



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:38 PM UTC

PDB ID : 8WSN / pdb_00008wsn
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 ⓘ 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

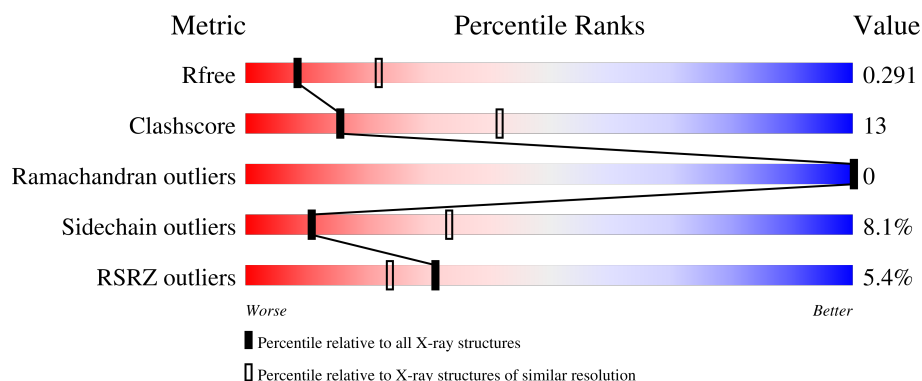
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	7% 57% 35% • 5%
1	D	327	9% 61% 32% • 5%
2	B	227	3% 66% 25% • 5%
2	E	227	3% 71% 21% • 6%
3	C	215	3% 69% 28% ••

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Mol	Chain	Length	Quality of chain
3	F	215	
4	G	2	
4	H	2	

2 Entry composition

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.

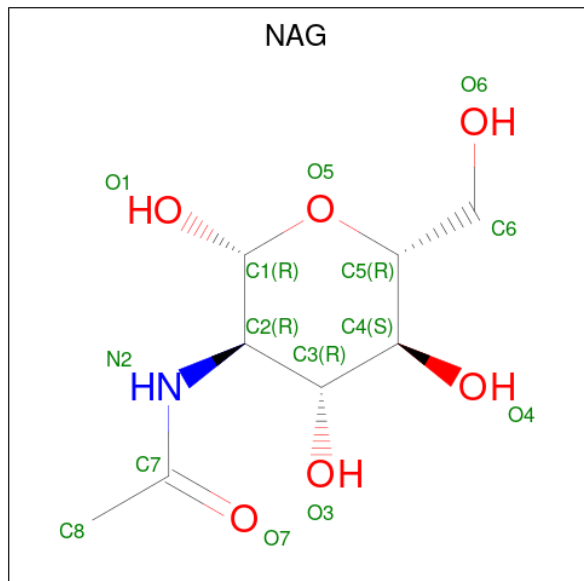
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1638	1029	282	323	4			
3	F	211	Total	C	N	O	S	0	0	0
			1628	1023	281	320	4			

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

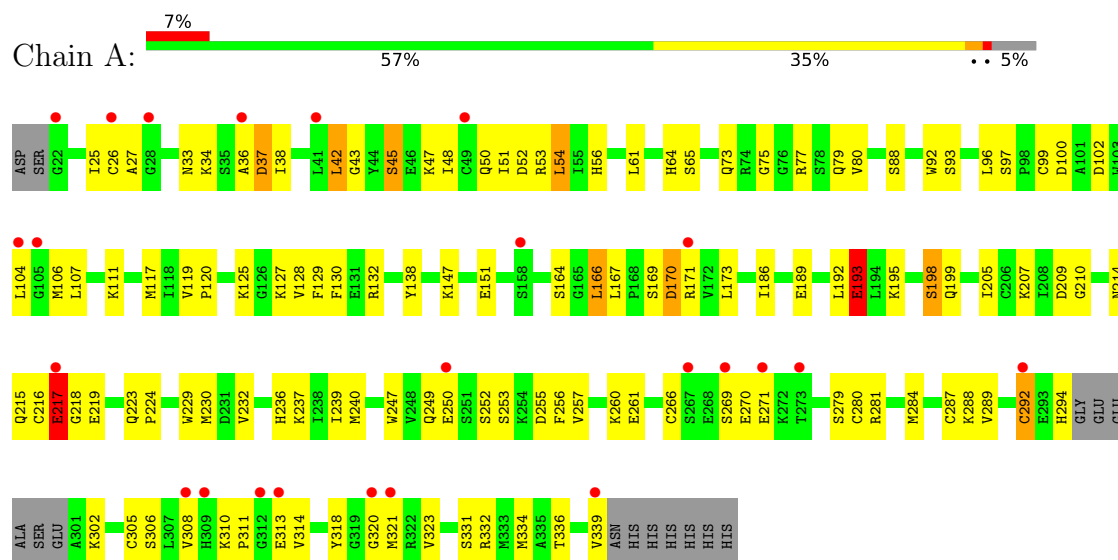
- Molecule 6 is water.

