



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 03:11 AM EDT

PDB ID : 1XKX
Title : Kinetic and crystallographic studies on 2-(beta-D-glucopyranosyl)-5-methyl-1,3,4-oxadiazole,-benzothiazole, and-benzimidazole, inhibitors of muscle glycogen phosphorylase b. Evidence for a new binding site.
Authors : Chrysina, E.D.; Kosmopoulou, M.N.; Tiraidis, C.; Kardakaris, R.; Bischler, N.; Leonidas, D.D.; Hadady, Z.; Somsak, L.; Docsa, T.; Gergely, P.; Oikonomakos, N.G.
Deposited on : 2004-09-30
Resolution : 1.93 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

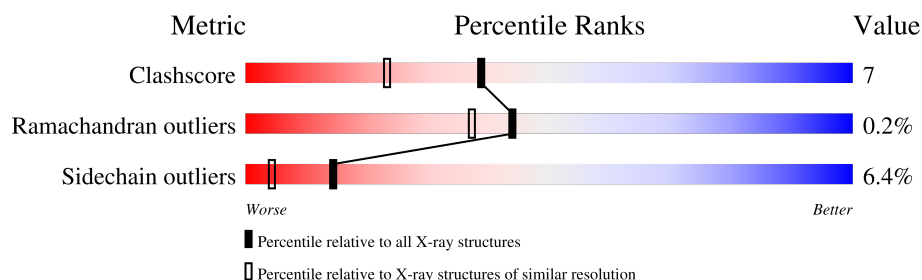
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)

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](#)

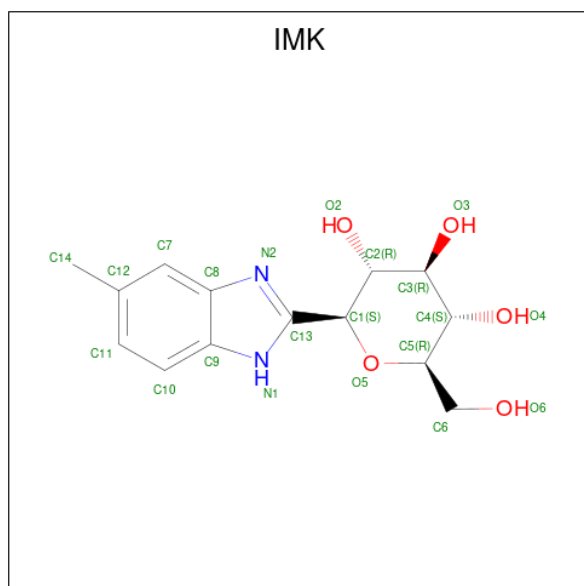
There are 4 unique types of molecules in this entry. The entry contains 7009 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

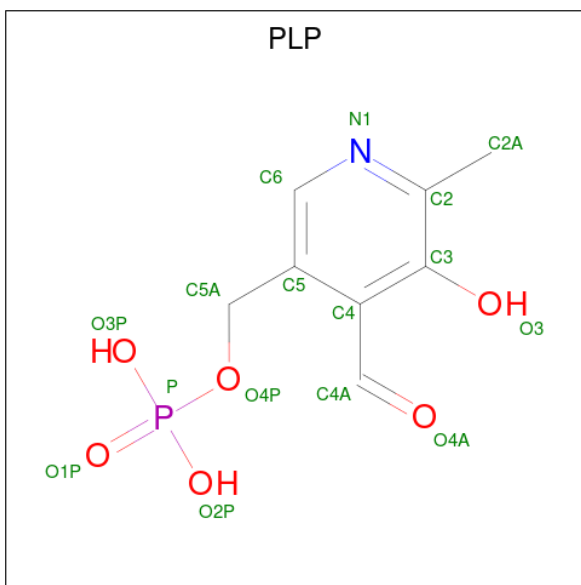
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	S	0	0	0
			6589	4201	1160	1199	29			

- Molecule 2 is 2-(BETA-D-GLUCOPYRANOSYL)-5-METHYL-1-BENZIMIDAZOLE (three-letter code: IMK) (formula: C₁₄H₁₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	13	2	5		
2	A	1	Total	C	N	O	0	0
			20	13	2	5		
2	A	1	Total	C	N	O	0	0
			20	13	2	5		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is water.

