



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:36 AM UTC

PDB ID : 3AMV / pdb_00003amv
Title : ALLOSTERIC INHIBITION OF GLYCOGEN PHOSPHORYLASE A BY A
POTENTIAL ANTIDIABETIC DRUG
Authors : Oikonomakos, N.G.; Tsitsanou, K.E.; Zographos, S.E.; Skamnaki, V.T.
Deposited on : 1999-02-18
Resolution : 2.10 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

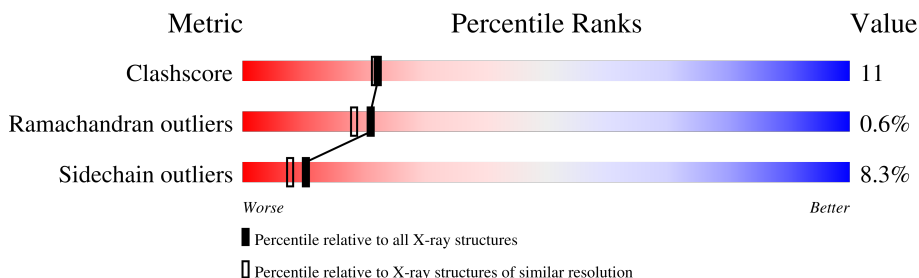
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 6 unique types of molecules in this entry. The entry contains 7425 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.

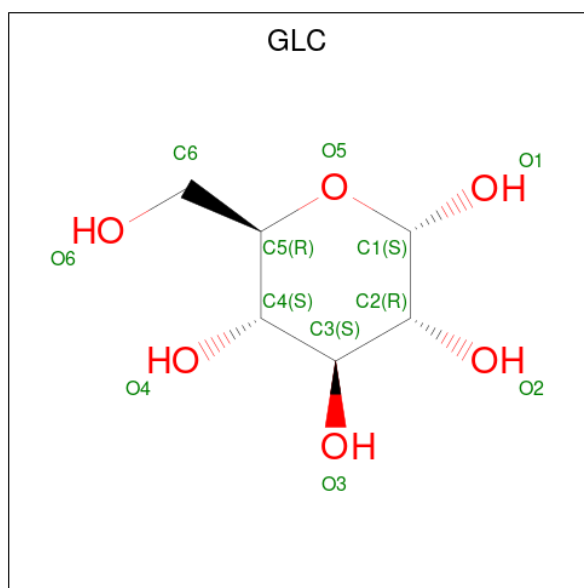
- Molecule 1 is a protein called PROTEIN (GLYCOGEN PHOSPHORYLASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	812	6611	4208	1167	1206	1	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	609	ALA	PRO	conflict	UNP P00489

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



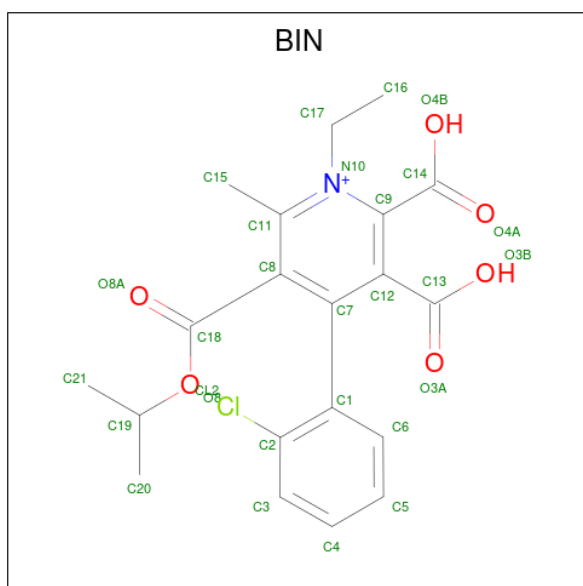
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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 2,3-DICARBOXY-4-(2-CHLORO-PHENYL)-1-ETHYL-5-ISOPROPOXYCARBONYL-6-METHYL-PYRIDINIUM (CCD ID: BIN) (formula: $C_{20}H_{21}ClNO_6$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

