



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:25 am BST

PDB ID : 6I33
Title : Crystal structure of human glycine decarboxylase (P-protein)
Authors : Van Laer, B.; Kapp, U.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on : 2018-11-05
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

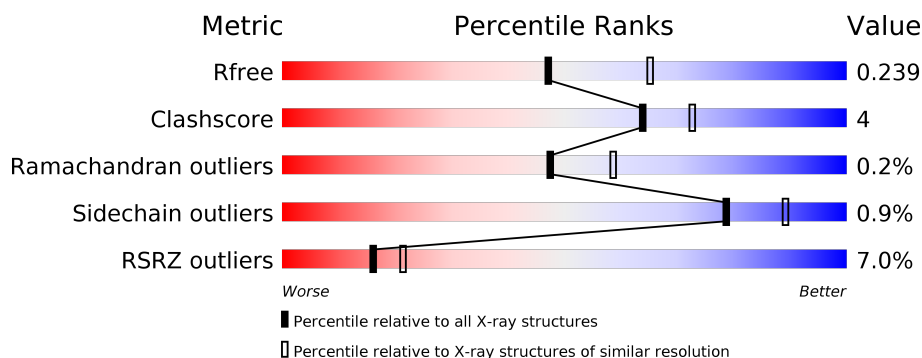
1 Overall quality at a glance

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))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 ≥ 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	984	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>••</div> </div> </div>
1	B	984	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>

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	EDO	A	1103	-	-	-	X
3	EDO	A	1106	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14852 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 Glycine dehydrogenase (decarboxylating), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	950	Total	C	N	O	S	0	0	0
			7403	4668	1310	1370	55			
1	B	925	Total	C	N	O	S	0	0	0
			7214	4553	1269	1339	53			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP P23378
A	1021	GLY	-	expression tag	UNP P23378
A	1022	HIS	-	expression tag	UNP P23378
A	1023	HIS	-	expression tag	UNP P23378
A	1024	HIS	-	expression tag	UNP P23378
A	1025	HIS	-	expression tag	UNP P23378
A	1026	HIS	-	expression tag	UNP P23378
A	1027	HIS	-	expression tag	UNP P23378
B	44	MET	-	initiating methionine	UNP P23378
B	1021	GLY	-	expression tag	UNP P23378
B	1022	HIS	-	expression tag	UNP P23378
B	1023	HIS	-	expression tag	UNP P23378
B	1024	HIS	-	expression tag	UNP P23378
B	1025	HIS	-	expression tag	UNP P23378
B	1026	HIS	-	expression tag	UNP P23378
B	1027	HIS	-	expression tag	UNP P23378

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



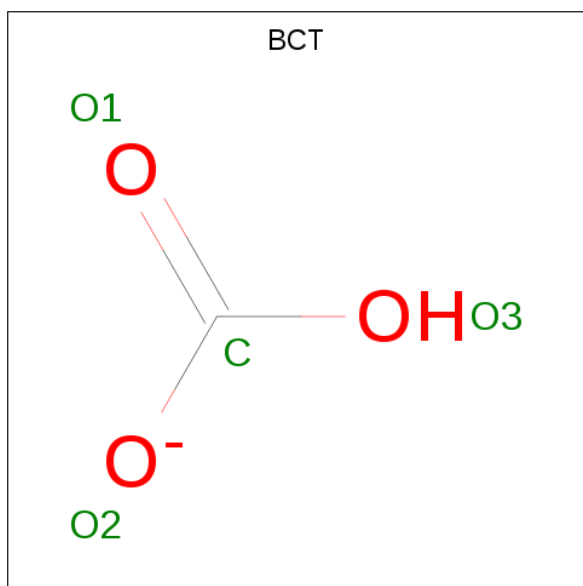
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3^-).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		

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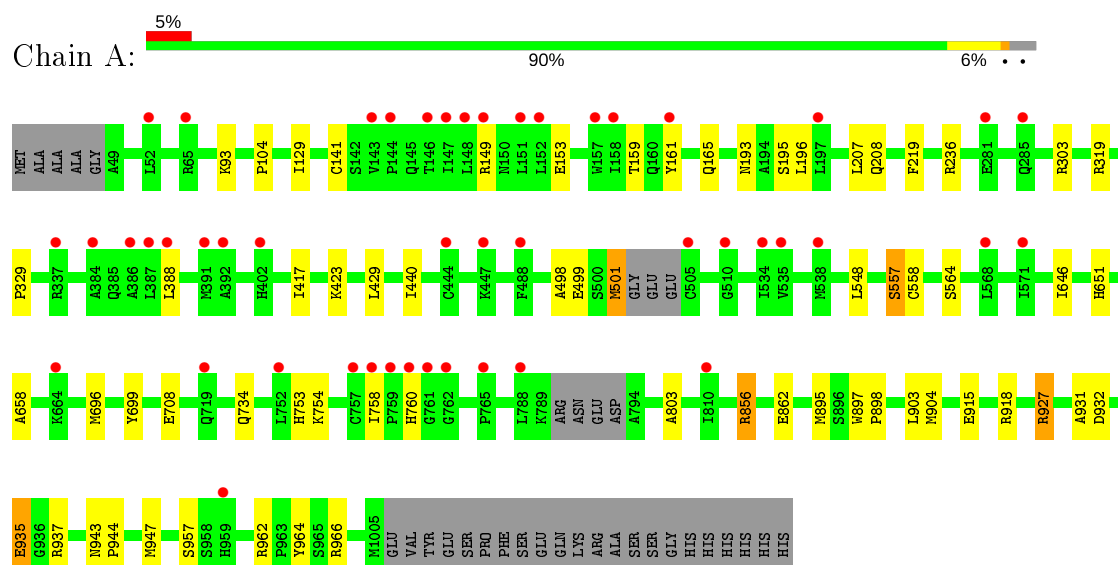
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	43	Total	O	0	0
			43	43		

