



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:55 pm BST

PDB ID : 3C2U  
Title : Structure of the two subsite D-xylosidase from *Selenomonas ruminantium* in complex with 1,3-bis[tris(hydroxymethyl)methylamino]propane  
Authors : Brunzelle, J.S.; Jordan, D.B.; McCaslin, D.R.; Olczak, A.; Wawrzak, A.  
Deposited on : 2008-01-25  
Resolution : 1.30 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

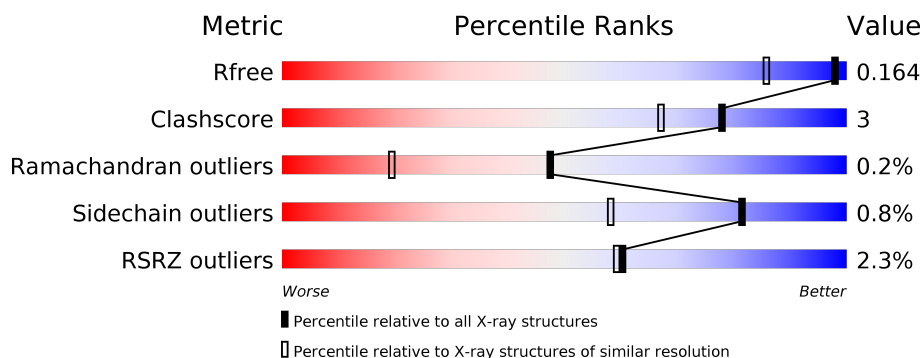
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	538	<div> <div>2%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
1	B	538	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	C	538	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	D	538	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

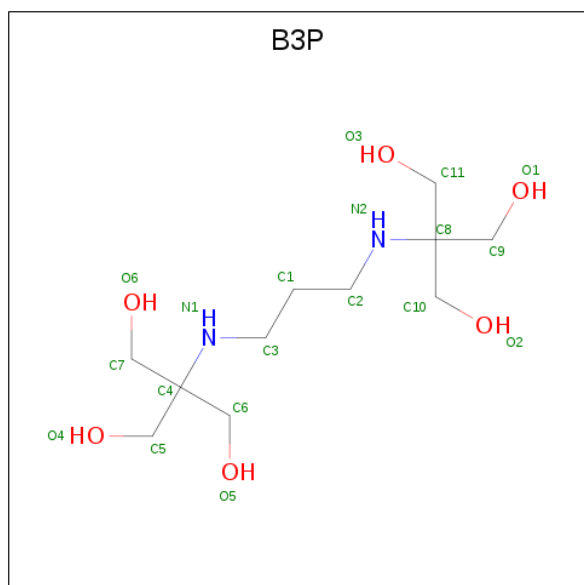
There are 3 unique types of molecules in this entry. The entry contains 19963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xylosidase/arabinosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	11	0
			4424	2849	731	832	12			
1	B	537	Total	C	N	O	S	0	17	0
			4462	2875	736	839	12			
1	C	537	Total	C	N	O	S	0	20	0
			4487	2885	741	849	12			
1	D	537	Total	C	N	O	S	0	16	0
			4459	2873	739	835	12			

- 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	A	1	Total	C	N	O	0	1
			20	11	2	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			20	11	2	7		
2	C	1	Total	C	N	O	0	1
			20	11	2	7		
2	D	1	Total	C	N	O	0	1
			21	11	2	8		

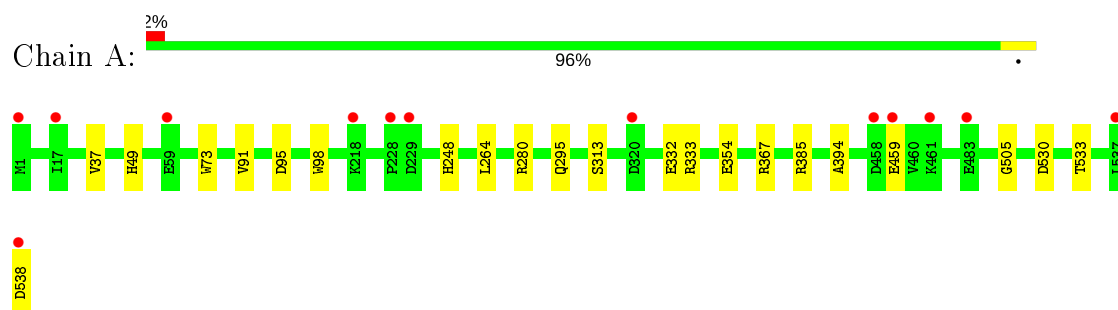
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	503	Total	O	0	1
			503	503		
3	B	503	Total	O	0	1
			503	503		
3	C	507	Total	O	0	1
			507	507		
3	D	536	Total	O	0	1
			537	537		

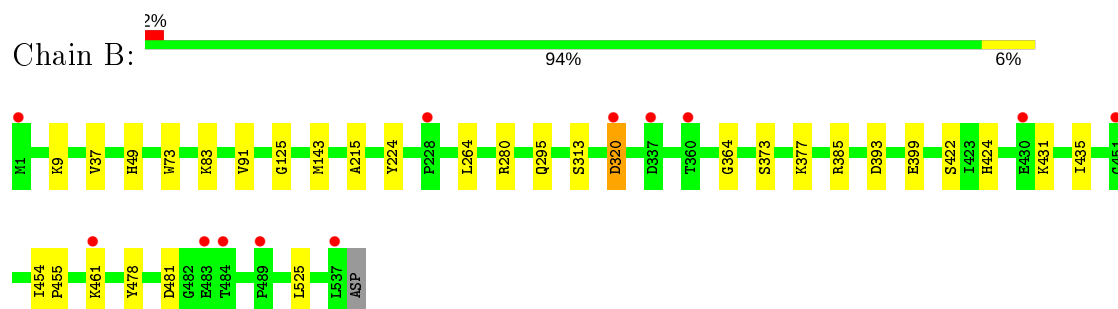
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

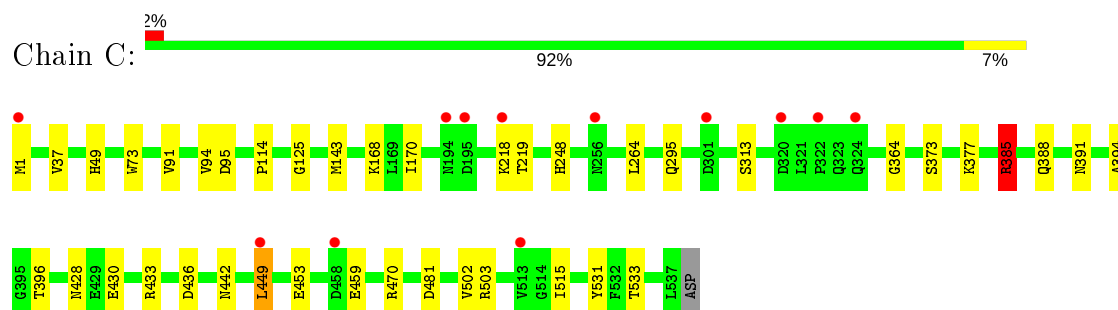
- Molecule 1: Xylosidase/arabinosidase



- Molecule 1: Xylosidase/arabinosidase

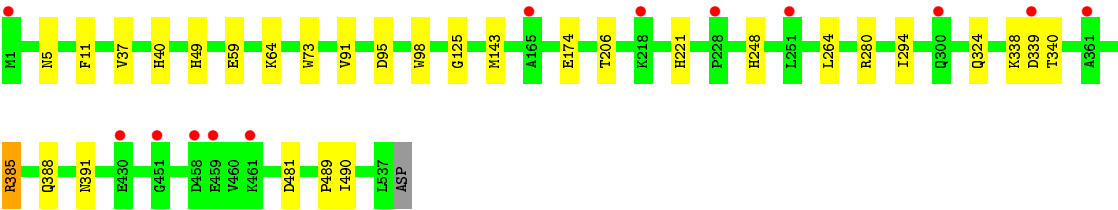


- Molecule 1: Xylosidase/arabinosidase



- Molecule 1: Xylosidase/arabinosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.58Å 84.40Å 94.04Å 67.84° 81.31° 75.08°	Depositor
Resolution (Å)	87.04 – 1.30 28.78 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (87.04-1.30) 94.5 (28.78-1.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.134 , 0.163 0.136 , 0.164	Depositor DCC
$R_{free}$ test set	31514 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	19963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B3P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.72	0/4569	0.82	4/6231 (0.1%)
1	B	0.75	0/4607	0.84	3/6283 (0.0%)
1	C	0.75	0/4632	0.84	4/6313 (0.1%)
1	D	0.75	0/4604	0.82	4/6278 (0.1%)
All	All	0.74	0/18412	0.83	15/25105 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	433	ARG	NE-CZ-NH2	9.28	124.94	120.30
1	C	433	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	D	11	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	A	530	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	D	481	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	280	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	385	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	11	PHE	CB-CG-CD1	5.33	124.53	120.80
1	A	333	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	280	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	393	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	367	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	D	280	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	481	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	481	ASP	CB-CG-OD1	5.03	122.83	118.30

