Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:27 AM UTC

PDB ID	:	4P1V / pdb_00004p1v
Title	:	Structure of the P domain from a GI.7 Norovirus variant in complex with H-type 2 HBGA
Authors	:	Shanker, S.; Czako, R.; Sankaran, B.; Atmar, R.; Estes, M.; Prasad, B.V.V.
Deposited on	:	2014-02-27
Resolution	:	1.55 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:

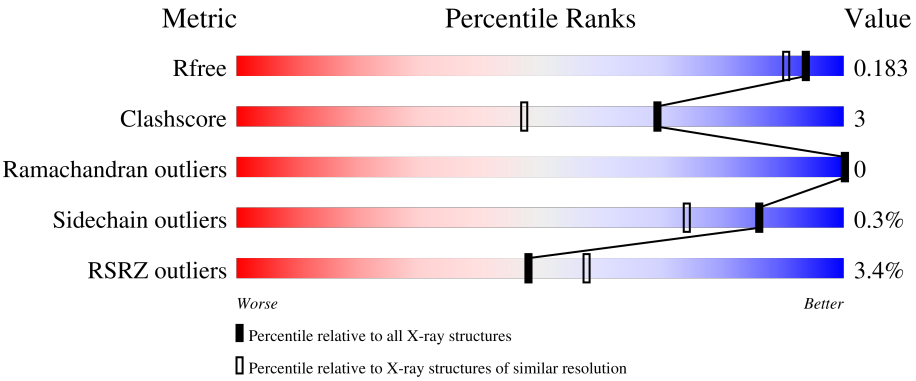
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.55 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	301	3% 92%
1	B	301	4% 86% 6% 7%
1	C	301	3% 90% 7%
1	D	301	3% 91% 6%
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	67% 33%
2	G	3	67% 33%
2	H	3	33% 67%

2 Entry composition (i)

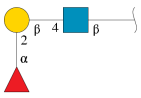
There are 3 unique types of molecules in this entry. The entry contains 10441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P domain of VPI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2203	1405	369	421	8			
1	B	280	Total	C	N	O	S	0	1	0
			2146	1372	362	404	8			
1	C	291	Total	C	N	O	S	0	0	0
			2218	1412	375	423	8			
1	D	290	Total	C	N	O	S	0	0	0
			2205	1407	369	421	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	F	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	G	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	H	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	388	Total	O	0	0
			388	388		

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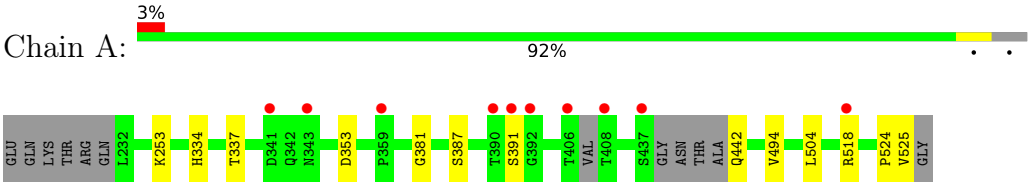
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	364	Total O 364 364	0	0
3	C	395	Total O 395 395	0	0
3	D	378	Total O 378 378	0	0

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.

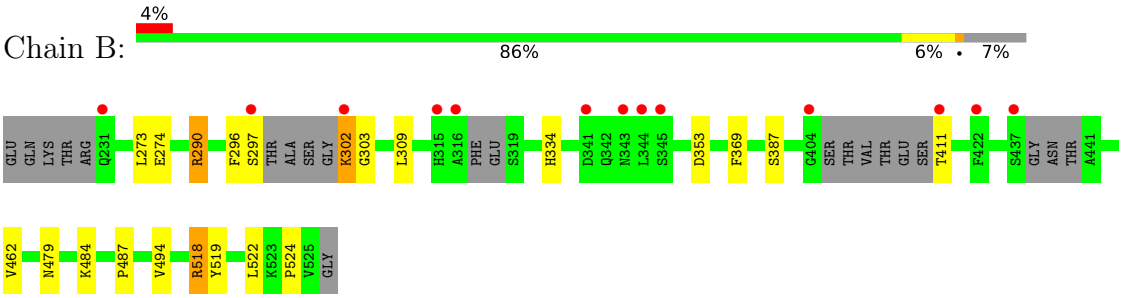
• Molecule 1: P domain of VPI

Chain A:



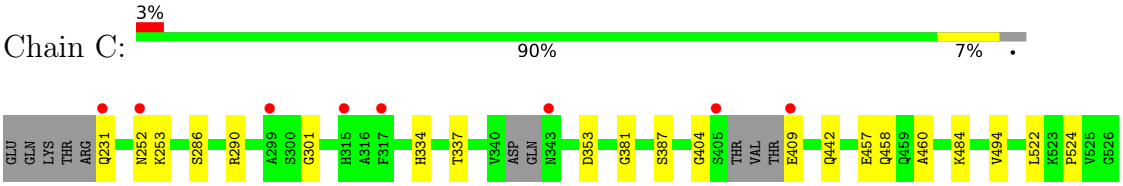
• Molecule 1: P domain of VPI

Chain B:



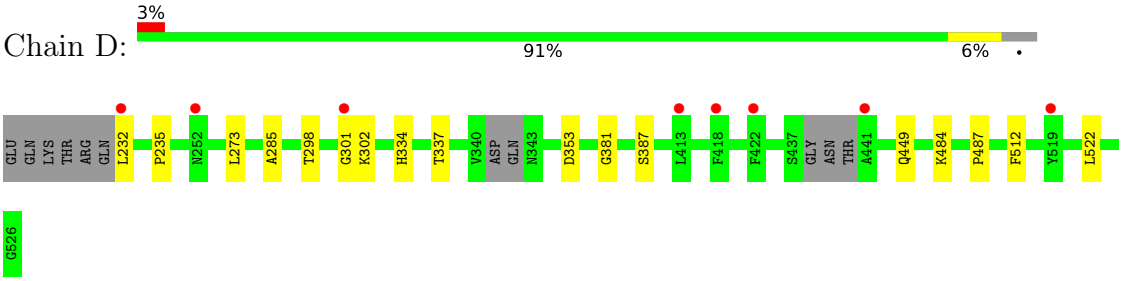
• Molecule 1: P domain of VPI

Chain C:



