



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:37 AM UTC

PDB ID : 1C8L / pdb_00001c8l
Title : SYNERGISTIC INHIBITION OF GLYCOGEN PHOSPHORYLASE A BY A
POTENTIAL ANTIDIABETIC DRUG AND CAFFEINE
Authors : Tsitsanou, K.E.; Skamnaki, V.T.; Oikonomakos, N.G.
Deposited on : 2000-05-16
Resolution : 2.30 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

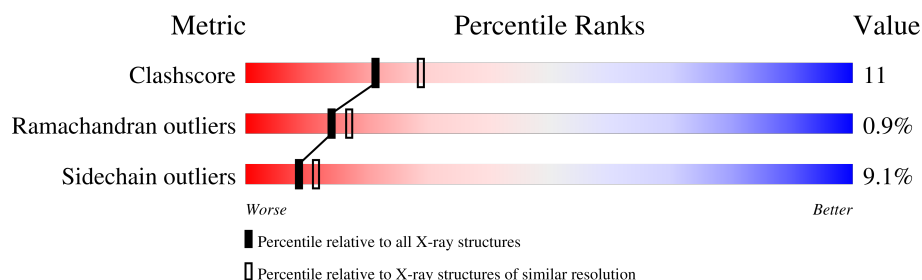
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	 68% 24% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BIN	A	930	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7378 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

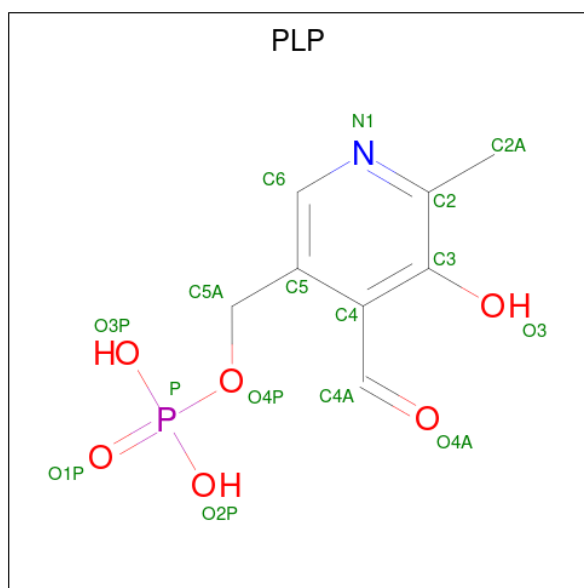
- Molecule 1 is a protein called PROTEIN (GLYCOGEN PHOSPHORYLASE).

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

There is a discrepancy between the modelled and reference sequences:

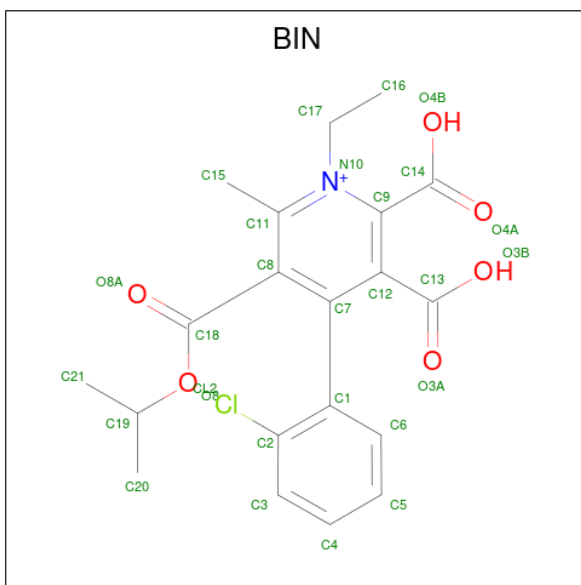
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	modified residue	UNP P00489

