



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:00 PM UTC

PDB ID : 6BPL / pdb_00006bpl
Title : E. coli MsbA in complex with LPS and inhibitor G907
Authors : Ho, H.; Koth, C.M.; Payandeh, J.
Deposited on : 2017-11-23
Resolution : 2.91 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

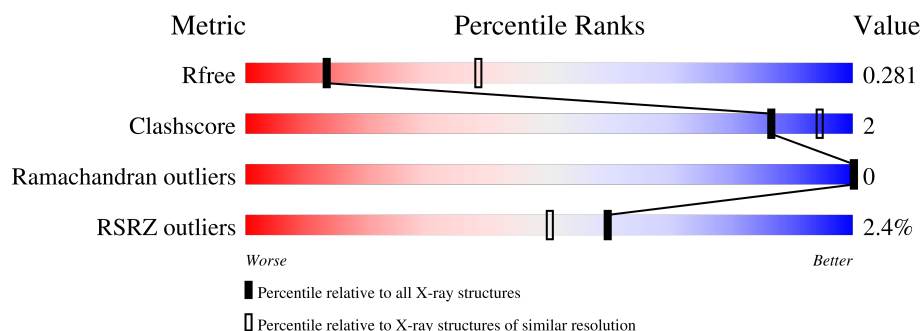
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	582	2% 95% ..
1	B	582	2% 94% ..
2	C	5	40% 60%
3	D	4	50% 50%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9180 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.

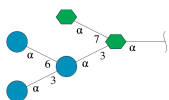
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein MsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4469	2829	778	835	27			
1	B	565	Total	C	N	O	S	0	0	0
			4358	2764	757	812	25			

There are 6 discrepancies between the modelled and reference sequences:

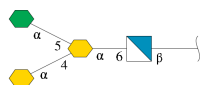
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q8FJB1
A	65	VAL	MET	conflict	UNP Q8FJB1
A	84	VAL	ILE	conflict	UNP Q8FJB1
B	1	SER	-	expression tag	UNP Q8FJB1
B	65	VAL	MET	conflict	UNP Q8FJB1
B	84	VAL	ILE	conflict	UNP Q8FJB1

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-heptopyranose-(1-7)]L-glycero-alpha-D-manno-heptopyranose.



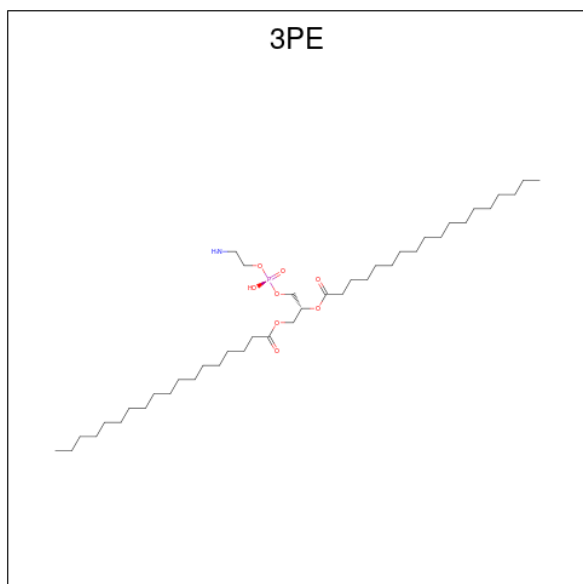
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			59	32	27			

- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose.



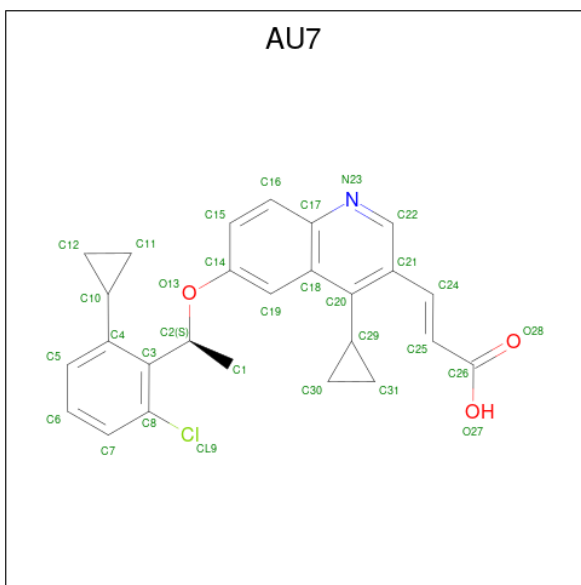
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			54	29	1	24			

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



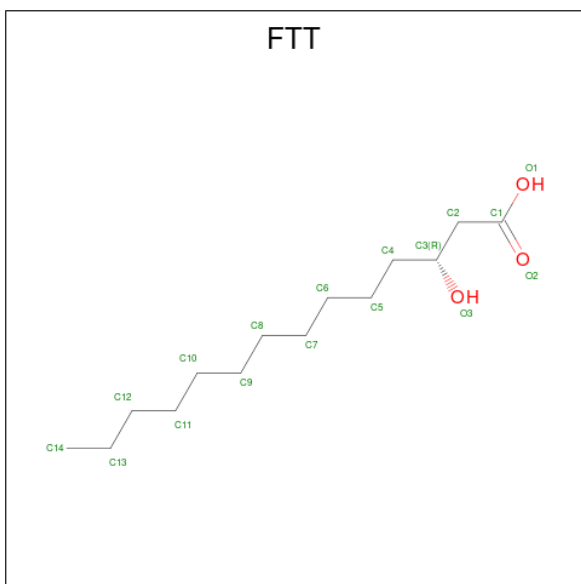
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total 22	C 12	N 1	O 8	P 1	0	0	
4	B	1	Total 19	C 9	N 1	O 8	P 1	0	0	
4	B	1	Total 10		C 10		0			0
4	B	1	Total 7		C 7		0			0

- Molecule 5 is (2E)-3-{6-[(1S)-1-(2-chloro-6-cyclopropylphenyl)ethoxy]-4-cyclopropylquinolin-3-yl}prop-2-enoic acid (CCD ID: AU7) (formula: $C_{26}H_{24}ClNO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			31	26	1	1	3		
5	B	1	Total	C	Cl	N	O	0	0
			31	26	1	1	3		

- Molecule 6 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: $C_{14}H_{28}O_3$).



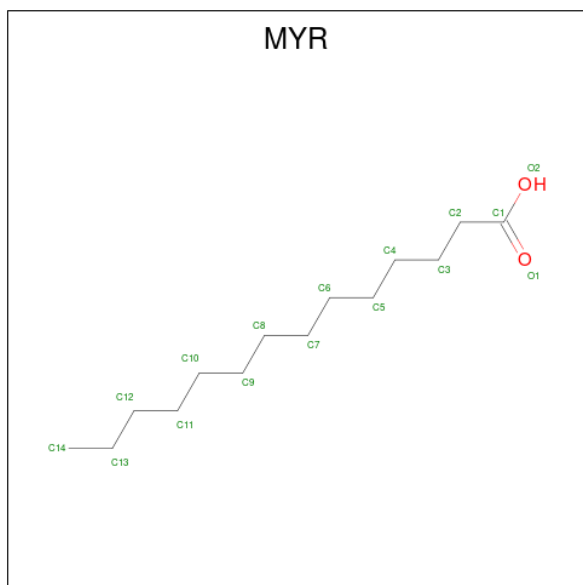
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	14	2		

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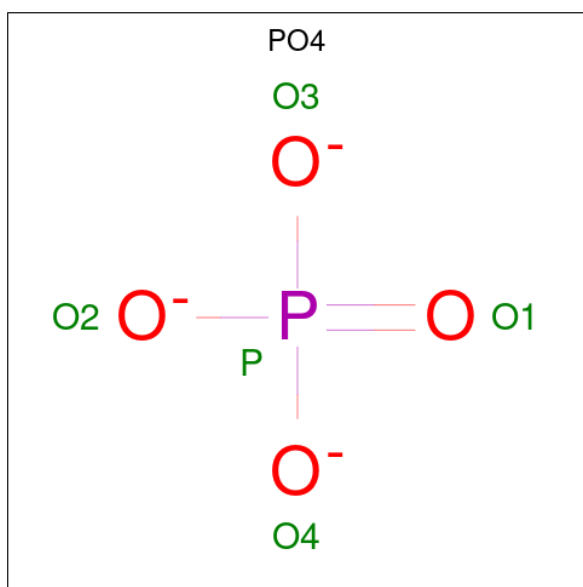
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	14	2		
6	A	1	Total	C	O	0	0
			16	14	2		
6	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



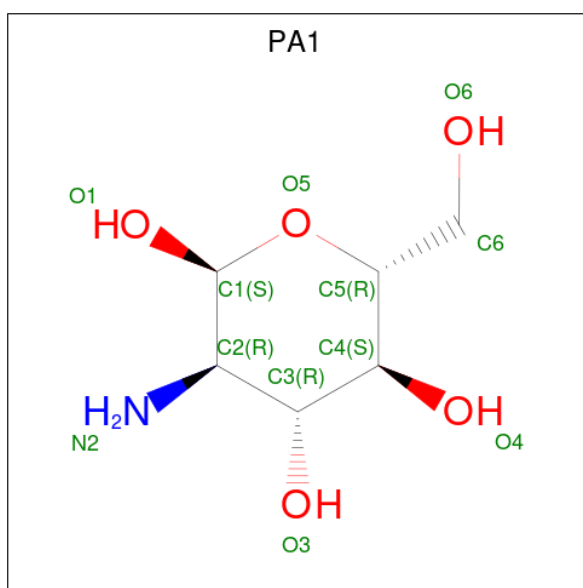
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



