wwPDB X-ray Structure Validation Summary Report (i)

Nov 27, 2023 – 12:23 pm GMT

PDB ID	:	8P20
Title	:	TarM(Se)_G117R-UDP-4RboP-glucose
Authors	:	Guo, Y.; Stehle, T.
Deposited on	:	2023-05-14
Resolution	:	2.85 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:

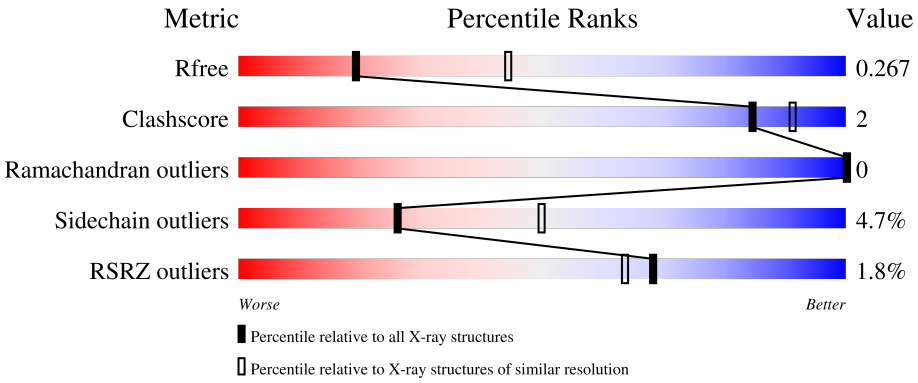
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	AAA	508	89% 8%
1	BBB	508	91% 6%
1	CCC	508	90% 7%
1	DDD	508	89% 8%

2 Entry composition (i)

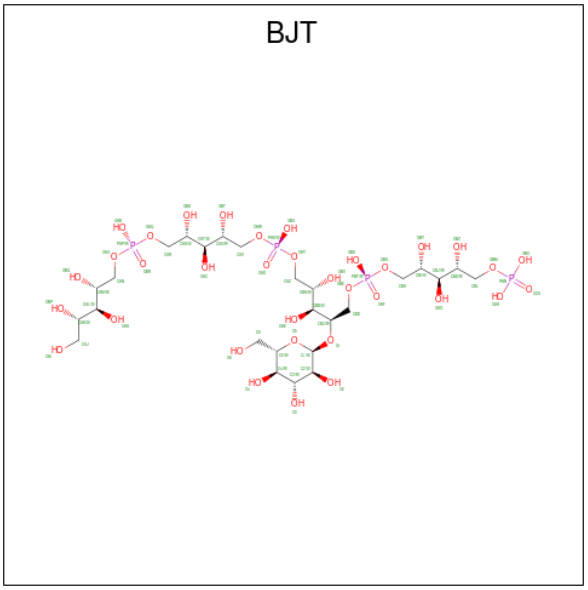
There are 7 unique types of molecules in this entry. The entry contains 15161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TarM(Se)_G117R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	492	Total	C	N	O	S	0	0	0
			3535	2264	590	666	15			
1	BBB	492	Total	C	N	O	S	0	0	0
			3507	2245	581	666	15			
1	CCC	492	Total	C	N	O	S	0	0	0
			3486	2214	592	667	13			
1	DDD	491	Total	C	N	O	S	0	0	0
			3476	2221	581	662	12			

- Molecule 2 is [(2 {R},3 {S},4 {S})-2-[(2 {S},3 {S},4 {R},5 {R},6 {S})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)-5-[oxidanyl-[(2 {R},3 {S},4 {S})-2,3,4-tris(oxidanyl)-5-[oxidanyl-[(2 {R},3 {S},4 {S})-2,3,4,5-tetrakis(oxidanyl)pentoxy]phosphoryl]oxy-pentoxy]phosphoryl]oxy-pentyl] [(2 {S},3 {R},4 {R})-2,3,4-tris(oxidanyl)-5-phosphonooxy-pentyl] hydrogen phosphate (three-letter code: BJT) (formula: $C_{26}H_{56}O_{34}P_4$) (labeled as "Ligand of Interest" by depositor).

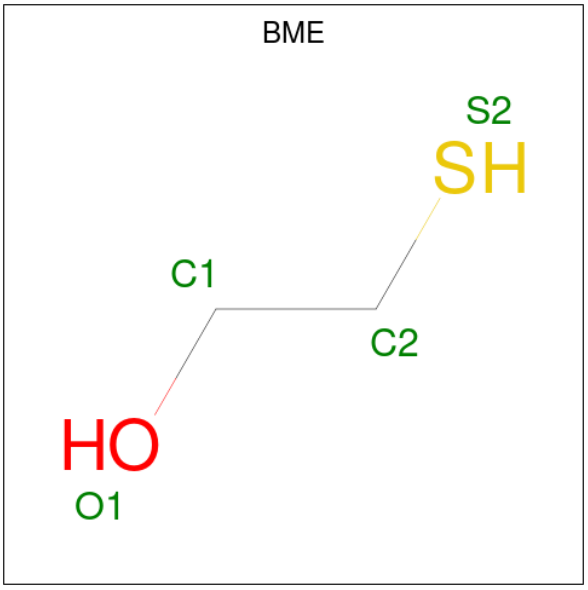


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	O	P	0	0
			64	26	34	4		
2	BBB	1	Total	C	O	P	0	0
			64	26	34	4		
2	CCC	1	Total	C	O	P	0	0
			64	26	34	4		
2	DDD	1	Total	C	O	P	0	0
			64	26	34	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Cl	0	0
			1	1		
3	CCC	1	Total	Cl	0	0
			1	1		
3	DDD	1	Total	Cl	0	0
			1	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		

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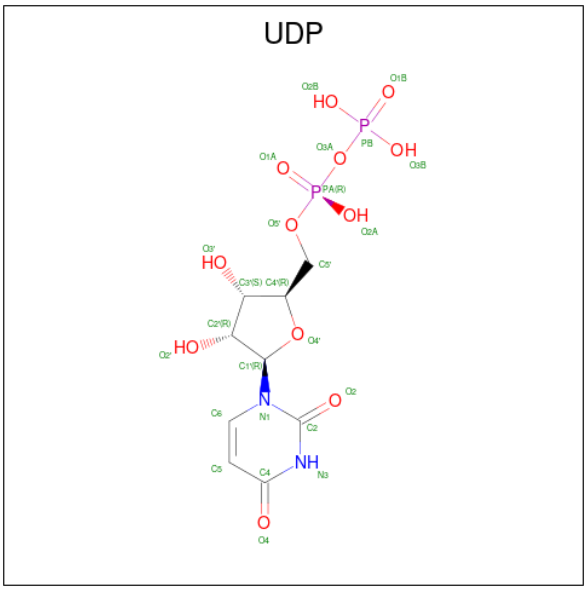
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C O S 4 2 1 1	0	0
4	BBB	1	Total C O S 4 2 1 1	0	0
4	CCC	1	Total C O S 4 2 1 1	0	0
4	CCC	1	Total C O S 4 2 1 1	0	0
4	CCC	1	Total C O S 4 2 1 1	0	0
4	CCC	1	Total C O S 4 2 1 1	0	0
4	CCC	1	Total C O S 4 2 1 1	0	0
4	DDD	1	Total C O S 4 2 1 1	0	0
4	DDD	1	Total C O S 4 2 1 1	0	0
4	DDD	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C N O P 25 9 2 12 2	0	0

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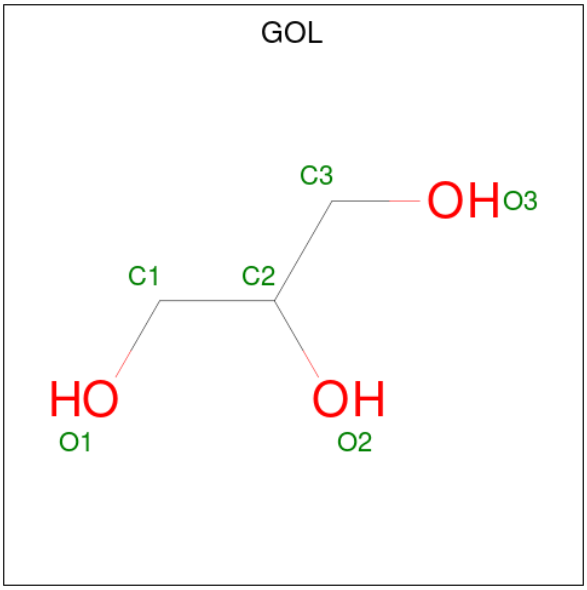
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	BBB	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	CCC	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	DDD	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			6	3	3		
6	BBB	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

