wwPDB X-ray Structure Validation Summary Report (i)

Mar 20, 2026 – 04:12 AM UTC

PDB ID	:	8JYC / pdb_00008jyc
Title	:	Crystal Structure of Intracellular B30.2 Domain of BTN3A1 and BTN2A1 in Complex with DMAPP
Authors	:	Yuan, L.J.; Yang, Y.Y.; Li, X.; Cai, N.N.; Chen, C.-C.; Guo, R.-T.; Zhang, Y.H.
Deposited on	:	2023-07-03
Resolution	:	2.29 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

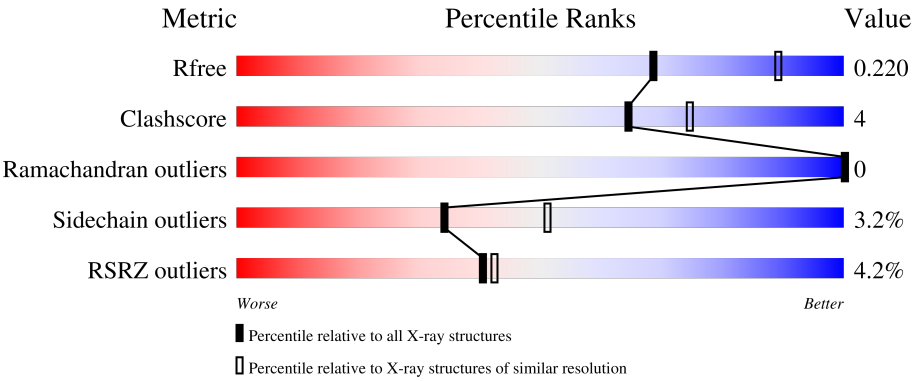
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 <=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	218	2% 79% 12% 8%
1	B	218	3% 83% 7% 9%
2	C	196	3% 83% 10% 6%
2	D	196	9% 73% 17% 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6669 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	1	0
			1614	1020	290	295	9			
1	B	199	Total	C	N	O	S	0	0	0
			1596	1009	285	293	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP Q7KYR7
A	311	ALA	-	expression tag	UNP Q7KYR7
A	312	GLY	-	expression tag	UNP Q7KYR7
A	313	ALA	-	expression tag	UNP Q7KYR7
A	314	GLY	-	expression tag	UNP Q7KYR7
A	315	ALA	-	expression tag	UNP Q7KYR7
B	310	GLY	-	expression tag	UNP Q7KYR7
B	311	ALA	-	expression tag	UNP Q7KYR7
B	312	GLY	-	expression tag	UNP Q7KYR7
B	313	ALA	-	expression tag	UNP Q7KYR7
B	314	GLY	-	expression tag	UNP Q7KYR7
B	315	ALA	-	expression tag	UNP Q7KYR7

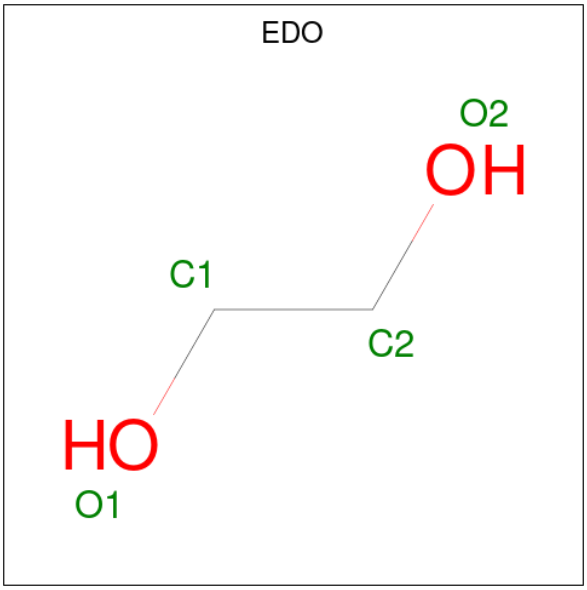
- Molecule 2 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	184	Total	C	N	O	S	0	1	0
			1498	967	252	273	6			
2	D	178	Total	C	N	O	S	0	0	0
			1437	926	242	263	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	296	MET	-	expression tag	UNP O00481
C	297	GLY	-	expression tag	UNP O00481
C	484	LEU	-	expression tag	UNP O00481
C	485	GLU	-	expression tag	UNP O00481
C	486	HIS	-	expression tag	UNP O00481
C	487	HIS	-	expression tag	UNP O00481
C	488	HIS	-	expression tag	UNP O00481
C	489	HIS	-	expression tag	UNP O00481
C	490	HIS	-	expression tag	UNP O00481
C	491	HIS	-	expression tag	UNP O00481
D	296	MET	-	expression tag	UNP O00481
D	297	GLY	-	expression tag	UNP O00481
D	484	LEU	-	expression tag	UNP O00481
D	485	GLU	-	expression tag	UNP O00481
D	486	HIS	-	expression tag	UNP O00481
D	487	HIS	-	expression tag	UNP O00481
D	488	HIS	-	expression tag	UNP O00481
D	489	HIS	-	expression tag	UNP O00481
D	490	HIS	-	expression tag	UNP O00481
D	491	HIS	-	expression tag	UNP O00481

