



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:26 PM UTC

PDB ID : 6D0K / pdb_00006d0k
Title : Crystal structure of a CLC-type fluoride/proton antiporter, E118Q mutant
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 : 3.35 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

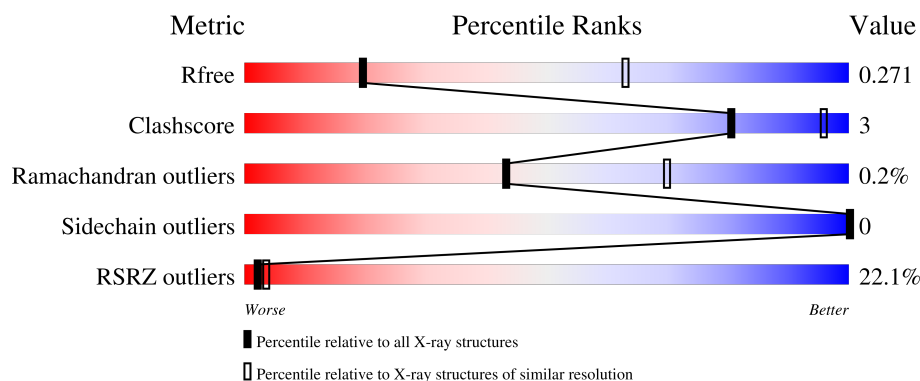
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	20% 86% 8% 6%
1	B	421	22% 88% 6% 6%
2	C	93	25% 88% 9% .
2	D	93	15% 90% . 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 7604 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	468	512	11			
1	B	396	Total	C	N	O	S	0	0	0
			3033	2037	472	513	11			

There are 36 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	118	GLN	GLU	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	118	GLN	GLU	engineered mutation	UNP C9CPP6
B	407	THR	-	expression tag	UNP C9CPP6

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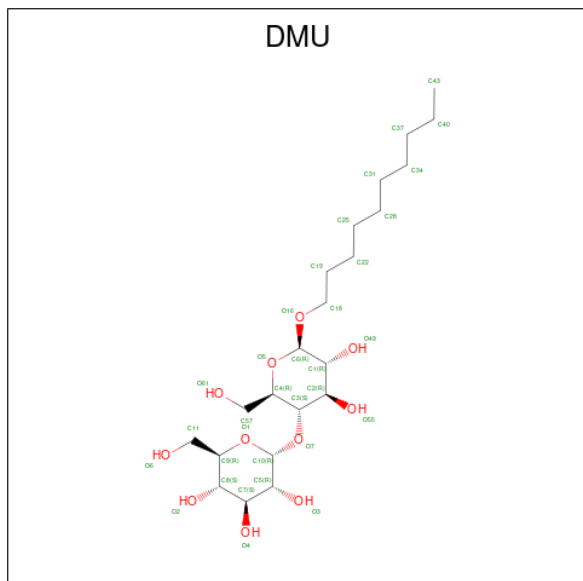
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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	ARG	-	expression tag	UNP C9CPP6
B	409	GLY	-	expression tag	UNP C9CPP6
B	410	SER	-	expression tag	UNP C9CPP6
B	411	GLY	-	expression tag	UNP C9CPP6
B	412	GLY	-	expression tag	UNP C9CPP6
B	413	HIS	-	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		

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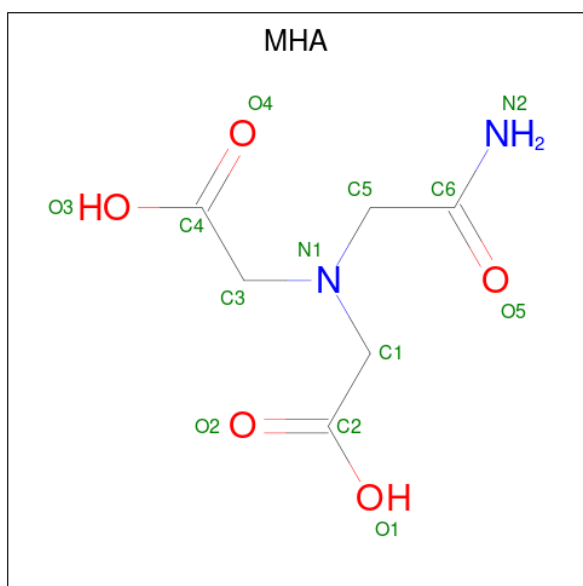
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			33	22	11		
3	A	1	Total	C	O	0	0
			33	22	11		
3	A	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			26	15	11		

- 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		

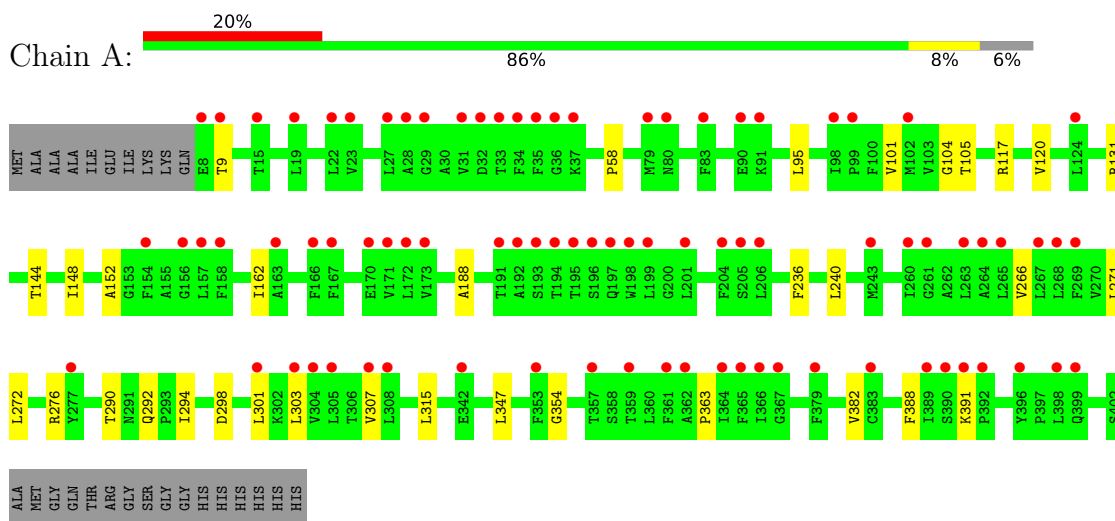
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	6	Total 6	O 6	0	0

