



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:15 PM UTC

PDB ID : 5YYL / pdb_00005yyL
Title : Structure of Major Royal Jelly Protein 1 Oligomer
Authors : Tian, W.; Chen, Z.
Deposited on : 2017-12-10
Resolution : 2.65 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

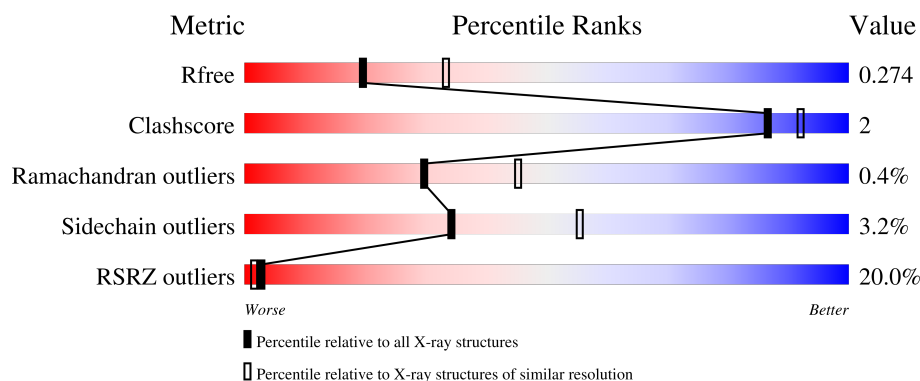
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	432	9% 87% 6% 6%
1	B	432	31% 81% 5% 13%
2	C	78	50% • 47%
2	D	78	4% 53% • 45%
3	E	2	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6562 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 Major royal jelly protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3054	1944	508	585	17			
1	B	375	Total	C	N	O	S	0	0	0
			2624	1665	453	492	14			

- Molecule 2 is a protein called Apisimin.

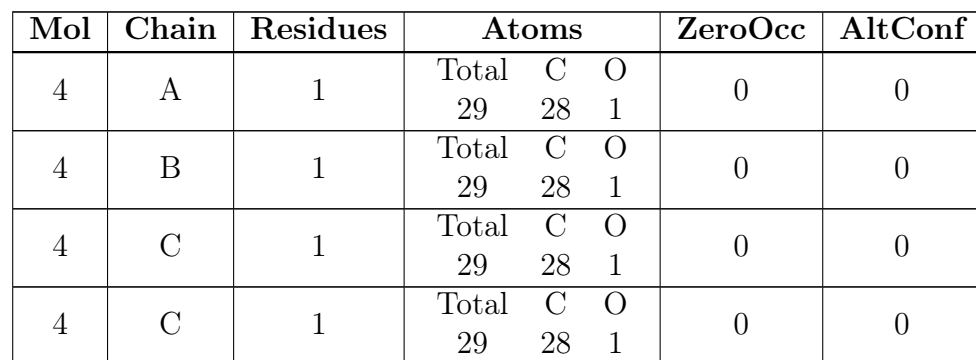
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	41	Total	C	N	O	0	0	0
			296	190	48	58			
2	D	43	Total	C	N	O	0	0	0
			298	191	49	58			

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			21	12	2	7			

- Molecule 4 is (3beta,14beta,17alpha)-ergosta-5,24(28)-dien-3-ol (CCD ID: 94R) (formula: C₂₈H₄₆O).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			9	5	1	3		

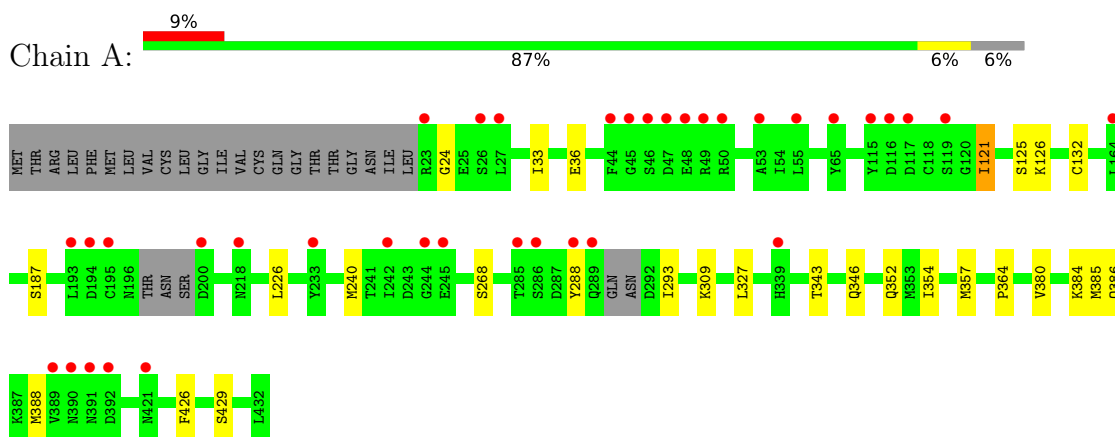
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total	O	0	0
			74	74		
6	B	46	Total	O	0	0
			46	46		
6	C	11	Total	O	0	0
			11	11		
6	D	13	Total	O	0	0
			13	13		

