



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:07 PM UTC

PDB ID : 1E1Y / pdb_00001e1y
Title : Flavopiridol inhibits glycogen phosphorylase by binding at the inhibitor site
Authors : Oikonomakos, N.G.; Zographos, S.E.; Skamnaki, V.T.; Tsitsanou, K.E.; Johnson, L.N.
Deposited on : 2000-05-11
Resolution : 2.23 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

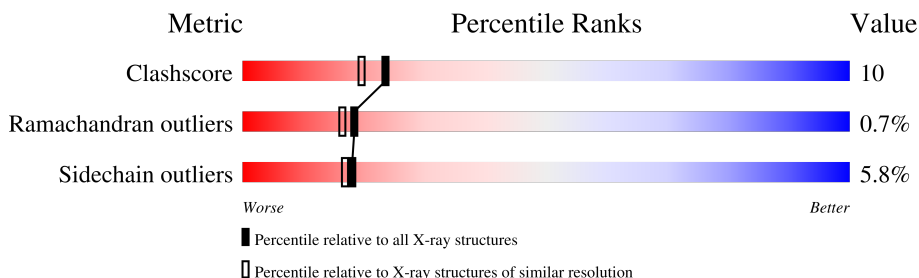
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)

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	 73% 20% . .

2 Entry composition [i](#)

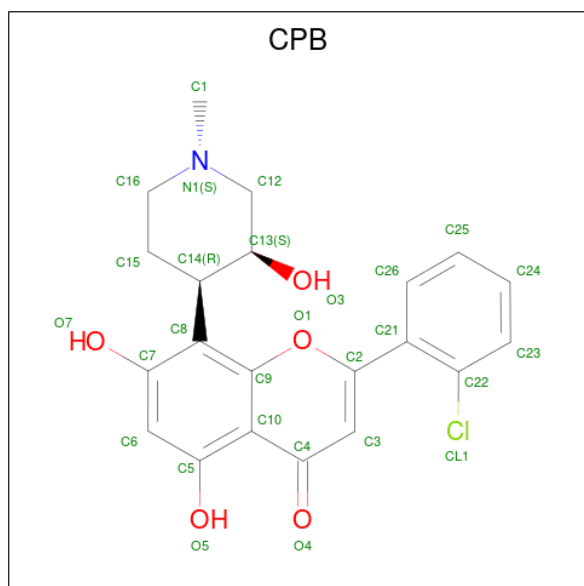
There are 6 unique types of molecules in this entry. The entry contains 7320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

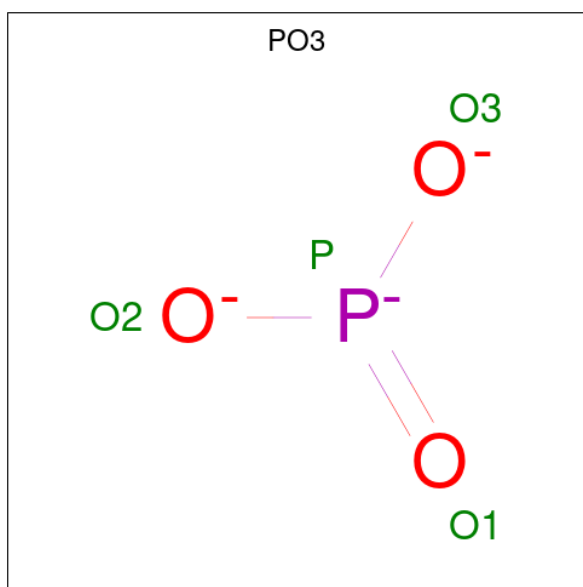
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	813	Total	C	N	O	S	0	0	0
			6617	4215	1168	1205	29			

- Molecule 2 is 2-(2-CHLORO-PHENYL)-5,7-DIHYDROXY-8-(3-HYDROXY-1-METHYL-PIPERIDIN-4-YL)-4H-BENZOPYRAN-4-ONE (CCD ID: CPB) (formula: C₂₁H₂₀ClNO₅).