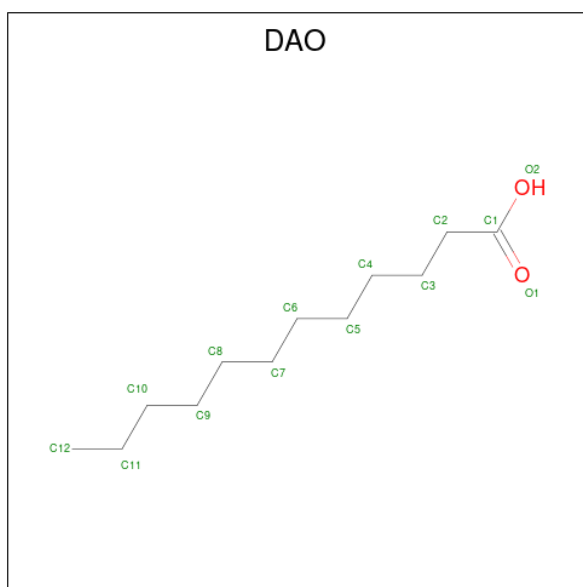
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			4	3	1		
8	B	1	Total	O	P	0	0
			4	3	1		

- Molecule 9 is 2-amino-2-deoxy-alpha-D-glucopyranose (CCD ID: PA1) (formula: $C_6H_{13}NO_5$).



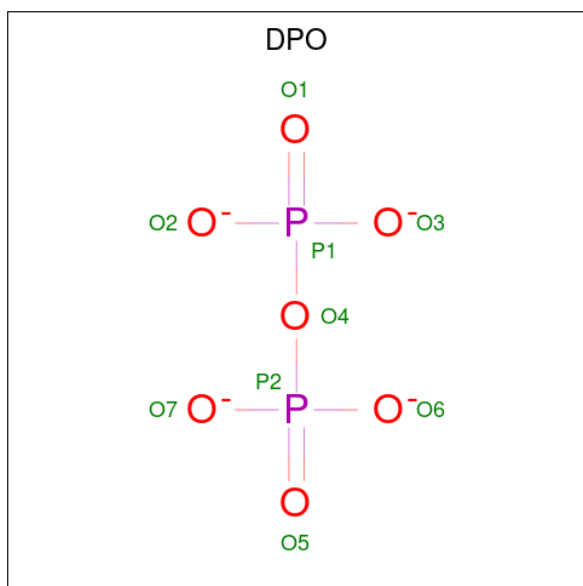
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 10 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	12	1		

- Molecule 11 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2).

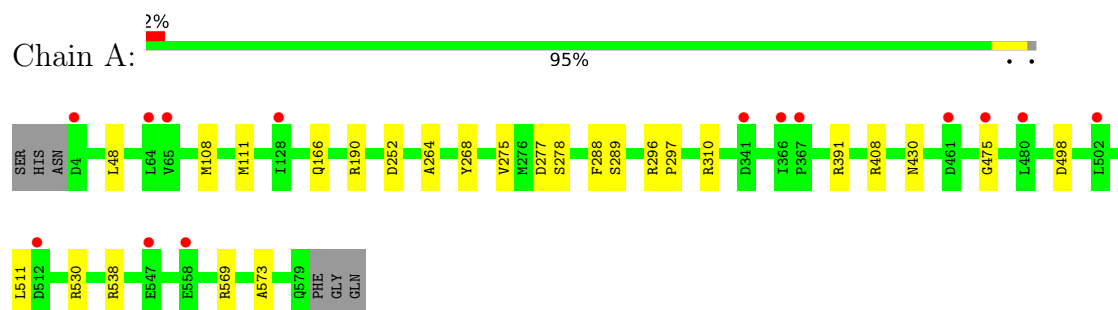


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	O	P	0	0
			8	6	2		

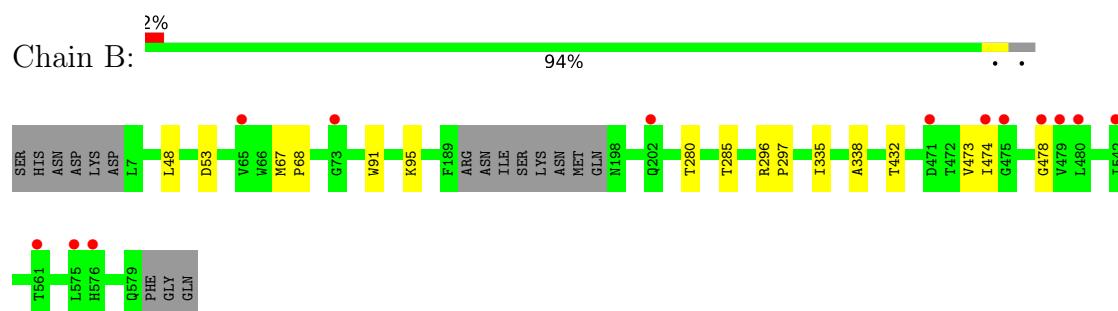
3 Residue-property plots [i](#)

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: Lipid A export ATP-binding/permease protein MsbA



- Molecule 1: Lipid A export ATP-binding/permease protein MsbA



- Molecule 2: alpha-D-glucopyranose-(1-3)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-heptopyranose-(1-7)]L-glycero-alpha-D-manno-heptopyranose



- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.75Å 91.61Å 111.01Å 90.00° 89.39° 90.00°	Depositor
Resolution (Å)	39.90 – 2.91 39.90 – 2.91	Depositor EDS
% Data completeness (in resolution range)	89.6 (39.90-2.91) 89.3 (39.90-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.90Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.233 , 0.283 (Not available) , 0.281	Depositor DCC
R_{free} test set	1482 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9180	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: MYR, PO4, PA1, GCS, DPO, GMH, DAO, 3PE, GLC, FTT, AU7, KDO

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	0.15	0/4534	0.33	0/6127
1	B	0.15	0/4421	0.33	0/5978
All	All	0.15	0/8955	0.33	0/12105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4469	0	4592	19	0
1	B	4358	0	4471	10	0
2	C	59	0	50	2	0
3	D	54	0	39	3	0
4	A	22	0	18	0	0
4	B	36	0	44	0	0
5	A	31	0	0	1	0
5	B	31	0	0	2	0
6	A	48	0	79	5	0
6	B	16	0	27	0	0
7	A	15	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	4	0	0	0	0
8	B	4	0	0	0	0
9	B	12	0	10	4	0
10	B	13	0	23	2	0
11	B	8	0	0	0	0
All	All	9180	0	9380	38	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 (38) 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)
9:B:605:PA1:H62	3:D:2:KDO:H81	1.63	0.80
1:A:498:ASP:OD1	1:A:530:ARG:NH2	2.22	0.72
1:A:288:PHE:CD2	6:A:603:FTT:H141	2.25	0.71
1:A:289:SER:HB3	10:B:608:DAO:H92	1.81	0.63
1:B:296:ARG:HB2	1:B:297:PRO:HD3	1.82	0.60
1:A:430:ASN:HA	1:A:475:GLY:HA3	1.88	0.55
3:D:2:KDO:H7	3:D:4:GMH:C1	2.37	0.53
1:A:277:ASP:OD1	1:A:278:SER:N	2.39	0.52
2:C:2:GLC:H4	2:C:4:GLC:C1	2.40	0.52
1:A:296:ARG:HB3	1:A:297:PRO:HD3	1.91	0.52
1:B:432:THR:HA	1:B:473:VAL:HA	1.93	0.51
6:A:605:FTT:H131	7:A:606:MYR:H132	1.93	0.50
1:B:67:MET:HB2	1:B:68:PRO:HD3	1.94	0.50
1:B:474:ILE:CG2	1:B:478:GLY:HA2	2.43	0.49
1:A:288:PHE:CG	6:A:603:FTT:H141	2.49	0.47
1:A:296:ARG:NH2	9:B:605:PA1:H2	2.30	0.47
1:A:296:ARG:HH22	9:B:605:PA1:C1	2.29	0.46
1:A:310:ARG:NH2	2:C:3:GLC:O2	2.48	0.46
3:D:1:GCS:H62	3:D:2:KDO:H32	1.64	0.46
1:A:48:LEU:HD21	6:A:605:FTT:H122	1.98	0.46
1:A:264:ALA:O	1:A:268:TYR:N	2.44	0.45
1:A:569:ARG:HA	1:A:573:ALA:HB2	1.99	0.44
1:A:166:GLN:HB2	1:A:275:VAL:HG21	2.00	0.44
6:A:605:FTT:C13	7:A:606:MYR:H132	2.48	0.44
1:B:335:ILE:HG21	1:B:338:ALA:HB2	1.99	0.44
5:A:602:AU7:O13	5:A:602:AU7:C10	2.66	0.43
1:A:190:ARG:NH1	1:A:252:ASP:OD1	2.51	0.43
1:B:53:ASP:OD2	1:B:280:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH21	9:B:605:PA1:H2	1.84	0.42
1:B:474:ILE:HG22	1:B:478:GLY:HA2	2.02	0.42
1:B:48:LEU:HD21	1:B:285:THR:HG22	2.02	0.41
5:B:604:AU7:C24	5:B:604:AU7:C31	2.97	0.41
1:A:108:MET:HA	1:A:111:MET:HG2	2.01	0.41
1:A:391:ARG:NH2	1:A:408:ARG:HA	2.36	0.41
1:A:511:LEU:HD21	1:A:538:ARG:HG2	2.03	0.41
5:B:604:AU7:O13	5:B:604:AU7:C10	2.69	0.41
1:B:48:LEU:HD11	10:B:608:DAO:C10	2.51	0.41
1:B:91:TRP:O	1:B:95:LYS:HG2	2.22	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	498/582 (86%)	479 (96%)	19 (4%)	0	100	100
1	B	419/582 (72%)	400 (96%)	19 (4%)	0	100	100
All	All	917/1164 (79%)	879 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GMH	C	1	2	13,13,14	0.48	0	16,18,20	1.07	1 (6%)
2	GLC	C	2	2	11,11,12	0.82	0	15,15,17	1.25	3 (20%)
2	GLC	C	3	2	11,11,12	0.39	0	15,15,17	3.08	2 (13%)
2	GLC	C	4	2	11,11,12	0.49	0	15,15,17	1.40	3 (20%)
2	GMH	C	5	2	13,13,14	0.60	0	16,18,20	1.40	2 (12%)
3	GCS	D	1	6,8,3	11,11,12	0.33	0	13,15,17	0.73	0
3	KDO	D	2	3	15,15,16	0.67	0	17,21,24	1.73	6 (35%)
3	KDO	D	3	3	15,15,16	0.67	0	17,21,24	1.38	4 (23%)
3	GMH	D	4	11,3	13,13,14	0.41	0	16,18,20	1.93	4 (25%)

