



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:59 AM UTC

PDB ID : 6NIH / pdb_00006nih
Title : Crystal structure of human TLR1
Authors : Su, L.; Zhang, H.
Deposited on : 2018-12-27
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

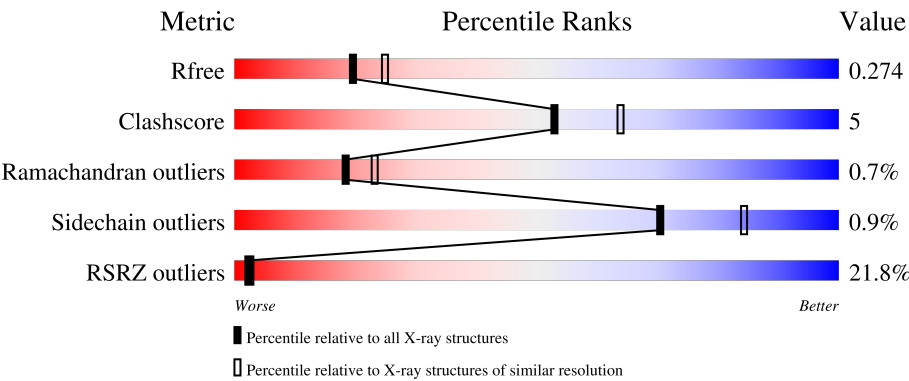
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	545	29% 84% 11% 5%
1	B	545	12% 83% 12% 5%
2	C	2	100%
2	D	2	50% 50%
2	F	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	3	 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17381 atoms, of which 8624 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 Toll-like receptor 1, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	519	Total	C	H	N	O	S	0	3	0
			8413	2677	4232	700	784	20			
1	B	520	Total	C	H	N	O	S	0	3	0
			8434	2686	4242	701	785	20			

There are 2 discrepancies between the modelled and reference sequences:

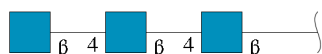
Chain	Residue	Modelled	Actual	Comment	Reference
A	476	ALA	-	linker	UNP Q15399
B	476	ALA	-	linker	UNP Q15399

- Molecule 2 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
2	C	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
2	D	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
2	F	2	Total	C	H	N	O		0	0	0
			52	16	24	2	10				

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
3	E	3	Total	C	H	N	O	0	0	0
			79	24	37	3	15			

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



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

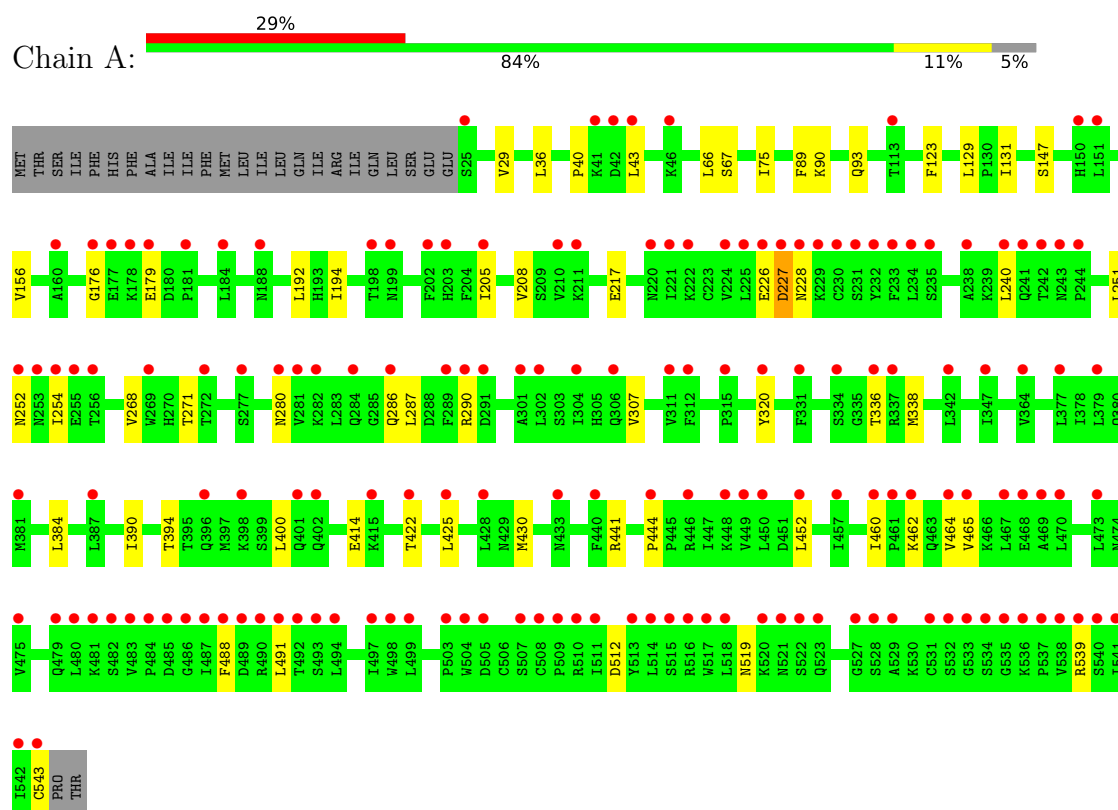
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	B	139	Total O 139 139	0	0

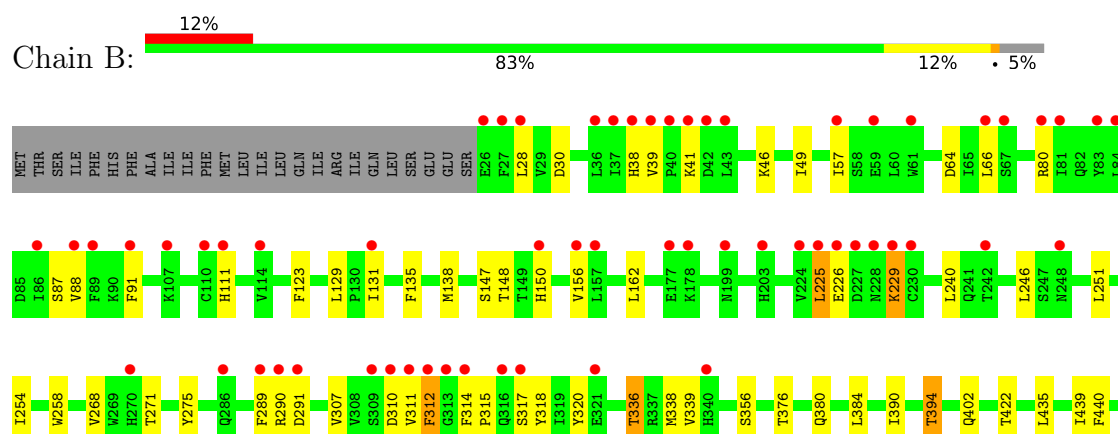
3 Residue-property plots [i](#)

