Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:06 PM GMT

PDB ID	:	1E1Y
Title	:	FLAVOPIRIDOL INHIBITS GLYCOGEN PHOSPHORYLASE BY BINDING AT THE INHIBITOR SITE
Authors	:	Oikonomakos, N.G.; Zographos, S.E.; Skamnaki, V.T.; Tsitsanou, K.E.; Johnson, L.N.
Deposited on	:	2000-05-11
Resolution	:	2.23 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 (i) symbol.

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

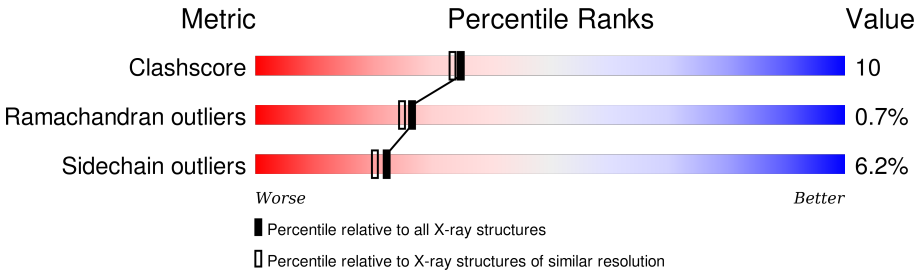
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.23 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	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)

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 <=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	75% 18%

2 Entry composition

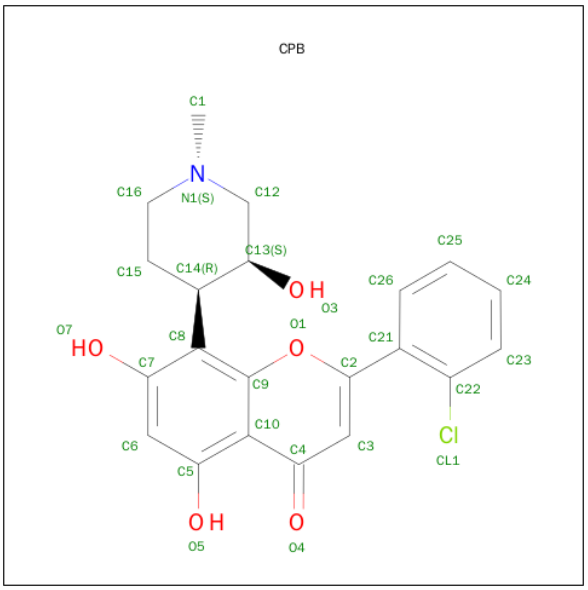
There are 6 unique types of molecules in this entry. The entry contains 7320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

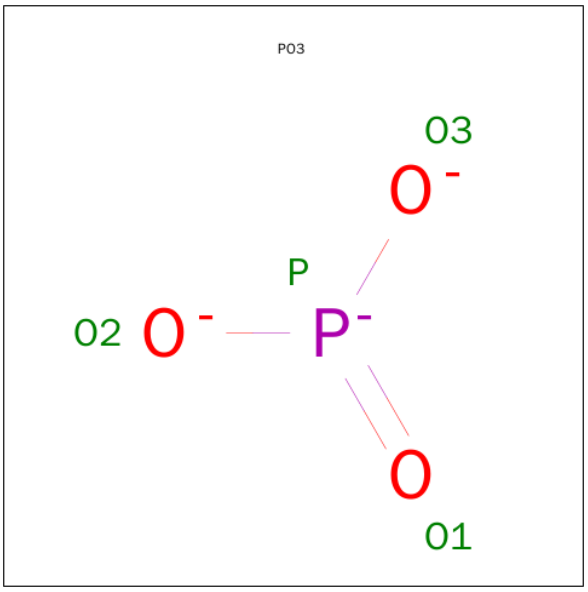
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	813	Total	C	N	O	S	0	0	0
			6617	4215	1168	1205	29			

- Molecule 2 is 2-(2-CHLORO-PHENYL)-5,7-DIHYDROXY-8-(3-HYDROXY-1-METHYL-PIPERIDIN-4-YL)-4H-BENZOPYRAN-4-ONE (three-letter code: CPB) (formula: $C_{21}H_{20}ClNO_5$).