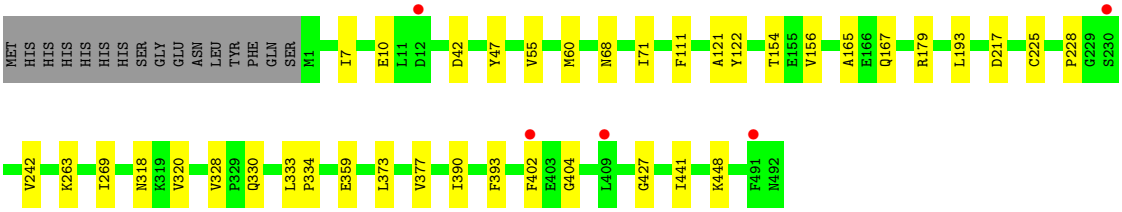
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	189	Total	O	0	0
			189	189		
7	BBB	191	Total	O	0	0
			191	191		
7	CCC	173	Total	O	0	0
			173	173		
7	DDD	181	Total	O	0	0
			181	181		

3 Residue-property plots (i)

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

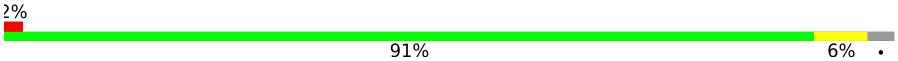
• Molecule 1: TarM(Se)_G117R

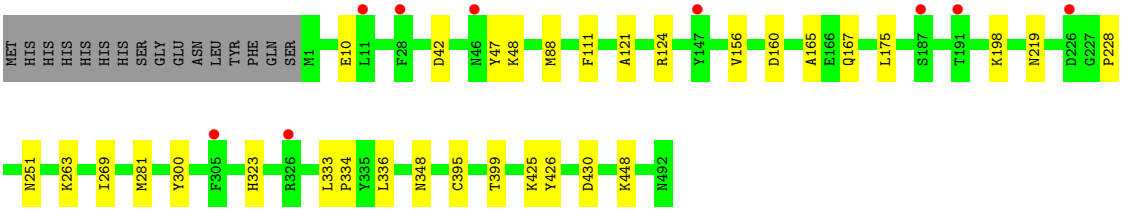
Chain AAA:



• Molecule 1: TarM(Se)_G117R

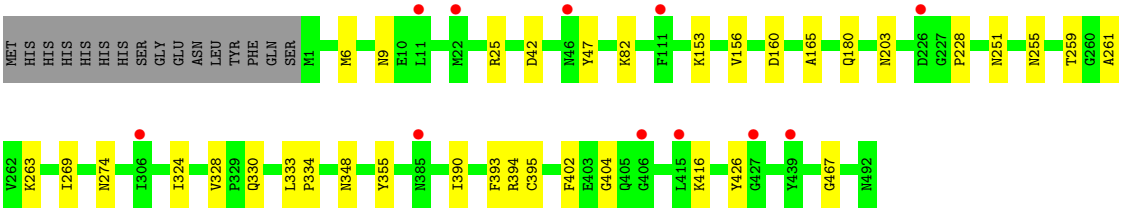
Chain BBB:





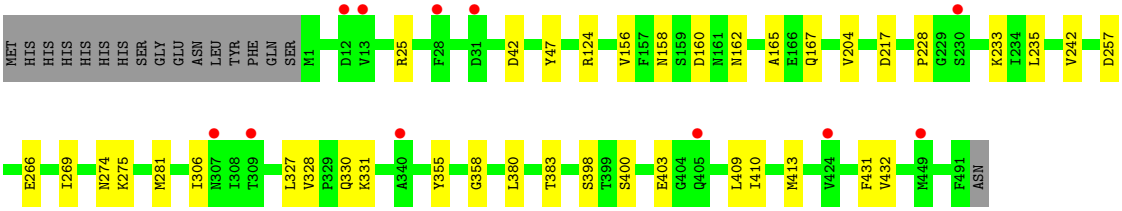
• Molecule 1: TarM(Se)_G117R

Chain CCC:



• Molecule 1: TarM(Se)_G117R

Chain DDD:


MET HIS HIS HIS HIS HIS SER GLY GLU ASN LEU TYR PHE GLN SER M1 D12 V13 R25 F28 D31 D42 Y47 R124 V156 F157 N158 S159 D160 N161 N162 A165 E166 Q167 V204 D217 P228 G229 S230 K233 I234 L235 V242 D257
E266 I269 N274 K275 M281 I306 N307 I308 T309 L327 V328 P329 Q330 K331 A340 Y355 G358 L380 T383 S398 T399 S400 E403 G404 Q405 L409 I410 M413 V424 F431 V432 M449 F491 ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.62Å 75.75Å 129.40Å 90.02° 90.04° 90.03°	Depositor
Resolution (Å)	49.20 – 2.85 49.20 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-2.85) 99.7 (49.20-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.266 0.232 , 0.267	Depositor DCC
R_{free} test set	2599 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 85.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l 0.398 for -h,k,-l 0.399 for -h,-k,l	Xtriage
Reported twinning fraction	0.414 for H, K, L 0.151 for -H, K, -L 0.163 for -h,-k,l 0.273 for h,-k,-l	Depositor
Outliers	0 of 51972 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15161	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: BJT, GOL, CL, BME, UDP

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	AAA	0.64	0/3601	0.65	0/4902
1	BBB	0.64	0/3574	0.65	0/4861
1	CCC	0.64	0/3551	0.67	0/4837
1	DDD	0.63	0/3540	0.67	0/4820
All	All	0.64	0/14266	0.66	0/19420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3535	0	2847	18	0
1	BBB	3507	0	2822	9	0
1	CCC	3486	0	2775	12	0
1	DDD	3476	0	2769	19	0
2	AAA	64	0	0	0	0
2	BBB	64	0	0	0	0
2	CCC	64	0	0	0	0
2	DDD	64	0	0	0	0
3	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	12	0	18	0	0
4	BBB	8	0	12	0	0
4	CCC	20	0	30	0	0
4	DDD	12	0	18	0	0
5	AAA	25	0	11	0	0
5	BBB	25	0	11	0	0
5	CCC	25	0	11	0	0
5	DDD	25	0	11	0	0
6	BBB	12	0	16	0	0
7	AAA	189	0	0	0	0
7	BBB	191	0	0	0	0
7	CCC	173	0	0	0	0
7	DDD	181	0	0	0	0
All	All	15161	0	11351	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 2.

The worst 5 of 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:BBB:167:GLN:HB3	1:BBB:175:LEU:HD11	1.73	0.70
1:CCC:255:ASN:HD21	1:CCC:263:LYS:NZ	1.95	0.64
1:DDD:413:MET:HE3	1:DDD:431:PHE:CD1	2.35	0.61
1:AAA:156:VAL:HB	1:AAA:165:ALA:HB3	1.82	0.61
1:DDD:413:MET:CE	1:DDD:431:PHE:CD1	2.84	0.60

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	AAA	490/508 (96%)	454 (93%)	36 (7%)	0	100	100
1	BBB	490/508 (96%)	452 (92%)	38 (8%)	0	100	100
1	CCC	490/508 (96%)	458 (94%)	32 (6%)	0	100	100
1	DDD	489/508 (96%)	447 (91%)	42 (9%)	0	100	100
All	All	1959/2032 (96%)	1811 (92%)	148 (8%)	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	AAA	262/471 (56%)	255 (97%)	7 (3%)	44	69
1	BBB	260/471 (55%)	245 (94%)	15 (6%)	20	38
1	CCC	256/471 (54%)	241 (94%)	15 (6%)	19	37
1	DDD	252/471 (54%)	241 (96%)	11 (4%)	28	53
All	All	1030/1884 (55%)	982 (95%)	48 (5%)	26	50