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



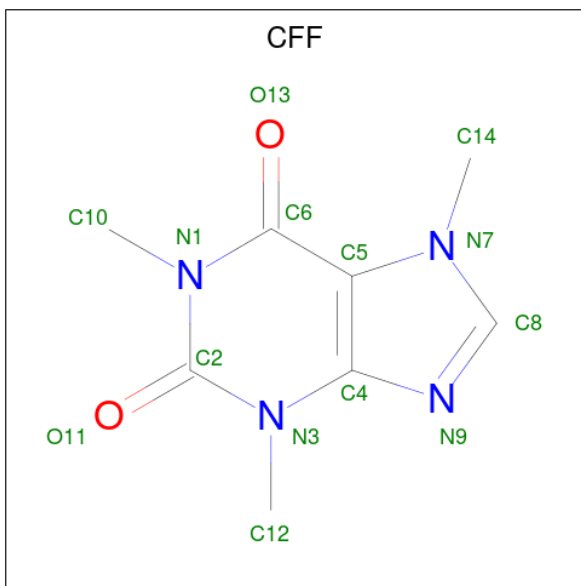
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	20	1	1	6		

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

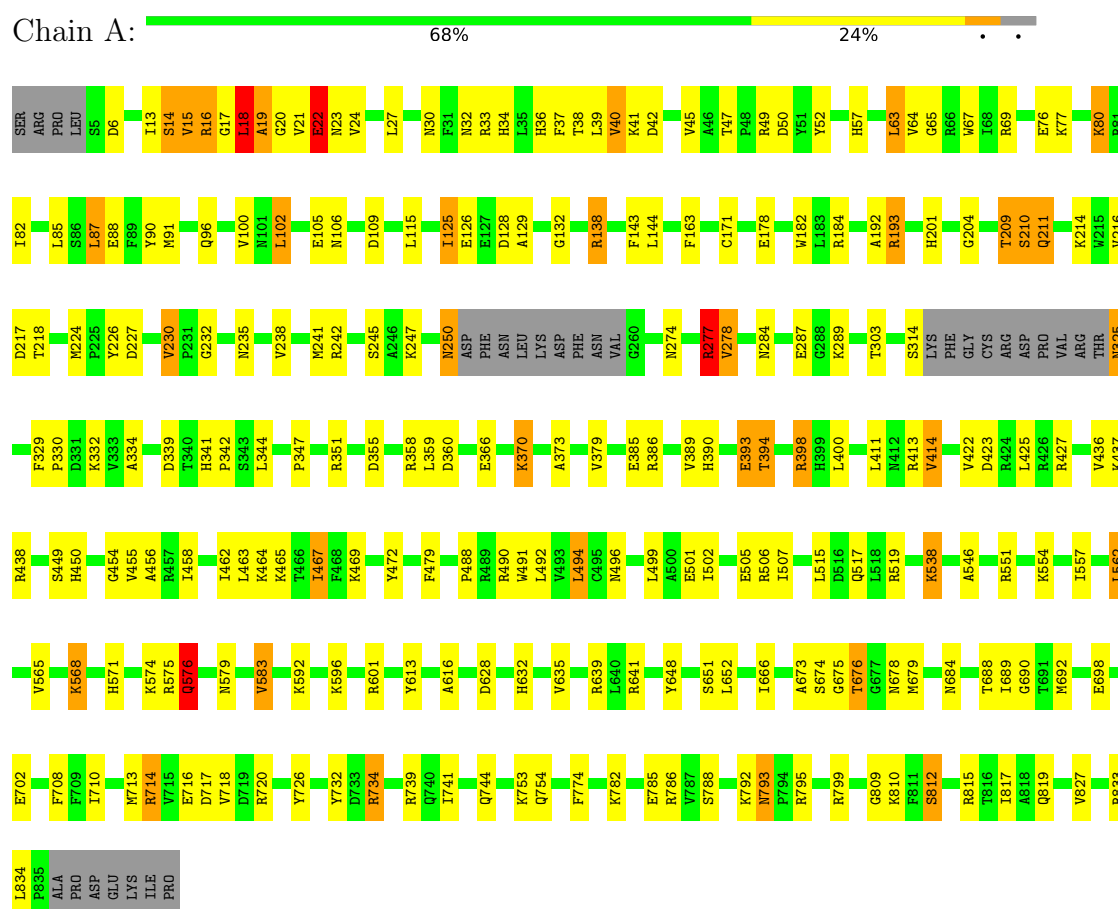
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	704	Total	O	0	0
			704	704		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROTEIN (GLYCOGEN PHOSPHORYLASE)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.69Å 126.69Å 115.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.50 – 2.30	Depositor
% Data completeness (in resolution range)	98.4 (26.50-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.210 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7378	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, GOL, SEP, CFF, BIN

