



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:37 PM GMT

PDB ID : 1L7X  
Title : Human liver glycogen phosphorylase b complexed with caffeine, N-acetyl-beta-D-glucopyranosylamine, and CP-403,700  
Authors : Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszkowski, D.G.; Rath, V.L.  
Deposited on : 2002-03-18  
Resolution : 2.30 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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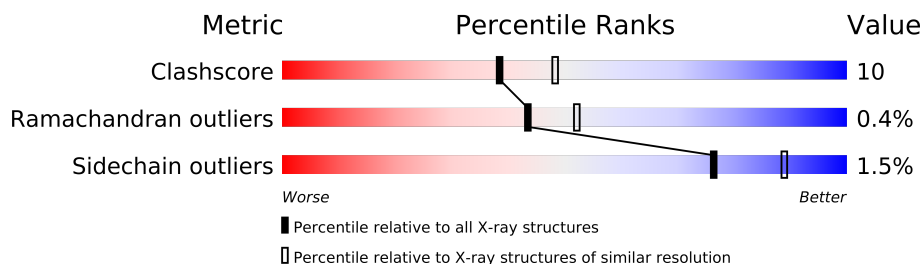
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	
1	B	847	

## 2 Entry composition i

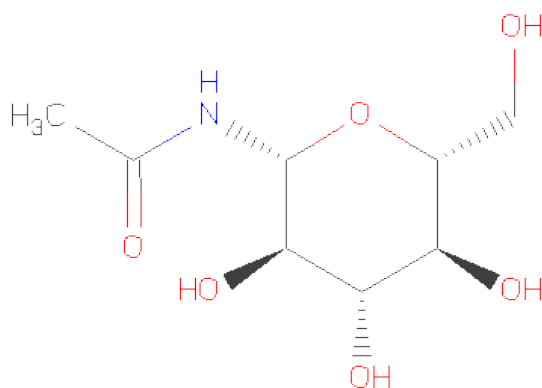
There are 7 unique types of molecules in this entry. The entry contains 13542 atoms, of which 0 are hydrogen and 0 are deuterium.

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, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	793	Total	C	N	O	S	0	0	0
			6436	4135	1092	1180	29			
1	B	795	Total	C	N	O	S	0	0	0
			6446	4141	1094	1182	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



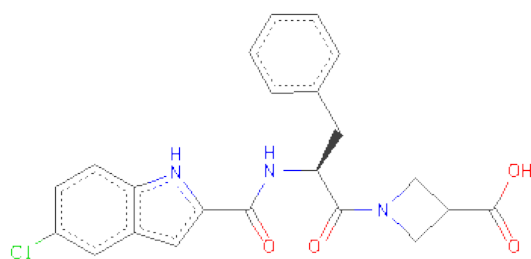
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLICACID (three-letter code: 700) (formula: C<sub>22</sub>H<sub>20</sub>ClN<sub>3</sub>O<sub>4</sub>).



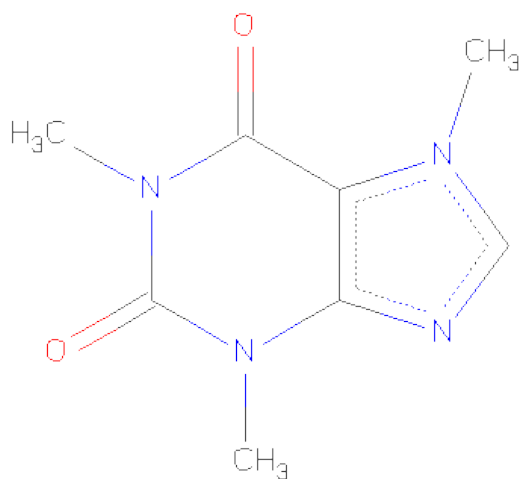
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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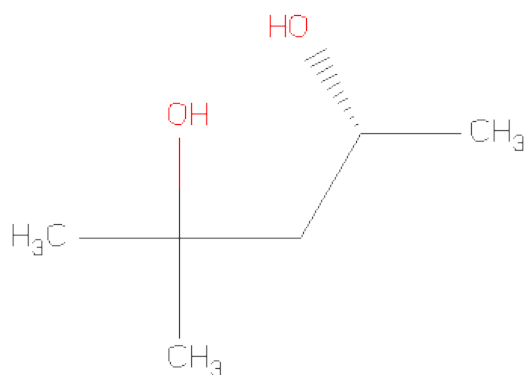
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula:  $C_8H_{10}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	4	2		
5	B	1	Total	C	N	O	0	0
			14	8	4	2		
5	A	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	252	Total	O	0	0
			252	252		
7	B	222	Total	O	0	0
			222	222		