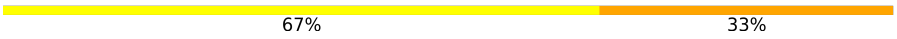
• Molecule 1: P domain of VPI

Chain D:



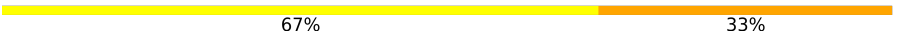
• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



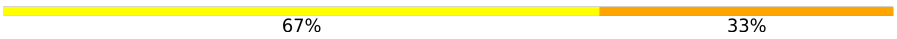
• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



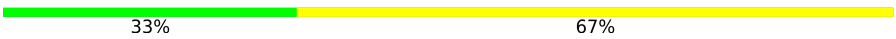
• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.40Å 63.15Å 90.32Å 72.71° 82.24° 60.75°	Depositor
Resolution (Å)	38.95 – 1.55 38.95 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.95-1.55) 96.7 (38.95-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.154 , 0.173 0.166 , 0.183	Depositor DCC
R_{free} test set	8109 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	10.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.006 for h-k,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10441	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: NAG, FUC, GAL

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	0.56	0/2268	0.81	0/3105
1	B	0.55	1/2210 (0.0%)	0.84	0/3022
1	C	0.52	0/2283	0.80	1/3122 (0.0%)
1	D	0.52	0/2270	0.81	0/3107
All	All	0.54	1/9031 (0.0%)	0.82	1/12356 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	479	ASN	CA-C	-5.70	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	GLY	N-CA-C	5.35	119.50	111.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	290[A]	ARG	Mainchain

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	2203	0	2117	11	0
1	B	2146	0	2075	16	0
1	C	2218	0	2139	19	0
1	D	2205	0	2127	11	0
2	E	36	0	33	1	0
2	F	36	0	33	2	0
2	G	36	0	33	2	0
2	H	36	0	33	0	0
3	A	388	0	0	3	1
3	B	364	0	0	6	0
3	C	395	0	0	1	1
3	D	378	0	0	1	0
All	All	10441	0	8590	61	1

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 (61) 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:518:ARG:NH1	3:A:1070:HOH:O	1.73	1.21
1:A:391:SER:O	3:A:1019:HOH:O	1.87	0.92
1:C:404:GLY:HA3	1:C:409:GLU:HG3	1.51	0.90
1:C:252:ASN:HD21	1:C:253:LYS:CE	1.92	0.82
1:A:253:LYS:HE3	1:A:442:GLN:HE22	1.44	0.81
1:C:252:ASN:HD21	1:C:253:LYS:HE3	1.45	0.78
1:A:253:LYS:HE3	1:A:442:GLN:NE2	1.99	0.78
1:C:252:ASN:ND2	1:C:253:LYS:HE3	1.97	0.77
1:C:252:ASN:HD21	1:C:253:LYS:NZ	1.83	0.77
1:C:252:ASN:HD21	1:C:253:LYS:HZ1	1.34	0.74
1:B:518:ARG:HD3	3:B:735:HOH:O	1.86	0.74
1:C:458:GLN:HG2	1:C:460:ALA:HB2	1.78	0.66
1:B:411:THR:N	3:B:1025:HOH:O	2.30	0.65
1:D:334:HIS:HE1	1:D:387:SER:OG	1.81	0.64
1:A:391:SER:O	3:A:1002:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ARG:HD2	1:B:519:TYR:CZ	2.32	0.63
1:B:334:HIS:HE1	1:B:387:SER:OG	1.82	0.62
1:D:273:LEU:HG	1:D:487:PRO:HA	1.81	0.62
1:C:253:LYS:NZ	1:C:442:GLN:OE1	2.32	0.62
1:C:334:HIS:HE1	1:C:387:SER:OG	1.84	0.61
1:A:334:HIS:HE1	1:A:387:SER:OG	1.84	0.61
1:C:404:GLY:HA3	1:C:409:GLU:CG	2.27	0.58
1:B:274:GLU:HG3	1:B:462:VAL:HG23	1.87	0.56
1:C:457:GLU:OE2	1:D:235:PRO:HA	2.09	0.53
3:B:704:HOH:O	2:F:1:NAG:H81	2.09	0.52
1:A:494:VAL:O	1:A:524:PRO:HA	2.11	0.51
1:D:484:LYS:HG3	1:D:522:LEU:HD21	1.93	0.50
1:A:504:LEU:HD11	1:A:525:VAL:HG21	1.93	0.50
1:C:231:GLN:N	3:C:974:HOH:O	2.44	0.50
2:F:1:NAG:H61	2:F:3:FUC:H5	1.94	0.49
1:C:484:LYS:HG3	1:C:522:LEU:HD21	1.94	0.49
1:B:411:THR:HA	3:B:1025:HOH:O	2.13	0.49
1:B:518:ARG:HG2	1:B:519:TYR:CD1	2.48	0.49
1:C:409:GLU:O	1:C:409:GLU:HG2	2.12	0.48
1:B:296:PHE:CZ	1:B:303:GLY:HA3	2.48	0.48
1:D:298:THR:HG1	1:D:301:GLY:C	2.21	0.48
1:C:404:GLY:CA	1:C:409:GLU:HG3	2.35	0.48
1:B:302:LYS:HD3	1:B:369:PHE:CE1	2.47	0.48
2:G:1:NAG:H61	2:G:2:GAL:C1	2.44	0.48
2:E:1:NAG:O4	2:E:3:FUC:H5	2.14	0.47
1:B:273:LEU:HG	1:B:487:PRO:HA	1.97	0.47
1:D:232:LEU:HD23	1:D:512:PHE:CD1	2.50	0.46
1:D:337:THR:HG22	1:D:381:GLY:HA3	1.98	0.46
1:D:302:LYS:NZ	3:D:1023:HOH:O	2.05	0.46
1:B:484:LYS:HG3	1:B:522:LEU:HD21	1.99	0.45
1:A:337:THR:HG22	1:A:381:GLY:HA3	1.98	0.45
1:B:290[B]:ARG:NH2	3:B:1018:HOH:O	2.49	0.44
1:B:334:HIS:HD2	1:B:353:ASP:OD1	2.00	0.44
1:D:334:HIS:HD2	1:D:353:ASP:OD1	2.00	0.44
1:A:334:HIS:HD2	1:A:353:ASP:OD1	2.02	0.43
1:B:411:THR:CA	3:B:1025:HOH:O	2.66	0.43
1:C:337:THR:HG22	1:C:381:GLY:HA3	2.00	0.43
1:D:285:ALA:HA	1:D:449:GLN:HG2	2.01	0.43
1:C:334:HIS:HD2	1:C:353:ASP:OD1	2.01	0.42
1:B:494:VAL:O	1:B:524:PRO:HA	2.19	0.42
1:B:290[B]:ARG:HB3	1:B:309:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:NAG:H5	2:G:3:FUC:C6	2.51	0.41
1:C:286:SER:O	1:C:290:ARG:HD2	2.21	0.41
1:C:494:VAL:O	1:C:524:PRO:HA	2.20	0.41
1:D:298:THR:OG1	1:D:301:GLY:O	2.30	0.41
1:A:504:LEU:HD11	1:A:525:VAL:CG2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:707:HOH:O	3:C:756:HOH:O[1_654]	2.03	0.17

