



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:09 PM UTC

PDB ID : 1WUT / pdb_00001wut
Title : Acyl Ureas as Human Liver Glycogen Phosphorylase Inhibitors for the Treatment of Type 2 Diabetes
Authors : Klabunde, T.; Wendt, K.U.; Kadereit, D.; Brachvogel, V.; Burger, H.-J.; Herling, A.W.; Oikonomakos, N.G.; Kosmopoulou, M.N.; Schmoll, D.; Sarubbi, E.; von Roedern, E.; Schonafinger, K.; Defossa, E.
Deposited on : 2004-12-08
Resolution : 2.26 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)
Xtrriage (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

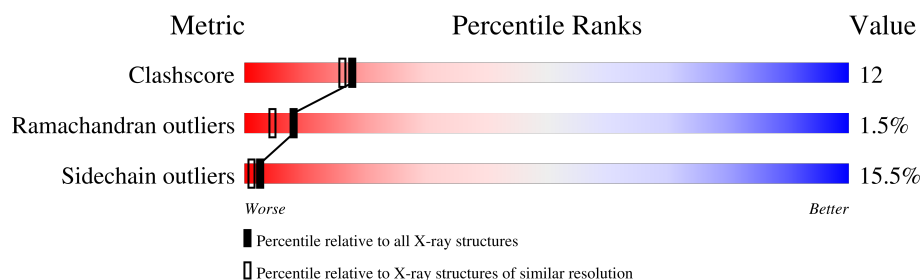
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	 66% 24% 6% ••

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6920 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.

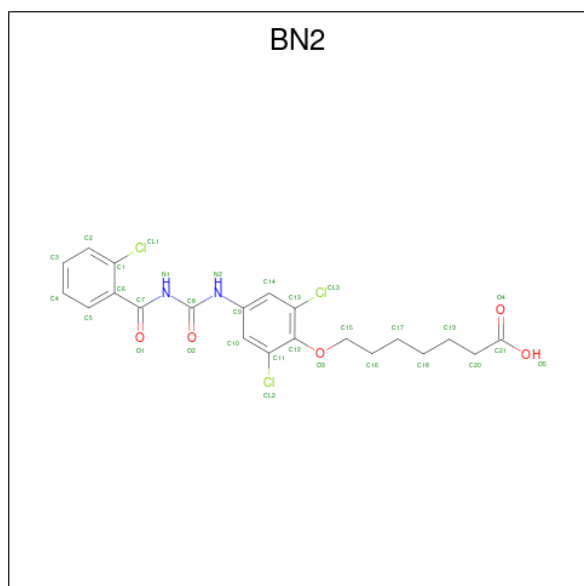
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	816	6649	4239	1168	1212	1	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is 7-[2,6-DICHLORO-4-({[(2-CHLOROBENZOYL)AMINO]CARBONYL}AMINO)PHENOXY]HEPTANOIC ACID (CCD ID: BN2) (formula: C₂₁H₂₁Cl₃N₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	31	21	3	2	5	0	0

- Molecule 3 is water.