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	A	4424	0	4179	14	0
1	B	4462	0	4219	19	0
1	C	4487	0	4229	39	0
1	D	4459	0	4221	21	0
2	A	20	0	6	1	0
2	B	20	0	6	1	0
2	C	20	0	6	1	0
2	D	21	0	12	1	0
3	A	503	0	0	7	0
3	B	503	0	0	7	0
3	C	507	0	0	12	0
3	D	537	0	0	9	0
All	All	19963	0	16878	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (98) 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:C:95[B]:ASP:OD1	3:C:854:HOH:O	1.59	1.21
1:D:95[B]:ASP:OD1	3:D:805:HOH:O	1.68	1.11
1:D:40:HIS:HD2	3:D:1022:HOH:O	1.60	0.85
1:C:396[A]:THR:HG23	1:C:531:TYR:O	1.80	0.82
1:D:40:HIS:CD2	3:D:1022:HOH:O	2.31	0.82
1:A:95[B]:ASP:OD1	1:A:505:GLY:HA3	1.79	0.82
1:C:385:ARG:HH12	1:C:388:GLN:HE21	1.28	0.81
1:D:385:ARG:HH22	1:D:388:GLN:HE21	1.28	0.81
1:C:436:ASP:OD1	1:C:449[A]:LEU:HD22	1.80	0.80
1:C:1:MET:SD	3:C:1002:HOH:O	2.39	0.80
1:C:449[A]:LEU:HD21	1:C:453:GLU:HA	1.63	0.79
1:A:354:GLU:OE1	3:A:931:HOH:O	2.03	0.75
1:A:95[B]:ASP:OD2	3:A:985:HOH:O	2.02	0.75
2:A:539[B]:B3P:H71	3:A:1042:HOH:O	1.87	0.72
1:B:320:ASP:O	1:B:320:ASP:CG	2.31	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377[B]:LYS:NZ	3:B:1014:HOH:O	2.29	0.66
1:A:295:GLN:HE22	1:A:313:SER:H	1.44	0.64
1:D:5:ASN:HD21	1:D:294:ILE:H	1.46	0.63
1:D:174:GLU:OE1	1:D:221[A]:HIS:HD2	1.82	0.63
1:C:218:LYS:HG3	1:C:219:THR:HG23	1.80	0.62
1:D:324[A]:GLN:NE2	3:D:851:HOH:O	2.33	0.62
1:B:295:GLN:HE22	1:B:313:SER:H	1.49	0.60
2:B:539[A]:B3P:H51	3:B:1040:HOH:O	2.01	0.58
1:C:449[A]:LEU:O	1:C:449[A]:LEU:HD23	2.03	0.58
1:C:295:GLN:HE22	1:C:313:SER:H	1.52	0.56
1:B:422:SER:OG	1:B:424:HIS:HD2	1.90	0.55
1:C:248:HIS:HE1	3:C:644:HOH:O	1.90	0.55
1:C:442:ASN:HD21	1:C:503:ARG:H	1.54	0.54
1:C:533[A]:THR:HG22	3:C:883:HOH:O	2.07	0.54
1:C:396[A]:THR:HG21	1:C:515:ILE:HG21	1.90	0.53
1:A:295:GLN:NE2	1:A:313:SER:H	2.05	0.53
1:C:442:ASN:ND2	1:C:503:ARG:H	2.07	0.52
1:C:377[B]:LYS:NZ	3:C:1032:HOH:O	2.41	0.52
1:D:5:ASN:ND2	1:D:294:ILE:H	2.05	0.52
1:C:449[A]:LEU:CD2	1:C:453:GLU:HG3	2.40	0.52
1:B:525[B]:LEU:HD23	3:B:934:HOH:O	2.10	0.52
1:D:174:GLU:OE1	1:D:221[A]:HIS:CD2	2.63	0.52
1:C:364:GLY:O	3:C:598:HOH:O	2.19	0.51
1:B:454[B]:ILE:HD13	1:B:478:TYR:CE2	2.44	0.51
1:C:248:HIS:HD2	3:C:583:HOH:O	1.92	0.51
1:C:449[A]:LEU:HD21	1:C:453:GLU:HG3	1.92	0.51
1:B:320:ASP:O	1:B:320:ASP:OD1	2.28	0.51
1:B:424:HIS:HE1	3:B:618:HOH:O	1.92	0.50
1:A:248:HIS:HE1	3:A:632:HOH:O	1.94	0.50
1:A:248:HIS:HD2	3:A:606:HOH:O	1.94	0.50
1:C:449[A]:LEU:C	1:C:449[A]:LEU:HD23	2.32	0.50
2:C:539[A]:B3P:H111	3:C:986:HOH:O	2.12	0.49
1:A:332:GLU:O	1:A:533[B]:THR:HG23	2.12	0.49
1:C:442:ASN:HD21	1:C:502:VAL:HA	1.78	0.49
1:D:391[A]:ASN:ND2	3:D:994:HOH:O	2.22	0.48
1:C:94[B]:VAL:O	1:C:94[B]:VAL:HG12	2.12	0.48
1:B:295:GLN:NE2	1:B:313:SER:H	2.11	0.48
1:B:364:GLY:O	3:B:716:HOH:O	2.20	0.48
1:B:431[A]:LYS:HD3	1:B:455:PRO:HG3	1.95	0.48
1:C:385:ARG:HH12	1:C:388:GLN:NE2	2.05	0.48
1:C:295:GLN:NE2	1:C:313:SER:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLY:HA3	1:B:143:MET:O	2.15	0.47
1:B:399:GLU:OE1	1:B:461:LYS:HE3	2.14	0.47
1:C:73:TRP:CD2	1:C:91:VAL:HG21	2.50	0.46
1:D:248:HIS:CE1	2:D:539[A]:B3P:HO3	2.33	0.46
1:B:73:TRP:CD2	1:B:91:VAL:HG21	2.52	0.45
1:D:264:LEU:HD12	1:D:264:LEU:C	2.36	0.45
1:D:339:ASP:OD1	1:D:340:THR:HG23	2.15	0.45
1:C:264:LEU:C	1:C:264:LEU:HD12	2.37	0.45
1:A:394:ALA:HA	1:A:533[B]:THR:O	2.17	0.45
1:C:394:ALA:HA	1:C:533[A]:THR:O	2.17	0.45
1:D:59:GLU:HG3	3:D:1005:HOH:O	2.16	0.45
1:C:428:ASN:ND2	1:C:430[A]:GLU:H	2.15	0.44
1:C:168[B]:LYS:HE3	1:C:170:ILE:HG22	1.99	0.44
1:A:98:TRP:CE3	1:B:373:SER:HB2	2.53	0.44
1:B:264:LEU:HD12	1:B:264:LEU:C	2.37	0.44
1:D:59:GLU:CG	3:D:1005:HOH:O	2.66	0.44
1:D:73:TRP:CD2	1:D:91:VAL:HG21	2.53	0.44
1:A:538:ASP:HB3	3:A:894:HOH:O	2.18	0.42
1:D:489:PRO:C	1:D:490:ILE:HG13	2.39	0.42
1:C:125:GLY:HA3	1:C:143:MET:O	2.19	0.42
1:A:95[B]:ASP:CG	1:A:505:GLY:HA3	2.39	0.42
1:A:73:TRP:CD2	1:A:91:VAL:HG21	2.54	0.42
1:A:264:LEU:HD12	1:A:264:LEU:C	2.40	0.42
1:C:1:MET:CG	3:C:1002:HOH:O	2.66	0.42
1:C:436:ASP:OD1	1:C:449[A]:LEU:CD2	2.62	0.41
1:C:373:SER:HB2	1:D:98:TRP:CE3	2.56	0.41
1:C:114:PRO:HG2	3:C:1035:HOH:O	2.20	0.41
1:C:248:HIS:CD2	3:C:986:HOH:O	2.73	0.41
1:C:449[A]:LEU:HD21	1:C:453:GLU:CA	2.43	0.41
1:C:391:ASN:HD22	1:C:470:ARG:HA	1.86	0.40
1:B:435:ILE:HB	1:B:454[A]:ILE:HB	2.03	0.40
1:B:215:ALA:HB1	1:B:224:TYR:HB3	2.03	0.40
1:B:9:LYS:HD3	3:B:841:HOH:O	2.21	0.40
1:D:125:GLY:HA3	1:D:143:MET:O	2.22	0.40
1:D:338[A]:LYS:HE2	3:D:834:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/538 (102%)	526 (96%)	20 (4%)	1 (0%)	47	19
1	B	552/538 (103%)	529 (96%)	22 (4%)	1 (0%)	47	19
1	C	555/538 (103%)	530 (96%)	24 (4%)	1 (0%)	47	19
1	D	551/538 (102%)	531 (96%)	19 (3%)	1 (0%)	47	19
All	All	2205/2152 (102%)	2116 (96%)	85 (4%)	4 (0%)	47	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	C	37	VAL
1	D	37	VAL
1	B	37	VAL

