wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 07:13 PM BST

PDB ID	:	6ZIV
Title	:	Crystal structure of a Beta-glucosidase from Alicyclobacillus acidiphilus
Authors	:	Gourlay, L.J.
Deposited on	:	2020-06-26
Resolution	:	1.95 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 following versions of software and data (see references (i)) were used in the production of this report:

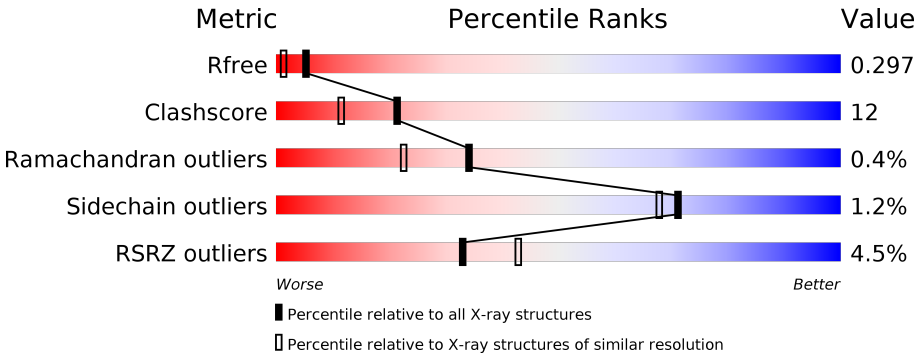
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	477	3% 73% 15% • 11%
1	BBB	477	3% 81% 11% • 6%
1	CCC	477	2% 80% 13% • 6%
1	DDD	477	2% 81% 12% • 6%
1	EEE	477	2% 80% 12% • 7%
1	FFF	477	% 76% 16% • 8%

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Mol	Chain	Length	Quality of chain
1	GGG	477	8% 80% 11% • 8%
1	HHH	477	12% 68% 14% • 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	AAA	502	-	-	X	-
3	EDO	BBB	502	-	-	X	-
3	EDO	GGG	502	-	-	X	-
3	EDO	GGG	503	-	-	X	-
5	IOD	CCC	504	-	-	X	-

2 Entry composition (i)

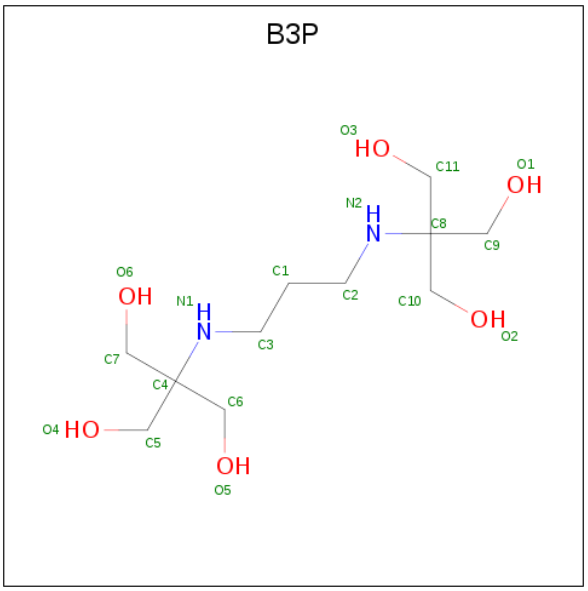
There are 6 unique types of molecules in this entry. The entry contains 30782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-glucosidase.

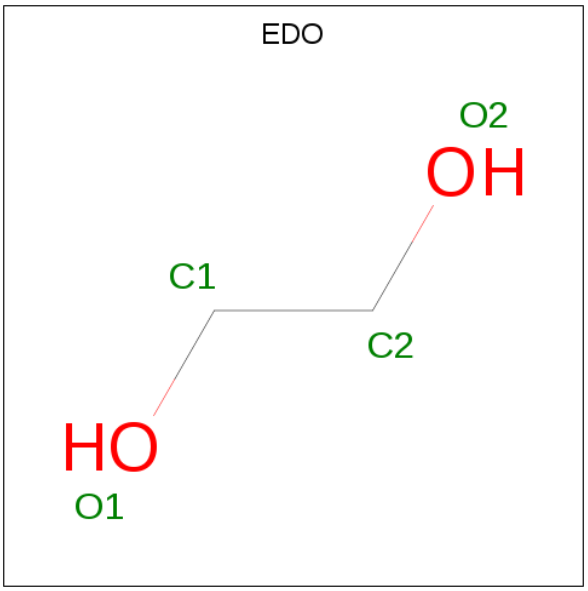
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	426	Total	C	N	O	S	0	5	0
			3493	2251	594	639	9			
1	BBB	447	Total	C	N	O	S	0	10	0
			3669	2362	619	679	9			
1	CCC	446	Total	C	N	O	S	0	4	0
			3638	2340	618	671	9			
1	DDD	448	Total	C	N	O	S	0	1	0
			3632	2333	616	674	9			
1	EEE	443	Total	C	N	O	S	0	8	0
			3629	2337	614	668	10			
1	FFF	441	Total	C	N	O	S	0	7	0
			3613	2325	613	666	9			
1	GGG	440	Total	C	N	O	S	0	5	0
			3599	2320	612	658	9			
1	HHH	401	Total	C	N	O	S	0	4	0
			3314	2145	561	599	9			

- Molecule 2 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			19	11	2	6		
2	BBB	1	Total	C	N	O	0	0
			19	11	2	6		
2	CCC	1	Total	C	N	O	0	0
			19	11	2	6		
2	DDD	1	Total	C	N	O	0	0
			19	11	2	6		
2	EEE	1	Total	C	N	O	0	0
			19	11	2	6		
2	FFF	1	Total	C	N	O	0	0
			19	11	2	6		
2	GGG	1	Total	C	N	O	0	0
			19	11	2	6		
2	HHH	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	FFF	1	Total C O 4 2 2	0	0
3	GGG	1	Total C O 4 2 2	0	0
3	GGG	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	FFF	2	Total Na 2 2	0	0
4	CCC	2	Total Na 2 2	0	0
4	EEE	1	Total Na 1 1	0	0
4	GGG	2	Total Na 2 2	0	0
4	AAA	1	Total Na 1 1	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total I 1 1	0	0

- Molecule 6 is water.

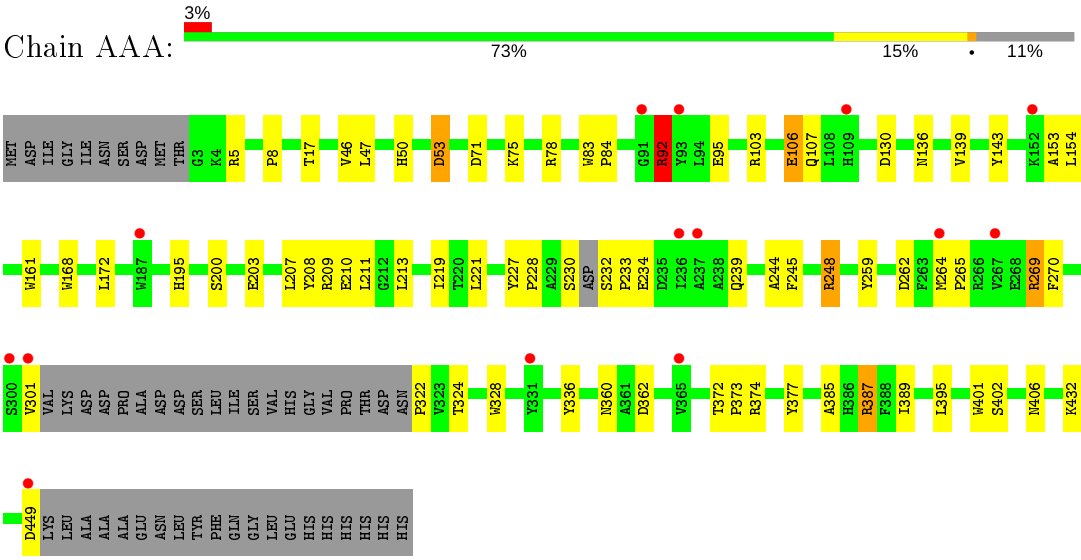
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	188	Total O 199 199	0	11
6	BBB	276	Total O 284 284	0	8
6	CCC	299	Total O 310 310	0	11
6	DDD	267	Total O 270 270	0	3
6	EEE	299	Total O 306 306	0	7
6	FFF	294	Total O 301 301	0	7
6	GGG	183	Total O 189 189	0	6
6	HHH	146	Total O 147 147	0	1

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.

