



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 23, 2026 – 02:15 PM EDT

PDB ID : 9NVE / pdb_00009nve
Title : Crystal structure of NP203 TCR in complex with NP366-H-2Db
Authors : Tan, K.; Reinherz, E.L.; Mallis, R.J.
Deposited on : 2025-03-20
Resolution : 2.10 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

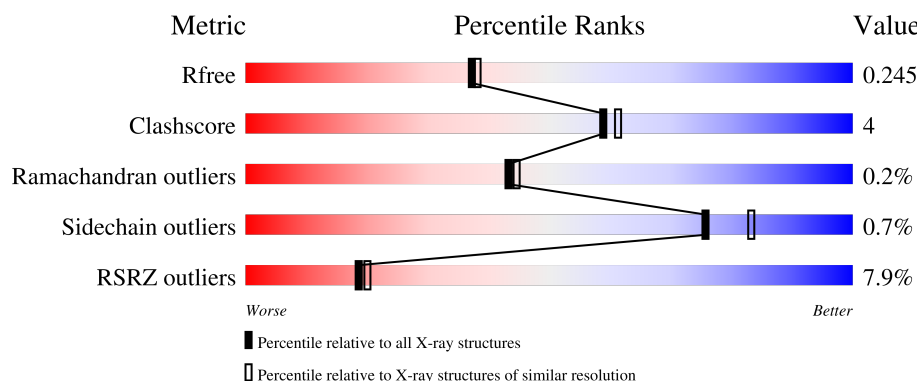
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	223	7% 87% 8% 5%
2	B	254	2% 85% 10% 5%
3	C	281	15% 86% 12% ..
4	D	100	5% 86% 14%
5	P	9	11% 89% 11%

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Mol	Chain	Length	Quality of chain
6	E	2	50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6963 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 NP203 TCR alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1656	1038	270	338	10			

- Molecule 2 is a protein called NP203 TCR beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1944	1235	333	368	8			

- Molecule 3 is a protein called H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	277	Total	C	N	O	S	0	0	0
			2250	1423	399	418	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P01899

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	100	Total	C	N	O	S	0	0	0
			826	527	139	153	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P01887
D	85	ASP	ALA	conflict	UNP P01887

- Molecule 5 is a protein called Nucleoprotein peptide.

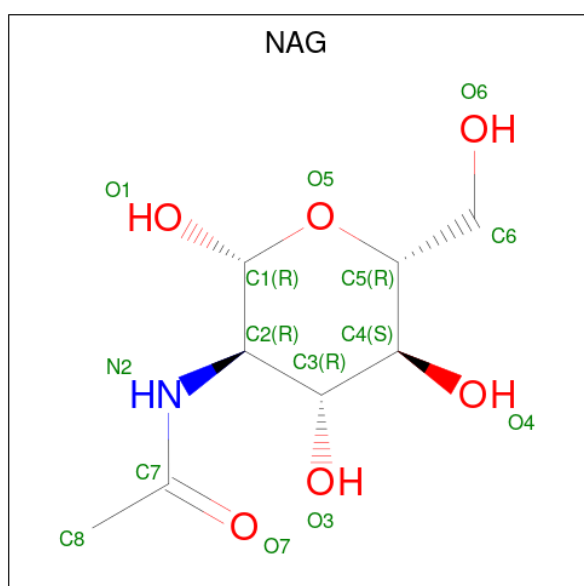
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			69	38	11	18	2			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



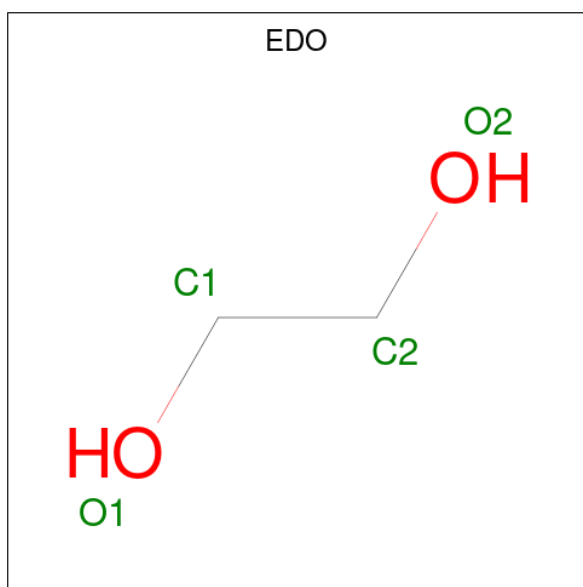
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	B	1	Total Cl 1 1	0	0
9	D	1	Total Cl 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	21	Total O 21 21	0	0
10	B	60	Total O 60 60	0	0

