Full wwPDB X-ray Structure Validation Report (i)

Nov 27, 2024 – 12:19 pm GMT

PDB ID	:	9FMB
Title	:	Crystal structure of human IgD-Fc
Authors	:	Davies, A.M.; McDonnell, J.M.
Deposited on	:	2024-06-05
Resolution	:	3.00 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 (1)) were used in the production of this report:

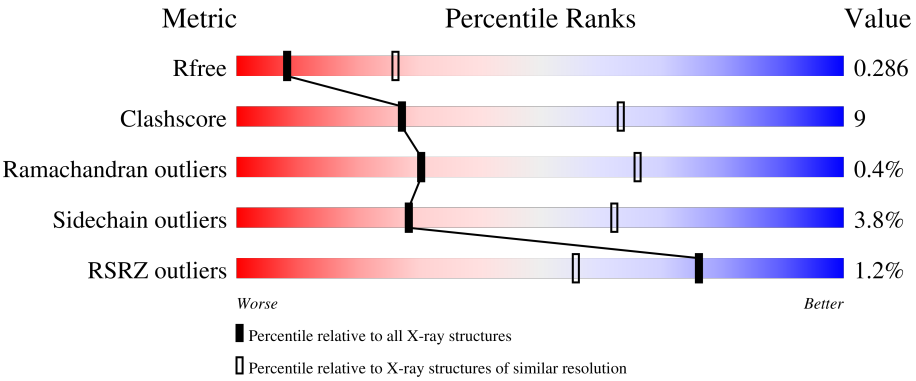
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	62% 20% · 17%
1	B	234	66% 15% 18%
1	C	234	63% 18% · 18%
1	D	234	59% 22% · 18%
2	E	7	29% 71%

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Mol	Chain	Length	Quality of chain
3	F	9	33% 67%
3	H	9	22% 78%
4	G	6	33% 67%

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
7	ACT	C	603	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6302 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 Isoform 1 of Immunoglobulin heavy constant delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1474	938	255	275	6			
1	B	192	Total	C	N	O	S	0	0	0
			1452	926	251	269	6			
1	C	193	Total	C	N	O	S	0	0	0
			1459	931	253	269	6			
1	D	192	Total	C	N	O	S	0	0	0
			1460	929	253	272	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	514	HIS	-	expression tag	UNP P01880
A	515	HIS	-	expression tag	UNP P01880
A	516	HIS	-	expression tag	UNP P01880
A	517	HIS	-	expression tag	UNP P01880
A	518	HIS	-	expression tag	UNP P01880
A	519	HIS	-	expression tag	UNP P01880
B	514	HIS	-	expression tag	UNP P01880
B	515	HIS	-	expression tag	UNP P01880
B	516	HIS	-	expression tag	UNP P01880
B	517	HIS	-	expression tag	UNP P01880
B	518	HIS	-	expression tag	UNP P01880
B	519	HIS	-	expression tag	UNP P01880
C	514	HIS	-	expression tag	UNP P01880
C	515	HIS	-	expression tag	UNP P01880
C	516	HIS	-	expression tag	UNP P01880
C	517	HIS	-	expression tag	UNP P01880
C	518	HIS	-	expression tag	UNP P01880
C	519	HIS	-	expression tag	UNP P01880
D	514	HIS	-	expression tag	UNP P01880
D	515	HIS	-	expression tag	UNP P01880
D	516	HIS	-	expression tag	UNP P01880

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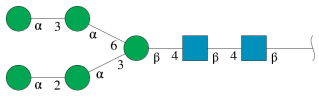
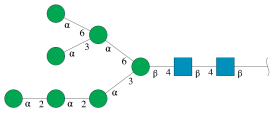
Chain	Residue	Modelled	Actual	Comment	Reference
D	517	HIS	-	expression tag	UNP P01880
D	518	HIS	-	expression tag	UNP P01880
D	519	HIS	-	expression tag	UNP P01880

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



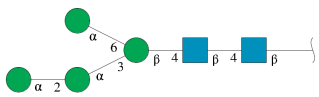
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



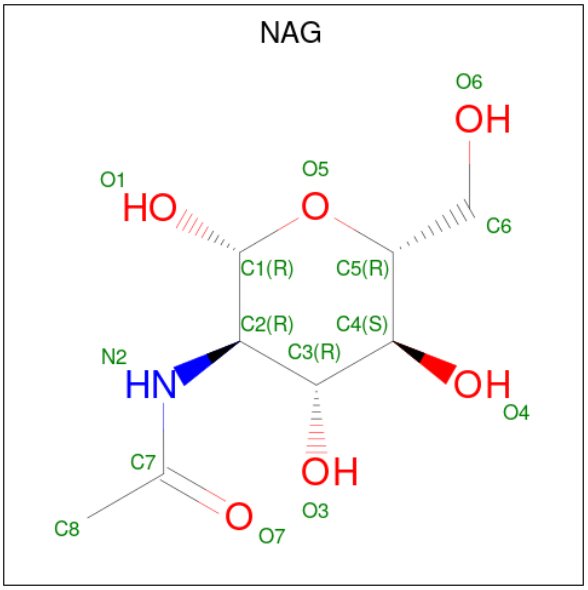
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	9	Total	C	N	O	0	0	0
			105	58	2	45			
3	H	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



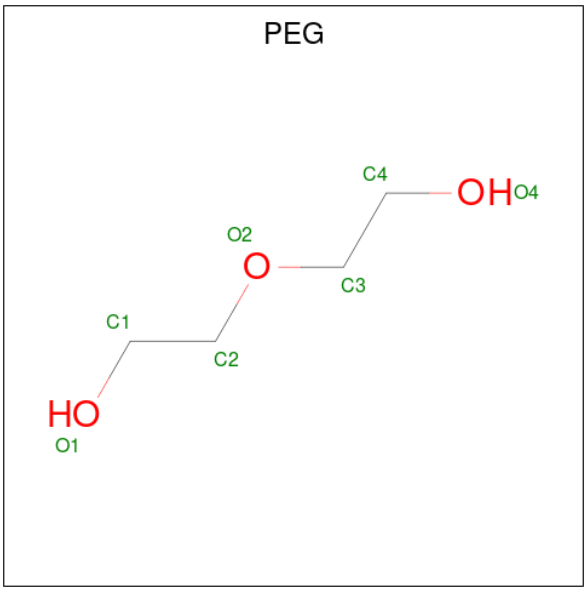
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



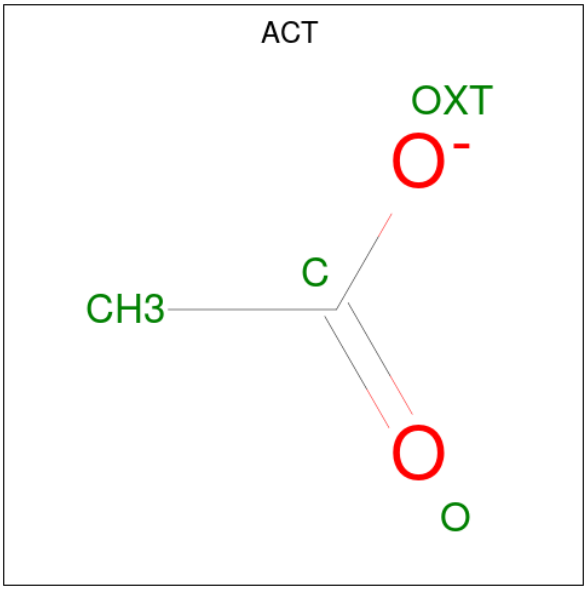
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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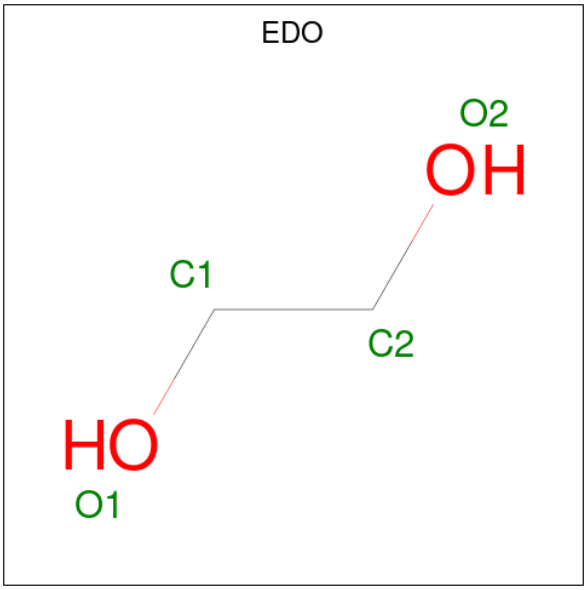
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