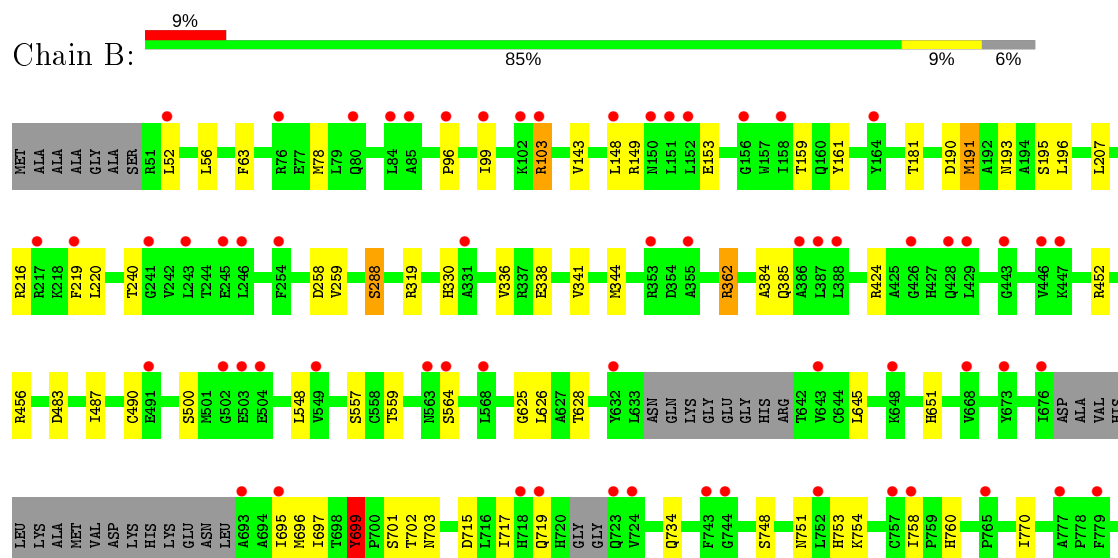
3 Residue-property plots

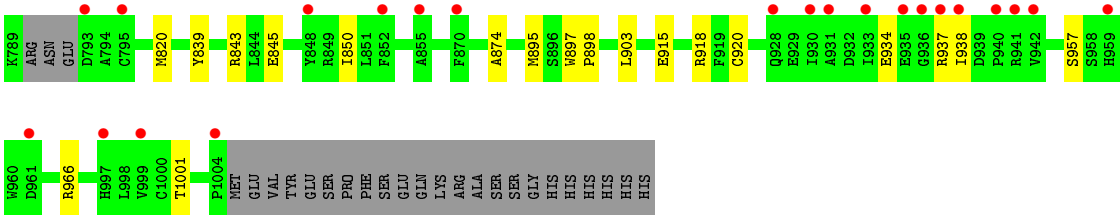
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial



- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.81Å 123.51Å 99.51Å 90.00° 97.87° 90.00°	Depositor
Resolution (Å)	46.08 – 2.30 46.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.08-2.30) 99.2 (46.08-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.212 , 0.235 0.217 , 0.239	Depositor DCC
R_{free} test set	4521 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: BCT, EDO, 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	0.61	0/7568	0.74	0/10248
1	B	0.53	0/7374	0.73	1/9988 (0.0%)
All	All	0.57	0/14942	0.74	1/20236 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	699	TYR	C-N-CD	-14.11	89.55	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	699	TYR	Peptide

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	7403	0	7346	54	0
1	B	7214	0	7144	76	0
2	A	15	0	6	1	0
2	B	15	0	6	3	0
3	A	20	0	30	4	0
3	B	16	0	24	0	0
4	A	4	0	0	0	0
5	A	122	0	0	3	0
5	B	43	0	0	1	0
All	All	14852	0	14556	122	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 4.