### 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	A	470/459 (102%)	467 (99%)	3 (1%)	86	65
1	B	474/459 (103%)	470 (99%)	4 (1%)	81	58
1	C	478/459 (104%)	473 (99%)	5 (1%)	76	48
1	D	474/459 (103%)	470 (99%)	4 (1%)	81	58
All	All	1896/1836 (103%)	1880 (99%)	16 (1%)	81	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	385	ARG
1	A	459	GLU
1	B	49	HIS
1	B	83	LYS
1	B	320	ASP
1	B	385	ARG
1	C	49	HIS
1	C	385	ARG
1	C	449[A]	LEU
1	C	449[B]	LEU
1	C	459	GLU
1	D	49	HIS
1	D	64[A]	LYS
1	D	64[B]	LYS
1	D	385	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	142	ASN
1	A	221	HIS
1	A	248	HIS
1	A	295	GLN
1	A	300	GLN
1	A	323	GLN
1	A	324	GLN
1	A	391	ASN
1	B	103	ASN
1	B	142	ASN
1	B	256	ASN
1	B	295	GLN
1	B	424	HIS
1	C	103	ASN
1	C	142	ASN
1	C	241	ASN
1	C	248	HIS
1	C	295	GLN
1	C	300	GLN
1	C	388	GLN

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Mol	Chain	Res	Type
1	C	391	ASN
1	C	428	ASN
1	C	442	ASN
1	D	4	GLN
1	D	5	ASN
1	D	38	GLN
1	D	103	ASN
1	D	142	ASN
1	D	153	ASN
1	D	323	GLN
1	D	388	GLN
1	D	475	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	B3P	D	539[B]	-	18,18,18	1.84	3 (16%)	21,23,23	3.17	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	B3P	C	539[B]	-	18,18,18	1.28	3 (16%)	21,23,23	2.10	4 (19%)
2	B3P	B	539[A]	-	18,18,18	1.39	3 (16%)	21,23,23	2.39	5 (23%)
2	B3P	D	539[A]	-	18,18,18	1.57	3 (16%)	21,23,23	2.59	7 (33%)
2	B3P	B	539[B]	-	18,18,18	1.25	2 (11%)	21,23,23	2.23	5 (23%)
2	B3P	A	539[B]	-	18,18,18	1.46	4 (22%)	21,23,23	2.72	8 (38%)
2	B3P	A	539[A]	-	18,18,18	1.29	3 (16%)	21,23,23	2.18	7 (33%)
2	B3P	C	539[A]	-	18,18,18	1.44	4 (22%)	21,23,23	2.29	5 (23%)

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	D	539[B]	-	-	4/28/28/28	-
2	B3P	C	539[B]	-	-	4/28/28/28	-
2	B3P	B	539[A]	-	-	3/28/28/28	-
2	B3P	D	539[A]	-	-	4/28/28/28	-
2	B3P	B	539[B]	-	-	5/28/28/28	-
2	B3P	A	539[B]	-	-	1/28/28/28	-
2	B3P	A	539[A]	-	-	4/28/28/28	-
2	B3P	C	539[A]	-	-	2/28/28/28	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	539[B]	B3P	O2-C10	4.22	1.56	1.42
2	D	539[B]	B3P	C3-N1	-3.82	1.42	1.46
2	D	539[A]	B3P	C3-N1	-3.82	1.42	1.46
2	A	539[B]	B3P	C5-C4	-3.55	1.49	1.53
2	A	539[A]	B3P	C5-C4	-3.55	1.49	1.53
2	D	539[B]	B3P	C9-C8	3.53	1.57	1.53
2	D	539[A]	B3P	C9-C8	3.53	1.57	1.53
2	C	539[B]	B3P	C9-C8	-2.96	1.50	1.53
2	C	539[A]	B3P	C9-C8	-2.96	1.50	1.53
2	A	539[B]	B3P	O6-C7	2.94	1.52	1.42
2	C	539[A]	B3P	O3-C11	2.85	1.51	1.42
2	B	539[A]	B3P	O4-C5	2.58	1.50	1.42
2	B	539[A]	B3P	C2-N2	-2.56	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	539[B]	B3P	C2-N2	-2.56	1.43	1.46
2	A	539[B]	B3P	O4-C5	2.34	1.50	1.42
2	A	539[A]	B3P	O4-C5	2.34	1.50	1.42
2	C	539[B]	B3P	C3-N1	-2.11	1.44	1.46
2	C	539[A]	B3P	C3-N1	-2.11	1.44	1.46
2	B	539[A]	B3P	C5-C4	-2.11	1.51	1.53
2	B	539[B]	B3P	C5-C4	-2.11	1.51	1.53
2	D	539[A]	B3P	O3-C11	2.10	1.49	1.42
2	A	539[B]	B3P	C2-N2	-2.07	1.44	1.46
2	A	539[A]	B3P	C2-N2	-2.07	1.44	1.46
2	C	539[B]	B3P	C2-N2	2.04	1.49	1.46
2	C	539[A]	B3P	C2-N2	2.04	1.49	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	539[B]	B3P	O2-C10-C8	8.19	128.22	111.63
2	A	539[B]	B3P	O6-C7-C4	7.46	126.73	111.63
2	D	539[B]	B3P	C3-N1-C4	6.85	125.80	116.08
2	D	539[A]	B3P	C3-N1-C4	6.85	125.80	116.08
2	B	539[A]	B3P	C3-N1-C4	6.60	125.44	116.08
2	B	539[B]	B3P	C3-N1-C4	6.60	125.44	116.08
2	A	539[B]	B3P	C2-N2-C8	6.28	124.99	116.08
2	A	539[A]	B3P	C2-N2-C8	6.28	124.99	116.08
2	C	539[B]	B3P	C3-N1-C4	6.17	124.83	116.08
2	C	539[A]	B3P	C3-N1-C4	6.17	124.83	116.08
2	D	539[B]	B3P	O3-C11-C8	-5.97	99.54	111.63
2	D	539[A]	B3P	O3-C11-C8	-5.60	100.31	111.63
2	D	539[B]	B3P	C2-N2-C8	5.55	123.95	116.08
2	D	539[A]	B3P	C2-N2-C8	5.55	123.95	116.08
2	B	539[A]	B3P	O4-C5-C4	5.16	122.09	111.63
2	C	539[A]	B3P	O3-C11-C8	4.22	120.17	111.63
2	C	539[B]	B3P	C2-N2-C8	4.14	121.95	116.08
2	C	539[A]	B3P	C2-N2-C8	4.14	121.95	116.08
2	C	539[B]	B3P	C11-C8-C10	3.76	117.99	110.04
2	C	539[A]	B3P	C11-C8-C10	3.76	117.99	110.04
2	B	539[A]	B3P	C2-N2-C8	3.67	121.29	116.08
2	B	539[B]	B3P	C2-N2-C8	3.67	121.29	116.08
2	A	539[B]	B3P	C7-C4-C6	3.64	117.75	110.04
2	A	539[A]	B3P	C7-C4-C6	3.64	117.75	110.04
2	B	539[B]	B3P	O4-C5-C4	3.28	118.27	111.63
2	B	539[A]	B3P	C6-C4-C5	3.21	116.84	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	539[B]	B3P	C6-C4-C5	3.21	116.84	110.04
2	A	539[B]	B3P	C3-N1-C4	3.18	120.59	116.08
2	A	539[A]	B3P	C3-N1-C4	3.18	120.59	116.08
2	D	539[B]	B3P	C10-C8-C9	2.84	116.06	110.04
2	D	539[A]	B3P	C10-C8-C9	2.84	116.06	110.04
2	D	539[B]	B3P	C11-C8-C10	-2.43	104.89	110.04
2	D	539[A]	B3P	C11-C8-C10	-2.43	104.89	110.04
2	B	539[A]	B3P	C9-C8-N2	-2.42	101.75	109.03
2	B	539[B]	B3P	C9-C8-N2	-2.42	101.75	109.03
2	A	539[B]	B3P	O1-C9-C8	2.38	116.46	111.63
2	A	539[A]	B3P	O1-C9-C8	2.38	116.46	111.63
2	C	539[B]	B3P	C7-C4-N1	-2.30	102.12	109.03
2	C	539[A]	B3P	C7-C4-N1	-2.30	102.12	109.03
2	A	539[B]	B3P	C10-C8-C9	-2.28	105.23	110.04
2	A	539[A]	B3P	C10-C8-C9	-2.28	105.23	110.04
2	D	539[B]	B3P	O6-C7-C4	2.22	116.14	111.63
2	D	539[A]	B3P	O6-C7-C4	2.22	116.14	111.63
2	A	539[B]	B3P	C7-C4-C5	-2.09	105.63	110.04
2	A	539[A]	B3P	C7-C4-C5	-2.09	105.63	110.04
2	A	539[B]	B3P	C6-C4-C5	-2.07	105.67	110.04
2	A	539[A]	B3P	C6-C4-C5	-2.07	105.67	110.04
2	D	539[B]	B3P	C6-C4-N1	-2.01	102.99	109.03
2	D	539[A]	B3P	C6-C4-N1	-2.01	102.99	109.03

