Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 01:30 AM EDT

PDB ID	:	3SDD
Title	:	Crystal structure of autoreactive-Valpha14-Vbeta6 NKT TCR in complex with CD1d-beta-lactosylceramide
Authors	:	Clarke, A.J.; Rossjohn, J.
Deposited on	:	2011-06-09
Resolution	:	3.00 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 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:

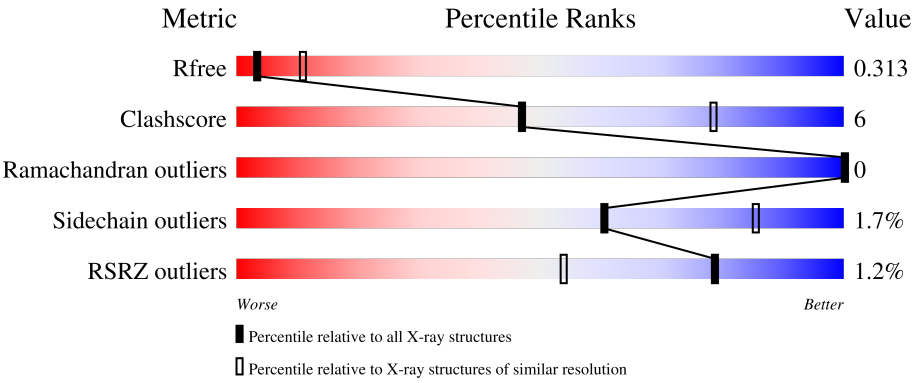
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	302	80% 16% .
2	B	99	96% .
3	C	207	4% 76% 14% . 9%
4	D	245	81% 15% . .
5	E	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6647 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	6	0	0
			2333	1486	406	427	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	expression tag	UNP P11609
A	281	SER	-	expression tag	UNP P11609
A	282	LEU	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	ILE	-	expression tag	UNP P11609
A	286	LEU	-	expression tag	UNP P11609
A	287	ASP	-	expression tag	UNP P11609
A	288	ALA	-	expression tag	UNP P11609
A	289	GLN	-	expression tag	UNP P11609
A	290	LYS	-	expression tag	UNP P11609
A	291	MET	-	expression tag	UNP P11609
A	292	VAL	-	expression tag	UNP P11609
A	293	TRP	-	expression tag	UNP P11609
A	294	ASN	-	expression tag	UNP P11609
A	295	HIS	-	expression tag	UNP P11609
A	296	ARG	-	expression tag	UNP P11609
A	297	HIS	-	expression tag	UNP P11609
A	298	HIS	-	expression tag	UNP P11609
A	299	HIS	-	expression tag	UNP P11609
A	300	HIS	-	expression tag	UNP P11609
A	301	HIS	-	expression tag	UNP P11609
A	302	HIS	-	expression tag	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	1	0	0
			814	520	138	149	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887

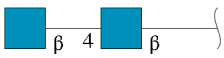
- Molecule 3 is a protein called NKT TCR Valpha14 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	189	Total	C	N	O	S	3	0	0
			1462	905	252	298	7			

- Molecule 4 is a protein called NKT TCR autoreactive-Vbeta6 chain.

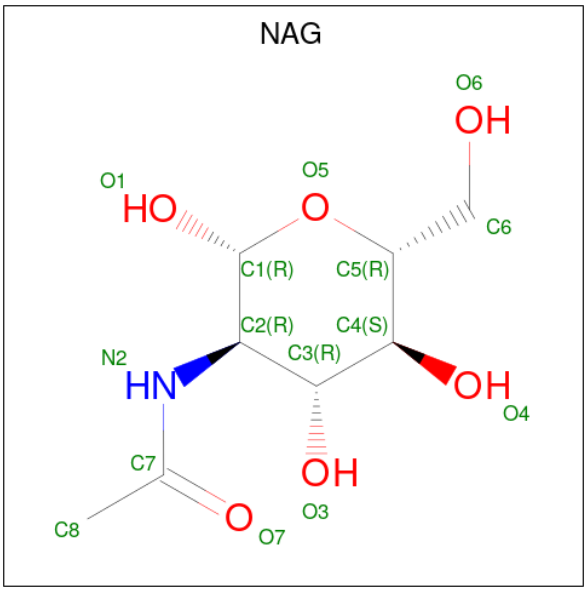
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	238	Total	C	N	O	S	6	0	0
			1886	1191	324	364	7			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



