



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 1LWO / pdb_00001lwo
Title : Crystal structure of rabbit muscle glycogen phosphorylase a in complex with a potential hypoglycaemic drug at 2.0 Å resolution
Authors : Oikonomakos, N.G.; Chrysina, E.D.; Kosmopoulou, M.N.; Leonidas, D.D.
Deposited on : 2002-06-01
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

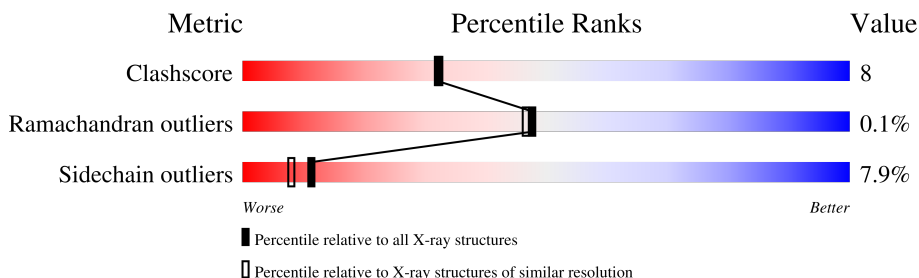
1 Overall quality at a glance

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	 76% 17% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7002 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.

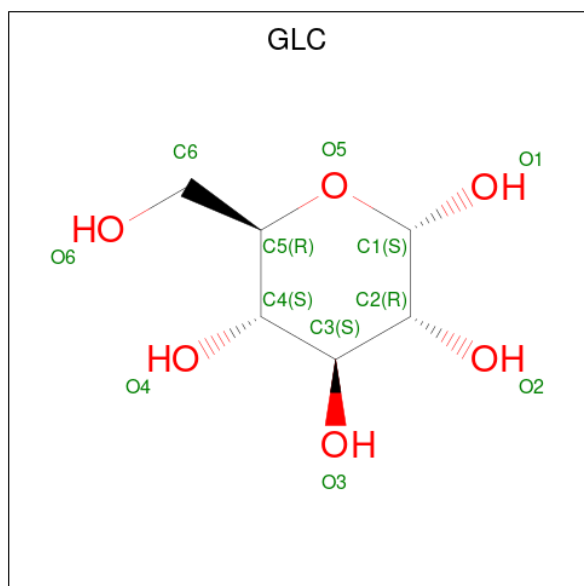
- Molecule 1 is a protein called glycogen phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	815	6635	4222	1170	1213	1	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	modified residue	UNP P00489

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



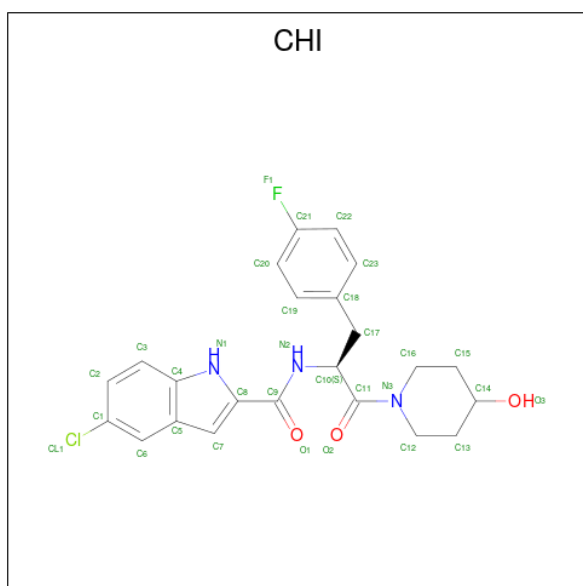
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- 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 5-CHLORO-1H-INDOLE-2-CARBOXYLIC ACID [1-(4-FLUOROBENZYL)-2-(4-HYDROXYPIPERIDIN-1YL)-2-OXOETHYL]AMIDE (CCD ID: CHI) (formula: $C_{23}H_{23}ClFN_3O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			31	23	1	1	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total 309	O 309	0	0

