



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:55 am BST

PDB ID : 2Z20
Title : Crystal structure of LL-Diaminopimelate Aminotransferase from *Arabidopsis thaliana*
Authors : Watanabe, N.; Cherney, M.M.; van Belkum, M.J.; Marcus, S.L.; Flegel, M.D.; Clay, M.D.; Deyholos, M.K.; Vederas, J.C.; James, M.N.G.
Deposited on : 2007-05-17
Resolution : 1.95 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
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

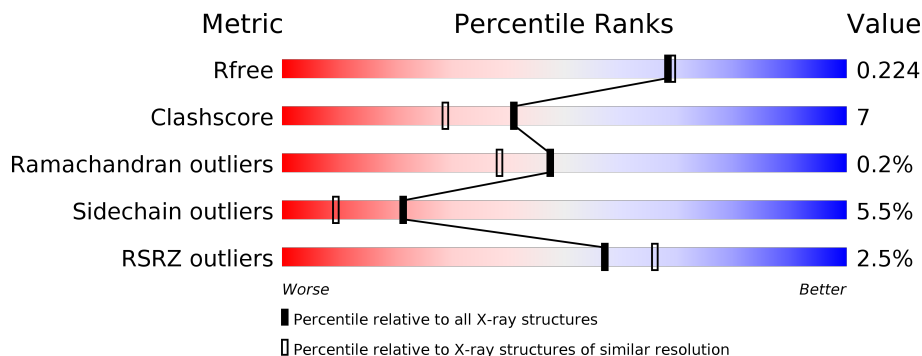
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	432	<p>3% (red), 81% (green), 13% (yellow), 5% (grey)</p>
1	B	432	<p>2% (red), 79% (green), 13% (yellow), 5% (grey)</p>

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
4	GOL	A	703	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7035 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 LL-diaminopimelate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	412	3184	2027	536	605	7	9	0	0	0
1	B	409	3154	2009	527	602	7	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

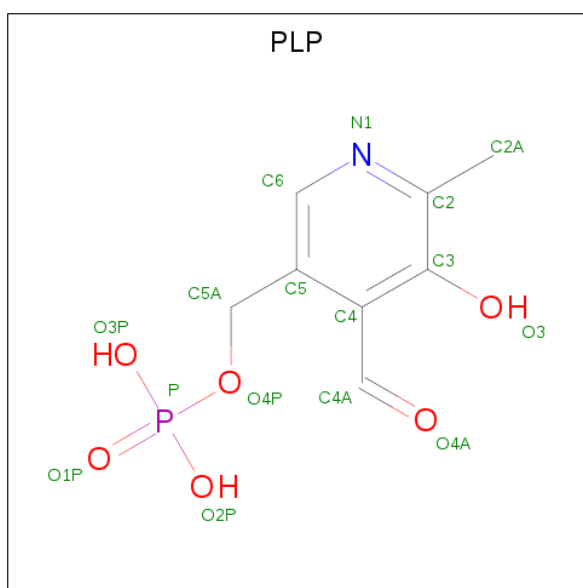
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	EXPRESSION TAG	UNP O81885
A	428	HIS	-	EXPRESSION TAG	UNP O81885
A	429	HIS	-	EXPRESSION TAG	UNP O81885
A	430	HIS	-	EXPRESSION TAG	UNP O81885
A	431	HIS	-	EXPRESSION TAG	UNP O81885
A	432	HIS	-	EXPRESSION TAG	UNP O81885
B	427	HIS	-	EXPRESSION TAG	UNP O81885
B	428	HIS	-	EXPRESSION TAG	UNP O81885
B	429	HIS	-	EXPRESSION TAG	UNP O81885
B	430	HIS	-	EXPRESSION TAG	UNP O81885
B	431	HIS	-	EXPRESSION TAG	UNP O81885
B	432	HIS	-	EXPRESSION TAG	UNP O81885

