Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:17 AM BST

PDB ID	:	6P7S
Title	:	Crystal Structure of the Cedar henipavirus Attachment G Glycoprotein globular domain in complex with the receptor ephrin-B1
Authors	:	Xu, K.; Nikolov, D.B.; Xu, Y.
Deposited on	:	2019-06-06
Resolution	:	3.49 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 following versions of software and data (see references ①) were used in the production of this report:

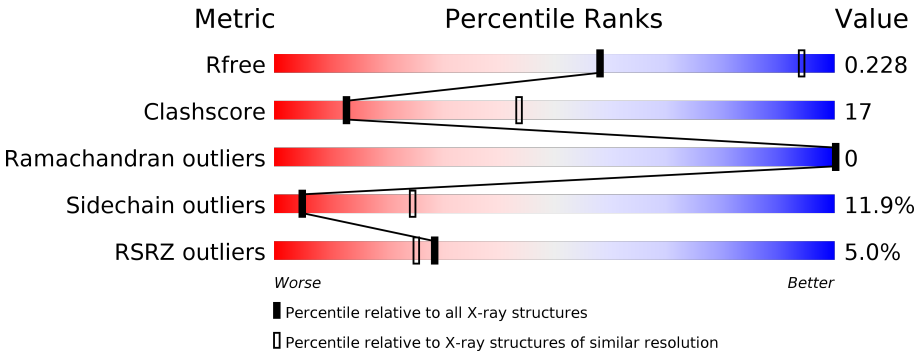
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.49 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.



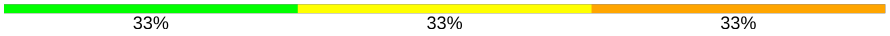
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	429	58% 34%
1	C	429	2% 53% 38% 6%
2	B	142	13% 63% 32%
2	D	142	15% 56% 35% 6%
3	E	2	50% 50%
3	G	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	2	
4	F	3	

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
3	NAG	G	1	X	-	-	-
5	NAG	A	702	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9114 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 Attachment glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3334	2118	550	642	24			
1	C	415	Total	C	N	O	S	0	0	0
			3334	2118	550	642	24			

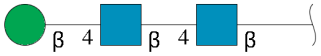
- Molecule 2 is a protein called Ephrin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1108	710	188	203	7			
2	D	138	Total	C	N	O	S	0	0	0
			1103	707	187	202	7			

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

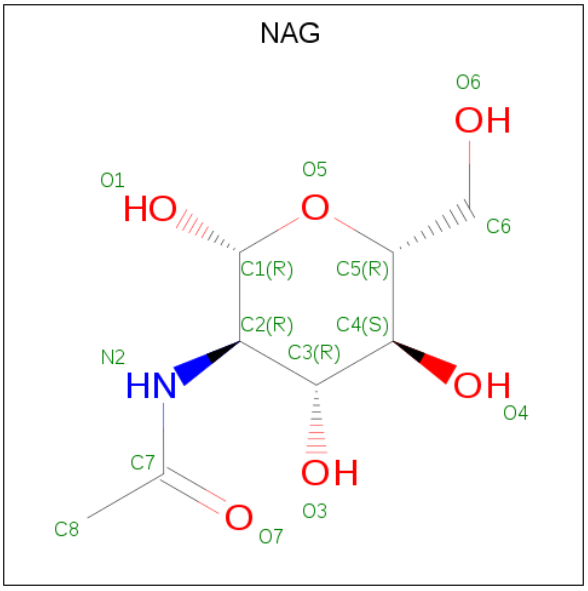
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 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	F	3	Total C N O 39 22 2 15	0	0	0

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



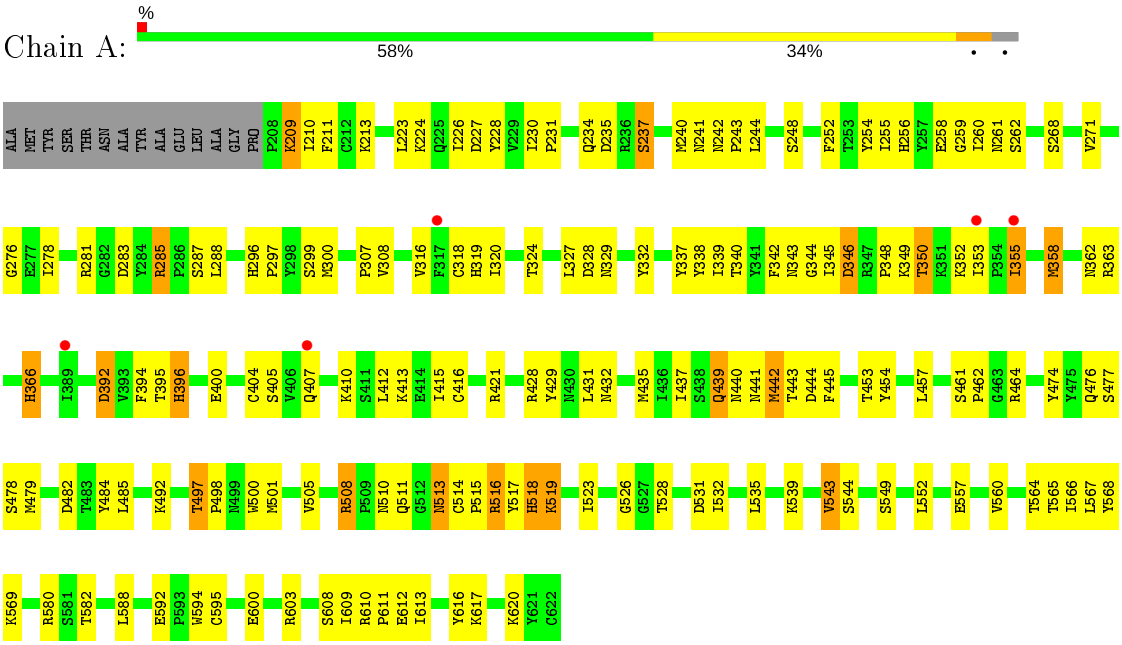
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

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.

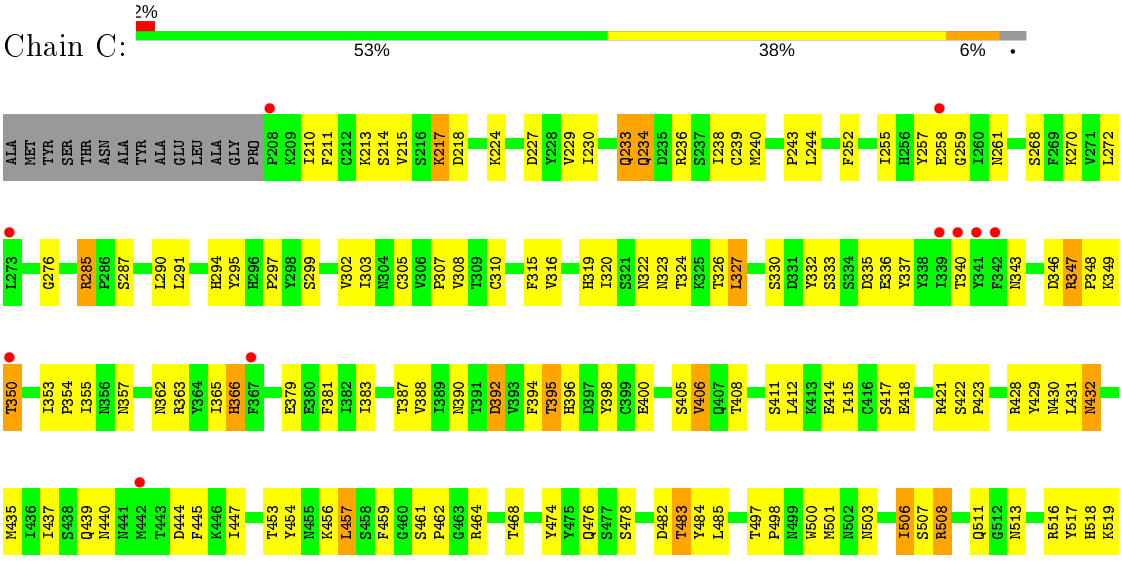
- Molecule 1: Attachment glycoprotein

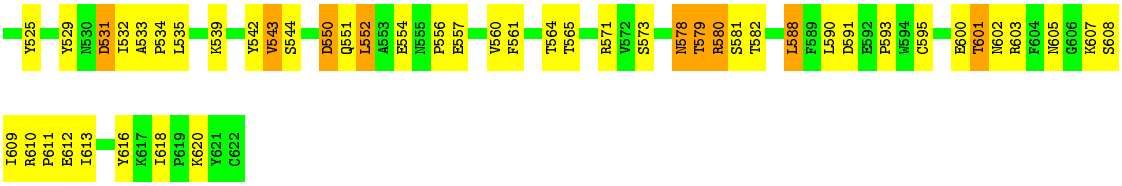
Chain A:



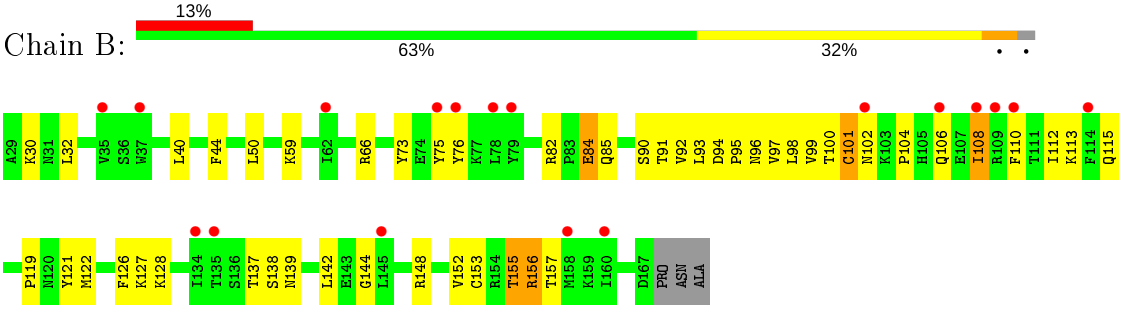
- Molecule 1: Attachment glycoprotein

Chain C:

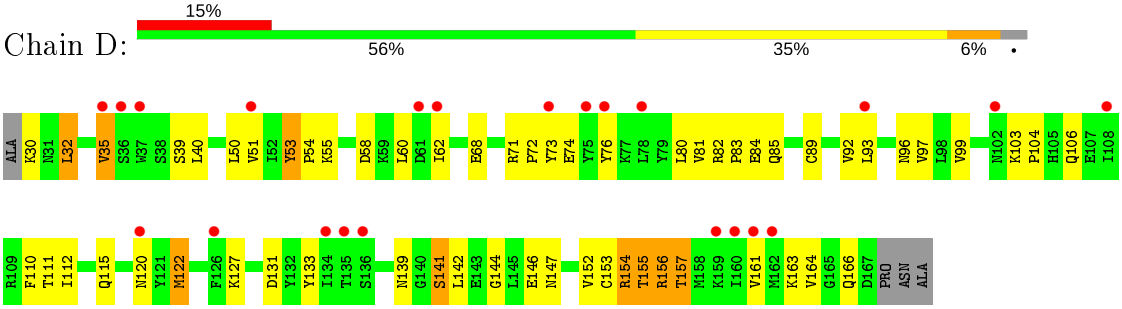




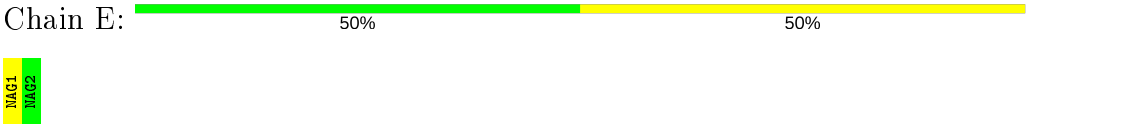
• Molecule 2: Ephrin-B1



• Molecule 2: Ephrin-B1

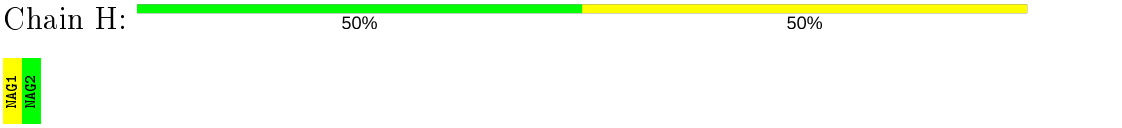


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



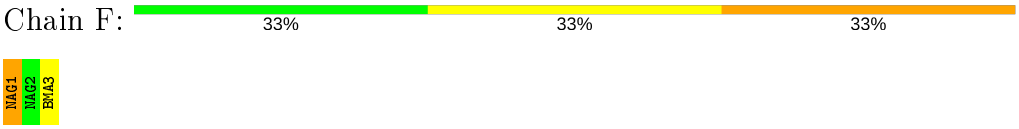
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	207.57Å 207.57Å 119.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.94 – 3.49 49.72 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.94-3.49) 91.0 (49.72-3.49)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.196 , 0.228 0.196 , 0.228	Depositor DCC
R_{free} test set	2009 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å^2)	120.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 21.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9114	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: BMA, 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	0.59	0/3418	0.76	1/4637 (0.0%)
1	C	0.55	0/3418	0.74	2/4637 (0.0%)
2	B	0.50	0/1134	0.73	0/1532
2	D	0.44	0/1129	0.70	0/1525
All	All	0.55	0/9099	0.74	3/12331 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	392	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	327	LEU	CA-CB-CG	5.42	127.76	115.30
1	C	392	ASP	CB-CG-OD1	5.09	122.88	118.30

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	3334	0	3216	102	0
1	C	3334	0	3215	129	0
2	B	1108	0	1108	37	0
2	D	1103	0	1102	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
4	F	39	0	34	1	0
5	A	42	0	39	1	0
5	C	56	0	52	5	0
5	D	14	0	13	1	0
All	All	9114	0	8854	297	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 17.