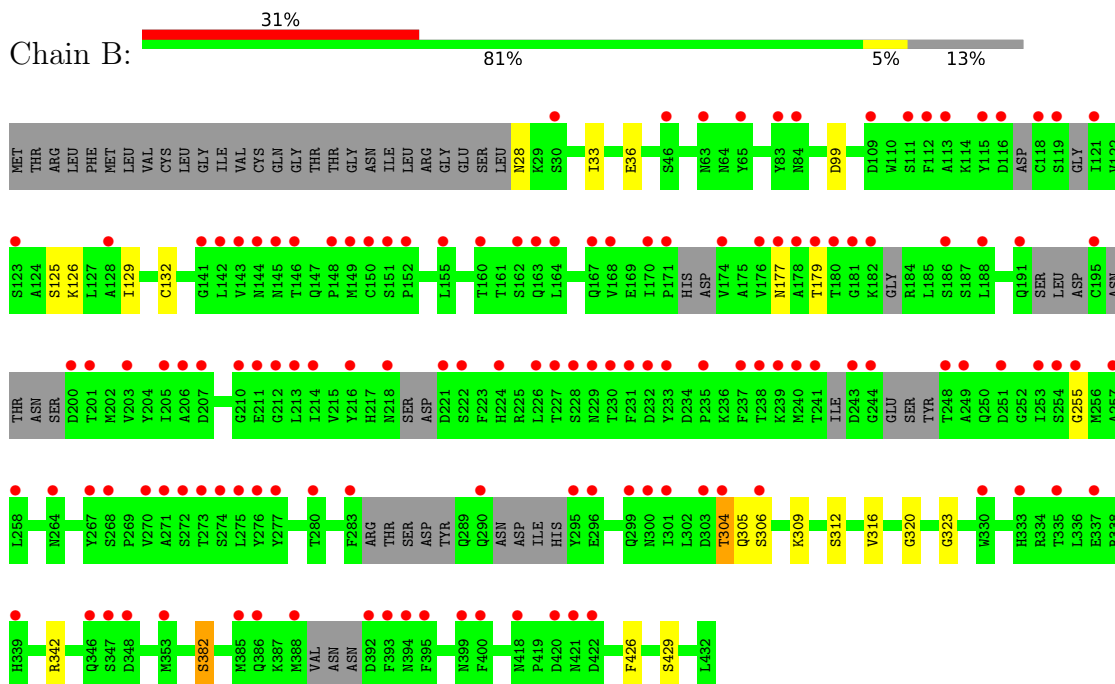
3 Residue-property plots [i](#)

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.

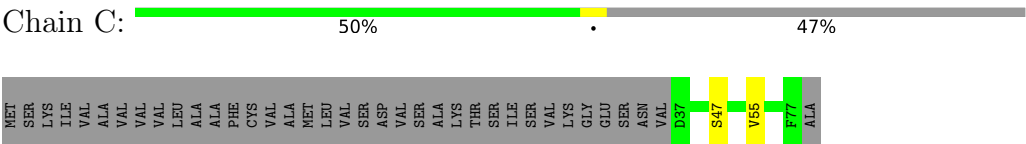
- Molecule 1: Major royal jelly protein 1



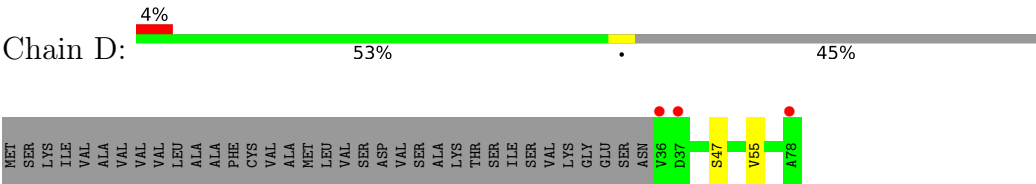
- Molecule 1: Major royal jelly protein 1



- Molecule 2: Apisimin



• Molecule 2: Apisimin



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	211.58Å 211.58Å 149.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.3 (50.00-2.65) 86.3 (50.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.239 , 0.275 0.241 , 0.274	Depositor DCC
R_{free} test set	1605 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6562	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: NAG, 94R

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	0.69	0/3123	0.86	1/4248 (0.0%)
1	B	0.66	0/2670	0.84	1/3609 (0.0%)
2	C	0.58	0/296	0.96	0/406
2	D	0.70	0/298	0.99	0/407
All	All	0.67	0/6387	0.86	2/8670 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ASN	N-CA-C	6.28	118.93	111.71
1	A	24	GLY	N-CA-C	5.56	118.33	111.93

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	3054	0	2784	17	0
1	B	2624	0	2209	10	0
2	C	296	0	314	0	0
2	D	298	0	307	0	0
3	E	21	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	29	0	0	1	0
4	B	29	0	0	0	0
4	C	58	0	0	0	0
5	B	9	0	5	0	0
6	A	74	0	0	0	0
6	B	46	0	0	0	0
6	C	11	0	0	0	0
6	D	13	0	0	0	0
All	All	6562	0	5634	25	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 2.

