



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:23 pm BST

PDB ID : 2VTF  
Title : X-ray crystal structure of the Endo-beta-N-acetylglucosaminidase from *Arthrobacter protophormiae* E173Q mutant reveals a TIM barrel catalytic domain and two ancillary domains  
Authors : Ling, Z.; Bingham, R.J.; Suits, M.D.L.; Moir, J.W.B.; Fairbanks, A.J.; Taylor, E.J.  
Deposited on : 2008-05-14  
Resolution : 1.79 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

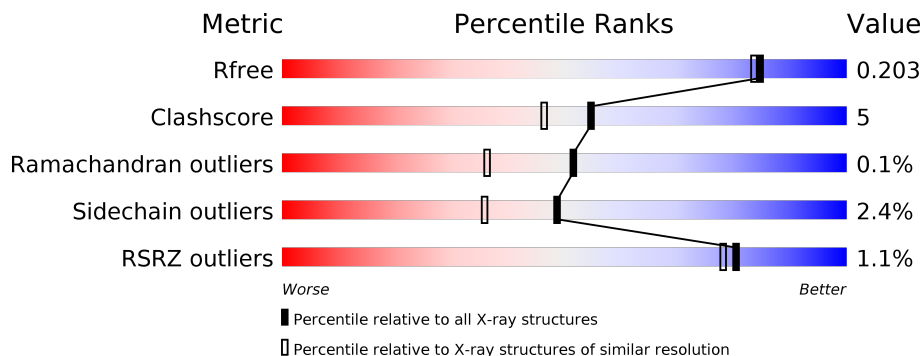
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	626	 2% 89% 9% ..
1	B	626	 90% 8% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11414 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.

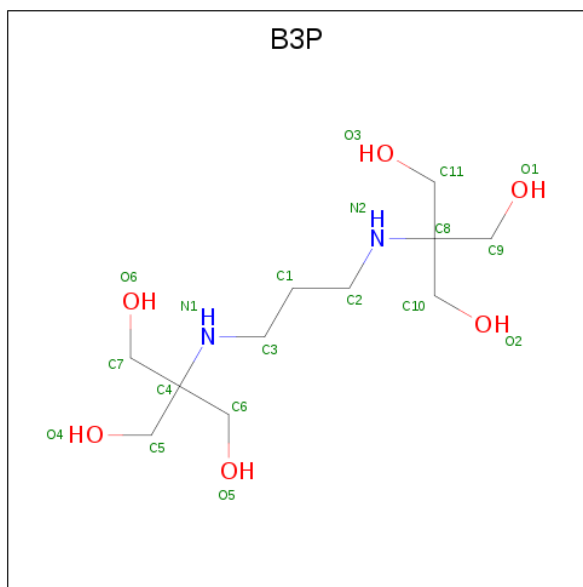
- Molecule 1 is a protein called ENDO-BETA-N-ACETYLGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	616	4932	3125	824	972	11	0	9	0
1	B	616	4870	3087	814	957	12	0	4	0

There are 6 discrepancies between the modelled and reference sequences:

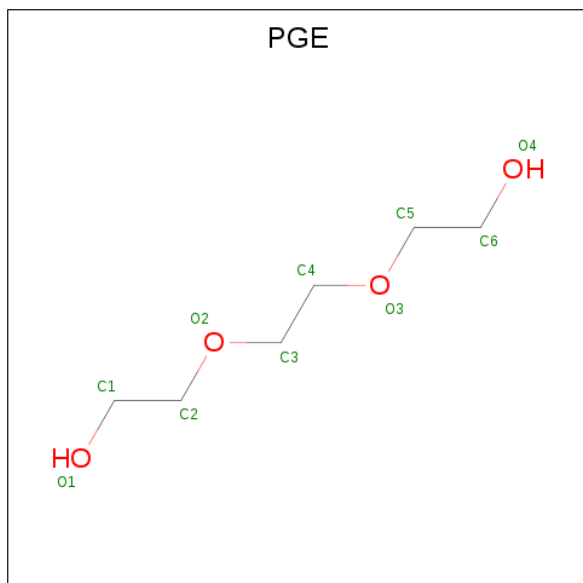
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ASP	ASN	engineered mutation	UNP Q9ZB22
A	51	THR	LYS	engineered mutation	UNP Q9ZB22
A	173	GLN	GLU	engineered mutation	UNP Q9ZB22
B	43	ASP	ASN	engineered mutation	UNP Q9ZB22
B	51	THR	LYS	engineered mutation	UNP Q9ZB22
B	173	GLN	GLU	engineered mutation	UNP Q9ZB22

- 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<sub>11</sub>H<sub>26</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			19	11	2	6		
2	A	1	Total	C	N	O	0	0
			19	11	2	6		
2	B	1	Total	C	N	O	0	0
			15	9	2	4		
2	B	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

