



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 2Z1Z / pdb_00002z1z
Title : Crystal structure of LL-Diaminopimelate Aminotransferase from Arabidopsis thaliana complexed with L-malate ion
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 : 2007-05-16
Resolution : 2.40 Å(reported)

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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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

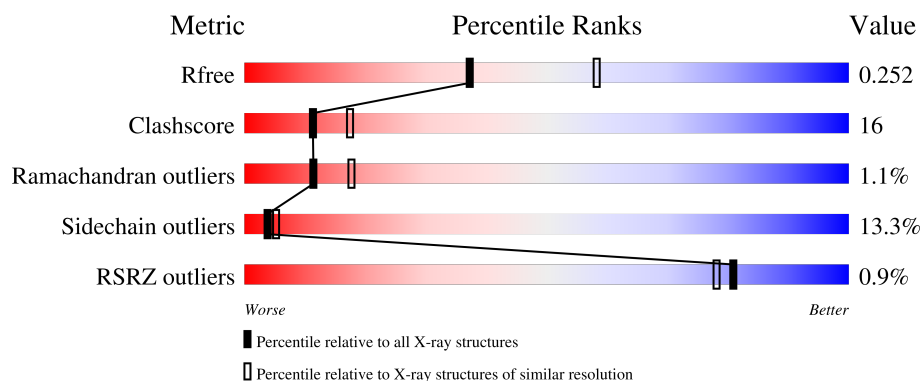
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	
1	B	432	

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
2	MLT	A	433	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6550 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.

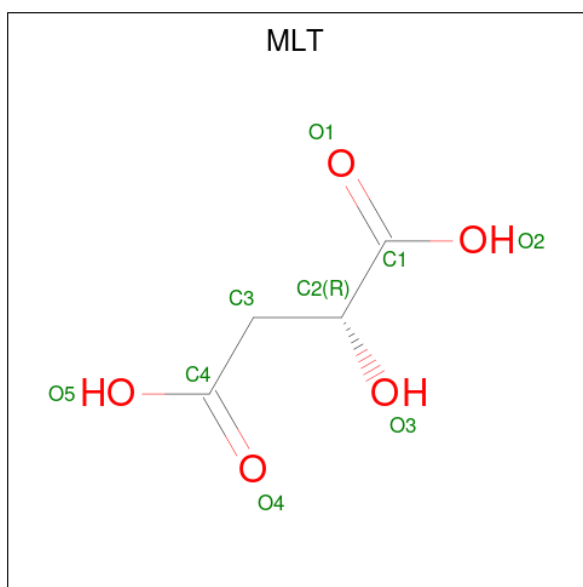
- Molecule 1 is a protein called LL-diaminopimelate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3144	2003	524	601	16			
1	B	408	Total	C	N	O	S	0	0	0
			3144	2003	524	601	16			

There are 12 discrepancies between the modelled and reference sequences:

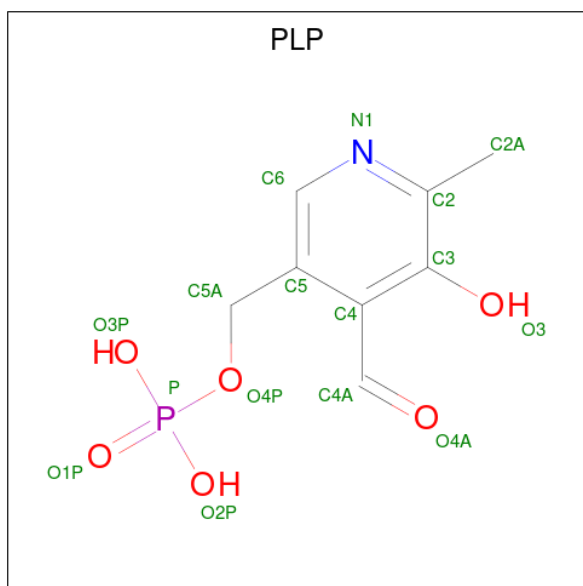
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP O81885
A	428	HIS	-	expression tag	UNP O81885
A	429	HIS	-	expression tag	UNP O81885
A	430	HIS	-	expression tag	UNP O81885
A	431	HIS	-	expression tag	UNP O81885
A	432	HIS	-	expression tag	UNP O81885
B	427	HIS	-	expression tag	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 D-MALATE (CCD ID: MLT) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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		

