Full wwPDB X-ray Structure Validation Report (i)

May 15, 2024 – 04:11 PM EDT

PDB ID	:	8G8C
Title	:	Crystal structure of DH1322.1 Fab in complex with HIV proximal MPER peptide
Authors	:	Niyongabo, A.; Janus, B.M.; Ofek, G.
Deposited on	:	2023-02-17
Resolution	:	2.08 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

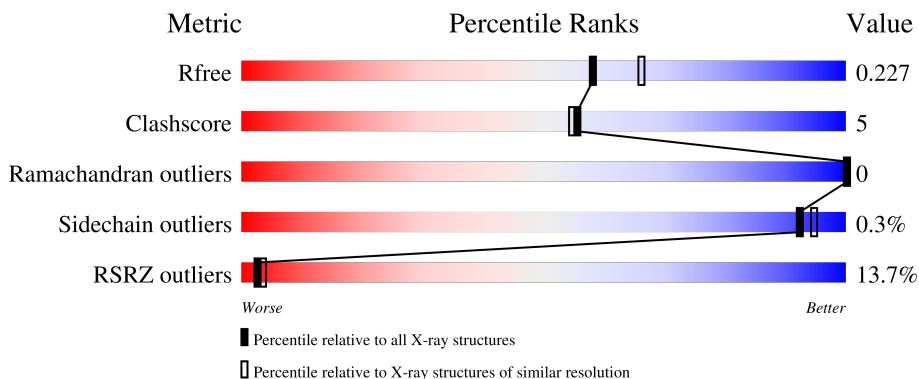|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.08 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		13.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	233	15% / 90% / 7% / ·
1	H	233	20% / 84% / 12% / ·
2	B	217	10% / 91% / 8%
2	L	217	6% / 89% / 10%
3	C	23	17% / 57% / 13% / 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	23	17% �— 74% — 22%
4	D	3	100%

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
4	BMA	D	3	-	-	-	X
5	NAG	H	301	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 14036 atoms, of which 6740 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 DH1322.1 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	225	Total 3303	C 1073	H 1619	N 280	O 326	S 5	0	0	0
1	A	226	Total 3315	C 1073	H 1629	N 282	O 326	S 5	0	0	0

- Molecule 2 is a protein called DH1322.1 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	216	Total 3209	C 1023	H 1574	N 280	O 328	S 4	0	0	0
2	B	216	Total 3244	C 1030	H 1598	N 282	O 330	S 4	0	0	0

- Molecule 3 is a protein called Env polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total 276	C 92	H 135	N 22	O 27	0	0	0
3	P	18	Total 266	C 88	H 125	N 23	O 30	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	650	LYS	-	expression tag	UNP A4UIY1
C	672	LYS	-	expression tag	UNP A4UIY1
P	650	LYS	-	expression tag	UNP A4UIY1
P	672	LYS	-	expression tag	UNP A4UIY1

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
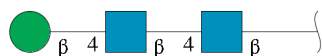
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total 73	C 22	H 34	N 2	O 15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total 27	C 8	H 13	N 1	O 5	0	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	47	Total 47	O 47	0	0
6	L	99	Total 99	O 99	0	0
6	A	44	Total 44	O 44	0	0
6	B	101	Total 101	O 101	0	0

Continued on next page...

Continued from previous page...

