Full wwPDB X-ray Structure Validation Report (i)

Jun 5, 2024 – 02:09 PM JST

PDB ID	:	8WSN
Title	:	Crystal structure of SFTSV Gn and antibody SF1
Authors	:	Chang, Z.; Gao, F.; Wu, Y.
Deposited on	:	2023-10-17
Resolution	:	2.80 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:

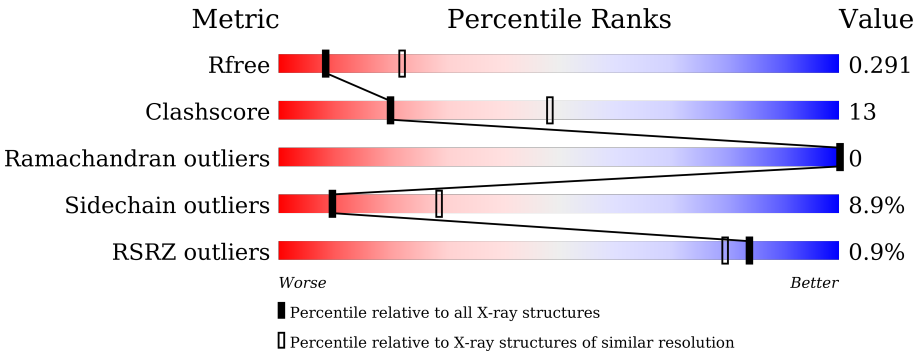
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	327	60% 32% • • 5%
1	D	327	61% 31% • 5%
2	B	227	70% 19% 5% 5%
2	E	227	70% 22% • 6%
3	C	215	69% 27% ••
3	F	215	64% 33% ••

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Mol	Chain	Length	Quality of chain
4	G	2	50% 50%
4	H	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11643 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 Gn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2403	1508	415	454	26			
1	D	312	Total	C	N	O	S	0	0	0
			2399	1504	414	455	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	HIS	-	expression tag	UNP F1BWV6
A	342	HIS	-	expression tag	UNP F1BWV6
A	343	HIS	-	expression tag	UNP F1BWV6
A	344	HIS	-	expression tag	UNP F1BWV6
A	345	HIS	-	expression tag	UNP F1BWV6
A	346	HIS	-	expression tag	UNP F1BWV6
D	341	HIS	-	expression tag	UNP F1BWV6
D	342	HIS	-	expression tag	UNP F1BWV6
D	343	HIS	-	expression tag	UNP F1BWV6
D	344	HIS	-	expression tag	UNP F1BWV6
D	345	HIS	-	expression tag	UNP F1BWV6
D	346	HIS	-	expression tag	UNP F1BWV6

- Molecule 2 is a protein called Ab1-H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1658	1062	275	315	6			
2	E	214	Total	C	N	O	S	0	0	0
			1658	1062	275	315	6			

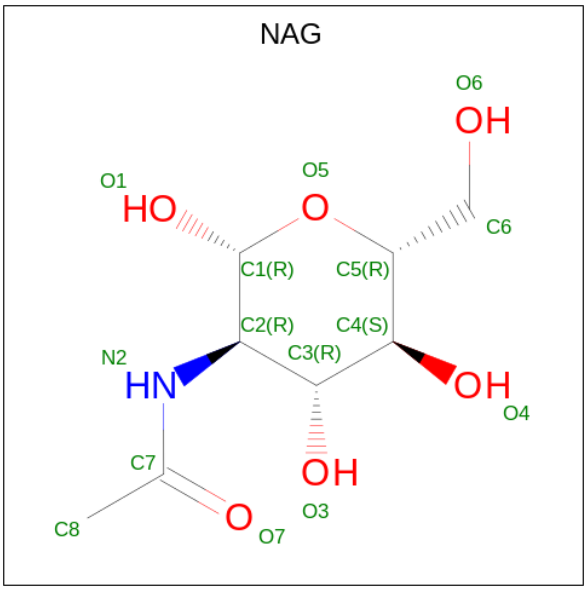
- Molecule 3 is a protein called Ab1-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1638	1029	282	323	4			
3	F	211	Total	C	N	O	S	0	0	0
			1628	1023	281	320	4			

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is water.

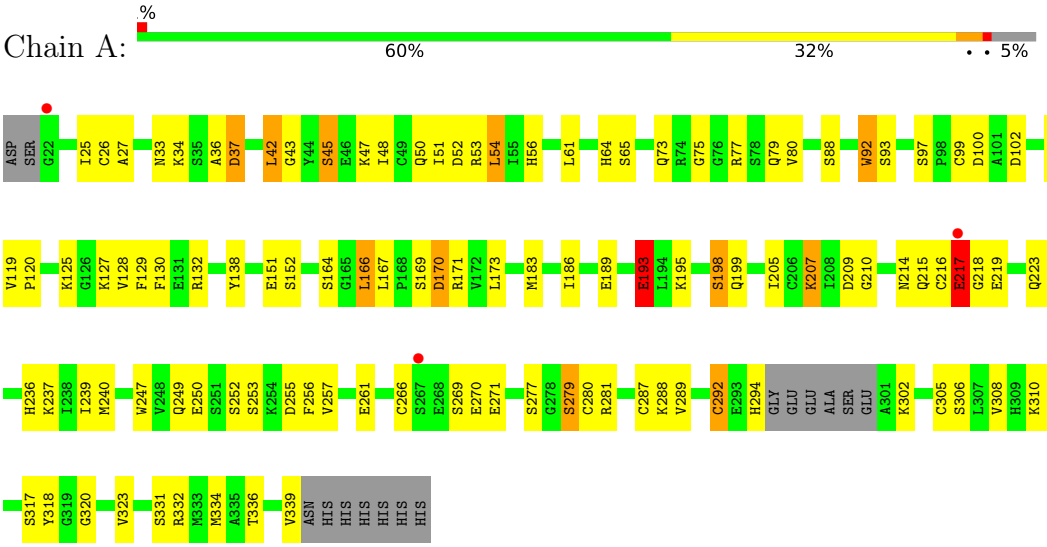
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	31	Total O 31 31	0	0
6	B	18	Total O 18 18	0	0
6	C	30	Total O 30 30	0	0
6	D	19	Total O 19 19	0	0
6	E	16	Total O 16 16	0	0
6	F	33	Total O 33 33	0	0

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.

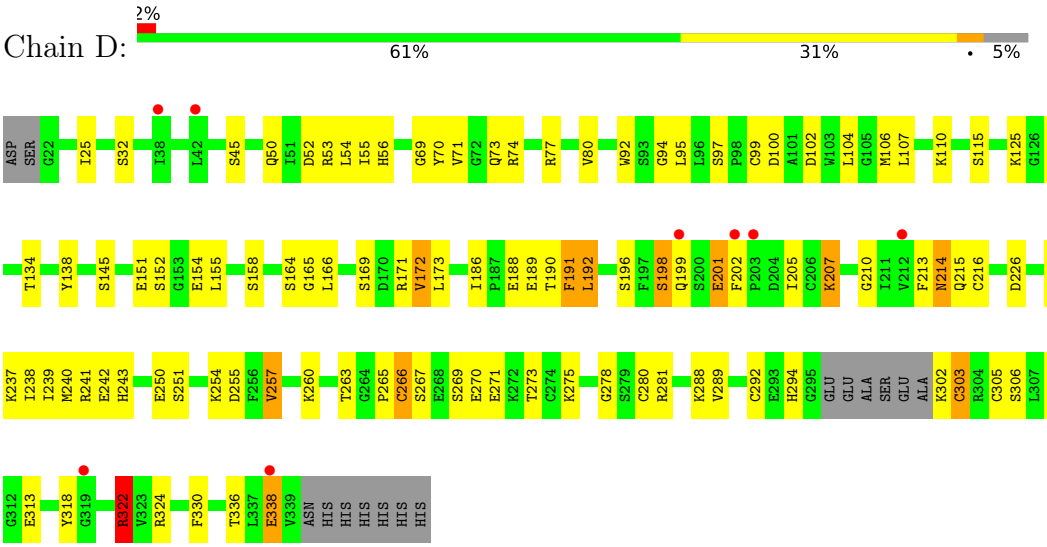
• Molecule 1: Gn

Chain A:



