



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:43 AM EDT

PDB ID : 7OJ1 / pdb_00007oj1
Title : Bacillus subtilis IMPDH in complex with Ap4A
Authors : Giammarinaro, P.I.; Bange, G.
Deposited on : 2021-05-13
Resolution : 2.44 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

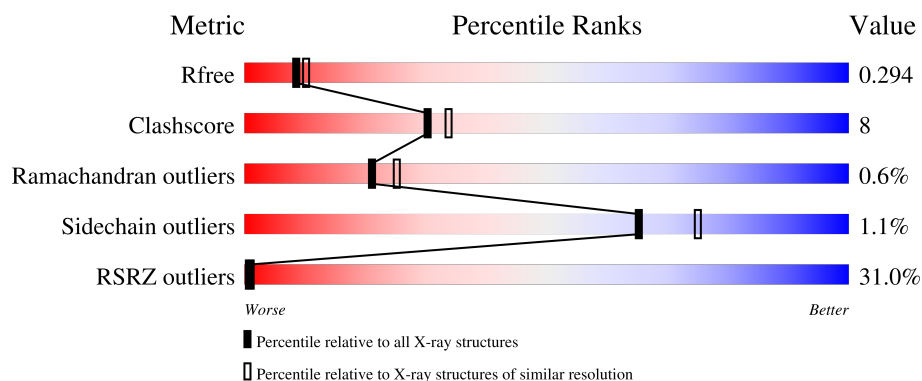
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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 of 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	401	33% 83% 16%
2	B	425	29% 81% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6255 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.

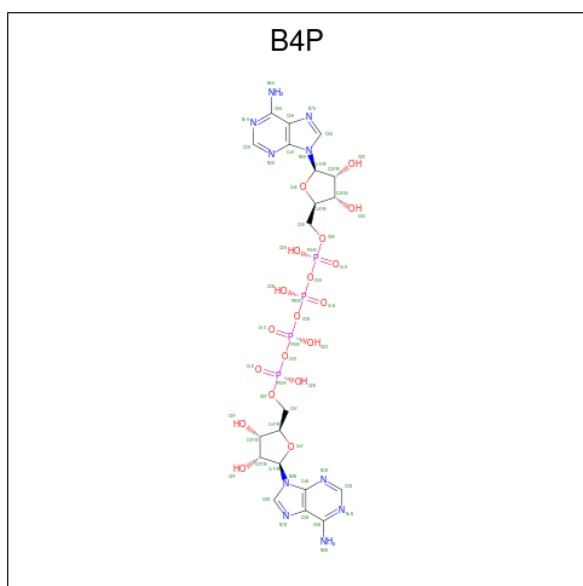
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	2963	1863	515	571	14	0	0	0

- Molecule 2 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3149	1978	544	613	14	0	0	0

- Molecule 3 is BIS(ADENOSINE)-5'-TETRAPHOSPHATE (CCD ID: B4P) (formula: $C_{20}H_{28}N_{10}O_{19}P_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	20	10	19	4	0	0
3	B	1	53	20	10	19	4	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

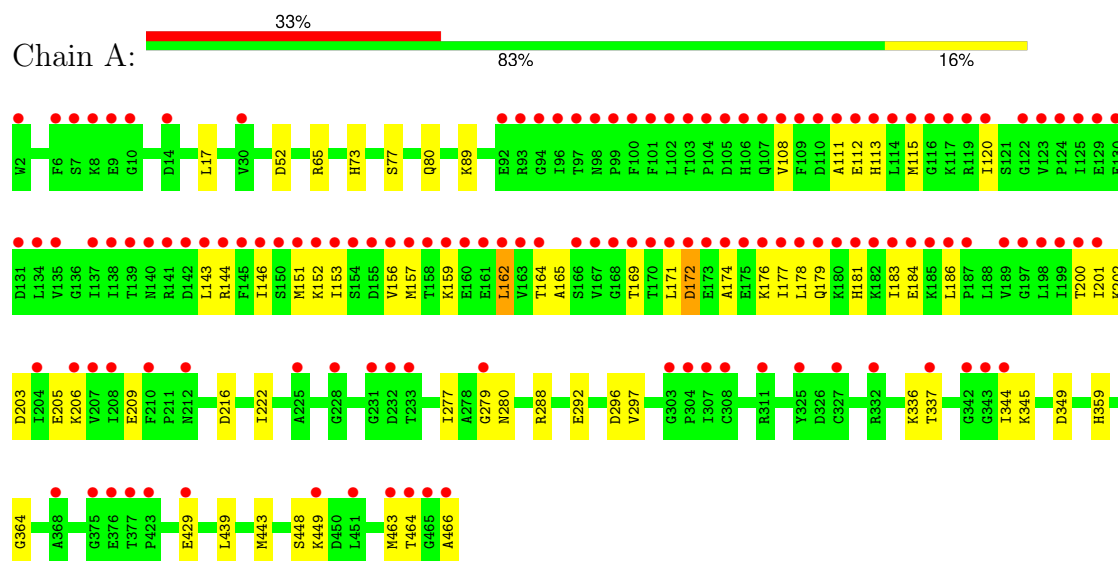
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	15	Total 15	O 15	0	0