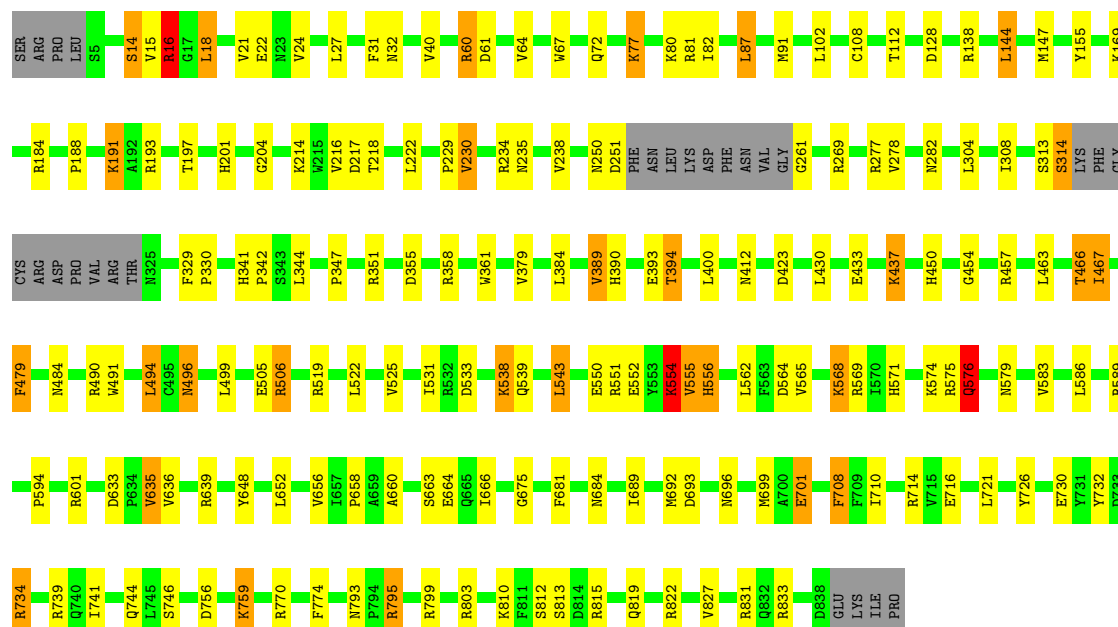
3 Residue-property plots

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

Chain A:  76% 17% . .



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	128.65Å 128.65Å 116.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.00	Depositor
% Data completeness (in resolution range)	97.6 (29.36-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.207 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7002	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: CHI, PLP, SEP, GLC

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	0.46	0/6771	0.93	24/9159 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	N-CA-C	8.59	121.72	111.33
1	A	467	ILE	N-CA-C	7.43	119.09	110.62
1	A	565	VAL	N-CA-C	7.02	117.94	108.11
1	A	675	GLY	N-CA-C	-6.77	104.29	112.48
1	A	466	THR	N-CA-C	6.54	118.51	108.30
1	A	91	MET	N-CA-C	6.42	120.32	112.23
1	A	556	HIS	N-CA-C	6.28	119.44	107.75
1	A	575	ARG	N-CA-C	6.26	120.28	111.52
1	A	80	LYS	N-CA-C	-6.12	100.02	109.76
1	A	454	GLY	N-CA-C	-5.98	103.13	112.58
1	A	714	ARG	N-CA-C	-5.92	101.70	110.46
1	A	656	VAL	N-CA-C	5.87	116.65	110.72
1	A	576	GLN	N-CA-C	-5.68	105.24	111.82
1	A	24	VAL	N-CA-C	5.65	116.39	110.62
1	A	77	LYS	N-CA-C	5.57	118.28	111.82
1	A	216	VAL	N-CA-C	5.51	116.78	108.96
1	A	72	GLN	N-CA-C	-5.48	105.22	111.14
1	A	479	PHE	N-CA-C	5.42	118.37	109.76
1	A	31	PHE	N-CA-C	-5.32	105.38	111.07
1	A	491	TRP	N-CA-C	5.22	119.36	113.15
1	A	361	TRP	N-CA-C	5.21	117.37	111.11
1	A	278	VAL	N-CA-C	5.17	117.18	108.81
1	A	666	ILE	N-CA-C	5.09	119.93	109.34
1	A	430	LEU	N-CA-C	-5.04	106.64	112.89

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	6635	0	6571	107	0
2	A	12	0	12	0	0
3	A	15	0	7	0	0
4	A	31	0	23	3	0
5	A	309	0	0	12	0
All	All	7002	0	6613	107	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 8.