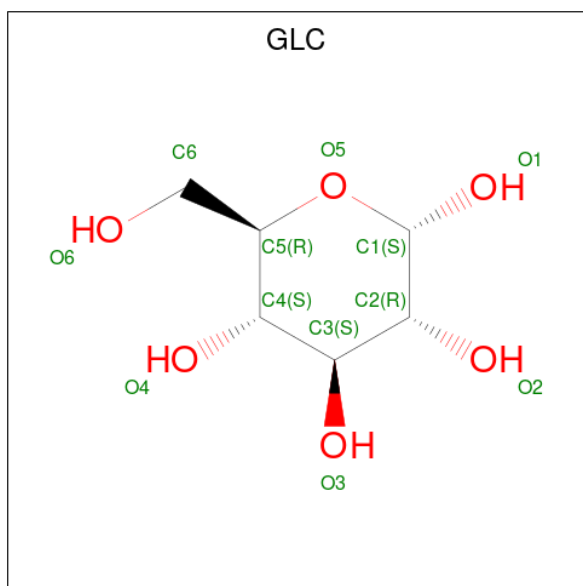
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	21	1	1	5		

- Molecule 3 is PHOSPHITE ION (CCD ID: PO3) (formula: O₃P).



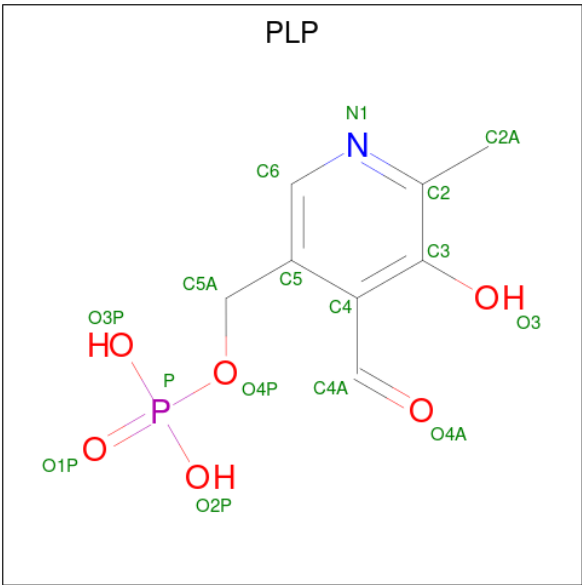
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			4	3	1		