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



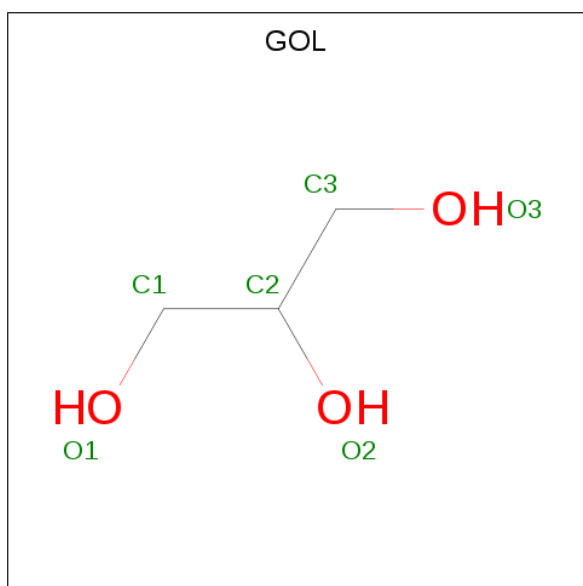
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S	0	0	
			5	4	1			
2	B	1	Total	O	S	0	0	
			5	4	1			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

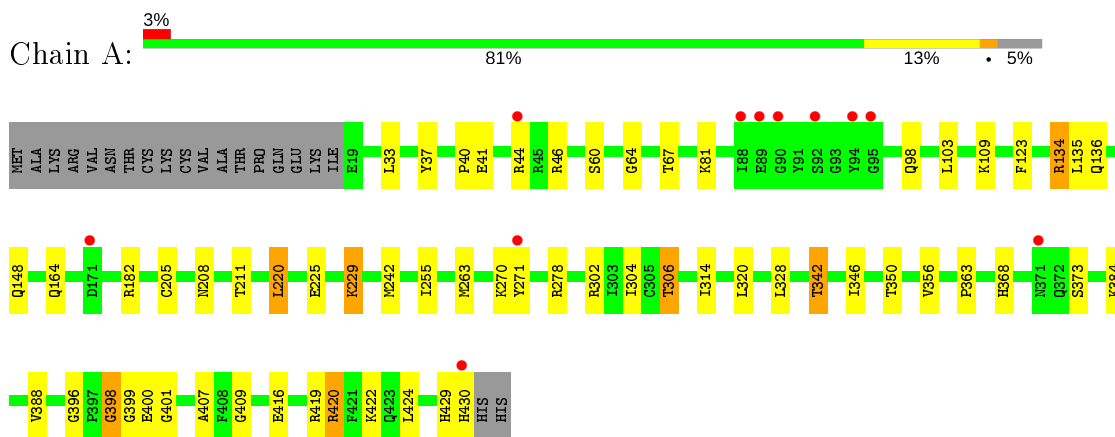
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	334	Total O 334 334	0	0
5	B	299	Total O 299 299	0	0

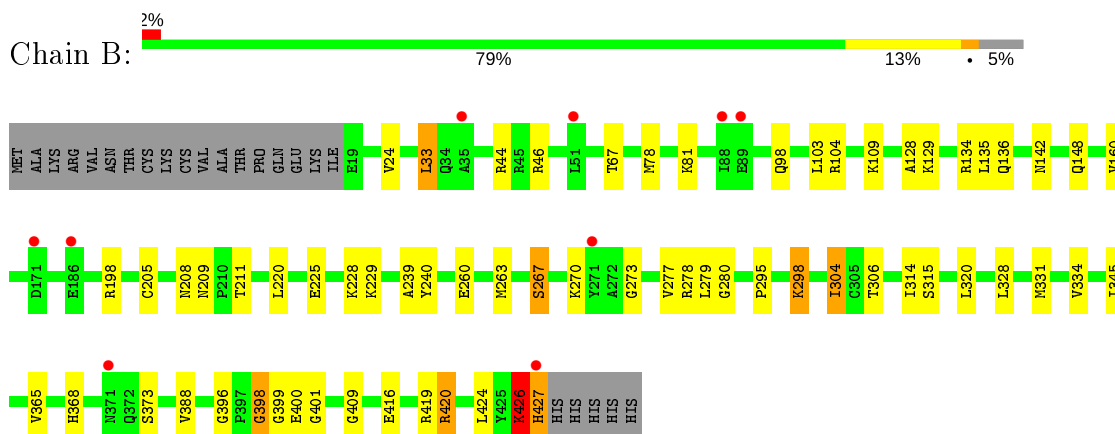
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: LL-diaminopimelate aminotransferase