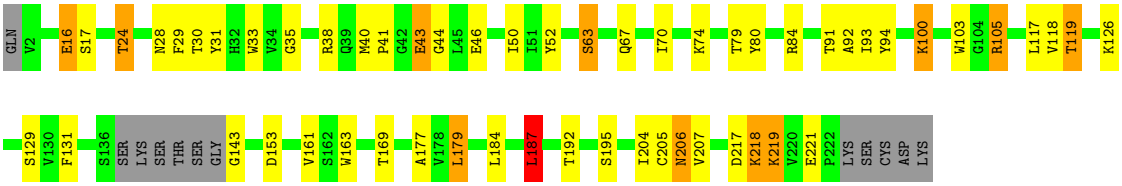
• Molecule 1: Gn

Chain D:



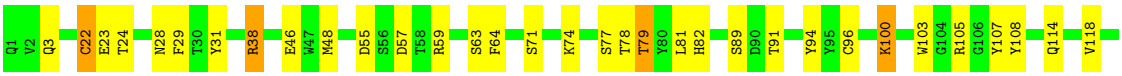
• Molecule 2: Ab1-H

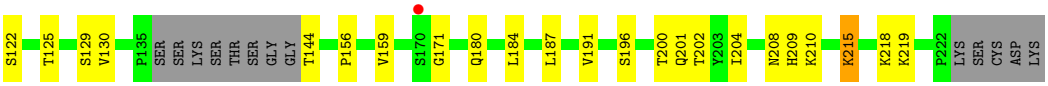
Chain B:



• Molecule 2: Ab1-H

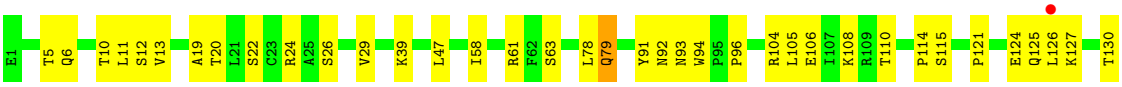
Chain E:





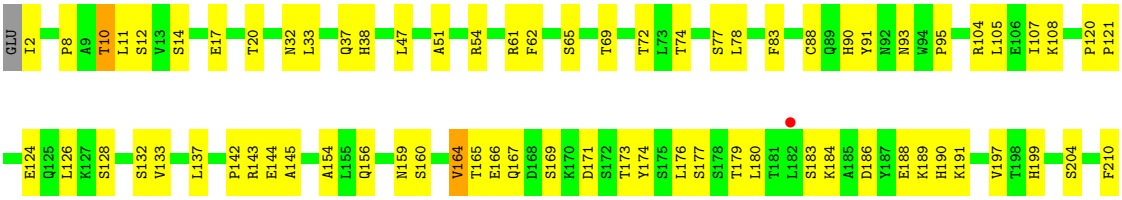
• Molecule 3: Ab1-L

Chain C:



• Molecule 3: Ab1-L

Chain F:



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

Chain G:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.06Å 97.25Å 133.09Å 90.00° 124.62° 90.00°	Depositor
Resolution (Å)	46.71 – 2.80 46.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.71-2.80) 99.4 (46.71-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.240 , 0.291 0.240 , 0.291	Depositor DCC
R_{free} test set	2942 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11643	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7800e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.57	2/2464 (0.1%)	0.80	7/3322 (0.2%)
1	D	0.53	1/2460 (0.0%)	0.70	2/3317 (0.1%)
2	B	0.56	0/1707	0.69	1/2331 (0.0%)
2	E	0.58	1/1707 (0.1%)	0.70	2/2331 (0.1%)
3	C	0.55	1/1677 (0.1%)	0.73	2/2281 (0.1%)
3	F	0.51	0/1667	0.68	0/2268
All	All	0.55	5/11682 (0.0%)	0.72	14/15850 (0.1%)

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	A	0	2
1	D	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	GLU	CB-CG	7.65	1.66	1.52
1	A	217	GLU	CB-CG	5.75	1.63	1.52
3	C	135	CYS	CB-SG	-5.66	1.72	1.81
1	D	322	ARG	CG-CD	5.24	1.65	1.51
2	E	22	CYS	CB-SG	-5.11	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	GLU	OE1-CD-OE2	-12.78	107.97	123.30
1	A	217	GLU	CG-CD-OE1	10.25	138.80	118.30
1	A	217	GLU	CG-CD-OE2	-9.91	98.49	118.30
1	A	193	GLU	N-CA-CB	-8.77	94.81	110.60
1	D	322	ARG	CB-CG-CD	-7.08	93.19	111.60
2	E	215	LYS	CD-CE-NZ	7.07	127.96	111.70
1	A	193	GLU	CB-CA-C	6.51	123.41	110.40
1	D	322	ARG	N-CA-CB	5.63	120.73	110.60
2	B	187	LEU	CA-CB-CG	5.60	128.18	115.30
3	C	39	LYS	CB-CG-CD	5.56	126.06	111.60
3	C	39	LYS	CG-CD-CE	5.42	128.16	111.90
2	E	187	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	193	GLU	CA-CB-CG	5.11	124.63	113.40
1	A	217	GLU	N-CA-C	5.08	124.71	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	CYS	Peptide
1	A	217	GLU	Sidechain
1	D	322	ARG	Sidechain

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	2403	0	2306	77	0
1	D	2399	0	2296	78	0
2	B	1658	0	1607	35	1
2	E	1658	0	1613	28	1
3	C	1638	0	1585	40	1
3	F	1628	0	1577	40	1
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	28	0	26	1	0
5	D	28	0	26	0	0
6	A	31	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	0	1	0
6	C	30	0	0	6	0
6	D	19	0	0	3	0
6	E	16	0	0	0	0
6	F	33	0	0	10	0
All	All	11643	0	11086	285	2

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 13.