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	644	Total	O	0	0
			644	644		

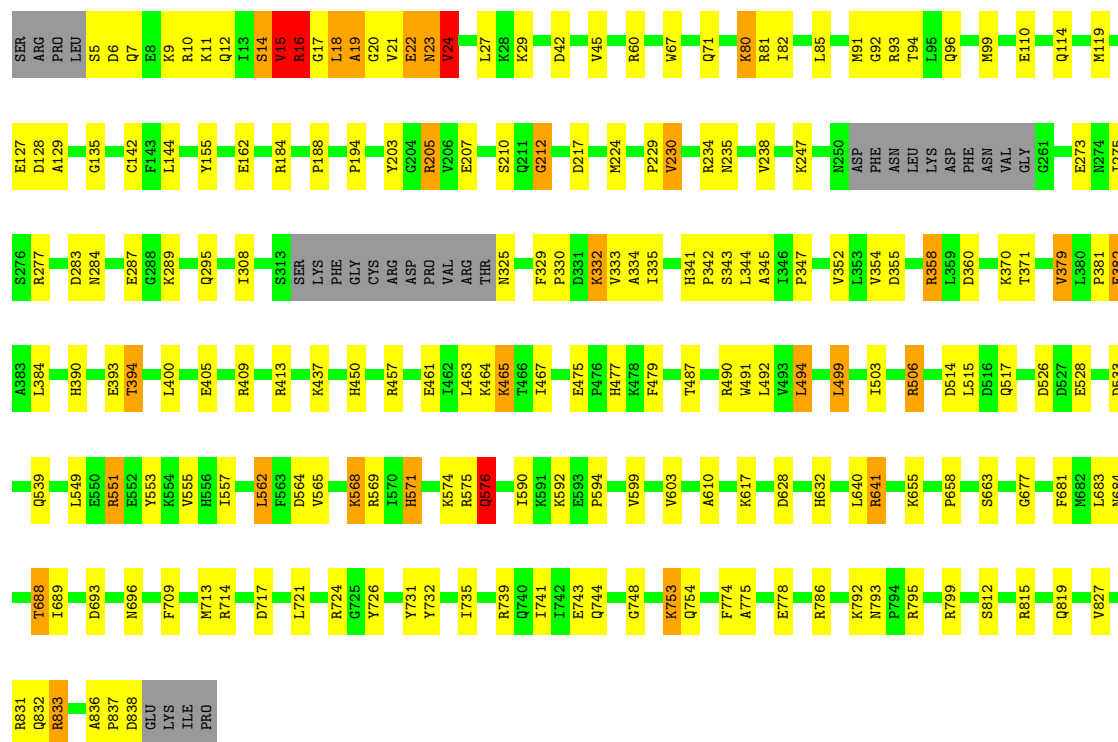
3 Residue-property plots

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

Chain A:  73% 20% . .



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	126.76 Å 126.76 Å 116.02 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.23	Depositor
% Data completeness (in resolution range)	87.3 (29.90-2.23)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.195 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7320	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: GLC, PO3, PLP, CPB

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	0.41	0/6764	0.94	26/9151 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	VAL	N-CA-C	8.68	120.26	108.11
1	A	91	MET	N-CA-C	8.00	121.10	111.82
1	A	576	GLN	N-CA-C	-6.87	103.85	111.82
1	A	714	ARG	N-CA-C	-6.54	100.29	110.17
1	A	575	ARG	N-CA-C	6.21	119.81	111.24
1	A	24	VAL	N-CA-C	6.21	122.25	109.34
1	A	754	GLN	CA-C-N	6.19	127.58	119.84
1	A	754	GLN	C-N-CA	6.19	127.58	119.84
1	A	15	VAL	N-CA-C	-6.06	104.83	113.07
1	A	333	VAL	N-CA-C	5.98	116.73	108.12
1	A	688	THR	N-CA-C	5.87	118.53	109.07
1	A	610	ALA	N-CA-C	-5.72	102.37	109.64
1	A	479	PHE	N-CA-C	5.69	118.81	109.76
1	A	748	GLY	N-CA-C	-5.62	107.23	115.72
1	A	129	ALA	N-CA-C	-5.61	96.07	107.41
1	A	491	TRP	N-CA-C	5.60	119.20	112.93
1	A	677	GLY	N-CA-C	-5.53	106.09	112.73
1	A	14	SER	CA-CB-OG	5.48	122.06	111.10
1	A	203	TYR	CB-CA-C	-5.37	110.40	116.63
1	A	80	LYS	N-CA-C	-5.20	102.69	110.23
1	A	212	GLY	N-CA-C	5.17	117.58	111.63
1	A	684	ASN	N-CA-C	5.15	119.25	112.92
1	A	135	GLY	N-CA-C	5.14	118.46	112.50
1	A	836	ALA	CA-C-N	5.08	126.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	836	ALA	C-N-CA	5.08	126.18	119.84
1	A	355	ASP	N-CA-C	5.06	116.87	111.36

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	6617	0	6563	135	0
2	A	28	0	20	0	0
3	A	4	0	0	0	0
4	A	12	0	12	0	0
5	A	15	0	7	0	0
6	A	644	0	0	25	4
All	All	7320	0	6602	135	4

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 10.

