



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:36 AM UTC

PDB ID : 1B4D / pdb_00001b4d
Title : AMIDOCARBAMATE INHIBITOR OF GLYCOGEN PHOSPHORYLASE
Authors : Tsitsanou, K.E.; Oikonomakos, N.G.; Zographos, S.E.; Skamnaki, V.T.; Gregoriou, M.; Watson, K.A.; Johnson, L.N.; Fleet, G.W.J.
Deposited on : 1998-12-18
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

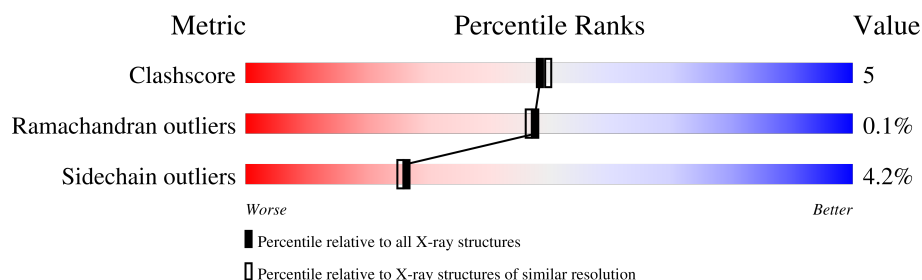
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7419 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.

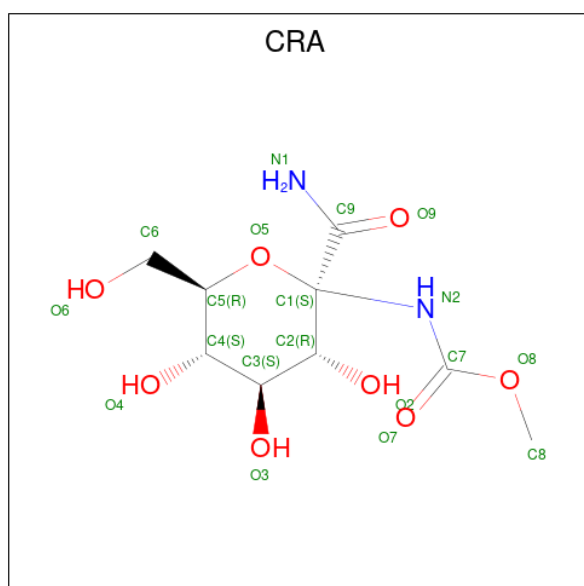
- Molecule 1 is a protein called PROTEIN (GLYCOGEN PHOSPHORYLASE B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6542	4172	1153	1188	29			

There are 2 discrepancies between the modelled and reference sequences:

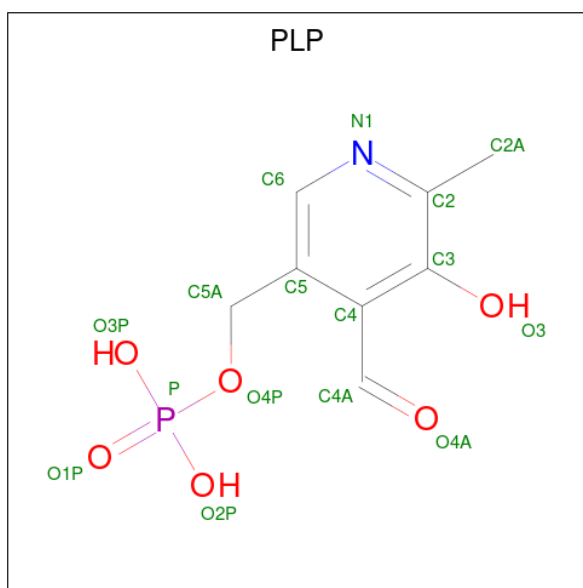
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489
A	609	ALA	PRO	SEE REMARK 999	UNP P00489

- Molecule 2 is 1-DEOXY-1-METHOXYCARBAMIDO-BETA-D-GLUCO-2-HEPTULOPYRANOSONAMIDE (CCD ID: CRA) (formula: $C_9H_{16}N_2O_8$).