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	0.45	0/6746	0.98	29/9123 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	VAL	N-CA-C	7.97	119.27	108.11
1	A	24	VAL	N-CA-C	7.66	118.40	110.36
1	A	64	VAL	N-CA-C	7.41	117.93	110.23
1	A	576	GLN	N-CA-C	-7.37	103.23	111.71
1	A	491	TRP	N-CA-C	7.12	121.62	113.15
1	A	575	ARG	N-CA-C	6.77	120.73	111.39
1	A	639	ARG	N-CA-C	6.61	119.49	111.82
1	A	507	ILE	N-CA-C	6.54	119.44	113.10
1	A	688	THR	N-CA-C	6.54	119.89	109.24
1	A	385	GLU	N-CA-C	6.38	119.01	109.25
1	A	467	ILE	N-CA-C	6.36	117.87	110.62
1	A	809	GLY	N-CA-C	6.13	121.42	113.27
1	A	129	ALA	N-CA-C	-5.97	98.17	108.56
1	A	666	ILE	N-CA-C	5.90	121.61	109.34
1	A	37	PHE	N-CA-C	5.81	119.55	112.23
1	A	479	PHE	N-CA-C	5.81	119.00	109.76
1	A	676	THR	N-CA-C	-5.77	108.05	114.62
1	A	455	VAL	N-CA-C	5.76	117.71	112.29
1	A	182	TRP	N-CA-C	5.69	119.70	112.87
1	A	834	LEU	N-CA-C	-5.69	102.95	110.40
1	A	80	LYS	N-CA-C	-5.62	101.97	110.28
1	A	454	GLY	N-CA-C	-5.51	104.18	112.89
1	A	277	ARG	N-CA-C	5.47	117.10	111.03
1	A	675	GLY	N-CA-C	-5.38	105.97	112.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	MET	N-CA-C	-5.36	99.67	108.41
1	A	18	LEU	CA-CB-CG	5.19	134.47	116.30
1	A	232	GLY	N-CA-C	-5.01	104.85	112.51
1	A	115	LEU	N-CA-C	-5.01	107.32	112.93
1	A	91	MET	N-CA-C	5.00	119.09	112.89

