Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:29 PM BST

PDB ID	:	4LEO
Title	:	Crystal structure of anti-HER3 Fab RG7116 in complex with the extracellular domains of human Her3 (ERBB3)
Authors	:	Schiller, C.B.; Hopfner, K.P.
Deposited on	:	2013-06-26
Resolution	:	2.64 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:

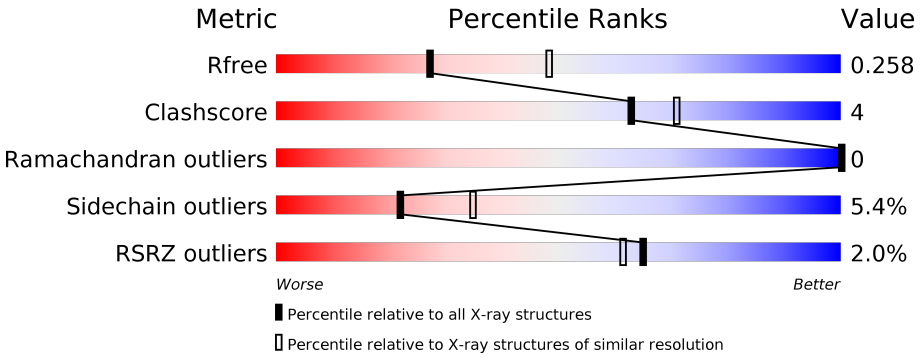
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	227	2% 83% 10% • 6%
2	B	220	88% 11%
3	C	621	2% 83% 13% • •
4	D	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8185 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 RG7116 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	60	0	0
			1618	1020	273	318	7			

- Molecule 2 is a protein called RG7116 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	61	0	0
			1697	1062	282	348	5			

- Molecule 3 is a protein called Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	601	Total	C	N	O	S	257	0	0
			4622	2861	834	868	59			

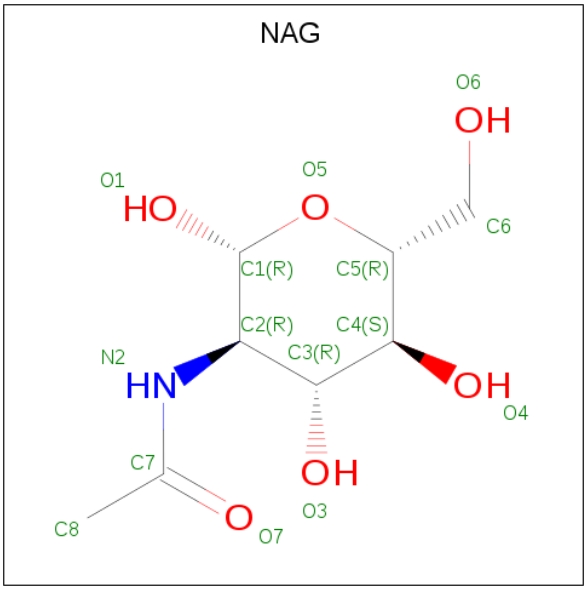
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	613	ALA	-	expression tag	UNP P21860
C	614	ALA	-	expression tag	UNP P21860
C	615	ALA	-	expression tag	UNP P21860
C	616	LEU	-	expression tag	UNP P21860
C	617	GLU	-	expression tag	UNP P21860
C	618	VAL	-	expression tag	UNP P21860
C	619	LEU	-	expression tag	UNP P21860
C	620	PHE	-	expression tag	UNP P21860
C	621	GLN	-	expression tag	UNP P21860

- 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	D	2	Total C N O 28 16 2 10	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	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	5	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0

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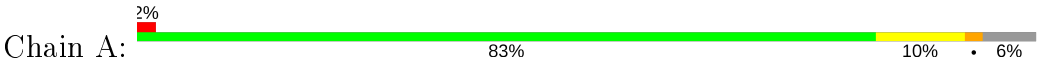
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	38	Total O 38 38	0	0
6	C	83	Total O 83 83	0	0