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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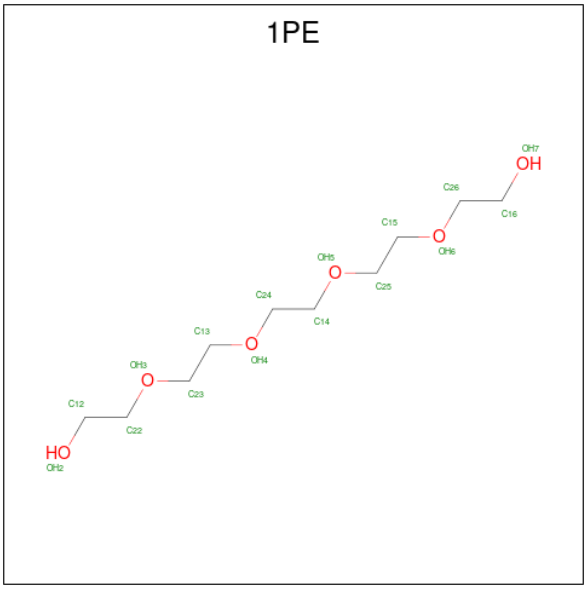
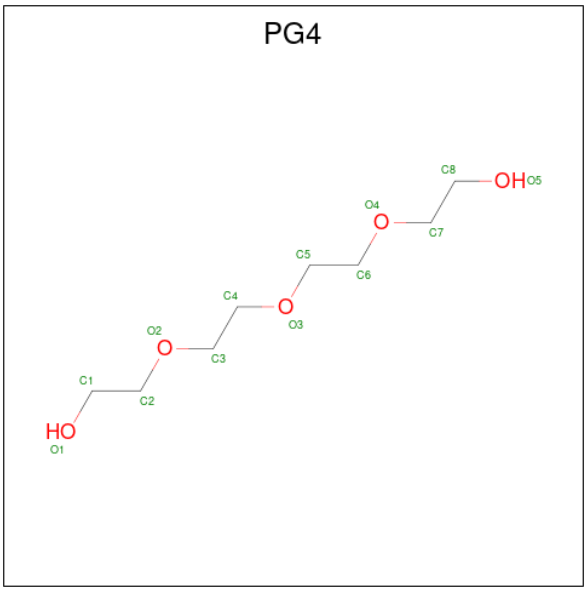
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



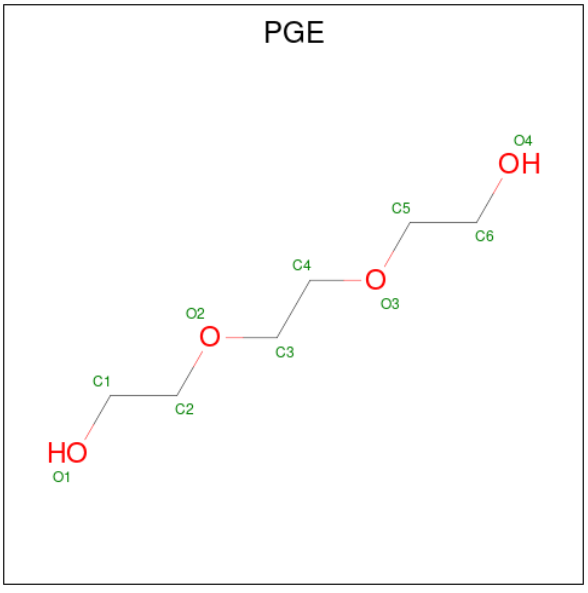
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 10 6	0	0
4	A	1	Total C O 16 10 6	0	0
4	A	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



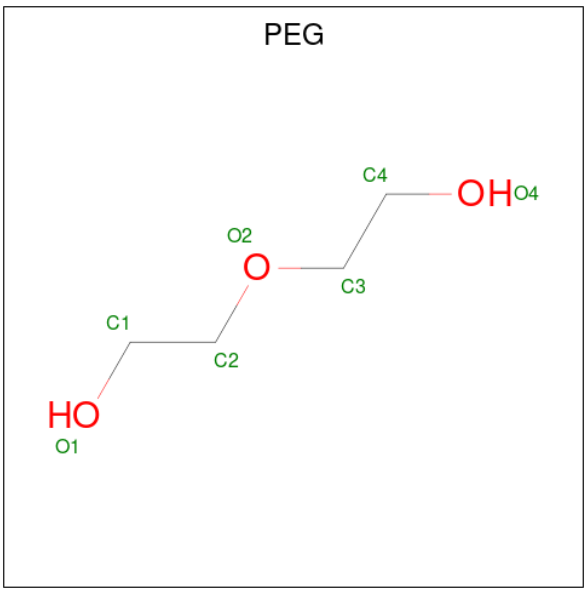
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	C	1	Total C O 13 8 5	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