- Molecule 1: LL-diaminopimelate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.91Å 102.91Å 171.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.00-1.95) 93.6 (19.89-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.227 0.183 , 0.224	Depositor DCC
R_{free} test set	3658 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7035	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, SO4, 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	0.79	0/3254	0.80	5/4395 (0.1%)
1	B	0.76	0/3221	0.84	7/4350 (0.2%)
All	All	0.78	0/6475	0.82	12/8745 (0.1%)

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	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	420	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	B	420	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	426	LYS	N-CA-C	7.67	131.69	111.00
1	B	398	GLY	N-CA-C	7.31	131.38	113.10
1	A	134	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	420	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	134	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	398	GLY	CA-C-N	5.54	127.28	116.20
1	A	398	GLY	CA-C-N	5.41	127.02	116.20
1	B	24	VAL	CG1-CB-CG2	5.26	119.32	110.90
1	B	401	GLY	N-CA-C	-5.26	99.95	113.10
1	A	420	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	GLY	Peptide
1	A	400	GLU	Peptide
1	B	398	GLY	Peptide
1	B	400	GLU	Peptide
1	B	426	LYS	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	3184	0	3092	49	0
1	B	3154	0	3071	41	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	15	0	6	1	0
3	B	15	0	6	3	0
4	A	12	0	16	10	0
4	B	12	0	16	2	0
5	A	334	0	0	11	0
5	B	299	0	0	15	0
All	All	7035	0	6207	90	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 7.