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	GMH	C	1	2	-	5/6/23/26	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GMH	C	5	2	-	4/6/23/26	0/1/1/1
3	GCS	D	1	6,8,3	-	2/2/19/22	0/1/1/1
3	KDO	D	2	3	-	1/10/26/30	0/1/1/1
3	KDO	D	3	3	-	4/10/26/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GMH	D	4	11,3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLC	C1-O5-C5	10.69	126.51	112.19
3	D	4	GMH	C1-C2-C3	5.31	117.37	109.64
2	C	5	GMH	C1-C2-C3	3.86	115.27	109.64
3	D	2	KDO	O6-C6-C7	3.85	114.08	106.60
2	C	3	GLC	C1-C2-C3	3.83	115.22	109.64
3	D	2	KDO	C4-C5-C6	-3.23	103.97	110.51
3	D	4	GMH	C2-C3-C4	3.14	116.38	110.86
3	D	4	GMH	C1-O5-C5	2.99	116.38	111.48
3	D	3	KDO	O6-C2-C3	2.66	114.13	110.56
3	D	3	KDO	C3-C4-C5	2.60	114.41	110.67
2	C	5	GMH	C1-O5-C5	2.60	115.73	111.48
2	C	4	GLC	O3-C3-C2	-2.47	105.01	110.05
3	D	2	KDO	O1A-C1-C2	-2.44	117.58	122.85
2	C	4	GLC	C3-C4-C5	2.33	114.45	110.23
2	C	1	GMH	C3-C4-C5	2.30	114.90	109.68
3	D	2	KDO	O1B-C1-C2	2.28	118.65	112.71
2	C	2	GLC	C1-O5-C5	2.27	115.23	112.19
3	D	2	KDO	O5-C5-C6	2.26	115.72	109.94
3	D	3	KDO	O1B-C1-C2	2.17	118.37	112.71
3	D	4	GMH	C3-C4-C5	2.17	114.60	109.68
2	C	4	GLC	O5-C5-C6	-2.16	103.46	107.66
2	C	2	GLC	O3-C3-C2	2.14	114.41	110.05
3	D	3	KDO	O6-C2-C1	2.13	111.74	107.72
3	D	2	KDO	O6-C2-C3	2.11	113.39	110.56
2	C	2	GLC	C1-C2-C3	2.10	112.71	109.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GMH	C4-C5-C6-C7
2	C	1	GMH	C4-C5-C6-O6
2	C	1	GMH	O5-C5-C6-C7
2	C	1	GMH	O5-C5-C6-O6
2	C	5	GMH	C4-C5-C6-C7

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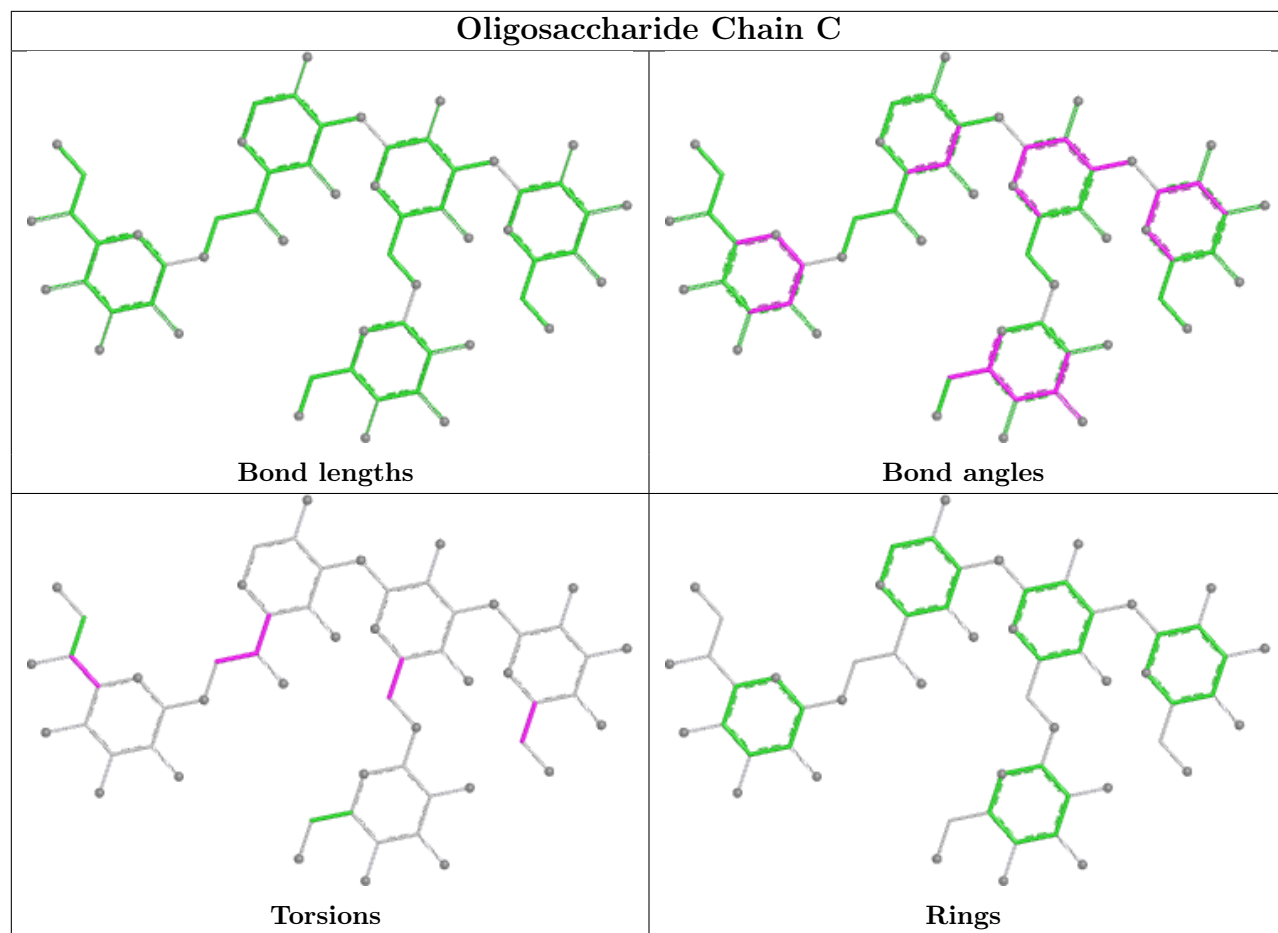
Mol	Chain	Res	Type	Atoms
2	C	5	GMH	C4-C5-C6-O6
2	C	5	GMH	O5-C5-C6-C7
2	C	5	GMH	O5-C5-C6-O6
3	D	3	KDO	C5-C6-C7-O7
3	D	3	KDO	C5-C6-C7-C8
3	D	3	KDO	O6-C6-C7-O7
3	D	3	KDO	O6-C6-C7-C8
3	D	4	GMH	C4-C5-C6-C7
3	D	4	GMH	C4-C5-C6-O6
3	D	4	GMH	O5-C5-C6-C7
3	D	4	GMH	O5-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
3	D	1	GCS	C4-C5-C6-O6
3	D	1	GCS	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	C	1	GMH	O6-C6-C7-O7
3	D	2	KDO	O1A-C1-C2-O6