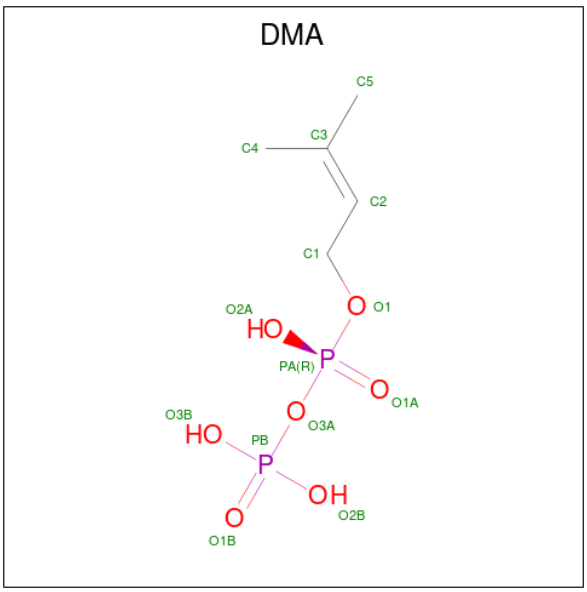
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0

- Molecule 8 is DIMETHYLALLYL DIPHOSPHATE (CCD ID: DMA) (formula: $C_5H_{12}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	O	P	0	0
			14	5	7	2		
8	D	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 9 is water.

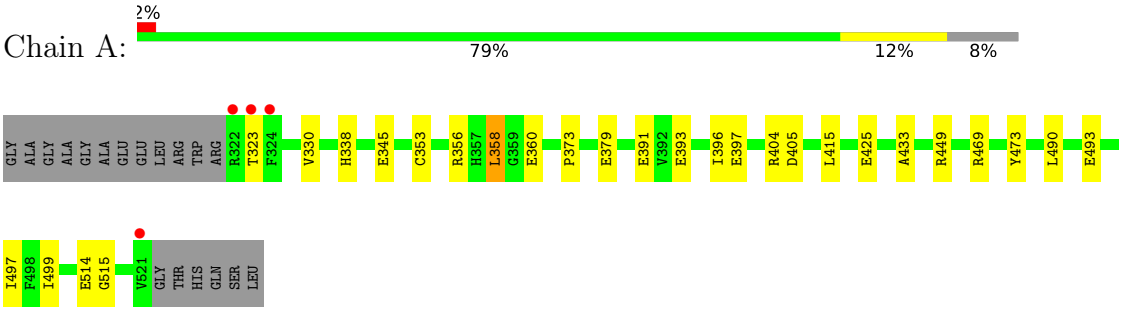
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	104	Total	O	0	0
			104	104		
9	B	94	Total	O	0	0
			94	94		
9	C	77	Total	O	0	0
			77	77		
9	D	55	Total	O	0	0
			55	55		

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.

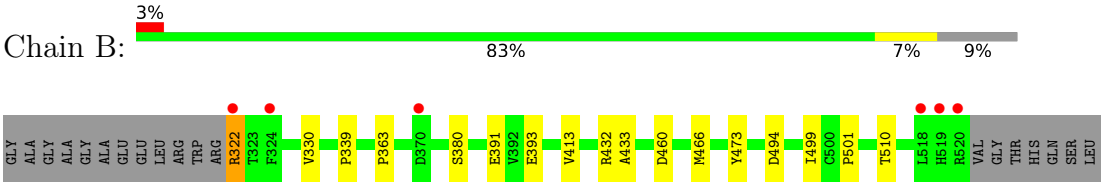
• Molecule 1: Butyrophilin subfamily 2 member A1

Chain A:



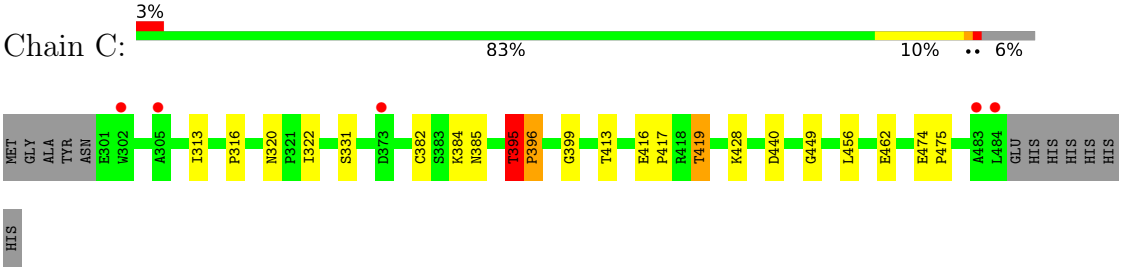
• Molecule 1: Butyrophilin subfamily 2 member A1

Chain B:



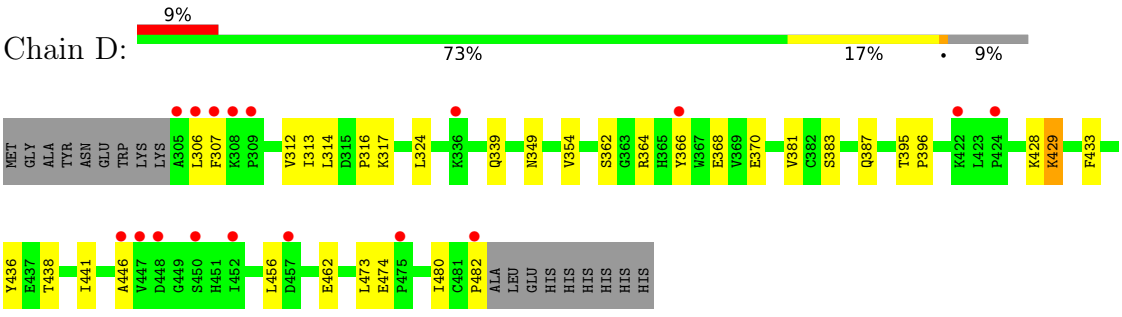
• Molecule 2: Butyrophilin subfamily 3 member A1

