



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:05 PM UTC

PDB ID : 8P20 / pdb_00008p20
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

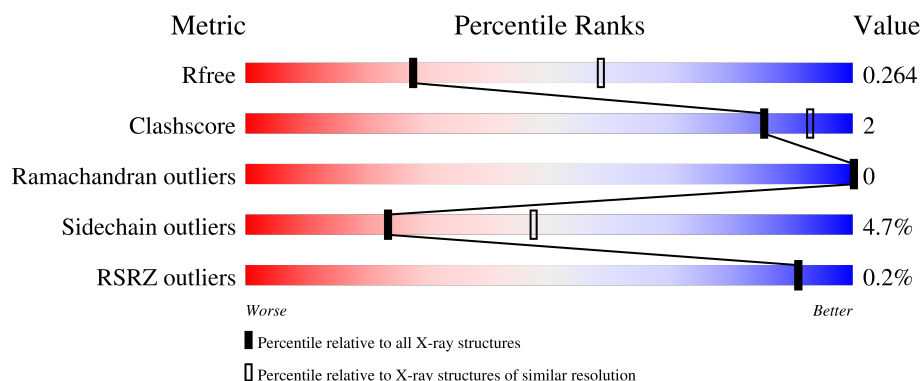
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

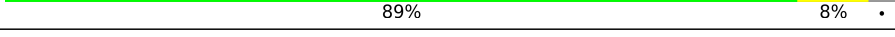
The reported resolution of this entry is 2.85 Å.

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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (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 $\leq 5\%$. 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	AAA	508	
1	BBB	508	
1	CCC	508	
1	DDD	508	

2 Entry composition [i](#)

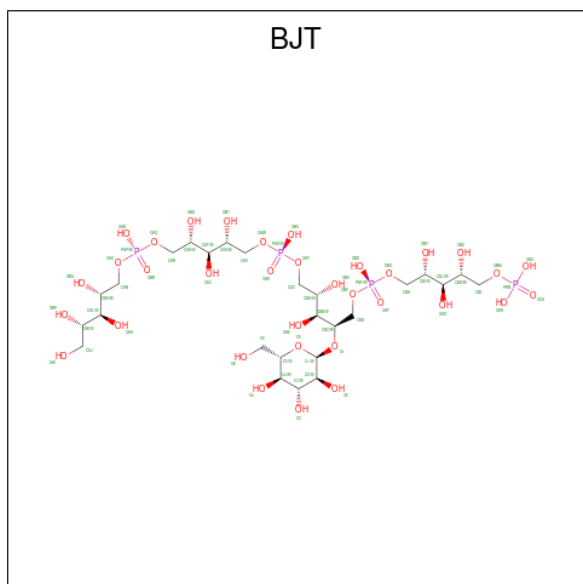
There are 7 unique types of molecules in this entry. The entry contains 15161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: BJT) (formula: C₂₆H₅₆O₃₄P₄) (labeled as "Ligand of Interest" by depositor).

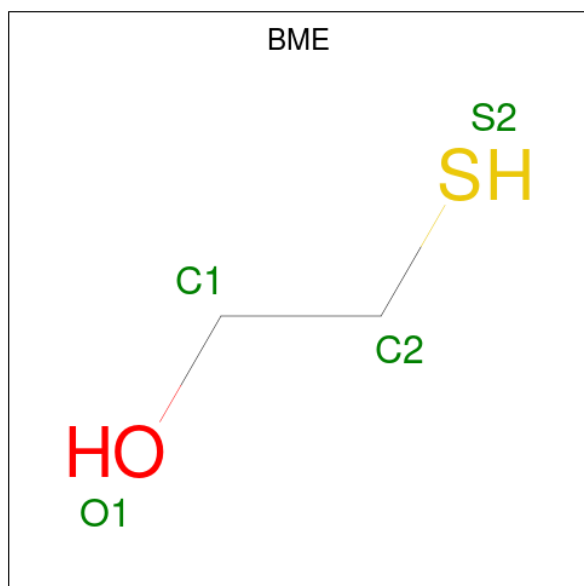


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	O	P	0	0
			64	26	34	4		
2	BBB	1	Total	C	O	P	0	0
			64	26	34	4		
2	CCC	1	Total	C	O	P	0	0
			64	26	34	4		
2	DDD	1	Total	C	O	P	0	0
			64	26	34	4		

- Molecule 3 is CHLORIDE ION (CCD ID: 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 (CCD ID: BME) (formula: C₂H₆OS).



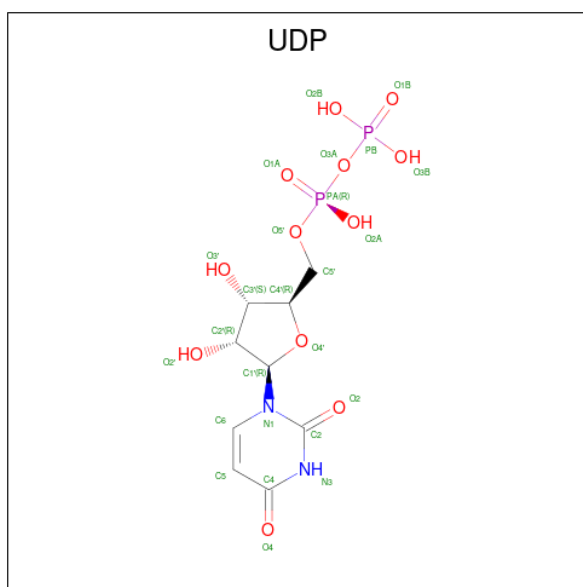
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		

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

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



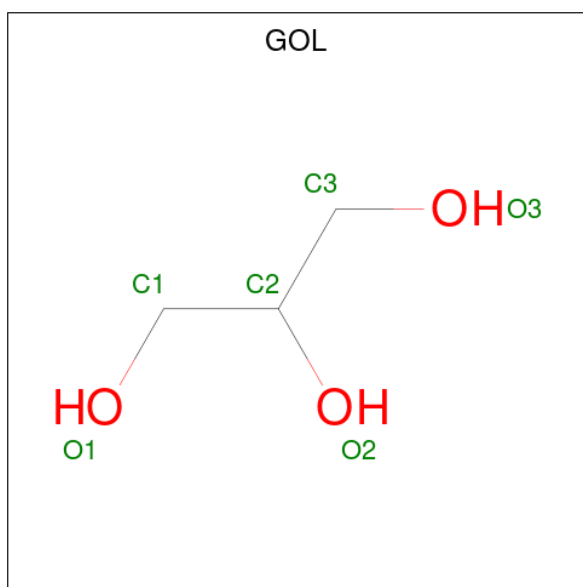
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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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 (CCD ID: 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.

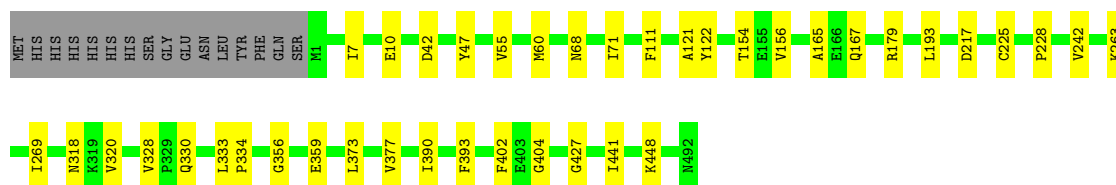
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	189	Total	O	0	0
			189	189		
7	BBB	191	Total	O	0	0
			191	191		
7	CCC	173	Total	O	0	0
			173	173		
7	DDD	181	Total	O	0	0
			181	181		

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.

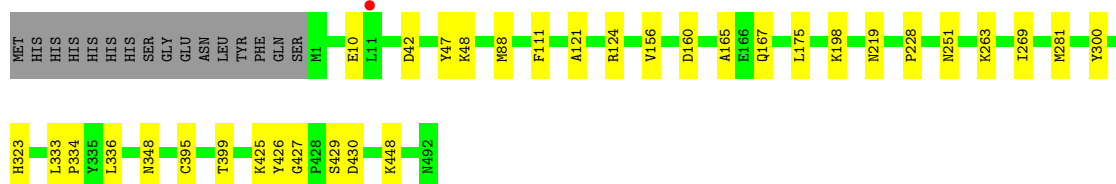
• Molecule 1: TarM(Se)_G117R

Chain AAA:  89% 8% .



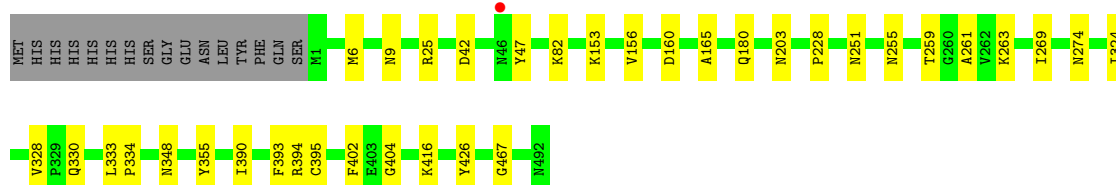
• Molecule 1: TarM(Se)_G117R

Chain BBB:  90% 7% .



• Molecule 1: TarM(Se)_G117R

Chain CCC:  90% 7% .



• Molecule 1: TarM(Se)_G117R

Chain DDD:  89% 8% .





4 Data and refinement statistics

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) 99.8 (49.20-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.266 0.229 , 0.264	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 , 101.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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	0.95	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.*

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: CL, GOL, BJT, 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	0.99	0/3601	1.30	1/4902 (0.0%)
1	BBB	0.99	0/3574	1.30	0/4861
1	CCC	0.98	0/3551	1.31	0/4837
1	DDD	0.97	0/3540	1.30	0/4820
All	All	0.99	0/14266	1.30	1/19420 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	356	GLY	CA-C-O	-5.43	118.69	122.22

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	AAA	3535	0	2847	18	0
1	BBB	3507	0	2822	10	0
1	CCC	3486	0	2775	12	0
1	DDD	3476	0	2769	17	0
2	AAA	64	0	0	0	0
2	BBB	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	64	0	0	0	0
2	DDD	64	0	0	0	0
3	AAA	1	0	0	0	0
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	57	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.