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	153	LYS
1	CCC	394	ARG
1	CCC	160	ASP
1	CCC	251	ASN
1	DDD	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 3 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
4	BME	CCC	505	-	3,3,3	0.13	0	1,2,2	0.09	0
4	BME	DDD	504	-	3,3,3	0.14	0	1,2,2	0.11	0
4	BME	AAA	504	-	3,3,3	0.12	0	1,2,2	0.08	0
4	BME	BBB	502	-	3,3,3	0.13	0	1,2,2	0.16	0
4	BME	CCC	507	-	3,3,3	0.13	0	1,2,2	0.10	0
5	UDP	BBB	506	-	24,26,26	1.13	3 (12%)	37,40,40	1.61	4 (10%)
5	UDP	CCC	508	-	24,26,26	1.13	3 (12%)	37,40,40	1.61	4 (10%)
5	UDP	DDD	506	-	24,26,26	1.12	3 (12%)	37,40,40	1.65	6 (16%)
2	BJT	DDD	501	-	64,64,64	0.91	2 (3%)	89,93,93	0.86	4 (4%)
2	BJT	BBB	501	-	64,64,64	0.90	2 (3%)	89,93,93	0.93	5 (5%)
4	BME	AAA	505	-	3,3,3	0.13	0	1,2,2	0.13	0
4	BME	BBB	503	-	3,3,3	0.13	0	1,2,2	0.11	0
6	GOL	BBB	505	-	5,5,5	0.08	0	5,5,5	0.24	0
4	BME	CCC	503	-	3,3,3	0.13	0	1,2,2	0.05	0
4	BME	CCC	506	-	3,3,3	0.13	0	1,2,2	0.06	0
4	BME	AAA	503	-	3,3,3	0.14	0	1,2,2	0.17	0
4	BME	DDD	505	-	3,3,3	0.13	0	1,2,2	0.17	0
2	BJT	CCC	501	-	64,64,64	0.89	3 (4%)	89,93,93	0.85	4 (4%)
4	BME	DDD	503	-	3,3,3	0.14	0	1,2,2	0.08	0
4	BME	CCC	504	-	3,3,3	0.13	0	1,2,2	0.12	0
5	UDP	AAA	506	-	24,26,26	1.15	3 (12%)	37,40,40	1.57	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	BBB	504	-	5,5,5	0.09	0	5,5,5	0.22	0
2	BJT	AAA	501	-	64,64,64	0.89	2 (3%)	89,93,93	0.89	3 (3%)

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
4	BME	CCC	505	-	-	0/1/1/1	-
4	BME	DDD	504	-	-	1/1/1/1	-
4	BME	AAA	504	-	-	1/1/1/1	-
4	BME	BBB	502	-	-	1/1/1/1	-
4	BME	CCC	507	-	-	0/1/1/1	-
5	UDP	BBB	506	-	-	4/16/32/32	0/2/2/2
5	UDP	CCC	508	-	-	3/16/32/32	0/2/2/2
5	UDP	DDD	506	-	-	4/16/32/32	0/2/2/2
2	BJT	DDD	501	-	-	42/82/102/102	0/1/1/1
2	BJT	BBB	501	-	-	52/82/102/102	0/1/1/1
4	BME	AAA	505	-	-	1/1/1/1	-
4	BME	BBB	503	-	-	1/1/1/1	-
6	GOL	BBB	505	-	-	2/4/4/4	-
4	BME	CCC	503	-	-	0/1/1/1	-
4	BME	CCC	506	-	-	1/1/1/1	-
4	BME	AAA	503	-	-	1/1/1/1	-
4	BME	DDD	505	-	-	1/1/1/1	-
2	BJT	CCC	501	-	-	42/82/102/102	0/1/1/1
4	BME	DDD	503	-	-	0/1/1/1	-
4	BME	CCC	504	-	-	1/1/1/1	-
5	UDP	AAA	506	-	-	3/16/32/32	0/2/2/2
6	GOL	BBB	504	-	-	0/4/4/4	-
2	BJT	AAA	501	-	-	43/82/102/102	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	501	BJT	PBN-OCA	3.73	1.62	1.50
2	AAA	501	BJT	PBN-OCA	3.68	1.62	1.50
2	DDD	501	BJT	PBN-OCA	3.60	1.62	1.50
2	BBB	501	BJT	PBN-OCA	3.58	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	501	BJT	PAP-OBR	3.20	1.62	1.50

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AAA	506	UDP	C4-N3-C2	-4.87	120.16	126.58
5	BBB	506	UDP	C4-N3-C2	-4.83	120.22	126.58
5	CCC	508	UDP	C4-N3-C2	-4.82	120.22	126.58
5	DDD	506	UDP	C4-N3-C2	-4.75	120.32	126.58
5	BBB	506	UDP	N3-C2-N1	4.34	120.65	114.89

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

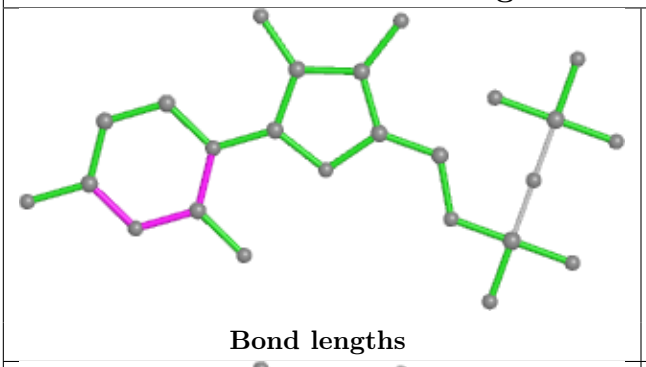
Mol	Chain	Res	Type	Atoms
2	AAA	501	BJT	CBL-OBM-PBN-OBO
2	AAA	501	BJT	CBL-OBM-PBN-OAH
2	AAA	501	BJT	CBI-CBJ-CBK-CBL
2	AAA	501	BJT	OBG-CBH-CBI-CBJ
2	AAA	501	BJT	OBG-CBH-CBI-OBY

There are no ring outliers.

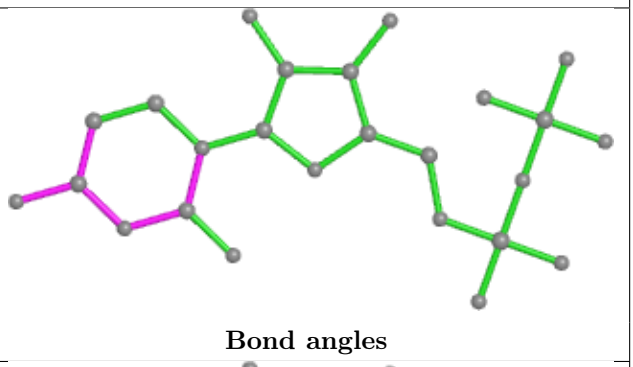
No monomer is involved in short contacts.

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.