Chain C:



• Molecule 2: Butyrophilin subfamily 3 member A1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	90.15Å 90.15Å 167.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.29 47.60 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.60-2.29) 99.9 (47.60-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.171 , 0.216 0.179 , 0.220	Depositor DCC
R_{free} test set	3016 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, PGE, PEG, PG4, EDO, DMA

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	1.06	0/1658	1.27	3/2253 (0.1%)
1	B	1.07	1/1640 (0.1%)	1.27	5/2229 (0.2%)
2	C	1.06	2/1543 (0.1%)	1.33	3/2099 (0.1%)
2	D	1.03	1/1480 (0.1%)	1.36	3/2014 (0.1%)
All	All	1.05	4/6321 (0.1%)	1.31	14/8595 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	396	PRO	C-O	-5.87	1.16	1.24
2	C	316	PRO	C-O	-5.81	1.17	1.24
2	D	354	VAL	C-O	5.35	1.29	1.24
1	B	339	PRO	C-O	-5.33	1.17	1.24

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	395	THR	CB-CA-C	-7.65	98.11	109.97
2	C	428	LYS	N-CA-C	-6.80	105.27	113.97
2	D	438	THR	CB-CA-C	6.43	120.97	110.88
1	B	363	PRO	CB-CA-C	6.41	119.74	111.21
2	C	440	ASP	CA-CB-CG	6.27	118.87	112.60

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	1614	0	1563	18	0
1	B	1596	0	1542	7	0
2	C	1498	0	1469	9	0
2	D	1437	0	1407	14	0
3	A	8	0	12	1	0
3	B	16	0	24	0	0
3	C	8	0	12	1	0
4	A	48	0	66	3	0
4	C	16	0	22	0	0
5	A	26	0	36	4	0
5	C	13	0	18	0	0
6	A	10	0	14	0	0
7	B	21	0	30	1	0
8	C	14	0	9	0	0
8	D	14	0	9	0	0
9	A	104	0	0	2	0
9	B	94	0	0	3	0
9	C	77	0	0	1	0
9	D	55	0	0	2	0
All	All	6669	0	6233	49	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 4.

The worst 5 of 49 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)
2:D:387:GLN:HG3	9:D:636:HOH:O	1.83	0.78
1:A:404:ARG:HH11	4:A:603:1PE:H121	1.65	0.61
1:A:425:GLU:OE1	5:A:606:PG4:H71	2.03	0.59
1:B:432:ARG:HD3	9:B:747:HOH:O	2.03	0.59
2:D:312:VAL:HG12	2:D:480:ILE:HD13	1.85	0.58

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	199/218 (91%)	192 (96%)	7 (4%)	0	100	100
1	B	197/218 (90%)	191 (97%)	6 (3%)	0	100	100
2	C	183/196 (93%)	174 (95%)	9 (5%)	0	100	100
2	D	176/196 (90%)	160 (91%)	16 (9%)	0	100	100
All	All	755/828 (91%)	717 (95%)	38 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	180/190 (95%)	176 (98%)	4 (2%)	45	65
1	B	178/190 (94%)	174 (98%)	4 (2%)	45	65
2	C	166/175 (95%)	160 (96%)	6 (4%)	31	47
2	D	160/175 (91%)	152 (95%)	8 (5%)	22	33
All	All	684/730 (94%)	662 (97%)	22 (3%)	34	51

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	313	ILE
2	D	429	LYS
2	D	396	PRO

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Mol	Chain	Res	Type
2	D	456	LEU
1	B	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	519	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