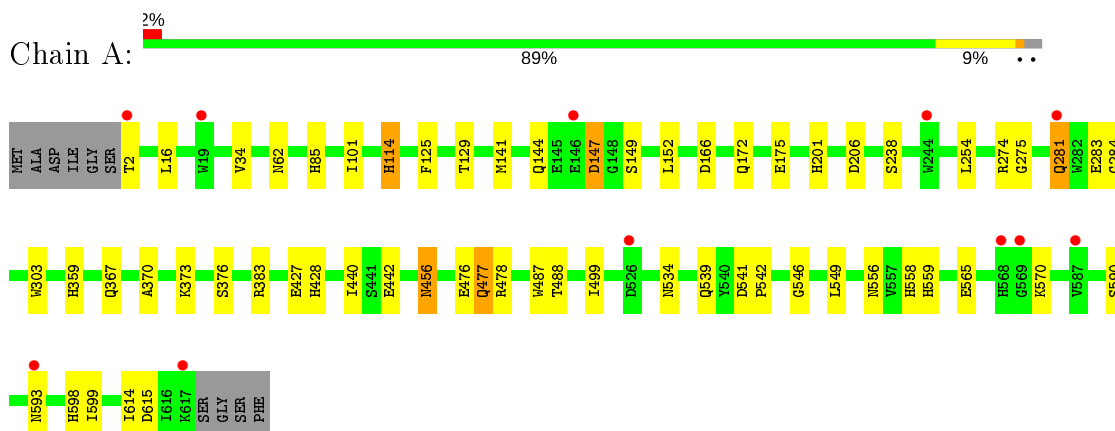
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	767	Total	O	0	0
			767	767		
4	B	733	Total	O	0	0
			733	733		

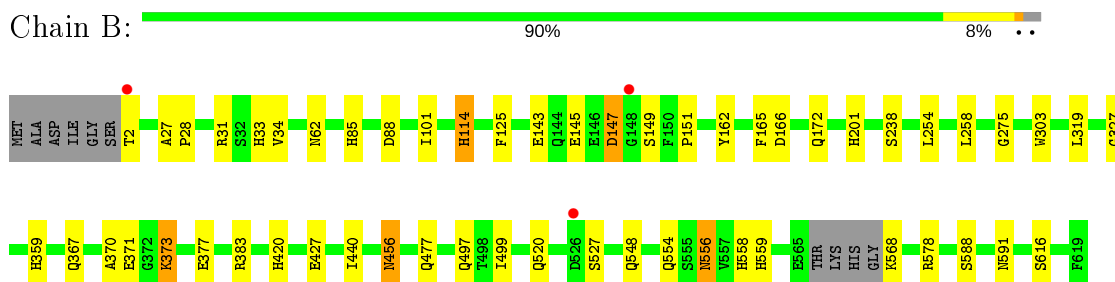
### 3 Residue-property plots [i](#)

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: ENDO-BETA-N-ACETYLGLUCOSAMINIDASE



- Molecule 1: ENDO-BETA-N-ACETYLGLUCOSAMINIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.84Å 226.76Å 68.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 1.79 49.04 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.03-1.79) 99.9 (49.04-1.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.164 , 0.202 0.165 , 0.203	Depositor DCC
$R_{free}$ test set	6652 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 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	0.49	0/5083	0.61	0/6938
1	B	0.49	0/5018	0.61	1/6845 (0.0%)
All	All	0.49	0/10101	0.61	1/13783 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	258	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	165	PHE	Peptide

### 5.2 Too-close contacts [i](#)

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



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4932	0	4493	47	0
1	B	4870	0	4441	50	0
2	A	38	0	52	0	0
2	B	34	0	46	0	0
3	A	20	0	28	1	0
3	B	20	0	28	7	0
4	A	767	0	0	11	0
4	B	733	0	0	10	0
All	All	11414	0	9088	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 5.