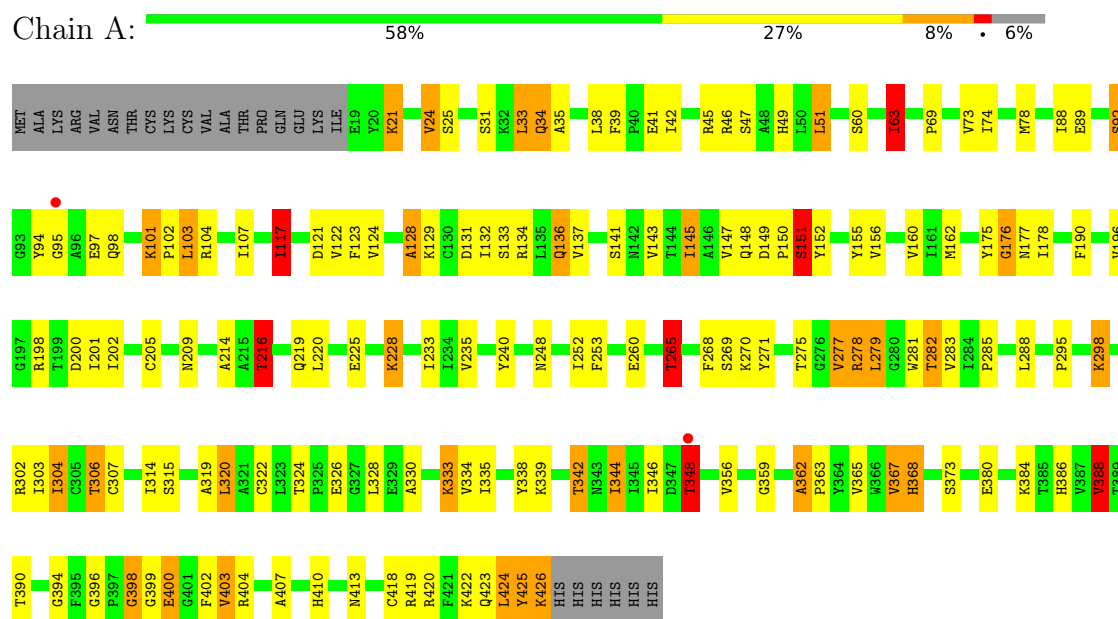
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	0	0
4	B	118	Total 118	O 118	0	0

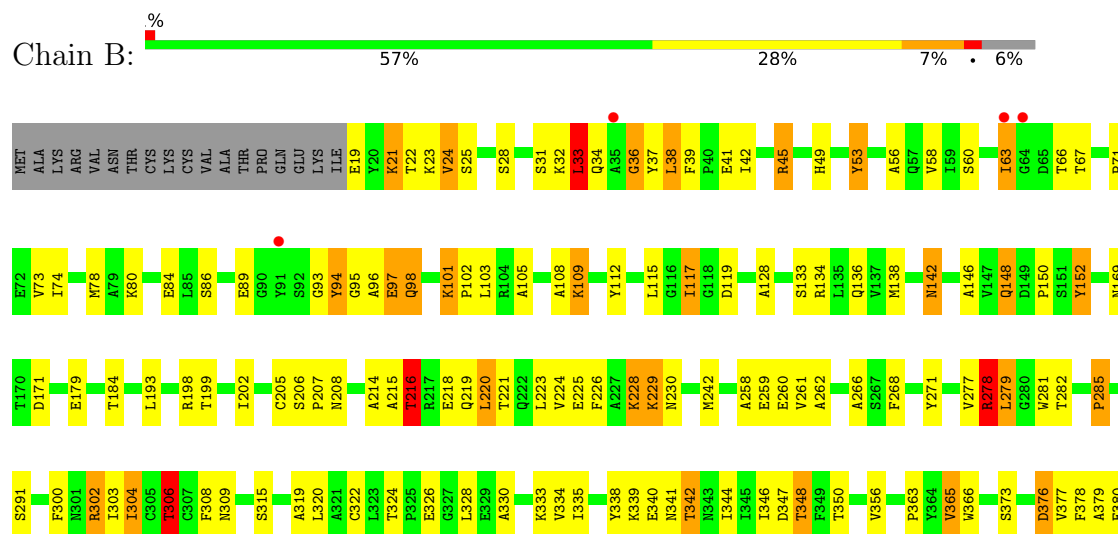
3 Residue-property plots

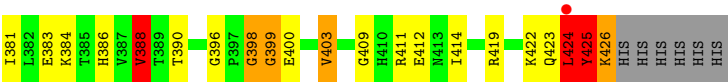
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	102.59Å 102.59Å 172.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.40) 90.1 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.251 0.179 , 0.252	Depositor DCC
R_{free} test set	1916 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, MLT

