



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:43 PM UTC

PDB ID : 6LVX / pdb_00006lvx
Title : Crystal structure of TLR7/Cpd-1 (SM-374527) complex
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on : 2020-02-06
Resolution : 2.77 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 : 9.0.010 (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

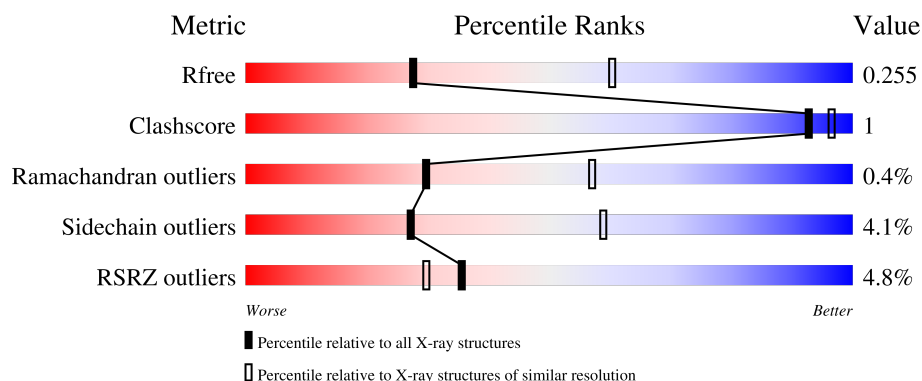
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

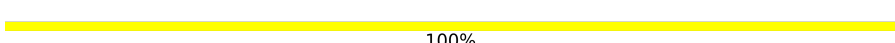
The reported resolution of this entry is 2.77 Å.

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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	823	
1	B	823	
2	C	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12774 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total	C	N	O	S	0	0	0
			6235	3996	1061	1148	30			
1	B	771	Total	C	N	O	S	0	0	0
			6235	3996	1061	1148	30			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	440	LEU	SER	engineered mutation	UNP B3Y653
A	441	VAL	GLU	engineered mutation	UNP B3Y653
A	442	PRO	VAL	engineered mutation	UNP B3Y653
A	443	ARG	GLY	engineered mutation	UNP B3Y653
A	444	GLY	PHE	engineered mutation	UNP B3Y653
A	445	SER	CYS	engineered mutation	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
A	840	GLU	-	expression tag	UNP B3Y653
A	841	PHE	-	expression tag	UNP B3Y653
A	842	LEU	-	expression tag	UNP B3Y653
A	843	VAL	-	expression tag	UNP B3Y653
A	844	PRO	-	expression tag	UNP B3Y653
A	845	ARG	-	expression tag	UNP B3Y653
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653

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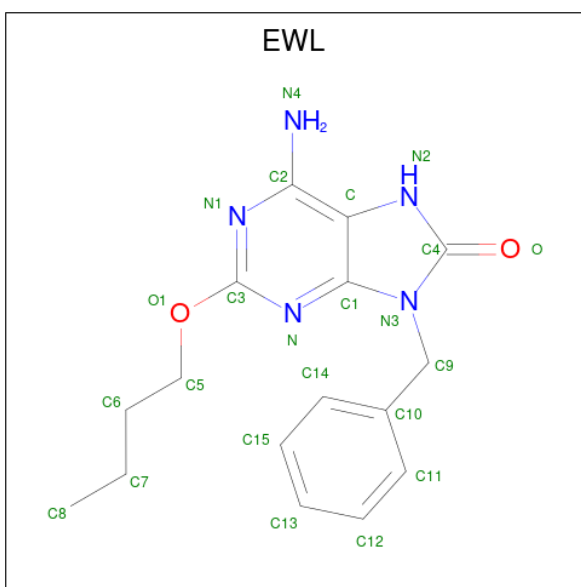
Chain	Residue	Modelled	Actual	Comment	Reference
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	440	LEU	SER	engineered mutation	UNP B3Y653
B	441	VAL	GLU	engineered mutation	UNP B3Y653
B	442	PRO	VAL	engineered mutation	UNP B3Y653
B	443	ARG	GLY	engineered mutation	UNP B3Y653
B	444	GLY	PHE	engineered mutation	UNP B3Y653
B	445	SER	CYS	engineered mutation	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653
B	840	GLU	-	expression tag	UNP B3Y653
B	841	PHE	-	expression tag	UNP B3Y653
B	842	LEU	-	expression tag	UNP B3Y653
B	843	VAL	-	expression tag	UNP B3Y653
B	844	PRO	-	expression tag	UNP B3Y653
B	845	ARG	-	expression tag	UNP B3Y653

- 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	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 6-azanyl-2-butoxy-9-(phenylmethyl)-7H-purin-8-one (CCD ID: EWL) (formula: C₁₆H₁₉N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	16	5	2		
3	B	1	Total	C	N	O	0	0
			23	16	5	2		

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



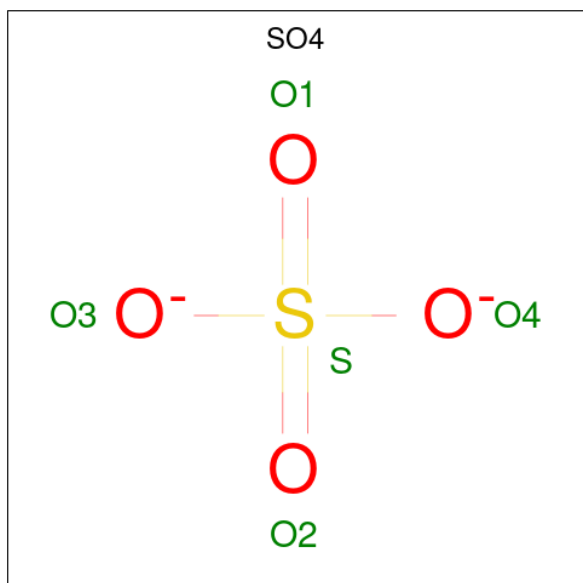
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