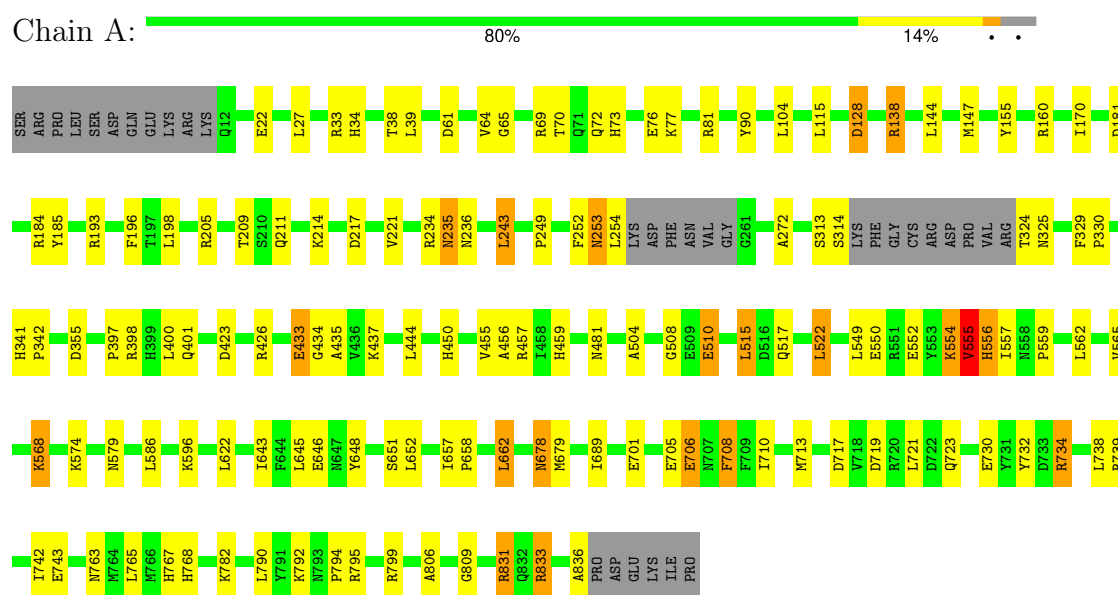
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	345	Total	O	0	0
			345	345		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Glycogen phosphorylase, muscle form



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	128.08 Å 128.08 Å 115.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.31 – 1.93	Depositor
% Data completeness (in resolution range)	99.8 (29.31-1.93)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.198	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7009	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: PLP, IMK

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	0.32	0/6736	0.60	0/9116

There are no bond length outliers.

There are no bond angle outliers.

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	6589	0	6533	89	0
2	A	60	0	45	3	0
3	A	15	0	7	0	0
4	A	345	0	0	7	0
All	All	7009	0	6585	89	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 7.