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total 4	O 4	0	0
6	P	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
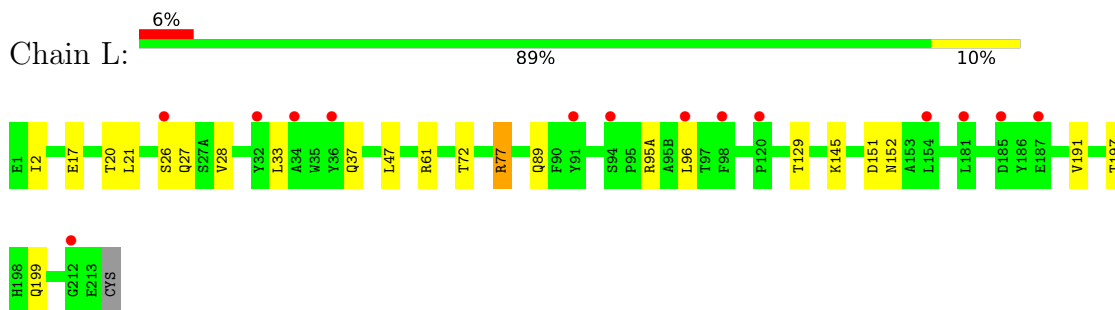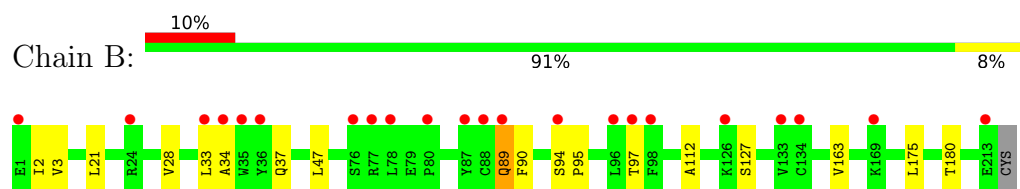
- Molecule 1: DH1322.1 heavy chain
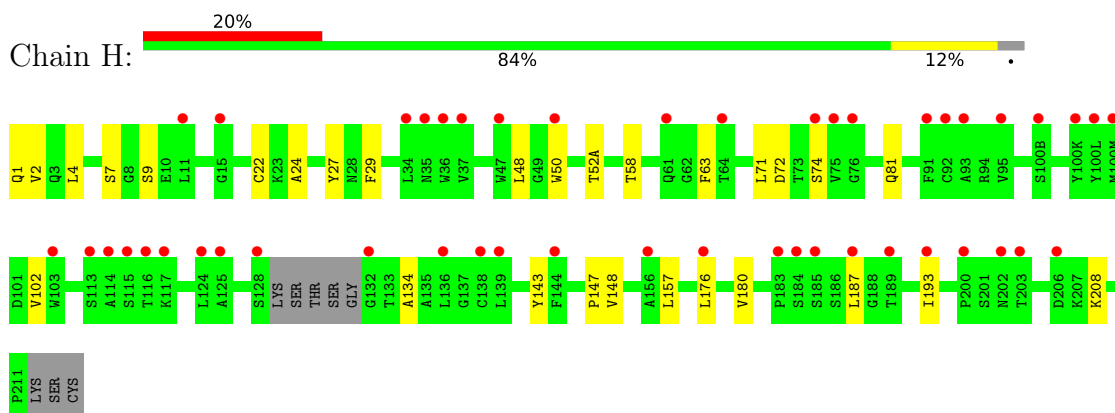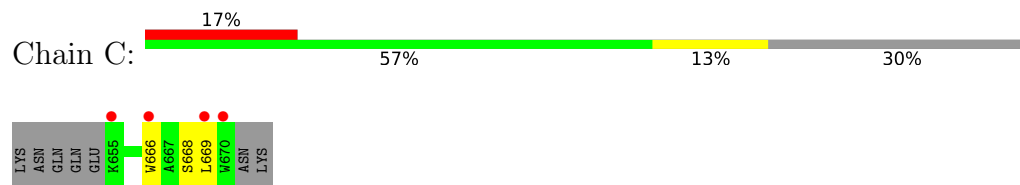

- Molecule 1: DH1322.1 heavy chain
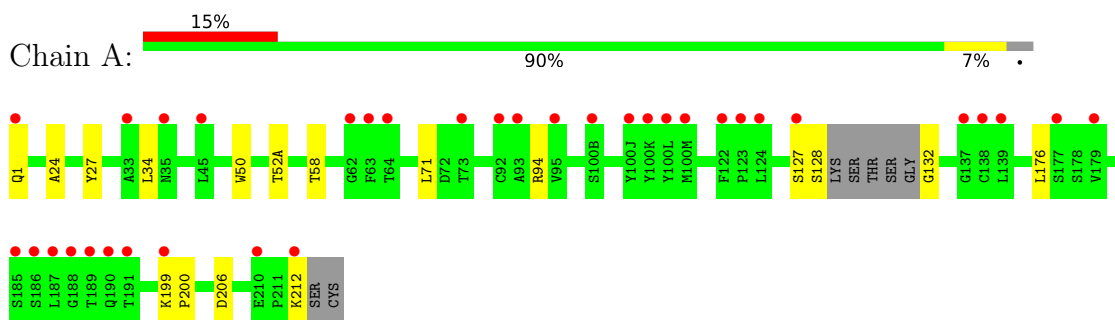
- Molecule 2: DH1322.1 light chain

