



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:33 PM UTC

PDB ID : 6D0J / pdb_00006d0j
Title : Crystal structure of a CLC-type fluoride/proton antiporter
Authors : Last, N.B.; Stockbridge, R.B.; Wilson, A.E.; Shane, T.; Kolmakova-Partensky, L.; Koide, A.; Koide, S.; Miller, C.
Deposited on : 2018-04-10
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

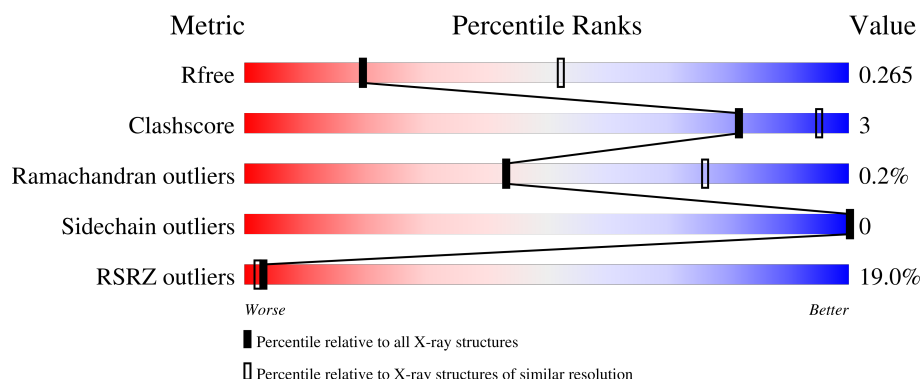
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	421	19% 87% 7% 6%
1	B	421	18% 87% 7% 6%
2	C	93	14% 90% 6% .
2	D	93	18% 88% . 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F	B	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7611 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 CLC-type fluoride/proton antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3022	2031	467	513	11			
1	B	396	Total	C	N	O	S	0	0	0
			3033	2037	471	514	11			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP C9CPP6
A	-1	ALA	-	expression tag	UNP C9CPP6
A	0	ALA	-	expression tag	UNP C9CPP6
A	1	ALA	-	expression tag	UNP C9CPP6
A	4	ILE	MET	engineered mutation	UNP C9CPP6
A	407	THR	-	expression tag	UNP C9CPP6
A	408	ARG	-	expression tag	UNP C9CPP6
A	409	GLY	-	expression tag	UNP C9CPP6
A	410	SER	-	expression tag	UNP C9CPP6
A	411	GLY	-	expression tag	UNP C9CPP6
A	412	GLY	-	expression tag	UNP C9CPP6
A	413	HIS	-	expression tag	UNP C9CPP6
A	414	HIS	-	expression tag	UNP C9CPP6
A	415	HIS	-	expression tag	UNP C9CPP6
A	416	HIS	-	expression tag	UNP C9CPP6
A	417	HIS	-	expression tag	UNP C9CPP6
A	418	HIS	-	expression tag	UNP C9CPP6
B	-2	MET	-	expression tag	UNP C9CPP6
B	-1	ALA	-	expression tag	UNP C9CPP6
B	0	ALA	-	expression tag	UNP C9CPP6
B	1	ALA	-	expression tag	UNP C9CPP6
B	4	ILE	MET	engineered mutation	UNP C9CPP6
B	407	THR	-	expression tag	UNP C9CPP6
B	408	ARG	-	expression tag	UNP C9CPP6
B	409	GLY	-	expression tag	UNP C9CPP6

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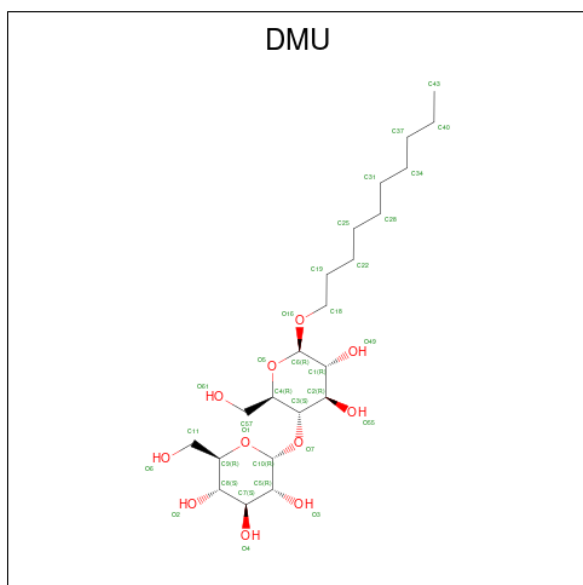
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Chain	Residue	Modelled	Actual	Comment	Reference
B	410	SER	-	expression tag	UNP C9CPP6
B	411	GLY	-	expression tag	UNP C9CPP6
B	412	GLY	-	expression tag	UNP C9CPP6
B	413	HIS	-	expression tag	UNP C9CPP6
B	414	HIS	-	expression tag	UNP C9CPP6
B	415	HIS	-	expression tag	UNP C9CPP6
B	416	HIS	-	expression tag	UNP C9CPP6
B	417	HIS	-	expression tag	UNP C9CPP6
B	418	HIS	-	expression tag	UNP C9CPP6

- Molecule 2 is a protein called Monobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	86	Total	C	N	O	S	0	0	0
			653	418	100	134	1			
2	C	90	Total	C	N	O	S	0	0	0
			679	434	104	140	1			

- Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			33	22	11		
3	A	1	Total	C	O	0	0
			33	22	11		

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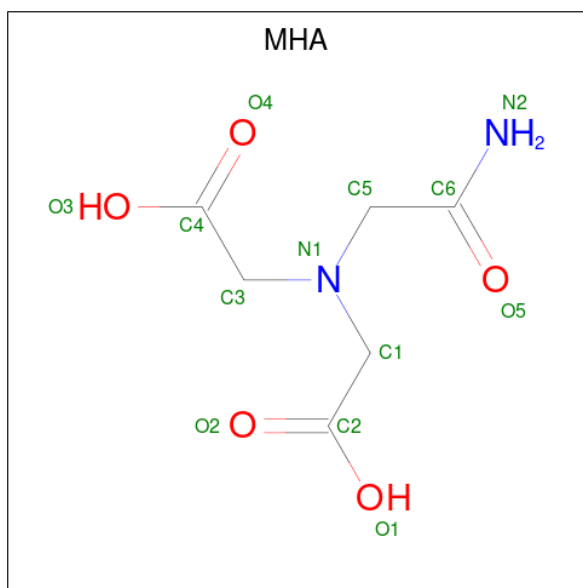
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			33	22	11		
3	A	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			26	15	11		

- Molecule 4 is FLUORIDE ION (CCD ID: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	F	0	0
			2	2		
4	B	2	Total	F	0	0
			2	2		

- Molecule 5 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (CCD ID: MHA) (formula: C₆H₁₀N₂O₅).