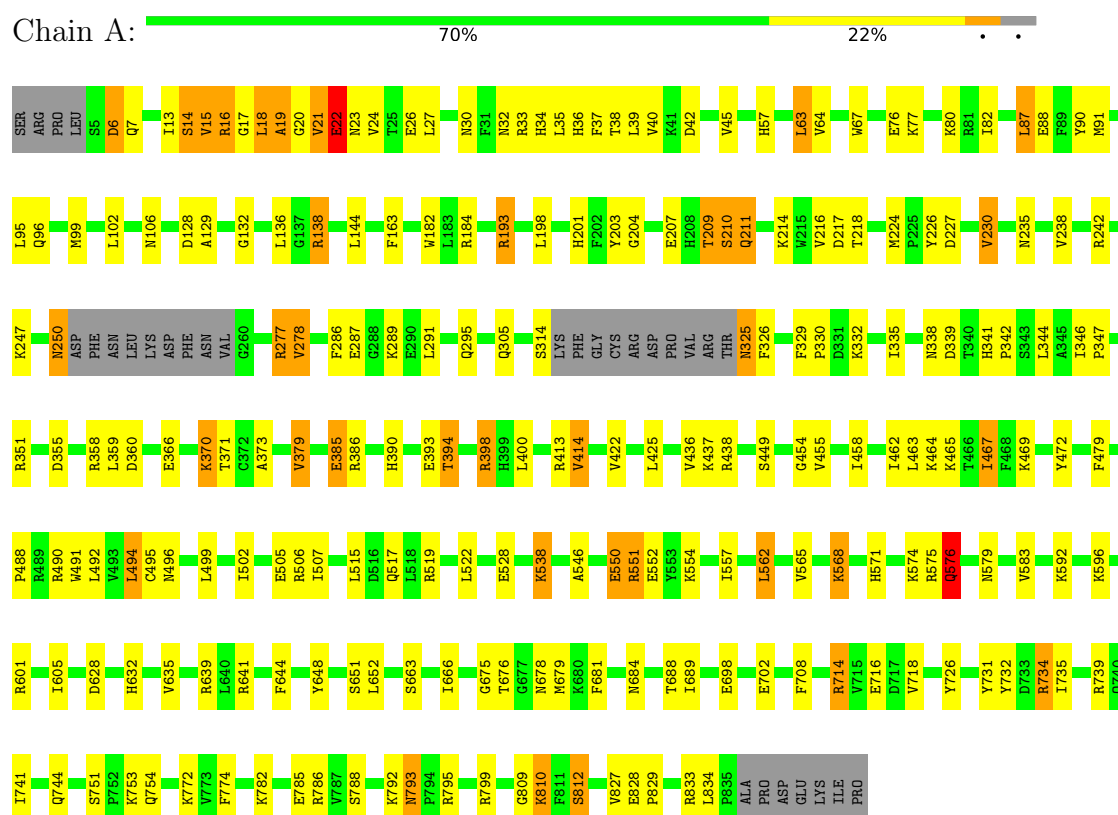
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	753	Total	O	0	0
			753	753		

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: PROTEIN (GLYCOGEN PHOSPHORYLASE)



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	127.20Å 127.20Å 115.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.9 (13.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.189 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7425	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: GOL, GLC, SEP, BIN, PLP