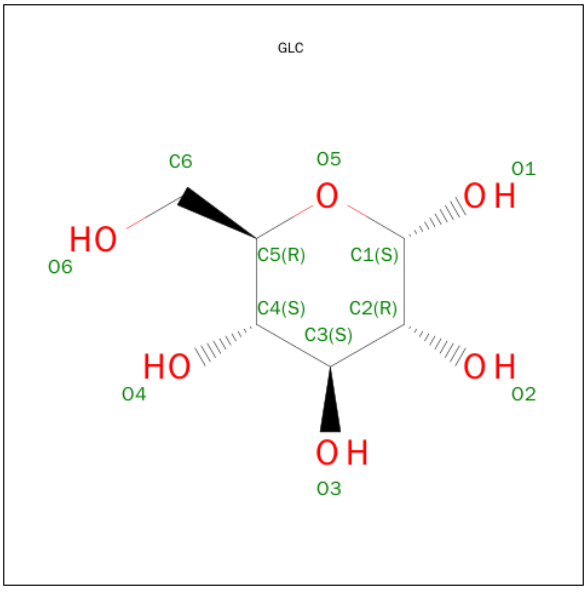
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	21	1	1	5		

- Molecule 3 is PHOSPHITE ION (three-letter code: PO3) (formula: O_3P).



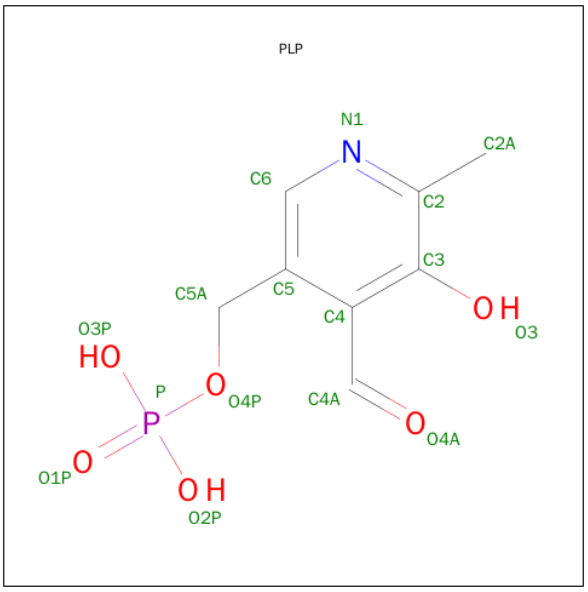
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 4 3 1	0	0

- Molecule 4 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	644	Total	O	0	0
			644	644		

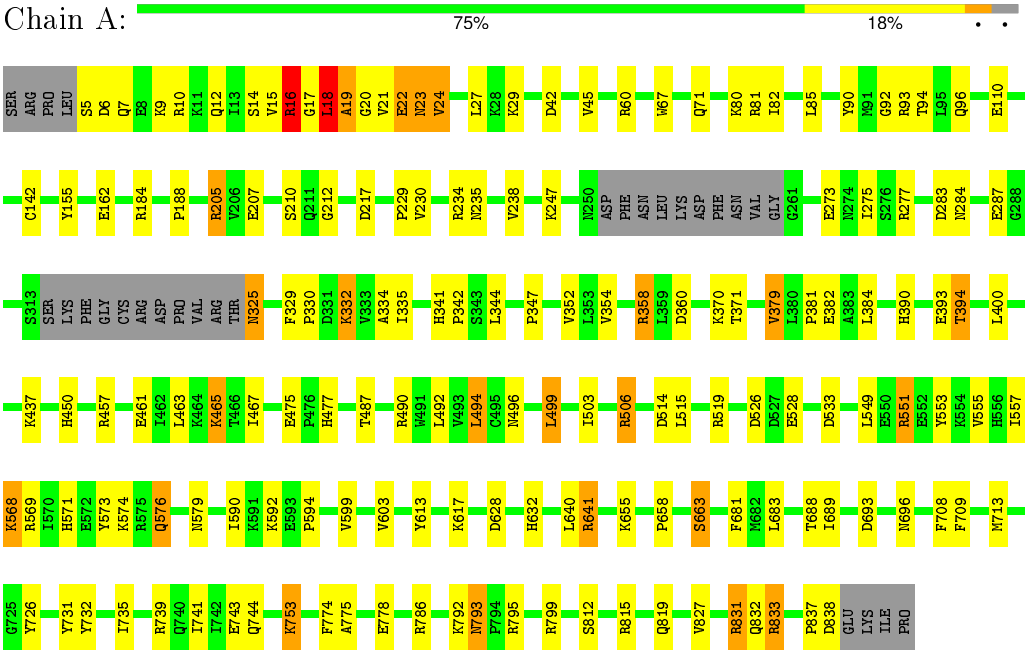
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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	126.76Å 126.76Å 116.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.23	Depositor
% Data completeness (in resolution range)	87.3 (29.90-2.23)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.195 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7320	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: CPB, GLC, PO3, 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	0.34	0/6764	0.60	3/9151 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	129	ALA	N-CA-C	-5.53	96.07	111.00
1	A	562	LEU	CA-CB-CG	5.48	127.90	115.30