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	1.57	26/3219 (0.8%)	1.47	33/4362 (0.8%)
1	B	1.60	25/3219 (0.8%)	1.52	33/4362 (0.8%)
All	All	1.58	51/6438 (0.8%)	1.49	66/8724 (0.8%)

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	3
1	B	0	4
All	All	0	7

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	302	ARG	C-O	-8.37	1.14	1.24
1	A	248	ASN	N-CA	8.21	1.52	1.45
1	B	184	THR	CA-CB	8.08	1.63	1.53
1	A	156	VAL	CA-CB	7.92	1.63	1.54
1	B	261	VAL	CA-CB	7.66	1.64	1.54
1	B	66	THR	CA-C	7.51	1.62	1.52
1	B	388	VAL	CA-CB	7.31	1.63	1.54
1	B	309	ASN	N-CA	7.00	1.54	1.46
1	A	235	VAL	C-O	-6.97	1.16	1.24
1	B	108	ALA	CA-C	6.94	1.61	1.52
1	A	92	SER	CA-C	6.71	1.58	1.52
1	A	136	GLN	C-O	-6.44	1.16	1.24
1	A	88	ILE	CA-CB	6.12	1.61	1.54
1	B	202	ILE	CA-CB	6.05	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	VAL	C-O	6.04	1.31	1.23
1	A	403	VAL	CA-CB	6.02	1.63	1.54
1	B	63	ILE	CA-CB	5.98	1.62	1.54
1	A	176	GLY	C-O	5.95	1.30	1.23
1	A	42	ILE	CA-CB	5.89	1.61	1.54
1	A	143	VAL	CA-CB	5.88	1.62	1.54
1	B	22	THR	CA-CB	5.86	1.62	1.53
1	A	314	ILE	C-O	-5.81	1.17	1.24
1	B	414	ILE	CA-CB	5.73	1.61	1.54
1	A	117	ILE	CG1-CD1	-5.72	1.29	1.51
1	A	285	PRO	N-CA	-5.66	1.40	1.46
1	B	303	ILE	CA-CB	5.64	1.61	1.54
1	B	224	VAL	CA-CB	5.54	1.61	1.54
1	B	63	ILE	C-O	5.47	1.30	1.24
1	A	252	ILE	CA-CB	5.46	1.62	1.54
1	B	425	TYR	CA-C	5.43	1.59	1.52
1	A	122	VAL	CA-CB	5.37	1.60	1.54
1	B	376	ASP	CA-C	-5.30	1.45	1.52
1	B	379	ALA	CA-CB	5.30	1.61	1.53
1	B	258	ALA	CA-CB	-5.29	1.45	1.53
1	B	24	VAL	CA-CB	5.26	1.61	1.54
1	B	226	PHE	CA-C	5.25	1.59	1.52
1	A	214	ALA	CA-CB	-5.25	1.45	1.53
1	A	330	ALA	CA-CB	5.24	1.61	1.53
1	B	306	THR	CA-CB	5.21	1.61	1.54
1	A	107	ILE	CA-CB	5.19	1.60	1.54
1	A	253	PHE	CA-C	5.18	1.60	1.52
1	A	367	VAL	CA-CB	5.11	1.60	1.54
1	A	73	VAL	CA-CB	5.11	1.61	1.54
1	B	214	ALA	CA-CB	-5.10	1.45	1.53
1	B	228	LYS	N-CA	5.10	1.52	1.46
1	A	202	ILE	CA-CB	5.08	1.60	1.54
1	A	344	ILE	CA-CB	5.06	1.60	1.54
1	B	73	VAL	CA-CB	5.06	1.61	1.54
1	B	319	ALA	CA-CB	-5.06	1.45	1.53
1	A	265	THR	CA-CB	5.05	1.62	1.53
1	A	128	ALA	CA-CB	5.04	1.61	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	TYR	N-CA-C	9.94	123.36	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	GLY	N-CA-C	9.78	131.60	115.66
1	B	365	VAL	CB-CA-C	8.91	123.54	110.98
1	A	190	PHE	CA-C-N	-8.82	111.30	120.03
1	A	190	PHE	C-N-CA	-8.82	111.30	120.03
1	B	398	GLY	N-CA-C	8.21	128.78	115.73