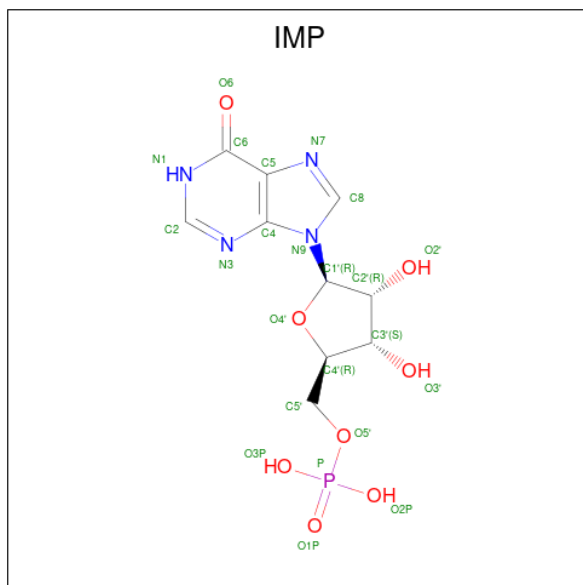
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	9	2	8		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

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



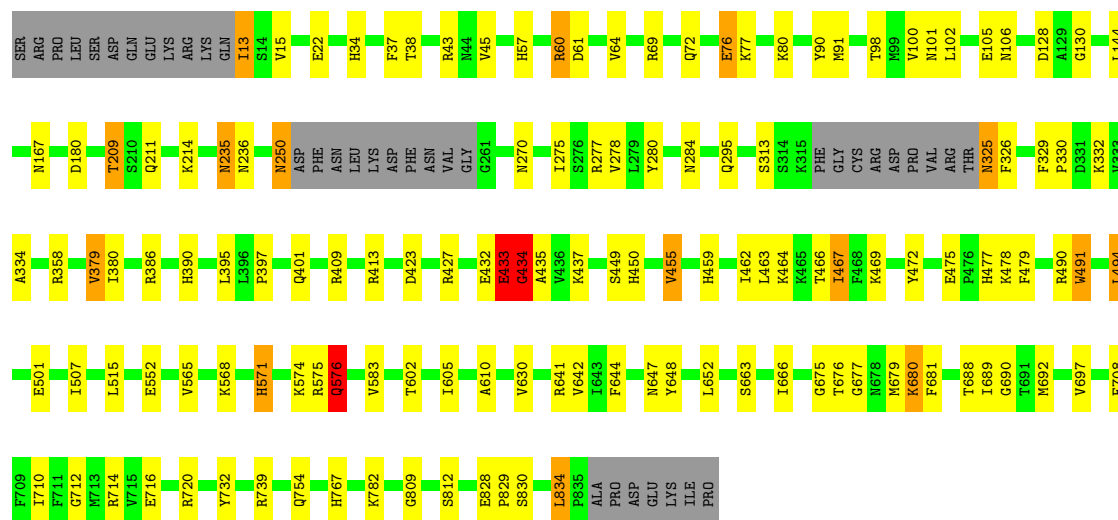
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	820	Total 820	O 820	0	0

Note EDS was not executed.