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	6611	0	6554	143	0
2	A	15	0	7	0	0
3	A	28	0	19	2	0
4	A	14	0	10	1	0
5	A	6	0	8	1	0
6	A	704	0	0	15	0
All	All	7378	0	6598	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:CD2	1:A:19:ALA:H	1.58	1.17
1:A:18:LEU:HD22	1:A:19:ALA:N	1.60	1.15
1:A:211:GLN:HB3	1:A:358:ARG:NH2	1.76	1.01
1:A:18:LEU:HD22	1:A:19:ALA:H	0.80	0.96
1:A:250:ASN:H	1:A:250:ASN:HD22	1.10	0.94
1:A:389:VAL:O	1:A:393:GLU:HG2	1.69	0.91
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.33	0.90
1:A:171:CYS:SG	6:A:1699:HOH:O	2.37	0.82
1:A:211:GLN:HB3	1:A:358:ARG:HH21	1.43	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD13	1:A:102:LEU:HD21	1.63	0.81
1:A:250:ASN:H	1:A:250:ASN:ND2	1.77	0.80
1:A:714:ARG:HD3	6:A:1233:HOH:O	1.83	0.77
1:A:393:GLU:OE1	6:A:1561:HOH:O	2.05	0.74
1:A:325:ASN:HB3	6:A:1544:HOH:O	1.88	0.74
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.69	0.73
1:A:250:ASN:HD22	1:A:250:ASN:N	1.81	0.72
1:A:250:ASN:ND2	1:A:250:ASN:N	2.36	0.72
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.53	0.72
1:A:138:ARG:O	1:A:138:ARG:HD3	1.88	0.72
1:A:390:HIS:O	1:A:394:THR:HG23	1.89	0.72
1:A:464:LYS:HG2	1:A:472:TYR:CD1	2.26	0.71
1:A:413:ARG:HD2	6:A:1674:HOH:O	1.93	0.68
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.75	0.68
1:A:314:SER:HA	6:A:1662:HOH:O	1.92	0.68
1:A:786:ARG:HD3	6:A:1363:HOH:O	1.93	0.67
1:A:506:ARG:HG2	1:A:506:ARG:HH11	1.61	0.66
1:A:18:LEU:HD22	1:A:19:ALA:CB	2.25	0.65
1:A:19:ALA:HB1	1:A:30:ASN:ND2	2.12	0.65
1:A:562:LEU:C	1:A:562:LEU:HD12	2.24	0.62
1:A:344:LEU:C	1:A:347:PRO:HD2	2.24	0.61
1:A:16:ARG:HG3	1:A:17:GLY:H	1.66	0.61
1:A:36:HIS:HB3	6:A:1694:HOH:O	2.00	0.60
1:A:386:ARG:HD3	6:A:1427:HOH:O	2.02	0.59
1:A:732:TYR:O	1:A:739:ARG:HG3	2.01	0.59
1:A:351:ARG:O	1:A:355:ASP:HB2	2.04	0.58
1:A:163:PHE:HB2	1:A:278:VAL:HG13	1.86	0.57
1:A:138:ARG:HB3	6:A:1034:HOH:O	2.03	0.57
1:A:414:VAL:HG22	1:A:425:LEU:CD2	2.35	0.57
1:A:810:LYS:O	1:A:810:LYS:HG3	2.04	0.57
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.87	0.57
1:A:414:VAL:HG22	1:A:425:LEU:HD23	1.86	0.56
1:A:138:ARG:HD3	1:A:138:ARG:C	2.30	0.56
1:A:36:HIS:O	1:A:40:VAL:HA	2.05	0.56
1:A:18:LEU:HD22	1:A:19:ALA:CA	2.34	0.55
1:A:21:VAL:C	1:A:22:GLU:HG2	2.31	0.55
1:A:36:HIS:CE1	1:A:42:ASP:HA	2.42	0.55
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.11	0.54
1:A:502:ILE:HA	1:A:505:GLU:HG2	1.89	0.54
1:A:734:ARG:HD2	6:A:1257:HOH:O	2.08	0.53
1:A:67:TRP:HA	1:A:238:VAL:HB	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLU:HB3	1:A:400:LEU:HD23	1.92	0.52
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.10	0.52
1:A:52:TYR:CZ	1:A:126:GLU:HB2	2.45	0.52
1:A:436:VAL:O	1:A:438:ARG:HG3	2.10	0.51
1:A:793:ASN:HD22	1:A:793:ASN:C	2.17	0.51
1:A:14:SEP:HB2	1:A:16:ARG:HG2	1.92	0.51
1:A:678:ASN:OD1	1:A:679:MET:HG3	2.11	0.51
1:A:716:GLU:H	1:A:716:GLU:CD	2.17	0.51
1:A:366:GLU:HG3	1:A:370:LYS:HD2	1.93	0.51
1:A:274:ASN:OD1	1:A:277:ARG:HD2	2.11	0.51
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.11	0.50
1:A:344:LEU:O	1:A:347:PRO:HD2	2.11	0.50
1:A:227:ASP:CG	1:A:242:ARG:HH21	2.19	0.50
1:A:501:GLU:HG3	1:A:502:ILE:N	2.27	0.50
1:A:571:HIS:H	1:A:576:GLN:HE22	1.60	0.49
1:A:230:VAL:HG22	1:A:230:VAL:O	2.11	0.49
1:A:538:LYS:NZ	1:A:684:ASN:O	2.45	0.49
1:A:450:HIS:HD2	6:A:1202:HOH:O	1.96	0.49
1:A:34:HIS:CE1	1:A:57:HIS:HB3	2.48	0.48
1:A:373:ALA:HA	1:A:449:SER:HB3	1.95	0.48
1:A:184:ARG:NH2	6:A:1087:HOH:O	2.47	0.47
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.49	0.47
1:A:204:GLY:HA2	1:A:217:ASP:O	2.14	0.47