All (57) 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:DDD:413:MET:HE1	1:DDD:431:PHE:CD1	1.91	1.05
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:AAA:156:VAL:HB	1:AAA:165:ALA:HB3	1.82	0.61
1:DDD:156:VAL:HB	1:DDD:165:ALA:HB3	1.84	0.59
1:DDD:398:SER:HB2	1:DDD:409:LEU:HD21	1.86	0.57
1:DDD:431:PHE:CD1	1:DDD:432:VAL:HG23	2.41	0.56
1:BBB:156:VAL:HB	1:BBB:165:ALA:HB3	1.88	0.55
1:AAA:404:GLY:O	1:AAA:427:GLY:HA2	2.09	0.53
1:DDD:327:LEU:HB2	1:DDD:358:GLY:HA3	1.91	0.53
1:BBB:333:LEU:N	1:BBB:334:PRO:HD2	2.25	0.52
1:AAA:333:LEU:N	1:AAA:334:PRO:HD2	2.25	0.51
1:DDD:355:TYR:CZ	1:DDD:380:LEU:HD12	2.47	0.49
1:AAA:7:ILE:HB	1:AAA:225:CYS:HA	1.94	0.49
1:CCC:324:ILE:HG23	1:CCC:355:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:404:GLY:O	1:CCC:426:TYR:O	2.32	0.48
1:CCC:333:LEU:N	1:CCC:334:PRO:HD2	2.28	0.48
1:AAA:55:VAL:HG12	1:AAA:60:MET:HB3	1.96	0.48
1:AAA:154:THR:OG1	1:AAA:167:GLN:HB2	2.15	0.46
1:AAA:390:ILE:HA	1:AAA:393:PHE:CD2	2.50	0.46
1:BBB:48:LYS:HE3	1:BBB:48:LYS:HB3	1.84	0.46
1:CCC:259:THR:HG23	1:CCC:261:ALA:H	1.81	0.45
1:AAA:193:LEU:HD23	1:AAA:193:LEU:HA	1.82	0.45
1:BBB:111:PHE:HB2	1:BBB:121:ALA:HB3	1.99	0.44
1:AAA:330:GLN:HA	1:AAA:402:PHE:CE1	2.53	0.44
1:CCC:390:ILE:HA	1:CCC:393:PHE:CD2	2.52	0.43
1:DDD:355:TYR:CD2	1:DDD:383:THR:CG2	3.01	0.43
1:AAA:320:VAL:HG13	1:AAA:393:PHE:HA	2.00	0.43
1:BBB:251:ASN:ND2	1:BBB:425:LYS:HB3	2.34	0.43
1:AAA:42:ASP:H	1:AAA:68:ASN:HD21	1.65	0.43
1:AAA:373:LEU:HB3	1:AAA:377:VAL:HG23	2.00	0.43
1:DDD:158:ASN:HD21	1:DDD:162:ASN:HB2	1.84	0.43
1:DDD:331:LYS:HA	1:DDD:400:SER:HA	2.00	0.43
1:AAA:111:PHE:HB2	1:AAA:121:ALA:HB3	2.01	0.43
1:CCC:228:PRO:HA	1:CCC:269:ILE:HD11	2.01	0.43
1:CCC:156:VAL:HB	1:CCC:165:ALA:HB3	2.00	0.43
1:DDD:228:PRO:HA	1:DDD:269:ILE:HD11	2.01	0.43
1:DDD:217:ASP:HA	1:DDD:242:VAL:HG23	1.99	0.42
1:AAA:441:ILE:HG23	1:AAA:448:LYS:HB3	2.01	0.42
1:AAA:228:PRO:HA	1:AAA:269:ILE:HD11	2.02	0.42
1:CCC:255:ASN:HD21	1:CCC:263:LYS:HZ2	1.63	0.42
1:DDD:355:TYR:CD2	1:DDD:383:THR:HG23	2.55	0.42
1:DDD:355:TYR:HD2	1:DDD:383:THR:HG23	1.84	0.42
1:DDD:306:ILE:HG21	1:DDD:410:ILE:HG22	2.02	0.41
1:BBB:228:PRO:HA	1:BBB:269:ILE:HD11	2.03	0.41
1:BBB:427:GLY:C	1:BBB:429:SER:H	2.28	0.41
1:DDD:204:VAL:HG13	1:DDD:233:LYS:HA	2.01	0.41
1:AAA:68:ASN:HB3	1:AAA:71:ILE:HG13	2.03	0.41
1:AAA:328:VAL:HG12	1:AAA:330:GLN:H	1.85	0.41
1:BBB:336:LEU:CB	1:BBB:399:THR:HG21	2.51	0.41
1:DDD:235:LEU:HD11	1:DDD:275:LYS:HB2	2.02	0.41
1:CCC:328:VAL:HG22	1:CCC:330:GLN:H	1.84	0.40
1:DDD:328:VAL:HG23	1:DDD:330:GLN:HB3	2.03	0.40
1:AAA:217:ASP:HA	1:AAA:242:VAL:HG23	2.02	0.40
1:CCC:330:GLN:HA	1:CCC:402:PHE:CE1	2.57	0.40
1:CCC:416:LYS:HA	1:CCC:467:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:281:MET:HG2	1:BBB:300:TYR:O	2.22	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	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%)	39	63
1	BBB	260/471 (55%)	245 (94%)	15 (6%)	18	38
1	CCC	256/471 (54%)	241 (94%)	15 (6%)	18	37
1	DDD	252/471 (54%)	241 (96%)	11 (4%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1030/1884 (55%)	982 (95%)	48 (5%)	23	47

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	10	GLU
1	AAA	47	TYR
1	AAA	122	TYR
1	AAA	179	ARG
1	AAA	263	LYS
1	AAA	318	ASN
1	AAA	359	GLU
1	BBB	10	GLU
1	BBB	42	ASP
1	BBB	47	TYR
1	BBB	88	MET
1	BBB	124	ARG
1	BBB	160	ASP
1	BBB	198	LYS
1	BBB	219	ASN
1	BBB	263	LYS
1	BBB	323	HIS
1	BBB	348	ASN
1	BBB	395	CYS
1	BBB	426	TYR
1	BBB	430	ASP
1	BBB	448	LYS
1	CCC	6	MET
1	CCC	9	ASN
1	CCC	25	ARG
1	CCC	42	ASP
1	CCC	47	TYR
1	CCC	82	LYS
1	CCC	153	LYS
1	CCC	160	ASP
1	CCC	180	GLN
1	CCC	203	ASN
1	CCC	251	ASN
1	CCC	274	ASN
1	CCC	348	ASN
1	CCC	394	ARG
1	CCC	395	CYS

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Mol	Chain	Res	Type
1	DDD	25	ARG
1	DDD	42	ASP
1	DDD	47	TYR
1	DDD	124	ARG
1	DDD	160	ASP
1	DDD	167	GLN
1	DDD	257	ASP
1	DDD	266	GLU
1	DDD	274	ASN
1	DDD	281	MET
1	DDD	403	GLU

