WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 11:49 pm GMT

PDB ID	:	6GH3
Title	:	Paenibacillus sp. YM1 laminaribiose phosphorylase with alpha-man-1-phosphate bound
Authors	:	Kuhaudomlarp, S.; Walpole, S.; Stevenson, C.E.M.; Nepogodiev, S.A.; Lawson, D.M.; Angulo, J.; Field, R.A.
Deposited on	:	2018-05-04
Resolution	:	1.82 Å(reported)

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

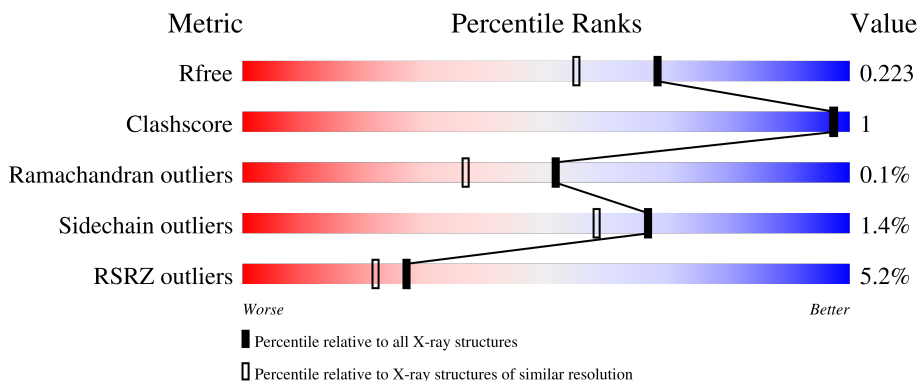|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

Full wwPDB X-ray Structure Validation Report

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 1.82 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		0.223
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		1.4%
RSRZ outliers		5.2%

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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 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 <=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	913	7% / 95%
1	B	913	3% / 95%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 14874 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 Laminaribiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	8	0
			6985	4432	1220	1310	23			
1	B	899	Total	C	N	O	S	0	7	0
			7076	4483	1241	1328	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP D7UT17
A	0	PRO	-	expression tag	UNP D7UT17
B	-1	GLY	-	expression tag	UNP D7UT17
B	0	PRO	-	expression tag	UNP D7UT17

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total O S			0	0
			5 4	1			
2	B	1	Total O S			0	0
			5 4	1			

- Molecule 3 is 1-O-phosphono-alpha-D-mannopyranose (three-letter code: M1P) (formula: $C_6H_{13}O_9P$).
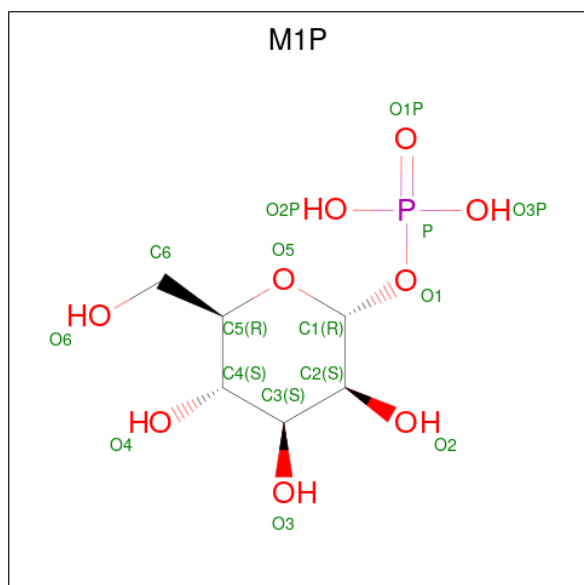
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total C O P				0	0
			16 6 9	1				
3	B	1	Total C O P				0	0
			16 6 9	1				

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 8	C 4	O 4	0	1
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Cl 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Cl 2	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total 252	O 252	0	9
6	B	452	Total 467	O 467	0	15

3 Residue-property plots ⓘ

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: Laminaribiose phosphorylase

Chain A:

