



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:55 PM BST

PDB ID : 5T0B
Title : Crystal structure of H6 hemagglutinin G225D mutant from Taiwan (2013)
H6N1 influenza virus in complex with 6'-SLN
Authors : Wilson, I.A.; Tzarum, N.; Zhu, X.
Deposited on : 2016-08-15
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

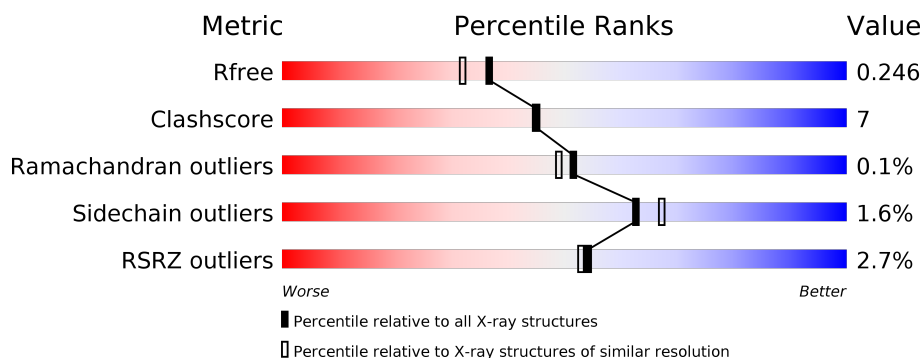
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



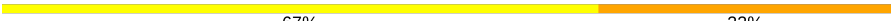
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	333	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	333	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	E	333	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
2	B	180	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>.</div> </div> </div>
2	D	180	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
2	F	180	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	3	 <div>67% 33%</div>

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12607 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2604	1650	443	498	13			
1	C	326	Total	C	N	O	S	0	0	0
			2573	1631	437	492	13			
1	E	325	Total	C	N	O	S	0	0	0
			2569	1629	437	490	13			

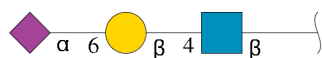
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASP	GLY	engineered mutation	UNP A0A0J9X268
C	225	ASP	GLY	engineered mutation	UNP A0A0J9X268
E	225	ASP	GLY	engineered mutation	UNP A0A0J9X268

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

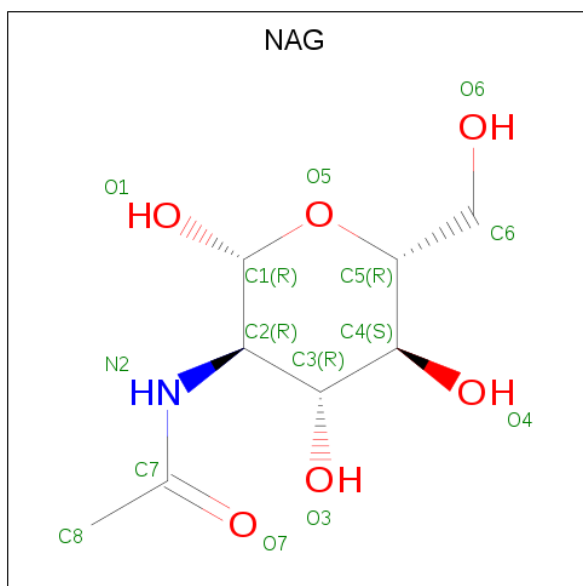
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1393	868	244	274	7			
2	D	172	Total	C	N	O	S	0	0	0
			1385	862	243	273	7			
2	F	172	Total	C	N	O	S	0	0	0
			1385	862	243	273	7			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total	O	0	0
			113	113		
5	B	86	Total	O	0	0
			86	86		
5	C	135	Total	O	0	0
			135	135		

Continued on next page...

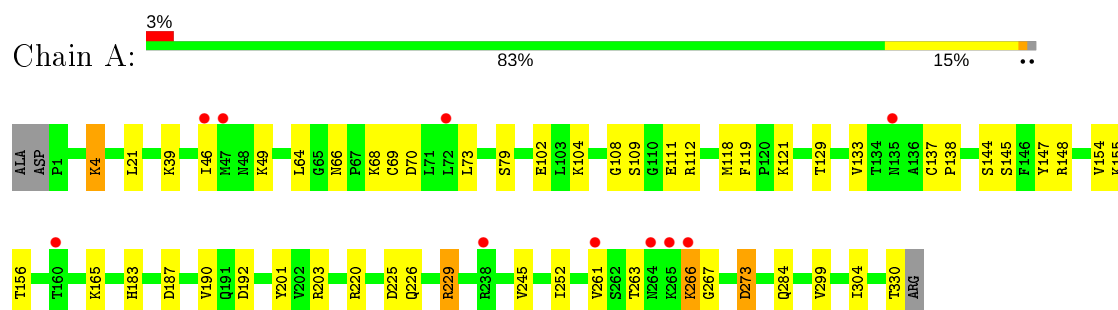
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	65	Total 65	O 65	0	0
5	E	114	Total 114	O 114	0	0
5	F	69	Total 69	O 69	0	0