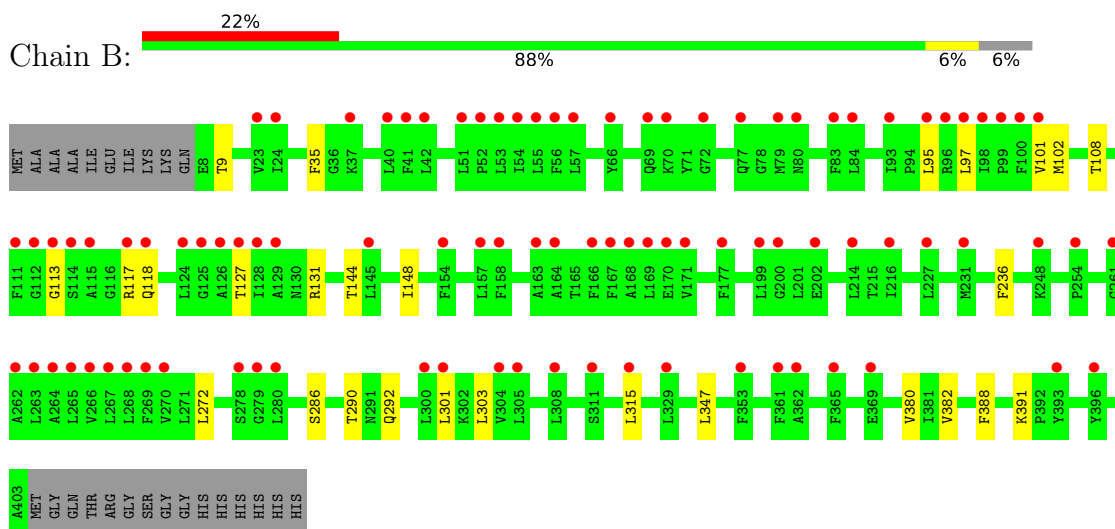
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

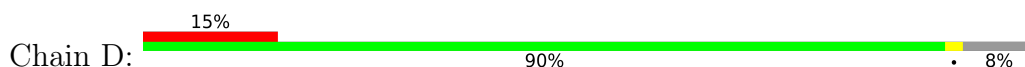
• Molecule 1: CLC-type fluoride/proton antiporter

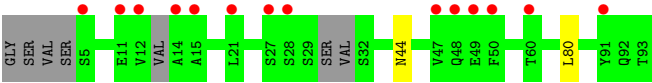


• Molecule 1: CLC-type fluoride/proton antiporter

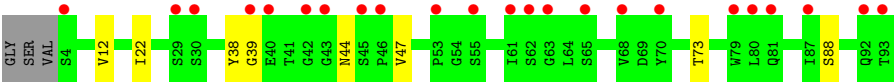
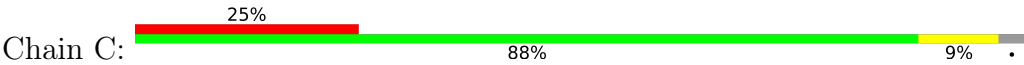


• Molecule 2: Monobody





● 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	118.32Å 125.99Å 134.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.35 49.73 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.73-3.35) 99.7 (49.73-3.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.244 , 0.266 0.251 , 0.271	Depositor DCC
R_{free} test set	1442 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	161.2	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 119.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: DMU, MHA, F

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	0.07	0/699	0.24	0/963
2	D	0.07	0/671	0.23	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	3139	19	0
1	B	3033	0	3155	15	0
2	C	679	0	648	5	0
2	D	653	0	618	2	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	3	0	0	0	0
6	B	6	0	0	0	0
All	All	7604	0	7803	40	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 (40) 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:B:118:GLN:N	4:B:503:F:F	2.23	0.61
1:A:101:VAL:HA	1:A:315:LEU:HD13	1.84	0.60
1:A:272:LEU:HD23	1:A:301:LEU:HD13	1.87	0.57
1:B:272:LEU:HD23	1:B:301:LEU:HD13	1.90	0.54
1:A:347:LEU:HD13	1:A:382:VAL:HG21	1.91	0.52
1:B:117:ARG:N	4:B:503:F:F	2.33	0.51
1:B:95:LEU:HD13	1:B:131:ARG:HG3	1.93	0.51
1:A:117:ARG:N	4:A:505:F:F	2.35	0.50
1:B:101:VAL:HA	1:B:315:LEU:HD13	1.94	0.49
1:B:290:THR:HG23	1:B:292:GLN:HG3	1.94	0.48
1:A:104:GLY:HA3	1:A:315:LEU:HD12	1.96	0.47
1:A:58:PRO:HD3	1:A:266:VAL:HG21	1.97	0.47
1:A:95:LEU:HD13	1:A:131:ARG:HG3	1.97	0.47
1:A:276:ARG:HH12	1:A:294:ILE:HG22	1.80	0.46
1:B:347:LEU:HD13	1:B:382:VAL:HG21	1.98	0.46
1:A:290:THR:HG23	1:A:292:GLN:HG3	1.97	0.46
2:C:73:THR:HG23	2:C:88:SER:HB2	1.98	0.45
1:B:286:SER:O	1:B:290:THR:HG22	2.17	0.45
3:A:502:DMU:H8	3:A:502:DMU:H5	1.53	0.45
1:A:144:THR:O	1:A:148:ILE:HG12	2.17	0.45
2:C:38:TYR:OH	5:C:101:MHA:O2	2.34	0.44
1:A:276:ARG:NH2	1:A:298:ASP:OD2	2.50	0.44
1:B:35:PHE:HB2	1:B:102:MET:HE3	1.98	0.44
1:B:97:LEU:HD23	1:B:127:THR:OG1	2.18	0.44
1:B:236:PHE:HD2	1:B:303:LEU:HG	1.82	0.44
2:C:44:ASN:OD1	2:C:44:ASN:N	2.51	0.44
1:B:388:PHE:HA	1:B:391:LYS:HE3	2.00	0.44
1:A:240:LEU:HA	1:A:307:VAL:HG13	2.00	0.43
2:D:44:ASN:OD1	2:D:44:ASN:N	2.51	0.43
1:A:152:ALA:HB2	1:A:188:ALA:HB1	2.01	0.42
1:A:162:ILE:HG23	1:B:380:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:THR:OG1	1:A:120:VAL:HG21	2.20	0.42
1:A:388:PHE:HA	1:A:391:LYS:HE3	2.01	0.41
2:C:12:VAL:HG22	2:C:22:ILE:HG22	2.03	0.41
2:C:39:GLY:HA3	2:C:47:VAL:HG12	2.02	0.41
1:B:144:THR:O	1:B:148:ILE:HG12	2.20	0.41
1:A:236:PHE:HD2	1:A:303:LEU:HG	1.86	0.41
1:A:271:LEU:HG	2:D:80:LEU:HA	2.03	0.41
1:A:354:GLY:HA3	1:A:363:PRO:HG3	2.02	0.41
1:B:108:THR:O	1:B:113:GLY:N	2.54	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%)	379 (96%)	13 (3%)	1 (0%)	36	63
1	B	394/421 (94%)	380 (96%)	13 (3%)	1 (0%)	36	63
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%)	921 (96%)	32 (3%)	2 (0%)	43	70

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	B	501	-	34,34,34	0.14	0	45,45,45	0.47	1 (2%)
3	DMU	A	504	-	34,34,34	0.13	0	45,45,45	0.31	0
3	DMU	A	501	-	34,34,34	0.13	0	45,45,45	0.42	0
3	DMU	B	502	-	27,27,34	0.12	0	38,38,45	0.18	0
3	DMU	A	502	-	34,34,34	0.12	0	45,45,45	0.39	0
3	DMU	A	503	-	34,34,34	0.14	0	45,45,45	0.47	0
5	MHA	C	101	-	12,12,12	1.58	4 (33%)	15,15,15	1.41	5 (33%)

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	B	501	-	-	1/19/59/59	0/2/2/2
3	DMU	A	504	-	-	5/19/59/59	0/2/2/2
3	DMU	A	501	-	-	7/19/59/59	0/2/2/2
3	DMU	B	502	-	-	2/12/52/59	0/2/2/2
3	DMU	A	502	-	-	2/19/59/59	0/2/2/2
3	DMU	A	503	-	-	5/19/59/59	0/2/2/2
5	MHA	C	101	-	-	6/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	101	MHA	O2-C2	2.79	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	-2.79	109.31	114.42
5	C	101	MHA	O3-C4-C3	2.44	123.00	113.38
5	C	101	MHA	O1-C2-C1	2.43	122.95	113.38
5	C	101	MHA	O4-C4-C3	-2.18	113.28	122.38
5	C	101	MHA	O2-C2-C1	-2.14	113.42	122.38
3	B	501	DMU	C6-O5-C4	2.06	117.75	113.72

There are no chirality outliers.

