0	2,2,2	0.14	0
5	NAG	B	501	1	14,14,15	0.45	0	17,19,21	0.55	0
4	EDO	B	502	-	3,3,3	0.39	0	2,2,2	0.38	0
4	EDO	F	504	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	A	508	-	3,3,3	0.36	0	2,2,2	0.67	0
4	EDO	C	503	-	3,3,3	0.45	0	2,2,2	0.19	0
4	EDO	D	510	-	3,3,3	0.43	0	2,2,2	0.53	0
4	EDO	B	506	-	3,3,3	0.44	0	2,2,2	0.45	0
5	NAG	D	501	1	14,14,15	0.80	1 (7%)	17,19,21	0.66	0
4	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.09	0
4	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.28	0
4	EDO	B	503	-	3,3,3	0.36	0	2,2,2	0.32	0
4	EDO	F	508	-	3,3,3	0.39	0	2,2,2	0.31	0
5	NAG	C	501	1	14,14,15	0.46	0	17,19,21	0.44	0
4	EDO	D	508	-	3,3,3	0.62	0	2,2,2	0.05	0
4	EDO	A	507	-	3,3,3	0.36	0	2,2,2	0.55	0
4	EDO	D	507	-	3,3,3	0.54	0	2,2,2	0.28	0
4	EDO	D	504	-	3,3,3	0.37	0	2,2,2	0.25	0
4	EDO	F	505	-	3,3,3	0.35	0	2,2,2	0.68	0
4	EDO	A	506	-	3,3,3	0.27	0	2,2,2	0.38	0
4	EDO	E	501	-	3,3,3	0.50	0	2,2,2	0.47	0
4	EDO	C	505	-	3,3,3	0.35	0	2,2,2	0.66	0
4	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.38	0
4	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.26	0
4	EDO	D	502	-	3,3,3	0.33	0	2,2,2	0.73	0
4	EDO	D	509	-	3,3,3	0.52	0	2,2,2	0.16	0
4	EDO	F	503	-	3,3,3	0.41	0	2,2,2	0.82	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
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	F	506	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	505	-	-	1/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	F	507	-	-	0/1/1/1	-
4	EDO	C	502	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
5	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	EDO	B	502	-	-	0/1/1/1	-
4	EDO	F	504	-	-	0/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	F	508	-	-	0/1/1/1	-
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	F	505	-	-	0/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	E	501	-	-	1/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	F	503	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	NAG	O5-C1	2.66	1.48	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501	NAG	O5-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
4	D	505	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
4	E	501	EDO	O1-C1-C2-O2
4	F	503	EDO	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2
4	A	509	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	506	EDO	1	0
4	D	505	EDO	1	0
4	D	506	EDO	1	0
4	C	502	EDO	1	0
4	A	509	EDO	1	0
4	F	504	EDO	3	0
4	D	508	EDO	3	0
4	A	507	EDO	1	0
4	A	506	EDO	3	0
4	E	501	EDO	1	0
4	C	504	EDO	1	0
4	D	502	EDO	1	0
4	D	509	EDO	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	390/417 (93%)	-1.29	0 100 100	20, 41, 74, 99	7 (1%)
1	B	391/417 (93%)	-1.36	0 100 100	13, 36, 69, 96	12 (3%)
1	C	392/417 (94%)	-1.28	0 100 100	18, 41, 76, 96	10 (2%)
1	D	392/417 (94%)	-1.22	0 100 100	17, 44, 78, 101	8 (2%)
1	E	389/417 (93%)	-1.12	1 (0%) 90 89	20, 44, 93, 134	11 (2%)
1	F	389/417 (93%)	-1.26	0 100 100	22, 40, 76, 110	8 (2%)
All	All	2343/2502 (93%)	-1.26	1 (0%) 100 100	13, 41, 78, 134	56 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	ALA	2.1

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.