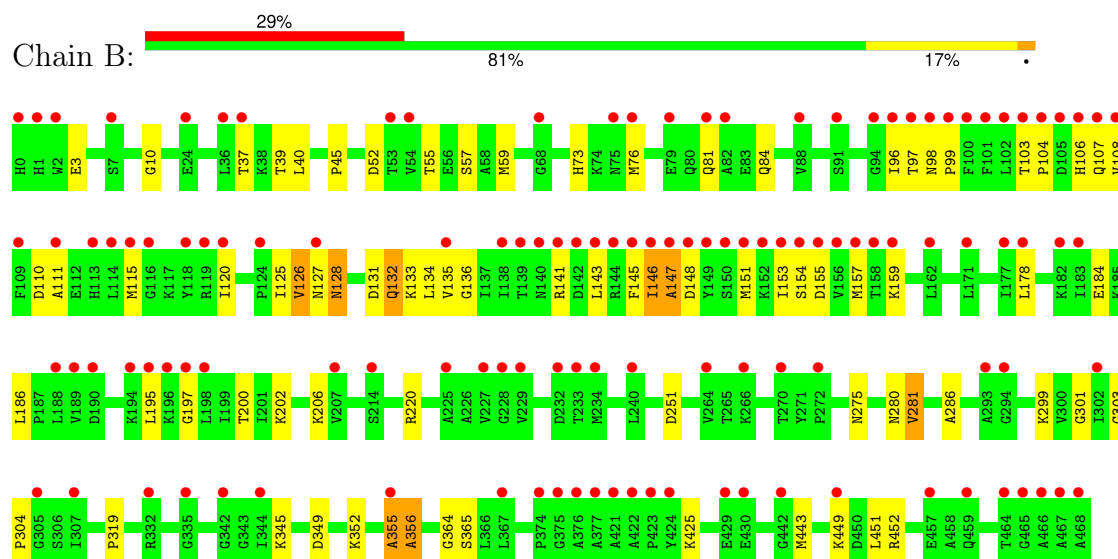
3 Residue-property plots [i](#)

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

- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 2: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	133.75Å 133.75Å 149.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.88 – 2.44 66.88 – 2.44	Depositor EDS
% Data completeness (in resolution range)	92.9 (66.88-2.44) 85.7 (66.88-2.44)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.268 , 0.287 0.273 , 0.294	Depositor DCC
R_{free} test set	2531 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6255	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: MG, B4P

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	0.34	0/2989	0.65	4/4029 (0.1%)
2	B	0.47	1/3185 (0.0%)	0.73	4/4305 (0.1%)
All	All	0.41	1/6174 (0.0%)	0.69	8/8334 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	355	ALA	C-O	-6.57	1.15	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	355	ALA	N-CA-C	-6.88	100.10	110.28
1	A	279	GLY	N-CA-C	6.33	119.29	112.33
1	A	177	ILE	N-CA-C	-5.86	104.64	110.62
1	A	280	ASN	CB-CA-C	5.61	117.51	109.71
2	B	147	ALA	N-CA-C	-5.51	103.26	110.53
2	B	355	ALA	CA-C-O	-5.37	115.14	121.16
2	B	141	ARG	N-CA-C	-5.21	105.72	111.71
1	A	172	ASP	N-CA-C	-5.15	105.66	111.28

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	2963	0	3051	42	4
2	B	3149	0	3232	62	4
3	A	53	0	24	4	0
3	B	53	0	24	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	0	2	0
5	B	15	0	0	2	0
All	All	6255	0	6331	105	4

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 8.