- Molecule 2: DH1322.1 light chain

Chain B:

• Molecule 3: Env polyprotein

Chain C:
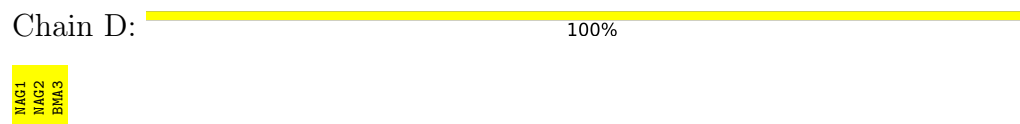

• Molecule 3: Env polyprotein

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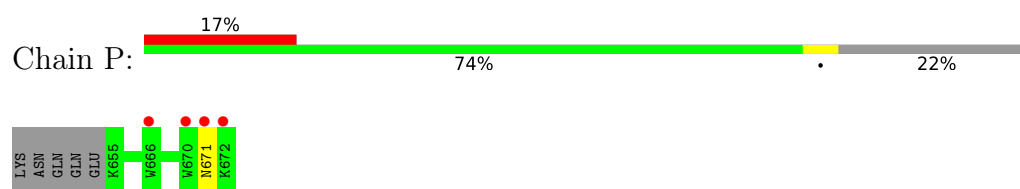
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	75.31Å 182.95Å 84.41Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	28.68 – 2.08 28.68 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.68-2.08) 97.0 (28.68-2.08)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.199 , 0.229 0.206 , 0.227	Depositor DCC
R_{free} test set	2023 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.1	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14036	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.61	0/1732	0.79	0/2364
1	H	0.61	1/1731 (0.1%)	0.79	1/2365 (0.0%)
2	B	0.67	0/1682	0.76	0/2283
2	L	0.72	0/1671	0.83	1/2271 (0.0%)
3	C	0.55	0/144	0.69	0/194
3	P	0.63	0/142	0.53	0/192
All	All	0.65	1/7102 (0.0%)	0.79	2/9669 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	147	PRO	N-CD	-7.12	1.37	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	77	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	H	147	PRO	CA-N-CD	5.44	119.31	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1686	1629	1628	12	1
1	H	1684	1619	1618	24	1
2	B	1646	1598	1598	12	2
2	L	1635	1574	1574	18	2
3	C	141	135	135	2	0
3	P	141	125	124	1	0
4	D	39	34	34	3	0
5	A	14	13	13	2	0
5	H	14	13	13	0	0
6	A	44	0	0	5	0
6	B	101	0	0	3	0
6	C	4	0	0	0	0
6	H	47	0	0	3	0
6	L	99	0	0	5	0
6	P	1	0	0	1	0
All	All	7296	6740	6737	70	3