All (122) 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:B:915:GLU:OE1	1:B:918:ARG:NH2	1.95	0.98
1:B:216:ARG:HB3	1:B:258:ASP:O	1.66	0.95
1:B:220:LEU:HD12	1:B:259:VAL:HG11	1.49	0.94
1:B:220:LEU:CD1	1:B:259:VAL:HG11	1.98	0.94
1:B:701:SER:HB2	1:B:703:ASN:OD1	1.68	0.93
1:B:63:PHE:CG	1:B:820:MET:HE2	2.05	0.91
1:B:626:LEU:HD11	1:B:696:MET:CE	2.00	0.91
1:B:557:SER:OG	2:B:1101:PLP:O3	1.89	0.91
1:A:129:ILE:HG21	3:A:1105:EDO:H11	1.57	0.85
1:B:220:LEU:HD12	1:B:259:VAL:CG1	2.06	0.85
1:A:931:ALA:O	1:A:935:GLU:HG2	1.80	0.82
1:B:559:THR:HB	1:B:754:LYS:O	1.80	0.81
1:A:935:GLU:HG3	1:A:937:ARG:NH2	1.98	0.78
1:B:651:HIS:HB2	2:B:1101:PLP:H2A3	1.65	0.78
1:A:501:MET:CE	1:B:56:LEU:HD13	2.15	0.77
1:B:645:LEU:HB2	1:B:695:ILE:HG22	1.68	0.76
1:A:501:MET:CE	1:B:56:LEU:CD1	2.65	0.74
1:A:658:ALA:HB2	1:A:696:MET:HE1	1.72	0.69
1:B:258:ASP:OD1	1:B:258:ASP:N	2.25	0.67
1:A:658:ALA:HB2	1:A:696:MET:CE	2.26	0.66
1:B:362:ARG:HH21	1:B:362:ARG:HG2	1.62	0.65
1:B:760:HIS:ND1	5:B:1204:HOH:O	2.29	0.63
1:B:751:ASN:HB3	1:B:754:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HG21	3:A:1105:EDO:C1	2.28	0.63
1:B:96:PRO:O	1:B:99:ILE:HG13	1.98	0.63
1:B:330:HIS:O	1:B:385:GLN:OE1	2.17	0.62
1:B:63:PHE:CD1	1:B:820:MET:HE2	2.34	0.62
1:B:424:ARG:NH2	1:B:500:SER:OG	2.33	0.62
1:B:695:ILE:HD12	1:B:697:ILE:HG23	1.81	0.61
1:A:501:MET:HE1	1:B:56:LEU:HD13	1.81	0.61
1:B:181:THR:HG23	1:B:1001:THR:HG23	1.83	0.60
1:B:559:THR:CB	1:B:754:LYS:O	2.50	0.59
1:A:423:LYS:HE2	1:A:429:LEU:HD22	1.85	0.58
1:A:93:LYS:O	1:A:856:ARG:NH1	2.35	0.58
1:A:932:ASP:OD1	1:A:937:ARG:NH1	2.37	0.58
1:B:220:LEU:CD1	1:B:259:VAL:CG1	2.71	0.57
1:A:557:SER:O	1:A:754:LYS:HE2	2.04	0.57
1:B:220:LEU:HD11	1:B:259:VAL:HG21	1.85	0.57
1:B:626:LEU:HD11	1:B:696:MET:HE1	1.85	0.57
1:B:336:VAL:HG22	1:B:344:MET:HE1	1.85	0.57
1:A:935:GLU:HG3	1:A:937:ARG:CZ	2.34	0.56
1:A:129:ILE:CG2	3:A:1105:EDO:H11	2.35	0.56
1:A:957:SER:O	1:A:966:ARG:NH2	2.40	0.55
1:B:843:ARG:NH1	1:B:920:CYS:HB2	2.21	0.54
1:A:895:MET:SD	1:A:903:LEU:HD22	2.48	0.54
1:B:625:GLY:O	1:B:628:THR:HG22	2.07	0.54
1:B:957:SER:O	1:B:966:ARG:NH2	2.40	0.54
1:A:947:MET:SD	1:A:962:ARG:NH1	2.80	0.54
1:A:329:PRO:HB2	1:A:388:LEU:HD13	1.90	0.53
1:A:753:HIS:HA	1:A:758:ILE:HB	1.90	0.53
1:A:862:GLU:CD	1:A:904:MET:HE2	2.29	0.53
1:B:362:ARG:HH21	1:B:362:ARG:CG	2.22	0.53
1:A:193:ASN:HD21	1:A:196:LEU:HG	1.74	0.53
1:B:699:TYR:O	1:B:734:GLN:NE2	2.41	0.53
1:B:559:THR:CG2	1:B:754:LYS:O	2.57	0.53
1:A:498:ALA:HA	1:A:501:MET:HE2	1.92	0.52
1:A:943:ASN:HB2	1:A:944:PRO:HD2	1.92	0.52
1:B:843:ARG:HH11	1:B:920:CYS:HB2	1.75	0.52
1:B:78:MET:HE3	1:B:839:TYR:CD2	2.45	0.51
1:B:220:LEU:HD12	1:B:259:VAL:HG13	1.91	0.51
1:B:103:ARG:HG3	1:B:103:ARG:O	2.10	0.50
1:A:699:TYR:O	1:A:734:GLN:NE2	2.44	0.50
1:A:501:MET:HE3	1:B:56:LEU:CD1	2.42	0.50