1	B	96	ALA	N-CA-C	-7.97	101.59	110.91
1	B	390	THR	CA-C-N	-7.36	112.40	119.76
1	B	390	THR	C-N-CA	-7.36	112.40	119.76
1	A	35	ALA	N-CA-C	-7.20	98.81	108.74
1	A	362	ALA	CA-C-N	7.01	128.60	119.84
1	A	362	ALA	C-N-CA	7.01	128.60	119.84
1	B	108	ALA	CA-C-N	7.00	129.89	120.65
1	B	108	ALA	C-N-CA	7.00	129.89	120.65
1	B	142	ASN	N-CA-C	6.96	121.47	112.92
1	A	41	GLU	N-CA-C	6.95	119.45	111.11
1	A	388	VAL	CB-CA-C	6.65	118.86	111.08
1	B	36	GLY	N-CA-C	-6.59	94.19	113.30
1	B	148	GLN	N-CA-C	-6.45	101.84	110.55
1	B	193	LEU	N-CA-C	6.40	120.18	112.38
1	A	388	VAL	N-CA-C	6.38	117.99	108.54
1	B	414	ILE	N-CA-C	-6.29	104.72	110.82
1	A	271	TYR	CA-CB-CG	6.22	125.09	113.90
1	A	314	ILE	N-CA-C	-6.18	104.82	110.82
1	A	390	THR	CA-C-N	-6.10	113.40	119.99
1	A	390	THR	C-N-CA	-6.10	113.40	119.99
1	B	39	PHE	CA-C-N	6.08	126.25	119.32
1	B	39	PHE	C-N-CA	6.08	126.25	119.32
1	B	94	TYR	N-CA-C	6.05	118.52	110.53
1	B	285	PRO	CA-C-N	6.00	128.32	120.28
1	B	285	PRO	C-N-CA	6.00	128.32	120.28
1	A	39	PHE	CA-C-N	-5.92	113.09	119.24
1	A	39	PHE	C-N-CA	-5.92	113.09	119.24
1	A	324	THR	N-CA-C	-5.91	101.39	108.25
1	B	53	TYR	CA-C-N	5.89	125.58	119.05
1	B	53	TYR	C-N-CA	5.89	125.58	119.05
1	A	400	GLU	CA-C-N	5.80	132.15	121.70
1	A	400	GLU	C-N-CA	5.80	132.15	121.70
1	B	399	GLY	CA-C-N	5.71	128.97	120.87
1	B	399	GLY	C-N-CA	5.71	128.97	120.87
1	B	36	GLY	CA-C-N	5.68	132.38	121.54
1	B	36	GLY	C-N-CA	5.68	132.38	121.54
1	B	373	SER	N-CA-C	-5.62	102.17	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	GLU	N-CA-CB	-5.60	101.77	110.29
1	B	152	TYR	CA-C-N	5.55	125.65	119.32
1	B	152	TYR	C-N-CA	5.55	125.65	119.32
1	A	63	ILE	CB-CA-C	5.53	118.33	111.15
1	A	24	VAL	CB-CA-C	5.52	117.76	110.91
1	B	216	THR	N-CA-CB	-5.51	102.56	110.44
1	A	348	THR	N-CA-CB	5.42	117.87	110.01
1	B	324	THR	N-CA-C	-5.39	102.00	108.25
1	A	216	THR	OG1-CB-CG2	5.38	120.06	109.30
1	B	425	TYR	N-CA-C	5.36	118.47	109.95
1	A	196	VAL	CA-C-N	5.34	125.76	120.31
1	A	196	VAL	C-N-CA	5.34	125.76	120.31
1	A	216	THR	N-CA-CB	-5.34	101.91	110.46
1	A	151	SER	N-CA-C	5.30	116.85	108.96
1	B	388	VAL	CB-CA-C	5.26	117.99	111.15
1	A	403	VAL	CB-CA-C	5.25	118.59	110.50
1	A	277	VAL	N-CA-C	5.22	117.11	111.58
1	A	152	TYR	CA-C-N	5.17	125.25	119.87
1	A	152	TYR	C-N-CA	5.17	125.25	119.87
1	A	117	ILE	N-CA-C	5.12	115.95	108.58
1	B	262	ALA	N-CA-C	5.09	117.55	109.50
1	B	223	LEU	N-CA-C	5.04	116.47	111.07
1	B	424	LEU	N-CA-C	5.02	117.40	111.33