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 oligosaccharides 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	0.17	0	2,2,2	0.21	0
4	BME	CCC	504	-	3,3,3	0.17	0	2,2,2	0.22	0
4	BME	DDD	504	-	3,3,3	0.17	0	2,2,2	0.21	0
2	BJT	DDD	501	-	64,64,64	0.93	2 (3%)	88,93,93	0.92	5 (5%)
2	BJT	AAA	501	-	64,64,64	0.91	2 (3%)	88,93,93	0.94	5 (5%)
4	BME	BBB	502	-	3,3,3	0.17	0	2,2,2	0.29	0
6	GOL	BBB	505	-	5,5,5	0.07	0	5,5,5	0.23	0
4	BME	CCC	507	-	3,3,3	0.17	0	2,2,2	0.19	0
4	BME	CCC	503	-	3,3,3	0.17	0	2,2,2	0.19	0
2	BJT	CCC	501	-	64,64,64	0.91	3 (4%)	88,93,93	0.90	4 (4%)
4	BME	AAA	505	-	3,3,3	0.16	0	2,2,2	0.21	0
4	BME	AAA	504	-	3,3,3	0.16	0	2,2,2	0.18	0
5	UDP	BBB	506	-	25,26,26	1.27	4 (16%)	38,40,40	1.64	4 (10%)
6	GOL	BBB	504	-	5,5,5	0.09	0	5,5,5	0.21	0
5	UDP	DDD	506	-	25,26,26	1.20	4 (16%)	38,40,40	1.65	5 (13%)
4	BME	BBB	503	-	3,3,3	0.17	0	2,2,2	0.19	0
4	BME	DDD	505	-	3,3,3	0.17	0	2,2,2	0.29	0
5	UDP	CCC	508	-	25,26,26	1.25	5 (20%)	38,40,40	1.64	4 (10%)
4	BME	CCC	506	-	3,3,3	0.17	0	2,2,2	0.18	0
5	UDP	AAA	506	-	25,26,26	1.28	4 (16%)	38,40,40	1.61	4 (10%)
2	BJT	BBB	501	-	64,64,64	0.92	2 (3%)	88,93,93	0.97	6 (6%)
4	BME	AAA	503	-	3,3,3	0.17	0	2,2,2	0.23	0
4	BME	DDD	503	-	3,3,3	0.18	0	2,2,2	0.20	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
4	BME	CCC	505	-	-	0/1/1/1	-
4	BME	CCC	504	-	-	1/1/1/1	-
4	BME	DDD	504	-	-	1/1/1/1	-
2	BJT	DDD	501	-	-	42/82/102/102	0/1/1/1
2	BJT	AAA	501	-	-	44/82/102/102	0/1/1/1
4	BME	BBB	502	-	-	1/1/1/1	-
6	GOL	BBB	505	-	-	2/4/4/4	-
4	BME	CCC	507	-	-	0/1/1/1	-
4	BME	CCC	503	-	-	0/1/1/1	-
2	BJT	CCC	501	-	-	45/82/102/102	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	AAA	505	-	-	1/1/1/1	-
4	BME	AAA	504	-	-	1/1/1/1	-
5	UDP	BBB	506	-	-	4/16/32/32	0/2/2/2
6	GOL	BBB	504	-	-	0/4/4/4	-
5	UDP	DDD	506	-	-	5/16/32/32	0/2/2/2
4	BME	BBB	503	-	-	1/1/1/1	-
4	BME	DDD	505	-	-	1/1/1/1	-
5	UDP	CCC	508	-	-	3/16/32/32	0/2/2/2
4	BME	CCC	506	-	-	1/1/1/1	-
5	UDP	AAA	506	-	-	3/16/32/32	0/2/2/2
2	BJT	BBB	501	-	-	54/82/102/102	0/1/1/1
4	BME	AAA	503	-	-	1/1/1/1	-
4	BME	DDD	503	-	-	0/1/1/1	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	501	BJT	PBN-OCA	3.89	1.62	1.50
2	AAA	501	BJT	PBN-OCA	3.84	1.62	1.50
2	DDD	501	BJT	PBN-OCA	3.76	1.62	1.50
2	BBB	501	BJT	PBN-OCA	3.74	1.62	1.50
2	BBB	501	BJT	PAP-OBP	3.30	1.62	1.50
2	AAA	501	BJT	PAP-OBP	3.26	1.62	1.50
2	CCC	501	BJT	PAP-OBP	3.15	1.61	1.50
2	DDD	501	BJT	PAP-OBP	3.14	1.61	1.50
5	BBB	506	UDP	PA-O3A	2.82	1.62	1.59
5	AAA	506	UDP	PA-O3A	2.75	1.62	1.59
5	AAA	506	UDP	C4-N3	-2.73	1.33	1.38
5	BBB	506	UDP	C4-N3	-2.68	1.34	1.38
5	CCC	508	UDP	C4-N3	-2.65	1.34	1.38
5	DDD	506	UDP	C4-N3	-2.61	1.34	1.38
5	CCC	508	UDP	PA-O3A	2.54	1.62	1.59
5	DDD	506	UDP	C2-N3	-2.36	1.33	1.38
5	AAA	506	UDP	C2-N3	-2.36	1.33	1.38
5	AAA	506	UDP	C2-N1	2.27	1.42	1.38
5	BBB	506	UDP	C2-N3	-2.27	1.34	1.38
5	CCC	508	UDP	C2-N3	-2.24	1.34	1.38
5	BBB	506	UDP	C2-N1	2.24	1.42	1.38
5	CCC	508	UDP	C2-N1	2.20	1.41	1.38
5	DDD	506	UDP	C2-N1	2.15	1.41	1.38
2	CCC	501	BJT	PBN-OBP	2.09	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	CCC	508	UDP	C5-C4	-2.04	1.39	1.43
5	DDD	506	UDP	PA-O3A	2.02	1.61	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	506	UDP	C4-N3-C2	-5.20	120.16	126.61
5	BBB	506	UDP	C4-N3-C2	-5.15	120.22	126.61
5	CCC	508	UDP	C4-N3-C2	-5.15	120.22	126.61
5	DDD	506	UDP	C4-N3-C2	-5.07	120.32	126.61
5	BBB	506	UDP	N3-C2-N1	4.42	120.65	114.89
5	DDD	506	UDP	N3-C2-N1	4.33	120.53	114.89
5	AAA	506	UDP	N3-C2-N1	4.33	120.52	114.89
5	CCC	508	UDP	N3-C2-N1	4.32	120.51	114.89
5	AAA	506	UDP	C5-C4-N3	4.19	120.67	114.80
5	DDD	506	UDP	C5-C4-N3	4.12	120.56	114.80
5	BBB	506	UDP	C5-C4-N3	4.10	120.55	114.80
5	CCC	508	UDP	C5-C4-N3	3.97	120.36	114.80
5	CCC	508	UDP	O4-C4-C5	-3.19	119.66	125.16
5	DDD	506	UDP	O4-C4-C5	-3.16	119.70	125.16
2	CCC	501	BJT	CAS-CAT-CAU	-3.14	108.35	113.57
2	DDD	501	BJT	OAH-PBN-OBM	3.09	114.72	106.67
2	BBB	501	BJT	OAH-PBN-OBM	3.04	114.60	106.67
5	BBB	506	UDP	O4-C4-C5	-3.04	119.92	125.16
2	AAA	501	BJT	CAK-CAL-CAM	-2.96	108.65	113.57
2	DDD	501	BJT	CAS-CAT-CAU	-2.94	108.69	113.57
5	AAA	506	UDP	O4-C4-C5	-2.92	120.13	125.16
2	AAA	501	BJT	OAH-PBN-OBM	2.85	114.11	106.67
2	BBB	501	BJT	O1-CBC-CBB	2.76	112.71	107.47
2	DDD	501	BJT	CBI-CBJ-CBK	-2.63	109.19	113.57
2	AAA	501	BJT	O1-CBC-CBB	2.61	112.44	107.47
2	AAA	501	BJT	CAS-CAT-CAU	-2.59	109.26	113.57
2	CCC	501	BJT	O1-CBC-CBB	2.49	112.20	107.47
2	CCC	501	BJT	CAK-CAL-CAM	-2.48	109.44	113.57
2	DDD	501	BJT	O1-CBC-CBB	2.39	112.02	107.47
2	CCC	501	BJT	OAH-PBN-OBM	2.33	112.75	106.67
2	DDD	501	BJT	CAK-CAL-CAM	-2.32	109.71	113.57
5	DDD	506	UDP	C3'-C2'-C1'	2.23	105.68	101.46
2	BBB	501	BJT	CAK-CAL-CAM	-2.21	109.90	113.57
2	BBB	501	BJT	O1-C1-C2	2.17	113.44	108.09
2	BBB	501	BJT	C1-O5-C5	-2.11	109.60	113.72
2	BBB	501	BJT	C1-O1-CBC	2.03	118.67	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	BJT	CAR-CAS-CAT	-2.00	108.44	112.22

There are no chirality outliers.

All (211) 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
2	AAA	501	BJT	CBD-OBE-PBF-OBG
2	AAA	501	BJT	CBD-OBE-PBF-OBX
2	AAA	501	BJT	CBB-CBC-O1-C1
2	AAA	501	BJT	OAE-CBB-CBC-CBD
2	AAA	501	BJT	OAE-CBB-CBC-O1
2	AAA	501	BJT	CAZ-OAY-PAX-OBU
2	AAA	501	BJT	CAZ-OAY-PAX-OAD
2	AAA	501	BJT	CAZ-OAY-PAX-OAW
2	AAA	501	BJT	OAQ-CAR-CAS-OBS
2	AAA	501	BJT	CAN-OAO-PAP-OAQ
2	AAA	501	BJT	CAN-OAO-PAP-OBP
2	BBB	501	BJT	CBH-CBI-CBJ-CBK
2	BBB	501	BJT	CBH-CBI-CBJ-OAG
2	BBB	501	BJT	CBH-OBG-PBF-OAF
2	BBB	501	BJT	CBH-OBG-PBF-OBE
2	BBB	501	BJT	CBD-OBE-PBF-OBX
2	BBB	501	BJT	O1-CBC-CBD-OBE
2	BBB	501	BJT	CBB-CBC-CBD-OBE
2	BBB	501	BJT	OAE-CBB-CBC-CBD
2	BBB	501	BJT	CBA-CBB-CBC-O1
2	BBB	501	BJT	OBV-CBA-CBB-CBC
2	BBB	501	BJT	OBV-CBA-CBB-OAE
2	BBB	501	BJT	CAZ-CBA-CBB-OAE
2	BBB	501	BJT	OAY-CAZ-CBA-OBV
2	BBB	501	BJT	CAZ-OAY-PAX-OBU
2	BBB	501	BJT	CAZ-OAY-PAX-OAD
2	BBB	501	BJT	CAZ-OAY-PAX-OAW
2	BBB	501	BJT	OAC-CAT-CAU-OBT
2	BBB	501	BJT	CAS-CAT-CAU-OBT
2	BBB	501	BJT	OBQ-CAM-CAN-OAO
2	BBB	501	BJT	CAL-CAM-CAN-OAO

