



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:59 PM EDT

PDB ID : 4GEY / pdb_00004gey
Title : High pH structure of Pseudomonas putida OprB
Authors : van den Berg, B.
Deposited on : 2012-08-02
Resolution : 2.70 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

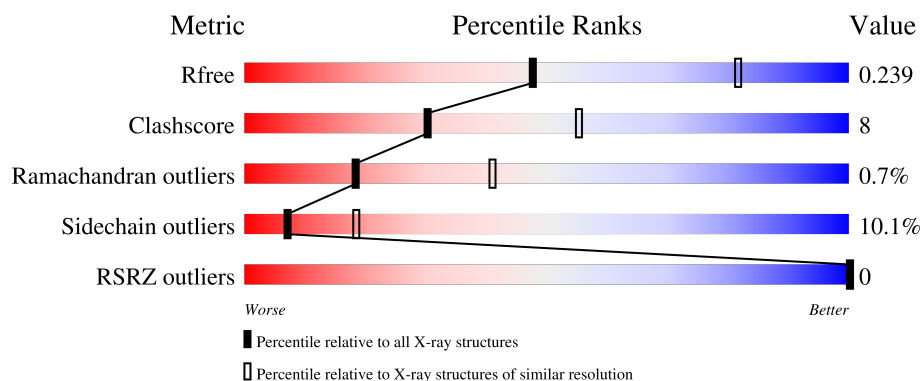
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	436	 75% 18% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3597 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.

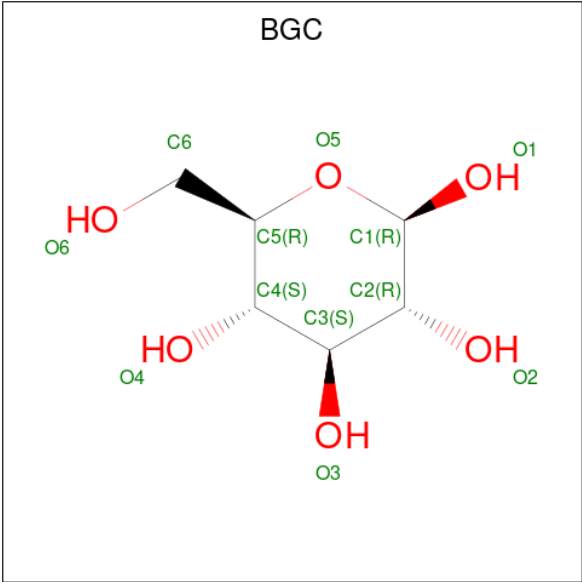
- Molecule 1 is a protein called Porin B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	Se	0	0	0
			3309	2104	570	629	2	4			

There are 17 discrepancies between the modelled and reference sequences:

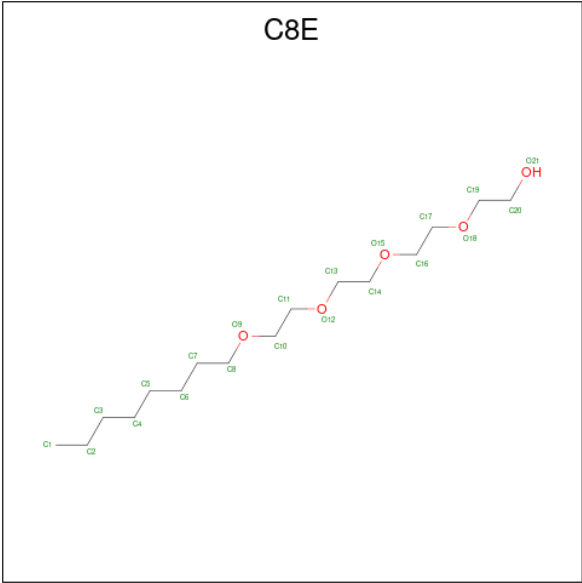
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP E4R6F8
A	-13	ASN	-	expression tag	UNP E4R6F8
A	-12	VAL	-	expression tag	UNP E4R6F8
A	-11	ARG	-	expression tag	UNP E4R6F8
A	-10	LEU	-	expression tag	UNP E4R6F8
A	-9	GLN	-	expression tag	UNP E4R6F8
A	-8	HIS	-	expression tag	UNP E4R6F8
A	-7	HIS	-	expression tag	UNP E4R6F8
A	-6	HIS	-	expression tag	UNP E4R6F8
A	-5	HIS	-	expression tag	UNP E4R6F8
A	-4	HIS	-	expression tag	UNP E4R6F8
A	-3	HIS	-	expression tag	UNP E4R6F8
A	-2	HIS	-	expression tag	UNP E4R6F8
A	-1	LEU	-	expression tag	UNP E4R6F8
A	0	GLU	-	expression tag	UNP E4R6F8
A	220	MSE	LEU	engineered mutation	UNP E4R6F8
A	222	MSE	VAL	engineered mutation	UNP E4R6F8

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



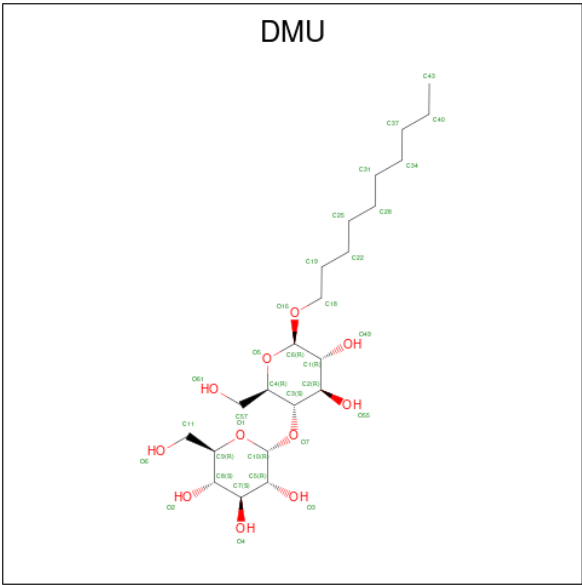
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			21	16	5		

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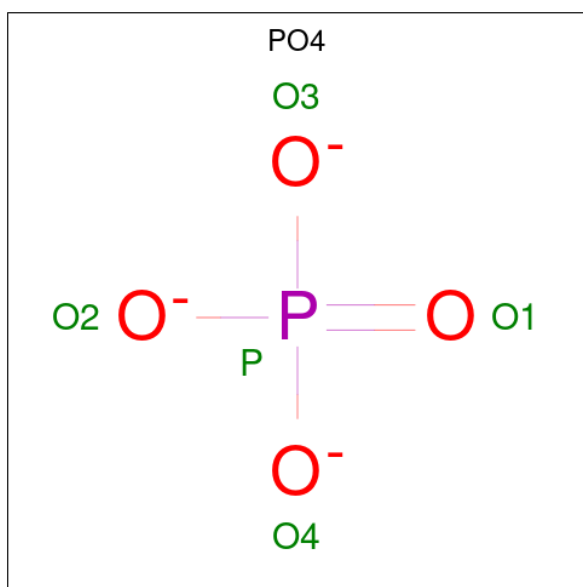
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	8	4		
3	A	1	Total	C	O	0	0
			15	10	5		
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C	O	0	0
			13	11	2		
3	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			30	19	11		
4	A	1	Total	C	O	0	0
			31	20	11		
4	A	1	Total	C	O	0	0
			30	19	11		
4	A	1	Total	C	O	0	0
			29	18	11		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