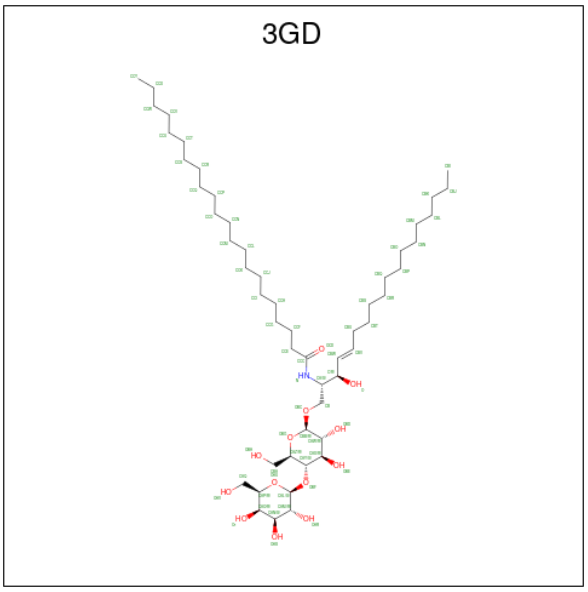
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is N-[(2S,3R,4E)-1-{[4-O-(beta-D-galactopyranosyl)-beta-D-glucopyranosyl]oxy}-3-hydroxyoctadec-4-en-2-yl]docosanamide (three-letter code: 3GD) (formula: $C_{52}H_{99}NO_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 66 52 1 13	0	0

- Molecule 8 is water.

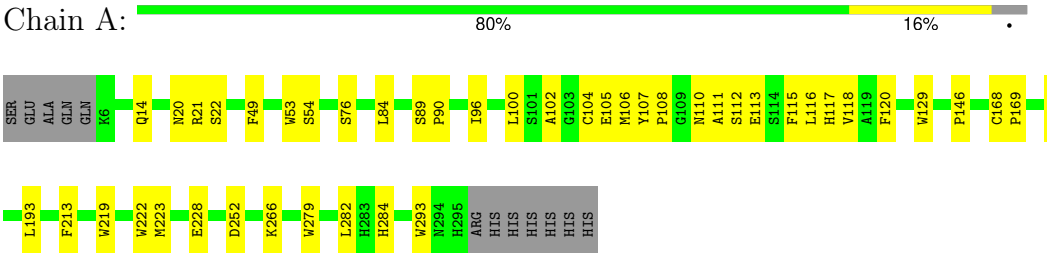
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	14	Total O 14 14	0	0
8	B	2	Total O 2 2	0	0
8	C	3	Total O 3 3	0	0
8	D	11	Total O 11 11	0	0

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.

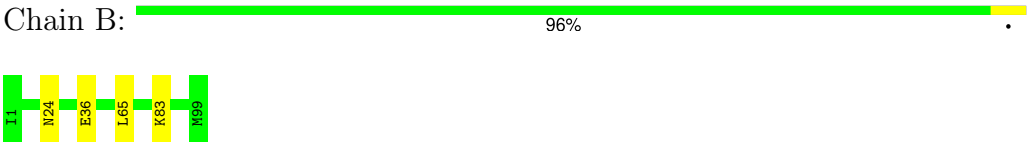
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain A:



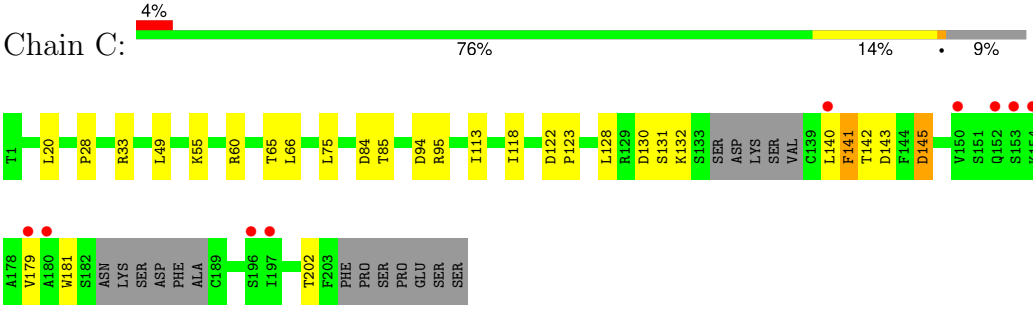
• Molecule 2: Beta-2-microglobulin

Chain B:



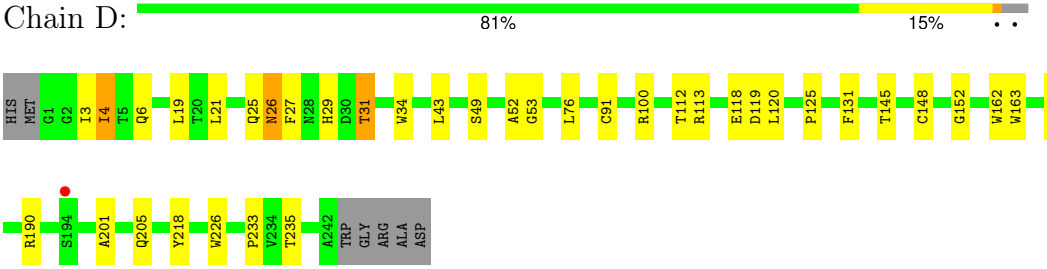
• Molecule 3: NKT TCR Valpha14 chain

Chain C:



• Molecule 4: NKT TCR autoreactive-Vbeta6 chain

Chain D:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.47Å 94.47Å 291.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.85 – 3.00 89.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.85-3.00) 99.7 (89.85-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.318 0.256 , 0.313	Depositor DCC
R_{free} test set	1373 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: 3GD, 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	0.62	2/2403 (0.1%)	0.55	2/3266 (0.1%)
2	B	0.49	0/840	0.49	0/1140
3	C	0.41	1/1485 (0.1%)	0.48	0/2015
4	D	0.48	2/1931 (0.1%)	0.52	0/2617
All	All	0.52	5/6659 (0.1%)	0.52	2/9038 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	TRP	CD2-CE2	5.03	1.47	1.41
1	A	293	TRP	CD2-CE2	5.02	1.47	1.41
4	D	34	TRP	CD2-CE2	5.02	1.47	1.41
4	D	163	TRP	CD2-CE2	5.01	1.47	1.41
1	A	53	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	SER	N-CA-CB	-5.55	102.18	110.50
1	A	22	SER	N-CA-C	5.18	124.98	111.00

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	2333	0	2233	26	0
2	B	814	0	788	2	0
3	C	1462	0	1413	20	0
4	D	1886	0	1820	37	0
5	E	28	0	25	0	0
6	A	28	0	26	0	0
7	A	66	0	99	0	0
8	A	14	0	0	0	0
8	B	2	0	0	0	0
8	C	3	0	0	0	0
8	D	11	0	0	1	0
All	All	6647	0	6404	80	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 6.