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Mol	Chain	Res	Type	Atoms
2	BBB	501	BJT	OAA-CAL-CAM-OBQ
2	BBB	501	BJT	CAK-CAL-CAM-OBQ
2	CCC	501	BJT	CBH-OBG-PBF-OAF
2	CCC	501	BJT	CBH-OBG-PBF-OBE
2	CCC	501	BJT	CBD-OBE-PBF-OAF
2	CCC	501	BJT	CBB-CBC-CBD-OBE
2	CCC	501	BJT	CBB-CBC-O1-C1
2	CCC	501	BJT	OAE-CBB-CBC-CBD
2	CCC	501	BJT	CBA-CBB-CBC-CBD
2	CCC	501	BJT	OAE-CBB-CBC-O1
2	CCC	501	BJT	OBS-CAS-CAT-CAU
2	CCC	501	BJT	OBS-CAS-CAT-OAC
2	CCC	501	BJT	CAR-CAS-CAT-OAC
2	CCC	501	BJT	OAQ-CAR-CAS-CAT
2	CCC	501	BJT	OAQ-CAR-CAS-OBS
2	CCC	501	BJT	CAL-CAM-CAN-OAO
2	CCC	501	BJT	OBP-CAK-CAL-CAM
2	CCC	501	BJT	OBP-CAK-CAL-OAA
2	CCC	501	BJT	CAJ-CAK-CAL-OAA
2	DDD	501	BJT	CBL-OBM-PBN-OBO
2	DDD	501	BJT	CBL-OBM-PBN-OCA
2	DDD	501	BJT	CBL-OBM-PBN-OAH
2	DDD	501	BJT	OBG-CBH-CBI-OBV
2	DDD	501	BJT	CBH-OBG-PBF-OAF
2	DDD	501	BJT	CBD-OBE-PBF-OBG
2	DDD	501	BJT	CBD-OBE-PBF-OBX
2	DDD	501	BJT	CBB-CBC-O1-C1
2	DDD	501	BJT	OAE-CBB-CBC-CBD
2	DDD	501	BJT	OAE-CBB-CBC-O1
2	DDD	501	BJT	OBV-CBA-CBB-CBC
2	DDD	501	BJT	OBV-CBA-CBB-OAE
2	DDD	501	BJT	OAY-CAZ-CBA-CBB
2	DDD	501	BJT	OAY-CAZ-CBA-OBV
2	DDD	501	BJT	CAV-OAW-PAX-OAY
2	DDD	501	BJT	CAV-OAW-PAX-OBV
2	DDD	501	BJT	OAQ-CAR-CAS-OBS
2	DDD	501	BJT	CAN-OAO-PAP-OAQ
2	DDD	501	BJT	CAN-OAO-PAP-OBV
2	DDD	501	BJT	CAN-OAO-PAP-OAB
2	DDD	501	BJT	CAL-CAM-CAN-OAO
4	AAA	503	BME	O1-C1-C2-S2
4	AAA	505	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
4	BBB	502	BME	O1-C1-C2-S2
4	BBB	503	BME	O1-C1-C2-S2
4	DDD	505	BME	O1-C1-C2-S2
5	CCC	508	UDP	PB-O3A-PA-O5'
5	DDD	506	UDP	C5'-O5'-PA-O1A
6	BBB	505	GOL	C1-C2-C3-O3
2	BBB	501	BJT	O5-C1-O1-CBC
2	DDD	501	BJT	OAI-CAJ-CAK-OBP
2	BBB	501	BJT	C2-C1-O1-CBC
2	AAA	501	BJT	CBI-CBJ-CBK-OBZ
2	BBB	501	BJT	OBY-CBI-CBJ-CBK
2	CCC	501	BJT	C4-C5-C6-O6
2	DDD	501	BJT	CBA-CBB-CBC-CBD
2	AAA	501	BJT	OAG-CBJ-CBK-CBL
2	BBB	501	BJT	OAC-CAT-CAU-CAV
2	BBB	501	BJT	OAA-CAL-CAM-CAN
2	DDD	501	BJT	CAZ-CBA-CBB-OAE
2	BBB	501	BJT	CAZ-CBA-CBB-CBC
2	BBB	501	BJT	CAS-CAT-CAU-CAV
2	BBB	501	BJT	CAK-CAL-CAM-CAN
2	CCC	501	BJT	CAR-CAS-CAT-CAU
2	CCC	501	BJT	CAJ-CAK-CAL-CAM
2	DDD	501	BJT	CAZ-CBA-CBB-CBC
2	DDD	501	BJT	CAJ-CAK-CAL-CAM
2	BBB	501	BJT	OBY-CBI-CBJ-OAG
5	AAA	506	UDP	O4'-C4'-C5'-O5'
5	CCC	508	UDP	O4'-C4'-C5'-O5'
2	DDD	501	BJT	C4-C5-C6-O6
2	DDD	501	BJT	OAI-CAJ-CAK-CAL
2	CCC	501	BJT	O5-C5-C6-O6
2	AAA	501	BJT	OAG-CBJ-CBK-OBZ
5	AAA	506	UDP	C3'-C4'-C5'-O5'
5	CCC	508	UDP	C3'-C4'-C5'-O5'
2	DDD	501	BJT	CAJ-CAK-CAL-OAA
2	BBB	501	BJT	CAJ-CAK-CAL-CAM
2	DDD	501	BJT	OBP-CAK-CAL-OAA
2	DDD	501	BJT	OBP-CAK-CAL-CAM
2	BBB	501	BJT	OBT-CAU-CAV-OAW
2	CCC	501	BJT	OBG-CBH-CBI-OBY
2	AAA	501	BJT	CBA-CBB-CBC-CBD
4	CCC	504	BME	O1-C1-C2-S2
4	DDD	504	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
2	CCC	501	BJT	O1-CBC-CBD-OBE
2	DDD	501	BJT	O5-C5-C6-O6
5	BBB	506	UDP	O4'-C4'-C5'-O5'
2	BBB	501	BJT	OBP-CAK-CAL-CAM
2	BBB	501	BJT	OAY-CAZ-CBA-CBB
2	BBB	501	BJT	CAT-CAU-CAV-OAW
2	CCC	501	BJT	OBG-CBH-CBI-CBJ
2	CCC	501	BJT	OAA-CAL-CAM-OBQ
2	AAA	501	BJT	OBS-CAS-CAT-CAU
2	CCC	501	BJT	CAK-CAL-CAM-OBQ
2	AAA	501	BJT	CAZ-CBA-CBB-OAE
2	CCC	501	BJT	CAK-CAL-CAM-CAN
2	AAA	501	BJT	CBL-OBM-PBN-OCA
5	BBB	506	UDP	PA-O3A-PB-O1B
5	BBB	506	UDP	C3'-C4'-C5'-O5'
2	BBB	501	BJT	CAJ-CAK-CAL-OAA
2	CCC	501	BJT	OAA-CAL-CAM-CAN
2	AAA	501	BJT	OBS-CAS-CAT-OAC
2	BBB	501	BJT	OBP-CAK-CAL-OAA
2	DDD	501	BJT	OBQ-CAM-CAN-OAO
4	AAA	504	BME	O1-C1-C2-S2
4	CCC	506	BME	O1-C1-C2-S2
2	AAA	501	BJT	CAR-CAS-CAT-OAC
2	AAA	501	BJT	OAA-CAL-CAM-CAN
2	AAA	501	BJT	OAI-CAJ-CAK-OBP
2	AAA	501	BJT	OAA-CAL-CAM-OBQ
2	AAA	501	BJT	CAR-CAS-CAT-CAU
2	AAA	501	BJT	CAK-CAL-CAM-OBQ
2	BBB	501	BJT	CBA-CBB-CBC-CBD
5	AAA	506	UDP	PB-O3A-PA-O5'
2	BBB	501	BJT	OAE-CBB-CBC-O1
6	BBB	505	GOL	O2-C2-C3-O3
2	AAA	501	BJT	CAK-CAL-CAM-CAN
2	AAA	501	BJT	OBV-CBA-CBB-CBC
2	CCC	501	BJT	OBV-CBA-CBB-CBC
2	CCC	501	BJT	CAS-CAT-CAU-OBT
2	CCC	501	BJT	CBL-OBM-PBN-OAH
5	BBB	506	UDP	PA-O3A-PB-O2B
2	BBB	501	BJT	CBD-CBC-O1-C1
2	DDD	501	BJT	OBG-CBH-CBI-CBJ
2	DDD	501	BJT	CAT-CAU-CAV-OAW
2	DDD	501	BJT	OBS-CAS-CAT-CAU

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Mol	Chain	Res	Type	Atoms
2	CCC	501	BJT	OBV-CBA-CBB-OAE
2	DDD	501	BJT	OBS-CAS-CAT-OAC
2	AAA	501	BJT	CAZ-CBA-CBB-CBC
2	AAA	501	BJT	CBH-OBG-PBF-OBX
2	AAA	501	BJT	CBH-OBG-PBF-OAF
2	AAA	501	BJT	CBH-OBG-PBF-OBE
2	AAA	501	BJT	CAV-OAW-PAX-OAY
2	AAA	501	BJT	CAV-OAW-PAX-OBU
2	AAA	501	BJT	CAN-OAO-PAP-OAB
2	BBB	501	BJT	CBD-OBE-PBF-OBG
2	BBB	501	BJT	CBD-OBE-PBF-OAF
2	BBB	501	BJT	CAN-OAO-PAP-OBZ
2	CCC	501	BJT	CBD-OBE-PBF-OBG
2	CCC	501	BJT	CBD-OBE-PBF-OBX
2	CCC	501	BJT	CAZ-OAY-PAX-OBZ
2	CCC	501	BJT	CAZ-OAY-PAX-OAW
5	DDD	506	UDP	C5'-O5'-PA-O3A
2	BBB	501	BJT	CAU-CAV-OAW-PAX
2	BBB	501	BJT	CAM-CAN-OAO-PAP
2	AAA	501	BJT	OAI-CAJ-CAK-CAL
2	AAA	501	BJT	C4-C5-C6-O6
2	DDD	501	BJT	CAR-CAS-CAT-OAC
2	CCC	501	BJT	OAG-CBJ-CBK-CBL
2	CCC	501	BJT	CAZ-CBA-CBB-OAE
5	DDD	506	UDP	O4'-C4'-C5'-O5'
2	AAA	501	BJT	OBV-CBA-CBB-OAE
2	CCC	501	BJT	OAC-CAT-CAU-CAV
2	AAA	501	BJT	CBA-CBB-CBC-O1
2	CCC	501	BJT	CBA-CBB-CBC-O1
2	DDD	501	BJT	CBA-CBB-CBC-O1
2	CCC	501	BJT	CAZ-CBA-CBB-CBC
2	CCC	501	BJT	CAS-CAT-CAU-CAV
2	BBB	501	BJT	CBI-CBJ-CBK-OBZ
2	BBB	501	BJT	OBG-CBH-CBI-OBZ
2	BBB	501	BJT	OAG-CBJ-CBK-OBZ
2	DDD	501	BJT	CAR-CAS-CAT-CAU
2	BBB	501	BJT	CBB-CBC-O1-C1
2	BBB	501	BJT	OBG-CBH-CBI-CBJ
2	DDD	501	BJT	CBA-CAZ-OAY-PAX
5	DDD	506	UDP	PB-O3A-PA-O1A
2	AAA	501	BJT	OAC-CAT-CAU-CAV
2	BBB	501	BJT	OAG-CBJ-CBK-CBL