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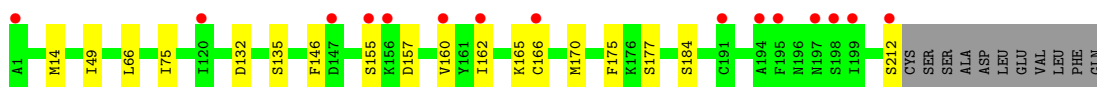
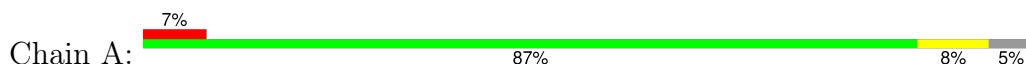
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	48	Total 48	O 48	0	0
10	D	8	Total 8	O 8	0	0
10	P	6	Total 6	O 6	0	0

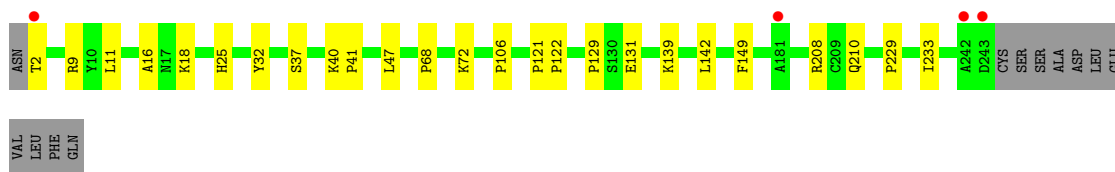
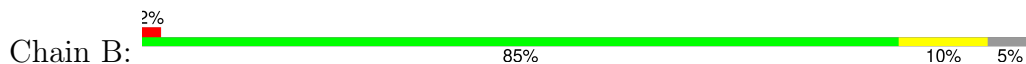
3 Residue-property plots [i](#)

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.

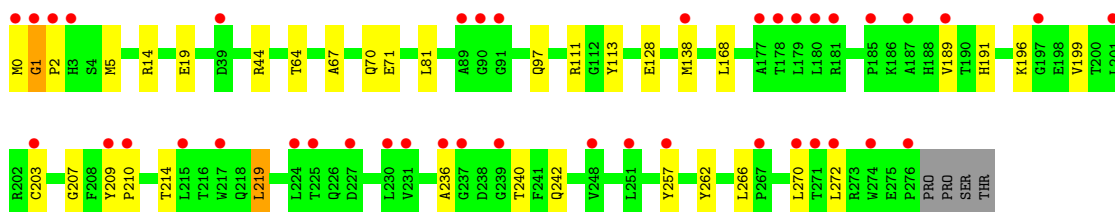
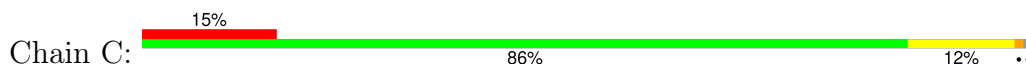
- Molecule 1: NP203 TCR alpha-chain



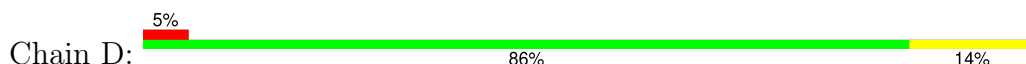
- Molecule 2: NP203 TCR beta-chain



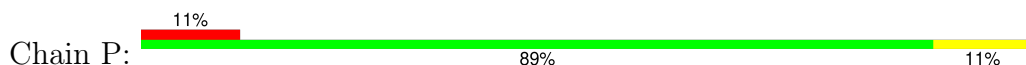
- Molecule 3: H-2 class I histocompatibility antigen, D-B alpha chain

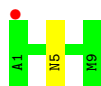


- Molecule 4: Beta-2-microglobulin



- Molecule 5: Nucleoprotein peptide





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.78Å 66.62Å 76.78Å 68.78° 89.27° 66.42°	Depositor
Resolution (Å)	49.94 – 2.10 49.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.94-2.10) 95.8 (49.94-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.211 , 0.245 0.211 , 0.245	Depositor DCC
R_{free} test set	2637 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, 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	0.09	0/1689	0.26	0/2286
2	B	0.09	0/1999	0.29	0/2723
3	C	0.10	0/2317	0.27	0/3148
4	D	0.14	0/852	0.31	0/1155
5	P	0.14	0/68	0.26	0/88
All	All	0.10	0/6925	0.28	0/9400

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 [i](#)