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	6617	0	6563	131	0
2	A	28	0	20	0	0
3	A	4	0	0	0	0
4	A	12	0	12	0	0
5	A	15	0	7	0	0
6	A	644	0	0	25	4
All	All	7320	0	6602	131	4

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 10.

All (131) 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:HD22	1:A:19:ALA:H	1.31	0.95
1:A:93:ARG:NH1	6:A:2092:HOH:O	1.98	0.90
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.54	0.90
1:A:212:GLY:HA3	1:A:358:ARG:HH12	1.37	0.88
1:A:18:LEU:HD22	1:A:19:ALA:N	1.94	0.82
1:A:18:LEU:HD13	1:A:20:GLY:H	1.43	0.81
1:A:212:GLY:HA3	1:A:358:ARG:NH1	2.01	0.75
1:A:22:GLU:HG3	6:A:2019:HOH:O	1.88	0.74
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.73	0.71
1:A:358:ARG:HA	1:A:358:ARG:HE	1.56	0.70
1:A:325:ASN:HB3	6:A:2289:HOH:O	1.91	0.69
1:A:22:GLU:HB3	6:A:2020:HOH:O	1.93	0.68
1:A:5:SER:HB3	1:A:9:LYS:HE3	1.76	0.66
1:A:390:HIS:O	1:A:394:THR:HG23	1.95	0.65
1:A:732:TYR:O	1:A:739:ARG:HG3	1.97	0.64
1:A:60:ARG:HD2	1:A:188:PRO:O	1.97	0.64
1:A:16:ARG:HG3	1:A:17:GLY:H	1.65	0.62
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.33	0.62
1:A:382:GLU:N	1:A:382:GLU:OE1	2.33	0.62
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.80	0.61
1:A:18:LEU:HD13	1:A:20:GLY:N	2.16	0.61
1:A:382:GLU:CD	1:A:382:GLU:H	2.03	0.61
1:A:247:LYS:HA	1:A:273:GLU:HG2	1.82	0.61
1:A:571:HIS:H	1:A:576:GLN:HE22	1.49	0.60
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.84	0.60
1:A:592:LYS:HE2	6:A:2441:HOH:O	2.01	0.59
1:A:640:LEU:O	1:A:641:ARG:NH1	2.36	0.59
1:A:655:LYS:O	1:A:658:PRO:HD2	2.02	0.59
1:A:753:LYS:H	1:A:753:LYS:NZ	2.00	0.59
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.85	0.58
1:A:506:ARG:NH2	1:A:533:ASP:OD2	2.34	0.58
1:A:628:ASP:O	1:A:632:HIS:HD2	1.87	0.58
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.86	0.58
1:A:127:GLU:HG2	6:A:2124:HOH:O	2.04	0.57
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.87	0.57
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.70	0.56
1:A:461:GLU:O	1:A:465:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:HG2	1:A:382:GLU:OE1	2.06	0.56