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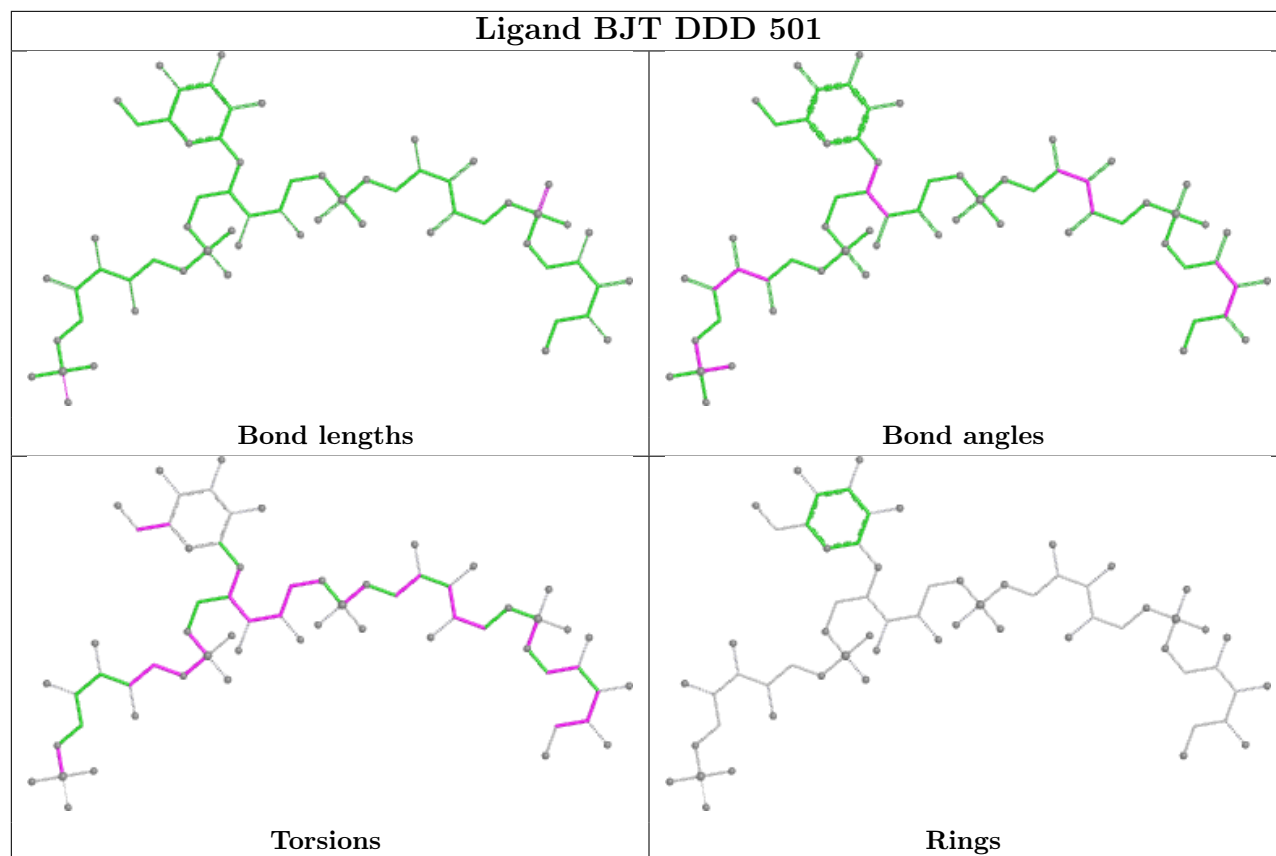
Mol	Chain	Res	Type	Atoms
2	CCC	501	BJT	OAG-CBJ-CBK-OBZ
2	CCC	501	BJT	OAC-CAT-CAU-OBT
2	CCC	501	BJT	CBI-CBJ-CBK-OBZ
2	BBB	501	BJT	CBC-CBD-OBE-PBF
2	DDD	501	BJT	CBI-CBH-OBG-PBF
2	BBB	501	BJT	OAI-CAJ-CAK-OBP
5	DDD	506	UDP	PB-O3A-PA-O2A

There are no ring outliers.

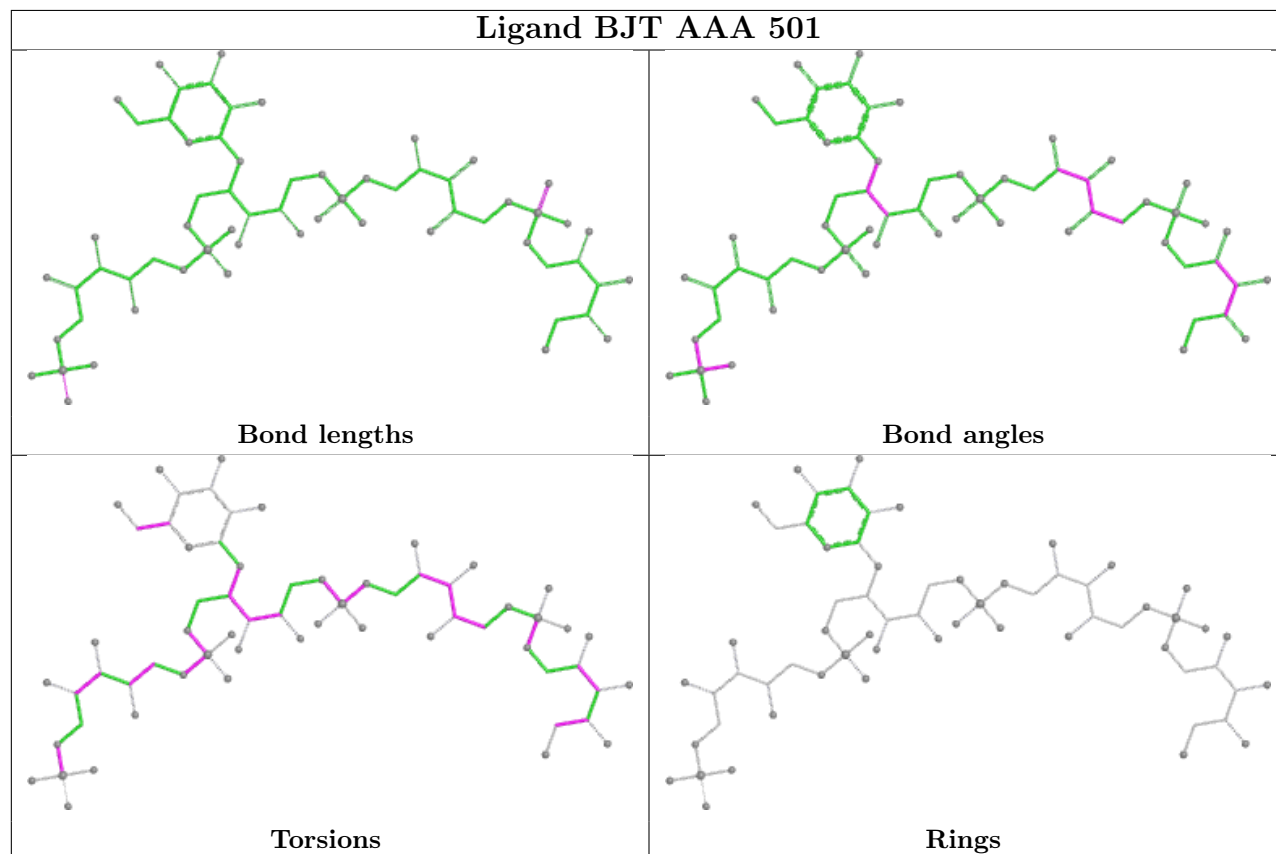
No monomer is involved in short contacts.

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 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.