All (25) 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:327:LEU:HD13	1:A:357:MET:HE1	1.41	0.98
1:A:327:LEU:CD1	1:A:357:MET:HE1	2.19	0.71
1:B:304:THR:HG22	1:B:305:GLN:H	1.65	0.59
1:A:384:LYS:HB3	1:A:386:GLN:HE22	1.68	0.58
1:A:385:MET:HE2	1:A:388:MET:HE1	1.85	0.58
1:A:357:MET:HE2	1:A:380:VAL:HG22	1.88	0.56
1:A:354:ILE:HG21	1:A:357:MET:HE3	1.90	0.53
1:A:352:GLN:OE1	1:A:386:GLN:NE2	2.45	0.50
1:A:125:SER:O	1:A:126:LYS:HD2	2.11	0.50
1:A:288:TYR:HB2	1:A:293:ILE:HD11	1.93	0.50
1:B:125:SER:O	1:B:126:LYS:HD2	2.12	0.49
1:B:312:SER:HG	1:B:316:VAL:H	1.63	0.47
1:B:304:THR:HG21	1:B:323:GLY:HA3	1.96	0.47
1:A:268:SER:OG	1:A:309:LYS:NZ	2.47	0.46
1:A:364:PRO:O	4:A:503:94R:O1	2.33	0.46
1:B:382:SER:O	1:B:382:SER:OG	2.34	0.45
1:A:384:LYS:HB3	1:A:386:GLN:NE2	2.30	0.45
1:A:33:ILE:HD13	1:A:36:GLU:OE2	2.17	0.45
1:B:33:ILE:HD13	1:B:36:GLU:OE2	2.17	0.44
1:A:384:LYS:HD2	1:A:386:GLN:HE22	1.83	0.43
1:A:33:ILE:HG21	1:A:36:GLU:HG3	2.01	0.42
1:B:33:ILE:HG21	1:B:36:GLU:HG3	2.03	0.41
1:B:306:SER:HA	1:B:320:GLY:O	2.21	0.40
1:A:426:PHE:HA	1:B:429:SER:O	2.21	0.40
1:A:429:SER:O	1:B:426:PHE:HA	2.21	0.40

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	399/432 (92%)	376 (94%)	22 (6%)	1 (0%)	36	52
1	B	350/432 (81%)	334 (95%)	14 (4%)	2 (1%)	21	34
2	C	39/78 (50%)	39 (100%)	0	0	100	100
2	D	41/78 (53%)	41 (100%)	0	0	100	100
All	All	829/1020 (81%)	790 (95%)	36 (4%)	3 (0%)	30	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	B	179	THR
1	B	255	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	308/391 (79%)	301 (98%)	7 (2%)	44	66
1	B	222/391 (57%)	214 (96%)	8 (4%)	31	51
2	C	35/66 (53%)	33 (94%)	2 (6%)	18	32
2	D	32/66 (48%)	30 (94%)	2 (6%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	597/914 (65%)	578 (97%)	19 (3%)	34 55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	A	132	CYS
1	A	187	SER
1	A	226	LEU
1	A	240	MET
1	A	343	THR
1	A	346	GLN
1	B	28	ASN
1	B	99	ASP
1	B	129	ILE
1	B	132	CYS
1	B	304	THR
1	B	309	LYS
1	B	342	ARG
1	B	382	SER
2	C	47	SER
2	C	55	VAL
2	D	47	SER
2	D	55	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	340	ASN
1	A	386	GLN
1	B	365	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$
3	NAG	E	1	1,3	14,14,15	0.57	0	17,19,21	1.50	3 (17%)
3	NAG	E	2	3	6,6,15	0.61	0	5,5,21	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/4/4/26	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O5-C1-C2	-3.04	106.59	111.29
3	E	1	NAG	C1-O5-C5	2.32	115.30	112.19
3	E	1	NAG	C1-C2-N2	2.32	114.09	110.43

There are no chirality outliers.