All (105) 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)
2:B:157:MET:SD	2:B:159:LYS:CE	2.39	1.11
2:B:157:MET:SD	2:B:159:LYS:HE3	1.95	1.05
2:B:157:MET:SD	2:B:159:LYS:HE2	2.02	0.96
1:A:203:ASP:HA	1:A:206:LYS:HE2	1.54	0.90
1:A:162:LEU:HD22	1:A:164:THR:HG23	1.65	0.79
2:B:220:ARG:HD3	5:B:606:HOH:O	1.83	0.78
2:B:281:VAL:HG13	2:B:286:ALA:HB3	1.67	0.76
2:B:157:MET:CG	2:B:159:LYS:HE3	2.16	0.75
2:B:443:MET:HE1	2:B:451:LEU:HD12	1.70	0.74
1:A:17:LEU:HD12	1:A:463:MET:SD	2.29	0.72
1:A:174:ALA:C	1:A:176:LYS:H	1.97	0.70
1:A:17:LEU:CD1	1:A:463:MET:SD	2.81	0.69
2:B:352:LYS:O	2:B:355:ALA:O	2.13	0.67
1:A:174:ALA:C	1:A:176:LYS:N	2.46	0.67
2:B:76:MET:HE3	2:B:81:GLN:HA	1.77	0.66
2:B:104:PRO:HB3	2:B:154:SER:HB3	1.79	0.65
1:A:165:ALA:HB1	1:A:169:THR:HG21	1.78	0.65
2:B:355:ALA:O	2:B:356:ALA:CB	2.45	0.65
2:B:154:SER:HA	2:B:157:MET:HE3	1.79	0.64
1:A:162:LEU:HD23	3:A:501:B4P:H62B	1.62	0.63
1:A:439:LEU:O	1:A:443:MET:HG3	1.99	0.63
2:B:120:ILE:HG23	3:B:501:B4P:C8A	2.29	0.63
2:B:125:ILE:CD1	2:B:157:MET:HE2	2.29	0.63
1:A:277:ILE:HG12	1:A:297:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ALA:O	2:B:356:ALA:HB3	2.00	0.61
1:A:464:THR:HG1	1:A:466:ALA:N	1.98	0.61
2:B:96:ILE:CG2	2:B:98:ASN:O	2.48	0.61
2:B:200:THR:HG21	3:B:501:B4P:H2E	1.83	0.60
2:B:202:LYS:O	2:B:206:LYS:HG2	2.01	0.60
3:B:501:B4P:H8A	3:B:501:B4P:H52A	1.82	0.59
2:B:76:MET:HE1	2:B:84:GLN:HG3	1.85	0.59
2:B:37:THR:HG22	2:B:40:LEU:HB3	1.85	0.58
1:A:111:ALA:O	1:A:115:MET:HG3	2.03	0.58
1:A:152:LYS:HG2	1:A:153:ILE:HG12	1.87	0.57
2:B:125:ILE:HD13	2:B:157:MET:HE2	1.86	0.57
1:A:443:MET:HB3	1:A:448:SER:HB2	1.88	0.56
2:B:281:VAL:CG1	2:B:286:ALA:HB3	2.35	0.56
1:A:345:LYS:HG2	1:A:349:ASP:OD2	2.05	0.56
1:A:171:LEU:O	1:A:174:ALA:HB3	2.06	0.55
1:A:89:LYS:NZ	1:A:216:ASP:OD2	2.40	0.55
2:B:45:PRO:HG3	2:B:451:LEU:HD21	1.88	0.54
2:B:126:VAL:HG11	2:B:132:GLN:HA	1.88	0.54
1:A:200:THR:HG21	3:A:501:B4P:H2E	1.89	0.54
1:A:172:ASP:C	1:A:174:ALA:H	2.16	0.54
2:B:143:LEU:O	2:B:146:ILE:HG13	2.07	0.54
2:B:365:SER:O	2:B:425:LYS:NZ	2.42	0.52
1:A:205:GLU:O	1:A:209:GLU:HG3	2.09	0.52
2:B:155:ASP:O	2:B:155:ASP:OD1	2.27	0.52
2:B:126:VAL:CG1	2:B:132:GLN:HA	2.39	0.52
1:A:77:SER:OG	1:A:80:GLN:HG3	2.10	0.51
2:B:131:ASP:O	2:B:133:LYS:N	2.44	0.49
2:B:303:GLY:N	2:B:304:PRO:HD3	2.27	0.49
1:A:184:GLU:HB3	1:A:201:ILE:HG22	1.94	0.49
1:A:162:LEU:HD23	3:A:501:B4P:N6B	2.28	0.48
2:B:39:THR:OG1	2:B:275:ASN:ND2	2.39	0.48
2:B:154:SER:HB2	2:B:159:LYS:NZ	2.28	0.48
2:B:108:VAL:HG23	2:B:151:MET:O	2.13	0.48
2:B:147:ALA:O	2:B:148:ASP:C	2.56	0.48
2:B:443:MET:CE	2:B:451:LEU:HD12	2.42	0.48
2:B:134:LEU:HD13	2:B:195:LEU:HD13	1.94	0.48
2:B:345:LYS:HG2	2:B:349:ASP:OD2	2.14	0.48
1:A:449:LYS:HD3	1:A:449:LYS:H	1.79	0.48
2:B:125:ILE:HD12	2:B:157:MET:HE2	1.94	0.47
1:A:172:ASP:C	1:A:174:ALA:N	2.71	0.47
2:B:127:ASN:OD1	2:B:128:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:O	5:A:601:HOH:O	2.20	0.47
2:B:107:GLN:N	2:B:110:ASP:OD2	2.42	0.47
2:B:449:LYS:NZ	2:B:452:ARG:HH22	2.12	0.47
1:A:181:HIS:O	1:A:183:ILE:HG23	2.15	0.47
1:A:120:ILE:HB	3:A:501:B4P:C8A	2.46	0.46
2:B:37:THR:HG23	2:B:39:THR:H	1.79	0.46
1:A:112:GLU:HG3	1:A:113:HIS:N	2.30	0.46
1:A:178:LEU:HD21	1:A:186:LEU:HB2	1.98	0.46
1:A:162:LEU:HD22	1:A:164:THR:CG2	2.41	0.46
2:B:10:GLY:HA3	2:B:319:PRO:HG2	1.97	0.46
1:A:108:VAL:HB	1:A:151:MET:O	2.16	0.46
2:B:178:LEU:HD21	2:B:186:LEU:HB2	1.98	0.46
2:B:103:THR:O	2:B:153:ILE:HD11	2.16	0.45
2:B:97:THR:O	2:B:99:PRO:HD3	2.17	0.45
1:A:288:ARG:NE	1:A:292:GLU:OE2	2.49	0.45
2:B:52:ASP:HA	2:B:73:HIS:CD2	2.51	0.45
2:B:136:GLY:HA3	2:B:157:MET:SD	2.56	0.45
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.52	0.44
1:A:337:THR:HG23	1:A:359:HIS:HB2	1.99	0.44
1:A:202:LYS:HA	1:A:205:GLU:HG2	1.99	0.44
1:A:344:ILE:HG23	1:A:349:ASP:HB2	1.98	0.44
2:B:57:SER:N	2:B:84:GLN:OE1	2.51	0.44
2:B:96:ILE:HG22	2:B:98:ASN:O	2.16	0.44
1:A:143:LEU:O	1:A:146:ILE:HG22	2.18	0.44
2:B:127:ASN:ND2	2:B:133:LYS:HB2	2.33	0.44
1:A:65:ARG:NH2	1:A:206:LYS:HD2	2.33	0.44
2:B:127:ASN:CG	2:B:133:LYS:HB2	2.44	0.43
2:B:96:ILE:HG22	2:B:98:ASN:C	2.43	0.43
2:B:55:THR:HA	2:B:59:MET:HB3	2.01	0.43
2:B:251:ASP:OD2	5:B:601:HOH:O	2.21	0.43
2:B:111:ALA:O	2:B:115:MET:HG3	2.19	0.42
1:A:157:MET:HE2	1:A:159:LYS:HD2	2.02	0.42
1:A:429:GLU:OE1	5:A:602:HOH:O	2.22	0.42
2:B:125:ILE:O	2:B:135:VAL:HG12	2.20	0.42
1:A:296:ASP:O	1:A:336:LYS:HD2	2.20	0.41
2:B:280:ASN:OD1	2:B:299:LYS:HE3	2.21	0.41
2:B:99:PRO:HG3	2:B:197:GLY:HA2	2.01	0.41
2:B:37:THR:HG21	2:B:275:ASN:OD1	2.21	0.41
2:B:106:HIS:HB3	2:B:110:ASP:OD2	2.21	0.41
2:B:120:ILE:HG23	3:B:501:B4P:N7A	2.35	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLN:OE1	2:B:145:PHE:O[6_544]	1.14	1.06
1:A:144:ARG:NH1	2:B:184:GLU:OE2[6_544]	2.06	0.14
1:A:179:GLN:OE1	2:B:145:PHE:C[6_544]	2.08	0.12
1:A:179:GLN:CD	2:B:145:PHE:O[6_544]	2.10	0.10