All (89) 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:138:ARG:O	1:A:138:ARG:HD3	1.77	0.85
1:A:455:VAL:H	1:A:459:HIS:HD2	1.28	0.82
1:A:708:PHE:HB3	1:A:710:ILE:CD1	2.12	0.79
1:A:708:PHE:HB3	1:A:710:ILE:HD11	1.67	0.76
1:A:678:ASN:HD22	1:A:679:MET:H	1.36	0.71
1:A:433:GLU:OE1	1:A:437:LYS:HD2	1.91	0.69
1:A:65:GLY:O	1:A:69:ARG:HG2	1.96	0.65
1:A:423:ASP:HB2	4:A:1232:HOH:O	1.95	0.65
1:A:355:ASP:OD1	1:A:398:ARG:HD3	1.97	0.64
1:A:61:ASP:O	1:A:64:VAL:HG22	1.98	0.63
1:A:235:ASN:H	1:A:235:ASN:HD22	1.45	0.62
1:A:236:ASN:CG	1:A:836:ALA:HB2	2.18	0.62
1:A:739:ARG:O	1:A:743:GLU:HG3	2.00	0.62
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.86	0.58
1:A:423:ASP:O	1:A:426:ARG:HG3	2.04	0.58
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.86	0.58
1:A:550:GLU:O	1:A:554:LYS:HD3	2.04	0.57
1:A:221:VAL:HG22	1:A:272:ALA:HB1	1.87	0.56
1:A:795:ARG:O	1:A:799:ARG:HG3	2.04	0.56
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.89	0.56
1:A:33:ARG:HH21	1:A:33:ARG:HG3	1.70	0.56
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.86	0.55
1:A:678:ASN:HD22	1:A:679:MET:N	2.04	0.55
1:A:221:VAL:HG23	2:A:910:IMK:C12	2.37	0.55
1:A:705:GLU:HG3	4:A:1029:HOH:O	2.07	0.55
1:A:708:PHE:HB3	1:A:710:ILE:HD12	1.87	0.55
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.08	0.54
1:A:510:GLU:HB2	4:A:1181:HOH:O	2.06	0.54
1:A:678:ASN:ND2	1:A:679:MET:H	2.04	0.54
1:A:138:ARG:HD3	1:A:138:ARG:C	2.27	0.54
1:A:556:HIS:CD2	1:A:556:HIS:N	2.74	0.54
1:A:568:LYS:HG3	1:A:574:LYS:HD3	1.90	0.52
1:A:763:ASN:OD1	1:A:767:HIS:HD2	1.92	0.52
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.90	0.52
1:A:678:ASN:HD22	1:A:678:ASN:N	2.07	0.52
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.13	0.51
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.92	0.51
1:A:170:ILE:HG12	1:A:646:GLU:HG3	1.93	0.51
1:A:144:LEU:HD12	1:A:147:MET:CE	2.41	0.50
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.93	0.50
1:A:556:HIS:CD2	1:A:556:HIS:H	2.29	0.50
1:A:554:LYS:O	1:A:555:VAL:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:SER:O	1:A:314:SER:C	2.50	0.50
1:A:710:ILE:HD12	1:A:710:ILE:N	2.27	0.49
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.43	0.48
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.95	0.48
1:A:549:LEU:HD12	1:A:557:ILE:HD13	1.95	0.47
1:A:235:ASN:H	1:A:235:ASN:ND2	2.12	0.47
1:A:181:ASP:HB3	1:A:184:ARG:NH2	2.30	0.47
1:A:738:LEU:O	1:A:742:ILE:HD13	2.16	0.46
1:A:434:GLY:O	1:A:435:ALA:C	2.54	0.46
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.98	0.46
1:A:450:HIS:HE1	4:A:1156:HOH:O	1.99	0.46
1:A:81:ARG:HG3	1:A:155:TYR:HE2	1.80	0.46
1:A:730:GLU:O	1:A:734:ARG:CG	2.65	0.45
1:A:253:ASN:ND2	4:A:1257:HOH:O	2.49	0.45
1:A:397:PRO:O	1:A:401:GLN:HG3	2.16	0.45
1:A:831:ARG:O	1:A:833:ARG:NH1	2.48	0.45
1:A:730:GLU:O	1:A:734:ARG:HG3	2.17	0.45
1:A:455:VAL:H	1:A:459:HIS:CD2	2.19	0.45
1:A:193:ARG:HB3	1:A:196:PHE:CD1	2.52	0.45
1:A:678:ASN:ND2	1:A:678:ASN:N	2.64	0.44
1:A:568:LYS:HE2	4:A:1123:HOH:O	2.18	0.43
1:A:456:ALA:C	1:A:481:ASN:HD21	2.22	0.43
1:A:72:GLN:O	1:A:76:GLU:HG2	2.19	0.43
1:A:73:HIS:NE2	1:A:77:LYS:HD2	2.34	0.43
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.99	0.43
1:A:205:ARG:NE	1:A:217:ASP:OD2	2.52	0.43
1:A:184:ARG:HE	1:A:185:TYR:HE2	1.66	0.43
1:A:450:HIS:HD2	4:A:1273:HOH:O	2.00	0.43
1:A:73:HIS:CE1	1:A:77:LYS:HD2	2.54	0.42
1:A:221:VAL:CG2	2:A:910:IMK:C12	2.97	0.42
1:A:557:ILE:O	1:A:559:PRO:HD3	2.19	0.42
1:A:209:THR:HG21	1:A:214:LYS:HZ2	1.85	0.42
1:A:678:ASN:ND2	1:A:679:MET:N	2.66	0.42
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.55	0.42
1:A:252:PHE:C	1:A:254:LEU:H	2.22	0.42
1:A:249:PRO:O	1:A:252:PHE:HB2	2.20	0.41
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.02	0.41
1:A:504:ALA:HA	1:A:508:GLY:O	2.20	0.41
1:A:70:THR:O	1:A:73:HIS:HB3	2.20	0.41
1:A:706:GLU:H	1:A:706:GLU:CD	2.24	0.41
1:A:719:ASP:O	1:A:723:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HG23	2:A:910:IMK:C11	2.51	0.41
1:A:792:LYS:O	1:A:794:PRO:HD3	2.21	0.41
1:A:193:ARG:HB3	1:A:196:PHE:HD1	1.84	0.41
1:A:510:GLU:HB3	1:A:517:GLN:HE22	1.85	0.41
1:A:689:ILE:HG23	1:A:689:ILE:O	2.20	0.41
1:A:235:ASN:HD22	1:A:235:ASN:N	2.07	0.41