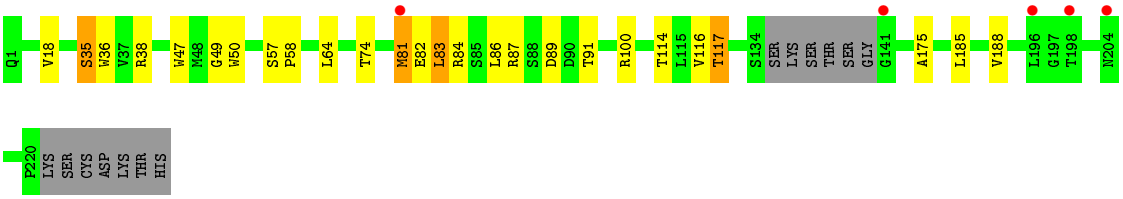
3 Residue-property plots (i)

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: RG7116 Fab heavy chain

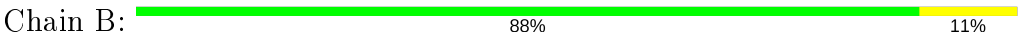
Chain A:

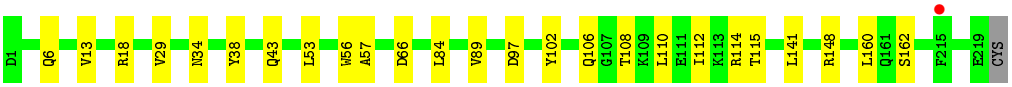




- Molecule 2: RG7116 Fab light chain

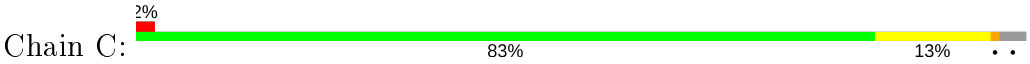
Chain B:

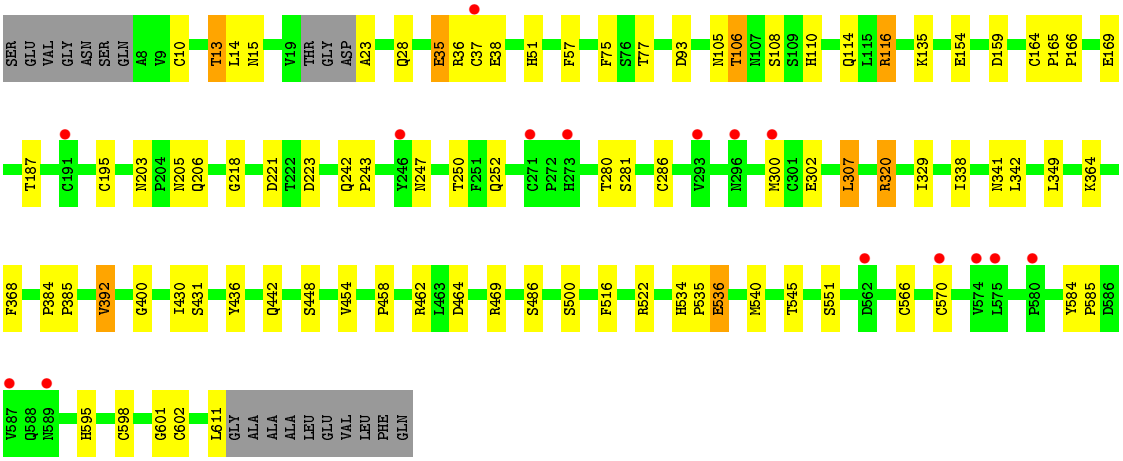




- Molecule 3: Receptor tyrosine-protein kinase erbB-3

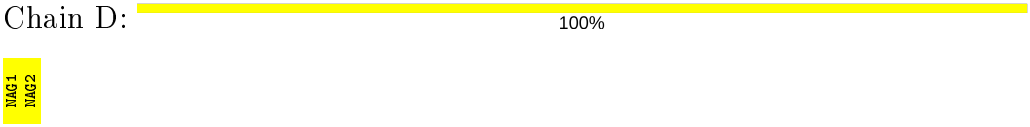
Chain C:





- Molecule 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	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.46Å 59.36Å 103.66Å 97.64° 106.85° 96.83°	Depositor
Resolution (Å)	48.83 – 2.64 48.83 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.83-2.64) 95.8 (48.83-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.228 , 0.258 0.228 , 0.258	Depositor DCC
R_{free} test set	1712 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8185	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: 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	0.23	0/1658	0.41	0/2261
2	B	0.32	0/1734	0.41	0/2356
3	C	0.28	0/4733	0.48	2/6422 (0.0%)
All	All	0.28	0/8125	0.45	2/11039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	116	ARG	NE-CZ-NH2	9.43	125.01	120.30
3	C	307	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1618	0	1583	11	0
2	B	1697	0	1638	11	0
3	C	4622	0	4386	45	0
4	D	28	0	25	0	0
5	C	70	0	65	0	0
6	A	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	38	0	0	0	0
6	C	83	0	0	2	0
All	All	8185	0	7697	63	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 4.

All (63) 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:B:34:ASN:HB3	3:C:154:GLU:HG2	1.60	0.84
1:A:18:VAL:HG23	1:A:86:LEU:HD11	1.67	0.76
3:C:247:ASN:HB3	3:C:250:THR:HG22	1.67	0.76
3:C:522:ARG:NH2	3:C:540:MET:O	2.20	0.75
2:B:34:ASN:CB	3:C:154:GLU:HG2	2.18	0.73
3:C:35:GLU:HB3	3:C:57:PHE:HB2	1.71	0.73
3:C:534:HIS:ND1	3:C:535:PRO:O	2.23	0.72
3:C:516:PHE:O	3:C:522:ARG:NH1	2.26	0.68
3:C:105:ASN:ND2	3:C:108:SER:OG	2.33	0.60
1:A:91:THR:HG23	1:A:117:THR:HA	1.86	0.58
3:C:601:GLY:HA3	3:C:611:LEU:HA	1.85	0.58
3:C:522:ARG:NH1	3:C:545:THR:OG1	2.38	0.57
3:C:77:THR:HG22	3:C:114:GLN:HB2	1.88	0.56
2:B:38:TYR:HB3	2:B:97:ASP:HB3	1.87	0.56
3:C:10:CYS:N	3:C:37:CYS:SG	2.79	0.55
3:C:37:CYS:SG	3:C:38:GLU:N	2.79	0.55
2:B:89:VAL:HG11	2:B:112:ILE:HG13	1.89	0.55
1:A:175:ALA:HA	1:A:185:LEU:HB3	1.90	0.54
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.44	0.53
3:C:250:THR:HG23	3:C:252:GLN:HG2	1.93	0.51
3:C:436:TYR:HD1	3:C:464:ASP:HB3	1.76	0.51
3:C:105:ASN:OD1	3:C:106:THR:N	2.45	0.50
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.94	0.50
3:C:320:ARG:NH2	6:C:861:HOH:O	2.44	0.50
3:C:486:SER:OG	3:C:500:SER:OG	2.26	0.49
3:C:329:ILE:HG12	3:C:364:LYS:HB3	1.95	0.49
3:C:535:PRO:O	3:C:536:GLU:HB2	2.13	0.49
2:B:13:VAL:HB	2:B:84:LEU:HD22	1.95	0.48
2:B:6:GLN:O	2:B:106:GLN:NE2	2.46	0.48
1:A:175:ALA:HB2	1:A:185:LEU:HD23	1.97	0.47
3:C:551:SER:HB2	3:C:566:CYS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:ALA:N	6:C:878:HOH:O	2.50	0.45
3:C:368:PHE:HB2	3:C:392:VAL:HG13	1.99	0.45
2:B:56:TRP:O	2:B:57:ALA:HB3	2.17	0.44
3:C:442:GLN:HA	3:C:469:ARG:HD2	1.99	0.44
1:A:36:TRP:CE2	1:A:81:MET:HB3	2.52	0.44
1:A:35:SER:OG	1:A:50:TRP:HB3	2.17	0.44
3:C:13:THR:HG23	3:C:15:ASN:H	1.83	0.44
3:C:105:ASN:CG	3:C:108:SER:OG	2.56	0.43
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.99	0.43
3:C:36:ARG:O	3:C:36:ARG:HG2	2.17	0.43
3:C:105:ASN:HD22	3:C:110:HIS:HB2	1.82	0.43
3:C:384:PRO:HA	3:C:385:PRO:HD3	1.82	0.43
2:B:102:TYR:OH	3:C:159:ASP:OD1	2.31	0.43
3:C:338:ILE:HD13	3:C:342:LEU:HD21	2.00	0.43
3:C:458:PRO:O	3:C:462:ARG:HD3	2.19	0.42
3:C:164:CYS:HA	3:C:165:PRO:HD3	1.87	0.42
3:C:242:GLN:HA	3:C:243:PRO:HD3	1.90	0.42
3:C:51:HIS:HA	3:C:75:PHE:HA	2.01	0.42
3:C:165:PRO:HA	3:C:166:PRO:HD3	1.94	0.42
3:C:584:TYR:HB3	3:C:602:CYS:SG	2.59	0.42
3:C:218:GLY:H	3:C:223:ASP:HB3	1.86	0.41
3:C:320:ARG:H	3:C:320:ARG:HG2	1.70	0.41
3:C:203:ASN:HB3	3:C:206:GLN:CD	2.41	0.41
3:C:203:ASN:HD22	3:C:206:GLN:HG3	1.85	0.41
2:B:114:ARG:HG2	2:B:115:THR:N	2.36	0.41
3:C:400:GLY:O	3:C:431:SER:HB2	2.21	0.41
1:A:188:VAL:HG11	2:B:141:LEU:HD22	2.03	0.41
3:C:595:HIS:HB3	3:C:598:CYS:SG	2.61	0.41
1:A:91:THR:HA	1:A:116:VAL:O	2.22	0.40
3:C:218:GLY:N	3:C:223:ASP:HB3	2.36	0.40
3:C:430:ILE:HG13	3:C:454:VAL:HG12	2.03	0.40
1:A:57:SER:HA	1:A:58:PRO:HD3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/227 (92%)	204 (97%)	6 (3%)	0	100	100
2	B	217/220 (99%)	212 (98%)	5 (2%)	0	100	100
3	C	597/621 (96%)	556 (93%)	41 (7%)	0	100	100
All	All	1024/1068 (96%)	972 (95%)	52 (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	182/194 (94%)	169 (93%)	13 (7%)	14	22
2	B	194/195 (100%)	186 (96%)	8 (4%)	30	47
3	C	521/535 (97%)	494 (95%)	27 (5%)	23	36
All	All	897/924 (97%)	849 (95%)	48 (5%)	22	35