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	382/401 (95%)	361 (94%)	20 (5%)	1 (0%)	36	44
2	B	419/425 (99%)	400 (96%)	15 (4%)	4 (1%)	12	13
All	All	801/826 (97%)	761 (95%)	35 (4%)	5 (1%)	21	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	132	GLN
2	B	356	ALA
1	A	364	GLY
2	B	301	GLY
2	B	364	GLY

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	318/328 (97%)	316 (99%)	2 (1%)	78	85
2	B	337/344 (98%)	332 (98%)	5 (2%)	57	69
All	All	655/672 (98%)	648 (99%)	7 (1%)	65	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	VAL
1	A	162	LEU
2	B	3	GLU
2	B	126	VAL
2	B	128	ASN
2	B	146	ILE
2	B	281	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	258	GLN
2	B	140	ASN
2	B	181	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B4P	B	501	4	58,58,58	0.48	0	84,91,91	0.67	0
3	B4P	A	501	4	58,58,58	0.52	0	84,91,91	0.56	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	B4P	B	501	4	-	8/38/70/70	0/6/6/6
3	B4P	A	501	4	-	14/38/70/70	0/6/6/6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	B4P	C5E-O5E-PA-O1A
3	A	501	B4P	C5E-O5E-PA-O3A
3	B	501	B4P	C5E-O5E-PA-O2A
3	B	501	B4P	C5E-O5E-PA-O3A
3	B	501	B4P	C3E-C4E-C5E-O5E
3	A	501	B4P	O4E-C4E-C5E-O5E
3	A	501	B4P	C3E-C4E-C5E-O5E
3	B	501	B4P	O4E-C4E-C5E-O5E
3	B	501	B4P	O4F-C4F-C5F-O5F
3	A	501	B4P	C3F-C4F-C5F-O5F
3	B	501	B4P	C4E-C5E-O5E-PA
3	A	501	B4P	O4F-C4F-C5F-O5F
3	A	501	B4P	PG-O3B-PB-O1B
3	B	501	B4P	C4F-C5F-O5F-PD
3	B	501	B4P	C3F-C4F-C5F-O5F

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Mol	Chain	Res	Type	Atoms
3	A	501	B4P	C5E-O5E-PA-O2A
3	A	501	B4P	PB-O3A-PA-O1A
3	A	501	B4P	PB-O3A-PA-O2A
3	A	501	B4P	PG-O3B-PB-O2B
3	A	501	B4P	PG-O3G-PD-O2D
3	A	501	B4P	PG-O3G-PD-O1D
3	A	501	B4P	C4E-C5E-O5E-PA

