Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 11:55 PM EDT

PDB ID	:	6MYA
Title	:	Crystal structure of InvbP.18715.a.KN11: Influenza hemagglutinin from strain A/Almaty/32/1998
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2018-11-01
Resolution	:	2.05 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

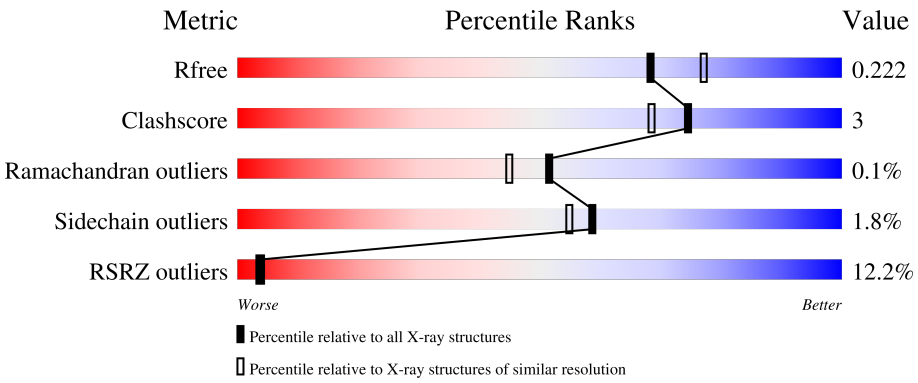
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	499	10% 89% 8% • •
1	B	499	10% 86% 10% •
1	C	499	4% 88% 9% •
1	D	499	19% 87% 8% • •
1	E	499	14% 91% 7% • •

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Mol	Chain	Length	Quality of chain
1	F	499	15% 88% 8%
2	G	2	50% 50%
2	H	2	100%
2	I	2	100%

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	G	2	-	-	-	X
2	NAG	H	2	-	-	-	X
2	NAG	I	1	-	-	-	X
2	NAG	I	2	-	-	-	X
3	NAG	A	502	-	-	-	X
3	NAG	A	503	-	-	-	X
3	NAG	A	504	-	-	-	X
3	NAG	B	501	-	-	-	X
3	NAG	B	504	-	-	-	X
3	NAG	C	501	-	-	-	X
3	NAG	C	503	-	-	-	X
3	NAG	F	501	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24594 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.

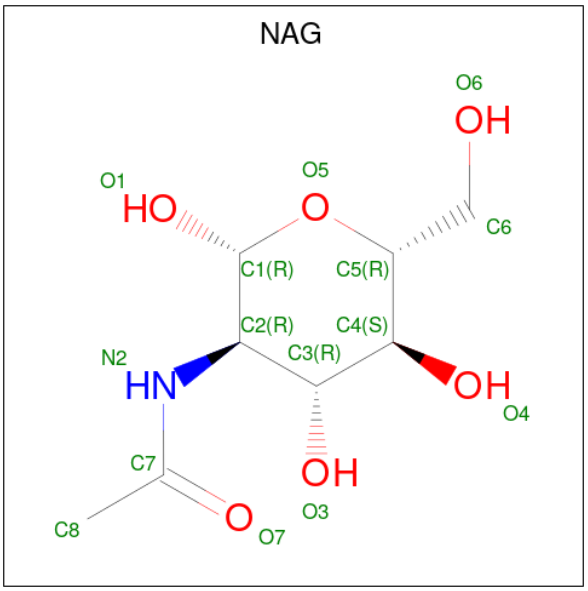
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3784	2384	651	730	19	0	8	0
1	B	482	3715	2345	640	711	19	0	4	0
1	C	486	3802	2395	647	741	19	0	9	0
1	D	478	3650	2300	626	705	19	0	7	0
1	E	489	3769	2377	647	725	20	0	7	0
1	F	484	3698	2328	637	713	20	0	5	0

- Molecule 2 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
			Total	C	N	O			
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0
2	I	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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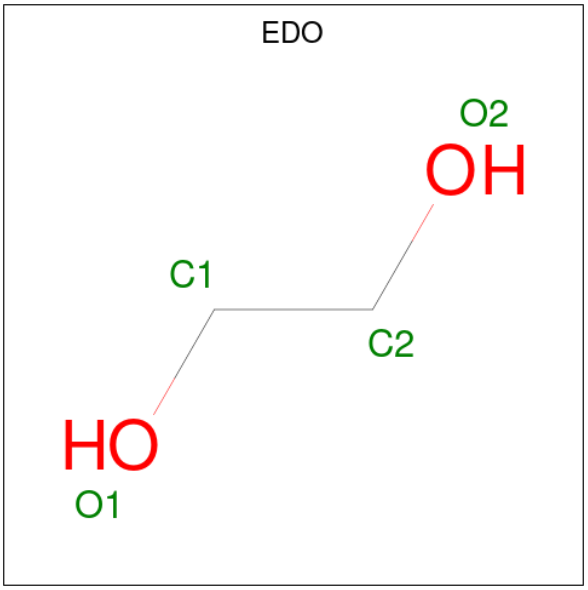
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	F	1	14	8	1	5	0	0
3	F	1	14	8	1	5	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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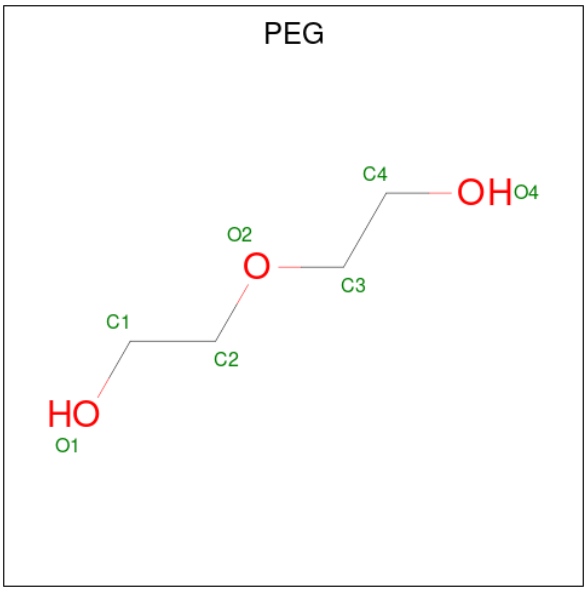
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	E	1	4	2	2	0	0
			Total	C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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	E	1	7	4	3	0	0

- Molecule 6 is water.

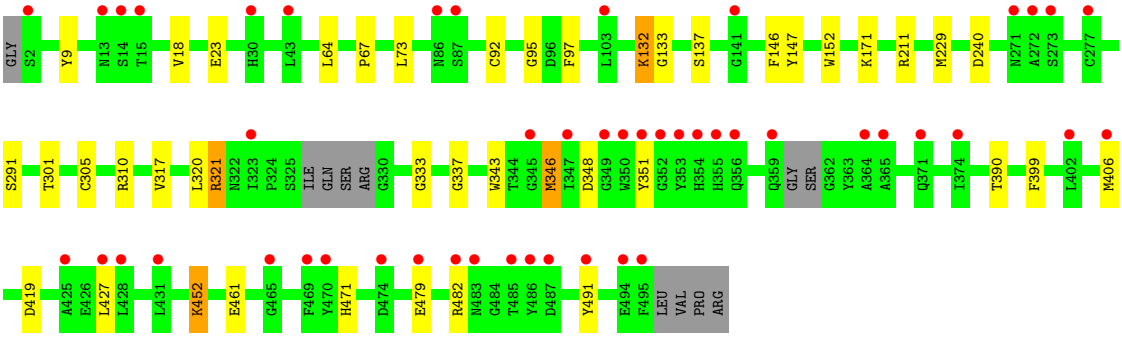
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	261	264	264	0	3
			Total	O		
6	B	295	299	299	0	4
			Total	O		
6	C	320	323	323	0	3
			Total	O		
6	D	309	312	312	0	3
			Total	O		
6	E	283	284	284	0	1
			Total	O		
6	F	289	291	291	0	2

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.