All (107) 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:756:ASP:HB2	1:A:759:LYS:HG3	1.45	0.97
1:A:313:SER:O	1:A:314:SER:HB2	1.77	0.83
1:A:390:HIS:O	1:A:394:THR:HG22	1.79	0.81
1:A:555:VAL:HB	5:A:1290:HOH:O	1.81	0.79
1:A:822:ARG:NH1	5:A:1238:HOH:O	2.14	0.79
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.49	0.76
1:A:554:LYS:O	1:A:554:LYS:HG2	1.86	0.75
1:A:191:LYS:C	1:A:191:LYS:HD3	2.14	0.73
1:A:795:ARG:O	1:A:799:ARG:HG3	1.90	0.72
1:A:250:ASN:HA	1:A:269:ARG:HH11	1.52	0.72
1:A:692:MET:HE3	1:A:710:ILE:HG12	1.73	0.71
1:A:191:LYS:HD2	1:A:193:ARG:NH1	2.06	0.70
1:A:64:VAL:HB	4:A:920:CHI:CL1	2.29	0.69
1:A:304:LEU:O	1:A:308:ILE:HG12	1.94	0.68
1:A:506:ARG:NH1	1:A:533:ASP:OD1	2.27	0.68
1:A:261:GLY:HA3	5:A:1266:HOH:O	1.93	0.68
1:A:191:LYS:HE3	4:A:920:CHI:O2	1.96	0.65
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:HG22	5:A:1095:HOH:O	1.99	0.62
1:A:250:ASN:HA	1:A:269:ARG:NH1	2.14	0.62
1:A:15:VAL:HA	1:A:18:LEU:HD22	1.82	0.61
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.31	0.61
1:A:793:ASN:HD22	1:A:793:ASN:C	2.09	0.60
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.83	0.60
1:A:770:ARG:HD3	5:A:1284:HOH:O	2.01	0.60
1:A:522:LEU:O	1:A:525:VAL:HG23	2.02	0.59
1:A:393:GLU:HB3	1:A:400:LEU:CD2	2.33	0.58
1:A:550:GLU:HG3	1:A:551:ARG:N	2.20	0.57
1:A:351:ARG:O	1:A:355:ASP:HB2	2.04	0.57
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.88	0.56
1:A:531:ILE:HD13	1:A:795:ARG:HD2	1.88	0.54
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.89	0.54
1:A:61:ASP:O	1:A:64:VAL:HG12	2.07	0.54
1:A:250:ASN:ND2	1:A:269:ARG:NH1	2.56	0.54
1:A:689:ILE:HG23	1:A:689:ILE:O	2.07	0.53
1:A:734:ARG:HD2	5:A:1228:HOH:O	2.08	0.53
1:A:313:SER:O	1:A:314:SER:CB	2.54	0.53
1:A:732:TYR:O	1:A:739:ARG:HG3	2.08	0.53
1:A:250:ASN:HD22	1:A:269:ARG:NH1	2.08	0.52
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.92	0.52
1:A:538:LYS:NZ	1:A:684:ASN:O	2.42	0.52
1:A:799:ARG:O	1:A:803:ARG:HG3	2.10	0.52
1:A:393:GLU:HB3	1:A:400:LEU:HD22	1.92	0.51
1:A:539:GLN:HE21	1:A:543:LEU:HD13	1.75	0.50
1:A:21:VAL:HG12	1:A:22:GLU:N	2.25	0.50
1:A:251:ASP:OD1	1:A:251:ASP:C	2.54	0.50
1:A:730:GLU:O	1:A:734:ARG:HD3	2.11	0.50
1:A:204:GLY:HA2	1:A:217:ASP:O	2.12	0.50
1:A:793:ASN:C	1:A:793:ASN:ND2	2.69	0.49
1:A:450:HIS:HE1	5:A:1010:HOH:O	1.94	0.49
1:A:463:LEU:HD22	1:A:467:ILE:HD11	1.94	0.49
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.11	0.49
1:A:14:SEP:OG	1:A:16:ARG:HB2	2.11	0.49
1:A:479:PHE:HB3	5:A:1111:HOH:O	2.11	0.49
1:A:496:ASN:HB2	1:A:684:ASN:ND2	2.28	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.96	0.48