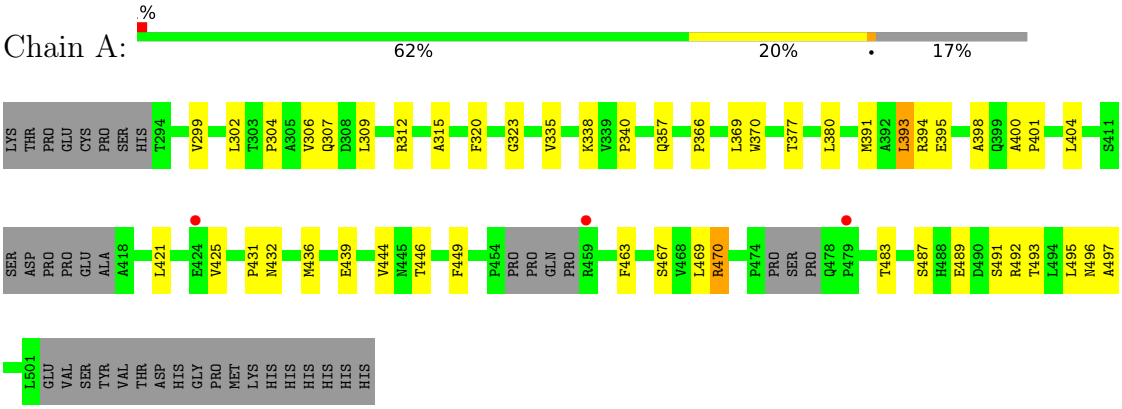
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total O 4 4	0	0
9	B	2	Total O 2 2	0	0
9	C	4	Total O 4 4	0	0
9	D	5	Total O 5 5	0	0

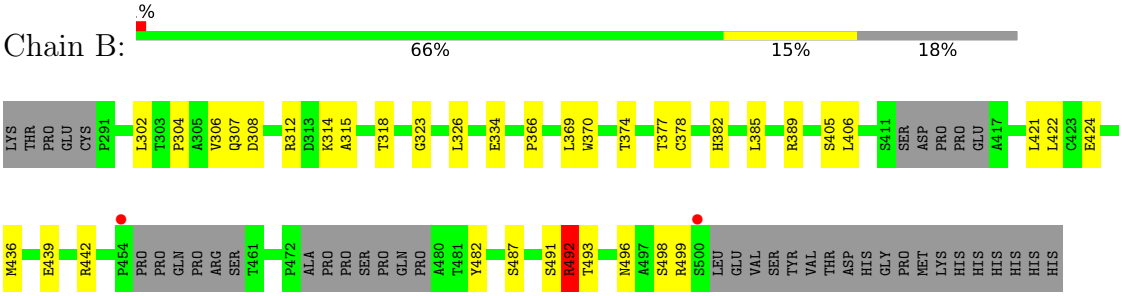
3 Residue-property plots (i)

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

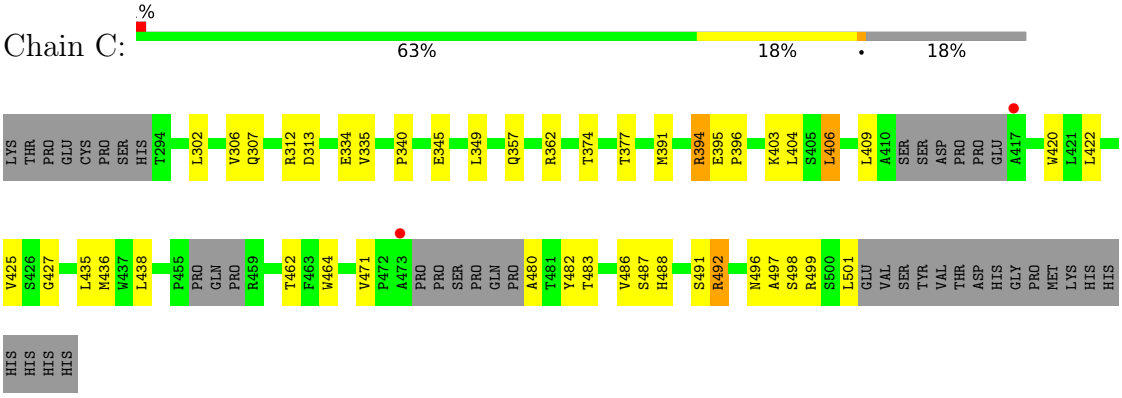
• Molecule 1: Isoform 1 of Immunoglobulin heavy constant delta



• Molecule 1: Isoform 1 of Immunoglobulin heavy constant delta

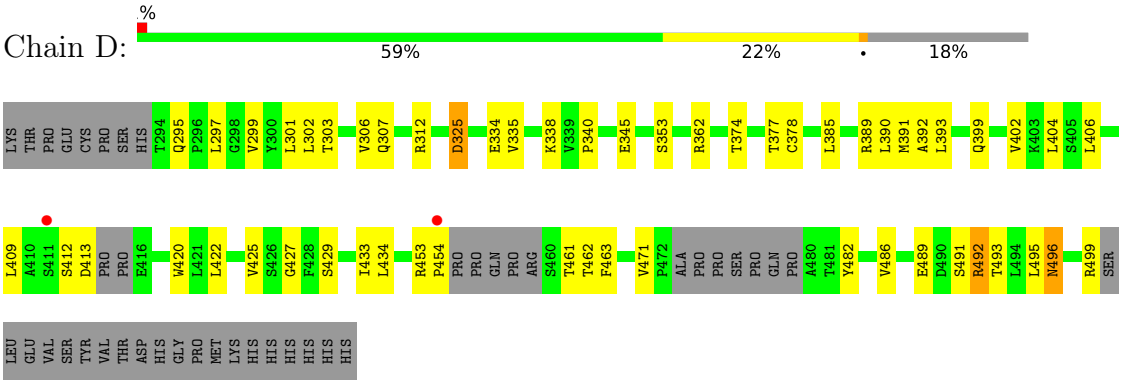


• Molecule 1: Isoform 1 of Immunoglobulin heavy constant delta



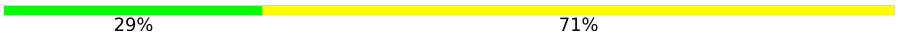
• Molecule 1: Isoform 1 of Immunoglobulin heavy constant delta

Chain D:



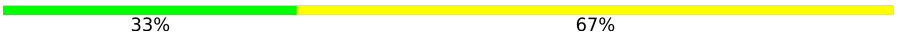
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



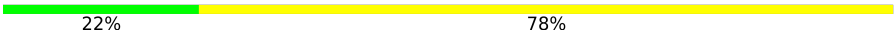
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



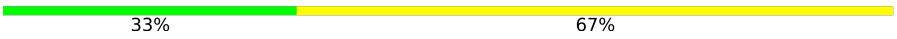
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

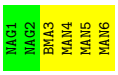
Chain H:



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

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.83Å 43.67Å 121.47Å 90.00° 107.96° 90.00°	Depositor
Resolution (Å)	52.45 – 3.00 52.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.45-3.00) 97.5 (52.45-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.228 , 0.288 0.229 , 0.286	Depositor DCC
R_{free} test set	20670 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	6302	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.94% 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

5.1 Standard geometry

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

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	0.26	0/1512	0.53	0/2074
1	B	0.25	0/1488	0.54	0/2038
1	C	0.25	0/1496	0.51	0/2049
1	D	0.25	0/1496	0.53	0/2048
All	All	0.25	0/5992	0.53	0/8209

There are no bond length outliers.

There are no bond angle outliers.

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	1474	0	1432	29	0
1	B	1452	0	1409	23	0
1	C	1459	0	1413	27	0
1	D	1460	0	1421	33	0
2	E	83	0	70	1	0
3	F	105	0	88	0	0
3	H	105	0	88	1	0
4	G	72	0	61	0	0
5	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	0	0
5	D	14	0	13	0	0
6	A	7	0	10	0	0
7	A	4	0	3	0	0
7	B	4	0	3	1	0
7	C	8	0	6	3	0
7	D	4	0	3	1	0
8	C	8	0	12	0	0
9	A	4	0	0	0	0
9	B	2	0	0	0	0
9	C	4	0	0	1	0
9	D	5	0	0	0	0
All	All	6302	0	6058	111	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 9.