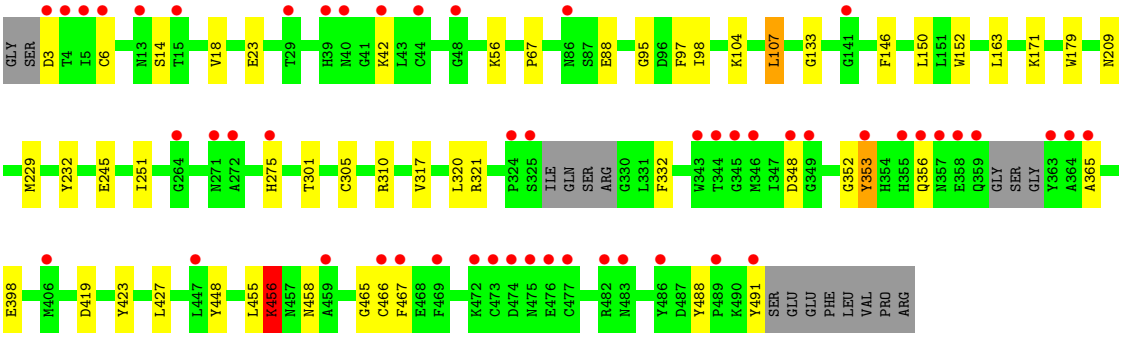
• Molecule 1: Hemagglutinin

Chain A:



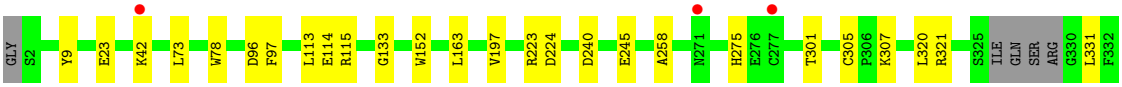
• Molecule 1: Hemagglutinin

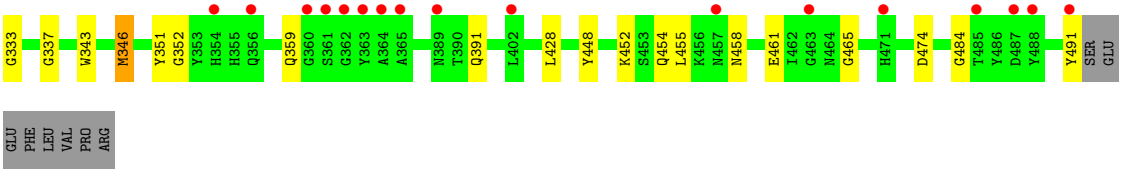
Chain B:



• Molecule 1: Hemagglutinin

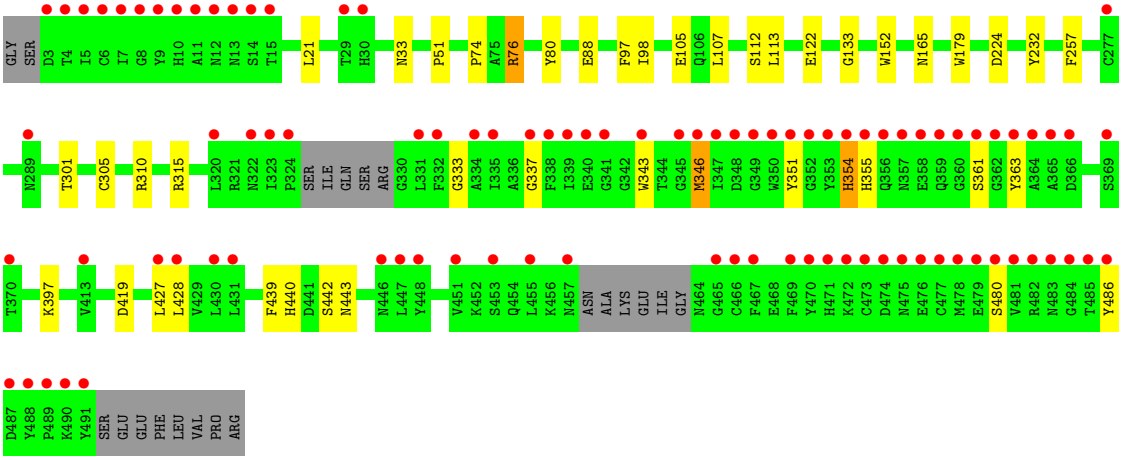
Chain C:





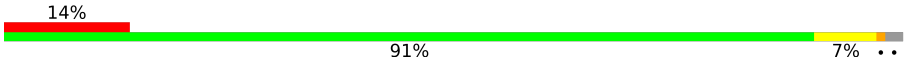
- Molecule 1: Hemagglutinin

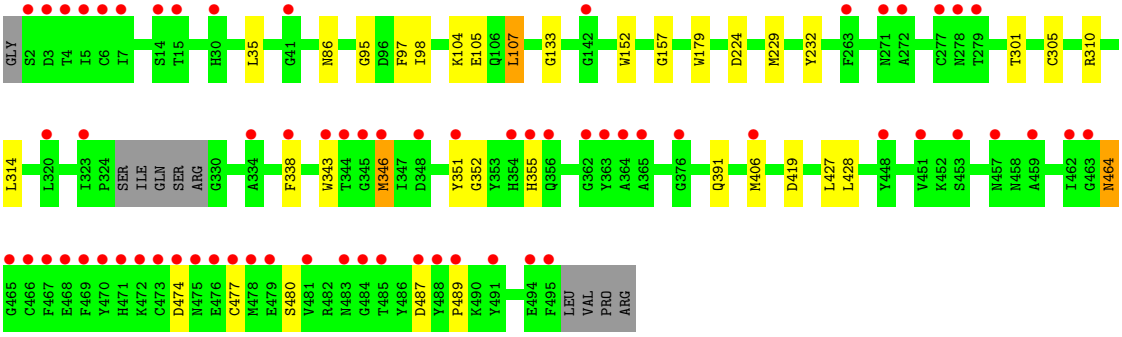
Chain D:



- Molecule 1: Hemagglutinin

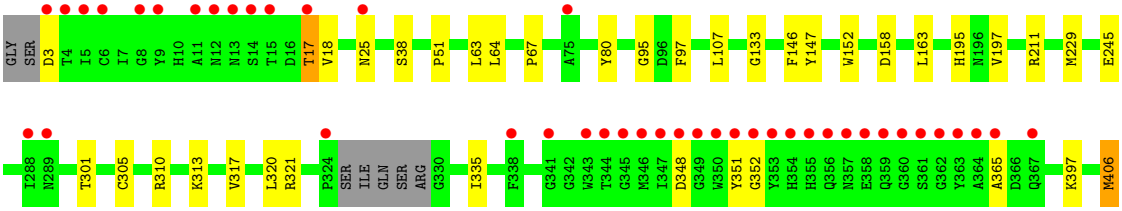
Chain E:

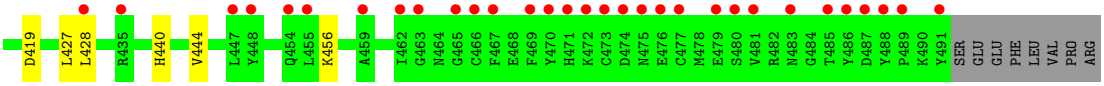




- Molecule 1: Hemagglutinin

Chain F:



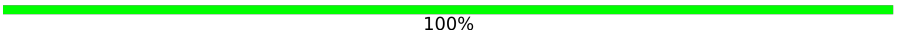


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

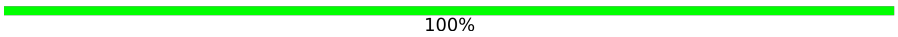
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.65Å 244.37Å 115.02Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	45.93 – 2.05 48.11 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.93-2.05) 96.5 (48.11-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_3283	Depositor
R, R_{free}	0.188 , 0.222 0.189 , 0.222	Depositor DCC
R_{free} test set	2003 reflections (0.87%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24594	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NAG, EDO

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	0.38	0/3899	0.55	0/5310
1	B	0.40	0/3817	0.59	1/5195 (0.0%)
1	C	0.41	0/3920	0.58	0/5332
1	D	0.43	0/3758	0.58	0/5118
1	E	0.40	0/3885	0.56	1/5294 (0.0%)
1	F	0.42	0/3804	0.58	0/5186
All	All	0.41	0/23083	0.57	2/31435 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	LEU	CA-CB-CG	-5.06	103.66	115.30
1	E	107	LEU	CA-CB-CG	-5.01	103.78	115.30

