WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 07:15 PM EDT

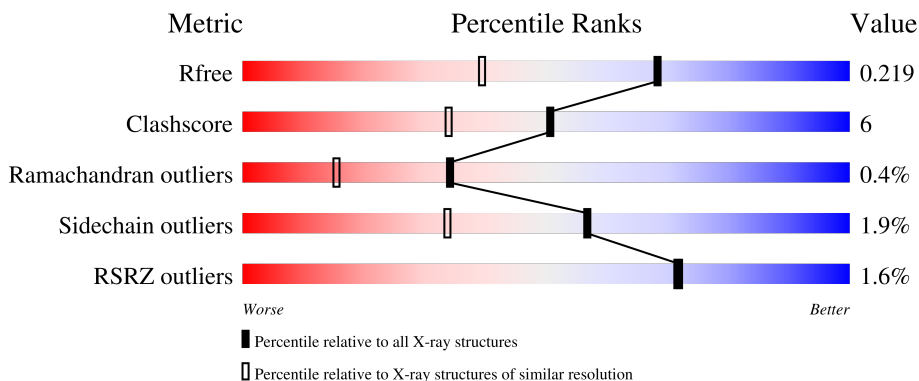|		
PDB ID	:	4GUW
Title	:	Crystal structure of type 1 Ribosome inactivating protein from Momordica balsamina with lipopolysaccharide at 1.6 Angstrom resolution
Authors	:	Singh, A.; Pandey, S.; Kushwaha, G.S.; Bhushan, A.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2012-08-30
Resolution	:	1.60 Å(reported)

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 1.60 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	Percentile Ranks	Value
Rfree		0.219
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		1.9%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	246	2% / 87% / 11% / •
2	B	2	100%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2217 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 rRNA N-glycosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total 1911	C 1215	N 328	O 365	S 3	0	0	0

- 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	B	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
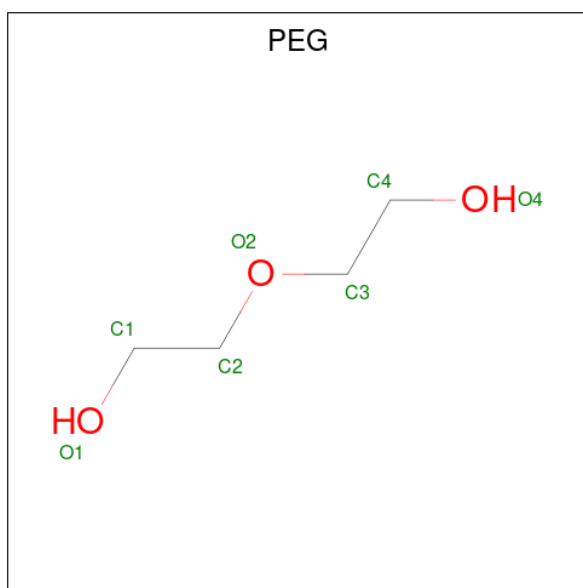
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 4	O 3	0	0

- Molecule 4 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R) -3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)TETRAHYDRO-2H- PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (three-letter code: LP5) (formula: $C_{34}H_{66}NO_{12}P$).

LP5
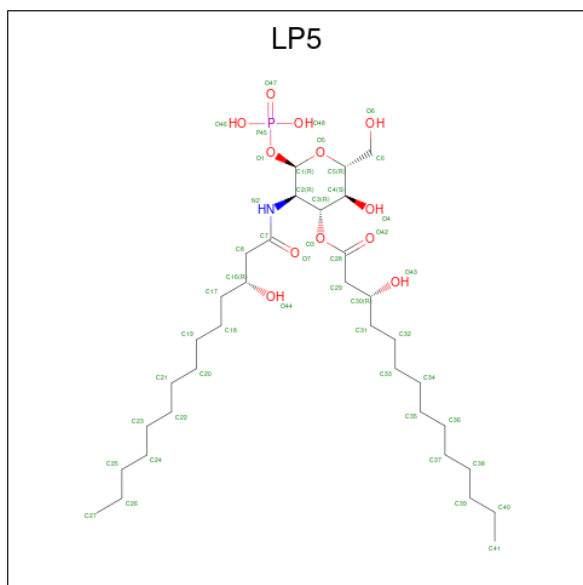
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 34	N 1	O 12	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total 223	O 223	0	0