All (90) 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:429:HIS:HB3	1:A:430:HIS:C	1.73	1.07
1:A:302:ARG:HH11	1:A:306:THR:HG21	1.23	1.04
1:A:401:GLY:HA3	5:A:962:HOH:O	1.69	0.93
3:B:801:PLP:H2A2	5:B:939:HOH:O	1.69	0.91
1:A:81:LYS:NZ	4:A:702:GOL:H12	1.86	0.90
1:A:422:LYS:NZ	4:A:703:GOL:H12	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LYS:HZ1	4:A:703:GOL:H12	1.38	0.88
1:A:225:GLU:HG3	5:A:869:HOH:O	1.74	0.86
1:A:342:THR:HG21	1:A:363:PRO:HA	1.59	0.84
1:A:422:LYS:HZ2	4:A:703:GOL:H31	1.43	0.83
1:A:81:LYS:HZ3	4:A:702:GOL:H12	1.43	0.78
1:B:78:MSE:HE2	1:B:314:ILE:HG22	1.66	0.78
1:A:416:GLU:OE2	1:A:420:ARG:HD2	1.85	0.77
1:B:142:ASN:HB2	5:B:1053:HOH:O	1.84	0.76
1:B:78:MSE:CE	1:B:314:ILE:HG22	2.17	0.74
1:A:302:ARG:NH1	1:A:306:THR:HG21	2.01	0.73
1:A:302:ARG:O	1:A:306:THR:HG23	1.88	0.72
1:B:270:LYS:HG2	5:B:981:HOH:O	1.89	0.72
1:B:228:LYS:NZ	1:B:260:GLU:OE1	2.23	0.69
1:B:239:ALA:HB2	5:B:913:HOH:O	1.92	0.68
1:A:242:MSE:HG2	1:A:271:TYR:CZ	2.28	0.68
1:B:416:GLU:OE2	1:B:420:ARG:HD2	1.94	0.67
1:A:422:LYS:NZ	4:A:703:GOL:H31	2.09	0.66
1:B:148:GLN:HE22	1:B:205:CYS:H	1.45	0.65
1:A:242:MSE:HB2	1:A:271:TYR:CE1	2.34	0.62
1:B:148:GLN:NE2	1:B:205:CYS:H	1.96	0.62
1:A:401:GLY:CA	5:A:962:HOH:O	2.39	0.60
1:B:427:HIS:HB2	5:B:937:HOH:O	2.01	0.60
1:A:342:THR:HG22	1:A:407:ALA:CB	2.32	0.60
1:A:60:SER:HB3	5:A:1006:HOH:O	2.00	0.60
1:A:368:HIS:HD2	5:A:790:HOH:O	1.84	0.59
1:A:81:LYS:HZ1	4:A:702:GOL:H12	1.66	0.59
1:B:136:GLN:HE21	1:B:136:GLN:HA	1.67	0.59
1:B:209:ASN:HD22	3:B:801:PLP:H2A1	1.67	0.59
1:B:396:GLY:O	1:B:399:GLY:HA3	2.01	0.59
1:A:134:ARG:NH2	5:A:714:HOH:O	2.32	0.59
1:B:128:ALA:HA	5:B:1080:HOH:O	2.03	0.59
1:B:98:GLN:HG2	1:B:104:ARG:HD3	1.83	0.59
1:A:302:ARG:HH11	1:A:306:THR:CG2	2.08	0.59
1:A:396:GLY:O	1:A:399:GLY:HA3	2.03	0.58
1:A:302:ARG:O	1:A:306:THR:CG2	2.52	0.58
1:B:427:HIS:CD2	5:B:868:HOH:O	2.56	0.58
1:B:78:MSE:HE1	1:B:277:VAL:HG13	1.86	0.58
1:A:422:LYS:CE	4:A:703:GOL:H31	2.36	0.56
1:A:37:TYR:HB2	5:B:1083:HOH:O	2.05	0.56
1:A:148:GLN:NE2	1:A:205:CYS:H	2.04	0.55
1:B:295:PRO:HG2	1:B:298:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HD12	1:B:78:MSE:HE2	1.90	0.54
1:B:81:LYS:NZ	4:B:802:GOL:O2	2.26	0.54
1:A:98:GLN:HG2	1:A:123:PHE:CD2	2.43	0.53
3:A:701:PLP:H5A1	5:B:1046:HOH:O	2.09	0.53
1:B:368:HIS:HD2	5:B:1067:HOH:O	1.91	0.53
1:A:422:LYS:HE3	4:A:703:GOL:H31	1.90	0.53
1:A:40:PRO:HB2	5:A:800:HOH:O	2.09	0.52
1:A:67:THR:HG21	1:A:409:GLY:HA2	1.92	0.52
1:A:148:GLN:HE22	1:A:205:CYS:H	1.58	0.52
1:B:67:THR:HG21	1:B:409:GLY:HA2	1.92	0.52
1:A:136:GLN:HA	1:A:136:GLN:HE21	1.75	0.51
1:A:64:GLY:O	1:A:270:LYS:HE3	2.10	0.51
1:B:208:ASN:HD22	1:B:211:THR:H	1.59	0.51
1:A:429:HIS:CB	1:A:430:HIS:C	2.65	0.48
1:A:208:ASN:HD22	1:A:211:THR:H	1.61	0.48
1:A:314:ILE:HD12	1:B:78:MSE:CE	2.44	0.47
5:A:714:HOH:O	1:B:134:ARG:NH2	2.46	0.47
1:B:135:LEU:HD22	1:B:263:MSE:SE	2.64	0.47
1:B:306:THR:OG1	5:B:1083:HOH:O	2.20	0.47
1:A:229:LYS:HD3	5:A:858:HOH:O	2.15	0.46
1:A:41:GLU:OE1	1:A:44:ARG:NH1	2.49	0.46
1:B:427:HIS:HD2	5:B:868:HOH:O	1.95	0.46
1:A:368:HIS:CD2	5:A:790:HOH:O	2.64	0.46
1:B:368:HIS:HE1	5:B:1056:HOH:O	1.98	0.46
1:B:129:LYS:N	3:B:801:PLP:H5A2	2.31	0.45
1:B:267:SER:HA	1:B:280:GLY:HA2	1.98	0.45
1:B:304:ILE:HD11	5:B:881:HOH:O	2.17	0.45
1:B:78:MSE:HE3	1:B:314:ILE:HG22	1.94	0.45
1:B:33:LEU:HD13	1:B:160:VAL:HG11	1.99	0.44
1:A:220:LEU:HB3	1:A:255:ILE:HG13	2.01	0.43
1:B:426:LYS:HE3	4:B:803:GOL:H2	2.00	0.43
1:B:78:MSE:HE3	1:B:315:SER:HA	2.00	0.43
1:A:342:THR:HG22	1:A:407:ALA:HB3	2.01	0.42
1:B:273:GLY:N	5:B:972:HOH:O	2.50	0.42
1:B:240:TYR:OH	2:B:800:SO4:O4	2.38	0.42
1:B:33:LEU:HD13	1:B:160:VAL:CG1	2.49	0.41
1:A:422:LYS:HZ2	4:A:703:GOL:H12	1.77	0.41
1:B:331:MSE:HA	1:B:334:VAL:HG22	2.02	0.41
1:B:345:ILE:HG22	1:B:365:VAL:HG21	2.01	0.41
1:A:136:GLN:NE2	1:A:164:GLN:HE22	2.18	0.41
1:A:182:ARG:NH1	5:A:733:HOH:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:O	1:A:350:THR:HG23	2.20	0.40
1:A:135:LEU:HD22	1:A:263:MSE:SE	2.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/432 (95%)	403 (98%)	6 (2%)	1 (0%)	47	38
1	B	407/432 (94%)	402 (99%)	4 (1%)	1 (0%)	47	38
All	All	817/864 (95%)	805 (98%)	10 (1%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	ARG
1	A	278	ARG