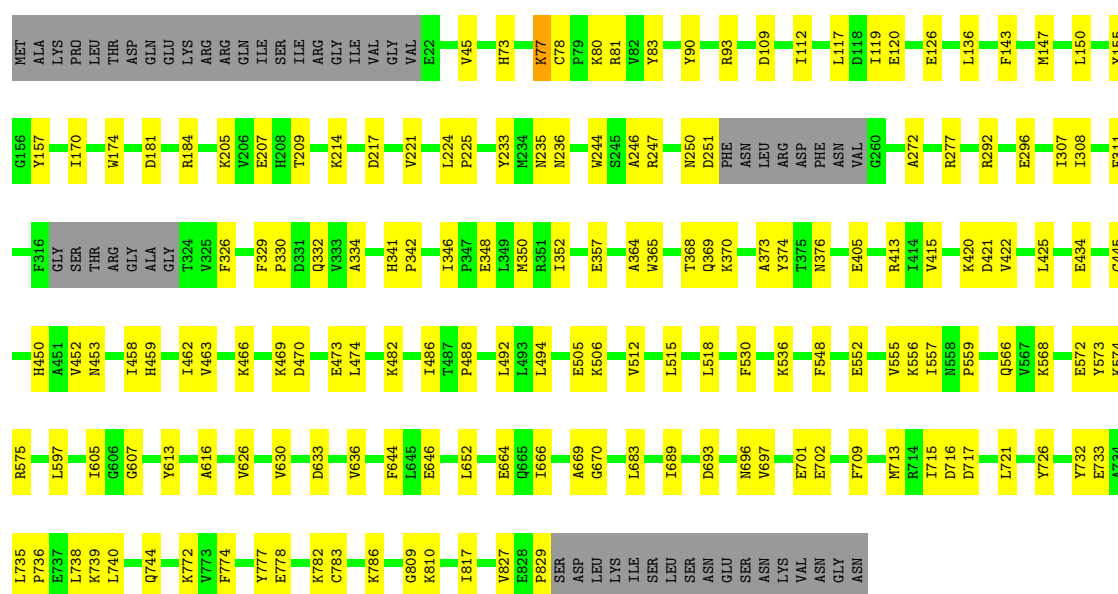
### 3 Residue-property plots

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.

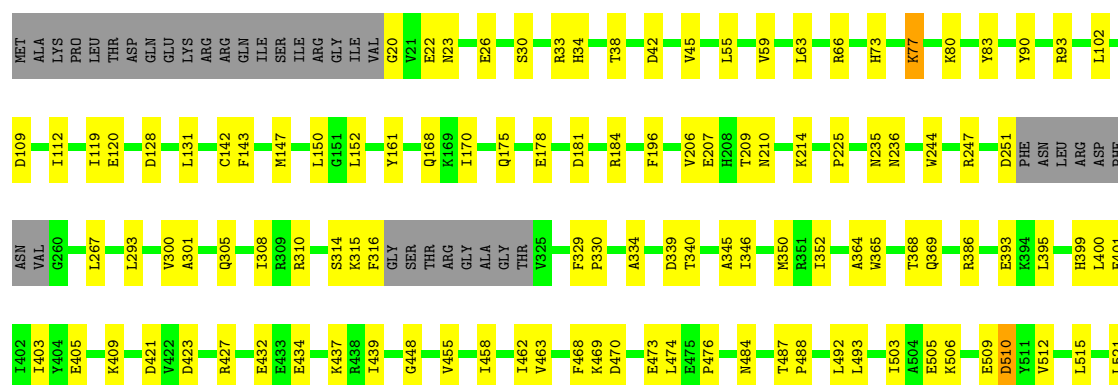
- Molecule 1: Glycogen phosphorylase, liver form

Chain A:



- Molecule 1: Glycogen phosphorylase, liver form

Chain B:



P829	S830	ASP	L662	F524
		LEU	I666	D528
		LYS	S667	F548
		ILE	T668	E552
		SER	L683	V555
		LEU	L689	K556
		SER	I689	I557
		ASN	R692	K568
		GLU	V697	Y573
		SER	E701	K574
		ASN	E702	R575
		LYS	A703	O576
		VAL	E706	L577
		ASN	L708	K591
		GLY	F709	K592
		ASN	I710	D593
S831	S832	LYS	M713	K596
		VAL	R714	L597
		ASN	I715	I605
		GLY	D716	K608
		ASN	D717	Y613
		LYS	V718	A616
		VAL	Y732	V626
		ASN	E733	A627
		GLY	K739	D628
		ASN	D743	V629
		LYS	N747	V630
		VAL	F750	N631
		ASN	L765	N632
		GLY	K772	D633
		ASN	D776	V636
		S833	S834	VAL
LYS	V781			I643
ASN	K782			F644
GLY	C783			L645
ASN	K786			E646
LYS	V787			V650
VAL	S812			S651
ASN	V827			L652
GLY	E828			I657
ASN				P658
LYS				
VAL				
ASN				
GLY				
ASN				