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	GLY	Peptide
1	A	400	GLU	Peptide
1	A	425	TYR	Peptide
1	B	398	GLY	Peptide
1	B	425	TYR	Peptide
1	B	94	TYR	Peptide
1	B	95	GLY	Peptide

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	3144	0	3064	101	0
1	B	3144	0	3061	106	0
2	A	9	0	4	0	0
3	A	15	0	6	2	0
3	B	15	0	6	2	0
4	A	105	0	0	6	0
4	B	118	0	0	8	0
All	All	6550	0	6141	202	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 16.

All (202) 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:78:MET:HE1	1:A:277:VAL:HG11	1.30	1.13
1:B:105:ALA:O	1:B:109:LYS:HE3	1.45	1.12
1:B:229:LYS:HD2	4:B:608:HOH:O	1.49	1.11
1:A:101:LYS:HG3	1:A:104:ARG:NH2	1.67	1.07
1:B:302:ARG:HH11	1:B:306:THR:HG21	1.13	1.07
1:B:78:MET:HE1	1:B:277:VAL:HG11	1.07	1.06
1:A:333:LYS:HD2	4:A:590:HOH:O	1.54	1.06
1:A:34:GLN:HE21	1:A:34:GLN:HA	1.20	1.06
1:B:98:GLN:HB2	4:B:507:HOH:O	1.53	1.05
1:B:78:MET:HE1	1:B:277:VAL:CG1	1.88	1.03
1:A:78:MET:HE1	1:A:277:VAL:CG1	1.89	1.01
1:B:49:HIS:NE2	1:B:386:HIS:HD2	1.56	1.01
1:A:216:THR:HG22	1:A:219:GLN:H	1.26	1.01
1:B:101:LYS:HD2	1:B:101:LYS:H	1.26	0.97
1:A:101:LYS:HG3	1:A:104:ARG:HH22	1.31	0.95
1:B:74:ILE:HD12	1:B:322:CYS:SG	2.07	0.94
1:B:302:ARG:NH1	1:B:306:THR:HG21	1.84	0.92
1:B:216:THR:HG21	4:B:515:HOH:O	1.74	0.86
1:A:426:LYS:HE2	1:A:426:LYS:HA	1.61	0.82
1:B:49:HIS:NE2	1:B:386:HIS:CD2	2.46	0.81
1:A:34:GLN:HA	1:A:34:GLN:NE2	1.94	0.81
1:A:302:ARG:HH11	1:A:306:THR:HG22	1.46	0.80
1:B:101:LYS:H	1:B:101:LYS:CD	1.95	0.80
1:B:105:ALA:O	1:B:109:LYS:CE	2.28	0.79
1:A:49:HIS:NE2	1:A:386:HIS:HD2	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ARG:O	1:B:306:THR:HG23	1.85	0.77
1:A:148:GLN:NE2	1:A:205:CYS:H	1.84	0.75
1:A:346:ILE:HD11	1:A:359:GLY:HA3	1.66	0.75
1:A:134:ARG:HD3	1:A:304:ILE:HD11	1.68	0.75
1:A:101:LYS:CG	1:A:104:ARG:NH2	2.47	0.75
1:A:348:THR:HG21	1:A:418:CYS:SG	2.26	0.75
1:B:338:TYR:O	1:B:342:THR:HG22	1.86	0.74
1:A:134:ARG:HD3	1:A:304:ILE:CD1	2.17	0.74
1:B:344:ILE:O	1:B:348:THR:HG23	1.88	0.74
1:A:265:THR:HG23	1:A:282:THR:HG22	1.70	0.73
1:B:228:LYS:NZ	1:B:260:GLU:OE1	2.24	0.70
1:A:148:GLN:HE22	1:A:205:CYS:H	1.40	0.70
1:B:148:GLN:HE22	1:B:205:CYS:H	1.40	0.69