All (80) 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)
4:D:52:ALA:CB	4:D:53:GLY:HA3	1.70	1.21
4:D:52:ALA:HB1	4:D:53:GLY:HA3	1.13	1.10
4:D:52:ALA:CB	4:D:53:GLY:CA	2.50	0.89
4:D:3:ILE:O	4:D:26:ASN:ND2	2.04	0.89
4:D:43:LEU:HD12	4:D:43:LEU:N	1.95	0.80
4:D:52:ALA:HB1	4:D:53:GLY:CA	2.07	0.79
4:D:43:LEU:HD12	4:D:43:LEU:H	1.49	0.77
4:D:26:ASN:ND2	4:D:26:ASN:H	1.86	0.74
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.69	0.74
1:A:107:TYR:CD2	1:A:111:ALA:HB3	2.24	0.71
1:A:110:ASN:HB2	1:A:173:ARG:NH1	2.05	0.71
1:A:107:TYR:HD2	1:A:111:ALA:HB3	1.55	0.70
4:D:26:ASN:H	4:D:26:ASN:HD22	1.38	0.69
4:D:25:GLN:NE2	4:D:29:HIS:HB2	2.08	0.68
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.77	0.67
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.77	0.67
1:A:102:ALA:HB2	1:A:116:LEU:HD13	1.78	0.65
1:A:89:SER:OG	1:A:90:PRO:HD3	1.98	0.64
4:D:3:ILE:H	4:D:26:ASN:ND2	1.94	0.63
4:D:52:ALA:HB3	4:D:53:GLY:HA3	1.74	0.60
3:C:123:PRO:HB2	3:C:202:THR:HG22	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:HB2	1:A:111:ALA:HB3	1.82	0.60
3:C:128:LEU:HB3	4:D:131:PHE:HB3	1.83	0.60
3:C:60:ARG:NH2	3:C:84:ASP:OD2	2.33	0.59
4:D:4:ILE:HD12	4:D:25:GLN:HB2	1.84	0.59
4:D:25:GLN:NE2	4:D:27:PHE:O	2.35	0.59
1:A:49:PHE:HD2	1:A:54:SER:HB2	1.67	0.58
3:C:85:THR:HG23	3:C:113:ILE:HA	1.85	0.58
1:A:76:SER:HA	3:C:95:ARG:HH21	1.69	0.58
4:D:201:ALA:O	4:D:205:GLN:HG2	2.05	0.56
4:D:26:ASN:ND2	4:D:26:ASN:N	2.54	0.56
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.42	0.55
1:A:279:TRP:O	1:A:284:HIS:ND1	2.39	0.55
4:D:52:ALA:HB3	4:D:53:GLY:CA	2.34	0.54
3:C:55:LYS:HG2	3:C:65:THR:HG22	1.90	0.54
3:C:130:ASP:N	3:C:131:SER:HA	2.23	0.53
4:D:6:GLN:HE22	4:D:91:CYS:H	1.57	0.53
4:D:43:LEU:H	4:D:43:LEU:CD1	2.18	0.53
3:C:20:LEU:HD12	3:C:75:LEU:HD23	1.91	0.53
3:C:49:LEU:HD13	3:C:66:LEU:HB2	1.92	0.52
4:D:43:LEU:N	4:D:43:LEU:CD1	2.69	0.52
1:A:106:MET:HE3	1:A:172:VAL:HG21	1.92	0.51
1:A:115:PHE:HB2	1:A:117:HIS:CD2	2.45	0.51
1:A:14:GLN:HB3	1:A:100:LEU:HB2	1.93	0.51
2:B:36:GLU:HB3	2:B:83:LYS:HB2	1.92	0.51
4:D:152:GLY:HA2	4:D:190:ARG:HD3	1.93	0.50
4:D:6:GLN:NE2	4:D:91:CYS:H	2.11	0.49
4:D:113:ARG:HG3	8:D:258:HOH:O	2.13	0.48
4:D:21:LEU:HD22	4:D:112:THR:HG21	1.95	0.48
3:C:128:LEU:HD11	3:C:140:LEU:HD12	1.96	0.48
1:A:49:PHE:CD2	1:A:54:SER:HB2	2.47	0.47
3:C:28:PRO:HG2	3:C:94:ASP:O	2.15	0.47
4:D:118:GLU:HA	4:D:119:ASP:HA	1.56	0.47
4:D:218:TYR:HA	4:D:235:THR:HG23	1.97	0.47
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.49	0.47
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.97	0.46
1:A:193:LEU:HD22	1:A:222:TRP:CH2	2.50	0.46
3:C:33:ARG:NH1	4:D:100:ARG:O	2.45	0.45
3:C:118:ILE:HD11	3:C:145:ASP:HA	1.99	0.45
3:C:131:SER:HB2	3:C:132:LYS:HA	1.98	0.45
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.99	0.44
1:A:84:LEU:HD22	1:A:146:PRO:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:MET:HG2	1:A:228:GLU:HA	2.00	0.43
4:D:125:PRO:HD3	4:D:233:PRO:HB3	2.00	0.43
3:C:166:LEU:HD13	3:C:166:LEU:H	1.83	0.43
1:A:100:LEU:HG	1:A:118:VAL:HG22	2.01	0.43
4:D:178:GLN:HA	4:D:179:PRO:HD3	1.91	0.43
3:C:140:LEU:HD11	4:D:145:THR:HB	2.00	0.42
1:A:20:ASN:O	1:A:21:ARG:C	2.57	0.42
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.01	0.42
3:C:141:PHE:O	3:C:177:SER:HA	2.19	0.42
3:C:122:ASP:O	3:C:143:ASP:HB2	2.20	0.42
3:C:142:THR:HG22	3:C:143:ASP:H	1.86	0.41
4:D:31:THR:HA	4:D:49:SER:O	2.21	0.41
1:A:104:CYS:HA	1:A:113:GLU:O	2.20	0.41
1:A:105:GLU:O	1:A:112:SER:HA	2.20	0.41
4:D:25:GLN:HE22	4:D:29:HIS:HB2	1.83	0.41
1:A:96:ILE:HG23	1:A:120:PHE:HE1	1.86	0.40
4:D:3:ILE:N	4:D:26:ASN:ND2	2.67	0.40
4:D:21:LEU:HD12	4:D:76:LEU:HD23	2.03	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	288/302 (95%)	279 (97%)	9 (3%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	183/207 (88%)	173 (94%)	10 (6%)	0	100	100
4	D	236/245 (96%)	224 (95%)	12 (5%)	0	100	100
All	All	804/853 (94%)	771 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	253/264 (96%)	251 (99%)	2 (1%)	81 93
2	B	92/93 (99%)	92 (100%)	0	100 100
3	C	169/186 (91%)	165 (98%)	4 (2%)	49 79
4	D	206/211 (98%)	200 (97%)	6 (3%)	42 76
All	All	720/754 (96%)	708 (98%)	12 (2%)	60 85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	282	LEU
3	C	141	PHE
3	C	145	ASP
3	C	166	LEU
3	C	179	VAL
4	D	4	ILE
4	D	19	LEU
4	D	26	ASN
4	D	31	THR
4	D	120	LEU
4	D	226	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	248	GLN
2	B	42	ASN
3	C	72	HIS
3	C	127	GLN
4	D	6	GLN
4	D	25	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	26	ASN
4	D	84	ASN
4	D	187	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
5	NAG	E	1	1,5	14,14,15	0.58	0	17,19,21	1.49	4 (23%)
5	NAG	E	2	5	14,14,15	0.61	0	17,19,21	0.92	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	E	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1	NAG	C4-C3-C2	4.07	116.99	111.02
5	E	1	NAG	O5-C1-C2	-2.56	107.33	111.29
5	E	1	NAG	C3-C4-C5	2.22	114.27	110.23
5	E	1	NAG	O4-C4-C3	-2.11	105.39	110.38
5	E	2	NAG	C4-C3-C2	2.05	114.03	111.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

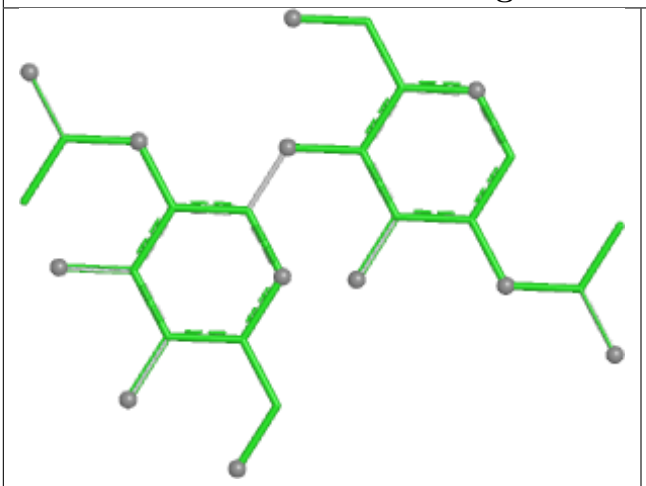
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