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:A:141:MET:SD	1:A:152:LEU:HD13	2.10	0.92
1:B:558:HIS:HD2	1:B:559:HIS:HD1	0.97	0.92
1:B:201:HIS:HD2	3:B:1622:PGE:H12	1.32	0.90
1:A:558:HIS:HD2	1:A:559:HIS:HD1	1.03	0.89
1:A:476:GLU:OE2	4:A:2632:HOH:O	1.92	0.87
1:B:556:ASN:HD22	1:B:556:ASN:H	1.18	0.87
1:B:558:HIS:CD2	1:B:559:HIS:HD1	1.90	0.87
1:B:62:ASN:HD21	1:B:383:ARG:HH22	1.29	0.78
1:A:62:ASN:HD21	1:A:383:ARG:HH22	1.32	0.76
1:B:370:ALA:O	1:B:373:LYS:HE3	1.85	0.76
1:B:114:HIS:HE1	1:B:166:ASP:OD2	1.71	0.73
1:A:558:HIS:CD2	1:A:559:HIS:HD1	1.96	0.73
1:A:129:THR:HG23	1:A:175:GLU:OE1	1.90	0.72
1:A:359:HIS:HE1	4:A:2485:HOH:O	1.73	0.71
1:A:558:HIS:HD2	1:A:559:HIS:ND1	1.84	0.71
1:B:558:HIS:HD2	1:B:559:HIS:ND1	1.81	0.71
1:B:147:ASP:HB3	1:B:149:SER:H	1.55	0.70
1:A:274[B]:ARG:HG2	4:A:2403:HOH:O	1.92	0.68
1:A:114:HIS:HE1	1:A:166:ASP:OD2	1.77	0.67
1:B:440:ILE:HD11	1:B:499:ILE:HG13	1.75	0.67
1:B:201:HIS:CD2	3:B:1622:PGE:H12	2.23	0.67
1:A:141:MET:HA	1:A:152:LEU:HD12	1.77	0.66
1:B:201:HIS:HE1	1:B:238:SER:OG	1.80	0.65
1:B:548:GLN:HE22	1:B:578:ARG:HH11	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:HIS:HE1	4:B:2426:HOH:O	1.80	0.64
1:B:568:LYS:HE3	3:B:1623:PGE:H5	1.81	0.62
1:A:201:HIS:HE1	1:A:238:SER:OG	1.82	0.62
1:B:568:LYS:HZ1	3:B:1623:PGE:H32	1.65	0.62
1:B:373:LYS:HE2	4:B:2586:HOH:O	2.01	0.61
1:B:556:ASN:H	1:B:556:ASN:ND2	1.95	0.61
1:A:283:GLU:HG2	4:A:2406:HOH:O	2.01	0.61
1:B:367:GLN:HG3	1:B:377:GLU:HA	1.82	0.60
1:A:456:ASN:HD22	1:A:456:ASN:H	1.49	0.60
1:B:62:ASN:ND2	1:B:383:ARG:HH22	2.00	0.60
1:A:147:ASP:CB	1:A:149:SER:H	2.16	0.58
1:B:456:ASN:ND2	1:B:456:ASN:H	2.02	0.56
1:A:62:ASN:ND2	1:A:383:ARG:HH22	2.01	0.56
1:A:367[B]:GLN:HB2	1:A:376:SER:O	2.06	0.56
1:B:359:HIS:HD2	4:B:2460:HOH:O	1.88	0.56
1:A:456:ASN:ND2	1:A:456:ASN:H	2.03	0.56
1:B:85:HIS:HD2	4:B:2146:HOH:O	1.88	0.54
1:B:456:ASN:HD22	1:B:456:ASN:H	1.56	0.54
1:A:370:ALA:O	1:A:373:LYS:HG2	2.08	0.54
1:A:478:ARG:HB2	1:A:487:TRP:CZ3	2.43	0.53
1:A:147:ASP:HB3	1:A:149:SER:H	1.72	0.53
1:A:85:HIS:HD2	4:A:2174:HOH:O	1.92	0.53
1:B:88:ASP:HB3	3:B:1622:PGE:H52	1.92	0.51
1:B:319:LEU:HD21	1:B:327:GLY:HA2	1.91	0.51
1:A:34:VAL:O	1:A:114:HIS:HD2	1.92	0.51
1:A:359:HIS:HD2	4:A:2516:HOH:O	1.93	0.51
1:A:281[B]:GLN:HE21	1:A:281[B]:GLN:HA	1.76	0.50
1:A:565:GLU:OE2	1:A:598:HIS:HE1	1.95	0.49
1:B:568:LYS:NZ	3:B:1623:PGE:H32	2.25	0.49
1:A:141:MET:HA	1:A:152:LEU:CD1	2.40	0.49
1:B:420:HIS:CE1	4:B:2501:HOH:O	2.65	0.49
1:B:2:THR:O	1:B:2:THR:HG23	2.14	0.48
1:B:371:GLU:HB2	1:B:373:LYS:HE3	1.95	0.48
1:B:588:SER:HA	1:B:591:ASN:O	2.14	0.48
1:B:27:ALA:HB3	1:B:28:PRO:HD3	1.94	0.48
1:B:554:GLN:HB3	1:B:556:ASN:HD21	1.79	0.47
1:B:34:VAL:O	1:B:114:HIS:HD2	1.97	0.47
1:A:427[A]:GLU:HG3	1:A:428:HIS:N	2.30	0.47
1:A:541:ASP:HB2	1:A:542:PRO:HD3	1.96	0.47
1:B:31:ARG:HD2	1:B:162:TYR:CZ	2.49	0.47
1:A:546:GLY:HA2	4:A:2735:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:SER:HA	1:A:593:ASN:O	2.15	0.46
1:B:556:ASN:HD22	1:B:556:ASN:N	1.97	0.46
1:A:570:LYS:HD2	3:A:1621:PGE:H32	1.98	0.46
1:A:440:ILE:HD11	1:A:499:ILE:HG13	1.97	0.46
1:B:33:HIS:HD2	4:B:2276:HOH:O	1.98	0.46
1:A:442:GLU:HG2	4:A:2653:HOH:O	2.15	0.45
1:B:275:GLY:HA3	1:B:303:TRP:CD2	2.52	0.44
1:A:144:GLN:NE2	4:A:2242:HOH:O	2.50	0.44
1:A:477:GLN:HG3	1:A:488:THR:HB	1.99	0.44
1:A:101:ILE:HB	1:A:125:PHE:O	2.17	0.44
1:B:367:GLN:CG	1:B:377:GLU:HA	2.47	0.44
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.76	0.44
1:B:143:GLU:O	1:B:151:PRO:HD2	2.18	0.44
1:B:554:GLN:HB3	1:B:556:ASN:ND2	2.34	0.43
1:A:281[A]:GLN:OE1	1:A:284:GLY:N	2.51	0.43
1:A:275:GLY:HA3	1:A:303:TRP:CD2	2.53	0.43
1:B:477:GLN:HG3	4:B:2597:HOH:O	2.17	0.43
1:B:568:LYS:N	4:B:2673:HOH:O	2.51	0.43
1:A:556[A]:ASN:ND2	4:A:2698:HOH:O	2.19	0.42
1:A:147:ASP:HB3	1:A:149:SER:N	2.34	0.42
1:B:588:SER:O	1:B:616:SER:HA	2.19	0.42
1:B:497:GLN:NE2	4:B:2606:HOH:O	2.52	0.42
1:B:370:ALA:O	1:B:373:LYS:CE	2.61	0.42
1:A:34:VAL:O	1:A:114:HIS:CD2	2.73	0.41
1:A:16:LEU:HD23	1:A:152:LEU:HD22	2.02	0.41
3:B:1622:PGE:H32	4:B:2281:HOH:O	2.21	0.41
1:B:101:ILE:HB	1:B:125:PHE:O	2.21	0.41
1:A:427[A]:GLU:CG	1:A:428:HIS:N	2.84	0.40
1:B:147:ASP:HB3	1:B:149:SER:N	2.31	0.40
1:B:201:HIS:CE1	1:B:238:SER:OG	2.67	0.40
1:A:558:HIS:HE1	4:A:2515:HOH:O	2.04	0.40
1:A:599:ILE:HD12	1:A:599:ILE:N	2.36	0.40
1:B:548:GLN:NE2	1:B:578:ARG:HH11	2.16	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	A	623/626 (100%)	609 (98%)	13 (2%)	1 (0%)	47	33
1	B	616/626 (98%)	602 (98%)	14 (2%)	0	100	100
All	All	1239/1252 (99%)	1211 (98%)	27 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/517 (98%)	494 (97%)	14 (3%)	43	30
1	B	500/517 (97%)	489 (98%)	11 (2%)	52	39
All	All	1008/1034 (98%)	983 (98%)	25 (2%)	49	34