All (285) 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)
2:E:130:VAL:O	2:E:218:LYS:NZ	1.91	1.02
1:D:196:SER:HA	1:D:199:GLN:HE21	1.21	0.99
3:F:20:THR:HG22	3:F:74:THR:HG22	1.48	0.96
1:A:127:LYS:HD2	1:A:173:LEU:HB2	1.49	0.93
1:A:27:ALA:O	1:A:53:ARG:NH1	2.06	0.89
1:A:77:ARG:NH1	1:A:100:ASP:OD2	2.07	0.87
1:D:201:GLU:O	1:D:241:ARG:NH2	2.10	0.85
3:C:188:GLU:OE2	6:C:301:HOH:O	1.95	0.84
2:E:208:ASN:HD22	2:E:215:LYS:HE2	1.43	0.81
2:E:208:ASN:ND2	2:E:215:LYS:HE2	1.97	0.79
1:A:120:PRO:HD2	1:A:334:MET:HE3	1.65	0.79
3:F:188:GLU:HG2	3:F:212:ARG:HH21	1.46	0.78
1:A:249:GLN:OE1	6:A:501:HOH:O	2.03	0.75
1:A:120:PRO:HD2	1:A:334:MET:CE	2.15	0.75
1:A:229:TRP:HE1	1:A:331:SER:HB3	1.52	0.75
1:D:201:GLU:OE2	1:D:318:TYR:OH	2.04	0.74
3:C:166:GLU:OE2	6:C:302:HOH:O	2.06	0.73
1:A:189:GLU:O	1:A:193:GLU:HB2	1.88	0.73
3:F:54:ARG:NH1	3:F:62:PHE:O	2.20	0.73
1:A:77:ARG:NH2	1:A:93:SER:O	2.23	0.72
1:D:53:ARG:HB2	1:D:55:ILE:HD12	1.72	0.72
3:F:17:GLU:O	6:F:302:HOH:O	2.07	0.71
1:D:271:GLU:O	6:D:501:HOH:O	2.09	0.71
1:A:125:LYS:HB2	1:A:151:GLU:HA	1.74	0.70
1:A:218:GLY:O	1:A:339:VAL:N	2.25	0.69
3:F:2:ILE:N	6:F:306:HOH:O	2.25	0.69
3:F:124:GLU:O	6:F:303:HOH:O	2.10	0.68
1:D:154:GLU:HG2	1:D:155:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:VAL:HG11	1:D:172:VAL:HG22	1.76	0.68
3:F:78:LEU:N	6:F:302:HOH:O	2.10	0.67
1:A:34:LYS:H	1:A:34:LYS:HD2	1.59	0.67
1:A:34:LYS:HE3	1:A:166:LEU:HD21	1.76	0.67
1:D:216:CYS:HB3	1:D:338:GLU:HG2	1.78	0.66
1:A:128:VAL:HG23	1:A:171:ARG:HB3	1.77	0.66
2:B:43:GLU:OE1	2:B:44:GLY:N	2.25	0.66
1:A:61:LEU:HD21	1:A:129:PHE:HB2	1.78	0.65
3:F:51:ALA:O	6:F:304:HOH:O	2.15	0.65
1:A:37:ASP:OD1	1:A:37:ASP:N	2.30	0.64
3:C:184:LYS:HE2	3:C:188:GLU:OE1	1.98	0.64
1:D:80:VAL:HG13	1:D:172:VAL:HB	1.79	0.63
1:D:207:LYS:HE3	1:D:336:THR:HG23	1.80	0.63
3:F:90:HIS:HE1	3:F:93:ASN:OD1	1.81	0.63
1:A:92:TRP:CD1	1:A:310:LYS:HA	2.33	0.63
1:D:202:PHE:HB2	1:D:213:PHE:HE2	1.63	0.63
2:B:63:SER:O	2:B:67:GLN:NE2	2.32	0.63
3:C:121:PRO:HD3	3:C:133:VAL:HG22	1.80	0.62
1:D:70:TYR:HB2	1:D:166:LEU:HD23	1.80	0.62
3:C:162:GLU:HG2	3:C:176:LEU:HD21	1.81	0.62
1:D:191:PHE:CE2	1:D:234:HIS:HB3	2.34	0.62
2:B:41:PRO:HD3	2:B:92:ALA:HA	1.82	0.62
1:D:127:LYS:HE2	1:D:173:LEU:HB2	1.82	0.62
1:D:196:SER:HA	1:D:199:GLN:NE2	2.03	0.61
1:A:43:GLY:O	1:A:47:LYS:HG2	2.01	0.61
1:A:64:HIS:HB3	1:A:111:LYS:HD2	1.82	0.61
2:B:143:GLY:O	2:B:195:SER:OG	2.08	0.61
1:D:198:SER:OG	1:D:239:ILE:O	2.17	0.61
2:B:163:TRP:CH2	2:B:205:CYS:HB3	2.36	0.60
1:D:214:ASN:OD1	1:D:214:ASN:N	2.33	0.60
3:C:104:ARG:NH2	6:C:302:HOH:O	2.35	0.60
1:D:186:ILE:HD12	1:D:190:THR:HG22	1.84	0.59
5:A:400:NAG:O7	5:A:400:NAG:O3	2.16	0.59
3:F:10:THR:HG23	3:F:104:ARG:HB3	1.83	0.59
1:A:56:HIS:NE2	1:A:100:ASP:OD1	2.34	0.59
1:A:120:PRO:O	1:A:332:ARG:NH1	2.33	0.59
3:F:93:ASN:OD1	3:F:95:PRO:HD3	2.01	0.59
1:D:254:LYS:HE2	1:D:310:LYS:HZ1	1.68	0.59
1:D:255:ASP:OD1	1:D:310:LYS:NZ	2.36	0.58
1:D:104:LEU:HB2	1:D:106:MET:HE2	1.86	0.57
1:D:189:GLU:CD	1:D:189:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HA	1:A:334:MET:HE3	1.86	0.57
1:D:188:GLU:HG3	1:D:192:LEU:HD11	1.87	0.57
1:D:25:ILE:HD11	1:D:257:VAL:HB	1.86	0.56
1:D:202:PHE:HB2	1:D:213:PHE:CE2	2.40	0.56
3:C:143:ARG:NH2	6:C:304:HOH:O	2.31	0.56
2:E:204:ILE:HD13	2:E:219:LYS:HA	1.86	0.56
3:F:171:ASP:OD1	3:F:173:THR:OG1	2.18	0.56
3:F:121:PRO:HD3	3:F:133:VAL:HG22	1.87	0.56
3:C:12:SER:O	3:C:108:LYS:HE2	2.05	0.56
3:C:19:ALA:HB2	3:C:78:LEU:HD11	1.87	0.55
1:A:207:LYS:HD3	1:A:210:GLY:H	1.71	0.55
1:A:33:ASN:HB3	1:A:36:ALA:HB2	1.87	0.55
1:D:229:TRP:HB3	1:D:239:ILE:HG22	1.89	0.55
1:D:240:MET:HB3	1:D:318:TYR:CE1	2.42	0.55
3:F:167:GLN:HB2	6:F:313:HOH:O	2.06	0.55
1:A:207:LYS:C	1:A:207:LYS:HD2	2.28	0.54
1:D:275:LYS:HG3	6:D:501:HOH:O	2.07	0.54
1:A:26:CYS:HB3	1:A:53:ARG:CZ	2.37	0.54
1:A:127:LYS:HE3	1:A:170:ASP:O	2.08	0.54
2:B:119:THR:OG1	6:B:301:HOH:O	2.18	0.54
1:A:320:GLY:HA2	3:C:5:THR:HG21	1.90	0.54
1:D:265:PRO:O	6:D:502:HOH:O	2.17	0.54
1:A:195:LYS:O	1:A:199:GLN:HG3	2.09	0.53
1:D:154:GLU:CD	1:D:154:GLU:H	2.12	0.53
1:A:128:VAL:HG21	1:A:167:LEU:HD13	1.91	0.52
1:D:130:PHE:HB3	1:D:173:LEU:HB3	1.90	0.52