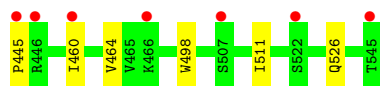
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Toll-like receptor 1, Variable lymphocyte receptor B



- Molecule 1: Toll-like receptor 1, Variable lymphocyte receptor B





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

Chain C:  100%



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

Chain D:  50% 50%



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

Chain F:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.03Å 74.38Å 106.08Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	46.40 – 2.30 46.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	74.7 (46.40-2.30) 74.7 (46.40-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.243 , 0.274 0.244 , 0.274	Depositor DCC
R_{free} test set	1958 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17381	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: 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	0.13	0/4275	0.38	0/5791
1	B	0.14	0/4288	0.40	0/5810
All	All	0.14	0/8563	0.39	0/11601

There are no bond length outliers.

There are no bond angle outliers.

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	4181	4232	4232	33	0
1	B	4192	4242	4241	53	0
2	C	28	25	25	0	0
2	D	28	25	25	0	0
2	F	28	24	25	0	0
3	E	42	37	37	1	0
4	A	14	13	13	1	0
4	B	28	26	26	0	0
5	A	77	0	0	0	0
5	B	139	0	0	2	0
All	All	8757	8624	8624	86	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 5.

All (86) 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:B:225:LEU:HD22	1:B:229:LYS:HG3	1.58	0.83
1:B:251:LEU:HB3	1:B:254:ILE:HD11	1.68	0.75
1:A:251:LEU:HB3	1:A:254:ILE:HD11	1.70	0.73
1:B:225:LEU:CD2	1:B:229:LYS:HG3	2.27	0.63
1:B:440:PHE:CD1	1:B:464:VAL:HG22	2.34	0.62
1:A:384:LEU:HB3	1:A:390:ILE:HD11	1.82	0.62
1:A:394:THR:HG23	1:A:400:LEU:HD23	1.81	0.62
1:B:148:THR:HG22	1:B:150[B]:HIS:H	1.65	0.61
1:B:148:THR:HG22	1:B:150[A]:HIS:H	1.65	0.61
1:B:275:TYR:HE1	3:E:1:NAG:H81	1.66	0.60
1:A:208:VAL:HG23	1:A:240:LEU:HD21	1.82	0.60
1:B:135:PHE:HA	1:B:138:MET:HE2	1.83	0.60
1:B:38:HIS:O	1:B:57:ILE:HG23	2.02	0.59
1:A:460:ILE:HG23	1:A:464:VAL:HG21	1.84	0.58
1:B:66:LEU:HD21	1:B:91:PHE:CD2	2.38	0.58
1:B:460:ILE:HG23	1:B:464:VAL:HG21	1.86	0.57
1:B:28:LEU:HD11	1:B:30:ASP:HB2	1.86	0.57
1:B:123:PHE:N	1:B:147:SER:OG	2.39	0.55
1:A:192:LEU:HD21	1:A:194:ILE:HD11	1.89	0.54
1:B:225:LEU:CD2	1:B:229:LYS:HA	2.38	0.53
1:B:226:GLU:HA	1:B:226:GLU:OE1	2.09	0.53
1:B:320:TYR:HE1	1:B:338:MET:HG3	1.75	0.52
1:B:384:LEU:HB3	1:B:390:ILE:HD11	1.91	0.52
1:A:66:LEU:HD12	1:A:67:SER:N	2.26	0.51
1:A:286:GLN:OE1	1:A:287:LEU:N	2.44	0.51
1:A:307:VAL:HB	1:A:336:THR:HG22	1.92	0.51
1:B:336:THR:HG22	1:B:338:MET:H	1.75	0.51
1:A:430:MET:HE3	1:A:452:LEU:HD21	1.92	0.50
1:A:29:VAL:HG11	1:A:43:LEU:HD22	1.93	0.50
1:B:240:LEU:HD22	1:B:246:LEU:HD22	1.94	0.50
1:B:336:THR:CG2	1:B:338:MET:HB2	2.42	0.49
1:A:123:PHE:N	1:A:147:SER:OG	2.45	0.49
1:B:251:LEU:CB	1:B:254:ILE:HD11	2.41	0.49
1:A:217:GLU:OE1	1:A:252:ASN:ND2	2.40	0.49
1:B:28:LEU:CD1	1:B:30:ASP:HB2	2.44	0.47
1:B:394:THR:CG2	1:B:422:THR:H	2.27	0.47
1:B:156:VAL:O	1:B:156:VAL:HG12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:TYR:OH	1:B:339:VAL:HG22	2.15	0.47
1:A:320:TYR:HE1	1:A:338:MET:HG3	1.81	0.46
1:A:425:LEU:HD23	1:A:444:PRO:HG3	1.96	0.46
1:A:462:LYS:O	1:A:465:VAL:HG22	2.15	0.46
1:B:511:ILE:O	1:B:511:ILE:HG13	2.15	0.46
1:B:402:GLN:NE2	5:B:824:HOH:O	2.47	0.46
1:A:75:ILE:CD1	4:A:601:NAG:H82	2.46	0.46
1:A:176:GLY:O	1:A:179:GLU:HG3	2.16	0.46
1:B:307:VAL:HB	1:B:336:THR:OG1	2.16	0.46
1:B:435:LEU:HD22	1:B:439:ILE:HD13	1.99	0.45
1:A:156:VAL:HG12	1:A:156:VAL:O	2.17	0.44
1:B:225:LEU:HD23	1:B:229:LYS:HA	1.99	0.44
1:B:310:ASP:OD1	1:B:311:VAL:N	2.51	0.44
1:B:87:SER:HB3	1:B:111:HIS:HB2	2.00	0.44
1:B:38:HIS:CG	1:B:39:VAL:H	2.35	0.44
1:A:394:THR:CG2	1:A:422:THR:HG22	2.48	0.43
1:A:251:LEU:CB	1:A:254:ILE:HD11	2.45	0.43
1:B:129:LEU:HD23	1:B:131:ILE:HD12	2.00	0.43
1:B:129:LEU:HD12	1:B:148:THR:OG1	2.19	0.43
1:B:38:HIS:O	1:B:57:ILE:HG12	2.19	0.43
1:A:414:GLU:OE2	1:A:441:ARG:NH1	2.51	0.43
1:A:488:PHE:HD1	1:A:491:LEU:HD12	1.84	0.43
1:B:258:TRP:CZ2	1:B:315:PRO:HD3	2.54	0.43
1:B:39:VAL:HG11	1:B:64:ASP:HB3	2.00	0.42
1:B:289:PHE:CE1	1:B:291:ASP:OD1	2.72	0.42
1:B:498:TRP:CD1	1:B:526:GLN:HB2	2.54	0.42
1:A:90:LYS:O	1:A:93:GLN:NE2	2.52	0.42
1:B:135:PHE:O	1:B:162:LEU:HD11	2.20	0.42
1:B:147:SER:O	1:B:148:THR:OG1	2.37	0.42
1:A:226:GLU:O	1:A:227:ASP:C	2.62	0.42
1:A:460:ILE:CG2	1:A:464:VAL:HG21	2.48	0.42
1:B:336:THR:CG2	1:B:338:MET:H	2.32	0.42
1:A:129:LEU:HD23	1:A:131:ILE:HD12	2.01	0.42
1:A:36:LEU:HD13	1:A:40:PRO:HD3	2.01	0.41
1:B:28:LEU:HD23	1:B:49:ILE:HB	2.03	0.41
1:B:310:ASP:O	1:B:312:PHE:N	2.53	0.41
1:A:512:ASP:OD1	1:A:543:CYS:HB2	2.20	0.41
1:B:268:VAL:HA	1:B:271:THR:HG23	2.01	0.41
1:B:28:LEU:C	1:B:28:LEU:HD13	2.46	0.41
1:B:80:ARG:NH2	5:B:832:HOH:O	2.52	0.41
1:B:356:SER:HA	1:B:380:GLN:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:HA	1:A:290:ARG:HD2	1.91	0.41
1:B:41:LYS:HD3	1:B:41:LYS:HA	1.95	0.41
1:B:290:ARG:HD2	1:B:318:TYR:CE1	2.56	0.41
1:A:268:VAL:HA	1:A:271:THR:HG23	2.03	0.40
1:A:394:THR:HG22	1:A:422:THR:HG22	2.03	0.40
1:A:519:ASN:HA	1:A:539:ARG:NE	2.37	0.40
1:B:394:THR:HG22	1:B:422:THR:H	1.87	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	520/545 (95%)	474 (91%)	43 (8%)	3 (1%)	21	27
1	B	521/545 (96%)	476 (91%)	40 (8%)	5 (1%)	12	15
All	All	1041/1090 (96%)	950 (91%)	83 (8%)	8 (1%)	18	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	229	LYS
1	B	312	PHE
1	A	227	ASP
1	A	280[A]	ASN
1	A	280[B]	ASN
1	B	225	LEU
1	B	317	SER
1	B	445	PRO