All (111) 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:374:THR:O	1:B:492:ARG:NH2	2.13	0.81
1:D:453:ARG:HD3	1:D:454:PRO:HD2	1.61	0.81
1:C:394:ARG:NH1	1:C:395:GLU:O	2.16	0.79
1:D:374:THR:O	1:D:492:ARG:NH1	2.20	0.74
1:D:392:ALA:O	1:D:492:ARG:NH2	2.22	0.72
1:C:335:VAL:HG23	1:C:340:PRO:HG3	1.72	0.72
1:B:491:SER:O	1:B:493:THR:N	2.22	0.72
1:D:491:SER:O	1:D:493:THR:N	2.23	0.71
1:C:306:VAL:HG22	1:C:487:SER:HB3	1.73	0.69
1:B:439:GLU:HG3	1:B:482:TYR:HE1	1.60	0.67
1:C:374:THR:O	1:C:492:ARG:NH1	2.29	0.65
1:A:366:PRO:HD2	1:A:369:LEU:HD12	1.80	0.64
1:B:366:PRO:HD2	1:B:369:LEU:HD12	1.80	0.64
1:C:425:VAL:HG21	1:C:486:VAL:HG21	1.80	0.62
1:B:312:ARG:HD2	1:B:314:LYS:HE2	1.82	0.62
1:D:345:GLU:HG3	1:D:362:ARG:HB3	1.82	0.61
1:A:491:SER:O	1:A:493:THR:N	2.35	0.60
1:B:306:VAL:HG12	1:B:436:MET:HE1	1.84	0.60
1:C:340:PRO:HA	7:C:603:ACT:H2	1.83	0.59
1:D:335:VAL:HG23	1:D:340:PRO:HG3	1.85	0.59
1:B:312:ARG:HB3	1:B:314:LYS:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HG23	1:A:340:PRO:HG3	1.85	0.59
1:A:401:PRO:HB2	1:A:495:LEU:HD11	1.85	0.58
1:B:406:LEU:HD21	1:B:421:LEU:HD23	1.84	0.58
1:D:302:LEU:HD11	3:H:3:BMA:H62	1.86	0.58
1:D:297:LEU:HD12	1:D:385:LEU:HD12	1.86	0.57
1:A:449:PHE:HD1	1:A:467:SER:HB2	1.70	0.56
1:B:306:VAL:HG22	1:B:487:SER:HB3	1.86	0.56
1:C:480:ALA:N	1:C:501:LEU:O	2.39	0.56
1:A:377:THR:HG23	1:A:391:MET:HG2	1.87	0.56
1:D:295:GLN:NE2	1:D:325:ASP:O	2.40	0.55
1:D:406:LEU:O	1:D:499:ARG:NE	2.40	0.55
1:D:454:PRO:HD3	1:D:463:PHE:CE2	2.42	0.54
1:A:483:THR:HA	1:A:497:ALA:O	2.08	0.54
1:A:421:LEU:HD12	1:A:469:LEU:HD23	1.90	0.54
1:B:323:GLY:HA3	1:B:326:LEU:HD21	1.89	0.54
1:D:461:THR:HG23	1:D:462:THR:HG23	1.90	0.54
1:B:439:GLU:N	1:B:442:ARG:O	2.40	0.53
1:C:349:LEU:HD11	1:C:357:GLN:HB3	1.90	0.53
1:C:334:GLU:HB2	1:C:377:THR:HB	1.89	0.52
1:A:446:THR:O	1:A:446:THR:OG1	2.28	0.52
1:D:399:GLN:HG3	1:D:429:SER:HB3	1.91	0.52
1:D:303:THR:HG21	1:D:489:GLU:HG2	1.92	0.52
1:C:496:ASN:N	1:C:496:ASN:OD1	2.42	0.51
1:C:471:VAL:HG11	1:C:482:TYR:CE1	2.46	0.50
1:A:491:SER:O	1:A:491:SER:OG	2.27	0.50
1:C:427:GLY:HA2	1:C:462:THR:HB	1.94	0.49
1:A:404:LEU:HB2	1:A:495:LEU:HD13	1.95	0.49
1:D:301:LEU:HD21	1:D:392:ALA:HB2	1.95	0.49
1:A:404:LEU:HD12	1:A:425:VAL:HB	1.95	0.49
1:D:402:VAL:HG23	1:D:427:GLY:HA3	1.94	0.48
1:D:489:GLU:O	1:D:492:ARG:HG2	2.13	0.48
1:C:420:TRP:CG	1:D:409:LEU:HD21	2.48	0.48
1:A:302:LEU:HD21	2:E:3:BMA:H62	1.93	0.48
1:B:334:GLU:HB2	1:B:377:THR:HB	1.96	0.48
1:A:370:TRP:NE1	1:A:489:GLU:OE2	2.29	0.48
1:B:307:GLN:HG3	1:B:436:MET:SD	2.53	0.48
1:C:483:THR:HA	1:C:497:ALA:O	2.13	0.48
1:C:409:LEU:HG	1:C:422:LEU:HB2	1.96	0.47
1:D:412:SER:HB2	1:D:420:TRP:HE1	1.79	0.47
1:D:404:LEU:HD21	1:D:486:VAL:HB	1.96	0.47
1:B:302:LEU:HB2	1:B:318:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:PRO:HD3	1:D:463:PHE:HE2	1.80	0.47
1:A:323:GLY:O	1:A:357:GLN:N	2.39	0.46
1:A:304:PRO:HG3	1:A:315:ALA:HB1	1.98	0.46
1:D:334:GLU:HB2	1:D:377:THR:HB	1.97	0.46
1:B:318:THR:OG1	7:B:602:ACT:OXT	2.26	0.46
1:A:400:ALA:HA	1:A:491:SER:OG	2.16	0.46
1:B:406:LEU:HD22	1:B:499:ARG:HB2	1.99	0.45
1:B:496:ASN:OD1	1:B:496:ASN:N	2.49	0.45
1:A:302:LEU:HD11	1:A:320:PHE:HE1	1.81	0.45
1:B:439:GLU:HG3	1:B:482:TYR:CE1	2.47	0.45
1:C:377:THR:OG1	1:C:391:MET:HG2	2.16	0.45
1:D:306:VAL:CG2	1:D:434:LEU:HB2	2.46	0.45
1:D:307:GLN:O	1:D:312:ARG:NH1	2.50	0.45
1:B:405:SER:HB2	1:B:424:GLU:HB2	2.00	0.44
1:A:431:PRO:HG3	1:A:463:PHE:CZ	2.52	0.44
1:C:482:TYR:O	1:C:498:SER:HA	2.18	0.44
1:D:299:VAL:HG13	1:D:390:LEU:HD11	1.99	0.44
1:C:307:GLN:HG3	1:C:436:MET:SD	2.58	0.43
1:D:378:CYS:O	1:D:389:ARG:HA	2.18	0.43
1:C:396:PRO:O	9:C:701:HOH:O	2.21	0.43
1:D:496:ASN:OD1	1:D:496:ASN:N	2.51	0.43
1:A:309:LEU:HD21	1:A:315:ALA:HB2	2.01	0.43
1:A:470:ARG:O	1:A:470:ARG:HG3	2.19	0.43
1:D:297:LEU:HD23	1:D:297:LEU:HA	1.78	0.43
1:A:306:VAL:HG22	1:A:487:SER:HB3	2.01	0.43
1:B:382:HIS:HB3	1:B:385:LEU:HB2	2.00	0.42
1:D:425:VAL:HG21	1:D:486:VAL:HG21	2.01	0.42
1:C:406:LEU:O	1:C:499:ARG:NE	2.45	0.42
1:C:488:HIS:ND1	1:C:491:SER:OG	2.48	0.42
1:A:439:GLU:HB2	1:A:444:VAL:HG21	2.01	0.42
1:C:403:LYS:HE2	1:C:403:LYS:HB3	1.93	0.42
1:C:335:VAL:HB	7:C:603:ACT:H1	2.00	0.42
1:C:302:LEU:HB3	7:C:604:ACT:H3	2.02	0.42
1:B:304:PRO:HG2	1:B:315:ALA:HB1	2.01	0.42
1:B:378:CYS:O	1:B:389:ARG:HA	2.20	0.42
1:C:438:LEU:HB2	1:C:483:THR:OG1	2.20	0.42
1:D:338:LYS:NZ	7:D:602:ACT:O	2.48	0.42
1:A:307:GLN:HG3	1:A:436:MET:SD	2.60	0.41
1:A:496:ASN:N	1:A:496:ASN:OD1	2.53	0.41
1:A:299:VAL:HB	1:A:380:LEU:HD22	2.01	0.41
1:C:345:GLU:HG2	1:C:362:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:MET:HB3	1:D:393:LEU:HG	2.03	0.41
1:A:302:LEU:HD11	1:A:320:PHE:CE1	2.55	0.41
1:A:391:MET:HB3	1:A:393:LEU:HD23	2.03	0.41
1:C:406:LEU:HD23	1:C:406:LEU:HA	1.93	0.41
1:B:370:TRP:O	1:B:492:ARG:HG2	2.20	0.40
1:A:395:GLU:HB2	1:A:398:ALA:HB2	2.04	0.40
1:D:471:VAL:HG21	1:D:482:TYR:OH	2.21	0.40
1:D:406:LEU:HA	1:D:422:LEU:O	2.20	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	187/234 (80%)	182 (97%)	4 (2%)	1 (0%)	25	61
1	B	184/234 (79%)	177 (96%)	6 (3%)	1 (0%)	25	61
1	C	185/234 (79%)	179 (97%)	6 (3%)	0	100	100
1	D	184/234 (79%)	178 (97%)	5 (3%)	1 (0%)	25	61
All	All	740/936 (79%)	716 (97%)	21 (3%)	3 (0%)	30	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	ARG
1	D	492	ARG
1	A	492	ARG