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	283/301 (94%)	273 (96%)	10 (4%)	0	100	100
1	B	271/301 (90%)	263 (97%)	8 (3%)	0	100	100
1	C	285/301 (95%)	275 (96%)	10 (4%)	0	100	100
1	D	284/301 (94%)	273 (96%)	11 (4%)	0	100	100
All	All	1123/1204 (93%)	1084 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	246/257 (96%)	246 (100%)	0	100 100
1	B	238/257 (93%)	235 (99%)	3 (1%)	61 31
1	C	247/257 (96%)	247 (100%)	0	100 100
1	D	246/257 (96%)	246 (100%)	0	100 100
All	All	977/1028 (95%)	974 (100%)	3 (0%)	86 74

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	SER
1	B	302	LYS
1	B	518	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	A	334	HIS
1	A	342	GLN
1	A	458	GLN
1	B	334	HIS
1	B	342	GLN
1	B	442	GLN
1	B	521	GLN
1	C	252	ASN
1	C	334	HIS
1	D	305	ASN
1	D	334	HIS

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)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2	15,15,15	0.64	0	21,21,21	0.81	1 (4%)
2	GAL	E	2	2	11,11,12	0.28	0	15,15,17	0.78	1 (6%)
2	FUC	E	3	2	10,10,11	0.34	0	14,14,16	0.77	0
2	NAG	F	1	2	15,15,15	0.64	0	21,21,21	0.81	1 (4%)
2	GAL	F	2	2	11,11,12	0.29	0	15,15,17	0.78	1 (6%)
2	FUC	F	3	2	10,10,11	0.33	0	14,14,16	0.77	0
2	NAG	G	1	2	15,15,15	0.64	0	21,21,21	0.81	1 (4%)
2	GAL	G	2	2	11,11,12	0.28	0	15,15,17	0.78	0
2	FUC	G	3	2	10,10,11	0.34	0	14,14,16	0.77	0
2	NAG	H	1	2	15,15,15	0.64	0	21,21,21	0.81	1 (4%)
2	GAL	H	2	2	11,11,12	0.29	0	15,15,17	0.78	1 (6%)
2	FUC	H	3	2	10,10,11	0.35	0	14,14,16	0.77	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	E	1	2	-	2/6/26/26	0/1/1/1
2	GAL	E	2	2	-	2/2/19/22	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
2	NAG	G	1	2	-	2/6/26/26	0/1/1/1
2	GAL	G	2	2	-	2/2/19/22	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1
2	NAG	H	1	2	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	H	2	2	-	1/2/19/22	0/1/1/1
2	FUC	H	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	C1-O5-C5	-2.16	109.47	113.65
2	E	1	NAG	C1-O5-C5	-2.15	109.48	113.65
2	F	1	NAG	C1-O5-C5	-2.15	109.48	113.65
2	H	1	NAG	C1-O5-C5	-2.14	109.51	113.65
2	H	2	GAL	C1-O5-C5	-2.03	109.47	112.19
2	E	2	GAL	C1-O5-C5	-2.01	109.49	112.19
2	F	2	GAL	C1-O5-C5	-2.01	109.49	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0
2	G	3	FUC	1	0
2	E	1	NAG	1	0
2	F	1	NAG	2	0