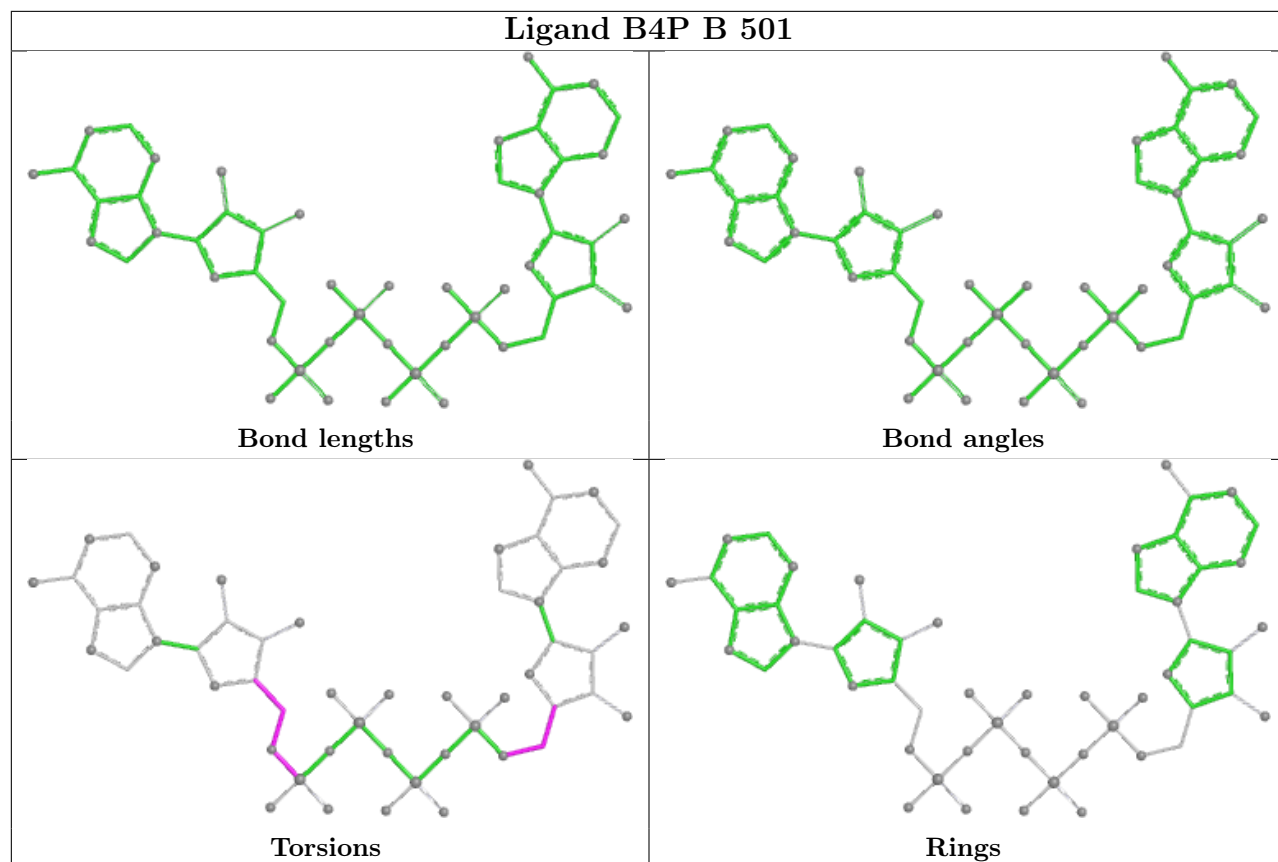
There are no ring outliers.

2 monomers are involved in 8 short contacts:

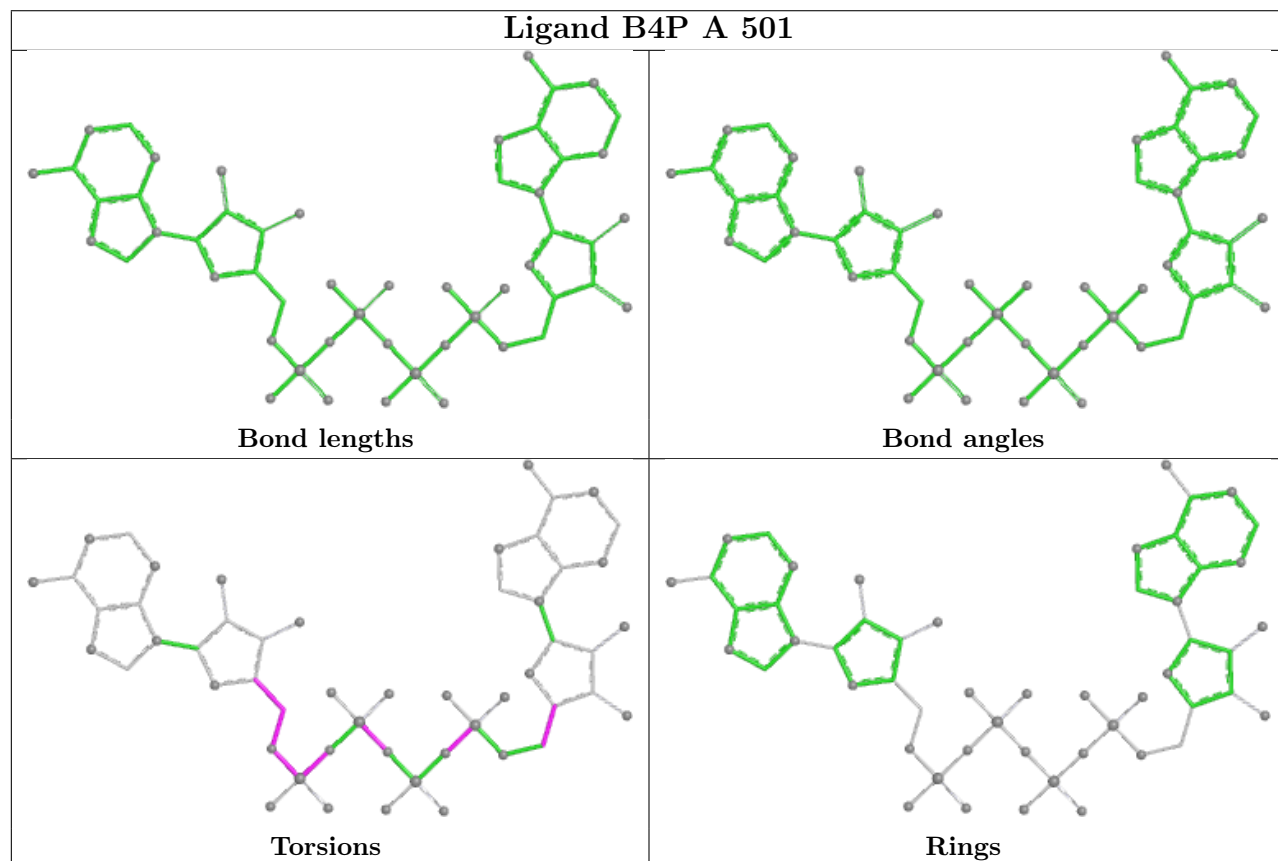
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	B4P	4	0
3	A	501	B4P	4	0