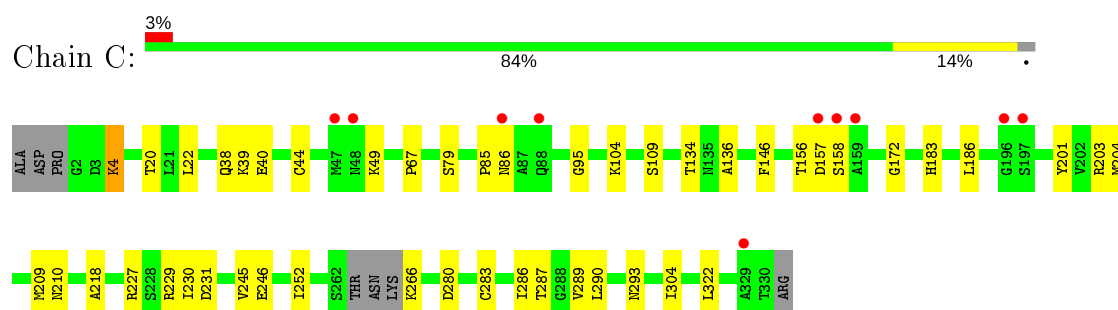
3 Residue-property plots [i](#)

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.

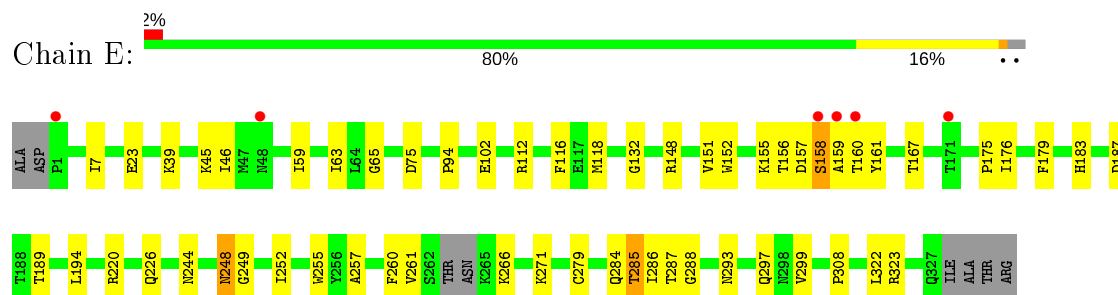
- Molecule 1: Hemagglutinin



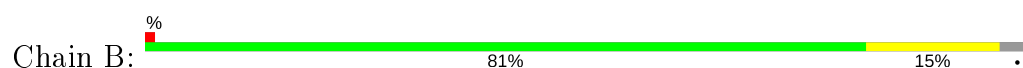
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

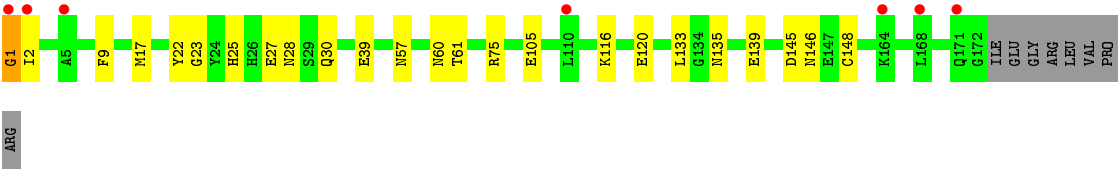
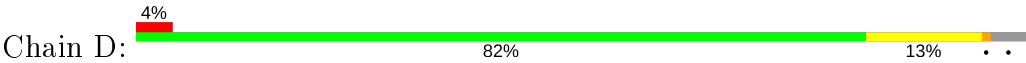


- Molecule 2: Hemagglutinin HA2 chain

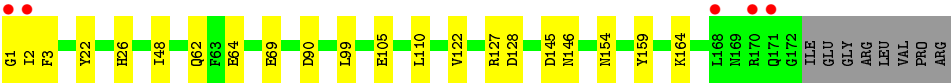
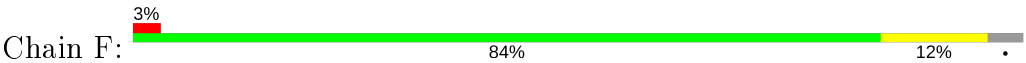




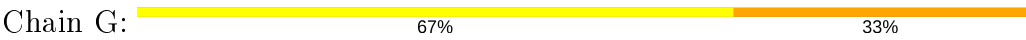
● Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



● Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.52Å 98.93Å 133.66Å 90.00° 126.63° 90.00°	Depositor
Resolution (Å)	49.54 – 2.00 49.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.54-2.00) 92.1 (49.54-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.214 , 0.246 0.215 , 0.246	Depositor DCC
R_{free} test set	6286 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12607	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SIA, GAL, 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	6/2666 (0.2%)	0.73	4/3628 (0.1%)
1	C	0.60	4/2633 (0.2%)	0.69	3/3582 (0.1%)
1	E	0.52	0/2630	0.68	0/3576
2	B	0.54	0/1421	0.61	0/1913
2	D	0.53	0/1413	0.65	1/1902 (0.1%)
2	F	0.50	0/1413	0.68	1/1902 (0.1%)
All	All	0.56	10/12176 (0.1%)	0.68	9/16503 (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	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	LYS	CD-CE	7.26	1.69	1.51
1	C	104	LYS	CE-NZ	7.18	1.67	1.49
1	A	104	LYS	CE-NZ	6.74	1.66	1.49
1	A	4	LYS	CB-CG	6.13	1.69	1.52
1	C	104	LYS	CD-CE	6.03	1.66	1.51
1	A	4	LYS	CE-NZ	5.93	1.63	1.49
1	C	4	LYS	CD-CE	5.87	1.66	1.51
1	A	4	LYS	CG-CD	5.55	1.71	1.52
1	A	104	LYS	CD-CE	5.37	1.64	1.51
1	C	4	LYS	CE-NZ	5.03	1.61	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	CD-CE-NZ	10.19	135.15	111.70
2	F	1	GLY	N-CA-C	-9.49	89.36	113.10
2	D	1	GLY	N-CA-C	-9.38	89.66	113.10
1	C	4	LYS	CD-CE-NZ	8.01	130.13	111.70
1	A	229	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	229	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	229	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	229	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	108	GLY	N-CA-C	-5.58	99.16	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LYS	Peptide

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	2604	0	2552	38	0
1	C	2573	0	2517	33	0
1	E	2569	0	2515	38	0
2	B	1393	0	1309	19	0
2	D	1385	0	1300	18	0
2	F	1385	0	1296	16	0
3	G	46	0	40	2	0
4	A	28	0	26	0	0
4	E	28	0	26	0	0
4	F	14	0	13	4	0
5	A	113	0	0	4	0
5	B	86	0	0	3	0
5	C	135	0	0	7	0
5	D	65	0	0	3	0
5	E	114	0	0	4	0
5	F	69	0	0	4	0
All	All	12607	0	11594	154	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 7.

