Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2026 – 01:48 PM UTC

PDB ID	:	4YI5 / pdb_00004yi5
Title	:	Crystal structure of Gpb in complex with 4b
Authors	:	Kantsadi, A.L.; Chatzileontiadou, D.S.M.; Stravodimos, G.A.; Leonidas, D.D.
Deposited on	:	2015-02-27
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 (i) 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 (i)) were used in the production of this report:

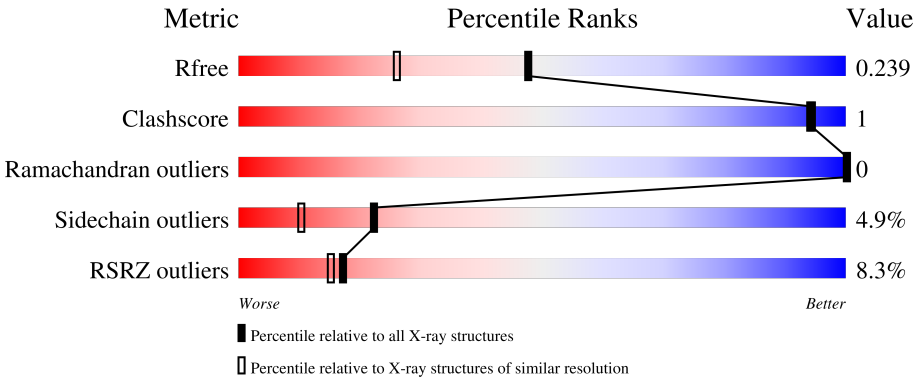
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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 <=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	843	8% 90% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMP	A	903	X	-	-	-

2 Entry composition

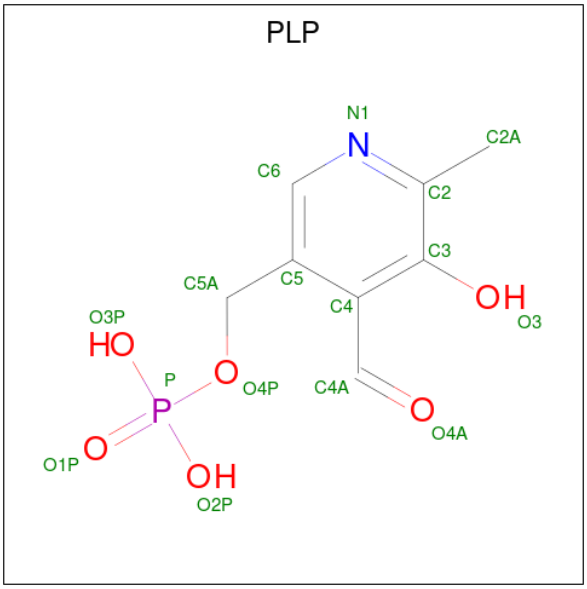
There are 5 unique types of molecules in this entry. The entry contains 7035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, muscle form.

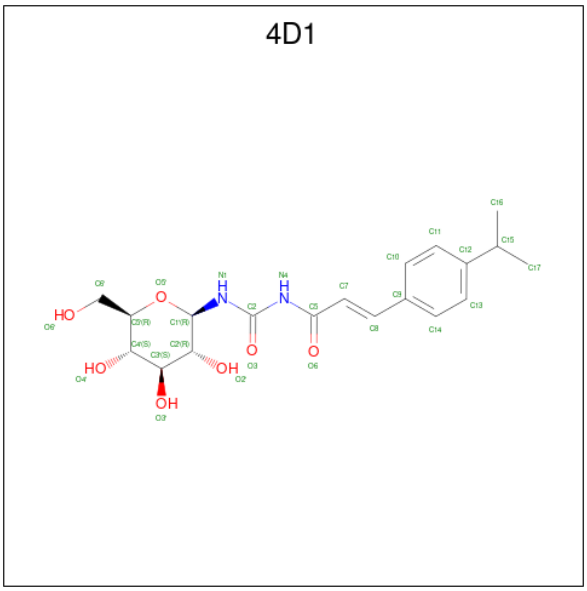
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	809	6585	4199	1159	1197	30	0	1	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