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	38	ARG
1	A	64	LEU
1	A	74	THR
1	A	81	MET
1	A	82	GLU
1	A	83	LEU
1	A	84	ARG
1	A	87	ARG
1	A	89	ASP
1	A	100	ARG

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Mol	Chain	Res	Type
1	A	114	THR
1	A	117	THR
2	B	18	ARG
2	B	29	VAL
2	B	66	ASP
2	B	108	THR
2	B	110	LEU
2	B	148	ARG
2	B	160	LEU
2	B	162	SER
3	C	13	THR
3	C	14	LEU
3	C	28	GLN
3	C	35	GLU
3	C	93	ASP
3	C	106	THR
3	C	116	ARG
3	C	135	LYS
3	C	169	GLU
3	C	187	THR
3	C	195	CYS
3	C	205	ASN
3	C	221	ASP
3	C	280	THR
3	C	281	SER
3	C	286	CYS
3	C	300	MET
3	C	302	GLU
3	C	307	LEU
3	C	320	ARG
3	C	341	ASN
3	C	349	LEU
3	C	392	VAL
3	C	448	SER
3	C	536	GLU
3	C	570	CYS
3	C	585	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	28	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

2 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	3,4	14,14,15	1.23	1 (7%)	17,19,21	1.34	2 (11%)
4	NAG	D	2	4	14,14,15	1.23	1 (7%)	17,19,21	1.46	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	D	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	2.60	1.56	1.52
4	D	2	NAG	C1-C2	2.32	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	NAG	O3-C3-C2	2.83	115.33	109.47
4	D	2	NAG	O3-C3-C2	2.79	115.25	109.47
4	D	2	NAG	C4-C3-C2	2.71	114.99	111.02
4	D	1	NAG	C4-C3-C2	2.27	114.35	111.02
4	D	2	NAG	C3-C4-C5	2.11	114.01	110.24
4	D	2	NAG	C6-C5-C4	-2.07	108.15	113.00

There are no chirality outliers.

