



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WV1
Title : Crystallographic studies on acyl ureas, a new class of inhibitors of glycogen phosphorylase. Broad specificity of the allosteric site
Authors : Oikonomakos, N.G.; Kosmopoulou, M.N.; Chrysina, E.D.; Leonidas, D.D.; Klabunde, T.; Wendt, K.U.; Defossa, E.
Deposited on : 2004-12-10
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

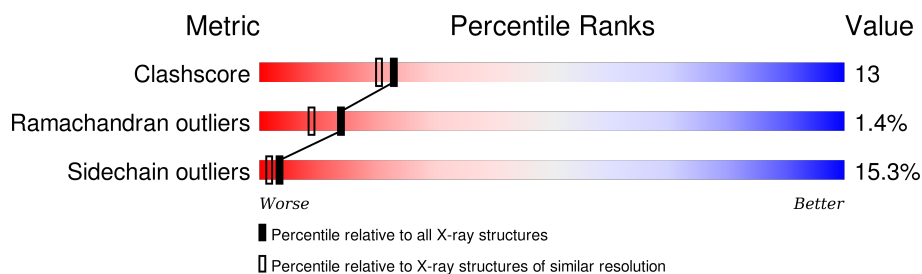
1 Overall quality at a glance

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	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6928 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.

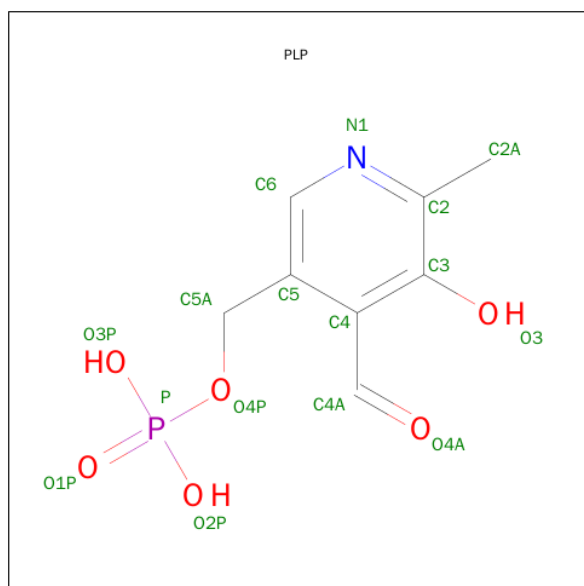
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	816	6634	4231	1167	1207	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

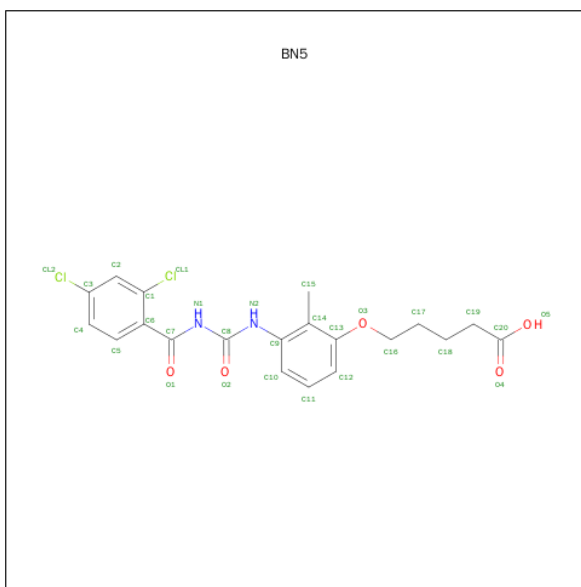
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is 5-[3-({[(2,4-DICHLOROBENZOYL)AMINO]CARBONYL}AMINO)-2-METHYLPHENOXY]PENTANOIC ACID (three-letter code: BN5) (formula: C₂₀H₂₀Cl₂N₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			29	20	2	2	5		

- Molecule 4 is water.