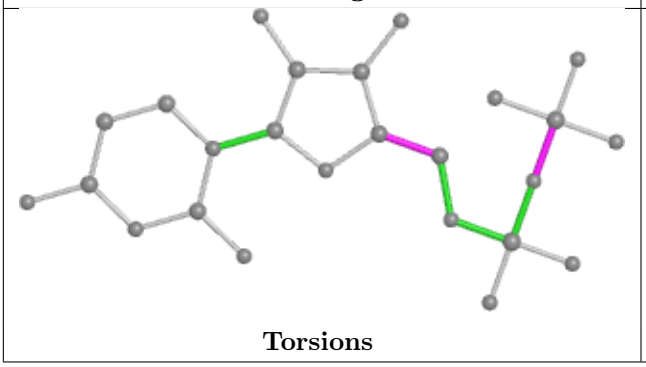
Ligand UDP BBB 506



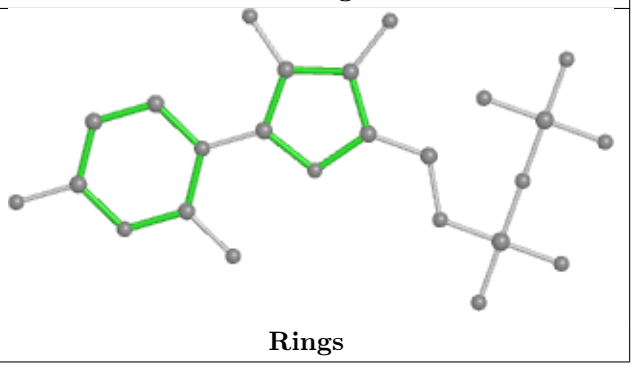
Bond lengths



Bond angles

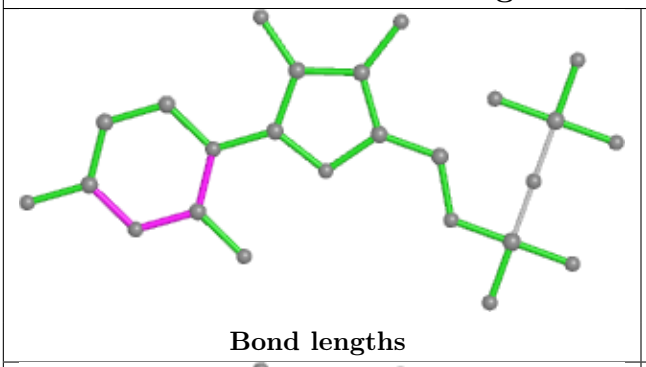


Torsions

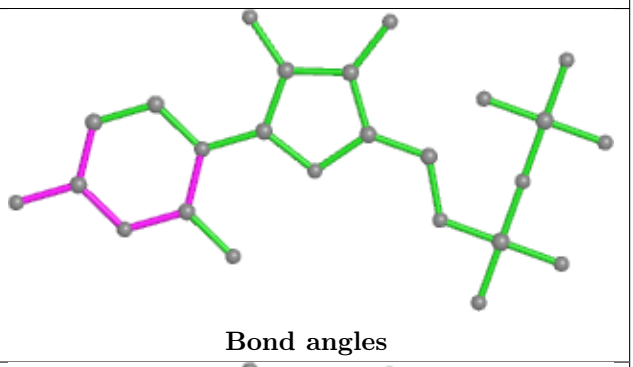


Rings

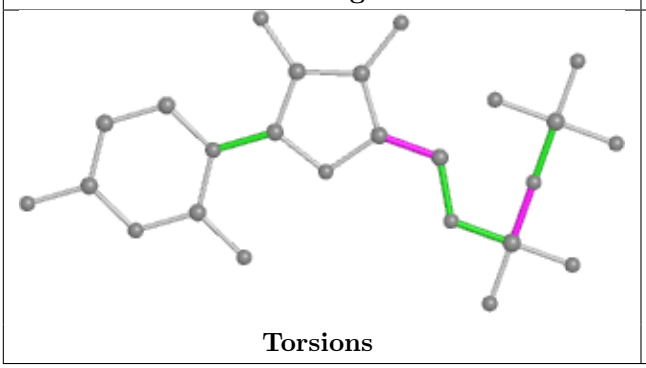
Ligand UDP CCC 508



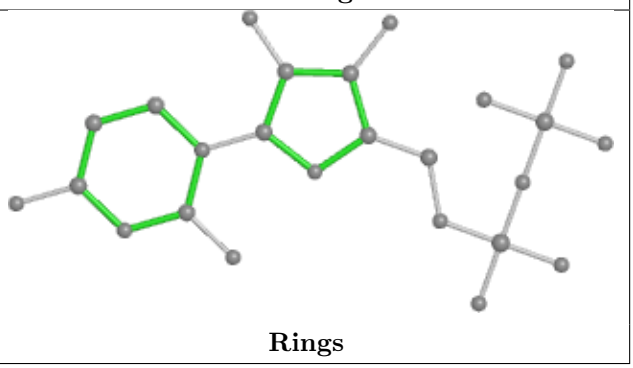
Bond lengths



Bond angles

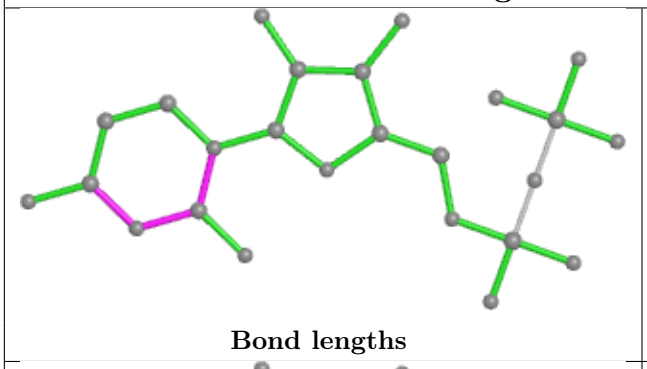


Torsions

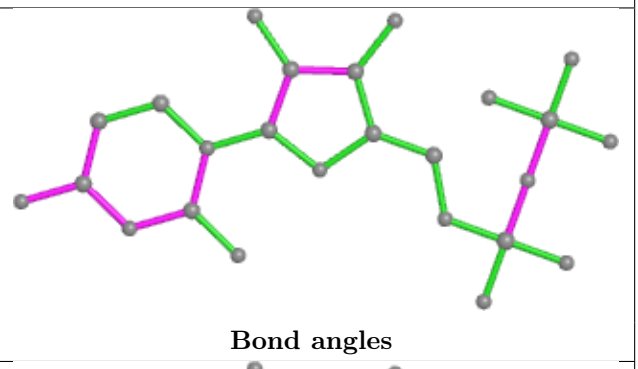


Rings

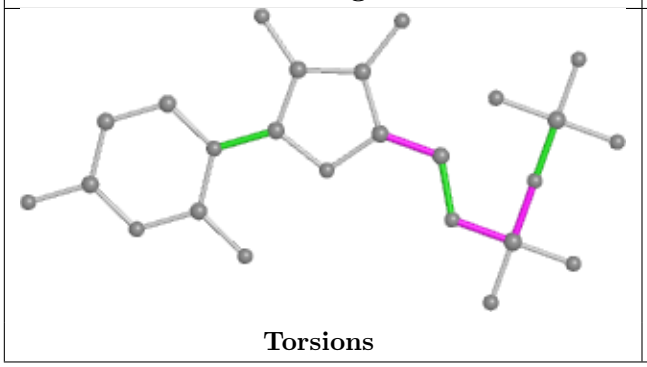
Ligand UDP DDD 506



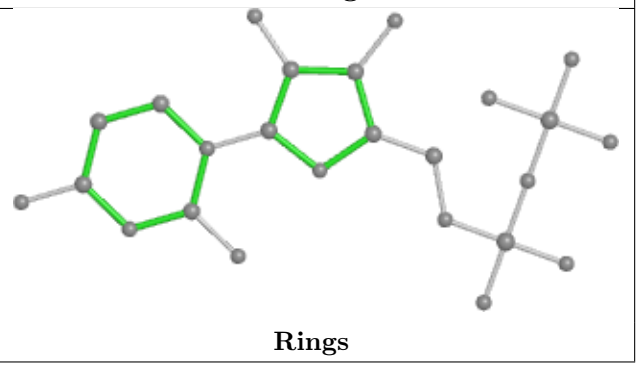
Bond lengths



Bond angles

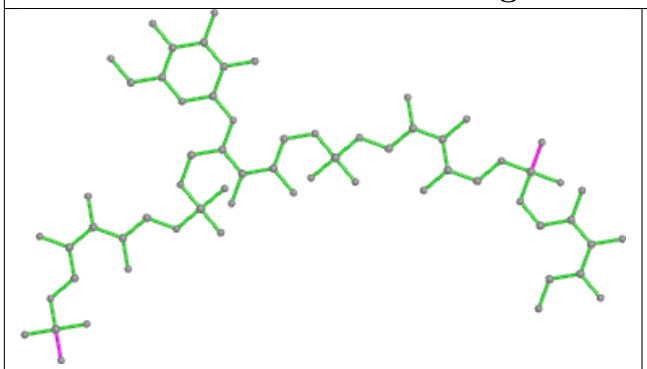


Torsions

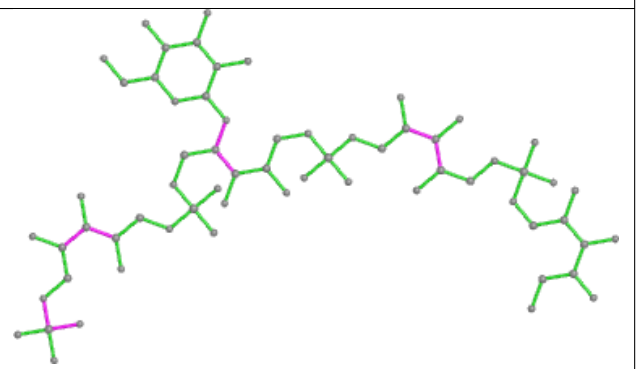


Rings

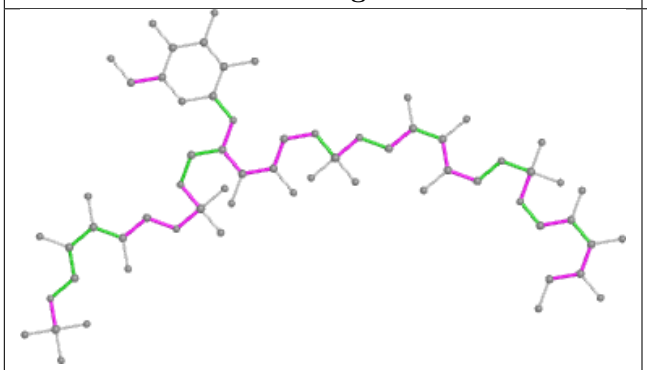
Ligand BJT DDD 501



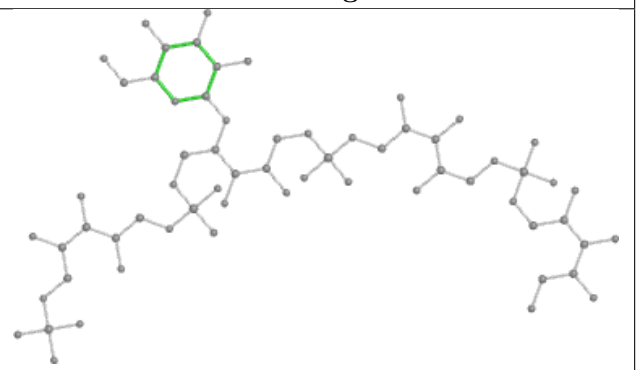
Bond lengths



Bond angles

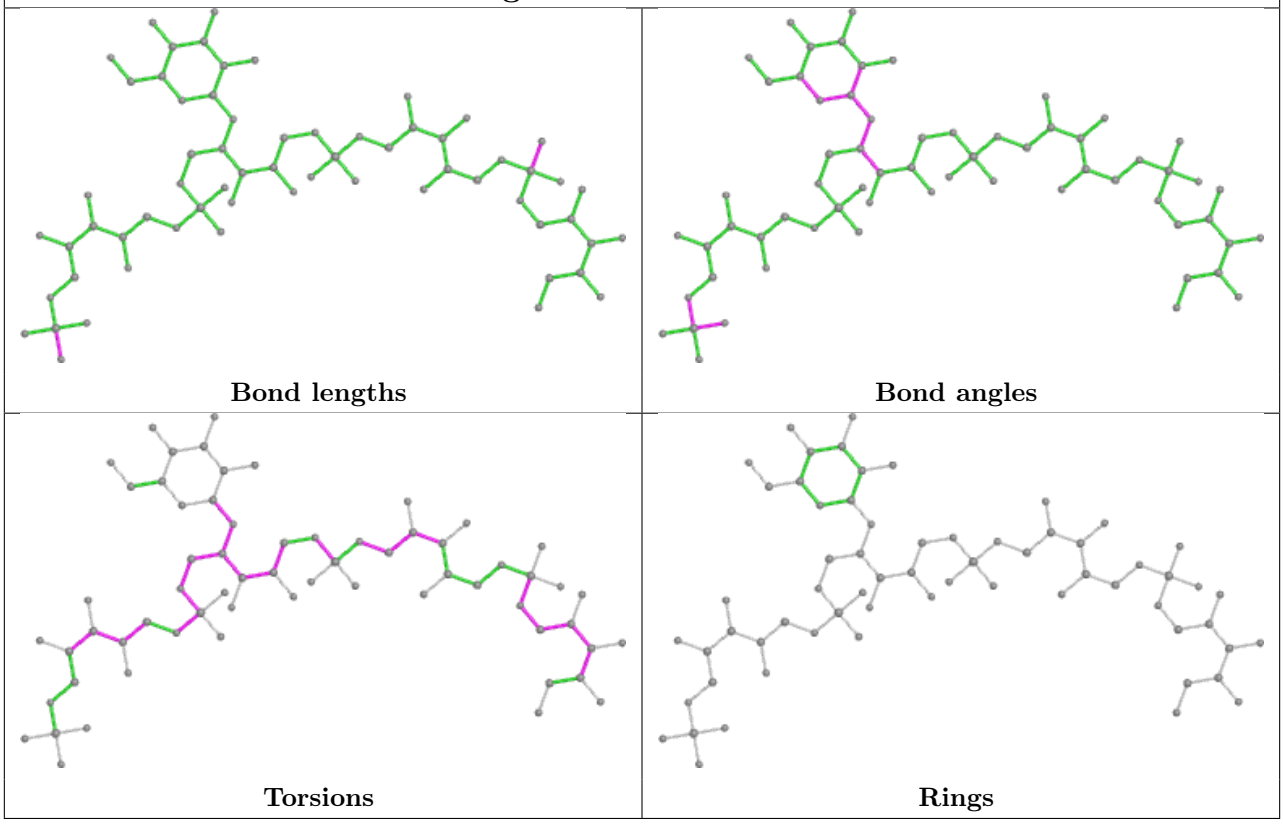


Torsions

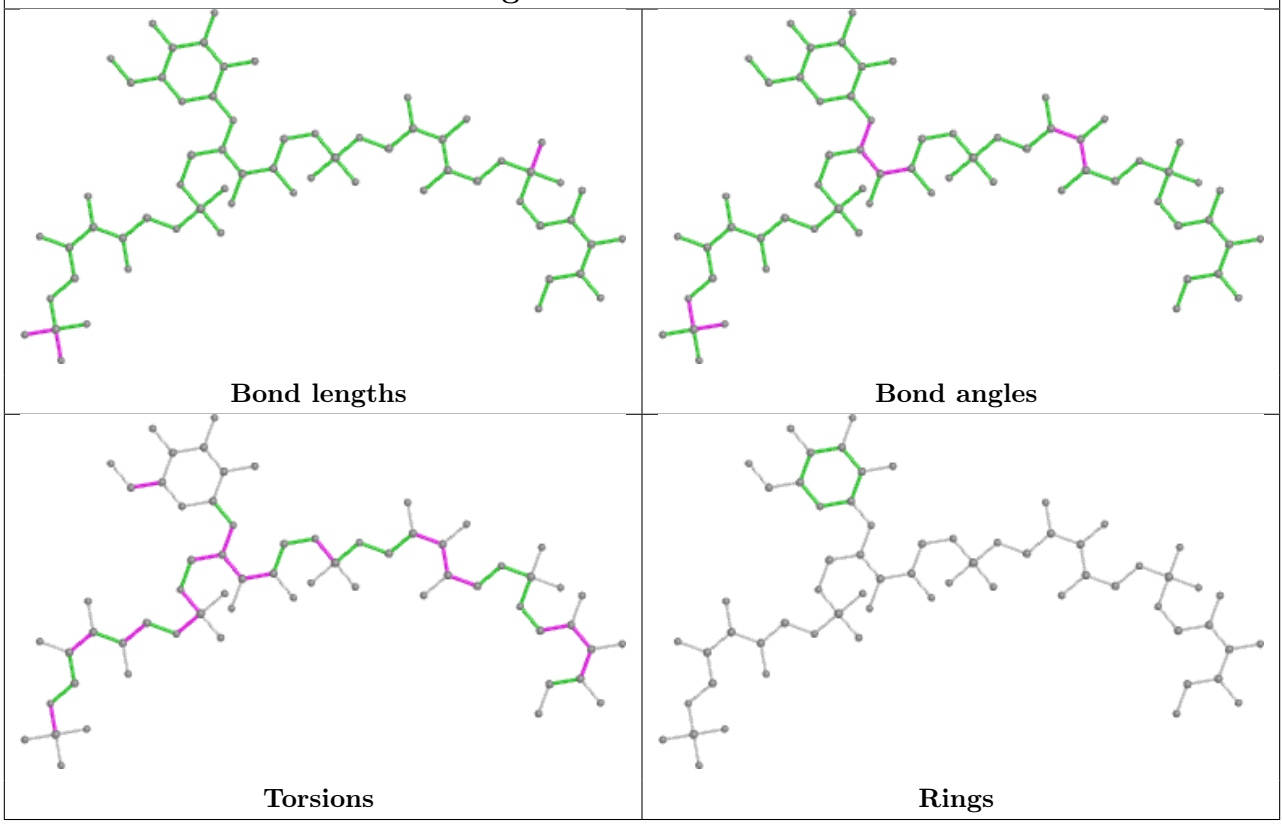


Rings

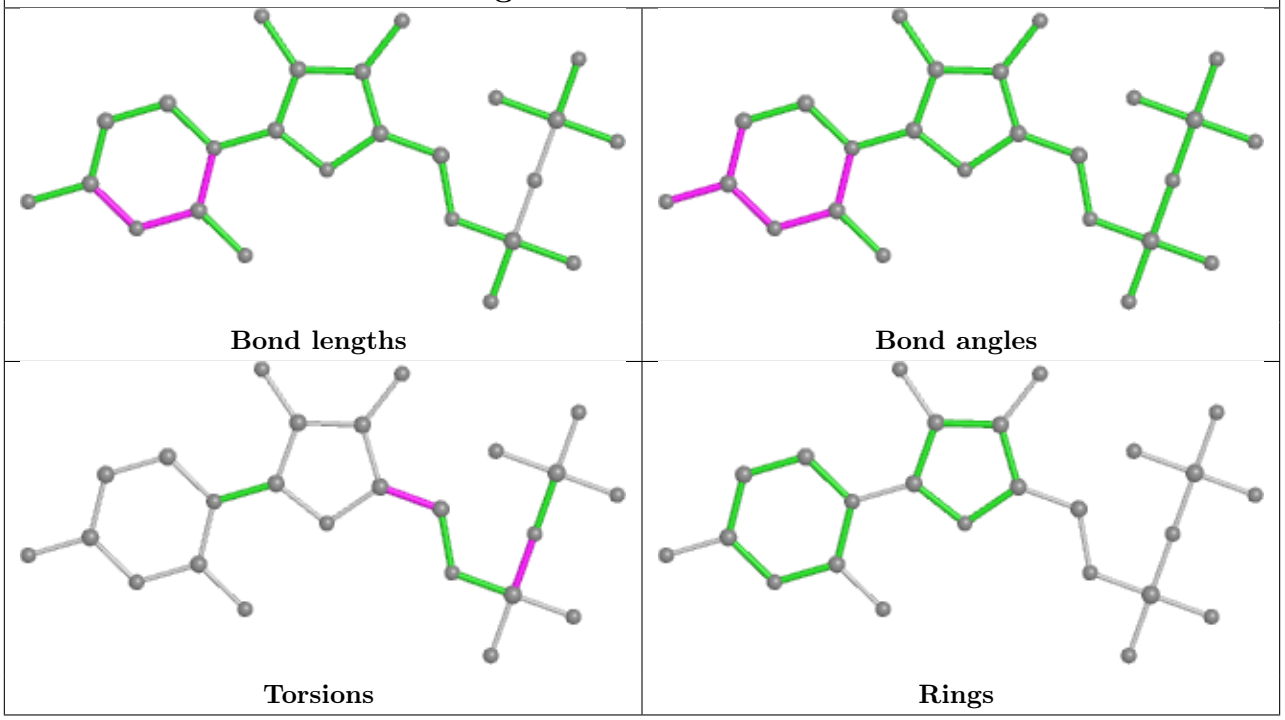
Ligand BJT BBB 501