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.07Å 124.07Å 122.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.39 – 2.30	Depositor
% Data completeness (in resolution range)	96.6 (34.39-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: CFF, MRD, 700, NBG, 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	0.36	0/6580	0.59	0/8899
1	B	0.35	0/6590	0.59	0/8912
All	All	0.35	0/13170	0.59	0/17811

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6436	0	6426	126	0
1	B	6446	0	6436	133	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	19	0	0
4	B	30	0	19	0	0
5	A	28	0	20	0	0
5	B	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	24	0	42	1	0
7	A	252	0	0	7	0
7	B	222	0	0	4	0
All	All	13542	0	13016	256	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (256) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:MET:HE1	1:A:364:ALA:HB1	1.56	0.86
1:B:77:LYS:HA	1:B:77:LYS:HE3	1.59	0.84
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.60	0.83
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.60	0.83
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.62	0.82
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.61	0.81
1:A:597:LEU:H	1:A:597:LEU:HD22	1.45	0.80
1:B:597:LEU:HD22	1:B:597:LEU:H	1.47	0.79
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.63	0.79
1:B:350:MET:HE1	1:B:364:ALA:HB1	1.64	0.78
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.64	0.78
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.14	0.77
1:B:633:ASP:O	1:B:636:VAL:HG12	1.84	0.76
1:B:181:ASP:OD2	1:B:184:ARG:HB2	1.85	0.76
1:B:30:SER:HA	1:B:33:ARG:NH1	2.02	0.75
1:B:575:ARG:HD3	1:B:666:ILE:O	1.88	0.74
1:A:209:THR:HG21	1:A:214:LYS:HE2	1.70	0.72
1:B:170:ILE:HG22	7:B:2366:HOH:O	1.89	0.71
1:A:77:LYS:HA	1:A:77:LYS:HE3	1.73	0.70
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.73	0.69
1:A:350:MET:HE3	1:A:364:ALA:O	1.92	0.69
1:B:568:LYS:HD3	1:B:574:LYS:HD3	1.74	0.69
1:A:633:ASP:O	1:A:636:VAL:HG12	1.94	0.68
1:A:350:MET:HA	1:A:350:MET:CE	2.24	0.67
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.09	0.67
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.78	0.66
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.61	0.65
1:B:247:ARG:HD2	7:B:2449:HOH:O	1.96	0.65
1:A:786:LYS:NZ	1:A:786:LYS:HB3	2.10	0.65
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.32	0.65
1:A:150:LEU:O	1:A:829:PRO:HB3	1.97	0.65
1:B:350:MET:HE3	1:B:364:ALA:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:142:CYS:SG	1:B:487:THR:HG22	2.37	0.64
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.80	0.63
1:B:93:ARG:HG3	1:B:128:ASP:OD2	1.97	0.63
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.33	0.62
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.81	0.62
1:B:548:PHE:O	1:B:552:GLU:HG2	2.01	0.61
1:A:515:LEU:HG	1:A:809:GLY:HA2	1.82	0.60
1:A:365:TRP:CD1	1:A:369:GLN:NE2	2.69	0.60
1:A:462:ILE:HG12	1:A:466:LYS:NZ	2.16	0.60
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.34	0.60
1:B:469:LYS:O	1:B:473:GLU:HG3	2.02	0.60
1:A:209:THR:CG2	1:A:214:LYS:HE2	2.32	0.59
1:B:109:ASP:OD1	1:B:119:ILE:HD13	2.03	0.58
1:B:207:GLU:HG2	1:B:209:THR:HG23	1.85	0.58
1:A:462:ILE:HA	1:A:466:LYS:HD2	1.84	0.58
1:B:386:ARG:HD2	1:B:432:GLU:OE2	2.04	0.58
1:B:697:VAL:O	1:B:701:GLU:HG3	2.03	0.58
1:A:548:PHE:O	1:A:552:GLU:HG2	2.03	0.58