All (297) 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:347:ARG:HG3	1:C:348:PRO:HD2	1.49	0.94
1:C:244:LEU:HD23	1:C:307:PRO:HD3	1.57	0.87
1:C:516:ARG:HD2	1:C:550:ASP:HA	1.60	0.83
1:C:573:SER:OG	1:C:603:ARG:NH1	2.14	0.80
1:C:337:TYR:O	1:C:353:ILE:HG22	1.85	0.77
1:A:227:ASP:OD1	1:A:610:ARG:NH2	2.20	0.75
1:C:332:TYR:HB3	1:C:366:HIS:HA	1.70	0.74
1:A:297:PRO:HG3	1:A:350:THR:HG21	1.68	0.73
1:A:482:ASP:OD1	1:A:519:LYS:HD2	1.88	0.73
2:B:139:ASN:HD22	2:B:144:GLY:HA3	1.54	0.72
1:C:578:ASN:HD21	2:D:115:GLN:CD	1.92	0.72
1:C:557:GLU:HG2	1:C:571:ARG:HG2	1.73	0.71
2:D:83:PRO:HG3	2:D:133:TYR:HE2	1.55	0.71
1:C:435:MET:HE3	1:C:437:ILE:HD11	1.70	0.71
1:A:211:PHE:HA	1:A:620:LYS:HA	1.73	0.70
2:D:74:GLU:HB3	2:D:76:TYR:HE2	1.56	0.70
1:C:227:ASP:OD1	1:C:610:ARG:NH2	2.25	0.70
1:C:240:MET:HG2	1:C:258:GLU:HG2	1.71	0.70
1:A:454:TYR:HA	1:A:457:LEU:HD21	1.75	0.69
2:B:91:THR:O	2:B:148:ARG:NH1	2.23	0.69
1:A:362:ASN:OD1	1:A:363:ARG:N	2.26	0.69
1:A:244:LEU:HD23	1:A:307:PRO:HD3	1.75	0.69
1:C:211:PHE:HA	1:C:620:LYS:HA	1.75	0.69
1:C:240:MET:HE3	1:C:610:ARG:HG3	1.73	0.69
1:C:362:ASN:OD1	1:C:363:ARG:N	2.25	0.68
1:C:543:VAL:HG12	1:C:560:VAL:HG22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HD13	1:A:338:TYR:HD2	1.59	0.68
1:C:230:ILE:O	1:C:610:ARG:NH1	2.27	0.67
1:C:326:THR:O	1:C:327:LEU:HB2	1.94	0.67
1:C:482:ASP:OD1	1:C:519:LYS:NZ	2.28	0.67
1:C:588:LEU:HD13	1:C:591:ASP:HA	1.76	0.67
1:A:209:LYS:H	1:A:209:LYS:NZ	1.93	0.66
1:C:294:HIS:CE1	1:C:348:PRO:HD3	2.30	0.66
2:D:76:TYR:HE1	2:D:152:VAL:HG21	1.60	0.66
1:A:532:ILE:HG22	1:A:544:SER:HB2	1.78	0.66
2:D:85:GLN:HE21	2:D:93:LEU:HB2	1.61	0.65
1:A:346:ASP:OD1	1:A:346:ASP:N	2.26	0.65
1:C:319:HIS:CD2	1:C:337:TYR:HE1	2.14	0.65
1:C:603:ARG:NH2	1:C:612:GLU:OE1	2.29	0.65
2:D:54:PRO:HD2	2:D:163:LYS:O	1.96	0.65
1:C:435:MET:CE	1:C:437:ILE:HD11	2.27	0.65
1:C:340:THR:HG23	1:C:350:THR:HG22	1.77	0.65
1:A:230:ILE:O	1:A:610:ARG:NH1	2.30	0.65
2:D:74:GLU:HB3	2:D:76:TYR:CE2	2.31	0.64
1:C:297:PRO:HG3	1:C:350:THR:HG21	1.80	0.64
1:A:535:LEU:HD11	1:A:543:VAL:HG13	1.80	0.63
1:A:392:ASP:HB2	1:A:429:TYR:CZ	2.34	0.63
1:C:330:SER:O	1:C:428:ARG:NH1	2.31	0.63
1:A:543:VAL:HG12	1:A:560:VAL:HG22	1.81	0.62
2:B:153:CYS:O	2:B:157:THR:HA	1.99	0.62
1:A:319:HIS:CD2	1:A:337:TYR:CE1	2.88	0.62
1:C:421:ARG:HG2	1:C:429:TYR:CE1	2.35	0.61
1:C:542:TYR:HB2	1:C:561:PHE:CE1	2.34	0.61
1:C:430:ASN:HB2	1:C:459:PHE:CE1	2.36	0.61
1:A:439:GLN:HB2	1:A:445:PHE:CE1	2.36	0.60
1:A:343:ASN:HB3	1:A:346:ASP:OD1	2.02	0.60
1:C:578:ASN:ND2	2:D:115:GLN:OE1	2.34	0.60
1:C:392:ASP:HB2	1:C:429:TYR:CZ	2.37	0.60
2:B:30:LYS:HE3	2:B:32:LEU:HD23	1.84	0.60
1:C:257:TYR:OH	1:C:305:CYS:HB2	2.02	0.59
1:A:567:LEU:HD21	4:F:1:NAG:H61	1.85	0.59
1:A:319:HIS:HD2	1:A:337:TYR:CE1	2.20	0.59
1:C:319:HIS:CD2	1:C:337:TYR:CE1	2.91	0.59
1:C:535:LEU:HD11	1:C:543:VAL:HG13	1.85	0.59
1:C:213:LYS:HB3	1:C:539:LYS:HD3	1.84	0.58
1:A:343:ASN:OD1	1:A:344:GLY:N	2.34	0.58
1:A:580:ARG:NH2	1:A:600:GLU:OE2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ILE:HD11	1:C:316:VAL:HG22	1.86	0.58
2:B:96:ASN:ND2	2:B:122:MET:HB2	2.20	0.57
1:C:252:PHE:CE1	1:C:276:GLY:HA3	2.40	0.57
1:C:516:ARG:HG3	1:C:517:TYR:CD2	2.39	0.57
1:C:392:ASP:OD2	1:C:417:SER:OG	2.23	0.57
1:C:468:THR:HG21	1:C:534:PRO:HD2	1.86	0.57
1:A:608:SER:O	1:A:608:SER:OG	2.22	0.56
1:C:230:ILE:HD11	1:C:613:ILE:HG13	1.87	0.56
1:C:430:ASN:HB2	1:C:459:PHE:HE1	1.70	0.56
1:C:428:ARG:NH2	3:H:1:NAG:H61	2.21	0.56
1:A:396:HIS:HD2	1:A:416:CYS:HB3	1.70	0.56
1:A:209:LYS:H	1:A:209:LYS:HZ3	1.53	0.56
1:C:578:ASN:HB3	1:C:602:ASN:HB3	1.87	0.56
2:B:139:ASN:HB2	2:B:144:GLY:HA3	1.86	0.56
1:C:243:PRO:O	1:C:244:LEU:HD12	2.06	0.55
1:A:235:ASP:OD1	1:A:237:SER:N	2.35	0.55
2:B:138:SER:O	2:B:152:VAL:HG13	2.06	0.55
1:C:379:GLU:CD	1:C:379:GLU:H	2.09	0.55
1:A:508:ARG:NH2	1:A:514:CYS:O	2.39	0.55
1:C:454:TYR:HA	1:C:457:LEU:HD13	1.89	0.55
2:B:76:TYR:HE1	2:B:152:VAL:HG11	1.72	0.54
2:B:85:GLN:HE21	2:B:93:LEU:HB2	1.72	0.54
1:C:445:PHE:HB3	1:C:447:ILE:HD11	1.89	0.54
1:C:498:PRO:HG2	1:C:500:TRP:CZ2	2.42	0.54
1:C:478:SER:O	1:C:508:ARG:NE	2.30	0.54
1:C:529:TYR:CE2	1:C:531:ASP:HB3	2.43	0.54
1:A:332:TYR:HB3	1:A:366:HIS:HA	1.90	0.54
2:B:101:CYS:HA	2:B:108:ILE:HD11	1.90	0.54
1:C:336:GLU:HB2	5:C:702:NAG:H83	1.90	0.54
2:D:82:ARG:HG2	2:D:85:GLN:OE1	2.08	0.53
1:A:231:PRO:O	1:A:610:ARG:HD2	2.07	0.53
1:C:353:ILE:HD12	1:C:354:PRO:HD2	1.89	0.53
2:B:73:TYR:CD2	2:B:104:PRO:HB3	2.44	0.53
1:C:483:THR:HG21	1:C:518:HIS:H	1.73	0.53
1:A:224:LYS:HB2	1:A:285:ARG:NH1	2.24	0.52
1:A:516:ARG:HD2	1:A:517:TYR:CZ	2.44	0.52
2:B:66:ARG:HB2	2:B:104:PRO:O	2.10	0.52
2:D:85:GLN:HG2	2:D:93:LEU:HD13	1.91	0.52
1:C:406:VAL:HG22	1:C:415:ILE:HD12	1.90	0.52
1:C:511:GLN:HA	1:C:551:GLN:NE2	2.25	0.52
2:D:83:PRO:HG3	2:D:133:TYR:CE2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:LEU:HD11	2:B:59:LYS:HD3	1.91	0.52
1:C:276:GLY:HA2	1:C:291:LEU:HD13	1.92	0.52
1:C:302:VAL:HG22	1:C:320:ILE:CD1	2.40	0.52
1:A:453:THR:HB	1:A:497:THR:HG23	1.92	0.52
1:C:400:GLU:HA	1:C:412:LEU:HD23	1.92	0.52
1:A:252:PHE:CE1	1:A:276:GLY:HA3	2.45	0.51
1:C:233:GLN:HB3	1:C:240:MET:HE2	1.92	0.51
1:A:439:GLN:HG3	1:A:442:MET:SD	2.50	0.51
1:A:603:ARG:NH2	1:A:612:GLU:OE1	2.44	0.51
1:A:340:THR:HG23	1:A:350:THR:HG22	1.92	0.51
2:B:98:LEU:HB3	2:B:110:PHE:CE1	2.46	0.51
2:D:139:ASN:HB2	2:D:144:GLY:HA3	1.93	0.51
1:A:528:THR:HG23	2:B:119:PRO:HB3	1.93	0.50
1:C:210:ILE:HG12	1:C:620:LYS:HG3	1.93	0.50
1:C:418:GLU:HB3	1:C:421:ARG:NH2	2.26	0.50
1:A:560:VAL:HG21	1:A:568:TYR:CE1	2.45	0.50
1:C:468:THR:OG1	1:C:534:PRO:HG2	2.11	0.50
1:A:342:PHE:HB3	1:A:348:PRO:HA	1.93	0.50
1:C:322:ASN:ND2	5:C:702:NAG:O7	2.43	0.50
1:A:255:ILE:HD11	1:A:316:VAL:HG22	1.93	0.50
1:C:387:THR:O	1:C:430:ASN:HA	2.11	0.50
1:A:394:PHE:HD1	1:A:454:TYR:CE2	2.29	0.50
1:C:579:THR:HG23	1:C:601:THR:HG23	1.93	0.50
1:C:485:LEU:HB2	1:C:506:ILE:HD12	1.94	0.50
2:D:54:PRO:HG2	2:D:164:VAL:HG12	1.93	0.50
1:A:338:TYR:CE1	1:A:352:LYS:HB2	2.47	0.49
1:C:398:TYR:CG	1:C:456:LYS:HG2	2.47	0.49
2:D:68:GLU:O	2:D:71:ARG:HB2	2.11	0.49
1:A:552:LEU:HD22	2:B:113:LYS:HB2	1.93	0.49
1:C:394:PHE:HA	1:C:454:TYR:HE2	1.78	0.49
1:A:400:GLU:OE2	1:A:413:LYS:HG3	2.13	0.49
1:A:394:PHE:HA	1:A:454:TYR:HE2	1.78	0.49
2:B:155:THR:OG1	2:B:156:ARG:N	2.46	0.49
1:C:302:VAL:HG22	1:C:320:ILE:HD12	1.95	0.49
2:B:44:PHE:HD1	2:B:50:LEU:HB2	1.78	0.48
1:C:395:THR:OG1	1:C:395:THR:O	2.31	0.48
1:A:439:GLN:HB2	1:A:445:PHE:HE1	1.77	0.48
2:B:73:TYR:HD2	2:B:75:TYR:CE1	2.30	0.48
2:B:75:TYR:CE2	2:B:142:LEU:HD13	2.48	0.48
1:C:319:HIS:CG	1:C:337:TYR:HE1	2.31	0.48
1:A:400:GLU:HA	1:A:412:LEU:HD23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:CYS:HB2	2:D:154:ARG:HH21	1.78	0.48
1:C:230:ILE:HG21	1:C:611:PRO:HG2	1.95	0.48
2:D:53:TYR:HB2	2:D:166:GLN:O	2.13	0.47
1:A:421:ARG:HG2	1:A:429:TYR:CE1	2.49	0.47
2:B:40:LEU:HD23	2:B:40:LEU:O	2.13	0.47