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	114	HIS
1	A	147	ASP
1	A	172	GLN
1	A	254	LEU

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Mol	Chain	Res	Type
1	A	281[A]	GLN
1	A	281[B]	GLN
1	A	456	ASN
1	A	477	GLN
1	A	534	ASN
1	A	539	GLN
1	A	549	LEU
1	A	614	ILE
1	A	615	ASP
1	B	114	HIS
1	B	145	GLU
1	B	147	ASP
1	B	172	GLN
1	B	254	LEU
1	B	373	LYS
1	B	427	GLU
1	B	456	ASN
1	B	520	GLN
1	B	527	SER
1	B	556	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	71	GLN
1	A	85	HIS
1	A	114	HIS
1	A	144	GLN
1	A	201	HIS
1	A	242	ASN
1	A	359	HIS
1	A	456	ASN
1	A	482	ASN
1	A	486	GLN
1	A	497	GLN
1	A	534	ASN
1	A	558	HIS
1	A	598	HIS
1	B	33	HIS
1	B	62	ASN
1	B	71	GLN

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Mol	Chain	Res	Type
1	B	85	HIS
1	B	114	HIS
1	B	116	ASN
1	B	134	GLN
1	B	144	GLN
1	B	201	HIS
1	B	242	ASN
1	B	359	HIS
1	B	378	GLN
1	B	456	ASN
1	B	482	ASN
1	B	497	GLN
1	B	520	GLN
1	B	548	GLN
1	B	556	ASN
1	B	558	HIS

### 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	B	1621	-	18,18,18	0.60	0	21,23,23	1.45	3 (14%)
3	PGE	A	1621	-	9,9,9	0.51	0	8,8,8	0.23	0
2	B3P	A	1618	-	18,18,18	0.60	0	21,23,23	1.24	3 (14%)
2	B3P	A	1619	-	18,18,18	0.57	0	21,23,23	1.38	2 (9%)
2	B3P	B	1620	-	14,14,18	0.58	0	14,16,23	1.89	2 (14%)
3	PGE	B	1623	-	9,9,9	0.46	0	8,8,8	0.26	0
3	PGE	B	1622	-	9,9,9	0.49	0	8,8,8	0.46	0
3	PGE	A	1620	-	9,9,9	0.50	0	8,8,8	0.15	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	B	1621	-	-	4/28/28/28	-
3	PGE	A	1621	-	-	3/7/7/7	-
2	B3P	A	1618	-	-	2/28/28/28	-
2	B3P	A	1619	-	-	0/28/28/28	-
2	B3P	B	1620	-	-	9/18/18/28	-
3	PGE	B	1623	-	-	5/7/7/7	-
3	PGE	B	1622	-	-	5/7/7/7	-
3	PGE	A	1620	-	-	1/7/7/7	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1620	B3P	C2-N2-C8	6.01	124.61	116.08
2	B	1621	B3P	C3-N1-C4	4.77	122.84	116.08
2	A	1619	B3P	C2-N2-C8	4.44	122.38	116.08
2	A	1618	B3P	C3-N1-C4	3.41	120.92	116.08
2	A	1619	B3P	C3-N1-C4	3.30	120.76	116.08
2	B	1621	B3P	C2-N2-C8	2.41	119.50	116.08
2	B	1621	B3P	O1-C9-C8	-2.39	106.80	111.63
2	A	1618	B3P	O3-C11-C8	-2.38	106.81	111.63
2	A	1618	B3P	O5-C6-C4	-2.27	107.04	111.63
2	B	1620	B3P	O1-C9-C8	-2.22	107.13	111.63