All (28) torsion outliers are listed below:

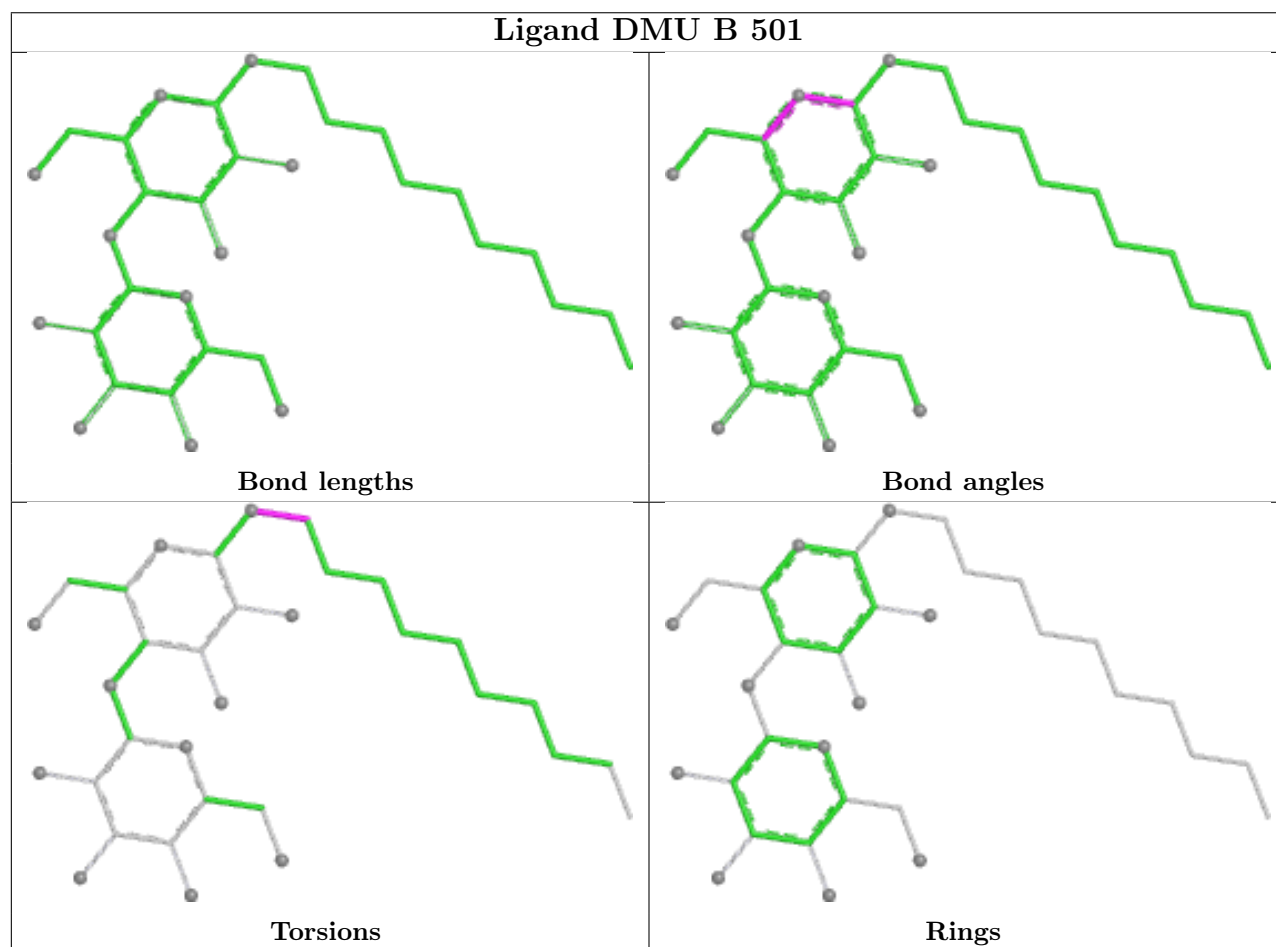
Mol	Chain	Res	Type	Atoms
3	A	502	DMU	C19-C18-O16-C6
3	A	504	DMU	O5-C6-O16-C18
5	C	101	MHA	C2-C1-N1-C3
5	C	101	MHA	N1-C1-C2-O1
5	C	101	MHA	N1-C1-C2-O2
5	C	101	MHA	N1-C5-C6-O5
5	C	101	MHA	N1-C5-C6-N2
3	A	501	DMU	O1-C10-O7-C3
3	A	501	DMU	C19-C18-O16-C6
3	B	502	DMU	C19-C18-O16-C6
3	A	504	DMU	C1-C6-O16-C18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