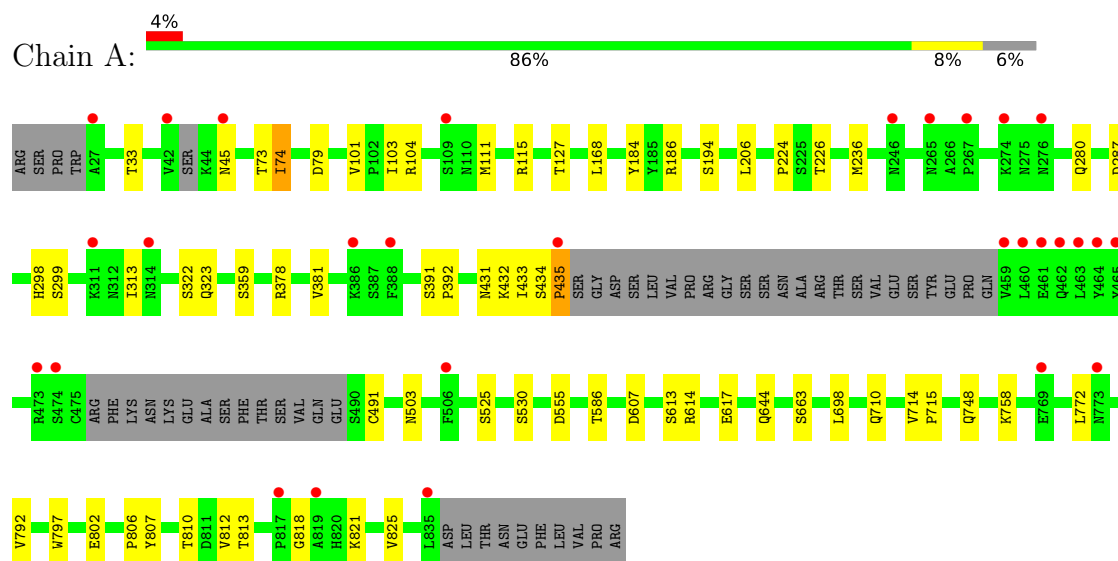
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	17	Total	O	0	0
			17	17		

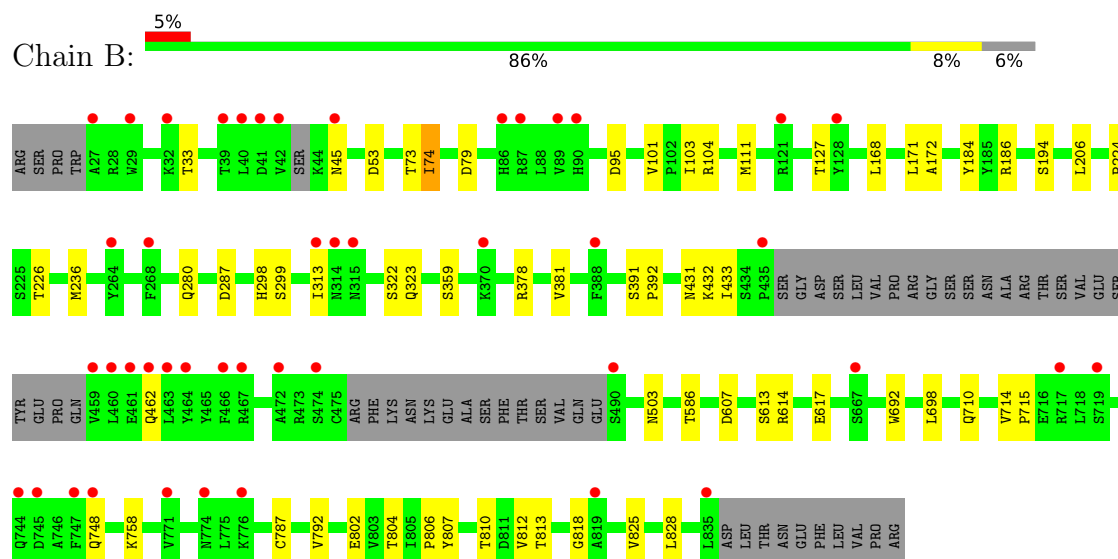
3 Residue-property plots [i](#)

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 7



• Molecule 1: Toll-like receptor 7



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

Chain C:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.75Å 138.50Å 148.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.77 50.01 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-2.77) 99.9 (50.01-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.79 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.212 , 0.252 0.216 , 0.255	Depositor DCC
R_{free} test set	2550 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12774	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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, EWL, SO4

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	0.86	1/6365 (0.0%)	0.95	3/8623 (0.0%)
1	B	0.84	0/6365	0.94	2/8623 (0.0%)
All	All	0.85	1/12730 (0.0%)	0.94	5/17246 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	SER	C-O	-5.79	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ASP	N-CA-C	5.75	117.81	109.07
1	A	287	ASP	N-CA-C	5.43	117.90	111.33
1	A	79	ASP	N-CA-C	5.41	117.29	109.07
1	A	115	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	B	287	ASP	N-CA-C	5.35	117.81	111.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	530	SER	Peptide
1	A	812	VAL	Peptide
1	B	812	VAL	Peptide

