Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2020 – 11:25 am BST

PDB ID	:	2JE8
Title	:	Structure of a beta-mannosidase from Bacteroides thetaiotaomicron
Authors	:	Tailford, L.E.; Money, V.A.; Smith, N.L.; Dumon, C.; Davies, G.J.; Gilbert, H.J.
Deposited on	:	2007-01-16
Resolution	:	1.70 Å(reported)

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

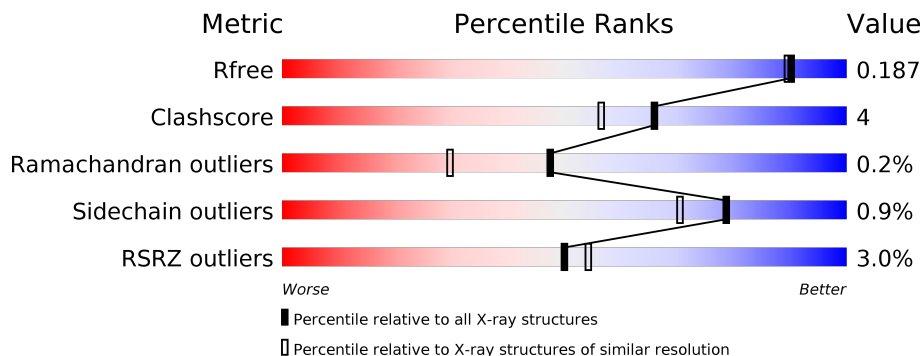|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
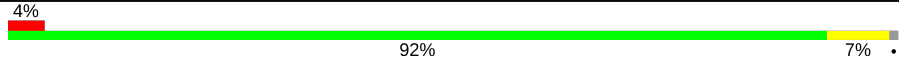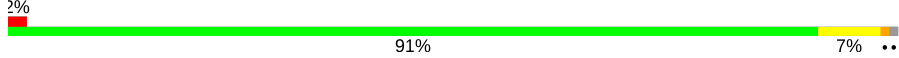*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Rfree		0.187
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		0.9%
RSRZ outliers		3.0%

Worse　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	A	848	4% 92% 7% •
1	B	848	2% 91% 7% ••

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	GOL	A	1867	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15992 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-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	837	Total 6944	C 4461	N 1165	O 1284	S 34	0	24	0
1	B	841	Total 7077	C 4548	N 1190	O 1302	S 37	0	42	0

- Molecule 2 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).
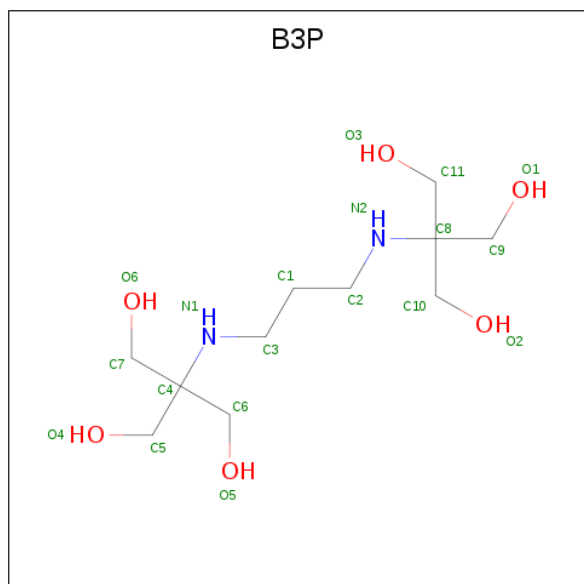
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 19	C 11	N 2	O 6	0	0
2	B	1	Total 19	C 11	N 2	O 6	0	0
2	B	1	Total 19	C 11	N 2	O 6	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	A	3	Total 3	Cl 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	870	Total 870	O 870	0	0
5	B	986	Total 986	O 986	0	0