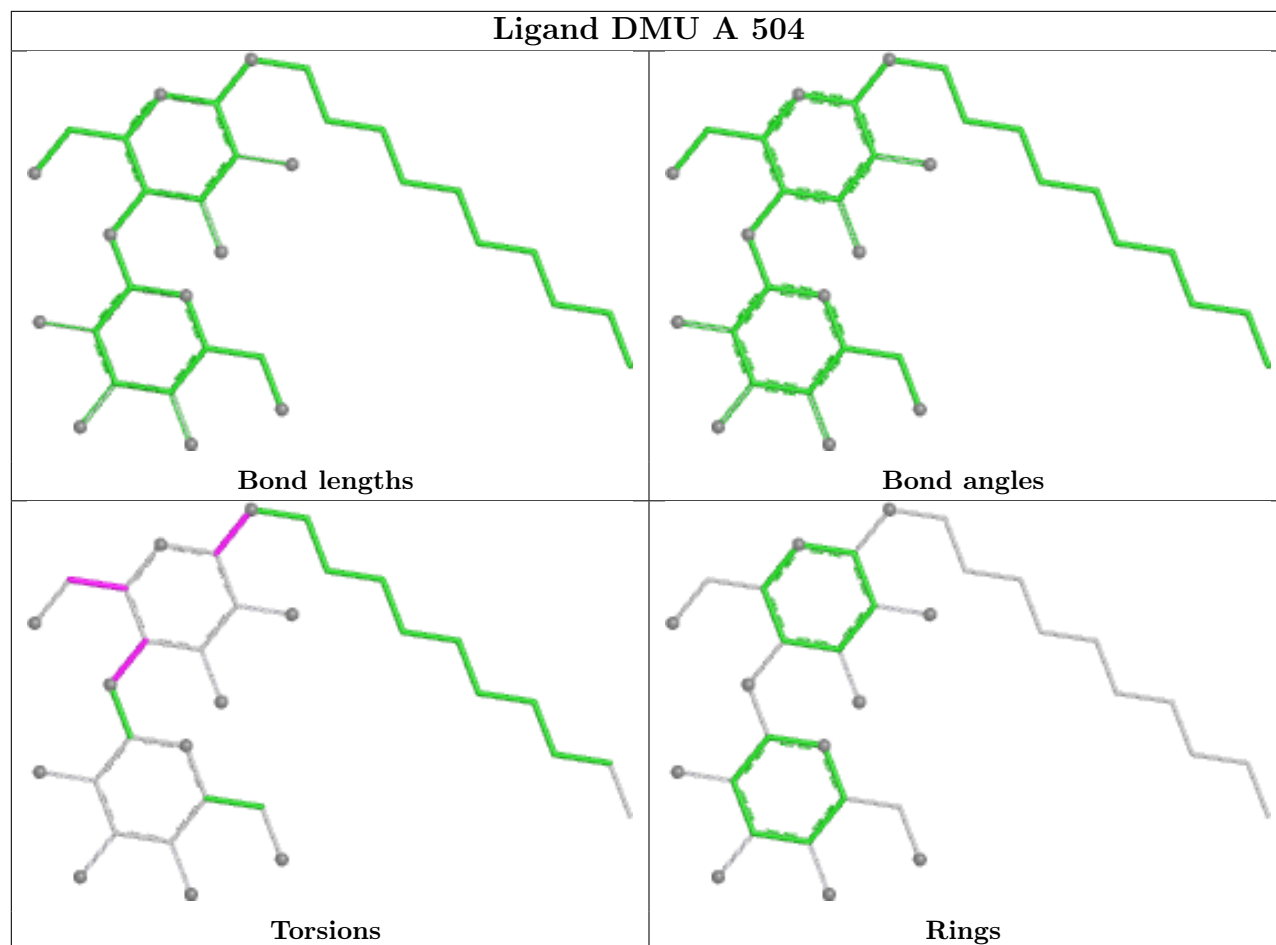
There are no ring outliers.

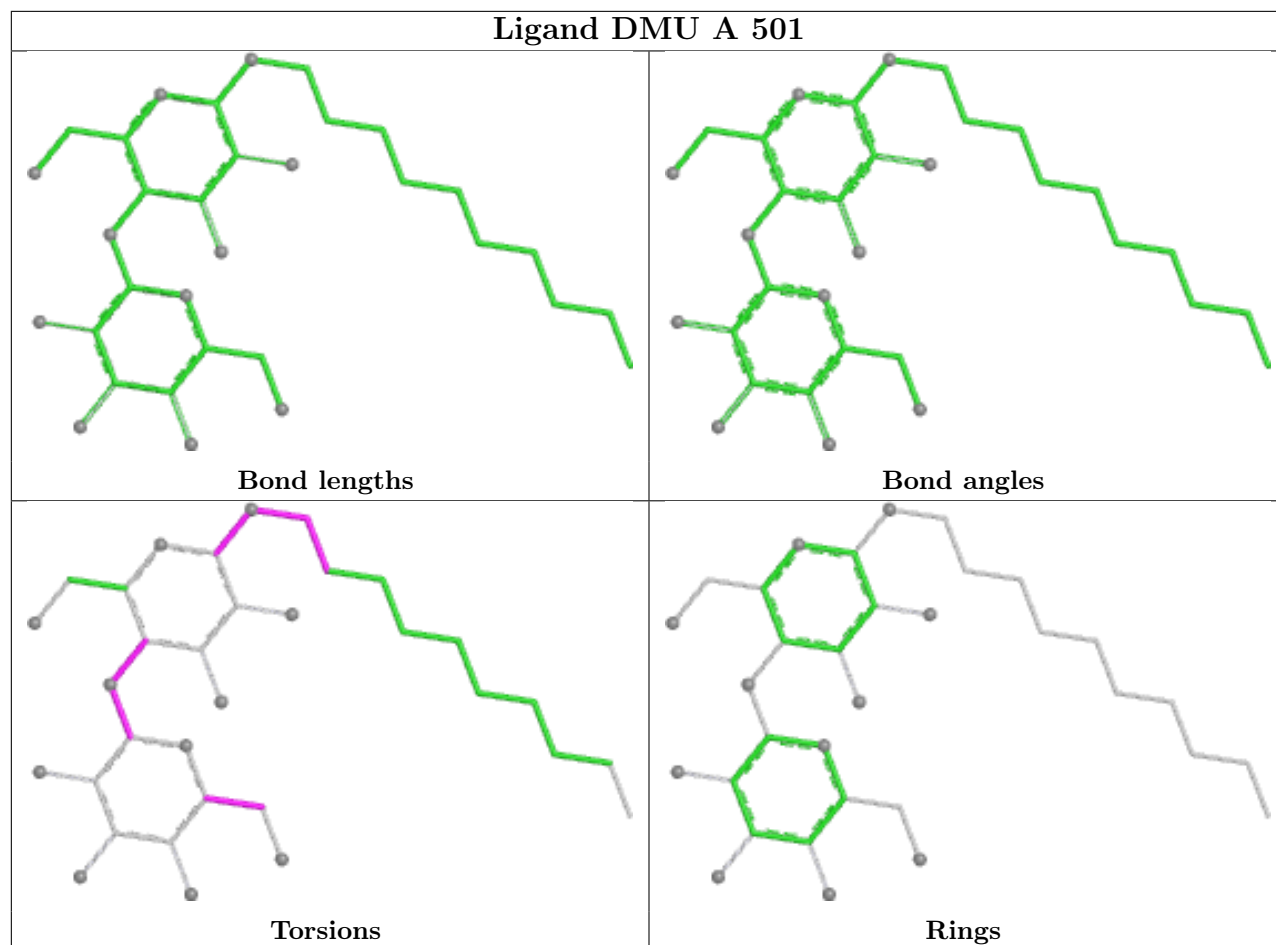
2 monomers are involved in 2 short contacts:

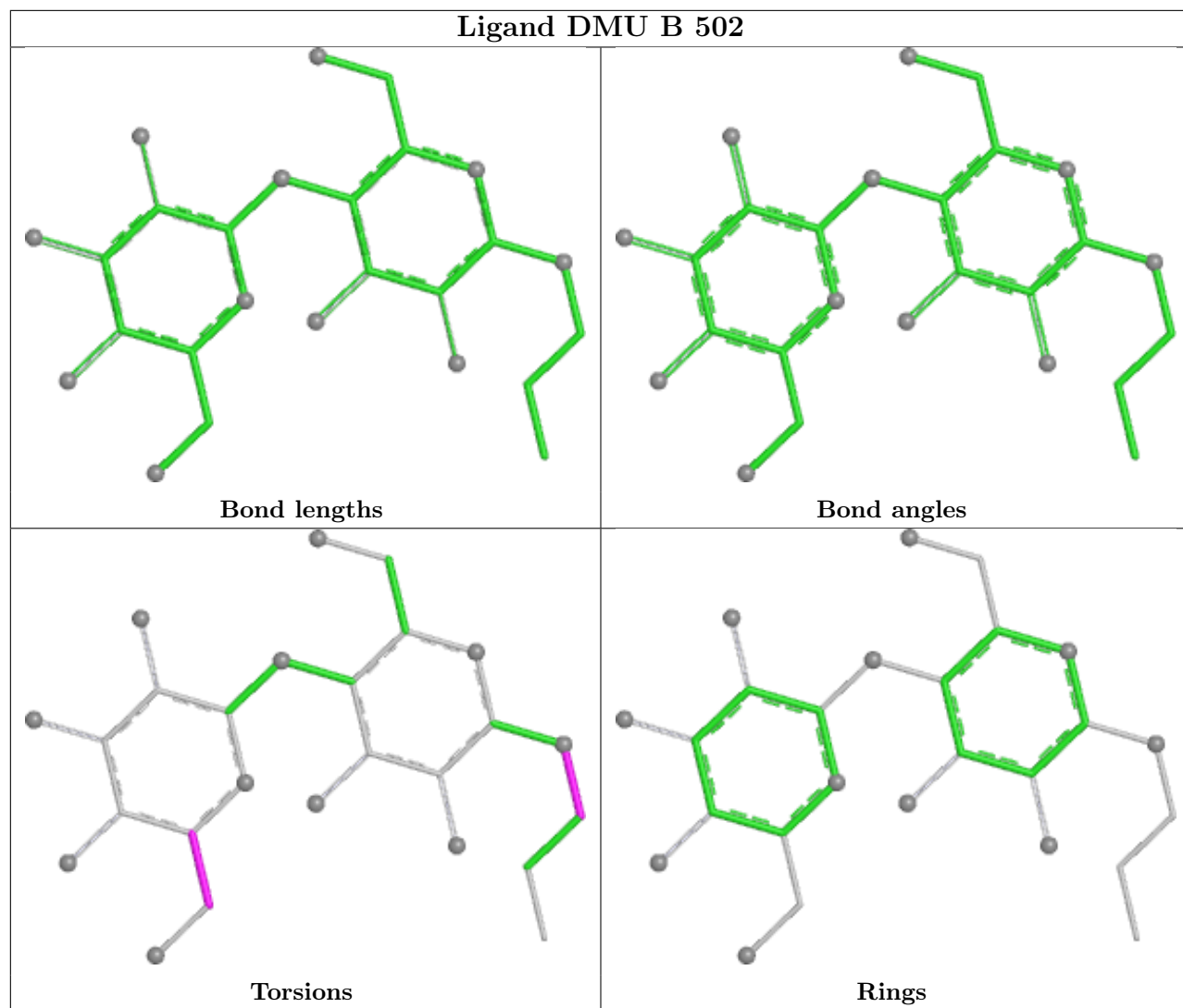
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	DMU	1	0
5	C	101	MHA	1	0

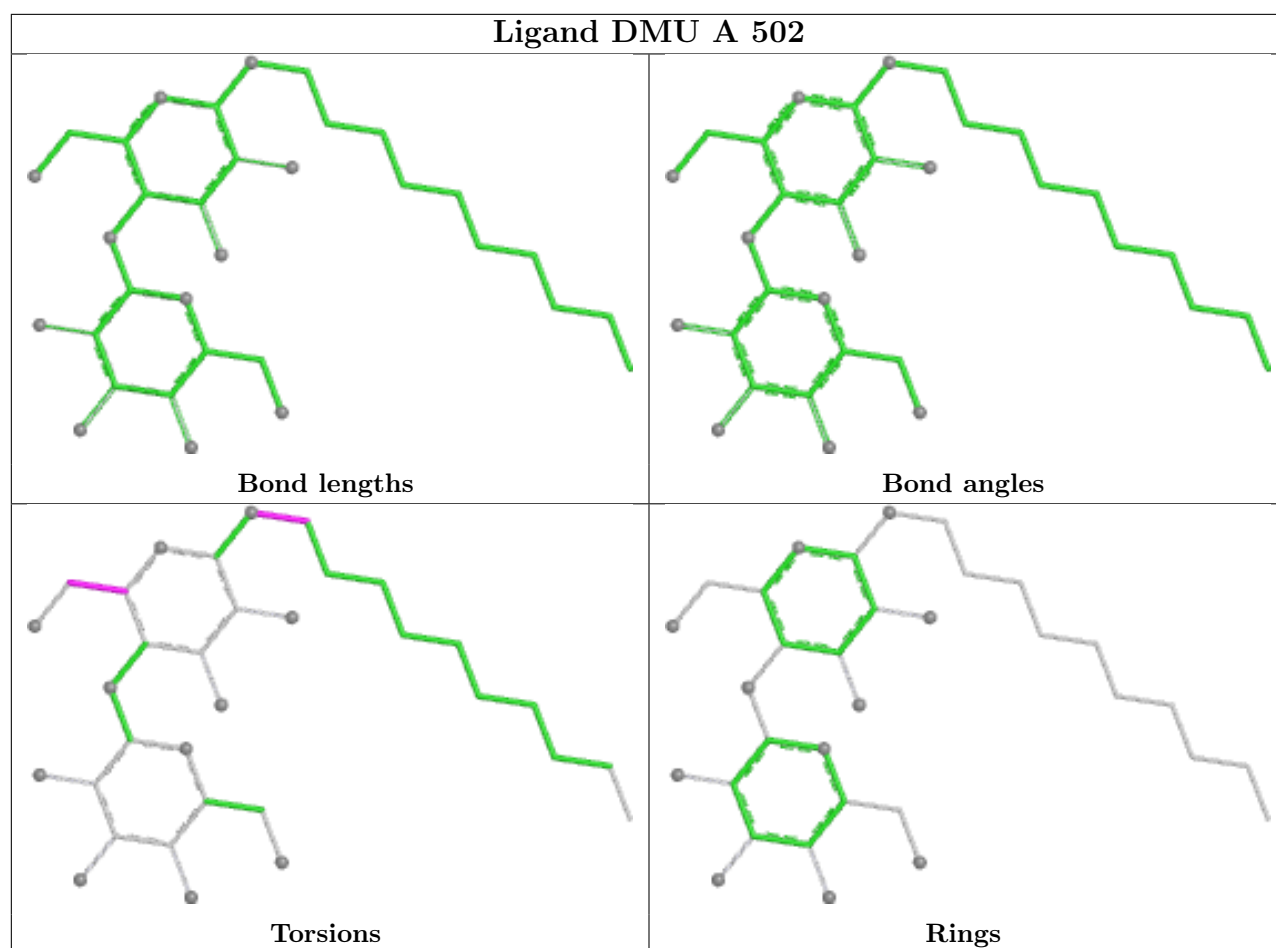
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