- Chain A:  79% 14% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.68Å 126.68Å 115.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.4 (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.182 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7419	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRA, 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	0.97	1/6688 (0.0%)	1.02	44/9049 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LYS	N-CA	69.36	2.31	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	GLU	N-CA-C	14.40	130.74	112.89
1	A	680	LYS	N-CA-CB	-13.94	89.15	110.06
1	A	565	VAL	N-CA-C	8.73	120.33	108.11
1	A	64	VAL	N-CA-C	7.81	117.92	110.42
1	A	679	MET	CA-C-N	-7.80	109.69	120.38
1	A	679	MET	C-N-CA	-7.80	109.69	120.38
1	A	479	PHE	N-CA-C	7.45	120.65	109.25
1	A	507	ILE	N-CA-C	7.04	118.86	112.17
1	A	37	PHE	N-CA-C	7.02	119.01	111.36
1	A	575	ARG	N-CA-C	7.00	121.04	111.39
1	A	675	GLY	N-CA-C	-6.82	104.23	112.48
1	A	680	LYS	CD-CE-NZ	-6.73	90.38	111.90
1	A	714	ARG	N-CA-C	-6.64	100.64	110.46
1	A	576	GLN	N-CA-C	-6.39	104.36	111.71
1	A	676	THR	N-CA-C	-6.39	107.34	114.62
1	A	455	VAL	N-CA-C	6.38	118.23	112.17
1	A	209	THR	N-CA-C	6.38	114.87	108.75
1	A	435	ALA	N-CA-C	-6.30	104.41	111.28
1	A	326	PHE	N-CA-C	5.92	119.98	112.87
1	A	666	ILE	N-CA-C	5.92	121.65	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	TYR	CA-C-N	5.90	127.22	119.84
1	A	280	TYR	C-N-CA	5.90	127.22	119.84
1	A	552	GLU	N-CA-C	5.88	119.63	112.23
1	A	809	GLY	N-CA-C	5.79	119.89	112.83
1	A	379	VAL	N-CA-C	-5.73	107.68	113.47
1	A	712	GLY	N-CA-C	5.68	122.62	112.22
1	A	754	GLN	CA-C-N	5.61	126.85	119.84
1	A	754	GLN	C-N-CA	5.61	126.85	119.84
1	A	105	GLU	N-CA-C	5.57	117.80	111.11
1	A	43	ARG	N-CA-C	5.51	118.80	111.75
1	A	688	THR	N-CA-C	5.46	117.87	109.07
1	A	834	LEU	N-CA-C	-5.43	103.33	110.39
1	A	767	HIS	N-CA-C	5.43	121.45	114.56
1	A	278	VAL	N-CA-C	5.42	116.18	108.42
1	A	209	THR	CB-CA-C	-5.42	108.57	116.53
1	A	677	GLY	N-CA-C	-5.39	106.18	113.24
1	A	491	TRP	N-CA-C	5.38	119.48	113.02
1	A	91	MET	N-CA-C	5.37	119.00	112.23
1	A	602	THR	N-CA-C	-5.32	98.72	108.02
1	A	630	VAL	N-CA-C	5.28	115.91	110.36
1	A	434	GLY	N-CA-C	5.26	125.65	113.18
1	A	395	LEU	N-CA-C	5.12	116.94	111.36
1	A	680	LYS	N-CA-C	-5.05	105.22	111.33
1	A	610	ALA	N-CA-C	-5.02	103.26	109.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6542	0	6498	71	0
2	A	19	0	16	0	0
3	A	15	0	7	0	0
4	A	23	0	11	0	0
5	A	820	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7419	0	6532	71	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 5.