All (135) 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:18:LEU:HD22	1:A:19:ALA:H	1.31	0.95
1:A:93:ARG:NH1	6:A:2092:HOH:O	1.98	0.90
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.54	0.90
1:A:212:GLY:HA3	1:A:358:ARG:HH12	1.37	0.88
1:A:18:LEU:HD22	1:A:19:ALA:N	1.94	0.82
1:A:18:LEU:HD13	1:A:20:GLY:H	1.43	0.81
1:A:212:GLY:HA3	1:A:358:ARG:NH1	2.01	0.75
1:A:22:GLU:HG3	6:A:2019:HOH:O	1.88	0.74
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.73	0.71
1:A:358:ARG:HA	1:A:358:ARG:HE	1.56	0.70
1:A:325:ASN:HB3	6:A:2289:HOH:O	1.91	0.69
1:A:22:GLU:HB3	6:A:2020:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:H	1:A:382:GLU:CD	2.03	0.67
1:A:5:SER:HB3	1:A:9:LYS:HE3	1.76	0.66
1:A:390:HIS:O	1:A:394:THR:HG23	1.95	0.65
1:A:732:TYR:O	1:A:739:ARG:HG3	1.97	0.64
1:A:60:ARG:HD2	1:A:188:PRO:O	1.97	0.64
1:A:16:ARG:HG3	1:A:17:GLY:H	1.65	0.62
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.33	0.62
1:A:382:GLU:OE1	1:A:382:GLU:N	2.33	0.62
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.80	0.61
1:A:18:LEU:HD13	1:A:20:GLY:N	2.16	0.61
1:A:247:LYS:HA	1:A:273:GLU:HG2	1.82	0.61
1:A:571:HIS:H	1:A:576:GLN:HE22	1.49	0.60
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.84	0.60
1:A:592:LYS:HE2	6:A:2441:HOH:O	2.01	0.59
1:A:640:LEU:O	1:A:641:ARG:NH1	2.36	0.59
1:A:18:LEU:HD13	1:A:18:LEU:C	2.28	0.59
1:A:655:LYS:O	1:A:658:PRO:HD2	2.02	0.59
1:A:753:LYS:NZ	1:A:753:LYS:H	2.00	0.59
1:A:793:ASN:HD22	1:A:793:ASN:C	2.09	0.58
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.85	0.58
1:A:506:ARG:NH2	1:A:533:ASP:OD2	2.34	0.58
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.86	0.58
1:A:628:ASP:O	1:A:632:HIS:HD2	1.87	0.58
1:A:127:GLU:HG2	6:A:2124:HOH:O	2.04	0.57
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.87	0.57
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.70	0.56
1:A:461:GLU:O	1:A:465:LYS:HG2	2.05	0.56
1:A:381:PRO:HG2	1:A:382:GLU:OE1	2.06	0.56
1:A:12:GLN:O	1:A:16:ARG:NH2	2.38	0.55
1:A:127:GLU:HG3	6:A:2127:HOH:O	2.05	0.55
1:A:332:LYS:NZ	1:A:332:LYS:HB3	2.20	0.55
1:A:753:LYS:H	1:A:753:LYS:HZ2	1.54	0.55
1:A:344:LEU:C	1:A:347:PRO:HD2	2.31	0.55
1:A:562:LEU:C	1:A:562:LEU:HD12	2.33	0.54
1:A:308:ILE:HD13	1:A:352:VAL:HG11	1.89	0.54
1:A:568:LYS:CD	1:A:574:LYS:HD3	2.38	0.53
1:A:393:GLU:HB3	1:A:400:LEU:CD2	2.38	0.53
1:A:457:ARG:NH1	6:A:2362:HOH:O	2.26	0.53
1:A:18:LEU:CD2	1:A:19:ALA:H	2.15	0.53
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.39	0.52
1:A:528:GLU:CD	1:A:795:ARG:HH12	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:HG3	1:A:114:GLN:HE21	1.74	0.52
1:A:641:ARG:HA	1:A:641:ARG:HH11	1.74	0.52
1:A:393:GLU:HB3	1:A:400:LEU:HD23	1.92	0.52
1:A:450:HIS:HE1	6:A:2305:HOH:O	1.92	0.51
1:A:641:ARG:HH11	1:A:641:ARG:CG	2.23	0.51
1:A:212:GLY:CA	1:A:358:ARG:HH12	2.17	0.51
1:A:663:SER:HB2	1:A:681:PHE:CG	2.46	0.51
1:A:815:ARG:O	1:A:819:GLN:HG3	2.10	0.51
1:A:553:TYR:O	1:A:555:VAL:HG23	2.11	0.51
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.51
1:A:81:ARG:NE	6:A:2080:HOH:O	2.44	0.50