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	161/205 (78%)	155 (96%)	6 (4%)	29	63
1	B	155/205 (76%)	151 (97%)	4 (3%)	41	72
1	C	155/205 (76%)	147 (95%)	8 (5%)	19	52
1	D	159/205 (78%)	153 (96%)	6 (4%)	28	62
All	All	630/820 (77%)	606 (96%)	24 (4%)	28	62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	ARG
1	A	338	LYS
1	A	393	LEU
1	A	394	ARG
1	A	432	ASN
1	A	470	ARG
1	B	308	ASP
1	B	422	LEU
1	B	492	ARG
1	B	498	SER
1	C	312	ARG
1	C	313	ASP
1	C	394	ARG
1	C	404	LEU
1	C	406	LEU
1	C	435	LEU
1	C	464	TRP
1	C	492	ARG
1	D	325	ASP
1	D	353	SER
1	D	413	ASP
1	D	433	ILE
1	D	495	LEU
1	D	496	ASN

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

Mol	Chain	Res	Type
1	B	399	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

31 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	1,2	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.40	0
2	BMA	E	3	2	11,11,12	0.54	0	15,15,17	0.99	0
2	MAN	E	4	2	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
2	MAN	E	5	2	11,11,12	0.65	0	15,15,17	1.20	2 (13%)
2	MAN	E	6	2	11,11,12	0.87	1 (9%)	15,15,17	1.04	1 (6%)
2	MAN	E	7	2	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.25	0	17,19,21	0.34	0
3	NAG	F	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	BMA	F	3	3	11,11,12	0.49	0	15,15,17	0.99	0
3	MAN	F	4	3	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
3	MAN	F	5	3	11,11,12	0.64	0	15,15,17	1.19	2 (13%)
3	MAN	F	6	3	11,11,12	1.20	1 (9%)	15,15,17	1.22	2 (13%)
3	MAN	F	7	3	11,11,12	0.75	0	15,15,17	1.17	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	F	8	3	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
3	MAN	F	9	3	11,11,12	0.61	0	15,15,17	1.13	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	G	2	4	14,14,15	0.30	0	17,19,21	0.39	0
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	1.19	2 (13%)
4	MAN	G	4	4	11,11,12	0.68	0	15,15,17	0.95	2 (13%)
4	MAN	G	5	4	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
4	MAN	G	6	4	11,11,12	0.72	0	15,15,17	0.88	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.20	0	17,19,21	0.34	0
3	NAG	H	2	3	14,14,15	0.17	0	17,19,21	0.46	0
3	BMA	H	3	3	11,11,12	0.58	0	15,15,17	0.93	0
3	MAN	H	4	3	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
3	MAN	H	5	3	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
3	MAN	H	6	3	11,11,12	0.68	0	15,15,17	0.89	1 (6%)
3	MAN	H	7	3	11,11,12	0.81	0	15,15,17	1.24	3 (20%)
3	MAN	H	8	3	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
3	MAN	H	9	3	11,11,12	0.66	0	15,15,17	1.20	2 (13%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
2	MAN	E	7	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	2/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	F	8	3	-	0/2/19/22	0/1/1/1
3	MAN	F	9	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	1/2/19/22	0/1/1/1
4	MAN	G	6	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
3	MAN	H	7	3	-	0/2/19/22	0/1/1/1
3	MAN	H	8	3	-	0/2/19/22	0/1/1/1
3	MAN	H	9	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	MAN	O5-C1	-2.89	1.39	1.43
2	E	6	MAN	C1-C2	2.02	1.56	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	MAN	C1-O5-C5	3.55	117.01	112.19
3	H	9	MAN	C1-O5-C5	3.43	116.84	112.19
3	F	5	MAN	O2-C2-C3	-3.10	103.94	110.14
3	F	9	MAN	C1-O5-C5	3.03	116.30	112.19
3	F	5	MAN	C1-O5-C5	2.87	116.08	112.19
3	H	5	MAN	O2-C2-C3	-2.76	104.61	110.14
3	F	4	MAN	C1-O5-C5	2.65	115.78	112.19
3	F	6	MAN	O2-C2-C3	-2.62	104.90	110.14
3	H	7	MAN	C1-O5-C5	2.53	115.62	112.19
4	G	5	MAN	C1-O5-C5	2.51	115.59	112.19
3	H	4	MAN	O2-C2-C3	-2.51	105.12	110.14
3	F	8	MAN	C1-O5-C5	2.45	115.51	112.19
3	F	7	MAN	C1-O5-C5	2.41	115.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	4	MAN	O2-C2-C3	-2.40	105.32	110.14
3	H	8	MAN	C1-O5-C5	2.39	115.44	112.19
3	H	4	MAN	C1-O5-C5	2.39	115.42	112.19
2	E	7	MAN	O2-C2-C3	-2.35	105.43	110.14
3	F	7	MAN	O2-C2-C3	-2.33	105.47	110.14
2	E	5	MAN	O2-C2-C3	-2.32	105.48	110.14
3	F	8	MAN	O2-C2-C3	-2.27	105.59	110.14
3	H	7	MAN	O2-C2-C3	-2.25	105.63	110.14
4	G	3	BMA	C1-O5-C5	2.23	115.22	112.19
2	E	4	MAN	C1-O5-C5	2.23	115.21	112.19
3	H	7	MAN	C1-C2-C3	2.22	112.40	109.67
3	H	9	MAN	O2-C2-C3	-2.21	105.70	110.14
3	H	6	MAN	O2-C2-C3	-2.21	105.71	110.14
4	G	5	MAN	O2-C2-C3	-2.21	105.72	110.14
4	G	3	BMA	C1-C2-C3	2.21	112.38	109.67
2	E	7	MAN	C1-O5-C5	2.19	115.16	112.19
3	H	8	MAN	O2-C2-C3	-2.18	105.77	110.14
3	H	5	MAN	C1-O5-C5	2.18	115.14	112.19
3	F	9	MAN	O2-C2-C3	-2.17	105.80	110.14
2	E	6	MAN	O2-C2-C3	-2.16	105.80	110.14
4	G	6	MAN	O2-C2-C3	-2.16	105.81	110.14
2	E	4	MAN	O2-C2-C3	-2.16	105.82	110.14
3	F	4	MAN	O2-C2-C3	-2.13	105.88	110.14
3	F	6	MAN	C1-C2-C3	-2.04	107.16	109.67
4	G	4	MAN	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	6	MAN	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	F	9	MAN	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	F	9	MAN	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
3	F	6	MAN	C4-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
2	E	6	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
2	E	6	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6

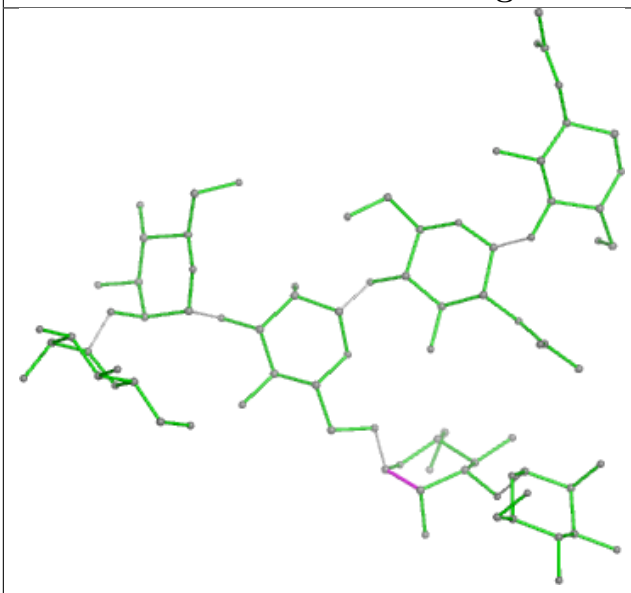
There are no ring outliers.