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 5.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:OG	6:A:401:HOH:O	1.81	0.99
2:L:129:THR:OG1	6:L:301:HOH:O	1.81	0.96
1:H:148:VAL:CG2	1:H:176:LEU:HD21	1.97	0.94
2:B:34:ALA:HB3	2:B:89:GLN:HG2	1.58	0.85
1:H:52(A):THR:HA	1:H:71:LEU:HD11	1.60	0.83
6:H:447:HOH:O	4:D:3:BMA:O6	1.99	0.81
2:L:17:GLU:OE2	6:L:302:HOH:O	2.00	0.80
3:P:671:ASN:O	6:P:701:HOH:O	2.02	0.78
2:L:2:ILE:HD13	2:L:27:GLN:HG2	1.67	0.77
2:L:61:ARG:NH2	6:L:303:HOH:O	2.16	0.77
1:A:127:SER:CB	6:A:401:HOH:O	2.38	0.70
2:B:127:SER:HB2	6:B:302:HOH:O	1.94	0.68
1:H:81:GLN:HB2	4:D:1:NAG:H82	1.76	0.66
1:H:143:TYR:OH	1:H:176:LEU:HD23	1.96	0.64
2:B:180:THR:OG1	6:B:301:HOH:O	2.15	0.63
1:H:2:VAL:CG1	1:H:102:VAL:HG21	2.29	0.63
2:B:34:ALA:HB3	2:B:89:GLN:CG	2.29	0.61
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.82	0.60
1:H:148:VAL:HG22	1:H:176:LEU:HD21	1.81	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:GLN:CB	4:D:1:NAG:H82	2.32	0.59
1:A:1:GLN:OE1	1:A:1:GLN:N	2.33	0.58
1:A:212:LYS:N	6:A:404:HOH:O	2.36	0.57
1:H:148:VAL:HG23	1:H:176:LEU:HD21	1.82	0.57
2:B:97:THR:CG2	6:B:311:HOH:O	2.53	0.56
2:B:21:LEU:HD12	2:B:21:LEU:N	2.21	0.55
1:H:134:ALA:CB	1:H:187:LEU:HD11	2.36	0.55
2:L:2:ILE:HD12	2:L:26:SER:OG	2.06	0.55
1:A:24:ALA:HB1	1:A:27:TYR:CE1	2.42	0.54
2:L:28:VAL:CG1	2:L:33:LEU:HD11	2.37	0.54
1:A:176:LEU:C	1:A:176:LEU:HD12	2.29	0.53
2:L:17:GLU:OE1	6:L:304:HOH:O	2.18	0.53
1:H:2:VAL:HG12	1:H:102:VAL:HG21	1.90	0.52
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.91	0.51
1:H:48:LEU:HD22	1:H:63:PHE:CE1	2.45	0.51