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 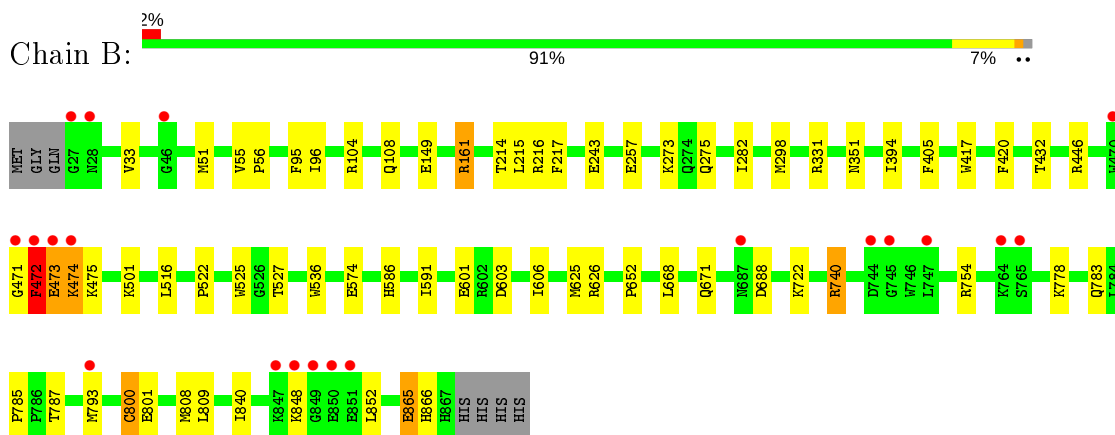one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: BETA-MANNOSIDASE
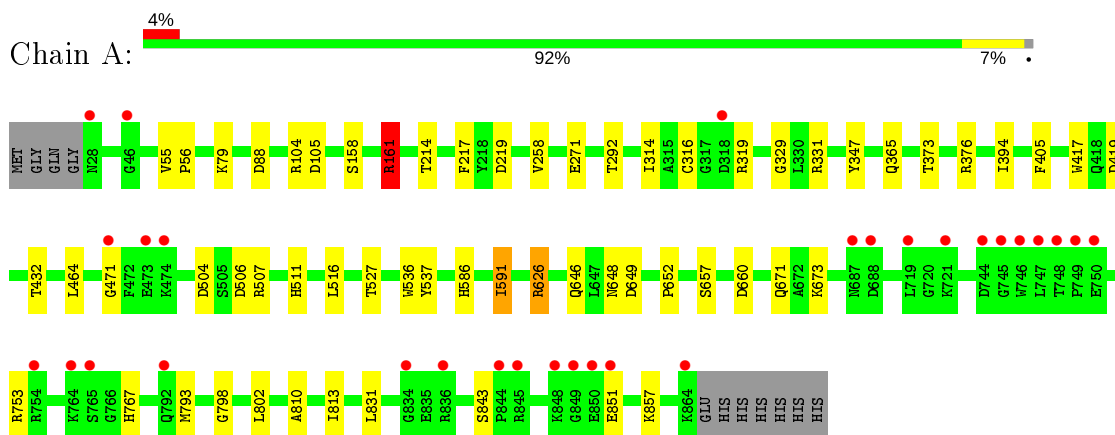
- Molecule 1: BETA-MANNOSIDASE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.46Å 116.00Å 99.15Å 90.00° 113.42° 90.00°	Depositor
Resolution (Å)	39.56 – 1.70 38.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.56-1.70) 100.0 (38.80-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.155 , 0.188 0.153 , 0.187	Depositor DCC
R_{free} test set	10324 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15992	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.85	0/7204	0.82	3/9778 (0.0%)
1	B	0.89	5/7390 (0.1%)	0.84	5/10022 (0.0%)
All	All	0.87	5/14594 (0.0%)	0.83	8/19800 (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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	865	GLU	CG-CD	-9.70	1.37	1.51
1	B	865	GLU	CB-CG	-9.46	1.34	1.52
1	B	800[A]	CYS	CB-SG	-6.56	1.71	1.82
1	B	800[B]	CYS	CB-SG	-6.56	1.71	1.82
1	B	420	PHE	CE2-CZ	5.05	1.47	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161[A]	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	161[B]	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	161[B]	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	865	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	A	419	ASP	CB-CG-OD2	-5.68	113.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161[A]	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	161[B]	ARG	NE-CZ-NH2	-5.32	117.64	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	GLY	Peptide
1	B	472	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	6944	0	6815	52	0
1	B	7077	0	6991	56	0
2	A	19	0	26	0	0
2	B	38	0	52	1	0
3	A	18	0	24	11	0
3	B	36	0	48	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
5	A	870	0	0	17	0
5	B	986	0	0	20	0
All	All	15992	0	13956	112	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 4.