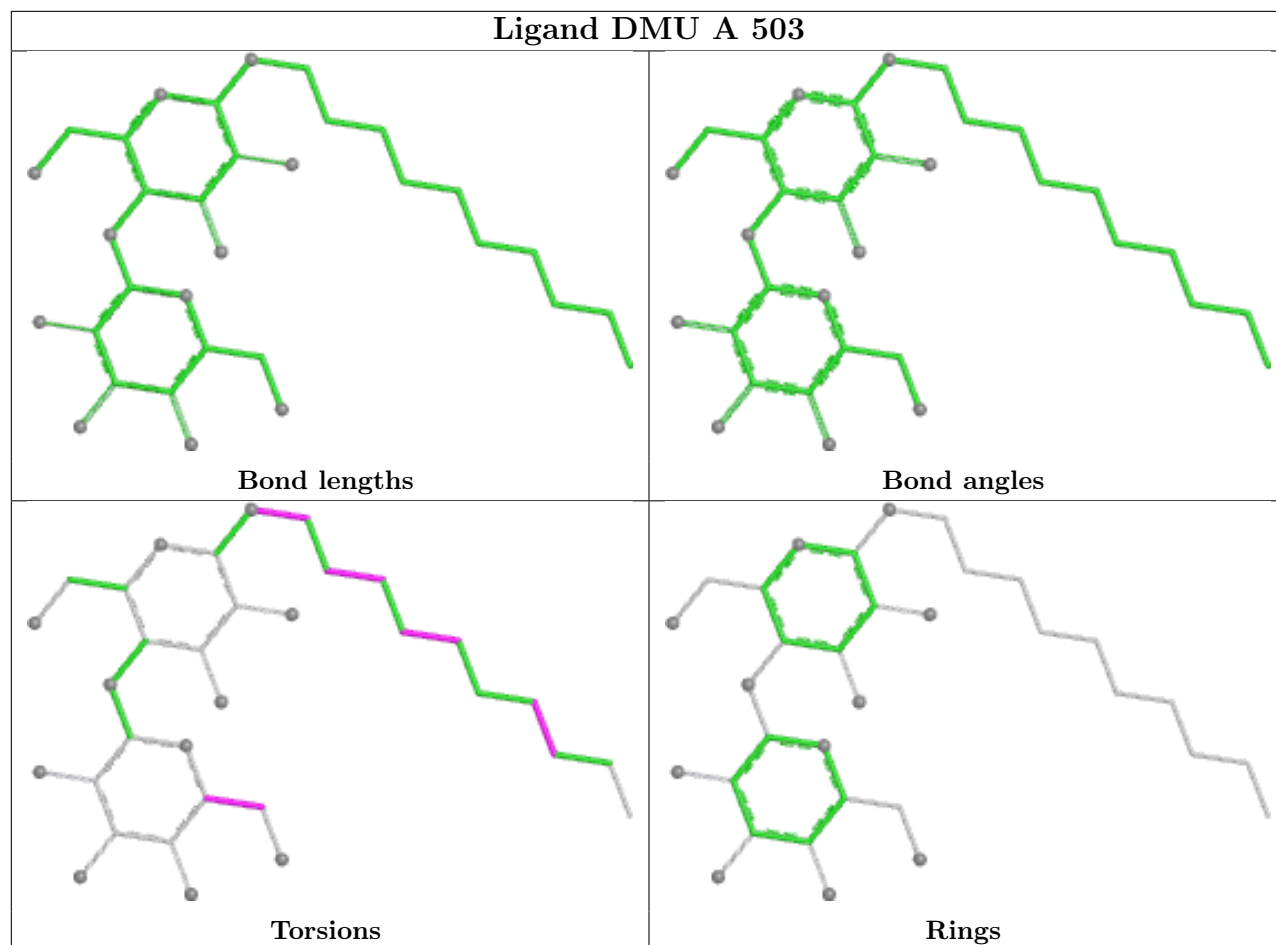












5.7 Other polymers [i](#)

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(Å ²)	Q<0.9
1	A	395/421 (93%)	0.89	84 (21%)	2 4	148, 178, 229, 272	0
1	B	396/421 (94%)	1.09	93 (23%)	2 3	145, 173, 216, 269	0
2	C	90/93 (96%)	1.01	23 (25%)	1 2	178, 205, 284, 338	0
2	D	86/93 (92%)	0.73	14 (16%)	4 5	198, 248, 304, 338	0
All	All	967/1028 (94%)	0.97	214 (22%)	2 3	145, 181, 257, 338	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	14	ALA	12.2
1	B	55	LEU	11.1
1	A	171	VAL	10.5
1	A	304	VAL	10.3
1	B	263	LEU	9.6
1	A	268	LEU	8.9
2	D	21	LEU	8.8
1	B	265	LEU	8.1
1	B	267	LEU	8.0
1	B	264	ALA	7.9
1	A	305	LEU	7.8
1	B	269	PHE	7.6
2	D	12	VAL	7.6
1	A	265	LEU	7.6
1	B	167	PHE	7.5
2	C	40	GLU	7.5
1	B	113	GLY	7.3
1	A	308	LEU	7.3
1	A	83	PHE	7.2
1	B	112	GLY	7.2
1	A	170	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	202	GLU	7.1
1	A	172	LEU	7.1
1	B	177	PHE	7.1
1	B	80	ASN	6.7
1	B	308	LEU	6.7
2	C	80	LEU	6.6
1	B	304	VAL	6.6
1	B	166	PHE	6.5
1	A	264	ALA	6.4
1	B	268	LEU	6.2
1	A	267	LEU	6.2
1	B	118	GLN	6.1
1	B	170	GLU	6.0
1	A	19	LEU	5.9
2	D	60	THR	5.6
1	B	56	PHE	5.6
1	A	260	ILE	5.5
1	A	167	PHE	5.5
1	B	163	ALA	5.4
2	C	55	SER	5.4
1	A	396	TYR	5.3
1	B	248	LYS	5.3
1	A	91	LYS	5.3
2	C	68	VAL	5.3
1	B	171	VAL	5.2
1	A	263	LEU	5.2
1	B	266	VAL	5.1
1	A	361	PHE	5.1
1	B	362	ALA	5.0
1	A	166	PHE	5.0
1	A	163	ALA	4.8
1	B	168	ALA	4.8
2	C	46	PRO	4.8
1	B	305	LEU	4.8
1	B	169	LEU	4.7
1	B	66	TYR	4.7
2	D	11	GLU	4.7
2	C	79	TRP	4.6
1	B	97	LEU	4.6
1	A	353	PHE	4.6
1	A	31	VAL	4.6
1	B	53	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	15	THR	4.5
2	D	49	GLU	4.5
1	B	54	ILE	4.5
1	B	214	LEU	4.5
1	A	261	GLY	4.5
1	A	32	ASP	4.4
1	A	301	LEU	4.3
2	C	62	SER	4.3
1	B	279	GLY	4.3
1	A	197	GLN	4.3
2	D	15	ALA	4.2
1	A	362	ALA	4.2
2	C	29	SER	4.1
1	B	42	LEU	4.1
1	A	392	PRO	3.9
1	B	158	PHE	3.9
1	A	195	THR	3.9
1	B	79	MET	3.9
1	A	389	ILE	3.9
1	A	379	PHE	3.9
1	B	200	GLY	3.9
1	A	194	THR	3.8
1	A	80	ASN	3.8
1	B	154	PHE	3.8
1	A	90	GLU	3.7
1	B	95	LEU	3.7
2	C	45	SER	3.6
1	B	114	SER	3.6
1	B	57	LEU	3.6
1	A	28	ALA	3.6
1	B	231	MET	3.6
1	A	193	SER	3.6
1	B	98	ILE	3.6
1	A	243	MET	3.5
1	A	399	GLN	3.5
1	A	23	VAL	3.5
2	C	63	GLY	3.5
1	A	79	MET	3.5
1	B	353	PHE	3.4
1	B	52	PRO	3.4
1	B	278	SER	3.3
2	D	5	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	111	PHE	3.3
1	B	361	PHE	3.3
1	B	41	PHE	3.3
1	A	173	VAL	3.3
2	D	48	GLN	3.3
1	A	33	THR	3.2
1	B	227	LEU	3.2
1	A	196	SER	3.2
1	B	115	ALA	3.2
1	B	84	LEU	3.1
2	C	61	ILE	3.1
2	C	81	GLN	3.1
2	C	65	SER	3.1
2	C	93	THR	3.1
1	B	101	VAL	3.1
1	A	29	GLY	3.0
1	A	364	ILE	3.0
1	A	124	LEU	3.0
1	B	124	LEU	3.0
1	B	300	LEU	3.0
1	A	307	VAL	3.0
1	A	36	GLY	3.0
1	B	51	LEU	3.0
1	A	192	ALA	2.9
1	A	201	LEU	2.9
1	B	261	GLY	2.9
1	A	27	LEU	2.9
1	B	125	GLY	2.8
2	D	27	SER	2.8
1	A	156	GLY	2.8
1	B	70	LYS	2.8
1	B	262	ALA	2.7
2	C	30	SER	2.7
1	B	280	LEU	2.7
1	B	301	LEU	2.7
2	D	50	PHE	2.7
1	B	127	THR	2.7
1	B	37	LYS	2.6
1	A	98	ILE	2.6
1	A	398	LEU	2.6
1	A	198	TRP	2.6
1	A	359	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	117	ARG	2.6
1	B	128	ILE	2.6
1	A	303	LEU	2.6
1	B	315	LEU	2.5
1	A	357	THR	2.5
1	A	158	PHE	2.5
1	A	22	LEU	2.5
1	A	206	LEU	2.5
1	A	277	TYR	2.5
1	B	126	ALA	2.5
1	A	35	PHE	2.5
2	C	53	PRO	2.5
2	D	91	TYR	2.5
1	B	77	GLN	2.5
1	B	24	ILE	2.4
1	B	40	LEU	2.4
2	D	47	VAL	2.4
1	B	164	ALA	2.4
1	A	204	PHE	2.4
1	B	96	ARG	2.4
1	B	365	PHE	2.4
1	B	311	SER	2.4
1	B	254	PRO	2.4
1	A	37	LYS	2.4
1	A	390	SER	2.4
1	A	269	PHE	2.3
1	A	383	CYS	2.3
1	B	93	ILE	2.3
1	B	129	ALA	2.3
1	B	145	LEU	2.3
1	A	8	GLU	2.3
1	B	369	GLU	2.2
1	B	329	LEU	2.2
1	A	9	THR	2.2
1	B	23	VAL	2.2
1	B	157	LEU	2.2
1	A	365	PHE	2.2
1	B	69	GLN	2.2
1	B	72	GLY	2.2
1	A	366	ILE	2.2
1	B	199	LEU	2.2
1	A	99	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	154	PHE	2.2
1	B	396	TYR	2.1
1	A	199	LEU	2.1
1	B	99	PRO	2.1
2	C	4	SER	2.1
2	C	39	GLY	2.1
1	B	83	PHE	2.1
1	A	102	MET	2.1
1	B	393	TYR	2.1
2	C	70	TYR	2.1
1	B	100	PHE	2.1
1	A	205	SER	2.1
1	A	391	LYS	2.1
1	A	367	GLY	2.1
1	A	34	PHE	2.1
1	A	342	GLU	2.1
2	D	28	SER	2.0
2	C	87	ILE	2.0
2	C	43	GLY	2.0
1	A	157	LEU	2.0
1	A	191	THR	2.0
2	C	42	GLY	2.0
2	C	92	GLN	2.0
1	B	270	VAL	2.0
1	B	216	ILE	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