1:B:895:MET:SD	1:B:903:LEU:HD22	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TRP:CD1	1:A:898:PRO:HA	2.48	0.49
1:B:193:ASN:HD21	1:B:196:LEU:HG	1.77	0.49
1:A:104:PRO:HA	5:A:1207:HOH:O	2.12	0.49
1:B:190:ASP:C	1:B:191:MET:HG2	2.32	0.49
1:B:897:TRP:CD1	1:B:898:PRO:HA	2.47	0.49
1:A:646:ILE:HD11	1:A:696:MET:HE3	1.93	0.49
1:B:645:LEU:CB	1:B:695:ILE:HG22	2.42	0.49
1:B:937:ARG:O	1:B:938:ILE:HG13	2.14	0.48
1:B:384:ALA:O	1:B:385:GLN:HG3	2.13	0.48
1:B:753:HIS:HA	1:B:758:ILE:HB	1.95	0.48
1:A:708:GLU:OE2	1:A:856:ARG:NH2	2.47	0.47
1:A:862:GLU:CG	1:A:904:MET:HE2	2.45	0.47
1:B:452:ARG:NH1	1:B:487:ILE:O	2.48	0.47
1:A:803:ALA:HB1	5:A:1268:HOH:O	2.14	0.47
1:A:915:GLU:OE1	1:A:918:ARG:NH1	2.47	0.47
1:A:862:GLU:CD	1:A:904:MET:CE	2.83	0.46
1:A:558:CYS:HA	1:A:754:LYS:HE2	1.98	0.46
1:B:626:LEU:HD11	1:B:696:MET:HE3	1.90	0.46
1:A:159:THR:HB	1:A:548:LEU:HD12	1.99	0.45
1:B:937:ARG:C	1:B:938:ILE:HG13	2.37	0.45
1:B:159:THR:HB	1:B:548:LEU:HD12	1.98	0.45
1:A:943:ASN:HB2	1:A:944:PRO:CD	2.47	0.45
1:A:501:MET:HE3	1:B:56:LEU:HD13	1.96	0.45
1:A:319:ARG:HG3	5:A:1294:HOH:O	2.17	0.44
1:A:208:GLN:NE2	1:A:236:ARG:HD2	2.32	0.44
1:A:927:ARG:O	1:A:927:ARG:HD2	2.17	0.44
1:B:143:VAL:HG11	1:B:148:LEU:HD13	1.99	0.44
1:A:651:HIS:HB2	2:A:1101:PLP:H2A3	1.99	0.44
1:B:701:SER:O	1:B:703:ASN:N	2.50	0.44
1:A:207:LEU:HD12	1:A:219:PHE:CD2	2.52	0.44
1:A:862:GLU:OE2	1:A:904:MET:HE1	2.17	0.43
1:A:161:TYR:CD1	1:A:760:HIS:HB3	2.53	0.43
1:B:701:SER:C	1:B:703:ASN:N	2.72	0.43
1:B:220:LEU:HD11	1:B:259:VAL:CG2	2.47	0.43
1:B:207:LEU:HD12	1:B:219:PHE:CG	2.53	0.43
1:B:362:ARG:NH2	1:B:362:ARG:CG	2.77	0.43
1:B:695:ILE:HG12	1:B:717:ILE:HG13	1.99	0.43
1:A:944:PRO:HD3	1:A:964:TYR:CD1	2.53	0.43
1:B:63:PHE:CD1	1:B:820:MET:CE	3.01	0.43
1:A:141:CYS:O	3:A:1106:EDO:H21	2.19	0.43
1:A:429:LEU:HD12	1:A:440:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LEU:HB2	1:B:695:ILE:CG2	2.44	0.42
1:B:751:ASN:ND2	2:B:1101:PLP:H5A1	2.34	0.42
1:A:558:CYS:O	1:A:754:LYS:HG2	2.19	0.42
1:B:715:ASP:O	1:B:719:GLN:HG3	2.19	0.42
1:B:161:TYR:CD1	1:B:760:HIS:HB3	2.55	0.42
1:B:845:GLU:HA	1:B:850:ILE:CD1	2.50	0.42
1:A:153:GLU:HA	1:B:149:ARG:NH2	2.35	0.42
1:A:499:GLU:HA	1:B:52:LEU:HD23	2.02	0.41
1:A:927:ARG:C	1:A:927:ARG:HD2	2.41	0.41
1:B:874:ALA:HB2	1:B:934:GLU:HG3	2.03	0.41
1:B:456:ARG:NH1	1:B:483:ASP:OD1	2.52	0.41
1:B:259:VAL:O	1:B:288:SER:HB3	2.21	0.41
1:A:417:ILE:CG1	1:A:501:MET:HE1	2.51	0.41
1:B:240:THR:O	1:B:240:THR:HG22	2.21	0.40
1:A:149:ARG:NH2	1:B:153:GLU:HA	2.36	0.40
1:B:338:GLU:O	1:B:341:VAL:HG23	2.22	0.40
1:B:748:SER:O	1:B:770:ILE:HA	2.22	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	944/984 (96%)	913 (97%)	29 (3%)	2 (0%)	47	58
1	B	915/984 (93%)	882 (96%)	31 (3%)	2 (0%)	47	58
All	All	1859/1968 (94%)	1795 (97%)	60 (3%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER