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	3784	0	3511	22	0
1	B	3715	0	3462	30	0
1	C	3802	0	3580	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3650	0	3355	22	0
1	E	3769	0	3480	18	0
1	F	3698	0	3399	26	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	56	0	52	0	0
3	B	42	0	39	0	0
3	C	56	0	52	0	0
3	D	14	0	13	0	0
3	E	28	0	26	0	0
3	F	28	0	26	0	0
4	A	12	0	18	1	0
4	C	36	0	54	4	0
4	D	16	0	24	0	0
4	E	16	0	24	2	0
4	F	8	0	12	1	0
5	E	7	0	10	0	0
6	A	264	0	0	2	0
6	B	299	0	0	1	0
6	C	323	0	0	1	0
6	D	312	0	0	1	0
6	E	284	0	0	1	0
6	F	291	0	0	2	0
All	All	24594	0	21212	139	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 (139) 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:C:23:GLU:OE1	1:C:321:ARG:NH2	2.13	0.77
1:A:399:PHE:CE1	1:A:406:MET:HG2	2.23	0.74
1:E:98[A]:ILE:HG13	1:E:232:TYR:CE2	2.31	0.65
1:F:335:ILE:HG13	1:F:444:VAL:HG21	1.79	0.64
1:F:351:TYR:OH	1:F:440:HIS:ND1	2.25	0.64
1:E:104:LYS:HB3	4:E:508:EDO:H12	1.78	0.64
1:F:63:LEU:HD11	1:F:107:LEU:HD11	1.80	0.64
1:E:310:ARG:NH1	1:E:419:ASP:OD1	2.29	0.62
1:C:454:GLN:HE22	1:C:484:GLY:HA2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ASN:ND2	1:B:491:TYR:HB2	2.16	0.61
1:C:133:GLY:HA3	1:C:152:TRP:HB3	1.82	0.60
1:B:56:LYS:NZ	1:B:88:GLU:OE2	2.35	0.59
1:B:310:ARG:NH1	1:B:419:ASP:OD1	2.25	0.59
1:E:133:GLY:HA3	1:E:152:TRP:HB3	1.85	0.58
1:A:427:LEU:HD21	1:C:428:LEU:HD13	1.84	0.58
1:B:98[A]:ILE:HG13	1:B:232:TYR:CE2	2.39	0.58
1:C:223:ARG:HH12	4:C:510:EDO:H22	1.70	0.56
1:B:23:GLU:OE1	1:B:321[B]:ARG:NH2	2.31	0.56
1:D:105:GLU:OE1	1:D:397:LYS:HE2	2.05	0.56
1:F:17:THR:OG1	1:F:25:ASN:HA	2.06	0.56
1:B:133:GLY:HA3	1:B:152:TRP:HB3	1.88	0.55
1:B:171:LYS:HE2	6:B:624:HOH:O	2.07	0.55
1:E:301:THR:HB	1:E:305:CYS:SG	2.47	0.55
1:B:3:ASP:N	1:B:356:GLN:O	2.40	0.54
1:D:480:SER:OG	1:D:486:TYR:HA	2.07	0.54
1:D:133:GLY:HA3	1:D:152:TRP:HB3	1.90	0.53
1:E:105:GLU:HA	4:E:508:EDO:H21	1.91	0.53
1:F:197:VAL:HG12	6:F:812:HOH:O	2.08	0.53
1:B:423:TYR:CZ	1:B:427:LEU:HD12	2.44	0.53
1:D:301:THR:HB	1:D:305:CYS:SG	2.49	0.53
1:D:439:PHE:O	1:D:443:ASN:ND2	2.42	0.53
1:C:240:ASP:HB2	4:C:513:EDO:H11	1.91	0.53
1:D:33:ASN:HB2	1:D:315:ARG:NH2	2.24	0.53
1:F:351:TYR:HH	1:F:440:HIS:HD1	1.53	0.53
1:B:67:PRO:HG3	1:B:146:PHE:O	2.10	0.52
1:C:454:GLN:NE2	1:C:484:GLY:HA2	2.23	0.52
1:A:133:GLY:HA3	1:A:152:TRP:HB3	1.90	0.52
1:F:440:HIS:O	1:F:444:VAL:HG22	2.10	0.52
1:E:343:TRP:HE3	1:E:346:MET:HE2	1.74	0.51
1:E:338:PHE:O	1:E:464:ASN:HA	2.09	0.51
1:C:301:THR:HB	1:C:305:CYS:SG	2.51	0.51
1:D:98[A]:ILE:HG13	1:D:232:TYR:CE2	2.45	0.51
1:D:427:LEU:HD21	1:F:428:LEU:HD13	1.91	0.51
1:B:95:GLY:HA3	1:B:229:MET:O	2.09	0.51
1:C:114:GLU:HG3	1:C:258:ALA:HB3	1.92	0.51
1:C:96:ASP:HB2	4:C:511:EDO:H21	1.92	0.50
1:C:197:VAL:HG12	6:C:771:HOH:O	2.10	0.50
1:B:104:LYS:NZ	1:B:398:GLU:OE1	2.26	0.50
1:A:301:THR:HB	1:A:305:CYS:SG	2.51	0.50
1:C:343:TRP:HE3	1:C:346:MET:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:ASP:N	1:F:3:ASP:OD1	2.45	0.49
1:B:18:VAL:HG21	1:B:317:VAL:HB	1.94	0.49
1:D:343:TRP:HE3	1:D:346:MET:HE2	1.77	0.49
1:F:17:THR:HG23	1:F:313:LYS:NZ	2.28	0.49
1:A:310:ARG:NH1	1:A:419:ASP:OD1	2.30	0.48
1:F:301:THR:HB	1:F:305:CYS:SG	2.53	0.48
1:F:133:GLY:HA3	1:F:152:TRP:HB3	1.95	0.48
1:E:406[B]:MET:HE3	1:F:406[B]:MET:HG3	1.95	0.48
1:A:348:ASP:OD1	1:A:348:ASP:N	2.47	0.48
1:B:42:LYS:HE2	1:B:275:HIS:ND1	2.29	0.48
1:A:67:PRO:HG3	1:A:146:PHE:O	2.14	0.48
1:A:479:GLU:HA	1:A:482:ARG:HD2	1.94	0.48
1:D:354:HIS:HB2	1:D:363:TYR:CD1	2.48	0.48
1:C:452:LYS:HE3	1:C:461:GLU:OE1	2.13	0.48
1:F:348:ASP:OD1	1:F:348:ASP:N	2.45	0.47
1:F:67:PRO:HG3	1:F:146:PHE:O	2.14	0.47
1:E:95:GLY:HA3	1:E:229:MET:O	2.14	0.47
1:F:95:GLY:HA3	1:F:229:MET:O	2.14	0.47
1:A:95:GLY:HA3	1:A:229:MET:O	2.15	0.47
1:A:211[B]:ARG:HD2	6:A:627:HOH:O	2.14	0.47
1:B:352:GLY:HA3	1:B:365:ALA:HA	1.95	0.47
1:B:301:THR:HB	1:B:305:CYS:SG	2.55	0.47
1:C:346:MET:SD	1:C:352:GLY:HA3	2.56	0.46
1:D:351:TYR:OH	1:D:440:HIS:ND1	2.37	0.46
1:A:343:TRP:HE3	1:A:346:MET:HE2	1.81	0.46
1:E:474:ASP:N	1:E:477:CYS:HB3	2.30	0.46
1:F:211[B]:ARG:NH1	4:F:503:EDO:O1	2.49	0.46
1:A:171:LYS:HE2	6:A:666:HOH:O	2.15	0.45
1:F:18:VAL:HG21	1:F:317:VAL:HB	1.98	0.45
1:F:352:GLY:HA3	1:F:365:ALA:HA	1.98	0.45
1:C:42:LYS:HD2	1:C:275:HIS:CD2	2.52	0.45
1:F:17:THR:HG22	6:F:603:HOH:O	2.16	0.45
1:F:310:ARG:NH1	1:F:419:ASP:OD1	2.38	0.45
1:B:209:ASN:HB3	4:C:505:EDO:H12	1.97	0.45
1:A:18:VAL:HG21	1:A:317:VAL:HB	1.98	0.45
1:D:113:LEU:HD22	1:D:257:PHE:HB3	1.98	0.44
1:A:132:LYS:HB2	1:A:132:LYS:HE2	1.77	0.44
1:D:343:TRP:CE3	1:D:346:MET:HE2	2.53	0.44
1:D:355:HIS:O	1:D:361:SER:HA	2.17	0.44
1:B:42:LYS:HE2	1:B:275:HIS:CE1	2.53	0.44
1:C:333:GLY:O	1:C:337:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ARG:NH1	1:D:419:ASP:OD1	2.34	0.44
1:F:163:LEU:O	1:F:245:GLU:HA	2.17	0.44
1:A:240:ASP:HB2	4:A:506:EDO:H12	2.00	0.44
1:F:64:LEU:O	1:F:147:TYR:HB3	2.18	0.43
1:B:448:TYR:CE1	1:B:465:GLY:HA2	2.53	0.43
1:A:23:GLU:OE2	1:A:321[B]:ARG:NH1	2.52	0.43
1:B:150:LEU:HB3	1:B:251:ILE:HG22	2.00	0.43
1:B:6:CYS:HA	1:B:466:CYS:HA	1.99	0.43
1:C:307:LYS:HD2	1:C:391:GLN:HB2	2.00	0.43
1:E:487:ASP:OD2	1:E:489:PRO:HD2	2.19	0.43
1:E:35:LEU:HB2	1:E:314:LEU:HB2	2.01	0.42
1:A:333:GLY:O	1:A:337:GLY:HA3	2.20	0.42
1:D:179:TRP:CE2	1:D:232:TYR:HB2	2.55	0.42
1:C:448:TYR:CE1	1:C:465:GLY:HA2	2.55	0.42
1:E:355:HIS:HD2	6:E:798:HOH:O	2.01	0.42
1:A:64:LEU:O	1:A:147:TYR:HB3	2.19	0.42
1:A:452:LYS:NZ	1:A:461:GLU:OE1	2.49	0.42
1:B:348:ASP:OD1	1:B:348:ASP:N	2.51	0.42
1:C:458:ASN:ND2	1:C:491:TYR:HB2	2.35	0.42
1:B:456:LYS:HB2	1:B:488:TYR:CE2	2.55	0.42
1:A:9:TYR:HB2	1:A:320:LEU:HD22	2.02	0.42
1:C:9:TYR:HB2	1:C:320:LEU:CD2	2.50	0.41
1:B:42:LYS:HG2	1:B:275:HIS:CD2	2.56	0.41
1:B:179:TRP:CE2	1:B:232:TYR:HB2	2.55	0.41
1:F:158:ASP:OD1	1:F:195:HIS:ND1	2.50	0.41
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.90	0.41
1:D:88:GLU:HB3	6:D:863:HOH:O	2.21	0.41
1:D:333:GLY:O	1:D:337:GLY:HA3	2.20	0.41
1:B:332:PHE:CZ	1:C:331:LEU:HG	2.56	0.41
1:A:471:HIS:CD2	1:A:491:TYR:HB3	2.56	0.41
1:C:73:LEU:HD22	1:C:115:ARG:CZ	2.50	0.41
1:B:6:CYS:O	1:B:353:TYR:HA	2.20	0.41
1:B:455:LEU:HD21	1:B:467:PHE:CG	2.56	0.41
1:C:359:GLN:OE1	1:C:474:ASP:HB2	2.21	0.41
1:E:346:MET:SD	1:E:352:GLY:HA3	2.61	0.41
1:E:428:LEU:HD13	1:F:427:LEU:HD21	2.03	0.41
1:D:428:LEU:HD13	1:E:427:LEU:HD21	2.03	0.41
1:C:114:GLU:CG	1:C:258:ALA:HB3	2.51	0.40
1:E:179:TRP:CE2	1:E:232:TYR:HB2	2.56	0.40
1:C:78:TRP:HH2	1:C:113:LEU:HG	1.86	0.40
1:C:455:LEU:O	1:C:458:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:CYS:HB2	1:A:137:SER:O	2.21	0.40
1:D:51:PRO:HB3	1:D:80:TYR:CZ	2.56	0.40
1:B:163:LEU:O	1:B:245:GLU:HA	2.22	0.40
1:B:320:LEU:N	1:B:320:LEU:HD12	2.36	0.40
1:C:163:LEU:O	1:C:245:GLU:HA	2.21	0.40
1:D:74:PRO:O	1:D:76:ARG:HG2	2.22	0.40
1:F:51:PRO:HB3	1:F:80:TYR:CZ	2.57	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	490/499 (98%)	480 (98%)	10 (2%)	0	100	100
1	B	480/499 (96%)	468 (98%)	11 (2%)	1 (0%)	47	39
1	C	491/499 (98%)	482 (98%)	9 (2%)	0	100	100
1	D	479/499 (96%)	468 (98%)	11 (2%)	0	100	100
1	E	492/499 (99%)	479 (97%)	11 (2%)	2 (0%)	34	24
1	F	485/499 (97%)	473 (98%)	11 (2%)	1 (0%)	47	39
All	All	2917/2994 (97%)	2850 (98%)	63 (2%)	4 (0%)	51	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	456	LYS
1	F	456	LYS
1	E	86	ASN
1	E	157	GLY