3 Residue-property plots ⓘ

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: rRNA N-glycosidase

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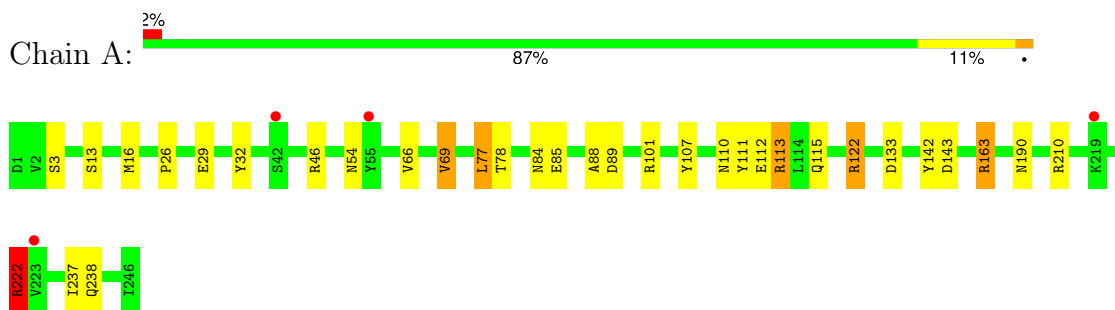
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	130.24Å 130.24Å 39.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.11 – 1.60 37.55 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.11-1.60) 99.7 (37.55-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.223 0.189 , 0.219	Depositor DCC
R_{free} test set	1681 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2217	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LP5, PEG, 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	1.47	8/1947 (0.4%)	1.22	13/2650 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ARG	CG-CD	-7.64	1.32	1.51
1	A	85	GLU	CD-OE2	-6.37	1.18	1.25
1	A	29	GLU	CB-CG	-6.26	1.40	1.52
1	A	32	TYR	CE1-CZ	-5.57	1.31	1.38
1	A	122	ARG	CB-CG	-5.54	1.37	1.52
1	A	88	ALA	CA-CB	5.53	1.64	1.52
1	A	3	SER	CA-CB	5.34	1.60	1.52
1	A	142	TYR	CD2-CE2	-5.26	1.31	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ARG	NE-CZ-NH1	10.19	125.40	120.30
1	A	46	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	A	122	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	A	101	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	163	ARG	NE-CZ-NH1	-7.73	116.43	120.30
1	A	210	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	A	46	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	89	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	143	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	143	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	163	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	113	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	222	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1911	0	1932	22	0
2	B	28	0	25	0	0
3	A	7	0	9	2	0
4	A	48	0	64	11	0
5	A	223	0	0	1	0
All	All	2217	0	2030	23	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (23) 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:115:GLN:OE1	1:A:122:ARG:HG3	1.80	0.81
1:A:112:GLU:HG2	4:A:304:LP5:H322	1.64	0.79
1:A:77:LEU:HD22	1:A:78:THR:HG23	1.69	0.75
1:A:163:ARG:NH1	4:A:304:LP5:H62	2.07	0.70
1:A:237:ILE:O	3:A:303:PEG:H41	1.92	0.69
1:A:111:TYR:HB2	4:A:304:LP5:H291	1.75	0.68
1:A:163:ARG:HH12	4:A:304:LP5:H62	1.58	0.65
1:A:54:ASN:HB2	1:A:133:ASP:OD1	1.99	0.62
1:A:112:GLU:OE2	1:A:112:GLU:HA	2.00	0.61
1:A:110:ASN:HB2	4:A:304:LP5:H292	1.84	0.59
4:A:304:LP5:O7	4:A:304:LP5:H3	2.07	0.53
1:A:238:GLN:HE22	3:A:303:PEG:H32	1.75	0.52
1:A:190:ASN:HB3	4:A:304:LP5:H381	1.91	0.51
1:A:111:TYR:N	4:A:304:LP5:H291	2.25	0.51
1:A:26:PRO:HD2	1:A:66:VAL:HB	1.94	0.48
1:A:13:SER:HA	1:A:16:MET:CE	2.43	0.48
1:A:112:GLU:HG2	4:A:304:LP5:H30	1.96	0.48
1:A:222:ARG:O	1:A:222:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HA	1:A:16:MET:HE3	1.95	0.47
1:A:84:ASN:O	4:A:304:LP5:H232	2.18	0.43
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.94	0.41
1:A:113:ARG:HD2	5:A:413:HOH:O	2.20	0.41
1:A:111:TYR:H	4:A:304:LP5:H291	1.85	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	244/246 (99%)	235 (96%)	8 (3%)	1 (0%)	34	15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	VAL