1:A:292:ARG:O	1:A:296:GLU:HG3	2.02	0.58
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.85	0.57
1:B:555:VAL:CG2	1:B:631:ASN:HD22	2.17	0.57
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.85	0.57
1:A:365:TRP:NE1	1:A:369:GLN:NE2	2.53	0.57
1:A:597:LEU:H	1:A:597:LEU:CD2	2.17	0.57
1:B:458:ILE:O	1:B:462:ILE:HG13	2.04	0.57
1:A:556:LYS:HD3	1:A:557:ILE:N	2.20	0.57
1:A:45:VAL:O	1:A:45:VAL:HG12	2.05	0.57
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.86	0.57
1:A:250:ASN:HD21	1:B:184:ARG:NH1	2.02	0.56
1:A:357:GLU:HA	1:A:357:GLU:OE2	2.04	0.56
1:A:458:ILE:HG22	7:A:2145:HOH:O	2.04	0.56
1:B:30:SER:HA	1:B:33:ARG:HH12	1.70	0.56
1:A:494:LEU:HD23	1:A:494:LEU:C	2.25	0.56
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.88	0.56
1:B:20:GLY:HA2	1:B:23:ASN:HD22	1.71	0.56
1:A:350:MET:HE3	1:A:364:ALA:C	2.26	0.56
1:B:150:LEU:O	1:B:829:PRO:HB3	2.07	0.55
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.05	0.55
1:A:505:GLU:HG3	7:A:2296:HOH:O	2.05	0.55
1:B:597:LEU:HD22	1:B:597:LEU:N	2.20	0.55
1:B:777:TYR:O	1:B:781:VAL:HG23	2.06	0.55
1:B:515:LEU:HD22	1:B:812:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:350:MET:CE	1:B:368:THR:OG1	2.56	0.54
1:A:73:HIS:CE1	1:A:77:LYS:HG3	2.43	0.54
1:A:469:LYS:O	1:A:473:GLU:HG3	2.07	0.54
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.20	0.54
1:B:597:LEU:CD2	1:B:597:LEU:H	2.17	0.54
1:A:350:MET:HA	1:A:350:MET:HE2	1.89	0.54
1:A:246:ALA:O	1:A:247:ARG:HD3	2.07	0.54
1:B:22:GLU:O	1:B:26:GLU:HG2	2.08	0.54
1:B:293:LEU:HD23	1:B:395:LEU:HD23	1.90	0.54
1:B:556:LYS:HD3	1:B:557:ILE:N	2.22	0.54
1:B:207:GLU:OE1	1:B:214:LYS:HE3	2.08	0.53
1:B:209:THR:OG1	1:B:214:LYS:HE2	2.08	0.53
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.44	0.53
1:B:786:LYS:HB3	1:B:786:LYS:NZ	2.24	0.53
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.44	0.53
1:A:536:LYS:HD3	7:A:2237:HOH:O	2.08	0.53
1:B:591:LYS:HD3	1:B:633:ASP:OD1	2.09	0.53
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.39	0.53
1:A:470:ASP:O	1:A:474:LEU:HD13	2.09	0.53
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.91	0.52
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.44	0.52
1:B:555:VAL:HG21	1:B:631:ASN:HD22	1.75	0.52
1:A:740:LEU:O	1:A:744:GLN:HG3	2.10	0.52
1:A:575:ARG:HD3	1:A:666:ILE:O	2.09	0.52
1:B:510:ASP:OD2	1:B:510:ASP:N	2.38	0.52
1:B:315:LYS:O	1:B:316:PHE:O	2.27	0.52
1:B:80:LYS:HB3	1:B:827:VAL:CG1	2.39	0.52
1:B:405:GLU:OE1	1:B:409:LYS:NZ	2.42	0.52
1:A:374:TYR:O	1:A:452:VAL:HA	2.10	0.52
1:B:492:LEU:HD22	1:B:683:LEU:HD11	1.92	0.51
1:B:45:VAL:HG12	1:B:45:VAL:O	2.10	0.51
1:B:575:ARG:HD2	1:B:668:THR:N	2.26	0.51
1:B:555:VAL:HG21	1:B:631:ASN:ND2	2.25	0.51
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.46	0.51
1:B:350:MET:HE3	1:B:368:THR:OG1	2.11	0.51
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.46	0.51
1:B:77:LYS:HA	1:B:77:LYS:CE	2.34	0.51
1:A:506:LYS:HE2	1:A:530:PHE:CD1	2.46	0.51
1:B:22:GLU:O	1:B:22:GLU:HG2	2.11	0.51
1:B:350:MET:HE3	1:B:364:ALA:C	2.30	0.50
1:B:301:ALA:O	1:B:305:GLN:HG3	2.11	0.50
1:B:470:ASP:O	1:B:474:LEU:HD13	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.93	0.50
1:A:506:LYS:HE2	1:A:530:PHE:HD1	1.77	0.50
1:A:515:LEU:HD11	1:A:518:LEU:HD11	1.94	0.50
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.92	0.49
1:A:786:LYS:HB3	1:A:786:LYS:HZ2	1.76	0.49