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	804/842 (96%)	769 (96%)	33 (4%)	2 (0%)	44 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	LYS
1	A	555	VAL

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	701/731 (96%)	656 (94%)	45 (6%)	14 4

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	27	LEU
1	A	39	LEU
1	A	90	TYR
1	A	104	LEU
1	A	115	LEU
1	A	128	ASP
1	A	138	ARG
1	A	198	LEU
1	A	211	GLN
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	253	ASN
1	A	324	THR
1	A	325	ASN
1	A	400	LEU
1	A	433	GLU
1	A	444	LEU
1	A	510	GLU
1	A	515	LEU
1	A	522	LEU
1	A	552	GLU
1	A	555	VAL
1	A	556	HIS
1	A	565	VAL
1	A	568	LYS
1	A	579	ASN
1	A	586	LEU
1	A	596	LYS
1	A	622	LEU
1	A	643	ILE
1	A	645	LEU
1	A	662	LEU
1	A	678	ASN
1	A	706	GLU
1	A	708	PHE
1	A	721	LEU
1	A	734	ARG
1	A	765	LEU
1	A	768	HIS
1	A	782	LYS

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Mol	Chain	Res	Type
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	73	HIS
1	A	211	GLN
1	A	235	ASN
1	A	264	GLN
1	A	270	ASN
1	A	325	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	556	HIS
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	767	HIS
1	A	832	GLN

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

4 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	IMK	A	998	-	19,22,23	1.56	4 (21%)	25,32,34	1.07	2 (8%)
2	IMK	A	910	-	19,22,23	1.52	4 (21%)	25,32,34	1.23	3 (12%)
3	PLP	A	999	1	15,15,16	1.36	1 (6%)	21,22,23	1.04	1 (4%)
2	IMK	A	920	-	19,22,23	1.58	4 (21%)	25,32,34	1.06	2 (8%)