All (71) 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:490:ARG:HA	1:A:494:LEU:HG	1.42	0.99
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.47	0.97
1:A:680:LYS:N	1:A:680:LYS:CA	2.31	0.93
1:A:463:LEU:HD23	1:A:467:ILE:HD13	1.53	0.89
1:A:270:ASN:HB2	5:A:1817:HOH:O	1.82	0.79
1:A:102:LEU:HG	5:A:1801:HOH:O	1.86	0.75
1:A:235:ASN:H	1:A:235:ASN:HD22	1.38	0.72
1:A:379:VAL:HG22	5:A:1651:HOH:O	1.89	0.71
1:A:455:VAL:H	1:A:459:HIS:HD2	1.39	0.70
1:A:98:THR:O	5:A:1801:HOH:O	2.10	0.69
1:A:692:MET:HE1	1:A:697:VAL:HG13	1.74	0.69
1:A:250:ASN:HA	5:A:1567:HOH:O	1.92	0.69
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.77	0.65
1:A:463:LEU:HA	1:A:467:ILE:HD12	1.80	0.63
1:A:716:GLU:HG3	1:A:720:ARG:HH21	1.64	0.63
1:A:60:ARG:HD3	5:A:1740:HOH:O	1.97	0.62
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.83	0.61
1:A:325:ASN:N	1:A:325:ASN:OD1	2.34	0.61
1:A:100:VAL:HG21	1:A:494:LEU:CD2	2.25	0.60
1:A:235:ASN:HD22	1:A:235:ASN:N	1.98	0.58
1:A:90:TYR:CE1	1:A:130:GLY:HA2	2.40	0.57
1:A:211:GLN:O	1:A:358:ARG:NH1	2.38	0.57
1:A:386:ARG:HD2	1:A:432:GLU:OE1	2.04	0.57
1:A:716:GLU:HG3	1:A:720:ARG:NH2	2.20	0.56
1:A:235:ASN:H	1:A:235:ASN:ND2	2.02	0.56
1:A:462:ILE:HG22	1:A:467:ILE:HD11	1.89	0.55
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.87	0.55
1:A:450:HIS:HD2	5:A:1075:HOH:O	1.89	0.54
1:A:732:TYR:O	1:A:739:ARG:HD3	2.08	0.54
1:A:692:MET:CE	1:A:697:VAL:HG13	2.38	0.54
1:A:167:ASN:ND2	1:A:647:ASN:HD21	2.07	0.53
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.91	0.52
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLU:OE1	1:A:478:LYS:HE3	2.10	0.51
1:A:101:ASN:HB2	5:A:1801:HOH:O	2.10	0.51
1:A:449:SER:O	1:A:478:LYS:HE2	2.11	0.51
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.50
1:A:277:ARG:HD2	5:A:1495:HOH:O	2.12	0.49
1:A:690:GLY:O	1:A:710:ILE:HA	2.13	0.49
1:A:680:LYS:N	1:A:680:LYS:CB	2.75	0.48
1:A:477:HIS:HB2	5:A:1770:HOH:O	2.13	0.48
1:A:464:LYS:HD2	1:A:472:TYR:CE1	2.49	0.47
1:A:397:PRO:O	1:A:401:GLN:HG3	2.14	0.47
1:A:455:VAL:H	1:A:459:HIS:CD2	2.26	0.47
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.44	0.47
1:A:409:ARG:O	1:A:413:ARG:HG3	2.15	0.46
1:A:13:ILE:CG2	1:A:15:VAL:HG22	2.46	0.45
1:A:72:GLN:NE2	1:A:76:GLU:OE2	2.49	0.45
1:A:571:HIS:HB2	1:A:574:LYS:HD2	1.98	0.45
1:A:491:TRP:CZ2	1:A:680:LYS:NZ	2.81	0.45
1:A:689:ILE:HG23	1:A:689:ILE:O	2.15	0.45
1:A:433:GLU:O	1:A:434:GLY:O	2.35	0.44
1:A:167:ASN:HD22	1:A:647:ASN:HD21	1.65	0.44
1:A:275:ILE:O	1:A:295:GLN:HG2	2.17	0.43
1:A:423:ASP:O	1:A:427:ARG:HG3	2.17	0.43
1:A:663:SER:HB2	1:A:681:PHE:CG	2.53	0.43
1:A:466:THR:OG1	1:A:467:ILE:N	2.47	0.43
1:A:455:VAL:N	1:A:459:HIS:HD2	2.13	0.43
1:A:209:THR:HG23	5:A:1694:HOH:O	2.19	0.42
1:A:463:LEU:HA	1:A:467:ILE:CD1	2.47	0.42
1:A:390:HIS:HD2	5:A:1606:HOH:O	2.02	0.42
1:A:332:LYS:HG3	5:A:1543:HOH:O	2.19	0.42
1:A:605:ILE:O	1:A:644:PHE:HA	2.19	0.42
1:A:69:ARG:HD2	5:A:1014:HOH:O	2.20	0.42
1:A:13:ILE:HG23	1:A:501:GLU:OE1	2.20	0.42
1:A:45:VAL:HG21	5:A:1775:HOH:O	2.19	0.41
1:A:57:HIS:HE1	5:A:1239:HOH:O	2.02	0.41
1:A:235:ASN:O	1:A:236:ASN:HB2	2.21	0.41
1:A:583:VAL:HG11	1:A:642:VAL:HG21	2.03	0.41
1:A:571:HIS:H	1:A:576:GLN:HE22	1.69	0.40
1:A:828:GLU:HA	1:A:829:PRO:HD2	1.97	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	798/842 (95%)	769 (96%)	28 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	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	696/731 (95%)	667 (96%)	29 (4%)	26	25

