



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:53 PM BST

PDB ID : 4ZEN
Title : Structure of Gan1D, a putative 6-phospho-beta-galactosidase from *Geobacillus stearothermophilus*, in complex with 6-phospho-beta-galactose
Authors : Lansky, S.; Zehavi, A.; Dvir, H.; Shoham, Y.; Shoham, G.
Deposited on : 2015-04-20
Resolution : 1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

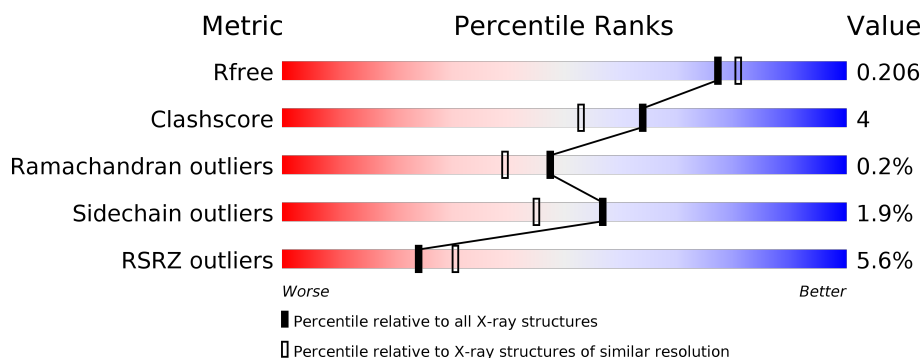
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 $\leq 5\%$. 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	485	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	B	485	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8374 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.

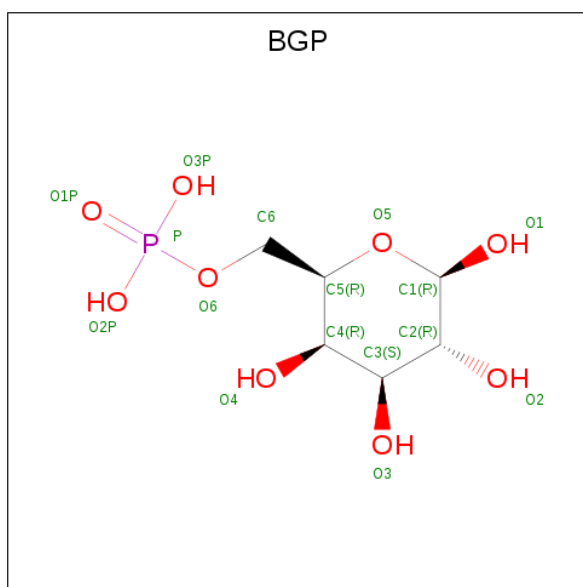
- Molecule 1 is a protein called Putative 6-phospho-beta-galactobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	3	0
			3890	2498	666	715	11			
1	B	474	Total	C	N	O	S	0	0	0
			3874	2486	664	713	11			

There are 16 discrepancies between the modelled and reference sequences:

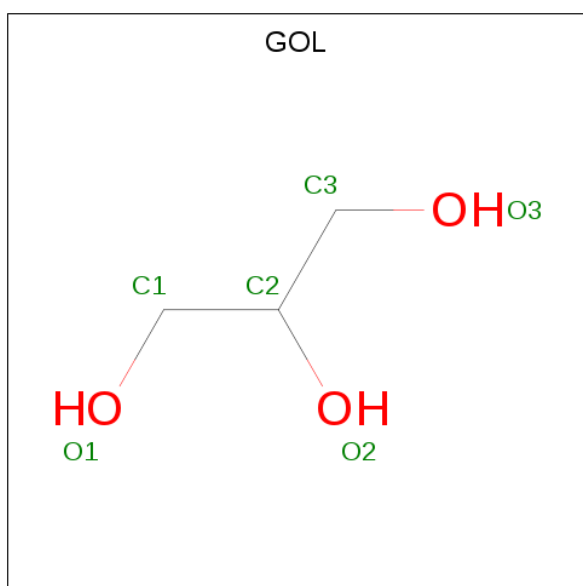
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	UNP W8QF82
A	1	HIS	-	expression tag	UNP W8QF82
B	-6	MET	-	initiating methionine	UNP W8QF82
B	-5	ILE	-	expression tag	UNP W8QF82
B	-4	HIS	-	expression tag	UNP W8QF82
B	-3	HIS	-	expression tag	UNP W8QF82
B	-2	HIS	-	expression tag	UNP W8QF82
B	-1	HIS	-	expression tag	UNP W8QF82
B	0	HIS	-	expression tag	UNP W8QF82
B	1	HIS	-	expression tag	UNP W8QF82