1:A:12:GLN:O	1:A:16:ARG:NH2	2.38	0.55
1:A:127:GLU:HG3	6:A:2127:HOH:O	2.05	0.55
1:A:332:LYS:HB3	1:A:332:LYS:NZ	2.20	0.55
1:A:18:LEU:C	1:A:18:LEU:HD13	2.28	0.54
1:A:793:ASN:C	1:A:793:ASN:HD22	2.09	0.54
1:A:308:ILE:HD13	1:A:352:VAL:HG11	1.89	0.54
1:A:568:LYS:CD	1:A:574:LYS:HD3	2.38	0.53
1:A:457:ARG:NH1	6:A:2362:HOH:O	2.26	0.53
1:A:393:GLU:HB3	1:A:400:LEU:CD2	2.38	0.53
1:A:18:LEU:CD2	1:A:19:ALA:H	2.15	0.53
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.39	0.52
1:A:641:ARG:HA	1:A:641:ARG:HH11	1.74	0.52
1:A:110:GLU:HG3	1:A:114:GLN:HE21	1.74	0.52
1:A:393:GLU:HB3	1:A:400:LEU:HD23	1.92	0.52
1:A:450:HIS:HE1	6:A:2305:HOH:O	1.92	0.51
1:A:641:ARG:CG	1:A:641:ARG:HH11	2.23	0.51
1:A:212:GLY:CA	1:A:358:ARG:HH12	2.17	0.51
1:A:815:ARG:O	1:A:819:GLN:HG3	2.10	0.51
1:A:663:SER:HB2	1:A:681:PHE:CG	2.46	0.51
1:A:553:TYR:O	1:A:555:VAL:HG23	2.11	0.51
1:A:753:LYS:H	1:A:753:LYS:HZ2	1.58	0.51
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.51
1:A:81:ARG:NE	6:A:2080:HOH:O	2.44	0.50
1:A:142:CYS:SG	1:A:487:THR:HG22	2.52	0.50
1:A:344:LEU:C	1:A:347:PRO:HD2	2.31	0.50
1:A:354:VAL:O	1:A:358:ARG:HA	2.12	0.50
1:A:16:ARG:O	1:A:838:ASP:HA	2.11	0.50
1:A:162:GLU:OE2	1:A:277:ARG:NH1	2.42	0.49
1:A:562:LEU:C	1:A:562:LEU:HD12	2.33	0.49
1:A:283:ASP:OD1	1:A:571:HIS:HE1	1.95	0.49
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.43	0.49
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.12	0.49
1:A:71:GLN:NE2	6:A:2069:HOH:O	2.34	0.49
1:A:413:ARG:NH1	6:A:2334:HOH:O	2.45	0.49
1:A:24:VAL:HG11	1:A:114:GLN:HE22	1.77	0.49
1:A:617:LYS:HE2	6:A:2157:HOH:O	2.13	0.49
1:A:18:LEU:HD12	6:A:2636:HOH:O	2.13	0.48
1:A:24:VAL:HG11	1:A:114:GLN:NE2	2.28	0.48
1:A:641:ARG:NH1	1:A:641:ARG:HG3	2.29	0.48
1:A:786:ARG:HD2	6:A:2595:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ARG:NH2	6:A:2597:HOH:O	2.28	0.48
1:A:492:LEU:HD22	1:A:683:LEU:HD11	1.94	0.48
1:A:528:GLU:CD	1:A:795:ARG:HH12	2.17	0.47
1:A:739:ARG:O	1:A:743:GLU:HG3	2.14	0.47
1:A:689:ILE:HG23	1:A:689:ILE:O	2.14	0.47