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	0.47	0/6746	1.00	33/9123 (0.4%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	VAL	N-CA-C	9.28	119.33	110.42
1	A	565	VAL	N-CA-C	8.80	120.42	108.11
1	A	64	VAL	N-CA-C	8.46	119.03	110.23
1	A	507	ILE	N-CA-C	7.61	120.49	113.10
1	A	467	ILE	N-CA-C	7.16	118.78	110.62
1	A	639	ARG	N-CA-C	6.99	119.93	111.82
1	A	834	LEU	N-CA-C	-6.64	101.70	110.40
1	A	576	GLN	N-CA-C	-6.62	104.09	111.71
1	A	688	THR	N-CA-C	6.32	119.53	109.24
1	A	575	ARG	N-CA-C	6.30	120.08	111.39
1	A	675	GLY	N-CA-C	-6.29	104.87	112.48
1	A	80	LYS	N-CA-C	-6.17	101.16	110.28
1	A	666	ILE	N-CA-C	6.12	122.06	109.34
1	A	455	VAL	N-CA-C	6.08	118.09	111.77
1	A	385	GLU	N-CA-C	6.06	118.52	109.25
1	A	37	PHE	N-CA-C	6.00	119.79	112.23
1	A	129	ALA	N-CA-C	-5.72	96.46	107.57
1	A	454	GLY	N-CA-C	-5.72	103.85	112.89
1	A	91	MET	N-CA-C	5.65	119.90	112.89
1	A	809	GLY	N-CA-C	5.59	120.70	113.27
1	A	495	CYS	N-CA-C	5.57	119.79	112.89
1	A	277	ARG	N-CA-C	5.52	118.14	111.40
1	A	491	TRP	N-CA-C	5.44	119.55	113.02
1	A	21	VAL	N-CA-C	5.41	118.39	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	THR	N-CA-C	-5.36	107.99	114.75
1	A	751	SER	CA-C-N	5.36	124.81	119.24
1	A	751	SER	C-N-CA	5.36	124.81	119.24
1	A	552	GLU	N-CA-C	5.36	118.98	112.23
1	A	479	PHE	N-CA-C	5.29	118.17	109.76
1	A	203	TYR	CB-CA-C	-5.24	110.51	116.54
1	A	772	LYS	N-CA-C	5.23	118.41	111.30
1	A	182	TRP	N-CA-C	5.22	118.74	112.38
1	A	326	PHE	N-CA-C	5.01	119.02	113.01

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	6611	0	6554	138	0
2	A	12	0	12	1	0
3	A	15	0	7	0	0
4	A	28	0	19	2	0
5	A	6	0	8	0	0
6	A	753	0	0	17	0
All	All	7425	0	6600	140	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 11.