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	402/438 (92%)	392 (98%)	10 (2%)	47	40
1	B	392/438 (90%)	387 (99%)	5 (1%)	69	67
1	C	414/438 (94%)	409 (99%)	5 (1%)	71	70
1	D	378/438 (86%)	367 (97%)	11 (3%)	42	35
1	E	398/438 (91%)	390 (98%)	8 (2%)	55	50
1	F	386/438 (88%)	378 (98%)	8 (2%)	53	48
All	All	2370/2628 (90%)	2323 (98%)	47 (2%)	59	50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	97	PHE
1	A	132	LYS
1	A	291	SER
1	A	321[A]	ARG
1	A	321[B]	ARG
1	A	346	MET
1	A	351	TYR
1	A	390	THR
1	A	452	LYS
1	B	14	SER
1	B	97	PHE
1	B	107	LEU
1	B	353	TYR
1	B	456	LYS
1	C	97	PHE
1	C	224[A]	ASP
1	C	224[B]	ASP
1	C	346	MET
1	C	351	TYR
1	D	76	ARG
1	D	97	PHE

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Mol	Chain	Res	Type
1	D	107	LEU
1	D	112	SER
1	D	122[A]	GLU
1	D	122[B]	GLU
1	D	165	ASN
1	D	224	ASP
1	D	346	MET
1	D	354	HIS
1	D	442	SER
1	E	97	PHE
1	E	107	LEU
1	E	224	ASP
1	E	346	MET
1	E	351	TYR
1	E	391	GLN
1	E	464	ASN
1	E	480	SER
1	F	17	THR
1	F	38	SER
1	F	97	PHE
1	F	320	LEU
1	F	321	ARG
1	F	397	LYS
1	F	406[A]	MET
1	F	406[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	443	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

6 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	0.39	0	17,19,21	0.41	0
2	NAG	G	2	2	14,14,15	0.27	0	17,19,21	0.75	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.31	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.75	0	17,19,21	0.70	0
2	NAG	I	1	2,1	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	I	2	2	14,14,15	0.34	0	17,19,21	0.81	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	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	C1-O5-C5	2.49	115.56	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

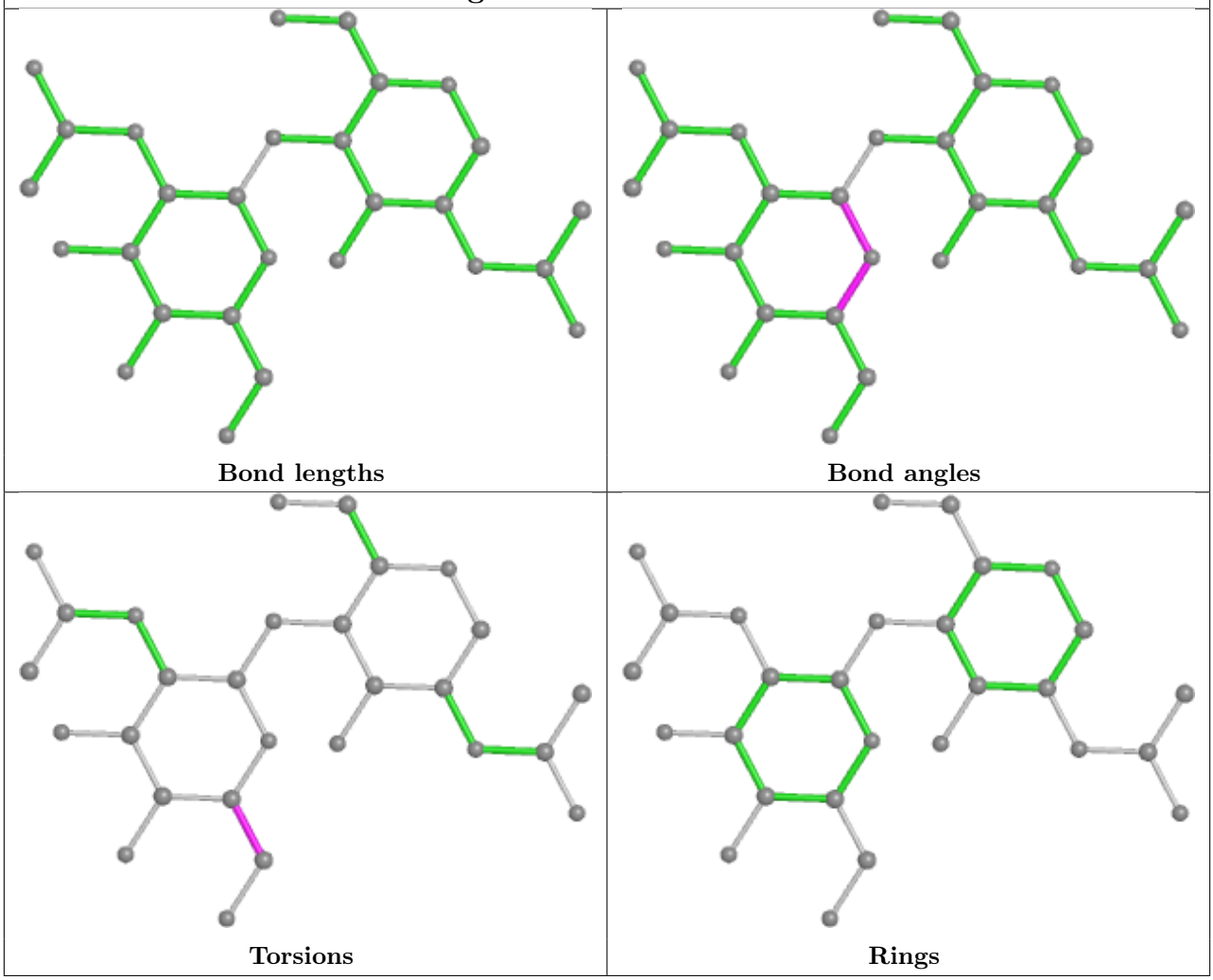
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	C1-C2-N2-C7
2	I	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
2	I	1	NAG	O5-C5-C6-O6

There are no ring outliers.

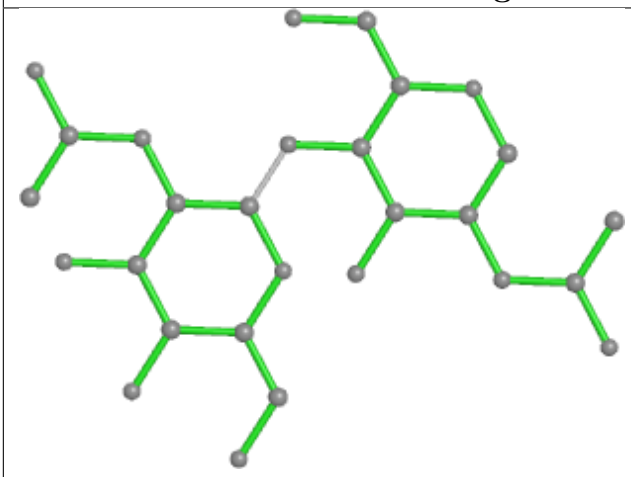
No monomer is involved in short contacts.