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Mol	Chain	Res	Type
1	B	195	SER
1	B	702	THR
1	A	165	GLN

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	802/829 (97%)	795 (99%)	7 (1%)	78	89
1	B	783/829 (94%)	776 (99%)	7 (1%)	78	89
All	All	1585/1658 (96%)	1571 (99%)	14 (1%)	78	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ARG
1	A	501	MET
1	A	557	SER
1	A	564	SER
1	A	856	ARG
1	A	927	ARG
1	A	935	GLU
1	B	103	ARG
1	B	191	MET
1	B	288	SER
1	B	319	ARG
1	B	362	ARG
1	B	490	CYS
1	B	564	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	EDO	A	1106	-	3,3,3	0.50	0	2,2,2	0.29	0
2	PLP	A	1101	1	15,15,16	2.85	5 (33%)	20,22,23	2.53	7 (35%)
3	EDO	A	1102	-	3,3,3	0.50	0	2,2,2	0.21	0
3	EDO	B	1104	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	B	1103	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	A	1103	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	B	1102	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	A	1104	-	3,3,3	0.60	0	2,2,2	0.33	0
4	BCT	A	1107	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EDO	A	1105	-	3,3,3	0.26	0	2,2,2	0.72	0
2	PLP	B	1101	1	15,15,16	2.80	4 (26%)	20,22,23	1.95	6 (30%)
3	EDO	B	1105	-	3,3,3	0.51	0	2,2,2	0.34	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
3	EDO	A	1106	-	-	1/1/1/1	-
2	PLP	A	1101	1	-	3/6/6/8	0/1/1/1
3	EDO	A	1102	-	-	1/1/1/1	-
3	EDO	B	1103	-	-	1/1/1/1	-
3	EDO	A	1103	-	-	1/1/1/1	-
2	PLP	B	1101	1	-	0/6/6/8	0/1/1/1
3	EDO	B	1102	-	-	0/1/1/1	-
3	EDO	A	1104	-	-	1/1/1/1	-
3	EDO	A	1105	-	-	0/1/1/1	-
3	EDO	B	1104	-	-	0/1/1/1	-
3	EDO	B	1105	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	PLP	C3-C2	7.29	1.48	1.40
2	A	1101	PLP	C3-C2	6.65	1.47	1.40
2	A	1101	PLP	C5-C4	6.64	1.47	1.40
2	B	1101	PLP	C5-C4	6.46	1.47	1.40
2	B	1101	PLP	C3-C4	3.04	1.46	1.40
2	A	1101	PLP	P-O3P	-2.78	1.44	1.54
2	A	1101	PLP	C3-C4	2.65	1.45	1.40
2	A	1101	PLP	P-O2P	-2.45	1.45	1.54
2	B	1101	PLP	C4A-C4	-2.27	1.46	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	PLP	C4A-C4-C5	7.35	128.50	120.94
2	B	1101	PLP	C5A-C5-C6	3.98	125.92	119.37
2	B	1101	PLP	O4P-C5A-C5	3.96	116.89	109.35
2	A	1101	PLP	O2P-P-O4P	-3.90	96.36	106.73
2	A	1101	PLP	O4P-C5A-C5	3.78	116.56	109.35
2	A	1101	PLP	C3-C4-C5	-3.32	115.16	118.74
2	B	1101	PLP	C2A-C2-C3	-2.83	117.39	120.89
2	B	1101	PLP	C2A-C2-N1	2.78	123.11	117.67
2	A	1101	PLP	O3P-P-O2P	2.71	117.98	107.64
2	B	1101	PLP	C6-N1-C2	2.54	123.87	119.17
2	A	1101	PLP	C4A-C4-C3	-2.45	116.34	120.50
2	B	1101	PLP	O3-C3-C2	2.31	122.52	117.49
2	A	1101	PLP	O3-C3-C2	2.22	122.33	117.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