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	496/518 (96%)	493 (99%)	3 (1%)	78	89
1	B	497/518 (96%)	491 (99%)	6 (1%)	63	79
All	All	993/1036 (96%)	984 (99%)	9 (1%)	70	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	PHE
1	A	205	ILE
1	A	228	ASN
1	B	46	LYS
1	B	88	VAL
1	B	314	PHE
1	B	336	THR
1	B	376	THR
1	B	394	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	340	HIS
1	A	380	GLN
1	B	45	GLN
1	B	78	HIS
1	B	102	HIS
1	B	253	ASN
1	B	284	GLN
1	B	401	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 ⓘ

9 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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.29	0	17,19,21	0.37	0
2	NAG	C	2	2	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	D	1	2,1	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	1.21	2 (14%)	17,19,21	1.22	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.21	0	17,19,21	0.56	0
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	E	3	3	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	F	1	2,1	14,14,15	0.50	0	17,19,21	0.67	0
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.39	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	E	3	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	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)
2	D	2	NAG	O5-C1	-2.67	1.39	1.43
2	D	2	NAG	C1-C2	-2.12	1.49	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	3.79	117.27	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

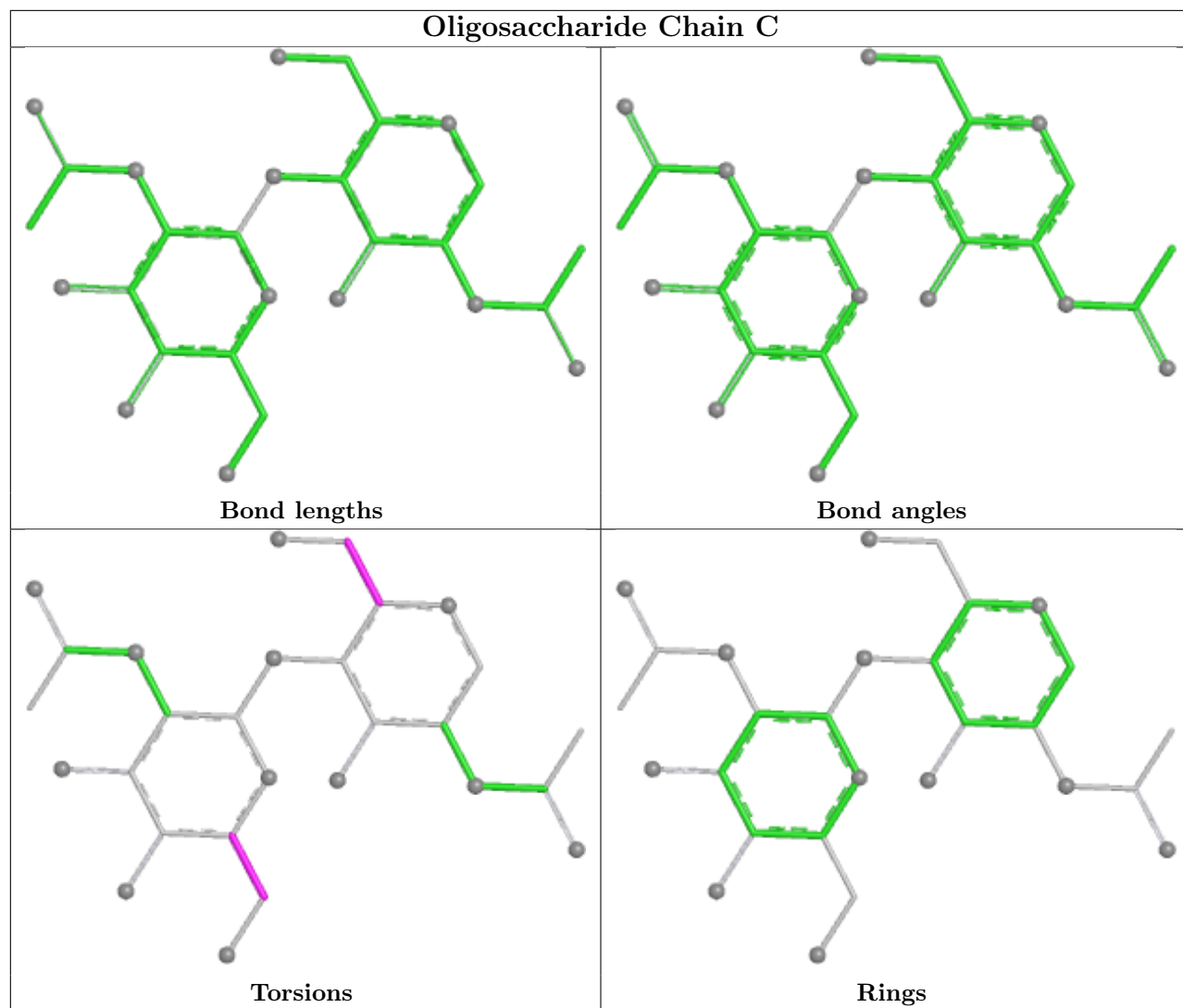
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7
2	F	1	NAG	O5-C5-C6-O6