1:A:67:TRP:CD2	1:A:229:PRO:HB3	2.49	0.47
1:A:457:ARG:NH2	6:A:2361:HOH:O	2.48	0.47
1:A:235:ASN:HB3	1:A:831:ARG:NH2	2.29	0.47
1:A:599:VAL:CG2	1:A:792:LYS:HG3	2.45	0.47
1:A:564:ASP:HB3	1:A:603:VAL:HA	1.97	0.47
1:A:688:THR:O	1:A:709:PHE:HB2	2.15	0.46
1:A:477:HIS:HB3	6:A:2380:HOH:O	2.15	0.46
1:A:230:VAL:HG22	1:A:230:VAL:O	2.16	0.46
1:A:475:GLU:HB3	1:A:477:HIS:CE1	2.50	0.46
1:A:21:VAL:O	1:A:22:GLU:CB	2.63	0.46
1:A:379:VAL:HG13	6:A:2309:HOH:O	2.16	0.46
1:A:205:ARG:NH2	1:A:207:GLU:OE1	2.49	0.46
1:A:569:ARG:O	1:A:574:LYS:HD2	2.16	0.45
1:A:21:VAL:O	1:A:22:GLU:HB2	2.16	0.45
1:A:15:VAL:O	1:A:16:ARG:C	2.54	0.45
1:A:42:ASP:OD1	1:A:45:VAL:HG22	2.17	0.45
1:A:528:GLU:OE2	1:A:795:ARG:NH1	2.46	0.45
1:A:358:ARG:CA	1:A:358:ARG:HE	2.21	0.45
1:A:230:VAL:CG2	1:A:230:VAL:O	2.65	0.45
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.99	0.44
1:A:67:TRP:HA	1:A:238:VAL:HB	2.00	0.44
1:A:568:LYS:HE3	6:A:2434:HOH:O	2.17	0.44
1:A:405:GLU:OE2	1:A:409:ARG:NH1	2.51	0.43
1:A:335:ILE:HD12	1:A:371:THR:CG2	2.49	0.43
1:A:344:LEU:O	1:A:347:PRO:HD2	2.19	0.43
1:A:549:LEU:HD12	1:A:557:ILE:HD13	2.00	0.43
1:A:833:ARG:H	1:A:833:ARG:HG3	1.67	0.43
1:A:641:ARG:CA	1:A:641:ARG:HH11	2.31	0.42
1:A:475:GLU:HB3	1:A:477:HIS:NE2	2.35	0.42
1:A:735:ILE:HD13	1:A:778:GLU:HG3	2.01	0.42
1:A:23:ASN:HA	1:A:23:ASN:HD22	1.55	0.42
1:A:731:TYR:CE2	1:A:775:ALA:HA	2.54	0.41
1:A:526:ASP:OD1	1:A:799:ARG:NH2	2.53	0.41
1:A:693:ASP:O	1:A:696:ASN:HB2	2.21	0.41
1:A:94:THR:HG23	6:A:2101:HOH:O	2.20	0.41
1:A:590:ILE:O	1:A:594:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HD2	6:A:2424:HOH:O	2.20	0.41
1:A:390:HIS:O	1:A:394:THR:CG2	2.67	0.41
1:A:14:SER:HB3	1:A:16:ARG:HG2	2.03	0.41
1:A:283:ASP:O	1:A:284:ASN:HB2	2.20	0.41
1:A:110:GLU:HG3	1:A:114:GLN:NE2	2.35	0.41
1:A:499:LEU:HD22	1:A:503:ILE:HG13	2.03	0.41
1:A:275:ILE:O	1:A:295:GLN:HG2	2.20	0.41
1:A:18:LEU:CD1	6:A:2636:HOH:O	2.67	0.40
1:A:96:GLN:NE2	6:A:2097:HOH:O	2.53	0.40
1:A:6:ASP:HB3	1:A:7:GLN:H	1.64	0.40
1:A:93:ARG:HD3	6:A:2092:HOH:O	2.22	0.40
1:A:92:GLY:HA2	1:A:128:ASP:OD1	2.22	0.40