All (154) 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:F:154:ASN:ND2	4:F:201:NAG:H82	1.78	0.98
1:C:134:THR:HG22	1:C:136:ALA:H	1.32	0.92
1:E:159:ALA:O	1:E:160:THR:OG1	1.90	0.89
1:C:266:LYS:O	1:C:304:ILE:HD11	1.84	0.78
1:C:156:THR:HG23	1:C:158:SER:H	1.49	0.78
1:C:20:THR:HG21	5:C:533:HOH:O	1.83	0.78
1:C:20:THR:HG22	1:C:22:LEU:H	1.50	0.77
1:C:201:TYR:OH	5:C:401:HOH:O	2.02	0.75
1:E:220:ARG:NH1	5:E:501:HOH:O	2.14	0.74
1:A:129:THR:O	5:A:502:HOH:O	2.08	0.72
2:B:17:MET:SD	2:B:23:GLY:HA3	2.29	0.72
2:F:90:ASP:OD2	5:F:301:HOH:O	2.06	0.72
1:A:4:LYS:HG2	2:B:27:GLU:HB3	1.72	0.71
1:A:111:GLU:HB3	1:A:263:THR:HB	1.71	0.71
1:C:4:LYS:NZ	2:D:25:HIS:NE2	2.37	0.70
5:C:480:HOH:O	2:D:61:THR:HG22	1.92	0.69
1:C:246:GLU:OE1	5:C:401:HOH:O	2.13	0.66
1:C:293:ASN:OD1	5:C:402:HOH:O	2.12	0.66
2:B:167:LYS:O	2:B:171:GLN:HG2	1.96	0.66
2:B:139:GLU:OE2	5:B:201:HOH:O	2.14	0.65
4:F:201:NAG:C1	4:F:201:NAG:H82	2.26	0.65
2:D:17:MET:SD	2:D:23:GLY:HA3	2.37	0.64
2:B:95:ASN:OD1	5:B:202:HOH:O	2.14	0.64
1:E:46:ILE:HD11	1:E:284:GLN:HB2	1.79	0.63
2:B:2:ILE:HG23	2:B:3:PHE:CD1	2.34	0.63
2:D:28:ASN:ND2	2:D:146:ASN:OD1	2.30	0.63
2:B:38:ARG:NE	5:B:207:HOH:O	2.31	0.62
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.82	0.61
2:F:145:ASP:OD1	2:F:146:ASN:N	2.33	0.61
3:G:3:SIA:O7	3:G:3:SIA:O10	2.09	0.60
2:D:145:ASP:HB3	2:D:148:CYS:H	1.67	0.59
2:F:154:ASN:CG	4:F:201:NAG:H82	2.23	0.59
1:E:285:THR:HB	1:E:288:GLY:O	2.03	0.59
1:E:285:THR:HG22	1:E:287:THR:H	1.67	0.59
2:F:2:ILE:HG23	2:F:3:PHE:CD1	2.38	0.59
2:D:133:LEU:HD11	2:D:139:GLU:HB2	1.83	0.59
1:E:156:THR:HG22	1:E:158:SER:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ASN:HB3	2:D:30:GLN:H	1.69	0.58
2:F:164:LYS:HG2	5:F:316:HOH:O	2.03	0.57
1:E:266:LYS:NZ	2:F:64:GLU:OE2	2.35	0.57
1:E:7:ILE:HD11	2:F:122:VAL:HG21	1.86	0.57
2:F:26:HIS:HD2	5:F:320:HOH:O	1.87	0.57
1:A:226:GLN:OE1	5:A:503:HOH:O	2.17	0.57
1:A:112:ARG:HB3	1:A:261:VAL:CG1	2.35	0.56
1:A:133:VAL:CG1	1:A:144:SER:HB3	2.35	0.56
2:B:30:GLN:OE1	2:B:145:ASP:HB2	2.06	0.56
1:C:156:THR:CG2	1:C:158:SER:HB3	2.35	0.56
1:E:158:SER:O	1:E:159:ALA:HB3	2.06	0.56
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.40	0.56
1:C:156:THR:HG23	1:C:158:SER:N	2.19	0.55
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.89	0.55
1:C:20:THR:HG22	1:C:22:LEU:N	2.20	0.54
1:A:192:ASP:OD2	5:A:504:HOH:O	2.18	0.54
2:B:98:LEU:HD21	2:F:99:LEU:HD13	1.90	0.53
4:F:201:NAG:C8	4:F:201:NAG:C1	2.86	0.53
1:C:4:LYS:HG2	2:D:27:GLU:HB3	1.91	0.53
1:E:285:THR:CG2	1:E:287:THR:H	2.20	0.53
1:C:209:MET:HG2	1:C:210:ASN:N	2.22	0.53
1:A:201:TYR:CD1	1:A:203:ARG:HG3	2.43	0.53
1:A:187:ASP:HB3	1:A:190:VAL:H	1.74	0.52
1:A:226:GLN:O	1:A:229:ARG:NH2	2.42	0.52
1:E:159:ALA:C	1:E:160:THR:HG1	2.02	0.52
1:E:118:MET:HE2	1:E:257:ALA:HB2	1.91	0.52
1:E:151:VAL:HG23	1:E:255:TRP:HB2	1.91	0.51
1:C:44:CYS:SG	1:C:289:VAL:HG21	2.50	0.51
1:A:46:ILE:CD1	1:A:304:ILE:HG23	2.40	0.51
1:A:49:LYS:HB3	1:A:79:SER:HB3	1.91	0.51
1:E:187:ASP:HB3	1:E:189:THR:H	1.76	0.50
1:A:64:LEU:O	1:A:147:TYR:HB3	2.12	0.50
1:C:20:THR:HG23	2:D:105:GLU:HB2	1.93	0.50
2:B:75:ARG:N	1:E:102:GLU:OE2	2.33	0.49
2:D:57:ASN:ND2	5:D:202:HOH:O	2.40	0.49
1:E:112:ARG:HB3	1:E:261:VAL:CG1	2.42	0.49
1:A:155:LYS:NZ	1:A:156:THR:O	2.34	0.49
1:E:132:GLY:HA3	1:E:152:TRP:HB3	1.96	0.48
1:C:186:LEU:HD13	1:C:227:ARG:HB2	1.94	0.48
1:A:118:MET:HE3	1:A:119:PHE:CD1	2.49	0.48