- Molecule 2 is 6-O-phosphono-beta-D-galactopyranose (three-letter code: BGP) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

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



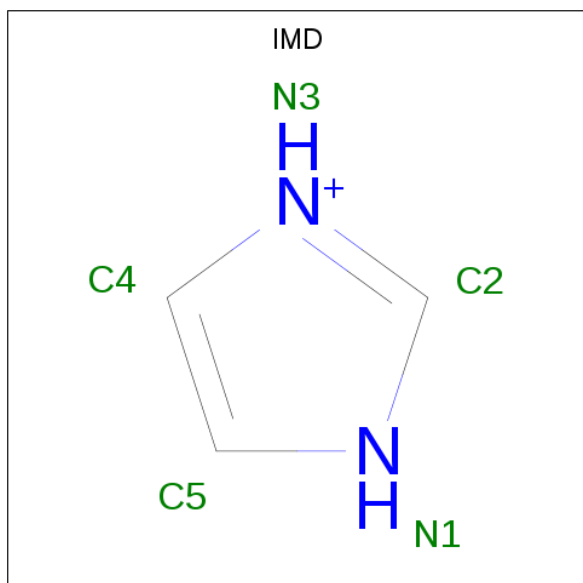
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total	O	0	0
			309	309		
5	B	177	Total	O	0	0
			177	177		

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A:
-
- 2% 90% 8%
- 0.15
0.10
0.05
0.00
- 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300
- MET ILE HIS HIS HIS HIS HIS HIS HIS HIS GLU ARG H5 L6 V24 Q44 K77 R80 V63 G92 V120 T121 I122 P128 F147 D148 K163 L168 N169 E170 Q171 H184 P185 K189 N198 V208 D218 D234 N245 H252 V253 V254
- Y258 A290 N299 P311 D312 L333 F337 R364 N368 E378 D385 D391 W425 S426 L430 W433 Q438 V444 R448 L478

- Chain B:
-

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.52Å 68.67Å 153.28Å 90.00° 99.03° 90.00°	Depositor
Resolution (Å)	26.22 – 1.93 26.21 – 1.93	Depositor EDS
% Data completeness (in resolution range)	91.3 (26.22-1.93) 91.4 (26.21-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.157 , 0.202 0.167 , 0.206	Depositor DCC
R_{free} test set	3831 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8374	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.02	0/4020	0.92	3/5472 (0.1%)
1	B	0.91	1/3995 (0.0%)	0.90	2/5437 (0.0%)
All	All	0.97	1/8015 (0.0%)	0.91	5/10909 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLY	N-CA	5.23	1.53	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	190	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	391	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	256	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	448	ARG	NE-CZ-NH2	-6.19	117.20	120.30