1:A:453:ASN:ND2	1:A:482:LYS:HB2	2.27	0.49
1:A:136:LEU:C	1:A:136:LEU:HD23	2.32	0.49
1:B:488:PRO:O	1:B:492:LEU:HB3	2.12	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.49
1:A:221:VAL:HG22	1:A:272:ALA:HB1	1.94	0.49
1:B:718:VAL:HG13	1:B:772:LYS:HE2	1.94	0.49
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.95	0.49
1:B:593:ASP:OD1	1:B:596:LYS:N	2.46	0.49
1:B:423:ASP:OD1	1:B:427:ARG:NH1	2.46	0.49
1:A:415:VAL:CG2	1:A:425:LEU:HD11	2.42	0.49
1:A:369:GLN:O	1:A:450:HIS:HB3	2.13	0.49
1:B:626:VAL:HA	1:B:750:PHE:CD1	2.48	0.49
1:B:196:PHE:CZ	6:B:903:MRD:H1C3	2.47	0.49
1:B:743:ASP:O	1:B:747:ASN:ND2	2.46	0.49
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.94	0.49
1:A:207:GLU:OE1	1:A:214:LYS:HE3	2.12	0.49
1:B:73:HIS:CE1	1:B:77:LYS:HG3	2.48	0.48
1:A:81:ARG:HD3	1:A:83:TYR:OH	2.13	0.48
1:B:613:TYR:CD2	1:B:616:ALA:HB2	2.48	0.48
1:A:462:ILE:HG12	1:A:466:LYS:HZ3	1.78	0.48
1:B:474:LEU:O	1:B:476:PRO:HD3	2.12	0.48
1:B:455:VAL:CG1	1:B:484:ASN:HD21	2.26	0.48
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.95	0.48
1:B:393:GLU:HB2	1:B:400:LEU:CD2	2.44	0.48
1:A:459:HIS:O	1:A:463:VAL:HG23	2.14	0.48
1:A:348:GLU:O	1:A:352:ILE:HG13	2.13	0.48
1:B:515:LEU:CD2	1:B:812:SER:HB2	2.44	0.48
1:B:493:LEU:HD21	1:B:512:VAL:HG11	1.96	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:B:350:MET:HA	1:B:350:MET:CE	2.44	0.47
1:B:63:LEU:HD23	1:B:102:LEU:HD11	1.96	0.47
1:A:350:MET:CE	1:A:368:THR:OG1	2.62	0.47
1:A:557:ILE:O	1:A:559:PRO:HD3	2.14	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:B:339:ASP:OD1	1:B:340:THR:N	2.43	0.47
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.95	0.47
1:B:568:LYS:HB3	1:B:568:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:386:ARG:HA	1:B:439:ILE:O	2.14	0.47
1:B:83:TYR:OH	1:B:310:ARG:HD2	2.15	0.47
1:A:205:LYS:HE2	1:A:217:ASP:OD2	2.14	0.47
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.83	0.47
1:B:505:GLU:HG2	1:B:505:GLU:O	2.15	0.47
1:B:66:ARG:CD	1:B:236:ASN:HA	2.44	0.47
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.63	0.47
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.96	0.47
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.15	0.47
1:B:577:LEU:HD13	1:B:765:LEU:HD21	1.96	0.47
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.50	0.46
1:A:308:ILE:HD12	1:A:352:ILE:HD13	1.96	0.46
1:A:626:VAL:O	1:A:630:VAL:HG23	2.16	0.46
1:A:492:LEU:HD22	1:A:683:LEU:HD11	1.97	0.46
1:A:78:CYS:HB3	1:A:332:GLN:HE22	1.80	0.46
1:B:630:VAL:O	1:B:636:VAL:HG11	2.14	0.46
1:B:605:ILE:O	1:B:644:PHE:HA	2.15	0.46
1:A:506:LYS:HG3	1:A:530:PHE:CE1	2.49	0.46
1:B:55:LEU:HD13	1:B:112:ILE:HD11	1.96	0.46
1:A:420:LYS:O	1:A:422:VAL:HG13	2.15	0.46
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.79	0.46
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.98	0.46
1:A:778:GLU:CG	1:A:782:LYS:HE2	2.46	0.46
1:B:55:LEU:O	1:B:59:VAL:HG23	2.15	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.97	0.45
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.49	0.45
1:A:693:ASP:O	1:A:696:ASN:HB2	2.16	0.45
1:A:376:ASN:O	1:A:459:HIS:HE1	1.98	0.45
1:B:293:LEU:HD23	1:B:395:LEU:CD2	2.47	0.45
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.52	0.45
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.52	0.45
1:A:405:GLU:HA	1:A:405:GLU:OE2	2.16	0.45
1:A:83:TYR:CD1	1:A:155:TYR:HB2	2.53	0.44