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	1656	0	1584	12	0
2	B	1944	0	1864	18	0
3	C	2250	0	2114	23	0
4	D	826	0	798	10	0
5	P	69	0	61	4	0
6	E	28	0	25	0	0
7	A	14	0	13	0	0
7	B	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	4	0	6	0	0
8	B	12	0	18	2	0
9	A	1	0	0	1	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	21	0	0	0	0
10	B	60	0	0	0	0
10	C	48	0	0	0	0
10	D	8	0	0	0	0
10	P	6	0	0	0	0
All	All	6963	0	6496	59	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 (59) 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)
3:C:97:GLN:HE22	5:P:5:ASN:HD21	1.22	0.85
3:C:236:ALA:HB1	4:D:12:ARG:HG3	1.66	0.76
2:B:37:SER:H	2:B:40:LYS:HE2	1.58	0.69
2:B:2:THR:HG21	2:B:25:HIS:HB2	1.74	0.69
2:B:16:ALA:HB3	7:B:301:NAG:H82	1.75	0.69
1:A:157:ASP:HB3	1:A:160:VAL:HG22	1.77	0.65
1:A:155:SER:HB3	1:A:162:ILE:HD13	1.80	0.63
2:B:11:LEU:HD11	2:B:18:LYS:HD3	1.83	0.61
2:B:40:LYS:HE3	2:B:41:PRO:O	2.01	0.60
3:C:214:THR:HB	3:C:262:TYR:HB2	1.86	0.58
3:C:266:LEU:HD13	3:C:270:LEU:HD13	1.87	0.57
2:B:40:LYS:HG2	2:B:41:PRO:HD2	1.86	0.56
3:C:209:TYR:HB3	3:C:210:PRO:HD3	1.87	0.56
2:B:106:PRO:HB2	8:B:303:EDO:H11	1.88	0.56
3:C:266:LEU:HD22	3:C:270:LEU:HD11	1.89	0.54
2:B:121:PRO:HD3	2:B:229:PRO:HB3	1.92	0.51
3:C:5:MET:HB2	3:C:168:LEU:HD13	1.93	0.51
1:A:177:SER:HA	9:A:303:CL:CL	2.47	0.51
2:B:32:TYR:CE2	2:B:47:LEU:HD13	2.47	0.50
4:D:12:ARG:HB2	4:D:22:ILE:HD11	1.95	0.48
4:D:54:MET:HE3	4:D:62:PHE:HB3	1.95	0.48
3:C:70:GLN:NE2	5:P:5:ASN:H	2.11	0.48
2:B:210:GLN:HG3	2:B:233:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:GLN:HE22	5:P:5:ASN:H	1.62	0.48
3:C:111:ARG:HG2	3:C:113:TYR:CZ	2.50	0.47
4:D:25:CYS:HB2	4:D:39:MET:HE3	1.96	0.47
1:A:146:PHE:HE2	1:A:165:LYS:HD3	1.80	0.46
4:D:23:LEU:O	4:D:67:HIS:HA	2.15	0.46
2:B:129:PRO:HD3	2:B:142:LEU:HG	1.98	0.46
1:A:49:ILE:HD13	1:A:66:LEU:HG	1.98	0.45
3:C:44:ARG:HG3	3:C:64:THR:OG1	2.16	0.45
1:A:212:SER:HB2	2:B:131:GLU:HG2	1.99	0.45
4:D:50:GLU:HB2	4:D:67:HIS:CE1	2.52	0.44
1:A:66:LEU:HD22	1:A:75:ILE:HD11	2.00	0.43
3:C:189:VAL:HG22	3:C:203:CYS:HB3	2.00	0.43
3:C:207:GLY:HA2	3:C:240:THR:HB	2.00	0.43
3:C:242:GLN:HE22	4:D:12:ARG:HA	1.83	0.43
4:D:28:THR:HG22	4:D:63:TYR:HB2	2.00	0.43
3:C:14:ARG:HH21	3:C:19:GLU:HB3	1.84	0.43
3:C:67:ALA:O	3:C:71:GLU:HG2	2.17	0.43
3:C:97:GLN:NE2	5:P:5:ASN:HD21	2.03	0.43
3:C:0:MET:HG3	3:C:1:GLY:H	1.84	0.43
3:C:14:ARG:NH2	3:C:19:GLU:HB3	2.34	0.43
3:C:219:LEU:HB3	3:C:257:TYR:CD2	2.53	0.43
2:B:9:ARG:HG3	8:B:303:EDO:H12	2.01	0.43
1:A:170:MET:HE2	1:A:170:MET:HB3	1.89	0.43
3:C:138:MET:HE2	3:C:138:MET:HB3	1.97	0.42
1:A:175:PHE:CD2	2:B:139:LYS:HE2	2.54	0.42
4:D:27:VAL:HG21	4:D:37:ILE:HD13	2.01	0.42
2:B:208:ARG:NH2	2:B:210:GLN:HB2	2.33	0.42
3:C:191:HIS:NE2	3:C:199:VAL:HG11	2.35	0.42
1:A:14:MET:HE2	1:A:14:MET:HB3	1.95	0.42
2:B:40:LYS:HE2	2:B:40:LYS:HB3	1.76	0.42
2:B:68:PRO:HG2	2:B:72:LYS:HB3	2.02	0.41
4:D:22:ILE:O	4:D:70:PHE:HE1	2.03	0.41
2:B:122:PRO:HB3	2:B:149:PHE:HB3	2.02	0.41
1:A:132:ASP:HB3	1:A:135:SER:O	2.21	0.41
1:A:160:VAL:HG12	1:A:184:SER:HB2	2.03	0.41
3:C:111:ARG:CZ	3:C:128:GLU:HG3	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/223 (94%)	199 (95%)	11 (5%)	0	100	100
2	B	240/254 (94%)	236 (98%)	4 (2%)	0	100	100
3	C	275/281 (98%)	258 (94%)	15 (6%)	2 (1%)	18	15
4	D	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
5	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	830/867 (96%)	794 (96%)	34 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	2	PRO
3	C	1	GLY