1:H:7:SER:CB	6:H:401:HOH:O	2.46	0.51
1:H:24:ALA:HB1	1:H:27:TYR:CE1	2.46	0.51
1:H:193:ILE:HG22	1:H:208:LYS:HA	1.94	0.50
1:A:50:TRP:CD1	1:A:58:THR:HB	2.47	0.49
2:B:94:SER:HB3	2:B:95:PRO:CD	2.42	0.49
1:A:52(A):THR:HA	1:A:71:LEU:HD11	1.95	0.49
1:H:48:LEU:HD22	1:H:63:PHE:CD1	2.48	0.49
2:L:191:VAL:HB	2:B:3:VAL:HG11	1.95	0.48
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.95	0.48
5:A:301:NAG:C1	5:A:301:NAG:H82	2.45	0.47
1:H:29:PHE:CE2	1:H:71:LEU:HD22	2.50	0.47
5:A:301:NAG:C1	5:A:301:NAG:C8	2.92	0.47
1:H:143:TYR:CE1	1:H:148:VAL:HG13	2.50	0.46
2:L:21:LEU:HD12	2:L:21:LEU:N	2.30	0.46
1:A:128:SER:N	6:A:401:HOH:O	2.48	0.46
2:B:2:ILE:HG12	2:B:90:PHE:CD1	2.51	0.45
1:H:50:TRP:CD1	1:H:58:THR:HB	2.51	0.44
1:H:157:LEU:HD21	1:H:180:VAL:HG21	1.98	0.44
2:L:28:VAL:HG13	2:L:33:LEU:HD11	2.00	0.44
1:H:72:ASP:OD1	1:H:74:SER:OG	2.33	0.44
1:A:132:GLY:N	6:A:405:HOH:O	2.50	0.44
1:A:199:LYS:N	1:A:200:PRO:HD2	2.32	0.44
1:H:7:SER:OG	6:H:401:HOH:O	1.88	0.44
2:L:199:GLN:HB2	6:L:309:HOH:O	2.17	0.43
2:L:151:ASP:O	2:L:152:ASN:HB2	2.18	0.43
2:L:95(A):ARG:HG2	3:C:668:SER:OG	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:LEU:HB3	1:H:22:CYS:SG	2.59	0.42
1:A:34:LEU:HD23	1:A:94:ARG:HA	2.02	0.42
2:L:145:LYS:HB3	2:L:197:THR:HB	2.00	0.42
1:H:143:TYR:CD1	1:H:148:VAL:HG13	2.54	0.42
2:B:28:VAL:CG1	2:B:33:LEU:HD11	2.49	0.42
2:L:28:VAL:HG12	2:L:33:LEU:HD11	2.03	0.41
2:L:20:THR:HG23	2:L:72:THR:CG2	2.51	0.41
2:L:89:GLN:HG3	2:L:96:LEU:HD21	2.03	0.40
1:H:29:PHE:CZ	1:H:71:LEU:HD22	2.56	0.40
3:C:666:TRP:HA	3:C:669:LEU:HD12	2.03	0.40