• Molecule 1: Laminaribiose phosphorylase

Chain B:
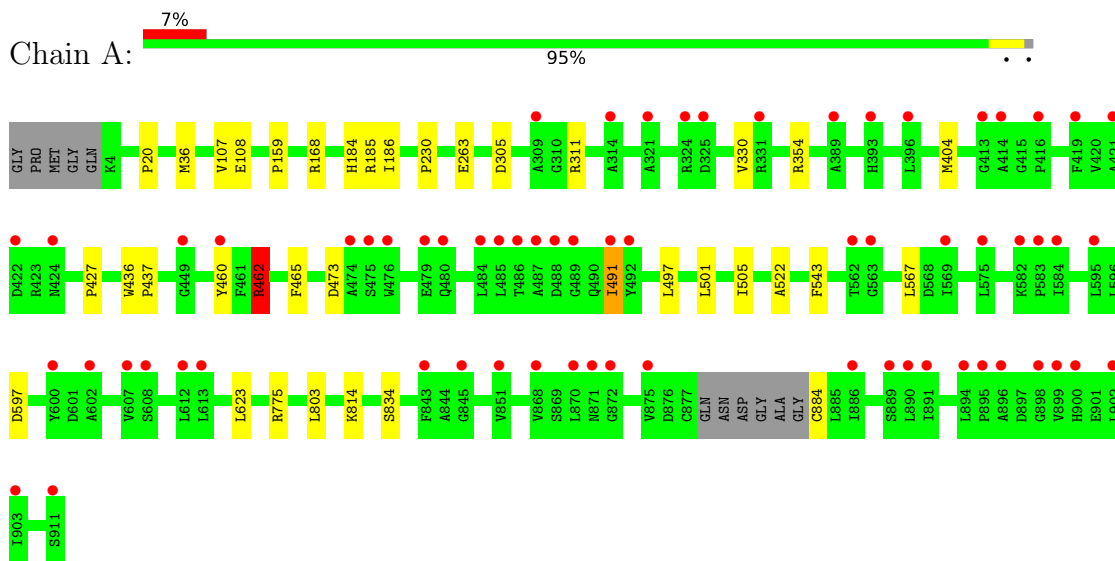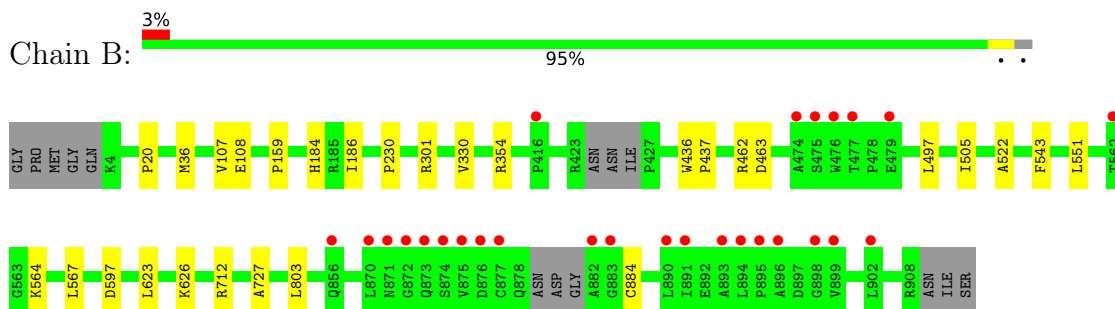
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.57Å 146.57Å 222.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.29 – 1.82 66.11 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (73.29-1.82) 100.0 (66.11-1.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.82Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.218 0.199 , 0.223	Depositor DCC
R_{free} test set	10878 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.3	EDS
L-test for twinning [2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14874	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5818e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, M1P, EDO, SO4

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	0.54	0/7152	0.73	6/9718 (0.1%)
1	B	0.58	0/7240	0.75	4/9812 (0.0%)
All	All	0.56	0/14392	0.74	10/19530 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	354	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	301	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	301	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	354	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	185	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	775	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	712	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	168	ARG	CG-CD-NE	5.12	122.55	111.80
1	A	462	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	354	ARG	NE-CZ-NH2	-5.02	117.79	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	6985	0	6584	13	0
1	B	7076	0	6805	10	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
4	A	24	0	36	0	0
4	B	24	0	36	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	252	0	0	0	0
6	B	467	0	0	0	0
All	All	14874	0	13483	22	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 1.