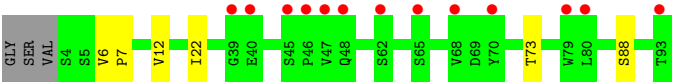
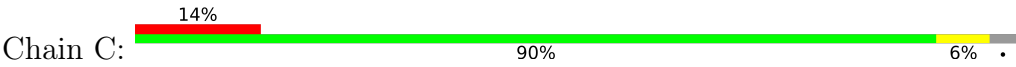
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			13	6	2	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	O 9	0	0
6	B	7	Total 7	O 7	0	0



● Molecule 2: Monobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.97Å 126.42Å 133.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 3.00 49.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.35-3.00) 99.3 (49.35-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.239 , 0.260 0.244 , 0.265	Depositor DCC
R_{free} test set	1965 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7611	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F, MHA, DMU

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	0.08	0/3102	0.24	0/4222
1	B	0.08	0/3113	0.24	0/4236
2	C	0.08	0/699	0.25	0/963
2	D	0.07	0/671	0.22	0/921
All	All	0.08	0/7585	0.24	0/10342

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 [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	3022	0	3137	17	0
1	B	3033	0	3153	17	0
2	C	679	0	648	3	0
2	D	653	0	618	3	0
3	A	132	0	168	1	0
3	B	59	0	67	0	0
4	A	2	0	0	1	0
4	B	2	0	0	2	0
5	C	13	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	9	0	0	0	0
6	B	7	0	0	1	0
All	All	7611	0	7799	39	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 3.

All (39) 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:101:VAL:HA	1:A:315:LEU:HD13	1.85	0.59
1:A:272:LEU:HD23	1:A:301:LEU:HD13	1.89	0.55
1:B:290:THR:HG23	1:B:292:GLN:HG3	1.90	0.54
1:A:104:GLY:HA3	1:A:315:LEU:HD12	1.90	0.53
1:B:272:LEU:HD23	1:B:301:LEU:HD13	1.91	0.53
1:B:118:GLU:N	4:B:503:F:F	2.33	0.51
1:A:347:LEU:HD13	1:A:382:VAL:HG21	1.92	0.51
1:B:71:TYR:O	6:B:601:HOH:O	2.20	0.49
1:B:117:ARG:N	4:B:503:F:F	2.35	0.49
1:A:296:SER:HA	1:A:332:VAL:HG21	1.95	0.49
1:A:290:THR:HG23	1:A:292:GLN:HG3	1.94	0.48
1:A:144:THR:O	1:A:148:ILE:HG12	2.15	0.47
1:B:101:VAL:HA	1:B:315:LEU:HD13	1.95	0.47
3:A:502:DMU:H8	3:A:502:DMU:H5	1.54	0.47
1:B:286:SER:O	1:B:290:THR:HG22	2.15	0.47
1:A:271:LEU:HG	2:D:80:LEU:HA	1.98	0.46
1:B:95:LEU:HD13	1:B:131:ARG:HG3	1.96	0.46
1:B:347:LEU:HD13	1:B:382:VAL:HG21	1.98	0.46
1:A:58:PRO:HD3	1:A:266:VAL:HG21	1.99	0.45
1:A:276:ARG:HH12	1:A:294:ILE:HG22	1.82	0.45
1:B:236:PHE:HD2	1:B:303:LEU:HG	1.81	0.45
1:A:46:ARG:HD3	1:A:109:HIS:O	2.18	0.43
2:D:44:ASN:OD1	2:D:44:ASN:N	2.51	0.43
1:B:97:LEU:HD23	1:B:127:THR:OG1	2.19	0.43
1:B:144:THR:O	1:B:148:ILE:HG12	2.19	0.42
1:B:296:SER:HA	1:B:332:VAL:HG21	2.02	0.42
2:D:39:GLY:HA3	2:D:47:VAL:HG12	2.00	0.42
2:C:12:VAL:HG22	2:C:22:ILE:HG22	2.02	0.42
2:C:6:VAL:HA	2:C:7:PRO:HA	1.89	0.41
1:A:276:ARG:NH2	1:A:298:ASP:OD2	2.52	0.41
1:A:27:LEU:HD12	1:A:132:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD13	1:A:131:ARG:HG3	2.02	0.41
1:A:391:LYS:HZ3	1:B:179:HIS:C	2.29	0.41
1:B:388:PHE:HA	1:B:391:LYS:HE3	2.03	0.41
1:A:117:ARG:N	4:A:505:F:F	2.44	0.41
1:B:27:LEU:HD12	1:B:132:LEU:HD11	2.03	0.41
1:B:33:THR:HG21	1:B:199:LEU:HB3	2.03	0.41
1:A:286:SER:O	1:A:290:THR:HG22	2.22	0.40
2:C:73:THR:HG23	2:C:88:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	393/421 (93%)	378 (96%)	14 (4%)	1 (0%)	36	70
1	B	394/421 (94%)	379 (96%)	14 (4%)	1 (0%)	36	70
2	C	88/93 (95%)	85 (97%)	3 (3%)	0	100	100
2	D	80/93 (86%)	77 (96%)	3 (4%)	0	100	100
All	All	955/1028 (93%)	919 (96%)	34 (4%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	B	9	THR

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	320/340 (94%)	320 (100%)	0	100	100
1	B	321/340 (94%)	321 (100%)	0	100	100
2	C	78/80 (98%)	78 (100%)	0	100	100
2	D	74/80 (92%)	74 (100%)	0	100	100
All	All	793/840 (94%)	793 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	ASN
1	B	77	GLN

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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	DMU	A	504	-	34,34,34	0.13	0	45,45,45	0.30	0
3	DMU	B	501	-	34,34,34	0.14	0	45,45,45	0.47	1 (2%)
3	DMU	A	501	-	34,34,34	0.13	0	45,45,45	0.43	0
3	DMU	A	503	-	34,34,34	0.14	0	45,45,45	0.46	0
3	DMU	A	502	-	34,34,34	0.12	0	45,45,45	0.39	0
5	MHA	C	101	-	12,12,12	1.58	4 (33%)	15,15,15	1.39	5 (33%)
3	DMU	B	502	-	27,27,34	0.12	0	38,38,45	0.18	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	DMU	A	504	-	-	5/19/59/59	0/2/2/2
3	DMU	B	501	-	-	1/19/59/59	0/2/2/2
3	DMU	A	501	-	-	7/19/59/59	0/2/2/2
3	DMU	A	503	-	-	5/19/59/59	0/2/2/2
3	DMU	A	502	-	-	2/19/59/59	0/2/2/2
5	MHA	C	101	-	-	6/12/12/12	-
3	DMU	B	502	-	-	2/12/52/59	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	101	MHA	O2-C2	2.78	1.31	1.22
5	C	101	MHA	O4-C4	2.76	1.31	1.22
5	C	101	MHA	O3-C4	-2.72	1.21	1.30
5	C	101	MHA	O1-C2	-2.68	1.21	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	101	MHA	C6-C5-N1	-2.74	109.41	114.42
5	C	101	MHA	O1-C2-C1	2.43	122.96	113.38
5	C	101	MHA	O3-C4-C3	2.40	122.86	113.38
5	C	101	MHA	O2-C2-C1	-2.15	113.40	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	101	MHA	O4-C4-C3	-2.14	113.42	122.38
3	B	501	DMU	C6-O5-C4	2.03	117.69	113.72

There are no chirality outliers.