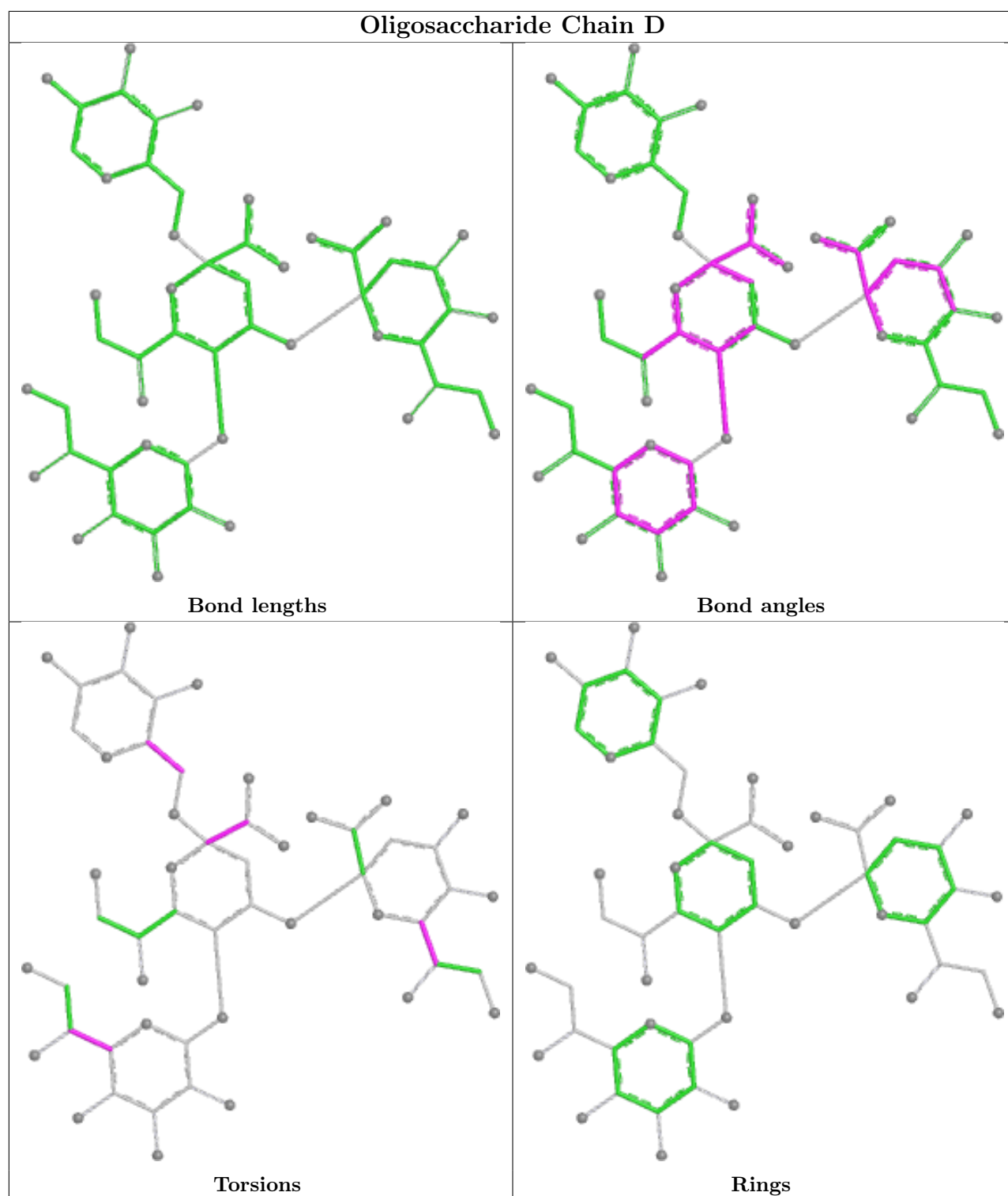
There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	GLC	1	0
2	C	4	GLC	1	0
3	D	4	GMH	1	0
3	D	2	KDO	3	0
3	D	1	GCS	1	0
2	C	2	GLC	1	0

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





5.6 Ligand geometry [i](#)

16 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
5	AU7	A	602	-	35,35,35	1.33	2 (5%)	48,51,51	1.43	7 (14%)
11	DPO	B	609	3	3,7,8	0.77	0	6,10,13	1.00	0
8	PO4	B	606	9	0,3,4	-	-	0,3,6	-	-
10	DAO	B	608	6	11,12,13	0.34	0	10,11,13	0.66	0
4	3PE	B	602	-	9,9,50	0.77	0	8,8,55	0.16	0
6	FTT	B	607	9	14,15,16	0.38	0	15,15,17	0.95	1 (6%)
4	3PE	B	603	-	6,6,50	0.70	0	5,5,55	0.18	0
5	AU7	B	604	-	35,35,35	1.31	3 (8%)	48,51,51	1.43	6 (12%)
9	PA1	B	605	6,8	12,12,12	0.74	0	16,17,17	1.43	2 (12%)
7	MYR	A	606	6	13,14,15	0.35	0	12,13,15	0.65	0
4	3PE	B	601	-	18,18,50	2.00	3 (16%)	21,23,55	1.88	5 (23%)
6	FTT	A	605	7,3	14,15,16	0.34	0	15,15,17	1.06	2 (13%)
6	FTT	A	604	3,10	14,15,16	0.36	0	15,15,17	1.07	1 (6%)
8	PO4	A	607	3	0,3,4	-	-	0,3,6	-	-
4	3PE	A	601	-	21,21,50	1.87	4 (19%)	24,26,55	1.58	4 (16%)
6	FTT	A	603	9	14,15,16	0.36	0	15,15,17	0.98	1 (6%)

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
5	AU7	A	602	-	-	1/21/25/25	0/5/5/5
11	DPO	B	609	3	-	1/2/5/6	-
10	DAO	B	608	6	-	8/10/10/11	-
4	3PE	B	602	-	-	4/7/7/54	-
6	FTT	B	607	9	-	3/14/14/15	-
4	3PE	B	603	-	-	2/4/4/54	-
5	AU7	B	604	-	-	2/21/25/25	0/5/5/5
9	PA1	B	605	6,8	-	2/2/22/22	0/1/1/1
7	MYR	A	606	6	-	4/12/12/13	-
4	3PE	B	601	-	-	10/20/20/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FTT	A	605	7,3	-	3/14/14/15	-
6	FTT	A	604	3,10	-	5/14/14/15	-
4	3PE	A	601	-	-	6/24/24/54	-
6	FTT	A	603	9	-	5/14/14/15	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	3PE	P-O13	6.09	1.83	1.59
4	A	601	3PE	P-O13	5.60	1.81	1.59
5	A	602	AU7	O28-C26	5.13	1.35	1.23
5	B	604	AU7	O28-C26	4.96	1.35	1.23
5	A	602	AU7	O27-C26	-3.32	1.21	1.30
5	B	604	AU7	O27-C26	-3.21	1.22	1.30
4	A	601	3PE	C3-C2	2.87	1.59	1.50
4	B	601	3PE	C3-C2	2.68	1.59	1.50
4	A	601	3PE	O13-C11	-2.44	1.35	1.44
5	B	604	AU7	C17-N23	-2.15	1.33	1.37
4	A	601	3PE	O21-C21	2.13	1.40	1.34
4	B	601	3PE	O13-C11	-2.13	1.36	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	3PE	O21-C21-C22	5.65	121.16	111.09
5	A	602	AU7	C21-C24-C25	-5.05	117.01	126.91
4	A	601	3PE	O21-C21-C22	4.46	121.14	111.48
5	B	604	AU7	C22-N23-C17	4.12	121.73	116.96
5	A	602	AU7	C22-N23-C17	4.06	121.66	116.96
5	B	604	AU7	C21-C24-C25	-3.85	119.36	126.91
4	B	601	3PE	O12-P-O14	3.62	129.30	112.44
4	A	601	3PE	O12-P-O14	3.62	129.29	112.44
9	B	605	PA1	C4-C3-C2	-3.44	105.29	110.99
5	B	604	AU7	C1-C2-C3	-2.91	108.97	113.20
5	B	604	AU7	C11-C10-C4	-2.89	116.35	121.75
6	A	604	FTT	O2-C1-C2	-2.61	117.78	125.38
4	B	601	3PE	O13-P-O14	-2.60	98.63	108.94
6	B	607	FTT	O2-C1-C2	-2.49	118.15	125.38
4	A	601	3PE	O13-P-O14	-2.45	99.22	108.94
5	A	602	AU7	C11-C10-C4	-2.43	117.20	121.75
9	B	605	PA1	O4-C4-C5	2.38	115.18	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	605	FTT	O2-C1-C2	-2.36	118.52	125.38
6	A	605	FTT	C3-C2-C1	-2.35	108.71	112.70
5	B	604	AU7	C18-C17-N23	-2.30	120.38	122.82
4	B	601	3PE	C2-O21-C21	2.29	121.89	117.85
6	A	603	FTT	O2-C1-C2	-2.27	118.78	125.38
5	A	602	AU7	C1-C2-C3	-2.26	109.92	113.20
4	B	601	3PE	O21-C21-O22	-2.25	118.64	122.99
5	A	602	AU7	C12-C10-C4	-2.24	117.56	121.75
5	A	602	AU7	C14-O13-C2	2.24	121.87	118.59
4	A	601	3PE	O21-C21-O22	-2.21	118.55	123.70
5	B	604	AU7	C21-C20-C18	-2.06	117.42	119.44
5	A	602	AU7	C21-C22-N23	-2.05	121.48	124.14