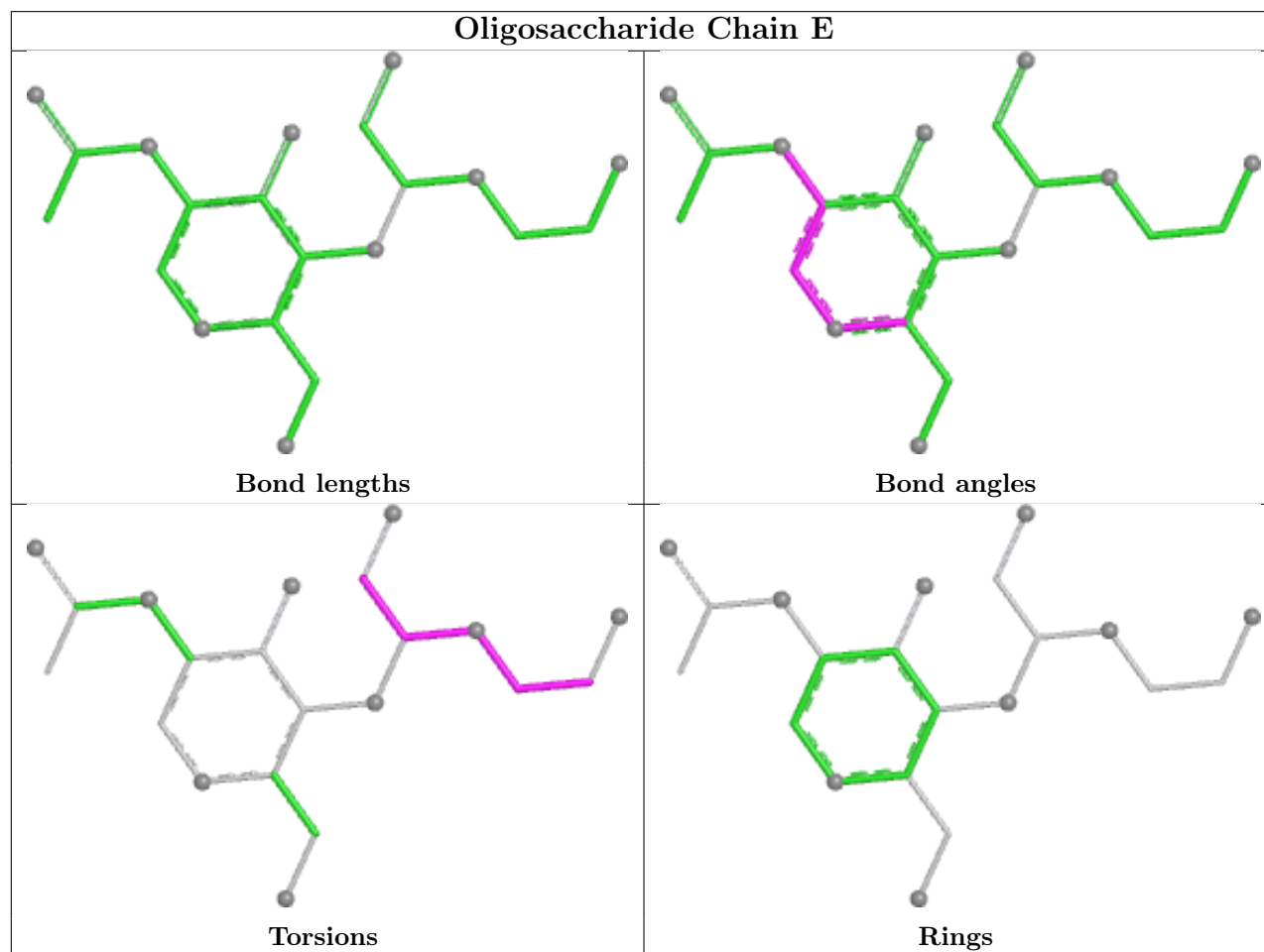
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C1-C2-N2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C2-C1-O5-C5
3	E	2	NAG	C6-C5-O5-C1

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](#)

5 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	94R	A	503	-	32,32,32	0.66	0	50,50,50	1.08	2 (4%)
4	94R	B	502	-	32,32,32	0.66	0	50,50,50	1.16	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	501	1	9,9,15	0.67	0	10,12,21	1.30	1 (10%)
4	94R	C	102	-	32,32,32	0.54	0	50,50,50	1.21	7 (14%)
4	94R	C	101	-	32,32,32	0.59	0	50,50,50	1.13	5 (10%)

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	94R	A	503	-	-	0/13/71/71	0/4/4/4
4	94R	B	502	-	-	2/13/71/71	0/4/4/4
5	NAG	B	501	1	-	-	0/1/1/1
4	94R	C	102	-	-	0/13/71/71	0/4/4/4
4	94R	C	101	-	-	0/13/71/71	0/4/4/4

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	94R	C4-C5-C10	3.98	121.52	116.42
4	B	502	94R	C23-C22-C20	-3.60	107.74	114.46
4	A	503	94R	C4-C5-C6	-3.44	115.90	120.57
4	A	503	94R	C4-C5-C10	3.44	120.82	116.42
5	B	501	NAG	C5-O5-C1	3.19	116.56	111.42
4	B	502	94R	C4-C5-C6	-3.16	116.29	120.57
4	C	101	94R	C12-C11-C9	3.06	118.33	113.14
4	C	102	94R	C12-C11-C9	2.66	117.66	113.14
4	C	102	94R	C7-C8-C9	-2.64	106.67	109.72
4	C	101	94R	C4-C5-C10	2.38	119.47	116.42
4	C	101	94R	C19-C10-C5	-2.33	104.83	108.38
4	C	101	94R	C21-C20-C17	-2.31	109.41	112.88
4	C	102	94R	C12-C13-C14	-2.20	103.96	107.25
4	C	102	94R	C21-C20-C17	-2.18	109.61	112.88
4	C	102	94R	C10-C9-C8	-2.17	109.54	112.71
4	C	102	94R	C22-C23-C24	-2.13	109.18	115.24
4	C	102	94R	C11-C9-C8	2.13	114.75	111.78
4	C	101	94R	C4-C5-C6	-2.05	117.79	120.57
4	B	502	94R	C21-C20-C17	2.00	115.89	112.88

There are no chirality outliers.