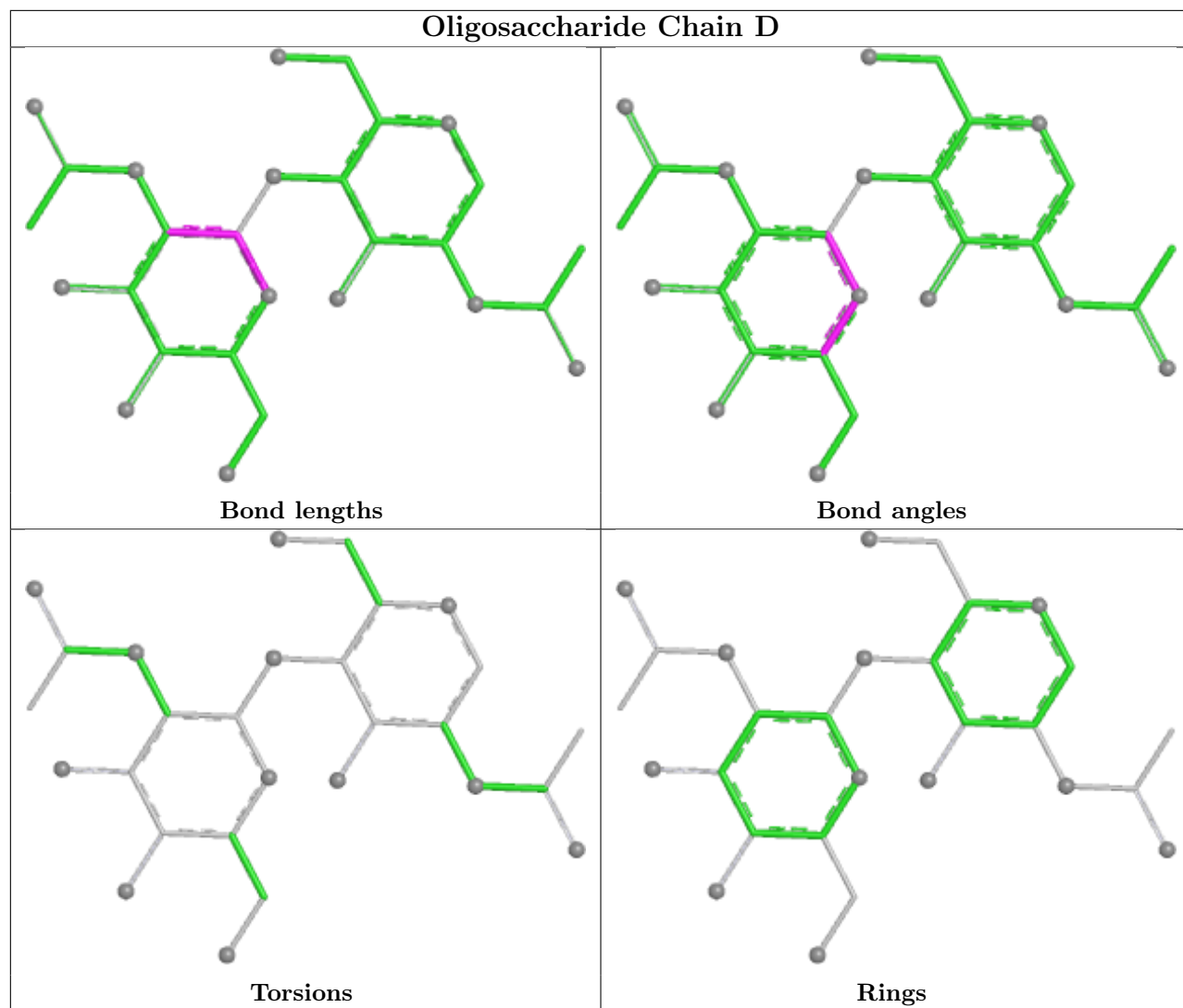
There are no ring outliers.

