



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:14 AM UTC

PDB ID : 4ZEV / pdb_00004zev
Title : Crystal structure of PfHAD1 in complex with mannose-6-phosphate
Authors : Park, J.; Tolia, N.H.
Deposited on : 2015-04-20
Resolution : 1.80 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

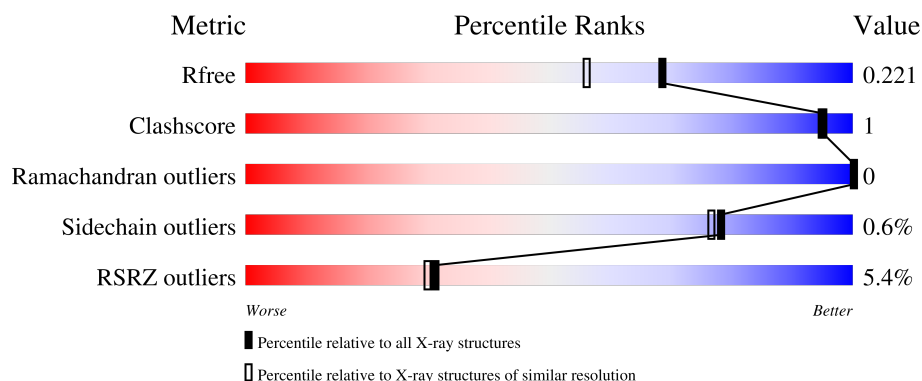
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	296	2% 94% • •
1	B	296	8% 87% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9449 atoms, of which 4535 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 PfHAD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	H	N	O	S	0	7	0
			4700	1485	2351	401	448	15			
1	B	270	Total	C	H	N	O	S	0	7	0
			4351	1379	2173	364	420	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q8IJ74
A	-6	ALA	-	expression tag	UNP Q8IJ74
A	-5	HIS	-	expression tag	UNP Q8IJ74
A	-4	HIS	-	expression tag	UNP Q8IJ74
A	-3	HIS	-	expression tag	UNP Q8IJ74
A	-2	HIS	-	expression tag	UNP Q8IJ74
A	-1	HIS	-	expression tag	UNP Q8IJ74
A	0	HIS	-	expression tag	UNP Q8IJ74
A	27	ALA	ASP	engineered mutation	UNP Q8IJ74
B	-7	MET	-	expression tag	UNP Q8IJ74
B	-6	ALA	-	expression tag	UNP Q8IJ74
B	-5	HIS	-	expression tag	UNP Q8IJ74
B	-4	HIS	-	expression tag	UNP Q8IJ74
B	-3	HIS	-	expression tag	UNP Q8IJ74
B	-2	HIS	-	expression tag	UNP Q8IJ74
B	-1	HIS	-	expression tag	UNP Q8IJ74
B	0	HIS	-	expression tag	UNP Q8IJ74
B	27	ALA	ASP	engineered mutation	UNP Q8IJ74

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

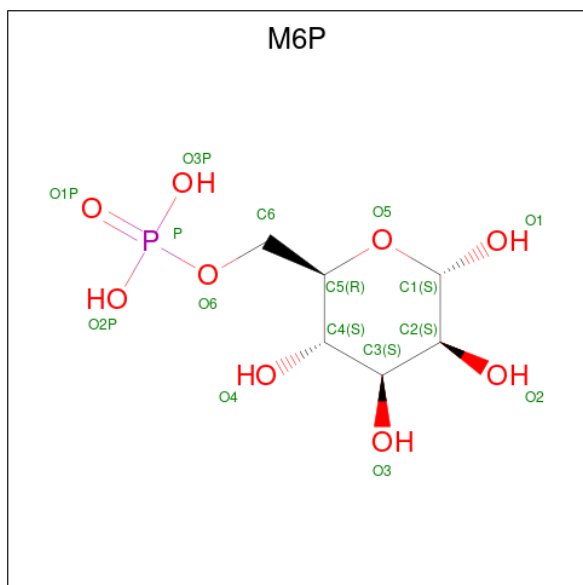
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