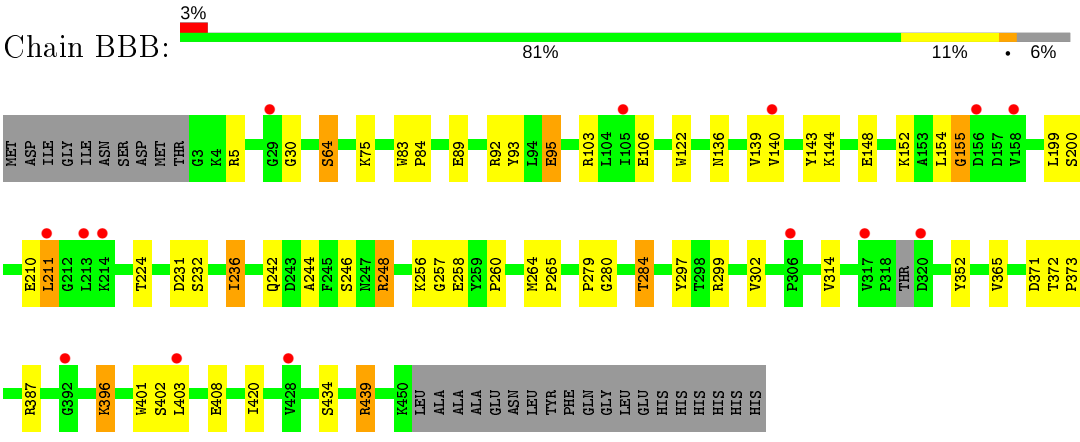
- Molecule 1: Beta-glucosidase

Chain AAA:



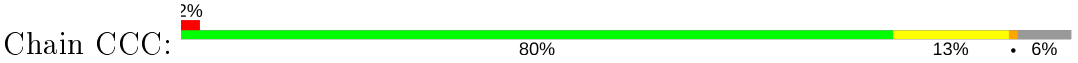
- Molecule 1: Beta-glucosidase

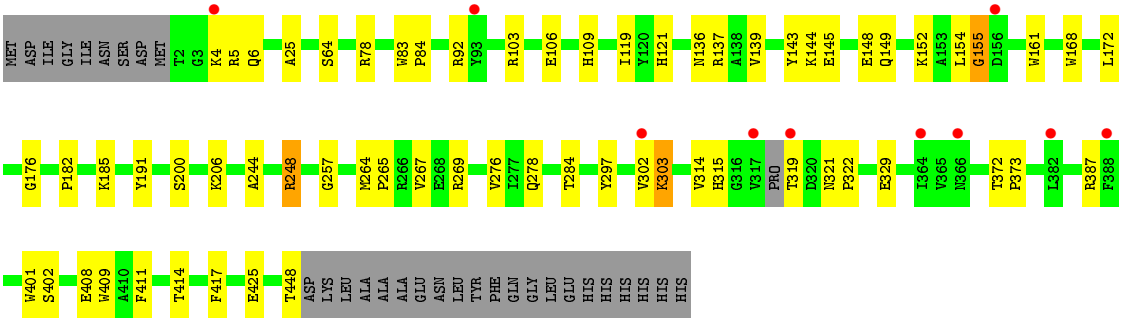
Chain BBB:



- Molecule 1: Beta-glucosidase

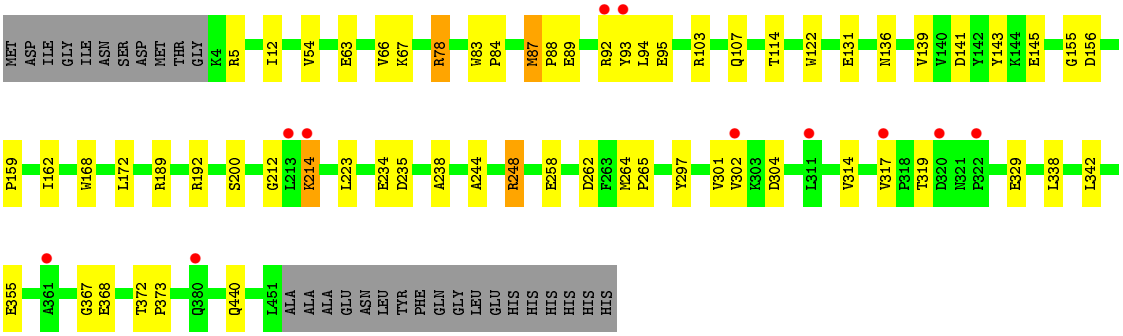
Chain CCC:





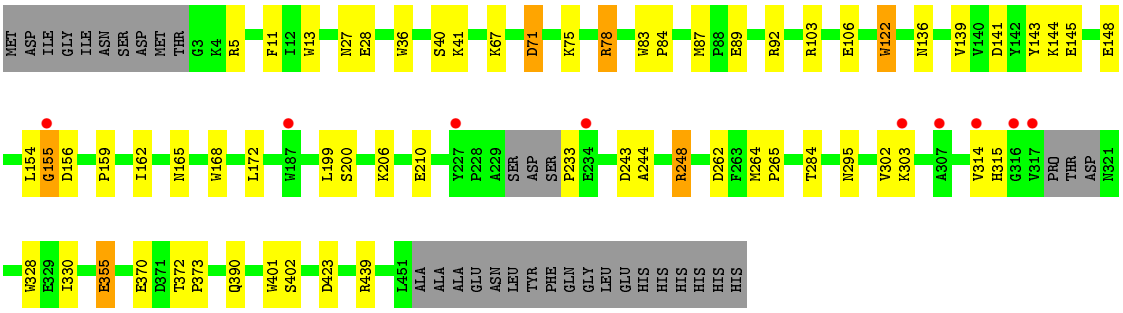
• Molecule 1: Beta-glucosidase

Chain DDD:



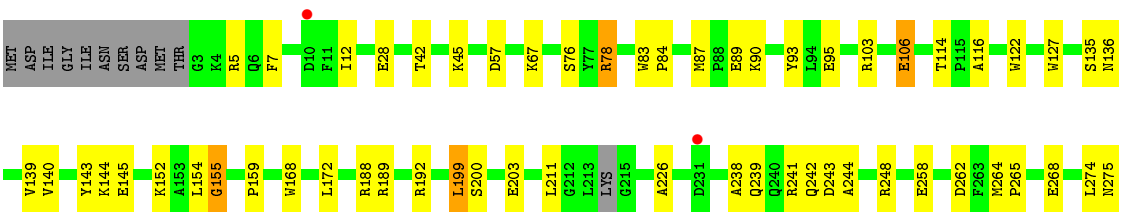
• Molecule 1: Beta-glucosidase

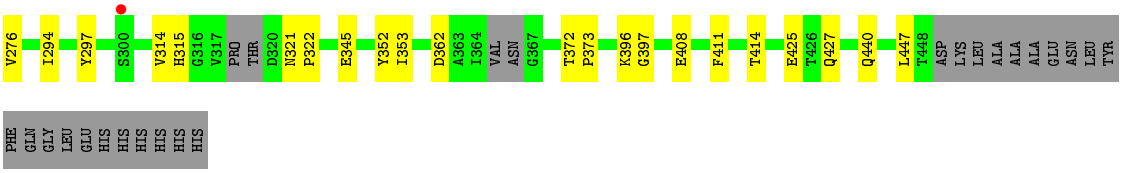
Chain EEE:



• Molecule 1: Beta-glucosidase

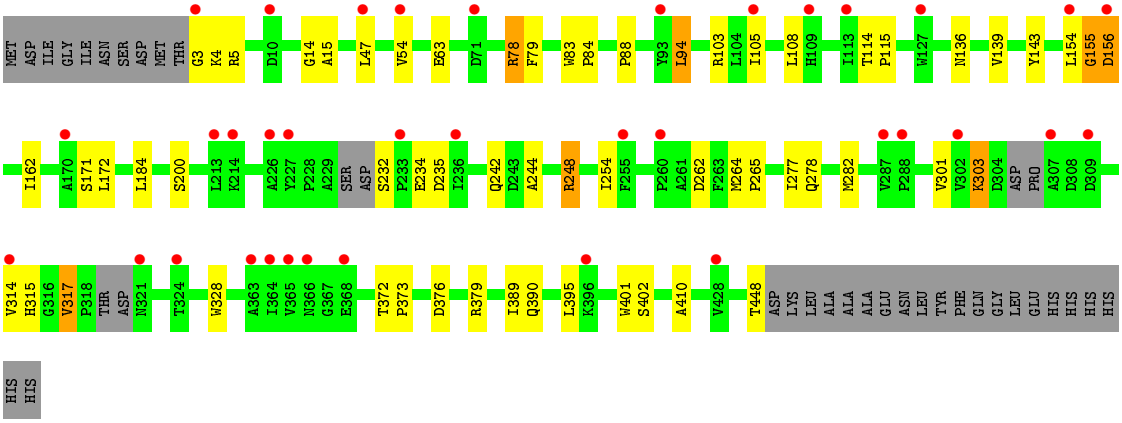
Chain FFF:





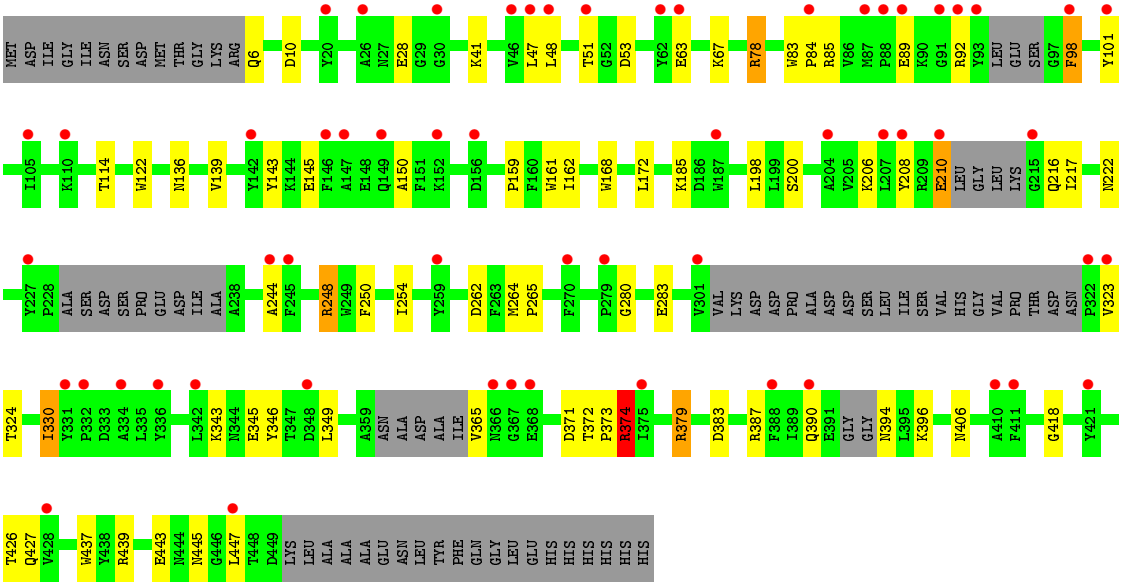
- Molecule 1: Beta-glucosidase

Chain GGG:



- Molecule 1: Beta-glucosidase

Chain HHH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.65Å 91.64Å 159.34Å 91.62° 90.42° 89.99°	Depositor
Resolution (Å)	46.55 – 1.95 46.51 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.55-1.95) 88.2 (46.51-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.262 , 0.296 0.263 , 0.297	Depositor DCC
R_{free} test set	24694 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 20.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-l 0.138 for -h,k,-l 0.058 for -h,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	30782	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: NA, IOD, B3P, EDO

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	0.49	1/3618 (0.0%)	0.73	10/4916 (0.2%)
1	BBB	0.41	0/3813	0.68	2/5187 (0.0%)
1	CCC	0.45	0/3763	0.69	3/5118 (0.1%)
1	DDD	0.45	1/3750 (0.0%)	0.71	4/5106 (0.1%)
1	EEE	1.68	3/3766 (0.1%)	1.61	9/5121 (0.2%)
1	FFF	0.46	2/3745 (0.1%)	0.69	1/5089 (0.0%)
1	GGG	0.37	0/3723	0.67	4/5060 (0.1%)
1	HHH	0.40	0/3431	0.76	8/4659 (0.2%)
All	All	0.73	7/29609 (0.0%)	0.87	41/40256 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	71[A]	ASP	CG-OD2	70.36	2.87	1.25
1	EEE	71[B]	ASP	CG-OD2	70.36	2.87	1.25
1	AAA	92	ARG	CD-NE	-15.33	1.20	1.46
1	FFF	345	GLU	CD-OE1	-6.71	1.18	1.25
1	EEE	355	GLU	CD-OE1	6.06	1.32	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	EEE	71[A]	ASP	CB-CG-OD2	-70.63	54.73	118.30
1	EEE	71[B]	ASP	CB-CG-OD2	-70.63	54.73	118.30
1	EEE	71[A]	ASP	OD1-CG-OD2	18.91	159.23	123.30
1	EEE	71[B]	ASP	OD1-CG-OD2	18.91	159.23	123.30
1	HHH	374	ARG	CB-CG-CD	-11.57	81.53	111.60

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	AAA	3493	0	3321	72	0
1	BBB	3669	0	3497	94	0
1	CCC	3638	0	3461	71	0
1	DDD	3632	0	3428	76	0
1	EEE	3629	0	3449	68	0
1	FFF	3613	0	3436	113	0
1	GGG	3599	0	3426	65	0
1	HHH	3314	0	3138	114	0
2	AAA	19	0	26	2	0
2	BBB	19	0	26	2	0
2	CCC	19	0	26	2	0
2	DDD	19	0	26	3	0
2	EEE	19	0	26	1	0
2	FFF	19	0	26	1	0
2	GGG	19	0	26	5	0
2	HHH	19	0	26	0	0
3	AAA	4	0	6	7	0
3	BBB	12	0	18	11	0
3	FFF	4	0	6	0	0
3	GGG	8	0	12	14	0
4	AAA	1	0	0	0	0
4	CCC	2	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	2	0	0	0	0
4	GGG	2	0	0	0	0
5	CCC	1	0	0	7	0
6	AAA	199	0	0	24	0
6	BBB	284	0	0	10	0
6	CCC	310	0	0	24	0
6	DDD	270	0	0	26	0
6	EEE	306	0	0	30	0
6	FFF	301	0	0	37	0
6	GGG	189	0	0	16	0
6	HHH	147	0	0	30	0
All	All	30782	0	27406	673	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 12.

The worst 5 of 673 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:AAA:389:ILE:HG12	6:AAA:602:HOH:O	1.29	1.28
1:BBB:210:GLU:OE2	1:HHH:280:GLY:HA2	1.27	1.28
1:FFF:57:ASP:HB2	6:FFF:603:HOH:O	1.16	1.26
1:AAA:402:SER:HB2	6:AAA:611:HOH:O	1.31	1.25
1:FFF:87:MET:HG3	6:FFF:758:HOH:O	1.11	1.24

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	425/477 (89%)	411 (97%)	12 (3%)	2 (0%)	29	17
1	BBB	453/477 (95%)	444 (98%)	7 (2%)	2 (0%)	34	22
1	CCC	446/477 (94%)	434 (97%)	11 (2%)	1 (0%)	47	38
1	DDD	447/477 (94%)	437 (98%)	8 (2%)	2 (0%)	34	22
1	EEE	445/477 (93%)	434 (98%)	9 (2%)	2 (0%)	34	22
1	FFF	440/477 (92%)	427 (97%)	11 (2%)	2 (0%)	29	17
1	GGG	437/477 (92%)	425 (97%)	11 (2%)	1 (0%)	47	38
1	HHH	391/477 (82%)	380 (97%)	10 (3%)	1 (0%)	41	30
All	All	3484/3816 (91%)	3392 (97%)	79 (2%)	13 (0%)	34	22

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	PRO
1	AAA	155	GLY

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Mol	Chain	Res	Type
1	BBB	155	GLY
1	CCC	155	GLY
1	DDD	155	GLY

5.3.2 Protein sidechains

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	360/399 (90%)	355 (99%)	5 (1%)	67	62
1	BBB	383/399 (96%)	374 (98%)	9 (2%)	50	42
1	CCC	377/399 (94%)	375 (100%)	2 (0%)	88	88
1	DDD	375/399 (94%)	371 (99%)	4 (1%)	73	71
1	EEE	376/399 (94%)	374 (100%)	2 (0%)	88	88
1	FFF	375/399 (94%)	372 (99%)	3 (1%)	81	80
1	GGG	372/399 (93%)	367 (99%)	5 (1%)	69	65
1	HHH	341/399 (86%)	335 (98%)	6 (2%)	59	53
All	All	2959/3192 (93%)	2923 (99%)	36 (1%)	71	68

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	67	LYS
1	EEE	144	LYS
1	HHH	365	VAL
1	DDD	214	LYS
1	EEE	390	GLN