All (140) 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:N	1.54	1.22
1:A:18:LEU:CD2	1:A:19:ALA:H	1.53	1.18
1:A:211:GLN:HB3	1:A:358:ARG:NH2	1.75	1.01
1:A:250:ASN:H	1:A:250:ASN:HD22	1.05	1.01
1:A:18:LEU:HD22	1:A:19:ALA:H	0.78	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.31	0.93
1:A:184:ARG:NH2	6:A:1089:HOH:O	2.07	0.88
1:A:413:ARG:HD2	6:A:1743:HOH:O	1.74	0.87
1:A:250:ASN:HD22	1:A:250:ASN:N	1.76	0.80
1:A:250:ASN:H	1:A:250:ASN:ND2	1.79	0.80
1:A:211:GLN:HB3	1:A:358:ARG:HH21	1.45	0.78
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.66	0.77
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.49	0.77
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.72	0.71
1:A:390:HIS:O	1:A:394:THR:HG23	1.91	0.70
1:A:250:ASN:N	1:A:250:ASN:ND2	2.36	0.70
1:A:138:ARG:O	1:A:138:ARG:HD3	1.92	0.69
1:A:18:LEU:CG	1:A:19:ALA:H	2.06	0.68
1:A:325:ASN:HB3	6:A:1580:HOH:O	1.94	0.67
1:A:26:GLU:OE1	6:A:1731:HOH:O	2.12	0.66
1:A:18:LEU:HD22	1:A:19:ALA:CB	2.24	0.66
1:A:506:ARG:HG2	1:A:506:ARG:HH11	1.60	0.65
1:A:714:ARG:HD3	6:A:1240:HOH:O	1.95	0.65
1:A:33:ARG:HD2	6:A:1450:HOH:O	1.97	0.64
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.09	0.63
1:A:63:LEU:HD13	1:A:102:LEU:HD21	1.80	0.63
1:A:16:ARG:HG3	1:A:17:GLY:H	1.64	0.62
1:A:18:LEU:HD22	1:A:19:ALA:CA	2.29	0.62
1:A:21:VAL:C	1:A:22:GLU:HG2	2.24	0.62
1:A:464:LYS:HG2	1:A:472:TYR:CD1	2.35	0.62
1:A:562:LEU:C	1:A:562:LEU:HD12	2.26	0.61
1:A:414:VAL:HG22	1:A:425:LEU:HD23	1.85	0.59
1:A:14:SEP:HB2	1:A:16:ARG:HG2	1.85	0.58
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.85	0.58
1:A:571:HIS:H	1:A:576:GLN:HE22	1.49	0.58
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.85	0.58
1:A:138:ARG:HB3	6:A:1035:HOH:O	2.04	0.57
1:A:314:SER:HA	6:A:1726:HOH:O	2.04	0.57
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.86	0.57
1:A:550:GLU:HG3	1:A:551:ARG:N	2.20	0.57
1:A:465:LYS:O	1:A:469:LYS:HD3	2.04	0.57
1:A:786:ARG:HD3	6:A:1375:HOH:O	2.03	0.57
1:A:235:ASN:HA	1:A:833:ARG:HG2	1.88	0.56
1:A:734:ARG:HD2	6:A:1265:HOH:O	2.04	0.56
1:A:21:VAL:O	1:A:22:GLU:HG2	2.06	0.56
1:A:67:TRP:HA	1:A:238:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:HB1	1:A:30:ASN:ND2	2.21	0.56
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.87	0.55
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.36	0.55
1:A:732:TYR:O	1:A:739:ARG:HG3	2.05	0.55
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.88	0.55
1:A:36:HIS:O	1:A:40:VAL:HA	2.06	0.54
1:A:207:GLU:OE2	6:A:1508:HOH:O	2.18	0.54
1:A:138:ARG:HD3	1:A:138:ARG:C	2.32	0.54
1:A:393:GLU:HB3	1:A:400:LEU:HD23	1.90	0.54
1:A:163:PHE:HB2	1:A:278:VAL:HG13	1.88	0.53
1:A:230:VAL:HG22	1:A:230:VAL:O	2.08	0.52
1:A:810:LYS:O	1:A:810:LYS:HG3	2.08	0.52
1:A:35:LEU:HA	1:A:39:LEU:HD12	1.92	0.52
1:A:36:HIS:CE1	1:A:42:ASP:HA	2.45	0.52
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.92	0.52
1:A:414:VAL:HG22	1:A:425:LEU:CD2	2.40	0.51
1:A:21:VAL:O	1:A:22:GLU:CG	2.58	0.51
1:A:227:ASP:CG	1:A:242:ARG:HH21	2.18	0.51
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.11	0.51
1:A:386:ARG:HD3	6:A:1444:HOH:O	2.10	0.51
1:A:502:ILE:HA	1:A:505:GLU:HG2	1.95	0.49
1:A:193:ARG:NH1	4:A:930:BIN:CL2	2.82	0.49
1:A:344:LEU:C	1:A:347:PRO:HD2	2.37	0.49
1:A:355:ASP:OD2	1:A:398:ARG:NE	2.46	0.49