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	209/209 (100%)	205 (98%)	4 (2%)	57	34

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	77	LEU
1	A	107	TYR
1	A	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	169	GLN
1	A	245	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	$\#|Z| > 2$
2	NAG	B	1	1,2	14,14,15	0.78	0	17,19,21	2.39	7 (41%)
2	NAG	B	2	2	14,14,15	0.97	1 (7%)	17,19,21	1.56	3 (17%)

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	B	1	1,2	-	<mark>2/6/23/26</mark>	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	2.15	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-O5-C5	5.52	119.58	112.19
2	B	1	NAG	C3-C4-C5	4.30	118.03	110.23
2	B	1	NAG	C1-C2-N2	-4.08	104.00	110.43
2	B	2	NAG	C1-C2-N2	3.55	116.03	110.43
2	B	2	NAG	O7-C7-C8	-3.24	116.28	122.05
2	B	1	NAG	O5-C1-C2	2.64	115.38	111.29
2	B	2	NAG	C8-C7-N2	2.60	120.42	116.12
2	B	1	NAG	C6-C5-C4	-2.30	107.38	113.02
2	B	1	NAG	O5-C5-C4	2.25	116.30	110.83
2	B	1	NAG	C4-C3-C2	2.06	114.03	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B
Bond lengths | Bond angles | Torsions | Rings
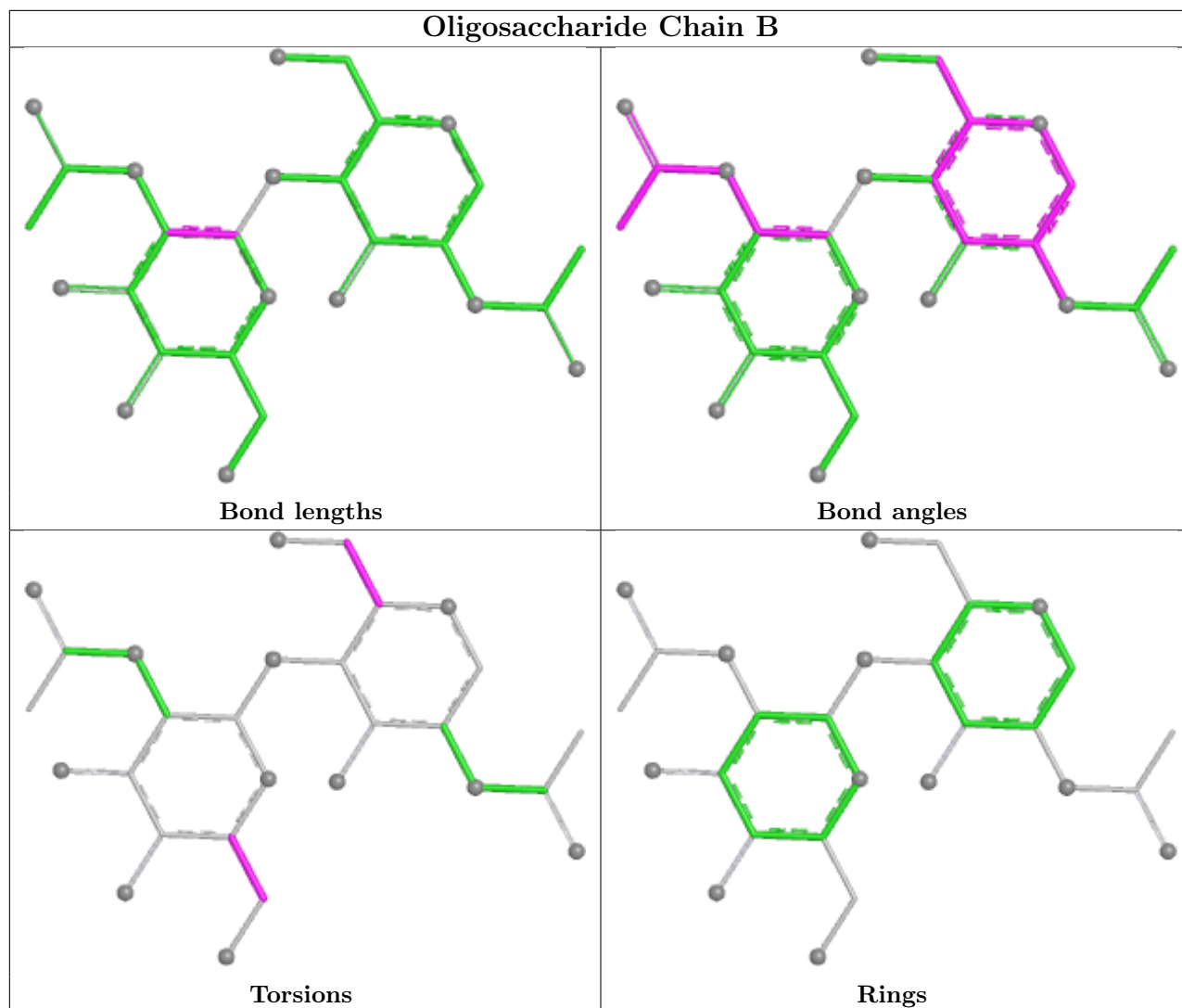
5.6 Ligand geometry ⓘ