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

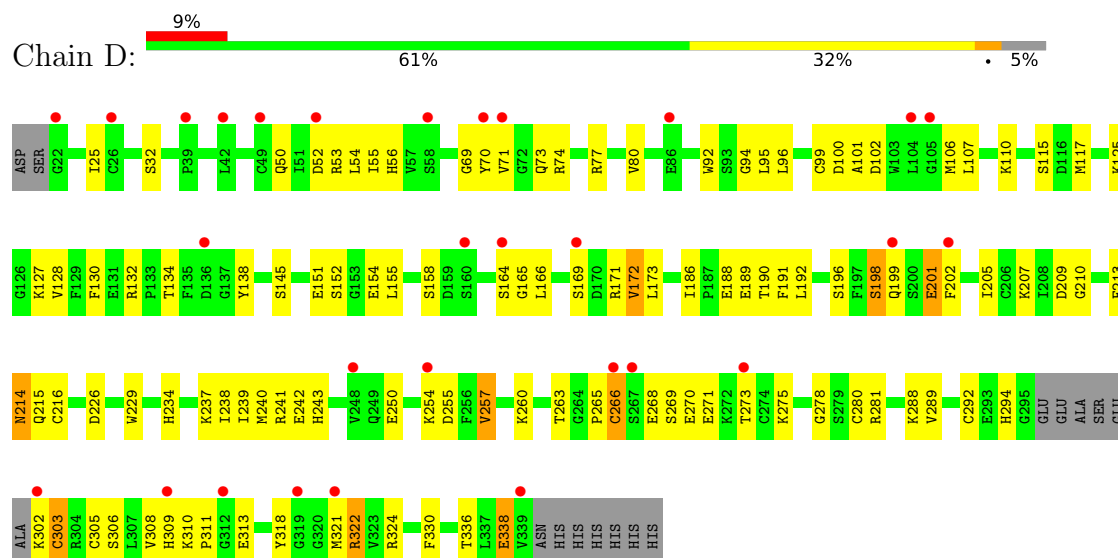
3 Residue-property plots

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: Gn

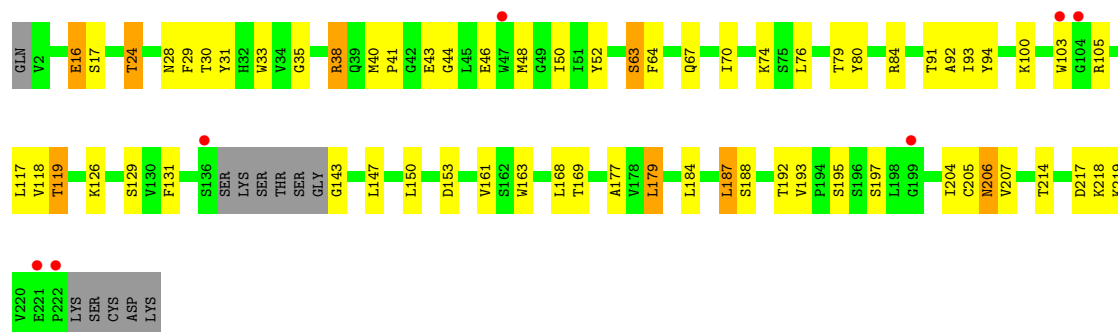


• Molecule 1: Gn

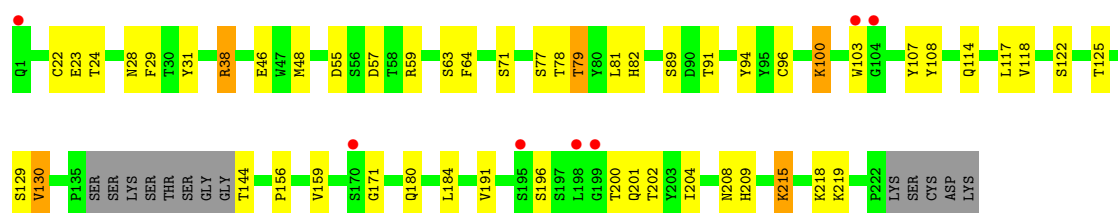


• Molecule 2: Ab1-H

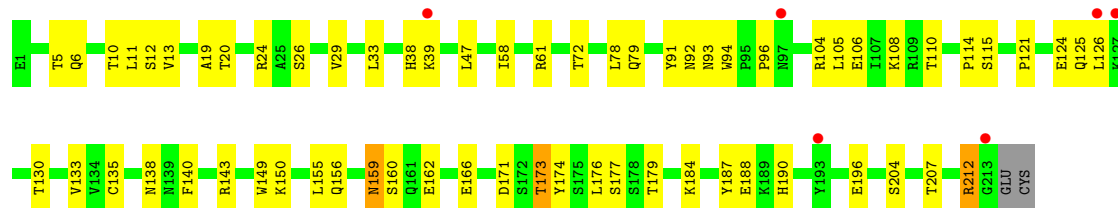




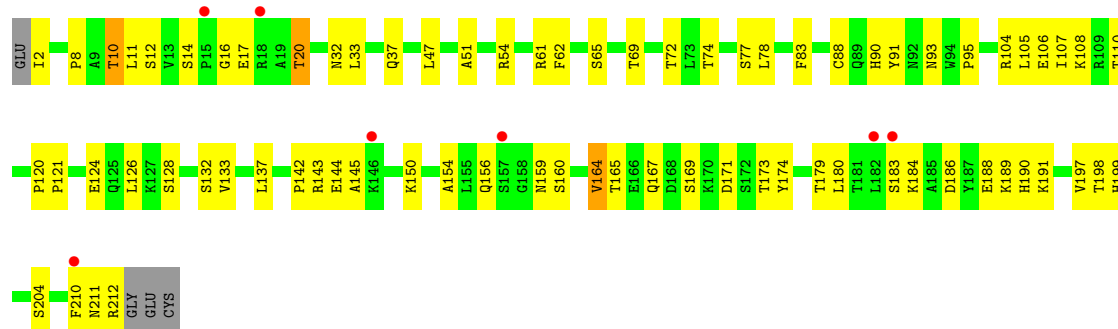
- Molecule 2: Ab1-H



- Molecule 3: Ab1-L



- Molecule 3: Ab1-L



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

Chain G:  50% 50%

 MAG1
MAG2

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

Chain H:  50% 50%

 MAG1
MAG2

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.99%)	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 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.47	0/2464	0.80	11/3322 (0.3%)
1	D	0.43	0/2460	0.64	3/3317 (0.1%)
2	B	0.48	0/1707	0.68	0/2331
2	E	0.48	0/1707	0.68	2/2331 (0.1%)
3	C	0.47	0/1677	0.71	4/2281 (0.2%)
3	F	0.45	0/1667	0.66	0/2268