1:A:198:LEU:HD13	1:A:305:GLN:HB2	1.94	0.48
1:A:579:ASN:C	1:A:579:ASN:HD22	2.19	0.48
1:A:528:GLU:CD	1:A:795:ARG:HH12	2.21	0.48
1:A:698:GLU:O	1:A:702:GLU:HG2	2.14	0.48
1:A:366:GLU:HG3	1:A:370:LYS:HD2	1.96	0.47
1:A:458:ILE:O	1:A:462:ILE:HG13	2.14	0.47
1:A:689:ILE:HG23	1:A:689:ILE:O	2.13	0.47
1:A:209:THR:O	1:A:210:SER:C	2.58	0.47
1:A:390:HIS:HA	1:A:393:GLU:HG2	1.96	0.47
1:A:793:ASN:HD22	1:A:793:ASN:C	2.21	0.47
1:A:568:LYS:CD	1:A:574:LYS:HD3	2.43	0.47
1:A:436:VAL:O	1:A:438:ARG:HG3	2.15	0.47
1:A:741:ILE:HA	1:A:744:GLN:NE2	2.24	0.47
1:A:224:MET:HE3	1:A:226:TYR:CE1	2.50	0.47
1:A:90:TYR:HE1	6:A:1561:HOH:O	1.97	0.46
1:A:351:ARG:O	1:A:355:ASP:HB2	2.16	0.46
1:A:291:LEU:O	1:A:295:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:CG2	1:A:425:LEU:HD23	2.46	0.46
1:A:425:LEU:HG	6:A:1252:HOH:O	2.15	0.46
1:A:678:ASN:OD1	1:A:679:MET:HG3	2.16	0.46
1:A:373:ALA:HA	1:A:449:SER:HB3	1.97	0.45
1:A:562:LEU:HG	1:A:601:ARG:HG2	1.98	0.45
1:A:42:ASP:OD1	1:A:45:VAL:HG22	2.16	0.45
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.52	0.45
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.88	0.45
2:A:998:GLC:H1	6:A:1218:HOH:O	2.17	0.44
1:A:716:GLU:H	1:A:716:GLU:CD	2.26	0.44
1:A:34:HIS:CE1	1:A:57:HIS:HB3	2.52	0.44
1:A:95:LEU:HG	1:A:99:MET:HE2	2.00	0.44
1:A:335:ILE:HD12	1:A:371:THR:CG2	2.48	0.43
1:A:795:ARG:O	1:A:799:ARG:HG3	2.17	0.43
1:A:18:LEU:CD2	1:A:19:ALA:N	2.38	0.43
1:A:528:GLU:OE1	1:A:795:ARG:NH1	2.42	0.43
1:A:379:VAL:HG13	6:A:1202:HOH:O	2.19	0.43
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.12	0.43
1:A:201:HIS:HD2	1:A:218:THR:OG1	2.00	0.43
1:A:18:LEU:C	1:A:20:GLY:H	2.27	0.42
1:A:214:LYS:HE2	1:A:216:VAL:HG12	2.02	0.42
1:A:393:GLU:HB3	1:A:400:LEU:CD2	2.48	0.42
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.86	0.42
1:A:731:TYR:O	1:A:735:ILE:HG13	2.19	0.42
1:A:18:LEU:CG	1:A:19:ALA:N	2.77	0.42
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.20	0.42
1:A:33:ARG:HE	1:A:33:ARG:HB2	1.67	0.42
1:A:538:LYS:NZ	1:A:684:ASN:O	2.52	0.42
1:A:554:LYS:HA	1:A:554:LYS:HD3	1.87	0.42
1:A:562:LEU:C	1:A:562:LEU:CD1	2.92	0.42
1:A:6:ASP:HB3	1:A:7:GLN:H	1.71	0.42
4:A:930:BIN:H151	4:A:930:BIN:H171	1.81	0.42
1:A:488:PRO:O	1:A:492:LEU:HB3	2.20	0.41
1:A:628:ASP:O	1:A:632:HIS:HD2	2.02	0.41
1:A:204:GLY:HA2	1:A:217:ASP:O	2.20	0.41
1:A:211:GLN:H	1:A:211:GLN:HG2	1.52	0.41
1:A:496:ASN:HB2	1:A:684:ASN:ND2	2.35	0.41
1:A:136:LEU:C	1:A:136:LEU:HD23	2.45	0.41
1:A:506:ARG:HG2	1:A:506:ARG:NH1	2.31	0.41
1:A:605:ILE:O	1:A:644:PHE:HA	2.21	0.41
1:A:106:ASN:HD22	1:A:106:ASN:HA	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:CG	1:A:398:ARG:NH1	2.76	0.41
1:A:663:SER:HB2	1:A:681:PHE:CG	2.55	0.41
1:A:230:VAL:O	1:A:230:VAL:CG2	2.69	0.41
1:A:517:GLN:HE21	1:A:517:GLN:HB3	1.69	0.41
1:A:338:ASN:O	1:A:339:ASP:CB	2.68	0.40
1:A:546:ALA:HA	1:A:557:ILE:HD11	2.02	0.40
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.03	0.40
1:A:15:VAL:HB	6:A:1120:HOH:O	2.21	0.40
1:A:88:GLU:HB3	1:A:132:GLY:HA2	2.02	0.40
1:A:782:LYS:O	1:A:785:GLU:HB2	2.22	0.40
1:A:34:HIS:O	1:A:38:THR:HB	2.21	0.40
1:A:346:ILE:HB	1:A:347:PRO:HD3	2.03	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	805/842 (96%)	772 (96%)	28 (4%)	5 (1%)	21	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	22	GLU
1	A	6	ASP
1	A	19	ALA
1	A	13	ILE