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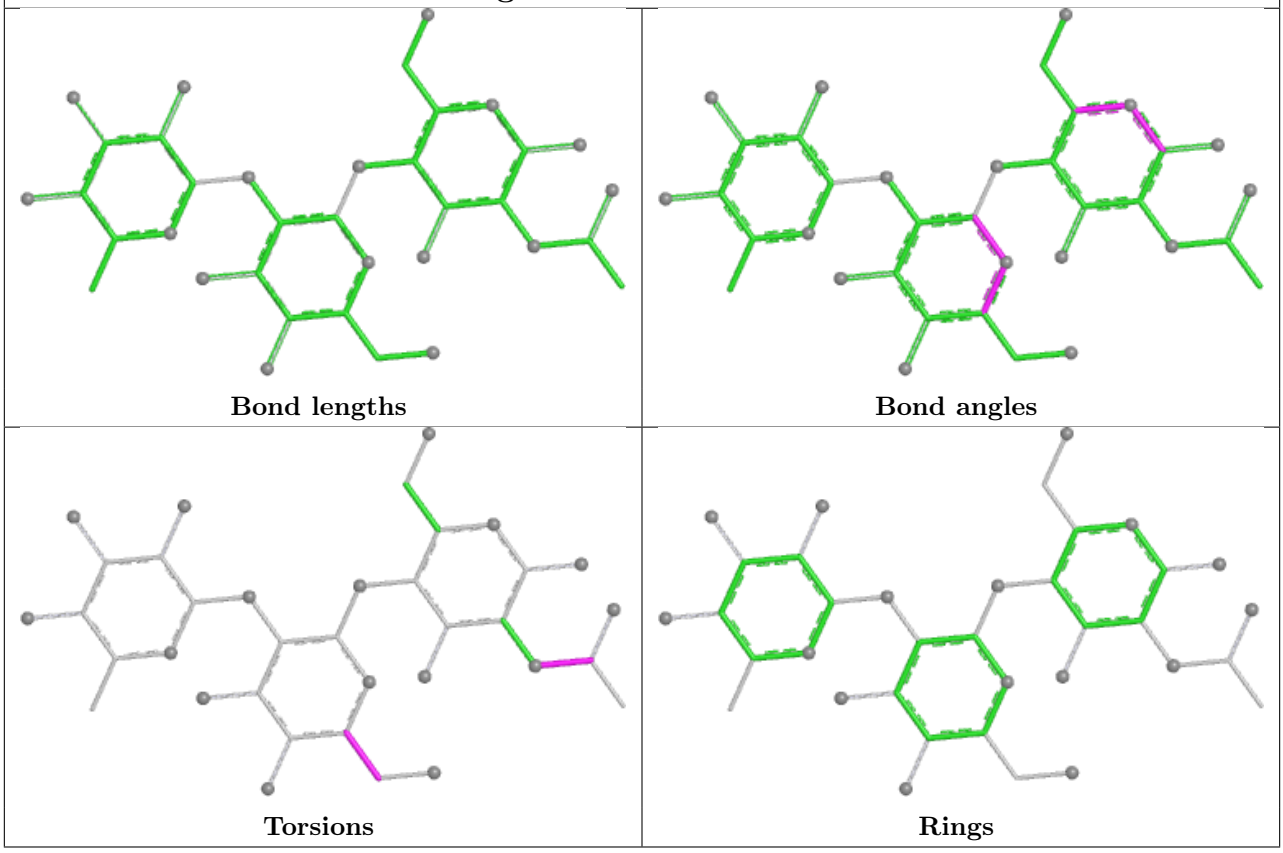
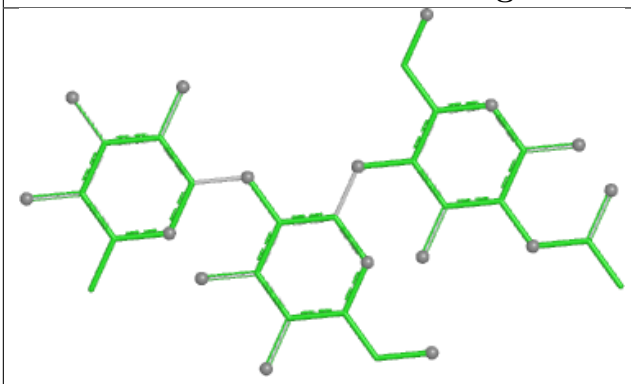
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	FUC	1	0
2	G	2	GAL	1	0
2	F	3	FUC	1	0