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	539[B]	B3P	C1-C3-N1-C4
2	C	539[B]	B3P	C1-C3-N1-C4
2	B	539[A]	B3P	C1-C2-N2-C8
2	D	539[A]	B3P	C1-C3-N1-C4
2	B	539[B]	B3P	C1-C2-N2-C8
2	A	539[B]	B3P	C1-C2-N2-C8
2	A	539[A]	B3P	C1-C2-N2-C8
2	C	539[A]	B3P	C1-C3-N1-C4
2	D	539[B]	B3P	N2-C8-C9-O1
2	D	539[A]	B3P	N2-C8-C9-O1
2	A	539[A]	B3P	C5-C4-C7-O6
2	C	539[B]	B3P	O3-C11-C8-C10
2	B	539[B]	B3P	C6-C4-C5-O4
2	C	539[B]	B3P	C1-C2-N2-C8

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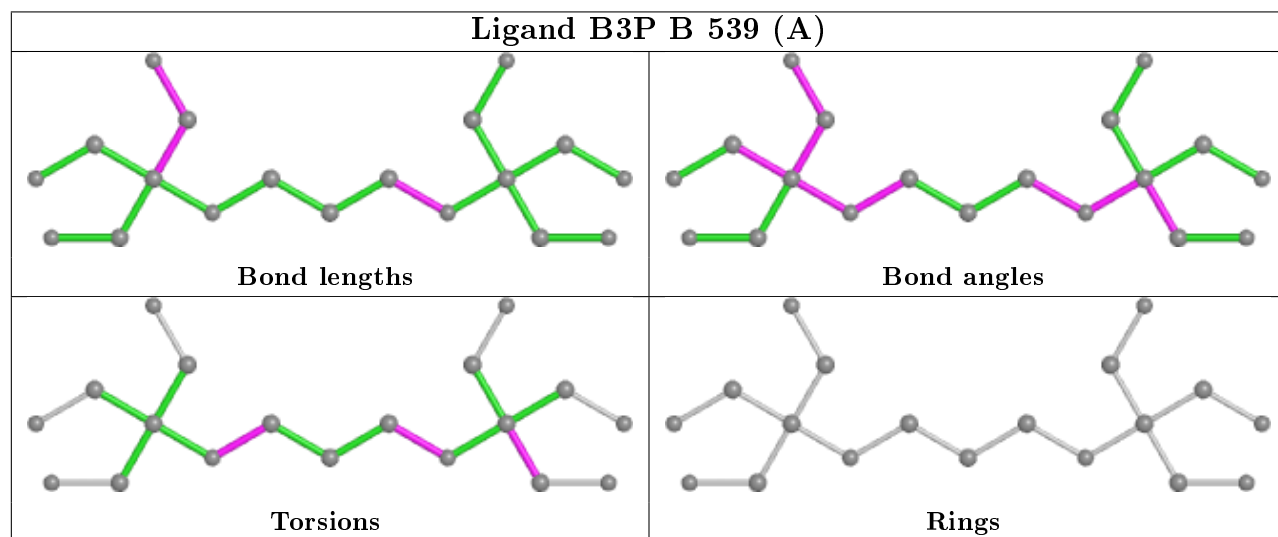
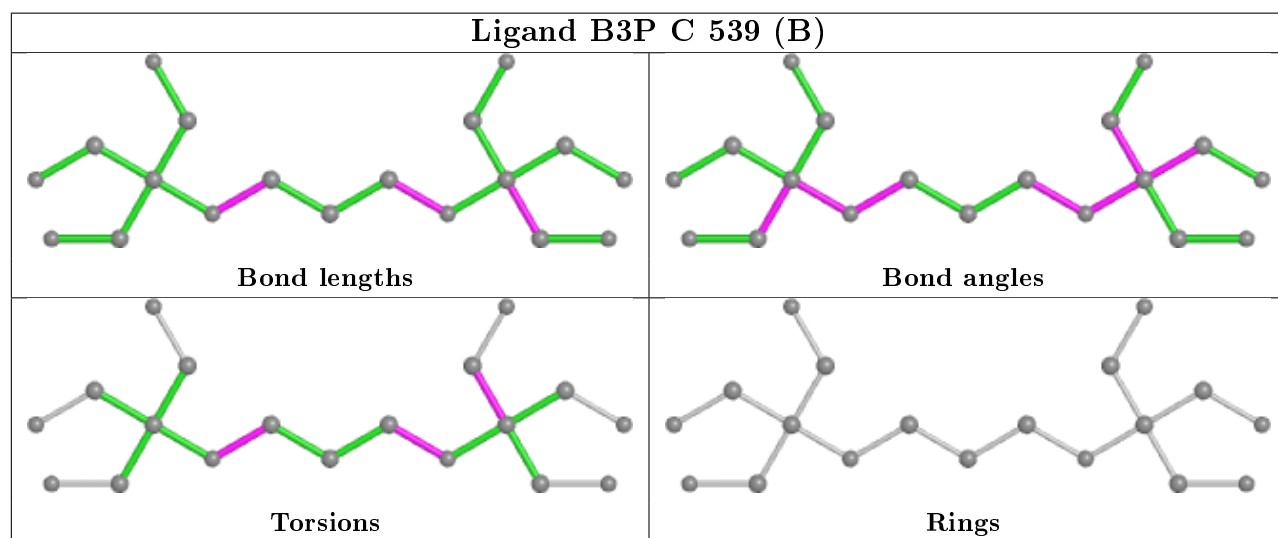
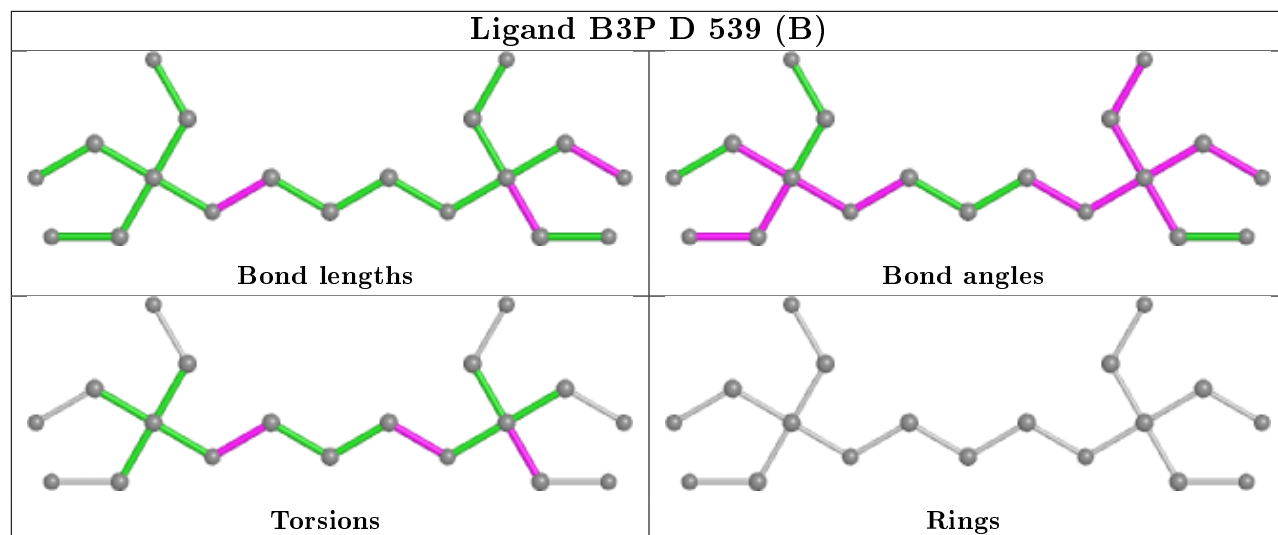
Mol	Chain	Res	Type	Atoms
2	B	539[A]	B3P	C1-C3-N1-C4
2	B	539[B]	B3P	C1-C3-N1-C4
2	C	539[A]	B3P	C1-C2-N2-C8
2	D	539[B]	B3P	C11-C8-C9-O1
2	C	539[B]	B3P	O3-C11-C8-C9
2	D	539[A]	B3P	C11-C8-C9-O1
2	B	539[B]	B3P	C7-C4-C5-O4
2	A	539[A]	B3P	C6-C4-C7-O6
2	D	539[B]	B3P	C1-C2-N2-C8
2	D	539[A]	B3P	C1-C2-N2-C8
2	B	539[A]	B3P	N2-C8-C9-O1
2	B	539[B]	B3P	N2-C8-C9-O1
2	A	539[A]	B3P	N1-C4-C7-O6