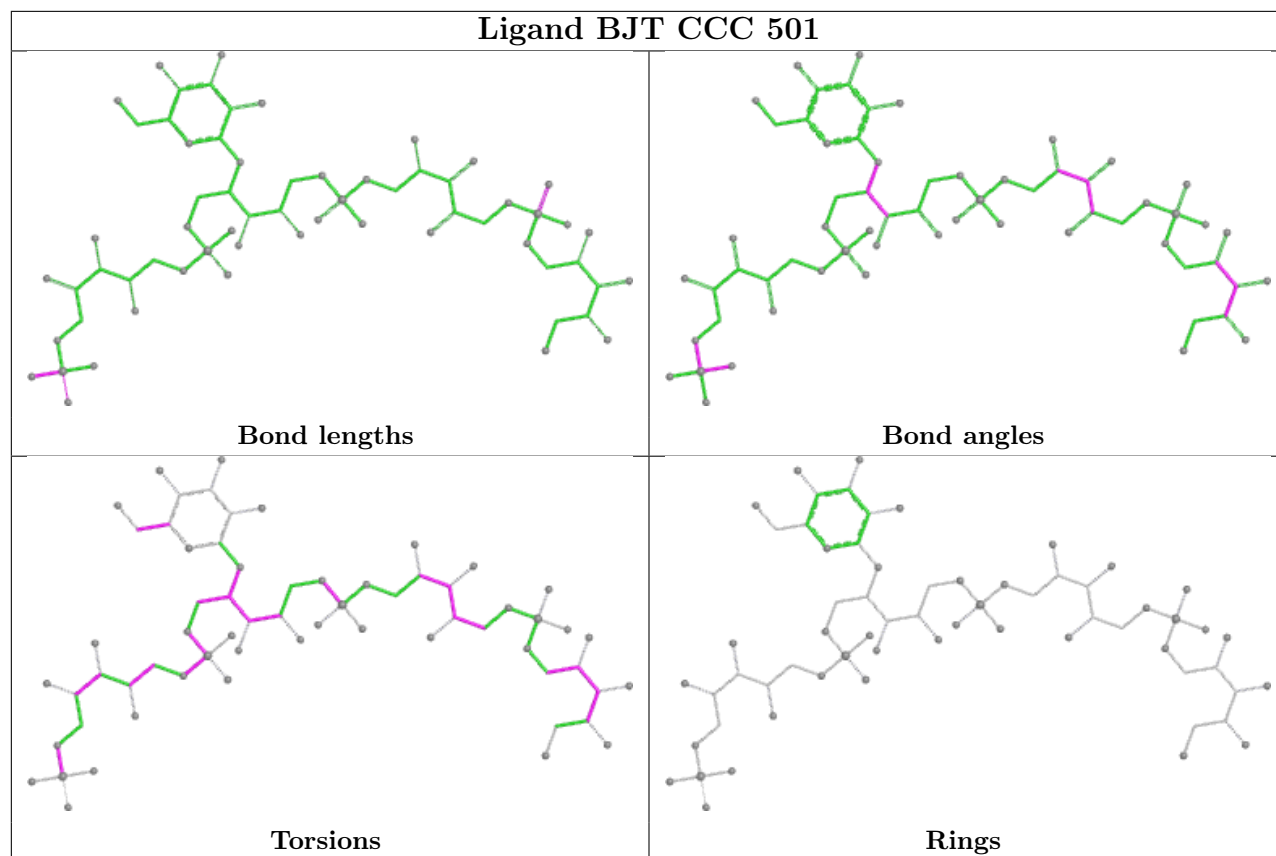
Ligand BJT DDD 501



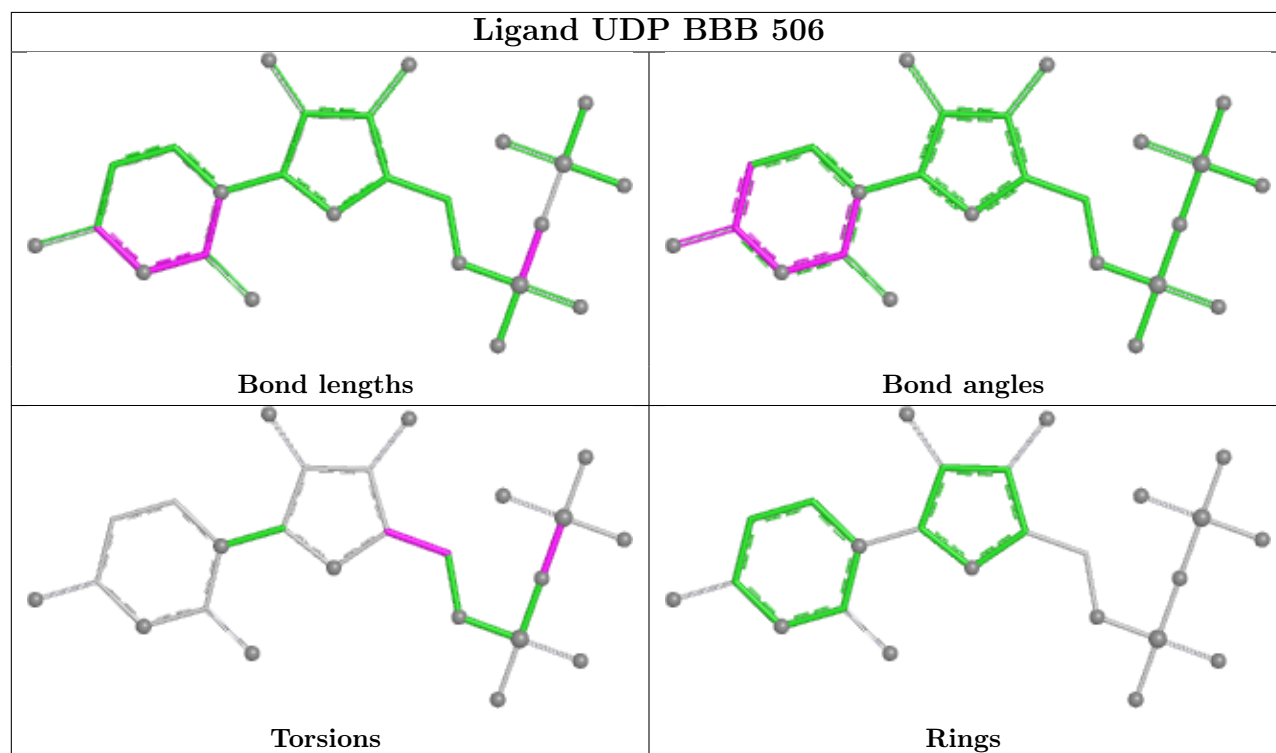
Ligand BJT AAA 501



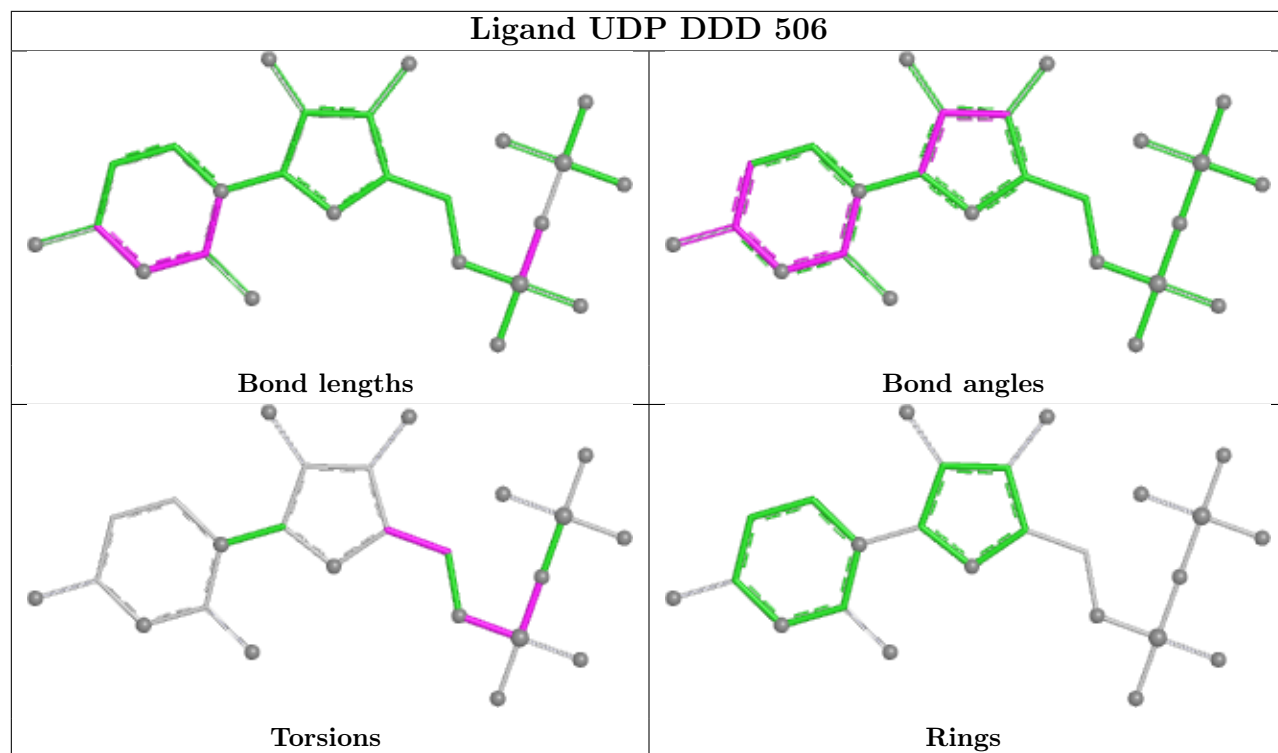
Ligand BJT CCC 501



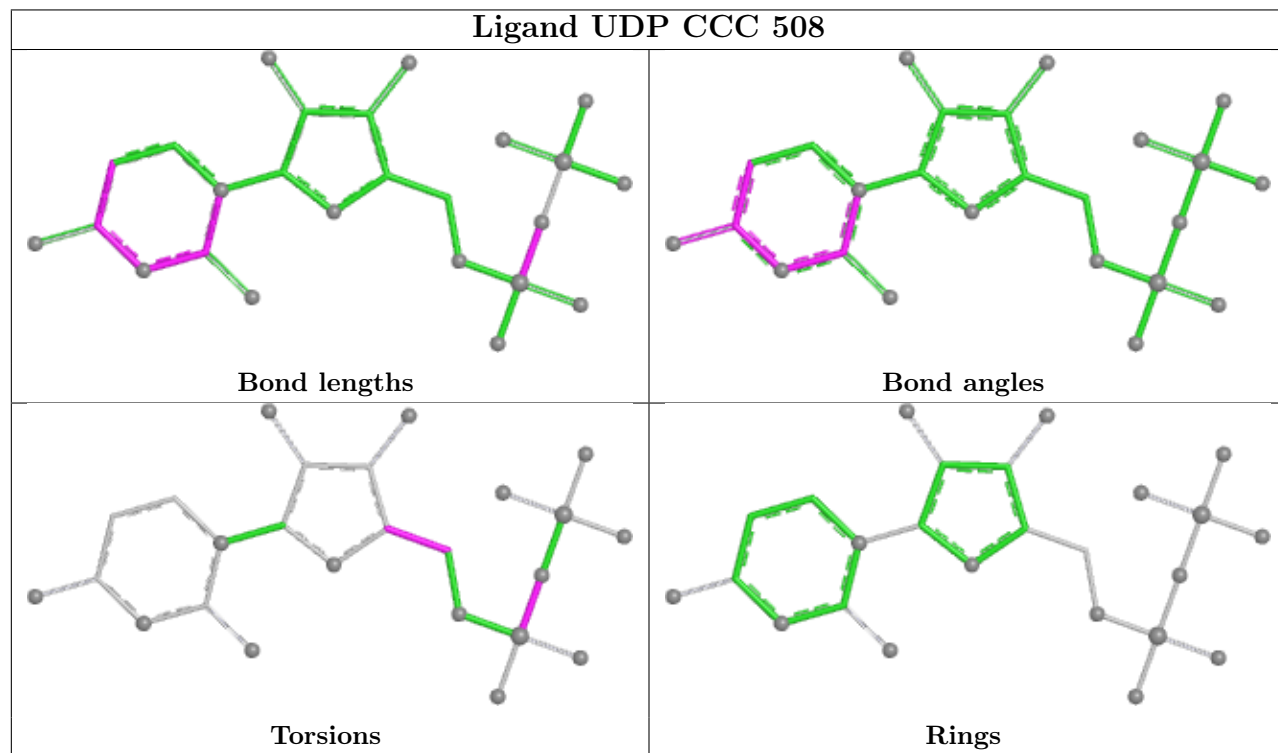
Ligand UDP BBB 506

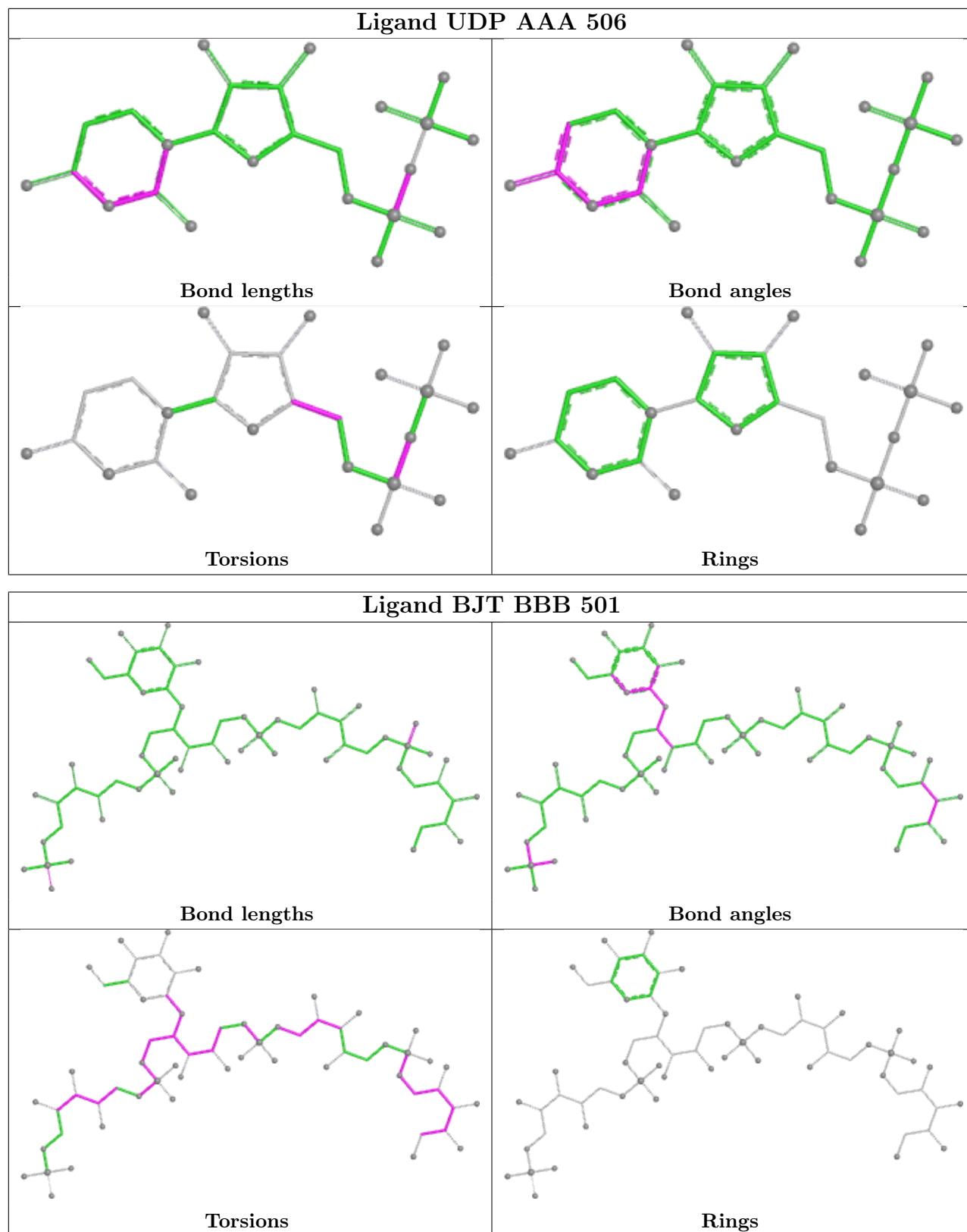


Ligand UDP DDD 506



Ligand UDP CCC 508





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	AAA	492/508 (96%)	-1.16	0	100 100	42, 58, 71, 84	0
1	BBB	492/508 (96%)	-1.11	1 (0%)	91 91	38, 60, 73, 87	0
1	CCC	492/508 (96%)	-1.14	1 (0%)	91 91	43, 61, 76, 85	0
1	DDD	491/508 (96%)	-1.17	1 (0%)	91 91	43, 61, 73, 79	0
All	All	1967/2032 (96%)	-1.15	3 (0%)	91 91	38, 60, 73, 87	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	11	LEU	2.5
1	CCC	46	ASN	2.2
1	DDD	12	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

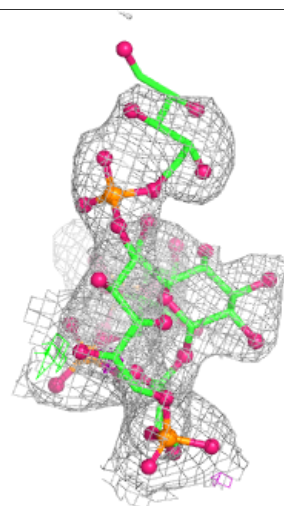
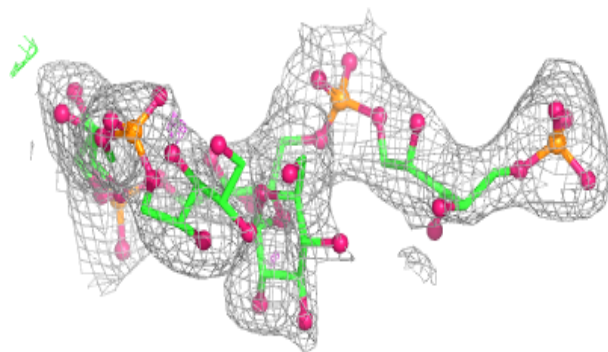
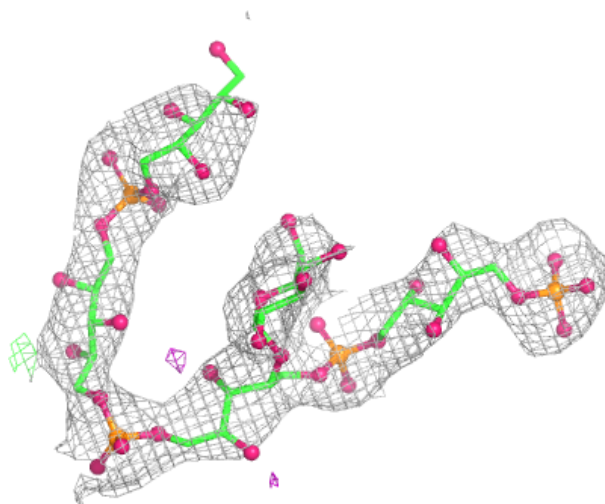
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BME	CCC	504	4/4	0.96	0.05	65,67,67,69	0
6	GOL	BBB	505	6/6	0.96	0.04	90,91,96,98	0
4	BME	BBB	502	4/4	0.97	0.04	67,70,72,75	0
4	BME	DDD	503	4/4	0.97	0.06	81,81,82,84	0
4	BME	DDD	504	4/4	0.97	0.06	95,99,102,104	0
6	GOL	BBB	504	6/6	0.97	0.05	78,82,83,84	0