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

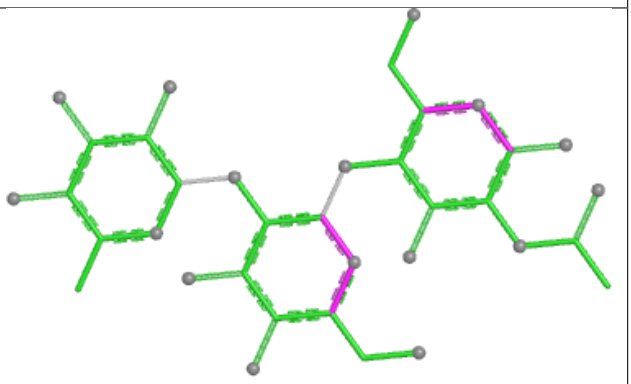
Oligosaccharide Chain E



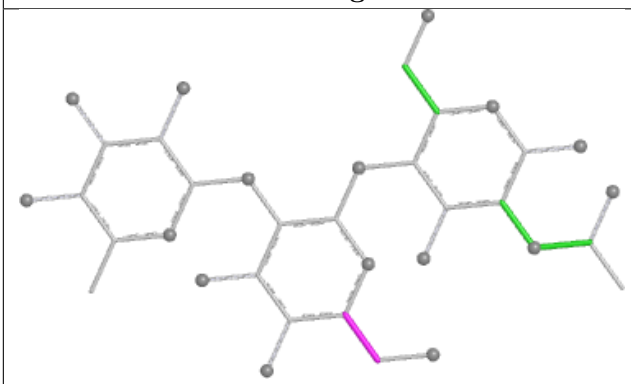
Oligosaccharide Chain F



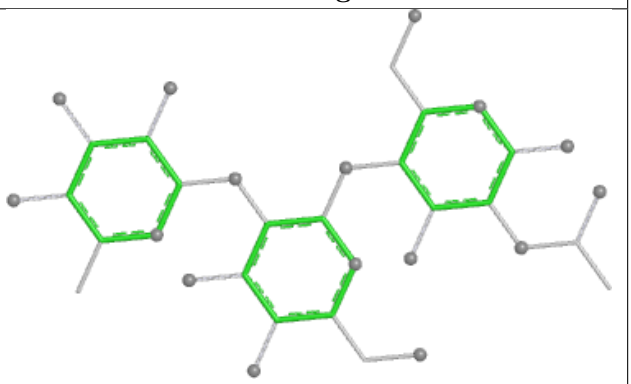
Bond lengths



Bond angles

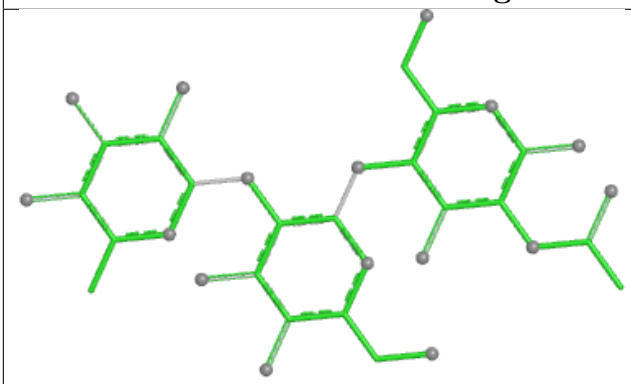


Torsions

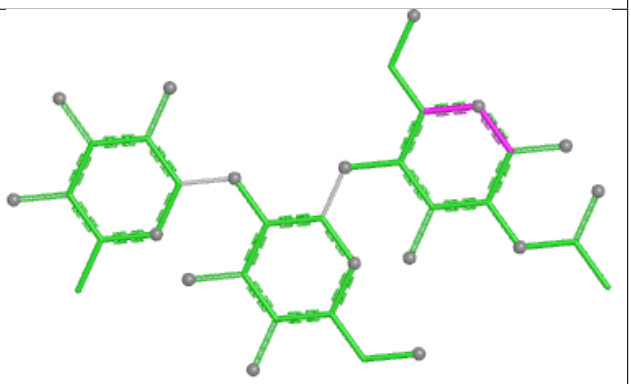


Rings

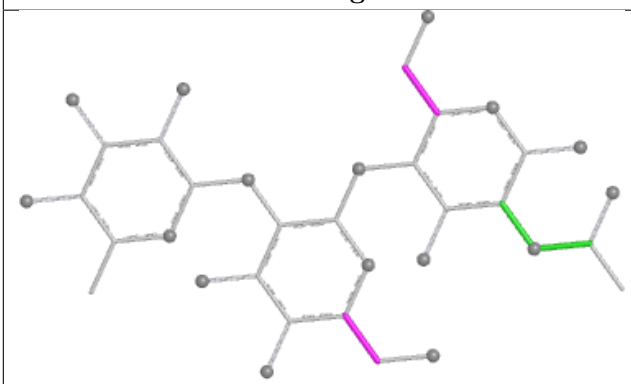
Oligosaccharide Chain G



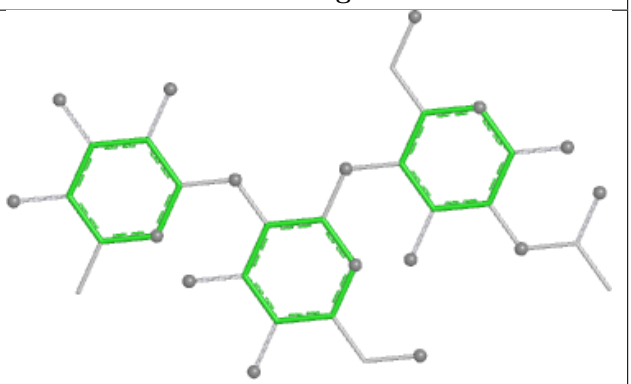
Bond lengths



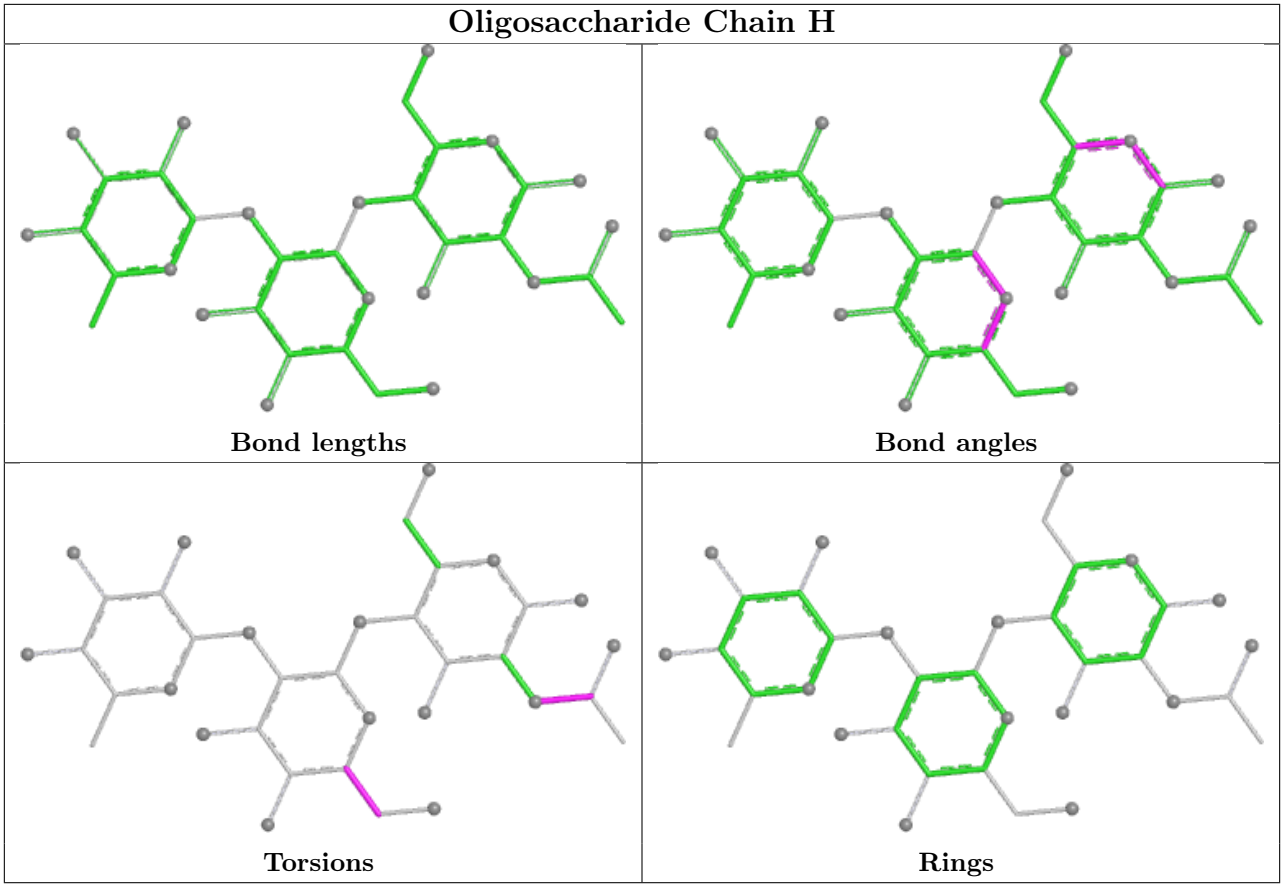
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	289/301 (96%)	-0.23	10 (3%) 47 56	3, 8, 23, 36	0
1	B	280/301 (93%)	-0.14	13 (4%) 37 45	4, 10, 27, 36	1 (0%)
1	C	291/301 (96%)	-0.29	8 (2%) 56 65	3, 8, 25, 39	0
1	D	290/301 (96%)	-0.27	8 (2%) 55 63	2, 8, 21, 39	0
All	All	1150/1204 (95%)	-0.23	39 (3%) 48 57	2, 9, 24, 39	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	SER	5.8
1	B	316	ALA	5.1
1	A	392	GLY	4.6
1	C	299	ALA	4.6
1	A	359	PRO	4.2
1	D	441	ALA	4.0