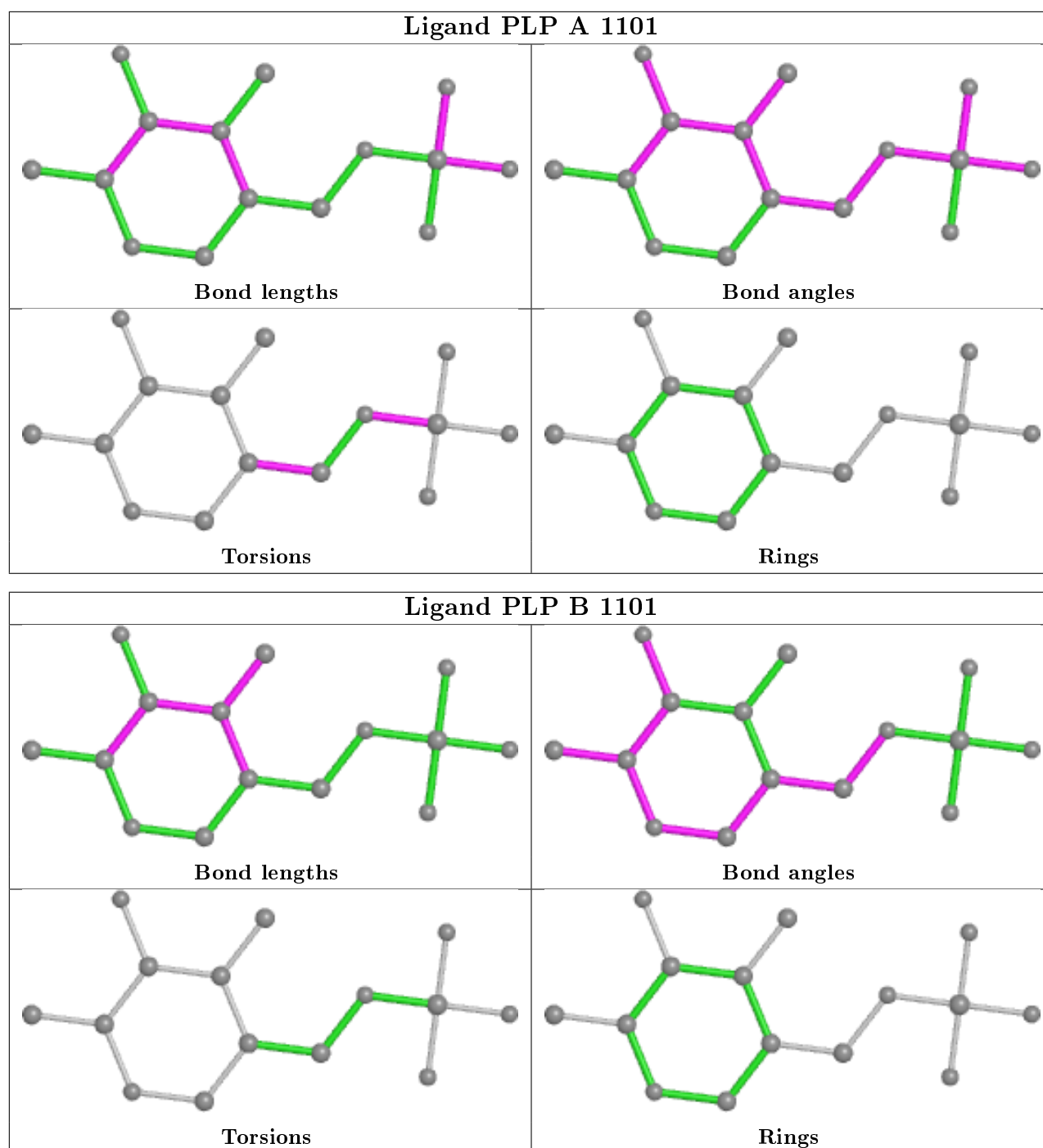
Mol	Chain	Res	Type	Atoms
2	A	1101	PLP	C4-C5-C5A-O4P
2	A	1101	PLP	C6-C5-C5A-O4P
2	A	1101	PLP	C5A-O4P-P-O2P
3	A	1102	EDO	O1-C1-C2-O2
3	B	1103	EDO	O1-C1-C2-O2
3	A	1103	EDO	O1-C1-C2-O2
3	A	1104	EDO	O1-C1-C2-O2
3	A	1106	EDO	O1-C1-C2-O2
3	B	1105	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1106	EDO	1	0
2	A	1101	PLP	1	0
3	A	1105	EDO	3	0
2	B	1101	PLP	3	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	950/984 (96%)	0.23	47 (4%) 29 36	35, 47, 65, 83	0
1	B	925/984 (94%)	0.55	85 (9%) 9 12	44, 65, 89, 99	0
All	All	1875/1968 (95%)	0.39	132 (7%) 16 21	35, 55, 85, 99	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	779	PHE	4.6
1	B	52	LEU	4.5
1	B	961	ASP	4.3
1	B	102	LYS	4.3
1	B	938	ILE	4.2
1	B	503	GLU	4.2
1	B	940	PRO	4.2
1	B	695	ILE	4.1
1	B	246	LEU	4.0
1	A	152	LEU	3.9
1	B	1004	PRO	3.9
1	B	959	HIS	3.9
1	B	777	ALA	3.6
1	A	147	ILE	3.5
1	B	502	GLY	3.5
1	A	337	ARG	3.5
1	B	848	TYR	3.4
1	B	504	GLU	3.4
1	A	387	LEU	3.4
1	B	152	LEU	3.4
1	A	758	ILE	3.3
1	B	937	ARG	3.3
1	A	959	HIS	3.3
1	B	388	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	158	ILE	3.2
1	A	664	LYS	3.2
1	B	930	ILE	3.2
1	B	795	CYS	3.1
1	B	942	VAL	3.1
1	B	429	LEU	3.1
1	A	761	GLY	3.1
1	B	941	ARG	3.1
1	B	724	VAL	3.0
1	B	928	GLN	3.0
1	B	997	HIS	3.0
1	A	510	GLY	3.0
1	A	759	PRO	2.9
1	B	158	ILE	2.9
1	B	96	PRO	2.9
1	B	743	PHE	2.9
1	B	870	PHE	2.9
1	B	723	GLN	2.9
1	A	388	LEU	2.9
1	B	855	ALA	2.8
1	B	76	ARG	2.8
1	B	254	PHE	2.8
1	B	245	GLU	2.8
1	B	744	GLY	2.7
1	A	535	VAL	2.7
1	B	387	LEU	2.7
1	A	810	ILE	2.7
1	A	765	PRO	2.7
1	B	446	VAL	2.7
1	A	151	LEU	2.7
1	B	428	GLN	2.7
1	B	103	ARG	2.6
1	A	788	LEU	2.6
1	B	568	LEU	2.6
1	B	217	ARG	2.6
1	B	243	LEU	2.6
1	B	668	VAL	2.6
1	B	752	LEU	2.6
1	B	999	VAL	2.6
1	B	718	HIS	2.5
1	A	392	ALA	2.5
1	B	693	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	391	MET	2.5
1	B	219	PHE	2.5
1	B	164	TYR	2.5
1	B	758	ILE	2.5
1	A	402	HIS	2.5
1	B	936	GLY	2.5
1	B	148	LEU	2.5
1	A	757	CYS	2.5
1	B	241	GLY	2.5
1	B	931	ALA	2.4
1	B	648	LYS	2.4
1	A	571	ILE	2.4
1	A	447	LYS	2.4
1	A	143	VAL	2.4
1	B	632	TYR	2.4
1	B	673	TYR	2.4
1	A	146	THR	2.4
1	B	549	VAL	2.4
1	A	52	LEU	2.4
1	A	505	CYS	2.4
1	B	719	GLN	2.4
1	A	384	ALA	2.4
1	B	563	ASN	2.4
1	A	157	TRP	2.3
1	A	149	ARG	2.3
1	B	353	ARG	2.3
1	B	765	PRO	2.3
1	B	852	PHE	2.3
1	A	568	LEU	2.3
1	A	144	PRO	2.3
1	B	426	GLY	2.3
1	A	488	PHE	2.2
1	A	719	GLN	2.2
1	B	355	ALA	2.2
1	B	643	VAL	2.2
1	A	386	ALA	2.2
1	A	281	GLU	2.2
1	B	386	ALA	2.2
1	B	84	LEU	2.2
1	A	161	TYR	2.2
1	B	793	ASP	2.2
1	B	491	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	331	ALA	2.2
1	A	534	ILE	2.2
1	B	757	CYS	2.2
1	A	148	LEU	2.2
1	B	564	SER	2.2
1	B	150	ASN	2.1
1	B	156	GLY	2.2
1	B	447	LYS	2.1
1	B	80	GLN	2.1
1	B	151	LEU	2.1
1	B	935	GLU	2.1
1	A	760	HIS	2.1
1	A	285	GLN	2.1
1	B	443	GLY	2.1
1	A	762	GLY	2.1
1	A	538	MET	2.1
1	B	99	ILE	2.1
1	B	85	ALA	2.1
1	A	444	CYS	2.1
1	A	197	LEU	2.0
1	A	752	LEU	2.0
1	B	676	ILE	2.0
1	B	933	ILE	2.0
1	A	65	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