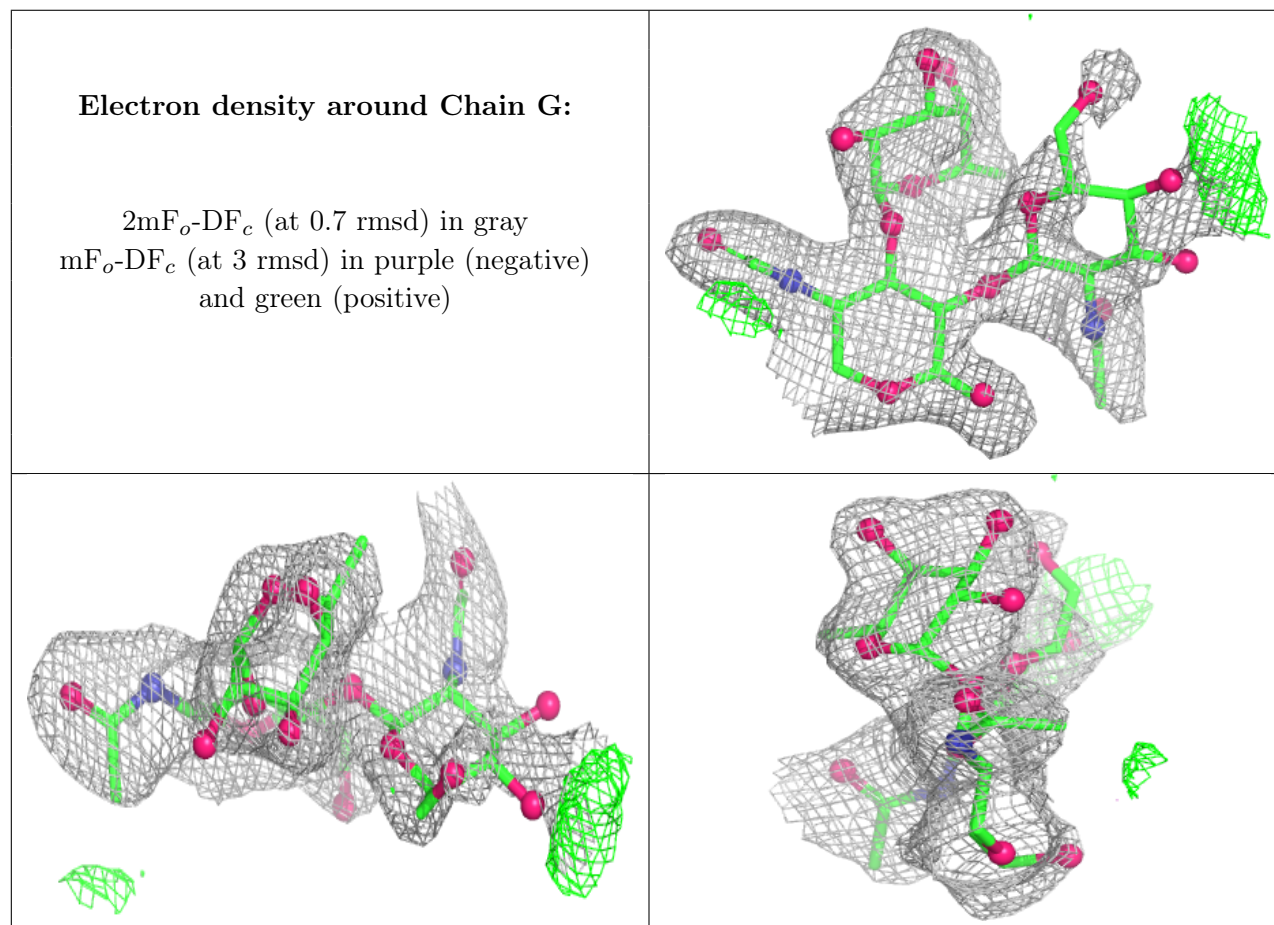
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	3	14/15	0.93	0.10	86,92,93,94	0
3	NAG	H	1	14/15	0.97	0.06	55,65,75,85	0
3	NAG	H	2	14/15	0.97	0.08	91,94,98,99	0

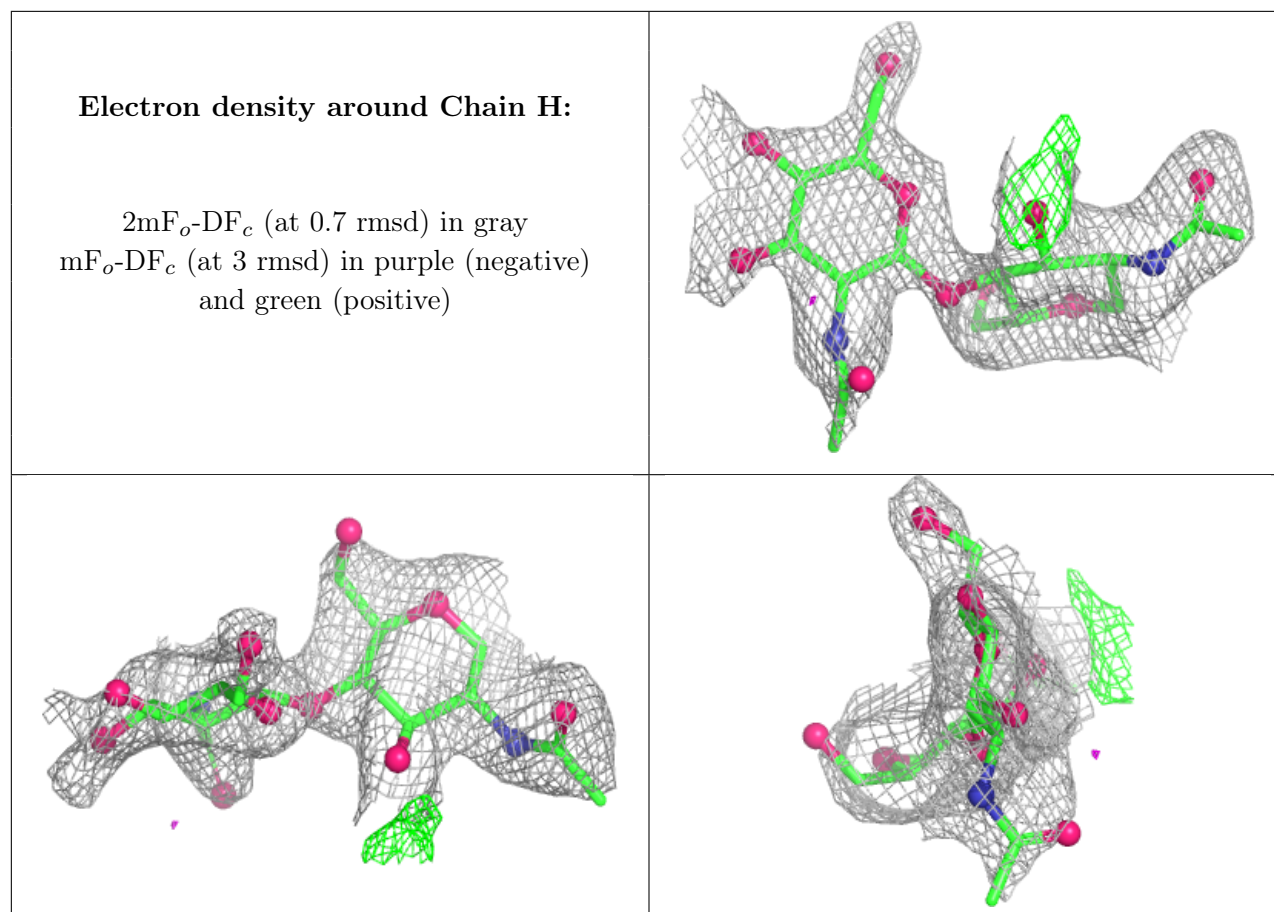
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	1	14/15	0.98	0.04	57,67,74,80	0
2	FUC	G	2	10/11	0.99	0.04	64,71,82,83	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	F	505	4/4	0.96	0.08	58,60,60,60	0
5	NAG	C	501	14/15	0.96	0.07	69,78,83,83	0
5	NAG	B	501	14/15	0.97	0.05	61,69,74,74	0
4	EDO	B	506	4/4	0.97	0.07	36,37,37,39	0
5	NAG	D	501	14/15	0.97	0.06	61,69,71,74	0
4	EDO	D	506	4/4	0.98	0.06	53,54,54,55	0
4	EDO	D	507	4/4	0.98	0.08	57,58,58,59	0
4	EDO	D	509	4/4	0.98	0.08	54,57,60,61	0
4	EDO	D	510	4/4	0.98	0.06	53,54,55,58	0
4	EDO	A	507	4/4	0.98	0.06	41,41,44,47	0
4	EDO	A	505	4/4	0.98	0.08	47,50,52,52	0
4	EDO	C	506	4/4	0.98	0.06	44,50,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	503	4/4	0.98	0.07	49,49,52,55	0