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	702/730 (96%)	644 (92%)	58 (8%)	10 8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	18	LEU
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	32	ASN
1	A	63	LEU
1	A	76	GLU
1	A	77	LYS
1	A	87	LEU
1	A	96	GLN
1	A	138	ARG
1	A	144	LEU
1	A	193	ARG
1	A	209	THR
1	A	210	SER
1	A	211	GLN
1	A	230	VAL
1	A	247	LYS
1	A	250	ASN
1	A	277	ARG
1	A	278	VAL
1	A	325	ASN
1	A	332	LYS
1	A	359	LEU
1	A	360	ASP
1	A	370	LYS
1	A	379	VAL
1	A	394	THR
1	A	398	ARG

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Mol	Chain	Res	Type
1	A	414	VAL
1	A	422	VAL
1	A	437	LYS
1	A	494	LEU
1	A	499	LEU
1	A	519	ARG
1	A	538	LYS
1	A	550	GLU
1	A	551	ARG
1	A	562	LEU
1	A	568	LYS
1	A	576	GLN
1	A	583	VAL
1	A	592	LYS
1	A	596	LYS
1	A	635	VAL
1	A	641	ARG
1	A	708	PHE
1	A	714	ARG
1	A	718	VAL
1	A	734	ARG
1	A	753	LYS
1	A	754	GLN
1	A	788	SER
1	A	792	LYS
1	A	793	ASN
1	A	810	LYS
1	A	812	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	30	ASN
1	A	57	HIS
1	A	97	ASN
1	A	101	ASN
1	A	106	ASN
1	A	201	HIS
1	A	208	HIS
1	A	250	ASN
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	325	ASN
1	A	408	GLN
1	A	412	ASN
1	A	443	HIS
1	A	450	HIS
1	A	484	ASN
1	A	496	ASN
1	A	517	GLN
1	A	541	ASN
1	A	556	HIS
1	A	566	GLN
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	767	HIS
1	A	793	ASN
1	A	832	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	SEP	A	14	-	8,9,10	1.11	1 (12%)	7,12,14	5.24	4 (57%)

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
1	SEP	A	14	-	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SEP	P-O3P	2.38	1.63	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SEP	OG-CB-CA	-13.12	95.38	108.14
1	A	14	SEP	O3P-P-OG	2.60	113.45	106.67
1	A	14	SEP	OG-P-O1P	-2.32	100.17	106.44
1	A	14	SEP	O2P-P-O1P	2.31	119.84	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	14	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	PLP	A	999	1	15,15,16	1.67	4 (26%)	21,22,23	1.09	2 (9%)
4	BIN	A	930	-	28,29,29	5.58	16 (57%)	34,42,42	2.61	12 (35%)
5	GOL	A	996	-	5,5,5	0.29	0	5,5,5	0.50	0
2	GLC	A	998	-	12,12,12	1.68	2 (16%)	17,17,17	1.24	1 (5%)