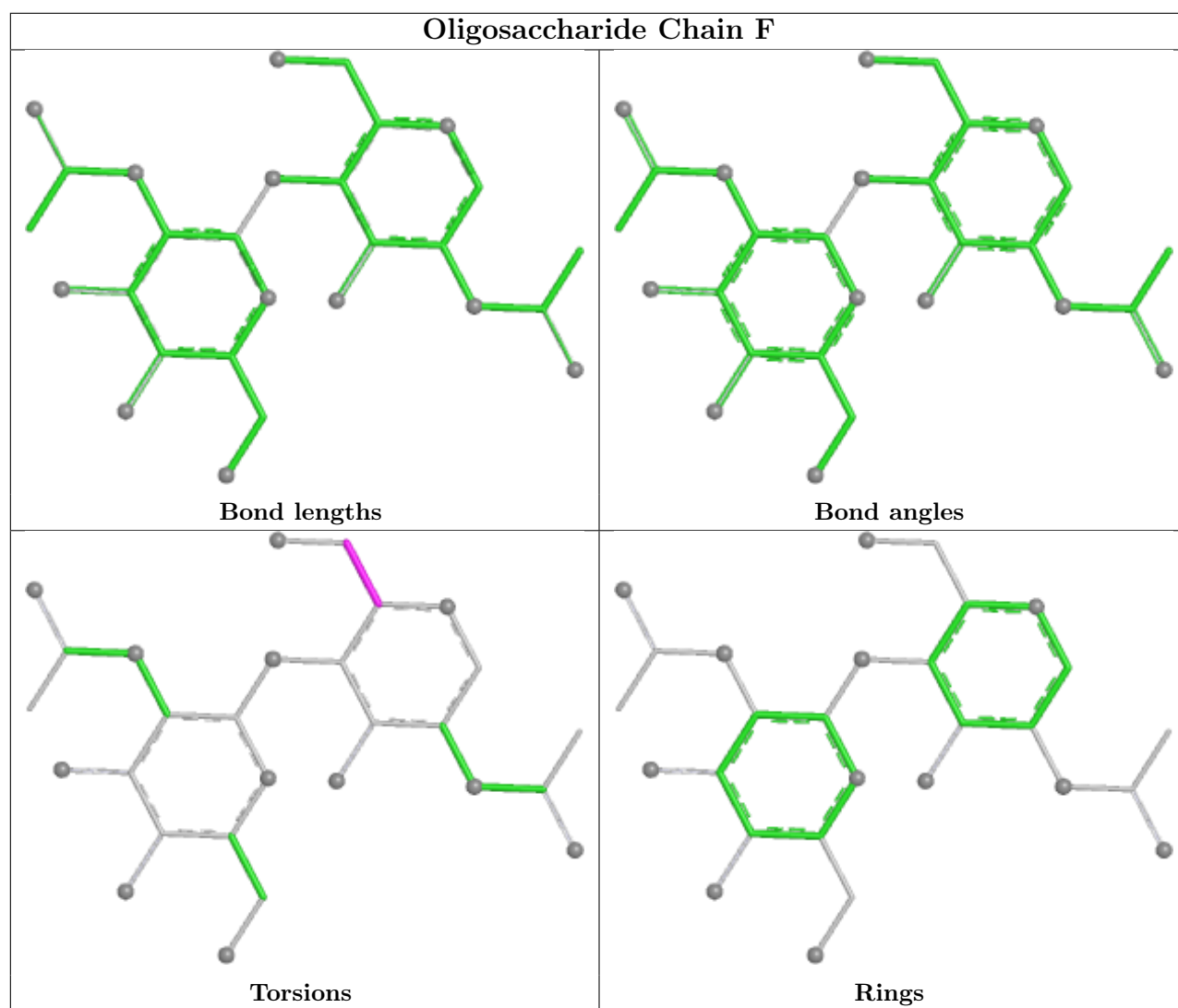
1 monomer is involved in 1 short contact:

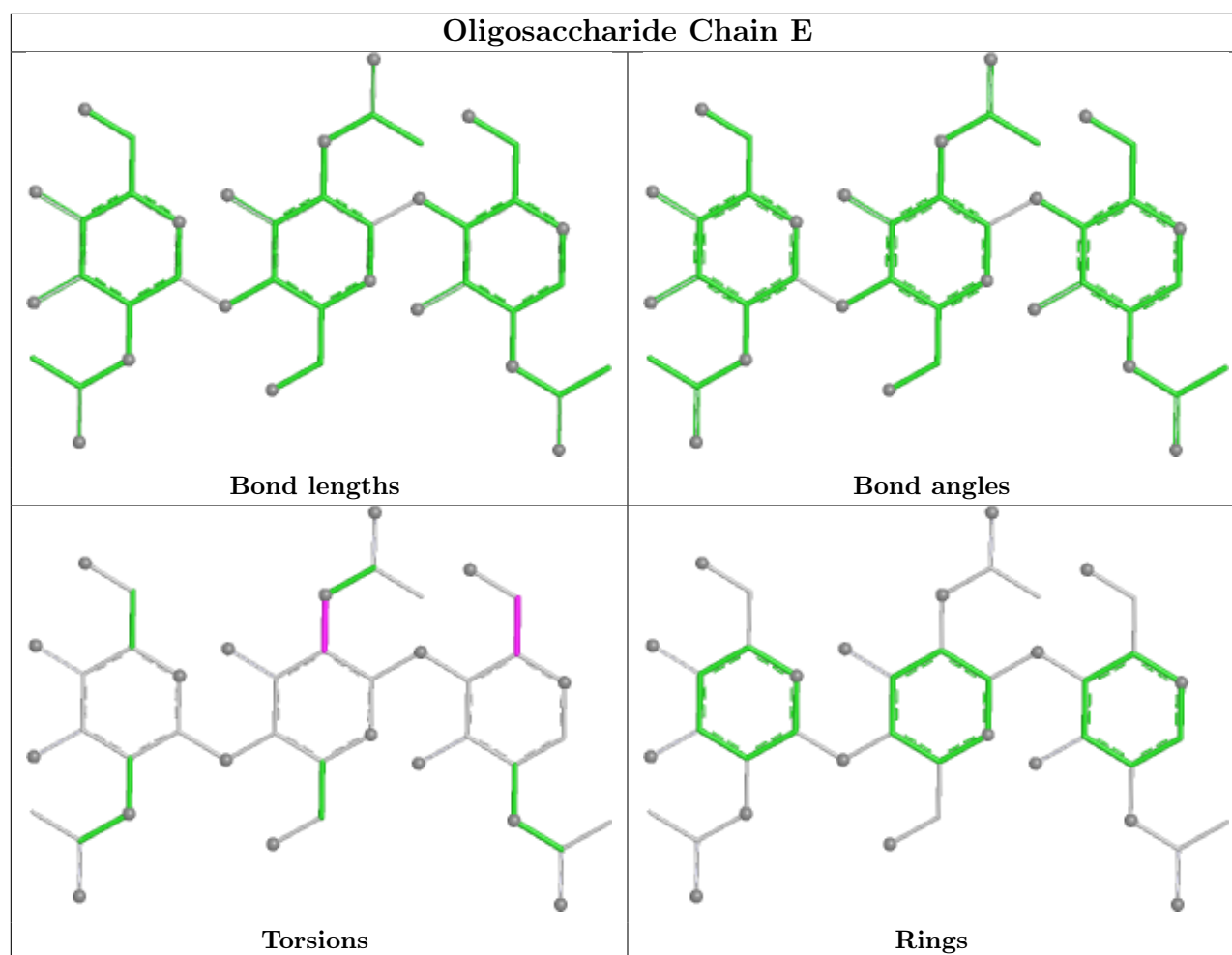
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0

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](#)