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	189/201 (94%)	188 (100%)	1 (0%)	81	88
2	B	214/225 (95%)	214 (100%)	0	100	100
3	C	229/239 (96%)	225 (98%)	4 (2%)	53	62
4	D	94/95 (99%)	94 (100%)	0	100	100
5	P	8/8 (100%)	8 (100%)	0	100	100
All	All	734/768 (96%)	729 (99%)	5 (1%)	76	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	CYS
3	C	81	LEU
3	C	196	LYS
3	C	219	LEU
3	C	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	GLN
2	B	183	ASN
3	C	70	GLN
3	C	86	ASN
3	C	97	GLN
3	C	188	HIS
5	P	3	ASN

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	$\# Z > 2$
6	NAG	E	1	6,2	14,14,15	0.72	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	2	6	14,14,15	0.72	0	17,19,21	0.78	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
6	NAG	E	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	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(°)	Ideal(°)
6	E	1	NAG	C1-O5-C5	2.17	115.09	112.19

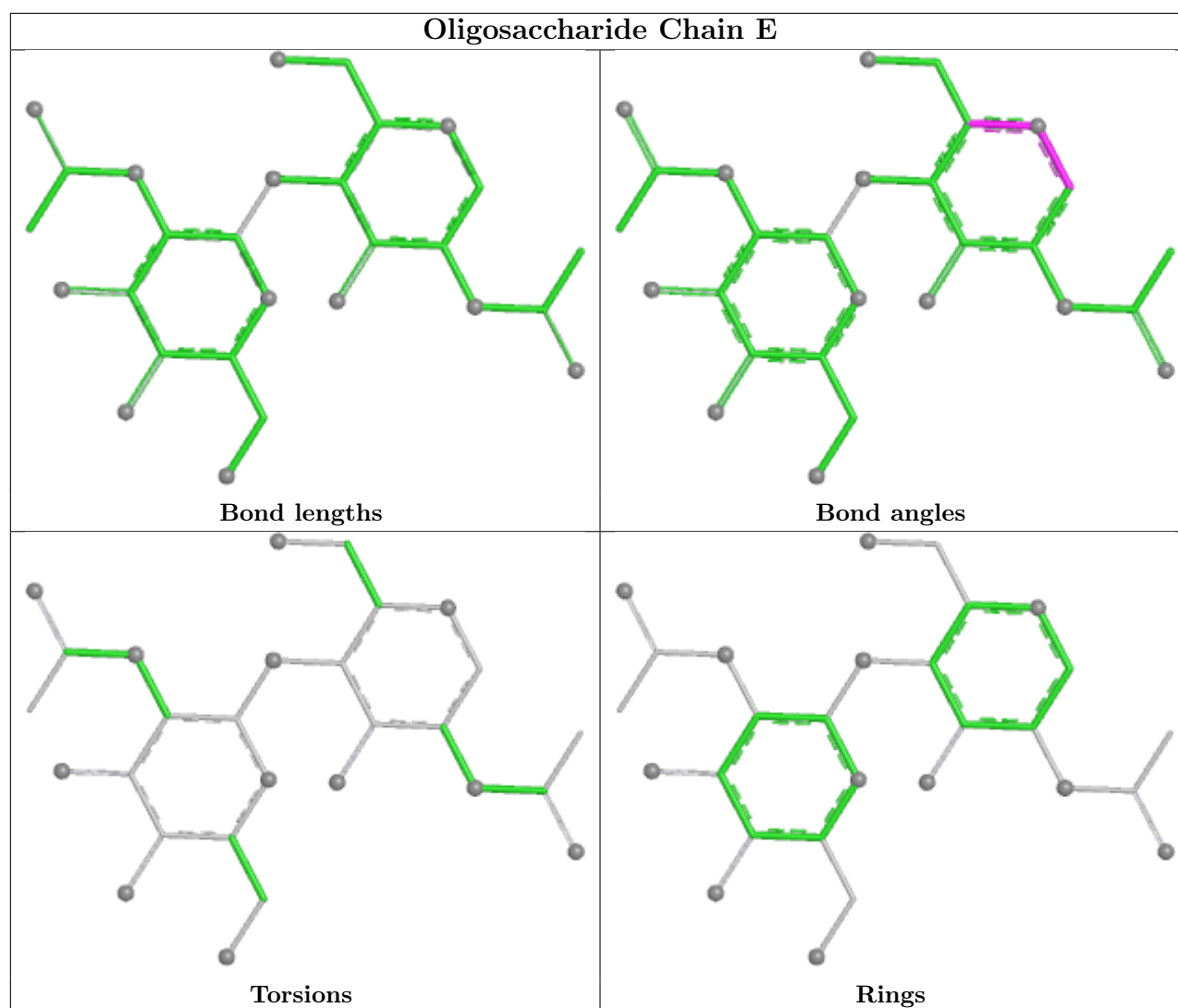
There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
8	EDO	B	304	-	3,3,3	0.25	0	2,2,2	0.37	0
7	NAG	B	301	2	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
8	EDO	B	302	-	3,3,3	0.25	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	301	1	14,14,15	0.66	0	17,19,21	0.95	0
8	EDO	B	303	-	3,3,3	0.26	0	2,2,2	0.29	0
8	EDO	A	302	-	3,3,3	0.25	0	2,2,2	0.34	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
8	EDO	B	304	-	-	0/1/1/1	-
7	NAG	B	301	2	-	1/6/23/26	0/1/1/1
8	EDO	B	302	-	-	0/1/1/1	-
7	NAG	A	301	1	-	0/6/23/26	0/1/1/1
8	EDO	B	303	-	-	1/1/1/1	-
8	EDO	A	302	-	-	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(°)	Ideal(°)
7	B	301	NAG	C1-O5-C5	2.31	115.28	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	301	NAG	O5-C5-C6-O6
8	B	303	EDO	O1-C1-C2-O2