2 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	LP5	A	304	-	47,48,48	1.61	8 (17%)	58,60,60	2.57	13 (22%)
3	PEG	A	303	-	6,6,6	0.77	0	5,5,5	1.49	1 (20%)

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	LP5	A	304	-	-	22/44/65/65	0/1/1/1
3	PEG	A	303	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	LP5	O3-C3	5.90	1.53	1.44
4	A	304	LP5	C29-C28	3.75	1.58	1.50
4	A	304	LP5	C4-C3	3.26	1.61	1.52
4	A	304	LP5	C4-C5	2.96	1.59	1.53
4	A	304	LP5	C3-C2	2.80	1.57	1.53
4	A	304	LP5	P45-O1	2.53	1.64	1.59
4	A	304	LP5	O5-C5	2.42	1.50	1.44
4	A	304	LP5	C2-N2	2.30	1.49	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	304	LP5	C25-C24-C23	8.86	159.14	114.37
4	A	304	LP5	C23-C22-C21	8.79	158.79	114.37
4	A	304	LP5	O46-P45-O1	7.38	134.59	105.85
4	A	304	LP5	O48-P45-O1	-6.10	82.06	105.85
4	A	304	LP5	O1-P45-O47	-4.39	93.69	109.33
4	A	304	LP5	O3-C3-C4	4.24	117.51	107.76
4	A	304	LP5	O5-C1-O1	-3.72	106.50	111.36
4	A	304	LP5	C8-C7-N2	-3.24	111.83	116.25
4	A	304	LP5	C2-N2-C7	2.90	127.17	122.90
3	A	303	PEG	O2-C3-C4	-2.89	97.38	110.11
4	A	304	LP5	O3-C28-C29	2.82	116.48	111.43
4	A	304	LP5	O42-C28-C29	-2.22	119.50	124.65
4	A	304	LP5	O7-C7-N2	2.10	126.50	122.95
4	A	304	LP5	C1-C2-N2	-2.07	107.45	110.92

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	LP5	O5-C1-O1-P45

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Mol	Chain	Res	Type	Atoms
4	A	304	LP5	C3-C2-N2-C7
4	A	304	LP5	O44-C16-C8-C7
4	A	304	LP5	C17-C16-C8-C7
4	A	304	LP5	C8-C16-C17-C18
4	A	304	LP5	C4-C5-C6-O6
4	A	304	LP5	O5-C5-C6-O6
4	A	304	LP5	C23-C24-C25-C26
4	A	304	LP5	O44-C16-C17-C18
4	A	304	LP5	C22-C23-C24-C25
4	A	304	LP5	C35-C36-C37-C38
4	A	304	LP5	C36-C37-C38-C39
4	A	304	LP5	C20-C21-C22-C23
4	A	304	LP5	C31-C32-C33-C34
4	A	304	LP5	C34-C35-C36-C37
4	A	304	LP5	C38-C39-C40-C41
3	A	303	PEG	C1-C2-O2-C3
4	A	304	LP5	C33-C34-C35-C36
4	A	304	LP5	C24-C25-C26-C27
4	A	304	LP5	O43-C30-C31-C32
4	A	304	LP5	C32-C33-C34-C35
4	A	304	LP5	C19-C20-C21-C22
4	A	304	LP5	C29-C30-C31-C32