1:A:142:CYS:SG	1:A:487:THR:HG22	2.52	0.50
1:A:16:ARG:O	1:A:838:ASP:HA	2.11	0.50
1:A:354:VAL:O	1:A:358:ARG:HA	2.12	0.50
1:A:15:VAL:O	1:A:16:ARG:C	2.54	0.49
1:A:162:GLU:OE2	1:A:277:ARG:NH1	2.42	0.49
1:A:283:ASP:OD1	1:A:571:HIS:HE1	1.95	0.49
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.43	0.49
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.12	0.49
1:A:71:GLN:NE2	6:A:2069:HOH:O	2.34	0.49
1:A:413:ARG:NH1	6:A:2334:HOH:O	2.45	0.49
1:A:24:VAL:HG11	1:A:114:GLN:HE22	1.77	0.49
1:A:617:LYS:HE2	6:A:2157:HOH:O	2.13	0.49
1:A:18:LEU:HD12	6:A:2636:HOH:O	2.13	0.48
1:A:24:VAL:HG11	1:A:114:GLN:NE2	2.28	0.48
1:A:194:PRO:HD3	1:A:224:MET:HE3	1.95	0.48
1:A:641:ARG:NH1	1:A:641:ARG:HG3	2.29	0.48
1:A:786:ARG:HD2	6:A:2595:HOH:O	2.13	0.48
1:A:786:ARG:NH2	6:A:2597:HOH:O	2.28	0.48
1:A:492:LEU:HD22	1:A:683:LEU:HD11	1.94	0.48
1:A:739:ARG:O	1:A:743:GLU:HG3	2.14	0.47
1:A:67:TRP:CD2	1:A:229:PRO:HB3	2.49	0.47
1:A:235:ASN:HB3	1:A:831:ARG:NH2	2.29	0.47
1:A:457:ARG:NH2	6:A:2361:HOH:O	2.48	0.47
1:A:599:VAL:CG2	1:A:792:LYS:HG3	2.45	0.47
1:A:689:ILE:HG23	1:A:689:ILE:O	2.14	0.47
1:A:564:ASP:HB3	1:A:603:VAL:HA	1.97	0.47
1:A:688:THR:O	1:A:709:PHE:HB2	2.15	0.46
1:A:230:VAL:HG22	1:A:230:VAL:O	2.16	0.46
1:A:477:HIS:HB3	6:A:2380:HOH:O	2.15	0.46
1:A:475:GLU:HB3	1:A:477:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:O	1:A:22:GLU:CB	2.63	0.46
1:A:379:VAL:HG13	6:A:2309:HOH:O	2.16	0.46
1:A:205:ARG:NH2	1:A:207:GLU:OE1	2.49	0.46
1:A:569:ARG:O	1:A:574:LYS:HD2	2.16	0.45
1:A:21:VAL:O	1:A:22:GLU:HB2	2.16	0.45
1:A:42:ASP:OD1	1:A:45:VAL:HG22	2.17	0.45
1:A:528:GLU:OE2	1:A:795:ARG:NH1	2.46	0.45
1:A:230:VAL:O	1:A:230:VAL:CG2	2.65	0.45
1:A:358:ARG:HE	1:A:358:ARG:CA	2.21	0.45
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.99	0.44
1:A:67:TRP:HA	1:A:238:VAL:HB	2.00	0.44
1:A:568:LYS:HE3	6:A:2434:HOH:O	2.17	0.44
1:A:515:LEU:C	1:A:517:GLN:H	2.27	0.43
1:A:405:GLU:OE2	1:A:409:ARG:NH1	2.51	0.43
1:A:335:ILE:HD12	1:A:371:THR:CG2	2.49	0.43
1:A:344:LEU:O	1:A:347:PRO:HD2	2.19	0.43
1:A:549:LEU:HD12	1:A:557:ILE:HD13	2.00	0.43
1:A:833:ARG:H	1:A:833:ARG:HG3	1.67	0.43
1:A:641:ARG:HH11	1:A:641:ARG:CA	2.31	0.42
1:A:475:GLU:HB3	1:A:477:HIS:NE2	2.35	0.42
1:A:99:MET:HE1	1:A:119:MET:HE3	2.02	0.42
1:A:735:ILE:HD13	1:A:778:GLU:HG3	2.01	0.42
1:A:23:ASN:HD22	1:A:23:ASN:HA	1.55	0.42
1:A:731:TYR:CE2	1:A:775:ALA:HA	2.54	0.41
1:A:526:ASP:OD1	1:A:799:ARG:NH2	2.53	0.41
1:A:94:THR:HG23	6:A:2101:HOH:O	2.20	0.41
1:A:590:ILE:O	1:A:594:PRO:HA	2.21	0.41
1:A:693:ASP:O	1:A:696:ASN:HB2	2.21	0.41
1:A:551:ARG:HD2	6:A:2424:HOH:O	2.20	0.41
1:A:14:SER:HB3	1:A:16:ARG:HG2	2.03	0.41
1:A:110:GLU:HG3	1:A:114:GLN:NE2	2.35	0.41
1:A:275:ILE:O	1:A:295:GLN:HG2	2.20	0.41
1:A:283:ASP:O	1:A:284:ASN:HB2	2.20	0.41
1:A:390:HIS:O	1:A:394:THR:CG2	2.67	0.41
1:A:499:LEU:HD22	1:A:503:ILE:HG13	2.03	0.41
1:A:18:LEU:CD1	6:A:2636:HOH:O	2.67	0.40
1:A:96:GLN:NE2	6:A:2097:HOH:O	2.53	0.40
1:A:6:ASP:HB3	1:A:7:GLN:H	1.64	0.40
1:A:343:SER:C	1:A:345:ALA:N	2.80	0.40
1:A:92:GLY:HA2	1:A:128:ASP:OD1	2.22	0.40
1:A:93:ARG:HD3	6:A:2092:HOH:O	2.22	0.40