1:A:699:MET:HE2	1:A:708:PHE:CZ	2.39	0.48
1:A:144:LEU:HD12	1:A:147:MET:CE	2.43	0.48
1:A:81:ARG:HG2	1:A:155:TYR:HE1	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:PRO:O	1:A:639:ARG:NH1	2.47	0.47
1:A:450:HIS:HD2	5:A:1273:HOH:O	1.97	0.47
1:A:633:ASP:OD2	1:A:635:VAL:HG13	2.14	0.47
1:A:692:MET:HA	1:A:692:MET:HE2	1.95	0.47
1:A:230:VAL:O	1:A:230:VAL:CG2	2.63	0.47
1:A:201:HIS:HD2	1:A:218:THR:OG1	1.98	0.46
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.97	0.46
1:A:663:SER:HB2	1:A:681:PHE:CG	2.51	0.45
1:A:389:VAL:HG13	1:A:437:LYS:HB3	1.99	0.45
1:A:191:LYS:HD2	1:A:193:ARG:HD3	1.99	0.45
1:A:191:LYS:HE2	5:A:1064:HOH:O	2.16	0.45
1:A:230:VAL:O	1:A:230:VAL:HG22	2.17	0.45
1:A:554:LYS:O	1:A:555:VAL:HG23	2.17	0.45
1:A:108:CYS:O	1:A:112:THR:HG23	2.17	0.44
1:A:564:ASP:OD2	1:A:664:GLU:OE2	2.35	0.44
1:A:61:ASP:O	1:A:64:VAL:CG1	2.65	0.44
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.98	0.44
1:A:538:LYS:HE3	1:A:658:PRO:O	2.16	0.44
1:A:692:MET:CE	1:A:710:ILE:HG12	2.45	0.44
1:A:538:LYS:HE2	1:A:660:ALA:O	2.18	0.44
1:A:815:ARG:O	1:A:819:GLN:HG3	2.18	0.44
1:A:810:LYS:O	1:A:810:LYS:HG2	2.17	0.43
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.34	0.43
1:A:457:ARG:NH1	1:A:701:GLU:OE2	2.43	0.43
1:A:235:ASN:HB3	1:A:831:ARG:NH1	2.34	0.43
1:A:433:GLU:OE2	1:A:437:LYS:HE2	2.18	0.43
1:A:496:ASN:HB2	1:A:684:ASN:HD21	1.84	0.43
1:A:579:ASN:C	1:A:579:ASN:HD22	2.26	0.43
1:A:60:ARG:HD2	1:A:188:PRO:O	2.19	0.43
1:A:201:HIS:CD2	1:A:218:THR:OG1	2.72	0.42
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.84	0.42
1:A:282:ASN:HB2	5:A:1076:HOH:O	2.19	0.42
1:A:191:LYS:HD2	1:A:193:ARG:HH11	1.82	0.42
1:A:15:VAL:HA	1:A:18:LEU:CD2	2.50	0.42
1:A:197:THR:CG2	1:A:222:LEU:HB3	2.50	0.42
1:A:569:ARG:O	1:A:574:LYS:HD2	2.20	0.42
1:A:412:ASN:HD22	1:A:412:ASN:HA	1.67	0.41
1:A:576:GLN:HE21	1:A:576:GLN:HB2	1.63	0.41
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.34	0.41
1:A:229:PRO:HG3	4:A:920:CHI:H21	2.03	0.41
1:A:344:LEU:C	1:A:347:PRO:HD2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:OG1	1:A:467:ILE:N	2.53	0.41
1:A:716:GLU:H	1:A:716:GLU:CD	2.28	0.41
1:A:484:ASN:ND2	5:A:1115:HOH:O	2.54	0.40
1:A:636:VAL:O	1:A:639:ARG:HD3	2.21	0.40
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.86	0.40
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.94	0.40
1:A:693:ASP:O	1:A:696:ASN:HB2	2.22	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	808/842 (96%)	776 (96%)	31 (4%)	1 (0%)	48 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	LYS