All (112) 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:B:787[B]:THR:HG22	1:B:808[B]:MET:HB2	1.27	1.10
1:A:648:ASN:HB2	3:A:1867:GOL:H31	1.43	1.01
1:B:51:MET:HE3	5:B:2021:HOH:O	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ARG:HG3	5:A:2733:HOH:O	1.63	0.98
1:B:51:MET:CE	5:B:2021:HOH:O	2.09	0.97
1:A:673:LYS:HE3	5:A:2480:HOH:O	1.69	0.92
1:A:158:SER:HB3	1:A:161[A]:ARG:CG	2.01	0.90
1:A:214[B]:THR:HG23	5:A:2157:HOH:O	1.71	0.90
1:B:472:PHE:O	1:B:475:LYS:HB2	1.76	0.85
3:A:1867:GOL:H2	5:A:2457:HOH:O	1.77	0.85
1:A:158:SER:HB3	1:A:161[A]:ARG:HG2	1.60	0.84
1:B:787[B]:THR:HG22	1:B:808[B]:MET:CB	2.11	0.79
1:B:787[B]:THR:CG2	1:B:808[B]:MET:HB2	2.13	0.76
1:B:432:THR:HG22	5:B:2575:HOH:O	1.85	0.75
1:B:33:VAL:HG13	1:B:214:THR:HG23	1.67	0.75
1:A:537:TYR:HA	1:A:591:ILE:HD11	1.70	0.73
1:A:158:SER:HB3	1:A:161[A]:ARG:HG3	1.70	0.72
1:A:376[A]:ARG:NH2	3:A:1867:GOL:O2	2.23	0.72
1:A:365:GLN:HG2	3:A:1867:GOL:H32	1.70	0.71
1:B:33:VAL:HG13	1:B:214:THR:CG2	2.21	0.70
1:B:472:PHE:H	1:B:473:GLU:HB3	1.56	0.70
1:B:787[B]:THR:HG21	1:B:809:LEU:O	1.90	0.70
1:B:591[A]:ILE:HD11	5:B:2733:HOH:O	1.92	0.69
1:A:214[B]:THR:CG2	5:A:2157:HOH:O	2.36	0.69
1:A:271:GLU:HG2	5:A:2362:HOH:O	1.95	0.67
1:B:257:GLU:OE2	1:B:275:GLN:NE2	2.29	0.66
1:A:88:ASP:OD1	1:A:161[A]:ARG:HD3	1.95	0.66
1:B:866:HIS:CD2	5:B:2961:HOH:O	2.50	0.65
1:B:722:LYS:HD2	5:B:2824:HOH:O	1.96	0.65
1:A:506:ASP:HB2	5:A:2577:HOH:O	1.97	0.64
1:A:347:TYR:CE2	3:A:1868:GOL:H31	2.33	0.64
1:A:373:THR:H	1:A:376[B]:ARG:HD3	1.62	0.64
1:A:432:THR:HG22	5:A:2521:HOH:O	1.98	0.62
1:B:51:MET:HE2	5:B:2021:HOH:O	1.85	0.62
1:A:793:MET:CE	1:A:851:GLU:HG3	2.31	0.61
1:B:866:HIS:HD2	5:B:2961:HOH:O	1.82	0.61
1:B:740[B]:ARG:HD2	5:B:2801:HOH:O	2.01	0.60
1:A:810:ALA:HB3	1:A:813[A]:ILE:HD11	1.82	0.60
1:B:351:ASN:HB2	5:B:2495:HOH:O	2.02	0.58
1:A:394:ILE:HD11	1:A:405:PHE:CE2	2.38	0.58
1:B:793[B]:MET:CE	1:B:800[B]:CYS:SG	2.92	0.58
1:B:472:PHE:CA	1:B:473:GLU:CB	2.83	0.57
1:B:472:PHE:CA	1:B:473:GLU:HB2	2.34	0.57
1:B:472:PHE:N	1:B:473:GLU:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446[A]:ARG:HD2	5:B:2582:HOH:O	2.04	0.56
1:A:516[A]:LEU:HD13	1:A:527:THR:HG21	1.87	0.55
1:A:79:LYS:HG3	5:A:2103:HOH:O	2.05	0.55
1:B:298[B]:MET:SD	5:B:2495:HOH:O	2.58	0.54
1:B:243:GLU:OE2	5:B:2349:HOH:O	2.18	0.53
1:B:472:PHE:N	1:B:473:GLU:CB	2.72	0.52
1:B:472:PHE:N	5:B:2599:HOH:O	2.42	0.52
1:A:214[B]:THR:HG21	5:A:2070:HOH:O	2.10	0.52
1:A:504:ASP:OD2	1:A:507:ARG:HD2	2.10	0.52
1:A:516[A]:LEU:HD22	1:A:527:THR:HB	1.91	0.52
1:A:464:LEU:HD22	1:A:511:HIS:HE1	1.75	0.51
1:B:95:PHE:CE1	1:B:215:LEU:HD11	2.46	0.51
1:A:79:LYS:CG	5:A:2103:HOH:O	2.58	0.51
1:B:161[A]:ARG:HG3	5:B:2239:HOH:O	2.11	0.50