All (28) torsion outliers are listed below:

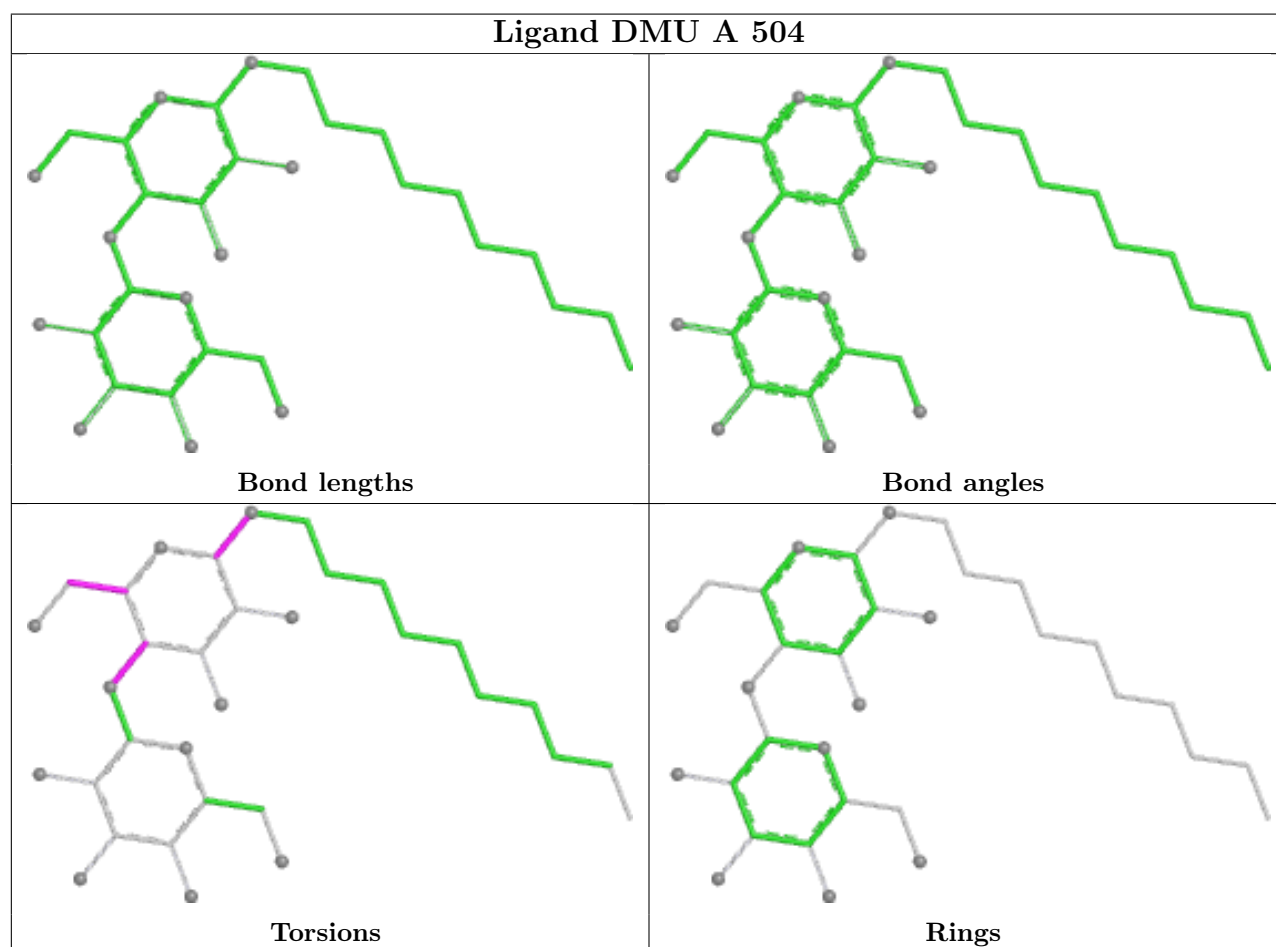
Mol	Chain	Res	Type	Atoms
3	A	502	DMU	C19-C18-O16-C6
3	A	504	DMU	O5-C6-O16-C18
5	C	101	MHA	C2-C1-N1-C3
5	C	101	MHA	N1-C1-C2-O1
5	C	101	MHA	N1-C1-C2-O2
5	C	101	MHA	N1-C5-C6-O5
3	A	501	DMU	O1-C10-O7-C3
5	C	101	MHA	N1-C5-C6-N2
3	A	501	DMU	C19-C18-O16-C6
3	B	502	DMU	C19-C18-O16-C6
3	A	504	DMU	C1-C6-O16-C18
3	A	503	DMU	O6-C11-C9-O1
3	B	502	DMU	O6-C11-C9-O1
3	A	502	DMU	O5-C4-C57-O61
3	A	504	DMU	O5-C4-C57-O61
3	A	501	DMU	O6-C11-C9-O1
3	A	501	DMU	C1-C6-O16-C18
3	A	501	DMU	C4-C3-O7-C10
3	A	501	DMU	C2-C3-O7-C10
3	A	503	DMU	C19-C18-O16-C6
3	B	501	DMU	C19-C18-O16-C6
5	C	101	MHA	C2-C1-N1-C5
3	A	504	DMU	C2-C3-O7-C10
3	A	503	DMU	C22-C25-C28-C31
3	A	504	DMU	C4-C3-O7-C10
3	A	503	DMU	C18-C19-C22-C25
3	A	501	DMU	O16-C18-C19-C22
3	A	503	DMU	C31-C34-C37-C40