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	338/347 (97%)	321 (95%)	17 (5%)	24	11
1	B	335/347 (96%)	315 (94%)	20 (6%)	19	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	673/694 (97%)	636 (94%)	37 (6%)	21 9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	46	ARG
1	A	103	LEU
1	A	109	LYS
1	A	220	LEU
1	A	229	LYS
1	A	304	ILE
1	A	306	THR
1	A	320	LEU
1	A	328	LEU
1	A	342	THR
1	A	356	VAL
1	A	373	SER
1	A	384	LYS
1	A	388	VAL
1	A	419	ARG
1	A	424	LEU
1	B	33	LEU
1	B	44	ARG
1	B	46	ARG
1	B	103	LEU
1	B	109	LYS
1	B	198	ARG
1	B	220	LEU
1	B	225	GLU
1	B	229	LYS
1	B	267	SER
1	B	279	LEU
1	B	298	LYS
1	B	304	ILE
1	B	320	LEU
1	B	328	LEU
1	B	373	SER
1	B	388	VAL
1	B	419	ARG
1	B	424	LEU
1	B	427	HIS

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	29	ASN
1	A	136	GLN
1	A	148	GLN
1	A	173	GLN
1	A	208	ASN
1	A	248	ASN
1	A	368	HIS
1	A	423	GLN
1	A	427	HIS
1	B	29	ASN
1	B	98	GLN
1	B	136	GLN
1	B	142	ASN
1	B	148	GLN
1	B	173	GLN
1	B	208	ASN
1	B	248	ASN
1	B	368	HIS
1	B	371	ASN
1	B	372	GLN

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](#)