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	3890	0	3693	26	0
1	B	3874	0	3668	39	0
2	A	16	0	11	2	0
2	B	16	0	11	2	0
3	A	42	0	56	2	0
3	B	30	0	40	1	0
4	A	15	0	15	2	0
4	B	5	0	5	0	0
5	A	309	0	0	11	0
5	B	177	0	0	4	0
All	All	8374	0	7499	64	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 (64) 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:44[B]:GLN:NE2	5:A:601:HOH:O	1.67	1.23
1:A:198:ASN:HD21	1:A:254:TRP:HE1	1.26	0.81
1:B:93:ASN:O	1:B:149:ARG:NH2	2.16	0.79
1:B:198:ASN:HD21	1:B:254:TRP:HE1	1.27	0.78
1:A:148:ASP:OD2	3:A:507:GOL:H32	1.91	0.70
1:A:163:LYS:HB2	5:A:867:HOH:O	1.93	0.68
1:A:245:ASN:ND2	5:A:602:HOH:O	2.24	0.66
1:A:252:HIS:CD2	1:B:368:ASN:HD21	2.17	0.62
1:A:438[B]:GLN:HG2	5:A:604:HOH:O	2.00	0.60
1:B:265:GLN:HE21	1:B:269:ASN:ND2	1.99	0.60
1:B:170:GLU:OE2	2:B:501:BGPO1	2.20	0.57
1:A:368:ASN:HD21	1:B:252:HIS:HD2	1.55	0.55
1:B:157:ARG:HD3	5:B:609:HOH:O	2.07	0.54
1:B:402:LEU:O	1:B:406:VAL:HG23	2.06	0.54
1:B:443:PHE:O	1:B:461:LYS:HG3	2.07	0.54
1:B:388:GLU:HB2	1:B:392:ILE:HB	1.91	0.53
1:A:252:HIS:HD2	1:B:368:ASN:HD21	1.55	0.53
1:B:68:VAL:HG11	1:B:110:GLU:HG3	1.91	0.51
1:B:93:ASN:C	1:B:149:ARG:HH21	2.14	0.51
1:A:218:ASP:HB2	5:A:774:HOH:O	2.11	0.51
1:B:198:ASN:ND2	1:B:254:TRP:HE1	2.05	0.50
1:B:426:SER:O	1:B:442:GLY:HA2	2.10	0.50
4:A:510:IMD:C4	5:A:857:HOH:O	2.59	0.50
1:B:148:ASP:HA	1:B:208:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:O	1:A:368:ASN:HB3	2.12	0.48
1:A:92:GLY:HA2	1:A:128:PRO:HG2	1.95	0.48
3:A:503:GOL:H32	5:A:783:HOH:O	2.13	0.48
1:B:93:ASN:C	1:B:93:ASN:HD22	2.17	0.47
1:B:171:GLN:HA	1:B:174:PHE:CE2	2.50	0.47
1:A:378:GLU:OE2	2:A:501:BGP:H1	2.14	0.47
1:A:5:HIS:CE1	5:A:606:HOH:O	2.67	0.47
1:B:252:HIS:HE1	5:B:701:HOH:O	1.97	0.46
1:B:73:GLU:OE2	1:B:460:LYS:NZ	2.43	0.46
1:B:85:TRP:HB2	5:B:705:HOH:O	2.15	0.46
1:B:79:TYR:CE2	1:B:81:PHE:HB3	2.51	0.45
1:A:80:ARG:HH22	1:A:169:ASN:ND2	2.14	0.45
1:A:333:ILE:HD12	1:A:337:PHE:CE2	2.52	0.45
1:B:378:GLU:OE2	2:B:501:BGP:H1	2.16	0.45
1:B:265:GLN:HE21	1:B:269:ASN:HD21	1.64	0.45
1:B:406:VAL:HA	1:B:409:ILE:HD12	1.97	0.45
1:A:425:TRP:HA	1:A:426:SER:HA	1.82	0.45
1:A:80:ARG:HH22	1:A:169:ASN:HD22	1.64	0.45
1:B:360:ARG:NH1	5:B:607:HOH:O	2.49	0.45
1:A:184:HIS:HB3	1:A:185:PRO:HD2	1.98	0.44
1:A:147:PHE:CE2	1:A:208[B]:VAL:HG21	2.53	0.44
1:A:433:TRP:HE1	2:A:501:BGP:HO4	1.66	0.44
1:A:171:GLN:NE2	1:A:258:TYR:OH	2.51	0.44
1:B:175:ILE:HG21	1:B:198:ASN:HB2	2.00	0.43
1:B:93:ASN:C	1:B:93:ASN:ND2	2.72	0.43
1:A:169:ASN:HD21	1:A:299:ASN:HD21	1.66	0.42
1:A:234:ASP:HA	1:B:234:ASP:HA	2.01	0.42
1:B:250:GLN:NE2	3:B:503:GOL:H31	2.34	0.42
1:B:368:ASN:O	1:B:371:GLN:NE2	2.52	0.42
1:A:438[B]:GLN:CG	5:A:604:HOH:O	2.62	0.42
4:A:510:IMD:H4	5:A:857:HOH:O	2.20	0.42
1:B:73:GLU:O	1:B:468:GLN:NE2	2.53	0.41
1:B:6:LEU:HD22	1:B:6:LEU:N	2.36	0.41
1:A:77:LYS:HE3	5:A:661:HOH:O	2.20	0.41
1:B:465:TYR:O	1:B:468:GLN:HB3	2.21	0.41
1:B:24:VAL:HG22	1:B:60:HIS:HB2	2.02	0.41
1:B:395:ASP:OD1	1:B:395:ASP:N	2.53	0.41
1:B:167:THR:OG1	1:B:205:ASN:ND2	2.54	0.41
1:B:166:VAL:HA	1:B:222:GLY:O	2.21	0.41
1:B:395:ASP:OD2	1:B:463:SER:OG	2.29	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	475/485 (98%)	457 (96%)	18 (4%)	0	100	100
1	B	472/485 (97%)	452 (96%)	18 (4%)	2 (0%)	34	24
All	All	947/970 (98%)	909 (96%)	36 (4%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	415	ASP
1	B	167	THR