All (3) 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)
2:L:77:ARG:NH2	2:B:112:ALA:O[2_555]	2.11	0.09
2:L:77:ARG:HH22	2:B:112:ALA:O[2_555]	1.52	0.08
1:H:1:GLN:NE2	1:A:206:ASP:O[1_655]	2.19	0.01

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	222/233 (95%)	216 (97%)	6 (3%)	0	100	100
1	H	221/233 (95%)	211 (96%)	10 (4%)	0	100	100
2	B	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
2	L	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
3	C	14/23 (61%)	14 (100%)	0	0	100	100
3	P	16/23 (70%)	15 (94%)	1 (6%)	0	100	100
All	All	901/946 (95%)	875 (97%)	26 (3%)	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	186/195 (95%)	186 (100%)	0	100	100
1	H	186/195 (95%)	185 (100%)	1 (0%)	88	92
2	B	181/183 (99%)	180 (99%)	1 (1%)	86	89
2	L	178/183 (97%)	178 (100%)	0	100	100
3	C	15/22 (68%)	15 (100%)	0	100	100
3	P	14/22 (64%)	14 (100%)	0	100	100
All	All	760/800 (95%)	758 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	9	SER
2	B	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\#|Z| > 2$
4	NAG	D	1	4,1	14,14,15	0.58	0	17,19,21	0.80	0
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
4	BMA	D	3	4	11,11,12	0.32	0	15,15,17	0.59	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	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	NAG	O5-C5-C6	2.20	110.66	107.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0
4	D	1	NAG	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.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
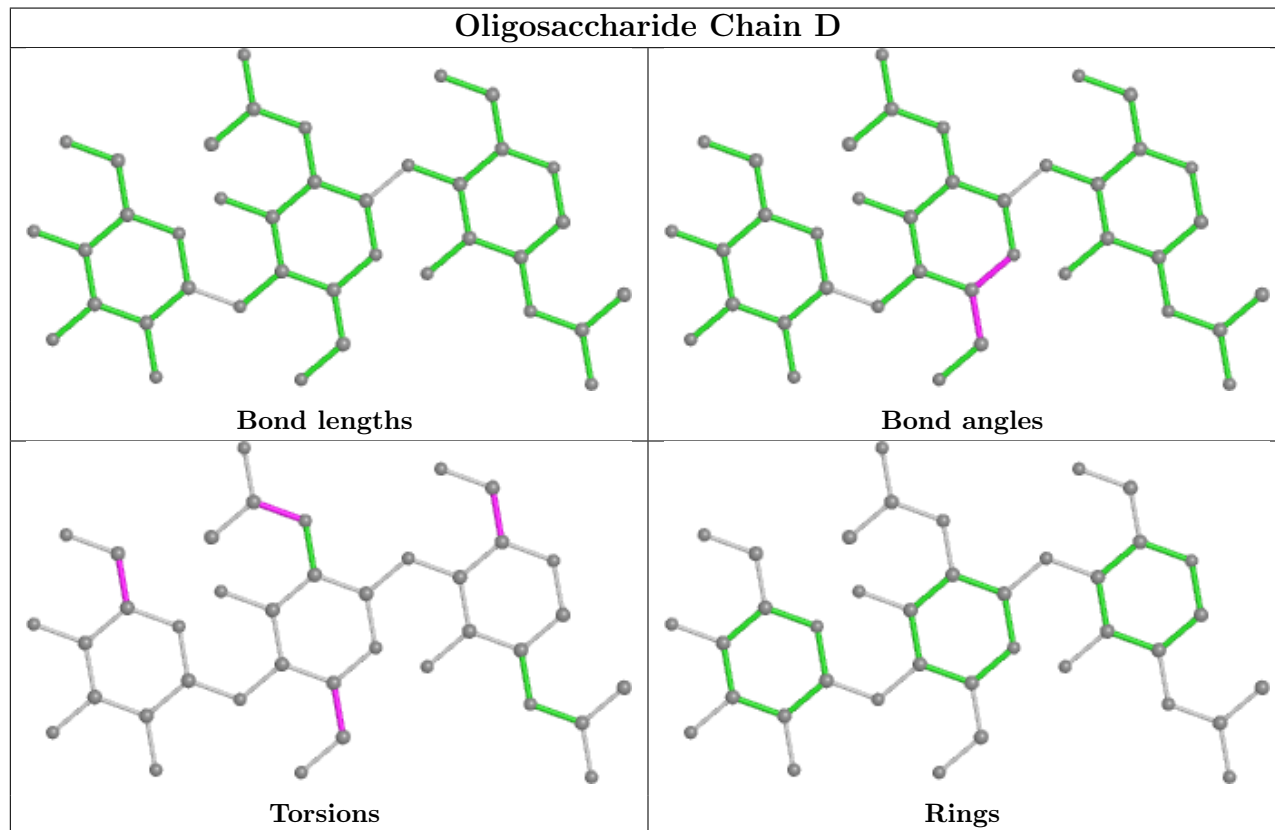
5.6 Ligand geometry (i)