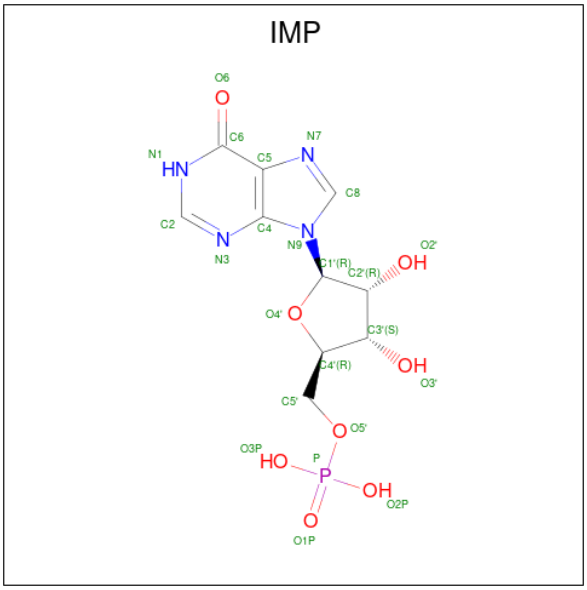
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is N-({(2E)-3-[4-(propan-2-yl)phenyl]prop-2-enoyl}carbamoyl)-beta-D-glucopyranosylamine (CCD ID: 4D1) (formula: $C_{19}H_{26}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	28	19	2	7	0	0

- Molecule 4 is INOSINIC ACID (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	23	10	4	8	1	0	0

- Molecule 5 is water.

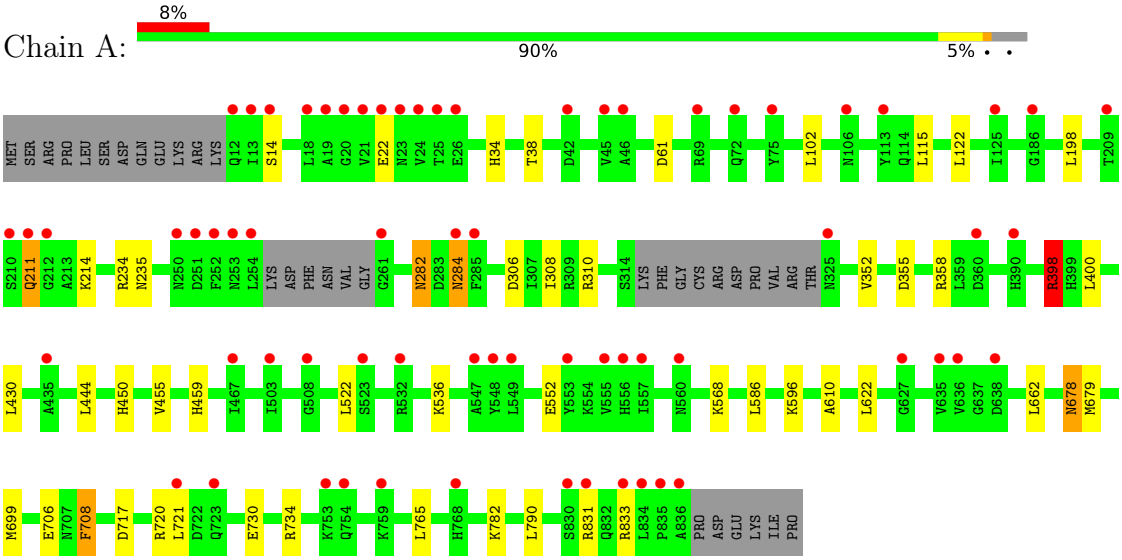
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	384	Total	O	0	0
			384	384		

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: Glycogen phosphorylase, muscle form

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.54Å 128.54Å 116.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 1.80 38.88 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.3 (38.88-1.80) 90.3 (38.88-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.230 0.204 , 0.239	Depositor DCC
R_{free} test set	4005 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7035	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 4D1, PLP, IMP

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	0.66	0/6735	0.87	2/9114 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	SER	N-CA-C	5.50	116.95	111.07
1	A	398	ARG	NE-CZ-NH2	5.20	123.88	119.20

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	6585	0	6531	17	0
2	A	15	0	7	0	0
3	A	28	0	26	0	0
4	A	23	0	11	0	0
5	A	384	0	0	1	1
All	All	7035	0	6575	17	1