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	3PE	C1-O11-P-O12
4	B	601	3PE	C1-O11-P-O14
4	B	601	3PE	C11-O13-P-O11
4	B	601	3PE	C11-O13-P-O14
4	B	601	3PE	C2-C1-O11-P
4	B	601	3PE	O13-C11-C12-N
4	B	601	3PE	O22-C21-O21-C2
5	B	604	AU7	C21-C20-C29-C31
6	A	604	FTT	O2-C1-C2-C3
7	A	606	MYR	O1-C1-C2-C3
10	B	608	DAO	O1-C1-C2-C3
4	B	601	3PE	C22-C21-O21-C2
9	B	605	PA1	C4-C5-C6-O6
4	A	601	3PE	O32-C31-O31-C3
9	B	605	PA1	O5-C5-C6-O6
4	A	601	3PE	C32-C31-O31-C3
10	B	608	DAO	C11-C10-C9-C8
6	A	604	FTT	C6-C7-C8-C9
4	A	601	3PE	C21-C22-C23-C24
10	B	608	DAO	C2-C3-C4-C5
6	A	603	FTT	C5-C6-C7-C8
7	A	606	MYR	C11-C10-C9-C8
6	A	603	FTT	O3-C3-C4-C5
6	B	607	FTT	C4-C5-C6-C7
6	B	607	FTT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	601	3PE	C2-C3-O31-C31
6	A	603	FTT	C2-C3-C4-C5
4	B	602	3PE	C2E-C2F-C2G-C2H
6	A	603	FTT	C6-C7-C8-C9
10	B	608	DAO	C5-C6-C7-C8
4	A	601	3PE	C22-C23-C24-C25
6	A	605	FTT	C11-C10-C9-C8
4	B	602	3PE	C29-C2A-C2B-C2C
6	A	605	FTT	C7-C8-C9-C10
4	B	602	3PE	C2A-C2B-C2C-C2D
4	B	603	3PE	C2F-C2G-C2H-C2I
10	B	608	DAO	C4-C5-C6-C7
6	A	603	FTT	C11-C12-C13-C14
7	A	606	MYR	C10-C11-C12-C13
10	B	608	DAO	C7-C8-C9-C10
7	A	606	MYR	C4-C5-C6-C7
10	B	608	DAO	C9-C10-C11-C12
6	A	604	FTT	C5-C6-C7-C8
6	B	607	FTT	O2-C1-C2-C3
10	B	608	DAO	C3-C4-C5-C6
6	A	604	FTT	C4-C5-C6-C7
4	B	601	3PE	C1-O11-P-O13
4	B	601	3PE	C2-C3-O31-C31
5	B	604	AU7	C18-C20-C29-C30
4	A	601	3PE	O21-C2-C3-O31
11	B	609	DPO	P1-O4-P2-O7
6	A	604	FTT	C10-C11-C12-C13
4	B	603	3PE	C2D-C2E-C2F-C2G
4	B	602	3PE	C2D-C2E-C2F-C2G
6	A	605	FTT	C3-C4-C5-C6
5	A	602	AU7	O13-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 14 short contacts:

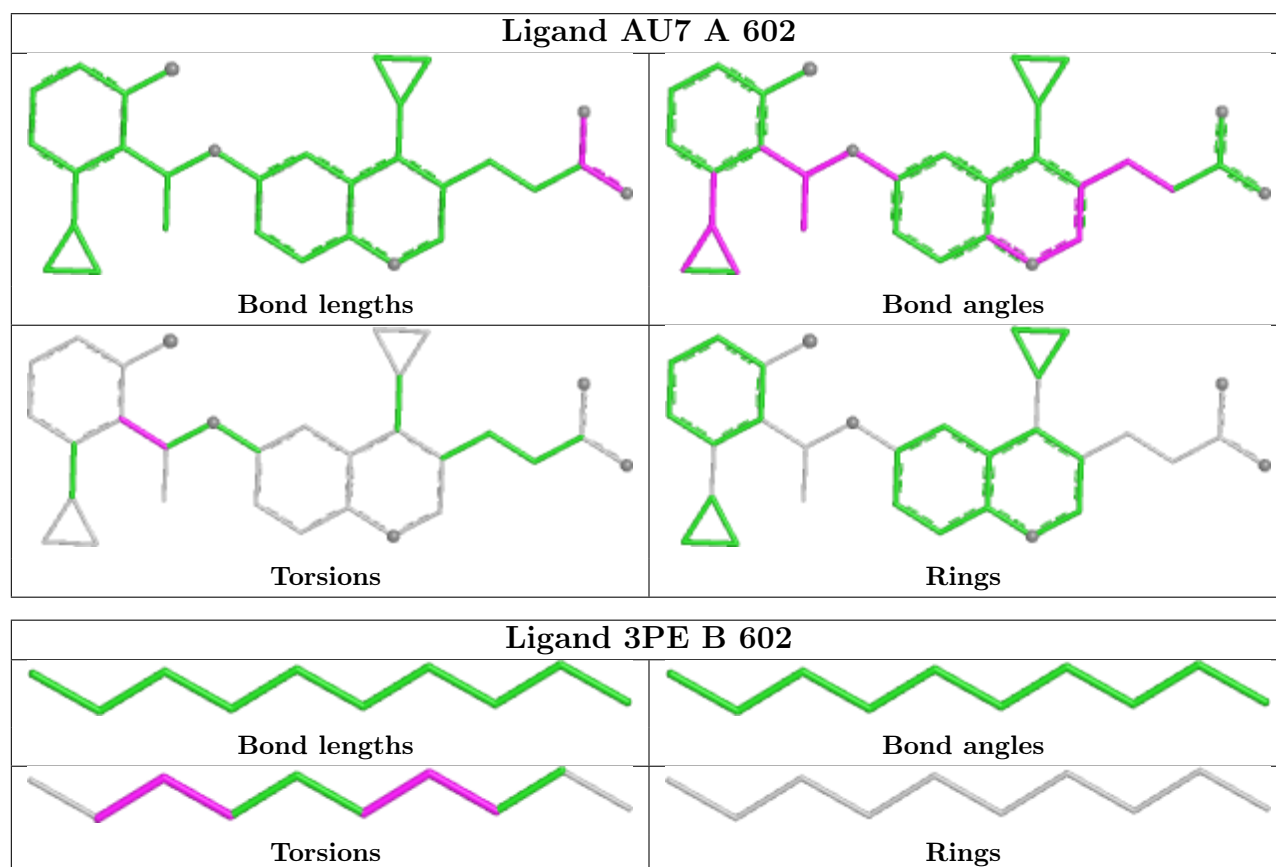
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	AU7	1	0
10	B	608	DAO	2	0
5	B	604	AU7	2	0
9	B	605	PA1	4	0
7	A	606	MYR	2	0
6	A	605	FTT	3	0