1:B:257:GLU:OE2	1:B:273:LYS:HD3	2.12	0.50
1:A:649:ASP:O	3:A:1867:GOL:O3	2.19	0.50
1:B:603:ASP:OD1	1:B:778[B]:LYS:HD3	2.11	0.50
1:B:501:LYS:HE2	5:B:2627:HOH:O	2.11	0.49
1:A:104:ARG:HG3	1:A:217:PHE:HB3	1.94	0.49
1:B:793[B]:MET:HE2	1:B:800[B]:CYS:SG	2.52	0.49
1:A:626:ARG:CG	5:A:2733:HOH:O	2.39	0.49
1:B:586:HIS:HD2	1:B:652:PRO:O	1.96	0.48
1:A:258:VAL:HG22	1:A:314:ILE:HD12	1.96	0.48
1:A:626:ARG:HB2	1:A:671:GLN:HB3	1.96	0.48
1:A:471:GLY:N	5:A:2546:HOH:O	2.40	0.47
1:B:754:ARG:HH11	1:B:783:GLN:NE2	2.11	0.47
1:A:365:GLN:HA	3:A:1867:GOL:O3	2.15	0.47
1:A:292:THR:HG22	5:A:2329:HOH:O	2.15	0.46
1:B:55:VAL:HA	1:B:56:PRO:C	2.35	0.46
2:B:1869:B3P:H32	2:B:1869:B3P:H62	1.60	0.46
1:A:214[A]:THR:HG21	5:A:2070:HOH:O	2.15	0.46
3:A:1867:GOL:C2	5:A:2457:HOH:O	2.47	0.46
1:A:793:MET:HE1	1:A:851:GLU:HG3	1.96	0.46
3:B:1874:GOL:H12	5:B:2984:HOH:O	2.14	0.45
1:B:96:ILE:HD11	1:B:149[B]:GLU:OE1	2.16	0.45
1:A:767[A]:HIS:HE1	5:B:2008:HOH:O	2.00	0.45
1:A:857:LYS:HA	5:A:2857:HOH:O	2.15	0.45
1:B:108:GLN:OE1	1:B:216[B]:ARG:NH1	2.49	0.45
1:B:282:ILE:HD12	5:B:2317:HOH:O	2.17	0.45
1:A:646:GLN:O	1:A:657:SER:HA	2.17	0.45
1:B:516[B]:LEU:HD23	1:B:527:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:PRO:HG2	1:B:787[B]:THR:CG2	2.47	0.44
1:B:785:PRO:HG2	1:B:787[B]:THR:HG23	1.99	0.44
1:A:316:CYS:O	1:A:319:ARG:HG2	2.17	0.44
1:A:648:ASN:HD22	3:A:1867:GOL:C3	2.31	0.43
1:A:626:ARG:HD3	1:A:626:ARG:HH11	1.66	0.43
1:B:104:ARG:HG3	1:B:217:PHE:HB3	2.01	0.43
1:A:793:MET:HE2	1:A:851:GLU:HG3	2.01	0.43
1:B:801[B]:GLU:HG2	1:B:840:ILE:HG12	2.01	0.43
1:A:586:HIS:HD2	1:A:652:PRO:O	2.01	0.42
1:B:474:LYS:HG3	5:B:2599:HOH:O	2.19	0.42
1:A:813[A]:ILE:HD13	1:A:831:LEU:HB2	2.01	0.42
1:B:472:PHE:O	1:B:475:LYS:CB	2.59	0.42
1:A:793:MET:HG3	1:A:802:LEU:HD23	2.00	0.42
1:A:329:GLY:O	3:A:1866:GOL:H12	2.19	0.42
1:A:55:VAL:HA	1:A:56:PRO:C	2.40	0.42
1:B:793[B]:MET:HE1	1:B:800[B]:CYS:SG	2.59	0.42
1:B:574:GLU:H	1:B:574:GLU:CD	2.24	0.41
1:B:601:GLU:HB2	1:B:606:ILE:HD11	2.02	0.41
1:B:793[B]:MET:HE1	1:B:852:LEU:HB3	2.03	0.41
1:B:516[B]:LEU:CD2	1:B:527:THR:HG21	2.51	0.41
1:B:625:MET:HB2	1:B:668:LEU:HD13	2.02	0.41
1:B:626[B]:ARG:HB3	1:B:671:GLN:HB3	2.01	0.41
1:B:522:PRO:HA	1:B:525:TRP:CE2	2.56	0.40
1:A:105:ASP:HB2	1:A:219:ASP:HA	2.03	0.40
1:A:660:ASP:O	3:A:1867:GOL:H12	2.22	0.40
1:A:798:GLY:HA2	1:A:843:SER:O	2.22	0.40
1:B:394:ILE:HD11	1:B:405:PHE:CE2	2.57	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	859/848 (101%)	838 (98%)	20 (2%)	1 (0%)	51	33
1	B	881/848 (104%)	859 (98%)	19 (2%)	3 (0%)	41	24
All	All	1740/1696 (103%)	1697 (98%)	39 (2%)	4 (0%)	47	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	TRP
1	B	473	GLU
1	B	536	TRP
1	B	472	PHE