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	LP5	11	0
3	A	303	PEG	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LP5 A 304

Bond lengths

Bond angles

Torsions

Rings
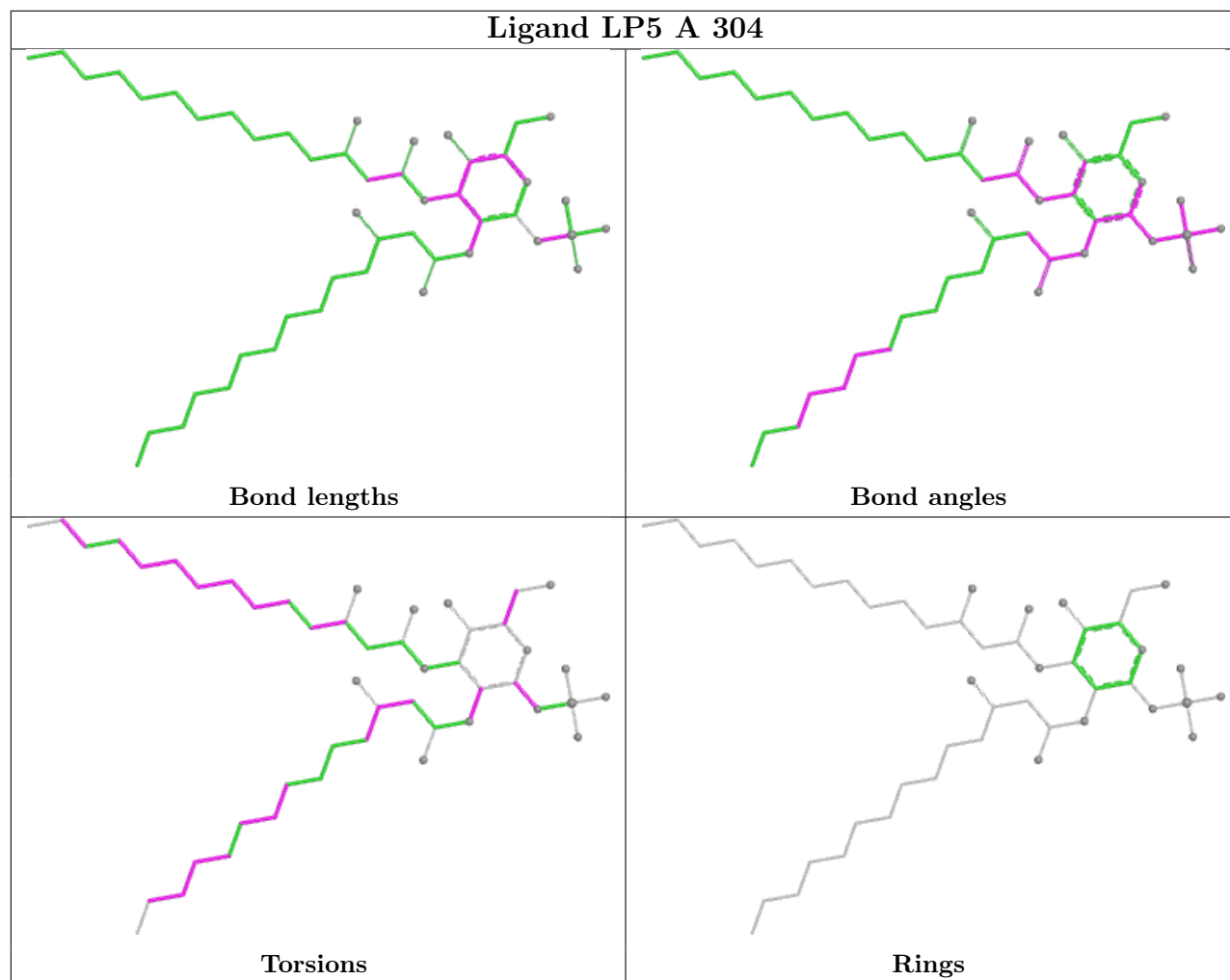
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	246/246 (100%)	-0.19	4 (1%)	72	71	16, 26, 41, 54	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	SER	3.0
1	A	55	TYR	2.9
1	A	219	LYS	2.5
1	A	223	VAL	2.4