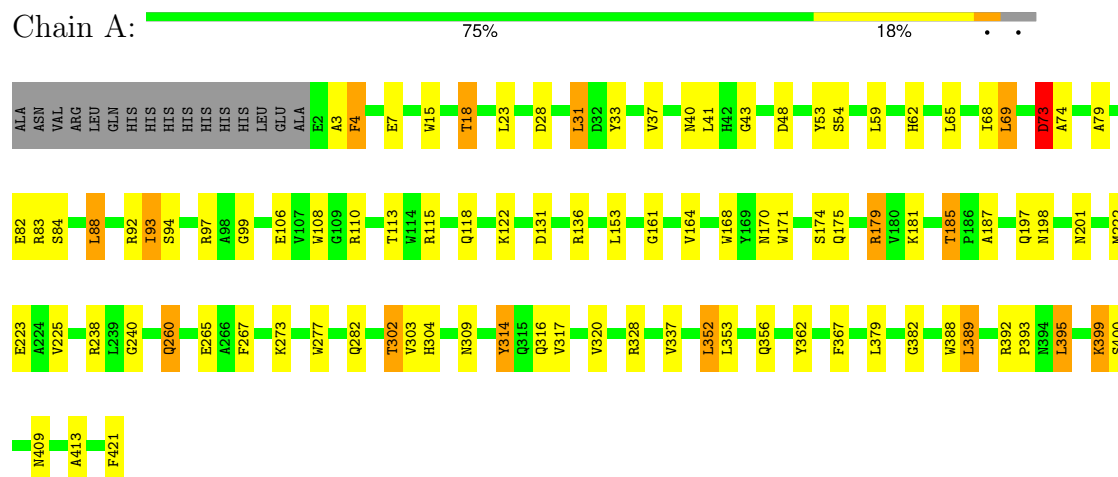
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		

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: Porin B



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.34Å 88.34Å 177.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.98-2.70) 96.5 (19.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.239 0.196 , 0.239	Depositor DCC
R_{free} test set	2007 reflections (8.85%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: C8E, DMU, BGC, PO4

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	0.50	0/3398	0.85	4/4609 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	328	ARG	CA-C-N	5.82	125.92	119.87
1	A	328	ARG	C-N-CA	5.82	125.92	119.87
1	A	198	ASN	CA-C-N	5.23	125.54	119.47
1	A	198	ASN	C-N-CA	5.23	125.54	119.47

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	3309	0	3085	55	0
2	A	12	0	12	4	0
3	A	104	0	156	7	0
4	A	120	0	132	2	0
5	A	5	0	0	0	0
6	A	47	0	0	0	0
All	All	3597	0	3385	58	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 8.

All (58) 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:185:THR:HG22	1:A:187:ALA:H	1.46	0.80
1:A:33:TYR:OH	1:A:53:TYR:OH	2.02	0.78
1:A:170:ASN:HB2	2:A:501:BGC:H6C1	1.66	0.77
1:A:106:GLU:O	2:A:501:BGC:O2	1.99	0.77
1:A:115:ARG:NH2	1:A:201:ASN:O	2.19	0.75
1:A:68:ILE:HG22	1:A:69:LEU:HD13	1.71	0.73
1:A:302:THR:HG23	1:A:304:HIS:NE2	2.08	0.68
1:A:395:LEU:HD12	3:A:503:C8E:H62	1.75	0.68
1:A:131:ASP:HB3	1:A:181:LYS:HB3	1.75	0.67
1:A:41:LEU:HD11	1:A:413:ALA:HB2	1.78	0.65
1:A:110:ARG:O	1:A:115:ARG:NH1	2.29	0.65
1:A:83:ARG:HH12	2:A:501:BGC:H2	1.63	0.63
1:A:382:GLY:HA2	1:A:392:ARG:HB3	1.82	0.62
1:A:28:ASP:HB3	1:A:62:HIS:HB3	1.84	0.59
1:A:65:LEU:HD22	1:A:69:LEU:HD22	1.84	0.58
1:A:260:GLN:HG2	1:A:267:PHE:CE2	2.40	0.57
1:A:48:ASP:OD1	1:A:92:ARG:NH1	2.39	0.56
1:A:223:GLU:OE2	1:A:238:ARG:HD3	2.06	0.55
1:A:302:THR:HG22	1:A:314:TYR:HB3	1.89	0.55
1:A:108:TRP:O	2:A:501:BGC:O2	2.23	0.55
1:A:79:ALA:HB3	1:A:118:GLN:HB2	1.89	0.54
1:A:15:TRP:O	1:A:18:THR:HG23	2.09	0.53
1:A:185:THR:CG2	1:A:187:ALA:H	2.20	0.53
1:A:302:THR:HB	1:A:314:TYR:HD1	1.73	0.53
1:A:379:LEU:HG	3:A:503:C8E:H82	1.90	0.53
1:A:37:VAL:HG22	1:A:53:TYR:HD1	1.74	0.53
1:A:94:SER:HB3	1:A:99:GLY:HA2	1.92	0.51
3:A:507:C8E:H72	4:A:513:DMU:H15	1.91	0.51
1:A:282:GLN:HB3	3:A:509:C8E:H192	1.93	0.51
1:A:240:GLY:HA3	1:A:277:TRP:CE2	2.47	0.50
1:A:161:GLY:HA2	1:A:168:TRP:CD1	2.47	0.50
3:A:507:C8E:H62	3:A:508:C8E:H71	1.94	0.49
1:A:222:MSE:HE2	3:A:502:C8E:H61	1.96	0.48
1:A:131:ASP:OD1	1:A:179:ARG:NH2	2.45	0.47
1:A:392:ARG:HA	1:A:393:PRO:HD2	1.82	0.46
1:A:136:ARG:HA	1:A:175:GLN:O	2.16	0.46
1:A:185:THR:HG22	1:A:187:ALA:N	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:HG22	1:A:238:ARG:HG2	1.98	0.45
1:A:48:ASP:O	1:A:92:ARG:HD2	2.17	0.45
1:A:161:GLY:HA3	1:A:170:ASN:HD21	1.82	0.44
1:A:31:LEU:HD13	1:A:421:PHE:CD2	2.52	0.44
1:A:362:TYR:HA	1:A:367:PHE:CD2	2.53	0.44
1:A:40:ASN:N	1:A:88:LEU:HD11	2.33	0.43
1:A:273:LYS:NZ	1:A:309:ASN:OD1	2.52	0.42
1:A:171:TRP:CD1	1:A:171:TRP:C	2.97	0.42
1:A:240:GLY:HA3	1:A:277:TRP:CZ2	2.54	0.42
1:A:74:ALA:HA	1:A:122:LYS:O	2.19	0.42
1:A:352:LEU:O	1:A:356:GLN:HG2	2.20	0.42
1:A:43:GLY:HA3	1:A:409:ASN:O	2.20	0.41
1:A:302:THR:CG2	1:A:314:TYR:HB3	2.49	0.41
1:A:388:TRP:CE3	1:A:389:LEU:HB2	2.55	0.41
1:A:161:GLY:HA3	1:A:170:ASN:ND2	2.35	0.41
1:A:73:ASP:OD1	1:A:73:ASP:N	2.54	0.41
1:A:136:ARG:HB3	1:A:174:SER:HB2	2.03	0.40
4:A:513:DMU:H35	4:A:513:DMU:H30	2.03	0.40
1:A:393:PRO:HB2	3:A:503:C8E:H52	2.04	0.40
1:A:88:LEU:HD13	1:A:93:ILE:HD11	2.04	0.40
1:A:399:LYS:HE3	1:A:400:SER:OG	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	418/436 (96%)	398 (95%)	17 (4%)	3 (1%)	18	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	4	PHE
1	A	73	ASP

5.3.2 Protein sidechains [i](#)

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	337/352 (96%)	303 (90%)	34 (10%)	7 18

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	7	GLU
1	A	18	THR
1	A	23	LEU
1	A	31	LEU
1	A	54	SER
1	A	59	LEU
1	A	69	LEU
1	A	73	ASP
1	A	82	GLU
1	A	84	SER
1	A	88	LEU
1	A	93	ILE
1	A	97	ARG
1	A	113	THR
1	A	153	LEU
1	A	164	VAL
1	A	179	ARG
1	A	185	THR
1	A	197	GLN
1	A	260	GLN
1	A	265	GLU
1	A	302	THR
1	A	303	VAL

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Mol	Chain	Res	Type
1	A	314	TYR
1	A	316	GLN
1	A	317	VAL
1	A	320	VAL
1	A	337	VAL
1	A	352	LEU
1	A	353	LEU
1	A	389	LEU
1	A	395	LEU
1	A	399	LYS