1:B:221:THR:O	1:B:225:GLU:HG3	1.91	0.69
1:B:383:GLU:HG3	1:B:384:LYS:HG3	1.73	0.69
1:A:380:GLU:HG2	1:A:384:LYS:HD2	1.74	0.69
1:B:229:LYS:CD	4:B:608:HOH:O	2.22	0.68
1:B:148:GLN:NE2	1:B:205:CYS:H	1.91	0.68
1:A:129:LYS:HE2	1:B:308:PHE:O	1.94	0.68
1:A:342:THR:HG21	1:A:363:PRO:HA	1.75	0.68
1:A:34:GLN:HE21	1:A:34:GLN:CA	1.98	0.67
1:B:216:THR:HG22	1:B:219:GLN:H	1.61	0.66
1:A:302:ARG:NH1	1:A:306:THR:CG2	2.59	0.66
1:A:302:ARG:HH11	1:A:306:THR:CG2	2.09	0.65
1:A:302:ARG:NH1	1:A:306:THR:HG22	2.13	0.64
1:B:208:ASN:ND2	4:B:563:HOH:O	2.30	0.64
1:A:384:LYS:HD3	1:A:424:LEU:HD21	1.80	0.64
1:B:101:LYS:HD2	1:B:101:LYS:N	2.08	0.64
1:B:33:LEU:O	1:B:34:GLN:CB	2.46	0.63
1:A:101:LYS:CD	1:A:104:ARG:HH21	2.11	0.63
1:A:33:LEU:HD13	1:A:160:VAL:HG11	1.80	0.62
1:A:33:LEU:HD13	1:A:160:VAL:CG1	2.30	0.61
1:B:282:THR:HG22	4:B:525:HOH:O	1.99	0.61
1:B:277:VAL:C	1:B:278:ARG:HG2	2.26	0.60
1:A:78:MET:CE	1:A:315:SER:HA	2.32	0.59
1:A:228:LYS:NZ	1:A:260:GLU:OE1	2.35	0.59
1:A:78:MET:HE3	1:A:315:SER:HA	1.84	0.59
1:A:233:ILE:HG12	1:A:288:LEU:HD11	1.85	0.58
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.69	0.58
1:A:117:ILE:HG12	1:A:283:VAL:HG11	1.85	0.58
1:A:63:ILE:HG23	4:A:517:HOH:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:THR:OG1	1:B:93:GLY:HA2	2.05	0.56
1:A:368:HIS:CD2	4:A:568:HOH:O	2.59	0.55
1:B:282:THR:HG21	1:B:300:PHE:CE2	2.42	0.55
1:A:410:HIS:HB2	1:A:413:ASN:HD22	1.71	0.55
1:A:320:LEU:HD22	4:A:548:HOH:O	2.07	0.55
1:B:136:GLN:HA	1:B:136:GLN:HE21	1.72	0.54
1:A:368:HIS:HD2	4:A:568:HOH:O	1.91	0.54
1:A:338:TYR:O	1:A:342:THR:HG23	2.08	0.53
1:B:109:LYS:NZ	1:B:119:ASP:OD1	2.37	0.53
1:B:215:ALA:CB	1:B:220:LEU:HD13	2.39	0.53
1:B:112:TYR:HB3	1:B:117:ILE:HD13	1.90	0.53
1:B:424:LEU:HD13	1:B:425:TYR:CZ	2.44	0.53
1:B:33:LEU:O	1:B:34:GLN:CG	2.57	0.53
1:A:101:LYS:N	1:A:102:PRO:CD	2.72	0.52
1:A:302:ARG:NH1	1:A:306:THR:HG21	2.24	0.52
1:B:38:LEU:HD11	1:B:42:ILE:HD11	1.92	0.52
1:B:142:ASN:CG	1:B:142:ASN:O	2.53	0.52
1:B:134:ARG:HD3	1:B:304:ILE:CD1	2.39	0.52
1:B:74:ILE:CD1	1:B:322:CYS:SG	2.91	0.52
1:A:47:SER:O	1:A:51:LEU:HD12	2.10	0.51
1:B:216:THR:CG2	1:B:218:GLU:H	2.22	0.51
1:B:19:GLU:N	4:B:579:HOH:O	2.43	0.51
1:A:268:PHE:CE2	1:A:319:ALA:HB1	2.46	0.51