1:C:474:TYR:HE2	1:C:476:GLN:HB2	1.79	0.47
1:C:556:PRO:HG3	1:C:579:THR:OG1	2.14	0.47
1:A:261:ASN:O	2:B:127:LYS:HE2	2.14	0.47
1:A:338:TYR:HE1	1:A:352:LYS:HB2	1.80	0.47
1:A:223:LEU:HD12	1:A:616:TYR:HB3	1.97	0.47
1:A:492:LYS:HB3	1:A:497:THR:OG1	2.15	0.47
1:C:327:LEU:HA	1:C:366:HIS:CD2	2.49	0.47
1:A:440:ASN:O	1:A:443:THR:HG22	2.14	0.47
1:C:532:ILE:HG22	1:C:544:SER:HB2	1.97	0.47
1:C:564:THR:HG22	1:C:565:THR:HG23	1.97	0.47
2:D:53:TYR:O	2:D:53:TYR:CG	2.67	0.47
2:B:139:ASN:ND2	2:B:144:GLY:HA3	2.27	0.47
1:C:336:GLU:HB2	5:C:702:NAG:C8	2.44	0.46
1:C:236:ARG:HG3	1:C:608:SER:OG	2.15	0.46
1:C:440:ASN:HB3	1:C:444:ASP:HB3	1.98	0.46
2:B:90:SER:OG	2:B:92:VAL:HG23	2.15	0.46
1:A:318:CYS:HB3	1:A:320:ILE:HD11	1.96	0.46
2:D:122:MET:HA	2:D:122:MET:HE3	1.97	0.46
1:C:229:VAL:HG13	1:C:290:LEU:HD22	1.98	0.46
2:D:120:ASN:OD1	2:D:122:MET:N	2.48	0.46
1:A:474:TYR:HE2	1:A:476:GLN:HB2	1.80	0.46
1:A:501:MET:HA	5:A:705:NAG:H82	1.98	0.46
1:A:505:VAL:HG21	1:A:566:ILE:HG13	1.98	0.46
1:A:320:ILE:HD13	1:A:338:TYR:CD2	2.46	0.45
1:C:310:CYS:HB3	1:C:315:PHE:CE1	2.50	0.45
1:A:444:ASP:OD2	1:A:445:PHE:N	2.49	0.45
2:D:127:LYS:O	2:D:164:VAL:HG21	2.16	0.45
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.76	0.45
2:D:51:VAL:HB	2:D:161:VAL:HG22	1.99	0.45
1:A:454:TYR:HA	1:A:457:LEU:CD2	2.46	0.45
1:C:484:TYR:CE1	1:C:517:TYR:HA	2.52	0.45
1:A:564:THR:HG22	1:A:565:THR:HG23	1.98	0.45
1:C:507:SER:OG	1:C:508:ARG:N	2.50	0.45
1:C:483:THR:OG1	1:C:508:ARG:NH2	2.50	0.45
1:C:506:ILE:C	1:C:506:ILE:HD13	2.37	0.45
1:A:254:TYR:HE1	1:A:256:HIS:HD1	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:MET:HE1	1:C:217:LYS:HE3	1.99	0.44
2:B:84:GLU:H	2:B:84:GLU:HG3	1.45	0.44
1:C:224:LYS:HB2	1:C:285:ARG:NH1	2.31	0.44
1:C:259:GLY:HA3	1:C:268:SER:HA	1.99	0.44
2:D:35:VAL:HG13	2:D:62:ILE:HG12	2.00	0.44
1:A:241:ASN:OD1	1:A:242:ASN:ND2	2.39	0.44
1:C:422:SER:HA	1:C:423:PRO:HD3	1.81	0.44
1:A:230:ILE:HD11	1:A:613:ILE:HG13	1.99	0.44
1:A:226:ILE:HG23	1:A:228:TYR:CE2	2.53	0.44
1:C:234:GLN:H	1:C:234:GLN:CD	2.21	0.44
1:A:557:GLU:OE1	1:A:569:LYS:HD2	2.18	0.44
2:D:71:ARG:HD2	2:D:72:PRO:HD2	2.00	0.44
1:A:510:ASN:OD1	1:A:511:GLN:N	2.51	0.44
2:D:32:LEU:HD11	2:D:58:ASP:OD2	2.17	0.44
1:A:485:LEU:HD11	1:A:532:ILE:HD13	2.00	0.43
1:A:595:CYS:HB2	1:A:616:TYR:CE2	2.52	0.43
1:C:501:MET:HA	5:C:705:NAG:H82	1.99	0.43
2:D:131:ASP:OD1	2:D:163:LYS:HA	2.18	0.43
1:C:218:ASP:N	1:C:218:ASP:OD1	2.51	0.43
1:C:327:LEU:HD12	1:C:366:HIS:CD2	2.53	0.43
1:C:365:ILE:HD11	1:C:428:ARG:CZ	2.48	0.43
1:C:396:HIS:NE2	1:C:417:SER:HA	2.33	0.43
1:C:593:PRO:HG2	1:C:618:ILE:HB	2.00	0.43
1:A:260:ILE:O	1:A:261:ASN:HB2	2.17	0.43
1:C:398:TYR:CD1	1:C:456:LYS:HG2	2.53	0.43
1:C:239:CYS:SG	1:C:609:ILE:HD11	2.59	0.43
1:A:243:PRO:O	1:A:244:LEU:HD12	2.19	0.43
2:D:153:CYS:O	2:D:157:THR:HA	2.19	0.43
1:A:518:HIS:CD2	1:A:518:HIS:C	2.92	0.43
1:C:239:CYS:O	1:C:258:GLU:HA	2.19	0.43
1:C:423:PRO:HG3	1:C:525:TYR:CZ	2.54	0.43
1:C:580:ARG:HG3	1:C:581:SER:H	1.83	0.43
1:A:339:ILE:HG13	1:A:353:ILE:HG12	2.01	0.43
1:A:410:LYS:HB2	1:A:410:LYS:HE3	1.87	0.43
2:B:122:MET:HA	2:B:122:MET:HE2	2.01	0.43
1:C:461:SER:HB2	1:C:462:PRO:HD2	2.00	0.43
1:A:355:ILE:O	1:A:358:MET:HB3	2.19	0.43
1:A:498:PRO:HG2	1:A:500:TRP:CZ2	2.53	0.42
1:A:543:VAL:CG1	1:A:560:VAL:HG22	2.49	0.42
1:C:243:PRO:C	1:C:244:LEU:HD12	2.39	0.42
1:C:552:LEU:HD12	1:C:554:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:CYS:HB2	1:C:616:TYR:CE2	2.54	0.42
1:C:214:SER:OG	1:C:215:VAL:N	2.51	0.42
1:C:453:THR:HG22	1:C:498:PRO:HD2	2.00	0.42
2:D:163:LYS:HB3	2:D:166:GLN:HB2	2.01	0.42
2:D:81:VAL:HB	2:D:85:GLN:HB2	2.01	0.42
1:A:484:TYR:CE1	1:A:517:TYR:HA	2.54	0.42
2:B:115:GLN:O	2:B:126:PHE:HB2	2.19	0.42
1:A:210:ILE:O	1:A:620:LYS:HG3	2.20	0.42
1:C:579:THR:HA	1:C:600:GLU:O	2.20	0.42
2:B:91:THR:HG23	2:B:137:THR:HG23	2.01	0.42
1:C:388:VAL:HG22	1:C:430:ASN:OD1	2.19	0.42
1:C:432:ASN:ND2	1:C:474:TYR:OH	2.53	0.42
1:C:506:ILE:HD13	1:C:507:SER:N	2.34	0.42
1:A:320:ILE:HD12	1:A:320:ILE:N	2.35	0.41
1:A:328:ASP:O	1:A:428:ARG:NH1	2.52	0.41
1:C:511:GLN:HB3	2:D:110:PHE:CE1	2.55	0.41
1:C:533:ALA:HA	1:C:534:PRO:HD3	1.74	0.41
2:D:141:SER:CB	5:D:201:NAG:H82	2.49	0.41
1:A:588:LEU:HD12	1:A:592:GLU:C	2.40	0.41
1:A:594:TRP:CZ2	1:A:617:LYS:HB2	2.55	0.41
2:B:110:PHE:HE2	2:B:112:ILE:HD11	1.85	0.41
1:C:483:THR:HG21	1:C:518:HIS:N	2.34	0.41
2:D:80:LEU:HB3	2:D:96:ASN:HB3	2.02	0.41
1:A:296:HIS:HB3	1:A:299:SER:HB3	2.02	0.41
1:C:340:THR:HA	1:C:350:THR:HA	2.03	0.41
1:C:381:PHE:HB3	1:C:383:ILE:HD11	2.03	0.41
2:B:44:PHE:CD1	2:B:50:LEU:HB2	2.55	0.41
1:C:291:LEU:HD12	1:C:291:LEU:N	2.36	0.41
1:C:303:ILE:HG21	1:C:319:HIS:CE1	2.55	0.41
1:C:323:ASN:OD1	1:C:326:THR:N	2.52	0.41
2:D:60:LEU:HB3	2:D:112:ILE:HG23	2.03	0.41
1:A:443:THR:HG23	1:A:444:ASP:H	1.86	0.41
2:B:121:TYR:CD2	2:B:122:MET:HE2	2.55	0.41
1:C:335:ASP:HA	5:C:702:NAG:H81	2.02	0.41
2:D:104:PRO:C	2:D:106:GLN:H	2.24	0.41
2:D:139:ASN:OD1	2:D:147:ASN:ND2	2.53	0.41
1:A:259:GLY:HA3	1:A:268:SER:HA	2.02	0.41
1:A:461:SER:HB2	1:A:477:SER:OG	2.20	0.41
1:A:516:ARG:NE	1:A:549:SER:O	2.53	0.41
2:B:115:GLN:HG2	2:B:115:GLN:H	1.64	0.41
1:C:270:LYS:HA	1:C:299:SER:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:LEU:HA	1:C:457:LEU:HD12	1.83	0.41
1:A:319:HIS:CD2	1:A:337:TYR:HE1	2.39	0.41
1:A:435:MET:HE3	1:A:437:ILE:CG1	2.51	0.41
1:A:478:SER:O	1:A:508:ARG:NH1	2.49	0.41
2:B:98:LEU:N	2:B:98:LEU:HD23	2.36	0.41
1:A:240:MET:O	1:A:611:PRO:HD3	2.21	0.41
1:A:281:ARG:HB2	1:A:283:ASP:HB2	2.03	0.41
1:C:411:SER:OG	1:C:414:GLU:HB2	2.20	0.41
1:A:479:MET:HA	1:A:526:GLY:O	2.21	0.41
1:C:270:LYS:HB3	1:C:295:TYR:CD2	2.56	0.41
1:C:503:ASN:OD1	1:C:506:ILE:HG22	2.21	0.41
2:B:94:ASP:HA	2:B:95:PRO:HD3	1.51	0.41
1:C:310:CYS:HB3	1:C:315:PHE:HE1	1.84	0.41
1:A:396:HIS:N	1:A:396:HIS:ND1	2.69	0.40
1:A:513:ASN:C	1:A:515:PRO:HD3	2.42	0.40
1:A:243:PRO:HG3	1:A:611:PRO:HB3	2.04	0.40
1:A:278:ILE:HD13	1:A:288:LEU:HD23	2.01	0.40
1:A:461:SER:HB2	1:A:462:PRO:HD2	2.03	0.40
1:A:407:GLN:HG3	2:B:102:ASN:HB2	2.03	0.40
1:C:543:VAL:CG1	1:C:560:VAL:HG22	2.47	0.40
2:D:30:LYS:HG2	2:D:55:LYS:NZ	2.36	0.40
2:D:152:VAL:HA	2:D:155:THR:HG23	2.04	0.40
2:B:73:TYR:CZ	2:B:104:PRO:HA	2.56	0.40
2:D:39:SER:HA	2:D:156:ARG:HH11	1.87	0.40
2:D:133:TYR:CE1	2:D:161:VAL:HB	2.56	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	413/429 (96%)	397 (96%)	16 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	413/429 (96%)	398 (96%)	15 (4%)	0	100	100
2	B	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
2	D	136/142 (96%)	129 (95%)	7 (5%)	0	100	100
All	All	1099/1142 (96%)	1056 (96%)	43 (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	389/398 (98%)	345 (89%)	44 (11%)	6	27
1	C	389/398 (98%)	342 (88%)	47 (12%)	5	24
2	B	122/125 (98%)	111 (91%)	11 (9%)	9	37
2	D	122/125 (98%)	102 (84%)	20 (16%)	2	13
All	All	1022/1046 (98%)	900 (88%)	122 (12%)	5	25