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	6235	0	6268	19	0
1	B	6235	0	6270	18	0
2	C	28	0	25	0	0
3	A	23	0	0	2	0
3	B	23	0	0	0	0
4	A	98	0	91	1	0
4	B	56	0	52	0	0
5	A	20	0	0	0	0
5	B	10	0	0	1	0
6	A	29	0	0	0	0
6	B	17	0	0	0	0
All	All	12774	0	12706	37	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 1.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:HB2	1:A:435:PRO:HD2	1.77	0.66
1:B:73:THR:HG22	1:B:74:ILE:HG13	1.81	0.63
1:A:663:SER:HB3	5:B:1007:SO4:O3	2.00	0.61
1:A:73:THR:HG22	1:A:74:ILE:HG13	1.81	0.61
1:A:206:LEU:O	1:A:226:THR:HG23	2.02	0.59
1:B:206:LEU:O	1:B:226:THR:HG23	2.03	0.59
1:A:298:HIS:CE1	1:A:323:GLN:HG3	2.43	0.53
1:A:714:VAL:HB	1:A:715:PRO:HD2	1.91	0.53
1:B:431:ASN:HB2	1:B:503:ASN:HD21	1.74	0.53
1:A:431:ASN:HB2	1:A:503:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:HIS:CE1	1:B:323:GLN:HG3	2.45	0.51
1:B:714:VAL:HB	1:B:715:PRO:HD2	1.92	0.51
1:A:772:LEU:HD13	1:A:797:TRP:CZ2	2.50	0.46
1:A:298:HIS:HA	1:A:322:SER:O	2.15	0.46
1:A:184:TYR:CZ	1:A:186:ARG:HB2	2.51	0.46
1:B:53:ASP:HA	1:B:74:ILE:O	2.17	0.45
1:A:433:ILE:H	1:A:503:ASN:HD22	1.66	0.44
1:B:298:HIS:HA	1:B:322:SER:O	2.17	0.44
1:B:95:ASP:C	1:B:95:ASP:OD1	2.60	0.44
1:A:555:ASP:OD1	3:A:1001:EWL:N4	2.51	0.43
1:B:184:TYR:CZ	1:B:186:ARG:HB2	2.53	0.43
1:A:224:PRO:HB2	1:A:226:THR:HG22	2.00	0.43
1:A:491:CYS:HB3	4:A:1003:NAG:H81	2.00	0.43
1:A:299:SER:HA	1:A:323:GLN:O	2.18	0.42
1:B:103:ILE:HD11	1:B:111:MET:SD	2.59	0.42
1:B:806:PRO:HB2	1:B:807:TYR:CD2	2.53	0.42
1:A:806:PRO:HB2	1:A:807:TYR:CD2	2.53	0.42
1:A:391:SER:N	1:A:392:PRO:CD	2.83	0.42
1:B:299:SER:HA	1:B:323:GLN:O	2.20	0.42
1:B:224:PRO:HB2	1:B:226:THR:HG22	2.02	0.41
1:B:692:TRP:CE2	1:B:715:PRO:HD3	2.55	0.41
1:B:787:CYS:HB3	1:B:828:LEU:HD21	2.01	0.41
1:A:103:ILE:HD11	1:A:111:MET:SD	2.60	0.41
1:B:433:ILE:H	1:B:503:ASN:HD22	1.68	0.41
1:B:391:SER:N	1:B:392:PRO:CD	2.84	0.41
1:A:555:ASP:OD2	3:A:1001:EWL:N2	2.54	0.41
1:B:171:LEU:O	1:B:172:ALA:C	2.64	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	763/823 (93%)	710 (93%)	50 (7%)	3 (0%)	30	57
1	B	763/823 (93%)	709 (93%)	51 (7%)	3 (0%)	30	57
All	All	1526/1646 (93%)	1419 (93%)	101 (7%)	6 (0%)	30	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	818	GLY
1	B	381	VAL
1	A	381	VAL
1	A	74	ILE
1	B	74	ILE
1	A	818	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	722/774 (93%)	692 (96%)	30 (4%)	26	58
1	B	722/774 (93%)	693 (96%)	29 (4%)	28	60
All	All	1444/1548 (93%)	1385 (96%)	59 (4%)	27	59

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	45	ASN
1	A	101	VAL
1	A	104	ARG
1	A	127	THR
1	A	168	LEU
1	A	194	SER
1	A	236	MET
1	A	280	GLN
1	A	313	ILE

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Mol	Chain	Res	Type
1	A	359	SER
1	A	378	ARG
1	A	432	LYS
1	A	435	PRO
1	A	586	THR
1	A	607	ASP
1	A	613	SER
1	A	614	ARG
1	A	617	GLU
1	A	644	GLN
1	A	698	LEU
1	A	710	GLN
1	A	748	GLN
1	A	758	LYS
1	A	792	VAL
1	A	802	GLU
1	A	810	THR
1	A	813	THR
1	A	821	LYS
1	A	825	VAL
1	B	33	THR
1	B	45	ASN
1	B	101	VAL
1	B	104	ARG
1	B	127	THR
1	B	168	LEU
1	B	194	SER
1	B	236	MET
1	B	280	GLN
1	B	313	ILE
1	B	359	SER
1	B	378	ARG
1	B	432	LYS
1	B	462	GLN
1	B	586	THR
1	B	607	ASP
1	B	613	SER
1	B	614	ARG
1	B	617	GLU
1	B	698	LEU
1	B	710	GLN
1	B	748	GLN

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Mol	Chain	Res	Type
1	B	758	LYS
1	B	792	VAL
1	B	802	GLU
1	B	804	THR
1	B	810	THR
1	B	813	THR
1	B	825	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	110	ASN
1	A	173	ASN
1	A	389	GLN
1	A	398	ASN
1	A	503	ASN
1	A	539	GLN
1	A	594	ASN
1	A	648	ASN
1	A	708	HIS
1	A	773	ASN
1	B	76	HIS
1	B	110	ASN
1	B	173	ASN
1	B	389	GLN
1	B	398	ASN
1	B	503	ASN
1	B	539	GLN
1	B	800	HIS

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
2	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	1.59	6 (35%)
2	NAG	C	2	2	14,14,15	0.54	0	17,19,21	1.67	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	4.46	118.17	112.19
2	C	2	NAG	C4-C3-C2	-2.84	106.86	111.02
2	C	1	NAG	O5-C1-C2	-2.82	106.93	111.29
2	C	1	NAG	O7-C7-N2	2.61	126.59	121.98
2	C	1	NAG	C3-C4-C5	-2.54	105.62	110.23
2	C	2	NAG	C3-C4-C5	-2.52	105.66	110.23
2	C	1	NAG	O5-C5-C6	-2.46	102.88	107.66
2	C	2	NAG	O4-C4-C5	2.44	115.33	109.32
2	C	1	NAG	C8-C7-N2	-2.07	112.68	116.12
2	C	1	NAG	O6-C6-C5	-2.03	104.42	111.33

There are no chirality outliers.