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	PLP	A	999	1	-	2/6/6/8	0/1/1/1
4	BIN	A	930	-	-	6/22/22/22	0/2/2/2
5	GOL	A	996	-	-	4/4/4/4	-
2	GLC	A	998	-	-	0/2/22/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	930	BIN	C7-C8	16.92	1.70	1.40
4	A	930	BIN	C11-N10	11.47	1.54	1.36
4	A	930	BIN	C1-C2	9.51	1.56	1.39
4	A	930	BIN	C4-C3	7.19	1.51	1.38
4	A	930	BIN	C1-C7	7.07	1.58	1.50
4	A	930	BIN	C7-C12	7.04	1.53	1.40
4	A	930	BIN	O8-C19	5.90	1.60	1.47
4	A	930	BIN	C8-C18	5.48	1.63	1.50
4	A	930	BIN	C6-C1	5.44	1.48	1.40
4	A	930	BIN	C8-C11	4.75	1.44	1.39
4	A	930	BIN	C12-C13	4.54	1.61	1.50
4	A	930	BIN	C3-C2	4.41	1.47	1.38
4	A	930	BIN	C2-CL2	-3.87	1.64	1.73
4	A	930	BIN	C5-C6	3.61	1.45	1.38
3	A	999	PLP	C3-C2	-3.57	1.37	1.41
2	A	998	GLC	C1-C2	3.53	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C4A-C4	3.47	1.58	1.51
2	A	998	GLC	C3-C2	3.14	1.60	1.52
4	A	930	BIN	C12-C9	2.93	1.50	1.41
4	A	930	BIN	O8-C18	2.05	1.38	1.34
3	A	999	PLP	P-O3P	-2.02	1.47	1.54
3	A	999	PLP	C2A-C2	2.02	1.53	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	930	BIN	C1-C7-C12	-7.36	109.23	121.34
4	A	930	BIN	C1-C7-C8	-5.68	111.99	121.34
4	A	930	BIN	C16-C17-N10	4.74	121.34	111.98
4	A	930	BIN	O3B-C13-O3A	-4.16	114.42	123.35
4	A	930	BIN	C5-C4-C3	3.85	124.99	120.24
4	A	930	BIN	O4B-C14-O4A	3.76	131.44	123.35
4	A	930	BIN	C15-C11-C8	3.68	128.44	122.76
4	A	930	BIN	O4B-C14-C9	-2.81	110.98	116.74
4	A	930	BIN	O4A-C14-C9	-2.74	117.56	121.17
2	A	998	GLC	O3-C3-C4	-2.36	104.82	110.38
4	A	930	BIN	O3A-C13-C12	2.35	126.80	121.18
4	A	930	BIN	C1-C2-CL2	2.26	123.76	120.67
3	A	999	PLP	O3P-P-O1P	2.19	119.37	110.83
4	A	930	BIN	C5-C6-C1	2.17	123.82	120.23
3	A	999	PLP	C5A-C5-C6	-2.01	116.08	119.36

There are no chirality outliers.

All (12) torsion outliers are listed below:

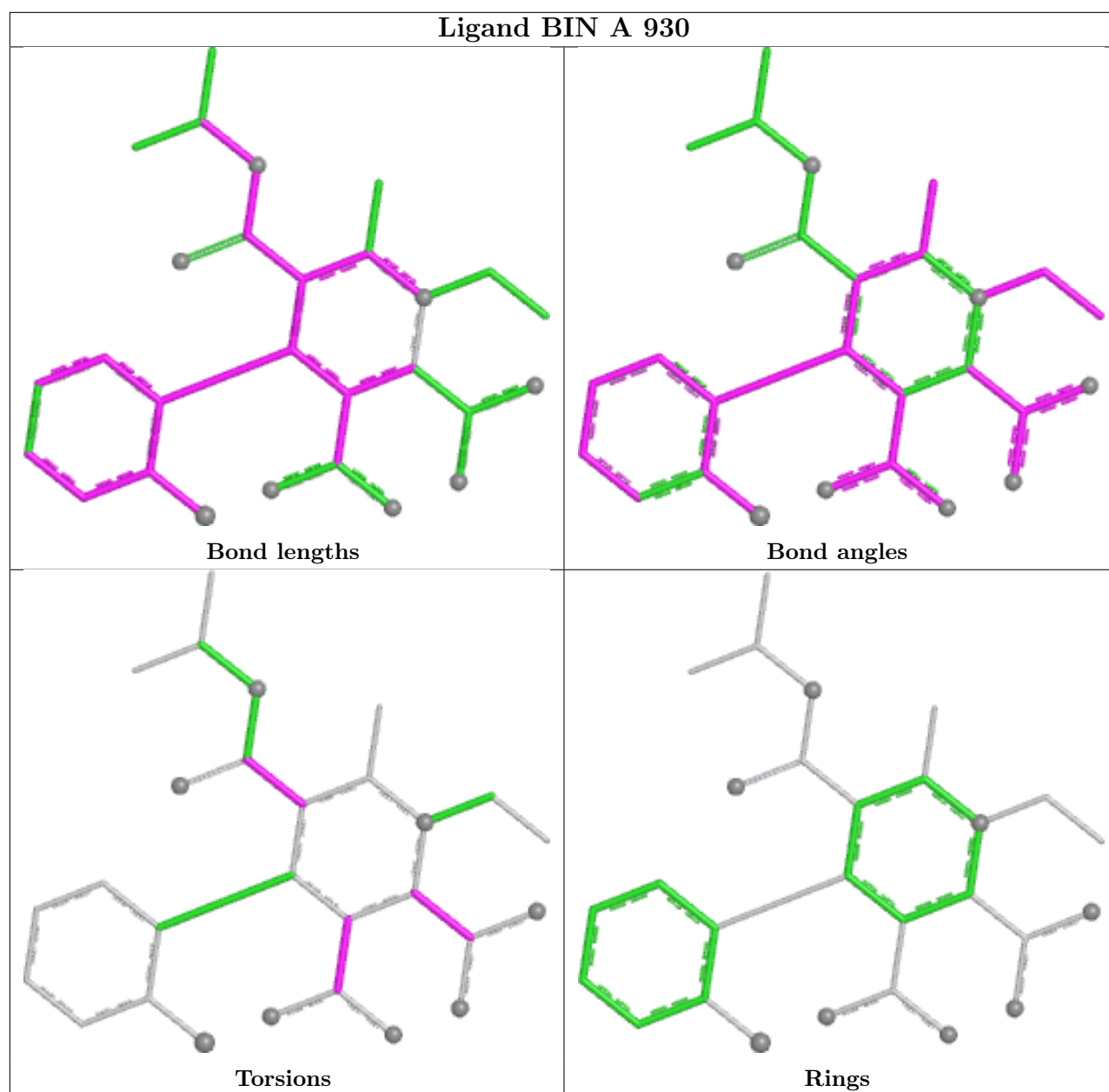
Mol	Chain	Res	Type	Atoms
5	A	996	GOL	O1-C1-C2-O2
5	A	996	GOL	O1-C1-C2-C3
5	A	996	GOL	C1-C2-C3-O3
5	A	996	GOL	O2-C2-C3-O3
4	A	930	BIN	O4B-C14-C9-N10
3	A	999	PLP	C4-C5-C5A-O4P
4	A	930	BIN	C7-C12-C13-O3B
4	A	930	BIN	C7-C12-C13-O3A
4	A	930	BIN	O8-C18-C8-C11
3	A	999	PLP	C6-C5-C5A-O4P
4	A	930	BIN	O8A-C18-C8-C7
4	A	930	BIN	C9-C12-C13-O3A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	930	BIN	2	0
2	A	998	GLC	1	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

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.