All (22) 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:404:MET:HE1	1:A:460:TYR:CZ	2.41	0.56
1:B:505[A]:ILE:HG23	1:B:626:LYS:HE2	1.91	0.51
1:A:305:ASP:O	1:A:311[A]:ARG:NE	2.46	0.49
1:A:330:VAL:HG11	1:A:803:LEU:HD11	1.94	0.49
1:B:330:VAL:HG11	1:B:803:LEU:HD11	1.94	0.49
1:A:497:LEU:HD23	1:A:567:LEU:HD22	1.95	0.48
1:B:497:LEU:HD23	1:B:567:LEU:HD22	1.96	0.47
1:A:462:ARG:NH2	1:A:473:ASP:OD2	2.48	0.46
1:A:404:MET:HE1	1:A:460:TYR:CE1	2.50	0.46
1:B:20:PRO:HG3	1:B:107:VAL:HG23	1.98	0.46
1:A:186:ILE:HG21	1:A:230:PRO:HB2	1.99	0.45
1:A:20:PRO:HG3	1:A:107:VAL:HG23	1.98	0.45
1:B:186:ILE:HG21	1:B:230:PRO:HB2	1.99	0.45
1:B:462:ARG:NH1	1:B:463:ASP:O	2.49	0.44
1:A:505:ILE:HD11	1:A:623:LEU:HD21	1.98	0.44
1:B:505[A]:ILE:HD11	1:B:623:LEU:HD21	2.01	0.41
1:A:263[A]:GLU:HG3	1:B:727:ALA:HB1	2.03	0.41
1:B:436:TRP:N	1:B:437:PRO:CD	2.84	0.41
1:A:427:PRO:HD3	1:A:465:PHE:CZ	2.56	0.41
1:A:436:TRP:N	1:A:437:PRO:CD	2.84	0.41
1:A:491:ILE:O	1:A:491:ILE:HG13	2.21	0.41
1:B:551:LEU:HB3	1:B:623:LEU:HD13	2.03	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	906/913 (99%)	884 (98%)	21 (2%)	1 (0%)	51	37
1	B	900/913 (99%)	876 (97%)	23 (3%)	1 (0%)	51	37
All	All	1806/1826 (99%)	1760 (98%)	44 (2%)	2 (0%)	51	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	522	ALA
1	B	522	ALA

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	689/740 (93%)	677 (98%)	12 (2%)	60	50
1	B	719/740 (97%)	711 (99%)	8 (1%)	73	67
All	All	1408/1480 (95%)	1388 (99%)	20 (1%)	67	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	GLU
1	A	159	PRO
1	A	184	HIS
1	A	462	ARG
1	A	491	ILE
1	A	501	LEU
1	A	543	PHE
1	A	597	ASP
1	A	814	LYS
1	A	834	SER
1	A	884	CYS
1	B	36	MET
1	B	108	GLU
1	B	159	PRO
1	B	184	HIS
1	B	543	PHE
1	B	564	LYS
1	B	597	ASP
1	B	884	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	378	GLN