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	175	GLN
1	A	197	GLN
1	A	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
3	C8E	A	507	-	9,9,20	0.29	0	8,8,19	0.46	0
3	C8E	A	508	-	12,12,20	0.47	0	11,11,19	0.38	0
3	C8E	A	509	-	8,8,20	0.47	0	7,7,19	0.35	0
4	DMU	A	513	-	30,30,34	2.33	11 (36%)	41,41,45	1.67	7 (17%)
5	PO4	A	514	-	4,4,4	0.90	0	6,6,6	0.50	0
3	C8E	A	502	-	11,11,20	0.31	0	10,10,19	0.49	0
3	C8E	A	506	-	11,11,20	0.34	0	10,10,19	0.40	0
3	C8E	A	503	-	20,20,20	0.47	0	19,19,19	0.40	0
4	DMU	A	510	-	31,31,34	2.34	10 (32%)	42,42,45	1.56	6 (14%)
4	DMU	A	511	-	32,32,34	2.20	9 (28%)	43,43,45	1.96	9 (20%)
2	BGC	A	501	-	12,12,12	2.63	5 (41%)	17,17,17	1.13	2 (11%)
3	C8E	A	504	-	11,11,20	0.49	0	10,10,19	0.23	0
4	DMU	A	512	-	31,31,34	2.26	11 (35%)	42,42,45	1.71	8 (19%)
3	C8E	A	505	-	14,14,20	0.47	0	13,13,19	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	C8E	A	507	-	-	5/7/7/18	-
3	C8E	A	508	-	-	5/10/10/18	-
3	C8E	A	509	-	-	3/6/6/18	-
4	DMU	A	513	-	-	6/15/55/59	0/2/2/2
3	C8E	A	502	-	-	6/9/9/18	-
3	C8E	A	506	-	-	3/9/9/18	-
3	C8E	A	503	-	-	13/18/18/18	-
4	DMU	A	510	-	-	4/16/56/59	0/2/2/2
4	DMU	A	511	-	-	7/17/57/59	0/2/2/2
2	BGC	A	501	-	-	2/2/22/22	0/1/1/1
3	C8E	A	504	-	-	7/9/9/18	-
4	DMU	A	512	-	-	4/16/56/59	0/2/2/2
3	C8E	A	505	-	-	5/12/12/18	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	511	DMU	C11-C9	-5.79	1.32	1.51
4	A	510	DMU	C11-C9	-5.66	1.32	1.51
4	A	513	DMU	C11-C9	-5.61	1.33	1.51
4	A	512	DMU	C11-C9	-5.60	1.33	1.51
4	A	513	DMU	C57-C4	-4.78	1.35	1.51
4	A	510	DMU	C57-C4	-4.77	1.35	1.51
4	A	511	DMU	C57-C4	-4.73	1.35	1.51
4	A	513	DMU	O1-C9	4.70	1.55	1.44
4	A	512	DMU	C57-C4	-4.68	1.36	1.51
2	A	501	BGC	C6-C5	-4.66	1.36	1.51
2	A	501	BGC	C3-C2	-4.63	1.40	1.52
4	A	510	DMU	O5-C4	4.62	1.55	1.44
4	A	512	DMU	O5-C4	4.44	1.55	1.44
4	A	511	DMU	O5-C4	4.31	1.54	1.44
4	A	510	DMU	O1-C9	4.27	1.54	1.44
4	A	512	DMU	O1-C9	4.16	1.54	1.44
4	A	513	DMU	O5-C4	4.13	1.54	1.44
4	A	511	DMU	O1-C9	3.97	1.54	1.44
4	A	510	DMU	C7-C5	-3.71	1.42	1.52
2	A	501	BGC	O5-C5	3.55	1.53	1.44
4	A	511	DMU	C7-C5	-3.48	1.43	1.52
4	A	510	DMU	C2-C1	-3.45	1.43	1.52
4	A	513	DMU	C7-C5	-3.43	1.43	1.52
2	A	501	BGC	C1-C2	-3.39	1.44	1.52
4	A	512	DMU	C7-C5	-3.36	1.43	1.52
4	A	512	DMU	C2-C1	-3.16	1.44	1.52
4	A	513	DMU	C2-C1	-2.94	1.44	1.52
4	A	511	DMU	C2-C1	-2.78	1.45	1.52
4	A	510	DMU	C6-C1	-2.64	1.44	1.52
4	A	511	DMU	O49-C1	2.61	1.49	1.43
4	A	513	DMU	C6-C1	-2.59	1.44	1.52
4	A	513	DMU	O49-C1	2.51	1.49	1.43
4	A	512	DMU	C6-C1	-2.40	1.45	1.52
4	A	513	DMU	C8-C9	2.39	1.58	1.53
4	A	511	DMU	O16-C6	2.30	1.44	1.40
4	A	512	DMU	O49-C1	2.29	1.48	1.43
2	A	501	BGC	C4-C3	-2.23	1.46	1.52
4	A	510	DMU	O49-C1	2.19	1.48	1.43
4	A	510	DMU	O3-C5	2.17	1.48	1.43
4	A	510	DMU	O16-C6	2.09	1.43	1.40
4	A	512	DMU	O3-C5	2.08	1.48	1.43
4	A	513	DMU	C10-C5	-2.07	1.46	1.52
4	A	513	DMU	O3-C5	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	512	DMU	O16-C6	2.02	1.43	1.40
4	A	511	DMU	C6-C1	-2.02	1.46	1.52
4	A	512	DMU	C8-C9	2.02	1.57	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	511	DMU	C10-O1-C9	5.49	124.44	113.72
4	A	510	DMU	C10-O1-C9	5.34	124.14	113.72
4	A	511	DMU	C1-C2-C3	5.12	121.31	109.68
4	A	512	DMU	C18-O16-C6	5.08	122.36	113.68
4	A	512	DMU	C10-O1-C9	4.91	123.31	113.72
4	A	513	DMU	C10-O1-C9	4.71	122.93	113.72
4	A	513	DMU	C18-O16-C6	4.27	120.97	113.68
4	A	511	DMU	C6-C1-C2	4.06	118.55	110.01
4	A	513	DMU	C7-C8-C9	3.83	117.18	110.23
4	A	511	DMU	C10-C5-C7	3.72	117.84	110.01
4	A	510	DMU	C18-O16-C6	3.48	119.62	113.68
4	A	513	DMU	C1-C2-C3	3.37	117.33	109.68
4	A	511	DMU	O16-C6-C1	3.21	113.15	108.27
4	A	510	DMU	O1-C10-C5	3.12	116.79	110.37
4	A	511	DMU	C18-O16-C6	2.85	118.56	113.68
4	A	511	DMU	O1-C10-C5	2.82	116.16	110.37
4	A	512	DMU	C1-C2-C3	2.72	115.85	109.68
4	A	510	DMU	O16-C18-C19	2.65	118.36	109.37
4	A	512	DMU	C7-C8-C9	2.61	114.96	110.23
4	A	511	DMU	O16-C18-C19	2.50	117.83	109.37
2	A	501	BGC	O6-C6-C5	2.47	119.75	111.33
4	A	512	DMU	O16-C18-C19	2.39	117.47	109.37
4	A	513	DMU	C6-O5-C4	2.33	118.27	113.72
4	A	513	DMU	C8-C7-C5	2.27	114.82	110.83
4	A	511	DMU	O7-C10-C5	2.19	113.47	108.09
4	A	512	DMU	O7-C10-C5	2.18	113.44	108.09
4	A	510	DMU	C6-O5-C4	2.16	117.94	113.72
4	A	513	DMU	C6-C1-C2	2.12	114.47	110.01
4	A	512	DMU	O1-C10-C5	2.11	114.70	110.37
4	A	512	DMU	O7-C10-O1	-2.07	105.24	110.69
2	A	501	BGC	O5-C5-C4	-2.04	106.02	109.70
4	A	510	DMU	O16-C6-C1	2.00	111.32	108.27