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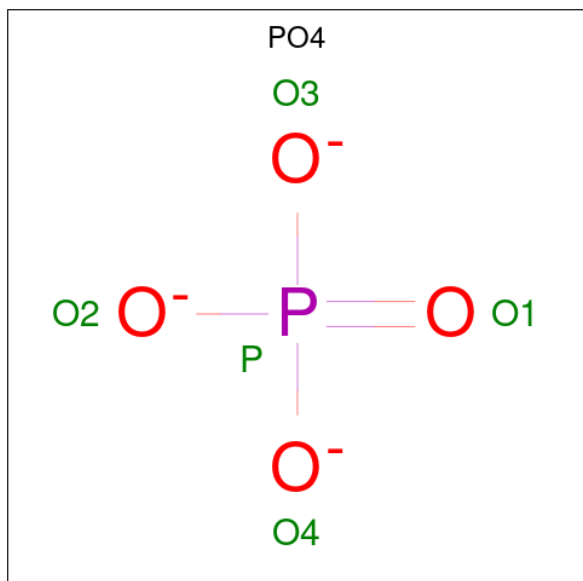
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 6-O-phosphono-alpha-D-mannopyranose (CCD ID: M6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			27	6	11	9	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	222	Total	O	0	0
			222	222		
5	B	142	Total	O	0	0
			142	142		

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- Molecule 1: PfHAD1



F202	L208	H212	A258	N284	S285	A266	A267	T288	V269	F283	T284	F285	C286	D287	ILE	RET	ALA	HIS	HIS	HIS	HIS	HIS	MET	HIS	GLU	TLE	VAL	ASP	LYS	ASN	GLY	LYS	LYS	VAL	GLN	LYS	ASN	ASN	LEU	M18	A27	A60	E97	I115	E134	I141	M142	D143	E147	V148	M149	E150	V151	E152	M153	L154	M155	P156	C188	F192	I196	N200	T204
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.60Å 44.50Å 84.50Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	19.60 – 1.80 19.60 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.60-1.80) 99.3 (19.60-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.188 , 0.219 0.190 , 0.221	Depositor DCC
R_{free} test set	2565 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9449	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: M6P, MG, PO4

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	0.55	0/2408	0.76	1/3243 (0.0%)
1	B	0.50	0/2234	0.75	1/3012 (0.0%)
All	All	0.53	0/4642	0.76	2/6255 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	192	PHE	N-CA-C	6.50	122.17	113.72
1	A	239	GLY	N-CA-C	5.02	120.51	112.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ASP	Mainchain

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	2349	2351	2365	5	0
1	B	2178	2173	2182	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	11	11	2	0
4	B	5	0	0	0	0
5	A	222	0	0	1	0
5	B	142	0	0	1	0
All	All	4914	4535	4558	11	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 (11) 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:192:PHE:HB3	1:A:196:ILE:HG22	1.81	0.62
1:B:97:GLU:N	5:B:403:HOH:O	2.34	0.60
1:B:188[B]:CYS:SG	1:B:208:LEU:HD21	2.55	0.47
1:A:202:PHE:HB2	3:A:302:M6P:O4	2.15	0.47
1:A:60:ALA:HA	1:A:87:ILE:HB	1.99	0.45
1:B:115:ILE:HD11	1:B:196[A]:ILE:HD13	1.99	0.43
1:A:146:ARG:HA	1:A:149:MET:HE2	2.01	0.42
3:A:302:M6P:H2	5:A:561:HOH:O	2.19	0.42
1:A:197:ASN:O	1:A:208:LEU:HA	2.20	0.41
1:B:149:MET:HE3	1:B:156:PRO:HD2	2.03	0.40
1:B:27:ALA:HA	1:B:60:ALA:O	2.22	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	295/296 (100%)	289 (98%)	6 (2%)	0	100	100
1	B	275/296 (93%)	268 (98%)	7 (2%)	0	100	100
All	All	570/592 (96%)	557 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	270/268 (101%)	270 (100%)	0	100	100
1	B	251/268 (94%)	247 (98%)	4 (2%)	55	47
All	All	521/536 (97%)	517 (99%)	4 (1%)	78	70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	GLU
1	B	196[A]	ILE
1	B	196[B]	ILE
1	B	200	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	155	ASN
1	A	194	HIS
1	A	200	ASN
1	A	256	HIS
1	B	37	ASN
1	B	232	ASN