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.91	0.52
3:F:137:LEU:HD11	3:F:197:VAL:HG21	1.91	0.52
3:F:167:GLN:HG3	3:F:174:TYR:CZ	2.45	0.52
1:D:243:HIS:HB3	1:D:318:TYR:CD1	2.45	0.52
1:D:243:HIS:HB3	1:D:318:TYR:HD1	1.74	0.52
1:D:254:LYS:HE2	1:D:310:LYS:NZ	2.23	0.52
2:B:33:TRP:CE3	2:B:50:ILE:HD12	2.44	0.52
1:D:269:SER:O	1:D:273:THR:HG23	2.09	0.52
2:B:30:THR:HG22	2:B:74:LYS:HD2	1.91	0.52
1:A:26:CYS:HB3	1:A:53:ARG:NH2	2.25	0.52
1:A:120:PRO:HD2	1:A:334:MET:HE1	1.91	0.51
3:C:171:ASP:OD1	3:C:173:THR:OG1	2.26	0.51
1:A:302:LYS:HA	6:A:502:HOH:O	2.11	0.51
1:D:92:TRP:CD1	1:D:311:PRO:HD3	2.46	0.51
2:B:52:TYR:CE2	1:D:288:LYS:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG12	1:A:334:MET:HG2	1.93	0.51
3:C:13:VAL:HG12	3:C:78:LEU:HD12	1.92	0.51
3:C:133:VAL:HG12	3:C:149:TRP:CH2	2.46	0.50
1:A:198:SER:HB3	1:A:239:ILE:O	2.11	0.50
3:C:94:TRP:HA	3:C:94:TRP:CE3	2.46	0.50
3:C:190:HIS:O	3:C:212:ARG:HD3	2.11	0.50
2:E:180:GLN:HG3	2:E:184:LEU:O	2.12	0.50
1:D:128:VAL:HG23	1:D:171:ARG:HB3	1.92	0.50
3:C:106:GLU:OE1	3:C:174:TYR:OH	2.20	0.50
1:D:250:GLU:OE1	1:D:324:ARG:NH1	2.38	0.50
3:F:186:ASP:HA	3:F:189:LYS:HD3	1.92	0.49
1:D:56:HIS:NE2	1:D:100:ASP:OD1	2.44	0.49
1:D:255:ASP:O	1:D:308:VAL:HG12	2.12	0.49
2:E:22:CYS:HB3	2:E:79:THR:HG23	1.95	0.49
2:E:38:ARG:HB2	2:E:94:TYR:CE1	2.47	0.49
1:A:261:GLU:CD	1:A:281:ARG:HH22	2.16	0.49
3:F:154:ALA:O	3:F:156:GLN:NE2	2.43	0.49
2:E:91:THR:HA	2:E:118:VAL:O	2.13	0.49
1:D:94:GLY:HA3	1:D:308:VAL:HG22	1.94	0.49
3:F:128:SER:N	6:F:303:HOH:O	2.46	0.49
1:A:266:CYS:HB3	1:A:270:GLU:HB2	1.95	0.48
2:B:192:THR:CG2	3:C:138:ASN:HD21	2.26	0.48
1:A:205:ILE:O	1:A:214:ASN:HB2	2.13	0.48
1:D:202:PHE:HB3	1:D:205:ILE:HD12	1.95	0.48
3:F:17:GLU:N	6:F:302:HOH:O	2.45	0.48
3:F:120:PRO:HB3	3:F:210:PHE:CE2	2.47	0.48
1:A:130:PHE:HA	1:A:173:LEU:O	2.14	0.48
3:C:93:ASN:OD1	3:C:93:ASN:N	2.45	0.48
3:F:142:PRO:HB2	3:F:144:GLU:OE2	2.13	0.48
1:A:229:TRP:NE1	1:A:331:SER:HB3	2.25	0.48
2:E:200:THR:OG1	2:E:201:GLN:N	2.46	0.48
1:A:34:LYS:HG3	1:A:166:LEU:HD21	1.95	0.48
1:A:207:LYS:HE3	1:A:336:THR:HG23	1.94	0.48
2:B:163:TRP:CZ3	2:B:205:CYS:HB3	2.49	0.48
1:D:107:LEU:HD22	1:D:138:TYR:CE2	2.49	0.48
1:D:281:ARG:HB3	1:D:294:HIS:CE1	2.49	0.48
1:A:288:LYS:NZ	2:E:55:ASP:OD2	2.44	0.47
1:D:125:LYS:HB2	1:D:151:GLU:HA	1.96	0.47
2:E:24:THR:HB	2:E:77:SER:O	2.14	0.47
1:A:45:SER:OG	1:A:271:GLU:OE2	2.32	0.47
1:A:223:GLN:HB2	1:A:224:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:MET:HG2	1:A:318:TYR:CD1	2.49	0.47
2:B:153:ASP:HA	2:B:184:LEU:HB3	1.96	0.47
2:B:105:ARG:HD3	3:C:92:ASN:HA	1.97	0.47
1:D:50:GLN:O	1:D:53:ARG:N	2.38	0.47
1:A:92:TRP:CD2	1:A:311:PRO:HD3	2.49	0.47
2:B:131:PHE:CG	3:C:125:GLN:HB2	2.50	0.47
1:D:73:GLN:HG3	1:D:74:ARG:HG2	1.96	0.47
1:A:250:GLU:OE1	1:A:250:GLU:HA	2.15	0.47
2:B:161:VAL:HG22	2:B:207:VAL:HG22	1.97	0.47
3:F:2:ILE:HG21	3:F:93:ASN:HD21	1.80	0.47
3:F:143:ARG:NE	6:F:311:HOH:O	2.48	0.47
1:A:34:LYS:HG3	1:A:166:LEU:HD11	1.97	0.46
1:A:47:LYS:HA	1:A:50:GLN:HG3	1.96	0.46
1:D:188:GLU:O	1:D:192:LEU:HD12	2.15	0.46
2:E:29:PHE:CD2	2:E:77:SER:HA	2.50	0.46
1:A:287:CYS:HB3	1:A:292:CYS:HB2	1.76	0.46
1:A:51:ILE:HA	1:A:56:HIS:ND1	2.30	0.46
2:B:17:SER:OG	2:B:84:ARG:NH1	2.39	0.46
1:A:186:ILE:HG21	1:A:323:VAL:HG23	1.97	0.46
1:D:130:PHE:HA	1:D:173:LEU:O	2.16	0.46
2:B:206:ASN:ND2	2:B:217:ASP:OD2	2.47	0.46
1:D:152:SER:OG	1:D:154:GLU:OE1	2.32	0.46
3:F:159:ASN:O	3:F:180:LEU:HD12	2.16	0.46
2:B:105:ARG:HB3	3:C:91:TYR:O	2.17	0.45
1:A:79:GLN:HB2	1:A:169:SER:HB2	1.97	0.45
1:A:75:GLY:O	1:A:79:GLN:HG2	2.16	0.45
3:C:96:PRO:O	6:C:303:HOH:O	2.21	0.45
2:B:103:TRP:HA	1:D:289:VAL:O	2.17	0.45
1:A:240:MET:HG2	1:A:318:TYR:CE1	2.52	0.45
1:A:54:LEU:HD11	1:A:80:VAL:HG22	1.98	0.45
1:D:54:LEU:HD23	1:D:54:LEU:HA	1.59	0.45
1:D:215:GLN:OE1	1:D:215:GLN:HA	2.17	0.44
2:B:40:MET:HE2	2:B:46:GLU:OE2	2.17	0.44
1:D:77:ARG:NH2	1:D:95:LEU:O	2.50	0.44
2:E:28:ASN:HB3	2:E:31:TYR:CE2	2.52	0.44
3:F:61:ARG:NH1	6:F:310:HOH:O	2.48	0.44
3:F:145:ALA:HB2	3:F:199:HIS:HD2	1.82	0.44
3:C:47:LEU:HA	3:C:58:ILE:HG12	1.99	0.44
1:D:77:ARG:NE	1:D:100:ASP:OD2	2.50	0.44