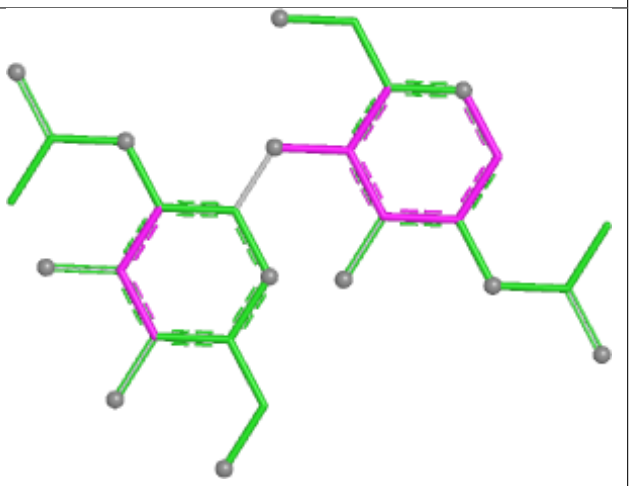
No monomer is involved in short contacts.

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

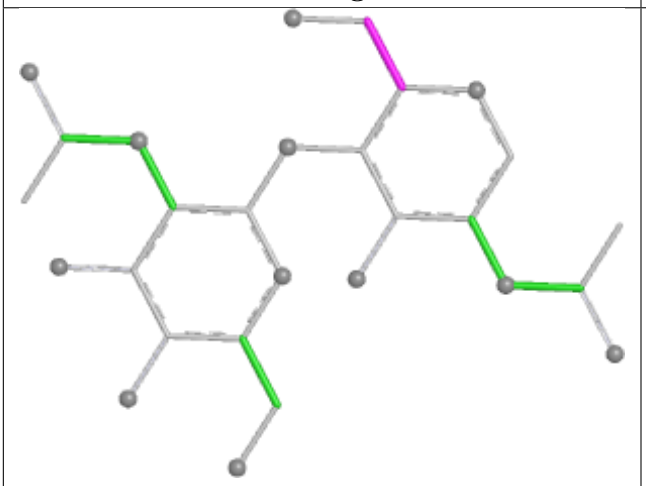
Oligosaccharide Chain E



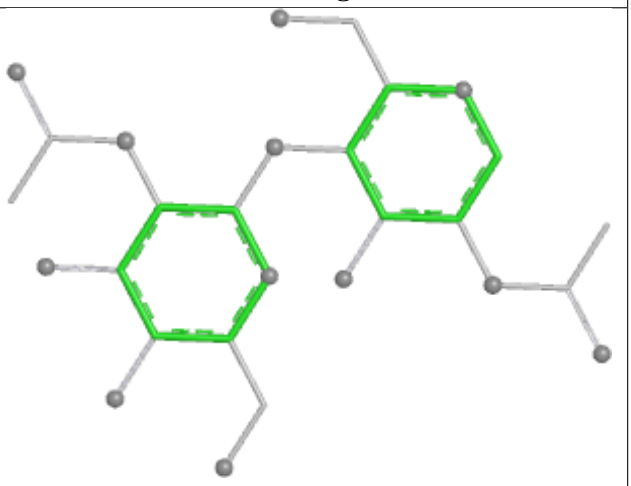
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

3 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	$\#\|Z\| > 2$
7	3GD	A	307	-	66,67,67	1.20	4 (6%)	79,81,81	1.11	5 (6%)
6	NAG	A	303	1	14,14,15	0.38	0	17,19,21	2.01	3 (17%)
6	NAG	A	304	1	14,14,15	0.49	0	17,19,21	0.87	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
7	3GD	A	307	-	-	33/57/97/97	0/2/2/2
6	NAG	A	303	1	-	2/6/23/26	0/1/1/1
6	NAG	A	304	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	307	3GD	O-C	5.57	1.53	1.43
7	A	307	3GD	CBW-CBV	5.42	1.53	1.31
7	A	307	3GD	OBC-CBB	2.99	1.45	1.40
7	A	307	3GD	C-CBW	2.44	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	303	NAG	C1-O5-C5	6.76	121.25	112.19
7	A	307	3GD	C-CBW-CBV	-4.97	114.40	124.69
6	A	303	NAG	O5-C1-C2	2.78	115.59	111.29
7	A	307	3GD	OBC-CBB-CAW	2.55	112.14	108.27
7	A	307	3GD	CBB-OBG-CAZ	-2.14	109.54	113.72
6	A	303	NAG	C3-C4-C5	2.09	114.02	110.23
7	A	307	3GD	CBU-CBV-CBW	-2.08	116.20	125.47
7	A	307	3GD	OBF-CAL-OAU	-2.02	105.38	110.69