1:E:155:LYS:HB2	1:E:194:LEU:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:CYS:SG	1:C:290:LEU:HB2	2.54	0.47
1:A:102:GLU:OE2	2:D:75:ARG:N	2.36	0.47
1:A:39:LYS:HD3	1:A:299:VAL:HG13	1.95	0.47
1:A:4:LYS:NZ	2:B:25:HIS:NE2	2.50	0.47
2:F:48:ILE:HD11	2:F:110:LEU:HD23	1.97	0.47
1:A:266:LYS:HB3	1:A:267:GLY:HA2	1.96	0.47
1:E:271:LYS:NZ	2:F:69:GLU:OE2	2.44	0.47
1:C:38:GLN:HG3	5:C:489:HOH:O	2.15	0.47
2:B:159:TYR:CZ	2:B:163:GLN:HG3	2.50	0.46
1:C:266:LYS:O	1:C:304:ILE:CD1	2.60	0.46
1:E:183:HIS:HB2	1:E:252:ILE:HD11	1.97	0.46
1:E:23:GLU:CD	1:E:323:ARG:HH22	2.18	0.46
1:E:75:ASP:OD2	5:E:502:HOH:O	2.20	0.46
1:C:49:LYS:HB3	1:C:79:SER:HB3	1.97	0.46
1:A:46:ILE:HD11	1:A:284:GLN:HB3	1.96	0.46
1:A:70:ASP:OD2	1:A:148:ARG:NH2	2.49	0.46
1:A:220:ARG:HB3	1:A:229:ARG:NH1	2.30	0.46
1:E:286:ILE:HG23	1:E:287:THR:HG23	1.98	0.46
1:E:63:ILE:HD13	1:E:179:PHE:CZ	2.51	0.46
1:A:121:LYS:CG	1:A:129:THR:HG21	2.46	0.46
2:D:116:LYS:HE3	2:D:120:GLU:OE2	2.16	0.46
2:F:127:ARG:HD2	2:F:159:TYR:CD1	2.51	0.45
1:A:273:ASP:OD1	5:A:505:HOH:O	2.21	0.45
1:E:116:PHE:HZ	1:E:176:ILE:HD13	1.82	0.45
1:A:121:LYS:CD	1:A:129:THR:HG21	2.47	0.45
2:D:1:GLY:CA	5:D:201:HOH:O	2.62	0.45
2:B:9:PHE:O	2:B:135:ASN:HA	2.18	0.44
2:D:1:GLY:N	5:D:201:HOH:O	2.22	0.44
1:C:40:GLU:HB2	1:C:289:VAL:HB	1.99	0.44
1:E:39:LYS:HD3	1:E:299:VAL:HG13	1.99	0.44
1:C:209:MET:CG	1:C:210:ASN:N	2.79	0.44
2:B:3:PHE:CE1	2:B:113:ALA:HB2	2.53	0.44
2:D:145:ASP:N	2:D:148:CYS:HB3	2.32	0.44
1:E:285:THR:HG22	1:E:287:THR:N	2.31	0.44
1:E:297:GLN:HG2	1:E:308:PRO:HD2	2.00	0.44
1:E:59:ILE:O	1:E:63:ILE:HG13	2.17	0.44
2:B:11:GLU:HG3	2:B:135:ASN:OD1	2.17	0.44
1:C:186:LEU:HA	1:C:218:ALA:O	2.18	0.44
2:F:127:ARG:HB2	2:F:159:TYR:CE1	2.52	0.44
1:C:172:GLY:HA3	5:C:445:HOH:O	2.18	0.44
1:C:286:ILE:HG23	1:C:287:THR:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:LYS:HG3	1:E:279:CYS:O	2.18	0.44
1:E:167:THR:HG22	1:E:244:ASN:ND2	2.33	0.44
2:B:124:SER:O	2:B:127:ARG:NE	2.50	0.43
1:E:102:GLU:HG3	5:E:547:HOH:O	2.16	0.43
1:E:94:PRO:HG3	1:E:226:GLN:HB2	2.00	0.43
2:B:18:ILE:HG12	2:B:18:ILE:H	1.60	0.43
1:A:183:HIS:HB2	1:A:252:ILE:CD1	2.48	0.43
2:B:141:TRP:HB2	2:B:166:SER:HB2	2.01	0.43
1:E:175:PRO:HD2	1:E:260:PHE:O	2.19	0.42
1:C:156:THR:HG23	1:C:158:SER:HB3	2.00	0.42
1:C:203:ARG:O	1:C:204:MET:HG3	2.18	0.42
1:A:68:LYS:HE2	1:A:138:PRO:HG2	2.01	0.42
2:F:105:GLU:OE1	5:F:302:HOH:O	2.21	0.42
2:D:9:PHE:O	2:D:135:ASN:HA	2.20	0.42
1:C:95:GLY:HA3	1:C:230:ILE:O	2.19	0.42
1:A:133:VAL:HG13	1:A:145:SER:N	2.35	0.41
1:C:204:MET:HG2	1:C:245:VAL:HG22	2.02	0.41
1:A:66:ASN:HB3	1:A:69:CYS:SG	2.60	0.41
2:D:133:LEU:HD11	2:D:139:GLU:CB	2.50	0.41
1:E:161:TYR:CD1	1:E:248:ASN:O	2.73	0.41
2:D:2:ILE:HG21	2:D:2:ILE:HD13	1.75	0.41
1:C:67:PRO:HG3	1:C:146:PHE:O	2.21	0.41
1:A:133:VAL:HG12	1:A:144:SER:HB3	2.01	0.41
1:A:109:SER:C	1:A:263:THR:HG22	2.41	0.41
1:C:85:PRO:HG2	1:C:86:ASN:ND2	2.36	0.41
1:E:65:GLY:O	1:E:148:ARG:HG2	2.20	0.41
1:A:154:VAL:HG12	1:A:155:LYS:O	2.20	0.41
1:A:229:ARG:HD2	5:E:528:HOH:O	2.21	0.41
2:B:19:ASP:N	2:B:19:ASP:OD1	2.54	0.41
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.26	0.40
1:A:109:SER:O	1:A:263:THR:HG22	2.21	0.40
1:A:165:LYS:HA	1:A:245:VAL:O	2.21	0.40
1:A:154:VAL:HG21	3:G:3:SIA:H111	2.04	0.40
1:E:285:THR:HG21	1:E:299:VAL:HG12	2.04	0.40
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