2 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	H	301	1	14,14,15	0.85	0	17,19,21	0.94	0
5	NAG	A	301	1	14,14,15	0.64	0	17,19,21	1.56	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
5	NAG	H	301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	301	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	NAG	C2-N2-C7	3.11	127.33	122.90
5	A	301	NAG	O4-C4-C5	-2.77	102.42	109.30
5	A	301	NAG	C1-C2-N2	2.51	114.78	110.49
5	A	301	NAG	C8-C7-N2	2.34	120.06	116.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	NAG	O5-C5-C6-O6
5	A	301	NAG	C4-C5-C6-O6
5	A	301	NAG	C8-C7-N2-C2
5	A	301	NAG	O7-C7-N2-C2
5	A	301	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	NAG	2	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	226/233 (96%)	0.82	35 (15%)	2	2	40, 61, 91, 118	0
1	H	225/233 (96%)	1.04	47 (20%)	1	0	37, 66, 101, 129	0
2	B	216/217 (99%)	0.50	22 (10%)	6	8	34, 51, 86, 108	0
2	L	216/217 (99%)	0.31	14 (6%)	18	22	33, 49, 98, 113	0
3	C	16/23 (69%)	1.23	4 (25%)	0	0	51, 66, 103, 127	0
3	P	18/23 (78%)	1.16	4 (22%)	0	0	65, 78, 86, 86	0
All	All	917/946 (96%)	0.69	126 (13%)	3	3	33, 58, 96, 129	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	670	TRP	6.0
2	L	94	SER	5.2
1	H	187	LEU	4.9
2	B	94	SER	4.7
2	B	88	CYS	4.5
1	A	62	GLY	4.4
1	H	100(K)	TYR	4.2
1	H	75	VAL	4.1
2	B	36	TYR	4.1
3	P	666	TRP	4.0
1	H	74	SER	3.9
2	B	34	ALA	3.9
1	A	95	VAL	3.9
1	A	189	THR	3.9
1	H	93	ALA	3.7
1	H	138	CYS	3.7
1	H	36	TRP	3.6
1	A	212	LYS	3.6
1	A	63	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	203	THR	3.5
2	L	96	LEU	3.5
1	H	116	THR	3.4
1	H	189	THR	3.4
2	B	98	PHE	3.4
1	H	47	TRP	3.4
2	B	213	GLU	3.3
1	H	37	VAL	3.3
2	B	77	ARG	3.3
1	H	35	ASN	3.3
1	H	100(B)	SER	3.2
1	H	115	SER	3.2
1	A	188	GLY	3.2
1	A	138	CYS	3.1
1	A	92	CYS	3.1
1	A	177	SER	3.0
2	L	36	TYR	3.0
1	A	100(B)	SER	3.0
1	A	191	THR	3.0
2	B	134	CYS	3.0
1	H	184	SER	2.9
1	A	139	LEU	2.9
1	A	64	THR	2.9
1	A	100(K)	TYR	2.9
1	A	185	SER	2.9
1	H	100(M)	MET	2.9
2	L	212	GLY	2.8
1	A	73	THR	2.8
1	A	1	GLN	2.8
1	H	114	ALA	2.8
1	A	190	GLN	2.8
1	H	176	LEU	2.8
3	C	669	LEU	2.8
1	H	132	GLY	2.7
1	H	95	VAL	2.7
1	H	200	PRO	2.7
1	H	117	LYS	2.7
2	B	133	VAL	2.7
3	P	671	ASN	2.7
1	H	124	LEU	2.7
2	B	87	TYR	2.7
2	B	96	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	113	SER	2.7
2	L	32	TYR	2.6
1	A	124	LEU	2.6
2	L	181	LEU	2.6
2	L	91	TYR	2.6
1	A	122	PHE	2.6
3	C	655	LYS	2.6
1	A	93	ALA	2.6
1	H	92	CYS	2.6
1	H	139	LEU	2.6
1	H	183	PRO	2.6
2	B	76	SER	2.6
3	P	670	TRP	2.5
1	H	61	GLN	2.5
2	L	98	PHE	2.5
1	H	11	LEU	2.5
1	H	34	LEU	2.5
2	B	1	GLU	2.5
1	H	50	TRP	2.5
1	H	64	THR	2.5
1	A	199	LYS	2.4
2	B	89	GLN	2.4
2	L	154	LEU	2.4
1	H	100(L)	TYR	2.4
1	H	202	ASN	2.3
1	A	35	ASN	2.3
3	C	666	TRP	2.3
1	A	127	SER	2.3
2	L	187	GLU	2.3
1	H	185	SER	2.3
1	A	186	SER	2.3
2	B	24	ARG	2.3
1	H	193	ILE	2.3
2	L	26	SER	2.3
1	H	103	TRP	2.3
2	B	35	TRP	2.3
1	A	45	LEU	2.2
2	B	126	LYS	2.2
3	P	672	LYS	2.2
1	A	100(M)	MET	2.2
1	H	136	LEU	2.2
1	A	100(L)	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	15	GLY	2.2
2	L	185	ASP	2.2
1	A	33	ALA	2.2
1	H	144	PHE	2.2
1	H	206	ASP	2.2
1	A	179	VAL	2.2
1	A	123	PRO	2.2
1	H	125	ALA	2.2
2	B	78	LEU	2.1
2	B	97	THR	2.1
2	B	80	PRO	2.1
2	B	33	LEU	2.1
1	H	91	PHE	2.1
1	H	156	ALA	2.1
2	L	120	PRO	2.1
1	H	128	SER	2.1
1	A	100(J)	TYR	2.1
1	H	76	GLY	2.1
2	L	34	ALA	2.1
1	A	187	LEU	2.0
1	A	137	GLY	2.0
1	A	210	GLU	2.0
2	B	169	LYS	2.0