1	B	297	SER	3.9
1	D	422	PHE	3.8
1	B	315	HIS	3.5
1	D	301	GLY	3.4
1	A	408	THR	3.3
1	B	341	ASP	3.2
1	A	390	THR	3.0
1	A	518	ARG	3.0
1	B	302	LYS	3.0
1	C	231	GLN	3.0
1	A	341	ASP	2.9
1	B	411	THR	2.7
1	A	343	ASN	2.7
1	C	315	HIS	2.6
1	B	231	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	405	SER	2.6
1	D	519	TYR	2.5
1	D	232	LEU	2.5
1	B	344	LEU	2.5
1	C	252	ASN	2.4
1	B	345	SER	2.4
1	C	409	GLU	2.4
1	B	437	SER	2.3
1	C	317	PHE	2.3
1	C	343	ASN	2.2
1	D	413	LEU	2.2
1	A	406	THR	2.1
1	A	437	SER	2.1
1	B	343	ASN	2.1
1	B	404	GLY	2.1
1	D	252	ASN	2.1
1	B	422	PHE	2.0
1	D	418	PHE	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	G	2	11/12	0.76	0.14	6,7,12,14	0
2	FUC	G	3	10/11	0.77	0.14	5,11,14,15	0
2	NAG	G	1	15/15	0.79	0.18	9,24,47,50	0
2	NAG	E	1	15/15	0.80	0.14	8,17,25,30	0
2	NAG	F	1	15/15	0.85	0.13	9,19,30,34	0
2	GAL	E	2	11/12	0.85	0.12	5,6,13,20	0
2	GAL	F	2	11/12	0.86	0.10	7,8,10,15	0
2	FUC	F	3	10/11	0.88	0.10	5,10,17,17	0
2	FUC	E	3	10/11	0.88	0.10	4,7,11,13	0
2	NAG	H	1	15/15	0.89	0.10	5,10,22,23	0