All (2) torsion outliers are listed below:

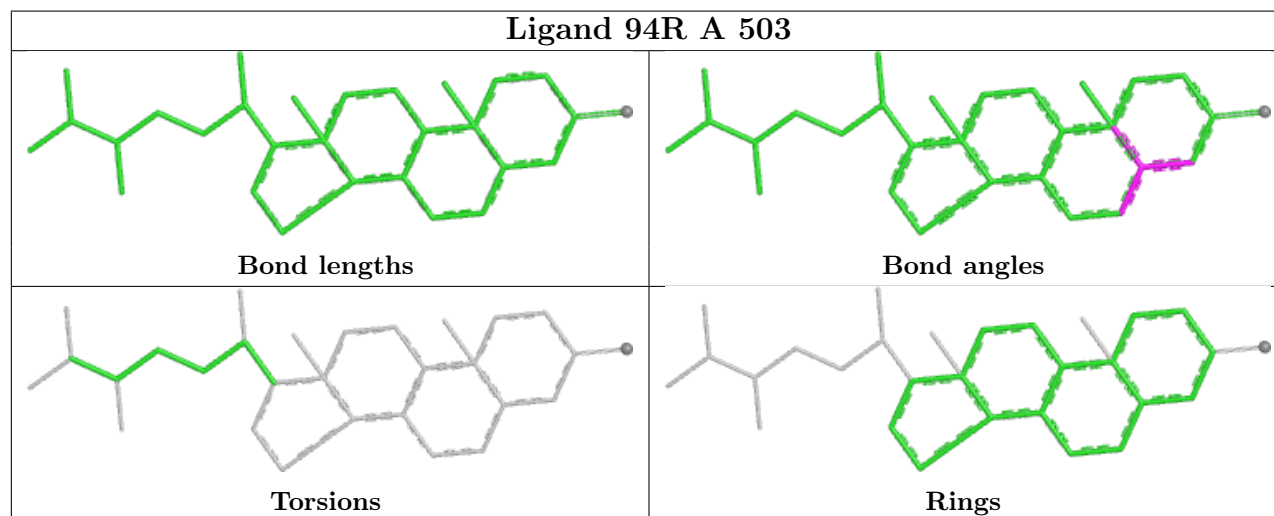
Mol	Chain	Res	Type	Atoms
4	B	502	94R	C17-C20-C22-C23
4	B	502	94R	C21-C20-C22-C23