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1621	B3P	O2-C10-C8-N2
2	B	1621	B3P	O2-C10-C8-C9
2	B	1621	B3P	O2-C10-C8-C11
2	B	1620	B3P	C9-C8-N2-C2
2	B	1620	B3P	C10-C8-N2-C2
2	B	1620	B3P	C11-C8-N2-C2
2	B	1620	B3P	N1-C4-C5-O4
2	B	1620	B3P	C2-C1-C3-N1
2	B	1620	B3P	C5-C4-N1-C3
3	A	1621	PGE	O2-C3-C4-O3
2	B	1620	B3P	O2-C10-C8-C9
3	B	1623	PGE	C6-C5-O3-C4
3	B	1623	PGE	O1-C1-C2-O2
3	B	1623	PGE	O3-C5-C6-O4
3	B	1622	PGE	O3-C5-C6-O4
3	B	1622	PGE	O1-C1-C2-O2
3	B	1622	PGE	C1-C2-O2-C3
3	A	1621	PGE	C1-C2-O2-C3
3	A	1621	PGE	O3-C5-C6-O4
2	A	1618	B3P	N1-C4-C6-O5
3	A	1620	PGE	C6-C5-O3-C4
3	B	1622	PGE	C3-C4-O3-C5
3	B	1623	PGE	O2-C3-C4-O3
3	B	1623	PGE	C1-C2-O2-C3
2	B	1620	B3P	O2-C10-C8-N2
2	B	1621	B3P	C5-C4-N1-C3
2	A	1618	B3P	C10-C8-N2-C2
2	B	1620	B3P	O2-C10-C8-C11
3	B	1622	PGE	O2-C3-C4-O3

There are no ring outliers.

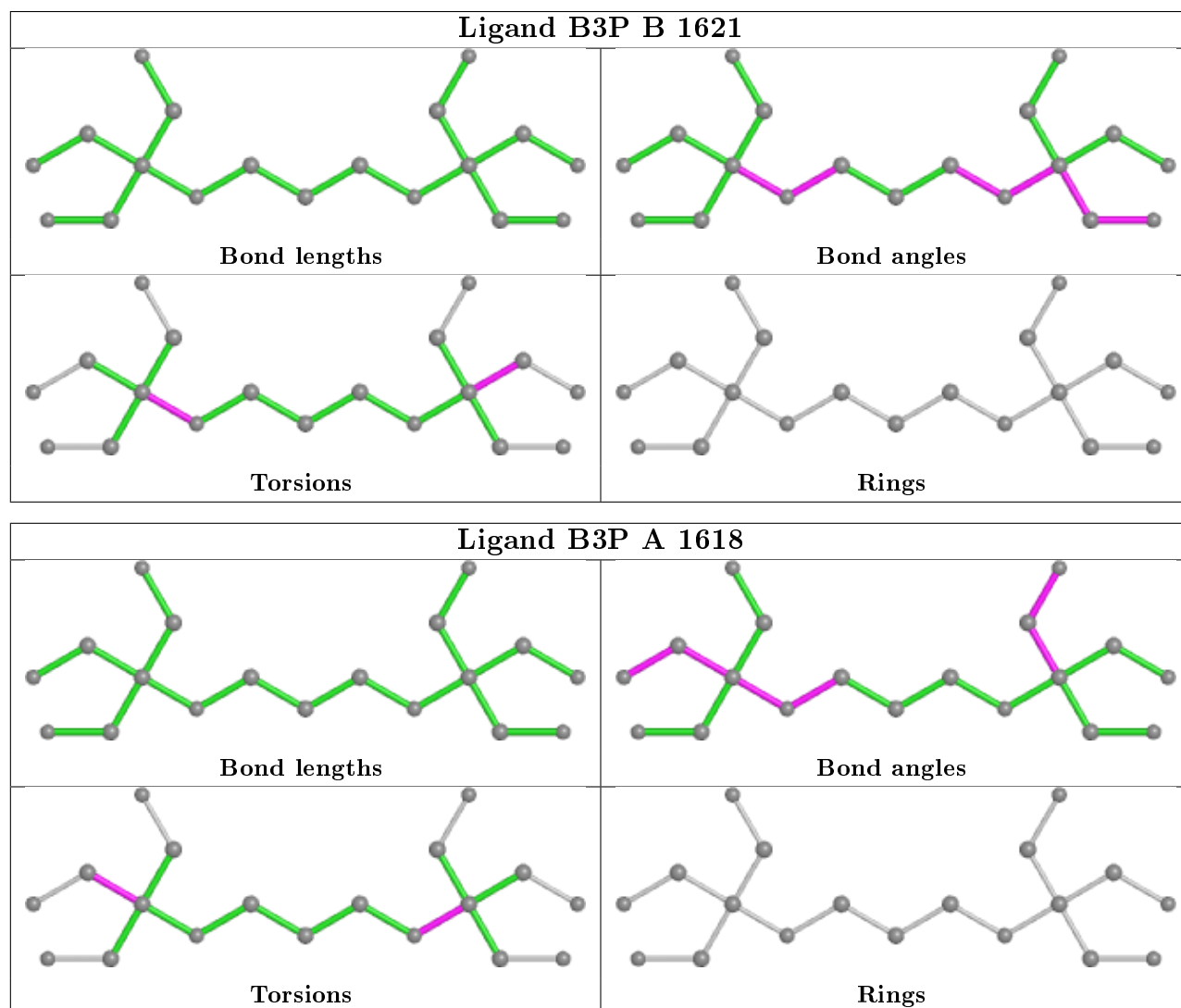
3 monomers are involved in 8 short contacts:

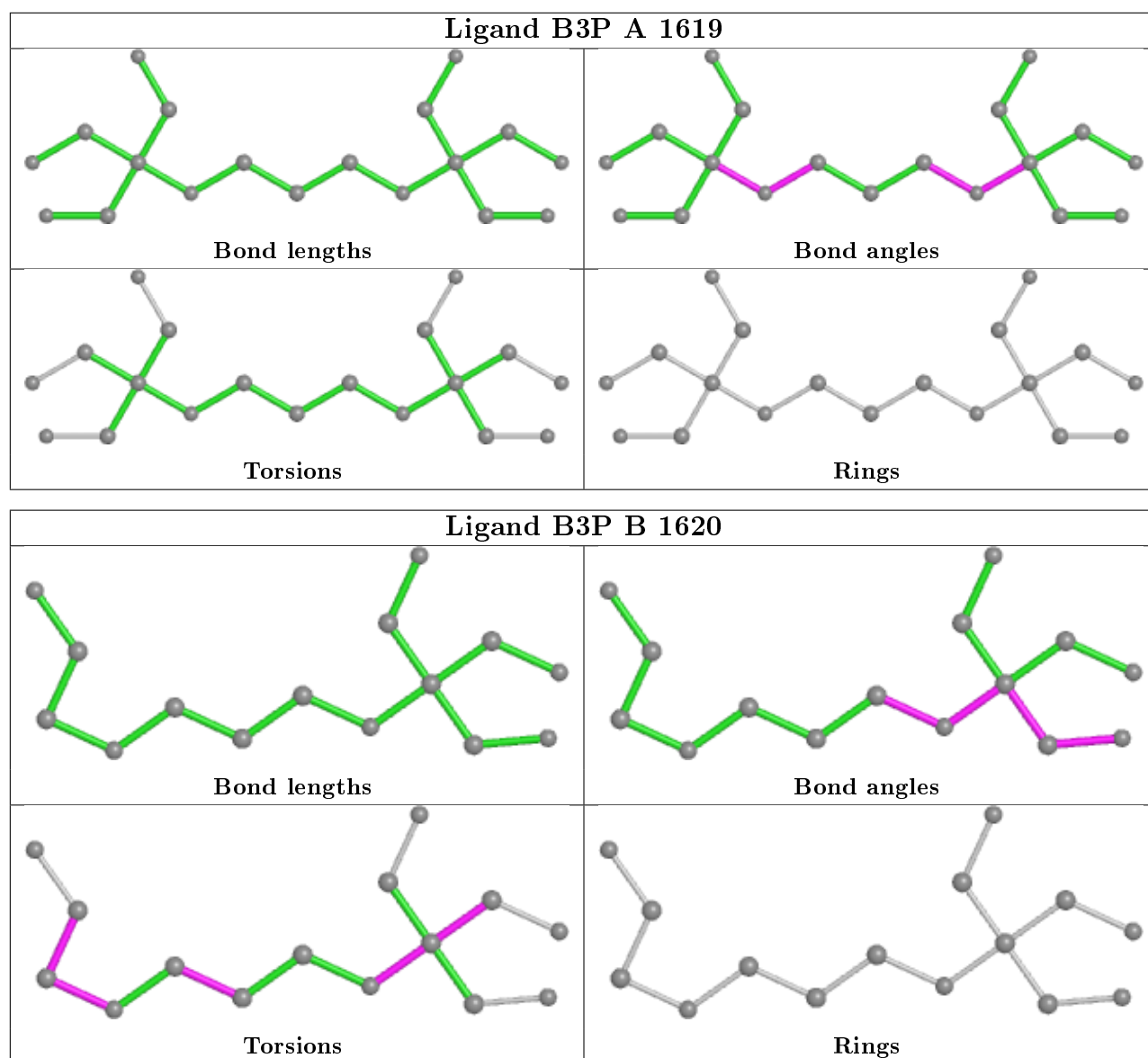
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1621	PGE	1	0
3	B	1623	PGE	3	0
3	B	1622	PGE	4	0

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 [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, 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	616/626 (98%)	-0.16	11 (1%) 68 64	9, 15, 31, 41	0
1	B	616/626 (98%)	-0.19	3 (0%) 91 89	8, 15, 27, 35	0
All	All	1232/1252 (98%)	-0.18	14 (1%) 80 78	8, 15, 29, 41	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	HIS	8.0
1	A	593	ASN	4.1
1	A	587	VAL	3.8
1	A	569	GLY	3.6
1	B	148	GLY	3.2
1	A	526	ASP	3.2
1	A	244[A]	TRP	3.0
1	B	526	ASP	2.7
1	A	281[A]	GLN	2.6
1	A	146	GLU	2.4
1	B	2	THR	2.3
1	A	19	TRP	2.2
1	A	2	THR	2.1
1	A	617	LYS	2.0