All	All	0.46	0/11682	0.70	20/15850 (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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	GLU	N-CA-CB	-10.41	94.81	110.12
1	A	217	GLU	CG-CD-OE1	8.86	138.77	118.40
1	A	217	GLU	CG-CD-OE2	-8.66	98.49	118.40
1	A	192	LEU	CA-C-N	8.44	131.59	120.28
1	A	192	LEU	C-N-CA	8.44	131.59	120.28
1	D	322	ARG	CB-CG-CD	-7.87	93.19	111.30
1	A	193	GLU	CB-CA-C	7.60	123.41	110.79
3	C	39	LYS	CG-CD-CE	7.33	128.16	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	GLU	CB-CG-CD	7.00	124.49	112.60
1	A	217	GLU	N-CA-C	6.53	124.71	110.80
1	D	322	ARG	N-CA-CB	6.49	120.73	110.55
3	C	39	LYS	CB-CG-CD	6.42	126.06	111.30
1	A	217	GLU	OE1-CD-OE2	-6.20	108.01	122.90
2	E	215	LYS	CG-CD-CE	-5.67	98.27	111.30
1	D	322	ARG	CB-CA-C	-5.31	101.48	110.19
1	A	193	GLU	CA-CB-CG	5.27	124.63	114.10
3	C	38	HIS	CA-C-N	5.04	129.10	121.03
3	C	38	HIS	C-N-CA	5.04	129.10	121.03
1	A	217	GLU	CA-CB-CG	-5.02	104.06	114.10
2	E	215	LYS	CD-CE-NZ	5.02	127.96	111.90