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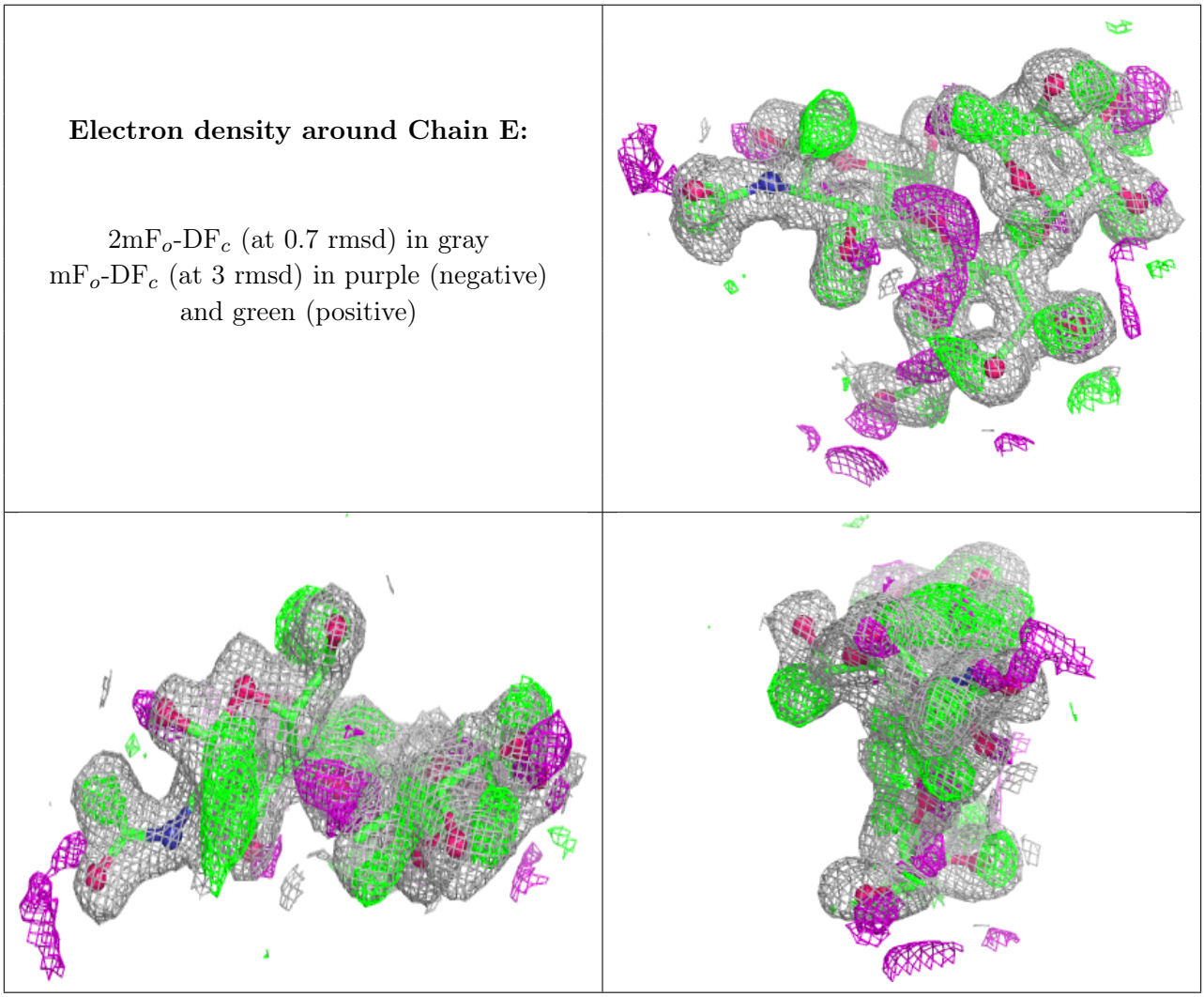
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	H	3	10/11	0.89	0.10	4,10,12,15	0
2	GAL	H	2	11/12	0.90	0.09	4,6,9,9	0

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

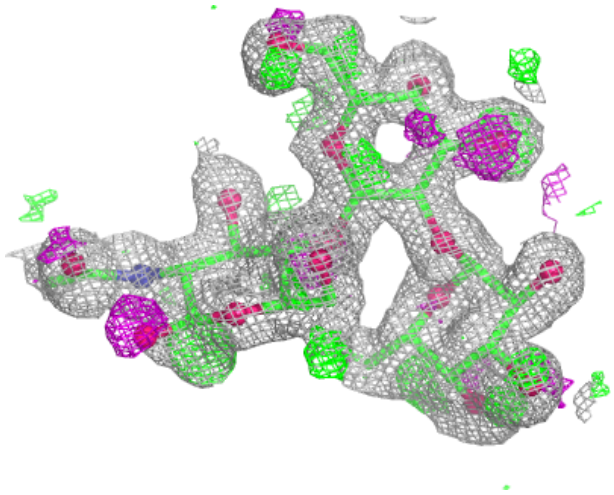
Electron density around Chain E:

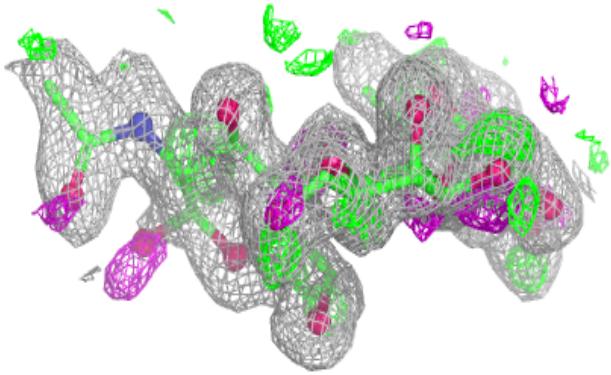
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