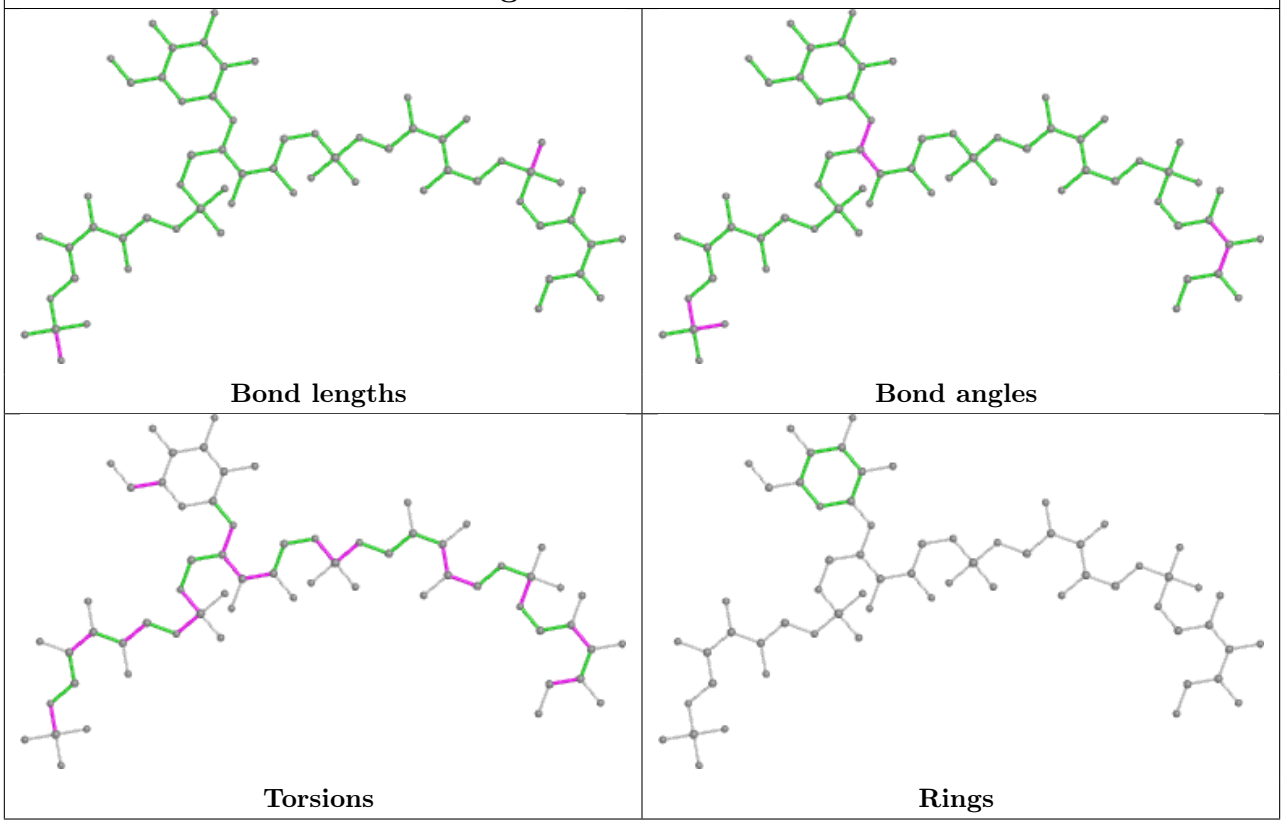
Ligand BJT CCC 501



Ligand UDP AAA 506



Ligand BJT AAA 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, 95^{th} 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	AAA	492/508 (96%)	-0.24	5 (1%)	82	79	42, 58, 71, 84	0
1	BBB	492/508 (96%)	-0.22	9 (1%)	68	63	38, 60, 73, 87	0
1	CCC	492/508 (96%)	-0.21	11 (2%)	62	57	43, 61, 76, 85	0
1	DDD	491/508 (96%)	-0.25	11 (2%)	62	57	43, 61, 73, 79	0
All	All	1967/2032 (96%)	-0.23	36 (1%)	68	63	38, 60, 73, 87	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	12	ASP	6.9
1	DDD	13	VAL	4.5
1	CCC	46	ASN	4.1
1	DDD	28	PHE	3.6
1	BBB	11	LEU	3.3

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 monosaccharides in this entry.

6.4 Ligands

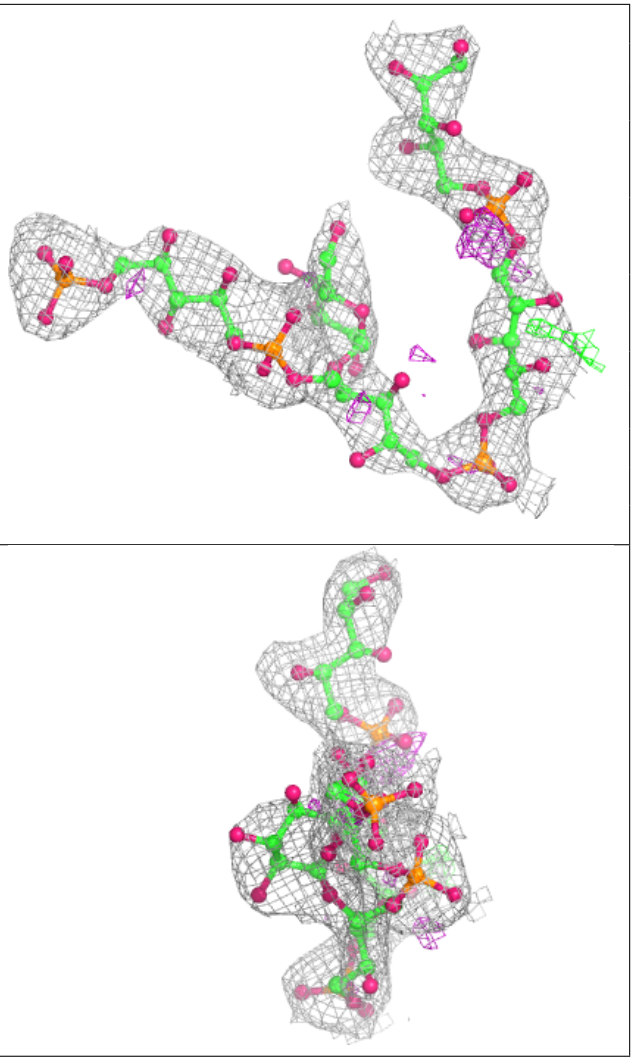
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GOL	BBB	504	6/6	0.83	0.18	78,82,83,84	0
4	BME	CCC	506	4/4	0.84	0.18	90,92,93,98	0
4	BME	CCC	503	4/4	0.86	0.24	74,79,82,86	0
2	BJT	DDD	501	64/64	0.86	0.30	52,66,82,88	0