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

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	84	0
1	D	2399	0	2296	84	0
2	B	1658	0	1607	36	1
2	E	1658	0	1613	28	1
3	C	1638	0	1585	42	1
3	F	1628	0	1577	42	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
6	B	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	11	0
All	All	11643	0	11086	303	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 (303) 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
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
1:D:71:VAL:HG11	1:D:172:VAL:HG22	1.76	0.68
1:A:120:PRO:HD2	1:A:334:MET:HE3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:LEU:HD13	1:D:106:MET:HE1	1.82	0.62
1:D:127:LYS:HE2	1:D:173:LEU:HB2	1.82	0.62
1:D:189:GLU:CD	1:D:189:GLU:H	2.07	0.61
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
1:A:120:PRO:HD2	1:A:334:MET:HE1	1.81	0.60
2:B:163:TRP:CH2	2:B:205:CYS:HB3	2.36	0.60
1:D:101:ALA:HA	1:D:106:MET:HE3	1.83	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:D:201:GLU:CD	1:D:318:TYR:HH	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:C	1:A:207:LYS:HD2	2.28	0.59
3:F:106:GLU:OE1	3:F:174:TYR:OH	2.20	0.59
1:D:255:ASP:OD1	1:D:310:LYS:NZ	2.36	0.58
1:A:117:MET:HE1	1:A:207:LYS:NZ	2.18	0.58
1:D:154:GLU:CD	1:D:154:GLU:H	2.12	0.58
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:121:PRO:HD3	3:F:133:VAL:HG22	1.87	0.56
3:C:106:GLU:OE1	3:C:174:TYR:OH	2.20	0.56
1:A:119:VAL:HA	1:A:334:MET:HE3	1.86	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:117:MET:HE1	1:A:207:LYS:HZ1	1.71	0.55
1:D:254:LYS:HE2	1:D:310:LYS:HZ1	1.73	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:261:GLU:CD	1:A:281:ARG:HH22	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:CYS:HB3	1:A:53:ARG:NH2	2.25	0.52
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
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
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
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
3:F:171:ASP:OD1	3:F:173:THR:OG1	2.18	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
2:B:40:MET:HE2	2:B:46:GLU:OE2	2.13	0.48
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
1:A:132:ARG:HH12	1:A:209:ASP:CG	2.19	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:D:190:THR:HG23	1:D:321:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:263:THR:O	1:D:263:THR:OG1	2.31	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:A:96:LEU:HD13	1:A:106:MET:HE1	1.97	0.46
1:D:117:MET:HE1	1:D:207:LYS:NZ	2.31	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:D:207:LYS:HD2	1:D:207:LYS:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:191:PHE:CD1	1:D:191:PHE:C	2.94	0.44
3:F:16:GLY:C	6:F:302:HOH:O	2.61	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
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:A:104:LEU:HB2	1:A:106:MET:HE3	1.99	0.43
3:C:171:ASP:CG	3:C:173:THR:HG1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:230:MET:HE3	1:A:232:VAL:HG11	2.00	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
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
1:A:284:MET:HE2	1:A:284:MET:HB2	1.77	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
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
2:B:177:ALA:HB2	2:B:187:LEU:HD12	2.02	0.42
2:B:48:MET:HE3	2:B:64:PHE:CE1	2.55	0.41
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:D:132:ARG:HH12	1:D:209:ASP:CG	2.29	0.41
1:A:99:CYS:O	1:A:102:ASP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:73:GLN:C	1:A:75:GLY:H	2.27	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
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
1:A:321:MET:HB2	1:A:321:MET:HE3	1.80	0.40
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:249:GLN:HE21	1:A:311:PRO:C	2.28	0.40
1:A:257:VAL:O	1:A:305:CYS:HA	2.22	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
3:C:176:LEU:HD23	3:C:177:SER:C	2.46	0.40
1:D:201:GLU:CD	1:D:201:GLU:H	2.29	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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	243 (91%)	25 (9%)	8	27
1	D	268/282 (95%)	249 (93%)	19 (7%)	13	39
2	B	183/195 (94%)	163 (89%)	20 (11%)	6	21
2	E	184/195 (94%)	171 (93%)	13 (7%)	13	39
3	C	182/186 (98%)	171 (94%)	11 (6%)	17	47
3	F	182/186 (98%)	168 (92%)	14 (8%)	12	36
All	All	1267/1326 (96%)	1165 (92%)	102 (8%)	11	33

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	38	ILE
1	A	42	LEU
1	A	45	SER
1	A	52	ASP
1	A	54	LEU
1	A	65	SER
1	A	88	SER
1	A	97	SER
1	A	147	LYS
1	A	164	SER
1	A	166	LEU
1	A	170	ASP
1	A	193	GLU
1	A	198	SER
1	A	217	GLU
1	A	219	GLU
1	A	252	SER
1	A	253	SER
1	A	260	LYS
1	A	269	SER
1	A	279	SER
1	A	280	CYS
1	A	292	CYS
1	A	313	GLU
2	B	16	GLU
2	B	24	THR
2	B	38	ARG
2	B	63	SER
2	B	76	LEU
2	B	79	THR
2	B	117	LEU
2	B	119	THR
2	B	129	SER
2	B	147	LEU
2	B	150	LEU
2	B	168	LEU
2	B	169	THR
2	B	179	LEU
2	B	187	LEU
2	B	188	SER
2	B	193	VAL