2:E:38:ARG:NE	2:E:46:GLU:OE1	2.40	0.44
2:E:100:LYS:HG2	2:E:108:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ARG:HB2	2:B:94:TYR:CE1	2.51	0.44
3:C:126:LEU:HD11	3:C:187:TYR:CE2	2.52	0.44
2:E:114:GLN:H	2:E:114:GLN:HG2	1.37	0.44
1:D:77:ARG:O	1:D:80:VAL:HG23	2.17	0.44
1:A:25:ILE:HD11	1:A:257:VAL:HB	1.99	0.44
2:B:131:PHE:CD1	3:C:125:GLN:HB2	2.53	0.44
1:D:92:TRP:CD1	1:D:309:HIS:NE2	2.86	0.44
1:D:266:CYS:SG	1:D:270:GLU:HB3	2.57	0.44
1:A:132:ARG:HH12	1:A:209:ASP:CG	2.19	0.43
2:B:218:LYS:HE2	3:C:124:GLU:OE1	2.17	0.43
3:F:33:LEU:HD11	3:F:88:CYS:HB2	1.98	0.43
1:A:92:TRP:CG	1:A:311:PRO:HD3	2.53	0.43
1:D:69:GLY:HA3	1:D:165:GLY:O	2.18	0.43
1:D:226:ASP:HB3	1:D:330:PHE:CZ	2.54	0.43
2:E:57:ASP:OD2	2:E:59:ARG:NH2	2.50	0.43
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.85	0.43
3:C:105:LEU:HD23	3:C:105:LEU:HA	1.81	0.43
3:F:189:LYS:O	3:F:190:HIS:ND1	2.51	0.43
1:A:215:GLN:HE21	1:A:215:GLN:HA	1.84	0.43
2:E:159:VAL:CG1	2:E:209:HIS:HD2	2.31	0.43
3:F:137:LEU:HD11	3:F:197:VAL:CG2	2.48	0.43
2:B:17:SER:OG	2:B:84:ARG:HD2	2.18	0.43
3:C:24:ARG:HH21	3:C:26:SER:HA	1.83	0.43
3:C:61:ARG:NE	3:C:79:GLN:HG3	2.33	0.43
1:D:257:VAL:O	1:D:305:CYS:HA	2.18	0.43
3:F:160:SER:HA	3:F:179:THR:O	2.19	0.43
1:D:92:TRP:CG	1:D:311:PRO:HD3	2.53	0.43
3:F:126:LEU:HD22	3:F:184:LYS:HG3	2.00	0.43
3:F:164:VAL:HG13	3:F:165:THR:O	2.19	0.43
3:C:12:SER:OG	3:C:106:GLU:OE2	2.26	0.43
3:C:160:SER:HA	3:C:179:THR:O	2.19	0.43
1:D:110:LYS:HB2	1:D:110:LYS:HE2	1.74	0.43
1:A:51:ILE:HD13	1:A:100:ASP:HB3	2.01	0.43
1:A:230:MET:HE3	1:A:323:VAL:HG11	2.01	0.43
2:B:204:ILE:HD13	2:B:219:LYS:HB2	2.01	0.43
1:A:42:LEU:N	1:A:42:LEU:HD12	2.34	0.42
1:A:256:PHE:HA	1:A:306:SER:O	2.19	0.42
1:D:169:SER:O	1:D:172:VAL:HG23	2.19	0.42
3:C:150:LYS:HE3	3:C:196:GLU:OE1	2.19	0.42
2:E:48:MET:HA	2:E:64:PHE:CD2	2.54	0.42
3:F:105:LEU:HD12	3:F:105:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:NZ	1:D:278:GLY:O	2.52	0.42
3:C:29:VAL:HA	3:C:92:ASN:ND2	2.33	0.42
2:B:126:LYS:HD3	2:B:153:ASP:O	2.19	0.42
1:D:191:PHE:CE1	1:D:238:ILE:HD11	2.54	0.42
1:A:130:PHE:HB3	1:A:173:LEU:HB3	2.02	0.42
1:D:45:SER:OG	1:D:271:GLU:OE2	2.37	0.42
3:F:32:ASN:HB3	3:F:91:TYR:CD2	2.55	0.42
1:D:99:CYS:O	1:D:102:ASP:HB3	2.19	0.42
2:E:171:GLY:O	2:E:191:VAL:HA	2.20	0.42
3:F:191:LYS:O	3:F:211:ASN:HA	2.20	0.42
1:D:229:TRP:CE3	1:D:237:LYS:HD3	2.54	0.42
1:D:260:LYS:HG3	1:D:303:CYS:SG	2.59	0.42
2:E:81:LEU:HD12	2:E:82:HIS:H	1.85	0.42
1:A:277:SER:HG	1:A:279:SER:CB	2.31	0.42
2:B:177:ALA:HB2	2:B:187:LEU:HD12	2.02	0.42
1:A:320:GLY:CA	3:C:5:THR:HG21	2.50	0.41
3:C:114:PRO:HB3	3:C:140:PHE:CD2	2.55	0.41
1:D:134:THR:O	1:D:237:LYS:HE2	2.19	0.41
1:D:207:LYS:HG3	1:D:336:THR:OG1	2.20	0.41
1:A:48:ILE:HD13	1:A:48:ILE:HA	1.96	0.41
1:A:255:ASP:O	1:A:308:VAL:HG22	2.20	0.41
1:A:236:HIS:ND1	1:A:237:LYS:O	2.43	0.41
1:A:247:TRP:CZ3	1:A:314:VAL:HB	2.56	0.41
2:B:70:ILE:HA	2:B:80:TYR:O	2.21	0.41
2:B:93:ILE:HD13	2:B:93:ILE:HG21	1.86	0.41
3:C:6:GLN:HB3	6:C:307:HOH:O	2.20	0.41
1:A:99:CYS:O	1:A:102:ASP:HB3	2.20	0.41
2:B:28:ASN:HB3	2:B:31:TYR:CZ	2.56	0.41
3:C:155:LEU:HG	3:C:156:GLN:N	2.36	0.41
1:D:207:LYS:CD	1:D:210:GLY:H	2.34	0.41
1:D:201:GLU:HG2	1:D:242:GLU:OE1	2.20	0.41
1:A:289:VAL:HG12	2:E:103:TRP:HA	2.02	0.41
2:B:91:THR:HA	2:B:118:VAL:O	2.21	0.41
3:C:11:LEU:HB3	3:C:105:LEU:HD23	2.02	0.41
1:D:207:LYS:HD2	1:D:207:LYS:C	2.41	0.41
2:E:107:TYR:CD1	2:E:107:TYR:N	2.88	0.41
2:E:125:THR:HG23	2:E:156:PRO:HD3	2.03	0.41
2:E:159:VAL:HG12	2:E:209:HIS:CD2	2.56	0.41
2:B:35:GLY:HA3	2:B:50:ILE:HG22	2.02	0.41
1:D:250:GLU:OE1	1:D:313:GLU:HG3	2.21	0.41
3:F:12:SER:O	3:F:108:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:THR:HG21	2:B:29:PHE:HD1	1.85	0.40
3:C:135:CYS:HB2	3:C:149:TRP:CZ2	2.57	0.40
1:A:257:VAL:O	1:A:305:CYS:HA	2.22	0.40
1:D:263:THR:O	1:D:263:THR:OG1	2.31	0.40
2:E:23:GLU:HG3	2:E:78:THR:HG22	2.03	0.40
3:F:8:PRO:HG2	3:F:11:LEU:HB2	2.03	0.40
3:F:83:PHE:CE2	3:F:107:ILE:HG13	2.56	0.40
1:A:294:HIS:HB2	2:E:31:TYR:OH	2.20	0.40
3:C:159:ASN:OD1	3:C:159:ASN:N	2.54	0.40
1:A:107:LEU:HD22	1:A:138:TYR:CE1	2.56	0.40
2:E:202:THR:HB	2:E:219:LYS:HE3	2.04	0.40