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	$\# Z > 2$
4	NAG	B	701	1	14,14,15	0.30	0	17,19,21	0.42	0
4	NAG	A	601	1	14,14,15	0.21	0	17,19,21	0.57	0
4	NAG	B	702	1	14,14,15	0.34	0	17,19,21	0.73	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	B	701	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	702	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	NAG	C3-C2-N2-C7
4	B	701	NAG	C1-C2-N2-C7
4	B	701	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/545 (95%)	1.60	160 (30%)  	18, 55, 128, 167	3 (0%)
1	B	520/545 (95%)	0.73	67 (12%)  	10, 34, 81, 120	3 (0%)
All	All	1039/1090 (95%)	1.16	227 (21%)  	10, 45, 110, 167	6 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	GLY	10.7
1	B	289	PHE	7.5
1	A	542	ILE	7.1
1	B	312	PHE	6.7
1	A	517	TRP	6.5
1	A	464	VAL	6.4
1	A	509	PRO	6.2
1	B	38	HIS	5.7
1	A	532	SER	5.2
1	A	538	VAL	5.2
1	A	507	SER	5.2
1	A	540	SER	5.2
1	A	483	VAL	5.2
1	A	518	LEU	5.0
1	B	39	VAL	4.9
1	A	232	TYR	4.8
1	A	485	ASP	4.7
1	B	225	LEU	4.6
1	A	503	PRO	4.6
1	A	531	CYS	4.6
1	A	25	SER	4.5
1	A	205	ILE	4.5
1	A	537	PRO	4.4
1	A	535	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	202	PHE	4.4
1	A	290	ARG	4.4
1	B	36	LEU	4.4
1	A	289	PHE	4.4
1	B	80	ARG	4.3
1	A	230	CYS	4.3
1	B	317	SER	4.3
1	A	460	ILE	4.3
1	A	491	LEU	4.2
1	B	311	VAL	4.1
1	B	310	ASP	4.1
1	A	227	ASP	4.1
1	B	199	ASN	4.1
1	A	543	CYS	4.0
1	A	381	MET	4.0
1	B	37	ILE	4.0
1	B	545	THR	4.0
1	A	541	ILE	3.9
1	A	467	LEU	3.9
1	B	28	LEU	3.9
1	A	252	ASN	3.9
1	A	494	LEU	3.8
1	A	504	TRP	3.8
1	A	242	THR	3.7
1	B	242	THR	3.7
1	A	488	PHE	3.7
1	A	487	ILE	3.7
1	A	241	GLN	3.7
1	A	42	ASP	3.7
1	A	244	PRO	3.7
1	A	527	GLY	3.6
1	A	514	LEU	3.6
1	A	243	ASN	3.6
1	A	499	LEU	3.6
1	B	43	LEU	3.6
1	B	42	ASP	3.6
1	B	230	CYS	3.6
1	B	446	ARG	3.6
1	A	425	LEU	3.6
1	A	179	GLU	3.6
1	A	225	LEU	3.5
1	A	473	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	86	ILE	3.5
1	A	522	SER	3.5
1	A	226	GLU	3.5
1	B	290	ARG	3.5
1	A	534	SER	3.4
1	A	452	LEU	3.4
1	B	309	SER	3.4
1	A	505	ASP	3.4
1	B	40	PRO	3.4
1	A	516	ARG	3.3
1	A	199	ASN	3.3
1	B	291	ASP	3.3
1	A	461	PRO	3.3
1	A	229	LYS	3.3
1	B	83	TYR	3.3
1	B	89	PHE	3.2
1	A	510	ARG	3.2
1	B	226	GLU	3.2
1	B	150[A]	HIS	3.2
1	B	203	HIS	3.1
1	A	302	LEU	3.1
1	A	523	GLN	3.1
1	B	316	GLN	3.1
1	A	490	ARG	3.1
1	A	521	ASN	3.1
1	B	227	ASP	3.1
1	A	238	ALA	3.1
1	A	469	ALA	3.1
1	A	398	LYS	3.1
1	A	457	ILE	3.0
1	A	211	LYS	3.0
1	A	486	GLY	3.0
1	A	312	PHE	3.0
1	A	181	PRO	3.0
1	A	150[A]	HIS	3.0
1	B	66	LEU	3.0
1	B	177	GLU	3.0
1	A	529	ALA	2.9
1	A	222	LYS	2.9
1	A	536	LYS	2.9
1	A	379	LEU	2.9
1	B	445	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	26	GLU	2.9
1	A	272	THR	2.9
1	A	489	ASP	2.9
1	B	229	LYS	2.8
1	A	291	ASP	2.8
1	A	539	ARG	2.8
1	A	342	LEU	2.8
1	A	41	LYS	2.8
1	B	41	LYS	2.8
1	A	428	LEU	2.8
1	B	314	PHE	2.8
1	A	520	LYS	2.8
1	A	277	SER	2.8
1	A	528	SER	2.8
1	A	465	VAL	2.8
1	A	254	ILE	2.7
1	A	450	LEU	2.7
1	A	513	TYR	2.7
1	A	221	ILE	2.7
1	B	67	SER	2.7
1	A	480	LEU	2.7
1	B	460	ILE	2.7
1	A	160	ALA	2.7
1	A	228	ASN	2.7
1	A	492	THR	2.7
1	B	466	LYS	2.7
1	A	484	PRO	2.7
1	A	446	ARG	2.6
1	A	497	ILE	2.6
1	A	508	CYS	2.6
1	B	286	GLN	2.6
1	B	228	ASN	2.5
1	B	61	TRP	2.5
1	A	481	LYS	2.5
1	B	340[A]	HIS	2.5
1	B	522	SER	2.5
1	A	306	GLN	2.5
1	A	320	TYR	2.5
1	B	178	LYS	2.5
1	A	364	VAL	2.5
1	A	422	THR	2.5
1	A	233	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	224	VAL	2.5
1	A	255	GLU	2.5
1	A	482	SER	2.5
1	B	59	GLU	2.5
1	A	304	ILE	2.5
1	A	43	LEU	2.5
1	A	184	LEU	2.5
1	A	234	LEU	2.5
1	A	448	LYS	2.5
1	A	315	PRO	2.5
1	A	336	THR	2.4
1	A	468	GLU	2.4
1	A	462	LYS	2.4
1	A	220	ASN	2.4
1	A	433	ASN	2.4
1	A	269	TRP	2.4
1	A	515	SER	2.4
1	B	107	LYS	2.4
1	A	176	GLY	2.4
1	B	57	ILE	2.4
1	B	81	ILE	2.4
1	B	114	VAL	2.4
1	A	240	LEU	2.4
1	A	235	SER	2.3
1	B	111	HIS	2.3
1	A	280[A]	ASN	2.3
1	A	475	VAL	2.3
1	A	387	LEU	2.3
1	A	444	PRO	2.3
1	A	203	HIS	2.3
1	A	396	GLN	2.3
1	A	256	THR	2.3
1	A	415	LYS	2.3
1	B	131	ILE	2.3
1	A	470	LEU	2.2
1	B	27	PHE	2.2
1	B	313	GLY	2.2
1	A	301	ALA	2.2
1	A	284	GLN	2.2
1	A	210	VAL	2.2
1	A	253	ASN	2.2
1	A	479	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	281	VAL	2.2
1	A	377	LEU	2.2
1	B	88	VAL	2.2
1	B	321	GLU	2.2
1	A	402	GLN	2.2
1	B	270	HIS	2.2
1	A	334	SER	2.2
1	A	337	ARG	2.1
1	A	498	TRP	2.1
1	A	188	ASN	2.1
1	A	311	VAL	2.1
1	A	449	VAL	2.1
1	B	224	VAL	2.1
1	A	331	PHE	2.1
1	A	286	GLN	2.1
1	B	91	PHE	2.1
1	A	231	SER	2.1
1	B	507	SER	2.1
1	A	282	LYS	2.1
1	A	511	ILE	2.1
1	B	157	LEU	2.1
1	B	248	ASN	2.1
1	A	440	PHE	2.1
1	A	178	LYS	2.1
1	B	156	VAL	2.1
1	A	401	GLN	2.0
1	A	151	LEU	2.0
1	A	113	THR	2.0
1	A	177	GLU	2.0
1	A	198	THR	2.0
1	A	493	SER	2.0
1	B	110	CYS	2.0
1	B	84	LEU	2.0
1	A	347	ILE	2.0
1	A	46	LYS	2.0