### 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](#)

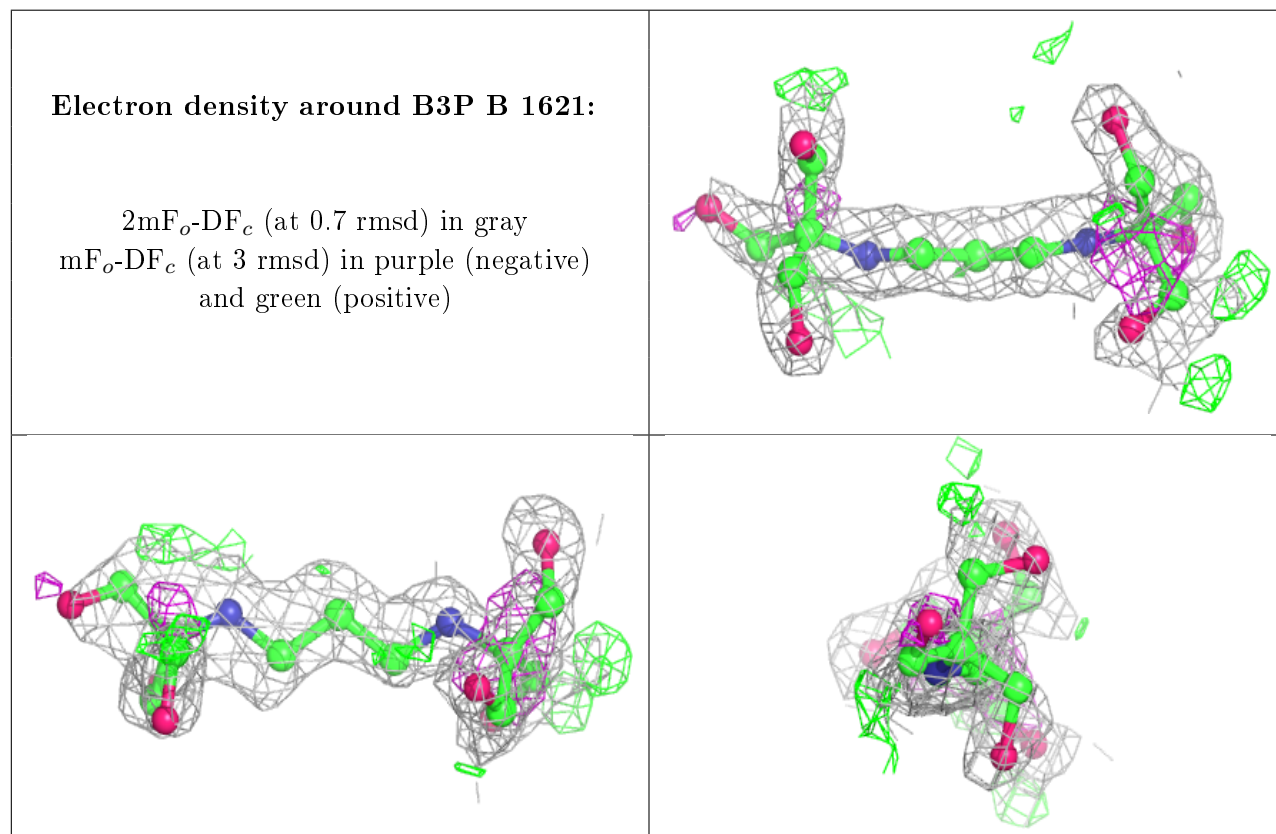
There are no carbohydrates in this entry.

## 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.

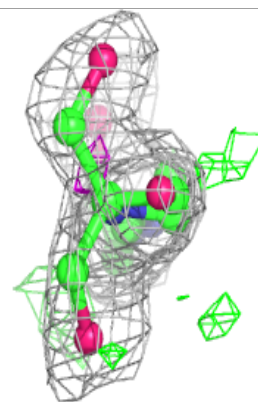
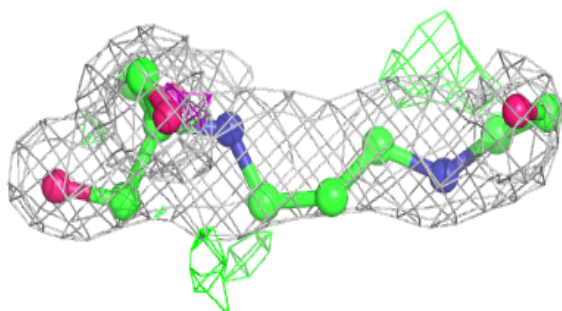
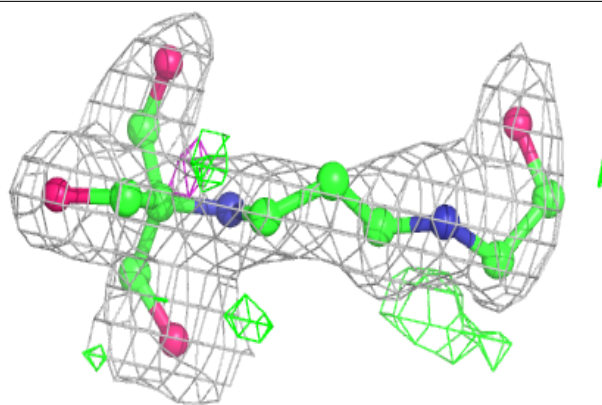
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	B3P	B	1621	19/19	0.72	0.27	26,34,43,44	0
3	PGE	A	1621	10/10	0.77	0.19	42,44,48,48	0
2	B3P	B	1620	15/19	0.81	0.22	37,39,42,42	0
3	PGE	B	1623	10/10	0.86	0.15	47,48,48,48	0
3	PGE	A	1620	10/10	0.86	0.15	24,26,34,35	0
3	PGE	B	1622	10/10	0.91	0.11	25,28,29,33	0
2	B3P	A	1619	19/19	0.93	0.12	26,29,32,32	0
2	B3P	A	1618	19/19	0.95	0.08	14,17,31,33	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.