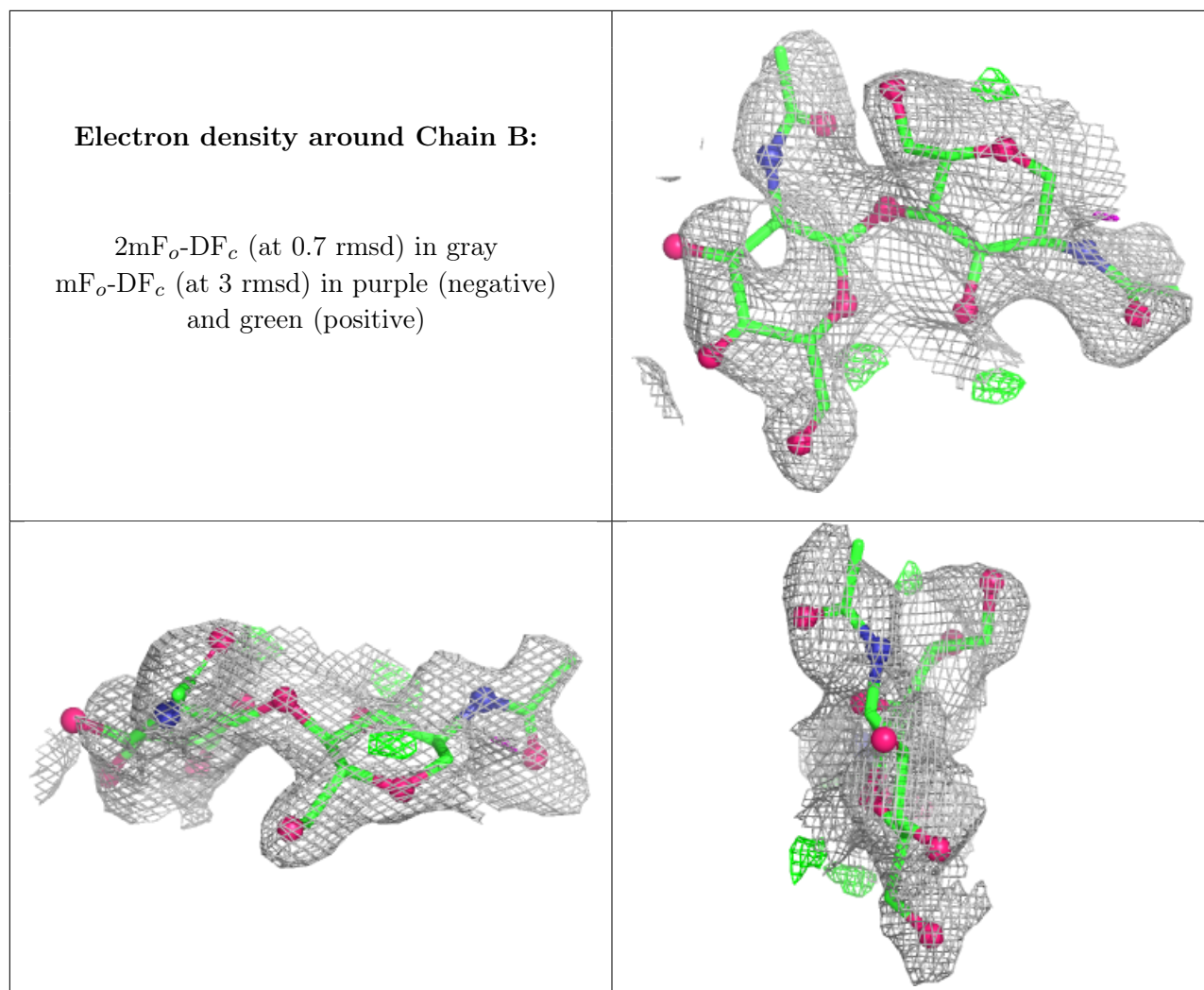## 6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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
2	NAG	B	2	14/15	0.61	0.30	79,82,83,84	0
2	NAG	B	1	14/15	0.78	0.21	57,67,71,76	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.
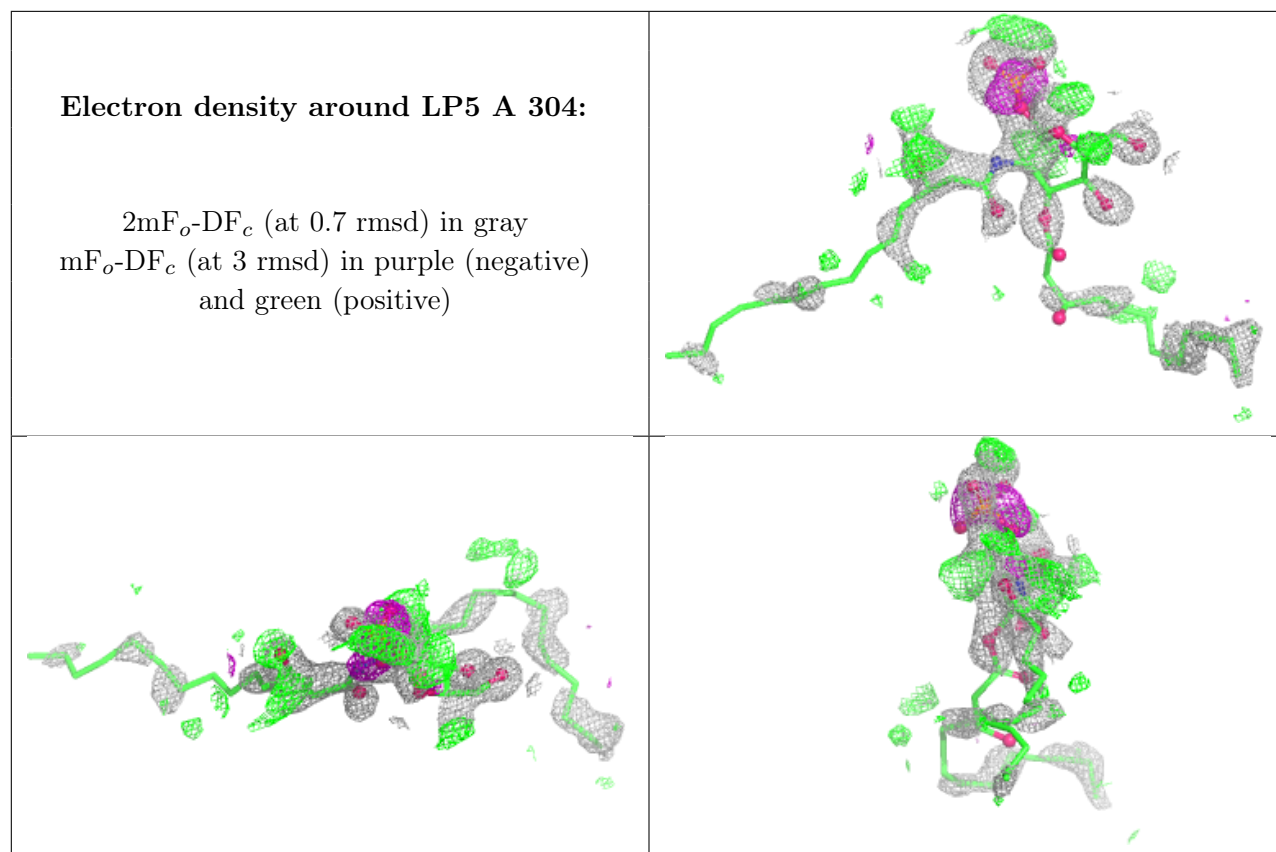
Electron density around Chain B:

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

6.4 Ligands ⓘ

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	LP5	A	304	48/48	0.53	0.36	23,48,57,60	48
3	PEG	A	303	7/7	0.89	0.21	28,37,50,57	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 LP5 A 304:

$2mF_o$-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 ⓘ

There are no such residues in this entry.