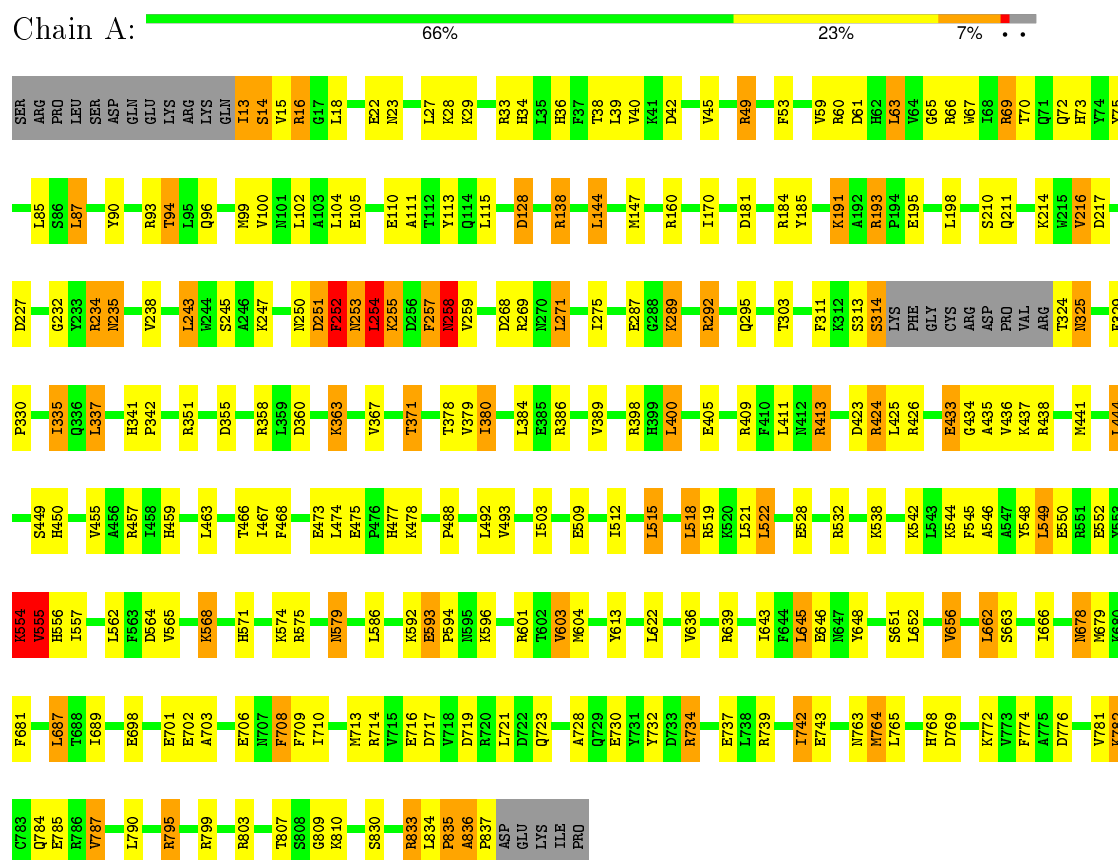
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	250	Total	O	0	0
			250	250		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.31Å 128.31Å 115.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.23 – 2.26	Depositor
% Data completeness (in resolution range)	95.6 (29.23-2.26)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6928	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BN5, 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	0.37	0/6784	0.63	2/9183 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	554	LYS	N-CA-C	5.70	126.38	111.00
1	A	63	LEU	CA-CB-CG	5.26	127.41	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6634	0	6577	179	0
2	A	15	0	7	0	0
3	A	29	0	19	2	0
4	A	250	0	0	19	0
All	All	6928	0	6603	179	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 13.