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 (17) 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:282:ASN:HD22	1:A:282:ASN:H	1.47	0.62
1:A:678:ASN:HD22	1:A:679:MET:H	1.49	0.61
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.93	0.52
1:A:455:VAL:H	1:A:459:HIS:HD2	1.58	0.51
1:A:282:ASN:H	1:A:282:ASN:ND2	2.10	0.48
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.97	0.47
1:A:730:GLU:O	1:A:734:ARG:HG3	2.14	0.46
1:A:717:ASP:OD1	1:A:720:ARG:NH1	2.47	0.46
1:A:282:ASN:HD22	1:A:282:ASN:N	2.13	0.46
1:A:308:ILE:HD13	1:A:352:VAL:HG11	2.01	0.43
1:A:450:HIS:HD2	5:A:1243:HOH:O	2.00	0.43
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.84	0.43
1:A:284:ASN:HD21	1:A:610:ALA:CB	2.32	0.42
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.20	0.41
1:A:211:GLN:O	1:A:358:ARG:NH1	2.53	0.41
1:A:678:ASN:HD22	1:A:679:MET:N	2.16	0.41
1:A:284:ASN:HD21	1:A:610:ALA:HB3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1046:HOH:O	5:A:1046:HOH:O[7_555]	1.50	0.70

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	804/843 (95%)	784 (98%)	20 (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	701/732 (96%)	667 (95%)	34 (5%)	22 10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	102	LEU
1	A	115	LEU
1	A	122	LEU
1	A	198	LEU
1	A	211	GLN
1	A	214	LYS
1	A	234	ARG
1	A	235	ASN
1	A	282	ASN
1	A	284	ASN
1	A	306	ASP
1	A	310	ARG
1	A	398	ARG
1	A	400	LEU
1	A	430	LEU
1	A	444	LEU
1	A	522	LEU
1	A	536	LYS
1	A	552	GLU
1	A	568	LYS
1	A	586	LEU
1	A	596	LYS
1	A	622	LEU
1	A	662	LEU
1	A	678	ASN
1	A	706	GLU

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Mol	Chain	Res	Type
1	A	708	PHE
1	A	721	LEU
1	A	765	LEU
1	A	782	LYS
1	A	790	LEU
1	A	831	ARG
1	A	833	ARG

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

Mol	Chain	Res	Type
1	A	34	HIS
1	A	96	GLN
1	A	211	GLN
1	A	235	ASN
1	A	270	ASN
1	A	282	ASN
1	A	284	ASN
1	A	390	HIS
1	A	412	ASN
1	A	450	HIS
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	571	HIS
1	A	579	ASN
1	A	678	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)

3 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	$\#\|Z\| > 2$
2	PLP	A	901	1	15,15,16	2.56	3 (20%)	21,22,23	1.62	4 (19%)
3	4D1	A	902	-	29,29,29	1.89	6 (20%)	40,40,40	1.53	6 (15%)
4	IMP	A	903	-	25,25,25	1.23	3 (12%)	37,38,38	2.09	9 (24%)

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
2	PLP	A	901	1	-	2/6/6/8	0/1/1/1
3	4D1	A	902	-	-	2/19/39/39	0/2/2/2
4	IMP	A	903	-	1/1/5/5	3/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	PLP	C5-C4	7.09	1.48	1.40
3	A	902	4D1	C7-C8	6.51	1.49	1.33
2	A	901	PLP	C3-C2	4.79	1.45	1.41
3	A	902	4D1	C12-C15	-4.05	1.43	1.53
2	A	901	PLP	C3-C4	3.49	1.46	1.40
4	A	903	IMP	C5-C4	3.31	1.47	1.38
3	A	902	4D1	C1'-N1	3.09	1.47	1.43
4	A	903	IMP	C2-N3	2.82	1.35	1.30
3	A	902	4D1	C7-C5	2.82	1.54	1.48
3	A	902	4D1	C4'-C5'	2.68	1.58	1.53
3	A	902	4D1	C9-C8	-2.48	1.40	1.47
4	A	903	IMP	C5-N7	-2.18	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	4D1	C5-N4-C2	-6.11	122.34	128.13
4	A	903	IMP	C5-C4-N3	-5.73	118.83	127.27
4	A	903	IMP	C2-N3-C4	5.48	121.17	111.53
4	A	903	IMP	C5-C6-N1	5.13	118.16	110.78
4	A	903	IMP	N9-C4-N3	3.51	134.90	126.90
4	A	903	IMP	C6-C5-N7	3.22	136.15	130.29
2	A	901	PLP	C2A-C2-C3	-3.12	117.14	120.80
3	A	902	4D1	O6-C5-N4	3.01	127.62	121.41
2	A	901	PLP	O4P-P-O1P	-2.93	98.53	106.44
2	A	901	PLP	C2A-C2-N1	2.61	122.57	117.64
3	A	902	4D1	C3'-C2'-C1'	-2.45	106.26	109.86
4	A	903	IMP	N1-C2-N3	-2.45	122.68	125.50
4	A	903	IMP	O6-C6-C5	-2.36	120.30	126.53
4	A	903	IMP	C4-C5-N7	-2.33	106.98	110.67
3	A	902	4D1	O5'-C1'-C2'	-2.22	107.23	109.72
3	A	902	4D1	C5'-O5'-C1'	-2.21	109.40	112.47
3	A	902	4D1	O5'-C5'-C6'	2.20	111.89	106.44
4	A	903	IMP	C2-N1-C6	-2.04	122.29	125.09
2	A	901	PLP	C6-N1-C2	2.02	122.86	119.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	903	IMP	C4'