8 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
4	GOL	A	702	-	5,5,5	0.37	0	5,5,5	0.47	0
2	SO4	B	800	-	4,4,4	0.51	0	6,6,6	0.59	0
3	PLP	B	801	-	15,15,16	1.48	1 (6%)	20,22,23	1.25	1 (5%)
4	GOL	B	803	-	5,5,5	0.30	0	5,5,5	0.36	0
4	GOL	A	703	-	5,5,5	0.50	0	5,5,5	0.71	0
3	PLP	A	701	-	15,15,16	1.61	2 (13%)	20,22,23	1.67	5 (25%)
4	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.54	0
2	SO4	A	700	-	4,4,4	0.30	0	6,6,6	0.28	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
4	GOL	A	702	-	-	2/4/4/4	-
3	PLP	B	801	-	-	3/6/6/8	0/1/1/1
4	GOL	B	803	-	-	0/4/4/4	-
4	GOL	A	703	-	-	4/4/4/4	-
3	PLP	A	701	-	-	2/6/6/8	0/1/1/1
4	GOL	B	802	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PLP	O3-C3	-4.65	1.26	1.37
3	B	801	PLP	O3-C3	-4.60	1.26	1.37
3	A	701	PLP	C3-C2	-2.06	1.38	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PLP	O4P-C5A-C5	3.10	115.26	109.35
3	A	701	PLP	C2A-C2-N1	2.82	123.19	117.67
3	A	701	PLP	C2A-C2-C3	-2.70	117.55	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PLP	O2P-P-O4P	-2.51	100.06	106.73
3	B	801	PLP	C2A-C2-N1	2.06	121.69	117.67
3	A	701	PLP	C4A-C4-C3	-2.04	117.04	120.50

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	PLP	C5A-O4P-P-O2P
4	A	703	GOL	O1-C1-C2-O2
4	A	703	GOL	O1-C1-C2-C3
4	B	802	GOL	C1-C2-C3-O3
4	A	702	GOL	C1-C2-C3-O3
4	A	703	GOL	C1-C2-C3-O3
4	A	703	GOL	O2-C2-C3-O3
3	B	801	PLP	C5A-O4P-P-O1P
4	B	802	GOL	O2-C2-C3-O3
3	B	801	PLP	C5A-O4P-P-O3P
3	A	701	PLP	C5A-O4P-P-O3P
4	A	702	GOL	O2-C2-C3-O3
3	A	701	PLP	C4-C5-C5A-O4P
4	B	802	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	GOL	3	0
2	B	800	SO4	1	0
3	B	801	PLP	3	0
4	B	803	GOL	1	0
4	A	703	GOL	7	0
3	A	701	PLP	1	0
4	B	802	GOL	1	0

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

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	403/432 (93%)	-0.19	11 (2%) 54 63	11, 18, 33, 42	0
1	B	400/432 (92%)	-0.12	9 (2%) 60 69	11, 19, 32, 41	0
All	All	803/864 (92%)	-0.16	20 (2%) 57 66	11, 19, 33, 42	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	4.4
1	A	89	GLU	4.3
1	A	430	HIS	3.3
1	B	371	ASN	3.2
1	B	88	ILE	3.1
1	A	94	TYR	3.1
1	A	90	GLY	3.1
1	B	89	GLU	3.0
1	A	95	GLY	3.0
1	B	51	LEU	2.9
1	B	271	TYR	2.6
1	A	44	ARG	2.6
1	A	92	SER	2.5
1	B	186	GLU	2.4
1	B	35	ALA	2.4
1	B	427	HIS	2.4
1	B	171	ASP	2.3
1	A	171	ASP	2.2
1	A	371	ASN	2.1
1	A	271	TYR	2.1

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
4	GOL	B	803	6/6	0.49	0.27	68,70,71,72	0
4	GOL	A	702	6/6	0.79	0.18	45,47,47,48	0
4	GOL	A	703	6/6	0.83	0.16	46,47,47,47	0
4	GOL	B	802	6/6	0.85	0.11	45,47,47,47	0
3	PLP	B	801	15/16	0.89	0.19	36,47,50,50	0
3	PLP	A	701	15/16	0.91	0.23	26,48,50,50	0
2	SO4	B	800	5/5	0.98	0.12	29,33,36,36	0
2	SO4	A	700	5/5	0.98	0.07	41,42,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.