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.99	0.44
1:A:670:GLY:H	1:A:693:ASP:CG	2.21	0.44
1:B:131:LEU:HD22	1:B:161:TYR:HB2	2.00	0.44
1:B:152:LEU:HD23	1:B:829:PRO:HA	1.99	0.44
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.58	0.44
1:B:393:GLU:HB2	1:B:400:LEU:HD22	2.00	0.44
1:B:715:ILE:HG23	1:B:716:ASP:N	2.32	0.44
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.99	0.44
1:A:568:LYS:O	1:A:607:GLY:HA3	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:650:VAL:HB	7:B:2328:HOH:O	2.18	0.43
1:A:209:THR:HG21	1:A:214:LYS:CE	2.43	0.43
1:A:778:GLU:HG3	1:A:782:LYS:HE2	2.00	0.43
1:A:486:ILE:O	1:A:486:ILE:HG13	2.16	0.43
1:A:307:ILE:HG23	7:A:2398:HOH:O	2.18	0.43
1:B:42:ASP:C	1:B:42:ASP:OD2	2.57	0.43
1:B:399:HIS:O	1:B:403:ILE:HG13	2.19	0.43
1:A:277:ARG:HG2	1:B:267:LEU:HD23	2.01	0.43
1:A:697:VAL:O	1:A:701:GLU:HG3	2.19	0.43
1:A:669:ALA:HA	1:A:693:ASP:HB2	2.00	0.43
1:B:432:GLU:O	1:B:437:LYS:HA	2.19	0.43
1:A:689:ILE:O	1:A:689:ILE:HG23	2.19	0.43
1:B:692:MET:HG2	1:B:710:ILE:HG21	2.01	0.43
1:A:373:ALA:HB3	7:A:2194:HOH:O	2.18	0.43
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.18	0.42
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.53	0.42
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.00	0.42
1:A:326:PHE:CZ	1:A:357:GLU:HG3	2.55	0.42
1:A:346:ILE:CD1	1:A:445:CYS:HA	2.49	0.42
1:B:350:MET:HE2	1:B:368:THR:OG1	2.19	0.42
1:A:515:LEU:CG	1:A:809:GLY:HA2	2.48	0.42
1:A:556:LYS:C	1:A:556:LYS:HD3	2.40	0.42
1:B:405:GLU:OE2	1:B:405:GLU:HA	2.20	0.42
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.39	0.42
1:B:235:ASN:O	1:B:236:ASN:HB2	2.19	0.42
1:B:143:PHE:O	1:B:147:MET:HG3	2.20	0.42
1:A:715:ILE:HG22	7:A:2297:HOH:O	2.19	0.42
1:B:34:HIS:O	1:B:38:THR:HB	2.20	0.42
1:B:315:LYS:O	1:B:316:PHE:C	2.58	0.42
1:A:702:GLU:CD	1:A:810:LYS:HD2	2.40	0.42
1:B:703:ALA:O	1:B:707:ASN:ND2	2.48	0.42
1:A:311:PHE:CE1	1:A:329:PHE:HA	2.55	0.42
1:B:350:MET:HE1	1:B:364:ALA:CB	2.44	0.42
1:A:235:ASN:O	1:A:236:ASN:HB2	2.19	0.41
1:B:503:ILE:HG23	1:B:521:LEU:HD21	2.02	0.41
1:A:548:PHE:CZ	1:A:552:GLU:HG3	2.55	0.41
1:A:143:PHE:O	1:A:147:MET:HG3	2.19	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.97	0.41
1:A:109:ASP:OD1	1:A:119:ILE:HG21	2.20	0.41
1:A:251:ASP:HA	1:B:178:GLU:OE1	2.20	0.41
1:B:314:SER:HB3	7:B:2199:HOH:O	2.20	0.41
1:A:170:ILE:HA	1:A:174:TRP:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:627:ALA:HA	1:B:642:VAL:HB	2.03	0.41
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.85	0.41
1:A:181:ASP:OD2	1:A:184:ARG:HB2	2.21	0.41
1:B:455:VAL:HG12	1:B:484:ASN:HD21	1.83	0.41
1:A:566:GLN:HA	7:A:2209:HOH:O	2.20	0.41
1:A:474:LEU:N	1:A:474:LEU:HD12	2.36	0.41
1:B:168:GLN:NE2	1:B:608:LYS:HA	2.35	0.41
1:A:715:ILE:HG23	1:A:716:ASP:OD1	2.20	0.41
1:B:206:VAL:HG11	1:B:401:GLU:OE1	2.20	0.41
1:B:555:VAL:HG22	1:B:631:ASN:HD22	1.86	0.40
1:A:136:LEU:O	1:A:136:LEU:HD23	2.21	0.40
1:B:509:GLU:O	1:B:512:VAL:HG23	2.21	0.40
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.61	0.40
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.50	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	787/847 (93%)	752 (96%)	32 (4%)	3 (0%)	43	52
1	B	789/847 (93%)	743 (94%)	43 (5%)	3 (0%)	43	52
All	All	1576/1694 (93%)	1495 (95%)	75 (5%)	6 (0%)	43	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	A	434	GLU
1	B	434	GLU
1	B	829	PRO