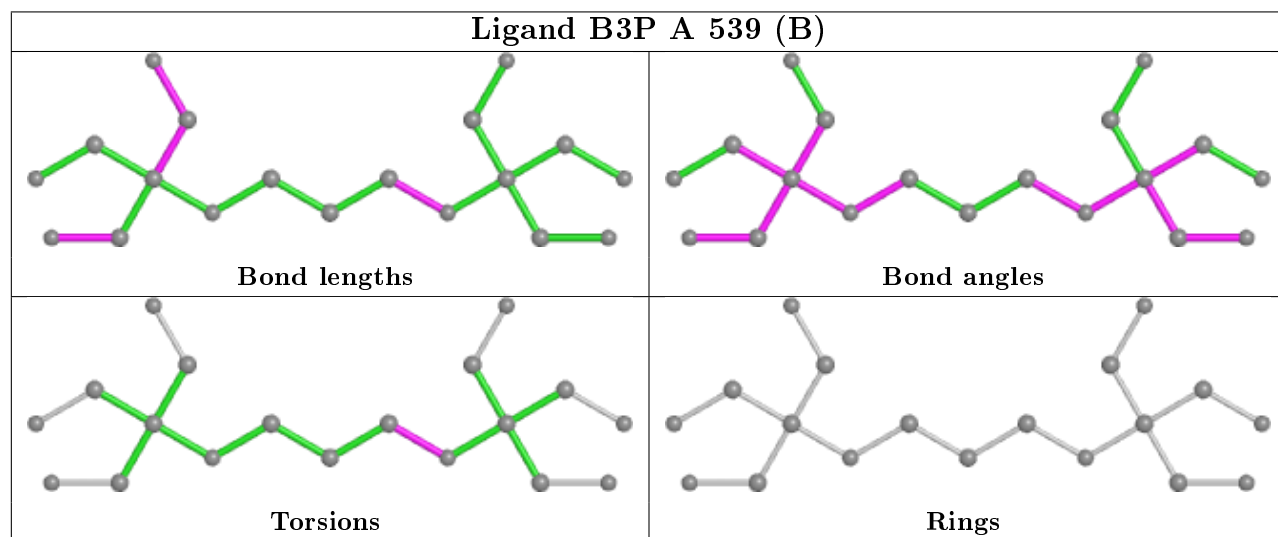
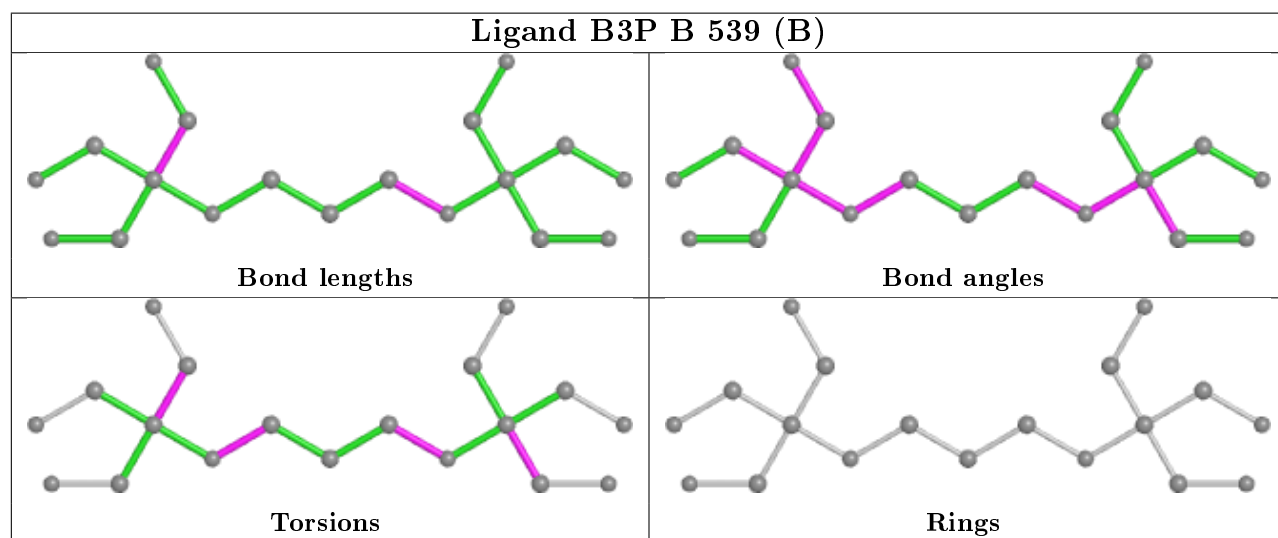
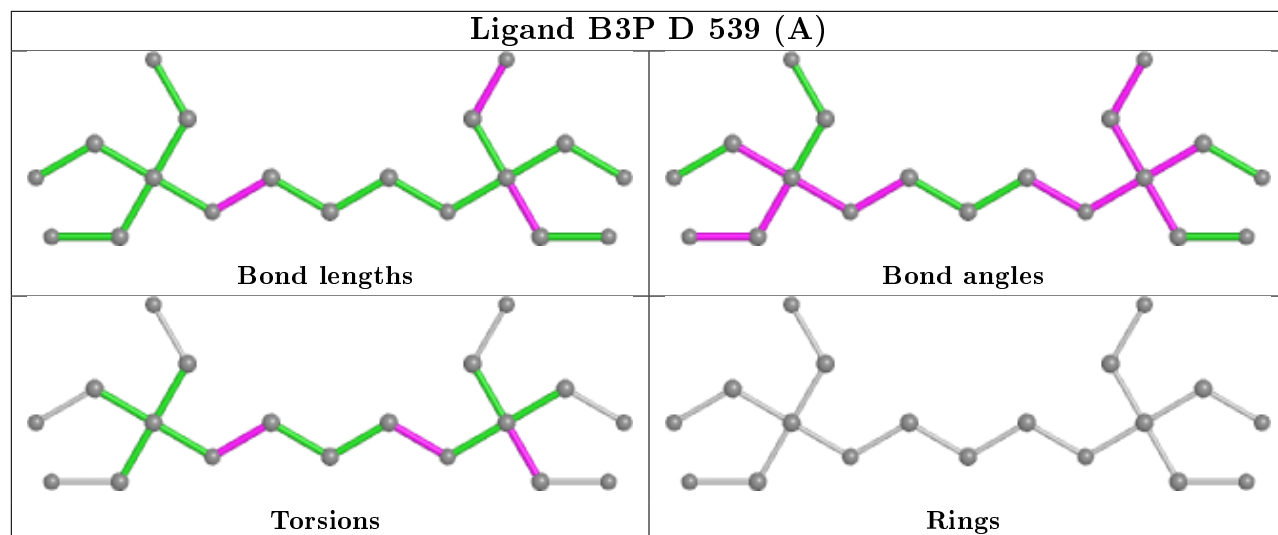
There are no ring outliers.