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	PLP	C4-C5-C5A-O4P
4	A	903	IMP	O4'-C4'-C5'-O5'
4	A	903	IMP	C3'-C4'-C5'-O5'
3	A	902	4D1	O3-C2-N4-C5
3	A	902	4D1	N1-C2-N4-C5
2	A	901	PLP	C6-C5-C5A-O4P
4	A	903	IMP	C4'-C5'-O5'-P

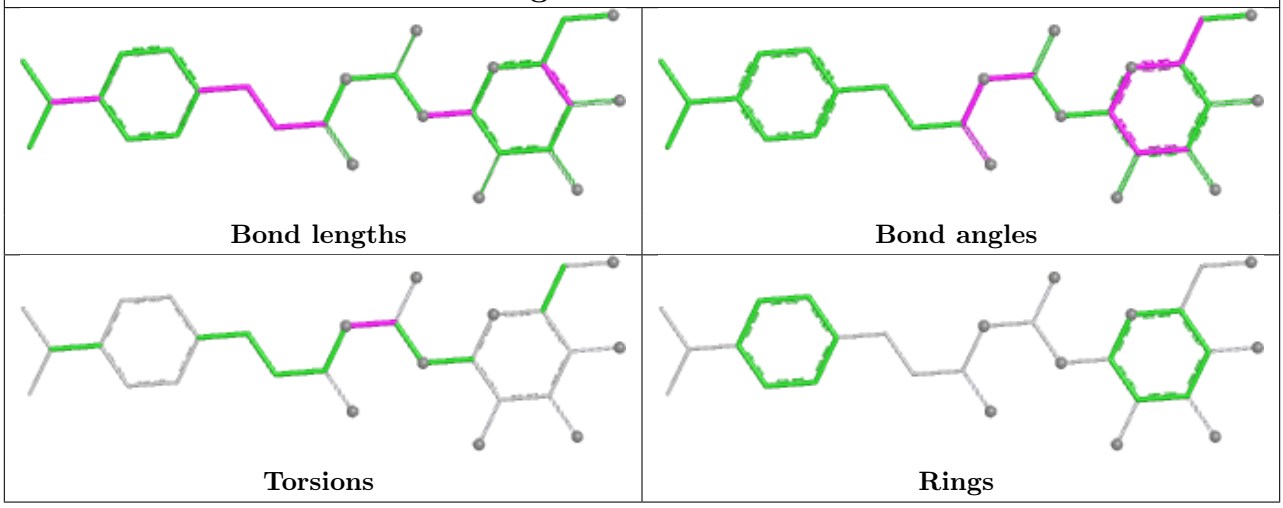
There are no ring outliers.

No monomer is involved in short contacts.