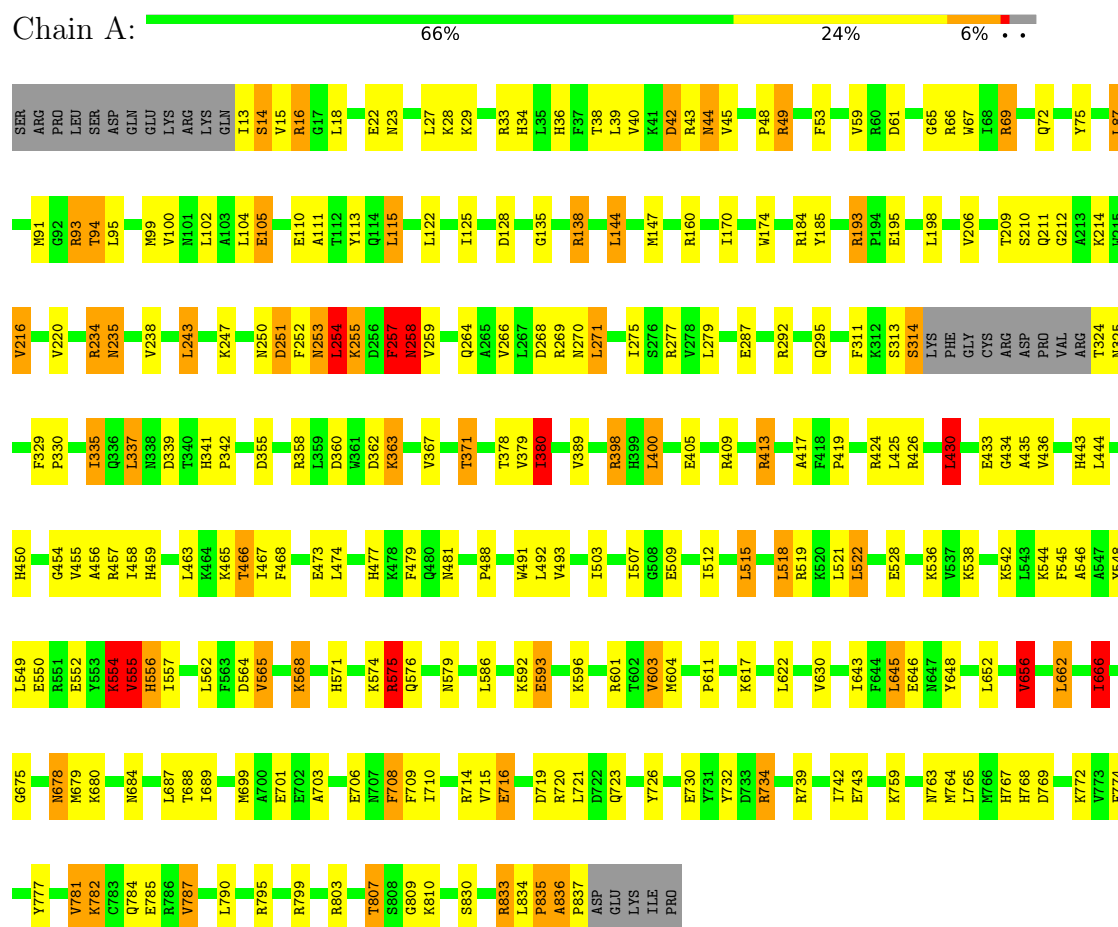
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total 240	O 240	0	0

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, 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	128.68Å 128.68Å 115.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.26	Depositor
% Data completeness (in resolution range)	95.7 (29.49-2.26)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.201 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6920	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: LLP, BN2

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	0.53	2/6774 (0.0%)	1.02	39/9169 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ASN	N-CA	-5.97	1.38	1.46
1	A	44	ASN	CA-CB	5.97	1.63	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASN	N-CA-C	9.07	122.34	111.82
1	A	554	LYS	N-CA-C	8.17	128.19	110.80
1	A	257	PHE	N-CA-C	8.13	120.28	110.19
1	A	91	MET	N-CA-C	7.55	121.74	112.23
1	A	576	GLN	N-CA-C	-7.40	103.20	111.71
1	A	212	GLY	N-CA-C	7.30	119.45	112.08
1	A	105	GLU	N-CA-C	6.86	119.34	111.11
1	A	565	VAL	N-CA-C	6.79	118.26	108.48
1	A	507	ILE	N-CA-C	6.56	118.40	112.17
1	A	714	ARG	N-CA-C	-6.55	100.77	110.46
1	A	630	VAL	N-CA-C	6.40	117.15	110.62
1	A	193	ARG	CA-C-N	6.37	127.80	119.84
1	A	193	ARG	C-N-CA	6.37	127.80	119.84
1	A	675	GLY	N-CA-C	-6.33	104.82	112.48
1	A	556	HIS	N-CA-C	6.29	124.19	110.80
1	A	656	VAL	CB-CA-C	-6.14	103.97	112.02
1	A	135	GLY	N-CA-C	6.02	119.93	112.64
1	A	466	THR	N-CA-C	5.89	117.49	108.12
1	A	209	THR	CA-C-N	5.81	128.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	THR	C-N-CA	5.81	128.07	120.28
1	A	362	ASP	N-CA-C	5.68	117.48	111.28
1	A	479	PHE	N-CA-C	5.67	117.93	109.25
1	A	491	TRP	N-CA-C	5.51	119.55	113.21
1	A	44	ASN	CA-C-O	5.50	126.30	119.97
1	A	430	LEU	N-CA-C	-5.50	106.08	112.89
1	A	380	ILE	CA-C-N	5.33	124.97	119.05
1	A	380	ILE	C-N-CA	5.33	124.97	119.05
1	A	220	VAL	N-CA-C	5.33	115.63	108.17
1	A	87	LEU	N-CA-C	-5.26	106.71	113.02
1	A	767	HIS	N-CA-C	5.25	121.08	114.31
1	A	454	GLY	N-CA-C	-5.21	103.61	112.51
1	A	216	VAL	N-CA-C	5.20	117.10	108.99
1	A	555	VAL	N-CA-C	5.11	119.97	109.34
1	A	666	ILE	N-CA-C	5.10	119.95	109.34
1	A	688	THR	N-CA-C	5.10	117.28	109.07
1	A	575	ARG	N-CA-C	5.08	118.63	111.52
1	A	684	ASN	N-CA-C	5.08	118.51	112.72
1	A	277	ARG	N-CA-C	5.06	116.60	111.14
1	A	206	VAL	N-CA-C	5.01	115.06	107.80