1:A:795:ARG:O	1:A:799:ARG:HG3	2.14	0.47
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.94	0.47
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.49	0.47
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.96	0.47
1:A:628:ASP:O	1:A:632:HIS:HD2	1.97	0.47
1:A:456:ALA:HB2	1:A:674:SER:HB2	1.97	0.47
1:A:414:VAL:CG2	1:A:425:LEU:HD23	2.43	0.47
1:A:235:ASN:HA	1:A:833:ARG:HG2	1.97	0.47
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.14	0.47
1:A:458:ILE:O	1:A:462:ILE:HG13	2.15	0.46
1:A:355:ASP:OD2	1:A:398:ARG:NE	2.45	0.46
1:A:579:ASN:C	1:A:579:ASN:HD22	2.22	0.46
1:A:698:GLU:O	1:A:702:GLU:HG2	2.16	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.97	0.46
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.45	0.46
1:A:689:ILE:HG23	1:A:689:ILE:O	2.15	0.46
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.98	0.46
1:A:214:LYS:HE2	1:A:216:VAL:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:C	1:A:562:LEU:CD1	2.89	0.45
1:A:47:THR:O	1:A:50:ASP:HB2	2.17	0.45
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.97	0.45
1:A:579:ASN:O	1:A:583:VAL:HG13	2.17	0.45
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.99	0.45
1:A:209:THR:O	1:A:210:SER:C	2.60	0.45
1:A:690:GLY:O	1:A:710:ILE:HA	2.17	0.45
1:A:39:LEU:O	1:A:40:VAL:C	2.59	0.44
1:A:65:GLY:O	1:A:69:ARG:HD3	2.17	0.44
1:A:562:LEU:HG	1:A:601:ARG:HG2	1.99	0.44
1:A:568:LYS:CD	1:A:574:LYS:HD3	2.46	0.44
1:A:496:ASN:HB2	1:A:684:ASN:ND2	2.32	0.44
1:A:18:LEU:CD2	1:A:19:ALA:N	2.43	0.44
1:A:517:GLN:HE21	1:A:517:GLN:HB3	1.63	0.44
1:A:741:ILE:HA	1:A:744:GLN:NE2	2.26	0.44
1:A:465:LYS:O	1:A:469:LYS:HD3	2.17	0.43
1:A:815:ARG:O	1:A:819:GLN:HG3	2.18	0.43
1:A:90:TYR:HE1	6:A:1529:HOH:O	2.01	0.43
1:A:782:LYS:O	1:A:785:GLU:HB2	2.19	0.43
1:A:192:ALA:C	1:A:193:ARG:HG2	2.43	0.43
1:A:18:LEU:CG	1:A:19:ALA:H	2.16	0.43
1:A:411:LEU:HA	1:A:414:VAL:HG13	2.01	0.42
1:A:571:HIS:CE1	4:A:940:CFF:C12	3.02	0.42
1:A:40:VAL:O	1:A:41:LYS:HG2	2.19	0.42
1:A:224:MET:HE3	1:A:226:TYR:CE1	2.54	0.42
1:A:227:ASP:OD2	1:A:242:ARG:NH2	2.42	0.42
1:A:224:MET:HE3	1:A:226:TYR:OH	2.19	0.42
1:A:423:ASP:O	1:A:427:ARG:HG3	2.19	0.42
1:A:673:ALA:HB3	5:A:998:GOL:C1	2.50	0.42
1:A:193:ARG:NH1	3:A:930:BIN:CL2	2.90	0.41
1:A:100:VAL:HG11	1:A:494:LEU:HD12	2.03	0.41
1:A:554:LYS:HA	1:A:554:LYS:HD3	1.86	0.41
1:A:15:VAL:O	1:A:16:ARG:C	2.63	0.41
1:A:34:HIS:O	1:A:38:THR:HB	2.19	0.41
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.02	0.41
1:A:506:ARG:HH11	1:A:506:ARG:CG	2.29	0.41
1:A:42:ASP:OD1	1:A:45:VAL:HG22	2.20	0.41
1:A:201:HIS:HD2	1:A:218:THR:OG1	2.02	0.41
1:A:106:ASN:HD22	1:A:106:ASN:HA	1.62	0.41
1:A:576:GLN:HE21	1:A:576:GLN:HB2	1.61	0.41
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:ARG:HG2	6:A:1436:HOH:O	2.20	0.41
1:A:287:GLU:HG2	1:A:289:LYS:HG2	2.03	0.41
1:A:678:ASN:OD1	1:A:679:MET:N	2.53	0.41
1:A:488:PRO:O	1:A:492:LEU:HB3	2.21	0.41
1:A:88:GLU:HB3	1:A:132:GLY:HA2	2.02	0.40
1:A:85:LEU:HD11	1:A:303:THR:HG21	2.03	0.40
3:A:930:BIN:H151	3:A:930:BIN:H171	1.90	0.40
1:A:18:LEU:C	1:A:20:GLY:H	2.29	0.40
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.02	0.40
1:A:105:GLU:O	1:A:109:ASP:HB2	2.22	0.40
1:A:19:ALA:HB1	1:A:30:ASN:HD21	1.85	0.40
1:A:692:MET:HG2	1:A:710:ILE:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	805/842 (96%)	767 (95%)	31 (4%)	7 (1%)	14 17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	22	GLU
1	A	6	ASP
1	A	19	ALA
1	A	339	ASP
1	A	13	ILE
1	A	40	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	702/730 (96%)	638 (91%)	64 (9%)	9 11