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

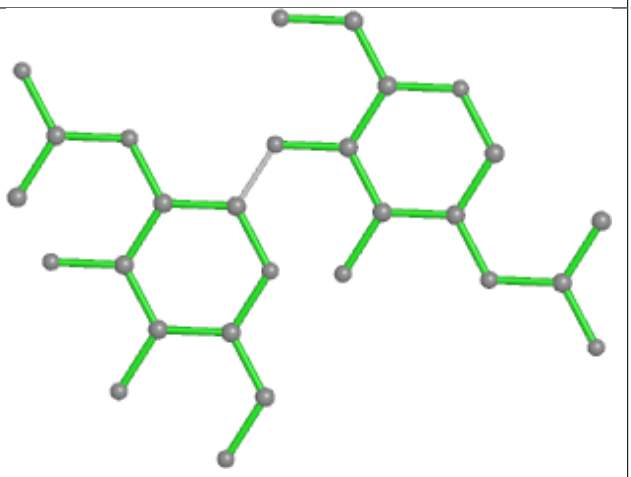
Oligosaccharide Chain G



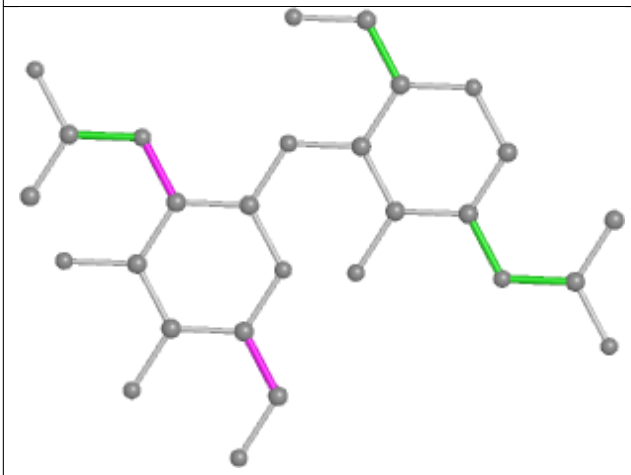
Oligosaccharide Chain H



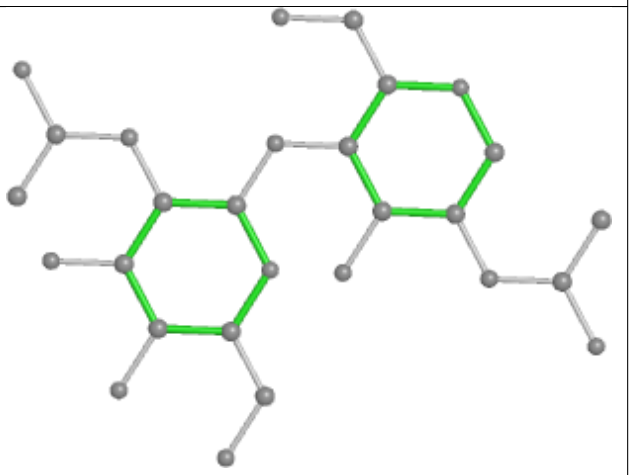
Bond lengths



Bond angles

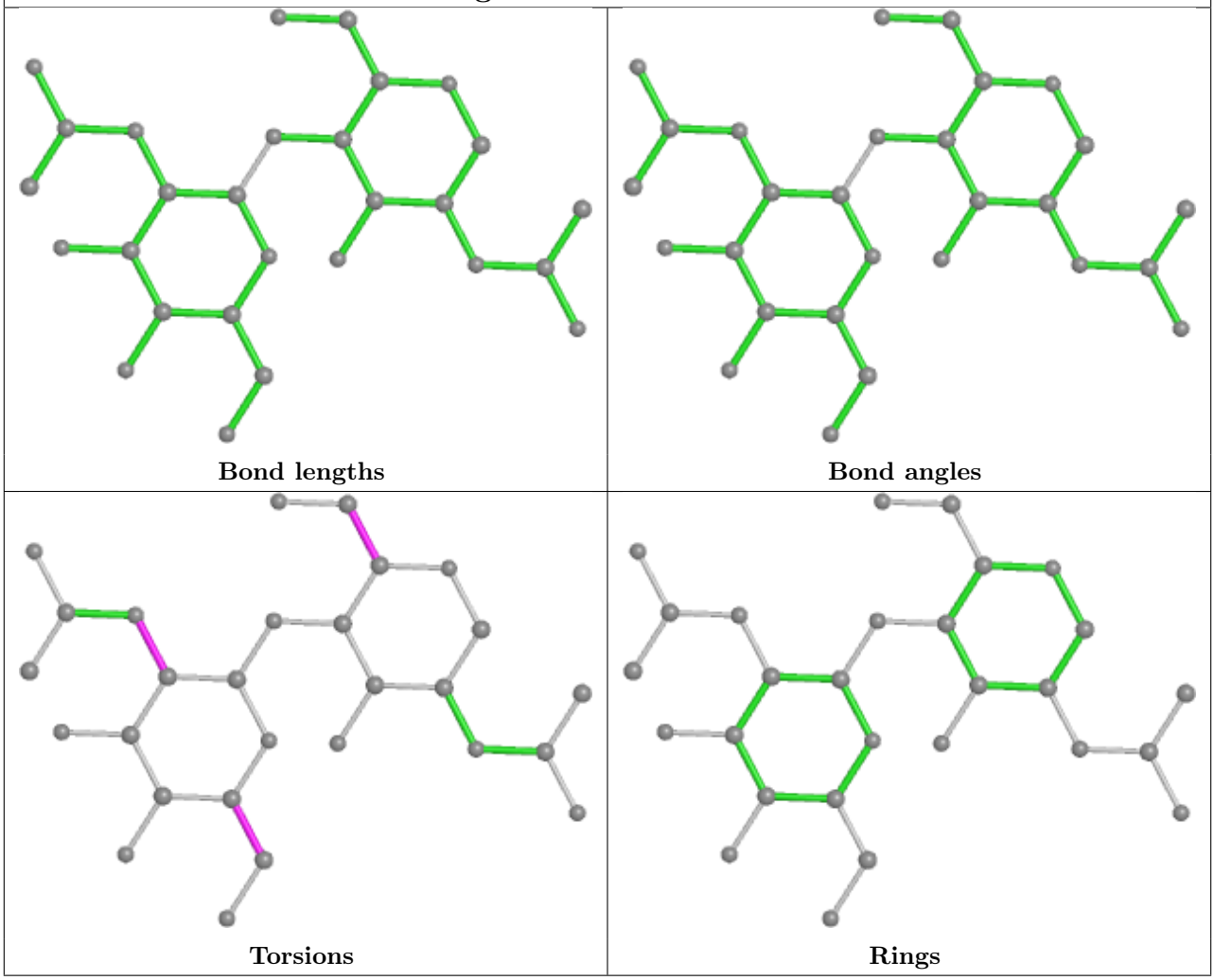


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

39 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	505	-	3,3,3	0.40	0	2,2,2	0.50	0
4	EDO	C	506	-	3,3,3	0.54	0	2,2,2	0.39	0
3	NAG	B	501	1	14,14,15	0.65	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	E	508	-	3,3,3	0.44	0	2,2,2	0.22	0
4	EDO	D	506	-	3,3,3	0.44	0	2,2,2	0.41	0
4	EDO	C	511	-	3,3,3	0.55	0	2,2,2	0.23	0
3	NAG	A	504	1	14,14,15	0.46	0	17,19,21	0.49	0
4	EDO	F	503	-	3,3,3	0.49	0	2,2,2	0.23	0
3	NAG	E	503	1	14,14,15	0.55	0	17,19,21	0.71	1 (5%)
4	EDO	C	508	-	3,3,3	0.44	0	2,2,2	0.32	0
3	NAG	C	501	1	14,14,15	0.33	0	17,19,21	0.55	0
4	EDO	C	505	-	3,3,3	0.82	0	2,2,2	0.57	0
3	NAG	B	505	1	14,14,15	0.34	0	17,19,21	0.53	0
4	EDO	E	505	-	3,3,3	0.50	0	2,2,2	0.23	0
3	NAG	E	504	1	14,14,15	0.32	0	17,19,21	0.47	0
4	EDO	D	507	-	3,3,3	0.63	0	2,2,2	0.07	0
3	NAG	A	501	1	14,14,15	0.53	0	17,19,21	0.63	0
3	NAG	D	501	1	14,14,15	0.71	0	17,19,21	0.61	1 (5%)
4	EDO	F	504	-	3,3,3	0.35	0	2,2,2	0.67	0
4	EDO	E	509	-	3,3,3	0.54	0	2,2,2	0.11	0
4	EDO	D	504	-	3,3,3	0.44	0	2,2,2	0.32	0
3	NAG	F	501	1	14,14,15	0.48	0	17,19,21	0.48	0
5	PEG	E	507	-	6,6,6	0.24	0	5,5,5	0.10	0
4	EDO	C	510	-	3,3,3	0.48	0	2,2,2	0.15	0
4	EDO	A	505	-	3,3,3	0.56	0	2,2,2	0.16	0
3	NAG	C	503	1	14,14,15	0.66	1 (7%)	17,19,21	0.57	0
4	EDO	A	507	-	3,3,3	0.45	0	2,2,2	0.42	0
3	NAG	A	503	1	14,14,15	0.42	0	17,19,21	0.46	0
4	EDO	E	506	-	3,3,3	0.40	0	2,2,2	0.37	0
4	EDO	C	507	-	3,3,3	0.35	0	2,2,2	0.60	0
3	NAG	A	502	1	14,14,15	0.46	0	17,19,21	0.55	0
3	NAG	F	502	1	14,14,15	0.47	0	17,19,21	0.49	0
3	NAG	C	504	1	14,14,15	0.44	0	17,19,21	0.60	0
4	EDO	C	513	-	3,3,3	0.54	0	2,2,2	0.25	0
4	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.25	0
3	NAG	C	502	1	14,14,15	0.37	0	17,19,21	0.40	0
4	EDO	C	509	-	3,3,3	0.51	0	2,2,2	0.20	0
4	EDO	C	512	-	3,3,3	0.50	0	2,2,2	0.23	0
3	NAG	B	504	1	14,14,15	0.46	0	17,19,21	0.47	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	505	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	EDO	E	508	-	-	1/1/1/1	-
4	EDO	D	506	-	-	1/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-
3	NAG	A	504	1	-	3/6/23/26	0/1/1/1
4	EDO	F	503	-	-	1/1/1/1	-
3	NAG	E	503	1	-	0/6/23/26	0/1/1/1
4	EDO	C	508	-	-	1/1/1/1	-
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
4	EDO	C	505	-	-	1/1/1/1	-
3	NAG	B	505	1	-	1/6/23/26	0/1/1/1
4	EDO	E	505	-	-	1/1/1/1	-
3	NAG	E	504	1	-	1/6/23/26	0/1/1/1
4	EDO	D	507	-	-	1/1/1/1	-
3	NAG	A	501	1	-	3/6/23/26	0/1/1/1
3	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	EDO	F	504	-	-	0/1/1/1	-
4	EDO	E	509	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
3	NAG	F	501	1	-	4/6/23/26	0/1/1/1
5	PEG	E	507	-	-	1/4/4/4	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-
3	NAG	C	503	1	-	0/6/23/26	0/1/1/1
4	EDO	A	507	-	-	0/1/1/1	-
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
4	EDO	E	506	-	-	0/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	F	502	1	-	2/6/23/26	0/1/1/1
3	NAG	C	504	1	-	2/6/23/26	0/1/1/1
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
3	NAG	C	502	1	-	2/6/23/26	0/1/1/1
4	EDO	C	509	-	-	1/1/1/1	-
4	EDO	C	512	-	-	1/1/1/1	-
3	NAG	B	504	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	NAG	O5-C1	2.16	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	503	NAG	C1-O5-C5	2.58	115.68	112.19
3	B	501	NAG	C1-O5-C5	2.11	115.05	112.19
3	D	501	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C4-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	C	502	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	C	502	NAG	C4-C5-C6-O6
3	F	501	NAG	C4-C5-C6-O6
3	F	502	NAG	C1-C2-N2-C7
3	A	504	NAG	O5-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	F	501	NAG	C1-C2-N2-C7
3	A	501	NAG	O5-C5-C6-O6
3	F	501	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	B	504	NAG	O5-C5-C6-O6
4	A	505	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
4	C	508	EDO	O1-C1-C2-O2
4	E	508	EDO	O1-C1-C2-O2
4	F	503	EDO	O1-C1-C2-O2
3	A	504	NAG	C4-C5-C6-O6
3	E	504	NAG	O5-C5-C6-O6
4	A	506	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
4	E	505	EDO	O1-C1-C2-O2
3	C	504	NAG	C4-C5-C6-O6
5	E	507	PEG	C1-C2-O2-C3
4	C	509	EDO	O1-C1-C2-O2
4	C	511	EDO	O1-C1-C2-O2
4	C	512	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C3-C2-N2-C7
3	A	504	NAG	C3-C2-N2-C7
3	B	505	NAG	O5-C5-C6-O6
3	C	504	NAG	O5-C5-C6-O6
3	F	501	NAG	C3-C2-N2-C7
3	F	502	NAG	C3-C2-N2-C7
4	D	506	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	508	EDO	2	0
4	C	511	EDO	1	0
4	F	503	EDO	1	0
4	C	505	EDO	1	0
4	C	510	EDO	1	0
4	C	513	EDO	1	0
4	A	506	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	488/499 (97%)	0.61	49 (10%)	7	7	20, 48, 91, 110	0
1	B	482/499 (96%)	0.60	52 (10%)	5	6	21, 42, 96, 124	0
1	C	486/499 (97%)	0.32	20 (4%)	37	40	20, 39, 70, 101	0
1	D	478/499 (95%)	1.05	93 (19%)	1	0	18, 42, 122, 154	0
1	E	489/499 (97%)	0.76	68 (13%)	2	2	19, 46, 96, 123	0
1	F	484/499 (96%)	0.80	74 (15%)	2	1	16, 43, 104, 130	0
All	All	2907/2994 (97%)	0.69	356 (12%)	4	3	16, 43, 99, 154	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451	VAL	9.3
1	D	362	GLY	9.0
1	F	345	GLY	8.7
1	D	476	GLU	8.7
1	D	6	CYS	8.4
1	E	463	GLY	7.9
1	F	473	CYS	7.6
1	D	485	THR	7.3
1	F	356	GLN	7.1
1	F	485	THR	7.1
1	D	489	PRO	7.0
1	D	354	HIS	6.8
1	F	364	ALA	6.8
1	D	365	ALA	6.7
1	D	453	SER	6.6
1	D	361	SER	6.6
1	D	345	GLY	6.5
1	D	364	ALA	6.5
1	D	469	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	471	HIS	6.1
1	F	343	TRP	6.1
1	D	475	ASN	6.0
1	D	353	TYR	6.0
1	F	361	SER	5.9