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.

Ligand B4P B 501



Ligand B4P A 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	9
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	377:THR	C	423:PRO	N	7.94
1	A	125:ILE	C	129:GLU	N	7.49
1	A	131:ASP	C	134:LEU	N	6.67
1	A	304:PRO	C	307:ILE	N	6.34
1	A	189:VAL	C	197:GLY	N	6.10
1	A	146:ILE	C	150:SER	N	5.39
1	A	94:GLY	C	96:ILE	N	4.48
1	B	377:ALA	C	421:ALA	N	4.44
1	B	94:GLY	C	96:ILE	N	3.99
1	A	117:LYS	C	119:ARG	N	3.41
1	A	465:GLY	C	466:ALA	N	3.00

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	401/401 (100%)	1.61	133 (33%) ⓘ ⓘ	30, 55, 137, 153	0
2	B	425/425 (100%)	1.54	123 (28%) ⓘ ⓘ	33, 61, 126, 145	0
All	All	826/826 (100%)	1.58	256 (30%) ⓘ ⓘ	30, 59, 134, 153	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	LEU	8.3
2	B	96	ILE	7.8
2	B	377	ALA	7.8
1	A	129	GLU	6.6
1	A	114	LEU	6.5
1	A	177	ILE	6.4
2	B	468	ALA	6.3
1	A	96	ILE	6.2
1	A	189	VAL	6.2
1	A	131	ASP	6.2
2	B	148	ASP	6.1
1	A	279	GLY	5.9
1	A	101	PHE	5.7
1	A	97	THR	5.7
1	A	94	GLY	5.6
2	B	149	TYR	5.5
1	A	466	ALA	5.5
1	A	146	ILE	5.4
1	A	2	TRP	5.4
1	A	174	ALA	5.2
1	A	161	GLU	5.2
1	A	100	PHE	5.0
2	B	147	ALA	4.9
2	B	151	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	156	VAL	4.9
1	A	105	ASP	4.7
1	A	377	THR	4.7
1	A	178	LEU	4.7
1	A	176	LYS	4.6
2	B	376	ALA	4.5
1	A	108	VAL	4.5
1	A	140	ASN	4.5
2	B	94	GLY	4.4
2	B	159	LYS	4.4
1	A	343	GLY	4.4
2	B	2	TRP	4.4
1	A	327	CYS	4.4
1	A	159	LYS	4.3
1	A	117	LYS	4.3
2	B	119	ARG	4.3
1	A	332	ARG	4.2
1	A	465	GLY	4.2
1	A	167	VAL	4.2
2	B	227	VAL	4.2
1	A	7	SER	4.2
1	A	150	SER	4.1
1	A	207	VAL	4.1
1	A	171	LEU	4.1
1	A	138	ILE	4.1
1	A	198	LEU	4.1
1	A	113	HIS	4.1
1	A	368	ALA	4.1
2	B	421	ALA	4.1
1	A	208	ILE	4.0
1	A	104	PRO	4.0
2	B	104	PRO	4.0
2	B	138	ILE	3.9
1	A	152	LYS	3.9
1	A	109	PHE	3.9
1	A	120	ILE	3.9
1	A	115	MET	3.8
1	A	197	GLY	3.8
1	A	172	ASP	3.8
1	A	143	LEU	3.8
1	A	124	PRO	3.8
2	B	158	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	175	GLU	3.8
1	A	187	PRO	3.8
2	B	144	ARG	3.7
2	B	82	ALA	3.7
1	A	125	ILE	3.7
1	A	464	THR	3.6
2	B	114	LEU	3.6
1	A	163	VAL	3.6
1	A	204	ILE	3.6
2	B	141	ARG	3.6
2	B	75	ASN	3.6
2	B	1	HIS	3.6
1	A	169	THR	3.6
1	A	102	LEU	3.6
2	B	100	PHE	3.6
2	B	342	GLY	3.5
2	B	307	ILE	3.5
2	B	228	GLY	3.5
2	B	108	VAL	3.5
2	B	101	PHE	3.5
1	A	160	GLU	3.5
1	A	134	LEU	3.5
2	B	105	ASP	3.4
2	B	98	ASN	3.4
2	B	97	THR	3.4
2	B	142	ASP	3.4
2	B	189	VAL	3.4
1	A	183	ILE	3.4
1	A	463	MET	3.3
2	B	109	PHE	3.3
1	A	135	VAL	3.3
1	A	111	ALA	3.3
2	B	467	ALA	3.3
2	B	68	GLY	3.3
2	B	152	LYS	3.3
1	A	116	GLY	3.3
1	A	185	LYS	3.3
1	A	142	ASP	3.2
1	A	122	GLY	3.2
2	B	442	GLY	3.2
2	B	120	ILE	3.2
2	B	466	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	151	MET	3.2