1:A:295:PRO:HG2	1:A:298:LYS:HD2	1.93	0.51
1:B:338:TYR:O	1:B:342:THR:CG2	2.57	0.51
1:A:101:LYS:CG	1:A:104:ARG:HH21	2.24	0.50
1:A:348:THR:HB	1:A:422:LYS:HE2	1.93	0.50
1:A:342:THR:HG22	1:A:407:ALA:CB	2.41	0.50
1:B:78:MET:CE	1:B:315:SER:HA	2.42	0.50
1:A:38:LEU:HD13	1:A:394:GLY:HA3	1.93	0.50
1:B:396:GLY:O	1:B:399:GLY:HA3	2.12	0.49
1:B:339:LYS:HA	1:B:342:THR:HG23	1.95	0.49
1:B:115:LEU:O	1:B:117:ILE:HD12	2.12	0.49
1:B:266:ALA:HB3	1:B:281:TRP:CE2	2.47	0.49
1:A:338:TYR:O	1:A:342:THR:CG2	2.61	0.49
1:B:33:LEU:C	1:B:34:GLN:HG3	2.38	0.49
1:B:105:ALA:C	1:B:109:LYS:HE3	2.30	0.49
1:B:146:ALA:HA	1:B:179:GLU:O	2.13	0.49
1:B:216:THR:HG22	1:B:218:GLU:H	1.76	0.49
1:A:74:ILE:HD12	1:A:322:CYS:SG	2.53	0.49
1:B:342:THR:HG21	1:B:363:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ARG:HG3	1:B:230:ASN:HB3	1.95	0.48
1:A:265:THR:HG23	1:A:282:THR:CG2	2.42	0.48
1:B:424:LEU:HD13	1:B:425:TYR:CE1	2.49	0.48
1:A:240:TYR:HE2	3:A:500:PLP:O3	1.96	0.48
1:B:33:LEU:O	1:B:34:GLN:HB3	2.13	0.48
1:A:339:LYS:HA	1:A:342:THR:HG23	1.95	0.48
1:B:344:ILE:O	1:B:348:THR:CG2	2.61	0.48
1:B:426:LYS:HB2	4:B:609:HOH:O	2.13	0.48
1:A:216:THR:CG2	1:A:219:GLN:H	2.13	0.47
1:B:268:PHE:CD2	1:B:279:LEU:HD22	2.49	0.47
1:A:176:GLY:O	1:A:177:ASN:HB3	2.14	0.47
1:B:150:PRO:HG3	1:B:366:TRP:CZ2	2.50	0.47
1:A:69:PRO:HB3	1:B:86:SER:C	2.39	0.47
1:A:21:LYS:NZ	1:B:291:SER:O	2.47	0.47
1:A:34:GLN:NE2	1:A:34:GLN:CA	2.64	0.47
1:A:60:SER:HA	1:A:388:VAL:HG13	1.96	0.47
1:A:198:ARG:NH1	1:A:200:ASP:OD1	2.40	0.47
1:A:335:ILE:O	1:A:339:LYS:HG3	2.15	0.47
1:B:377:VAL:HG12	1:B:381:ILE:HD12	1.95	0.47
1:A:117:ILE:HG23	1:A:121:ASP:HB2	1.97	0.47
1:A:38:LEU:HD13	1:A:394:GLY:CA	2.45	0.46
1:B:128:ALA:HB3	3:B:501:PLP:H5A1	1.97	0.46
1:B:348:THR:HB	1:B:422:LYS:HE3	1.98	0.46
1:A:367:VAL:O	1:A:402:PHE:HA	2.14	0.46
1:B:216:THR:HG22	1:B:218:GLU:N	2.30	0.46
1:B:206:SER:HA	1:B:207:PRO:C	2.40	0.46
1:B:33:LEU:O	1:B:34:GLN:HG3	2.16	0.46
1:A:148:GLN:O	1:A:151:SER:HB2	2.16	0.46
1:A:342:THR:HG22	1:A:407:ALA:HB3	1.97	0.46
1:A:131:ASP:CG	1:A:282:THR:CG2	2.89	0.45
1:A:123:PHE:O	1:A:281:TRP:HA	2.16	0.45
1:A:270:LYS:HB2	4:A:511:HOH:O	2.16	0.45
1:B:67:THR:HG21	1:B:409:GLY:HA2	1.99	0.45