1	F	362	GLY	5.8
1	B	469	PHE	5.8
1	B	365	ALA	5.8
1	F	351	TYR	5.7
1	D	359	GLN	5.7
1	D	3	ASP	5.6
1	F	477	CYS	5.6
1	F	363	TYR	5.5
1	B	364	ALA	5.5
1	D	5	ILE	5.4
1	D	491	TYR	5.3
1	E	459	ALA	5.1
1	F	365	ALA	5.1
1	D	482	ARG	5.1
1	D	360	GLY	5.0
1	D	351	TYR	5.0
1	F	469	PHE	5.0
1	F	447	LEU	5.0
1	E	485	THR	4.9
1	A	364	ALA	4.8
1	D	343	TRP	4.8
1	F	480	SER	4.7
1	E	477	CYS	4.7
1	F	357	ASN	4.7
1	F	475	ASN	4.7
1	D	483	ASN	4.6
1	D	477	CYS	4.6
1	E	365	ALA	4.6
1	D	473	CYS	4.6
1	F	476	GLU	4.5
1	D	363	TYR	4.5
1	A	323	ILE	4.5
1	F	355	HIS	4.5
1	D	348	ASP	4.5
1	F	472	LYS	4.5
1	D	486	TYR	4.5
1	D	472	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	349	GLY	4.4
1	F	466	CYS	4.4
1	F	353	TYR	4.4
1	D	448	TYR	4.3
1	F	481	VAL	4.3
1	E	488	TYR	4.3
1	B	475	ASN	4.3
1	B	472	LYS	4.3
1	E	481	VAL	4.3
1	D	334	ALA	4.3
1	F	348	ASP	4.3
1	B	356	GLN	4.2
1	E	345	GLY	4.2
1	D	487	ASP	4.2
1	E	483	ASN	4.2
1	A	277	CYS	4.2
1	B	345	GLY	4.1
1	D	370	THR	4.1
1	F	5	ILE	4.1
1	D	479	GLU	4.1
1	B	86	ASN	4.1
1	D	466	CYS	4.1
1	E	473	CYS	4.1
1	D	447	LEU	4.0
1	F	352	GLY	4.0
1	B	363	TYR	4.0
1	D	470	TYR	4.0
1	D	339	ILE	4.0
1	E	467	PHE	4.0
1	D	484	GLY	3.9
1	A	355	HIS	3.9
1	F	486	TYR	3.9
1	F	4	THR	3.9
1	A	2	SER	3.9
1	E	4	THR	3.9
1	E	5	ILE	3.9
1	B	489	PRO	3.9
1	D	366	ASP	3.9
1	E	470	TYR	3.9
1	F	489	PRO	3.8
1	F	3	ASP	3.8
1	A	141	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	431	LEU	3.8
1	E	451	VAL	3.8
1	B	275	HIS	3.8
1	D	358	GLU	3.8
1	E	2	SER	3.7
1	A	351	TYR	3.7
1	D	338	PHE	3.7
1	E	469	PHE	3.7
1	E	495	PHE	3.7
1	E	271	ASN	3.7
1	D	277	CYS	3.7
1	D	455	LEU	3.7
1	D	481	VAL	3.7
1	A	86	ASN	3.6
1	D	341	GLY	3.6
1	D	7	ILE	3.6
1	D	347	ILE	3.6
1	D	488	TYR	3.6
1	A	485	THR	3.6
1	F	465	GLY	3.6
1	F	75	ALA	3.5
1	A	14	SER	3.5
1	F	483	ASN	3.5
1	A	15	THR	3.4
1	B	325	SER	3.4
1	D	324	PRO	3.4
1	F	15	THR	3.4
1	F	463	GLY	3.4
1	D	478	MET	3.3
1	B	349	GLY	3.3
1	D	465	GLY	3.3
1	D	355	HIS	3.3
1	F	474	ASP	3.3
1	D	357	ASN	3.3
1	B	359	GLN	3.3
1	E	272	ALA	3.3
1	B	3	ASP	3.3
1	E	343	TRP	3.3
1	B	272	ALA	3.3
1	D	474	ASP	3.2
1	D	350	TRP	3.2
1	D	12	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	12	ASN	3.2
1	E	351	TYR	3.2
1	D	427	LEU	3.2
1	A	365	ALA	3.2
1	D	11	ALA	3.2
1	E	471	HIS	3.2
1	F	14	SER	3.2
1	D	457	ASN	3.2
1	E	363	TYR	3.2
1	D	352	GLY	3.2
1	D	30	HIS	3.2
1	A	483	ASN	3.2
1	D	480	SER	3.1
1	F	487	ASP	3.1
1	D	335	ILE	3.1
1	D	10	HIS	3.1
1	B	357	ASN	3.1
1	E	7	ILE	3.1
1	B	44	CYS	3.1
1	A	13	ASN	3.1
1	A	371	GLN	3.1
1	D	349	GLY	3.1
1	F	358	GLU	3.1
1	C	356	GLN	3.1
1	A	465	GLY	3.1
1	E	355	HIS	3.1
1	F	347	ILE	3.1
1	F	8	GLY	3.0
1	F	470	TYR	3.0
1	F	491	TYR	3.0
1	D	29	THR	3.0
1	E	476	GLU	3.0
1	F	471	HIS	3.0
1	F	448	TYR	3.0
1	F	428	LEU	3.0
1	F	360	GLY	3.0
1	A	350	TRP	2.9
1	A	353	TYR	2.9
1	B	476	GLU	2.9
1	A	428	LEU	2.9
1	E	362	GLY	2.9
1	D	9	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	484	GLY	2.9
1	B	5	ILE	2.9
1	E	263	PHE	2.9
1	D	490	LYS	2.9
1	E	475	ASN	2.9
1	B	39	HIS	2.9
1	B	343	TRP	2.9
1	F	13	ASN	2.9
1	A	354	HIS	2.9
1	C	485	THR	2.9
1	D	346	MET	2.9
1	E	320	LEU	2.9
1	B	474	ASP	2.8
1	E	323	ILE	2.8
1	E	364	ALA	2.8
1	A	359	GLN	2.8
1	B	491	TYR	2.8
1	E	474	ASP	2.8
1	B	353	TYR	2.8
1	D	323	ILE	2.8
1	B	13	ASN	2.8
1	E	348	ASP	2.8
1	A	427	LEU	2.8
1	A	272	ALA	2.7
1	F	344	THR	2.7
1	E	346	MET	2.7
1	B	467	PHE	2.7
1	D	356	GLN	2.7
1	E	465	GLY	2.7
1	B	15	THR	2.7
1	D	337	GLY	2.7
1	A	43	LEU	2.7
1	C	363	TYR	2.7
1	C	457	ASN	2.7
1	C	471	HIS	2.6
1	E	354[A]	HIS	2.6
1	B	466	CYS	2.6
1	C	271	ASN	2.6
1	D	4	THR	2.6
1	A	349	GLY	2.6
1	C	277	CYS	2.6
1	F	346	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	467	PHE	2.6
1	E	489	PRO	2.6
1	D	289	ASN	2.6
1	A	87	SER	2.6
1	B	482	ARG	2.6
1	E	487	ASP	2.6
1	B	486	TYR	2.6
1	C	491	TYR	2.6
1	D	8	GLY	2.6
1	F	6	CYS	2.6
1	C	488	TYR	2.5
1	A	345	GLY	2.5
1	A	487	ASP	2.5
1	F	354	HIS	2.5
1	A	470	TYR	2.5
1	B	4	THR	2.5
1	D	467	PHE	2.5
1	F	17	THR	2.5
1	E	491	TYR	2.5
1	A	347	ILE	2.5
1	E	406[A]	MET	2.5
1	F	324	PRO	2.5
1	A	491	TYR	2.5
1	E	462	ILE	2.5
1	A	271	ASN	2.5
1	F	341	GLY	2.5
1	D	322	ASN	2.4
1	F	11	ALA	2.4
1	F	459	ALA	2.4
1	A	474	ASP	2.4
1	B	42	LYS	2.4
1	E	466	CYS	2.4
1	D	446	ASN	2.4
1	C	402	LEU	2.4
1	B	48	GLY	2.4
1	F	367	GLN	2.4
1	C	364	ALA	2.4
1	E	457	ASN	2.4
1	A	431	LEU	2.4
1	D	430	LEU	2.4
1	A	425	ALA	2.4
1	C	354	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	334	ALA	2.4
1	A	494	GLU	2.4
1	A	402	LEU	2.4
1	B	324	PRO	2.4
1	F	479	GLU	2.4
1	D	15	THR	2.4
1	E	472	LYS	2.4
1	A	469	PHE	2.3
1	B	271	ASN	2.3
1	D	320	LEU	2.3
1	E	6	CYS	2.3
1	E	478	MET	2.3
1	B	29	THR	2.3
1	B	348	ASP	2.3
1	D	14	SER	2.3
1	E	14	SER	2.3
1	B	406	MET	2.3
1	A	374	ILE	2.3
1	E	3	ASP	2.3
1	F	289	ASN	2.3
1	F	9	TYR	2.3
1	C	463	GLY	2.3
1	D	13	ASN	2.3
1	B	473	CYS	2.3
1	B	141	GLY	2.3
1	F	25	ASN	2.3
1	B	344	THR	2.3
1	C	360	GLY	2.3
1	B	459	ALA	2.2
1	E	279	THR	2.2
1	D	369	SER	2.2
1	A	30	HIS	2.2
1	C	42	LYS	2.2
1	E	41	GLY	2.2
1	A	479	GLU	2.2
1	E	468	GLU	2.2
1	C	365	ALA	2.2
1	E	344[A]	THR	2.2
1	D	428	LEU	2.2
1	C	389	ASN	2.2
1	F	488	TYR	2.2
1	E	142	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	6	CYS	2.2
1	A	486	TYR	2.2
1	C	487	ASP	2.2
1	E	278	ASN	2.2
1	E	494	GLU	2.2
1	A	482	ARG	2.2
1	A	406	MET	2.2
1	B	264	GLY	2.2
1	E	15[A]	THR	2.2
1	A	103	LEU	2.1
1	F	455	LEU	2.1
1	F	288	ILE	2.1
1	B	447	LEU	2.1
1	E	277	CYS	2.1
1	B	40	ASN	2.1
1	F	462	ILE	2.1
1	A	495	PHE	2.1
1	E	448	TYR	2.1
1	B	483	ASN	2.1
1	B	355	HIS	2.1
1	D	340	GLU	2.1
1	F	454	GLN	2.1
1	A	273	SER	2.1
1	B	346	MET	2.1
1	D	332	PHE	2.1
1	F	350	TRP	2.1
1	F	359	GLN	2.1
1	D	413	VAL	2.1
1	E	30	HIS	2.1
1	E	376	GLY	2.1
1	B	358	GLU	2.0
1	E	356	GLN	2.0
1	E	338	PHE	2.0
1	A	352	GLY	2.0
1	E	479	GLU	2.0
1	C	361	SER	2.0
1	E	453	SER	2.0
1	B	477	CYS	2.0
1	D	331	LEU	2.0
1	F	338	PHE	2.0
1	F	435	ARG	2.0
1	A	356	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	362	GLY	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)