21 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	EDO	B	605	-	3,3,3	0.15	0	2,2,2	0.24	0
8	DMA	C	501	-	12,13,13	0.71	0	15,19,19	1.46	4 (26%)
4	1PE	A	602	-	15,15,15	1.01	0	14,14,14	0.96	0
3	EDO	C	502	-	3,3,3	0.12	0	2,2,2	0.19	0
3	EDO	B	603	-	3,3,3	0.09	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	DMA	D	501	-	12,13,13	0.94	1 (8%)	15,19,19	1.04	1 (6%)
3	EDO	C	505	-	3,3,3	0.24	0	2,2,2	0.13	0
5	PG4	A	606	-	12,12,12	0.44	0	11,11,11	0.38	0
3	EDO	A	608	-	3,3,3	0.06	0	2,2,2	0.25	0
5	PG4	A	605	-	12,12,12	0.29	0	11,11,11	0.35	0
7	PEG	B	607	-	6,6,6	0.28	0	5,5,5	0.25	0
3	EDO	B	606	-	3,3,3	0.13	0	2,2,2	0.23	0
3	EDO	A	601	-	3,3,3	0.16	0	2,2,2	0.24	0
4	1PE	C	503	-	15,15,15	0.71	0	14,14,14	0.46	0
7	PEG	B	601	-	6,6,6	0.51	0	5,5,5	0.35	0
5	PG4	C	504	-	12,12,12	0.22	0	11,11,11	0.21	0
3	EDO	B	604	-	3,3,3	0.15	0	2,2,2	0.21	0
4	1PE	A	604	-	15,15,15	0.65	0	14,14,14	0.59	0
4	1PE	A	603	-	15,15,15	0.75	0	14,14,14	0.82	1 (7%)
7	PEG	B	602	-	6,6,6	0.44	0	5,5,5	0.28	0
6	PGE	A	607	-	9,9,9	0.55	0	8,8,8	0.26	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	EDO	B	605	-	-	0/1/1/1	-
8	DMA	C	501	-	-	2/13/13/13	-
4	1PE	A	602	-	-	4/13/13/13	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	B	603	-	-	1/1/1/1	-
8	DMA	D	501	-	-	3/13/13/13	-
3	EDO	C	505	-	-	1/1/1/1	-
5	PG4	A	606	-	-	2/10/10/10	-
3	EDO	A	608	-	-	1/1/1/1	-
5	PG4	A	605	-	-	2/10/10/10	-
7	PEG	B	607	-	-	1/4/4/4	-
3	EDO	B	606	-	-	1/1/1/1	-
3	EDO	A	601	-	-	1/1/1/1	-
4	1PE	C	503	-	-	2/13/13/13	-
7	PEG	B	601	-	-	1/4/4/4	-
5	PG4	C	504	-	-	4/10/10/10	-
3	EDO	B	604	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	A	604	-	-	6/13/13/13	-
4	1PE	A	603	-	-	8/13/13/13	-
7	PEG	B	602	-	-	1/4/4/4	-
6	PGE	A	607	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	DMA	PB-O2B	-2.10	1.47	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	501	DMA	C1-C2-C3	2.80	131.30	126.76
8	C	501	DMA	O3B-PB-O2B	2.21	116.10	107.80
4	A	603	1PE	C23-OH3-C22	2.18	122.79	113.26
8	C	501	DMA	O2A-PA-O3A	2.16	113.12	107.27
8	D	501	DMA	O3B-PB-O2B	2.13	115.79	107.80

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	501	DMA	PA-O3A-PB-O2B
8	D	501	DMA	PA-O3A-PB-O3B
5	C	504	PG4	O3-C5-C6-O4
4	A	603	1PE	OH4-C13-C23-OH3
5	C	504	PG4	O2-C3-C4-O3

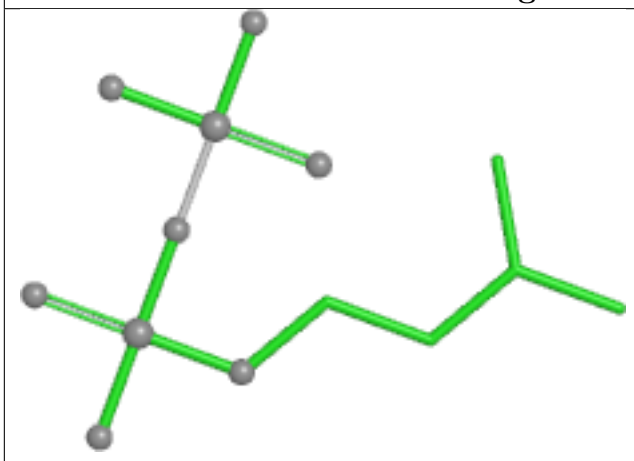
There are no ring outliers.

7 monomers are involved in 10 short contacts:

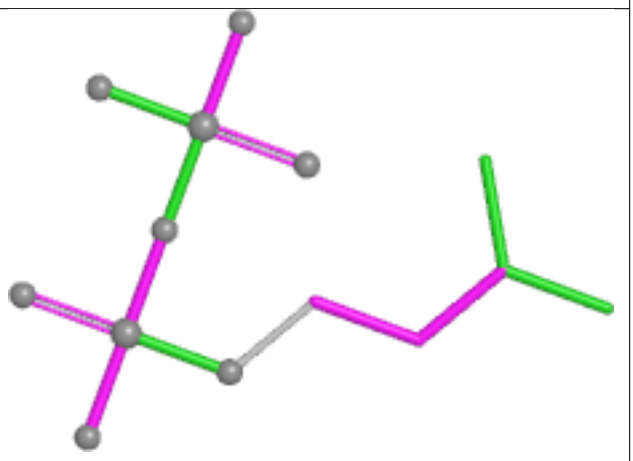
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	505	EDO	1	0
5	A	606	PG4	4	0
3	A	608	EDO	1	0
7	B	607	PEG	1	0
4	A	604	1PE	1	0
4	A	603	1PE	2	0
7	B	602	PEG	1	0

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 then 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.