All (4) 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)
6:A:2018:HOH:O	6:A:2172:HOH:O[7_556]	1.93	0.27
6:A:2039:HOH:O	6:A:2039:HOH:O[7_556]	2.04	0.16
6:A:2018:HOH:O	6:A:2176:HOH:O[7_556]	2.04	0.16
6:A:2220:HOH:O	6:A:2220:HOH:O[7_555]	2.19	0.01

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	807/842 (96%)	769 (95%)	32 (4%)	6 (1%)	26 25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG

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Mol	Chain	Res	Type
1	A	19	ALA
1	A	22	GLU
1	A	24	VAL
1	A	514	ASP
1	A	837	PRO

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	704/731 (96%)	660 (94%)	44 (6%)	22 20

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	16	ARG
1	A	18	LEU
1	A	23	ASN
1	A	27	LEU
1	A	29	LYS
1	A	90	TYR
1	A	184	ARG
1	A	205	ARG
1	A	210	SER
1	A	217	ASP
1	A	234	ARG
1	A	325	ASN
1	A	332	LYS
1	A	358	ARG
1	A	360	ASP
1	A	370	LYS
1	A	379	VAL
1	A	384	LEU
1	A	394	THR
1	A	437	LYS

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Mol	Chain	Res	Type
1	A	465	LYS
1	A	494	LEU
1	A	496	ASN
1	A	499	LEU
1	A	506	ARG
1	A	519	ARG
1	A	551	ARG
1	A	562	LEU
1	A	568	LYS
1	A	573	TYR
1	A	576	GLN
1	A	579	ASN
1	A	613	TYR
1	A	641	ARG
1	A	663	SER
1	A	708	PHE
1	A	721	LEU
1	A	724	ARG
1	A	753	LYS
1	A	793	ASN
1	A	831	ARG
1	A	832	GLN
1	A	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	36	HIS
1	A	97	ASN
1	A	106	ASN
1	A	201	HIS
1	A	325	ASN
1	A	450	HIS
1	A	484	ASN
1	A	496	ASN
1	A	517	GLN
1	A	541	ASN
1	A	560	ASN
1	A	566	GLN
1	A	571	HIS
1	A	576	GLN

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Mol	Chain	Res	Type
1	A	579	ASN
1	A	588	ASN
1	A	632	HIS
1	A	684	ASN
1	A	744	GLN
1	A	754	GLN
1	A	793	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	CPB	A	940	-	29,31,31	3.45	16 (55%)	33,46,46	2.02	7 (21%)
3	PO3	A	997	1	0,3,3	0.00	-	0,3,3	0.00	-
4	GLC	A	998	-	12,12,12	1.04	0	17,17,17	1.01	1 (5%)
5	PLP	A	999	1	15,15,16	1.32	2 (13%)	21,22,23	1.10	2 (9%)

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	CPB	A	940	-	-	0/7/21/21	0/4/4/4
3	PO3	A	997	1	-	0/0/0/0	0/0/0/0
4	GLC	A	998	-	-	0/2/22/22	0/1/1/1
5	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	PLP	P-O3P	-2.37	1.46	1.54
5	A	999	PLP	P-O2P	2.00	1.61	1.54
2	A	940	CPB	O5-C5	2.01	1.40	1.35
2	A	940	CPB	C24-C23	2.02	1.43	1.38
2	A	940	CPB	C21-C22	2.17	1.44	1.40
2	A	940	CPB	C25-C24	2.25	1.43	1.38
2	A	940	CPB	C12-C13	2.32	1.55	1.52
2	A	940	CPB	O1-C9	2.42	1.40	1.36
2	A	940	CPB	O7-C7	2.52	1.41	1.36
2	A	940	CPB	O1-C2	2.79	1.38	1.35
2	A	940	CPB	C10-C9	2.81	1.44	1.41
2	A	940	CPB	C26-C21	2.91	1.44	1.39
2	A	940	CPB	C6-C7	3.29	1.43	1.38
2	A	940	CPB	C14-C13	3.30	1.57	1.53
2	A	940	CPB	C3-C4	5.06	1.47	1.37
2	A	940	CPB	C21-C2	6.97	1.55	1.46
2	A	940	CPB	C7-C8	8.19	1.46	1.38
2	A	940	CPB	C4-C10	10.04	1.55	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	940	CPB	C3-C2-C21	-7.53	119.23	127.32
2	A	940	CPB	O3-C13-C12	-2.75	104.19	109.53
2	A	940	CPB	C16-C15-C14	-2.06	109.65	111.39
5	A	999	PLP	C6-C5-C4	2.09	119.92	118.15
4	A	998	GLC	O5-C5-C6	2.10	111.66	106.36
2	A	940	CPB	C1-N1-C16	2.17	114.01	110.63
2	A	940	CPB	C15-C16-N1	2.49	114.78	111.32
5	A	999	PLP	O3P-P-O1P	2.59	118.90	110.58
2	A	940	CPB	C16-N1-C12	2.84	113.07	110.17
2	A	940	CPB	O1-C2-C21	4.74	119.66	113.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.