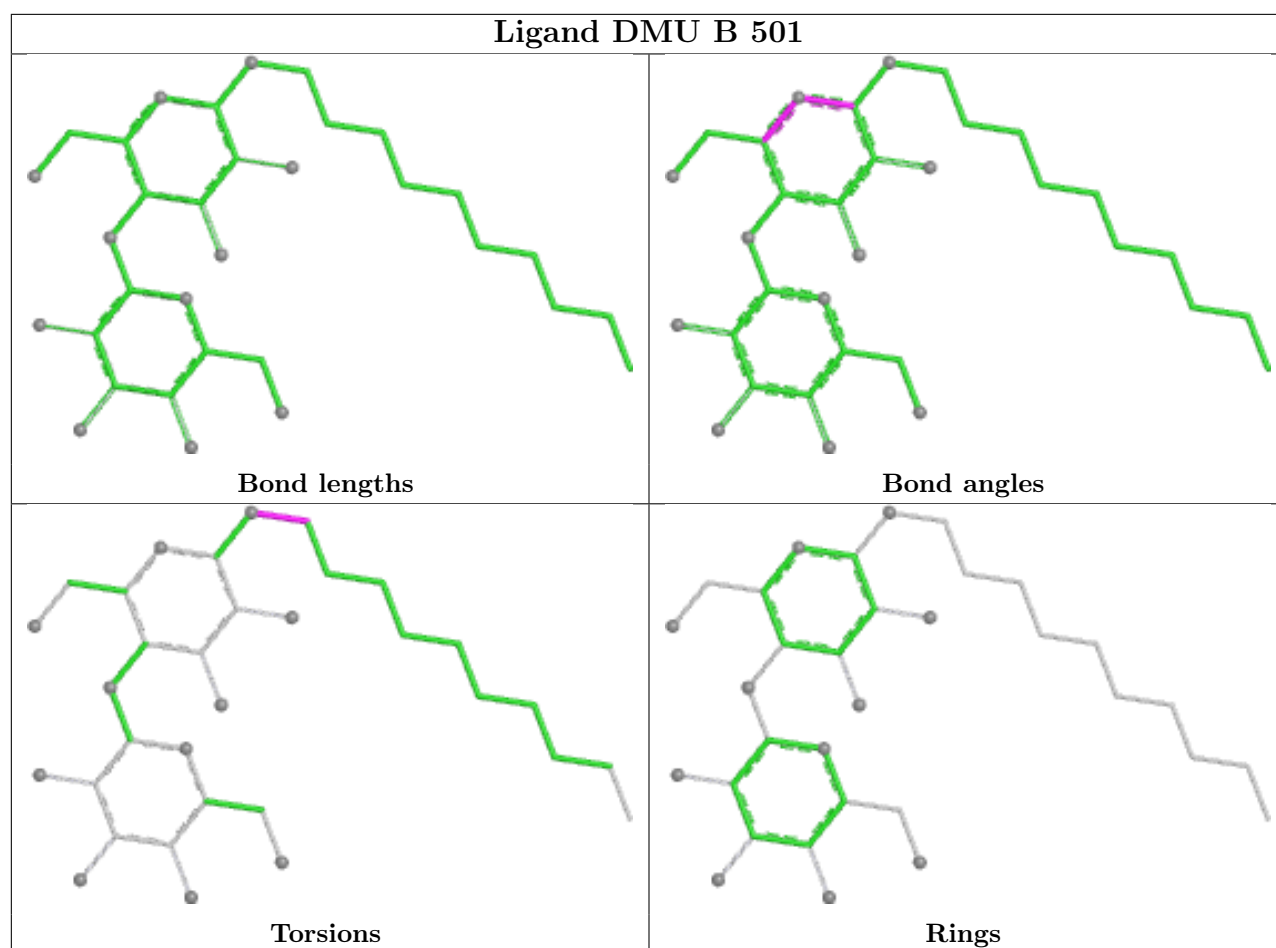
There are no ring outliers.

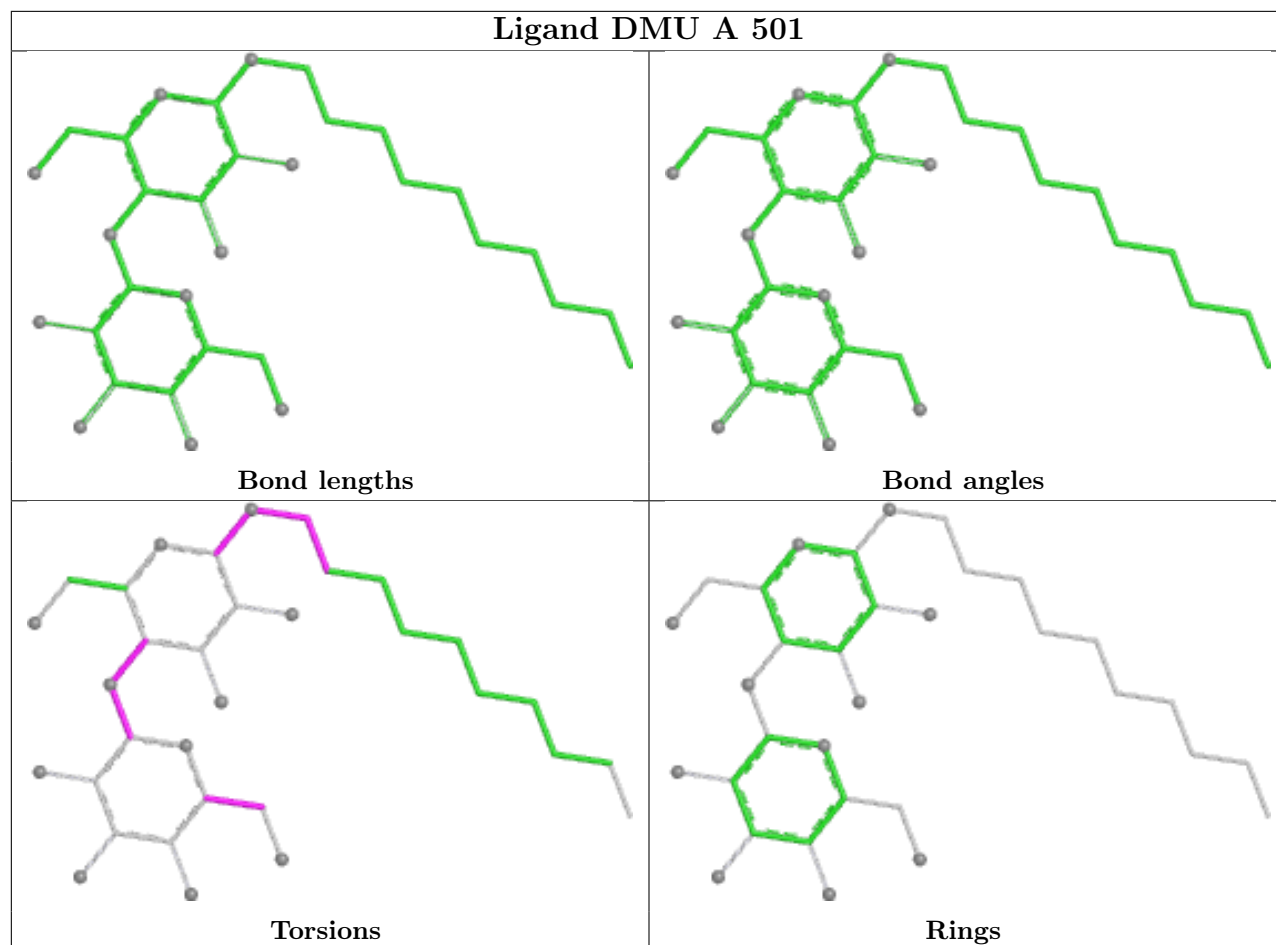
1 monomer is involved in 1 short contact:

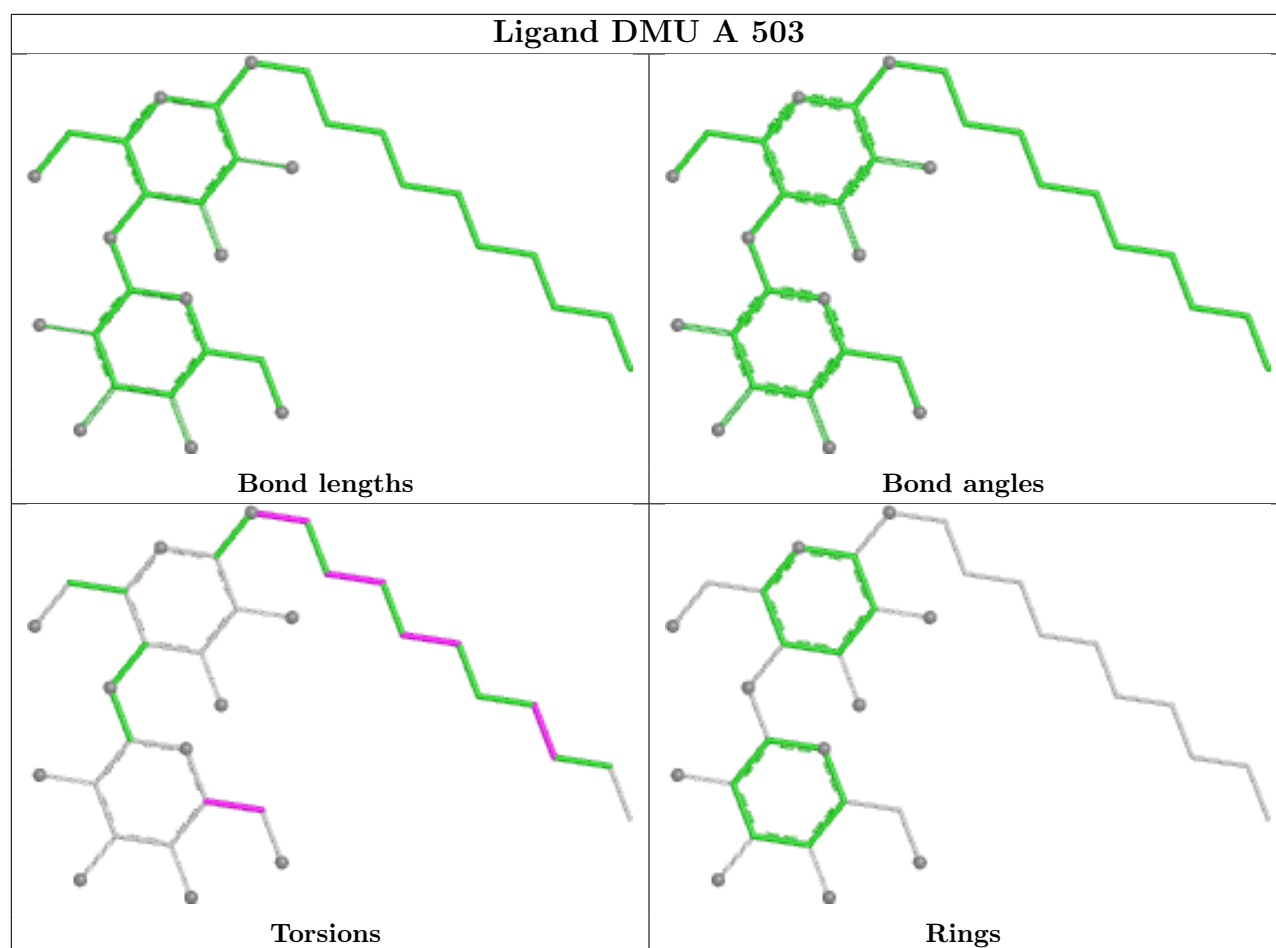
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	DMU	1	0

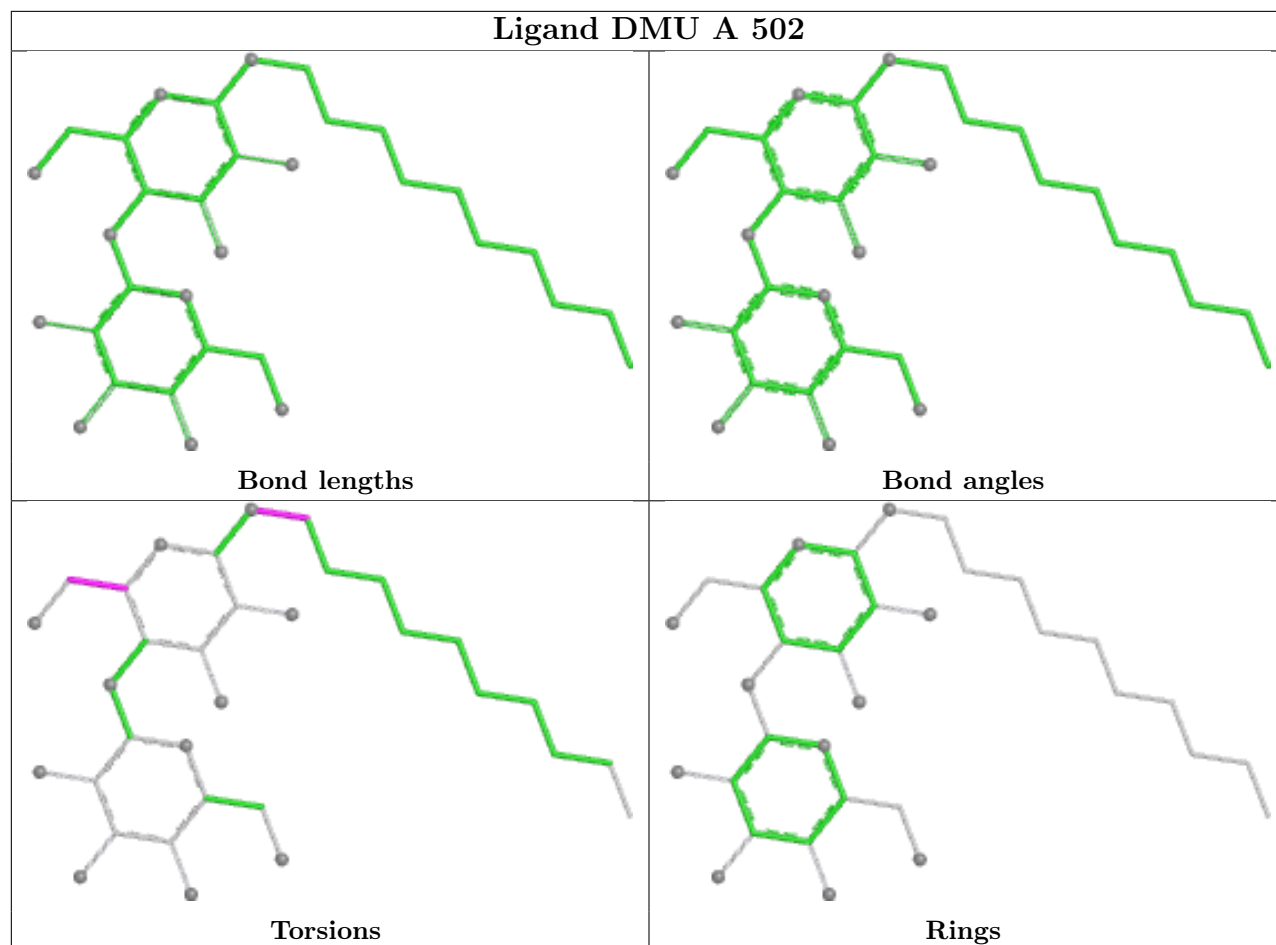
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