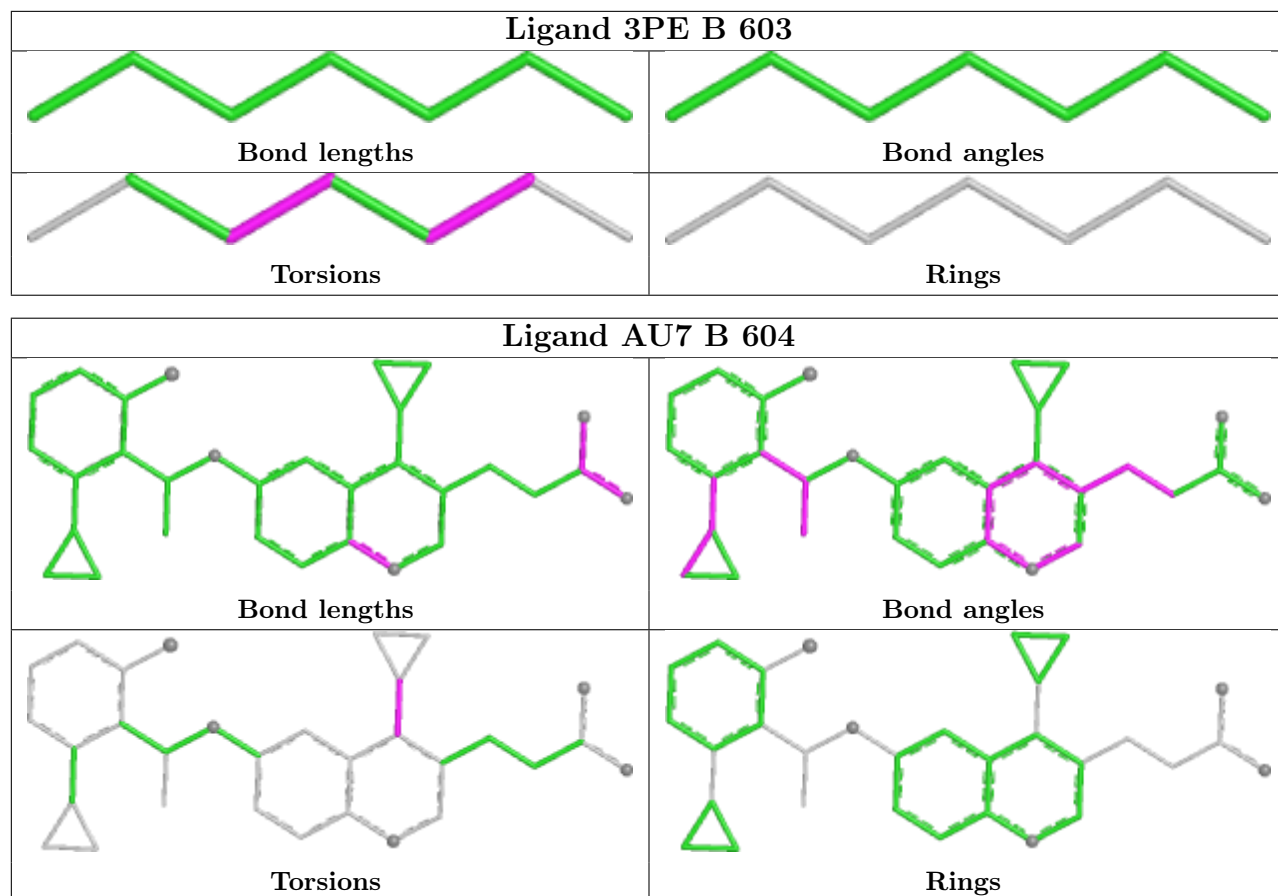
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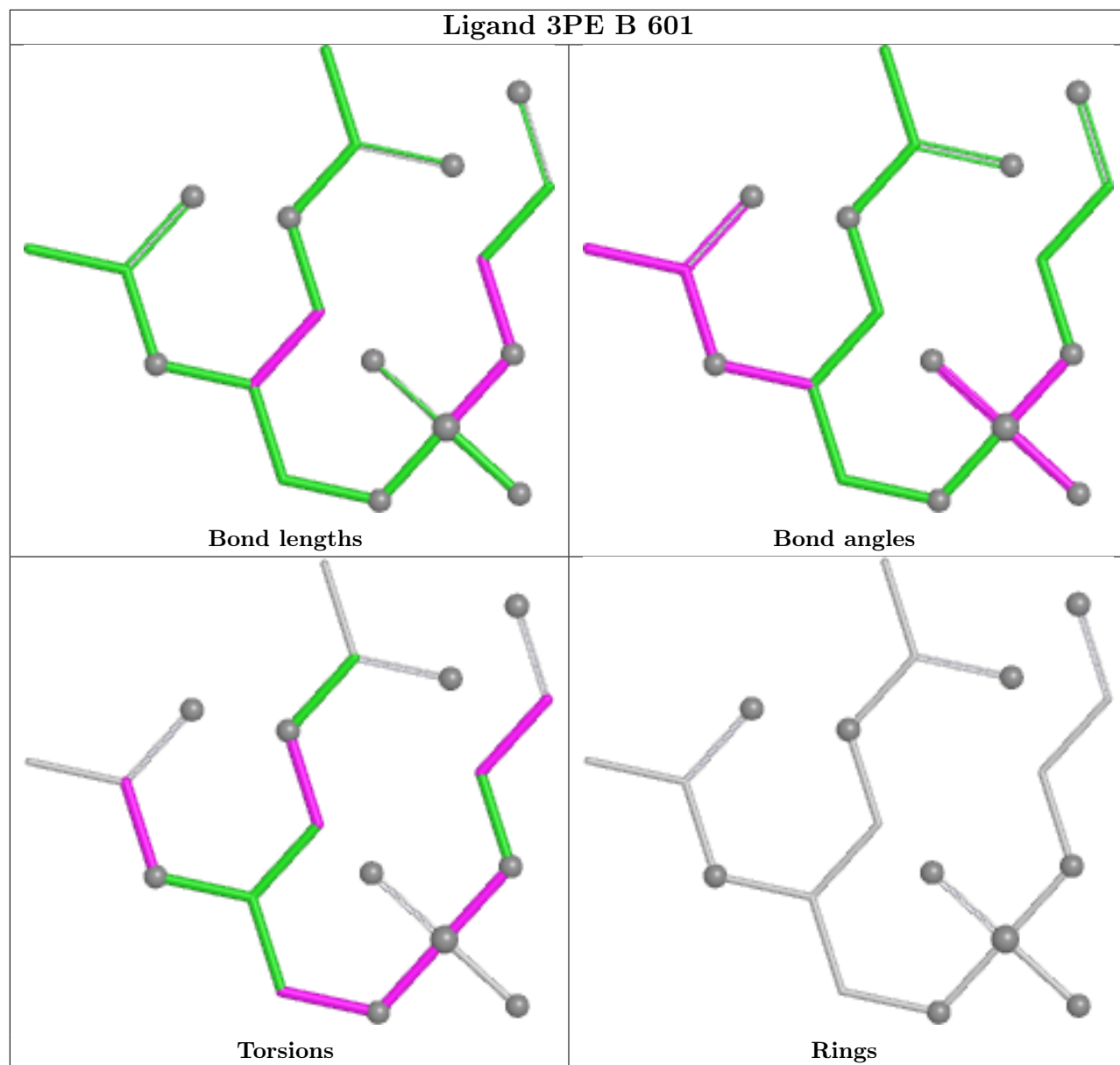
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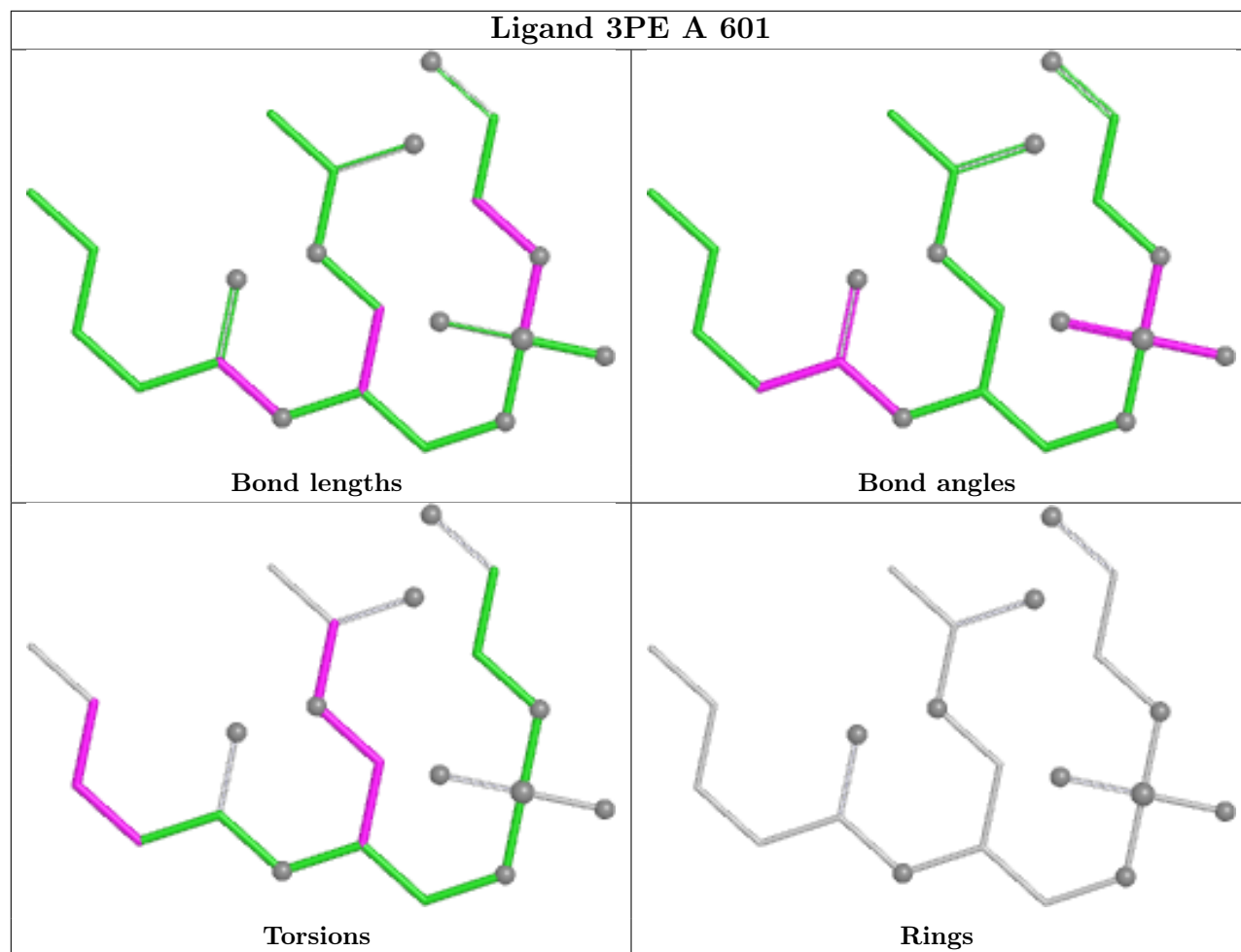
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	FTT	2	0