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

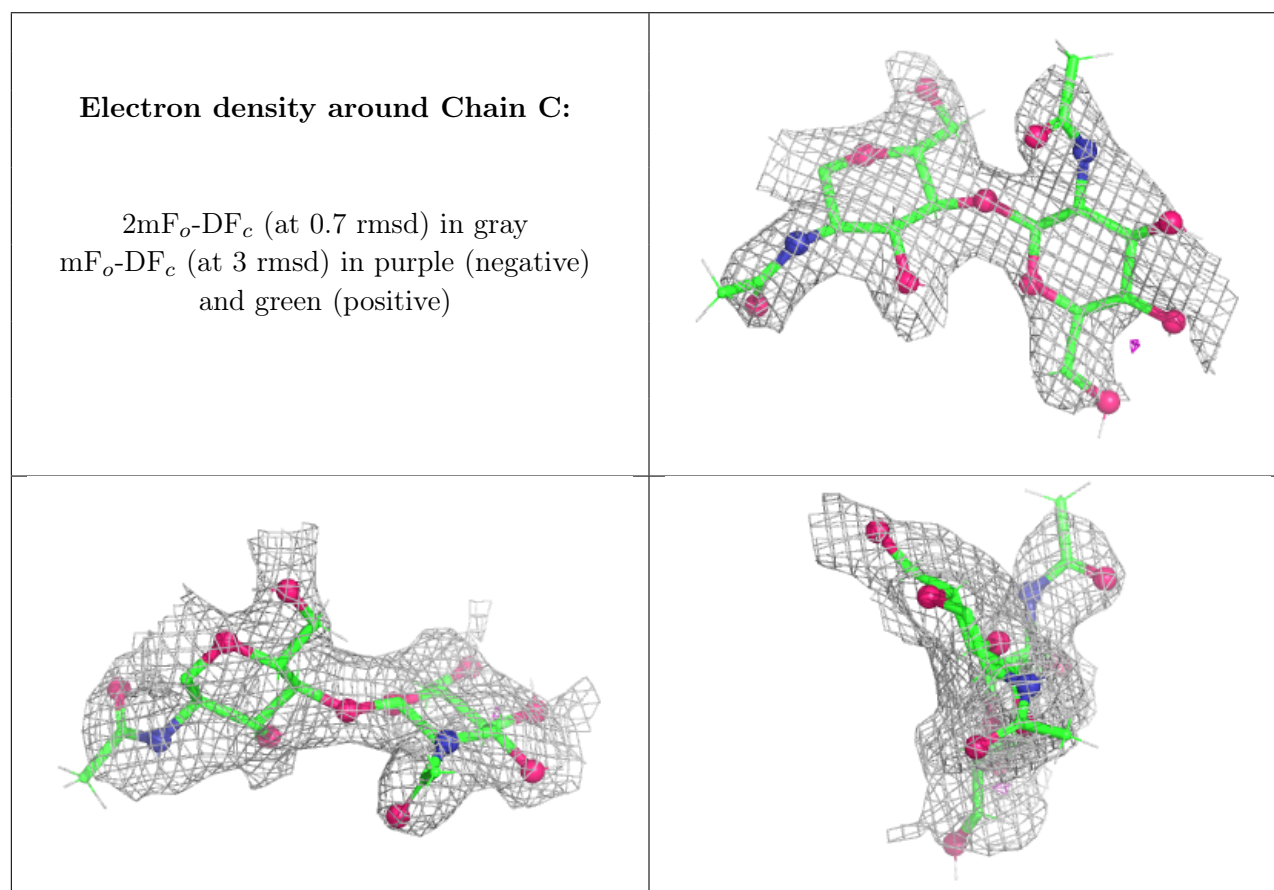
There are no non-standard protein/DNA/RNA residues in this entry.

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.

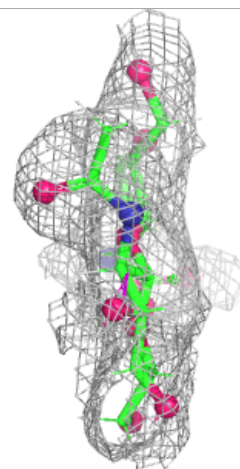
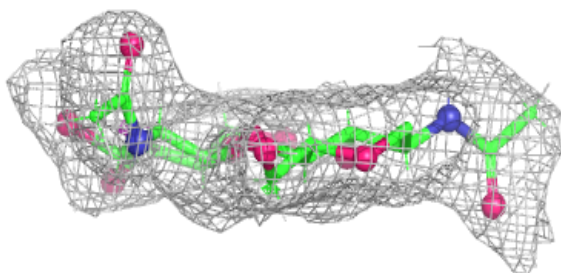
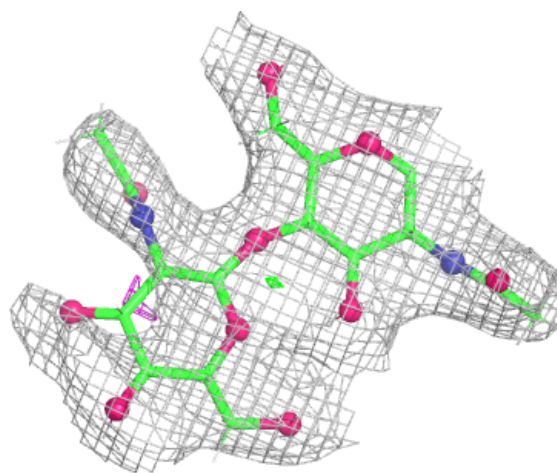
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	3	14/15	0.49	0.18	66,80,96,99	0
2	NAG	C	2	14/15	0.71	0.13	59,71,83,87	0
2	NAG	D	2	14/15	0.72	0.15	44,62,79,93	0
2	NAG	C	1	14/15	0.79	0.13	39,51,60,65	0
2	NAG	F	2	14/15	0.85	0.11	15,36,61,73	0
3	NAG	E	2	14/15	0.86	0.10	28,47,60,67	0
2	NAG	D	1	14/15	0.90	0.08	30,36,40,43	0
3	NAG	E	1	14/15	0.92	0.07	15,34,43,51	0
2	NAG	F	1	14/15	0.95	0.06	6,9,19,23	0