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	IMK	A	998	-	-	0/2/26/26	0/3/3/3
2	IMK	A	910	-	-	2/2/26/26	0/3/3/3
3	PLP	A	999	1	-	2/6/6/8	0/1/1/1
2	IMK	A	920	-	-	0/2/26/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	920	IMK	C12-C7	3.29	1.43	1.36
2	A	998	IMK	C12-C7	3.29	1.43	1.36
2	A	998	IMK	C11-C10	3.22	1.43	1.36
2	A	920	IMK	C11-C10	3.16	1.43	1.36
3	A	999	PLP	C3-C2	-2.85	1.38	1.41
2	A	910	IMK	C11-C10	2.69	1.42	1.36
2	A	920	IMK	C12-C11	2.49	1.43	1.38
2	A	910	IMK	C12-C11	2.47	1.43	1.38
2	A	910	IMK	C12-C7	2.34	1.41	1.36
2	A	910	IMK	C4-C5	2.33	1.58	1.53
2	A	998	IMK	C12-C11	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	920	IMK	O5-C1	2.30	1.46	1.43
2	A	998	IMK	O5-C1	2.28	1.46	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	910	IMK	C12-C7-C8	-3.34	115.52	120.09
2	A	910	IMK	C11-C10-C9	-3.02	115.96	120.09
2	A	998	IMK	C12-C7-C8	-3.02	115.96	120.09
2	A	998	IMK	C11-C10-C9	-2.90	116.12	120.09
2	A	920	IMK	C12-C7-C8	-2.86	116.18	120.09
2	A	920	IMK	C11-C10-C9	-2.46	116.73	120.09
3	A	999	PLP	O3P-P-O1P	2.40	120.19	110.83
2	A	910	IMK	C13-C1-C2	-2.11	108.40	113.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	910	IMK	C4-C5-C6-O6
2	A	910	IMK	O5-C5-C6-O6
3	A	999	PLP	C6-C5-C5A-O4P
3	A	999	PLP	C4-C5-C5A-O4P

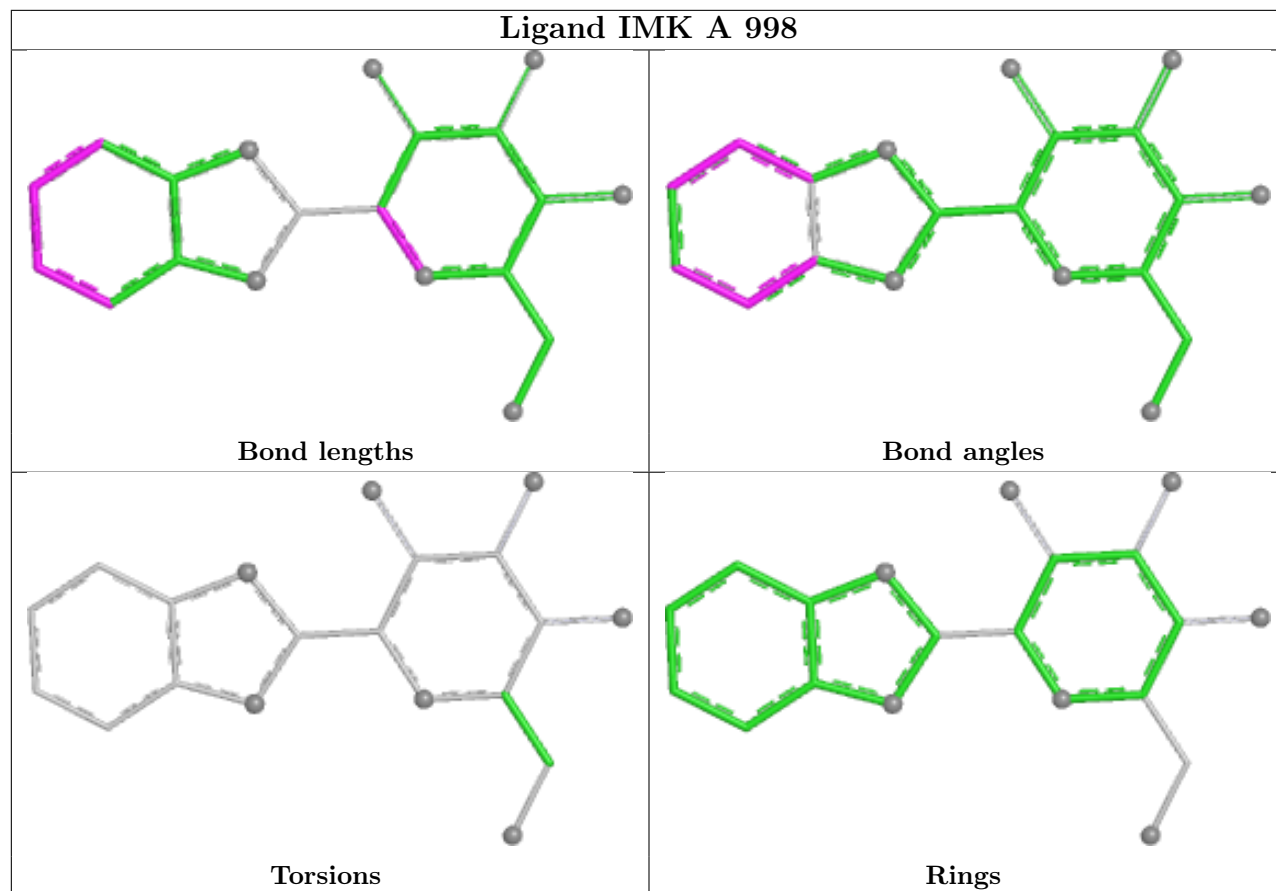
There are no ring outliers.