1	A	103	THR	3.2
2	B	103	THR	3.2
1	A	201	ILE	3.2
1	A	106	HIS	3.2
1	A	119	ARG	3.1
1	A	179	GLN	3.1
2	B	183	ILE	3.1
1	A	137	ILE	3.1
2	B	465	GLY	3.1
1	A	145	PHE	3.0
2	B	195	LEU	3.0
2	B	146	ILE	3.0
2	B	207	VAL	3.0
1	A	307	ILE	3.0
1	A	376	GLU	3.0
2	B	293	ALA	3.0
2	B	332	ARG	3.0
1	A	199	ILE	3.0
2	B	464	THR	2.9
1	A	168	GLY	2.9
2	B	140	ASN	2.9
1	A	153	ILE	2.9
1	A	164	THR	2.9
2	B	106	HIS	2.9
2	B	270	THR	2.9
2	B	162	LEU	2.9
1	A	303	GLY	2.9
1	A	337	THR	2.8
2	B	143	LEU	2.8
1	A	210	PHE	2.8
2	B	335	GLY	2.8
2	B	229	VAL	2.8
1	A	170	THR	2.8
1	A	173	GLU	2.8
2	B	156	VAL	2.8
1	A	180	LYS	2.8
1	A	110	ASP	2.8
2	B	0	HIS	2.8
1	A	233	THR	2.8
1	A	181	HIS	2.8
2	B	344	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	158	THR	2.7
2	B	233	THR	2.7
1	A	155	ASP	2.7
1	A	93	ARG	2.7
1	A	141	ARG	2.7
1	A	9	GLU	2.7
1	A	231	GLY	2.7
1	A	449	LYS	2.7
1	A	154	SER	2.7
1	A	423	PRO	2.6
1	A	144	ARG	2.6
2	B	91	SER	2.6
1	A	139	THR	2.6
2	B	272	PRO	2.6
2	B	182	LYS	2.6
2	B	225	ALA	2.6
1	A	166	SER	2.5
2	B	214	SER	2.5
2	B	99	PRO	2.5
1	A	14	ASP	2.5
2	B	305	GLY	2.5
1	A	130	GLU	2.5
1	A	429	GLU	2.5
2	B	79	GLU	2.5
2	B	36	LEU	2.5
2	B	355	ALA	2.5
2	B	422	ALA	2.5
2	B	124	PRO	2.5
2	B	375	GLY	2.5
1	A	10	GLY	2.5
2	B	430	GLU	2.5
2	B	459	GLN	2.5
2	B	88	VAL	2.5
1	A	228	GLY	2.4
1	A	342	GLY	2.4
1	A	6	PHE	2.4
2	B	157	MET	2.4
2	B	234	MET	2.4
1	A	8	LYS	2.4
2	B	196	LYS	2.4
1	A	344	ILE	2.4
2	B	102	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	178	LEU	2.4
2	B	113	HIS	2.4
1	A	30	VAL	2.4
2	B	194	LYS	2.4
2	B	457	GLU	2.4
2	B	424	TYR	2.4
2	B	145	PHE	2.4
1	A	308	CYS	2.4
2	B	37	THR	2.3
2	B	24	GLU	2.3
2	B	139	THR	2.3
1	A	451	LEU	2.3
2	B	155	ASP	2.3
2	B	127	ASN	2.3
2	B	81	GLN	2.3
2	B	76	MET	2.3
1	A	92	GLU	2.3
2	B	197	GLY	2.3
1	A	182	LYS	2.3
2	B	153	ILE	2.2
1	A	98	ASN	2.2
1	A	157	MET	2.2
2	B	54	VAL	2.2
2	B	423	PRO	2.2
2	B	302	ILE	2.2
1	A	232	ASP	2.2
2	B	135	VAL	2.2
1	A	225	ALA	2.2
2	B	111	ALA	2.2
2	B	188	LEU	2.2
2	B	7	SER	2.2
2	B	232	ASP	2.2
2	B	266	LYS	2.2
1	A	200	THR	2.1
2	B	116	GLY	2.1
2	B	118	TYR	2.1
2	B	190	ASP	2.1
1	A	123	VAL	2.1
2	B	115	MET	2.1
1	A	375	GLY	2.1
2	B	198	LEU	2.1
2	B	240	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	154	SER	2.1
1	A	206	LYS	2.1
1	A	304	PRO	2.1
1	A	186	LEU	2.1
2	B	294	GLY	2.1
1	A	311	ARG	2.1
2	B	177	ILE	2.1
1	A	99	PRO	2.1
2	B	374	PRO	2.1
1	A	212	ASN	2.1
1	A	112	GLU	2.1
1	A	107	GLN	2.0
2	B	107	GLN	2.0
2	B	171	LEU	2.0
2	B	367	LEU	2.0
1	A	184	GLU	2.0
2	B	429	GLU	2.0
2	B	53	THR	2.0
2	B	449	LYS	2.0
2	B	264	VAL	2.0
1	A	325	TYR	2.0
2	B	150	SER	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 oligosaccharides 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
4	MG	A	502	1/1	0.38	0.17	30,30,30,30	0