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Mol	Chain	Res	Type
2	B	197	SER
2	B	206	ASN
2	B	214	THR
3	C	10	THR
3	C	20	THR
3	C	33	LEU
3	C	72	THR
3	C	115	SER
3	C	130	THR
3	C	159	ASN
3	C	173	THR
3	C	204	SER
3	C	207	THR
3	C	212	ARG
1	D	32	SER
1	D	52	ASP
1	D	115	SER
1	D	145	SER
1	D	158	SER
1	D	164	SER
1	D	172	VAL
1	D	198	SER
1	D	201	GLU
1	D	214	ASN
1	D	257	VAL
1	D	266	CYS
1	D	268	GLU
1	D	280	CYS
1	D	292	CYS
1	D	302	LYS
1	D	303	CYS
1	D	306	SER
1	D	338	GLU
2	E	38	ARG
2	E	63	SER
2	E	71	SER
2	E	79	THR
2	E	89	SER
2	E	96	CYS
2	E	100	LYS
2	E	117	LEU
2	E	122	SER

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Mol	Chain	Res	Type
2	E	129	SER
2	E	130	VAL
2	E	144	THR
2	E	196	SER
3	F	10	THR
3	F	14	SER
3	F	20	THR
3	F	65	SER
3	F	69	THR
3	F	72	THR
3	F	110	THR
3	F	132	SER
3	F	150	LYS
3	F	164	VAL
3	F	169	SER
3	F	183	SER
3	F	198	THR
3	F	204	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	199	GLN
1	A	215	GLN
2	B	32	HIS
3	C	153	ASN
1	D	199	GLN
1	D	249	GLN
2	E	32	HIS
2	E	208	ASN
3	F	32	ASN
3	F	42	GLN
3	F	90	HIS
3	F	101	GLN
3	F	139	ASN
3	F	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.72	1 (7%)	17,19,21	0.73	0
4	NAG	G	2	4	14,14,15	0.58	0	17,19,21	0.58	0
4	NAG	H	1	2,4	14,14,15	1.14	1 (7%)	17,19,21	0.75	0
4	NAG	H	2	4	14,14,15	0.46	0	17,19,21	0.54	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	-	3/6/23/26	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	4.08	1.50	1.43
4	G	1	NAG	O5-C1	2.41	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

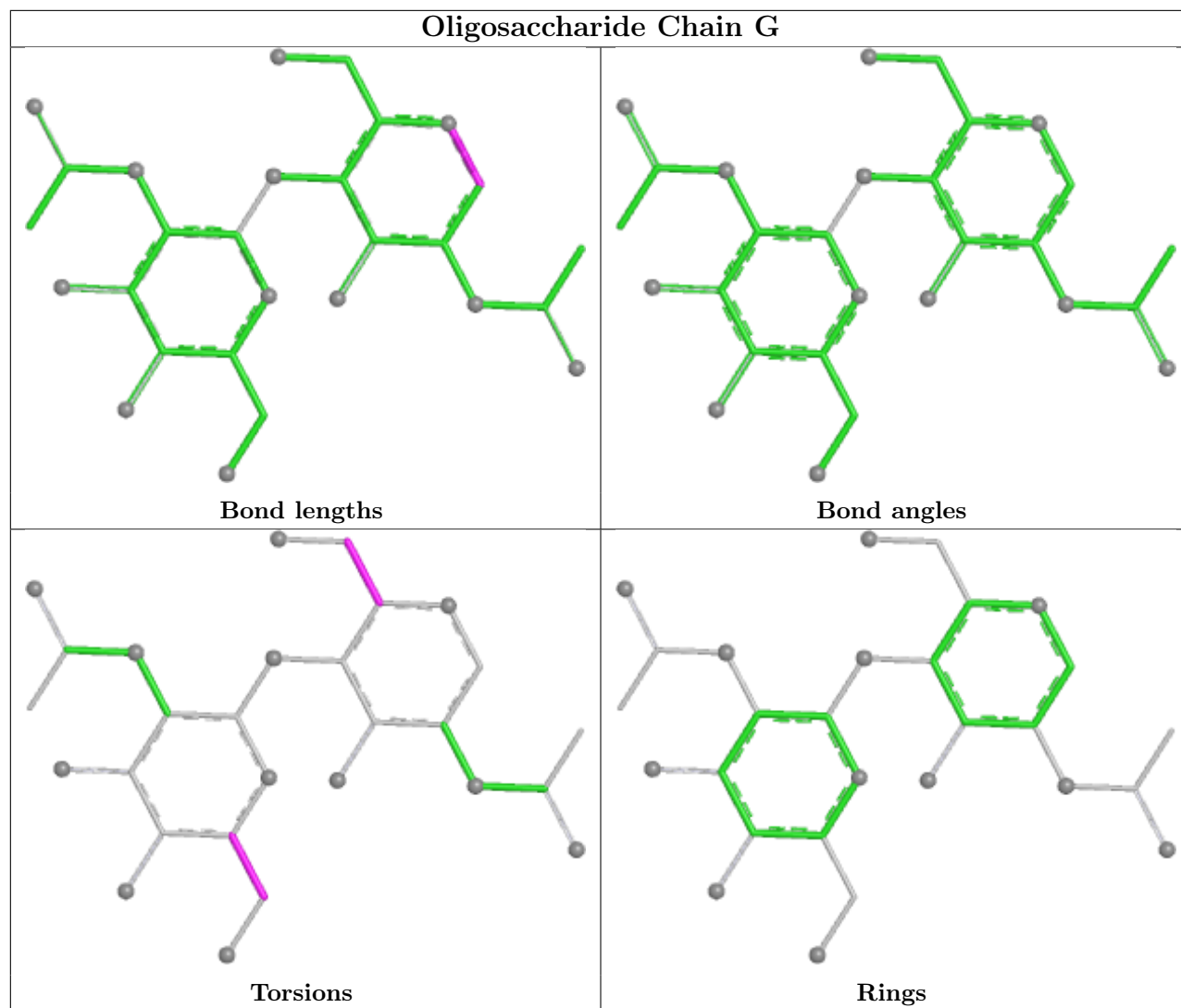
All (9) torsion outliers are listed below:

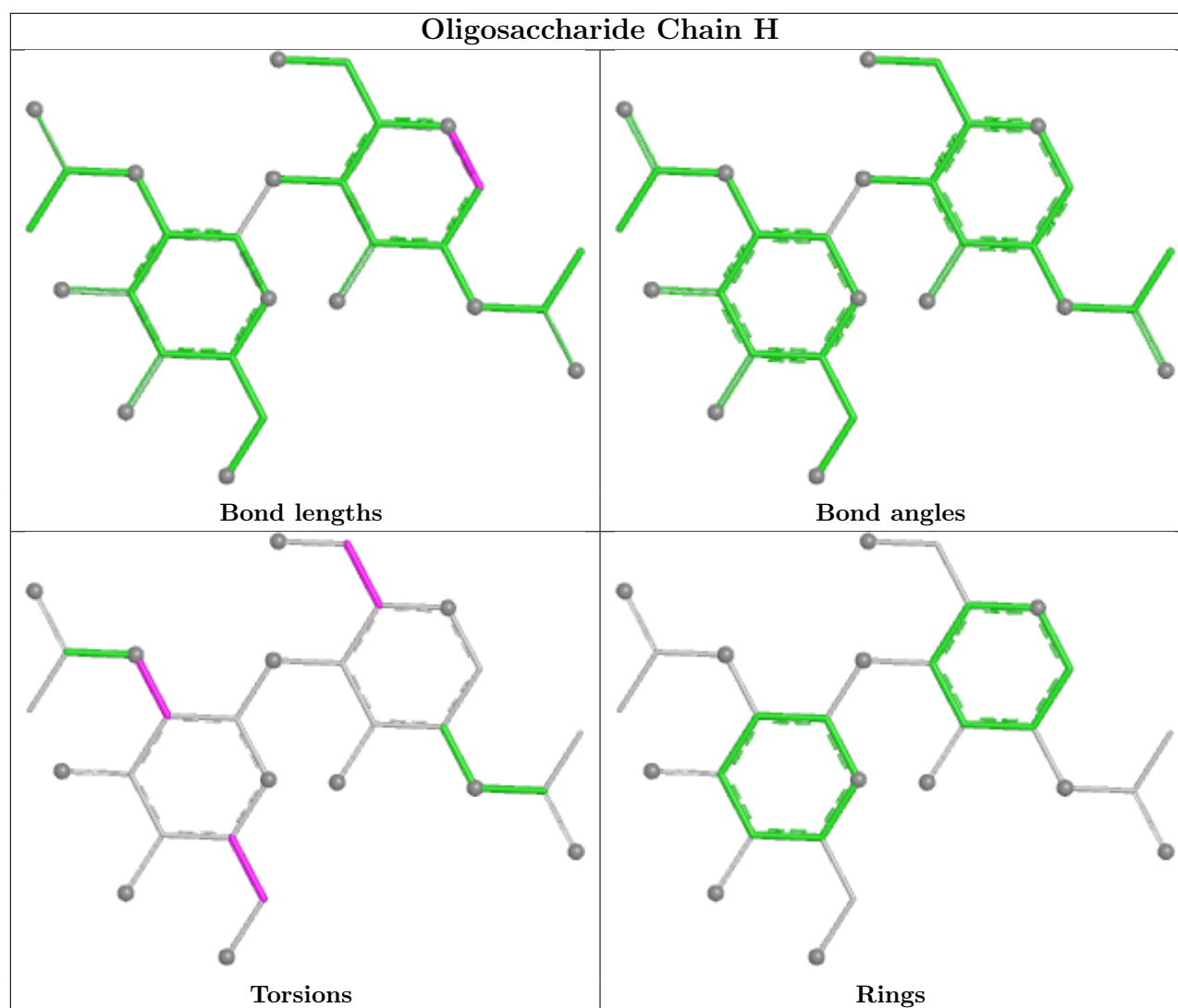
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7

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.