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	DMU	O1-C10-O7-C3
4	A	510	DMU	O1-C10-O7-C3
4	A	511	DMU	O5-C6-O16-C18
4	A	511	DMU	O5-C4-C57-O61
4	A	511	DMU	C1-C6-O16-C18
3	A	504	C8E	O12-C13-C14-O15
3	A	504	C8E	O18-C19-C20-O21
4	A	511	DMU	C3-C4-C57-O61
3	A	502	C8E	C6-C7-C8-O9
4	A	511	DMU	O16-C18-C19-C22
3	A	504	C8E	O15-C16-C17-O18
3	A	503	C8E	O12-C13-C14-O15
3	A	505	C8E	O18-C19-C20-O21
3	A	505	C8E	O12-C13-C14-O15
3	A	502	C8E	C4-C5-C6-C7
3	A	503	C8E	C2-C3-C4-C5
3	A	507	C8E	C2-C3-C4-C5
4	A	513	DMU	C19-C22-C25-C28
3	A	507	C8E	C6-C7-C8-O9
3	A	503	C8E	C6-C7-C8-O9
3	A	509	C8E	O15-C16-C17-O18
3	A	506	C8E	C3-C4-C5-C6
3	A	507	C8E	C4-C5-C6-C7
3	A	506	C8E	C5-C6-C7-C8
3	A	502	C8E	C2-C3-C4-C5
3	A	503	C8E	C3-C4-C5-C6
4	A	512	DMU	C18-C19-C22-C25
4	A	513	DMU	O1-C10-O7-C3
3	A	508	C8E	C4-C5-C6-C7
3	A	503	C8E	O18-C19-C20-O21
3	A	508	C8E	C3-C4-C5-C6
3	A	502	C8E	C3-C4-C5-C6
3	A	508	C8E	C6-C7-C8-O9
4	A	510	DMU	O6-C11-C9-O1
4	A	513	DMU	O6-C11-C9-O1
4	A	512	DMU	O16-C18-C19-C22
3	A	507	C8E	C3-C4-C5-C6
3	A	503	C8E	C1-C2-C3-C4
4	A	510	DMU	O16-C18-C19-C22
3	A	502	C8E	C1-C2-C3-C4
3	A	508	C8E	C2-C3-C4-C5
3	A	504	C8E	C13-C14-O15-C16
3	A	503	C8E	C17-C16-O15-C14

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Mol	Chain	Res	Type	Atoms
3	A	503	C8E	C13-C14-O15-C16
3	A	503	C8E	C16-C17-O18-C19
3	A	504	C8E	C14-C13-O12-C11
3	A	502	C8E	O9-C10-C11-O12
3	A	503	C8E	C4-C5-C6-C7
4	A	513	DMU	C5-C10-O7-C3
4	A	512	DMU	C25-C28-C31-C34
4	A	510	DMU	C19-C22-C25-C28
3	A	503	C8E	C7-C8-O9-C10
3	A	509	C8E	C16-C17-O18-C19
2	A	501	BGC	C4-C5-C6-O6
3	A	508	C8E	C7-C8-O9-C10
2	A	501	BGC	O5-C5-C6-O6
4	A	511	DMU	C28-C31-C34-C37
3	A	504	C8E	C10-C11-O12-C13
3	A	505	C8E	C7-C8-O9-C10
3	A	507	C8E	C7-C8-O9-C10
3	A	506	C8E	C2-C3-C4-C5
3	A	509	C8E	O18-C19-C20-O21
3	A	505	C8E	C13-C14-O15-C16
4	A	513	DMU	C1-C6-O16-C18
3	A	503	C8E	C10-C11-O12-C13
3	A	503	C8E	O15-C16-C17-O18
4	A	512	DMU	C19-C22-C25-C28
3	A	504	C8E	C20-C19-O18-C17
4	A	513	DMU	O5-C6-O16-C18
3	A	505	C8E	C16-C17-O18-C19

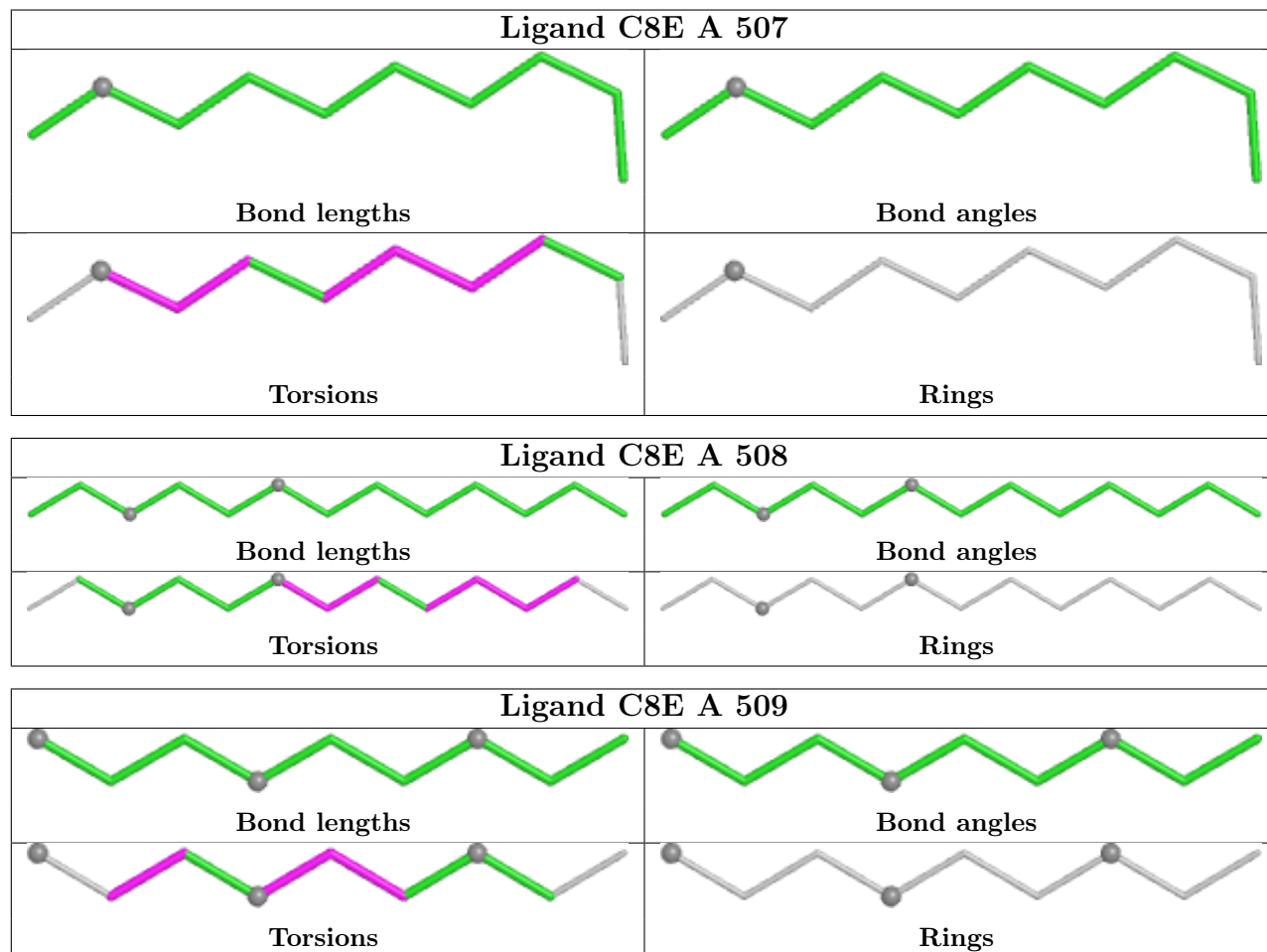
There are no ring outliers.