### 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	694/740 (94%)	688 (99%)	6 (1%)	87	95
1	B	695/740 (94%)	680 (98%)	15 (2%)	64	81
All	All	1389/1480 (94%)	1368 (98%)	21 (2%)	76	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	90	TYR
1	A	120	GLU
1	A	573	TYR
1	A	652	LEU
1	A	733	GLU
1	B	77	LYS
1	B	90	TYR
1	B	120	GLU
1	B	210	ASN
1	B	251	ASP
1	B	510	ASP
1	B	528	ASP
1	B	568	LYS
1	B	573	TYR
1	B	613	TYR
1	B	628	ASP
1	B	652	LEU
1	B	706	GLU
1	B	716	ASP
1	B	733	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	HIS
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	105	GLN
1	A	250	ASN
1	A	332	GLN
1	A	369	GLN
1	A	484	ASN
1	A	517	GLN
1	A	822	GLN
1	B	23	ASN
1	B	62	HIS
1	B	73	HIS
1	B	219	GLN
1	B	332	GLN
1	B	369	GLN
1	B	484	ASN
1	B	539	GLN
1	B	747	ASN
1	B	793	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

12 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	860	1	14,15,16	1.72	3 (21%)	20,22,23	1.17	1 (5%)
2	NBG	A	861	-	15,15,15	1.47	3 (20%)	21,21,21	1.17	1 (4%)
4	700	A	862	-	33,33,33	1.95	8 (24%)	47,47,47	1.16	4 (8%)
5	CFF	A	863	-	15,15,15	4.18	6 (40%)	18,23,23	3.17	5 (27%)
5	CFF	A	864	-	15,15,15	4.18	6 (40%)	18,23,23	3.20	4 (22%)
3	PLP	B	1860	1	14,15,16	1.20	3 (21%)	20,22,23	1.37	3 (15%)
2	NBG	B	1861	-	15,15,15	1.68	2 (13%)	21,21,21	1.32	1 (4%)
4	700	B	1862	-	33,33,33	2.03	9 (27%)	47,47,47	1.21	6 (12%)
5	CFF	B	1863	-	15,15,15	4.07	6 (40%)	18,23,23	3.04	6 (33%)
6	MRD	B	1902	-	7,7,7	0.51	0	10,10,10	0.73	0
6	MRD	B	902	-	7,7,7	0.54	0	10,10,10	0.72	0
6	MRD	B	903	-	7,7,7	0.64	0	10,10,10	0.94	1 (10%)