All (179) 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:N	1:A:716:GLU:OE1	2.02	0.92
1:A:13:ILE:HG22	4:A:1243:HOH:O	1.72	0.89
1:A:413:ARG:HG2	1:A:413:ARG:HH21	1.36	0.89
1:A:251:ASP:CG	1:A:252:PHE:H	1.73	0.87
1:A:138:ARG:O	1:A:138:ARG:HD3	1.75	0.86
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.58	0.85
1:A:423:ASP:HB2	4:A:1237:HOH:O	1.77	0.84
1:A:764:MET:HE2	1:A:769:ASP:HA	1.64	0.79
1:A:15:VAL:HG12	4:A:1173:HOH:O	1.84	0.78
1:A:235:ASN:H	1:A:235:ASN:HD22	1.29	0.77
1:A:335:ILE:HG13	1:A:335:ILE:O	1.85	0.77
1:A:719:ASP:O	1:A:723:GLN:HG2	1.86	0.76
1:A:764:MET:CE	1:A:769:ASP:HA	2.16	0.76
1:A:554:LYS:O	1:A:555:VAL:HG22	1.87	0.74
1:A:379:VAL:HG22	4:A:1095:HOH:O	1.88	0.74
1:A:15:VAL:HG13	1:A:15:VAL:O	1.87	0.73
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.72	0.72
1:A:708:PHE:HB3	1:A:710:ILE:HD12	1.71	0.72
1:A:335:ILE:HD11	1:A:337:LEU:HD11	1.73	0.70
1:A:678:ASN:HD22	1:A:679:MET:H	1.38	0.70
1:A:251:ASP:CG	1:A:252:PHE:N	2.45	0.70
1:A:795:ARG:O	1:A:799:ARG:HG3	1.91	0.70
1:A:455:VAL:H	1:A:459:HIS:HD2	1.37	0.69
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.23	0.69
1:A:65:GLY:O	1:A:69:ARG:HG2	1.91	0.69
1:A:571:HIS:HB2	1:A:574:LYS:HG3	1.74	0.69
1:A:66:ARG:HG3	1:A:837:PRO:HB3	1.75	0.69
1:A:59:VAL:HG21	1:A:99:MET:HE2	1.74	0.69
1:A:550:GLU:O	1:A:554:LYS:HG2	1.94	0.68
1:A:703:ALA:HA	1:A:807:THR:HG21	1.74	0.68
1:A:15:VAL:HG22	4:A:1027:HOH:O	1.93	0.68
1:A:360:ASP:OD1	1:A:363:LYS:HB2	1.95	0.67
1:A:257:PHE:O	1:A:258:ASN:HB2	1.93	0.67
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.30	0.67
1:A:413:ARG:NH2	1:A:413:ARG:HG2	2.07	0.66
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.78	0.66
1:A:708:PHE:HB3	1:A:710:ILE:CD1	2.25	0.65
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.80	0.63
1:A:739:ARG:O	1:A:743:GLU:HG3	2.00	0.62
1:A:554:LYS:O	1:A:555:VAL:HG13	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLU:O	1:A:734:ARG:HG2	1.99	0.61
1:A:678:ASN:HD22	1:A:678:ASN:N	1.98	0.61
1:A:36:HIS:O	1:A:40:VAL:HA	2.01	0.60
1:A:423:ASP:CB	4:A:1237:HOH:O	2.42	0.60
1:A:592:LYS:HG3	1:A:593:GLU:HG2	1.83	0.60
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.86	0.59
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.85	0.59
1:A:493:VAL:CG2	1:A:512:ILE:HD12	2.33	0.59
1:A:554:LYS:C	1:A:555:VAL:HG22	2.23	0.58
1:A:15:VAL:HB	4:A:1215:HOH:O	2.01	0.58
1:A:703:ALA:CA	1:A:807:THR:HG21	2.32	0.58
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.86	0.58
1:A:15:VAL:CG1	4:A:1173:HOH:O	2.48	0.58
1:A:15:VAL:HG21	1:A:509:GLU:OE1	2.03	0.58
1:A:235:ASN:HD22	1:A:235:ASN:N	1.96	0.57
1:A:128:ASP:OD2	1:A:651:SER:HB3	2.05	0.56
1:A:93:ARG:HH21	1:A:93:ARG:CG	2.18	0.56
1:A:268:ASP:O	1:A:271:LEU:HB2	2.06	0.56
1:A:678:ASN:ND2	1:A:679:MET:H	2.02	0.55
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.07	0.55