2 monomers are involved in 2 short contacts:

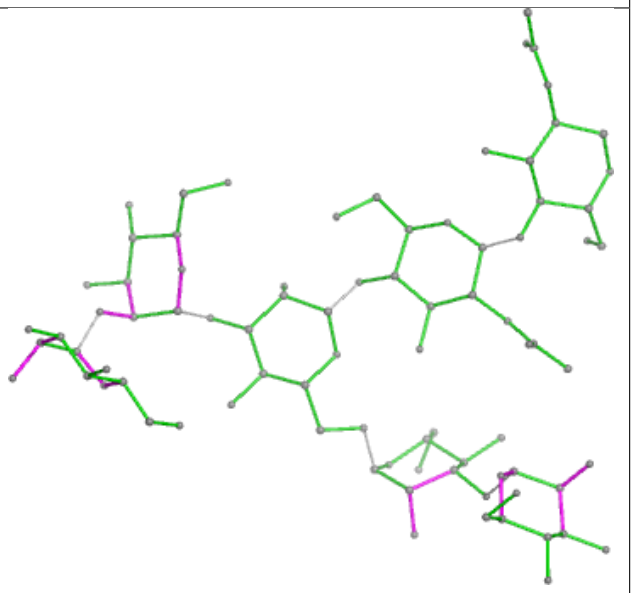
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3	BMA	1	0
2	E	3	BMA	1	0