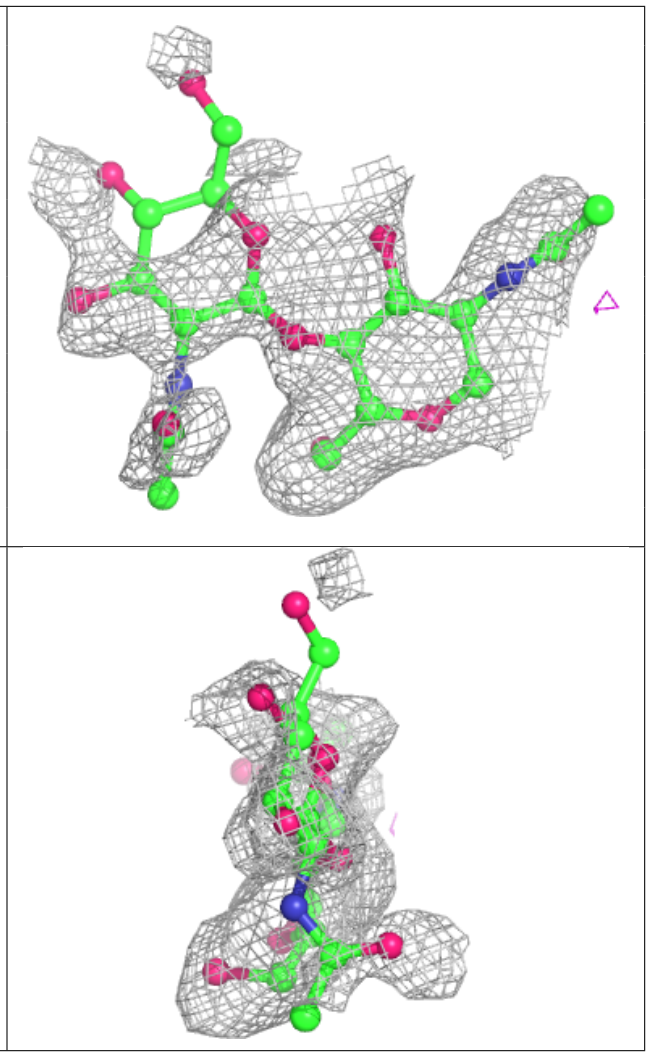
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2	14/15	0.45	0.47	106,112,117,119	0
2	NAG	H	2	14/15	0.47	0.64	97,121,126,127	0
2	NAG	H	1	14/15	0.61	0.35	78,92,108,112	0
2	NAG	I	2	14/15	0.66	0.45	107,114,122,125	0
2	NAG	I	1	14/15	0.76	0.42	71,91,98,105	0
2	NAG	G	1	14/15	0.77	0.29	66,86,95,102	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.