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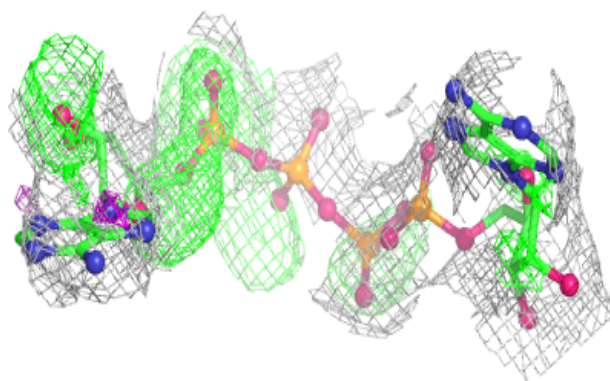
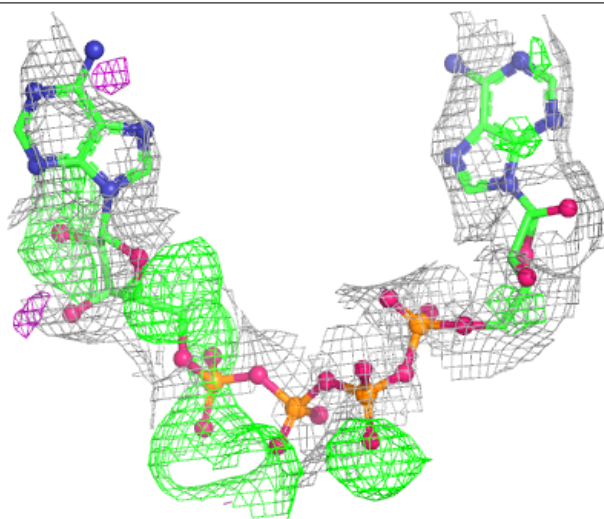
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	B4P	A	501	53/53	0.66	0.24	113,131,149,161	0
3	B4P	B	501	53/53	0.80	0.20	95,110,130,141	0
4	MG	B	502	1/1	0.88	0.07	30,30,30,30	0

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.

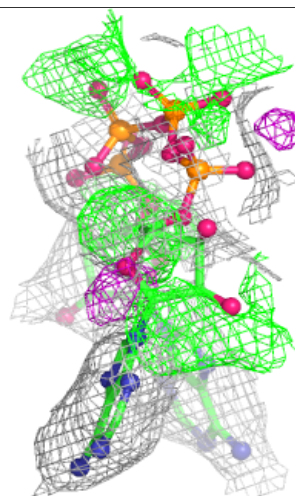
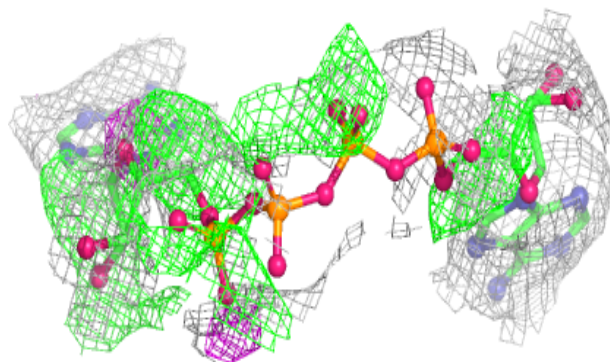
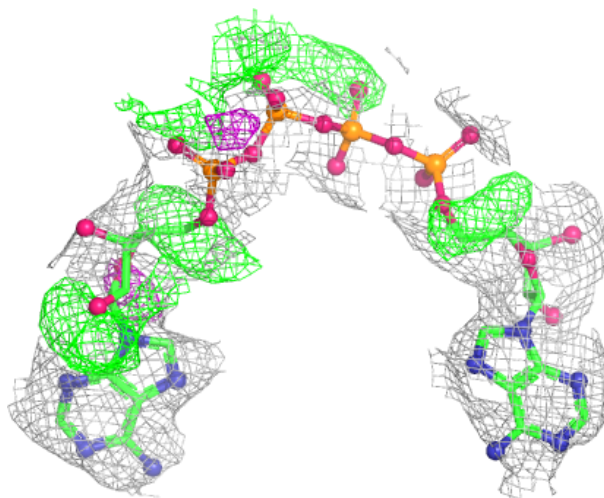
Electron density around B4P A 501:

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



Electron density around B4P 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.