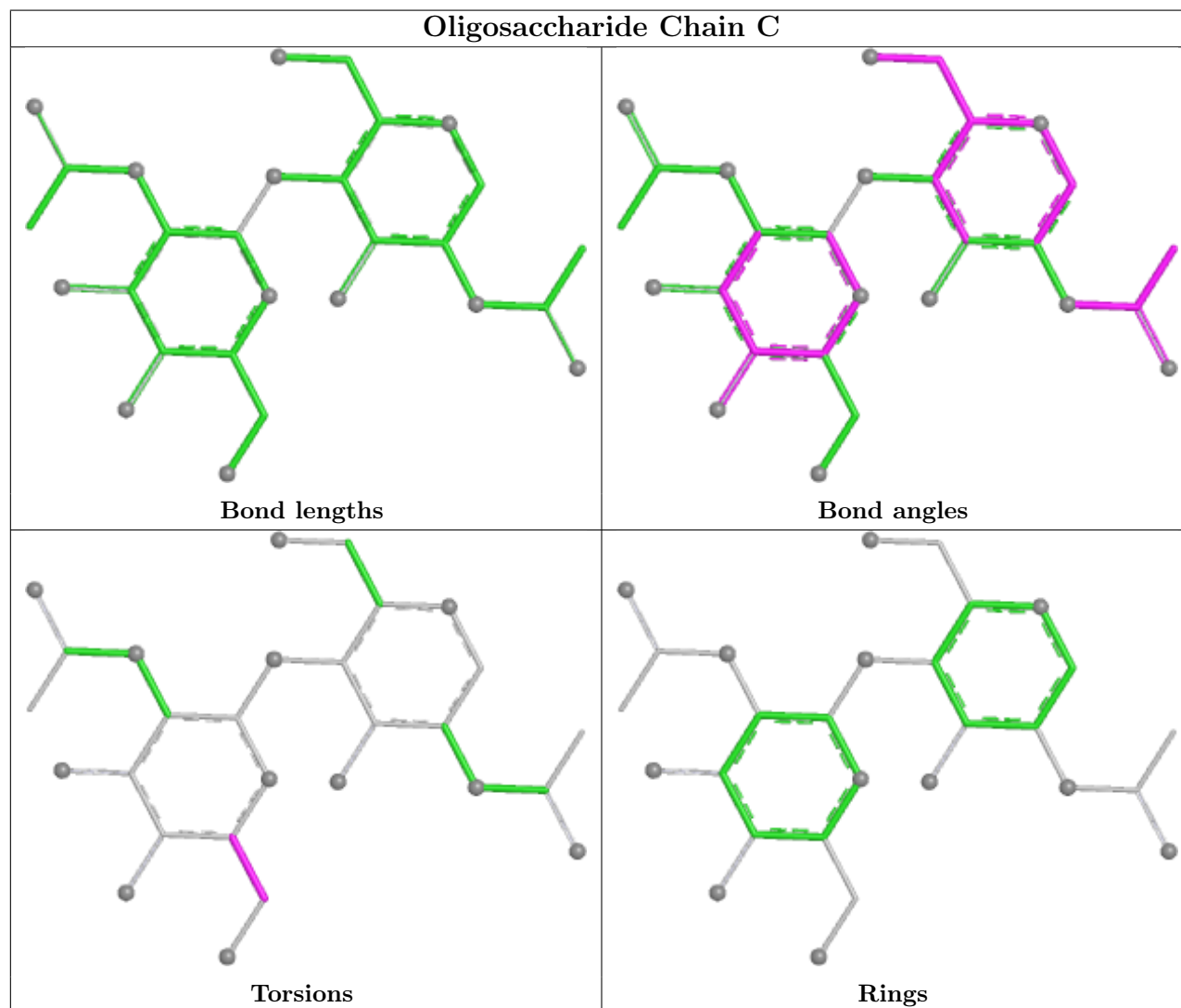
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	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 [i](#)