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	705/730 (97%)	649 (92%)	56 (8%)	11 8

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	18	LEU
1	A	27	LEU
1	A	32	ASN
1	A	40	VAL
1	A	60	ARG
1	A	77	LYS
1	A	87	LEU
1	A	102	LEU
1	A	128	ASP
1	A	144	LEU
1	A	169	LYS
1	A	184	ARG
1	A	191	LYS
1	A	214	LYS
1	A	230	VAL
1	A	234	ARG
1	A	277	ARG
1	A	314	SER
1	A	358	ARG
1	A	384	LEU
1	A	389	VAL
1	A	394	THR
1	A	423	ASP
1	A	437	LYS
1	A	494	LEU
1	A	496	ASN
1	A	499	LEU
1	A	505	GLU
1	A	506	ARG
1	A	519	ARG
1	A	538	LYS
1	A	543	LEU
1	A	552	GLU
1	A	554	LYS
1	A	555	VAL
1	A	556	HIS
1	A	562	LEU
1	A	568	LYS
1	A	571	HIS
1	A	576	GLN
1	A	583	VAL

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Mol	Chain	Res	Type
1	A	586	LEU
1	A	589	ARG
1	A	601	ARG
1	A	635	VAL
1	A	701	GLU
1	A	708	PHE
1	A	721	LEU
1	A	734	ARG
1	A	746	SER
1	A	759	LYS
1	A	795	ARG
1	A	812	SER
1	A	813	SER
1	A	833	ARG

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	12	GLN
1	A	30	ASN
1	A	32	ASN
1	A	36	HIS
1	A	57	HIS
1	A	71	GLN
1	A	106	ASN
1	A	201	HIS
1	A	211	GLN
1	A	250	ASN
1	A	412	ASN
1	A	450	HIS
1	A	453	ASN
1	A	484	ASN
1	A	496	ASN
1	A	517	GLN
1	A	539	GLN
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	588	ASN
1	A	614	HIS
1	A	632	HIS

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Mol	Chain	Res	Type
1	A	684	ASN
1	A	744	GLN
1	A	767	HIS
1	A	768	HIS
1	A	793	ASN
1	A	804	ASN

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	1	8,9,10	1.21	1 (12%)	7,12,14	6.00	2 (28%)

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	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SEP	P-O2P	2.30	1.63	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SEP	OG-CB-CA	15.63	123.35	108.14
1	A	14	SEP	O3P-P-O1P	2.48	120.49	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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](#)

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
4	CHI	A	920	-	34,34,34	3.79	23 (67%)	48,48,48	2.68	19 (39%)
3	PLP	A	999	1	15,15,16	1.53	2 (13%)	21,22,23	1.05	1 (4%)
2	GLC	A	998	-	12,12,12	1.28	1 (8%)	17,17,17	0.85	0

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
4	CHI	A	920	-	-	2/20/30/30	0/4/4/4
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1
2	GLC	A	998	-	-	0/2/22/22	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	920	CHI	C7-C8	8.82	1.51	1.37
4	A	920	CHI	O2-C11	8.16	1.36	1.22
4	A	920	CHI	C6-C1	6.84	1.49	1.38
4	A	920	CHI	C3-C4	6.68	1.50	1.39
4	A	920	CHI	C8-N1	-5.88	1.30	1.38
4	A	920	CHI	C20-C21	4.89	1.46	1.37
4	A	920	CHI	C3-C2	4.83	1.46	1.38
4	A	920	CHI	C4-N1	-4.15	1.31	1.38
4	A	920	CHI	C19-C18	3.89	1.46	1.38
4	A	920	CHI	C16-N3	3.79	1.53	1.47
4	A	920	CHI	C1-CL1	-3.63	1.65	1.74
4	A	920	CHI	C22-C21	3.47	1.44	1.37
4	A	920	CHI	C17-C10	3.41	1.62	1.54
4	A	920	CHI	C12-N3	3.40	1.53	1.47
4	A	920	CHI	C23-C18	3.26	1.45	1.38
3	A	999	PLP	C4A-C4	2.99	1.57	1.51
4	A	920	CHI	C13-C14	2.90	1.58	1.51
2	A	998	GLC	C4-C5	2.87	1.59	1.53
4	A	920	CHI	C20-C19	2.76	1.43	1.38
4	A	920	CHI	C9-N2	2.59	1.39	1.34
4	A	920	CHI	C5-C4	-2.54	1.37	1.41
4	A	920	CHI	C11-N3	2.38	1.38	1.35
3	A	999	PLP	C5A-C5	2.34	1.57	1.50
4	A	920	CHI	C6-C5	2.31	1.44	1.40
4	A	920	CHI	C10-C11	2.30	1.57	1.53
4	A	920	CHI	C10-N2	2.12	1.50	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	CHI	O1-C9-C8	-7.22	111.79	121.09
4	A	920	CHI	C6-C5-C4	6.03	122.86	119.13
4	A	920	CHI	C5-C7-C8	-5.91	102.12	107.41
4	A	920	CHI	C5-C6-C1	-5.44	113.87	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	CHI	C10-C11-N3	5.41	127.00	118.85
4	A	920	CHI	C8-C9-N2	5.17	123.76	116.86
4	A	920	CHI	C16-N3-C11	-4.18	107.62	123.30
4	A	920	CHI	C5-C4-N1	3.98	111.79	107.65
4	A	920	CHI	C3-C4-N1	-3.08	124.59	130.83
4	A	920	CHI	O2-C11-N3	-3.02	118.00	121.61
4	A	920	CHI	C17-C18-C23	-2.71	115.86	120.90
4	A	920	CHI	O2-C11-C10	-2.53	114.98	119.61
4	A	920	CHI	C9-C8-N1	2.53	128.12	120.04
4	A	920	CHI	C2-C1-C6	2.51	124.81	121.53
4	A	920	CHI	C12-N3-C11	-2.49	113.95	123.30
4	A	920	CHI	C2-C3-C4	-2.49	114.77	119.57
4	A	920	CHI	C2-C1-CL1	-2.41	115.80	119.36
3	A	999	PLP	O3P-P-O1P	2.38	120.12	110.83
4	A	920	CHI	C4-N1-C8	2.37	111.55	109.01
4	A	920	CHI	C17-C10-C11	-2.03	105.69	109.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	920	CHI	C10-C11-N3-C16
4	A	920	CHI	O2-C11-N3-C16
3	A	999	PLP	C4-C5-C5A-O4P