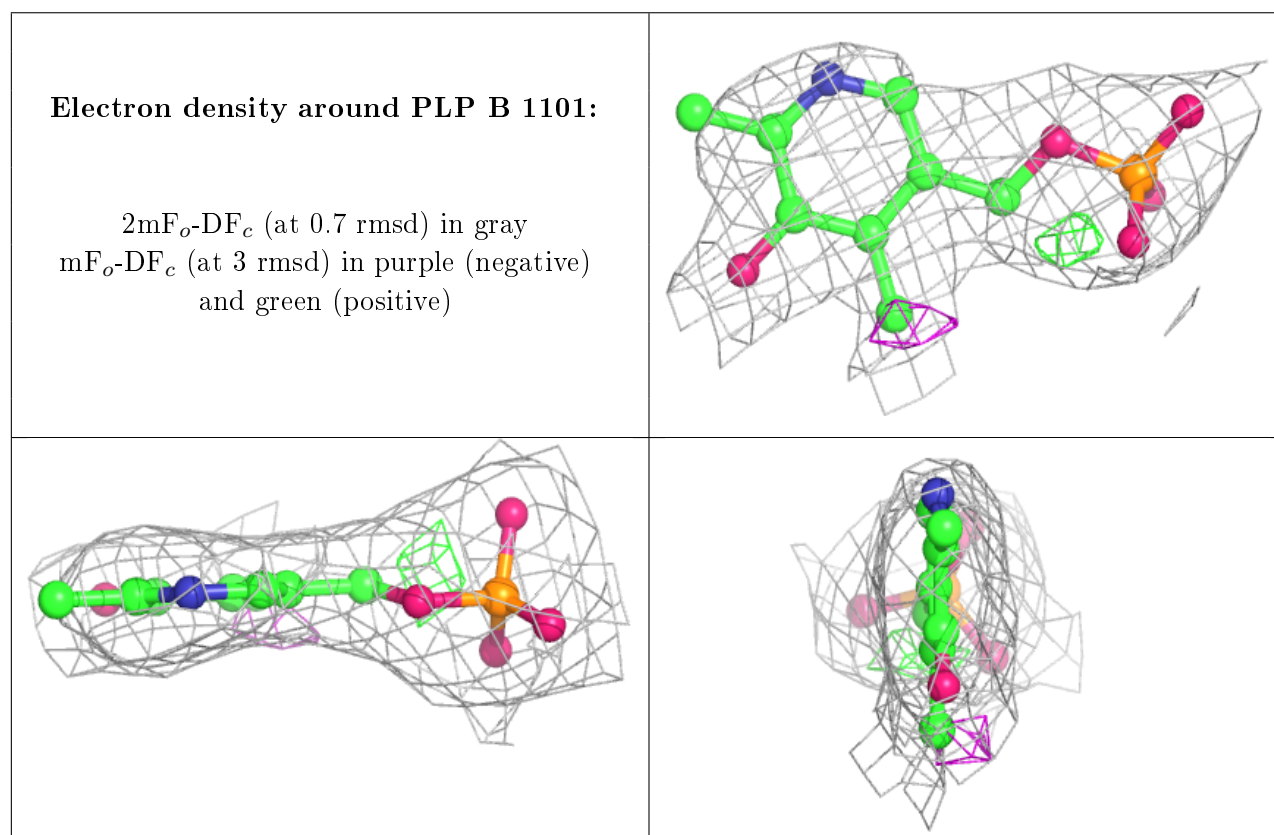
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