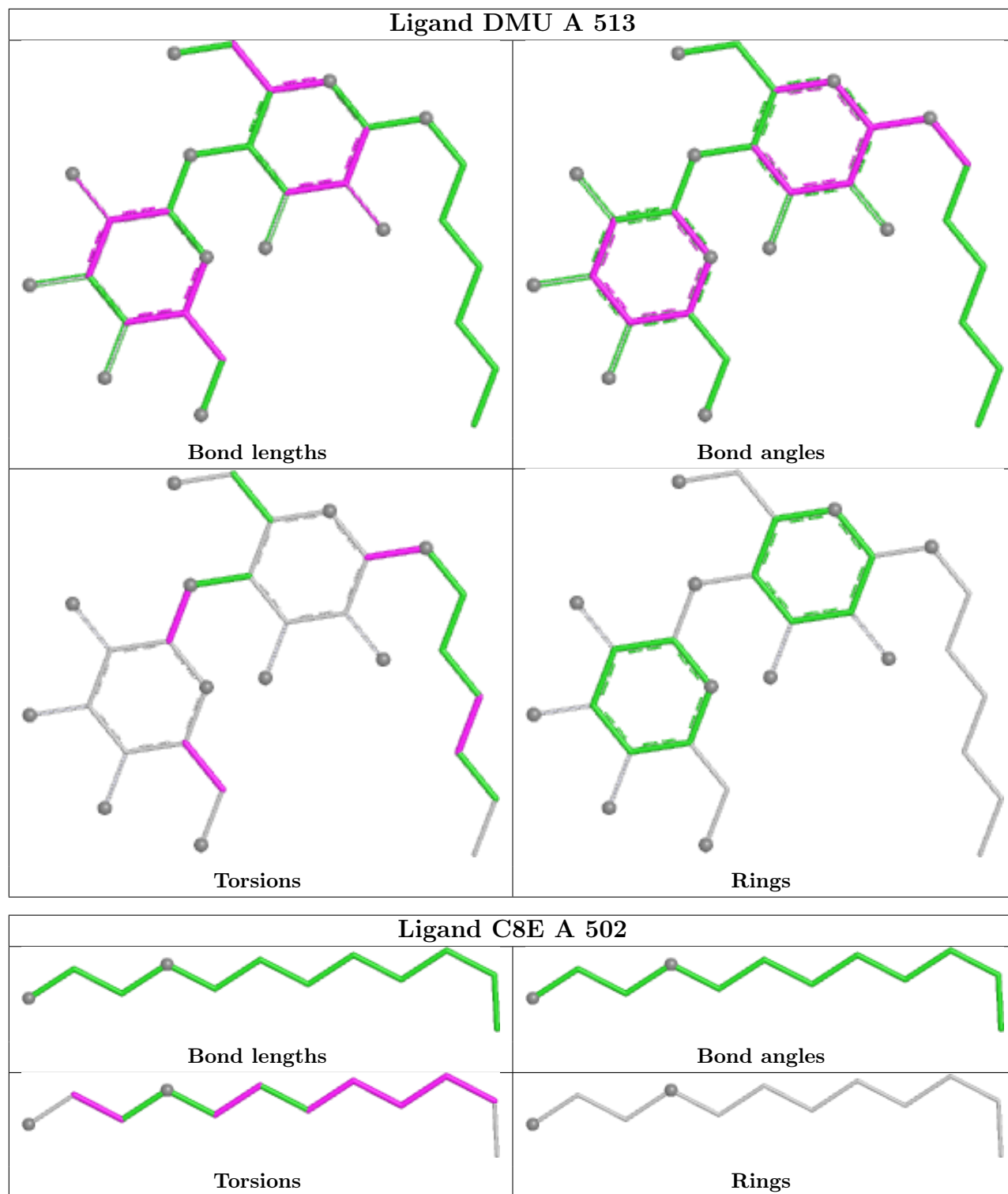
7 monomers are involved in 12 short contacts:

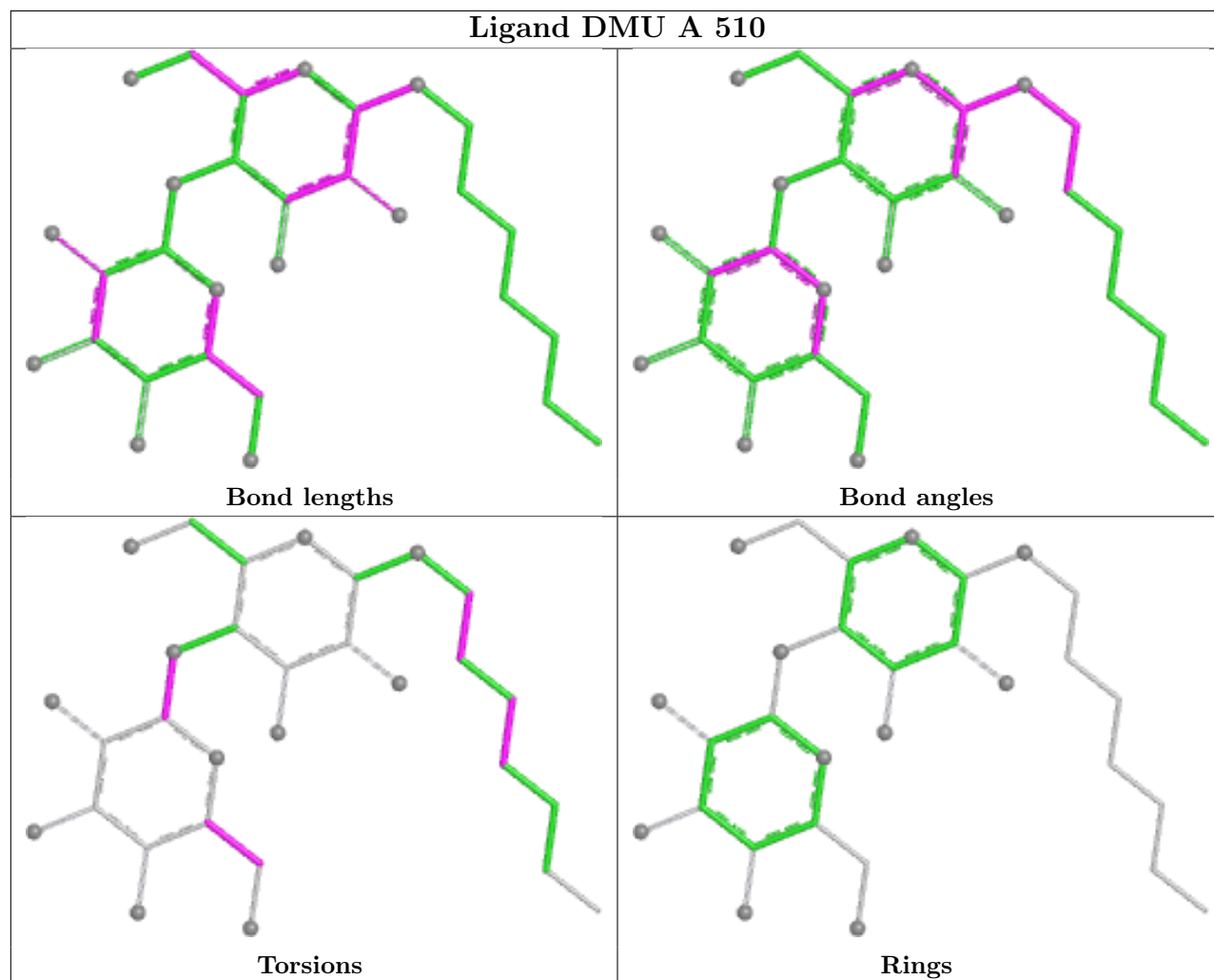
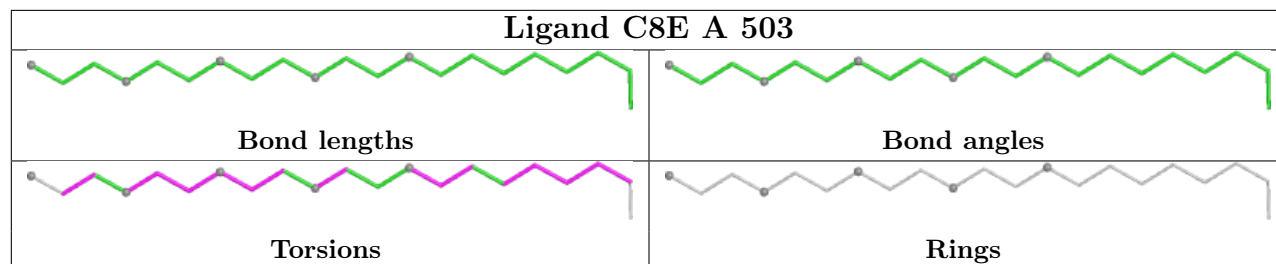
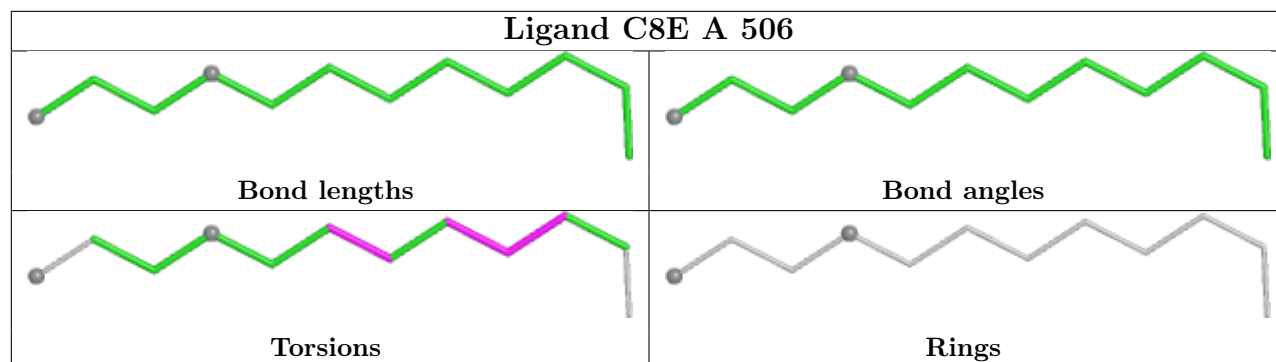
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	C8E	2	0
3	A	508	C8E	1	0
3	A	509	C8E	1	0
4	A	513	DMU	2	0
3	A	502	C8E	1	0
3	A	503	C8E	3	0
2	A	501	BGC	4	0