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	6649	0	6584	163	2
2	A	31	0	20	1	2
3	A	240	0	0	15	0
All	All	6920	0	6604	163	2

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 12.

All (163) 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:716:GLU:OE1	1:A:716:GLU:N	1.79	1.16
1:A:251:ASP:CG	1:A:252:PHE:H	1.68	0.99
1:A:413:ARG:HG2	1:A:413:ARG:HH21	1.27	0.98
1:A:764:MET:HE2	1:A:769:ASP:HA	1.45	0.98
1:A:554:LYS:O	1:A:555:VAL:HG22	1.77	0.85
1:A:15:VAL:HG22	3:A:1027:HOH:O	1.79	0.82
1:A:251:ASP:CG	1:A:252:PHE:N	2.40	0.80
1:A:66:ARG:HG3	1:A:837:PRO:HB3	1.63	0.79
1:A:138:ARG:O	1:A:138:ARG:HD3	1.83	0.78
1:A:379:VAL:HG22	3:A:1098:HOH:O	1.85	0.77
1:A:678:ASN:HD22	1:A:679:MET:H	1.31	0.77
1:A:764:MET:HE1	3:A:1198:HOH:O	1.83	0.76
1:A:15:VAL:HG12	3:A:1181:HOH:O	1.86	0.76
1:A:719:ASP:O	1:A:723:GLN:HG2	1.87	0.75
1:A:65:GLY:O	1:A:69:ARG:HG2	1.85	0.75
1:A:716:GLU:H	1:A:716:GLU:CD	1.90	0.75
1:A:795:ARG:O	1:A:799:ARG:HG3	1.87	0.73
1:A:184:ARG:HE	1:A:185:TYR:HE1	1.33	0.73
1:A:703:ALA:HA	1:A:807:THR:HG21	1.71	0.72
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.26	0.71
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.73	0.71
1:A:335:ILE:O	1:A:335:ILE:HG13	1.91	0.71
1:A:235:ASN:H	1:A:235:ASN:HD22	1.37	0.70
1:A:413:ARG:HG2	1:A:413:ARG:NH2	2.01	0.70
1:A:764:MET:CE	1:A:769:ASP:HA	2.22	0.70
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.74	0.70
1:A:601:ARG:HD2	3:A:1033:HOH:O	1.90	0.70
1:A:477:HIS:HD2	3:A:1239:HOH:O	1.75	0.69
1:A:571:HIS:HB2	1:A:574:LYS:HG3	1.74	0.69
1:A:455:VAL:H	1:A:459:HIS:HD2	1.40	0.68
1:A:730:GLU:O	1:A:734:ARG:HG2	1.93	0.68
1:A:708:PHE:HB3	1:A:710:ILE:HD12	1.74	0.67
1:A:184:ARG:NE	1:A:185:TYR:CE1	2.61	0.66
1:A:257:PHE:O	1:A:258:ASN:HB2	1.95	0.66
1:A:360:ASP:OD1	1:A:363:LYS:HB2	1.96	0.66
1:A:550:GLU:O	1:A:554:LYS:HG2	1.97	0.65
1:A:554:LYS:C	1:A:555:VAL:HG22	2.21	0.64
1:A:15:VAL:CG1	3:A:1181:HOH:O	2.44	0.63
1:A:15:VAL:HG21	1:A:509:GLU:CD	2.23	0.63
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.81	0.63
1:A:739:ARG:O	1:A:743:GLU:HG3	1.98	0.63
1:A:15:VAL:HG13	1:A:15:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ASN:ND2	1:A:679:MET:H	1.96	0.62
1:A:268:ASP:O	1:A:271:LEU:HB2	2.00	0.61
1:A:703:ALA:CA	1:A:807:THR:HG21	2.30	0.60
1:A:764:MET:HE3	3:A:1055:HOH:O	2.01	0.60
1:A:708:PHE:HB3	1:A:710:ILE:CD1	2.31	0.60
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.84	0.60
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.66	0.59
1:A:678:ASN:HD22	1:A:678:ASN:N	2.00	0.59