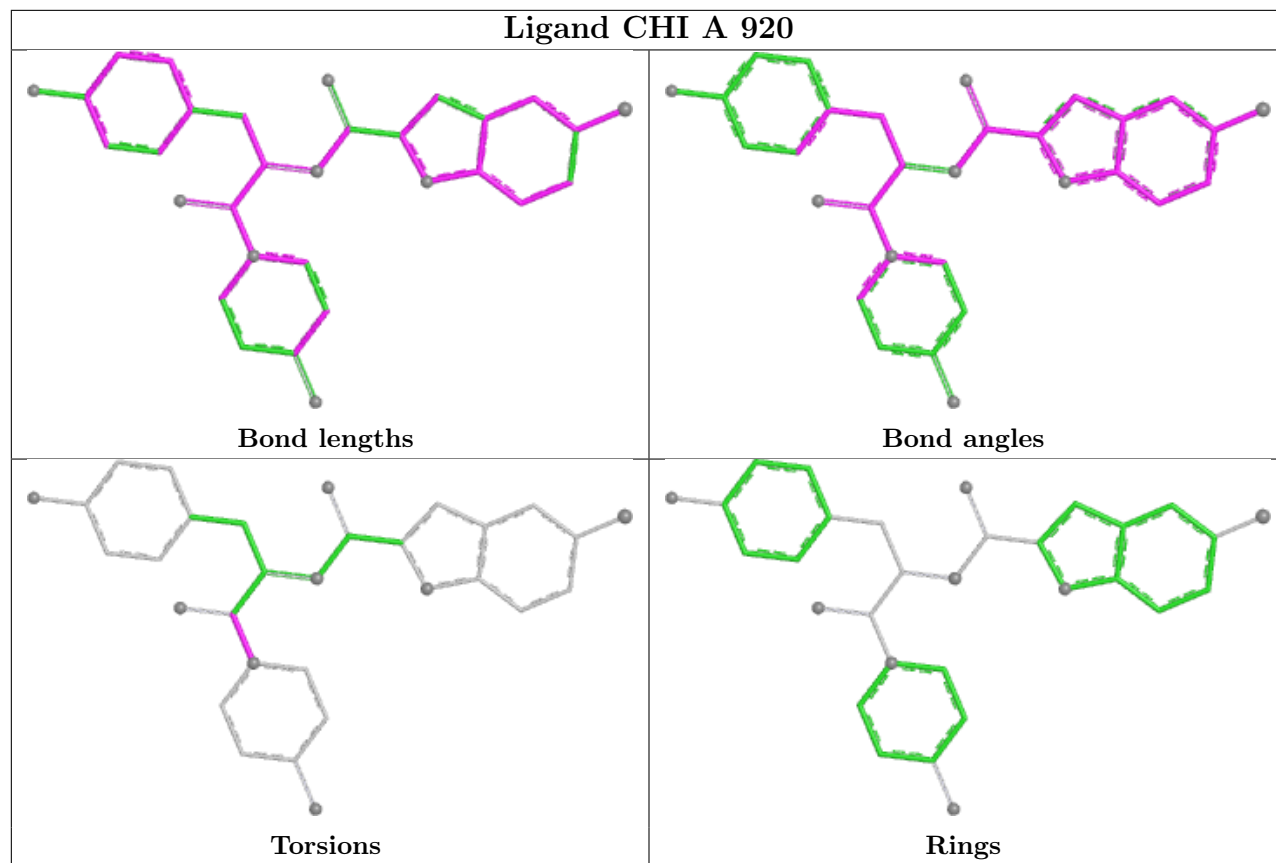
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	920	CHI	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.



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.