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



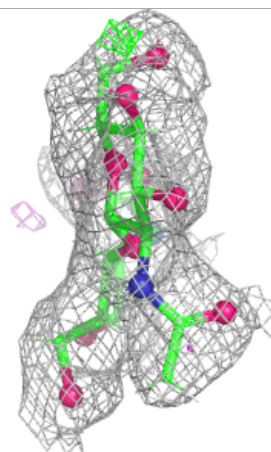
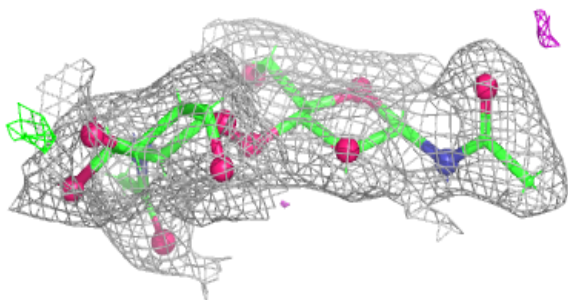
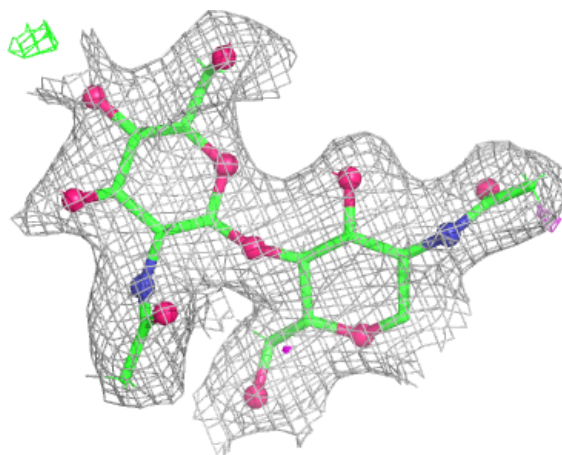
Electron density around Chain D:

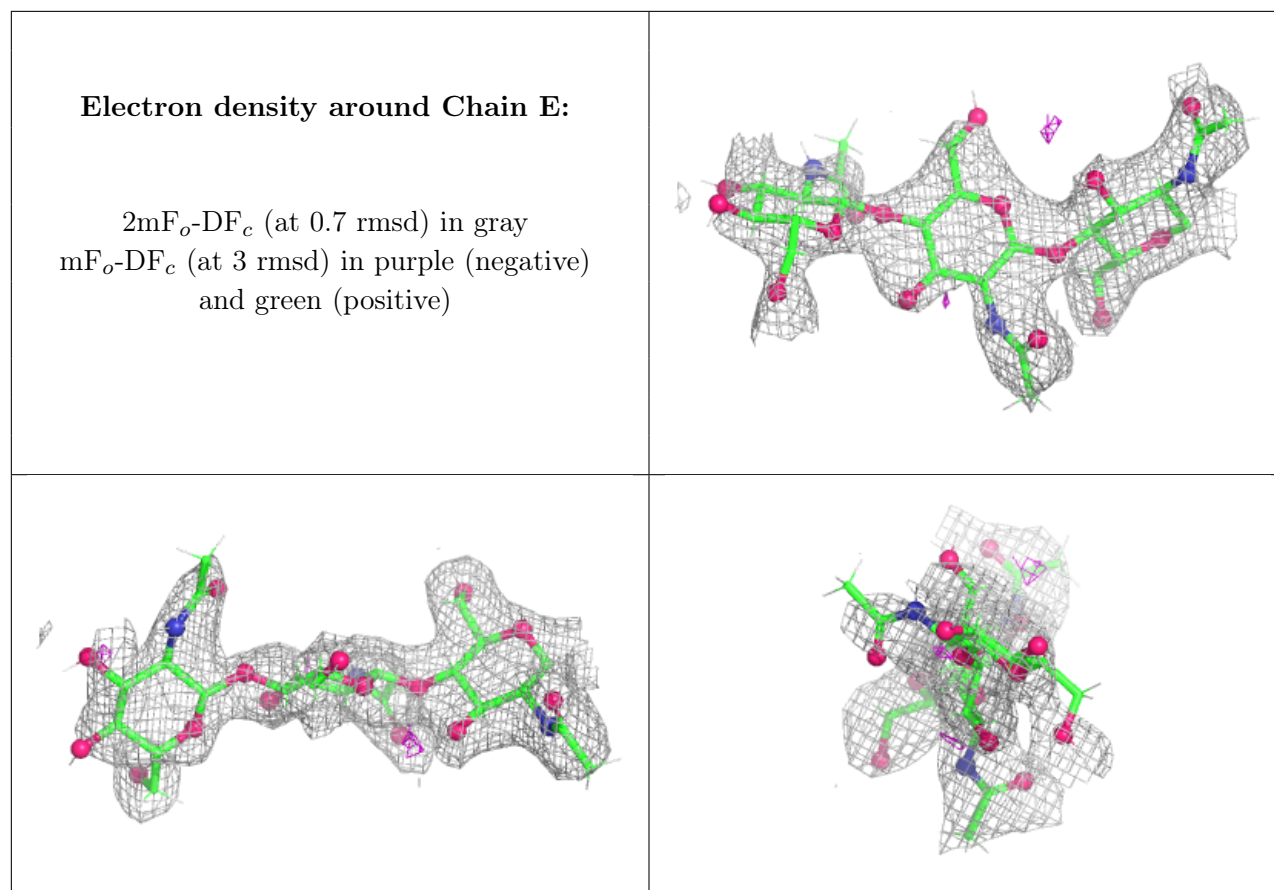
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	702	14/15	0.60	0.17	48,64,73,82	0
4	NAG	B	701	14/15	0.75	0.14	48,64,80,89	0
4	NAG	A	601	14/15	0.87	0.12	6,9,19,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.