1:A:678:ASN:HD22	1:A:679:MET:N	2.01	0.58
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.86	0.57
1:A:335:ILE:HD11	1:A:337:LEU:HD11	1.86	0.57
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.05	0.57
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.86	0.57
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.87	0.56
1:A:503:ILE:HG12	1:A:521:LEU:HD11	1.87	0.56
1:A:36:HIS:O	1:A:40:VAL:HA	2.06	0.56
1:A:367:VAL:O	1:A:371:THR:HG23	2.05	0.56
1:A:15:VAL:HG21	1:A:509:GLU:OE1	2.07	0.55
1:A:592:LYS:HG3	1:A:593:GLU:HG2	1.88	0.55
1:A:93:ARG:CG	1:A:93:ARG:HH21	2.20	0.55
1:A:554:LYS:O	1:A:555:VAL:HG13	2.07	0.54
1:A:49:ARG:HD2	1:A:53:PHE:HE1	1.72	0.54
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.37	0.54
1:A:235:ASN:HD22	1:A:235:ASN:N	2.01	0.54
1:A:413:ARG:HH21	1:A:413:ARG:CG	2.11	0.54
1:A:253:ASN:O	1:A:254:LEU:HB2	2.07	0.53
1:A:252:PHE:C	1:A:254:LEU:H	2.15	0.53
1:A:434:GLY:O	1:A:435:ALA:C	2.52	0.53
1:A:138:ARG:HD3	1:A:138:ARG:C	2.33	0.52
1:A:94:THR:CG2	3:A:1078:HOH:O	2.57	0.52
1:A:575:ARG:HD3	1:A:666:ILE:O	2.10	0.52
1:A:93:ARG:HH21	1:A:93:ARG:HG3	1.75	0.51
1:A:95:LEU:HD11	1:A:99:MET:HE3	1.91	0.51
1:A:493:VAL:CG2	1:A:512:ILE:HD12	2.40	0.51
1:A:413:ARG:NH2	1:A:413:ARG:CG	2.73	0.51
1:A:519:ARG:O	1:A:522:LEU:HB2	2.11	0.50
1:A:59:VAL:HG21	1:A:99:MET:HE2	1.92	0.50
1:A:250:ASN:HD22	1:A:269:ARG:HH22	1.59	0.50
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.93	0.50
1:A:75:TYR:CB	2:A:930:BN2:CL3	2.97	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ILE:HG23	1:A:689:ILE:O	2.11	0.49
1:A:378:THR:OG1	1:A:380:ILE:HG12	2.12	0.49
1:A:65:GLY:O	1:A:69:ARG:CG	2.58	0.49
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.20	0.49
1:A:810:LYS:O	1:A:810:LYS:HG2	2.13	0.49
1:A:715:VAL:HB	1:A:716:GLU:OE1	2.13	0.49
1:A:515:LEU:HD13	1:A:809:GLY:HA2	1.94	0.48
1:A:251:ASP:C	1:A:255:LYS:HB3	2.38	0.48
1:A:601:ARG:NH1	1:A:784:GLN:OE1	2.45	0.48
1:A:313:SER:O	1:A:314:SER:C	2.56	0.48
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.95	0.48
1:A:538:LYS:O	1:A:542:LYS:HG3	2.13	0.48
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.49	0.48
1:A:678:ASN:ND2	1:A:678:ASN:N	2.60	0.47
1:A:703:ALA:CB	1:A:807:THR:HG21	2.43	0.47
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.97	0.47
1:A:250:ASN:HA	1:A:269:ARG:HH22	1.79	0.47
1:A:405:GLU:O	1:A:409:ARG:HG3	2.16	0.46
1:A:456:ALA:C	1:A:481:ASN:HD21	2.24	0.46
1:A:367:VAL:O	1:A:371:THR:CG2	2.64	0.46
1:A:554:LYS:O	1:A:555:VAL:CG2	2.56	0.46
1:A:455:VAL:H	1:A:459:HIS:CD2	2.28	0.46