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	404/412 (98%)	400 (99%)	4 (1%)	76	71
1	B	401/412 (97%)	390 (97%)	11 (3%)	44	31
All	All	805/824 (98%)	790 (98%)	15 (2%)	57	45

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	24	VAL
1	A	189	LYS
1	A	430	LEU

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Mol	Chain	Res	Type
1	B	77	LYS
1	B	93	ASN
1	B	96	VAL
1	B	160	ASP
1	B	191	MET
1	B	192	LYS
1	B	243	PHE
1	B	331	SER
1	B	430	LEU
1	B	451	GLU
1	B	472	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	171	GLN
1	A	198	ASN
1	A	202	ASN
1	A	205	ASN
1	A	250	GLN
1	A	251	ASN
1	A	252	HIS
1	A	308	HIS
1	A	349	ASN
1	A	379	ASN
1	B	93	ASN
1	B	129	GLN
1	B	171	GLN
1	B	198	ASN
1	B	202	ASN
1	B	205	ASN
1	B	250	GLN
1	B	251	ASN
1	B	252	HIS
1	B	269	ASN
1	B	274	GLN
1	B	308	HIS
1	B	379	ASN
1	B	394	ASN
1	B	474	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	$\# Z > 2$
3	GOL	B	506	-	5,5,5	0.68	0	5,5,5	0.67	0
2	BGP	B	501	-	16,16,16	0.95	1 (6%)	24,24,24	2.93	8 (33%)
3	GOL	B	505	-	5,5,5	0.45	0	5,5,5	0.99	0
3	GOL	A	505	-	5,5,5	1.09	0	5,5,5	0.54	0
3	GOL	A	508	-	5,5,5	0.52	0	5,5,5	0.88	0
3	GOL	B	502	-	5,5,5	0.19	0	5,5,5	0.58	0
3	GOL	A	506	-	5,5,5	0.59	0	5,5,5	0.71	0
4	IMD	A	509	-	3,5,5	0.28	0	4,5,5	0.63	0
3	GOL	B	504	-	5,5,5	0.53	0	5,5,5	0.65	0
2	BGP	A	501	-	16,16,16	1.04	1 (6%)	24,24,24	2.00	6 (25%)
3	GOL	A	504	-	5,5,5	0.85	0	5,5,5	0.38	0
4	IMD	A	510	-	3,5,5	0.22	0	4,5,5	0.49	0
4	IMD	A	511	-	3,5,5	0.25	0	4,5,5	0.58	0
3	GOL	B	503	-	5,5,5	0.60	0	5,5,5	0.91	0
3	GOL	A	507	-	5,5,5	0.61	0	5,5,5	1.02	0
3	GOL	A	502	-	5,5,5	0.28	0	5,5,5	0.47	0
4	IMD	B	507	-	3,5,5	0.27	0	4,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.66	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	506	-	-	0/4/4/4	-
2	BGP	B	501	-	-	2/6/26/26	0/1/1/1
4	IMD	A	511	-	-	-	0/1/1/1
3	GOL	B	505	-	-	4/4/4/4	-
3	GOL	A	505	-	-	1/4/4/4	-
3	GOL	A	508	-	-	2/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	A	506	-	-	4/4/4/4	-
4	IMD	A	509	-	-	-	0/1/1/1
3	GOL	B	504	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
4	IMD	A	510	-	-	-	0/1/1/1
2	BGP	A	501	-	-	2/6/26/26	0/1/1/1
3	GOL	B	503	-	-	4/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
4	IMD	B	507	-	-	-	0/1/1/1
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	BGP	P-O1P	2.77	1.59	1.50
2	B	501	BGP	P-O1P	2.14	1.57	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	BGP	C1-O5-C5	-8.80	97.06	113.66
2	A	501	BGP	O1-C1-O5	-6.90	89.66	110.38
2	B	501	BGP	O5-C1-C2	-5.19	101.02	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	BGP	O6-P-O1P	4.65	119.51	106.47
2	B	501	BGP	O5-C5-C6	4.03	114.81	106.67
2	B	501	BGP	O2P-P-O6	-3.71	96.85	106.73
2	B	501	BGP	O6-C6-C5	-3.18	98.06	108.99
2	B	501	BGP	O5-C5-C4	-3.01	104.22	109.69
2	B	501	BGP	O4-C4-C3	-2.58	104.38	110.35
2	A	501	BGP	C1-O5-C5	-2.41	109.11	113.66
2	A	501	BGP	O3P-P-O6	2.38	113.06	106.73
2	A	501	BGP	O5-C5-C4	-2.37	105.39	109.69
2	A	501	BGP	O4-C4-C5	2.37	115.17	109.30
2	A	501	BGP	O5-C1-C2	-2.03	106.66	110.28