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	576/582 (98%)	0.09	14 (2%)	59 50	44, 68, 111, 135	0
1	B	565/582 (97%)	0.13	13 (2%)	61 52	43, 77, 112, 147	0
All	All	1141/1164 (98%)	0.11	27 (2%)	59 50	43, 72, 112, 147	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	LEU	4.7
1	B	474	ILE	4.4
1	B	480	LEU	3.8
1	A	128	ILE	3.7
1	B	478	GLY	3.3
1	A	480	LEU	2.9
1	B	65	VAL	2.9
1	A	366	ILE	2.8
1	A	547	GLU	2.8
1	A	4	ASP	2.6
1	B	202	GLN	2.6
1	B	73	GLY	2.6
1	B	576	HIS	2.5
1	B	561	THR	2.5
1	B	479	VAL	2.3
1	A	367	PRO	2.3
1	B	471	ASP	2.2
1	A	65	VAL	2.2
1	A	461	ASP	2.2
1	A	475	GLY	2.2
1	B	475	GLY	2.1
1	A	502	LEU	2.1
1	A	341	ASP	2.1
1	A	64	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	542	ILE	2.0
1	A	558	GLU	2.0
1	A	512	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](#)

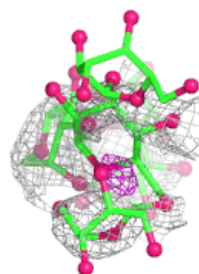
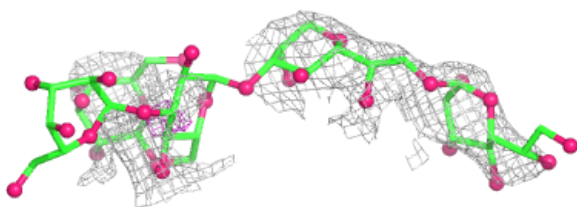
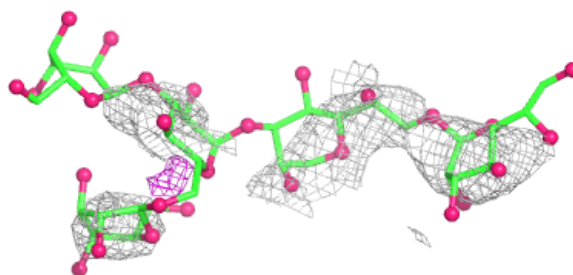
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

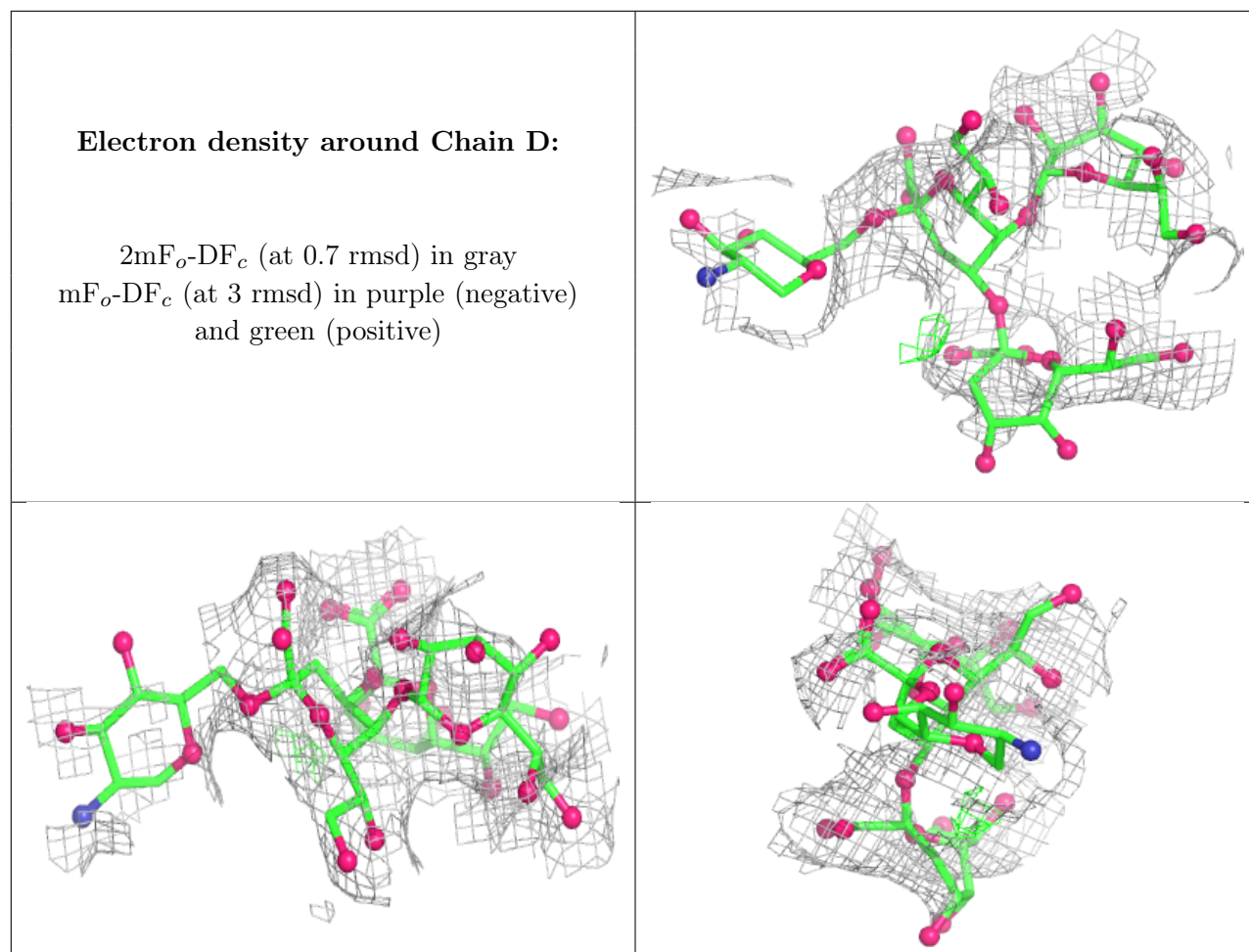
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	2	11/12	0.03	0.14	161,168,179,181	0
2	GMH	C	1	13/14	0.53	0.13	142,149,165,172	0
3	GMH	D	4	13/14	0.58	0.09	135,149,158,166	0
2	GLC	C	3	11/12	0.59	0.10	154,165,169,171	0
2	GLC	C	4	11/12	0.64	0.09	155,164,179,182	0
3	KDO	D	3	15/16	0.65	0.15	109,129,142,145	0
3	KDO	D	2	15/16	0.72	0.10	125,139,147,149	0
2	GMH	C	5	13/14	0.73	0.09	103,138,146,148	0
3	GCS	D	1	11/12	0.84	0.07	111,118,132,134	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 C:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	DPO	B	609	8/9	0.57	0.07	159,167,171,177	0
4	3PE	B	603	7/51	0.72	0.31	59,80,85,85	0
4	3PE	B	601	19/51	0.72	0.13	85,101,109,119	0
4	3PE	A	601	22/51	0.76	0.13	63,94,107,190	0
9	PA1	B	605	12/12	0.82	0.08	103,114,123,131	0
8	PO4	B	606	4/5	0.86	0.06	81,85,116,118	0
6	FTT	A	605	16/17	0.87	0.18	65,94,110,125	0
4	3PE	B	602	10/51	0.87	0.21	58,80,89,94	0
6	FTT	A	604	16/17	0.88	0.17	79,96,114,122	0
6	FTT	A	603	16/17	0.89	0.18	68,88,106,108	0
10	DAO	B	608	13/14	0.91	0.17	62,81,90,96	0

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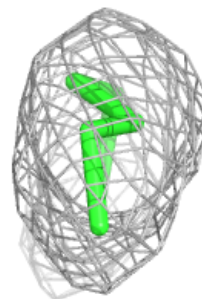
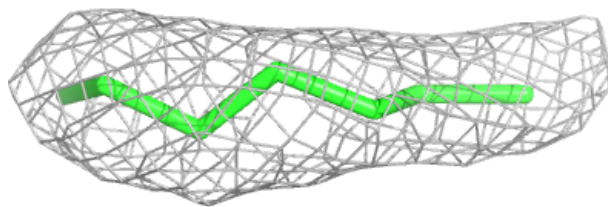
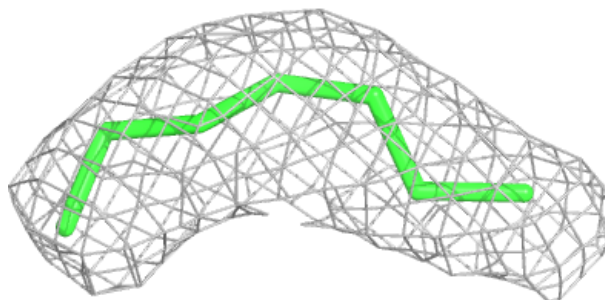
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FTT	B	607	16/17	0.92	0.15	69,94,113,114	0
7	MYR	A	606	15/16	0.92	0.16	65,75,95,101	0
5	AU7	A	602	31/31	0.93	0.08	43,54,67,70	0
8	PO4	A	607	4/5	0.93	0.05	85,90,96,112	0
5	AU7	B	604	31/31	0.93	0.08	50,69,81,82	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.