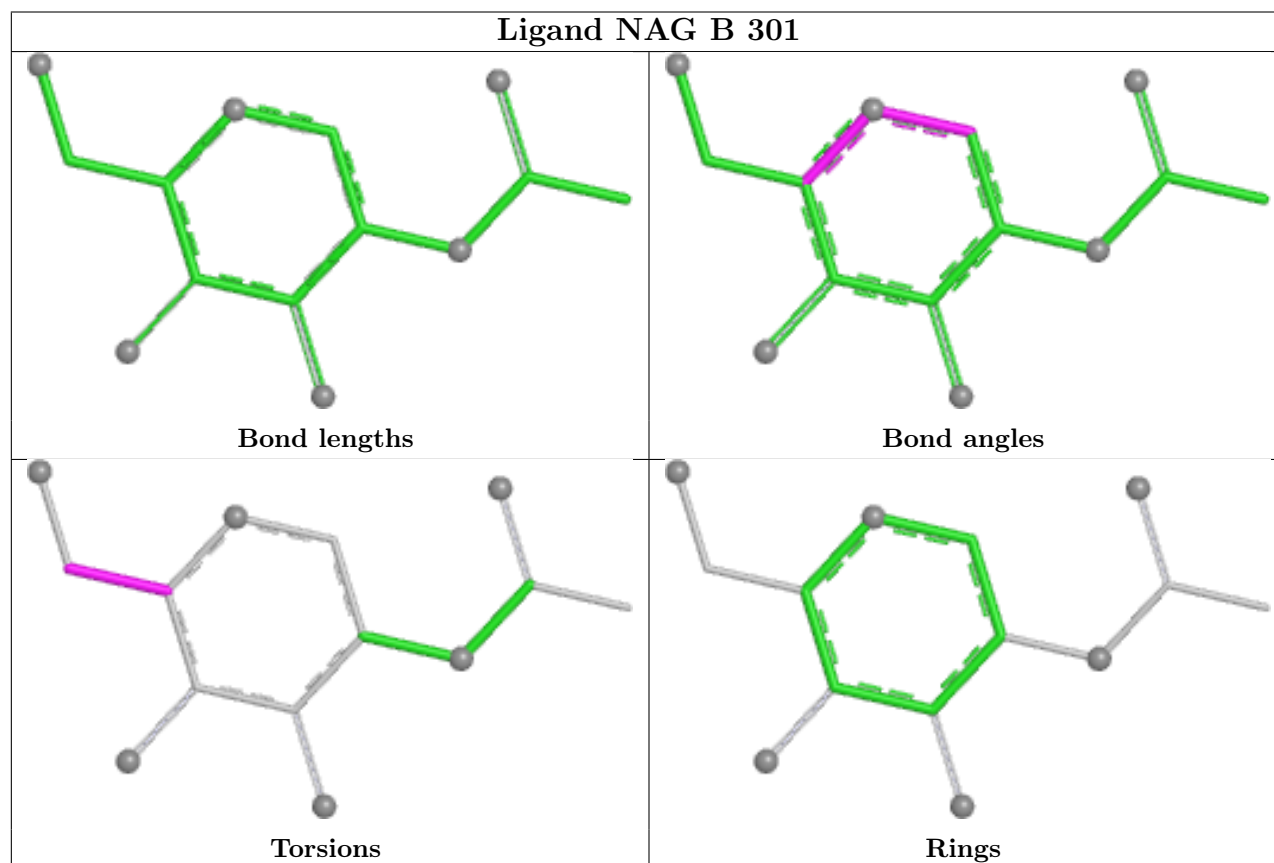
There are no ring outliers.