1:A:601:ARG:HD2	4:A:1032:HOH:O	2.05	0.55
1:A:93:ARG:HH21	1:A:93:ARG:HG3	1.72	0.55
1:A:191:LYS:HG2	3:A:930:BN5:CL2	2.43	0.55
1:A:519:ARG:O	1:A:522:LEU:HB2	2.08	0.54
1:A:737:GLU:HG3	4:A:1150:HOH:O	2.06	0.54
1:A:709:PHE:CD1	1:A:787:VAL:HG12	2.42	0.54
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.89	0.54
1:A:144:LEU:HA	1:A:147:MET:HE3	1.90	0.53
1:A:378:THR:OG1	1:A:380:ILE:HG12	2.09	0.53
1:A:40:VAL:O	1:A:40:VAL:HG12	2.09	0.52
1:A:678:ASN:HD22	1:A:679:MET:N	2.07	0.52
1:A:325:ASN:HA	4:A:1160:HOH:O	2.09	0.52
1:A:94:THR:CG2	4:A:1075:HOH:O	2.58	0.52
1:A:216:VAL:HG13	1:A:217:ASP:N	2.25	0.51
1:A:252:PHE:C	1:A:254:LEU:H	2.13	0.51
1:A:515:LEU:HD13	1:A:809:GLY:HA2	1.91	0.51
1:A:253:ASN:O	1:A:254:LEU:HB2	2.09	0.51
1:A:184:ARG:NE	1:A:185:TYR:CE1	2.74	0.51
1:A:678:ASN:N	1:A:678:ASN:ND2	2.57	0.50
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.41	0.50
1:A:49:ARG:HD2	1:A:53:PHE:HE1	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ILE:O	1:A:689:ILE:HG23	2.10	0.50
1:A:434:GLY:O	1:A:435:ALA:C	2.50	0.50
1:A:703:ALA:CB	1:A:807:THR:HG21	2.40	0.50
1:A:405:GLU:O	1:A:409:ARG:HG3	2.12	0.50
1:A:144:LEU:HD12	1:A:147:MET:CE	2.42	0.49
1:A:170:ILE:HG12	1:A:646:GLU:HG3	1.93	0.49
1:A:138:ARG:C	1:A:138:ARG:HD3	2.32	0.49
1:A:367:VAL:O	1:A:371:THR:HG23	2.13	0.49
1:A:75:TYR:CD2	3:A:930:BN5:H161	2.48	0.49
1:A:455:VAL:H	1:A:459:HIS:CD2	2.24	0.48
1:A:367:VAL:O	1:A:371:THR:CG2	2.62	0.48
1:A:424:ARG:NH1	1:A:473:GLU:OE1	2.41	0.48
1:A:477:HIS:HD2	4:A:1229:HOH:O	1.95	0.48
1:A:65:GLY:O	1:A:69:ARG:CG	2.59	0.48
1:A:66:ARG:HA	1:A:69:ARG:HG3	1.95	0.48
1:A:538:LYS:O	1:A:542:LYS:HG3	2.14	0.48
1:A:592:LYS:HD2	1:A:592:LYS:O	2.15	0.47
1:A:16:ARG:HB3	1:A:105:GLU:HB3	1.96	0.47
1:A:15:VAL:CG1	1:A:15:VAL:O	2.59	0.47
1:A:467:ILE:HG23	1:A:468:PHE:N	2.28	0.47
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.96	0.46
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.98	0.46
1:A:235:ASN:H	1:A:235:ASN:ND2	2.07	0.46
1:A:234:ARG:NH1	4:A:1027:HOH:O	2.49	0.46
1:A:782:LYS:O	1:A:785:GLU:HB2	2.16	0.46
1:A:575:ARG:HD3	1:A:666:ILE:O	2.16	0.46
1:A:601:ARG:NH1	1:A:784:GLN:OE1	2.45	0.46
1:A:488:PRO:O	1:A:492:LEU:HB3	2.16	0.46
1:A:550:GLU:HA	1:A:554:LYS:HA	1.98	0.45
1:A:250:ASN:HA	1:A:269:ARG:HH22	1.80	0.45
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.97	0.45
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.52	0.45
1:A:28:LYS:HG3	1:A:111:ALA:HB1	1.99	0.45
1:A:292:ARG:O	1:A:292:ARG:HD2	2.16	0.45
1:A:250:ASN:HD22	1:A:269:ARG:HH22	1.65	0.45
1:A:532:ARG:HG3	4:A:1153:HOH:O	2.16	0.45
1:A:467:ILE:HG23	1:A:468:PHE:CG	2.51	0.45
1:A:549:LEU:HD23	1:A:557:ILE:HD13	2.00	0.44
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.82	0.44
1:A:110:GLU:O	1:A:113:TYR:HB3	2.16	0.44
1:A:275:ILE:O	1:A:295:GLN:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ALA:HB1	1:A:837:PRO:HD2	1.98	0.44