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

5.3.3 RNA

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 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
2	B3P	HHH	501	-	18,18,18	0.22	0	21,23,23	0.76	0
3	EDO	GGG	502	-	3,3,3	0.25	0	2,2,2	0.52	0
2	B3P	EEE	501	-	18,18,18	0.56	0	21,23,23	0.79	0
3	EDO	GGG	503	-	3,3,3	0.02	0	2,2,2	0.43	0
2	B3P	CCC	501	-	18,18,18	0.29	0	21,23,23	1.11	2 (9%)
3	EDO	BBB	502	-	3,3,3	0.12	0	2,2,2	0.40	0
2	B3P	DDD	501	-	18,18,18	0.43	0	21,23,23	1.18	2 (9%)
2	B3P	FFF	501	-	18,18,18	0.53	0	21,23,23	1.08	1 (4%)
3	EDO	AAA	502	-	3,3,3	0.27	0	2,2,2	0.63	0
2	B3P	GGG	501	-	18,18,18	0.32	0	21,23,23	0.85	0
3	EDO	BBB	504	-	3,3,3	0.10	0	2,2,2	0.23	0
2	B3P	BBB	501	-	18,18,18	0.43	0	21,23,23	1.11	2 (9%)
2	B3P	AAA	501	-	18,18,18	0.23	0	21,23,23	1.25	2 (9%)
3	EDO	FFF	502	-	3,3,3	0.31	0	2,2,2	0.47	0
3	EDO	BBB	503	-	3,3,3	0.23	0	2,2,2	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
2	B3P	HHH	501	-	-	1/28/28/28	-
3	EDO	GGG	502	-	-	0/1/1/1	-
2	B3P	EEE	501	-	-	5/28/28/28	-
3	EDO	GGG	503	-	-	0/1/1/1	-
2	B3P	CCC	501	-	-	8/28/28/28	-
3	EDO	BBB	502	-	-	0/1/1/1	-
2	B3P	DDD	501	-	-	5/28/28/28	-
2	B3P	FFF	501	-	-	4/28/28/28	-
3	EDO	AAA	502	-	-	0/1/1/1	-
2	B3P	GGG	501	-	-	14/28/28/28	-
3	EDO	BBB	504	-	-	1/1/1/1	-
2	B3P	BBB	501	-	-	3/28/28/28	-
2	B3P	AAA	501	-	-	10/28/28/28	-
3	EDO	FFF	502	-	-	1/1/1/1	-
3	EDO	BBB	503	-	-	1/1/1/1	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	501	B3P	C7-C4-C5	-3.45	102.75	110.04
2	DDD	501	B3P	C10-C8-N2	2.79	117.41	109.03
2	CCC	501	B3P	O2-C10-C8	2.63	116.97	111.63
2	BBB	501	B3P	C2-N2-C8	2.62	119.80	116.08
2	FFF	501	B3P	O3-C11-C8	-2.56	106.46	111.63

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

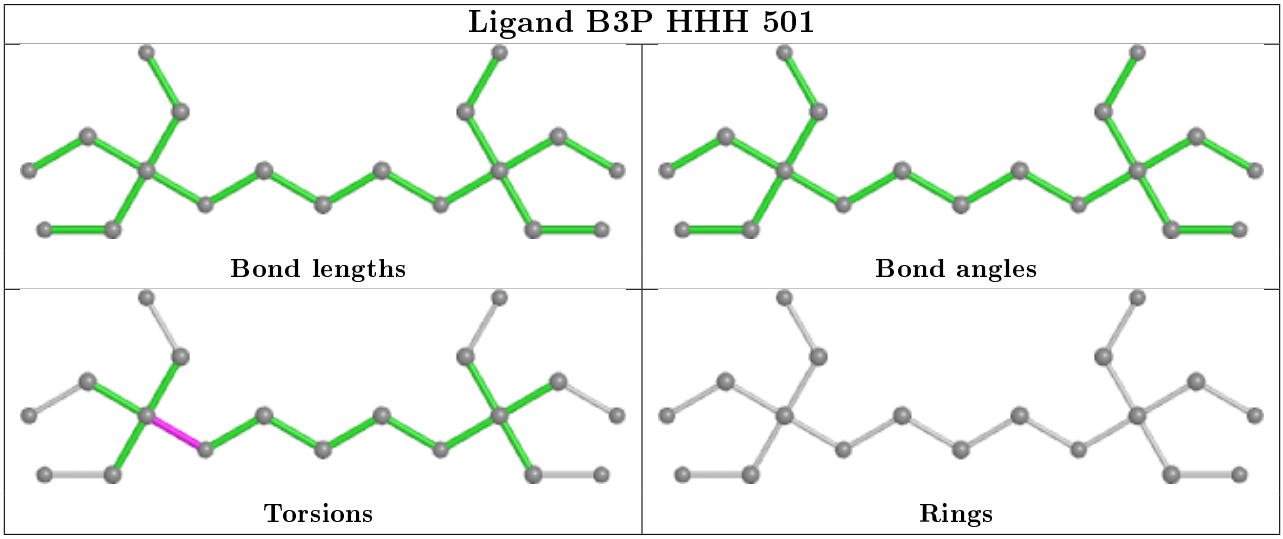
Mol	Chain	Res	Type	Atoms
2	GGG	501	B3P	C10-C8-N2-C2
2	GGG	501	B3P	C11-C8-N2-C2
2	GGG	501	B3P	N2-C8-C9-O1
2	GGG	501	B3P	C10-C8-C9-O1
2	GGG	501	B3P	C11-C8-C9-O1

There are no ring outliers.

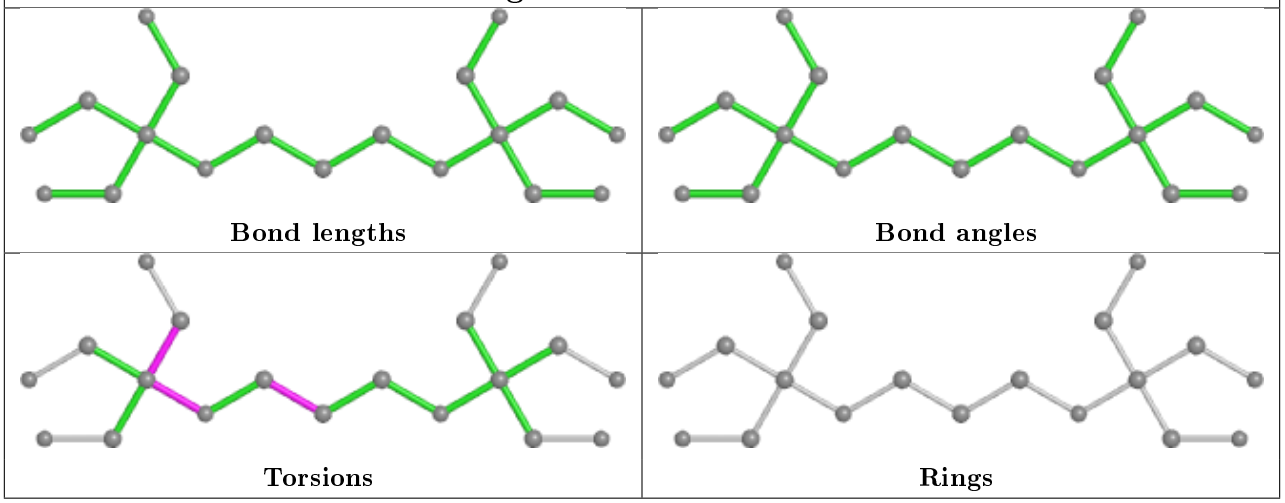
12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	GGG	502	EDO	10	0
2	EEE	501	B3P	1	0
3	GGG	503	EDO	4	0
2	CCC	501	B3P	2	0
3	BBB	502	EDO	10	0
2	DDD	501	B3P	3	0
2	FFF	501	B3P	1	0
3	AAA	502	EDO	7	0
2	GGG	501	B3P	5	0
2	BBB	501	B3P	2	0
2	AAA	501	B3P	2	0
3	BBB	503	EDO	1	0