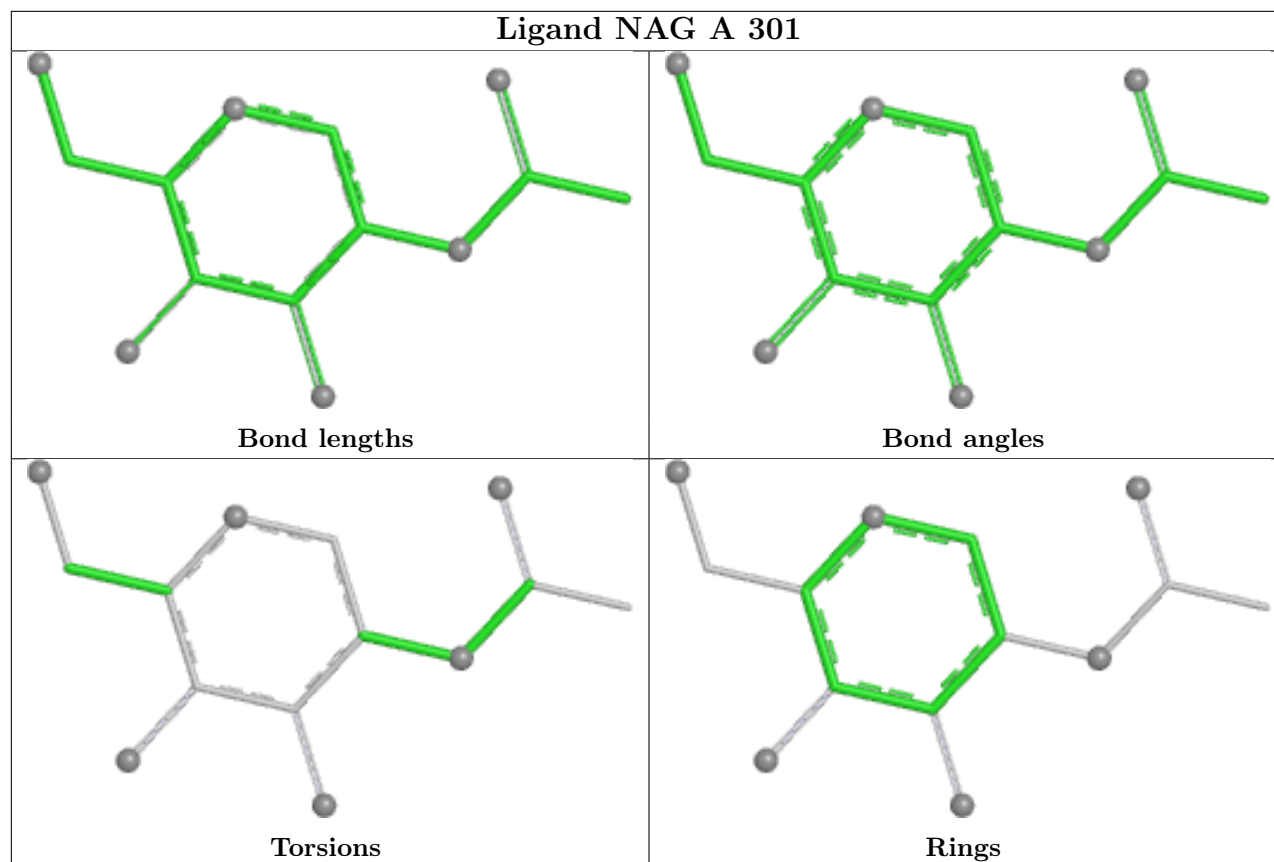
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	301	NAG	1	0
8	B	303	EDO	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 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 than 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.





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	212/223 (95%)	0.72	15 (7%) 22 23	30, 65, 125, 148	0
2	B	242/254 (95%)	0.23	4 (1%) 69 71	29, 50, 77, 123	0
3	C	277/281 (98%)	0.73	41 (14%) 5 6	30, 58, 152, 165	0
4	D	100/100 (100%)	0.78	5 (5%) 34 36	49, 64, 104, 106	0
5	P	9/9 (100%)	0.06	1 (11%) 10 10	30, 33, 45, 49	0
All	All	840/867 (96%)	0.58	66 (7%) 18 20	29, 56, 134, 165	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	276	PRO	4.6
1	A	194	ALA	4.3
3	C	2	PRO	4.3
3	C	209	TYR	4.1
1	A	195	PHE	4.1
3	C	180	LEU	4.0
1	A	199	ILE	4.0
1	A	160	VAL	3.9
2	B	243	ASP	3.8
3	C	215	LEU	3.5
2	B	2	THR	3.4
1	A	1	ALA	3.3
1	A	212	SER	3.3
3	C	89	ALA	3.2
3	C	248	VAL	3.1
3	C	271	THR	3.0
3	C	210	PRO	3.0
3	C	236	ALA	2.9
1	A	162	ILE	2.9
4	D	1	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	0	MET	2.9
3	C	203	CYS	2.9
4	D	49	VAL	2.9
3	C	177	ALA	2.9
3	C	274	TRP	2.9
3	C	225	THR	2.8
3	C	185	PRO	2.8
3	C	91	GLY	2.8
1	A	198	SER	2.7
3	C	179	LEU	2.7
4	D	22	ILE	2.7
2	B	242	ALA	2.7
3	C	227	ASP	2.6
4	D	54	MET	2.6
3	C	201	LEU	2.6
1	A	191	CYS	2.6
3	C	1	GLY	2.6
3	C	224	LEU	2.6
3	C	270	LEU	2.6
3	C	257	TYR	2.6
3	C	90	GLY	2.6
3	C	267	PRO	2.6
3	C	138	MET	2.5
3	C	189	VAL	2.5
2	B	181	ALA	2.4
4	D	0	MET	2.4
3	C	239	GLY	2.4
3	C	231	VAL	2.4
3	C	178	THR	2.4
3	C	197	GLY	2.3
3	C	237	GLY	2.3
3	C	187	ALA	2.3
1	A	166	CYS	2.3
3	C	272	LEU	2.3
5	P	1	ALA	2.2
1	A	155	SER	2.2
1	A	197	ASN	2.2
3	C	3	HIS	2.1
3	C	230	LEU	2.1
3	C	251	LEU	2.1
1	A	156	LYS	2.1
3	C	39	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	ILE	2.1
3	C	217	TRP	2.1
3	C	181	ARG	2.0
1	A	147	ASP	2.0