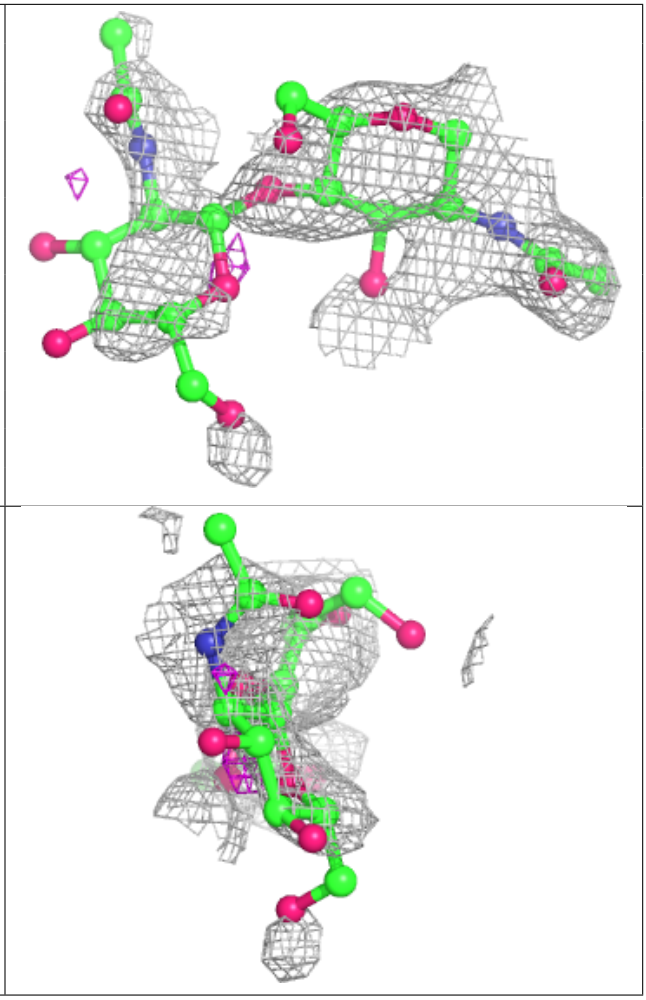
Electron density around Chain G:

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



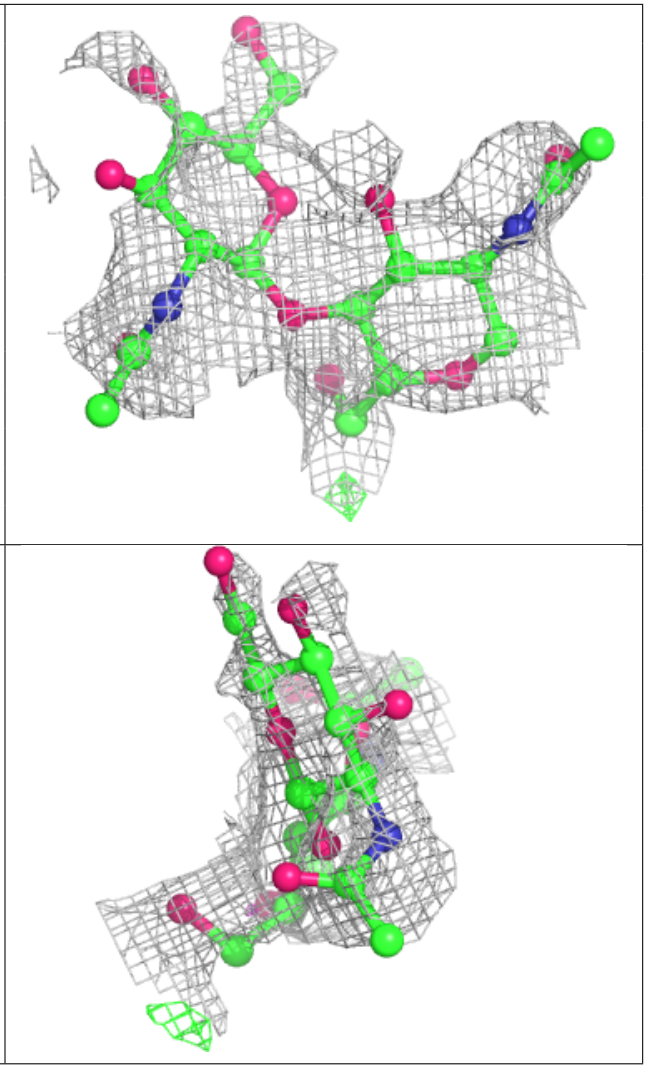
Electron density around Chain H:

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



Electron density around Chain I:

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



6.4 Ligands (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
3	NAG	A	503	14/15	0.41	0.53	95,111,120,122	0
3	NAG	A	504	14/15	0.57	0.55	76,100,106,111	0
3	NAG	C	503	14/15	0.58	0.50	77,86,92,94	0
3	NAG	D	501	14/15	0.59	0.29	87,102,109,112	0
4	EDO	D	507	4/4	0.61	0.29	46,54,57,58	0
3	NAG	A	502	14/15	0.65	0.54	87,102,107,109	0
3	NAG	F	501	14/15	0.66	0.48	82,100,109,109	0
3	NAG	B	501	14/15	0.68	0.41	84,100,106,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	505	4/4	0.69	0.20	60,62,62,64	0
3	NAG	F	502	14/15	0.70	0.35	85,100,111,112	0
3	NAG	E	503	14/15	0.70	0.30	78,91,101,101	0
3	NAG	C	501	14/15	0.70	0.49	79,99,104,107	0
4	EDO	E	509	4/4	0.70	0.27	63,67,69,70	0
5	PEG	E	507	7/7	0.72	0.16	51,58,63,69	0
3	NAG	B	504	14/15	0.73	0.47	82,95,104,104	0
4	EDO	C	506	4/4	0.74	0.25	44,46,52,55	0
4	EDO	A	506	4/4	0.74	0.20	71,74,75,75	0
3	NAG	E	504	14/15	0.78	0.39	77,99,104,105	0
3	NAG	B	505	14/15	0.80	0.41	74,87,96,97	0
4	EDO	C	509	4/4	0.81	0.15	52,52,54,55	0
3	NAG	C	502	14/15	0.81	0.30	69,88,99,99	0
4	EDO	C	512	4/4	0.82	0.17	65,67,67,70	0
4	EDO	A	507	4/4	0.83	0.38	65,65,68,69	0
3	NAG	A	501	14/15	0.84	0.23	65,81,96,101	0
4	EDO	C	505	4/4	0.84	0.26	33,43,46,50	0
3	NAG	C	504	14/15	0.85	0.32	67,78,91,92	0
4	EDO	E	505	4/4	0.85	0.20	47,48,52,60	0
4	EDO	D	505	4/4	0.86	0.22	61,66,69,71	0
4	EDO	F	503	4/4	0.87	0.13	64,70,70,72	0
4	EDO	C	513	4/4	0.87	0.17	54,56,59,61	0
4	EDO	C	508	4/4	0.90	0.25	64,66,69,74	0
4	EDO	C	510	4/4	0.91	0.18	47,59,64,66	0
4	EDO	D	504	4/4	0.91	0.16	50,54,57,67	0
4	EDO	D	506	4/4	0.92	0.12	57,59,62,62	0
4	EDO	C	511	4/4	0.92	0.30	38,46,57,60	0
4	EDO	F	504	4/4	0.93	0.12	46,48,56,57	0
4	EDO	E	506	4/4	0.93	0.26	60,61,63,63	0
4	EDO	C	507	4/4	0.94	0.12	40,45,47,52	0
4	EDO	E	508	4/4	0.97	0.17	37,39,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.