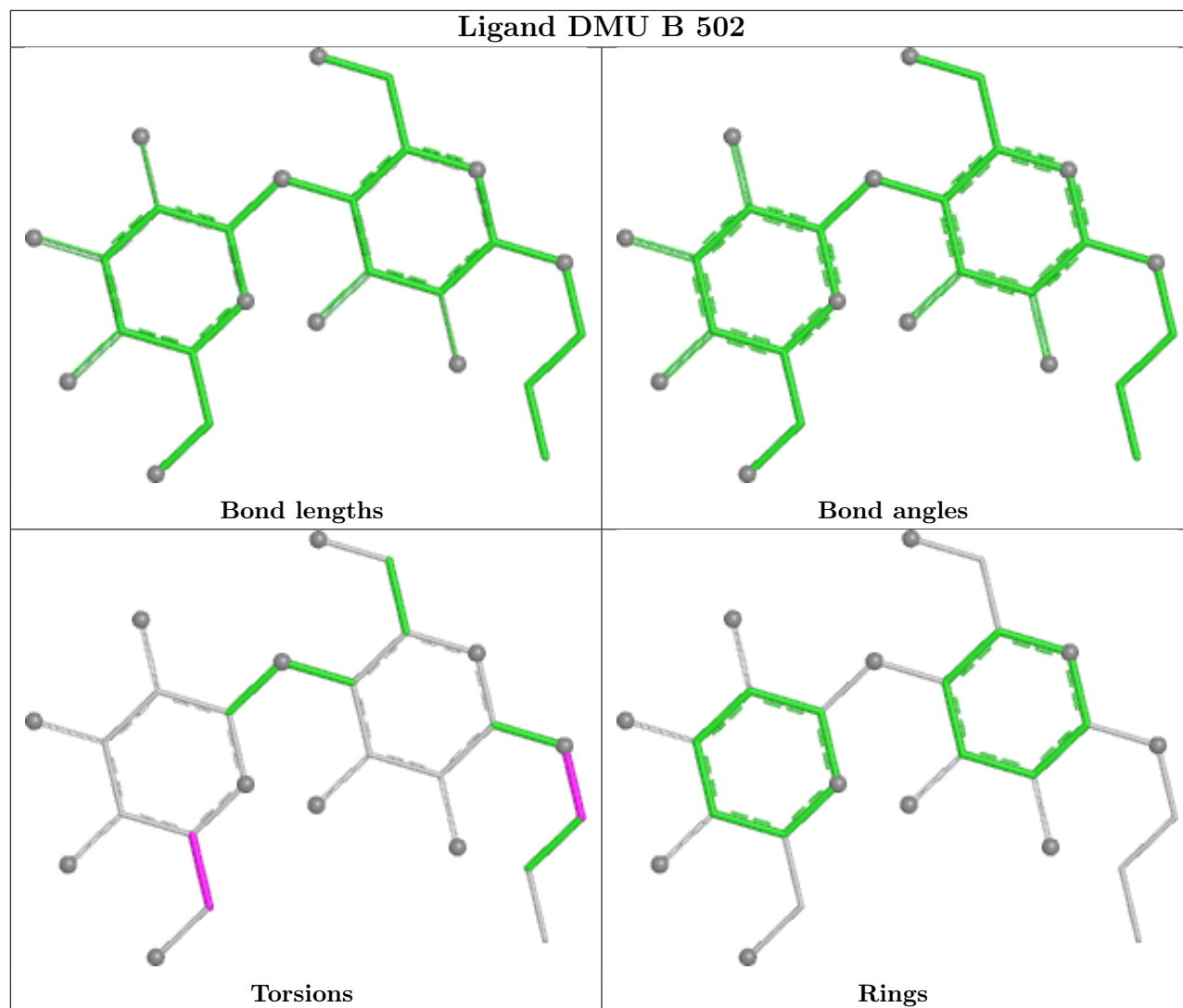












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	395/421 (93%)	0.92	78 (19%)	3	2	115, 142, 182, 230	0
1	B	396/421 (94%)	0.97	76 (19%)	3	2	113, 136, 174, 218	0
2	C	90/93 (96%)	0.67	13 (14%)	6	3	141, 164, 229, 256	0
2	D	86/93 (92%)	0.95	17 (19%)	3	2	163, 204, 271, 295	0
All	All	967/1028 (94%)	0.92	184 (19%)	3	2	113, 144, 216, 295	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	GLU	10.9
1	A	19	LEU	9.1
2	C	40	GLU	8.4
1	B	231	MET	8.3
1	B	227	LEU	8.3
2	C	80	LEU	7.9
1	B	224	VAL	7.6
1	A	107	LEU	7.5
1	B	248	LYS	7.3
1	A	59	ILE	7.3
1	B	304	VAL	7.2
1	A	342	GLU	7.2
1	A	22	LEU	7.0
1	A	171	VAL	6.8
1	B	267	LEU	6.7
1	A	23	VAL	6.7
1	A	211	SER	6.6
2	D	14	ALA	6.5
2	D	60	THR	6.4
2	C	79	TRP	6.4
2	C	70	TYR	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	228	ILE	6.3
2	C	45	SER	6.2
1	A	63	CYS	6.1
2	D	12	VAL	6.1
1	A	163	ALA	6.0
1	B	300	LEU	5.9
2	D	21	LEU	5.8
1	B	297	TYR	5.7
2	C	46	PRO	5.6
1	B	55	LEU	5.6
1	A	118	GLU	5.5
1	A	392	PRO	5.4
2	C	47	VAL	5.4
1	B	264	ALA	5.3
1	A	304	VAL	5.2
1	B	263	LEU	5.2
1	A	83	PHE	5.1
1	B	41	PHE	5.0
1	B	268	LEU	5.0
1	B	66	TYR	4.9
1	B	200	GLY	4.8
2	D	11	GLU	4.8
1	A	167	PHE	4.8
1	B	301	LEU	4.8
1	A	209	PRO	4.7
2	C	65	SER	4.6
1	B	19	LEU	4.6
2	C	39	GLY	4.5
1	A	170	GLU	4.5
1	A	291	ASN	4.5
1	A	60	ILE	4.5
1	A	62	ILE	4.5
1	A	15	THR	4.4
1	B	42	LEU	4.3
1	A	56	PHE	4.3
1	A	8	GLU	4.3
2	D	50	PHE	4.3
1	B	23	VAL	4.3
1	B	265	LEU	4.2
1	B	308	LEU	4.2
1	A	197	GLN	4.1
1	A	9	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	214	LEU	4.1
1	B	315	LEU	4.1
1	B	199	LEU	4.1
1	A	308	LEU	4.0
1	B	97	LEU	4.0
1	B	336	LEU	4.0
1	A	166	PHE	4.0
1	A	389	ILE	4.0
1	B	167	PHE	4.0
1	B	56	PHE	4.0
1	A	154	PHE	3.9
2	D	58	THR	3.9
1	A	396	TYR	3.9
1	A	187	LEU	3.9
2	D	5	SER	3.8
1	B	118	GLU	3.8
1	B	163	ALA	3.7