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	BGP	C4-C5-C6-O6
2	B	501	BGP	O5-C5-C6-O6
3	B	505	GOL	C1-C2-C3-O3
3	A	508	GOL	C1-C2-C3-O3
3	A	508	GOL	O2-C2-C3-O3
3	B	502	GOL	C1-C2-C3-O3
3	B	504	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-C3
2	A	501	BGP	C4-C5-C6-O6
2	A	501	BGP	O5-C5-C6-O6
3	B	503	GOL	O1-C1-C2-C3
3	A	507	GOL	O1-C1-C2-C3
3	A	504	GOL	C1-C2-C3-O3
3	A	503	GOL	C1-C2-C3-O3
3	A	506	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-O2
3	B	505	GOL	O1-C1-C2-C3
3	A	505	GOL	O1-C1-C2-C3
3	A	506	GOL	O1-C1-C2-C3
3	A	506	GOL	C1-C2-C3-O3
3	B	503	GOL	C1-C2-C3-O3
3	B	505	GOL	O2-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3

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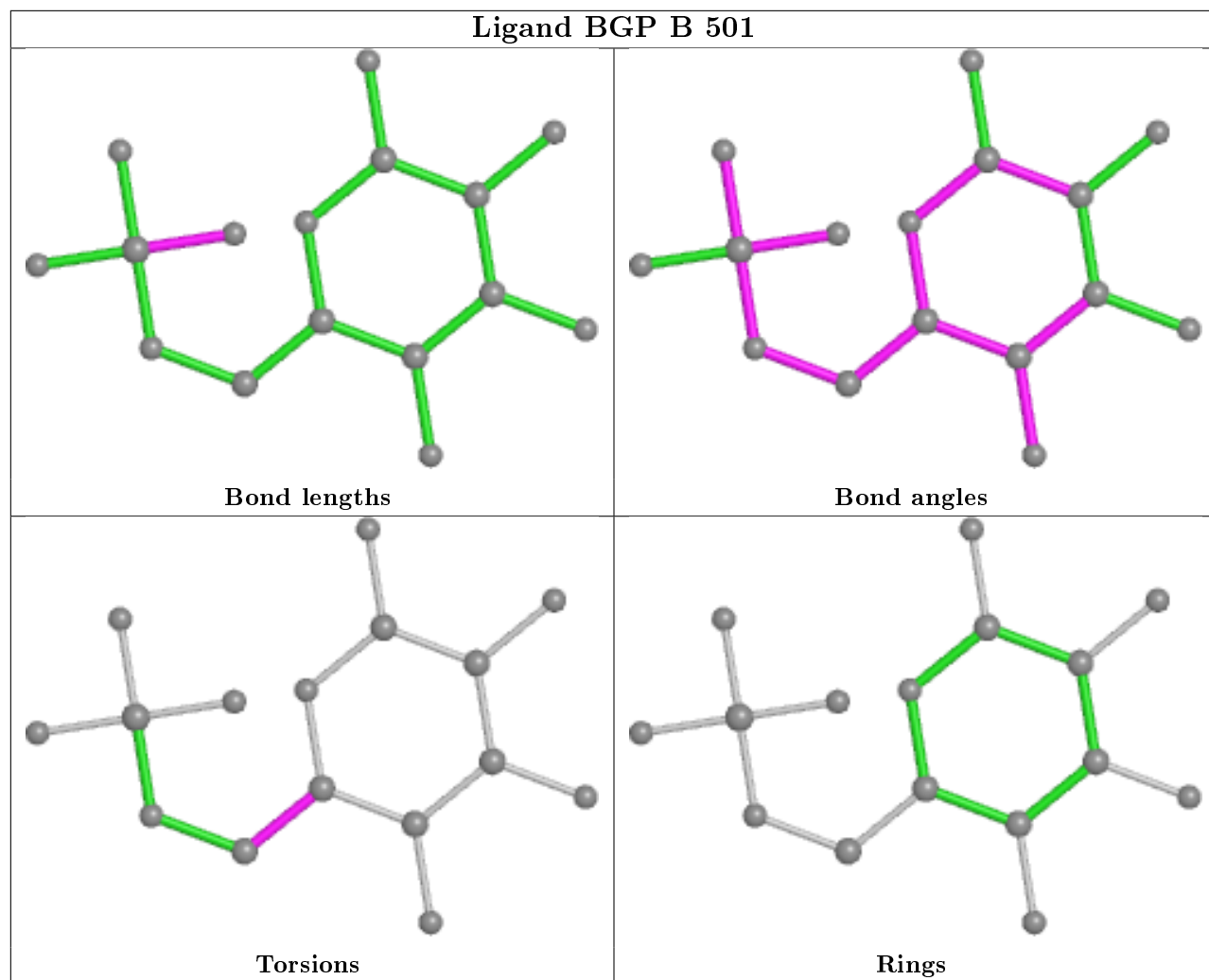
Mol	Chain	Res	Type	Atoms
3	A	507	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-O2
3	B	502	GOL	O2-C2-C3-O3
3	B	505	GOL	O1-C1-C2-O2