All (4) 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)
6:A:2018:HOH:O	6:A:2172:HOH:O[7_556]	1.93	0.27
6:A:2018:HOH:O	6:A:2176:HOH:O[7_556]	2.04	0.16
6:A:2039:HOH:O	6:A:2039:HOH:O[7_556]	2.04	0.16
6:A:2220:HOH:O	6:A:2220:HOH:O[7_555]	2.19	0.01

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	807/842 (96%)	769 (95%)	32 (4%)	6 (1%)	18 16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	ALA
1	A	22	GLU
1	A	24	VAL
1	A	514	ASP
1	A	837	PRO

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	704/731 (96%)	663 (94%)	41 (6%)	18	17

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	LYS
1	A	15	VAL
1	A	16	ARG
1	A	18	LEU
1	A	23	ASN
1	A	27	LEU
1	A	29	LYS
1	A	144	LEU
1	A	184	ARG
1	A	205	ARG
1	A	210	SER
1	A	217	ASP
1	A	230	VAL
1	A	234	ARG
1	A	332	LYS
1	A	358	ARG
1	A	360	ASP
1	A	370	LYS
1	A	379	VAL
1	A	382	GLU
1	A	384	LEU
1	A	394	THR
1	A	437	LYS
1	A	464	LYS
1	A	465	LYS
1	A	494	LEU
1	A	499	LEU
1	A	506	ARG
1	A	539	GLN
1	A	551	ARG
1	A	562	LEU
1	A	568	LYS
1	A	571	HIS
1	A	576	GLN
1	A	641	ARG
1	A	721	LEU
1	A	724	ARG