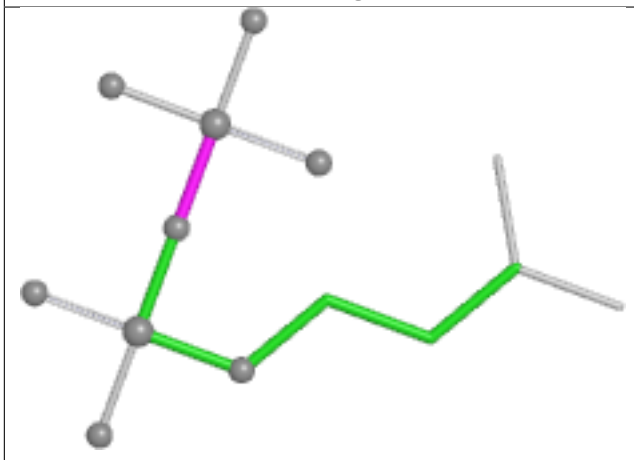
Ligand DMA C 501



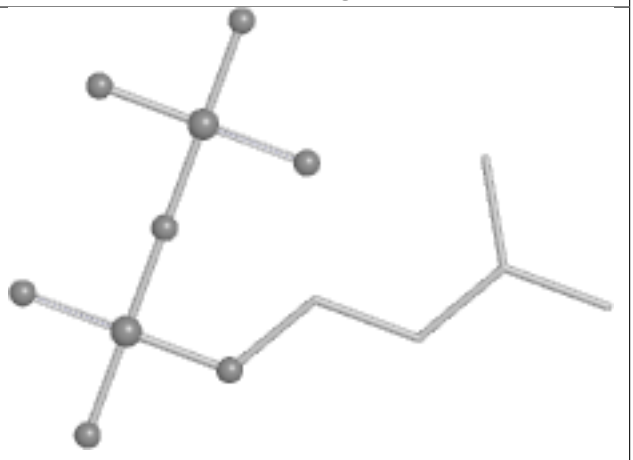
Bond lengths



Bond angles

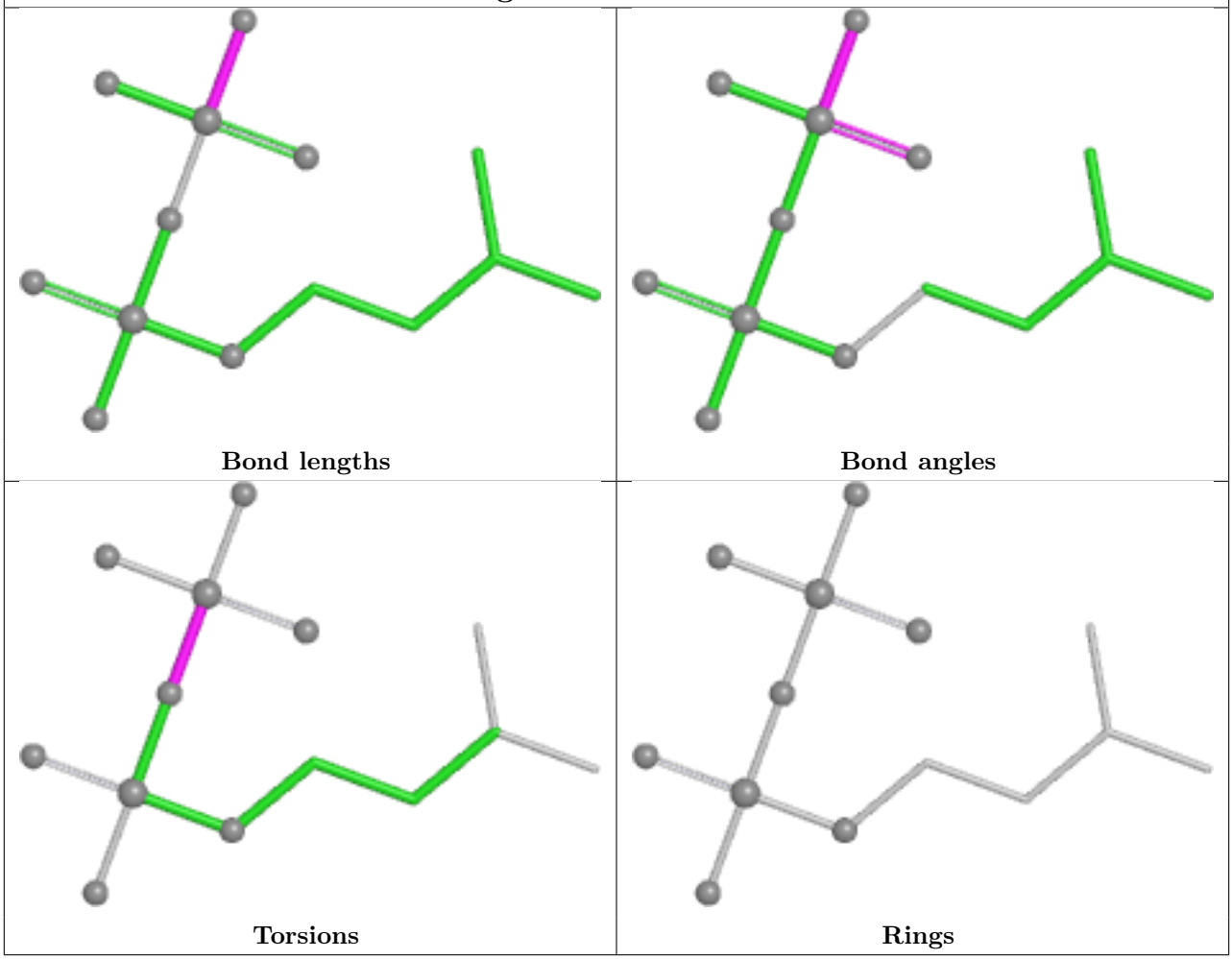


Torsions



Rings

Ligand DMA D 501



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	200/218 (91%)	-0.26	4 (2%)	65	66	15, 32, 54, 96	1 (0%)
1	B	199/218 (91%)	-0.14	6 (3%)	52	54	25, 36, 58, 85	0
2	C	184/196 (93%)	0.17	5 (2%)	56	58	17, 41, 65, 89	1 (0%)
2	D	178/196 (90%)	0.65	17 (9%)	13	15	31, 51, 76, 97	0
All	All	761/828 (91%)	0.09	32 (4%)	40	42	15, 38, 68, 97	2 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	306	LEU	6.6
1	A	521	VAL	5.4
2	C	484	LEU	5.2
2	D	305	ALA	5.0
1	A	324	PHE	3.9

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

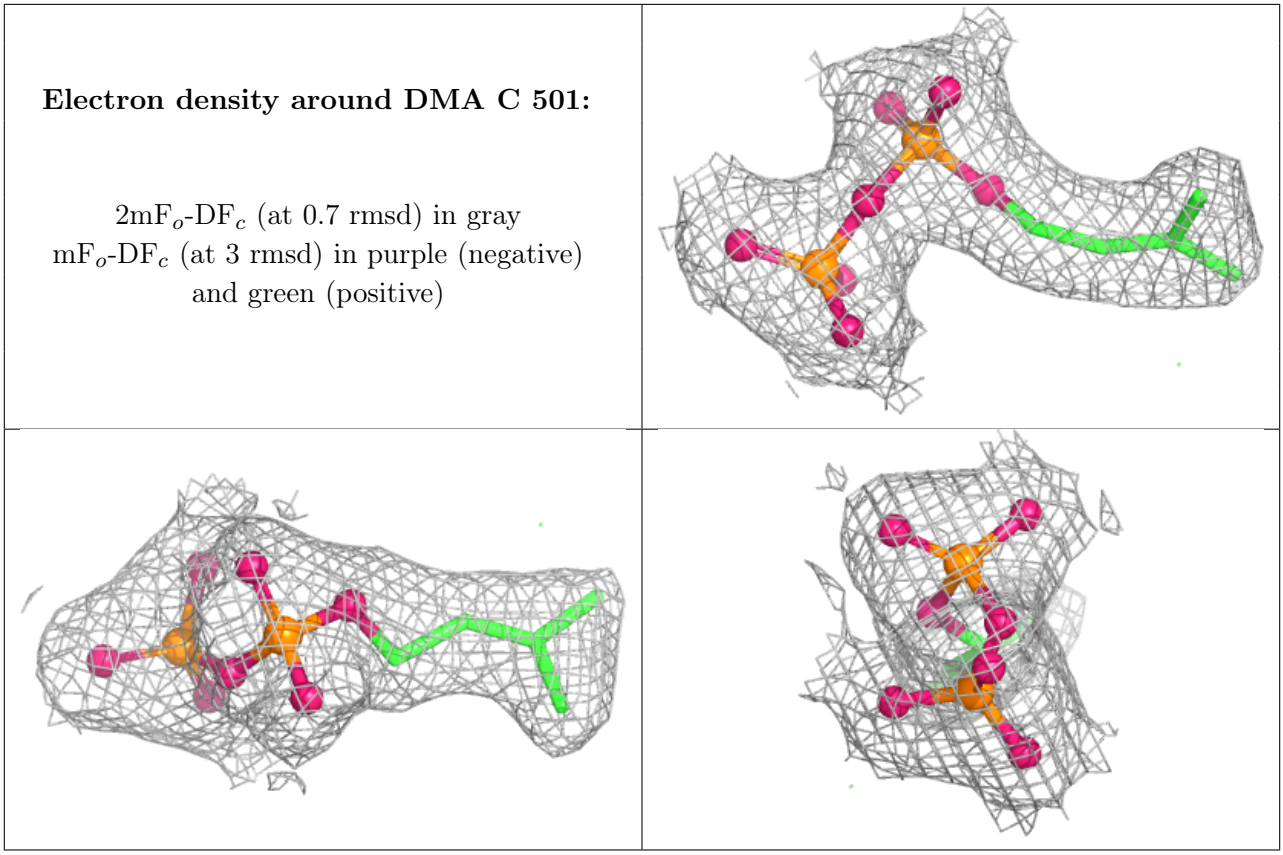
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PGE	A	607	10/10	0.79	0.20	47,60,68,68	0