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	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	1/22/32/32	0/1/4/4
5	CFF	A	863	-	-	0/0/0/0	0/0/2/2
5	CFF	A	864	-	-	0/0/0/0	0/0/2/2
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
4	700	B	1862	-	-	1/22/32/32	0/1/4/4
5	CFF	B	1863	-	-	0/0/0/0	0/0/2/2
6	MRD	B	1902	-	-	0/5/5/5	0/0/0/0
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0
6	MRD	B	903	-	-	0/5/5/5	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	863	CFF	C2-N1	14.13	1.53	1.38
5	A	864	CFF	C2-N1	13.96	1.53	1.38
5	B	1863	CFF	C2-N1	13.51	1.53	1.38
5	B	1863	CFF	C2-N3	-5.67	1.32	1.38
4	B	1862	700	C8-N2	-5.13	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	864	CFF	C2-N3	-4.98	1.33	1.38
4	A	862	700	C8-N2	-4.75	1.32	1.36
5	A	863	CFF	C2-N3	-4.63	1.33	1.38
2	B	1861	NBG	C2-C1	4.59	1.57	1.52
4	B	1862	700	C22-C20	4.31	1.60	1.54
3	A	860	PLP	C3-C2	-4.02	1.37	1.40
4	A	862	700	C22-C20	3.64	1.59	1.54
4	A	862	700	C20-C21	3.28	1.56	1.51
5	A	864	CFF	C4-N3	3.21	1.45	1.38
2	B	1861	NBG	C1-N1	3.14	1.46	1.43
2	A	861	NBG	C2-C1	3.05	1.56	1.52
4	B	1862	700	C5-C4	3.04	1.43	1.36
5	A	863	CFF	C4-N9	-2.98	1.31	1.33
4	A	862	700	C5-C4	2.98	1.43	1.36
4	B	1862	700	C12-C11	2.93	1.45	1.38
2	A	861	NBG	C1-N1	2.91	1.46	1.43
5	A	863	CFF	C4-N3	2.80	1.44	1.38
4	B	1862	700	C7-C8	-2.80	1.35	1.38
4	A	862	700	C2-C3	2.79	1.42	1.36
4	B	1862	700	C2-C3	2.74	1.42	1.36
4	A	862	700	C7-C6	2.72	1.51	1.41
4	B	1862	700	C7-C6	2.67	1.51	1.41
5	B	1863	CFF	C4-N3	2.55	1.44	1.38
4	A	862	700	C3-C4	2.47	1.42	1.38
4	B	1862	700	C20-C21	2.44	1.55	1.51
4	B	1862	700	C3-C4	2.43	1.42	1.38
5	B	1863	CFF	C5-C4	-2.38	1.36	1.40
5	B	1863	CFF	C4-N9	-2.34	1.31	1.33
5	A	864	CFF	O13-C6	2.32	1.29	1.24
2	A	861	NBG	C3-C2	2.32	1.58	1.52
5	A	863	CFF	C5-C4	-2.29	1.36	1.40
5	A	864	CFF	C5-N7	2.24	1.42	1.39
3	A	860	PLP	C4-C5	2.21	1.43	1.39
4	A	862	700	C7-C8	-2.19	1.36	1.38
5	A	864	CFF	C6-C5	2.19	1.44	1.41
5	A	863	CFF	O13-C6	2.15	1.28	1.24
3	B	1860	PLP	P-O2P	-2.13	1.46	1.54
3	B	1860	PLP	C3-C2	-2.11	1.39	1.40
5	B	1863	CFF	O13-C6	2.05	1.28	1.24
3	A	860	PLP	C2-N1	2.04	1.37	1.33
3	B	1860	PLP	P-O3P	-2.01	1.47	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	864	CFF	C6-N1-C2	11.30	125.65	121.69
5	A	863	CFF	C6-N1-C2	11.11	125.58	121.69
5	B	1863	CFF	C6-N1-C2	10.39	125.33	121.69
2	B	1861	NBG	C5-O5-C1	4.37	118.57	112.50
5	B	1863	CFF	C8-N7-C5	-4.16	103.97	107.07
5	A	864	CFF	C8-N7-C5	-4.02	104.08	107.07
5	A	863	CFF	C8-N7-C5	-3.94	104.14	107.07
2	A	861	NBG	C5-O5-C1	3.85	117.85	112.50
5	A	863	CFF	N3-C2-N1	-3.70	112.39	115.69
5	A	864	CFF	N3-C2-N1	-3.57	112.50	115.69
5	B	1863	CFF	N3-C2-N1	-3.54	112.53	115.69
4	B	1862	700	O3-C21-C20	-3.51	113.76	122.80
4	A	862	700	C8-C9-N1	3.01	123.43	116.55
4	B	1862	700	O4-C21-O3	2.85	130.52	124.07
4	B	1862	700	C4-C5-C6	-2.85	117.21	119.22
3	B	1860	PLP	O4P-C5A-C5	2.82	114.99	109.26
3	B	1860	PLP	O4P-P-O1P	-2.81	98.48	106.71
4	A	862	700	O3-C21-C20	-2.72	115.78	122.80
4	B	1862	700	C8-C9-N1	2.67	122.64	116.55
4	A	862	700	C4-C5-C6	-2.62	117.37	119.22
4	A	862	700	O4-C21-O3	2.56	129.87	124.07
3	B	1860	PLP	O2P-P-O1P	2.54	118.75	110.44
5	A	864	CFF	C10-N1-C2	-2.50	114.15	119.51
3	A	860	PLP	P-O4P-C5A	2.38	129.81	121.22
5	A	863	CFF	C10-N1-C2	-2.35	114.46	119.51
5	B	1863	CFF	C10-N1-C2	-2.27	114.64	119.51
5	B	1863	CFF	N9-C4-N3	-2.25	126.70	128.19
5	A	863	CFF	N9-C4-N3	-2.22	126.72	128.19
6	B	903	MRD	O2-C2-C3	2.17	116.76	109.16
4	B	1862	700	O2-C18-N3	2.03	124.07	121.65
4	B	1862	700	C22-C20-C21	2.03	121.30	116.40
5	B	1863	CFF	C2-N3-C4	2.02	124.48	118.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1862	700	C17-C18-N3-C22
4	A	862	700	C17-C18-N3-C22

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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