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.99	0.44
1:A:579:ASN:C	1:A:579:ASN:HD22	2.21	0.44
1:A:341:HIS:N	1:A:342:PRO:CD	2.81	0.44
1:A:313:SER:O	1:A:314:SER:C	2.56	0.44
1:A:466:THR:HG22	1:A:467:ILE:N	2.32	0.43
1:A:85:LEU:HD11	1:A:303:THR:HG21	2.00	0.43
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.20	0.43
1:A:554:LYS:O	1:A:555:VAL:CG2	2.63	0.43
1:A:604:MET:HB3	1:A:645:LEU:CD2	2.48	0.43
1:A:571:HIS:HB2	1:A:574:LYS:CG	2.46	0.43
1:A:15:VAL:HG21	1:A:509:GLU:CD	2.39	0.43
1:A:34:HIS:HE1	1:A:61:ASP:OD1	2.00	0.43
1:A:254:LEU:N	4:A:1186:HOH:O	2.51	0.43
1:A:636:VAL:O	1:A:639:ARG:HD3	2.19	0.43
1:A:193:ARG:HD3	1:A:227:ASP:OD1	2.19	0.43
1:A:433:GLU:OE1	1:A:437:LYS:HD2	2.19	0.43
1:A:441:MET:HE3	1:A:444:LEU:HD12	2.00	0.43
1:A:568:LYS:HE2	4:A:1106:HOH:O	2.18	0.42
1:A:389:VAL:HG13	1:A:400:LEU:HD11	2.00	0.42
1:A:93:ARG:CG	1:A:93:ARG:NH2	2.82	0.42
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.54	0.42
1:A:87:LEU:HD13	1:A:341:HIS:HB3	2.01	0.42
1:A:96:GLN:O	1:A:100:VAL:HG23	2.18	0.42
1:A:810:LYS:O	1:A:810:LYS:HG2	2.19	0.42
1:A:351:ARG:O	1:A:355:ASP:HB2	2.20	0.42
1:A:255:LYS:O	1:A:257:PHE:N	2.53	0.42
1:A:235:ASN:N	1:A:235:ASN:ND2	2.65	0.42
1:A:503:ILE:HG12	1:A:521:LEU:HD11	2.00	0.42
1:A:60:ARG:HA	1:A:63:LEU:CD2	2.49	0.42
1:A:467:ILE:CG2	1:A:468:PHE:N	2.82	0.42
1:A:594:PRO:O	1:A:639:ARG:NH1	2.50	0.41
1:A:67:TRP:HA	1:A:238:VAL:HB	2.00	0.41
1:A:386:ARG:HB3	1:A:438:ARG:HD3	2.01	0.41
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.02	0.41
1:A:548:TYR:CD1	1:A:548:TYR:C	2.92	0.41
1:A:564:ASP:O	1:A:603:VAL:HA	2.20	0.41
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.56	0.41
1:A:835:PRO:O	1:A:836:ALA:O	2.38	0.41
1:A:252:PHE:C	1:A:254:LEU:N	2.74	0.41
1:A:70:THR:O	1:A:73:HIS:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:HG22	4:A:1075:HOH:O	2.18	0.41
1:A:181:ASP:HB3	1:A:184:ARG:HH21	1.84	0.41
1:A:475:GLU:HB3	1:A:477:HIS:CE1	2.56	0.41
1:A:575:ARG:NH1	1:A:776:ASP:HB2	2.36	0.41
1:A:663:SER:HB2	1:A:681:PHE:CG	2.56	0.41
1:A:251:ASP:C	1:A:255:LYS:HB3	2.42	0.41
1:A:834:LEU:O	1:A:836:ALA:N	2.54	0.41
1:A:311:PHE:O	1:A:314:SER:HB2	2.21	0.41
1:A:698:GLU:O	1:A:702:GLU:HG2	2.20	0.41
1:A:449:SER:O	1:A:478:LYS:HE2	2.21	0.41
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.85	0.41
1:A:411:LEU:HA	1:A:411:LEU:HD23	1.91	0.40
1:A:450:HIS:HE1	4:A:1133:HOH:O	2.04	0.40
1:A:34:HIS:CD2	1:A:38:THR:OG1	2.70	0.40
1:A:289:LYS:HA	1:A:289:LYS:HD2	1.93	0.40
1:A:730:GLU:O	1:A:734:ARG:CG	2.66	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	812/842 (96%)	761 (94%)	40 (5%)	11 (1%)	14 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	254	LEU
1	A	258	ASN
1	A	259	VAL
1	A	555	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	556	HIS
1	A	554	LYS
1	A	835	PRO
1	A	836	ALA
1	A	251	ASP
1	A	252	PHE