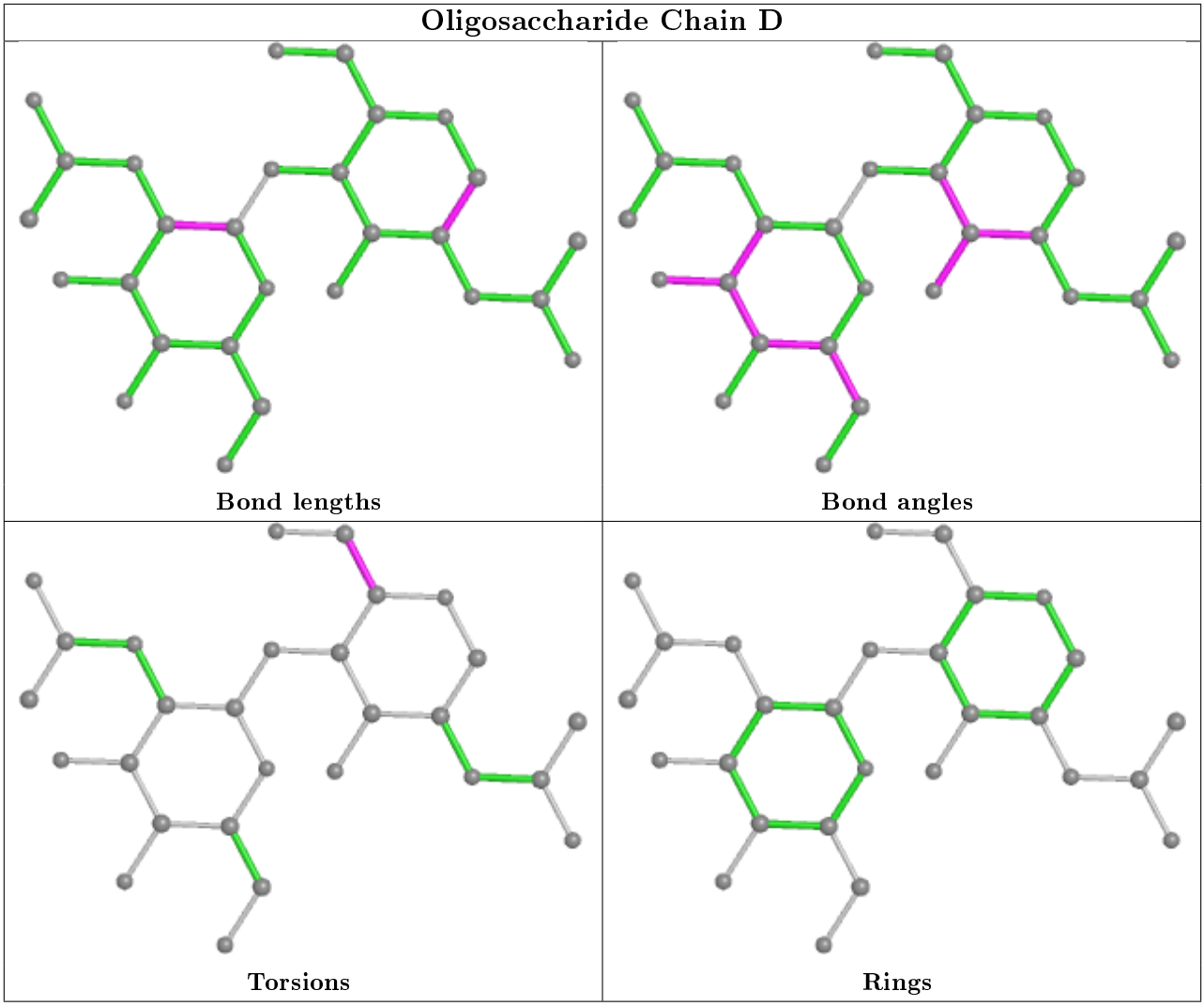
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	NAG	C	705	3	14,14,15	1.23	1 (7%)	17,19,21	1.50	4 (23%)
5	NAG	C	706	3	14,14,15	1.22	1 (7%)	17,19,21	1.50	5 (29%)
5	NAG	C	701	3	14,14,15	1.19	1 (7%)	17,19,21	1.44	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	702	3	14,14,15	1.23	0	17,19,21	1.48	4 (23%)
5	NAG	C	707	3	14,14,15	1.23	1 (7%)	17,19,21	1.44	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	C	705	3	-	0/6/23/26	0/1/1/1
5	NAG	C	706	3	-	0/6/23/26	0/1/1/1
5	NAG	C	701	3	-	0/6/23/26	0/1/1/1
5	NAG	C	702	3	-	0/6/23/26	0/1/1/1
5	NAG	C	707	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	705	NAG	C1-C2	2.33	1.55	1.52
5	C	707	NAG	C1-C2	2.21	1.55	1.52
5	C	701	NAG	C1-C2	2.14	1.55	1.52
5	C	706	NAG	C1-C2	2.05	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	705	NAG	C4-C3-C2	2.85	115.19	111.02
5	C	707	NAG	O3-C3-C2	2.84	115.33	109.47
5	C	701	NAG	O3-C3-C2	2.78	115.21	109.47
5	C	702	NAG	O3-C3-C2	2.76	115.19	109.47
5	C	705	NAG	O3-C3-C2	2.73	115.11	109.47
5	C	702	NAG	C4-C3-C2	2.68	114.94	111.02
5	C	706	NAG	O3-C3-C2	2.65	114.94	109.47
5	C	706	NAG	C4-C3-C2	2.56	114.77	111.02
5	C	701	NAG	C4-C3-C2	2.55	114.76	111.02