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LYS
1	A	213	LYS
1	A	234	GLN
1	A	237	SER
1	A	248	SER
1	A	258	GLU
1	A	262	SER
1	A	271	VAL
1	A	285	ARG
1	A	287	SER
1	A	308	VAL
1	A	324	THR
1	A	327	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	329	ASN
1	A	345	ILE
1	A	346	ASP
1	A	349	LYS
1	A	350	THR
1	A	355	ILE
1	A	358	MET
1	A	366	HIS
1	A	395	THR
1	A	396	HIS
1	A	404	CYS
1	A	405	SER
1	A	415	ILE
1	A	431	LEU
1	A	432	ASN
1	A	439	GLN
1	A	441	ASN
1	A	442	MET
1	A	464	ARG
1	A	497	THR
1	A	508	ARG
1	A	513	ASN
1	A	516	ARG
1	A	518	HIS
1	A	519	LYS
1	A	523	ILE
1	A	531	ASP
1	A	539	LYS
1	A	543	VAL
1	A	582	THR
1	A	609	ILE
2	B	82	ARG
2	B	84	GLU
2	B	97	VAL
2	B	99	VAL
2	B	100	THR
2	B	101	CYS
2	B	106	GLN
2	B	108	ILE
2	B	128	LYS
2	B	155	THR
2	B	156	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	217	LYS
1	C	233	GLN
1	C	234	GLN
1	C	238	ILE
1	C	261	ASN
1	C	272	LEU
1	C	285	ARG
1	C	287	SER
1	C	308	VAL
1	C	324	THR
1	C	333	SER
1	C	343	ASN
1	C	346	ASP
1	C	347	ARG
1	C	349	LYS
1	C	350	THR
1	C	355	ILE
1	C	357	ASN
1	C	366	HIS
1	C	390	ASN
1	C	395	THR
1	C	405	SER
1	C	406	VAL
1	C	408	THR
1	C	431	LEU
1	C	432	ASN
1	C	439	GLN
1	C	457	LEU
1	C	464	ARG
1	C	483	THR
1	C	497	THR
1	C	506	ILE
1	C	508	ARG
1	C	513	ASN
1	C	531	ASP
1	C	543	VAL
1	C	550	ASP
1	C	552	LEU
1	C	578	ASN
1	C	579	THR
1	C	580	ARG
1	C	582	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	588	LEU
1	C	590	LEU
1	C	601	THR
1	C	605	ASN
1	C	607	LYS
2	D	32	LEU
2	D	35	VAL
2	D	40	LEU
2	D	50	LEU
2	D	53	TYR
2	D	73	TYR
2	D	84	GLU
2	D	92	VAL
2	D	97	VAL
2	D	99	VAL
2	D	103	LYS
2	D	111	THR
2	D	122	MET
2	D	141	SER
2	D	142	LEU
2	D	146	GLU
2	D	154	ARG
2	D	155	THR
2	D	156	ARG
2	D	157	THR