3	EDO	B	603	4/4	0.85	0.18	64,64,69,74	0
4	1PE	A	604	16/16	0.86	0.22	59,81,92,92	0
4	1PE	A	603	16/16	0.86	0.20	42,75,90,91	0
4	1PE	A	602	16/16	0.88	0.19	43,67,82,83	0
7	PEG	B	602	7/7	0.88	0.16	50,51,63,64	0
7	PEG	B	607	7/7	0.88	0.17	48,63,73,75	0
5	PG4	A	606	13/13	0.89	0.17	47,58,72,78	0
5	PG4	C	504	13/13	0.90	0.15	52,68,82,82	0
7	PEG	B	601	7/7	0.91	0.17	56,61,70,74	0
3	EDO	B	604	4/4	0.91	0.16	61,61,62,69	0
3	EDO	C	505	4/4	0.91	0.17	62,64,64,70	0
3	EDO	A	608	4/4	0.92	0.14	63,64,64,69	0
3	EDO	B	606	4/4	0.92	0.18	56,60,62,64	0
3	EDO	A	601	4/4	0.92	0.11	40,47,49,52	0
3	EDO	B	605	4/4	0.93	0.13	50,55,56,62	0
3	EDO	C	502	4/4	0.93	0.15	63,64,67,69	0
4	1PE	C	503	16/16	0.94	0.10	40,50,57,58	0
5	PG4	A	605	13/13	0.95	0.12	35,45,66,66	0
8	DMA	C	501	14/14	0.99	0.05	24,28,32,36	0
8	DMA	D	501	14/14	0.99	0.05	27,32,38,42	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.