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	706/731 (97%)	598 (85%)	108 (15%)	3 2

All (108) 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	90	TYR
1	A	94	THR
1	A	102	LEU
1	A	104	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	LEU
1	A	128	ASP
1	A	138	ARG
1	A	144	LEU
1	A	191	LYS
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	245	SER
1	A	247	LYS
1	A	252	PHE
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	271	LEU
1	A	287	GLU
1	A	289	LYS
1	A	292	ARG
1	A	314	SER
1	A	324	THR
1	A	325	ASN
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	384	LEU
1	A	400	LEU
1	A	413	ARG
1	A	424	ARG
1	A	425	LEU
1	A	426	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	433	GLU
1	A	436	VAL
1	A	444	LEU
1	A	474	LEU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	528	GLU
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	579	ASN
1	A	586	LEU
1	A	593	GLU
1	A	596	LYS
1	A	603	VAL
1	A	613	TYR
1	A	622	LEU
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	678	ASN
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	714	ARG
1	A	721	LEU
1	A	734	ARG
1	A	742	ILE
1	A	763	ASN
1	A	764	MET
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	795	ARG
1	A	803	ARG
1	A	830	SER
1	A	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	235	ASN
1	A	250	ASN
1	A	270	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	763	ASN
1	A	768	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

2 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	BN5	A	930	-	27,30,30	1.73	8 (29%)	36,40,40	1.53	6 (16%)
2	PLP	A	999	1	15,15,16	1.52	3 (20%)	21,22,23	1.14	1 (4%)

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	BN5	A	930	-	-	0/18/20/20	0/2/2/2
2	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C3-C2	-2.72	1.38	1.40
3	A	930	BN5	C3-CL2	-2.39	1.69	1.74
3	A	930	BN5	C4-C3	2.03	1.42	1.38
3	A	930	BN5	C6-C1	2.49	1.43	1.39
3	A	930	BN5	C2-C1	2.49	1.42	1.38
3	A	930	BN5	C10-C9	2.51	1.44	1.39
3	A	930	BN5	C13-C14	2.63	1.43	1.40
3	A	930	BN5	C5-C4	2.81	1.43	1.38
2	A	999	PLP	C5A-C5	3.05	1.59	1.50
2	A	999	PLP	C4A-C4	3.05	1.57	1.51
3	A	930	BN5	C9-C14	3.51	1.46	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	930	BN5	C2-C1-C6	-2.88	119.67	121.59
3	A	930	BN5	C6-C1-CL1	2.04	124.09	120.97
3	A	930	BN5	O1-C7-N1	2.18	125.74	122.36
3	A	930	BN5	C9-N2-C8	2.67	131.17	125.57
2	A	999	PLP	O3P-P-O1P	3.01	120.27	110.58
3	A	930	BN5	O2-C8-N2	3.05	128.22	123.58
3	A	930	BN5	O3-C13-C14	5.07	118.71	115.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	930	BN5	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.