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

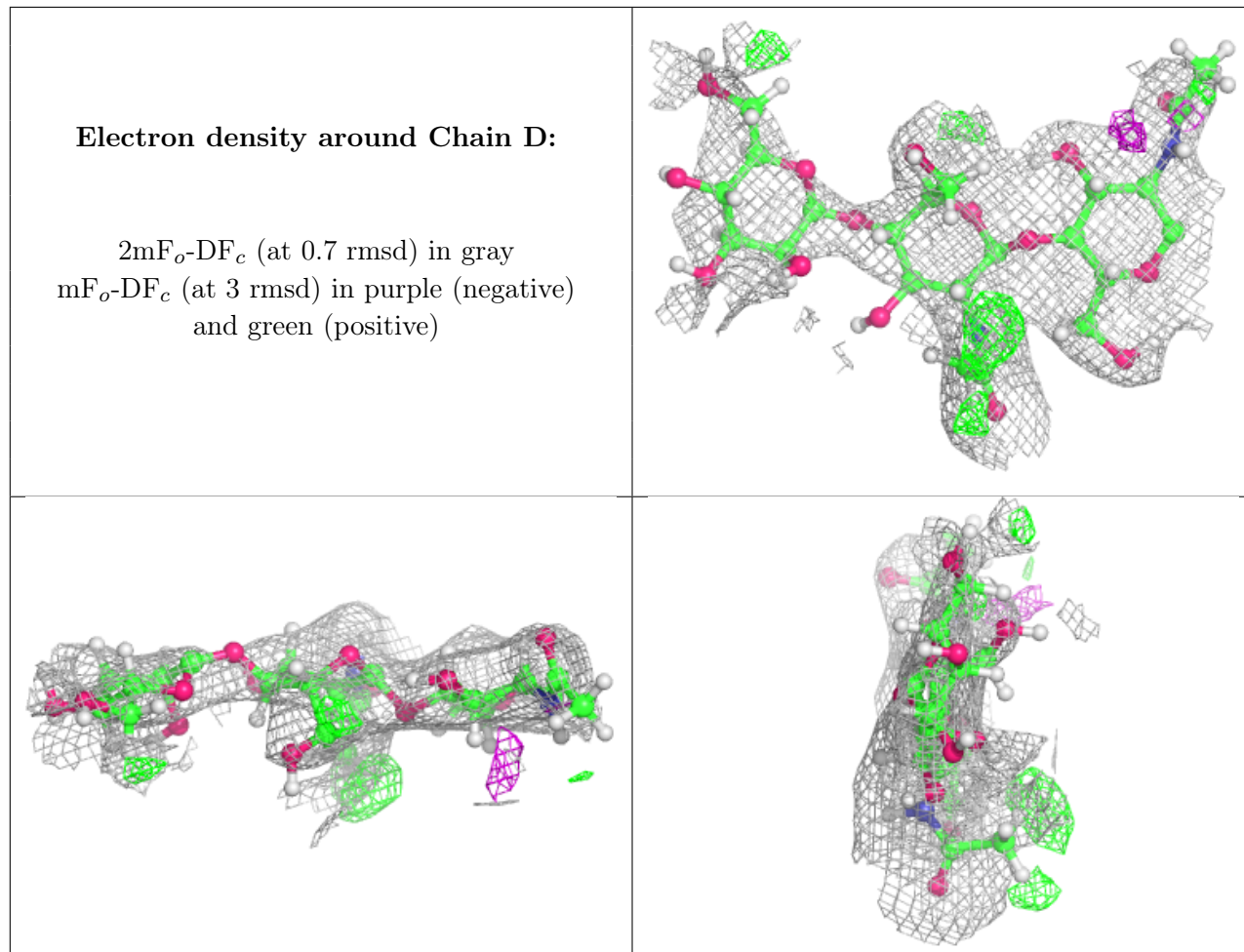There are no non-standard protein/DNA/RNA residues in this entry.

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(Å^2)	Q<0.9
4	NAG	D	2	14/15	0.50	0.36	83,111,134,138	0
4	BMA	D	3	11/12	0.67	0.48	105,124,147,150	0
4	NAG	D	1	14/15	0.78	0.20	64,77,91,98	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

$2mF_o$-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, 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
5	NAG	H	301	14/15	0.64	0.48	128,160,185,197	0
5	NAG	A	301	14/15	0.70	0.20	73,87,103,111	0

6.5 Other polymers ⓘ

There are no such residues in this entry.