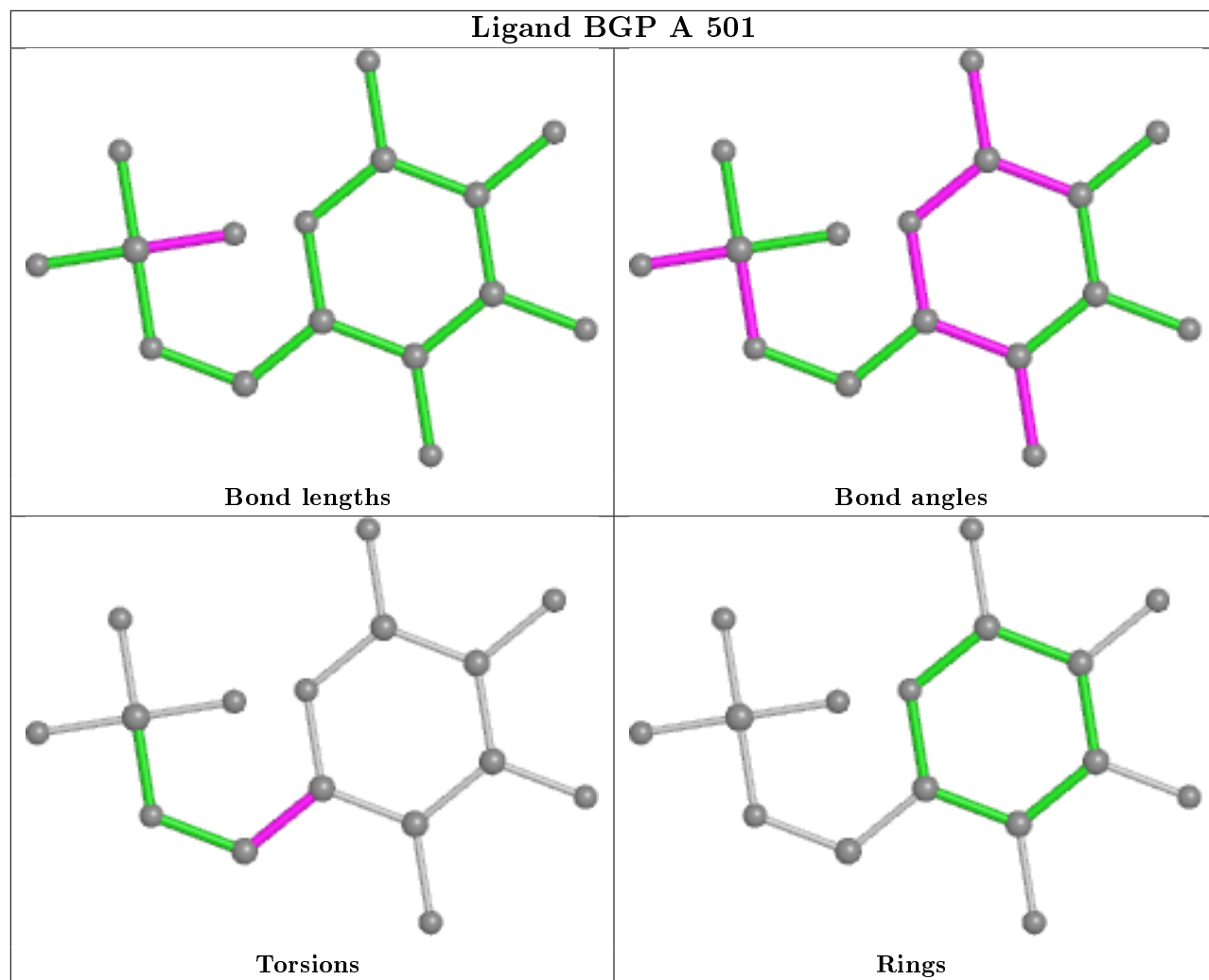
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	BGP	2	0
2	A	501	BGP	2	0
4	A	510	IMD	2	0
3	B	503	GOL	1	0
3	A	507	GOL	1	0
3	A	503	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 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, 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	474/485 (97%)	-0.10	11 (2%) 60 67	21, 30, 47, 92	0
1	B	474/485 (97%)	0.32	42 (8%) 9 14	27, 43, 63, 91	0
All	All	948/970 (97%)	0.11	53 (5%) 24 31	21, 37, 58, 92	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	HIS	5.9
1	B	5	HIS	5.3
1	B	214	HIS	4.9
1	B	122	LEU	4.7
1	B	312	ASP	4.7
1	B	217	PRO	4.2
1	A	312	ASP	4.0
1	B	282	PRO	4.0
1	A	311	PRO	3.8
1	B	275	GLY	3.6
1	B	311	PRO	3.6
1	B	166	VAL	3.3
1	B	83	VAL	3.3
1	B	45	PRO	3.2
1	B	313	GLY	3.2
1	B	11	PRO	3.1
1	B	160	ASP	3.1
1	A	122	LEU	3.1
1	B	17	ALA	3.1
1	B	120	VAL	3.0
1	B	215	TYR	2.9
1	B	119	ILE	2.8
1	B	218	ASP	2.8
1	B	451	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	12	GLU	2.6
1	B	168	LEU	2.6
1	B	274	GLN	2.6
1	B	392	ILE	2.6
1	A	120	VAL	2.5
1	B	290	ALA	2.5
1	B	147	PHE	2.5
1	B	121	THR	2.4
1	B	113	ASN	2.3
1	B	326	GLY	2.3
1	A	121	THR	2.3
1	B	79	TYR	2.3
1	A	168	LEU	2.3
1	B	465	TYR	2.2
1	B	81	PHE	2.2
1	B	472	GLU	2.2
1	B	201	ALA	2.2
1	B	396	ASP	2.2
1	B	446	VAL	2.2
1	B	167	THR	2.1
1	A	290	ALA	2.1
1	B	318	VAL	2.1
1	B	324	LYS	2.1
1	B	469	ARG	2.1
1	A	218	ASP	2.1
1	B	334	PRO	2.1
1	A	83	VAL	2.1
1	A	444	VAL	2.1
1	B	388	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