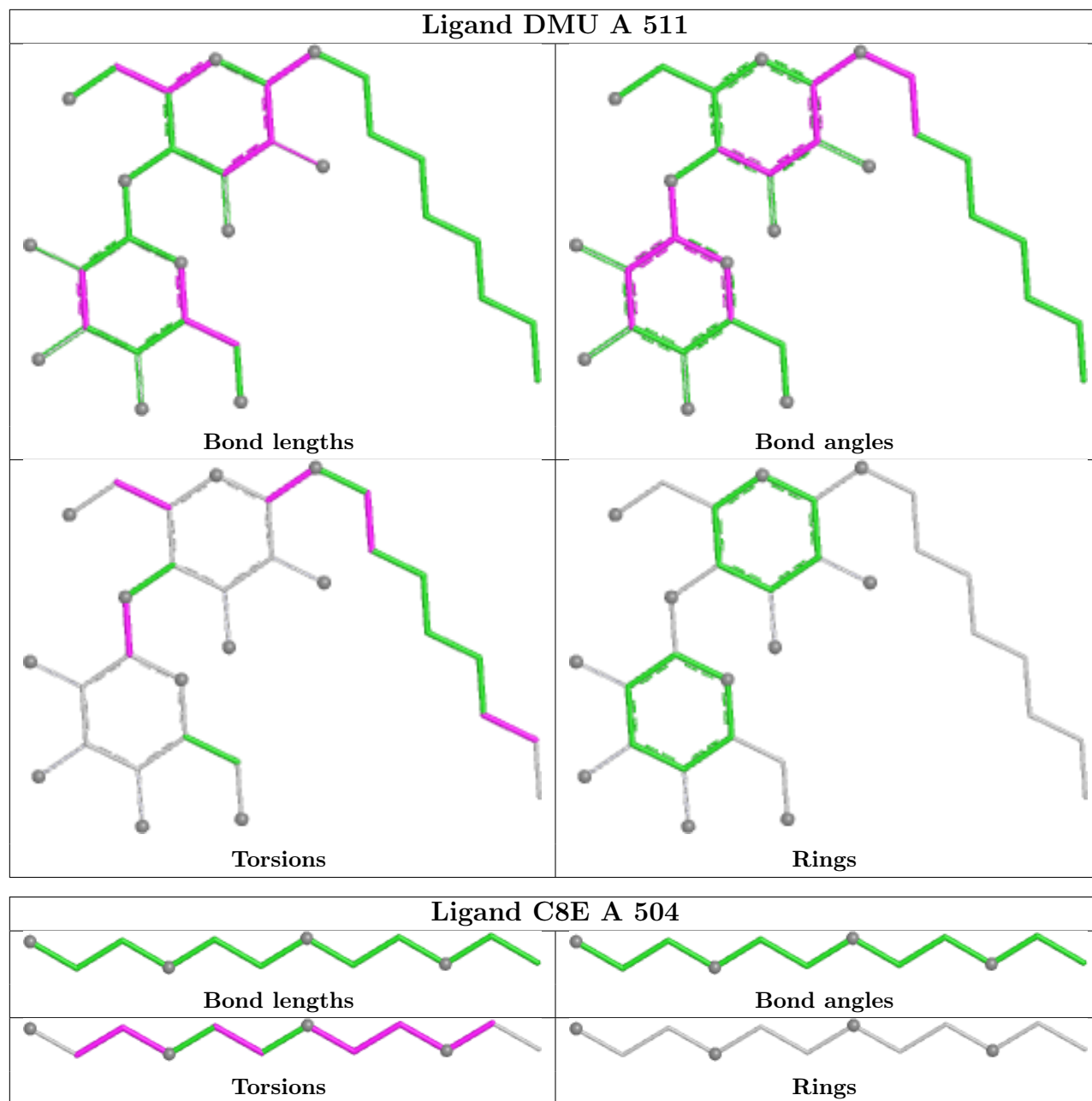
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

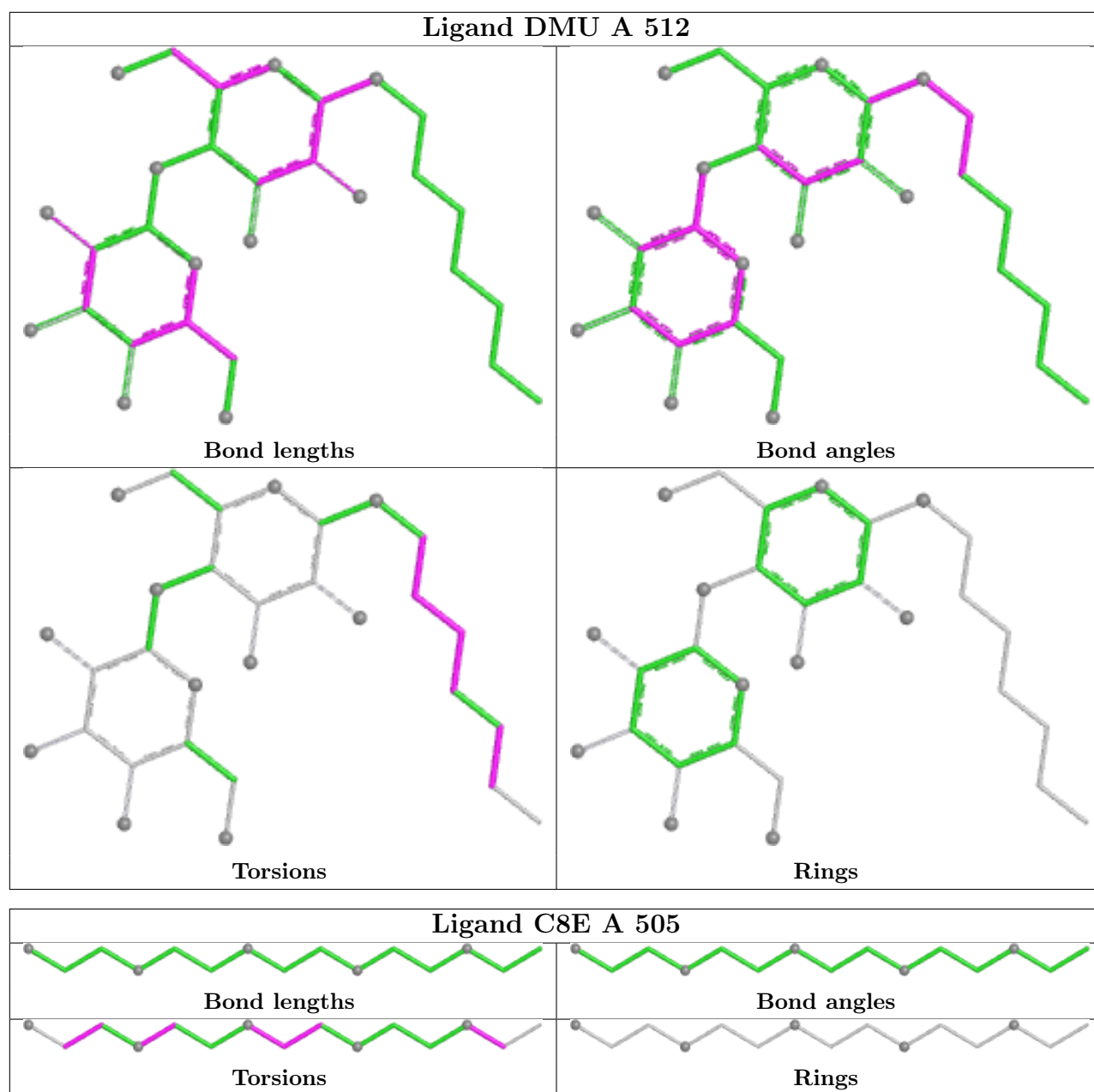
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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 [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	416/436 (95%)	-0.63	0 100 100	22, 35, 55, 65	0