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	328/333 (98%)	318 (97%)	9 (3%)	1 (0%)	41	37
1	C	322/333 (97%)	315 (98%)	7 (2%)	0	100	100
1	E	321/333 (96%)	312 (97%)	9 (3%)	0	100	100
2	B	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
2	D	170/180 (94%)	167 (98%)	3 (2%)	0	100	100
2	F	170/180 (94%)	170 (100%)	0	0	100	100
All	All	1482/1539 (96%)	1451 (98%)	30 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	CYS

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	290/292 (99%)	286 (99%)	4 (1%)	67	72
1	C	286/292 (98%)	280 (98%)	6 (2%)	53	57
1	E	286/292 (98%)	280 (98%)	6 (2%)	53	57
2	B	147/153 (96%)	147 (100%)	0	100	100
2	D	146/153 (95%)	143 (98%)	3 (2%)	53	57
2	F	146/153 (95%)	144 (99%)	2 (1%)	67	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1301/1335 (98%)	1280 (98%)	21 (2%)	62 67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	225	ASP
1	A	273	ASP
1	A	330	THR
1	C	39	LYS
1	C	109	SER
1	C	157	ASP
1	C	231	ASP
1	C	280	ASP
1	C	322	LEU
2	D	22	TYR
2	D	39	GLU
2	D	60	ASN
1	E	157	ASP
1	E	158	SER
1	E	248	ASN
1	E	285	THR
1	E	293	ASN
1	E	322	LEU
2	F	22	TYR
2	F	62	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	163	GLN
1	C	86	ASN
2	D	169	ASN
1	E	244	ASN
2	F	26	HIS

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 ⓘ

3 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	G	1	3	15,15,15	0.56	0	21,21,21	0.98	1 (4%)
3	GAL	G	2	3	11,11,12	0.64	0	15,15,17	0.77	1 (6%)
3	SIA	G	3	3	17,20,21	0.73	0	21,28,31	1.35	1 (4%)

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	G	1	3	-	2/6/26/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
3	SIA	G	3	3	-	2/14/34/38	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	G	3	SIA	C3-C2-C1	3.49	119.54	111.93
3	G	1	NAG	O5-C1-C2	2.22	111.75	109.52
3	G	2	GAL	O5-C1-C2	-2.09	107.55	110.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

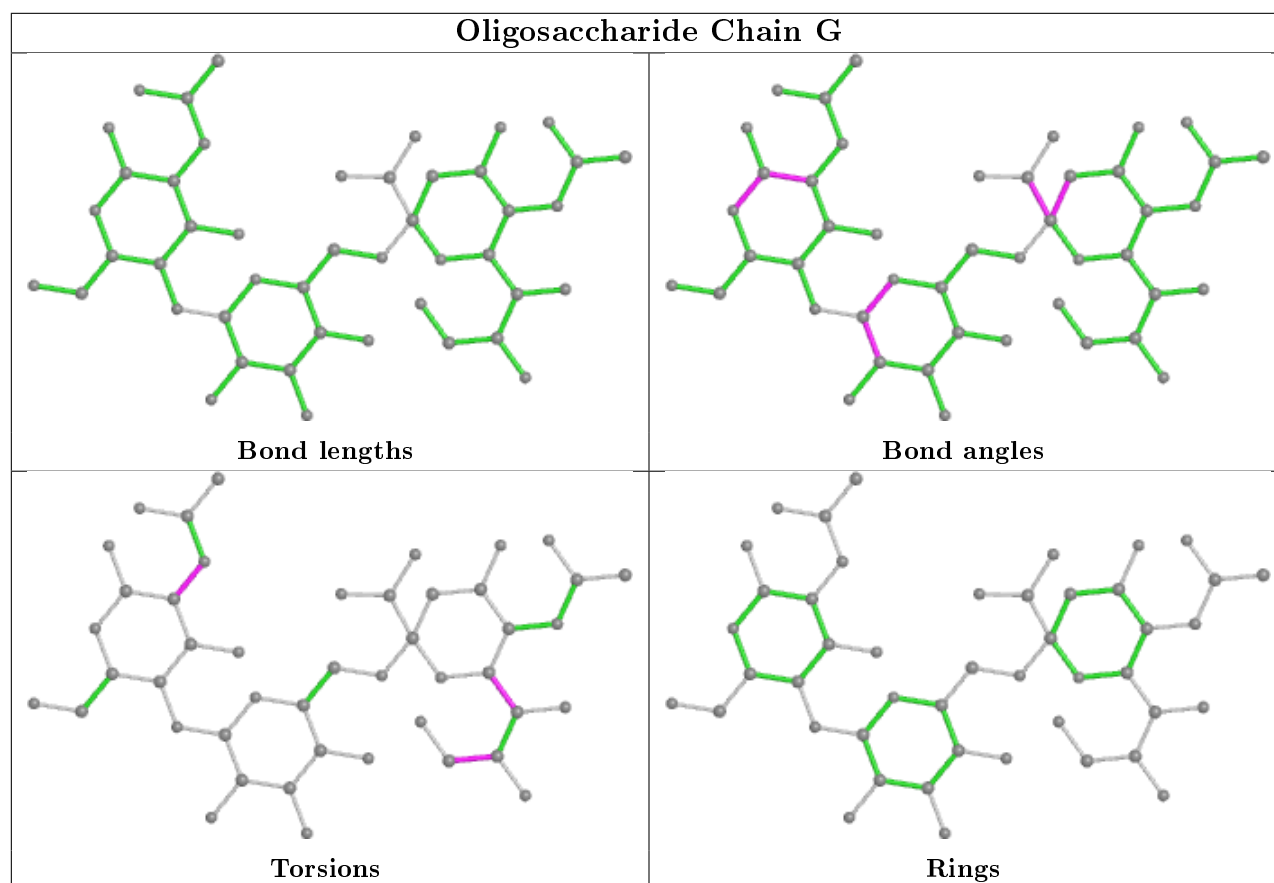
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C1-C2-N2-C7
3	G	3	SIA	O6-C6-C7-O7
3	G	3	SIA	C7-C8-C9-O9
3	G	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	SIA	2	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.