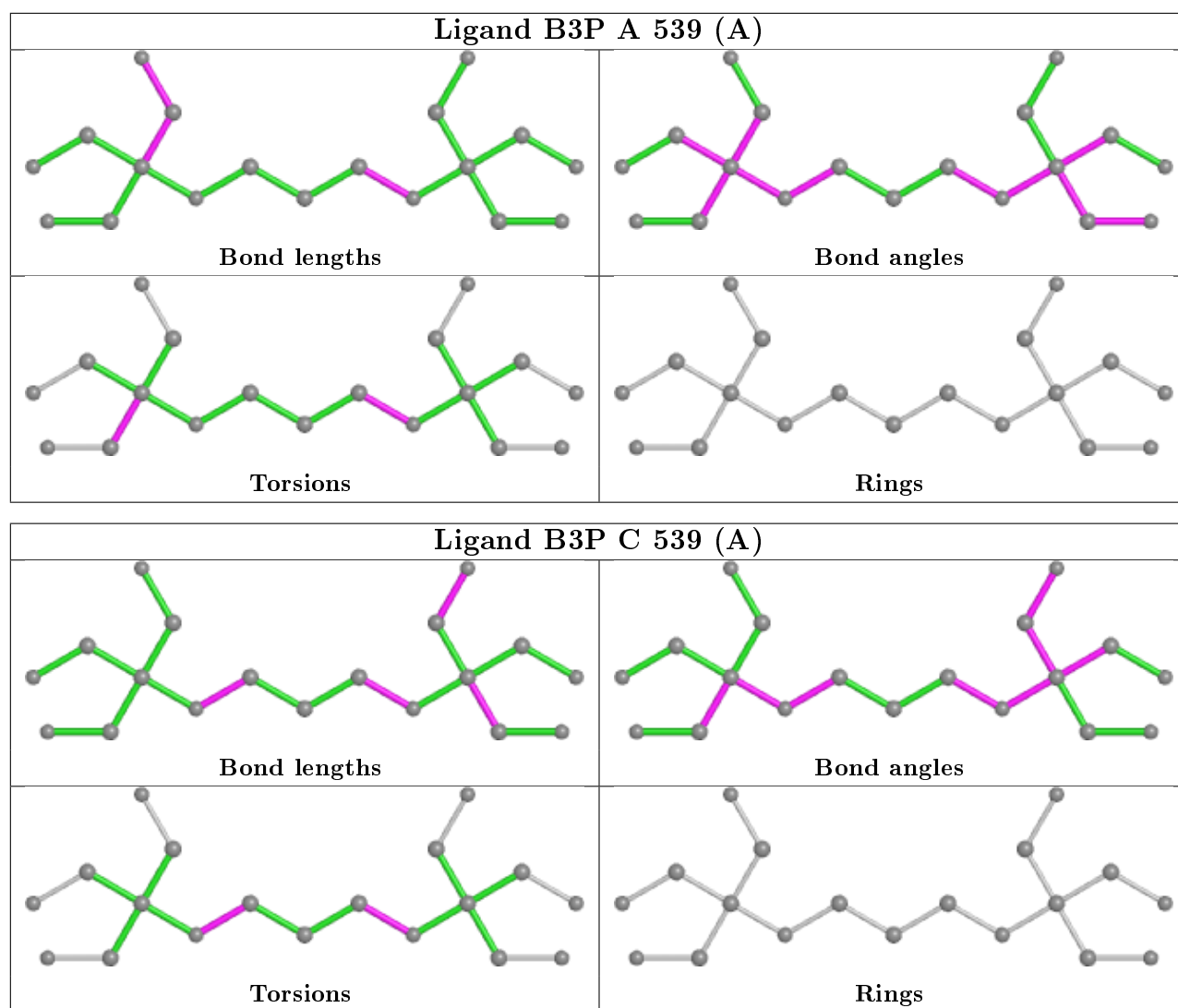
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	539[A]	B3P	1	0
2	D	539[A]	B3P	1	0
2	A	539[B]	B3P	1	0
2	C	539[A]	B3P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	538/538 (100%)	-0.04	13 (2%) 59 58	7, 13, 22, 36	0
1	B	537/538 (99%)	-0.03	12 (2%) 62 61	8, 13, 22, 31	0
1	C	537/538 (99%)	-0.11	12 (2%) 62 61	7, 11, 21, 30	0
1	D	537/538 (99%)	-0.09	13 (2%) 59 58	7, 11, 20, 29	0
All	All	2149/2152 (99%)	-0.07	50 (2%) 60 59	7, 12, 21, 36	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	ASP	6.3
1	C	1	MET	4.5
1	D	165	ALA	4.4
1	B	484	THR	4.2
1	A	458	ASP	4.0
1	B	483	GLU	3.9
1	A	320	ASP	3.8
1	D	458	ASP	3.7
1	D	1	MET	3.7
1	B	489	PRO	3.6
1	A	1	MET	3.6
1	B	1	MET	3.6
1	D	430	GLU	3.6
1	C	256	ASN	3.5
1	B	537	LEU	3.4
1	C	449[A]	LEU	3.4
1	B	320	ASP	2.9
1	B	360	THR	2.8
1	A	537	LEU	2.8
1	B	430	GLU	2.7
1	C	458	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	2.7
1	A	483	GLU	2.6
1	A	459	GLU	2.6
1	A	218	LYS	2.5
1	D	218	LYS	2.5
1	B	228	PRO	2.4
1	D	228	PRO	2.4
1	D	459	GLU	2.4
1	C	320	ASP	2.4
1	D	339	ASP	2.3
1	C	218	LYS	2.3
1	C	301	ASP	2.3
1	C	324[A]	GLN	2.3
1	D	300	GLN	2.3
1	B	451	GLY	2.2
1	D	451	GLY	2.2
1	D	461	LYS	2.2
1	A	59	GLU	2.2
1	D	361	ALA	2.1
1	C	194	ASN	2.1
1	D	251[A]	LEU	2.1
1	B	337	ASP	2.1
1	A	229	ASP	2.1
1	C	195	ASP	2.1
1	C	322	PRO	2.1
1	B	461	LYS	2.0
1	C	513	VAL	2.0
1	A	17	ILE	2.0
1	A	461	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