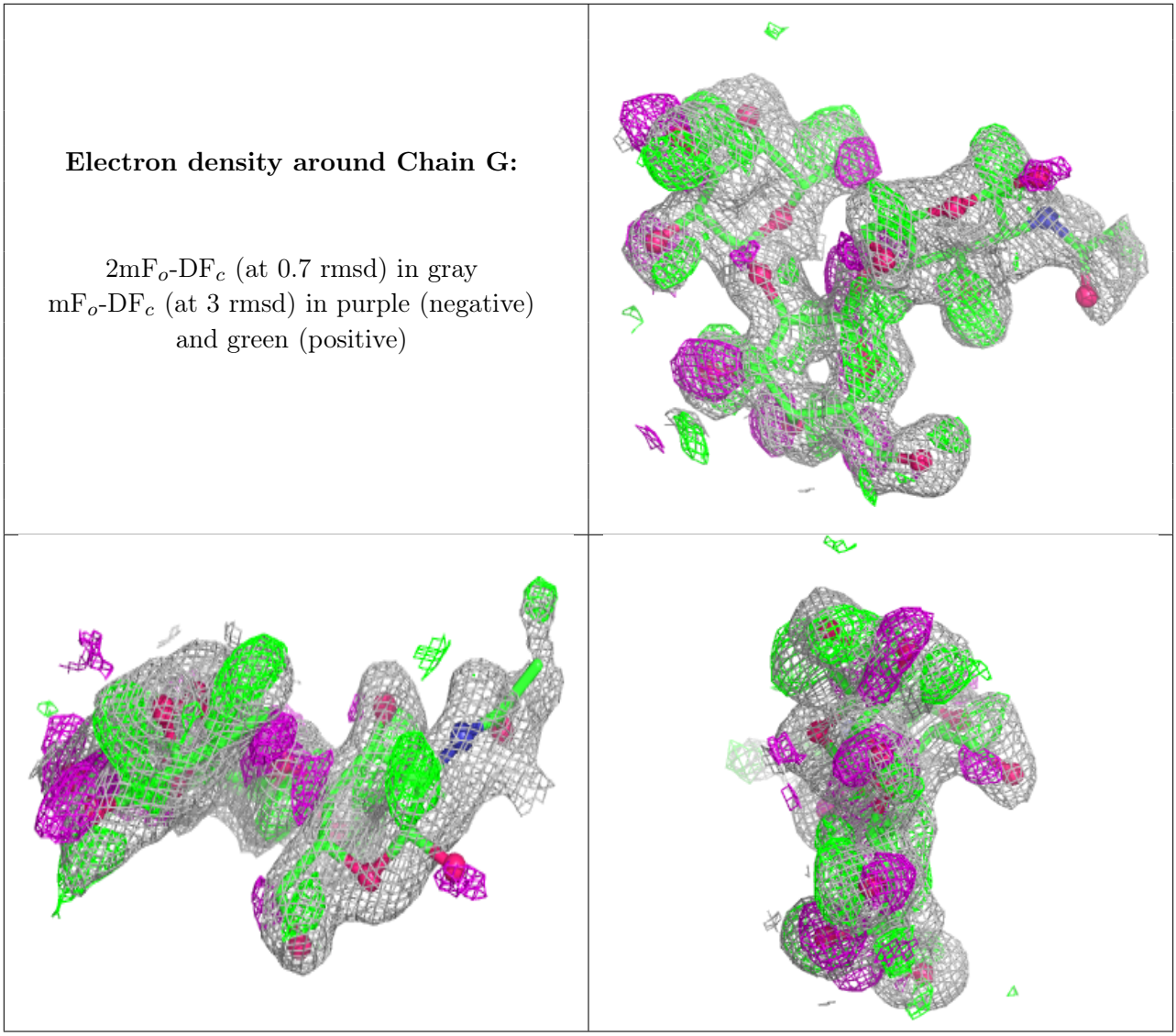
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





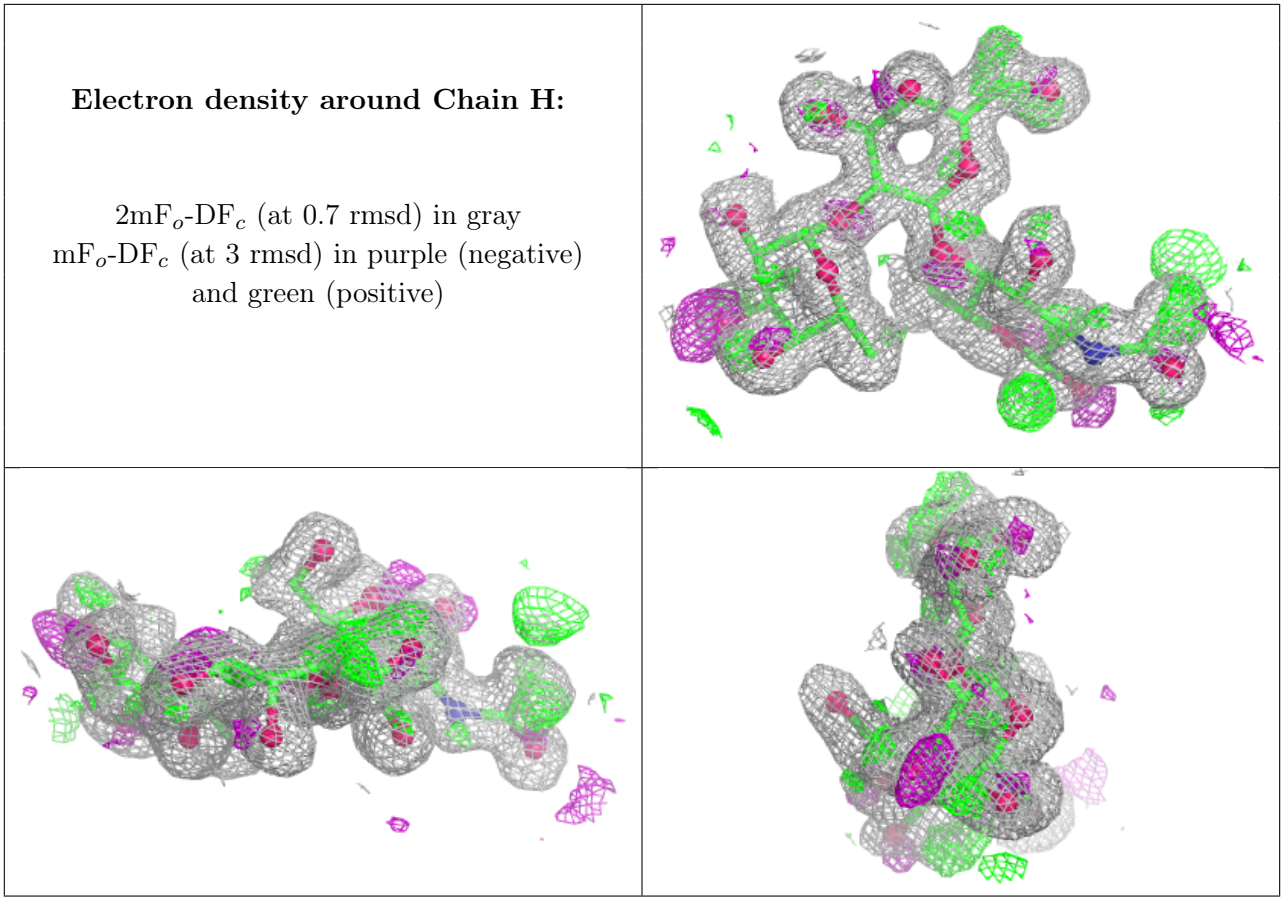
Electron density around Chain G:

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



Electron density around Chain H:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.