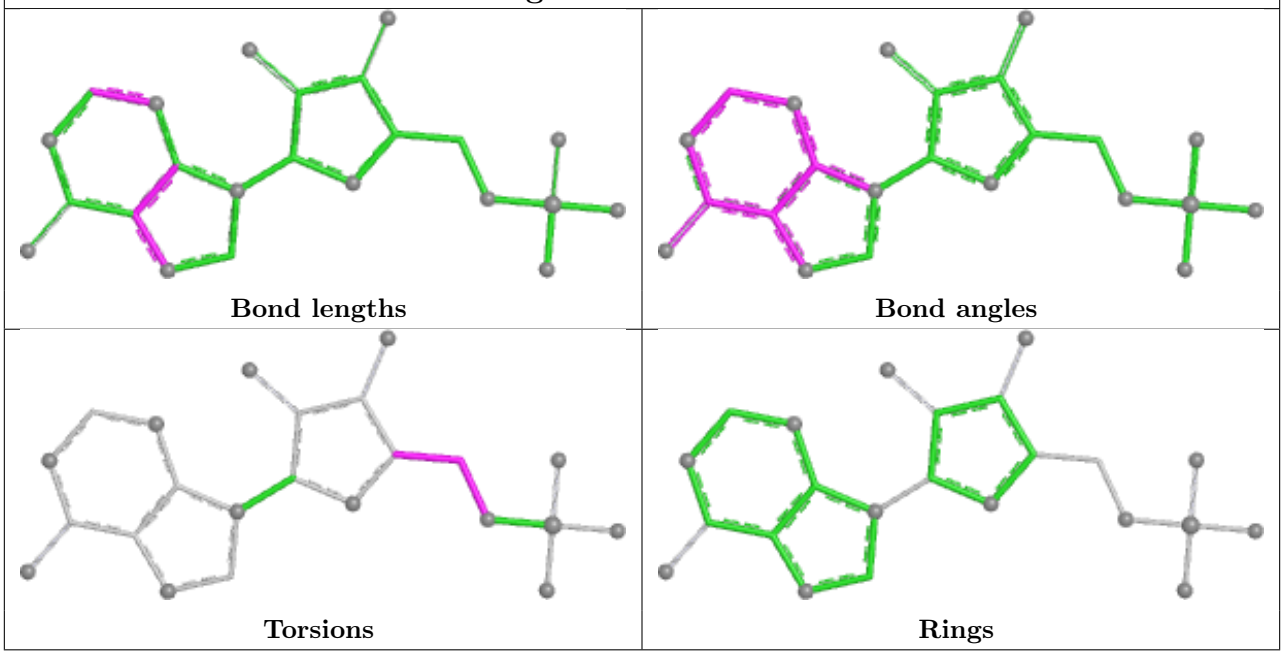
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 4D1 A 902



Ligand IMP A 903



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, 95^{th} 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	809/843 (95%)	0.64	67 (8%)	17	15	18, 30, 54, 90	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	VAL	6.5
1	A	836	ALA	6.0
1	A	252	PHE	5.4
1	A	556	HIS	4.7
1	A	13	ILE	4.3
1	A	211	GLN	4.1
1	A	830	SER	4.0
1	A	284	ASN	3.6
1	A	251	ASP	3.3
1	A	45	VAL	3.3
1	A	18	LEU	3.3
1	A	834	LEU	3.2
1	A	835	PRO	3.2
1	A	253	ASN	3.2
1	A	547	ALA	3.1
1	A	72	GLN	3.0
1	A	549	LEU	3.0
1	A	42	ASP	3.0
1	A	254	LEU	2.9
1	A	250	ASN	2.8
1	A	768	HIS	2.8
1	A	21	VAL	2.8
1	A	209	THR	2.8
1	A	325	ASN	2.7
1	A	532	ARG	2.7
1	A	635	VAL	2.7
1	A	390	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	723	GLN	2.6
1	A	106	ASN	2.6
1	A	548	TYR	2.6
1	A	553	TYR	2.6
1	A	14	SER	2.6
1	A	69	ARG	2.5
1	A	285	PHE	2.5
1	A	560	ASN	2.5
1	A	25	THR	2.5
1	A	210	SER	2.5
1	A	523	SER	2.4
1	A	20	GLY	2.4
1	A	508	GLY	2.4
1	A	125	ILE	2.4
1	A	186	GLY	2.4
1	A	22	GLU	2.3
1	A	46	ALA	2.3
1	A	75	TYR	2.2
1	A	627	GLY	2.2
1	A	360	ASP	2.2
1	A	503	ILE	2.2
1	A	12	GLN	2.2
1	A	638	ASP	2.2
1	A	467	ILE	2.2
1	A	113	TYR	2.2
1	A	753	LYS	2.2
1	A	636	VAL	2.1
1	A	261	GLY	2.1
1	A	754	GLN	2.1
1	A	557	ILE	2.1
1	A	831	ARG	2.1
1	A	833	ARG	2.1
1	A	24	VAL	2.1
1	A	721	LEU	2.1
1	A	212	GLY	2.0
1	A	19	ALA	2.0
1	A	435	ALA	2.0
1	A	26	GLU	2.0
1	A	759	LYS	2.0
1	A	23	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)