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	D	401	1	14,14,15	0.62	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	A	401	1	14,14,15	0.68	1 (7%)	17,19,21	0.74	1 (5%)
5	NAG	A	400	1	14,14,15	0.65	1 (7%)	17,19,21	1.05	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	400	1	14,14,15	0.36	0	17,19,21	0.65	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	D	401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	400	1	-	3/6/23/26	0/1/1/1
5	NAG	D	400	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	401	NAG	C1-C2	2.44	1.55	1.52
5	A	400	NAG	C1-C2	2.15	1.55	1.52
5	D	401	NAG	C1-C2	2.01	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	400	NAG	C2-N2-C7	3.20	127.19	122.90
5	D	401	NAG	C1-O5-C5	2.78	115.91	112.19
5	A	401	NAG	C1-O5-C5	2.58	115.65	112.19
5	D	400	NAG	C1-O5-C5	2.28	115.25	112.19
5	A	400	NAG	C1-O5-C5	2.21	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	D	401	NAG	O5-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
5	D	400	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	D	400	NAG	O5-C5-C6-O6

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	312/327 (95%)	0.56	24 (7%)	19 14	43, 61, 87, 141	0
1	D	312/327 (95%)	0.68	29 (9%)	14 10	44, 64, 93, 119	0
2	B	215/227 (94%)	0.17	7 (3%)	49 39	36, 49, 77, 106	0
2	E	214/227 (94%)	0.28	7 (3%)	49 39	38, 50, 81, 109	0
3	C	213/215 (99%)	0.26	6 (2%)	55 45	42, 53, 75, 112	0
3	F	211/215 (98%)	0.36	7 (3%)	49 39	41, 54, 72, 84	0
All	All	1477/1538 (96%)	0.42	80 (5%)	31 24	36, 56, 84, 141	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	319	GLY	5.6
3	C	39	LYS	4.8
2	B	136	SER	4.6
1	A	22	GLY	3.8
3	F	182	LEU	3.6
1	A	339	VAL	3.6
1	D	22	GLY	3.3
1	D	302	LYS	3.3
1	A	49	CYS	3.2
1	D	26	CYS	3.2
3	F	183	SER	3.1
1	A	267	SER	3.0
2	E	170	SER	3.0
1	A	271	GLU	2.9
2	E	198	LEU	2.9
1	A	312	GLY	2.9
1	D	339	VAL	2.9
1	D	39	PRO	2.8
1	D	58	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	104	GLY	2.7
2	E	195	SER	2.7
1	A	321	MET	2.6
1	A	313	GLU	2.6
1	D	248	VAL	2.6
3	F	146	LYS	2.5
3	C	126	LEU	2.5
3	C	193	TYR	2.5
1	D	71	VAL	2.5
1	A	104	LEU	2.5
3	F	15	PRO	2.5
1	D	105	GLY	2.5
1	D	104	LEU	2.4
2	B	103	TRP	2.4
1	D	202	PHE	2.4
1	A	250	GLU	2.4
1	A	26	CYS	2.4
1	D	312	GLY	2.4
1	D	52	ASP	2.4
3	C	127	LYS	2.4
1	A	309	HIS	2.3
1	D	160	SER	2.3
3	F	18	ARG	2.3
1	A	36	ALA	2.3
1	D	266	CYS	2.3
2	B	221	GLU	2.3
1	A	41	LEU	2.2
1	A	273	THR	2.2
1	D	254	LYS	2.2
1	D	309	HIS	2.2
1	D	321	MET	2.2
3	F	157	SER	2.2
3	F	210	PHE	2.2
1	A	28	GLY	2.2
1	A	320	GLY	2.2
1	D	49	CYS	2.2
2	B	222	PRO	2.1
1	A	105	GLY	2.1
3	C	213	GLY	2.1
2	E	103	TRP	2.1
1	A	269	SER	2.1
2	B	199	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	47	TRP	2.1
1	D	70	TYR	2.1
2	E	1	GLN	2.1
2	E	199	GLY	2.1
1	A	158	SER	2.1
2	B	104	GLY	2.1
1	A	171	ARG	2.1
1	D	136	ASP	2.1
1	D	164	SER	2.0
1	D	169	SER	2.0
1	D	42	LEU	2.0
1	A	217	GLU	2.0
1	A	308	VAL	2.0
1	D	199	GLN	2.0
1	D	267	SER	2.0
1	A	292	CYS	2.0
3	C	97	ASN	2.0
1	D	273	THR	2.0
1	D	86	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