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	307	3GD	O-C-CA-N
7	A	307	3GD	O-C-CA-CB
7	A	307	3GD	CBW-C-CA-N
7	A	307	3GD	CBW-C-CA-CB
7	A	307	3GD	CA-C-CBW-CBV
7	A	307	3GD	CCJ-CCK-CCL-CCM
7	A	307	3GD	OBG-CBB-OBC-CB
6	A	303	NAG	O5-C5-C6-O6
7	A	307	3GD	CAW-CBB-OBC-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	307	3GD	CBO-CBP-CBQ-CBR
6	A	304	NAG	C8-C7-N2-C2
6	A	304	NAG	O7-C7-N2-C2
6	A	303	NAG	C4-C5-C6-O6
7	A	307	3GD	O-C-CBW-CBV
7	A	307	3GD	CBK-CBL-CBM-CBN
7	A	307	3GD	CCL-CCM-CCN-CCO
7	A	307	3GD	CCR-CCS-CCT-CCU
7	A	307	3GD	CBN-CBO-CBP-CBQ
7	A	307	3GD	CCQ-CCR-CCS-CCT
7	A	307	3GD	CBQ-CBR-CBS-CBT
7	A	307	3GD	CCC-CCE-CCF-CCG
7	A	307	3GD	CCM-CCN-CCO-CCP
7	A	307	3GD	CCH-CCI-CCJ-CCK
7	A	307	3GD	CCG-CCH-CCI-CCJ
7	A	307	3GD	CCO-CCP-CCQ-CCR
7	A	307	3GD	CBL-CBM-CBN-CBO
7	A	307	3GD	CCT-CCU-CCV-CCW
7	A	307	3GD	CCU-CCV-CCW-CCX
7	A	307	3GD	CBI-CBJ-CBK-CBL
7	A	307	3GD	CBT-CBU-CBV-CBW
7	A	307	3GD	CBM-CBN-CBO-CBP
7	A	307	3GD	CAY-CAZ-CBA-OBH
7	A	307	3GD	CBP-CBQ-CBR-CBS
7	A	307	3GD	CCS-CCT-CCU-CCV
7	A	307	3GD	C-CA-CB-OBC
7	A	307	3GD	N-CA-CB-OBC
7	A	307	3GD	CBJ-CBK-CBL-CBM

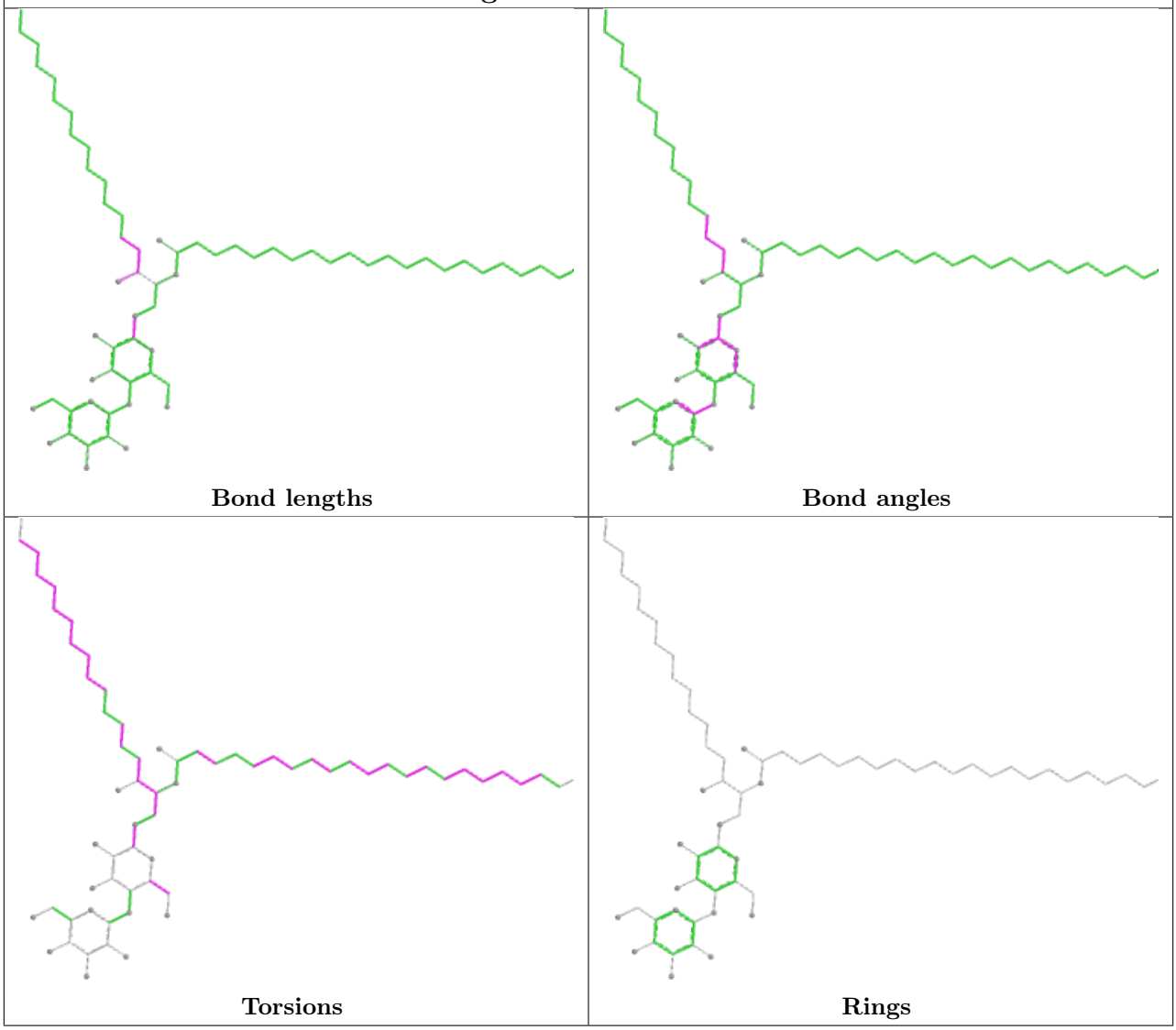
There are no ring outliers.