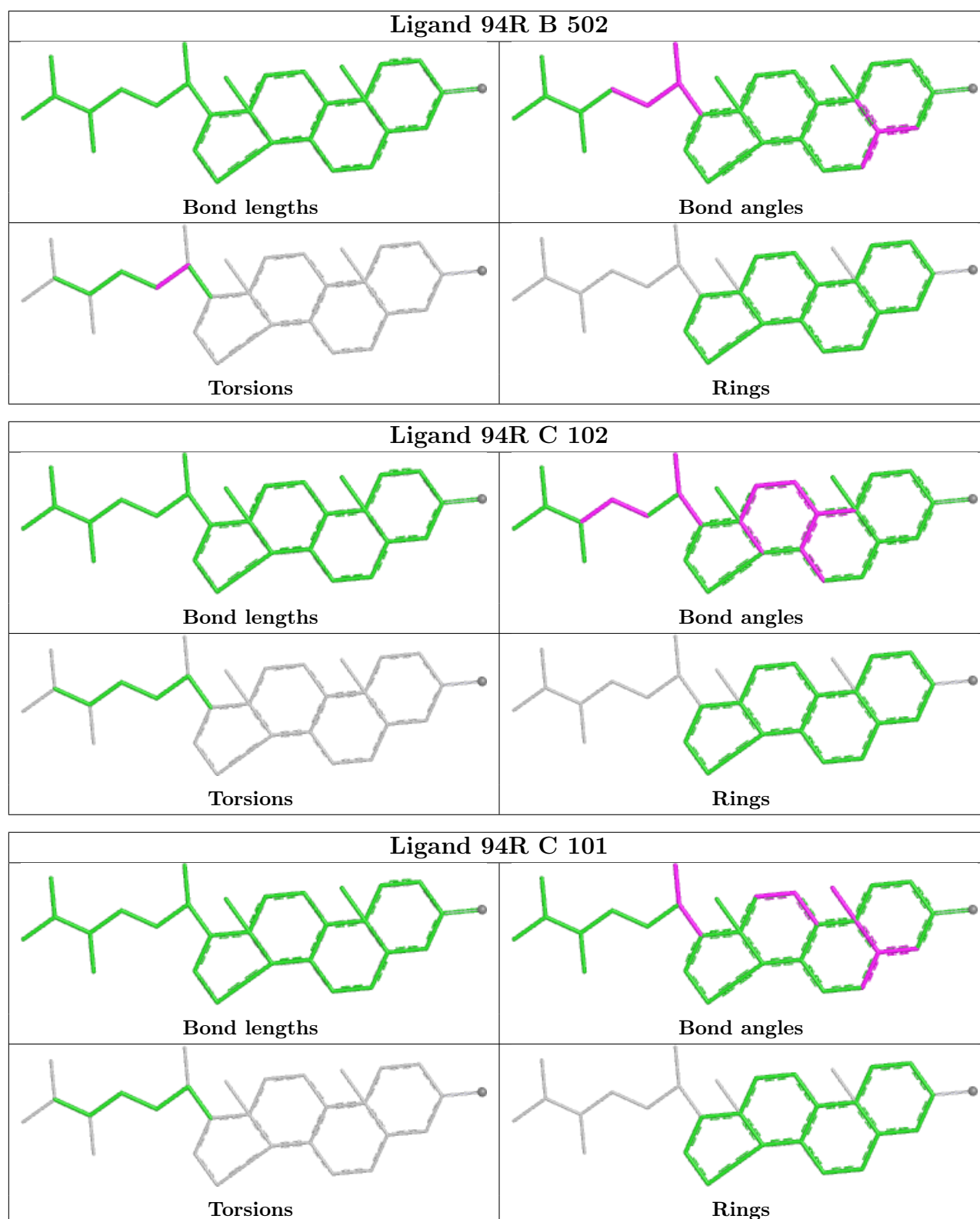
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	94R	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	405/432 (93%)	0.42	37 (9%) 15 11	18, 42, 83, 99	0
1	B	375/432 (86%)	1.59	133 (35%) 1 0	24, 61, 90, 120	2 (0%)
2	C	41/78 (52%)	-0.13	0 100 100	24, 30, 40, 58	0
2	D	43/78 (55%)	0.15	3 (6%) 22 17	26, 32, 52, 77	0
All	All	864/1020 (84%)	0.89	173 (20%) 3 1	18, 48, 88, 120	2 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	ASN	6.7
1	A	46	SER	5.6
1	A	116	ASP	5.3
1	B	385	MET	5.3
1	A	117	ASP	4.8
1	B	218	ASN	4.7
1	B	239	LYS	4.7
1	B	152	PRO	4.5
1	A	47	ASP	4.5
1	B	254	SER	4.4
1	B	119	SER	4.4
1	B	178	ALA	4.4
1	B	233	TYR	4.3
1	B	295	TYR	4.3
1	A	194	ASP	4.2
1	B	232	ASP	4.2
1	B	272	SER	4.2
1	B	155	LEU	4.2
1	B	207	ASP	4.1
1	A	200	ASP	4.1
1	B	264	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	393	PHE	4.0
1	B	177	ASN	4.0
1	B	83	TYR	3.9
1	B	271	ALA	3.8
1	B	420	ASP	3.8
1	B	386	GLN	3.8
1	B	339	HIS	3.8
1	B	237	PHE	3.8
1	B	230	THR	3.8
1	A	286	SER	3.8
1	B	116	ASP	3.7
1	A	49	ARG	3.7
1	B	418	ASN	3.7
1	A	193	LEU	3.6
1	B	231	PHE	3.6
1	B	268	SER	3.6
1	B	118	CYS	3.6
1	B	277	TYR	3.5
1	B	274	SER	3.5
1	B	150	CYS	3.5
1	B	180	THR	3.5
1	B	142	LEU	3.5
2	D	36	VAL	3.5
1	A	23	ARG	3.5
1	B	141	GLY	3.4
1	A	50	ARG	3.4
1	A	245	GLU	3.4
1	A	421	ASN	3.4
1	B	283	PHE	3.4
1	B	212	GLY	3.4
1	B	275	LEU	3.4
1	A	119	SER	3.3
1	B	46	SER	3.3
1	B	240	MET	3.2
1	B	30	SER	3.2
1	B	181	GLY	3.2
1	B	84	ASN	3.2
2	D	37	ASP	3.2
1	B	149	MET	3.2
1	A	195	CYS	3.1
1	B	421	ASN	3.1
1	A	392	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	251	ASP	3.1
1	B	392	ASP	3.1
1	B	112	PHE	3.1
1	A	53	ALA	3.1
1	B	300	ASN	3.0
1	B	109	ASP	3.0
1	B	290	GLN	3.0
1	B	186	SER	3.0
1	B	296	GLU	3.0
1	B	226	LEU	3.0
1	B	227	THR	3.0
1	B	394	ASN	3.0
1	B	205	ILE	3.0
1	B	179	THR	2.9
1	B	238	THR	2.9
1	B	241	THR	2.9
1	A	48	GLU	2.9
1	B	388	MET	2.9
1	B	195	CYS	2.9
1	B	333	HIS	2.9
1	B	148	PRO	2.8
1	A	339	HIS	2.8
1	B	270	VAL	2.8
1	B	221	ASP	2.8
1	B	273	THR	2.8
1	B	299	GLN	2.8
1	A	285	THR	2.8
1	B	348	ASP	2.8
1	B	228	SER	2.7
1	B	200	ASP	2.7
1	B	248	THR	2.7
1	B	243	ASP	2.7
1	B	216	TYR	2.7
1	B	276	TYR	2.7
1	B	253	ILE	2.7
1	B	258	LEU	2.7
1	B	144	ASN	2.7
1	A	288	TYR	2.6
1	B	65	TYR	2.6
1	B	115	TYR	2.6
1	B	63	ASN	2.6
1	B	111	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	222	SER	2.6
1	B	213	LEU	2.6
1	A	244	GLY	2.6
1	B	206	ALA	2.6
1	B	146	THR	2.6
1	B	335	THR	2.6
1	B	211	GLU	2.6
1	B	143	VAL	2.5
1	B	235	PRO	2.5
1	B	400	PHE	2.5
2	D	78	ALA	2.5
1	B	229	ASN	2.5
1	B	121	ILE	2.5
1	B	201	THR	2.4
1	A	218	ASN	2.4
1	B	267	TYR	2.4
1	A	164	LEU	2.4
1	B	151	SER	2.4
1	B	347	SER	2.4
1	A	289	GLN	2.4
1	B	249	ALA	2.4
1	B	280	THR	2.4
1	B	224	HIS	2.4
1	A	233	TYR	2.4
1	A	391	ASN	2.4
1	B	422	ASP	2.4
1	B	188	LEU	2.3
1	B	214	ILE	2.3
1	B	160	THR	2.3
1	A	55	LEU	2.3
1	B	304	THR	2.3
1	A	27	LEU	2.3
1	B	191	GLN	2.3
1	B	182	LYS	2.2
1	B	255	GLY	2.2
1	B	168	VAL	2.2
1	A	44	PHE	2.2
1	A	242	ILE	2.2
1	B	337	GLU	2.2
1	A	390	ASN	2.2
1	B	164	LEU	2.2
1	B	210	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	167	GLN	2.2
1	B	170	ILE	2.2
1	B	301	ILE	2.2
1	B	128	ALA	2.1
1	A	115	TYR	2.1
1	B	306	SER	2.1
1	B	171	PRO	2.1
1	B	303	ASP	2.1
1	A	26	SER	2.1
1	B	123	SER	2.1
1	B	257	ALA	2.1
1	B	163	GLN	2.1
1	B	399	ASN	2.1
1	B	113	ALA	2.0
1	B	330	TRP	2.0
1	B	353	MET	2.0
1	B	346	GLN	2.0
1	B	176	VAL	2.0
1	B	395	PHE	2.0
1	B	162	SER	2.0
1	A	45	GLY	2.0
1	B	244	GLY	2.0
1	A	389	VAL	2.0
1	B	174	VAL	2.0
1	B	203	VAL	2.0
1	A	65	TYR	2.0