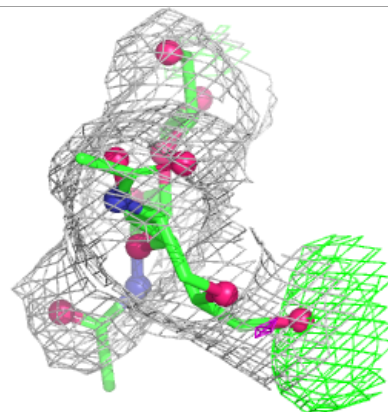
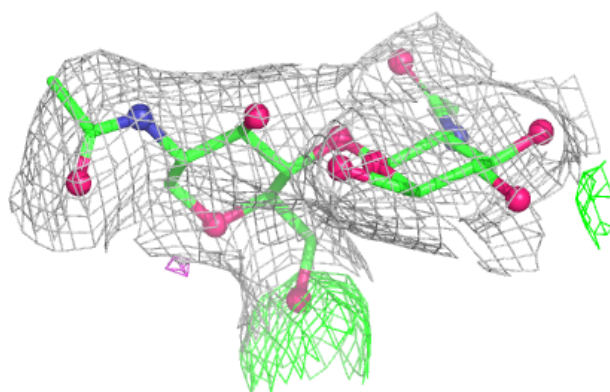
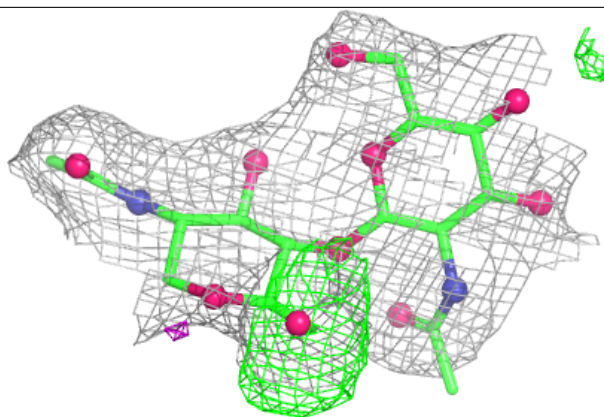
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	1	14/15	0.66	0.18	63,80,86,90	0
4	NAG	G	1	14/15	0.75	0.12	58,68,72,74	0
4	NAG	H	2	14/15	0.78	0.11	85,89,92,93	0
4	NAG	G	2	14/15	0.85	0.11	69,76,80,81	0

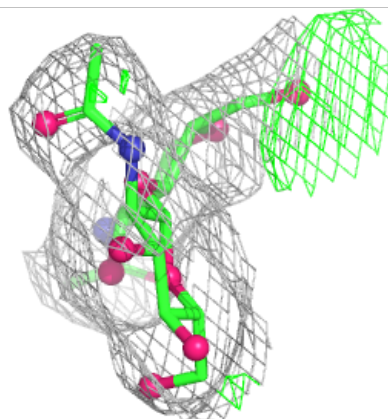
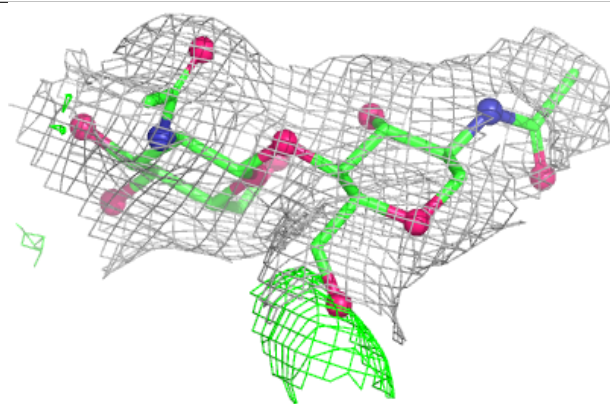
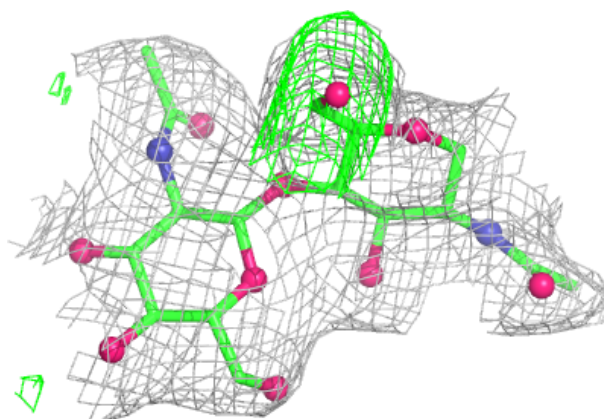
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	400	14/15	0.46	0.23	91,99,109,117	0
5	NAG	D	400	14/15	0.71	0.16	104,106,116,118	0
5	NAG	A	401	14/15	0.73	0.16	53,67,76,90	0
5	NAG	D	401	14/15	0.73	0.17	67,79,89,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.