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 ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	#$|Z| > 2$
4	EDO	B	1006	-	3,3,3	0.54	0	2,2,2	0.32	0
4	EDO	B	1004	-	3,3,3	0.54	0	2,2,2	0.09	0
4	EDO	A	1007	-	3,3,3	0.43	0	2,2,2	0.38	0
3	M1P	A	1002	-	15,16,16	0.51	0	23,24,24	0.67	0
4	EDO	A	1006	-	3,3,3	0.40	0	2,2,2	0.30	0
4	EDO	B	1003	-	3,3,3	0.62	0	2,2,2	0.05	0
4	EDO	B	1007	-	3,3,3	0.62	0	2,2,2	0.16	0
4	EDO	A	1004	-	3,3,3	0.52	0	2,2,2	0.56	0
4	EDO	B	1005	-	3,3,3	0.44	0	2,2,2	0.46	0
4	EDO	A	1005[A]	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	A	1005[B]	-	3,3,3	0.48	0	2,2,2	0.21	0
4	EDO	A	1003	-	3,3,3	0.48	0	2,2,2	0.14	0
2	SO4	A	1001	-	4,4,4	0.32	0	6,6,6	0.33	0
3	M1P	B	1002	-	15,16,16	0.74	0	23,24,24	0.95	0
2	SO4	B	1001	-	4,4,4	0.32	0	6,6,6	0.31	0
4	EDO	B	1008	-	3,3,3	0.53	0	2,2,2	0.30	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
4	EDO	B	1006	-	-	0/1/1/1	-
4	EDO	B	1004	-	-	0/1/1/1	-
4	EDO	A	1007	-	-	1/1/1/1	-
3	M1P	A	1002	-	-	2/7/27/27	0/1/1/1
4	EDO	A	1006	-	-	0/1/1/1	-
4	EDO	B	1003	-	-	0/1/1/1	-
4	EDO	B	1007	-	-	1/1/1/1	-
4	EDO	A	1004	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1005	-	-	0/1/1/1	-
4	EDO	A	1005[A]	-	-	1/1/1/1	-
4	EDO	A	1005[B]	-	-	0/1/1/1	-
4	EDO	A	1003	-	-	0/1/1/1	-
3	M1P	B	1002	-	-	2/7/27/27	0/1/1/1
4	EDO	B	1008	-	-	1/1/1/1	-

There are no bond length outliers.

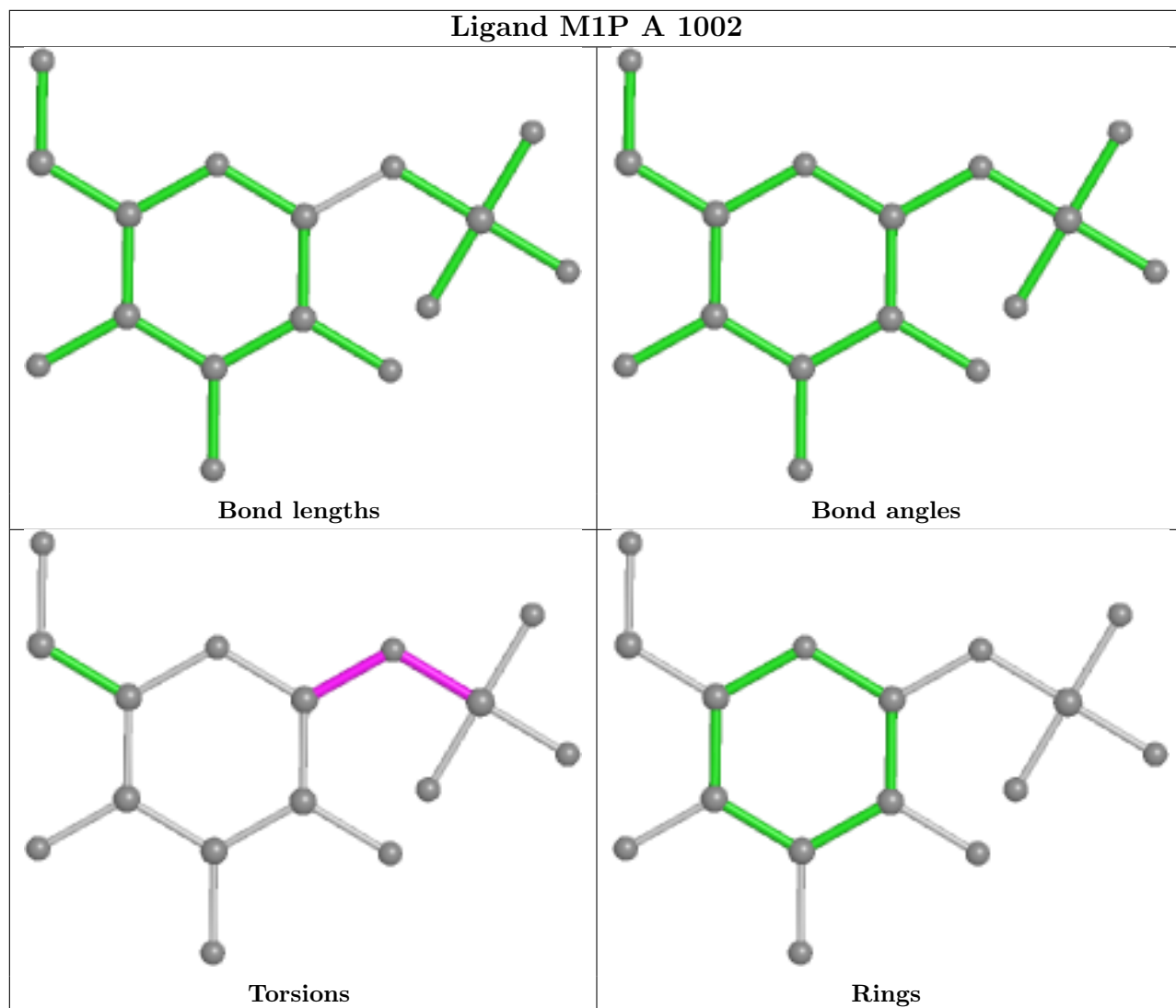There are no bond angle outliers.