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	18	LEU
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	32	ASN
1	A	33	ARG
1	A	63	LEU
1	A	76	GLU
1	A	77	LYS
1	A	87	LEU
1	A	96	GLN
1	A	102	LEU
1	A	125	ILE
1	A	138	ARG
1	A	144	LEU
1	A	178	GLU
1	A	193	ARG
1	A	209	THR
1	A	210	SER
1	A	211	GLN
1	A	230	VAL
1	A	245	SER
1	A	247	LYS
1	A	250	ASN
1	A	277	ARG
1	A	278	VAL
1	A	284	ASN
1	A	325	ASN
1	A	332	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	359	LEU
1	A	360	ASP
1	A	370	LYS
1	A	379	VAL
1	A	393	GLU
1	A	394	THR
1	A	398	ARG
1	A	414	VAL
1	A	422	VAL
1	A	437	LYS
1	A	494	LEU
1	A	499	LEU
1	A	519	ARG
1	A	538	LYS
1	A	551	ARG
1	A	562	LEU
1	A	568	LYS
1	A	576	GLN
1	A	583	VAL
1	A	592	LYS
1	A	596	LYS
1	A	635	VAL
1	A	641	ARG
1	A	676	THR
1	A	708	PHE
1	A	714	ARG
1	A	718	VAL
1	A	734	ARG
1	A	753	LYS
1	A	754	GLN
1	A	788	SER
1	A	792	LYS
1	A	793	ASN
1	A	812	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	ASN
1	A	30	ASN
1	A	57	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	GLN
1	A	97	ASN
1	A	101	ASN
1	A	106	ASN
1	A	201	HIS
1	A	250	ASN
1	A	282	ASN
1	A	284	ASN
1	A	295	GLN
1	A	325	ASN
1	A	408	GLN
1	A	412	ASN
1	A	450	HIS
1	A	484	ASN
1	A	496	ASN
1	A	517	GLN
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	588	ASN
1	A	632	HIS
1	A	684	ASN
1	A	727	ASN
1	A	744	GLN
1	A	763	ASN
1	A	767	HIS
1	A	793	ASN
1	A	804	ASN
1	A	832	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	14	1	8,9,10	1.14	1 (12%)	7,12,14	4.06	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	2.41	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	-10.38	98.04	108.14
1	A	14	SEP	O3P-P-O1P	2.23	119.53	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	CB-OG-P-O3P