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

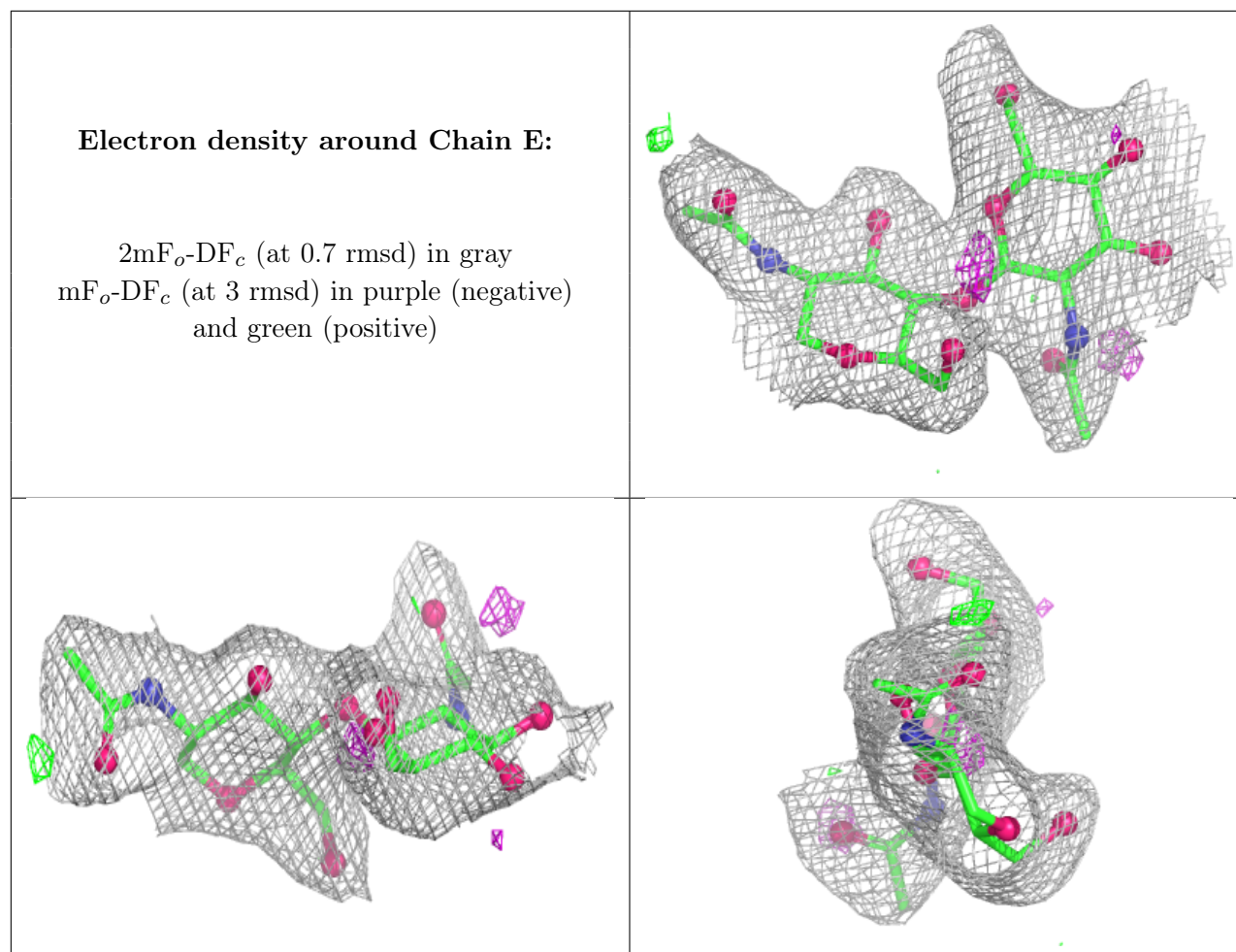
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
6	NAG	E	1	14/15	-	-	45,55,60,62	0
6	NAG	E	2	14/15	-	-	62,67,71,75	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, 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.