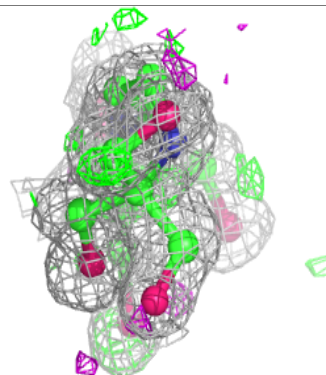
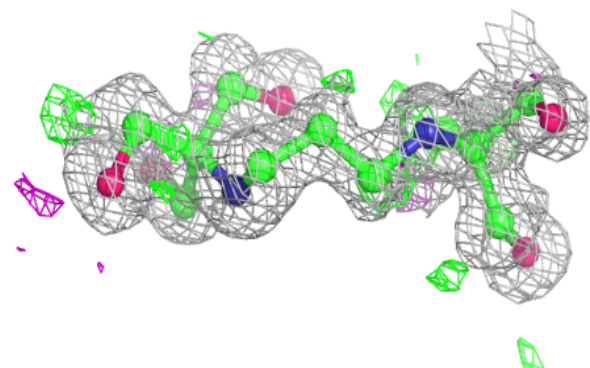
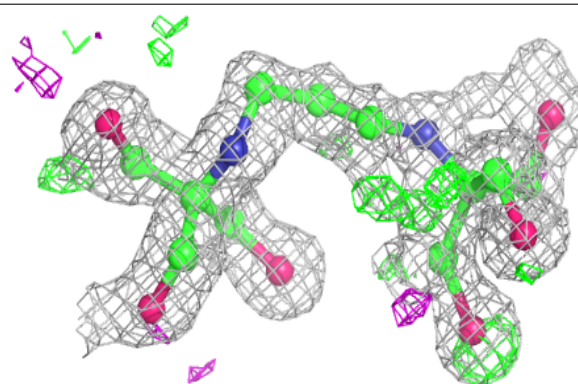
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	B3P	D	539[B]	19/19	0.93	0.10	8,15,18,21	2
2	B3P	D	539[A]	19/19	0.93	0.10	9,15,18,21	2
2	B3P	A	539[B]	19/19	0.93	0.10	10,15,19,21	1
2	B3P	A	539[A]	19/19	0.93	0.10	10,15,19,21	1
2	B3P	B	539[A]	19/19	0.94	0.09	10,14,18,20	1
2	B3P	B	539[B]	19/19	0.94	0.09	10,14,18,20	1
2	B3P	C	539[B]	19/19	0.95	0.09	10,16,20,22	1
2	B3P	C	539[A]	19/19	0.95	0.09	10,16,20,22	1

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 D 539 (B):

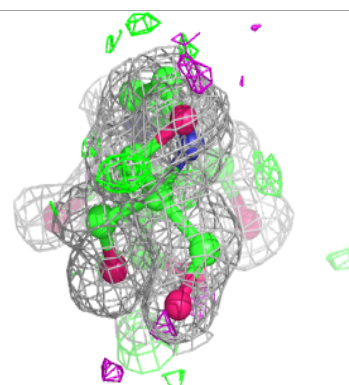
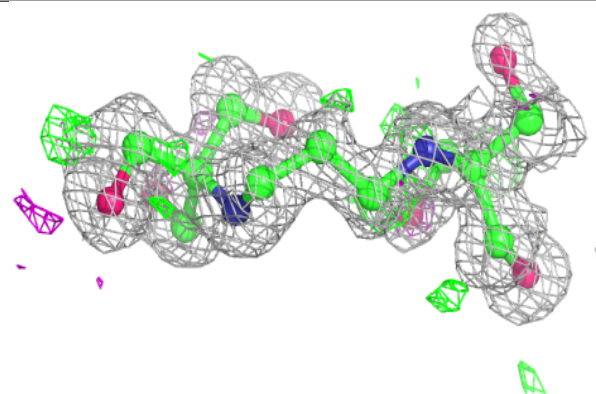
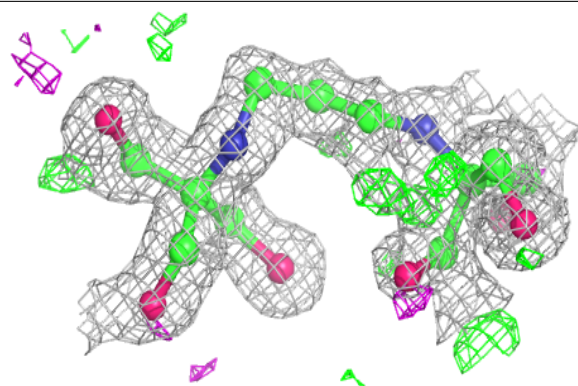
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



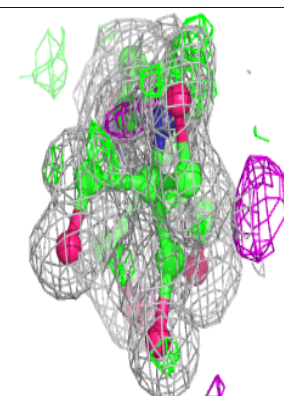
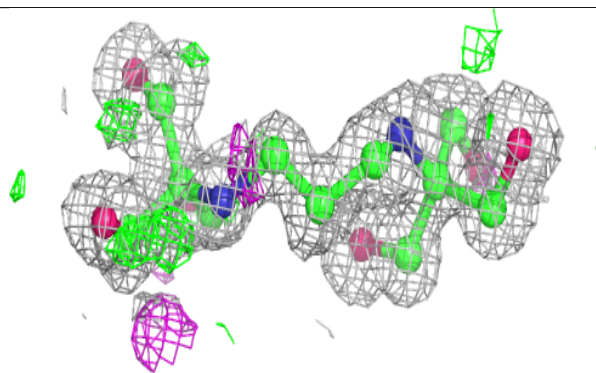
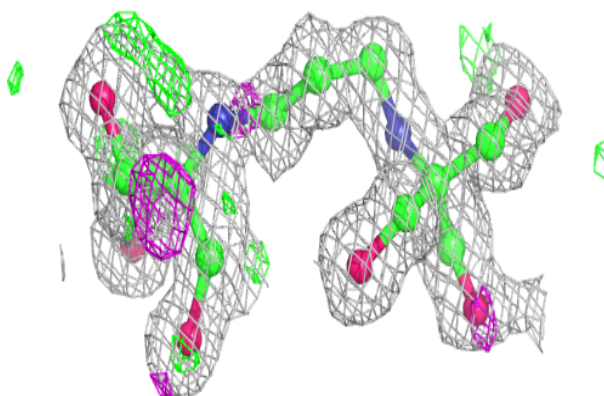


**Electron density around B3P D 539 (A):**

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

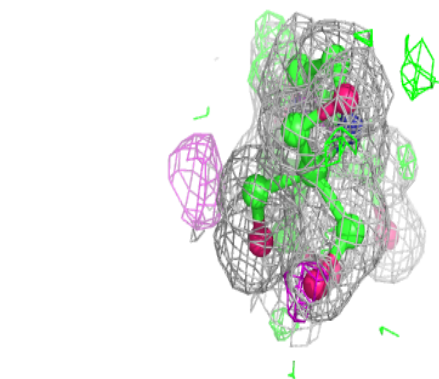
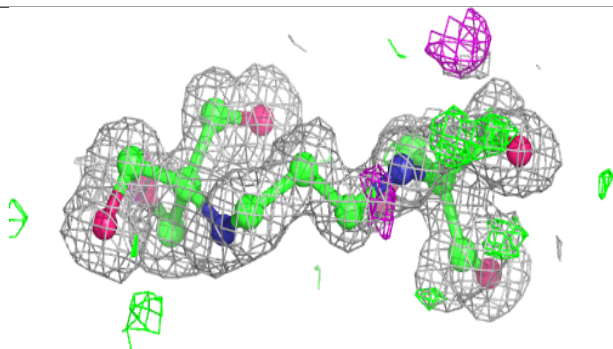
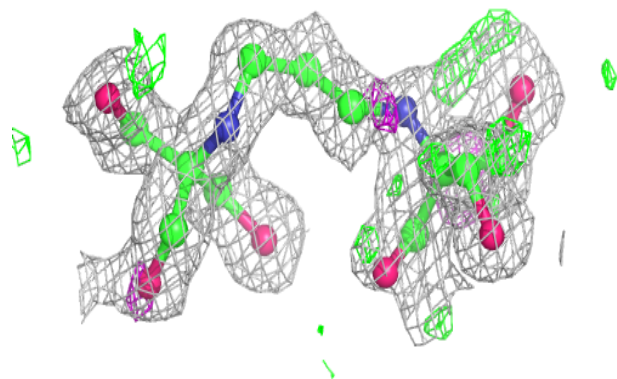
**Electron density around B3P A 539 (B):**