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	$\# Z > 2$
4	PO4	B	302	2	4,4,4	0.87	0	6,6,6	0.76	0
3	M6P	A	302	2	16,16,16	0.54	0	23,24,24	0.73	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	M6P	A	302	2	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

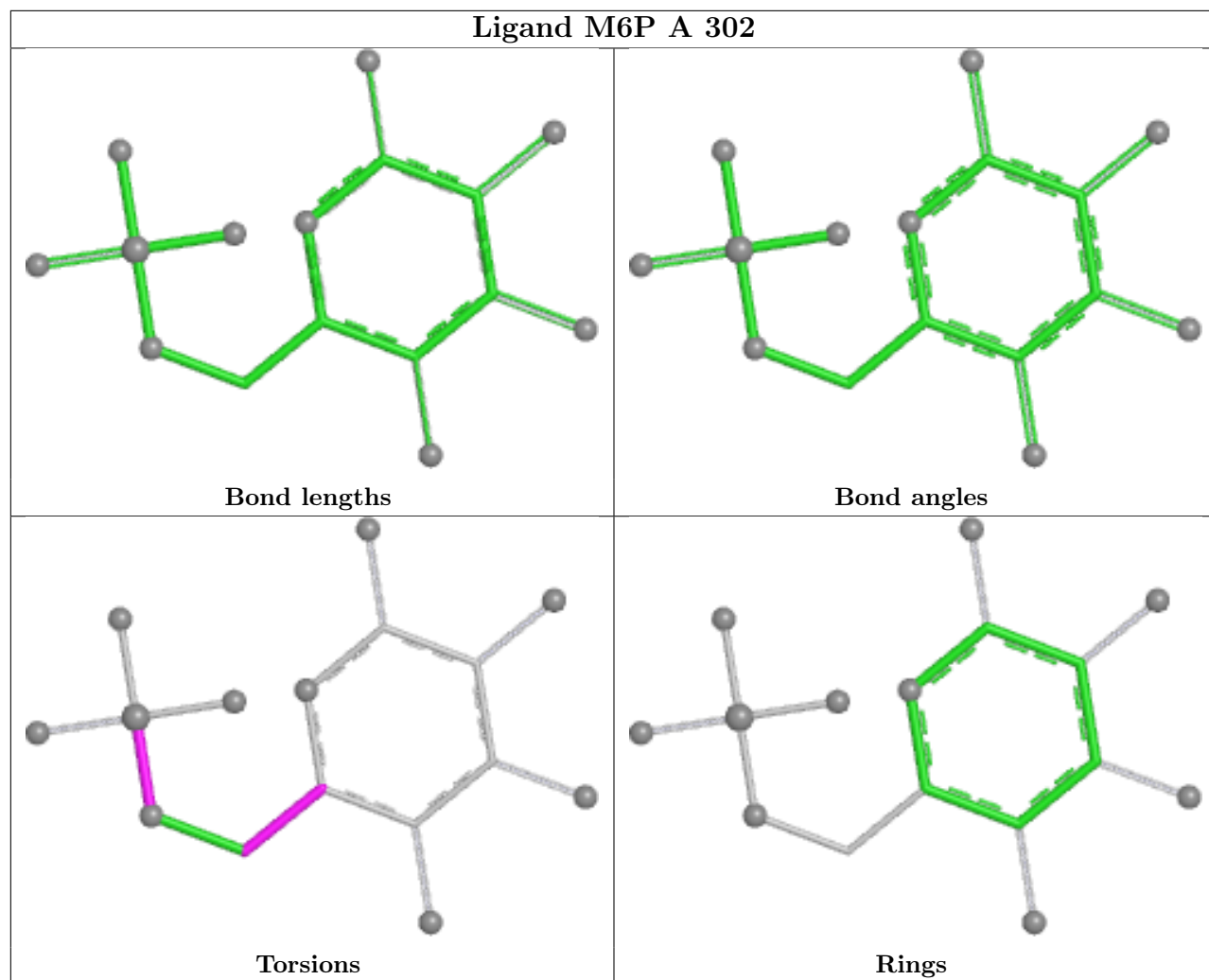
Mol	Chain	Res	Type	Atoms
3	A	302	M6P	C6-O6-P-O3P
3	A	302	M6P	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	M6P	2	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	290/296 (97%)	-0.28	6 (2%) 63 64	9, 23, 51, 91	7 (2%)
1	B	270/296 (91%)	0.32	24 (8%) 15 13	10, 32, 70, 109	7 (2%)
All	All	560/592 (94%)	0.01	30 (5%) 31 30	9, 27, 63, 109	14 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	PHE	6.8
1	B	148	TYR	6.2
1	A	288	ILE	5.7
1	B	151	VAL	4.6
1	B	154	LEU	4.2
1	B	153	ALA	3.9
1	B	202	PHE	3.4
1	B	201	THR	3.1
1	B	143	ASP	2.9
1	B	287	ASP	2.9
1	B	149	MET	2.8
1	B	258	ALA	2.7
1	B	286	CYS	2.7
1	B	267	ALA	2.6
1	B	283	LYS	2.6
1	B	268	TYR	2.5
1	B	18	ASN	2.5
1	A	205	TYR	2.4
1	B	212	HIS	2.4
1	B	150	GLU	2.4
1	B	147	GLU	2.3
1	B	264	ASN	2.3
1	B	266	ALA	2.3
1	B	284	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	7	LYS	2.2
1	B	269	VAL	2.2
1	A	-1	HIS	2.1
1	B	141	ILE	2.1
1	A	203	GLN	2.0
1	B	155	ASN	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](#)