1 monomer is involved in 3 short contacts:

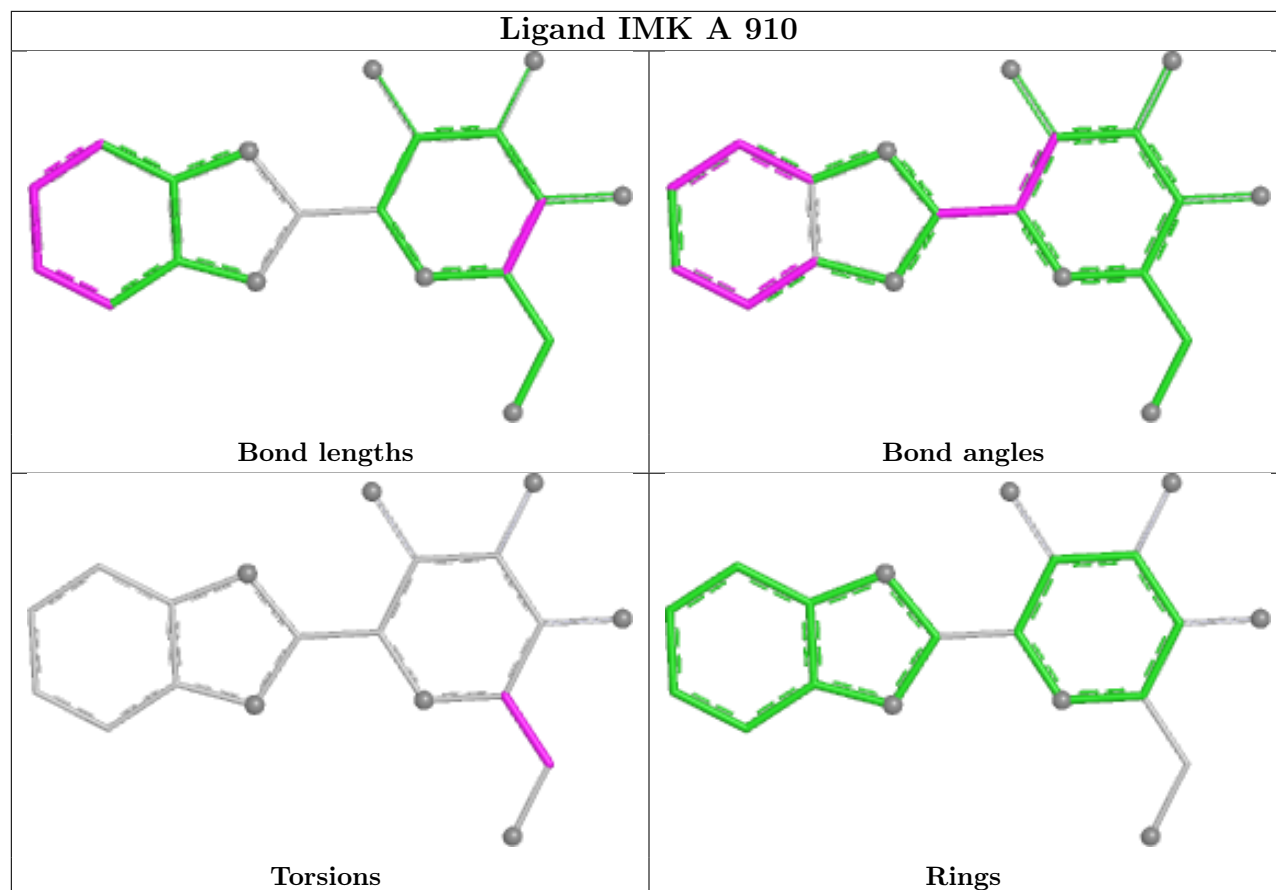
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	910	IMK	3	0