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

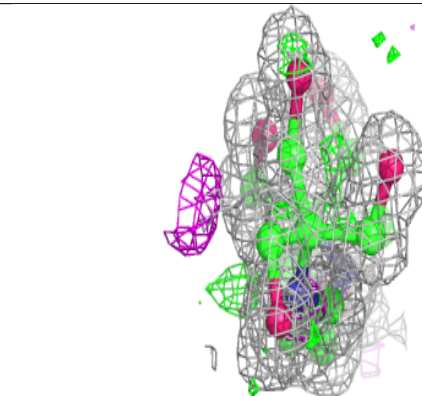
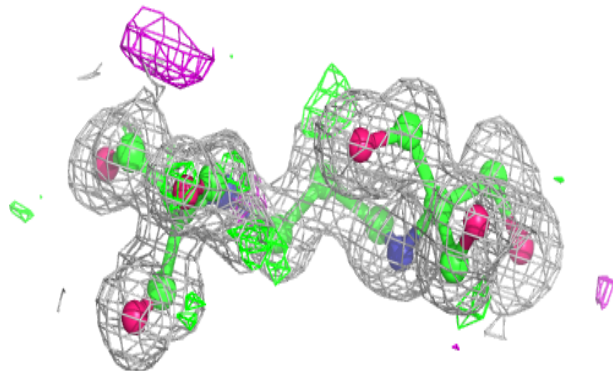
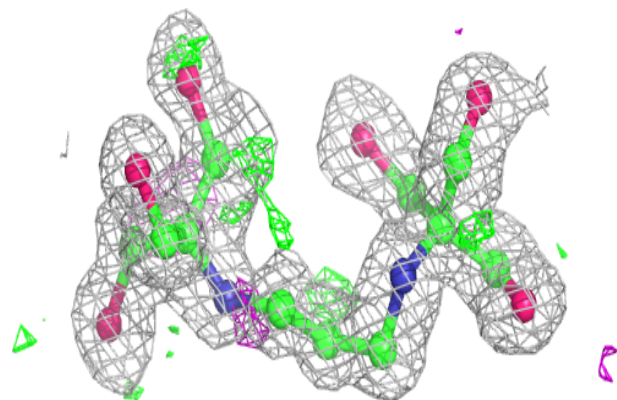


**Electron density around B3P A 539 (A):**

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

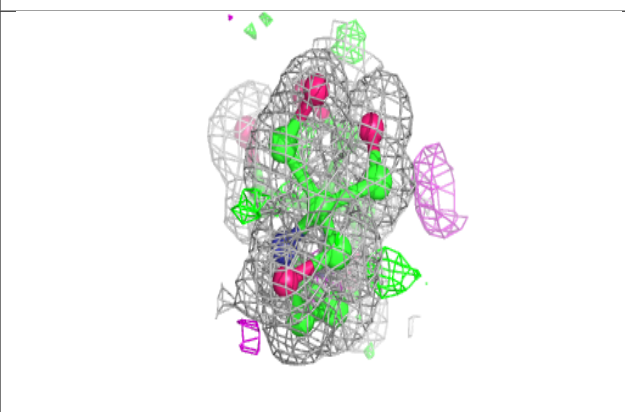
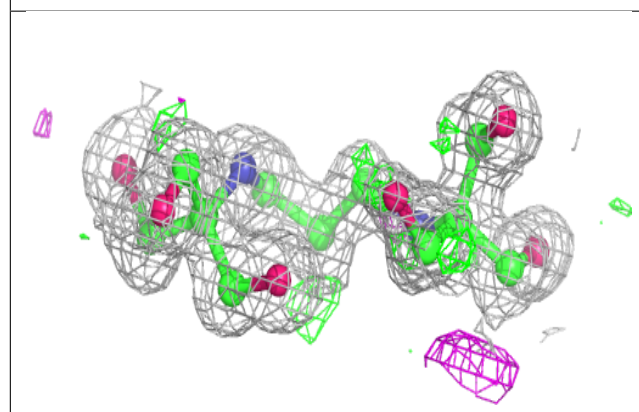
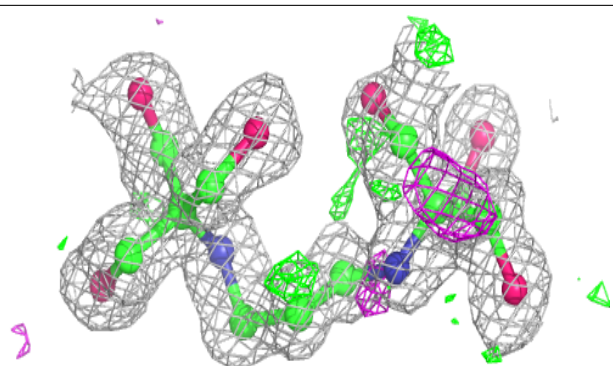
**Electron density around B3P B 539 (A):**

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

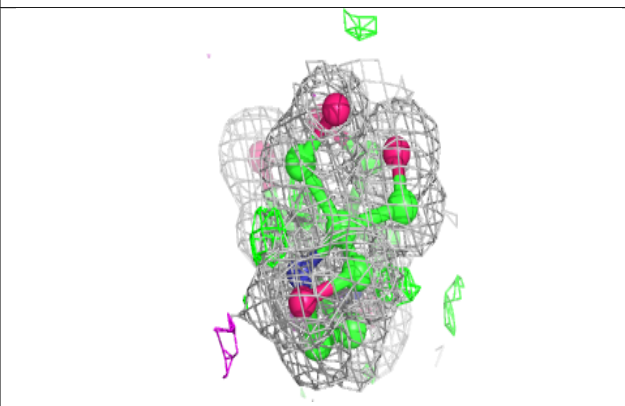
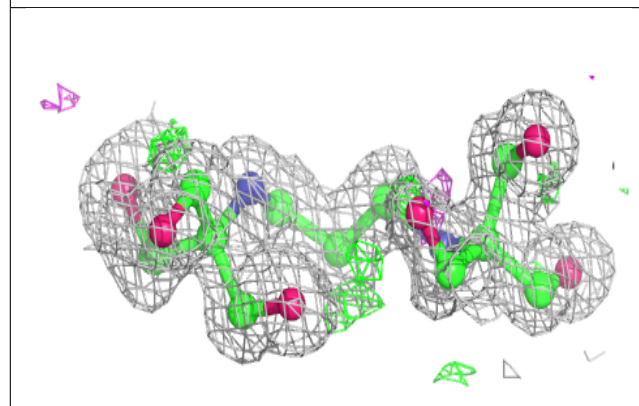
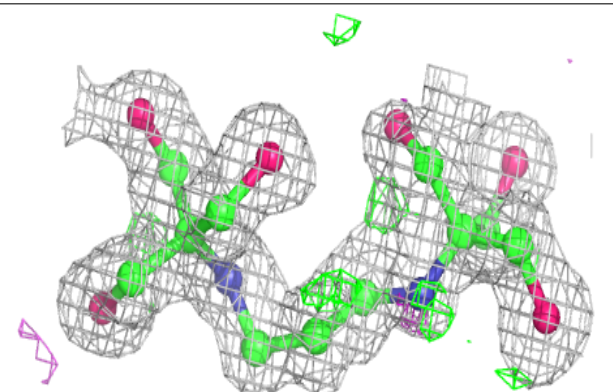


**Electron density around B3P B 539 (B):**

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

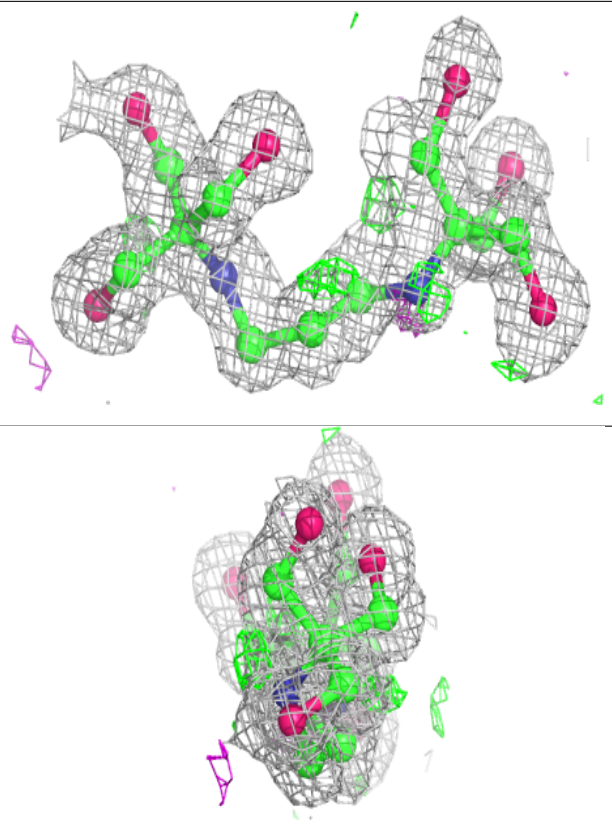
**Electron density around B3P C 539 (B):**

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



**Electron density around B3P C 539 (A):**

$2mF_o-DF_c$  (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.