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

Mol	Chain	Res	Type
1	A	294	HIS
1	A	319	HIS
1	A	396	HIS
1	A	439	GLN
1	C	294	HIS
1	C	319	HIS
1	C	357	ASN
1	C	407	GLN
1	C	471	GLN
1	C	551	GLN
1	C	578	ASN
2	D	31	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

9 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.88	1 (7%)	17,19,21	0.82	0
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	0.45	0
4	NAG	F	1	1,4	14,14,15	1.03	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	0.41	0
4	BMA	F	3	4	11,11,12	1.22	1 (9%)	15,15,17	0.95	0
3	NAG	G	1	3,2	14,14,15	1.20	1 (7%)	17,19,21	0.79	0
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.35	0
3	NAG	H	1	1,3	14,14,15	0.39	0	17,19,21	0.89	0
3	NAG	H	2	3	14,14,15	0.56	0	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3,2	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	3.95	1.50	1.43
4	F	1	NAG	O5-C1	-3.69	1.37	1.43
3	E	1	NAG	O5-C1	-2.57	1.39	1.43
4	F	3	BMA	C4-C3	2.36	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C1-O5-C5	2.03	114.95	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1	NAG	C1

All (13) torsion outliers are listed below:

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

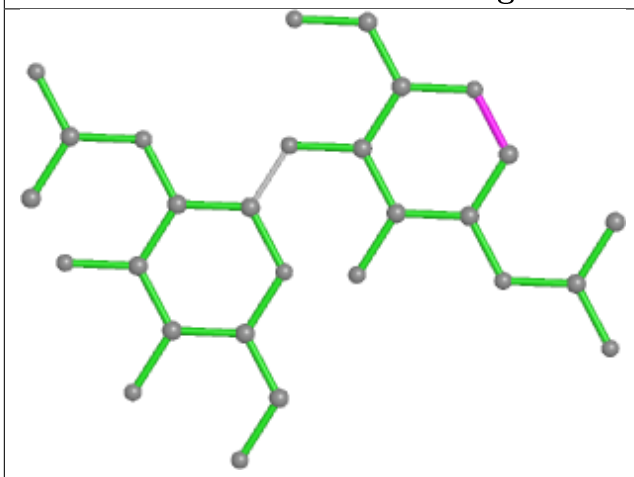
There are no ring outliers.

2 monomers are involved in 2 short contacts:

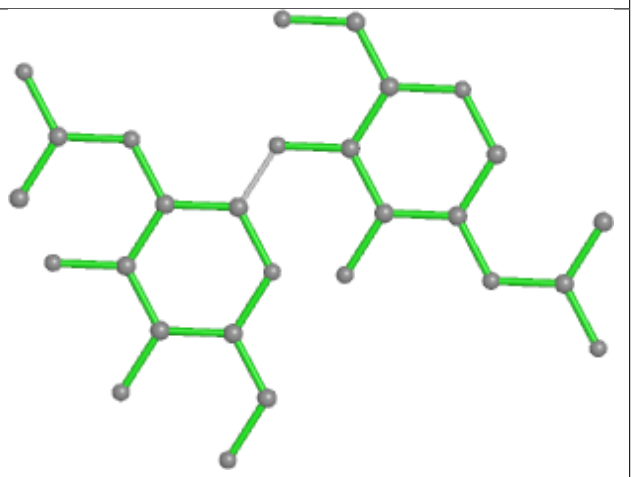
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
4	F	1	NAG	1	0