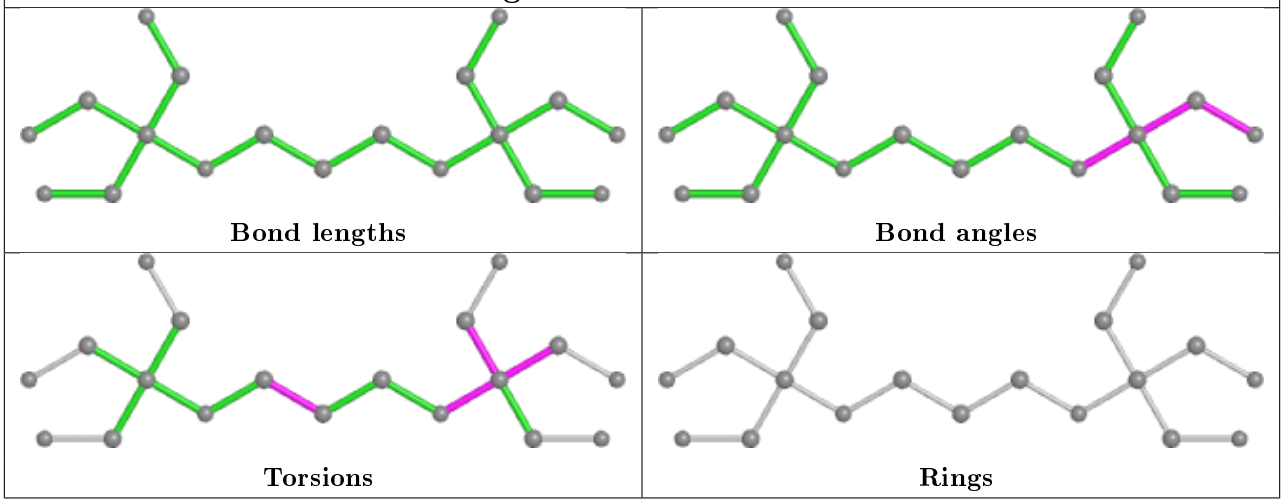
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