19 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	A	1004	1	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
4	NAG	A	1005	1	14,14,15	0.97	2 (14%)	17,19,21	1.75	4 (23%)
4	NAG	A	1007	1	14,14,15	0.73	0	17,19,21	2.09	6 (35%)
5	SO4	B	1007	-	4,4,4	0.75	0	6,6,6	0.54	0
4	NAG	B	1002	1	14,14,15	0.63	0	17,19,21	1.94	5 (29%)
4	NAG	A	1008	1	14,14,15	0.48	0	17,19,21	1.57	2 (11%)
4	NAG	B	1003	1	14,14,15	1.08	1 (7%)	17,19,21	2.52	7 (41%)
4	NAG	A	1002	1	14,14,15	0.94	0	17,19,21	1.89	3 (17%)
3	EWL	B	1001	-	24,25,25	1.98	7 (29%)	27,34,34	5.11	11 (40%)
4	NAG	B	1005	1	14,14,15	0.66	0	17,19,21	2.07	4 (23%)
5	SO4	A	1012	-	4,4,4	0.67	0	6,6,6	0.70	0
5	SO4	B	1006	-	4,4,4	0.62	0	6,6,6	0.55	0
3	EWL	A	1001	-	24,25,25	1.74	7 (29%)	27,34,34	5.01	11 (40%)
4	NAG	A	1006	1	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
5	SO4	A	1011	-	4,4,4	0.61	0	6,6,6	0.48	0
4	NAG	A	1003	1	14,14,15	0.76	0	17,19,21	1.55	3 (17%)
4	NAG	B	1004	1	14,14,15	0.67	0	17,19,21	1.13	2 (11%)
5	SO4	A	1010	-	4,4,4	0.62	0	6,6,6	0.85	0
5	SO4	A	1009	-	4,4,4	0.49	0	6,6,6	0.23	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	A	1004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1008	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EWL	A	1001	-	-	3/9/9/9	0/3/3/3
4	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
3	EWL	B	1001	-	-	1/9/9/9	0/3/3/3
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1005	1	-	1/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	EWL	C4-N3	-5.24	1.34	1.38
3	A	1001	EWL	O-C4	4.36	1.30	1.23
3	B	1001	EWL	O-C4	3.79	1.29	1.23
3	B	1001	EWL	O1-C3	3.39	1.38	1.34
3	A	1001	EWL	O1-C3	3.25	1.37	1.34
3	A	1001	EWL	C4-N3	-2.79	1.36	1.38
3	A	1001	EWL	C4-N2	-2.36	1.34	1.37
3	A	1001	EWL	C1-N3	-2.36	1.34	1.39
3	B	1001	EWL	C1-N	2.31	1.37	1.34
3	A	1001	EWL	C3-N	2.22	1.37	1.33
3	A	1001	EWL	C1-N	2.22	1.37	1.34
3	B	1001	EWL	C1-N3	-2.19	1.34	1.39
3	B	1001	EWL	C3-N1	2.16	1.37	1.33
4	B	1003	NAG	C1-C2	2.11	1.55	1.52
4	A	1005	NAG	O5-C5	2.10	1.47	1.43
4	A	1005	NAG	C3-C2	2.09	1.56	1.52
3	B	1001	EWL	C-C2	2.01	1.47	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	EWL	N2-C4-N3	20.33	116.01	106.76
3	A	1001	EWL	N2-C4-N3	19.26	115.53	106.76
3	A	1001	EWL	C-N2-C4	-12.04	103.31	109.82
3	B	1001	EWL	C-N2-C4	-10.79	103.99	109.82
3	A	1001	EWL	O-C4-N2	-6.57	121.81	127.49
4	B	1005	NAG	C1-O5-C5	6.52	120.92	112.19
4	B	1003	NAG	C8-C7-N2	6.04	126.13	116.12
3	B	1001	EWL	O-C4-N2	-5.85	122.43	127.49
3	B	1001	EWL	O-C4-N3	-5.50	121.53	125.82
3	A	1001	EWL	N-C1-N3	5.43	134.80	125.67
4	A	1008	NAG	C1-O5-C5	5.18	119.12	112.19
3	B	1001	EWL	N-C1-N3	5.07	134.18	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	NAG	C1-O5-C5	4.70	118.49	112.19
4	A	1005	NAG	O5-C1-C2	-4.60	104.17	111.29
3	B	1001	EWL	C3-N1-C2	4.57	122.67	115.42
4	B	1003	NAG	O7-C7-C8	-4.10	114.76	122.05
3	A	1001	EWL	O-C4-N3	-4.05	122.66	125.82
3	A	1001	EWL	C3-N1-C2	4.04	121.83	115.42
4	A	1002	NAG	O5-C1-C2	-4.01	105.08	111.29
3	B	1001	EWL	N4-C2-N1	3.94	122.35	117.03
4	B	1002	NAG	O5-C5-C6	3.93	115.31	107.66
4	A	1002	NAG	C3-C4-C5	-3.78	103.38	110.23
4	A	1002	NAG	O4-C4-C5	3.76	118.58	109.32
3	B	1001	EWL	N1-C3-N	-3.75	120.84	127.65
4	B	1003	NAG	C2-N2-C7	3.75	127.92	122.90
3	A	1001	EWL	C9-N3-C4	3.73	129.27	122.59
4	B	1003	NAG	O5-C1-C2	-3.38	106.05	111.29
3	A	1001	EWL	N1-C3-N	-3.30	121.66	127.65
4	B	1002	NAG	O4-C4-C3	-3.25	102.71	110.38
4	B	1005	NAG	O5-C1-C2	3.24	116.30	111.29
3	B	1001	EWL	C9-N3-C4	3.20	128.32	122.59
4	A	1003	NAG	C2-N2-C7	3.09	127.04	122.90
4	A	1003	NAG	C1-O5-C5	2.95	116.14	112.19
4	A	1007	NAG	C6-C5-C4	-2.72	106.35	113.02
4	B	1002	NAG	O5-C1-C2	-2.68	107.14	111.29
4	B	1002	NAG	C4-C3-C2	2.67	114.93	111.02
4	A	1007	NAG	O5-C5-C6	2.65	112.83	107.66
4	B	1003	NAG	O4-C4-C5	2.63	115.81	109.32
4	A	1007	NAG	C1-C2-N2	2.63	114.58	110.43
4	A	1007	NAG	O4-C4-C3	2.60	116.50	110.38
4	A	1007	NAG	O7-C7-N2	2.58	126.54	121.98
4	A	1004	NAG	C4-C3-C2	2.56	114.78	111.02
4	B	1005	NAG	C3-C4-C5	2.51	114.78	110.23
3	B	1001	EWL	C5-O1-C3	2.38	121.29	117.80
4	B	1002	NAG	C2-N2-C7	-2.37	119.72	122.90
4	B	1005	NAG	O7-C7-C8	-2.35	117.86	122.05
4	A	1003	NAG	C6-C5-C4	-2.31	107.36	113.02
4	A	1005	NAG	O5-C5-C6	2.20	111.94	107.66
4	B	1004	NAG	C1-C2-N2	2.18	113.86	110.43
4	A	1005	NAG	C3-C4-C5	-2.17	106.30	110.23
4	A	1006	NAG	C4-C3-C2	-2.16	107.85	111.02
4	B	1004	NAG	C2-N2-C7	2.16	125.79	122.90
4	A	1008	NAG	O5-C1-C2	2.15	114.62	111.29
3	A	1001	EWL	C14-C10-C11	2.10	121.36	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	EWL	N4-C2-N1	2.06	119.81	117.03
3	B	1001	EWL	C-C2-N4	-2.06	118.80	123.49
3	A	1001	EWL	O1-C3-N	2.03	122.60	116.17
4	B	1003	NAG	C3-C4-C5	-2.02	106.56	110.23
4	B	1003	NAG	O3-C3-C2	2.01	113.57	109.40
4	A	1005	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	EWL	C6-C5-O1-C3
4	B	1004	NAG	O5-C5-C6-O6
4	A	1002	NAG	O5-C5-C6-O6
4	B	1004	NAG	C4-C5-C6-O6
4	B	1003	NAG	C8-C7-N2-C2
4	B	1003	NAG	O7-C7-N2-C2
4	A	1004	NAG	C4-C5-C6-O6
4	A	1004	NAG	O5-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	A	1007	NAG	O5-C5-C6-O6
3	A	1001	EWL	C5-C6-C7-C8
4	B	1002	NAG	C4-C5-C6-O6
3	A	1001	EWL	O1-C5-C6-C7
3	B	1001	EWL	C6-C5-O1-C3
4	A	1008	NAG	C1-C2-N2-C7
4	B	1005	NAG	C3-C2-N2-C7
4	B	1002	NAG	O5-C5-C6-O6