There are no chirality outliers.
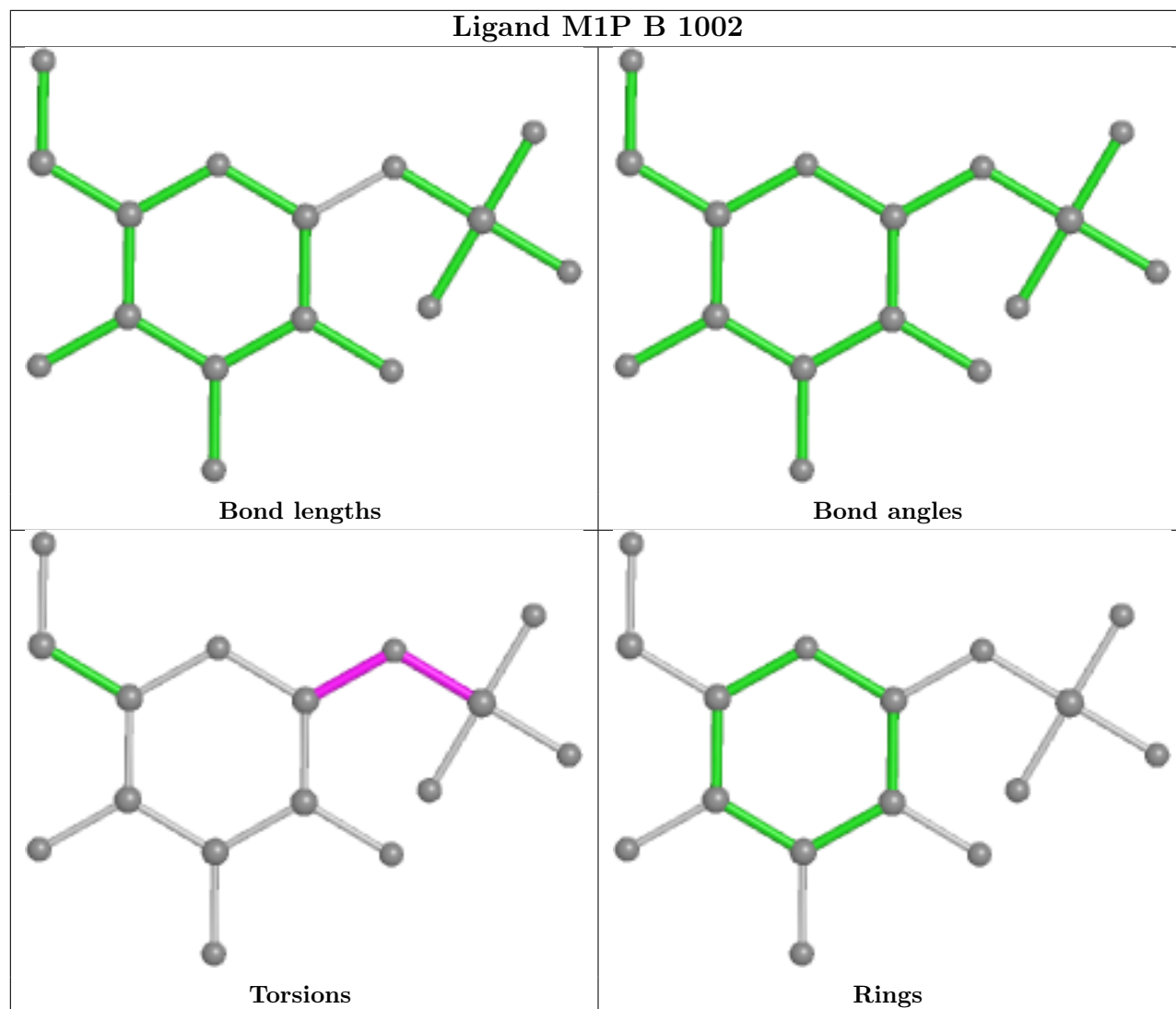
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	M1P	O5-C1-O1-P
3	A	1002	M1P	C1-O1-P-O1P
3	B	1002	M1P	O5-C1-O1-P
4	A	1005[A]	EDO	O1-C1-C2-O2
4	B	1007	EDO	O1-C1-C2-O2
4	B	1008	EDO	O1-C1-C2-O2
4	A	1007	EDO	O1-C1-C2-O2
3	B	1002	M1P	C1-O1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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 M1P A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand M1P B 1002