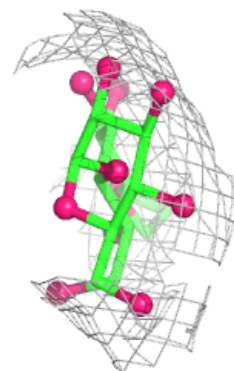
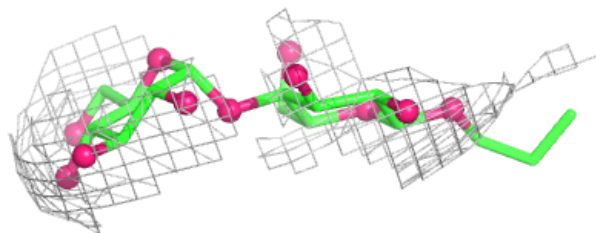
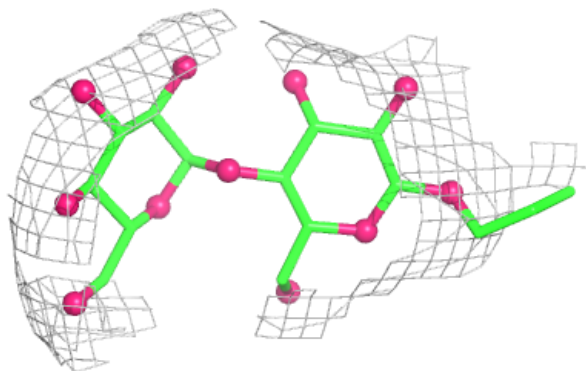
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMU	B	502	26/33	0.56	0.10	212,265,285,289	0
5	MHA	C	101	13/13	0.73	0.07	194,229,240,244	0
3	DMU	A	504	33/33	0.83	0.09	156,260,288,292	0
3	DMU	A	503	33/33	0.86	0.19	169,227,242,251	0
3	DMU	B	501	33/33	0.87	0.13	156,205,239,245	0
3	DMU	A	501	33/33	0.88	0.11	156,229,258,261	0
3	DMU	A	502	33/33	0.91	0.18	167,214,247,250	0
4	F	A	506	1/1	0.93	0.42	164,164,164,164	0
4	F	B	503	1/1	0.94	0.11	164,164,164,164	0
4	F	A	505	1/1	0.94	0.07	166,166,166,166	0
4	F	B	504	1/1	0.95	0.33	195,195,195,195	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.