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand 3GD A 307



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	290/302 (96%)	0.04	0 100 100	53, 66, 81, 97	4 (1%)
2	B	99/99 (100%)	0.12	0 100 100	54, 67, 80, 84	1 (1%)
3	C	189/207 (91%)	0.33	9 (4%) 30 11	57, 76, 136, 144	2 (1%)
4	D	238/245 (97%)	0.25	1 (0%) 92 79	57, 94, 119, 126	3 (1%)
All	All	816/853 (95%)	0.18	10 (1%) 79 54	53, 72, 121, 144	10 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	140	LEU	4.6
3	C	196	SER	4.1
3	C	150	VAL	4.0
3	C	152	GLN	3.4
3	C	153	SER	3.2
3	C	180	ALA	2.6
3	C	179	VAL	2.5
3	C	154	LYS	2.5
3	C	197	ILE	2.5
4	D	194	SER	2.1

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

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

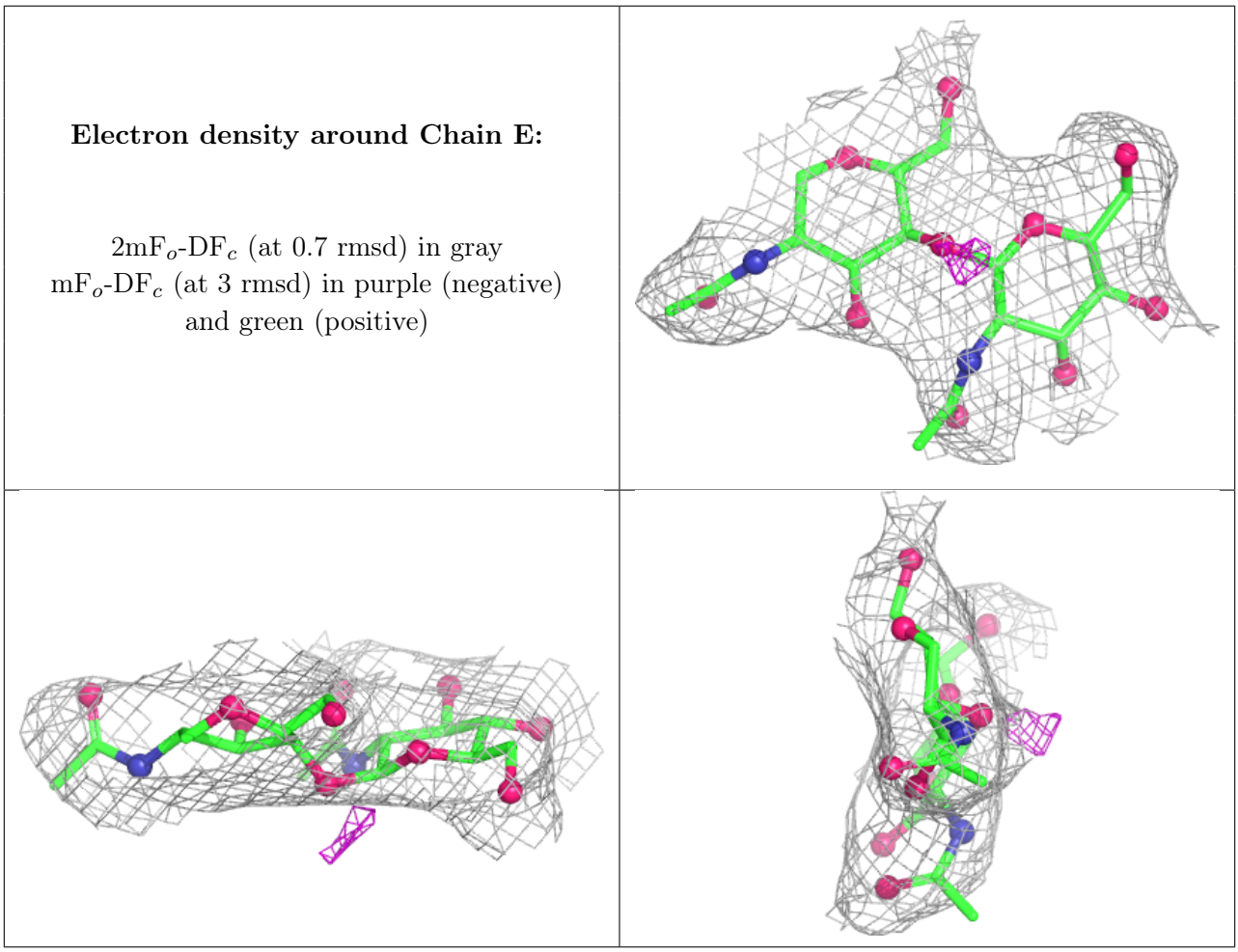