1:A:716:GLU:N	1:A:716:GLU:CD	2.63	0.46
1:A:270:ASN:ND2	3:A:1214:HOH:O	2.49	0.46
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.46	0.45
1:A:764:MET:HE2	1:A:769:ASP:CA	2.31	0.45
1:A:458:ILE:HD11	1:A:715:VAL:HG21	1.98	0.45
1:A:66:ARG:CG	1:A:837:PRO:HB3	2.41	0.45
1:A:571:HIS:HB2	1:A:574:LYS:CG	2.45	0.45
1:A:834:LEU:HG	1:A:835:PRO:HD2	1.99	0.45
1:A:715:VAL:CA	1:A:716:GLU:OE1	2.65	0.45
1:A:466:THR:HG22	1:A:467:ILE:N	2.31	0.45
1:A:28:LYS:HG3	1:A:111:ALA:HB1	1.99	0.44
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.17	0.44
1:A:548:TYR:CD1	1:A:548:TYR:C	2.95	0.44
1:A:67:TRP:HA	1:A:238:VAL:HB	1.98	0.44
1:A:144:LEU:HA	1:A:147:MET:HE3	1.99	0.44
1:A:15:VAL:HB	3:A:1224:HOH:O	2.16	0.44
1:A:252:PHE:C	1:A:254:LEU:N	2.75	0.44
1:A:678:ASN:ND2	1:A:679:MET:N	2.61	0.44
1:A:94:THR:HG22	3:A:1078:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD12	1:A:147:MET:CE	2.47	0.44
1:A:16:ARG:HB3	1:A:105:GLU:HB3	2.00	0.43
1:A:709:PHE:CD1	1:A:787:VAL:HG12	2.53	0.43
1:A:730:GLU:O	1:A:734:ARG:CG	2.64	0.43
1:A:715:VAL:C	1:A:716:GLU:OE1	2.55	0.43
1:A:254:LEU:HD21	1:A:266:VAL:HG23	2.01	0.43
1:A:311:PHE:O	1:A:314:SER:HB2	2.18	0.43
1:A:579:ASN:C	1:A:579:ASN:HD22	2.26	0.43
1:A:546:ALA:CA	1:A:557:ILE:HD11	2.47	0.42
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.88	0.42
1:A:550:GLU:HA	1:A:554:LYS:HA	2.01	0.42
1:A:703:ALA:HB2	1:A:807:THR:HG21	2.01	0.42
1:A:275:ILE:O	1:A:295:GLN:HG2	2.20	0.42
1:A:341:HIS:N	1:A:342:PRO:CD	2.82	0.42
1:A:424:ARG:HH12	1:A:473:GLU:CD	2.26	0.42
1:A:836:ALA:HB1	1:A:837:PRO:HD2	2.00	0.42
1:A:389:VAL:HG13	1:A:400:LEU:HD11	2.00	0.42
1:A:604:MET:HB3	1:A:645:LEU:CD2	2.48	0.42
1:A:100:VAL:O	1:A:234:ARG:NH2	2.51	0.42
1:A:170:ILE:HA	1:A:174:TRP:O	2.20	0.42
1:A:562:LEU:HD21	1:A:662:LEU:HB2	2.01	0.42
1:A:66:ARG:HA	1:A:69:ARG:HG3	2.01	0.42
1:A:515:LEU:HB3	1:A:809:GLY:HA2	2.02	0.41
1:A:34:HIS:HE1	1:A:61:ASP:OD1	2.03	0.41
1:A:835:PRO:O	1:A:836:ALA:O	2.38	0.41
1:A:325:ASN:HA	3:A:1167:HOH:O	2.21	0.41
1:A:568:LYS:HE2	3:A:1110:HOH:O	2.20	0.41
1:A:48:PRO:HB2	1:A:125:ILE:HD11	2.03	0.41
1:A:110:GLU:O	1:A:113:TYR:HB3	2.20	0.41
1:A:170:ILE:HG12	1:A:646:GLU:HG3	2.02	0.41
1:A:417:ALA:C	1:A:419:PRO:HD3	2.44	0.41
1:A:611:PRO:HA	1:A:617:LYS:HE3	2.03	0.41
1:A:467:ILE:HG23	1:A:468:PHE:N	2.35	0.41
1:A:777:TYR:O	1:A:781:VAL:HG13	2.21	0.41
1:A:450:HIS:HE1	3:A:1139:HOH:O	2.04	0.41
1:A:652:LEU:O	1:A:656:VAL:HG22	2.20	0.41
1:A:782:LYS:O	1:A:785:GLU:HB2	2.22	0.40
1:A:564:ASP:O	1:A:603:VAL:HA	2.22	0.40
1:A:42:ASP:OD2	1:A:44:ASN:ND2	2.51	0.40