There are no RSRZ outliers to report.

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](#)

There are no oligosaccharides in this entry.

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
3	C8E	A	508	13/21	0.68	0.23	40,70,73,73	0
3	C8E	A	507	10/21	0.72	0.17	44,51,59,63	0
5	PO4	A	514	5/5	0.73	0.13	106,108,110,111	0
3	C8E	A	504	12/21	0.74	0.18	66,76,87,88	0
3	C8E	A	503	21/21	0.76	0.18	50,67,79,80	0
2	BGC	A	501	12/12	0.80	0.24	48,55,61,71	12
4	DMU	A	510	30/33	0.81	0.11	43,57,85,92	0
3	C8E	A	505	15/21	0.82	0.14	50,62,89,90	0
4	DMU	A	512	30/33	0.83	0.10	38,66,91,95	0

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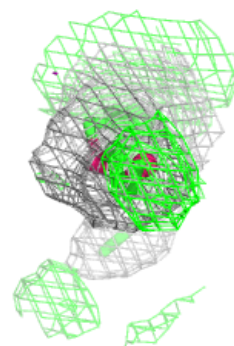
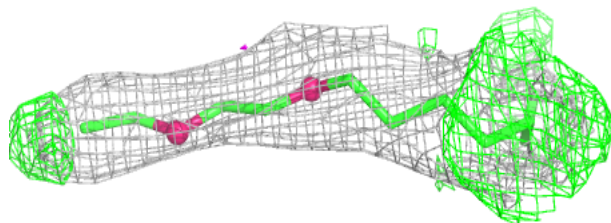
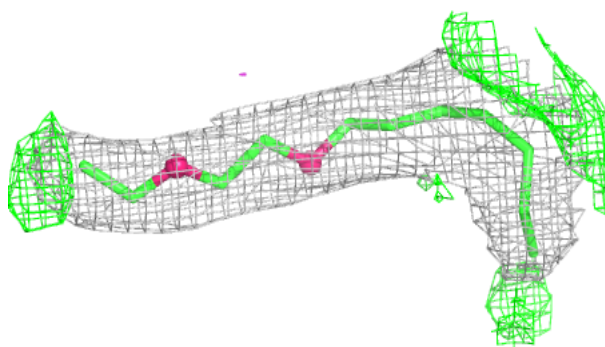
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C8E	A	509	9/21	0.85	0.17	47,50,69,70	0
4	DMU	A	513	29/33	0.85	0.12	43,69,110,113	0
3	C8E	A	506	12/21	0.85	0.17	54,60,67,72	0
4	DMU	A	511	31/33	0.90	0.10	31,53,64,69	0
3	C8E	A	502	12/21	0.93	0.10	34,43,52,55	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.

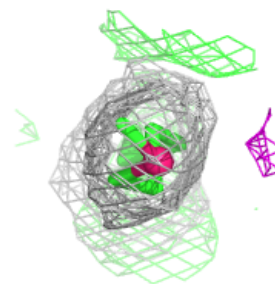
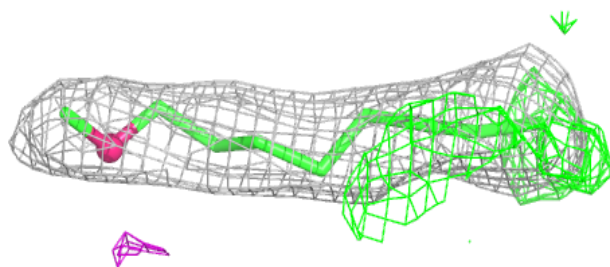
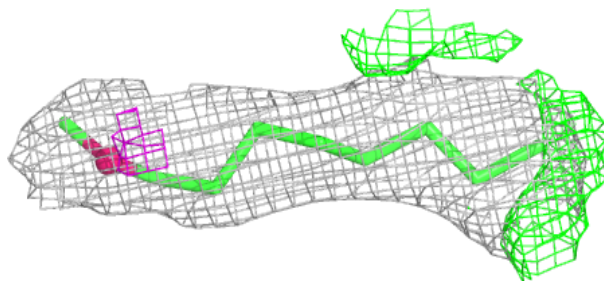
Electron density around C8E A 508:

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

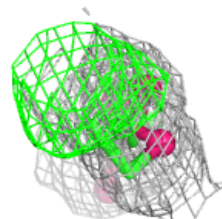
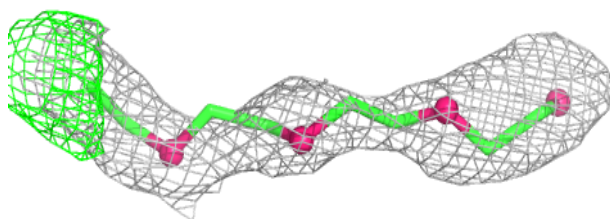
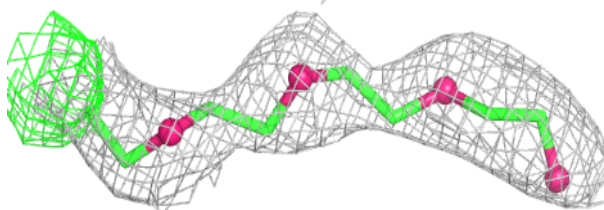


Electron density around C8E A 507:

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

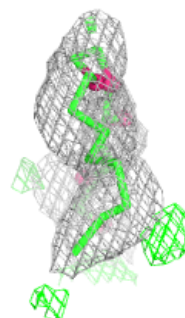
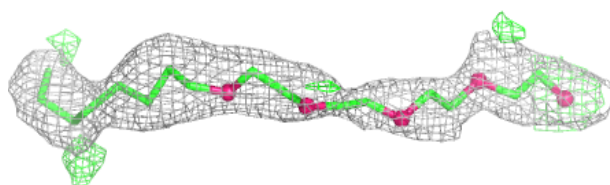
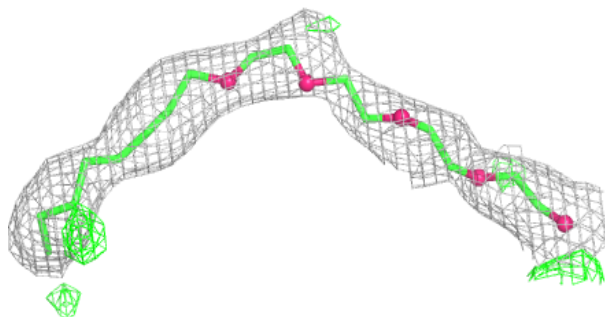
**Electron density around C8E A 504:**