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	902/913 (98%)	0.33	66 (7%)	15	11	20, 46, 86, 110	0
1	B	899/913 (98%)	-0.05	27 (3%)	50	44	17, 29, 65, 94	0
All	All	1801/1826 (98%)	0.14	93 (5%)	27	22	17, 37, 80, 110	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	ALA	6.0
1	A	562	THR	5.9
1	A	414	ALA	5.8
1	B	871	ASN	5.6
1	A	872	GLY	4.6
1	A	896	ALA	4.6
1	B	474	ALA	4.4
1	B	870	LEU	4.4
1	A	485	LEU	4.1
1	A	474	ALA	4.1
1	A	894	LEU	3.9
1	A	583	PRO	3.8
1	B	872	GLY	3.8
1	A	563	GLY	3.7
1	A	871	ASN	3.6
1	A	460	TYR	3.6
1	B	876	ASP	3.5
1	B	896	ALA	3.5
1	A	419	PHE	3.4
1	A	898	GLY	3.4
1	B	477	THR	3.4
1	A	389	ALA	3.3
1	B	875	VAL	3.3
1	A	321	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	479	GLU	3.2
1	A	492	TYR	3.2
1	A	602	ALA	3.2
1	B	890	LEU	3.1
1	A	899	VAL	3.1
1	B	899	VAL	3.1
1	B	894	LEU	3.1
1	B	562	THR	3.1
1	A	891	ILE	3.1
1	A	890	LEU	3.0
1	B	475	SER	3.0
1	A	484	LEU	2.9
1	A	595	LEU	2.9
1	A	488	ASP	2.9
1	A	889	SER	2.9
1	A	868	VAL	2.9
1	A	396	LEU	2.9
1	A	416	PRO	2.9
1	A	475	SER	2.8
1	A	476[A]	TRP	2.8
1	B	479	GLU	2.7
1	A	489	GLY	2.7
1	B	416	PRO	2.7
1	A	449	GLY	2.7