6.3 Carbohydrates

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, 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	E	2	14/15	0.83	0.19	81,82,84,84	0
5	NAG	E	1	14/15	0.93	0.21	74,76,77,80	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 (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
6	NAG	A	303	14/15	0.81	0.18	82,84,84,84	0

Continued on next page...

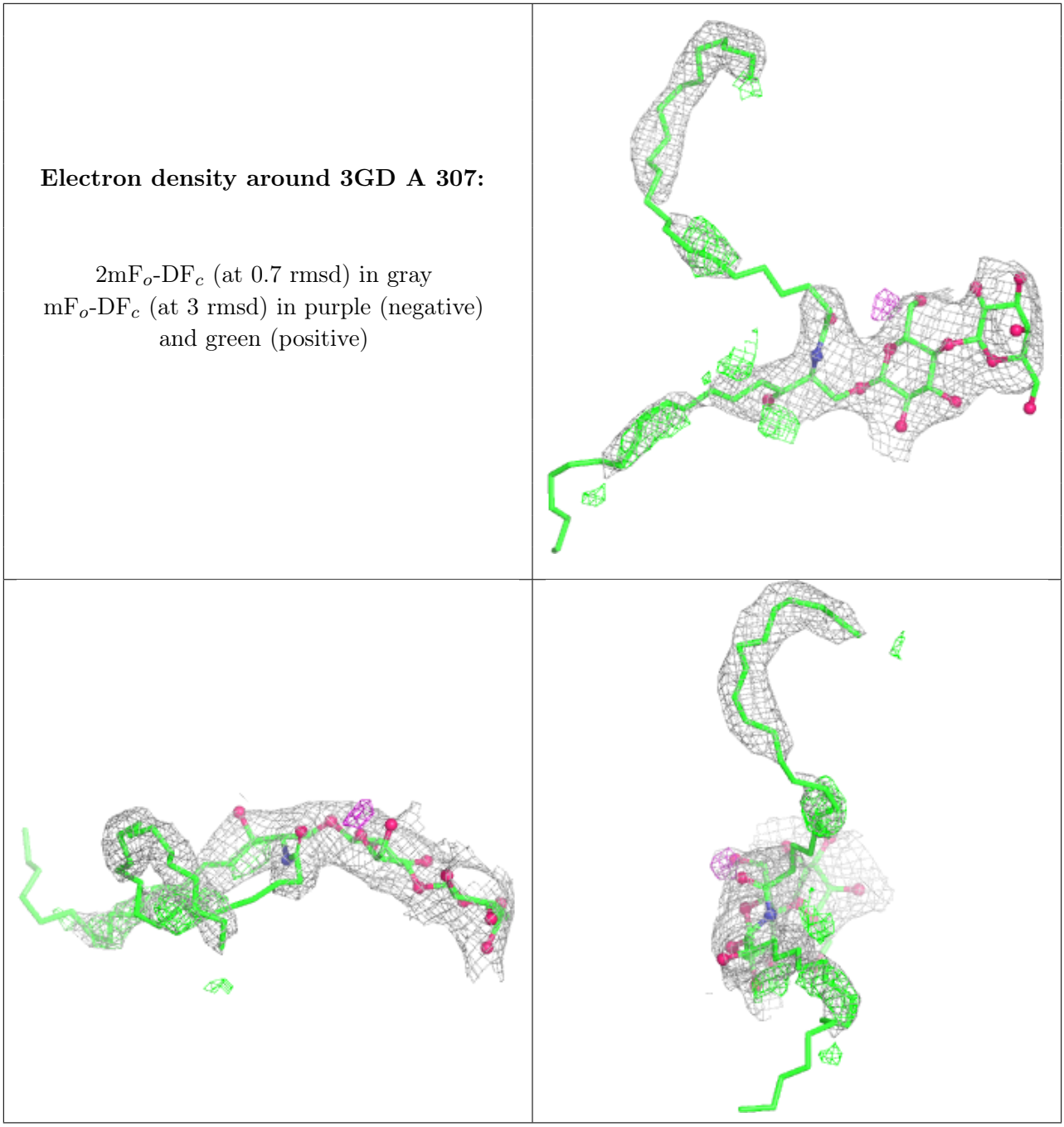
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	3GD	A	307	66/66	0.89	0.41	60,68,90,92	20
6	NAG	A	304	14/15	0.92	0.18	74,75,76,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3GD A 307:

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



6.5 Other polymers (i)

There are no such residues in this entry.