1	B	166	PHE	3.7
1	B	101	VAL	3.6
1	A	265	LEU	3.6
1	B	15	THR	3.6
1	B	223	LEU	3.5
1	B	80	ASN	3.5
2	D	67	GLY	3.5
1	A	362	ALA	3.5
1	A	289	PHE	3.5
1	B	362	ALA	3.5
1	B	305	LEU	3.4
1	A	208	LEU	3.4
1	B	168	ALA	3.4
1	A	168	ALA	3.2
1	B	170	GLU	3.2
2	D	52	VAL	3.2
1	B	164	ALA	3.2
1	B	220	LEU	3.2
1	B	269	PHE	3.2
1	B	385	VAL	3.2
1	A	21	SER	3.1
1	A	172	LEU	3.1
1	B	343	LEU	3.1
1	A	194	THR	3.1
1	A	361	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	391	LYS	3.1
1	A	138	LEU	3.0
2	C	68	VAL	3.0
1	B	111	PHE	3.0
1	A	260	ILE	3.0
1	B	53	LEU	3.0
1	B	159	GLU	3.0
1	B	296	SER	3.0
1	A	141	TYR	2.9
1	B	226	GLY	2.9
1	A	158	PHE	2.9
1	B	177	PHE	2.9
1	A	198	TRP	2.9
1	A	390	SER	2.9
1	B	27	LEU	2.9
1	B	165	THR	2.9
1	A	195	THR	2.9
1	B	63	CYS	2.8
1	A	268	LEU	2.8
1	A	353	PHE	2.8
1	A	164	ALA	2.8
2	D	53	PRO	2.8
1	A	42	LEU	2.8
1	B	37	LYS	2.7
1	A	213	ASP	2.7
1	A	375	ASN	2.7
1	A	379	PHE	2.7
1	B	154	PHE	2.7
1	A	89	GLU	2.7
1	B	393	TYR	2.7
1	A	305	LEU	2.7
1	B	169	LEU	2.7
2	D	55	SER	2.7
1	B	40	LEU	2.6
1	A	401	THR	2.6
1	A	402	SER	2.6
1	A	393	TYR	2.6
1	B	84	LEU	2.6
1	A	17	LEU	2.6
2	D	59	ALA	2.6
1	A	70	LYS	2.6
1	B	96	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	203	LYS	2.5
1	B	158	PHE	2.5
2	C	62	SER	2.5
1	A	73	ASP	2.5
1	B	215	THR	2.5
2	C	93	THR	2.5
1	A	201	LEU	2.5
1	A	264	ALA	2.4
2	D	51	THR	2.4
1	B	113	GLY	2.4
2	D	44	ASN	2.4
2	D	82	TRP	2.4
1	A	103	VAL	2.3
1	A	214	LEU	2.3
1	A	160	THR	2.3
1	A	243	MET	2.3
1	A	111	PHE	2.3
2	C	48	GLN	2.3
1	A	96	ARG	2.3
1	B	254	PRO	2.3
1	B	112	GLY	2.3
1	A	144	THR	2.3
1	A	364	ILE	2.2
1	A	290	THR	2.2
2	D	15	ALA	2.2
1	B	197	GLN	2.1
1	B	252	PRO	2.1
1	B	381	ILE	2.1
1	A	261	GLY	2.1
1	B	337	PHE	2.1
1	B	249	ARG	2.1
1	B	271	LEU	2.1
1	A	18	GLY	2.1
1	B	361	PHE	2.1
1	B	75	SER	2.0
1	A	341	ILE	2.0
1	A	256	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