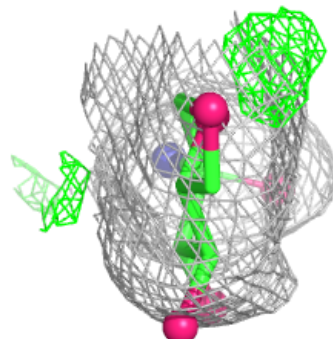
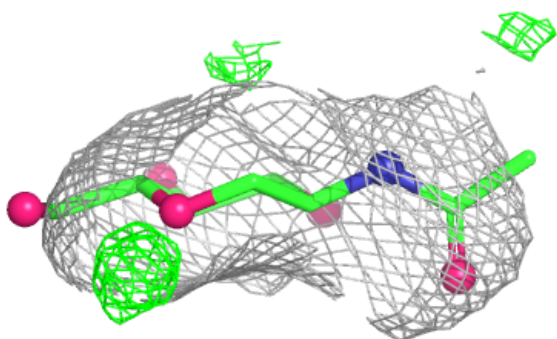
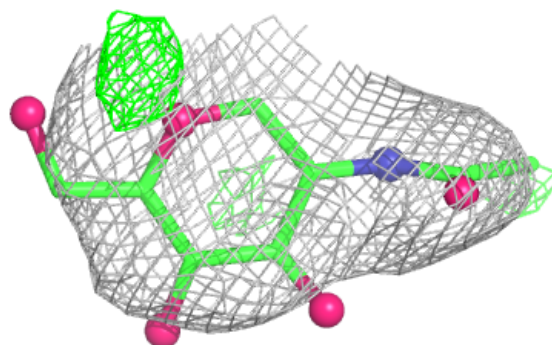
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	301	14/15	0.71	0.13	76,83,90,91	0
8	EDO	B	302	4/4	0.76	0.16	80,81,84,86	0
8	EDO	B	304	4/4	0.77	0.16	51,53,55,57	0
8	EDO	A	302	4/4	0.80	0.20	53,54,56,58	0
8	EDO	B	303	4/4	0.86	0.17	41,46,46,49	0
7	NAG	A	301	14/15	0.86	0.10	41,45,48,53	0
9	CL	B	305	1/1	0.87	0.12	74,74,74,74	0
9	CL	A	303	1/1	0.91	0.10	76,76,76,76	0
9	CL	D	101	1/1	0.92	0.11	78,78,78,78	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.

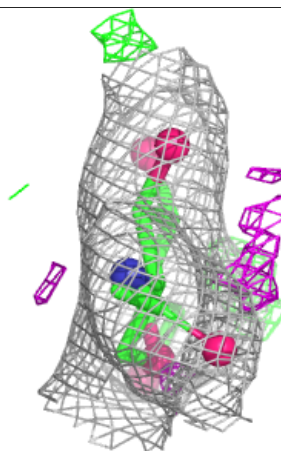
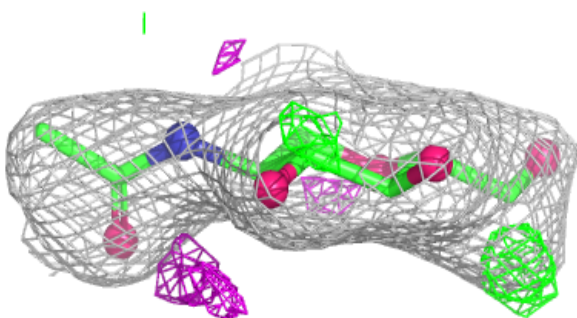
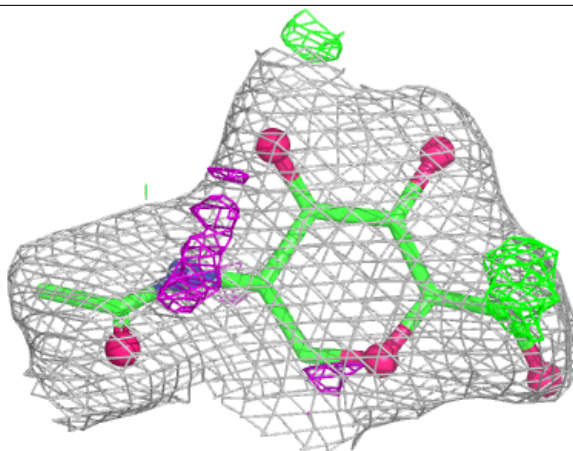
Electron density around NAG B 301:

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



Electron density around NAG A 301:

$2mF_o-DF_c$ (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.