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	22	GLU
1	A	60	ARG
1	A	76	GLU
1	A	77	LYS
1	A	106	ASN
1	A	128	ASP
1	A	144	LEU
1	A	180	ASP
1	A	214	LYS

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Mol	Chain	Res	Type
1	A	235	ASN
1	A	250	ASN
1	A	284	ASN
1	A	313	SER
1	A	325	ASN
1	A	380	ILE
1	A	433	GLU
1	A	437	LYS
1	A	467	ILE
1	A	469	LYS
1	A	494	LEU
1	A	568	LYS
1	A	571	HIS
1	A	576	GLN
1	A	641	ARG
1	A	708	PHE
1	A	782	LYS
1	A	830	SER
1	A	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	57	HIS
1	A	97	ASN
1	A	106	ASN
1	A	167	ASN
1	A	235	ASN
1	A	282	ASN
1	A	284	ASN
1	A	295	GLN
1	A	325	ASN
1	A	450	HIS
1	A	459	HIS
1	A	477	HIS
1	A	484	ASN
1	A	556	HIS
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	595	ASN

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Mol	Chain	Res	Type
1	A	614	HIS
1	A	767	HIS
1	A	768	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](#)

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	CRA	A	998	-	16,19,19	1.42	2 (12%)	19,28,28	1.68	2 (10%)
4	IMP	A	930	-	25,25,25	1.47	4 (16%)	37,38,38	1.41	8 (21%)
3	PLP	A	999	1	15,15,16	2.22	6 (40%)	21,22,23	2.15	8 (38%)

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	CRA	A	998	-	-	1/11/38/38	0/1/1/1
4	IMP	A	930	-	-	5/10/26/26	0/3/3/3
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C5A-C5	4.55	1.62	1.50
3	A	999	PLP	C3-C2	-4.31	1.36	1.41
2	A	998	CRA	O8-C7	3.90	1.40	1.34
4	A	930	IMP	C8-N7	3.87	1.43	1.32
4	A	930	IMP	C2-N1	3.35	1.41	1.35
3	A	999	PLP	O3-C3	3.29	1.44	1.36
4	A	930	IMP	C5'-C4'	2.83	1.60	1.51
3	A	999	PLP	C4A-C4	-2.67	1.46	1.51
3	A	999	PLP	P-O3P	-2.65	1.45	1.54
3	A	999	PLP	C2A-C2	2.38	1.54	1.50
4	A	930	IMP	P-O3P	-2.20	1.46	1.54
2	A	998	CRA	C3-C4	2.12	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	CRA	O8-C7-N2	5.55	114.51	109.65
3	A	999	PLP	C2A-C2-C3	3.74	125.18	120.80
3	A	999	PLP	C3-C4-C5	3.70	123.03	118.59
3	A	999	PLP	O4P-C5A-C5	-3.05	103.63	109.36
3	A	999	PLP	O3P-P-O1P	2.99	122.47	110.83
3	A	999	PLP	C4A-C4-C5	-2.86	117.99	120.94
3	A	999	PLP	O2P-P-O4P	-2.81	99.34	106.67
3	A	999	PLP	C6-N1-C2	2.81	124.29	119.20
4	A	930	IMP	C6-C5-N7	-2.69	125.39	130.29
4	A	930	IMP	O4'-C4'-C3'	-2.56	100.06	105.15
3	A	999	PLP	C6-C5-C4	-2.48	116.06	118.10
4	A	930	IMP	O4'-C4'-C5'	-2.47	101.44	109.33
4	A	930	IMP	C6-C5-C4	2.42	122.47	118.83
4	A	930	IMP	N9-C8-N7	-2.35	109.04	113.40
4	A	930	IMP	N1-C2-N3	-2.34	122.80	125.50
2	A	998	CRA	O5-C5-C6	2.17	109.39	106.53
4	A	930	IMP	C5-C6-N1	-2.14	107.70	110.78
4	A	930	IMP	C8-N9-C4	2.02	109.81	106.03

There are no chirality outliers.