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	770/755 (102%)	763 (99%)	7 (1%)	78	70
1	B	791/755 (105%)	782 (99%)	9 (1%)	73	63
All	All	1561/1510 (103%)	1545 (99%)	16 (1%)	78	67

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

Mol	Chain	Res	Type
1	A	161[A]	ARG
1	A	161[B]	ARG
1	A	331	ARG
1	A	417	TRP
1	A	591	ILE
1	A	626	ARG
1	A	753	ARG
1	B	331	ARG
1	B	417	TRP
1	B	474	LYS
1	B	688	ASP
1	B	740[A]	ARG

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Mol	Chain	Res	Type
1	B	740[B]	ARG
1	B	848[A]	LYS
1	B	848[B]	LYS
1	B	865	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	103	ASN
1	A	242	ASN
1	A	265	ASN
1	A	274	GLN
1	A	726	HIS
1	A	768	GLN
1	B	248	GLN
1	B	265	ASN
1	B	274	GLN
1	B	293	ASN
1	B	337	ASN
1	B	586	HIS
1	B	768	GLN
1	B	783	GLN
1	B	866	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)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#|Z| > 2$
3	GOL	B	1875	-	5,5,5	0.17	0	5,5,5	0.55	0
3	GOL	A	1868	-	5,5,5	0.15	0	5,5,5	0.79	0
3	GOL	B	1871	-	5,5,5	0.49	0	5,5,5	0.59	0
3	GOL	A	1867	-	5,5,5	0.62	0	5,5,5	1.19	0
3	GOL	B	1874	-	5,5,5	0.50	0	5,5,5	1.00	0
3	GOL	B	1870	-	5,5,5	0.54	0	5,5,5	0.36	0
3	GOL	B	1873	-	5,5,5	0.18	0	5,5,5	0.81	0
2	B3P	B	1869	-	18,18,18	0.77	0	21,23,23	3.69	9 (42%)
3	GOL	A	1866	-	5,5,5	0.61	0	5,5,5	0.69	0
2	B3P	A	1865	-	18,18,18	1.17	2 (11%)	21,23,23	1.44	2 (9%)
2	B3P	B	1868	-	18,18,18	1.49	2 (11%)	21,23,23	3.27	11 (52%)
3	GOL	B	1872	-	5,5,5	0.46	0	5,5,5	0.36	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
3	GOL	B	1875	-	-	4/4/4/4	-
3	GOL	A	1868	-	-	4/4/4/4	-
3	GOL	B	1871	-	-	2/4/4/4	-
3	GOL	A	1867	-	-	2/4/4/4	-
3	GOL	B	1874	-	-	0/4/4/4	-
3	GOL	B	1870	-	-	0/4/4/4	-
3	GOL	B	1873	-	-	2/4/4/4	-
2	B3P	B	1869	-	-	4/28/28/28	-
3	GOL	A	1866	-	-	2/4/4/4	-
2	B3P	A	1865	-	-	3/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B3P	B	1868	-	-	7/28/28/28	-
3	GOL	B	1872	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1868	B3P	C3-N1	5.09	1.53	1.46
2	A	1865	B3P	C2-N2	2.92	1.50	1.46
2	A	1865	B3P	C9-C8	2.35	1.56	1.53
2	B	1868	B3P	C7-C4	-2.29	1.50	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1869	B3P	C7-C4-N1	-7.37	86.87	109.03
2	B	1868	B3P	C3-N1-C4	6.90	125.87	116.08
2	B	1869	B3P	C3-N1-C4	6.70	125.59	116.08
2	B	1869	B3P	C7-C4-C6	6.38	123.54	110.04
2	B	1869	B3P	C6-C4-N1	-6.14	90.56	109.03
2	B	1868	B3P	O5-C6-C4	-6.12	99.25	111.63
2	B	1868	B3P	C6-C4-C5	5.26	121.16	110.04
2	B	1869	B3P	C2-N2-C8	5.04	123.23	116.08
2	B	1869	B3P	O6-C7-C4	-4.86	101.80	111.63
2	B	1868	B3P	C6-C4-N1	-4.37	95.88	109.03
2	B	1869	B3P	C6-C4-C5	4.26	119.05	110.04
2	B	1868	B3P	C7-C4-N1	-4.22	96.34	109.03
2	B	1869	B3P	C5-C4-N1	-3.99	97.03	109.03
2	A	1865	B3P	C3-N1-C4	3.72	121.36	116.08
2	B	1868	B3P	C7-C4-C6	3.69	117.84	110.04
2	B	1868	B3P	C11-C8-C10	-3.51	102.62	110.04
2	B	1868	B3P	C5-C4-N1	-3.44	98.69	109.03
2	B	1868	B3P	C2-N2-C8	3.41	120.92	116.08
2	B	1869	B3P	C7-C4-C5	3.40	117.24	110.04
2	B	1868	B3P	C7-C4-C5	3.12	116.63	110.04
2	B	1868	B3P	C11-C8-N2	2.28	115.88	109.03
2	A	1865	B3P	O4-C5-C4	-2.02	107.54	111.63

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1875	GOL	O1-C1-C2-O2
3	B	1875	GOL	O1-C1-C2-C3
3	B	1875	GOL	C1-C2-C3-O3
3	A	1868	GOL	O1-C1-C2-C3
3	B	1871	GOL	O1-C1-C2-O2
3	A	1867	GOL	C1-C2-C3-O3
2	B	1869	B3P	C7-C4-C6-O5
2	B	1869	B3P	C6-C4-C7-O6
3	A	1866	GOL	O1-C1-C2-C3
2	A	1865	B3P	C1-C2-N2-C8
2	B	1868	B3P	C1-C3-N1-C4
2	B	1868	B3P	C7-C4-N1-C3
2	B	1868	B3P	C6-C4-C5-O4
2	B	1868	B3P	C1-C2-N2-C8
3	B	1871	GOL	O1-C1-C2-C3
3	B	1873	GOL	C1-C2-C3-O3
3	A	1867	GOL	O2-C2-C3-O3
3	A	1866	GOL	O1-C1-C2-O2
2	A	1865	B3P	C11-C8-N2-C2
2	B	1868	B3P	C5-C4-N1-C3
3	B	1875	GOL	O2-C2-C3-O3
3	A	1868	GOL	O2-C2-C3-O3
3	B	1873	GOL	O2-C2-C3-O3
2	B	1869	B3P	C5-C4-C7-O6
3	A	1868	GOL	O1-C1-C2-O2
2	A	1865	B3P	C9-C8-N2-C2
2	B	1868	B3P	C6-C4-N1-C3
2	B	1868	B3P	N1-C4-C5-O4
3	A	1868	GOL	C1-C2-C3-O3
2	B	1869	B3P	C6-C4-C5-O4

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1868	GOL	1	0
3	A	1867	GOL	9	0
3	B	1874	GOL	1	0
2	B	1869	B3P	1	0
3	A	1866	GOL	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 B 1869