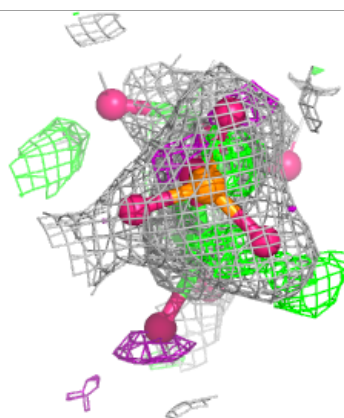
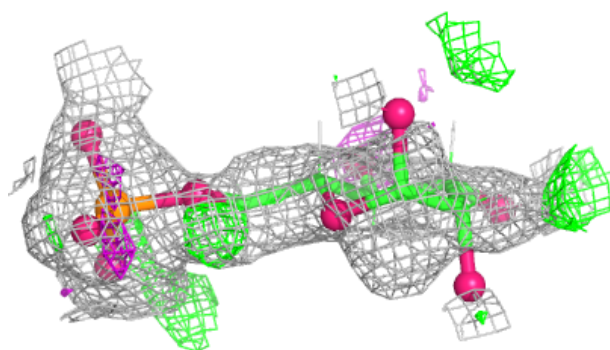
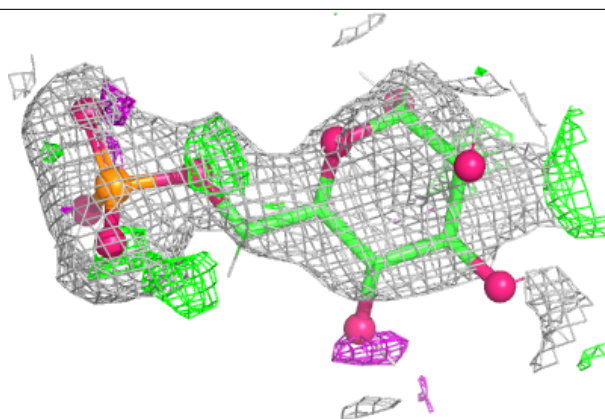
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	M6P	A	302	16/16	0.90	0.21	21,89,107,109	0
2	MG	B	301	1/1	0.95	0.06	27,27,27,27	0
2	MG	A	301	1/1	0.97	0.06	26,26,26,26	0
4	PO4	B	302	5/5	0.98	0.05	26,29,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around M6P A 302:

$2mF_o-DF_c$ (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.