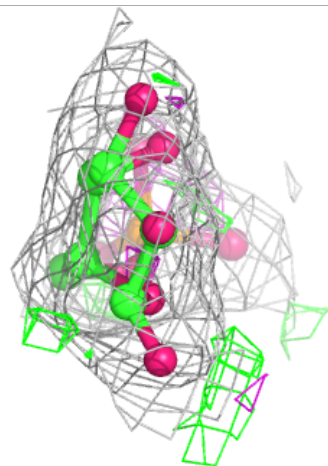
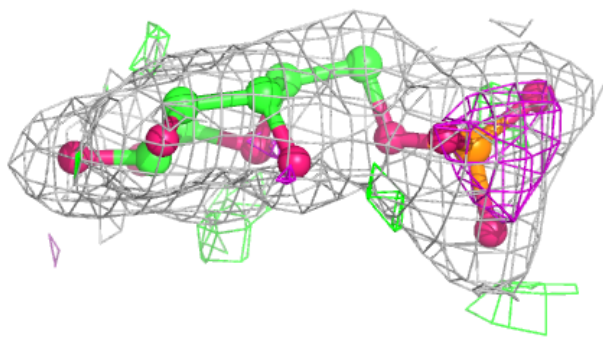
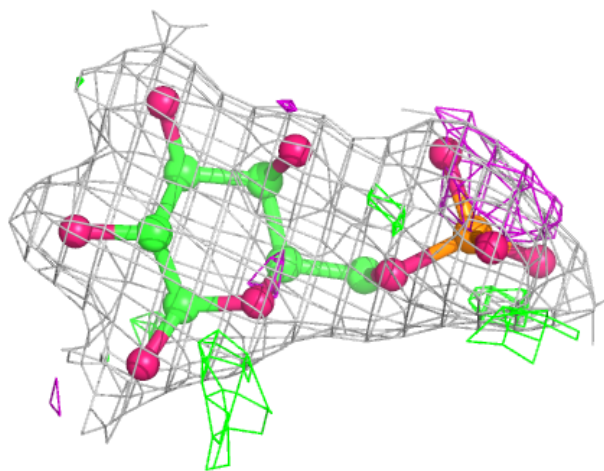
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	506	6/6	0.80	0.17	58,60,63,66	0
3	GOL	B	504	6/6	0.83	0.19	53,57,59,63	0
3	GOL	B	506	6/6	0.84	0.18	58,60,70,72	0
3	GOL	A	502	6/6	0.84	0.19	50,61,62,72	0
4	IMD	A	511	5/5	0.87	0.19	53,58,65,66	0
3	GOL	A	507	6/6	0.87	0.17	39,51,64,66	0
3	GOL	A	505	6/6	0.88	0.14	25,35,37,39	0
4	IMD	B	507	5/5	0.88	0.13	64,69,71,72	0
4	IMD	A	510	5/5	0.89	0.20	58,65,66,68	0
3	GOL	B	503	6/6	0.89	0.14	35,52,59,61	0
3	GOL	B	505	6/6	0.90	0.11	45,51,54,60	0
4	IMD	A	509	5/5	0.93	0.10	55,57,68,70	0
3	GOL	A	504	6/6	0.93	0.11	31,57,58,59	0
3	GOL	A	508	6/6	0.94	0.10	26,49,52,53	0
3	GOL	B	502	6/6	0.95	0.16	54,61,64,72	0
2	BGP	B	501	16/16	0.95	0.09	31,34,36,50	0
3	GOL	A	503	6/6	0.96	0.14	60,63,65,65	0
2	BGP	A	501	16/16	0.98	0.08	25,29,36,53	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.