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P A 1865

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P B 1868

Bond lengths

Bond angles

Torsions

Rings
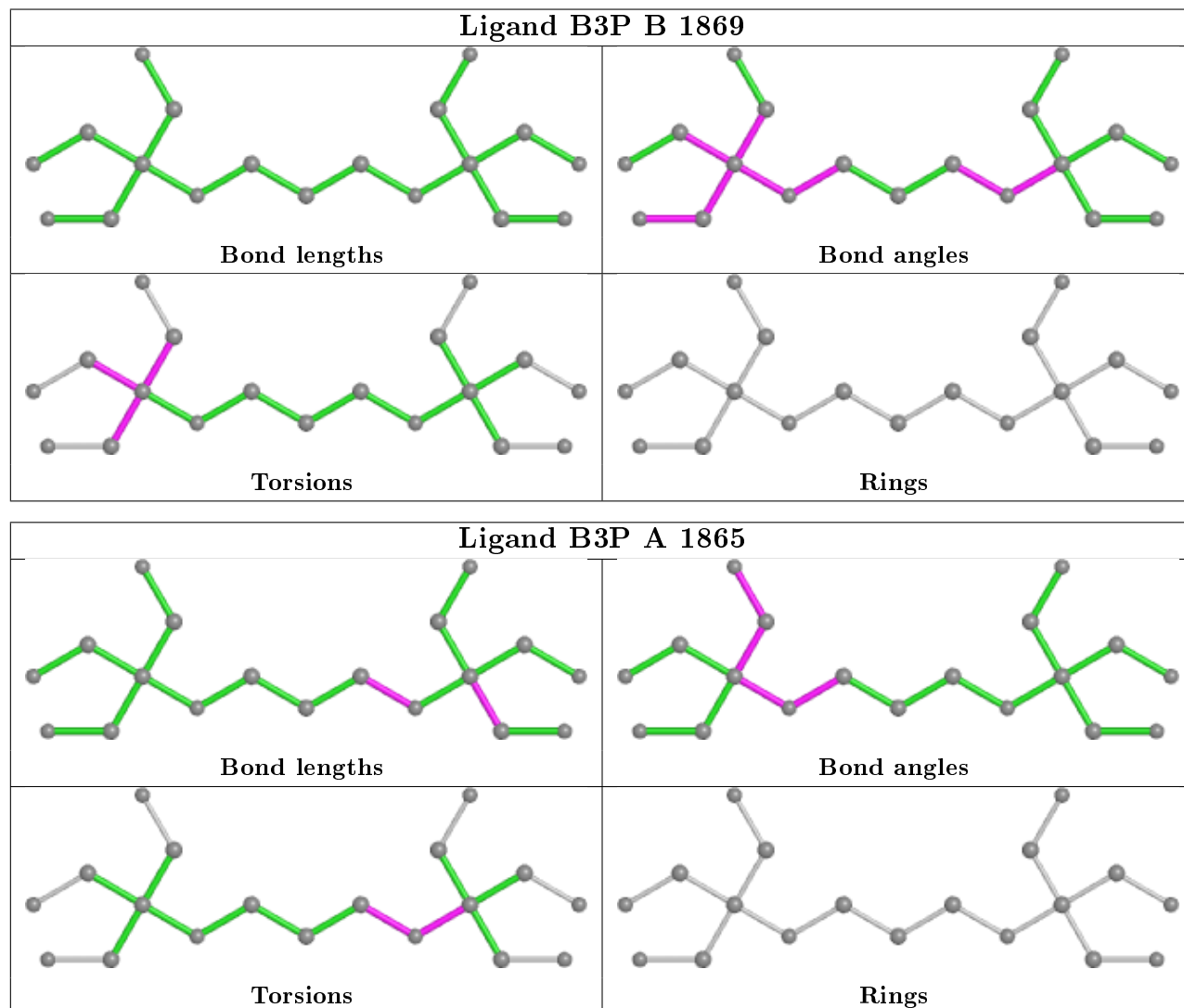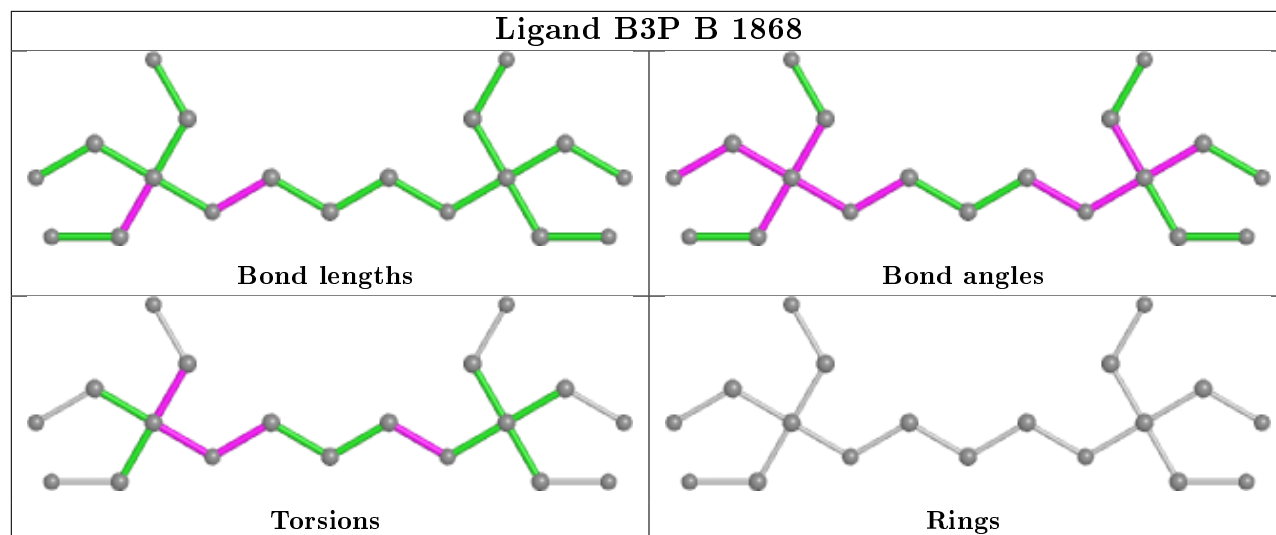
5.7 Other polymers (i)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	837/848 (98%)	-0.10	30 (3%)	42	47	7, 14, 34, 47	0
1	B	841/848 (99%)	-0.21	20 (2%)	59	63	7, 13, 28, 47	0
All	All	1678/1696 (98%)	-0.15	50 (2%)	50	54	7, 14, 31, 47	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ASP	4.1
1	A	471	GLY	4.1
1	A	721	LYS	3.7
1	A	474	LYS	3.7
1	B	471	GLY	3.6
1	A	754	ARG	3.6
1	B	849	GLY	3.5
1	A	849	GLY	3.4
1	B	851	GLU	3.4
1	A	473	GLU	3.3
1	B	28[A]	ASN	3.2
1	B	27	GLY	3.1
1	A	46	GLY	3.0
1	A	851	GLU	3.0
1	A	836	ARG	2.9
1	A	746	TRP	2.9
1	A	747	LEU	2.9
1	A	748	THR	2.8
1	B	850	GLU	2.8
1	B	472	PHE	2.8
1	A	687	ASN	2.7
1	B	46	GLY	2.7
1	B	848[A]	LYS	2.6