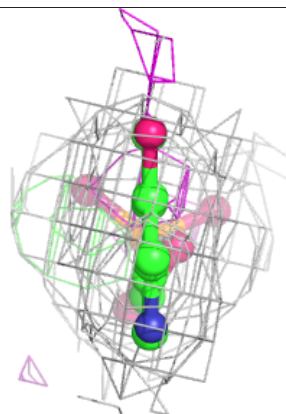
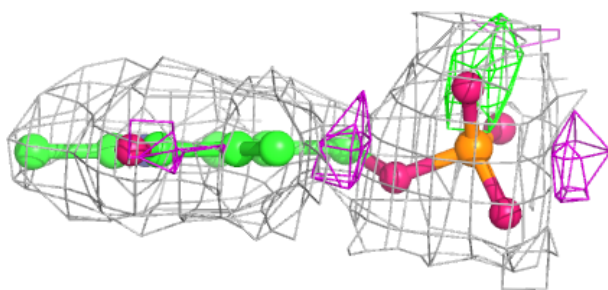
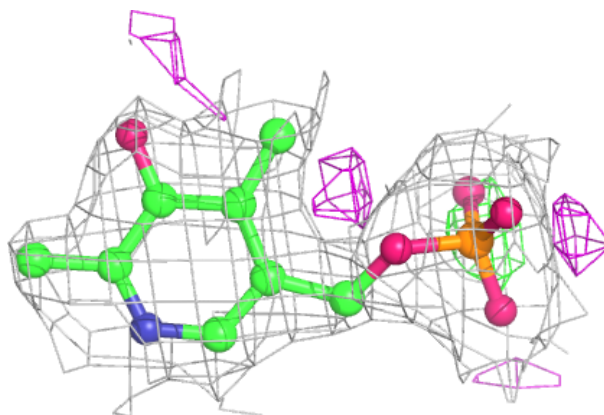
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	1102	4/4	0.53	0.31	70,72,73,73	0
4	BCT	A	1107	4/4	0.66	0.23	77,82,85,87	0
3	EDO	A	1104	4/4	0.71	0.28	60,65,67,67	0
3	EDO	B	1105	4/4	0.71	0.35	72,73,74,75	0
3	EDO	A	1106	4/4	0.78	0.47	64,69,73,77	0
3	EDO	A	1103	4/4	0.79	0.50	71,73,76,79	0
3	EDO	B	1104	4/4	0.81	0.55	68,72,72,73	0
3	EDO	B	1103	4/4	0.82	0.63	61,62,64,69	0
3	EDO	A	1105	4/4	0.83	0.24	69,69,73,75	0
2	PLP	B	1101	15/16	0.93	0.22	60,72,75,76	0
3	EDO	B	1102	4/4	0.94	0.28	59,60,61,65	0
2	PLP	A	1101	15/16	0.95	0.27	47,65,70,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around PLP A 1101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.