1	A	309	ALA	2.7
1	A	393	HIS	2.7
1	A	895	PRO	2.6
1	A	911	SER	2.6
1	A	584	ILE	2.6
1	A	886	ILE	2.5
1	B	856	GLN	2.5
1	A	607	VAL	2.5
1	A	851	VAL	2.5
1	B	877	CYS	2.5
1	A	422	ASP	2.5
1	A	491	ILE	2.5
1	A	413	GLY	2.5
1	B	898	GLY	2.5
1	A	903	ILE	2.4
1	B	902	LEU	2.4
1	A	900	HIS	2.4
1	A	486	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	883	GLY	2.4
1	B	891	ILE	2.4
1	A	582	LYS	2.4
1	A	424	ASN	2.3
1	A	421	ALA	2.3
1	B	873	GLN	2.3
1	A	569	ILE	2.3
1	A	870	LEU	2.2
1	B	893	ALA	2.2
1	A	324	ARG	2.2
1	A	575	LEU	2.2
1	A	902	LEU	2.2
1	A	480	GLN	2.2
1	B	476	TRP	2.1
1	B	874	SER	2.1
1	A	314	ALA	2.1
1	A	613	LEU	2.1
1	A	600	TYR	2.1
1	A	845	GLY	2.1
1	A	843	PHE	2.1
1	A	875	VAL	2.1
1	A	612	LEU	2.1
1	A	331	ARG	2.1
1	A	608	SER	2.0
1	B	882	ALA	2.0
1	A	325	ASP	2.0
1	B	895	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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,
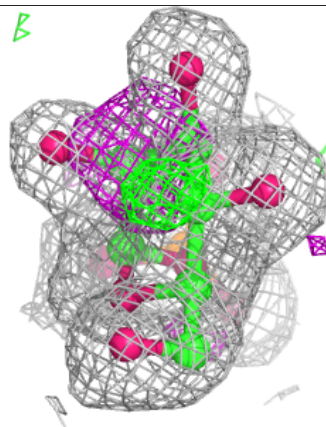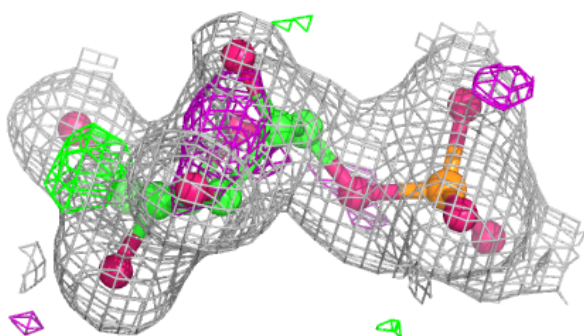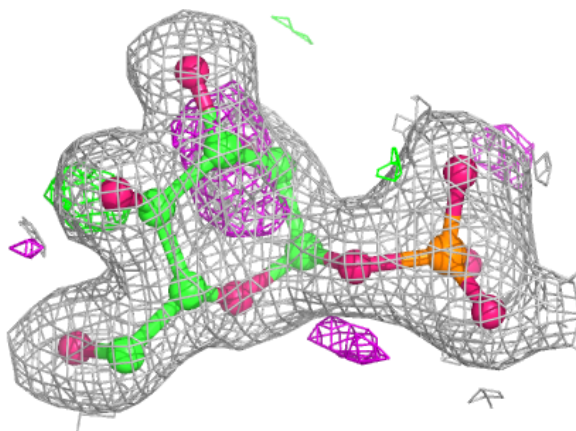
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
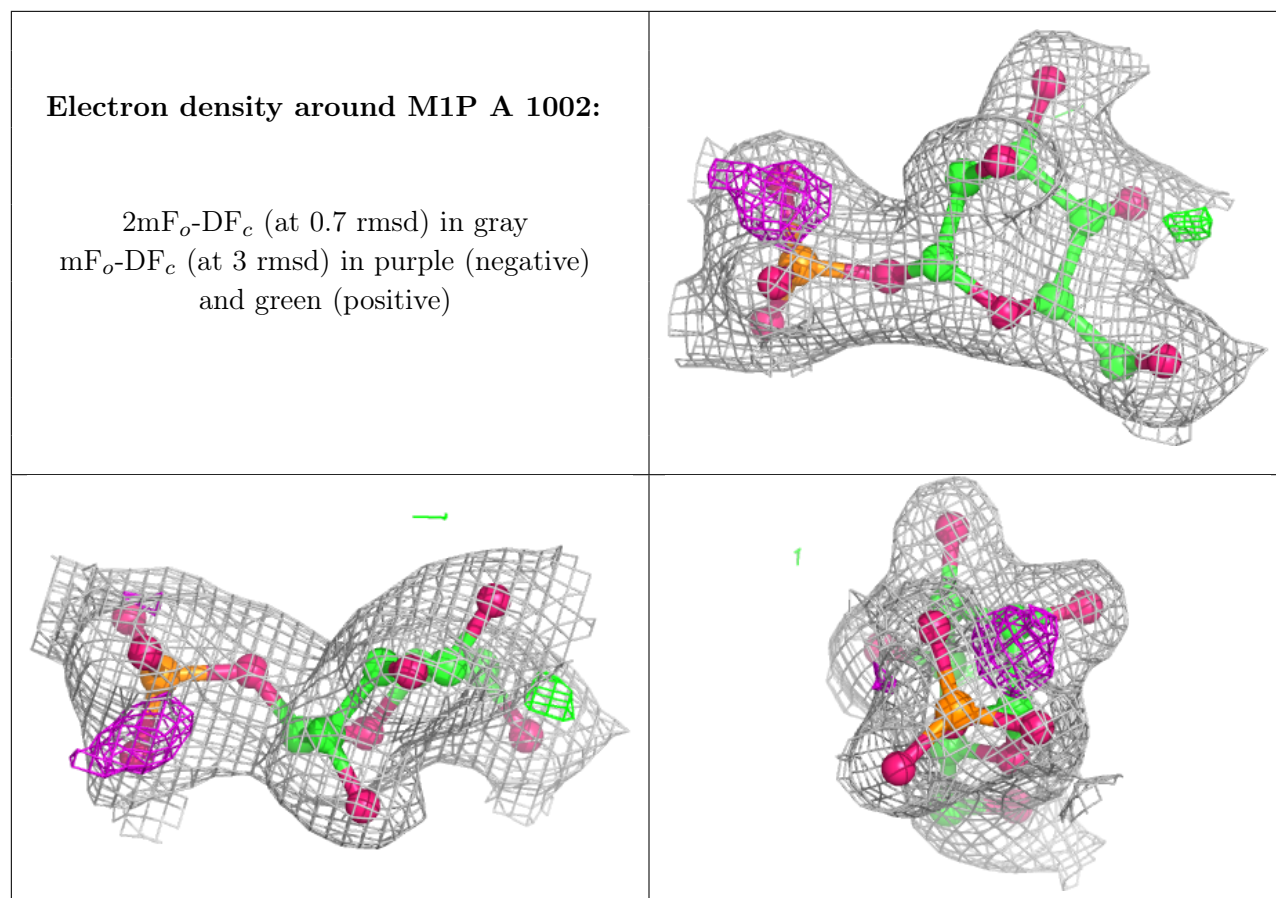