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

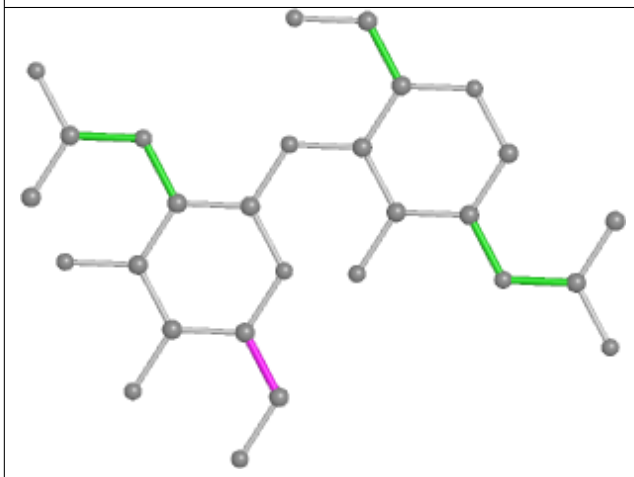
Oligosaccharide Chain E



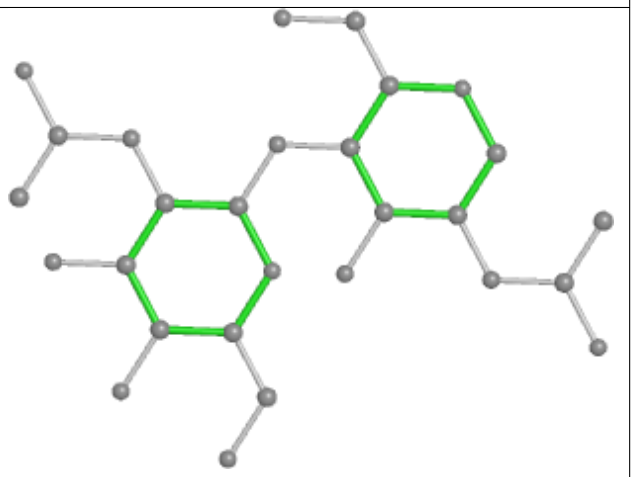
Bond lengths



Bond angles

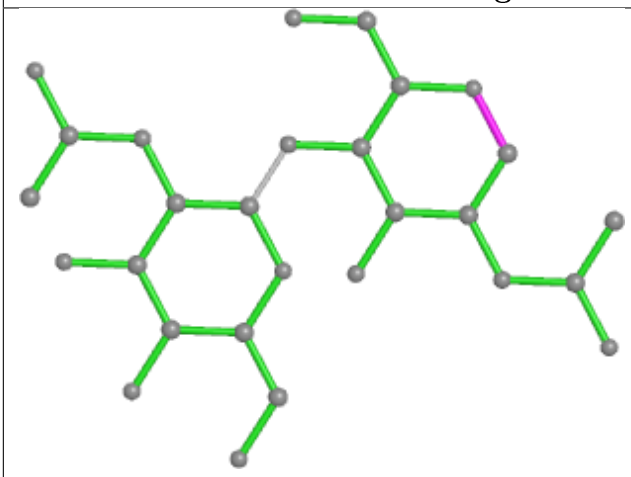


Torsions

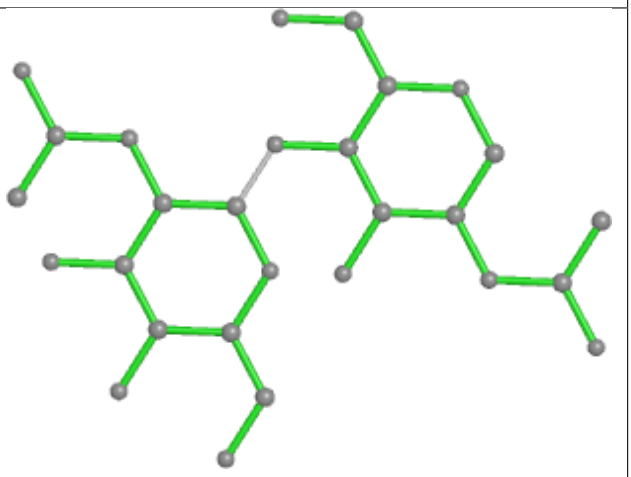


Rings

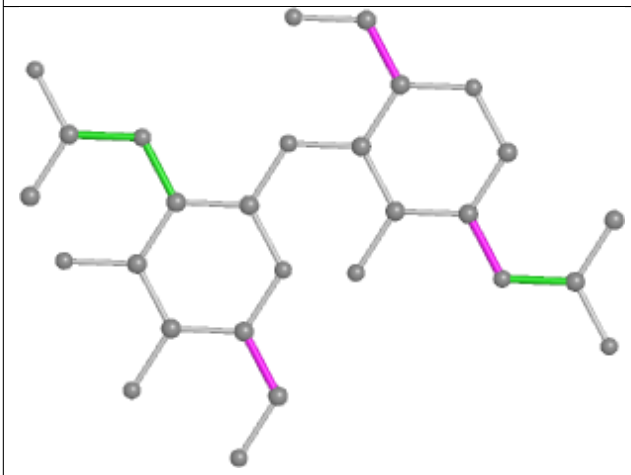
Oligosaccharide Chain G



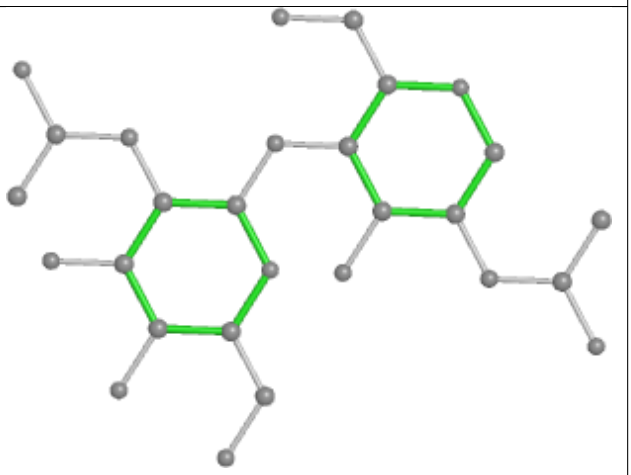
Bond lengths



Bond angles

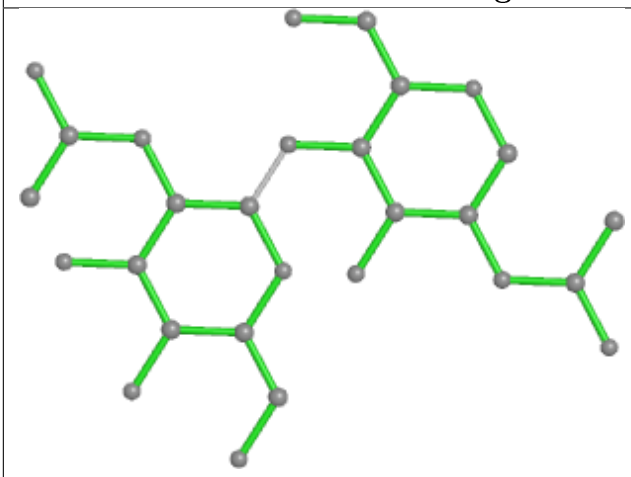


Torsions

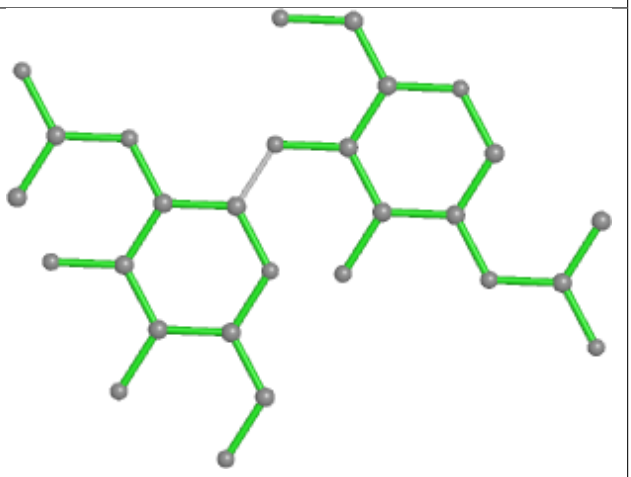


Rings

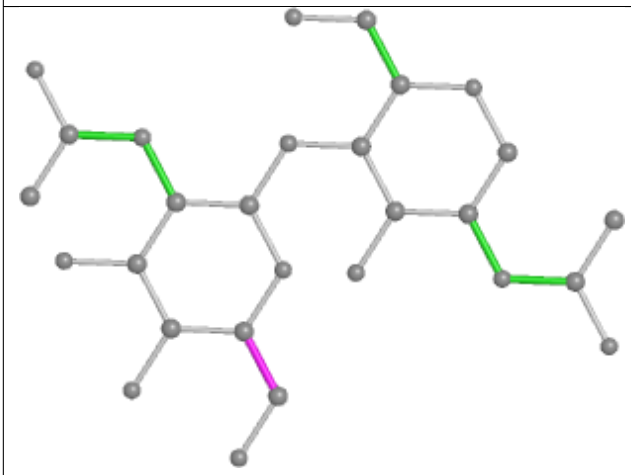
Oligosaccharide Chain H



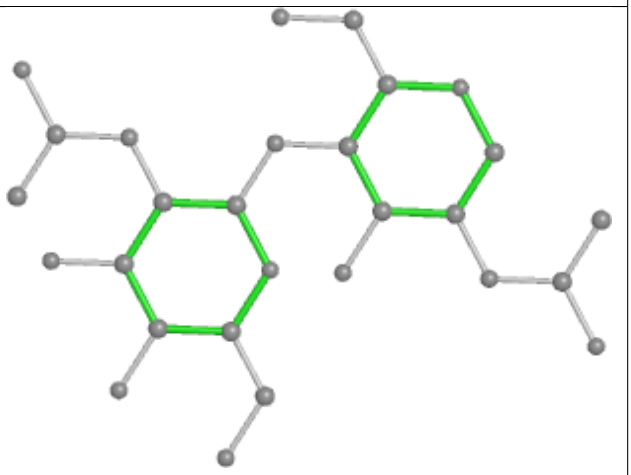
Bond lengths



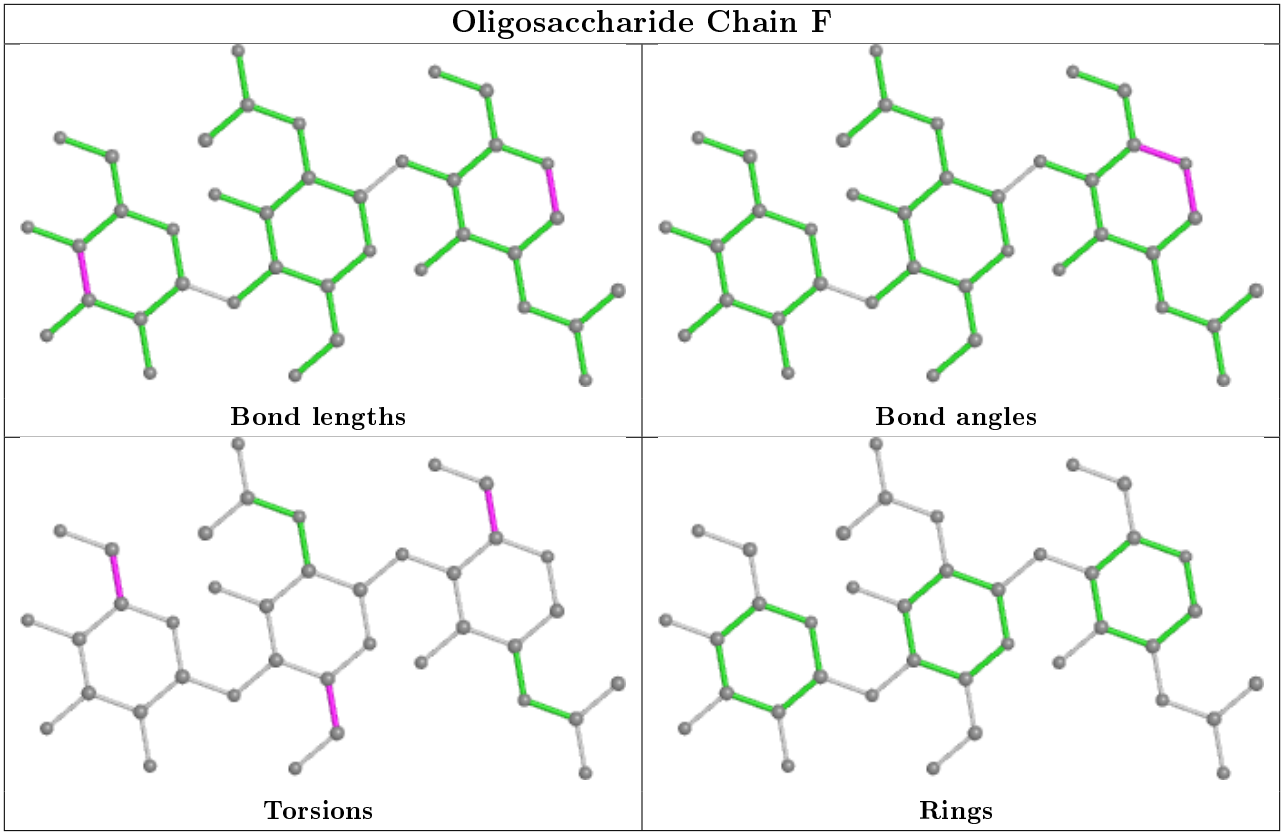
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
5	NAG	D	201	2	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	NAG	A	702	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	C	706	1	14,14,15	0.63	1 (7%)	17,19,21	0.72	0
5	NAG	C	702	1	14,14,15	0.62	0	17,19,21	0.58	0
5	NAG	A	705	1	14,14,15	1.08	1 (7%)	17,19,21	0.74	0
5	NAG	C	705	1	14,14,15	0.67	1 (7%)	17,19,21	0.53	0
5	NAG	A	701	1	14,14,15	0.52	0	17,19,21	0.48	0
5	NAG	C	701	1	14,14,15	0.24	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
5	NAG	D	201	2	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	C	706	1	-	0/6/23/26	0/1/1/1
5	NAG	C	702	1	-	1/6/23/26	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	C	705	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	705	NAG	O5-C1	-3.47	1.38	1.43
5	C	706	NAG	O5-C1	-2.23	1.40	1.43
5	C	705	NAG	O5-C1	-2.02	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	201	NAG	C1-O5-C5	3.19	116.52	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	702	NAG	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	NAG	O5-C5-C6-O6
5	A	705	NAG	C4-C5-C6-O6
5	D	201	NAG	O5-C5-C6-O6
5	C	701	NAG	O5-C5-C6-O6
5	D	201	NAG	C4-C5-C6-O6
5	A	702	NAG	C8-C7-N2-C2
5	A	702	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	701	NAG	C4-C5-C6-O6
5	C	705	NAG	O5-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	C	705	NAG	C4-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6
5	C	702	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	NAG	1	0
5	C	702	NAG	4	0
5	A	705	NAG	1	0
5	C	705	NAG	1	0

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	415/429 (96%)	0.01	5 (1%) 79 73	9, 30, 71, 100	0
1	C	415/429 (96%)	0.10	10 (2%) 59 53	12, 41, 80, 125	0
2	B	139/142 (97%)	0.63	18 (12%) 3 4	18, 61, 90, 110	0
2	D	138/142 (97%)	0.66	22 (15%) 1 2	48, 101, 133, 158	0
All	All	1107/1142 (96%)	0.20	55 (4%) 28 25	9, 42, 108, 158	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	73	TYR	5.0
2	B	135	THR	4.4
2	D	135	THR	4.3
2	D	36	SER	4.2
1	C	208	PRO	4.0
2	B	37	TRP	4.0
2	D	51	VAL	3.9
2	B	78	LEU	3.7
2	B	79	TYR	3.6
2	B	62	ILE	3.5
2	D	160	ILE	3.5
2	B	102	ASN	3.4
1	C	340	THR	3.4
2	D	37	TRP	3.2
2	B	110	PHE	3.2
2	B	134	ILE	3.2
2	D	35	VAL	3.1
2	D	93	LEU	2.9
1	C	342	PHE	2.8
2	D	61	ASP	2.7
2	B	106	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	136	SER	2.7
1	C	350	THR	2.7
2	D	161	VAL	2.6
1	C	339	ILE	2.6
2	D	62	ILE	2.6
2	B	35	VAL	2.6
2	B	160	ILE	2.6
2	D	134	ILE	2.6
1	A	355	ILE	2.5
2	D	162	MET	2.5
2	B	158	MET	2.4
1	C	273	LEU	2.4
2	B	108	ILE	2.4
2	D	120	ASN	2.3
2	D	102	ASN	2.3
2	D	75	TYR	2.3
2	D	126	PHE	2.3
2	B	145	LEU	2.3
2	B	114	PHE	2.3
2	B	76	TYR	2.3
2	B	109	ARG	2.2
1	C	442	MET	2.2
1	A	407	GLN	2.2
1	C	258	GLU	2.2
2	D	76	TYR	2.2
2	D	78	LEU	2.2
2	D	159	LYS	2.1
1	A	317	PHE	2.1
1	A	353	ILE	2.1
2	D	108	ILE	2.1
1	C	341	TYR	2.0
2	B	75	TYR	2.0
1	C	367	PHE	2.0
1	A	389	ILE	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)

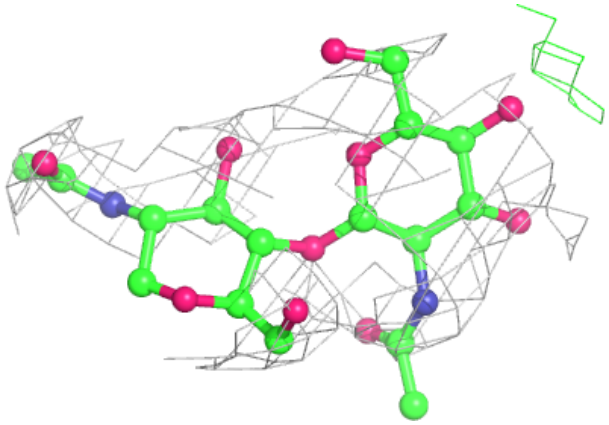
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

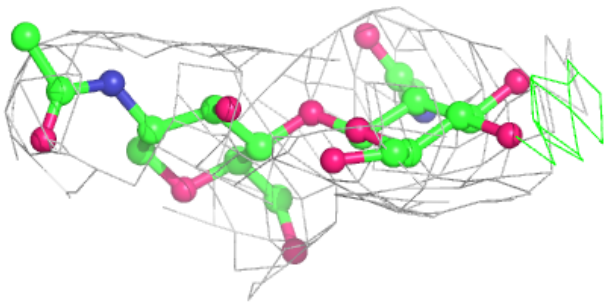
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	F	3	11/12	0.74	0.26	75,88,99,104	0
3	NAG	G	2	14/15	0.77	0.34	82,99,107,113	0
3	NAG	E	2	14/15	0.79	0.33	63,70,87,94	0
3	NAG	G	1	14/15	0.82	0.17	58,71,85,88	0
4	NAG	F	2	14/15	0.88	0.26	63,80,88,95	0
3	NAG	H	2	14/15	0.91	0.14	73,83,94,99	0
4	NAG	F	1	14/15	0.93	0.24	48,57,66,70	0
3	NAG	H	1	14/15	0.95	0.09	39,55,64,79	0
3	NAG	E	1	14/15	0.96	0.18	32,38,41,60	0

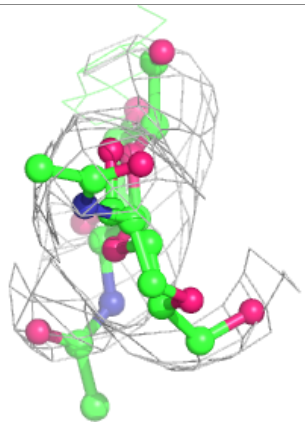
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