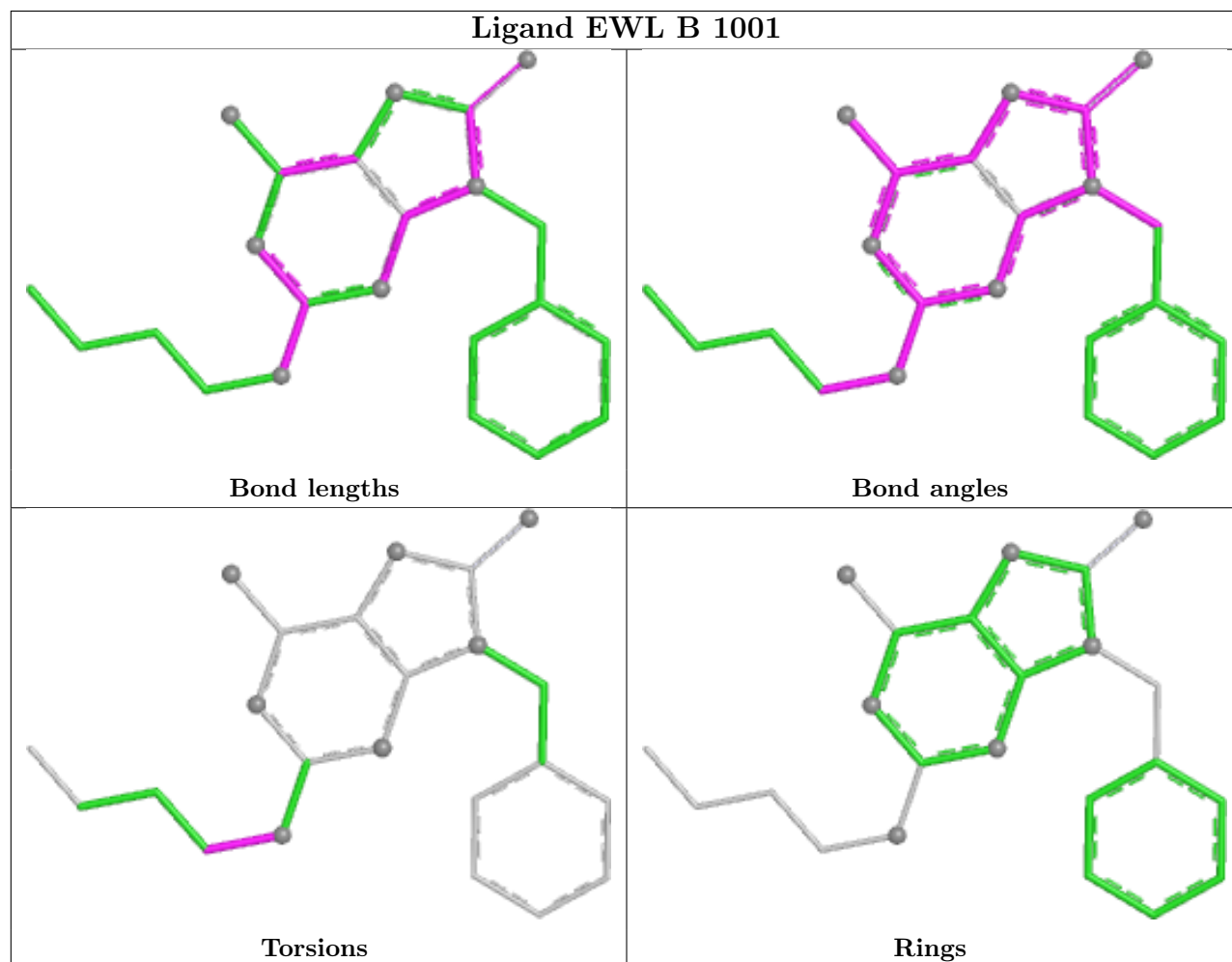
There are no ring outliers.

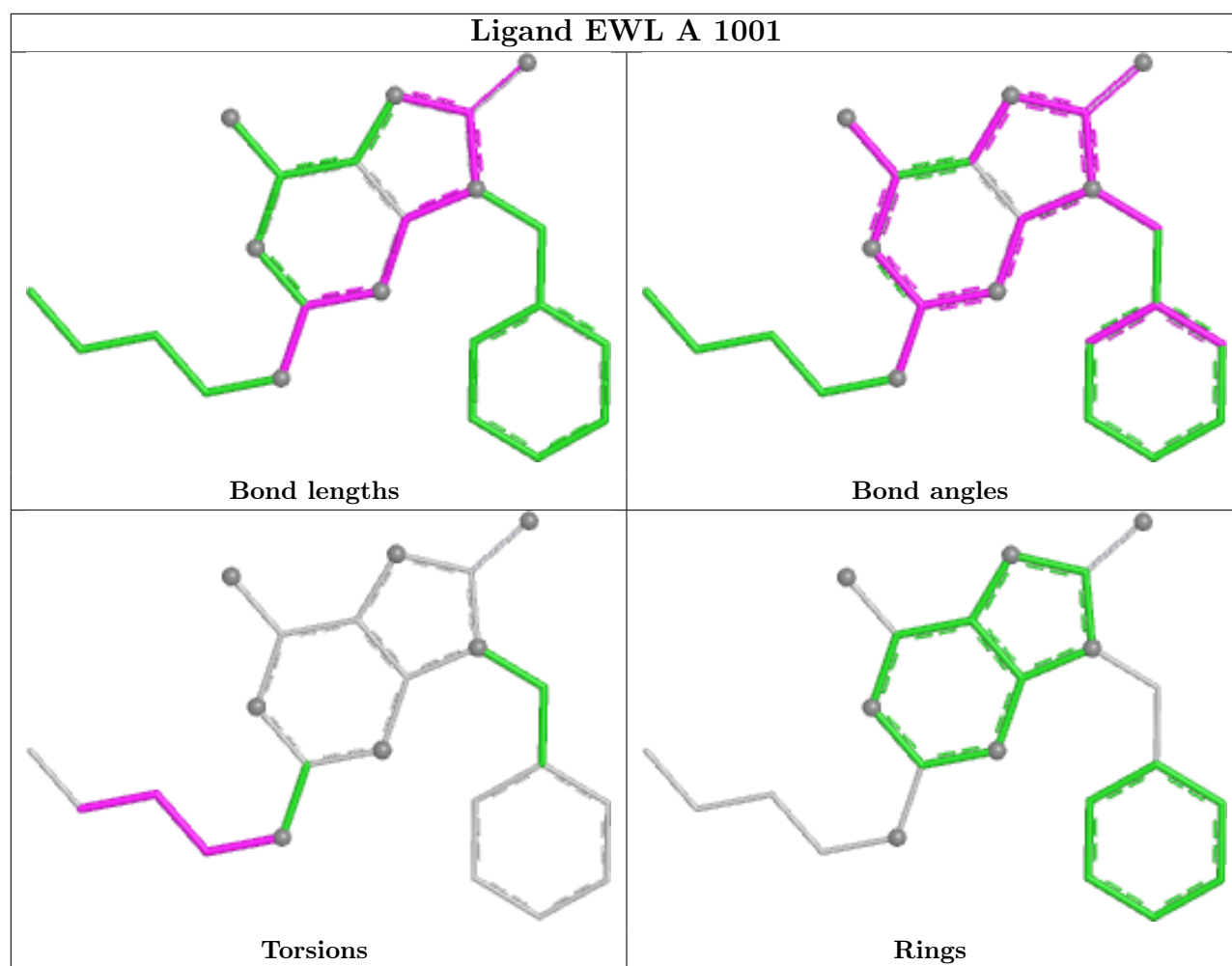
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1007	SO4	1	0
3	A	1001	EWL	2	0
4	A	1003	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 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	771/823 (93%)	0.12	29 (3%) 44 37	12, 27, 55, 107	0
1	B	771/823 (93%)	0.44	45 (5%) 29 24	17, 36, 65, 113	0
All	All	1542/1646 (93%)	0.28	74 (4%) 35 30	12, 31, 60, 113	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	VAL	5.6
1	A	463	LEU	5.5
1	B	42	VAL	5.4
1	B	744	GLN	5.4
1	B	45	ASN	5.3
1	A	45	ASN	4.9
1	B	90	HIS	4.7
1	B	747	PHE	4.5
1	A	27	ALA	4.5
1	B	717	ARG	4.3
1	A	835	LEU	4.2
1	B	463	LEU	4.2
1	B	462	GLN	4.2
1	A	461	GLU	3.9
1	B	461	GLU	3.8
1	B	460	LEU	3.6
1	B	89	VAL	3.6
1	B	435	PRO	3.5
1	B	748	GLN	3.4
1	A	474	SER	3.4
1	A	506	PHE	3.4
1	B	313	ILE	3.3
1	A	464	TYR	3.3
1	A	459	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	435	PRO	3.2
1	B	315	ASN	3.1
1	A	817	PRO	3.1
1	B	27	ALA	3.1
1	A	42	VAL	3.1
1	B	464	TYR	3.0
1	B	745	ASP	3.0
1	B	121	ARG	3.0
1	A	460	LEU	2.9
1	A	819	ALA	2.9
1	B	87	ARG	2.9
1	B	388	PHE	2.9
1	B	819	ALA	2.9
1	A	314	ASN	2.8
1	A	473	ARG	2.8
1	A	773	ASN	2.8
1	B	86	HIS	2.8
1	B	835	LEU	2.7
1	A	465	TYR	2.7
1	A	769	GLU	2.7
1	B	29	TRP	2.6
1	B	474	SER	2.6
1	B	39	THR	2.6
1	B	264	TYR	2.5
1	A	388	PHE	2.5
1	B	776	LYS	2.5
1	A	462	GLN	2.5
1	A	276	ASN	2.5
1	B	370	LYS	2.5
1	B	719	SER	2.4
1	A	267	PRO	2.3
1	B	771	VAL	2.3
1	B	774	ASN	2.3
1	B	41	ASP	2.2
1	B	32	LYS	2.2
1	B	128	TYR	2.2
1	B	40	LEU	2.2
1	B	268	PHE	2.2
1	A	265	ASN	2.2
1	B	466	PHE	2.2
1	B	314	ASN	2.1
1	A	109	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	472	ALA	2.1
1	B	667	SER	2.1
1	A	386	LYS	2.1
1	B	467	ARG	2.0
1	B	490	SER	2.0
1	A	274	LYS	2.0
1	A	311	LYS	2.0
1	A	246	ASN	2.0