All (2) 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:C:110:THR:OG1	3:F:77:SER:OG[1_545]	2.08	0.12
2:B:16:GLU:OE2	2:E:215:LYS:NZ[4_546]	2.16	0.04

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	308/327 (94%)	294 (96%)	14 (4%)	0	100	100
1	D	308/327 (94%)	294 (96%)	14 (4%)	0	100	100
2	B	211/227 (93%)	202 (96%)	9 (4%)	0	100	100
2	E	210/227 (92%)	198 (94%)	12 (6%)	0	100	100
3	C	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
3	F	209/215 (97%)	199 (95%)	10 (5%)	0	100	100
All	All	1457/1538 (95%)	1388 (95%)	69 (5%)	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	268/282 (95%)	240 (90%)	28 (10%)	7 21
1	D	268/282 (95%)	243 (91%)	25 (9%)	9 26
2	B	183/195 (94%)	166 (91%)	17 (9%)	9 26
2	E	184/195 (94%)	169 (92%)	15 (8%)	11 33
3	C	182/186 (98%)	168 (92%)	14 (8%)	13 35
3	F	182/186 (98%)	168 (92%)	14 (8%)	13 35
All	All	1267/1326 (96%)	1154 (91%)	113 (9%)	9 28

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	42	LEU
1	A	45	SER
1	A	52	ASP
1	A	54	LEU
1	A	65	SER
1	A	73	GLN
1	A	88	SER
1	A	92	TRP
1	A	97	SER
1	A	152	SER
1	A	164	SER
1	A	166	LEU
1	A	170	ASP
1	A	183	MET
1	A	193	GLU
1	A	198	SER
1	A	207	LYS
1	A	217	GLU

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Mol	Chain	Res	Type
1	A	219	GLU
1	A	252	SER
1	A	253	SER
1	A	269	SER
1	A	279	SER
1	A	280	CYS
1	A	292	CYS
1	A	313	GLU
1	A	317	SER
2	B	16	GLU
2	B	24	THR
2	B	43	GLU
2	B	63	SER
2	B	79	THR
2	B	100	LYS
2	B	105	ARG
2	B	117	LEU
2	B	119	THR
2	B	129	SER
2	B	169	THR
2	B	179	LEU
2	B	187	LEU
2	B	206	ASN
2	B	218	LYS
2	B	219	LYS
2	B	221	GLU
3	C	10	THR
3	C	20	THR
3	C	22	SER
3	C	63	SER
3	C	79	GLN
3	C	115	SER
3	C	127	LYS
3	C	130	THR
3	C	143	ARG
3	C	153	ASN
3	C	159	ASN
3	C	173	THR
3	C	189	LYS
3	C	204	SER
1	D	32	SER
1	D	52	ASP

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Mol	Chain	Res	Type
1	D	97	SER
1	D	115	SER
1	D	145	SER
1	D	158	SER
1	D	164	SER
1	D	172	VAL
1	D	191	PHE
1	D	192	LEU
1	D	198	SER
1	D	201	GLU
1	D	207	LYS
1	D	214	ASN
1	D	251	SER
1	D	257	VAL
1	D	266	CYS
1	D	267	SER
1	D	280	CYS
1	D	292	CYS
1	D	302	LYS
1	D	303	CYS
1	D	306	SER
1	D	322	ARG
1	D	338	GLU
2	E	3	GLN
2	E	38	ARG
2	E	63	SER
2	E	71	SER
2	E	74	LYS
2	E	79	THR
2	E	89	SER
2	E	96	CYS
2	E	100	LYS
2	E	105	ARG
2	E	122	SER
2	E	129	SER
2	E	144	THR
2	E	196	SER
2	E	210	LYS
3	F	10	THR
3	F	14	SER
3	F	38	HIS
3	F	65	SER

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Mol	Chain	Res	Type
3	F	69	THR
3	F	72	THR
3	F	132	SER
3	F	164	VAL
3	F	166	GLU
3	F	169	SER
3	F	176	LEU
3	F	177	SER
3	F	183	SER
3	F	204	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	D	199	GLN
1	D	294	HIS
2	E	208	ASN
3	F	42	GLN
3	F	90	HIS
3	F	101	GLN

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)

4 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	$\#\|Z\| > 2$
4	NAG	G	1	2,4	14,14,15	0.74	1 (7%)	17,19,21	0.75	0
4	NAG	G	2	4	14,14,15	0.58	0	17,19,21	0.56	0
4	NAG	H	1	2,4	14,14,15	1.19	1 (7%)	17,19,21	0.80	0
4	NAG	H	2	4	14,14,15	0.45	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	4.28	1.50	1.43
4	G	1	NAG	O5-C1	2.52	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

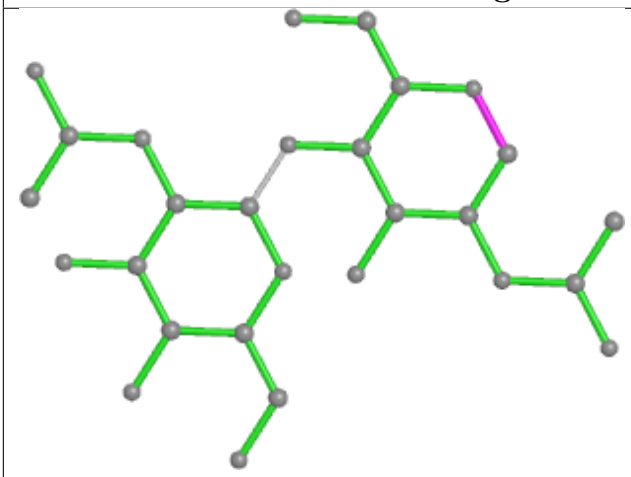
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

There are no ring outliers.

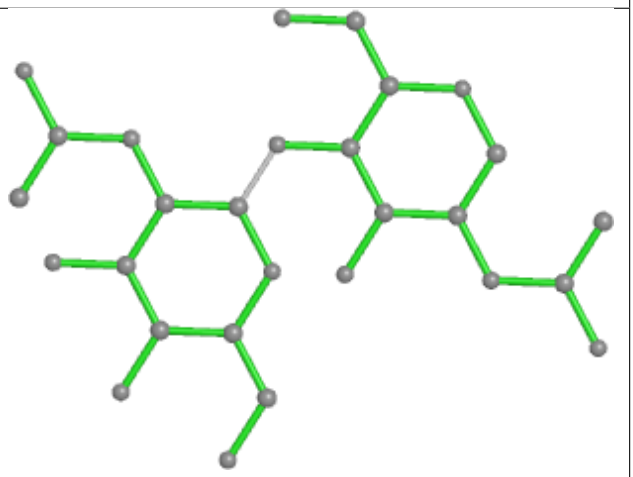
No monomer is involved in short contacts.