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	1006	4/4	0.74	0.14	52,55,59,59	0
4	EDO	A	1004	4/4	0.78	0.14	44,51,52,54	0
5	CL	A	1009	1/1	0.86	0.05	65,65,65,65	0
4	EDO	A	1007	4/4	0.87	0.14	50,54,55,59	0
4	EDO	A	1005[B]	4/4	0.89	0.20	50,50,51,51	4
4	EDO	B	1007	4/4	0.89	0.20	42,49,51,54	0
4	EDO	A	1005[A]	4/4	0.89	0.20	33,40,40,41	4
4	EDO	B	1005	4/4	0.91	0.13	36,36,37,37	0
4	EDO	B	1004	4/4	0.91	0.15	41,45,47,49	0
4	EDO	B	1003	4/4	0.94	0.12	28,32,37,37	0
5	CL	B	1010	1/1	0.94	0.04	65,65,65,65	0
4	EDO	B	1008	4/4	0.95	0.09	30,33,40,46	0
3	M1P	B	1002	16/16	0.96	0.11	22,32,36,37	0
5	CL	A	1008	1/1	0.96	0.14	59,59,59,59	0
3	M1P	A	1002	16/16	0.96	0.10	31,43,48,48	0
5	CL	B	1009	1/1	0.96	0.19	53,53,53,53	0
4	EDO	A	1006	4/4	0.96	0.14	34,36,43,50	0
4	EDO	A	1003	4/4	0.97	0.12	27,30,33,36	0
2	SO4	A	1001	5/5	0.97	0.17	50,53,56,67	0
2	SO4	B	1001	5/5	0.99	0.07	29,32,35,38	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 M1P B 1002:

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 M1P A 1002:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.