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

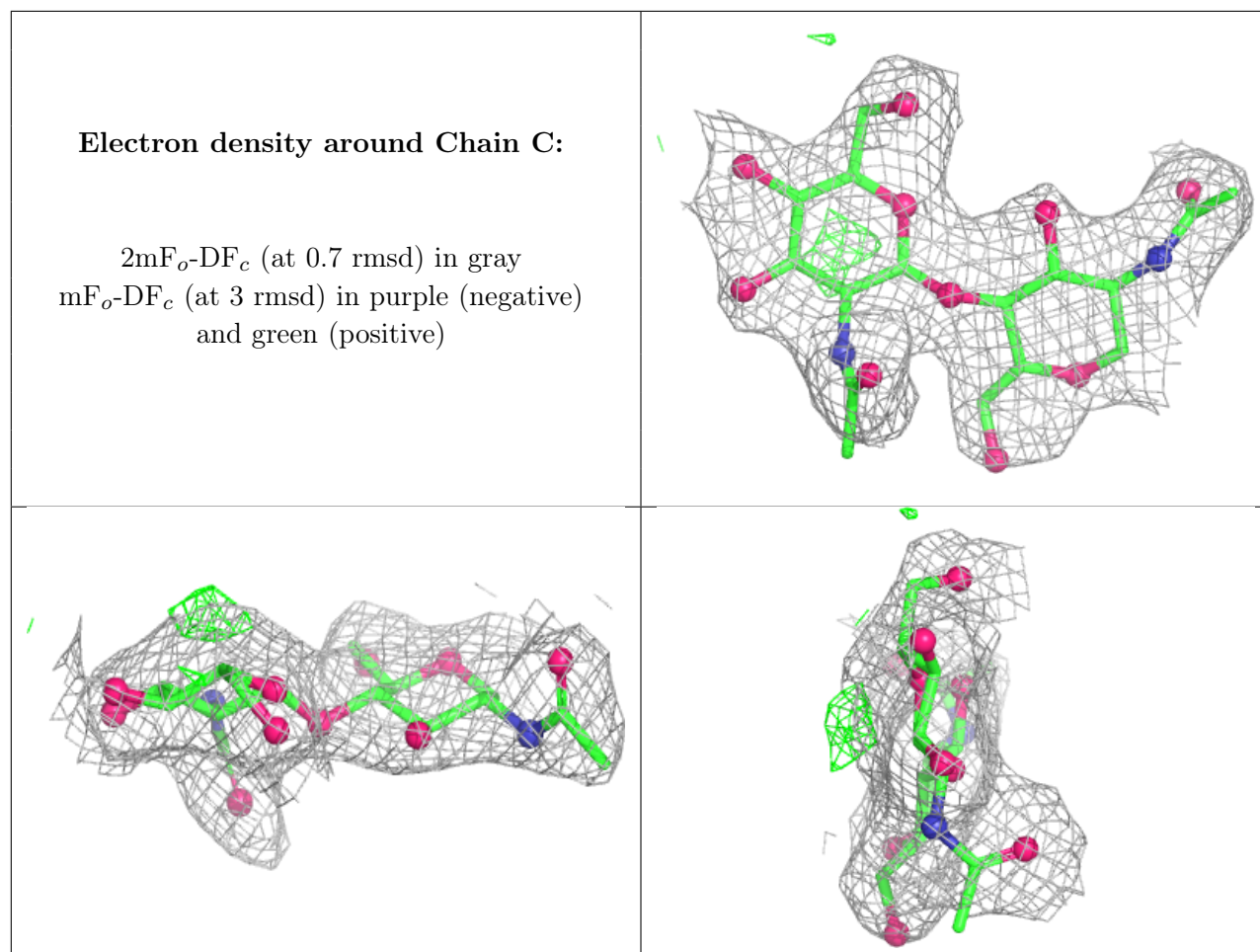
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	NAG	C	2	14/15	0.81	0.14	49,57,60,61	0
2	NAG	C	1	14/15	0.94	0.10	29,35,41,48	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1005	14/15	0.71	0.18	47,54,72,75	0
4	NAG	B	1004	14/15	0.73	0.17	57,69,78,85	0
5	SO4	A	1012	5/5	0.78	0.17	58,66,76,77	0
5	SO4	A	1010	5/5	0.79	0.20	58,67,71,79	0
5	SO4	A	1011	5/5	0.82	0.17	65,67,71,73	0
4	NAG	A	1007	14/15	0.83	0.13	52,54,57,59	0
5	SO4	B	1006	5/5	0.84	0.12	52,57,64,66	0
4	NAG	A	1008	14/15	0.86	0.12	41,46,53,55	0
4	NAG	B	1003	14/15	0.88	0.10	36,41,50,50	0
5	SO4	A	1009	5/5	0.89	0.13	56,57,64,64	0
4	NAG	A	1002	14/15	0.90	0.12	24,26,29,29	0