1	B	764	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	749	PRO	2.6
1	A	834	GLY	2.5
1	B	747	LEU	2.5
1	A	28	ASN	2.5
1	A	719	LEU	2.5
1	B	473	GLU	2.5
1	A	688	ASP	2.5
1	A	744	ASP	2.5
1	B	745	GLY	2.5
1	A	850	GLU	2.4
1	A	848	LYS	2.4
1	A	745	GLY	2.4
1	A	864	LYS	2.4
1	A	845	ARG	2.2
1	A	844	PRO	2.2
1	B	687	ASN	2.2
1	B	474	LYS	2.2
1	B	470	TRP	2.2
1	B	744	ASP	2.1
1	B	793[A]	MET	2.1
1	B	765	SER	2.1
1	A	792	GLN	2.1
1	A	764	LYS	2.0
1	B	847	LYS	2.0
1	A	765	SER	2.0
1	A	750	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	GOL	B	1875	6/6	0.79	0.13	39,42,42,43	0
2	B3P	B	1869	19/19	0.88	0.16	17,22,30,31	0
3	GOL	A	1867	6/6	0.89	0.18	12,20,24,29	0
3	GOL	B	1871	6/6	0.89	0.10	29,34,34,35	0
3	GOL	B	1873	6/6	0.91	0.14	22,28,29,32	0
3	GOL	A	1868	6/6	0.91	0.13	25,32,33,33	0
3	GOL	B	1872	6/6	0.92	0.12	18,29,30,31	0
3	GOL	B	1874	6/6	0.93	0.16	11,31,34,38	0
2	B3P	A	1865	19/19	0.94	0.13	6,10,22,25	0