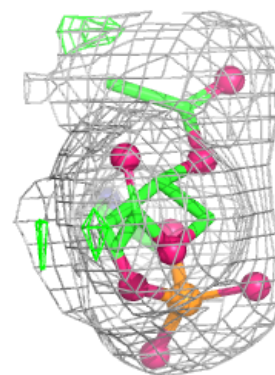
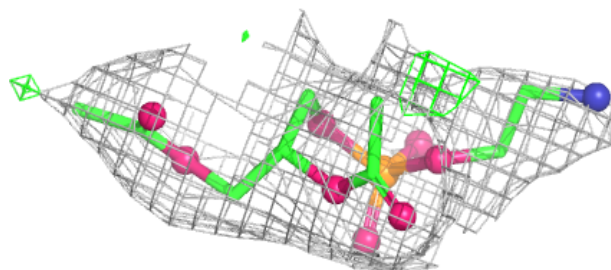
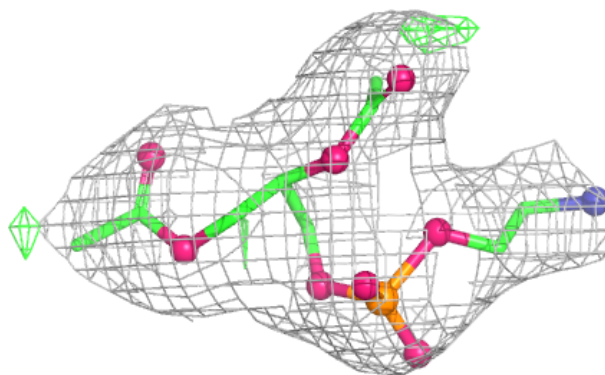
Electron density around 3PE B 603:

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



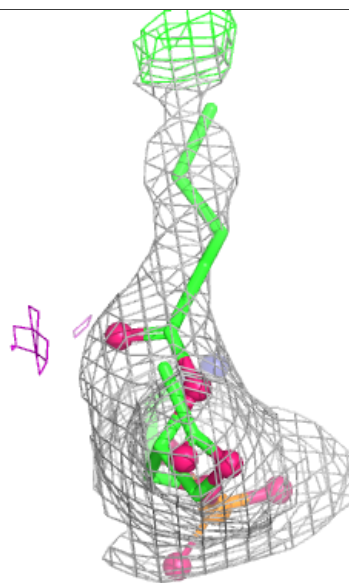
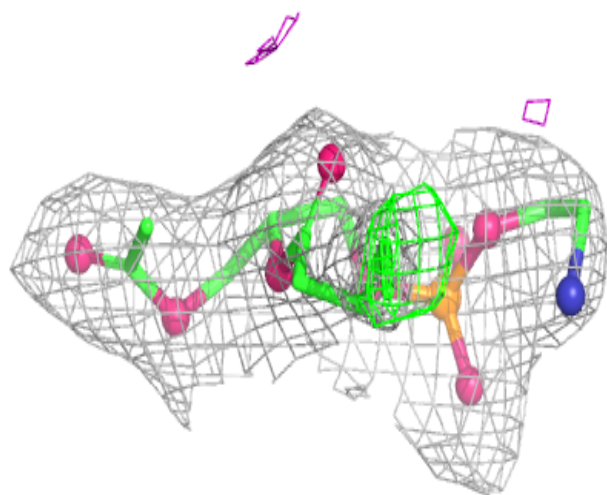
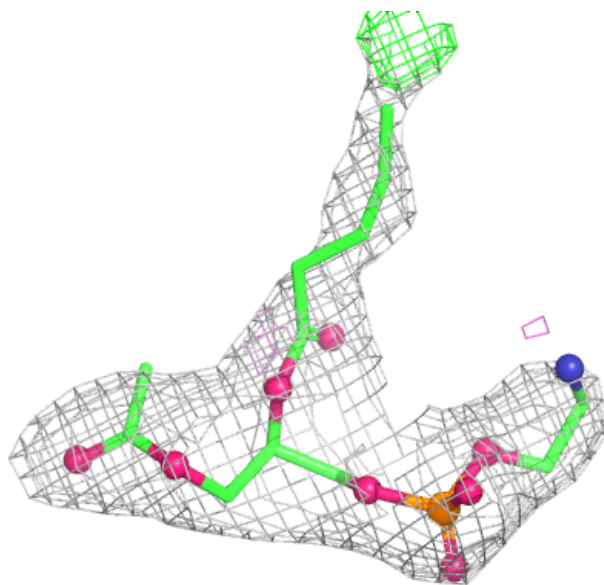
Electron density around 3PE B 601:

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



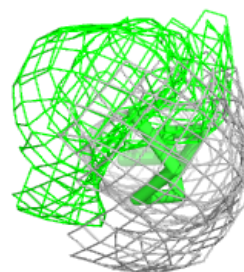
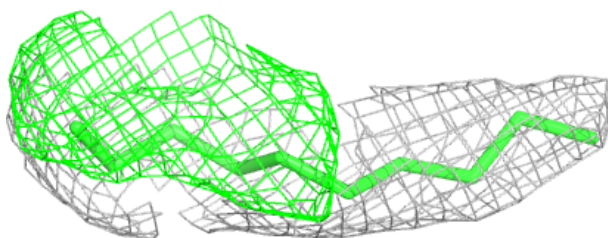
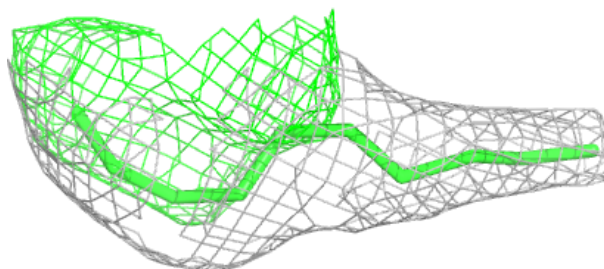
Electron density around 3PE A 601:

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

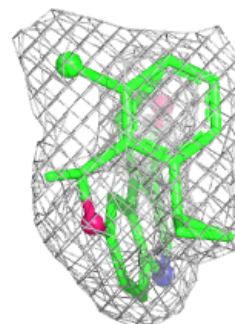
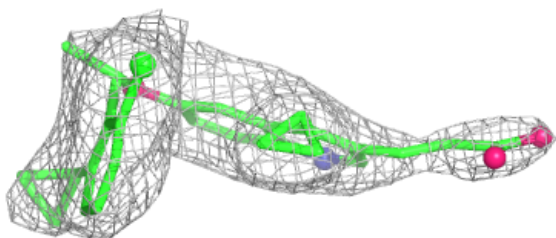
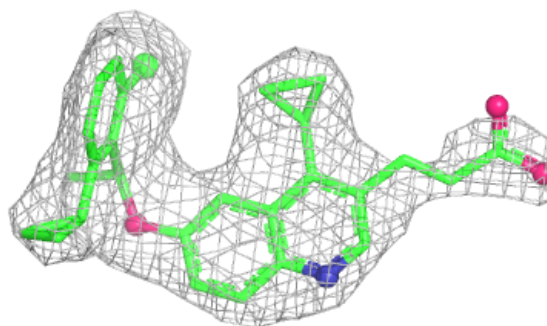


Electron density around 3PE B 602:

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

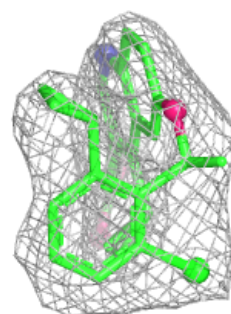
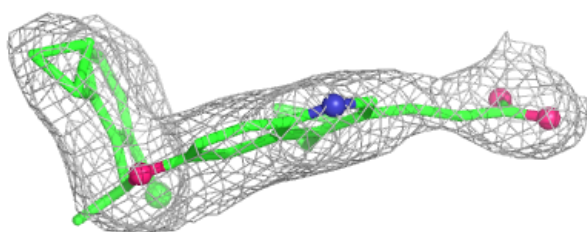
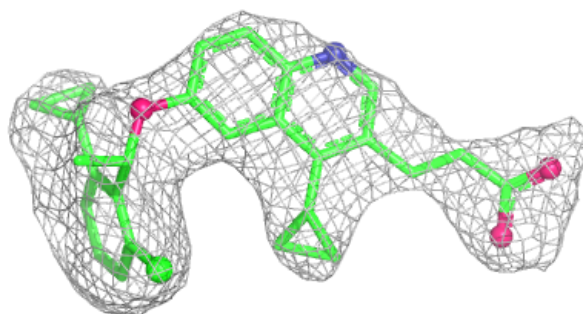
**Electron density around AU7 A 602:**

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



Electron density around AU7 B 604:

$2mF_o-DF_c$ (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.