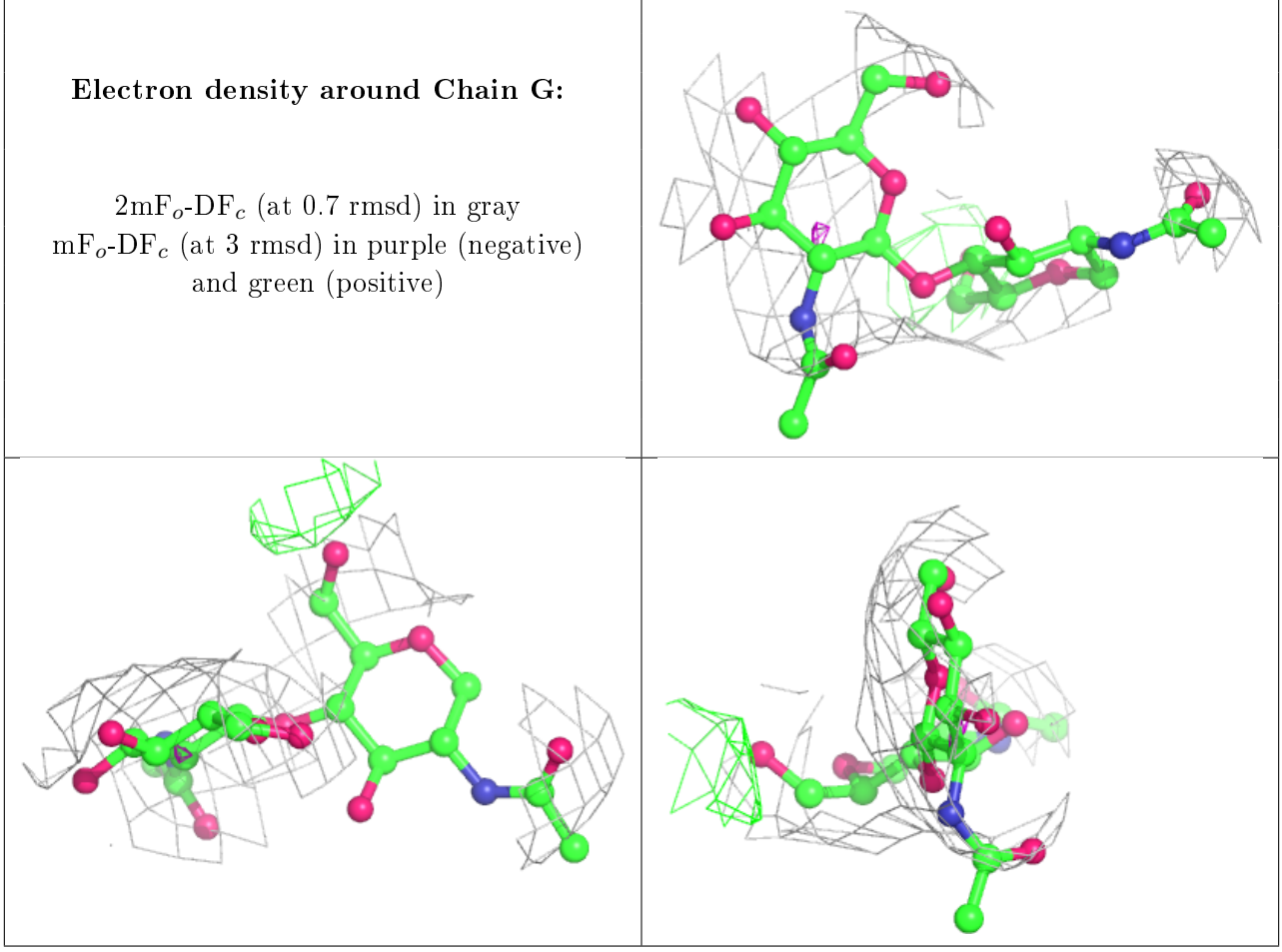






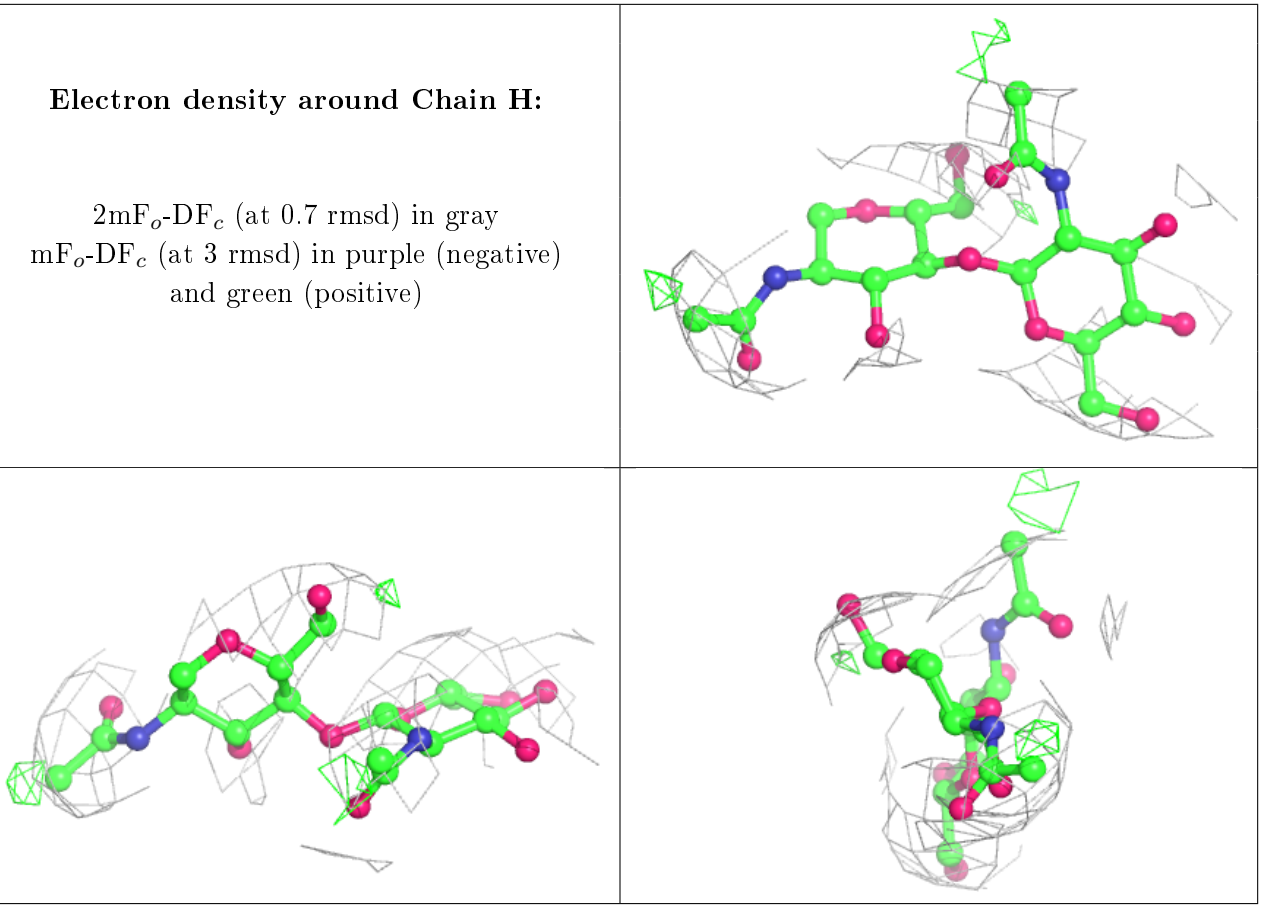
Electron density around Chain G:

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



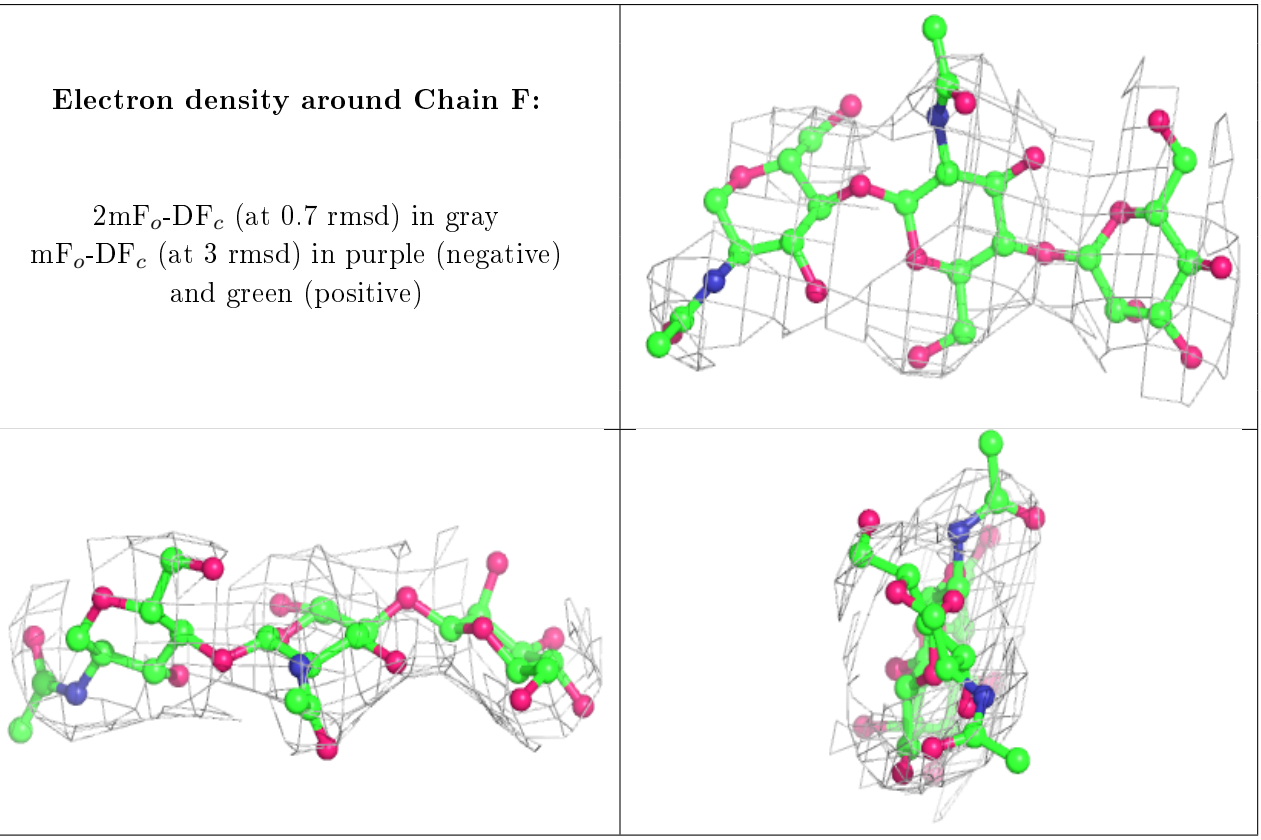
Electron density around Chain H:

$2mF_o$-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 F:

$2mF_o$-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	D	201	14/15	0.76	0.15	59,98,107,109	0
5	NAG	C	702	14/15	0.76	0.18	61,78,80,82	0
5	NAG	C	706	14/15	0.81	0.23	49,57,69,72	0
5	NAG	A	702	14/15	0.88	0.26	47,63,74,75	0
5	NAG	A	701	14/15	0.88	0.20	79,90,96,98	0
5	NAG	C	701	14/15	0.88	0.21	81,94,104,105	0
5	NAG	C	705	14/15	0.94	0.26	30,35,42,47	0
5	NAG	A	705	14/15	0.95	0.31	34,38,48,55	0

6.5 Other polymers

There are no such residues in this entry.