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

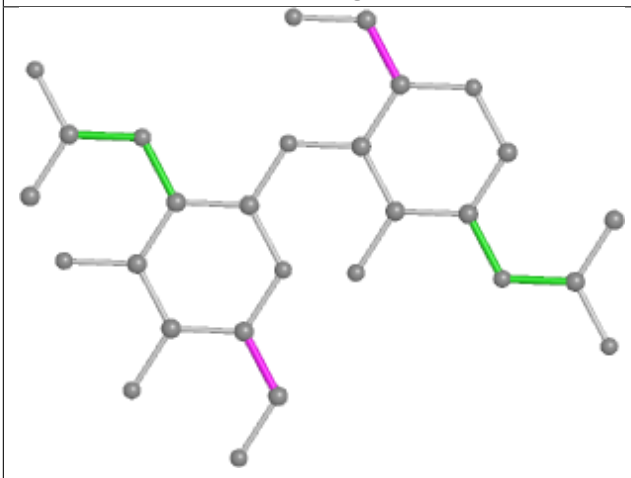
Oligosaccharide Chain G



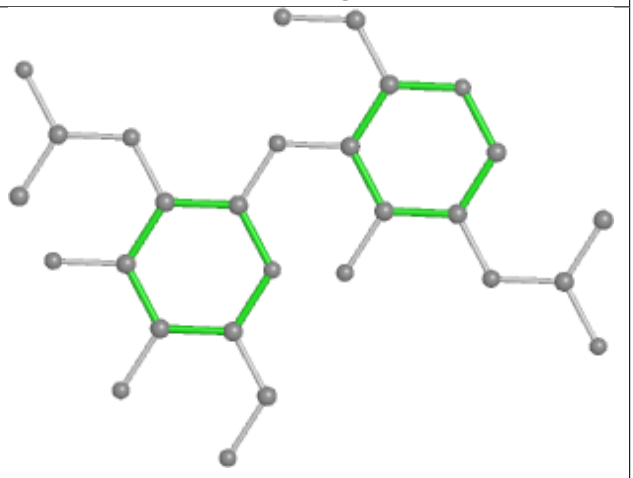
Bond lengths



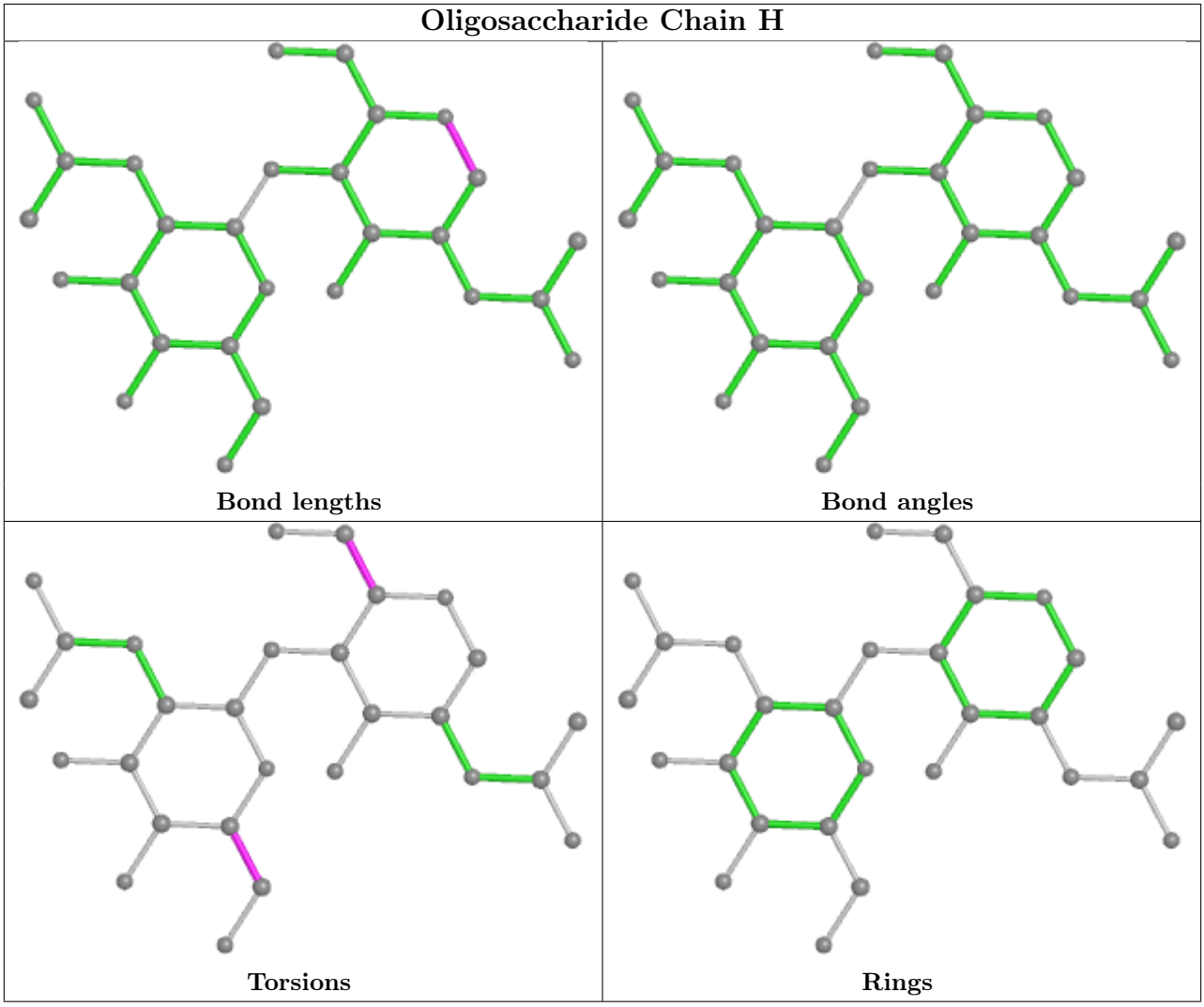
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 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	A	400	1	14,14,15	0.61	0	17,19,21	1.02	2 (11%)
5	NAG	D	401	1	14,14,15	0.58	0	17,19,21	0.86	1 (5%)
5	NAG	D	400	1	14,14,15	0.36	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	401	1	14,14,15	0.63	1 (7%)	17,19,21	0.72	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
5	NAG	A	400	1	-	4/6/23/26	0/1/1/1
5	NAG	D	401	1	-	2/6/23/26	0/1/1/1
5	NAG	D	400	1	-	2/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	NAG	C1-C2	2.23	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	400	NAG	C2-N2-C7	3.01	127.19	122.90
5	D	401	NAG	C1-O5-C5	2.74	115.91	112.19
5	A	401	NAG	C1-O5-C5	2.55	115.64	112.19
5	D	400	NAG	C1-O5-C5	2.25	115.25	112.19
5	A	400	NAG	C1-O5-C5	2.18	115.14	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	400	NAG	C3-C2-N2-C7
5	D	401	NAG	C4-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
5	D	401	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	D	400	NAG	C4-C5-C6-O6
5	D	400	NAG	O5-C5-C6-O6
5	A	400	NAG	C4-C5-C6-O6
5	A	400	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	A	400	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	400	NAG	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	312/327 (95%)	0.02	3 (0%) 82 77	43, 61, 87, 141	0
1	D	312/327 (95%)	0.14	8 (2%) 56 46	44, 64, 93, 119	0
2	B	215/227 (94%)	-0.19	0 100 100	36, 49, 77, 106	0
2	E	214/227 (94%)	-0.14	1 (0%) 91 88	38, 50, 81, 109	0
3	C	213/215 (99%)	-0.23	1 (0%) 91 88	42, 53, 75, 112	0
3	F	211/215 (98%)	-0.16	1 (0%) 91 88	41, 54, 72, 84	0
All	All	1477/1538 (96%)	-0.07	14 (0%) 84 80	36, 56, 84, 141	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	319	GLY	3.5
1	A	217	GLU	3.1
1	D	199	GLN	3.1
1	D	212	VAL	2.5
1	D	42	LEU	2.5
1	A	267	SER	2.4
3	F	182	LEU	2.3
1	D	338	GLU	2.3
2	E	170	SER	2.2
1	D	38	ILE	2.2
1	D	202	PHE	2.1
3	C	126	LEU	2.1
1	A	22	GLY	2.1
1	D	203	PRO	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 (i)