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	A	999	1	15,15,16	1.76	4 (26%)	21,22,23	1.08	1 (4%)
4	CFF	A	940	-	15,15,15	2.64	6 (40%)	23,23,23	2.33	7 (30%)
3	BIN	A	930	-	28,29,29	6.04	19 (67%)	34,42,42	3.20	15 (44%)
5	GOL	A	998	-	5,5,5	0.26	0	5,5,5	0.53	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
2	PLP	A	999	1	-	2/6/6/8	0/1/1/1
4	CFF	A	940	-	-	-	0/2/2/2
3	BIN	A	930	-	-	8/22/22/22	0/2/2/2
5	GOL	A	998	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	930	BIN	C7-C8	16.96	1.70	1.40
3	A	930	BIN	C11-N10	11.72	1.55	1.36
3	A	930	BIN	C1-C7	11.20	1.63	1.50
3	A	930	BIN	C1-C2	10.03	1.57	1.39
4	A	940	CFF	C2-N1	8.15	1.55	1.39
3	A	930	BIN	C7-C12	8.07	1.55	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	930	BIN	C4-C3	7.37	1.51	1.38
3	A	930	BIN	C6-C1	7.35	1.51	1.40
3	A	930	BIN	O8-C19	5.91	1.60	1.47
3	A	930	BIN	C8-C18	5.60	1.63	1.50
3	A	930	BIN	C5-C6	5.36	1.48	1.38
3	A	930	BIN	C3-C2	5.11	1.49	1.38
3	A	930	BIN	C8-C11	4.00	1.43	1.39
3	A	930	BIN	O4B-C14	-3.95	1.18	1.30
2	A	999	PLP	C4A-C4	3.51	1.58	1.51
4	A	940	CFF	O13-C6	3.21	1.29	1.23
2	A	999	PLP	C3-C2	-3.13	1.37	1.41
3	A	930	BIN	C12-C13	2.75	1.57	1.50
4	A	940	CFF	C4-N3	2.72	1.42	1.38
2	A	999	PLP	C5A-C5	2.50	1.57	1.50
3	A	930	BIN	C12-C9	2.48	1.49	1.41
3	A	930	BIN	C2-CL2	-2.41	1.67	1.73
3	A	930	BIN	O3B-C13	-2.38	1.23	1.30
4	A	940	CFF	C10-N1	2.36	1.51	1.47
4	A	940	CFF	C2-N3	-2.09	1.34	1.39
4	A	940	CFF	C4-N9	-2.07	1.31	1.36
3	A	930	BIN	C17-N10	2.05	1.52	1.47
3	A	930	BIN	O4A-C14	2.04	1.28	1.22
2	A	999	PLP	P-O2P	2.01	1.62	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	930	BIN	C1-C7-C12	-9.79	105.24	121.34
4	A	940	CFF	O11-C2-N3	6.67	130.56	121.33
3	A	930	BIN	O4A-C14-C9	-6.62	112.47	121.17
3	A	930	BIN	C1-C7-C8	-6.46	110.71	121.34
3	A	930	BIN	C16-C17-N10	5.25	122.35	111.98
4	A	940	CFF	C2-N3-C4	4.73	125.66	119.58
3	A	930	BIN	O3B-C13-C12	4.27	126.68	114.67
4	A	940	CFF	N3-C2-N1	-4.06	112.06	117.14
3	A	930	BIN	C17-N10-C9	-3.87	117.17	119.47
3	A	930	BIN	O3B-C13-O3A	-3.68	115.43	123.35
3	A	930	BIN	C15-C11-C8	3.50	128.16	122.76
3	A	930	BIN	C6-C1-C2	-3.26	113.93	117.60
4	A	940	CFF	C12-N3-C4	-3.21	116.02	120.75
3	A	930	BIN	C6-C1-C7	3.02	126.12	118.42
3	A	930	BIN	C5-C4-C3	3.00	123.94	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	930	BIN	C19-O8-C18	2.94	121.74	117.40
4	A	940	CFF	O11-C2-N1	-2.86	117.38	121.33
3	A	930	BIN	O4B-C14-O4A	2.73	129.21	123.35
2	A	999	PLP	O3P-P-O1P	2.54	120.74	110.83
3	A	930	BIN	C7-C8-C18	-2.53	115.33	120.37
4	A	940	CFF	C5-C6-N1	2.46	116.56	112.06
4	A	940	CFF	C6-C5-C4	-2.22	120.12	122.92
3	A	930	BIN	C7-C1-C2	-2.06	119.94	122.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	930	BIN	O4A-C14-C9-N10
5	A	998	GOL	C1-C2-C3-O3
5	A	998	GOL	O2-C2-C3-O3
2	A	999	PLP	C6-C5-C5A-O4P
3	A	930	BIN	C7-C12-C13-O3B
3	A	930	BIN	O4B-C14-C9-N10
3	A	930	BIN	C7-C12-C13-O3A
3	A	930	BIN	C9-C12-C13-O3A
3	A	930	BIN	O8-C18-C8-C11
3	A	930	BIN	C9-C12-C13-O3B
3	A	930	BIN	O8A-C18-C8-C7
2	A	999	PLP	C4-C5-C5A-O4P