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

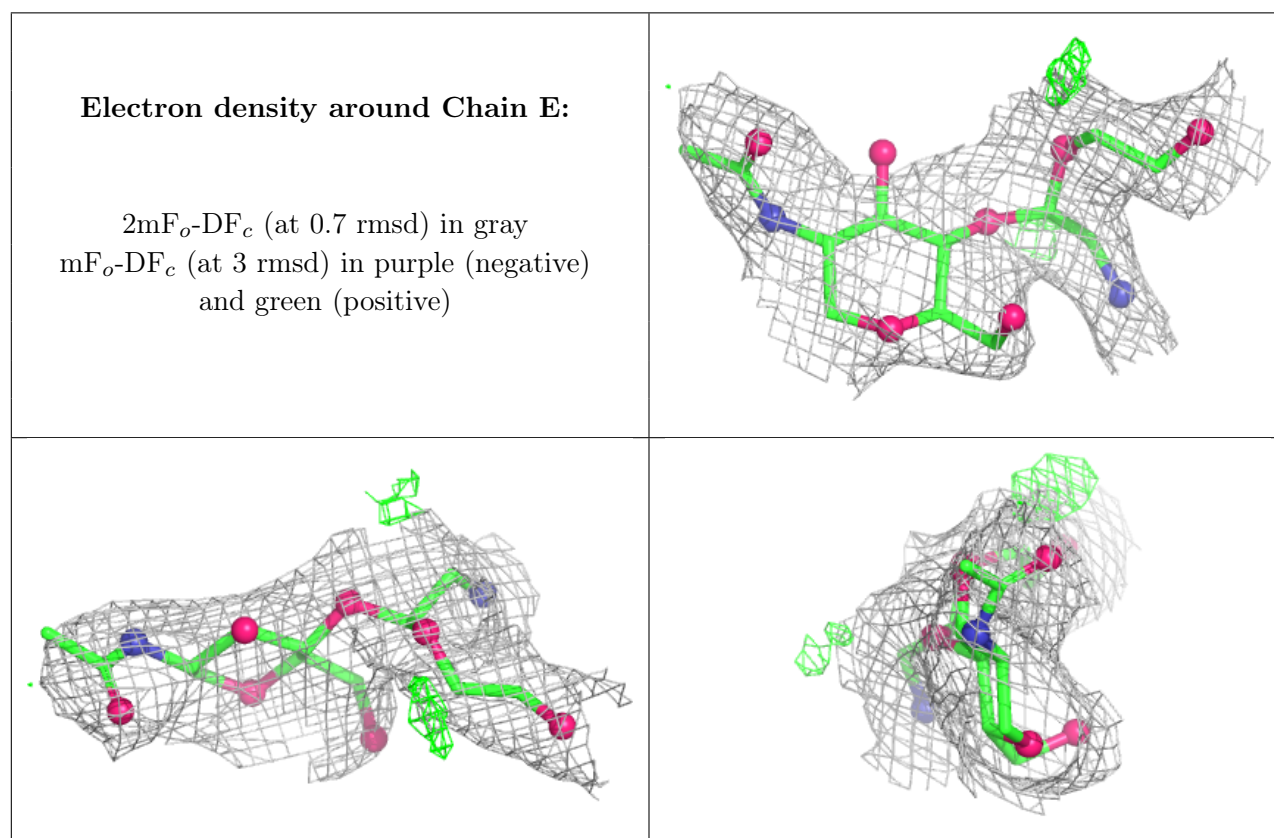
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	NAG	E	2	7/15	0.47	0.24	74,77,80,83	2
3	NAG	E	1	14/15	0.83	0.14	80,84,88,89	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 ⓘ