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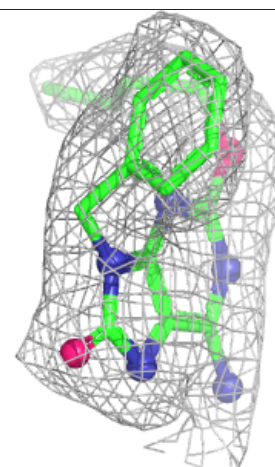
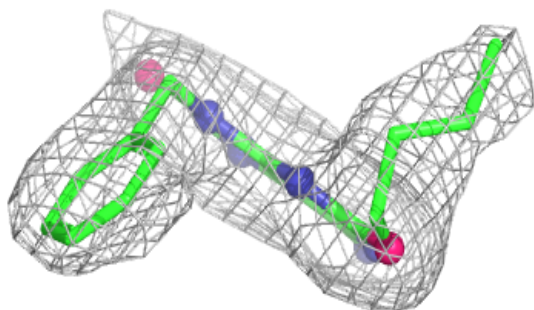
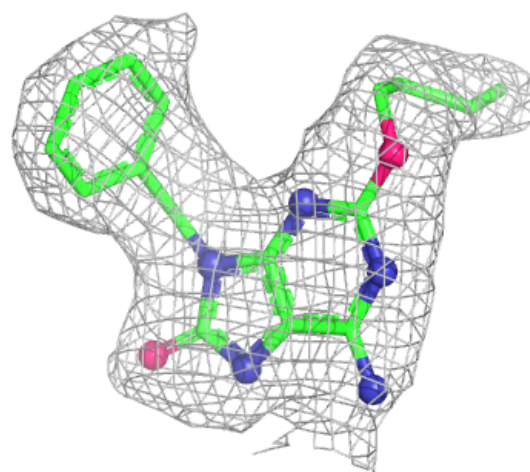
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	1005	14/15	0.90	0.10	36,40,43,45	0
5	SO4	B	1007	5/5	0.90	0.15	52,53,58,60	0
4	NAG	A	1006	14/15	0.91	0.09	34,37,40,40	0
4	NAG	A	1004	14/15	0.91	0.10	31,37,50,51	0
4	NAG	A	1003	14/15	0.92	0.09	17,20,22,24	0
4	NAG	B	1002	14/15	0.93	0.08	25,28,31,32	0
3	EWL	B	1001	23/23	0.95	0.09	26,31,34,35	0
3	EWL	A	1001	23/23	0.95	0.09	24,28,32,34	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.

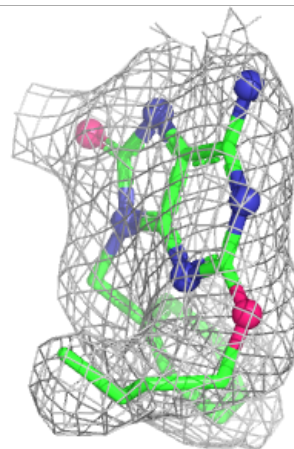
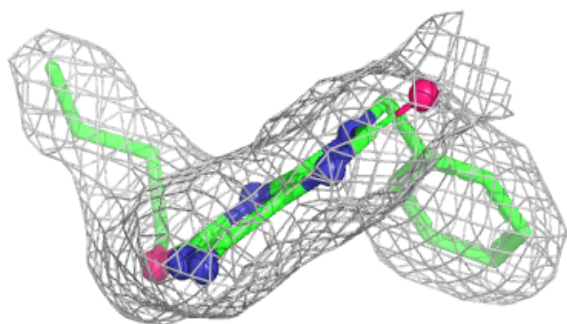
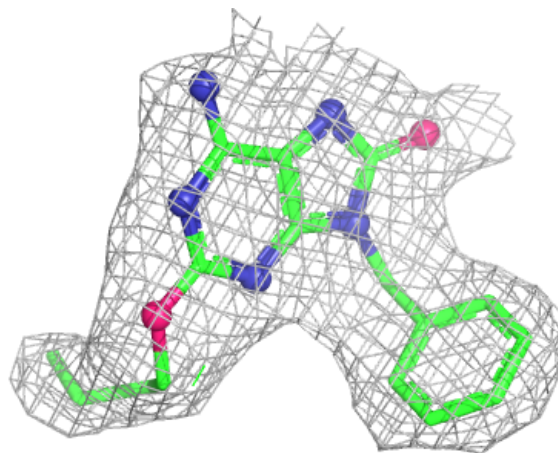
Electron density around EWL B 1001:

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 EWL A 1001:

$2mF_o-DF_c$ (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.