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

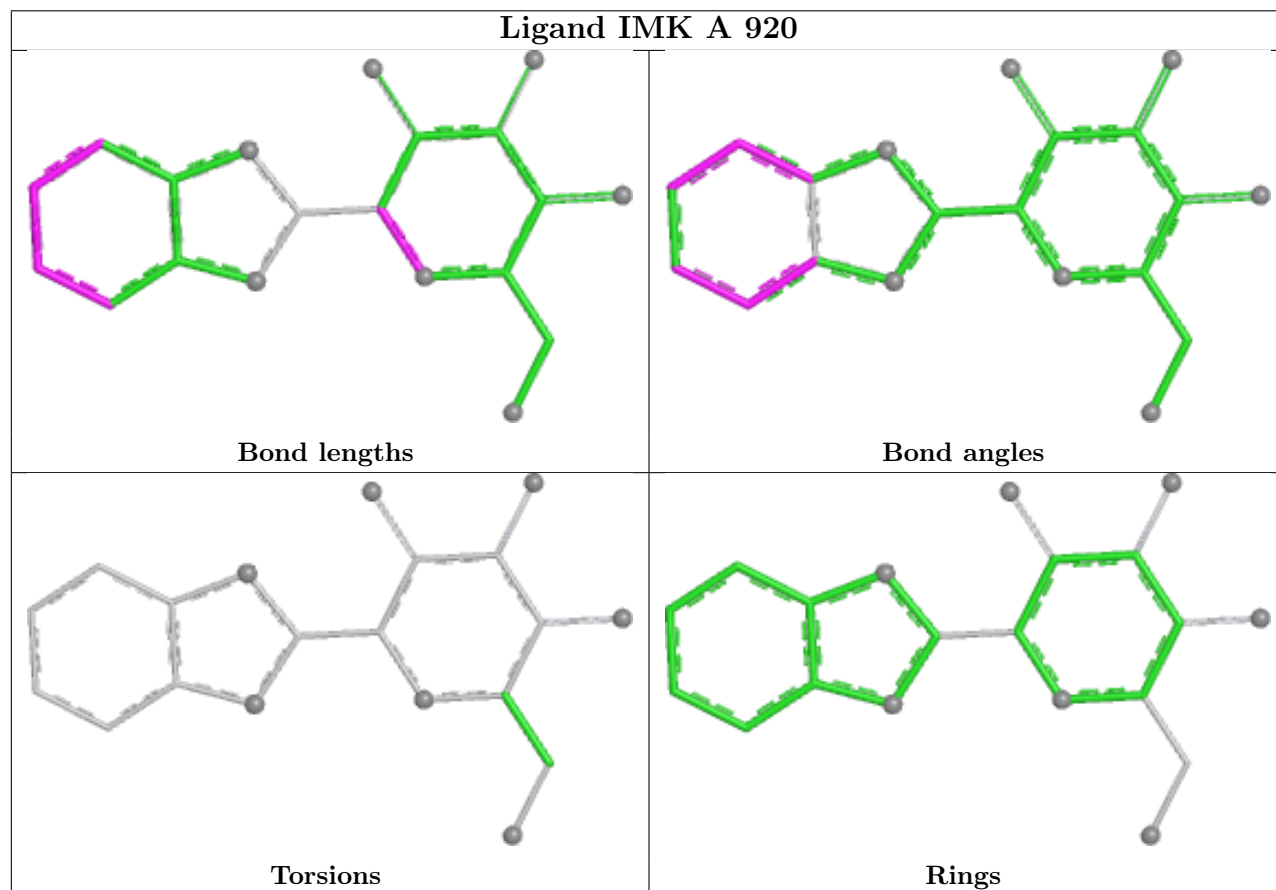
equivalents in the CSD to analyse the geometry.



Ligand IMK A 910



Ligand IMK A 920



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

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.