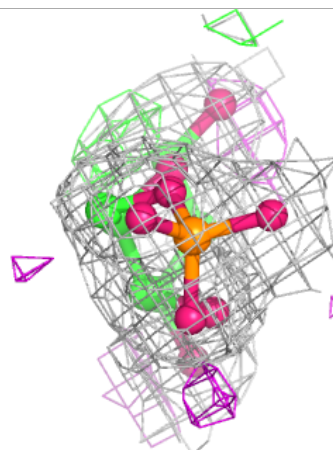
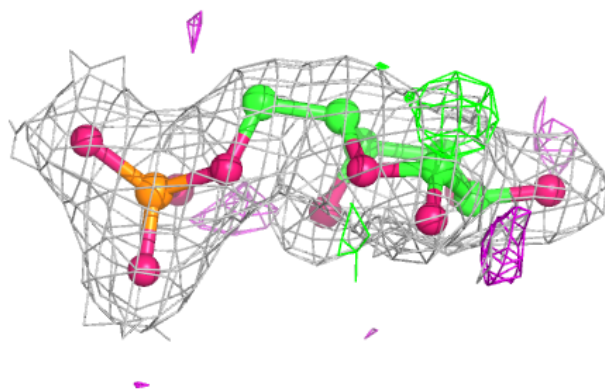
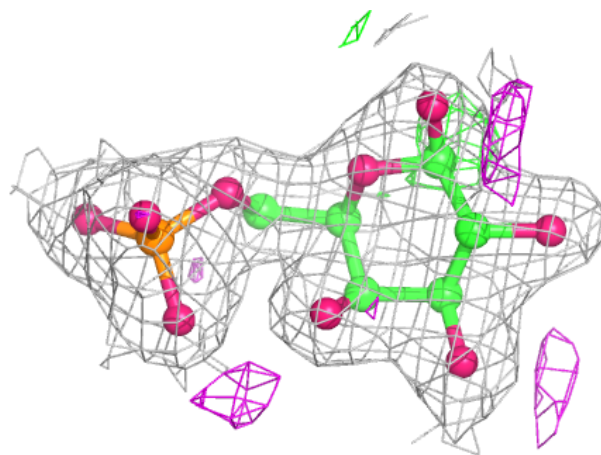
Electron density around BGP B 501:

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



Electron density around BGP A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.