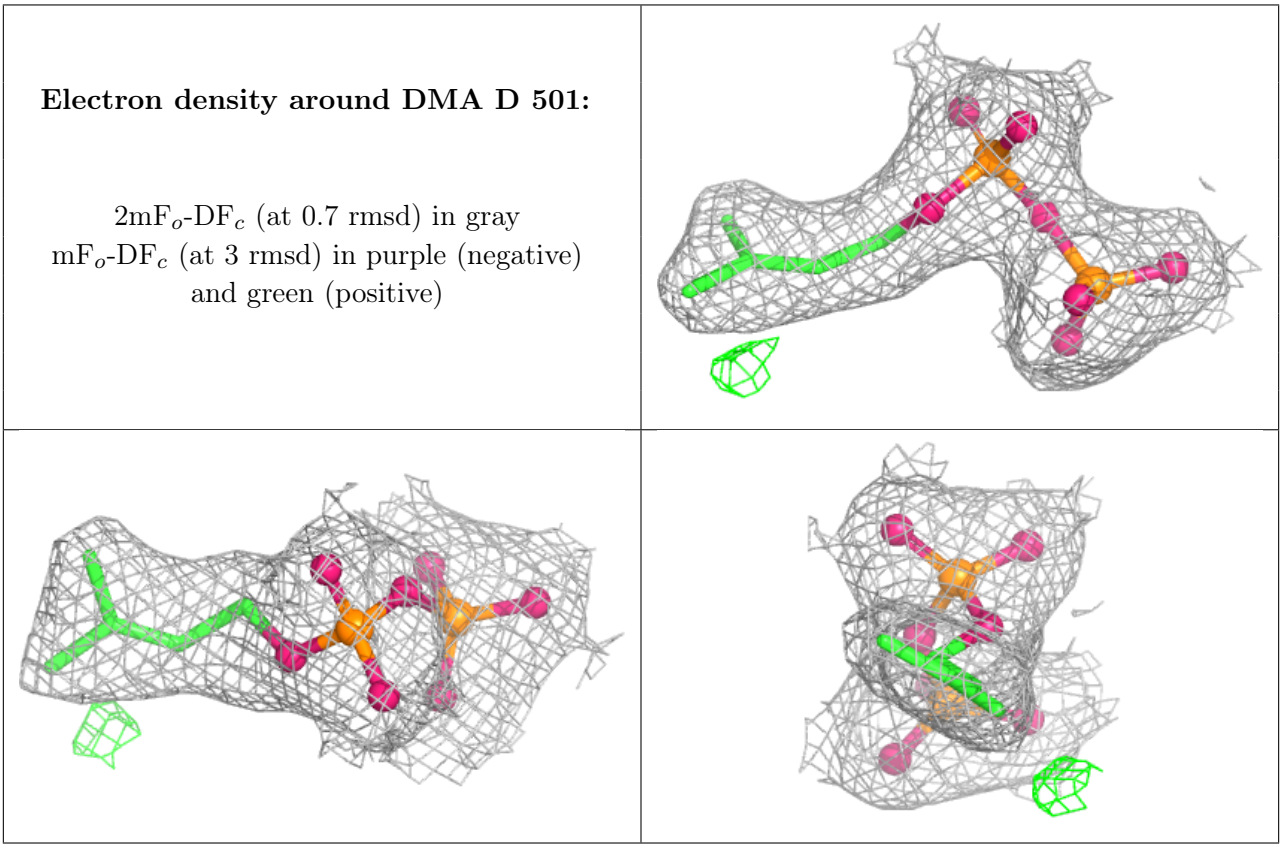
Electron density around DMA C 501:

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



Electron density around DMA D 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.