5	C	707	NAG	C4-C3-C2	2.48	114.66	111.02
5	C	706	NAG	C3-C4-C5	2.45	114.61	110.24
5	C	702	NAG	C3-C4-C5	2.42	114.55	110.24
5	C	705	NAG	C3-C4-C5	2.25	114.25	110.24
5	C	706	NAG	C2-N2-C7	-2.20	119.77	122.90
5	C	707	NAG	C3-C4-C5	2.14	114.06	110.24
5	C	702	NAG	C6-C5-C4	-2.08	108.14	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	705	NAG	C6-C5-C4	-2.07	108.16	113.00
5	C	701	NAG	C6-C5-C4	-2.07	108.16	113.00
5	C	706	NAG	C6-C5-C4	-2.07	108.16	113.00
5	C	707	NAG	C6-C5-C4	-2.05	108.20	113.00
5	C	701	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	214/227 (94%)	0.18	5 (2%)	60	57	29, 52, 77, 97	21 (9%)
2	B	219/220 (99%)	0.07	1 (0%)	91	90	29, 49, 80, 106	25 (11%)
3	C	601/621 (96%)	0.25	15 (2%)	57	53	28, 54, 88, 124	81 (13%)
All	All	1034/1068 (96%)	0.20	21 (2%)	65	61	28, 52, 86, 124	127 (12%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	587	VAL	4.8
3	C	37	CYS	3.7
3	C	296	ASN	3.7
3	C	574	VAL	3.6
3	C	300	MET	3.2
1	A	196	LEU	3.2
3	C	580	PRO	2.8
3	C	589	ASN	2.6
3	C	575	LEU	2.6
3	C	246	TYR	2.5
1	A	81	MET	2.4
1	A	198	THR	2.4
3	C	570	CYS	2.2
1	A	204	ASN	2.2
3	C	293	VAL	2.2
3	C	562	ASP	2.1
3	C	271	CYS	2.1
2	B	215	PHE	2.1
1	A	141	GLY	2.1
3	C	191	CYS	2.0
3	C	273	HIS	2.0