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Mol	Chain	Res	Type
1	A	753	LYS
1	A	832	GLN
1	A	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	23	ASN
1	A	36	HIS
1	A	106	ASN
1	A	201	HIS
1	A	325	ASN
1	A	412	ASN
1	A	450	HIS
1	A	477	HIS
1	A	484	ASN
1	A	496	ASN
1	A	517	GLN
1	A	541	ASN
1	A	560	ASN
1	A	566	GLN
1	A	571	HIS
1	A	576	GLN
1	A	579	ASN
1	A	588	ASN
1	A	632	HIS
1	A	684	ASN
1	A	744	GLN
1	A	754	GLN
1	A	767	HIS
1	A	793	ASN

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 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
5	PLP	A	999	1	15,15,16	1.34	1 (6%)	21,22,23	1.08	2 (9%)
4	GLC	A	998	-	12,12,12	1.01	0	17,17,17	0.98	1 (5%)
2	CPB	A	940	-	31,31,31	2.56	16 (51%)	42,46,46	2.04	10 (23%)
3	PO3	A	997	1	0,3,3	-	-	0,3,3	-	-

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
5	PLP	A	999	1	-	0/6/6/8	0/1/1/1
4	GLC	A	998	-	-	0/2/22/22	0/1/1/1
2	CPB	A	940	-	-	0/8/21/21	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	940	CPB	C14-C13	4.83	1.57	1.53
2	A	940	CPB	C8-C14	4.81	1.59	1.52
2	A	940	CPB	C7-C8	4.24	1.46	1.40
2	A	940	CPB	C21-C2	3.67	1.55	1.47
2	A	940	CPB	C10-C4	3.55	1.55	1.46
2	A	940	CPB	C9-C8	3.41	1.45	1.39
2	A	940	CPB	C21-C22	3.38	1.44	1.39
2	A	940	CPB	C26-C21	3.25	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	940	CPB	C6-C7	3.19	1.43	1.38
2	A	940	CPB	O7-C7	2.63	1.41	1.36
2	A	940	CPB	C12-C13	2.57	1.55	1.52
2	A	940	CPB	C25-C24	2.52	1.43	1.38
2	A	940	CPB	C24-C23	2.42	1.43	1.38
2	A	940	CPB	C6-C5	2.34	1.42	1.38
5	A	999	PLP	P-O3P	-2.32	1.46	1.54
2	A	940	CPB	O5-C5	2.24	1.40	1.36
2	A	940	CPB	C25-C26	2.19	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	940	CPB	O1-C2-C21	7.65	119.66	110.65
2	A	940	CPB	C9-O1-C2	3.93	124.44	120.04
2	A	940	CPB	O1-C9-C8	3.93	119.95	116.10
2	A	940	CPB	C15-C14-C13	3.11	112.17	109.35
2	A	940	CPB	C16-N1-C12	3.01	113.07	110.06
2	A	940	CPB	O3-C13-C14	2.92	115.69	110.81
2	A	940	CPB	O3-C13-C12	-2.86	104.19	109.66
2	A	940	CPB	C15-C16-N1	2.78	114.78	111.20
2	A	940	CPB	C5-C10-C9	2.35	120.79	117.04
5	A	999	PLP	C6-C5-C4	2.23	119.92	118.10
2	A	940	CPB	C9-C10-C4	-2.23	115.80	119.28
4	A	998	GLC	O5-C5-C6	2.11	111.66	106.44
5	A	999	PLP	O3P-P-O1P	2.07	118.90	110.83

There are no chirality outliers.