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

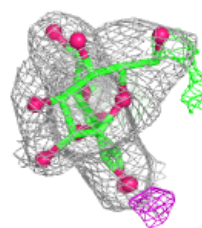
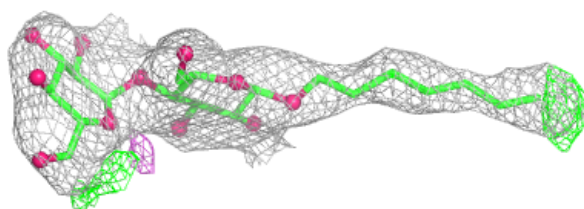
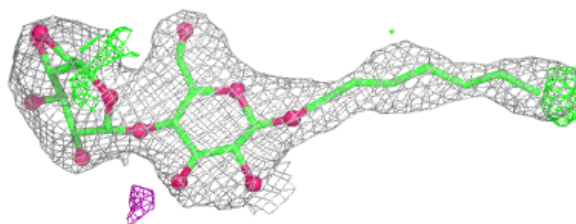


Electron density around C8E A 503:

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

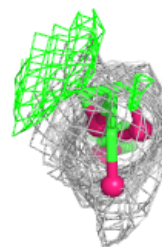
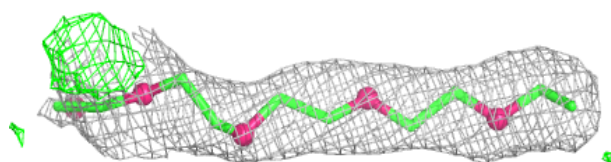
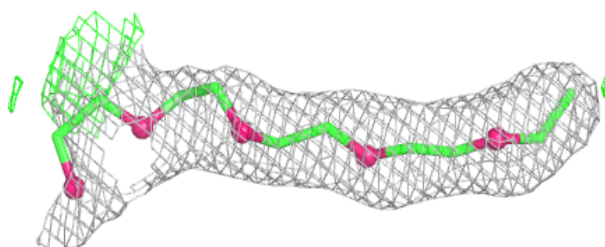
**Electron density around DMU A 510:**

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

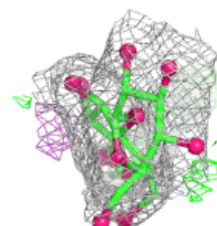
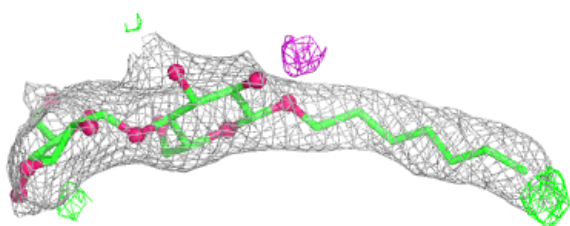
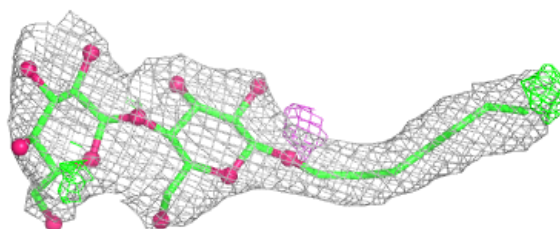


Electron density around C8E A 505:

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

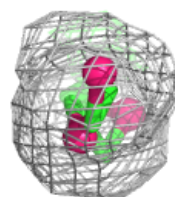
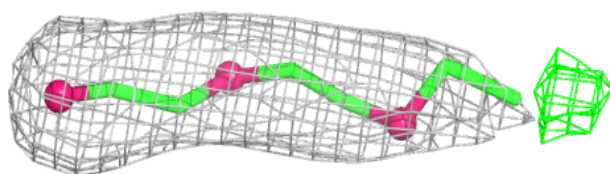
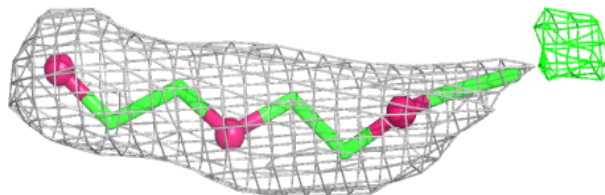
**Electron density around DMU A 512:**

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

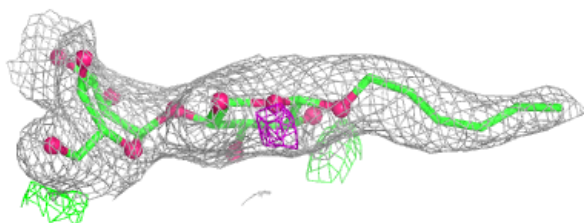
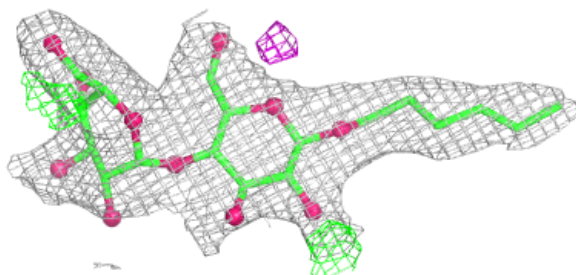


Electron density around C8E A 509:

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

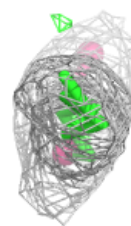
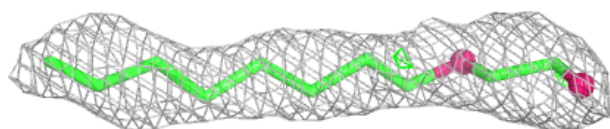
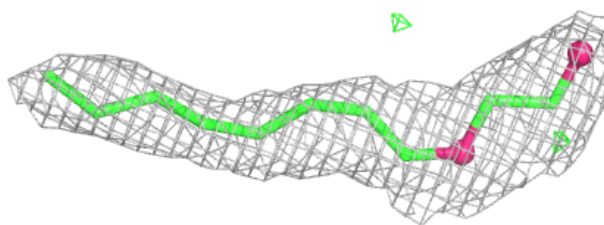
**Electron density around DMU A 513:**

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

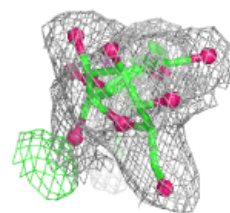
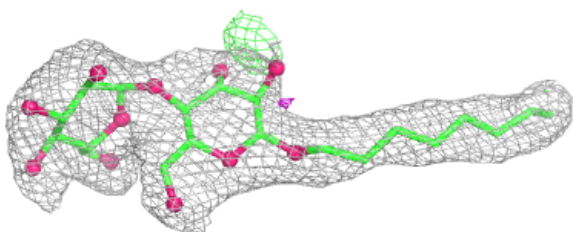
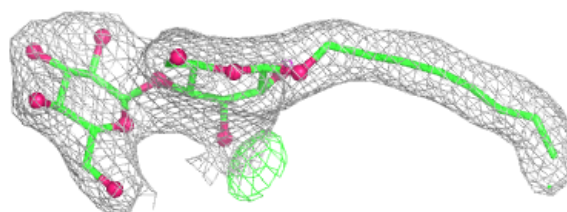


Electron density around C8E A 506:

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

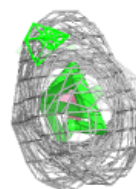
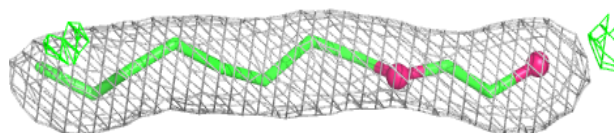
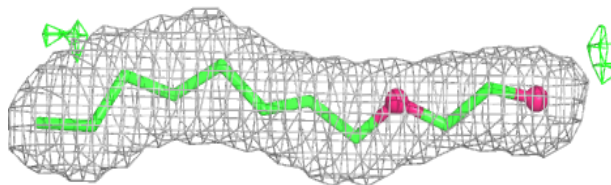
**Electron density around DMU A 511:**

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



Electron density around C8E A 502:

$2mF_o-DF_c$ (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.