3	GOL	A	1866	6/6	0.94	0.14	13,33,38,40	0
2	B3P	B	1868	19/19	0.95	0.11	8,12,25,27	0
3	GOL	B	1870	6/6	0.97	0.09	9,14,16,16	0
4	CL	A	1869	1/1	0.99	0.05	13,13,13,13	0
4	CL	B	1876	1/1	0.99	0.04	19,19,19,19	0
4	CL	A	1870	1/1	0.99	0.03	19,19,19,19	0
4	CL	A	1871	1/1	0.99	0.04	25,25,25,25	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.
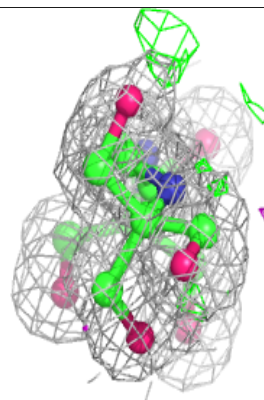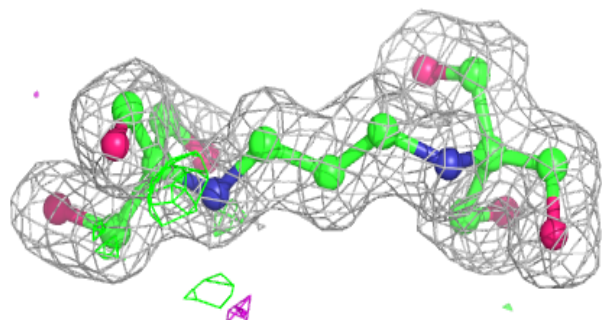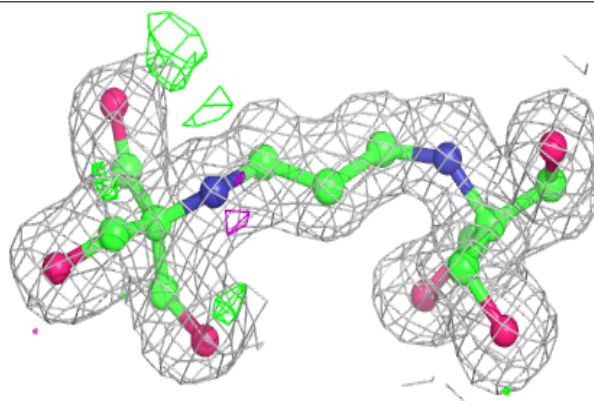
Electron density around B3P B 1869:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
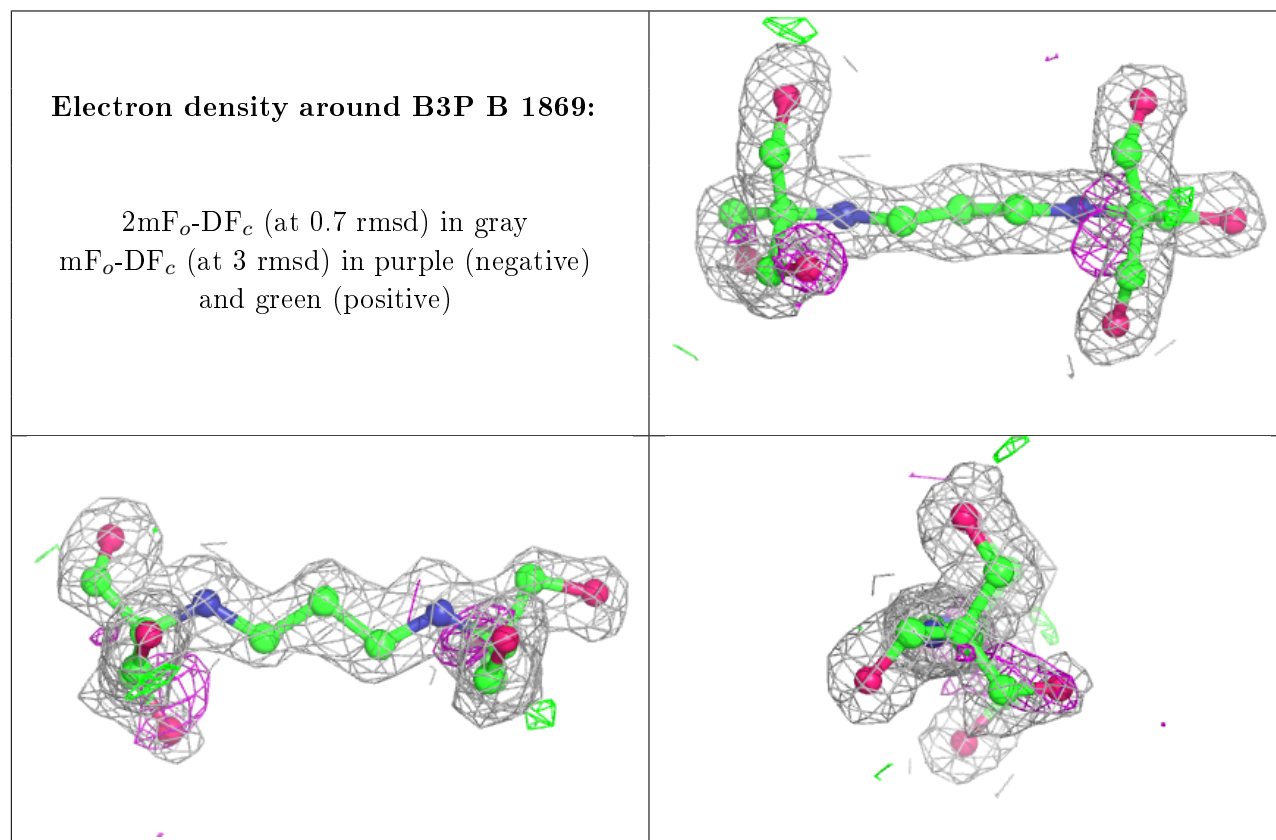
Electron density around B3P A 1865:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
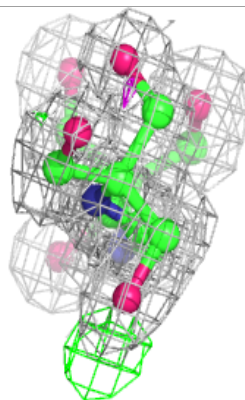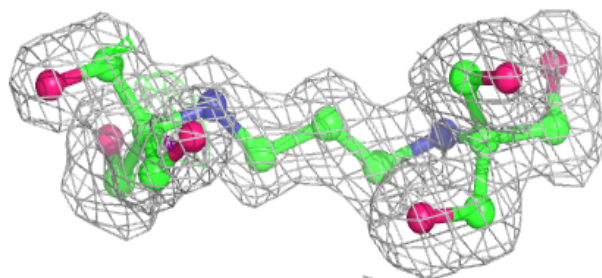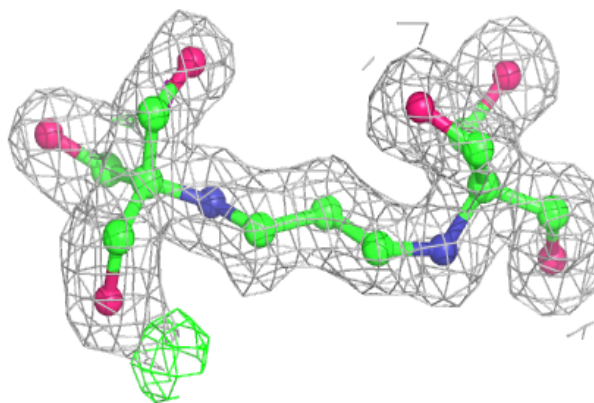
Electron density around B3P B 1868:

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.