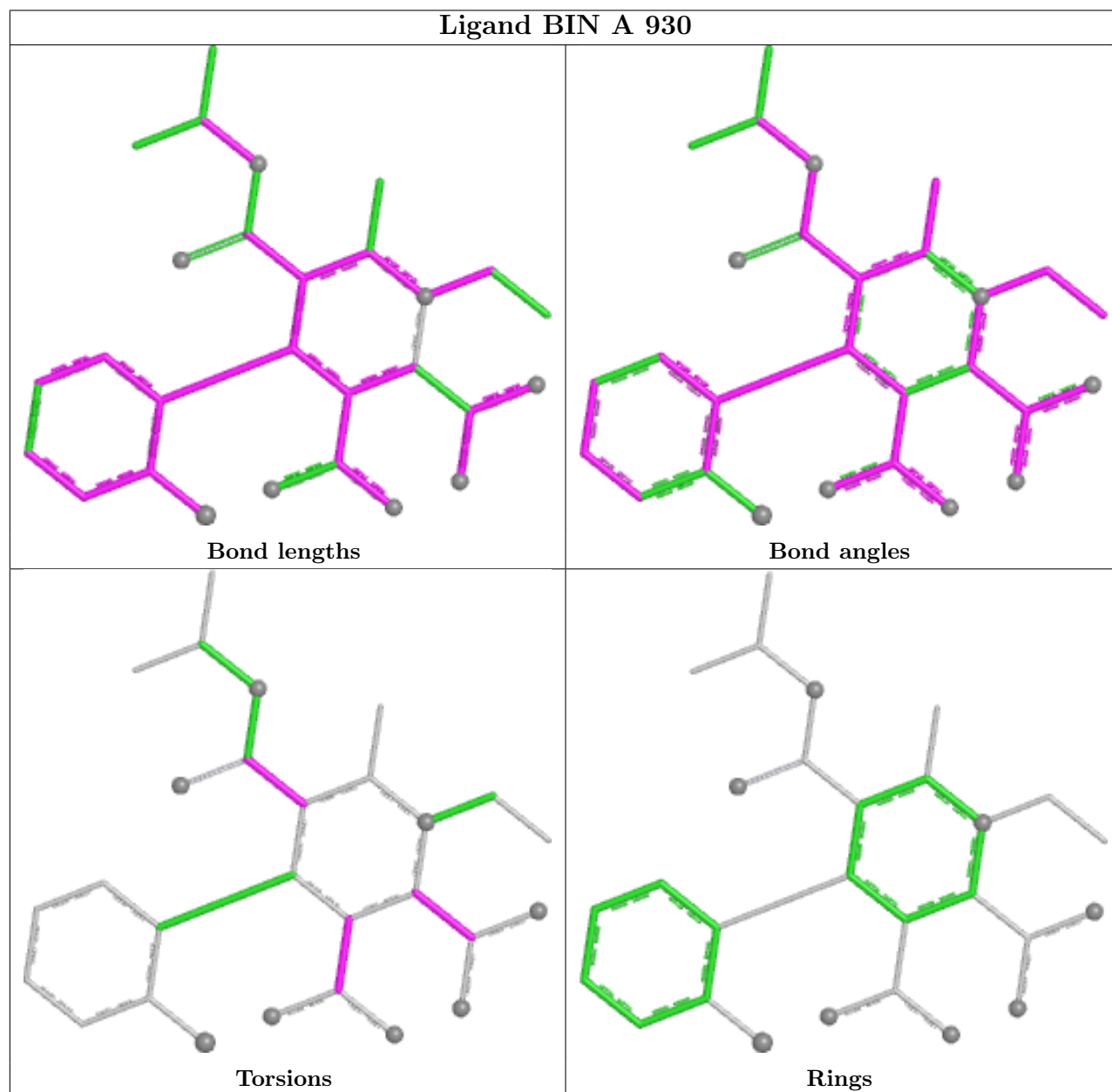
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	940	CFF	1	0
3	A	930	BIN	2	0
5	A	998	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.