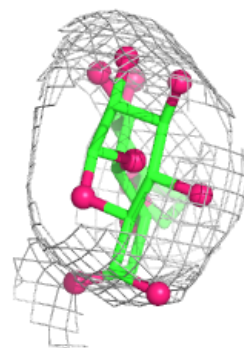
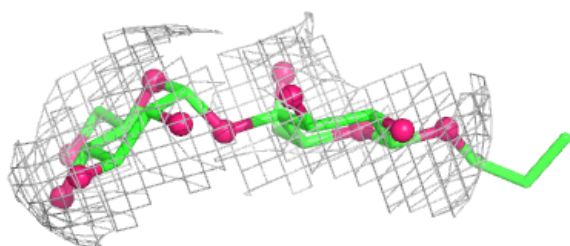
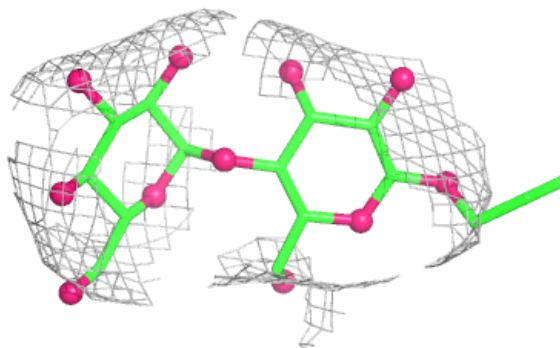
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DMU	B	502	26/33	0.63	0.12	190,220,228,237	0
4	F	B	503	1/1	0.75	0.12	173,173,173,173	0
5	MHA	C	101	13/13	0.81	0.06	146,184,192,197	0
3	DMU	A	501	33/33	0.82	0.16	125,179,201,202	0
3	DMU	A	504	33/33	0.84	0.14	120,226,252,254	0
4	F	B	504	1/1	0.88	0.57	117,117,117,117	0
3	DMU	B	501	33/33	0.89	0.13	119,166,186,192	0
3	DMU	A	502	33/33	0.90	0.23	143,178,195,198	0
3	DMU	A	503	33/33	0.90	0.18	158,194,202,205	0
4	F	A	506	1/1	0.92	0.31	125,125,125,125	0
4	F	A	505	1/1	0.94	0.10	197,197,197,197	0

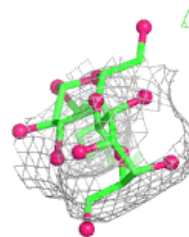
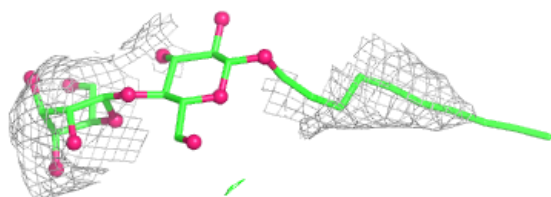
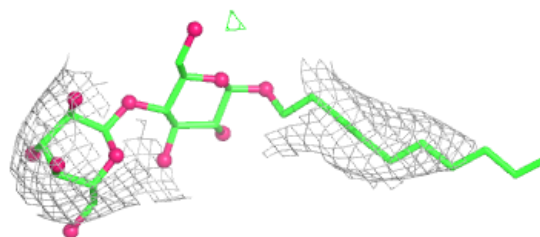
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU 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)

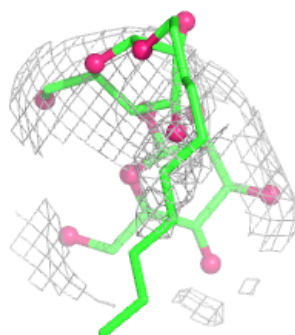
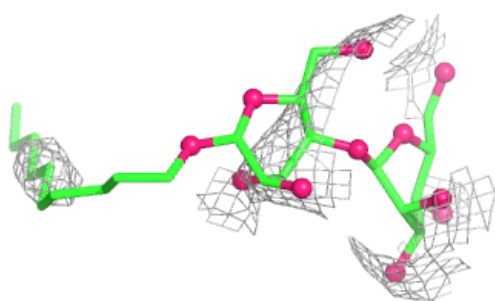
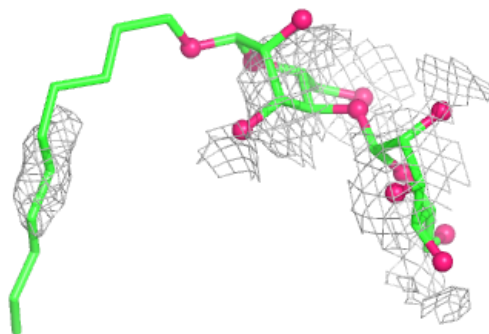
**Electron density around DMU A 501:**

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

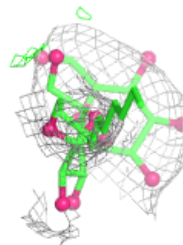
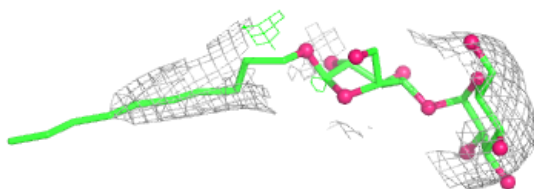
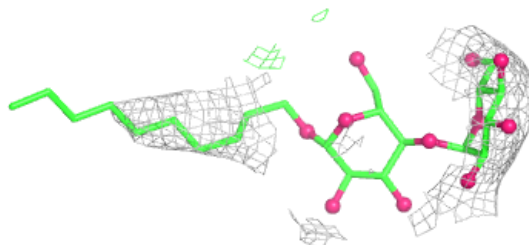


Electron density around DMU A 504:

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

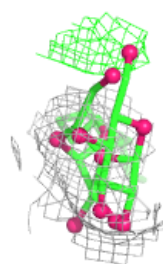
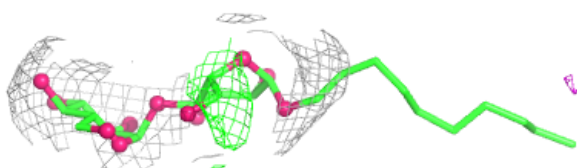
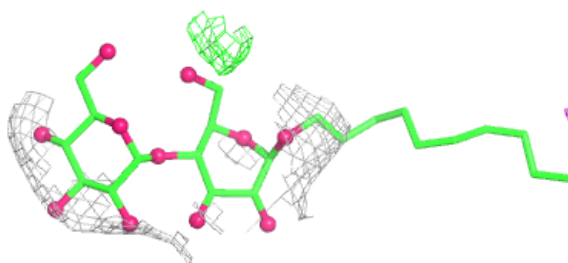
**Electron density around DMU B 501:**

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

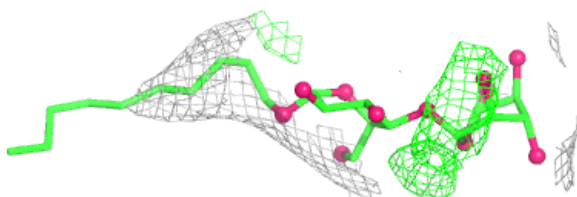
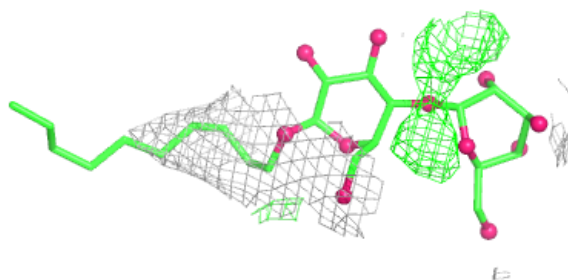


Electron density around DMU A 502:

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

**Electron density around DMU 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.