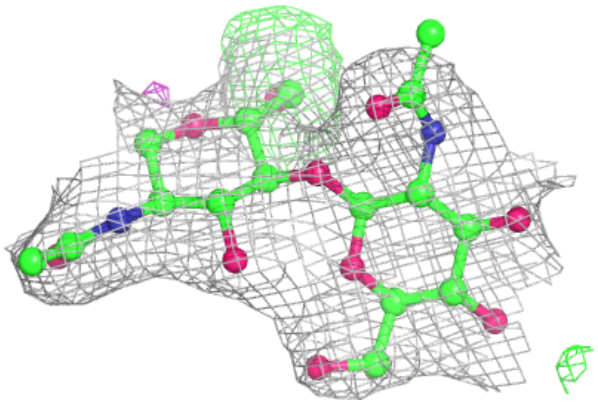
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

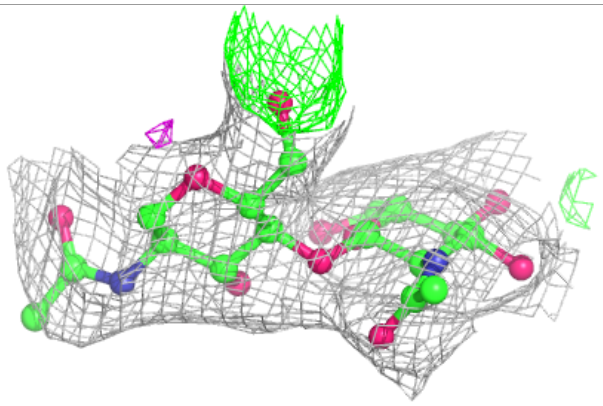
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	1	14/15	0.68	0.20	58,68,72,74	0
4	NAG	H	1	14/15	0.73	0.20	63,80,86,90	0
4	NAG	H	2	14/15	0.88	0.14	85,89,92,93	0
4	NAG	G	2	14/15	0.90	0.18	69,76,80,81	0

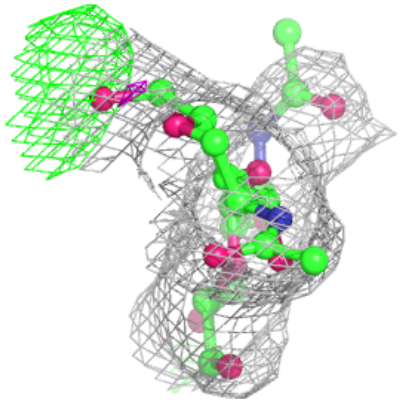
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

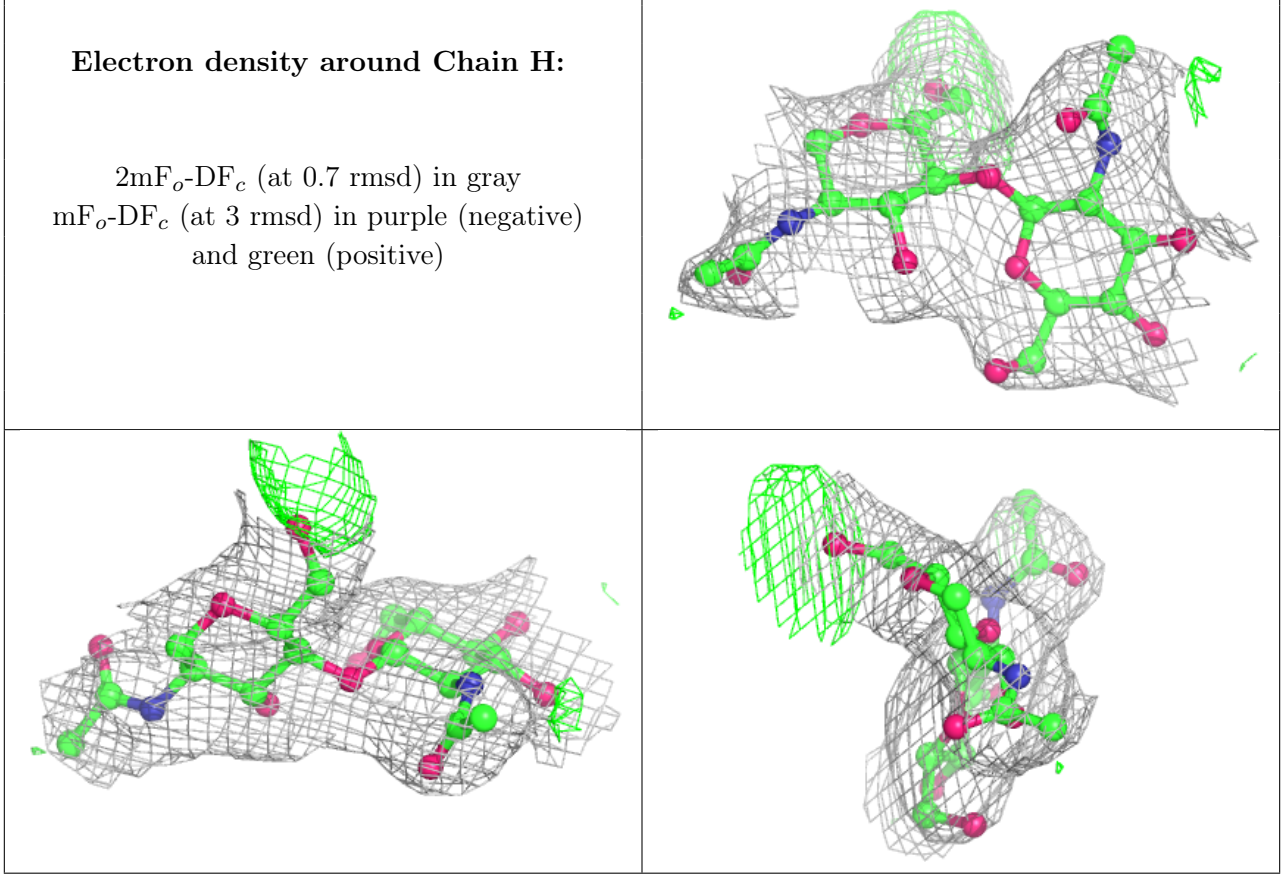






Electron density around Chain H:

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



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	400	14/15	0.68	0.19	91,99,109,117	0
5	NAG	D	400	14/15	0.81	0.27	104,106,116,118	0
5	NAG	A	401	14/15	0.83	0.36	53,67,76,90	0
5	NAG	D	401	14/15	0.89	0.29	67,79,89,97	0

6.5 Other polymers

There are no such residues in this entry.