4	EDO	D	502	4/4	0.99	0.04	46,47,48,48	0
4	EDO	A	508	4/4	0.99	0.06	51,55,56,56	0
4	EDO	D	504	4/4	0.99	0.03	34,35,36,36	0
4	EDO	D	505	4/4	0.99	0.05	47,47,50,54	0
4	EDO	B	502	4/4	0.99	0.07	52,52,53,55	0
4	EDO	B	504	4/4	0.99	0.04	49,49,51,56	0
4	EDO	D	508	4/4	0.99	0.05	51,51,52,52	0
4	EDO	A	506	4/4	0.99	0.05	37,37,40,40	0
4	EDO	C	502	4/4	0.99	0.04	57,57,57,58	0
4	EDO	E	501	4/4	0.99	0.04	32,35,39,41	0
4	EDO	F	503	4/4	0.99	0.05	44,45,49,53	0
4	EDO	F	504	4/4	0.99	0.05	44,45,45,48	0
4	EDO	C	503	4/4	0.99	0.03	27,28,30,32	0
4	EDO	F	507	4/4	0.99	0.05	53,53,55,55	0
4	EDO	F	508	4/4	0.99	0.04	46,47,50,52	0
4	EDO	C	504	4/4	0.99	0.06	48,51,54,58	0
4	EDO	C	505	4/4	0.99	0.04	36,38,38,40	0
4	EDO	A	504	4/4	0.99	0.04	33,34,36,39	0
4	EDO	B	505	4/4	1.00	0.03	27,31,33,33	0
4	EDO	B	503	4/4	1.00	0.03	32,32,33,34	0
4	EDO	F	506	4/4	1.00	0.03	28,29,30,31	0
4	EDO	A	509	4/4	1.00	0.04	40,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.