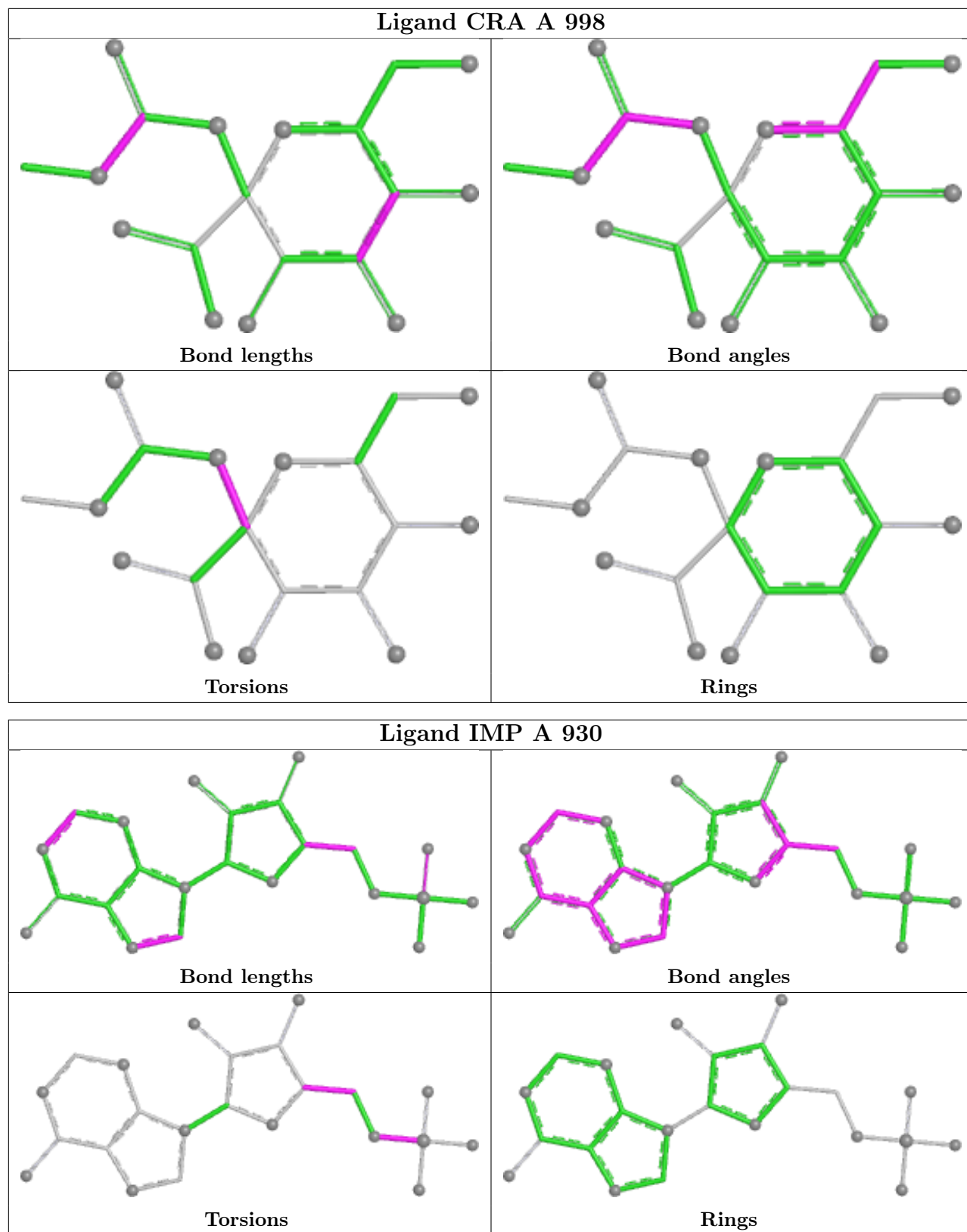
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	930	IMP	C5'-O5'-P-O1P
4	A	930	IMP	C5'-O5'-P-O2P
4	A	930	IMP	C5'-O5'-P-O3P
4	A	930	IMP	C3'-C4'-C5'-O5'
4	A	930	IMP	O4'-C4'-C5'-O5'
2	A	998	CRA	C2-C1-N2-C7

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 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 ⓘ

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.