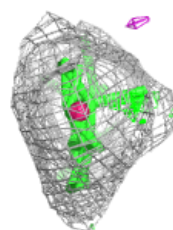
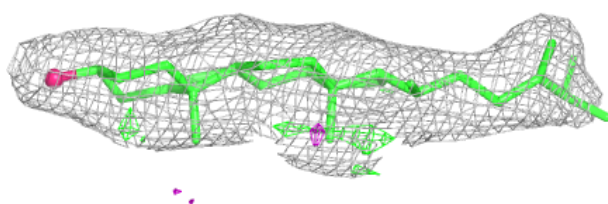
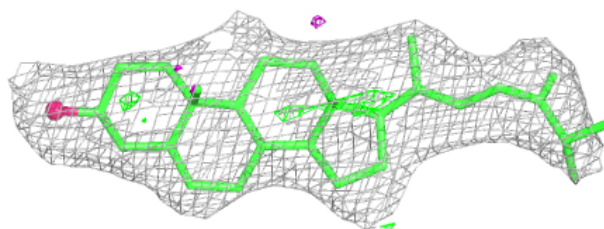
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	501	9/15	0.72	0.14	82,90,94,96	1
4	94R	C	102	29/29	0.89	0.17	53,59,64,67	0
4	94R	C	101	29/29	0.92	0.12	44,47,52,55	0
4	94R	B	502	29/29	0.93	0.11	29,31,34,41	0
4	94R	A	503	29/29	0.95	0.10	29,31,35,39	0

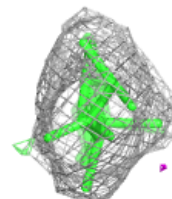
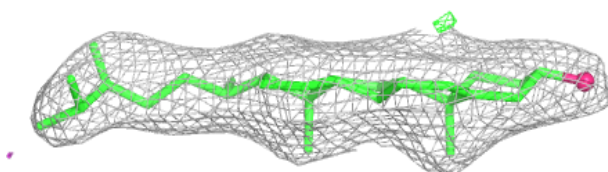
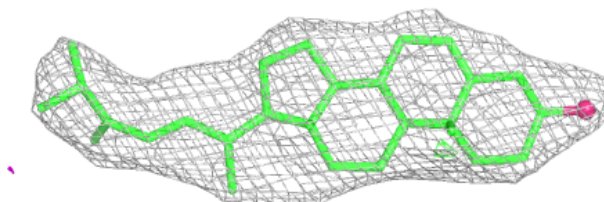
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 94R C 102:

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

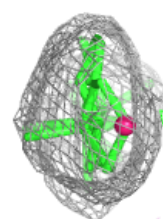
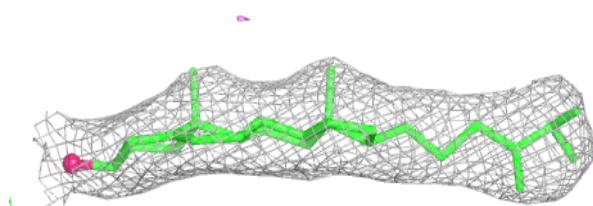
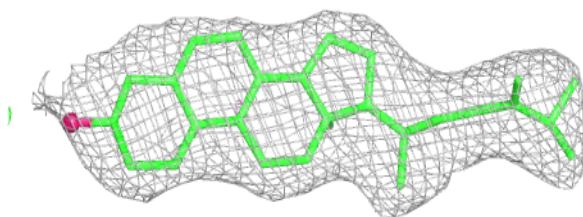
**Electron density around 94R C 101:**

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

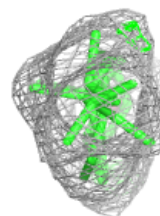
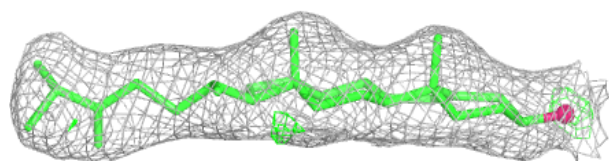
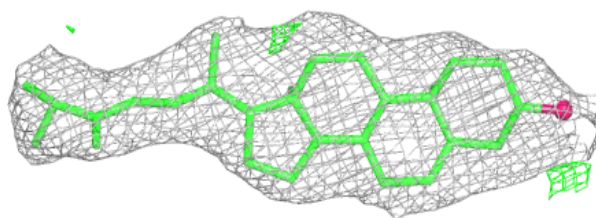


Electron density around 94R B 502:

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

**Electron density around 94R A 503:**

$2mF_o-DF_c$ (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.