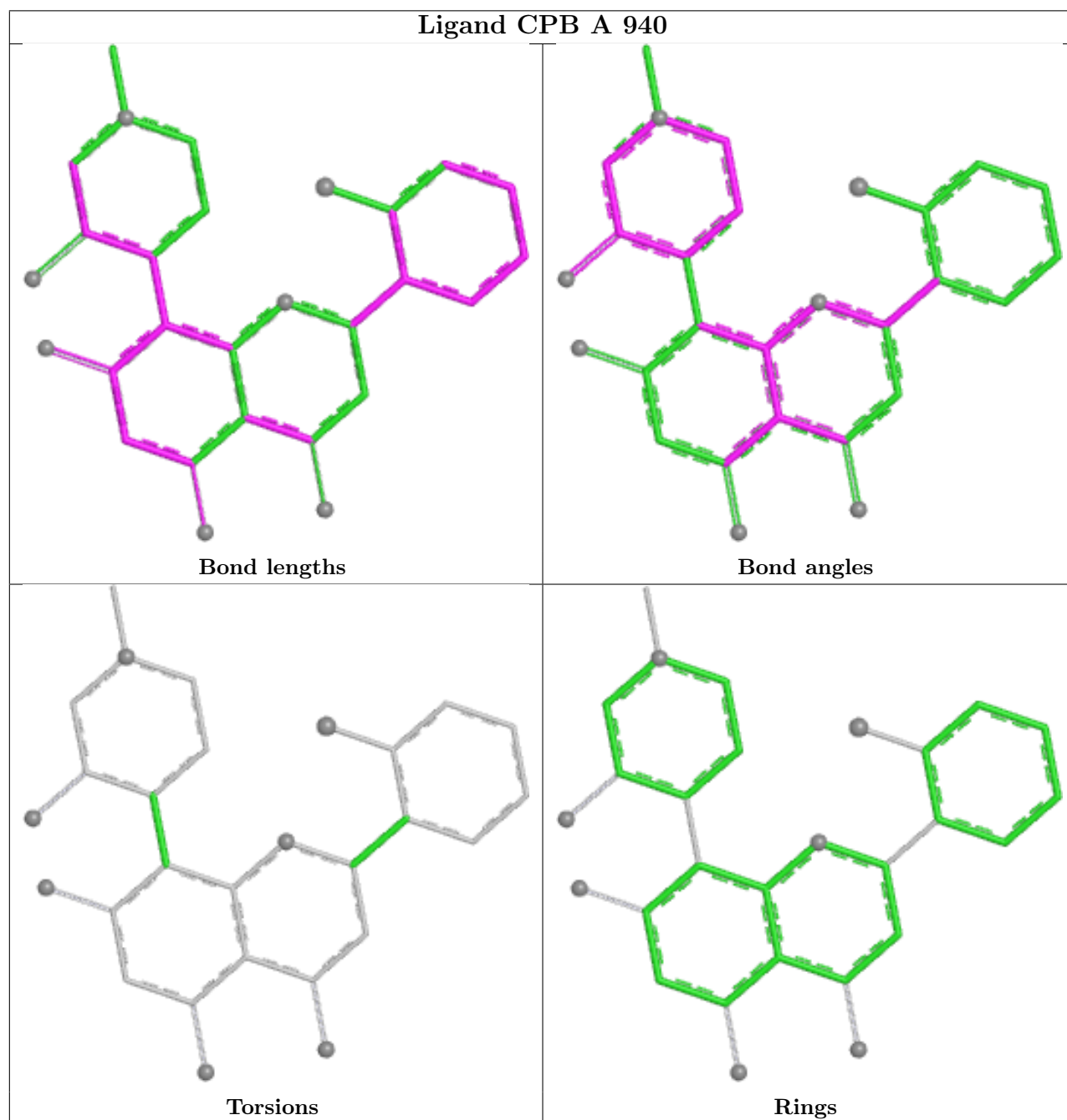
There are no torsion outliers.

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 [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.