5.6 Ligand geometry [i](#)

5 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
4	NAG	A	401	1	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
4	NAG	A	402	1	14,14,15	0.66	0	17,19,21	1.82	5 (29%)
4	NAG	F	201	2	14,14,15	0.50	0	17,19,21	2.17	6 (35%)
4	NAG	E	401	1	14,14,15	0.50	0	17,19,21	1.49	3 (17%)
4	NAG	E	402	1	14,14,15	0.75	0	17,19,21	1.72	4 (23%)

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	A	401	1	-	5/6/23/26	0/1/1/1
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	4/6/23/26	0/1/1/1
4	NAG	E	401	1	-	4/6/23/26	0/1/1/1
4	NAG	E	402	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	NAG	C2-N2-C7	5.79	131.15	122.90
4	A	402	NAG	C1-C2-N2	4.26	117.76	110.49
4	A	402	NAG	C6-C5-C4	-3.88	103.93	113.00
4	E	402	NAG	O5-C5-C6	3.75	113.09	107.20
4	E	402	NAG	C6-C5-C4	-3.69	104.35	113.00
4	A	401	NAG	O5-C5-C6	-3.66	101.47	107.20
4	E	401	NAG	C2-N2-C7	3.47	127.84	122.90
4	F	201	NAG	C1-C2-N2	3.40	116.30	110.49
4	E	402	NAG	O3-C3-C2	-3.08	103.10	109.47
4	E	401	NAG	C1-O5-C5	2.80	115.99	112.19
4	F	201	NAG	O4-C4-C5	2.80	116.24	109.30
4	E	401	NAG	C1-C2-N2	-2.76	105.78	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	NAG	C1-O5-C5	2.75	115.92	112.19
4	E	402	NAG	C1-O5-C5	2.75	115.91	112.19
4	F	201	NAG	C1-O5-C5	2.74	115.90	112.19
4	F	201	NAG	O5-C5-C6	-2.58	103.15	107.20
4	A	402	NAG	O5-C5-C6	-2.53	103.24	107.20
4	F	201	NAG	O6-C6-C5	-2.45	102.88	111.29
4	A	401	NAG	O6-C6-C5	-2.28	103.46	111.29
4	A	402	NAG	C2-N2-C7	-2.21	119.76	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	F	201	NAG	C1-C2-N2-C7
4	F	201	NAG	C8-C7-N2-C2
4	F	201	NAG	O7-C7-N2-C2
4	E	401	NAG	C8-C7-N2-C2
4	E	401	NAG	O7-C7-N2-C2
4	E	402	NAG	C8-C7-N2-C2
4	E	402	NAG	O7-C7-N2-C2
4	A	401	NAG	O5-C5-C6-O6
4	E	402	NAG	O5-C5-C6-O6
4	A	401	NAG	C4-C5-C6-O6
4	A	401	NAG	C1-C2-N2-C7
4	E	402	NAG	C4-C5-C6-O6
4	E	401	NAG	O5-C5-C6-O6
4	E	401	NAG	C4-C5-C6-O6
4	F	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	201	NAG	4	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, 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	330/333 (99%)	0.06	10 (3%) 50 49	28, 44, 60, 75	0
1	C	326/333 (97%)	0.01	10 (3%) 49 48	29, 38, 53, 75	0
1	E	325/333 (97%)	0.04	6 (1%) 68 66	29, 39, 52, 74	0
2	B	173/180 (96%)	0.16	2 (1%) 79 78	26, 34, 52, 74	0
2	D	172/180 (95%)	0.26	7 (4%) 37 36	26, 37, 55, 68	0
2	F	172/180 (95%)	0.13	5 (2%) 51 50	27, 36, 55, 71	0
All	All	1498/1539 (97%)	0.09	40 (2%) 54 53	26, 39, 56, 75	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	159	ALA	11.1
2	D	1	GLY	5.9
2	B	1	GLY	5.7
1	C	196	GLY	5.0
2	F	1	GLY	4.7
1	A	46	ILE	4.2
1	A	265	LYS	4.0
1	C	158	SER	3.6
1	C	159	ALA	3.5
1	E	1	PRO	3.5
2	D	168	LEU	3.5
2	D	171	GLN	3.4
1	C	48	ASN	3.4
2	F	168	LEU	3.3
1	A	264	ASN	3.2
2	B	2	ILE	3.1
1	C	329	ALA	3.1
1	E	158	SER	3.0
1	C	47	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	157	ASP	2.9
1	C	86	ASN	2.9
1	A	47	MET	2.9
2	F	170	ARG	2.5
1	E	171	THR	2.4
2	D	2	ILE	2.4
2	F	2	ILE	2.3
1	A	238	ARG	2.3
2	F	171	GLN	2.3
1	C	197	SER	2.3
2	D	110	LEU	2.2
1	A	160	THR	2.2
2	D	164	LYS	2.2
2	D	5	ALA	2.2
1	E	48	ASN	2.1
1	A	261	VAL	2.1
1	A	72	LEU	2.0
1	E	160	THR	2.0
1	A	135	ASN	2.0
1	A	266	LYS	2.0
1	C	88	GLN	2.0