All (2) 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)
1:A:44:ASN:CA	2:A:930:BN2:O4[7_556]	1.87	0.33
1:A:44:ASN:CB	2:A:930:BN2:O4[7_556]	2.00	0.20

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	811/842 (96%)	759 (94%)	40 (5%)	12 (2%)	8 4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	A	258	ASN
1	A	259	VAL
1	A	555	VAL
1	A	556	HIS
1	A	14	SER
1	A	43	ARG
1	A	554	LYS
1	A	251	ASP
1	A	835	PRO
1	A	836	ALA
1	A	339	ASP

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%)	596 (84%)	109 (16%)	2 1

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	14	SER
1	A	16	ARG
1	A	18	LEU
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	29	LYS
1	A	33	ARG
1	A	39	LEU
1	A	42	ASP
1	A	45	VAL
1	A	49	ARG
1	A	69	ARG
1	A	72	GLN
1	A	87	LEU
1	A	93	ARG
1	A	94	THR
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
1	A	128	ASP
1	A	138	ARG
1	A	144	LEU
1	A	193	ARG
1	A	195	GLU
1	A	198	LEU
1	A	210	SER
1	A	211	GLN
1	A	214	LYS
1	A	216	VAL
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	247	LYS
1	A	253	ASN
1	A	254	LEU

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Mol	Chain	Res	Type
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	264	GLN
1	A	271	LEU
1	A	279	LEU
1	A	287	GLU
1	A	292	ARG
1	A	314	SER
1	A	324	THR
1	A	335	ILE
1	A	337	LEU
1	A	358	ARG
1	A	363	LYS
1	A	371	THR
1	A	380	ILE
1	A	398	ARG
1	A	400	LEU
1	A	413	ARG
1	A	425	LEU
1	A	426	ARG
1	A	430	LEU
1	A	433	GLU
1	A	436	VAL
1	A	444	LEU
1	A	465	LYS
1	A	474	LEU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	528	GLU
1	A	536	LYS
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	555	VAL
1	A	565	VAL
1	A	568	LYS
1	A	575	ARG
1	A	586	LEU
1	A	593	GLU
1	A	596	LYS

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Mol	Chain	Res	Type
1	A	603	VAL
1	A	622	LEU
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	666	ILE
1	A	678	ASN
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	716	GLU
1	A	720	ARG
1	A	721	LEU
1	A	734	ARG
1	A	742	ILE
1	A	759	LYS
1	A	763	ASN
1	A	765	LEU
1	A	768	HIS
1	A	772	LYS
1	A	781	VAL
1	A	782	LYS
1	A	787	VAL
1	A	790	LEU
1	A	803	ARG
1	A	807	THR
1	A	830	SER
1	A	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	208	HIS
1	A	235	ASN
1	A	250	ASN
1	A	270	ASN
1	A	325	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS

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Mol	Chain	Res	Type
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	614	HIS
1	A	678	ASN
1	A	707	ASN
1	A	763	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	LLP	A	680	1	23,24,25	1.59	2 (8%)	25,32,34	1.29	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
1	LLP	A	680	1	-	1/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C4-C4'	5.13	1.57	1.46
1	A	680	LLP	C5'-C5	2.96	1.58	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	CD-CE-NZ	-3.81	100.74	110.83
1	A	680	LLP	OP3-P-OP1	2.63	121.08	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	680	LLP	C6-C5-C5'-OP4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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
2	BN2	A	930	-	32,32,32	1.78	12 (37%)	42,42,42	1.80	9 (21%)