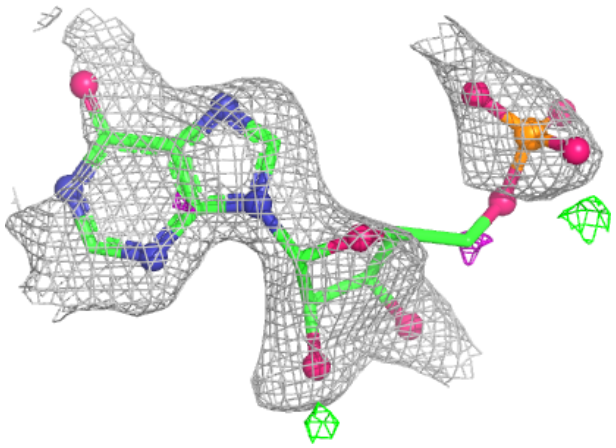
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

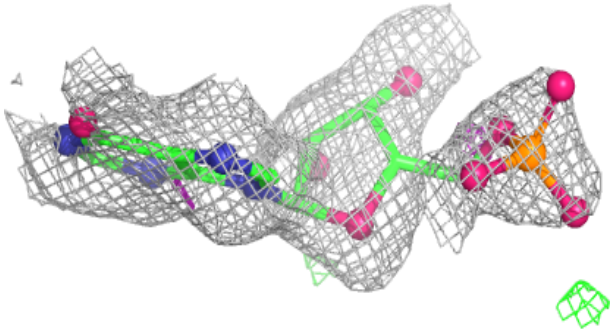
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IMP	A	903	23/23	0.77	0.16	68,74,76,77	0
3	4D1	A	902	28/28	0.94	0.08	18,21,25,27	0
2	PLP	A	901	15/16	0.97	0.06	19,19,22,23	0

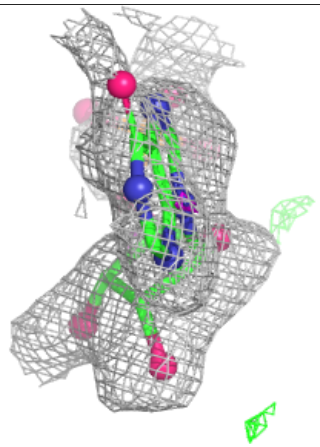
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IMP A 903:

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

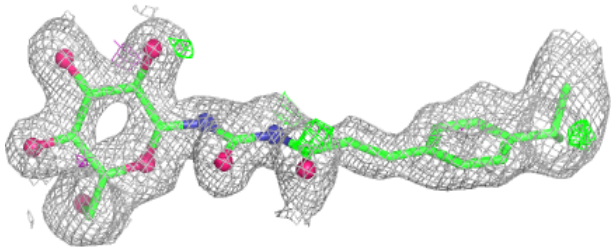


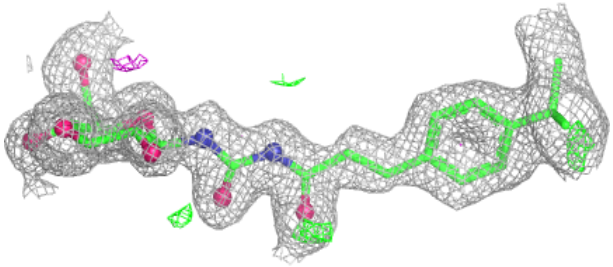


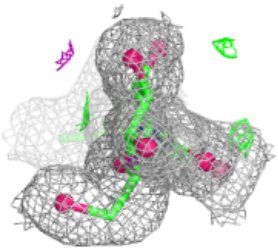


Electron density around 4D1 A 902:

$2mF_o$-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.