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

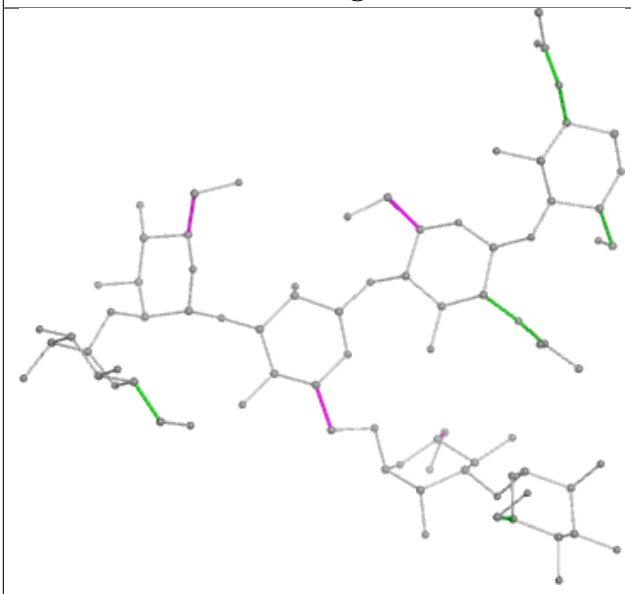
Oligosaccharide Chain E



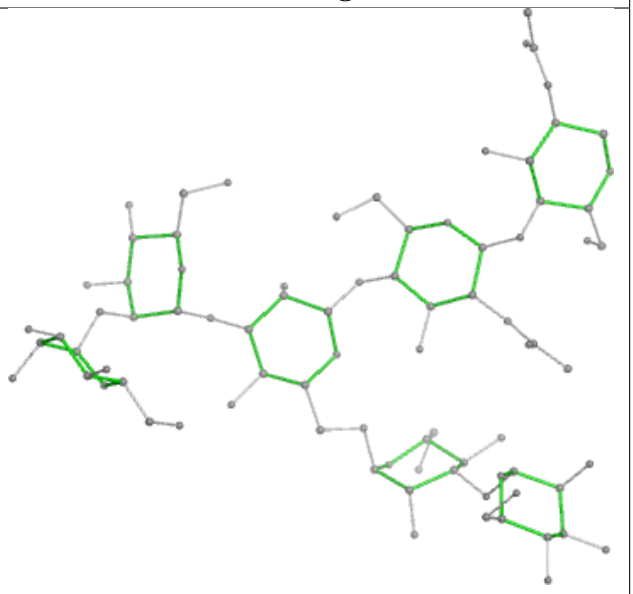
Bond lengths



Bond angles

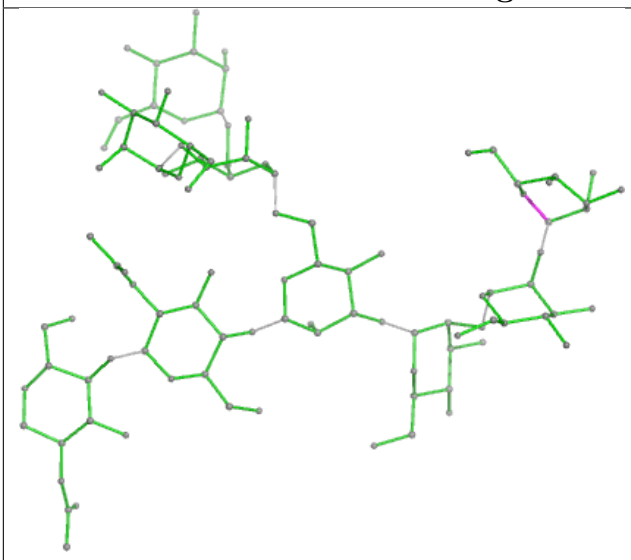


Torsions

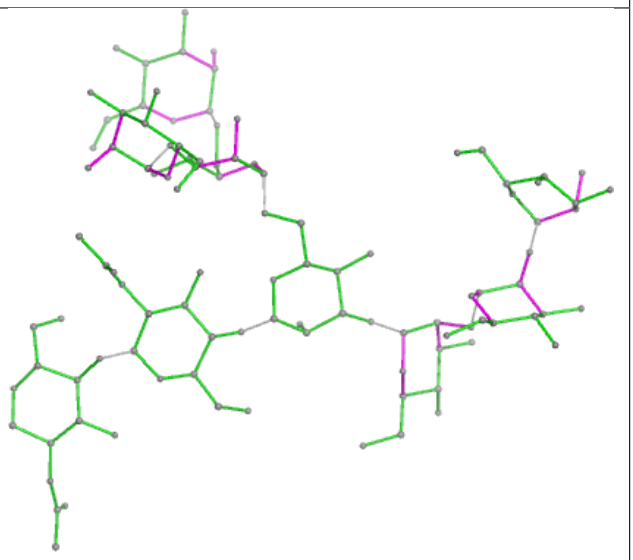


Rings

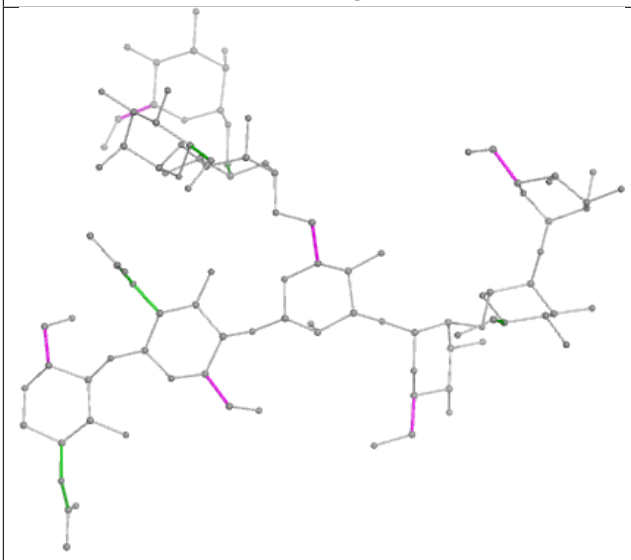
Oligosaccharide Chain F



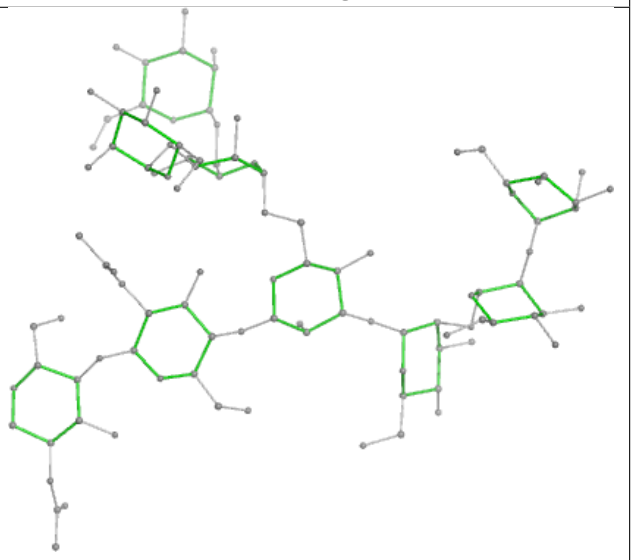
Bond lengths



Bond angles

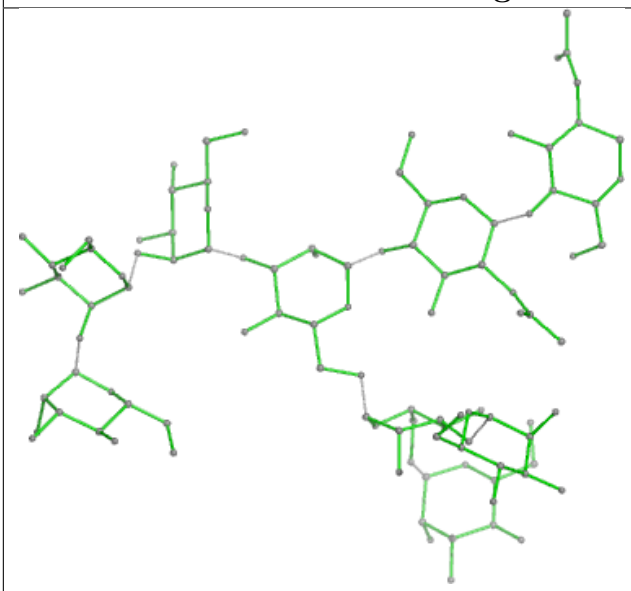


Torsions

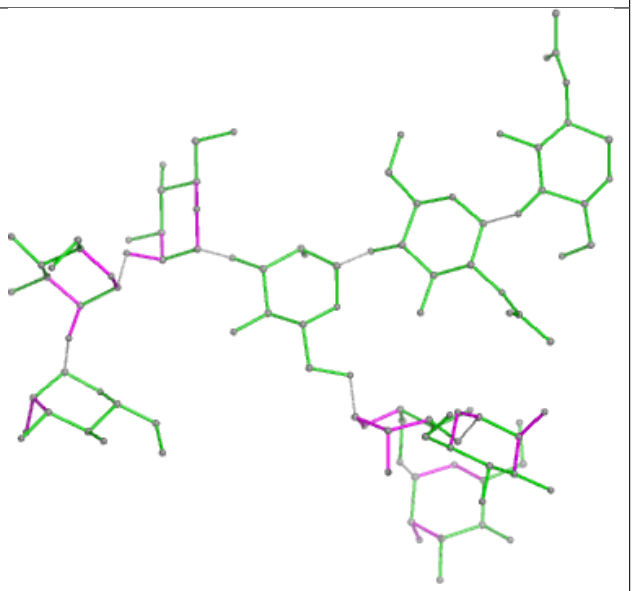


Rings

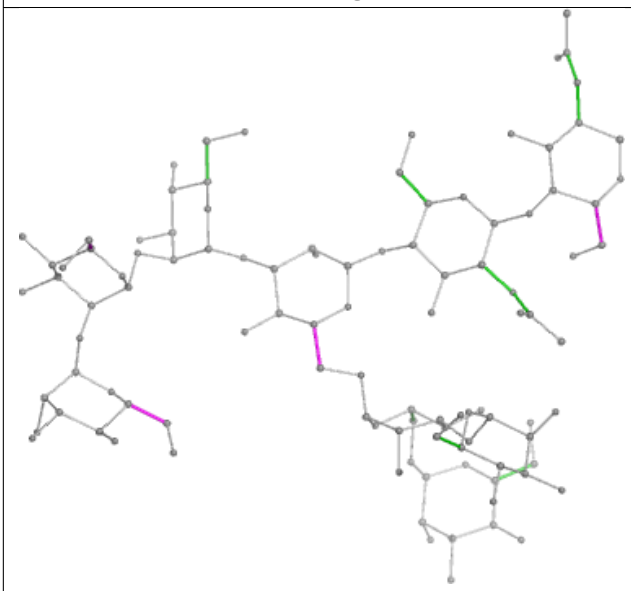
Oligosaccharide Chain H



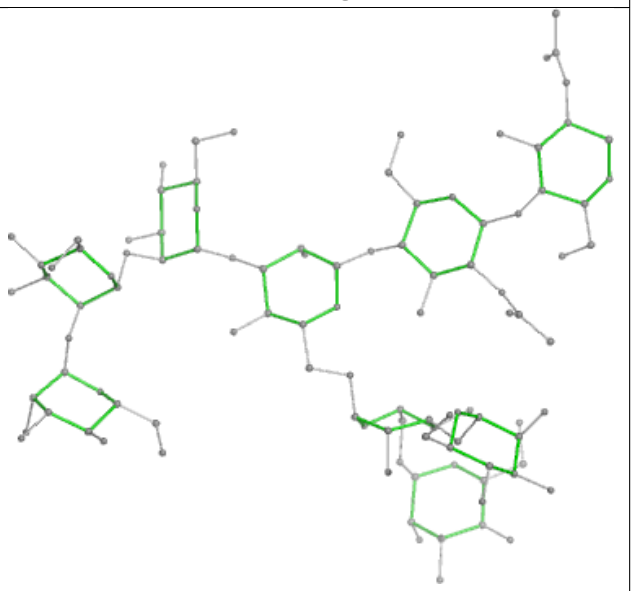
Bond lengths



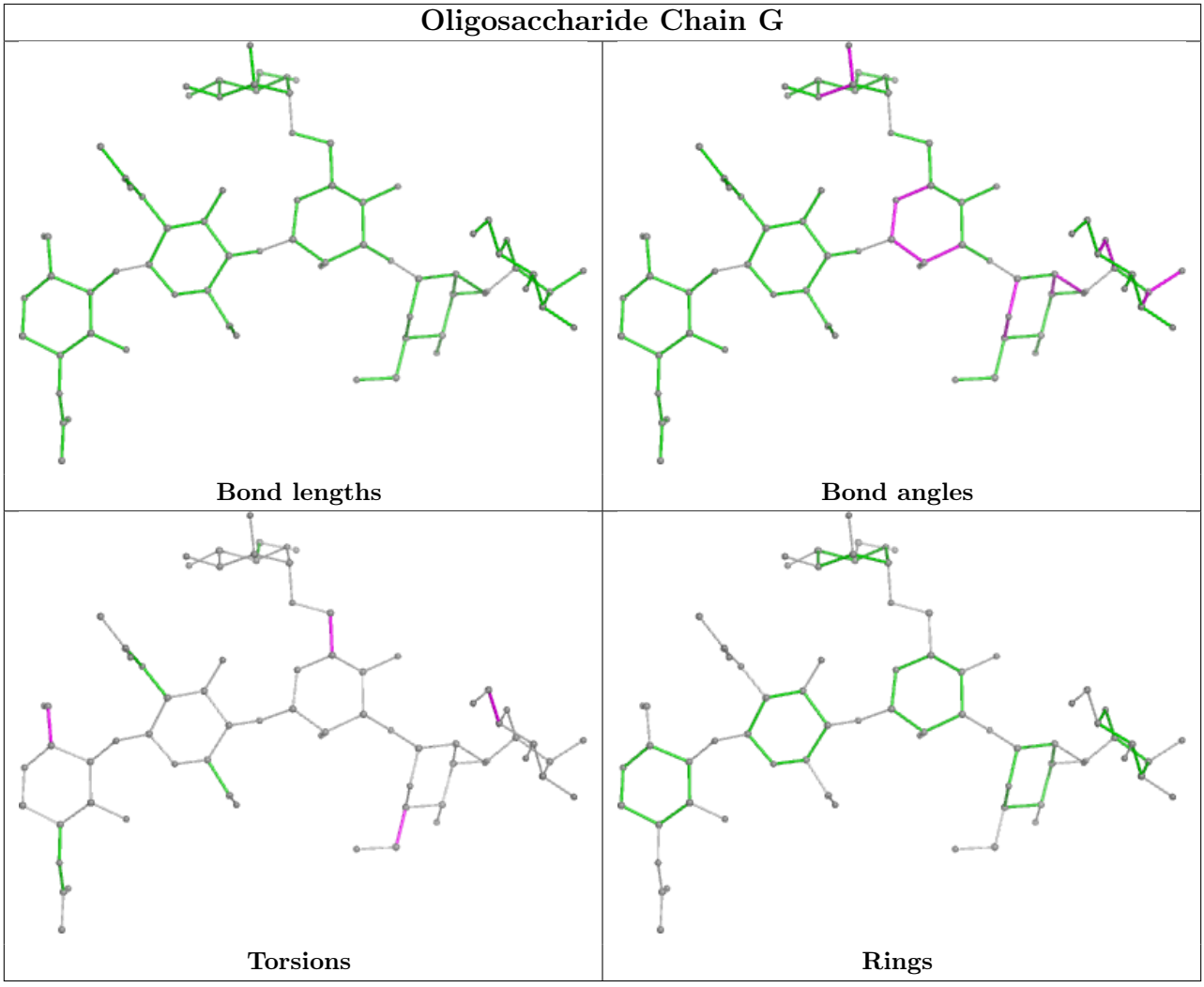
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
6	PEG	A	602	-	6,6,6	0.15	0	5,5,5	0.06	0
7	ACT	D	602	-	3,3,3	1.30	0	3,3,3	1.42	0
7	ACT	A	603	-	3,3,3	1.31	0	3,3,3	1.41	0
5	NAG	B	601	1	14,14,15	0.19	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	EDO	C	602	-	3,3,3	0.46	0	2,2,2	0.30	0
5	NAG	D	601	1	14,14,15	0.28	0	17,19,21	0.48	0
7	ACT	C	604	-	3,3,3	1.20	0	3,3,3	1.43	0
8	EDO	C	601	-	3,3,3	0.41	0	2,2,2	0.50	0
7	ACT	C	603	-	3,3,3	1.24	0	3,3,3	1.42	0
7	ACT	B	602	-	3,3,3	1.27	0	3,3,3	1.37	0
5	NAG	A	601	1	14,14,15	0.53	0	17,19,21	0.77	1 (5%)