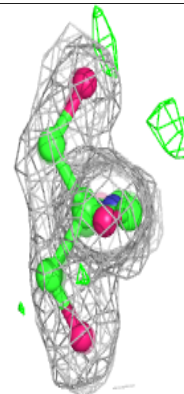
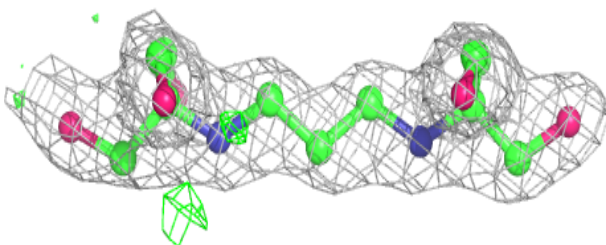
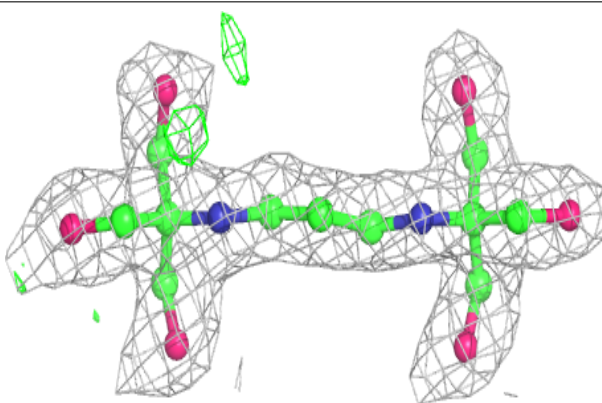


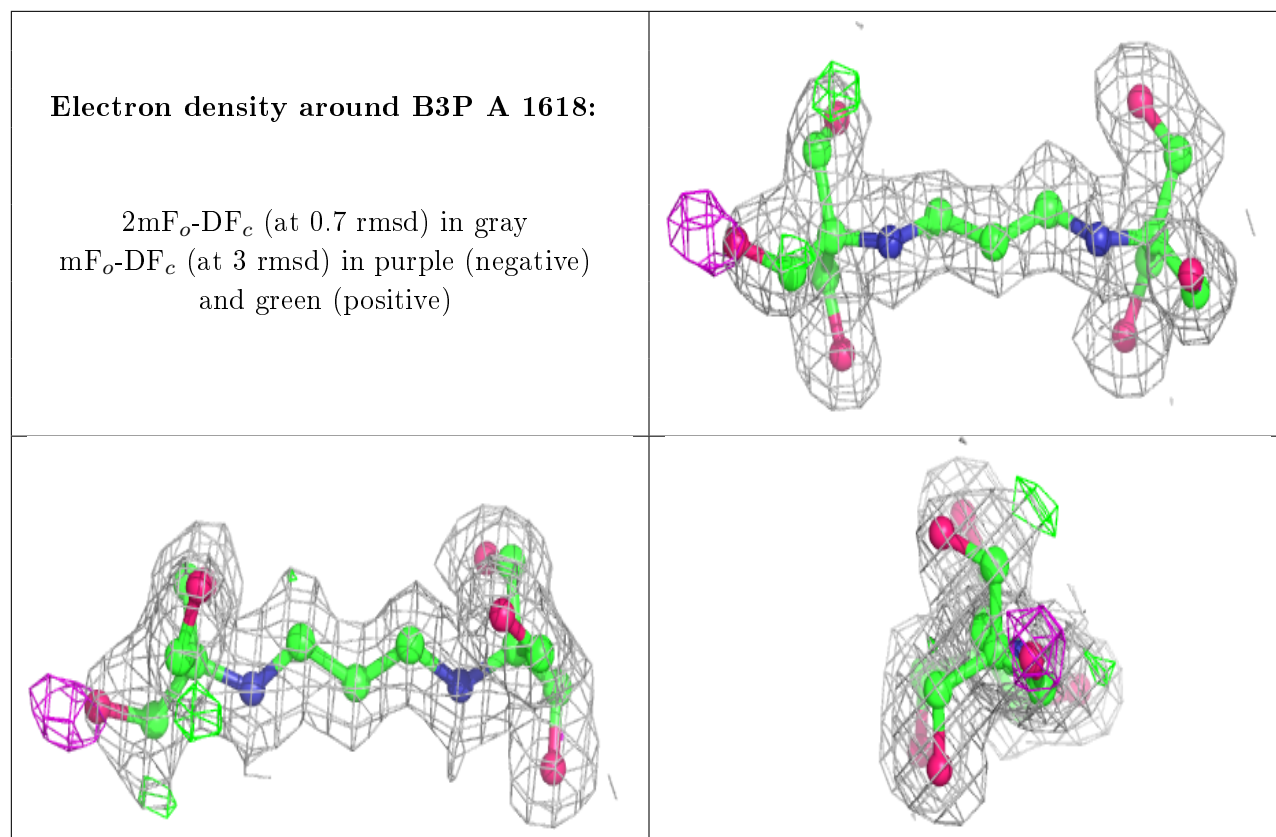
**Electron density around B3P B 1620:**

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

**Electron density around B3P A 1619:**

$2mF_o-DF_c$  (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.