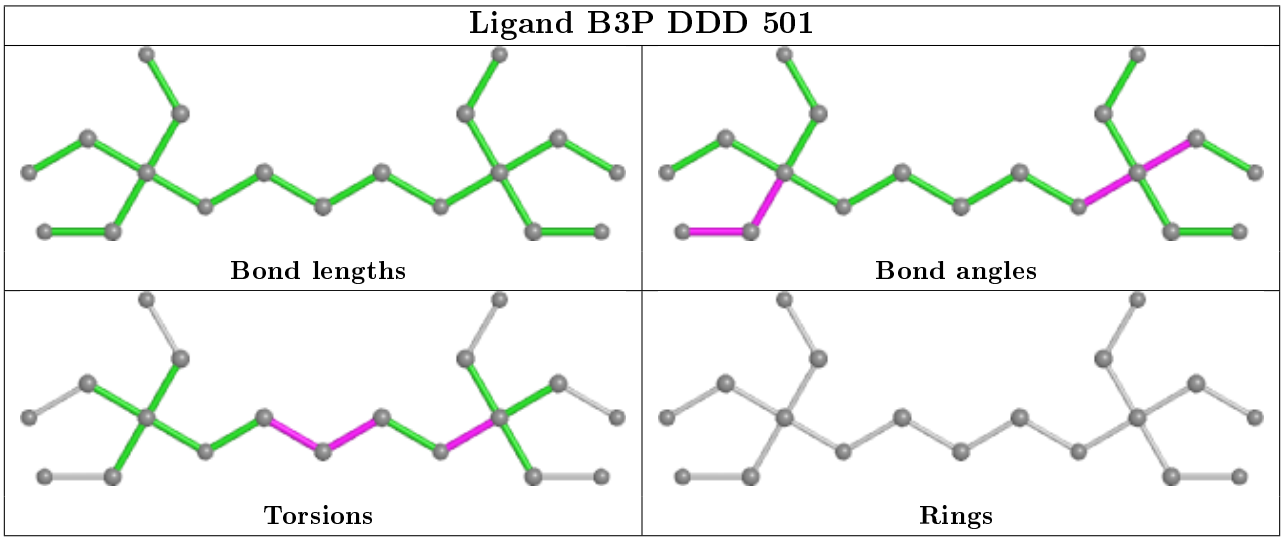
Ligand B3P EEE 501



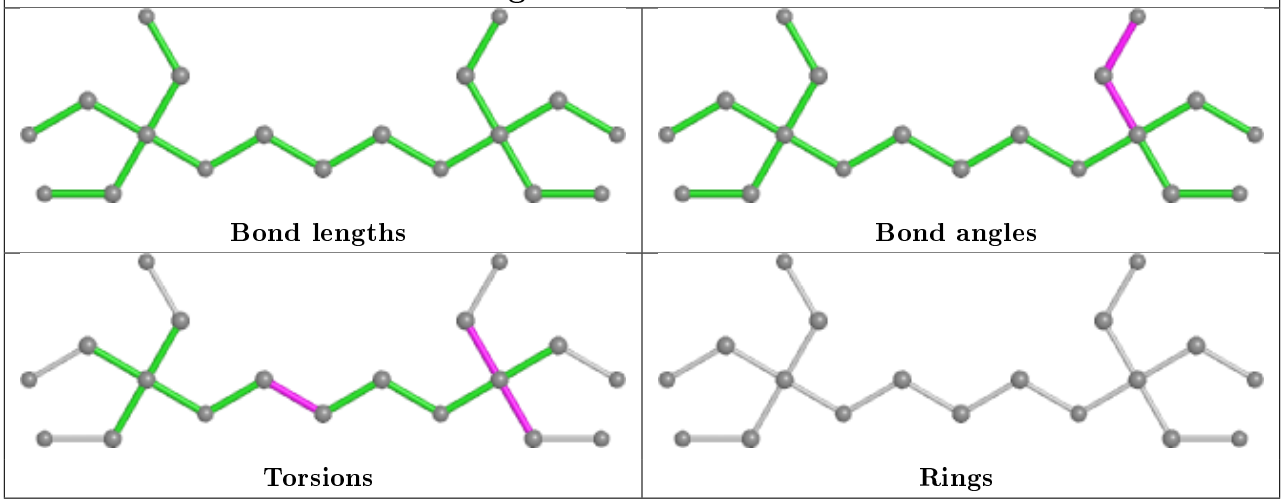
Ligand B3P CCC 501



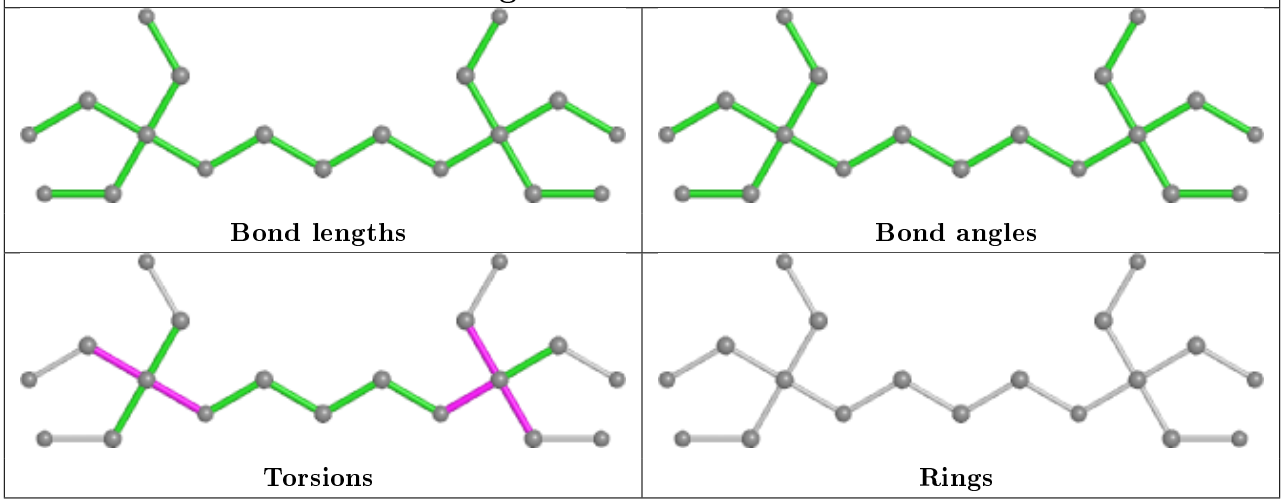
Ligand B3P DDD 501



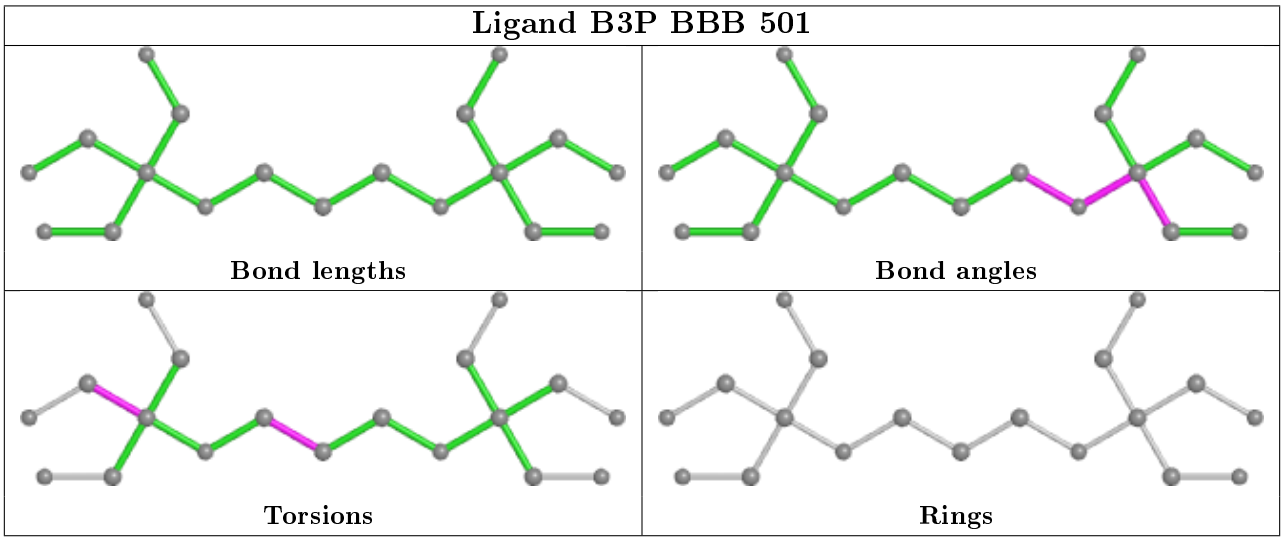
Ligand B3P FFF 501



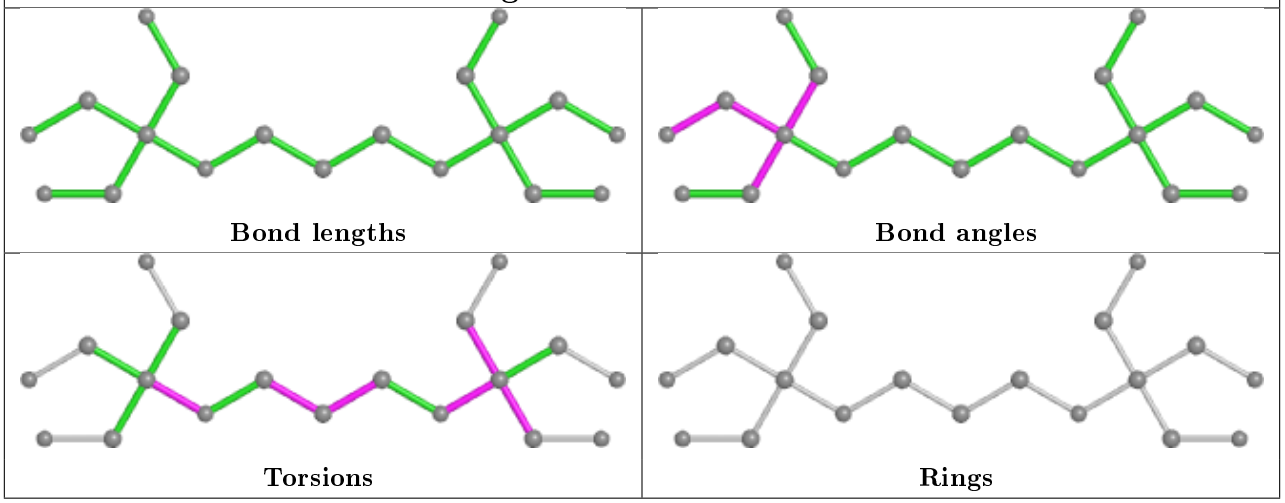
Ligand B3P GGG 501



Ligand B3P BBB 501



Ligand B3P 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	426/477 (89%)	0.74	15 (3%) 44 53	5, 11, 24, 37	6 (1%)
1	BBB	447/477 (93%)	0.71	14 (3%) 49 58	5, 12, 24, 33	5 (1%)
1	CCC	446/477 (93%)	0.55	10 (2%) 62 70	4, 7, 18, 37	5 (1%)
1	DDD	448/477 (93%)	0.57	11 (2%) 57 66	3, 8, 17, 29	2 (0%)
1	EEE	443/477 (92%)	0.49	9 (2%) 65 73	4, 7, 18, 35	3 (0%)
1	FFF	441/477 (92%)	0.52	3 (0%) 87 92	4, 7, 16, 26	6 (1%)
1	GGG	440/477 (92%)	0.99	36 (8%) 11 18	6, 15, 28, 37	5 (1%)
1	HHH	401/477 (84%)	1.16	58 (14%) 2 4	6, 17, 29, 45	8 (1%)
All	All	3492/3816 (91%)	0.71	156 (4%) 33 43	3, 10, 24, 45	40 (1%)

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	HHH	301	VAL	4.8
1	CCC	302	VAL	4.2
1	HHH	93	TYR	4.0
1	CCC	156	ASP	4.0
1	EEE	317	VAL	4.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

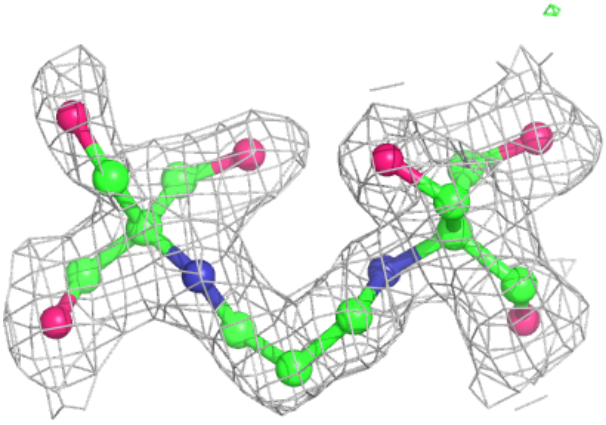
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

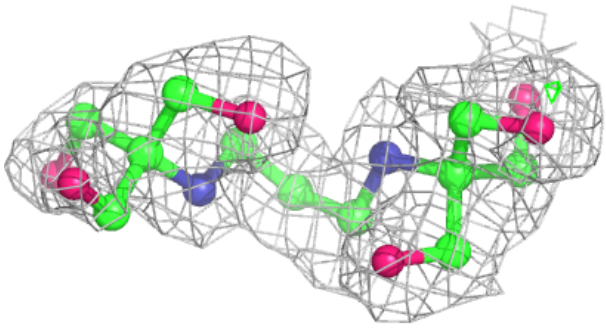
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IOD	CCC	504	1/1	0.77	0.26	189,189,189,189	0
3	EDO	GGG	503	4/4	0.82	0.33	17,20,20,23	0
3	EDO	BBB	504	4/4	0.84	0.16	19,20,20,22	0
3	EDO	BBB	502	4/4	0.84	0.29	27,30,31,33	0
2	B3P	HHH	501	19/19	0.86	0.15	16,20,26,28	0
3	EDO	GGG	502	4/4	0.87	0.17	17,18,20,20	0
2	B3P	GGG	501	19/19	0.88	0.18	10,11,13,14	0
4	NA	EEE	502	1/1	0.88	0.17	22,22,22,22	0
2	B3P	FFF	501	19/19	0.90	0.13	5,6,6,6	0
2	B3P	DDD	501	19/19	0.90	0.15	6,7,12,13	0
2	B3P	BBB	501	19/19	0.91	0.13	9,10,13,15	0
3	EDO	BBB	503	4/4	0.91	0.17	16,18,20,22	0
4	NA	CCC	502	1/1	0.93	0.11	17,17,17,17	0
3	EDO	FFF	502	4/4	0.93	0.19	12,16,16,17	0
4	NA	AAA	503	1/1	0.93	0.12	22,22,22,22	0
4	NA	FFF	504	1/1	0.93	0.18	19,19,19,19	0
3	EDO	AAA	502	4/4	0.94	0.15	6,7,7,8	0
2	B3P	AAA	501	19/19	0.94	0.11	6,7,11,13	0
2	B3P	EEE	501	19/19	0.94	0.11	5,6,8,9	0
2	B3P	CCC	501	19/19	0.94	0.11	5,6,9,11	0
4	NA	GGG	504	1/1	0.97	0.15	21,21,21,21	0
4	NA	GGG	505	1/1	0.97	0.06	21,21,21,21	0
4	NA	CCC	503	1/1	0.98	0.07	9,9,9,9	0
4	NA	FFF	503	1/1	0.99	0.10	13,13,13,13	0