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

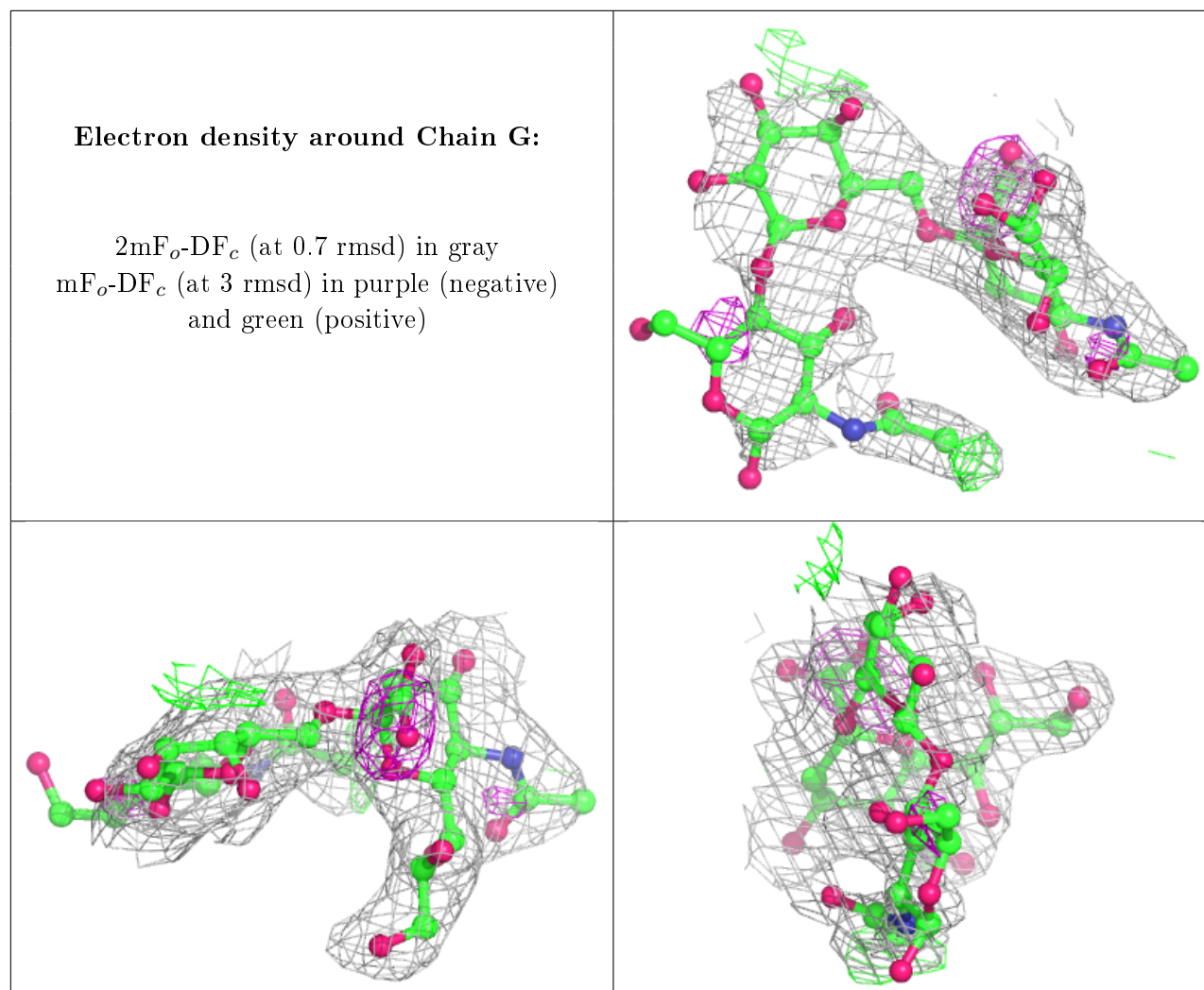
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
3	NAG	G	1	15/15	0.54	0.44	70,87,91,91	0
3	SIA	G	3	20/21	0.79	0.19	50,60,62,63	0
3	GAL	G	2	11/12	0.80	0.17	60,71,79,87	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.



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, 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(\AA^2)	Q<0.9
4	NAG	A	401	14/15	0.56	0.23	66,76,83,90	0
4	NAG	F	201	14/15	0.71	0.30	62,66,75,76	0
4	NAG	E	401	14/15	0.79	0.33	76,83,89,92	0
4	NAG	E	402	14/15	0.80	0.16	62,71,74,75	0
4	NAG	A	402	14/15	0.85	0.11	56,62,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.