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

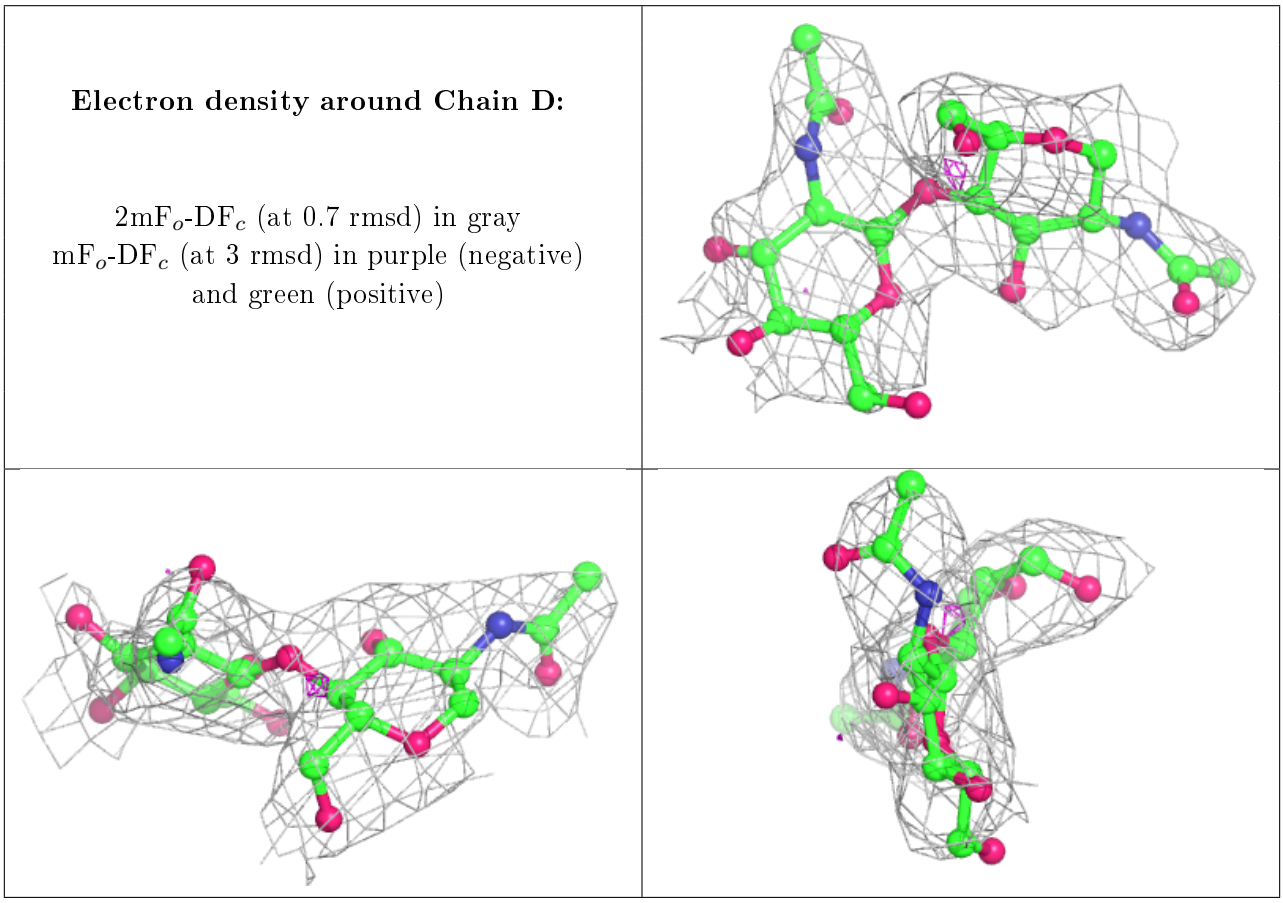
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	2	14/15	0.74	0.23	96,97,99,99	0
4	NAG	D	1	14/15	0.86	0.16	57,60,60,61	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	706	14/15	0.70	0.36	106,109,111,111	0
5	NAG	C	707	14/15	0.83	0.20	80,82,83,83	0
5	NAG	C	702	14/15	0.86	0.15	75,76,78,79	5
5	NAG	C	705	14/15	0.87	0.23	64,66,67,67	0
5	NAG	C	701	14/15	0.95	0.17	45,47,49,49	0

6.5 Other polymers

There are no such residues in this entry.