4	BME	BBB	502	4/4	0.86	0.15	67,70,72,75	0
2	BJT	CCC	501	64/64	0.87	0.24	55,67,86,90	0
2	BJT	BBB	501	64/64	0.87	0.27	58,69,83,86	0
3	CL	DDD	502	1/1	0.88	0.10	92,92,92,92	0
4	BME	DDD	504	4/4	0.89	0.17	95,99,102,104	0
4	BME	BBB	503	4/4	0.90	0.25	70,72,73,75	0
2	BJT	AAA	501	64/64	0.90	0.24	51,64,79,81	0
4	BME	CCC	504	4/4	0.90	0.15	65,67,67,69	0
6	GOL	BBB	505	6/6	0.91	0.14	90,91,96,98	0
3	CL	AAA	502	1/1	0.92	0.15	63,63,63,63	0
4	BME	AAA	503	4/4	0.92	0.14	75,75,77,77	0
4	BME	CCC	505	4/4	0.94	0.11	79,85,87,90	0
5	UDP	BBB	506	25/25	0.94	0.14	35,39,42,44	0
4	BME	DDD	503	4/4	0.96	0.18	81,81,82,84	0
5	UDP	DDD	506	25/25	0.96	0.14	38,41,50,50	0
3	CL	CCC	502	1/1	0.96	0.22	70,70,70,70	0
5	UDP	AAA	506	25/25	0.96	0.13	34,37,41,44	0
4	BME	CCC	507	4/4	0.97	0.07	40,40,41,42	0
4	BME	DDD	505	4/4	0.97	0.09	38,39,42,47	0
5	UDP	CCC	508	25/25	0.97	0.10	39,45,46,46	0
4	BME	AAA	504	4/4	0.98	0.11	41,41,42,44	0
4	BME	AAA	505	4/4	0.98	0.07	38,38,38,38	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.