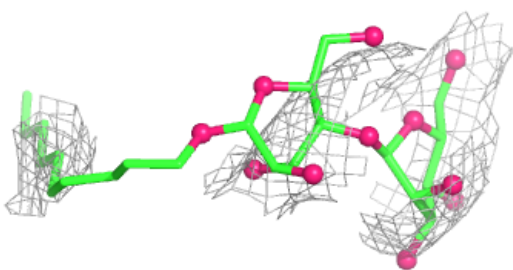
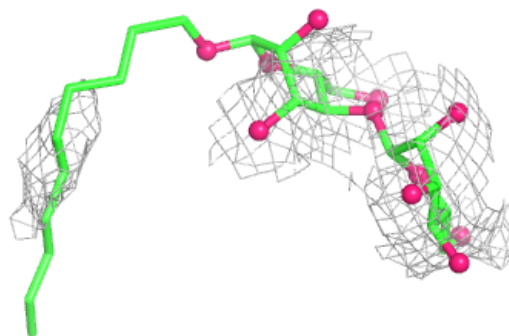
Electron density around DMU B 502:

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

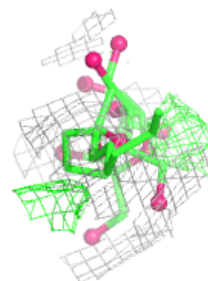
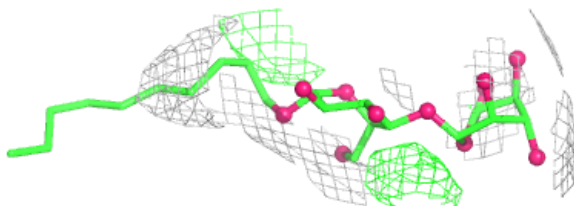
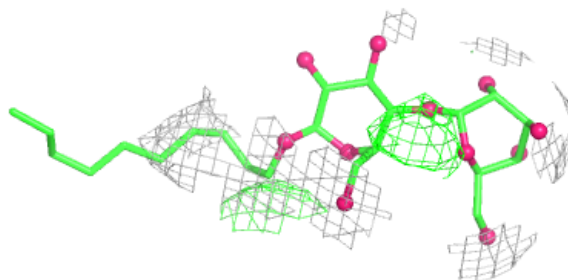


Electron density around DMU A 504:

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

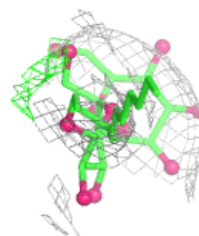
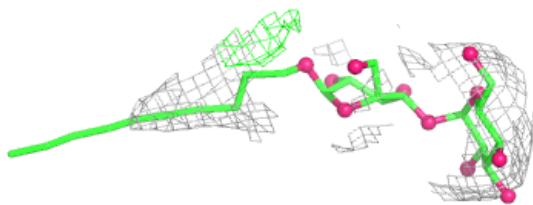
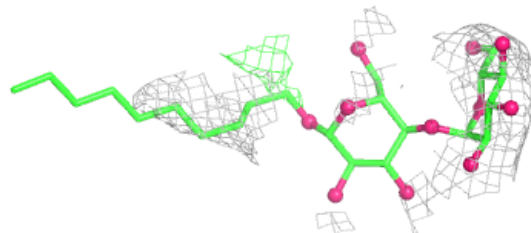
**Electron density around DMU A 503:**

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

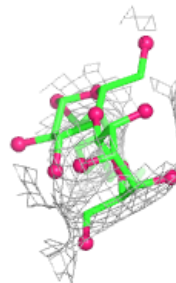
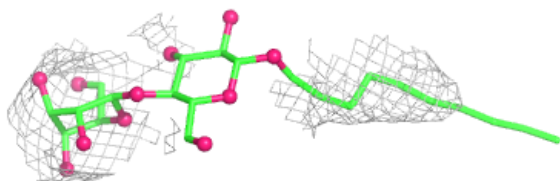
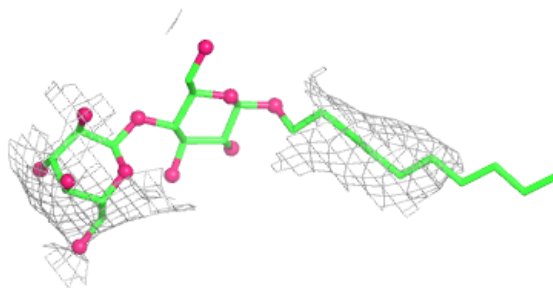


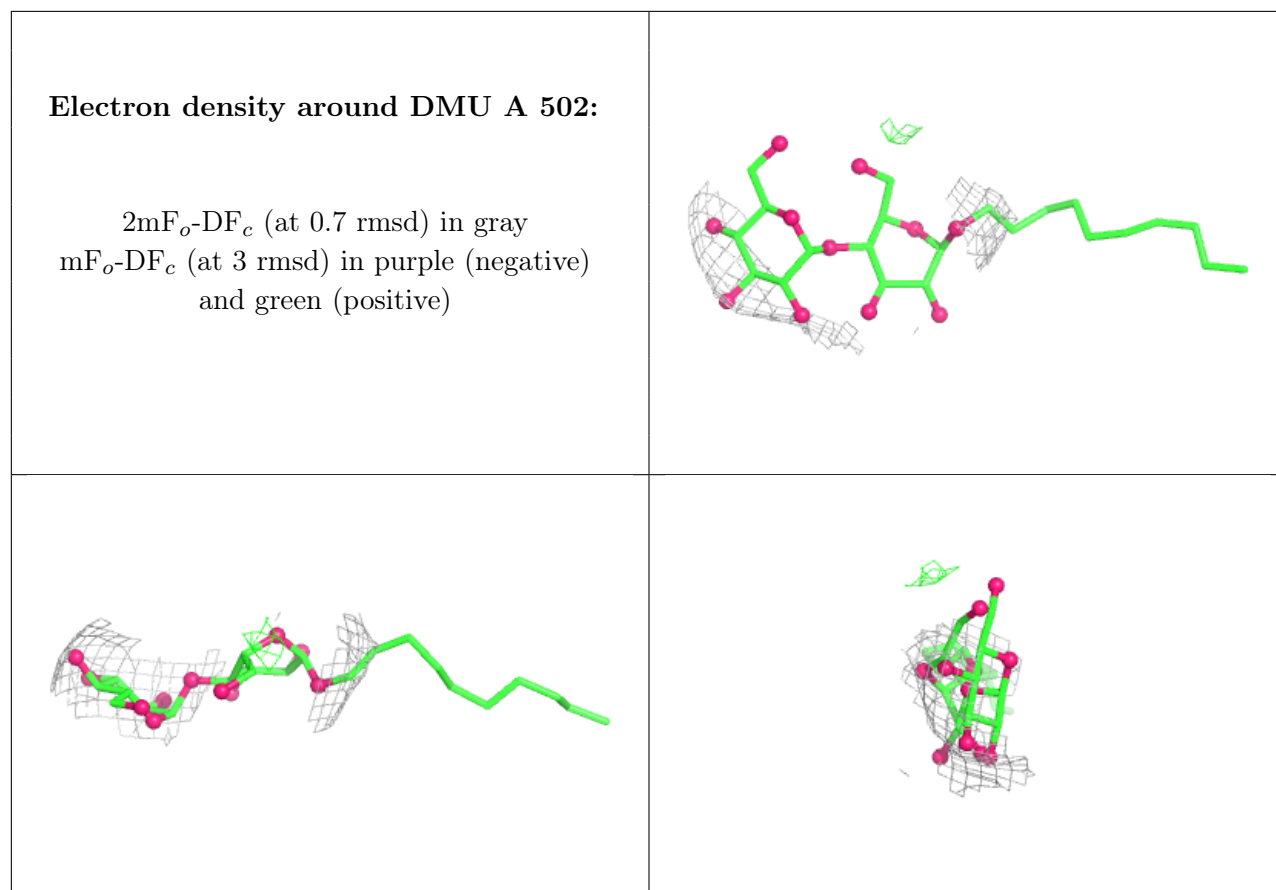
Electron density around DMU B 501:

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

**Electron density around DMU A 501:**

$2mF_o-DF_c$ (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.