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	BN2	A	930	-	-	4/22/22/22	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	930	BN2	C3-C2	3.50	1.44	1.38
2	A	930	BN2	O5-C21	-3.19	1.20	1.30
2	A	930	BN2	C14-C9	3.05	1.44	1.39
2	A	930	BN2	C5-C6	2.87	1.44	1.39
2	A	930	BN2	C10-C9	2.75	1.43	1.39
2	A	930	BN2	C4-C5	2.73	1.43	1.38
2	A	930	BN2	C3-C4	2.57	1.43	1.38
2	A	930	BN2	C2-C1	2.51	1.43	1.38
2	A	930	BN2	C13-CL3	-2.39	1.68	1.73
2	A	930	BN2	O2-C8	2.27	1.28	1.23
2	A	930	BN2	O3-C15	2.22	1.51	1.43
2	A	930	BN2	C10-C11	2.08	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	930	BN2	O5-C21-C20	6.53	134.64	114.00
2	A	930	BN2	O5-C21-O4	-4.17	112.61	123.33
2	A	930	BN2	C12-C11-CL2	3.91	123.56	118.40
2	A	930	BN2	O4-C21-C20	-3.27	112.73	123.09
2	A	930	BN2	O1-C7-N1	2.69	126.20	122.27
2	A	930	BN2	C12-C13-CL3	2.59	121.82	118.40
2	A	930	BN2	C5-C6-C1	2.44	120.64	117.79
2	A	930	BN2	C19-C20-C21	-2.25	108.62	114.51
2	A	930	BN2	C10-C11-CL2	-2.18	114.88	118.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

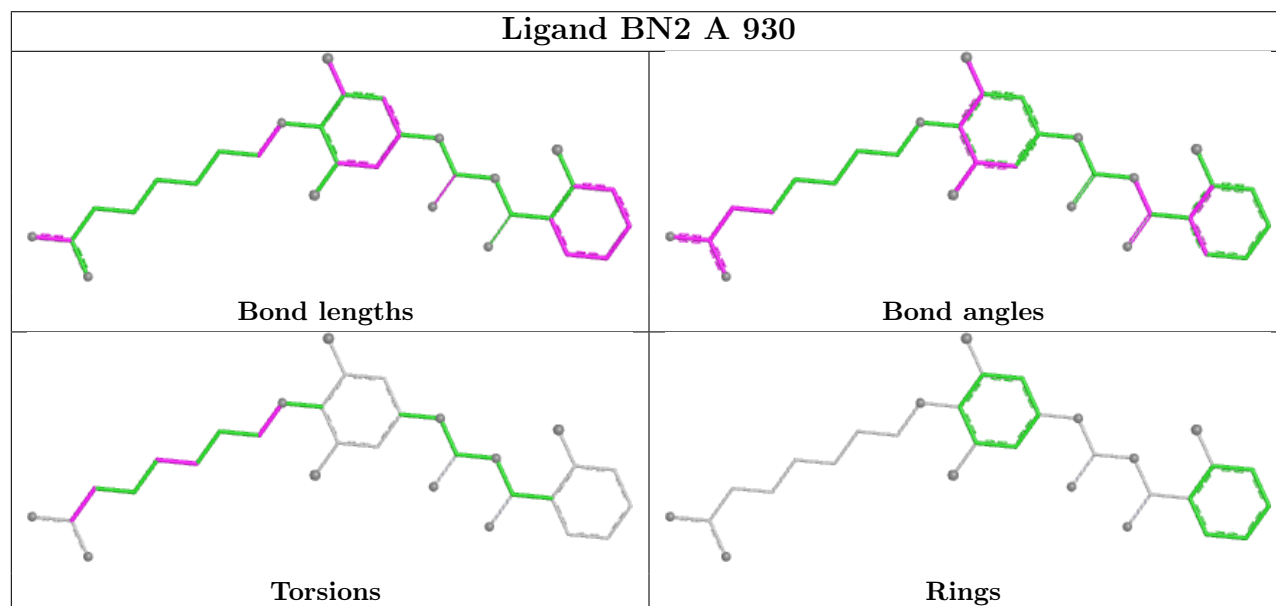
Mol	Chain	Res	Type	Atoms
2	A	930	BN2	C16-C17-C18-C19
2	A	930	BN2	C16-C15-O3-C12
2	A	930	BN2	C19-C20-C21-O5
2	A	930	BN2	C19-C20-C21-O4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	930	BN2	1	2

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.