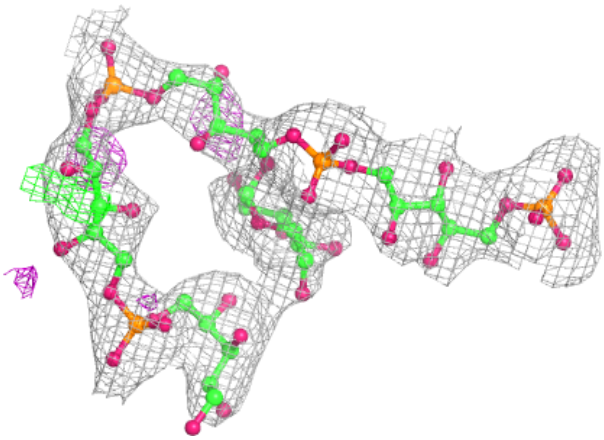
Electron density around BJT DDD 501:

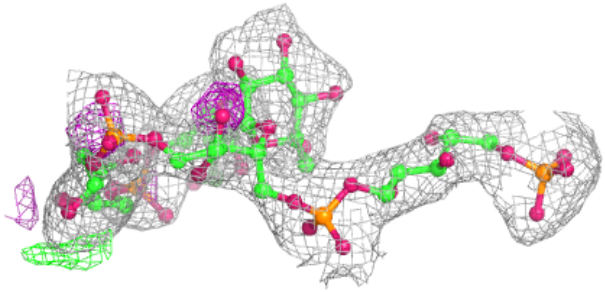
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

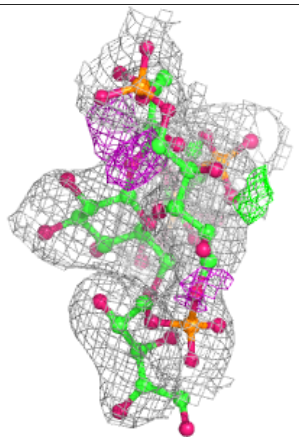


Electron density around BJT CCC 501:

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

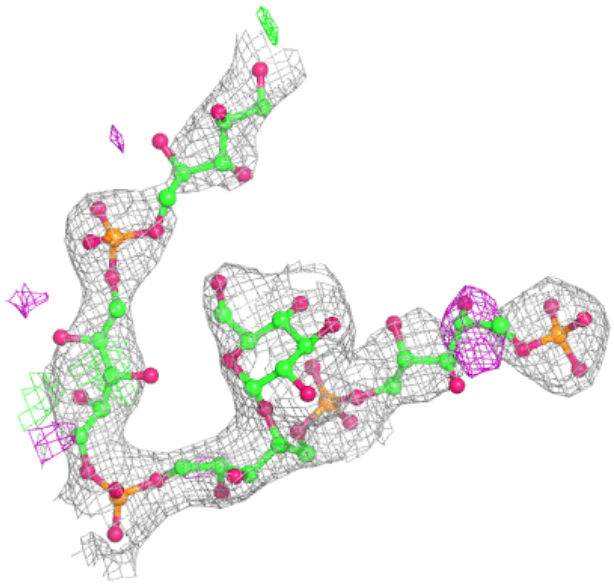


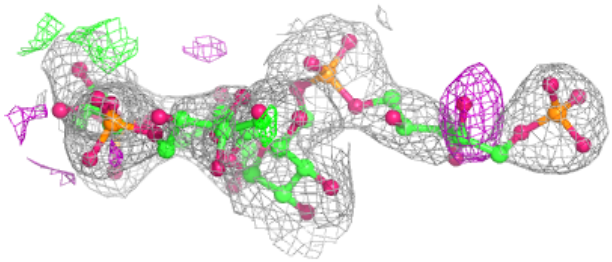




Electron density around BJT BBB 501:

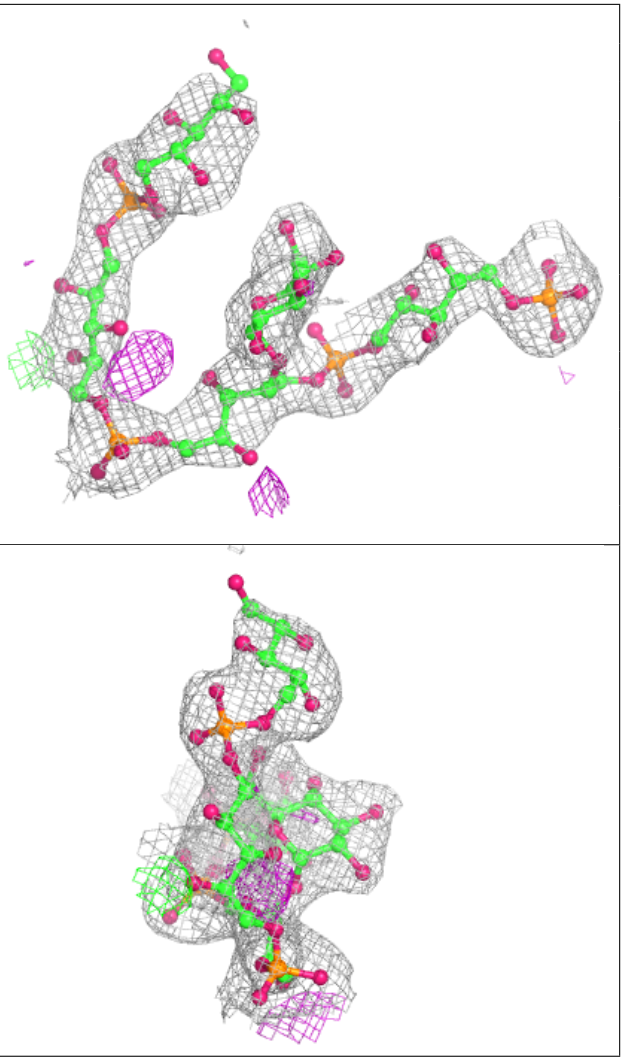
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





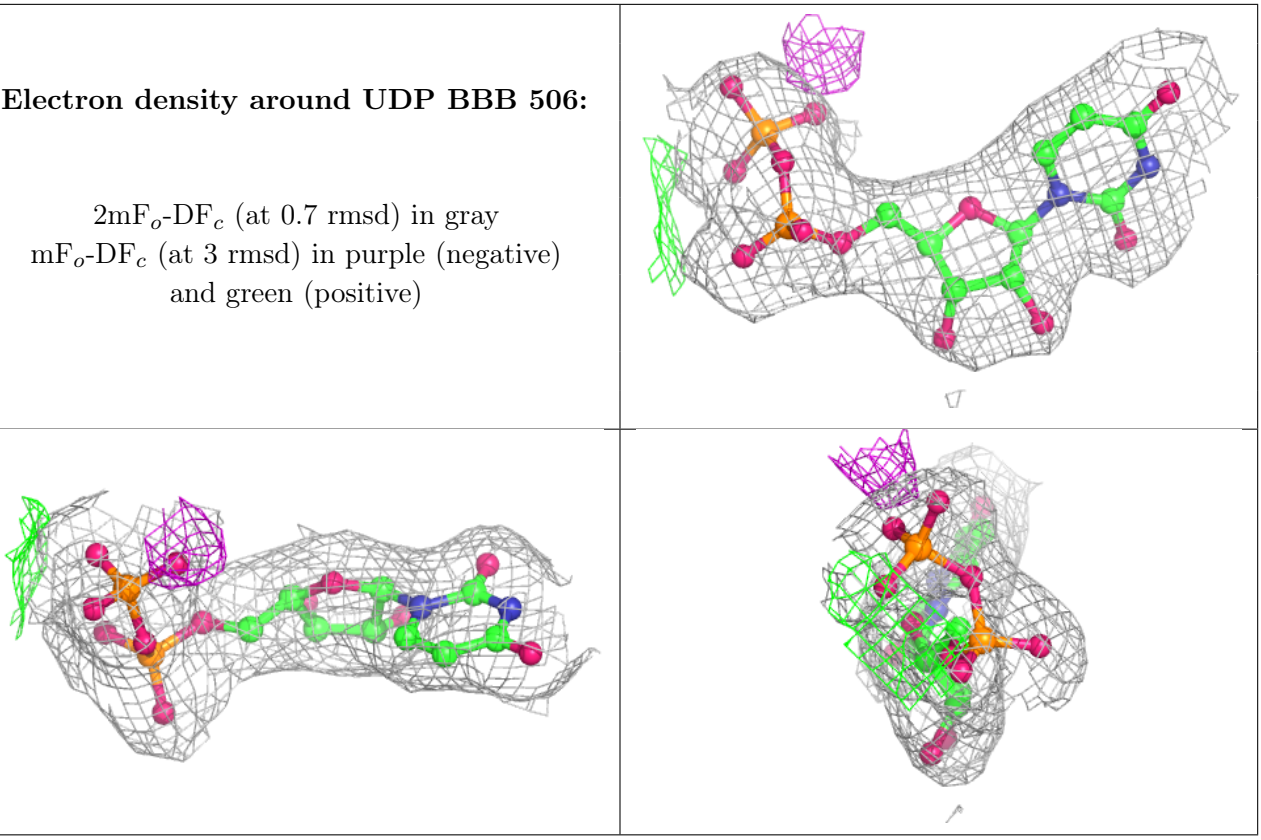
Electron density around BJT AAA 501:

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



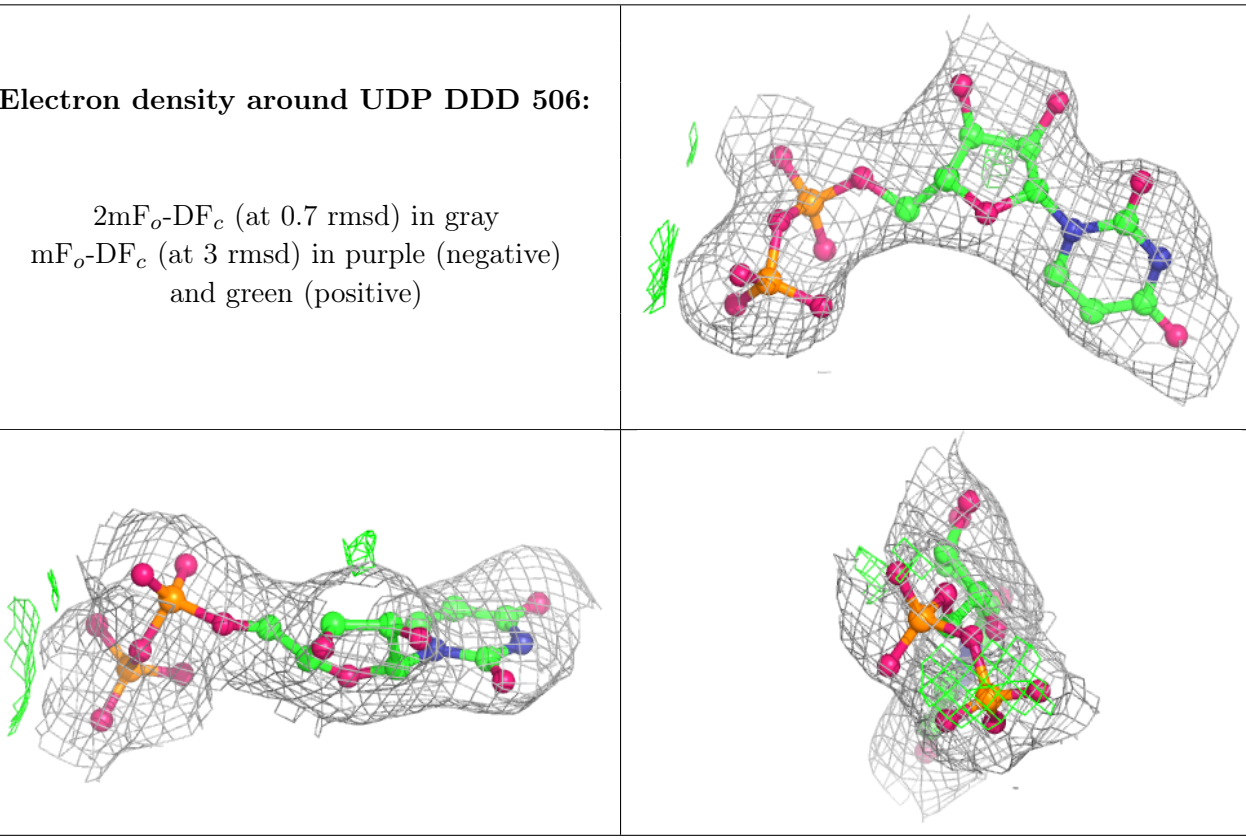
Electron density around UDP BBB 506:

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



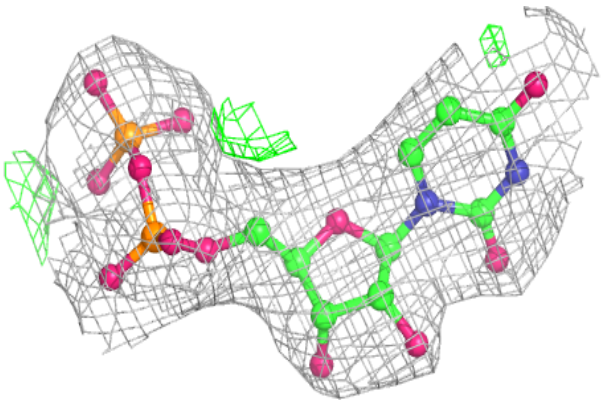
Electron density around UDP DDD 506:

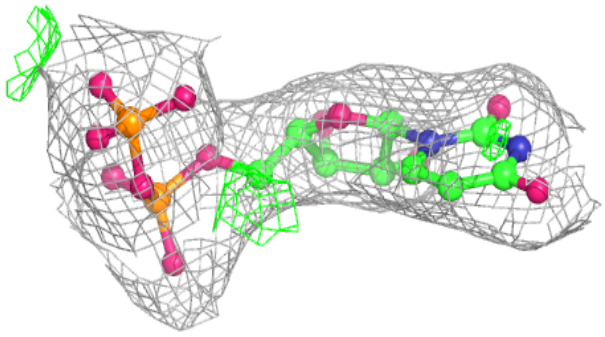
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

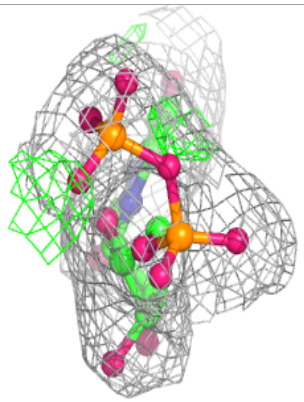


Electron density around UDP AAA 506:

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

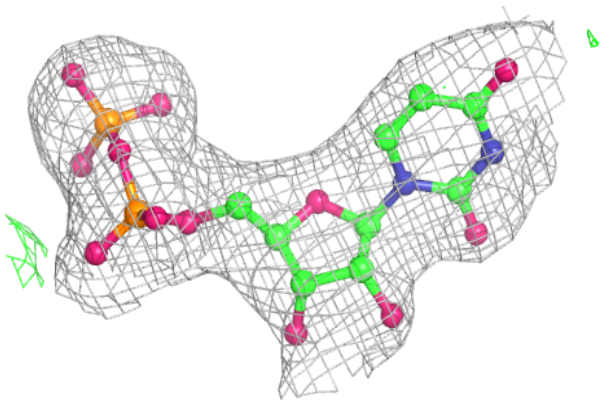


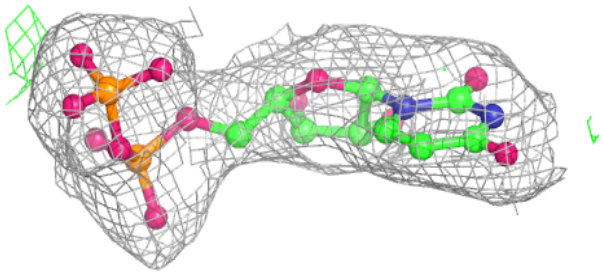


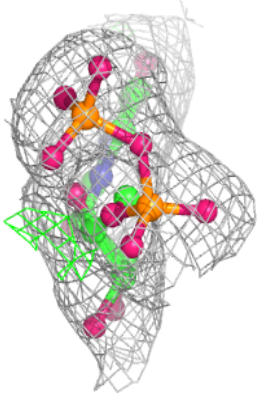


Electron density around UDP CCC 508:

$2mF_o$-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.