4	BME	CCC	503	4/4	0.97	0.07	74,79,82,86	0
2	BJT	AAA	501	64/64	0.98	0.05	51,64,79,81	0
2	BJT	BBB	501	64/64	0.98	0.07	58,69,83,86	0
2	BJT	CCC	501	64/64	0.98	0.05	55,67,86,90	0
4	BME	CCC	506	4/4	0.98	0.05	90,92,93,98	0
2	BJT	DDD	501	64/64	0.98	0.06	52,66,82,88	0
3	CL	CCC	502	1/1	0.98	0.05	70,70,70,70	0
5	UDP	CCC	508	25/25	0.98	0.04	39,45,46,46	0
5	UDP	DDD	506	25/25	0.98	0.04	38,41,50,50	0
3	CL	DDD	502	1/1	0.98	0.04	92,92,92,92	0
4	BME	AAA	503	4/4	0.98	0.07	75,75,77,77	0
4	BME	DDD	505	4/4	0.99	0.05	38,39,42,47	0
5	UDP	AAA	506	25/25	0.99	0.04	34,37,41,44	0
5	UDP	BBB	506	25/25	0.99	0.04	35,39,42,44	0
3	CL	AAA	502	1/1	0.99	0.03	63,63,63,63	0
4	BME	CCC	507	4/4	0.99	0.04	40,40,41,42	0
4	BME	BBB	503	4/4	0.99	0.07	70,72,73,75	0
4	BME	CCC	505	4/4	0.99	0.03	79,85,87,90	0
4	BME	AAA	504	4/4	1.00	0.02	41,41,42,44	0
4	BME	AAA	505	4/4	1.00	0.03	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.

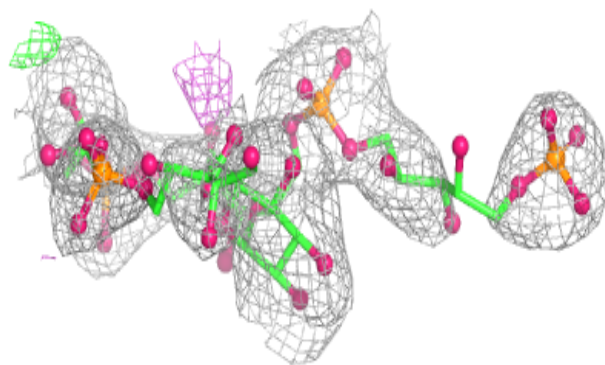
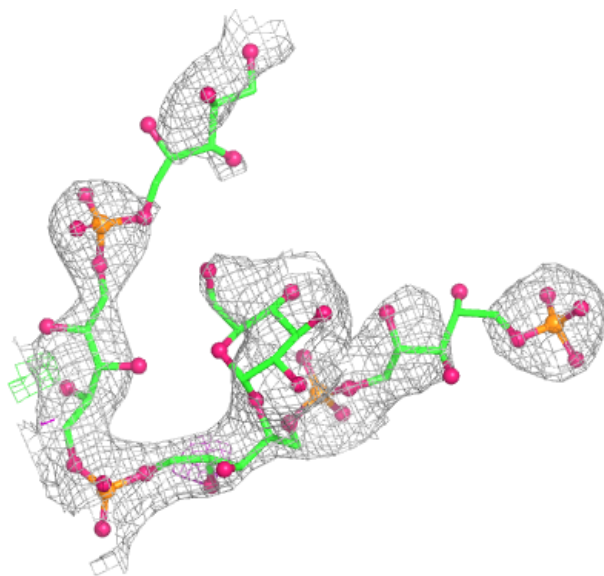
Electron density around BJT AAA 501:

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



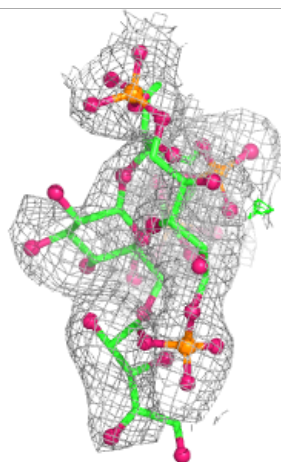
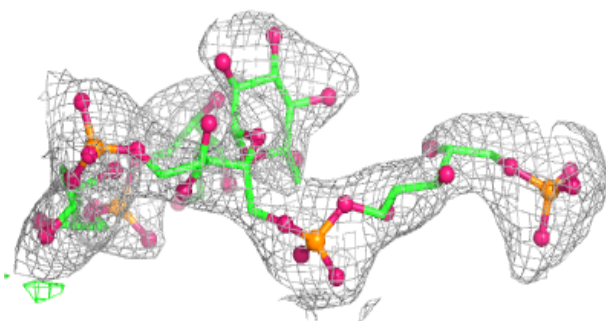
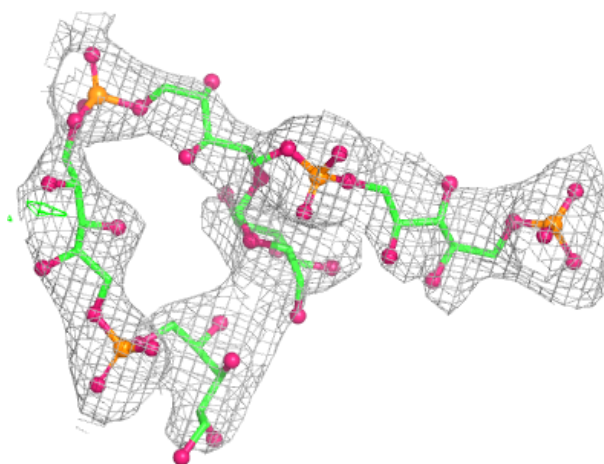
Electron density around BJT BBB 501:

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



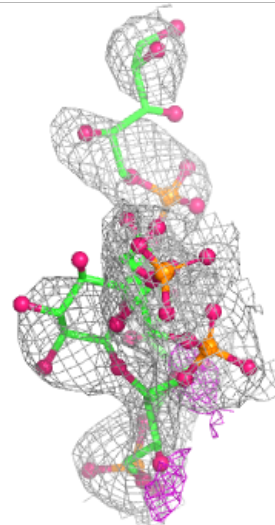
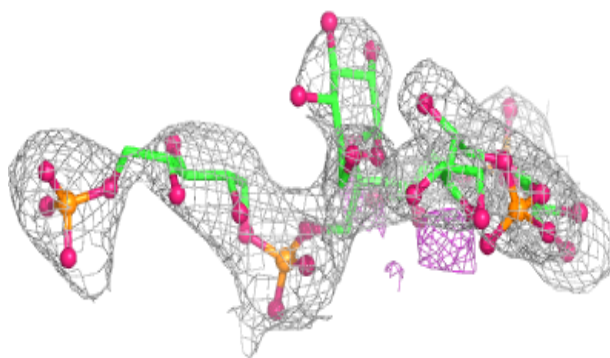
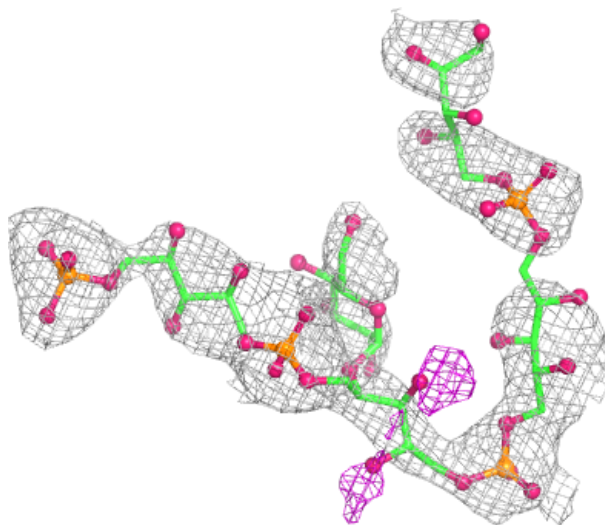
Electron density around BJT CCC 501:

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



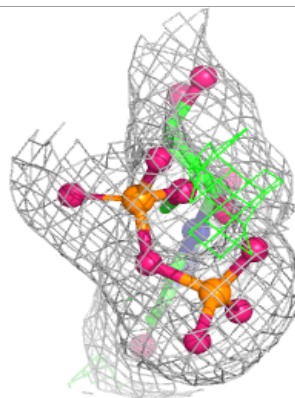
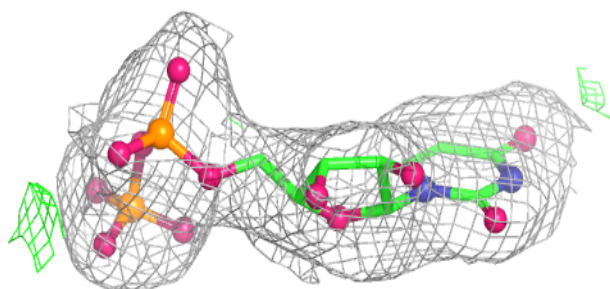
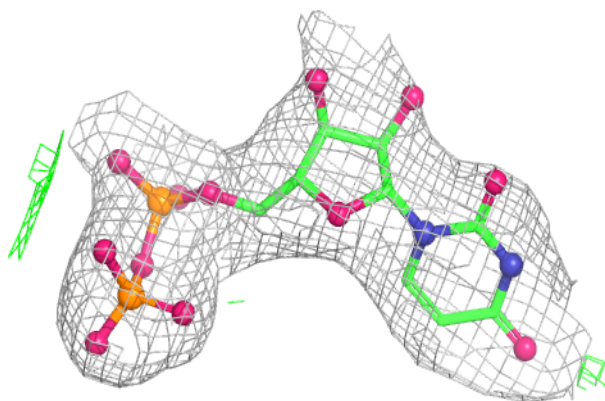
Electron density around BJT DDD 501:

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

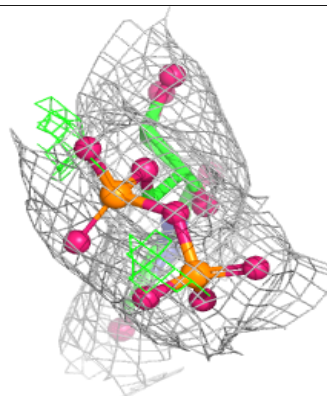
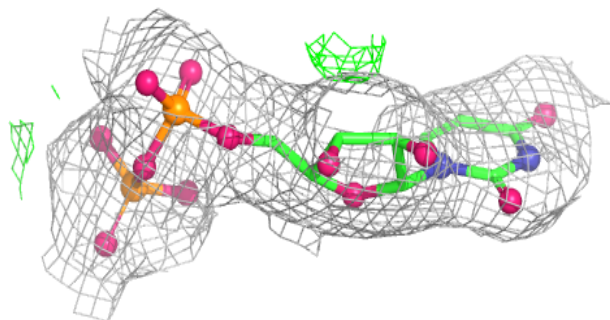
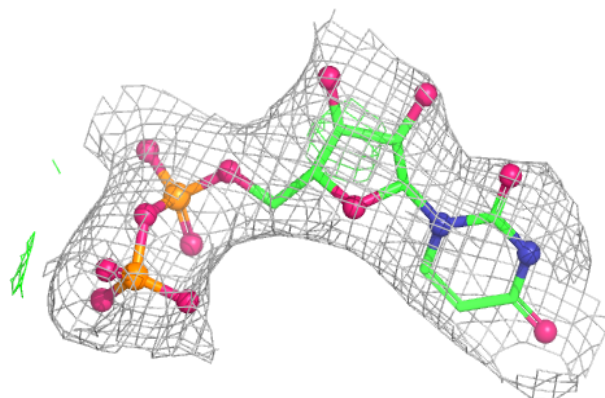


Electron density around UDP CCC 508:

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

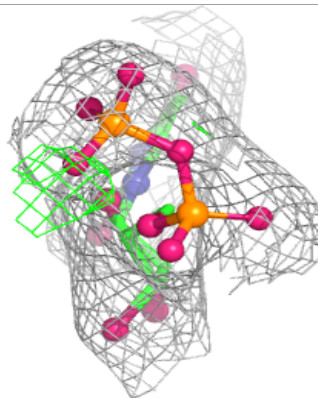
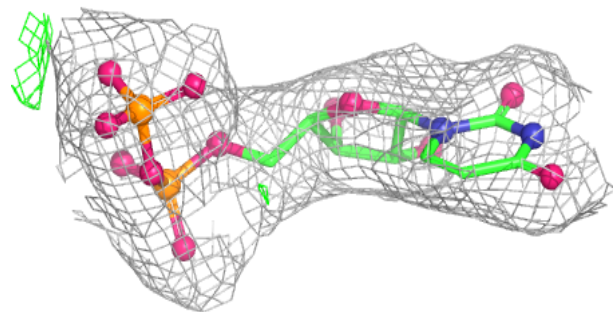
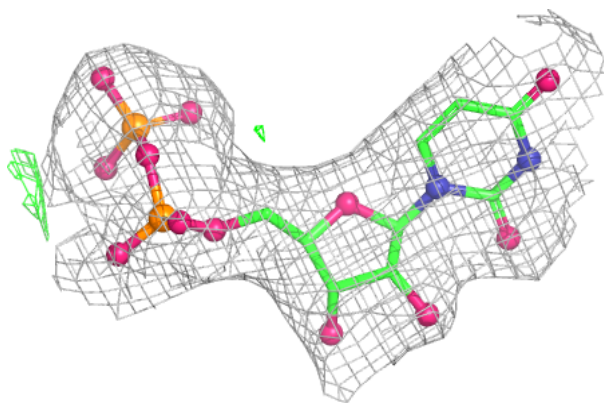
**Electron density around UDP DDD 506:**

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

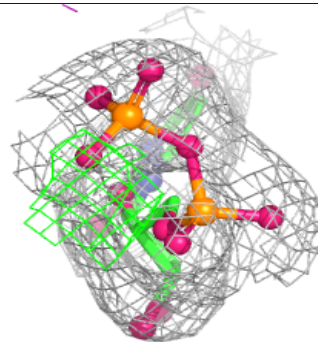
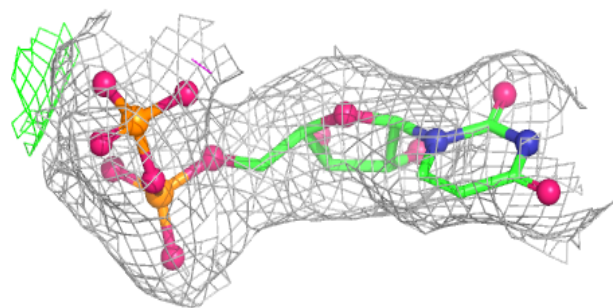
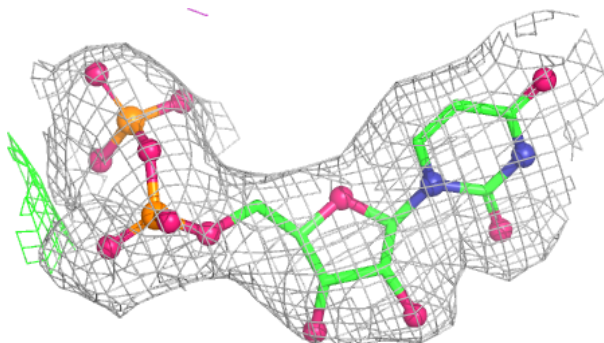


Electron density around UDP AAA 506:

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

**Electron density around UDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.