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
6	PEG	A	602	-	-	1/4/4/4	-
5	NAG	B	601	1	-	3/6/23/26	0/1/1/1
8	EDO	C	602	-	-	1/1/1/1	-
5	NAG	D	601	1	-	0/6/23/26	0/1/1/1
8	EDO	C	601	-	-	1/1/1/1	-
5	NAG	A	601	1	-	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})
5	A	601	NAG	C1-O5-C5	-2.79	108.42	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
6	A	602	PEG	O1-C1-C2-O2
5	B	601	NAG	O5-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6
8	C	602	EDO	O1-C1-C2-O2
8	C	601	EDO	O1-C1-C2-O2
5	B	601	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	602	ACT	1	0
7	C	604	ACT	1	0
7	C	603	ACT	2	0
7	B	602	ACT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	195/234 (83%)	0.09	3 (1%)	71	50	13, 38, 70, 113	0
1	B	192/234 (82%)	0.12	2 (1%)	79	60	17, 37, 70, 89	0
1	C	193/234 (82%)	0.20	2 (1%)	79	60	11, 42, 76, 94	0
1	D	192/234 (82%)	0.08	2 (1%)	79	60	14, 37, 72, 91	0
All	All	772/936 (82%)	0.12	9 (1%)	76	56	11, 38, 72, 113	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	473	ALA	2.7
1	B	500	SER	2.6
1	A	459	ARG	2.5
1	A	479	PRO	2.4
1	B	454	PRO	2.3
1	D	411	SER	2.2
1	D	454	PRO	2.2
1	A	424	GLU	2.0
1	C	417	ALA	2.0

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

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

6.3 Carbohydrates

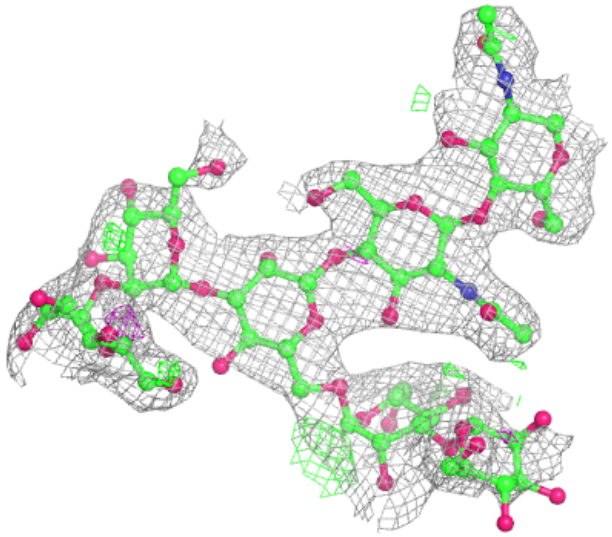
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

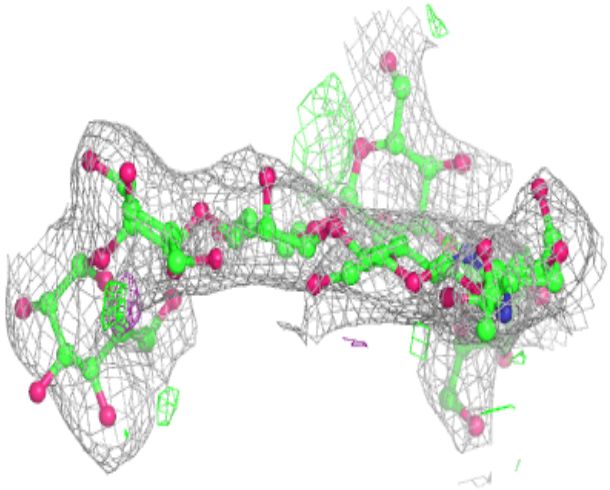
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	F	9	11/12	0.66	0.13	54,65,76,78	0
2	MAN	E	5	11/12	0.70	0.17	31,59,79,82	0
2	MAN	E	7	11/12	0.72	0.21	38,64,82,94	0
3	MAN	F	6	11/12	0.73	0.17	34,63,75,82	0
2	MAN	E	6	11/12	0.75	0.16	31,47,67,73	0
3	MAN	H	5	11/12	0.75	0.15	29,61,84,99	0
4	MAN	G	5	11/12	0.76	0.17	26,65,85,92	0
4	MAN	G	4	11/12	0.77	0.15	49,57,67,88	0
3	MAN	F	4	11/12	0.77	0.15	41,50,58,58	0
3	MAN	H	9	11/12	0.79	0.10	49,69,86,89	0
2	MAN	E	4	11/12	0.81	0.14	37,52,66,69	0
3	MAN	H	8	11/12	0.83	0.11	30,55,75,80	0
4	MAN	G	6	11/12	0.84	0.10	27,32,43,46	0
3	MAN	F	5	11/12	0.85	0.12	32,53,69,72	0
3	MAN	H	6	11/12	0.86	0.13	32,56,66,68	0
3	MAN	F	8	11/12	0.87	0.11	36,51,70,78	0
3	MAN	H	7	11/12	0.88	0.10	26,41,61,71	0
3	MAN	H	4	11/12	0.88	0.12	9,31,55,64	0
3	BMA	F	3	11/12	0.89	0.11	18,25,33,39	0
2	BMA	E	3	11/12	0.91	0.09	17,33,45,45	0
3	MAN	F	7	11/12	0.91	0.10	29,41,59,66	0
4	NAG	G	2	14/15	0.91	0.13	17,28,58,71	0
3	NAG	F	2	14/15	0.92	0.11	17,25,43,48	0
3	NAG	H	1	14/15	0.92	0.12	15,29,43,84	0
3	NAG	F	1	14/15	0.93	0.10	11,17,29,30	0
4	BMA	G	3	11/12	0.93	0.09	23,28,37,50	0
3	NAG	H	2	14/15	0.93	0.11	13,35,53,69	0
2	NAG	E	2	14/15	0.93	0.12	15,23,37,41	0
2	NAG	E	1	14/15	0.93	0.11	17,22,37,39	0
3	BMA	H	3	11/12	0.94	0.09	15,32,38,47	0
4	NAG	G	1	14/15	0.95	0.09	12,21,37,44	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:

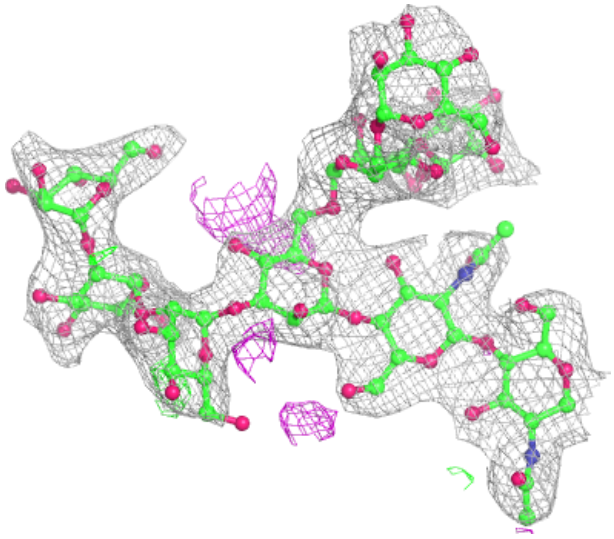
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

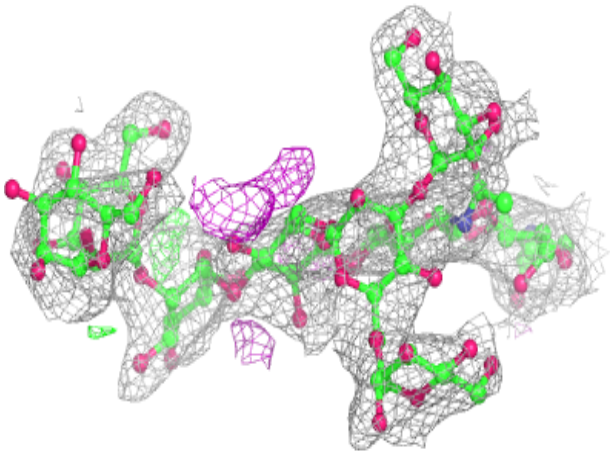


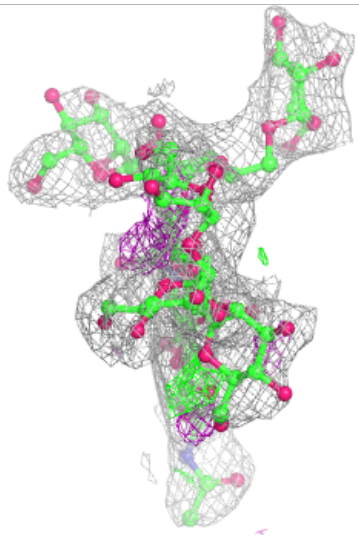


Electron density around Chain F:

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

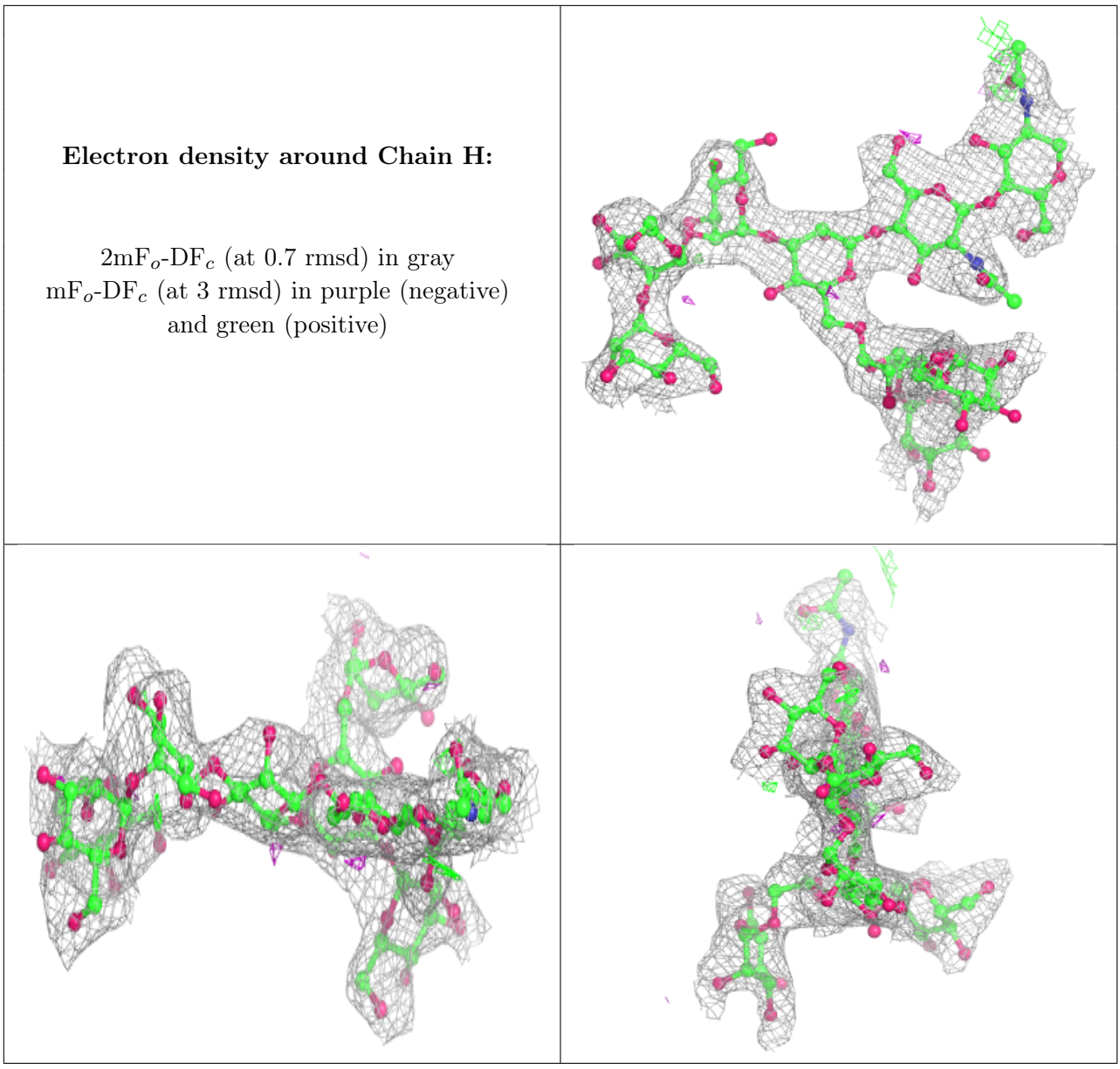






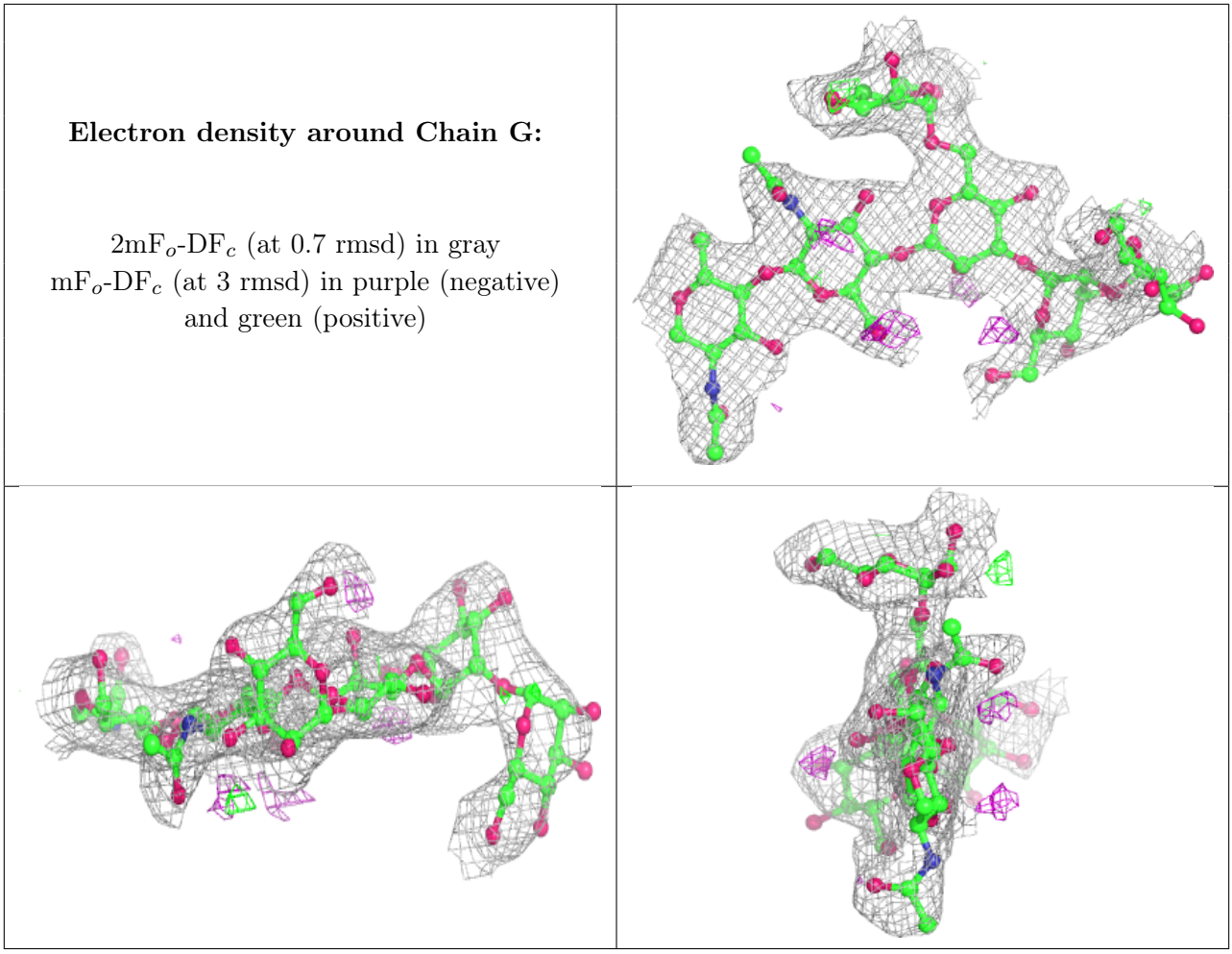
Electron density around Chain H:

$2mF_o$-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 G:

$2mF_o$-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
5	NAG	A	601	14/15	0.57	0.14	61,87,96,108	0
5	NAG	B	601	14/15	0.73	0.13	45,56,66,72	0
7	ACT	C	603	4/4	0.77	0.17	43,45,59,60	0
5	NAG	D	601	14/15	0.79	0.15	51,60,76,76	0
7	ACT	A	603	4/4	0.80	0.15	18,34,37,41	0
7	ACT	D	602	4/4	0.82	0.14	32,48,62,65	0
8	EDO	C	602	4/4	0.84	0.14	32,53,54,65	0
7	ACT	C	604	4/4	0.86	0.19	23,32,40,60	0
6	PEG	A	602	7/7	0.89	0.17	22,28,46,48	0
8	EDO	C	601	4/4	0.90	0.11	27,43,49,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ACT	B	602	4/4	0.91	0.16	24,27,37,54	0

6.5 Other polymers (i)

There are no such residues in this entry.