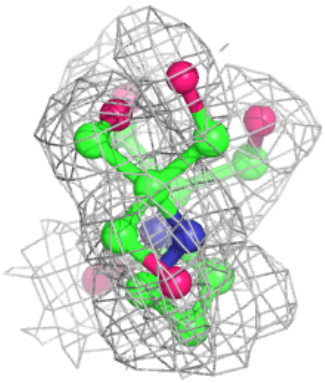
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P HHH 501:

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

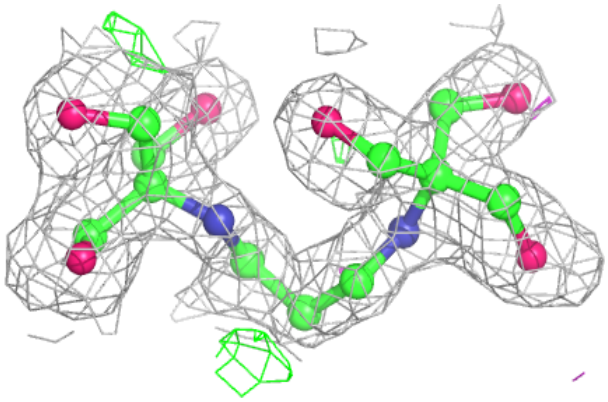


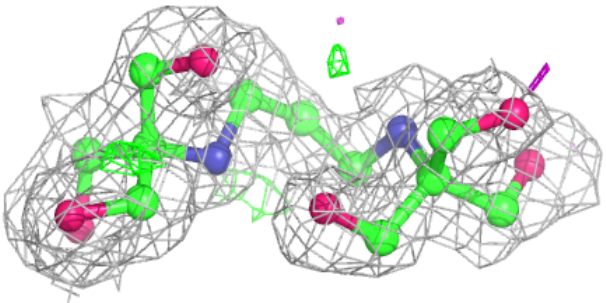


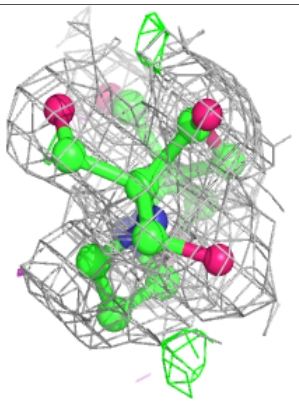


Electron density around B3P GGG 501:

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

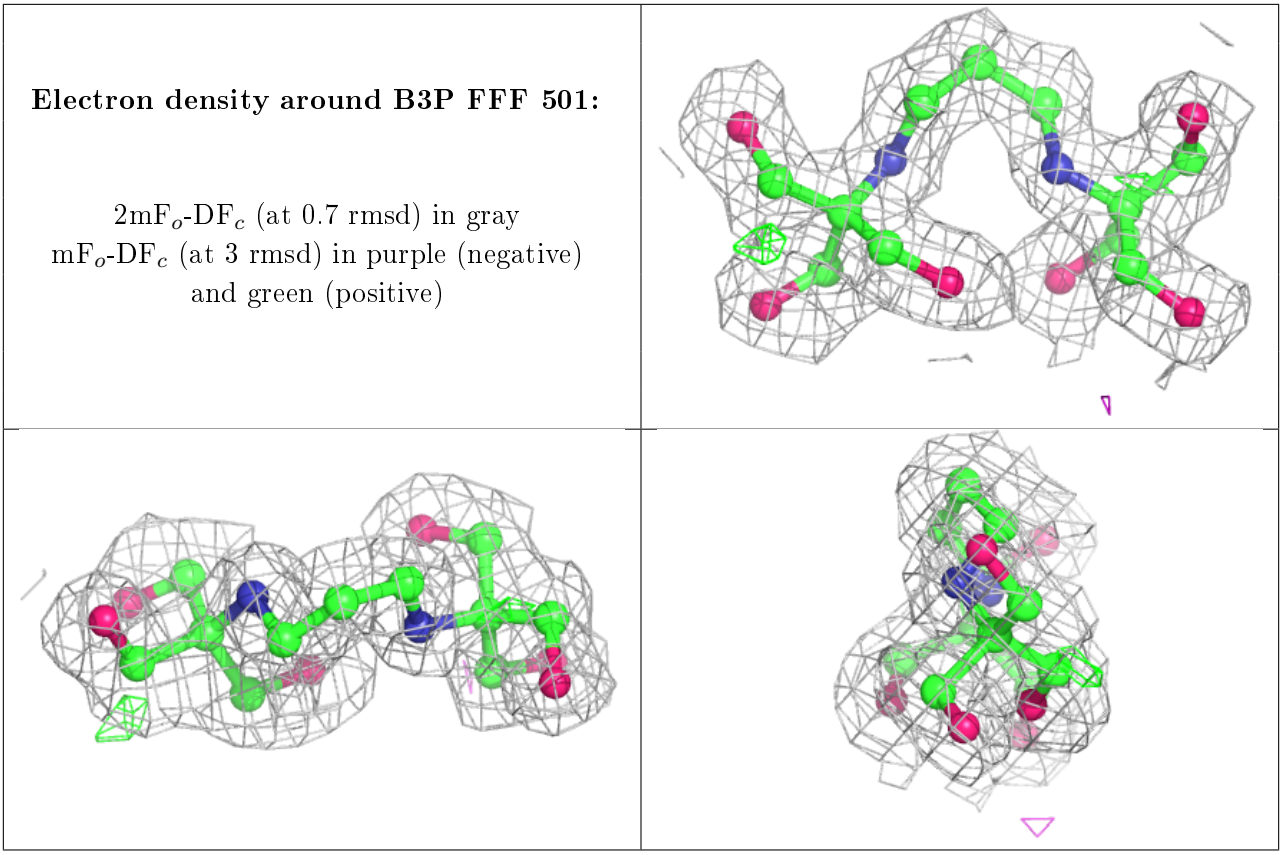






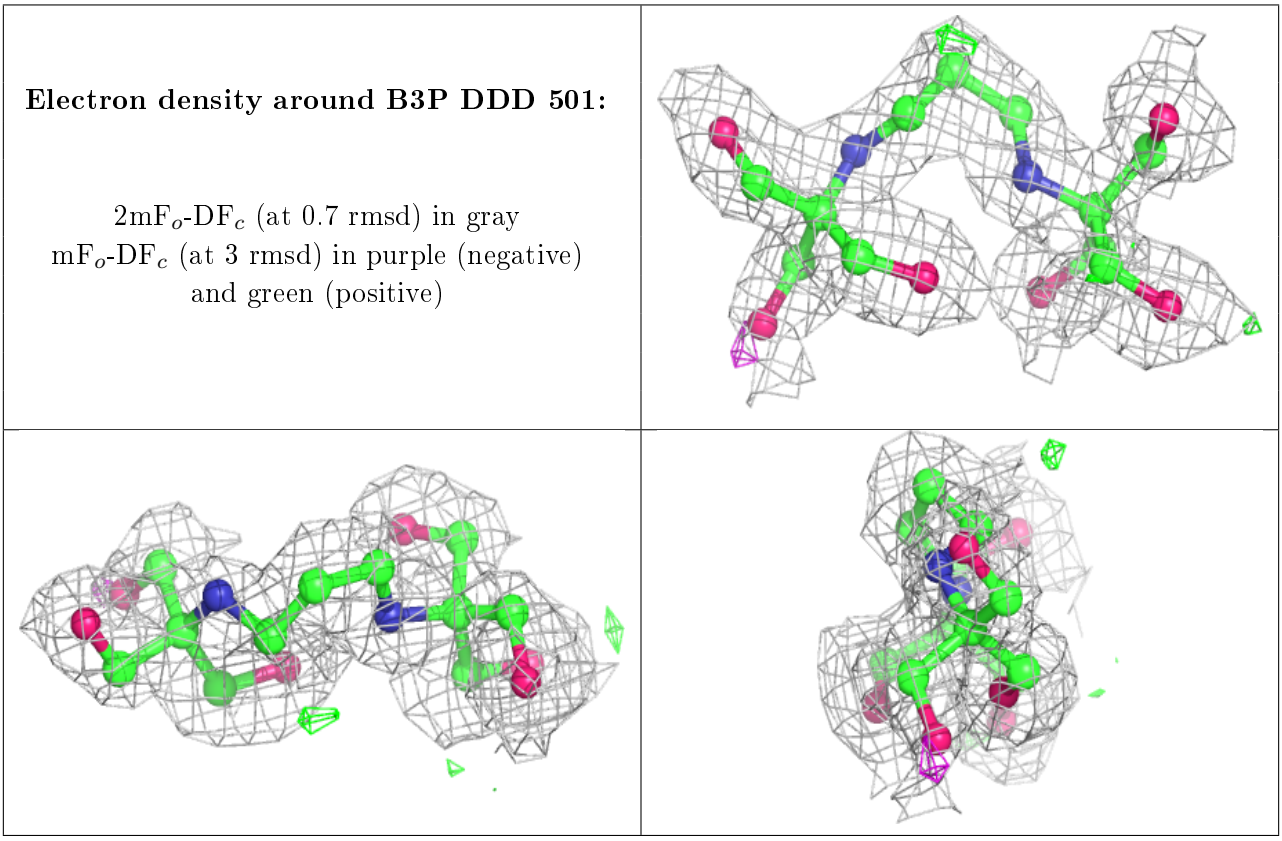
Electron density around B3P FFF 501:

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



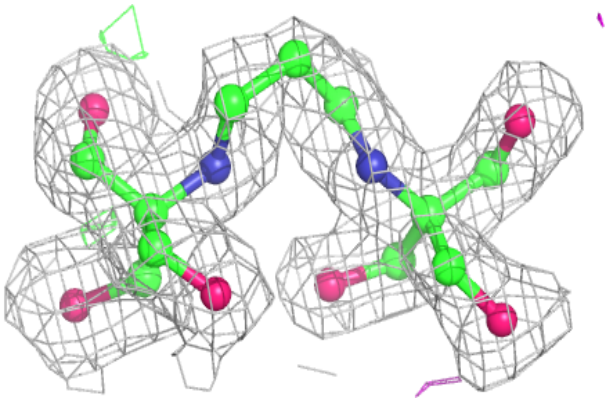
Electron density around B3P DDD 501:

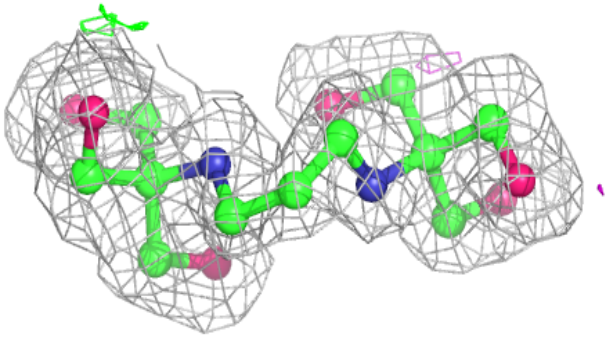
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

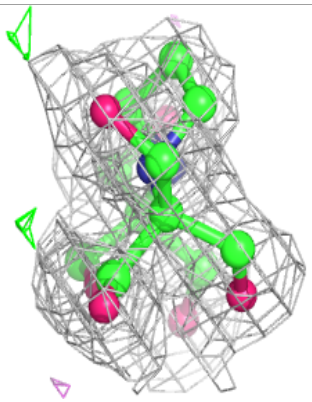


Electron density around B3P BBB 501:

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

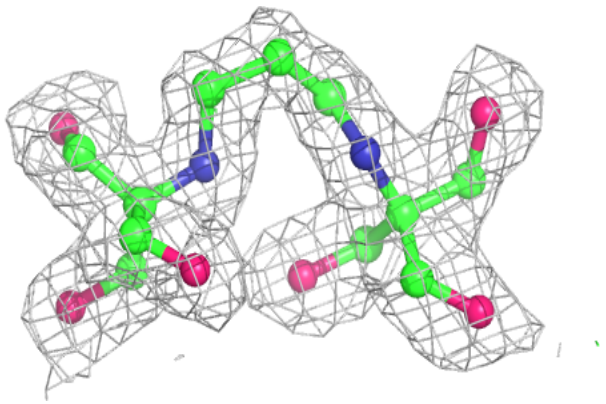


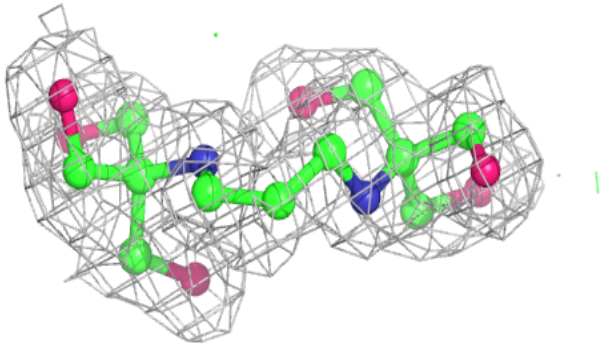


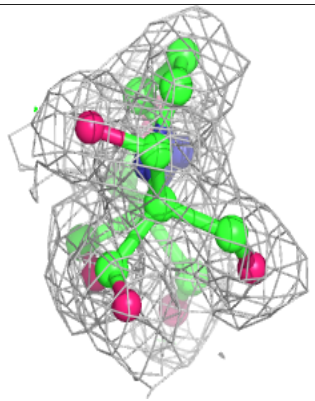


Electron density around B3P AAA 501:

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

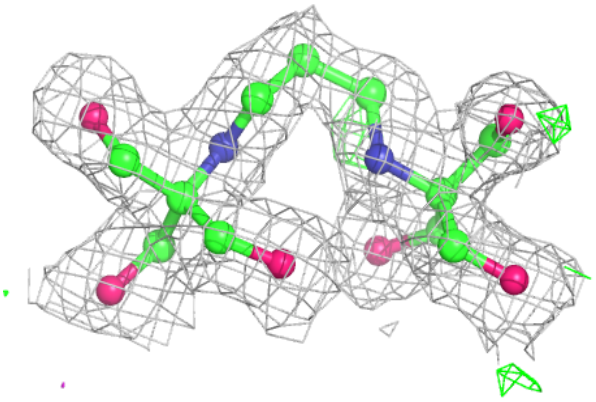


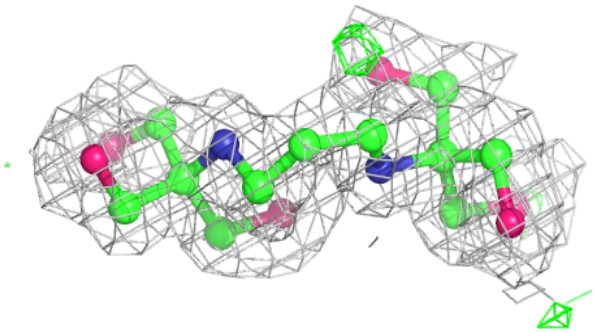


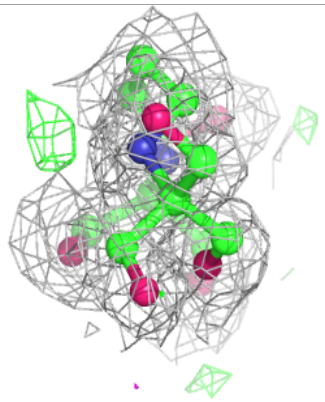


Electron density around B3P EEE 501:

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

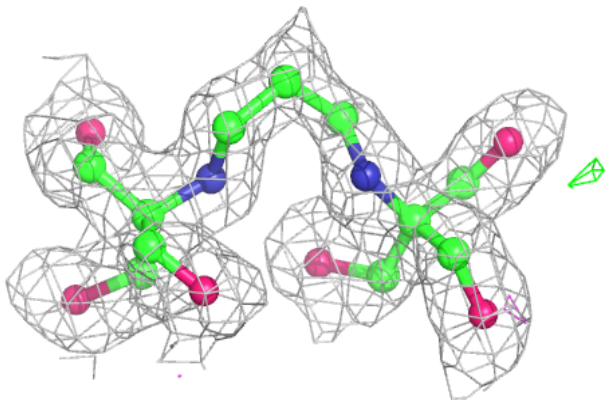


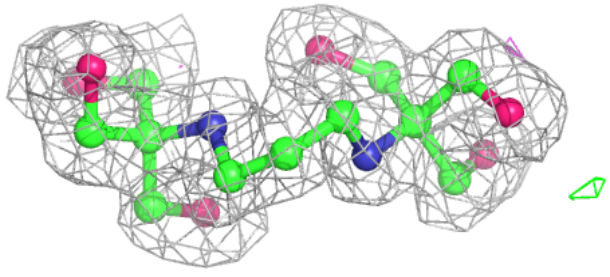


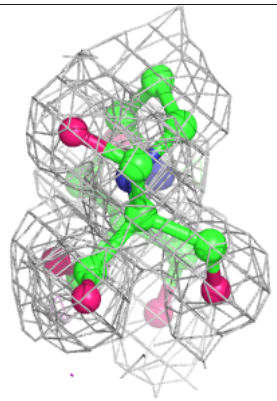


Electron density around B3P CCC 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.