1:A:141:SER:HB2	1:A:162:MET:O	2.16	0.45
1:A:128:ALA:O	1:A:132:ILE:HG13	2.17	0.45
1:B:97:GLU:H	1:B:97:GLU:HG2	1.17	0.45
1:B:215:ALA:HB1	1:B:220:LEU:HD13	1.99	0.45
1:B:346:ILE:O	1:B:347:ASP:C	2.60	0.45
1:B:78:MET:HE3	1:B:315:SER:HA	1.97	0.45
1:B:282:THR:HG21	1:B:300:PHE:CZ	2.52	0.45
1:A:175:TYR:HB2	1:A:178:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LYS:HB2	1:A:228:LYS:HE2	1.72	0.44
1:B:60:SER:HA	1:B:388:VAL:HG13	1.99	0.44
1:A:424:LEU:HD13	1:A:425:TYR:CZ	2.52	0.44
1:B:101:LYS:HB2	1:B:102:PRO:HD3	1.99	0.44
1:B:49:HIS:CE1	1:B:386:HIS:CD2	3.05	0.44
1:B:152:TYR:CG	3:B:501:PLP:H2A2	2.53	0.44
1:A:132:ILE:HD13	1:A:155:TYR:CE1	2.53	0.43
1:B:71:PRO:CB	1:B:330:ALA:HB1	2.47	0.43
1:A:124:VAL:HG13	1:A:279:LEU:HD21	1.99	0.43
1:B:377:VAL:CG1	1:B:403:VAL:HG11	2.48	0.43
1:A:362:ALA:HB1	1:A:363:PRO:HD2	2.01	0.43
1:B:346:ILE:HG21	1:B:346:ILE:HD13	1.79	0.43
1:A:269:SER:HB3	1:A:275:THR:HG22	2.00	0.43
1:B:53:TYR:HB3	1:B:56:ALA:HB2	2.01	0.43
1:B:58:VAL:HA	1:B:386:HIS:O	2.19	0.43
1:A:270:LYS:HA	1:A:270:LYS:HD3	1.72	0.43
1:B:32:LYS:O	1:B:33:LEU:O	2.37	0.43
1:B:38:LEU:O	1:B:42:ILE:HG13	2.19	0.42
1:B:376:ASP:O	1:B:380:GLU:HB2	2.19	0.42
1:B:49:HIS:CE1	1:B:386:HIS:HD2	2.31	0.42
1:B:134:ARG:HD3	1:B:304:ILE:HD13	2.02	0.42
1:B:378:PHE:CD1	1:B:378:PHE:C	2.97	0.42
1:B:411:ARG:HG2	1:B:411:ARG:HH11	1.84	0.42
1:A:344:ILE:O	1:A:348:THR:HG22	2.19	0.42
1:B:340:GLU:O	1:B:341:ASN:C	2.62	0.42
1:A:141:SER:CB	1:A:162:MET:O	2.68	0.42
1:A:131:ASP:CG	1:A:282:THR:HG22	2.45	0.42
1:A:304:ILE:HD13	1:A:304:ILE:HA	1.80	0.42
1:B:21:LYS:CB	1:B:21:LYS:NZ	2.83	0.42
1:B:205:CYS:O	1:B:208:ASN:HB2	2.20	0.42
1:A:103:LEU:HD13	1:A:124:VAL:HG21	2.02	0.41
1:A:145:ILE:HD12	1:A:147:VAL:HG13	2.02	0.41
1:B:377:VAL:CG1	1:B:381:ILE:HD12	2.50	0.41
1:A:149:ASP:HA	1:A:150:PRO:HA	1.89	0.41
1:B:45:ARG:HH11	1:B:45:ARG:HB3	1.86	0.41
1:B:242:MET:HB3	1:B:335:ILE:HD13	2.02	0.41
1:A:117:ILE:HG12	1:A:283:VAL:CG1	2.50	0.41
1:A:132:ILE:HD13	1:A:155:TYR:CD1	2.55	0.41
1:A:209:ASN:OD1	1:A:404:ARG:NH1	2.50	0.41
1:A:270:LYS:NZ	3:A:500:PLP:C4A	2.84	0.41
1:A:89:GLU:H	1:A:89:GLU:CD	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:TYR:CB	1:B:56:ALA:HB2	2.51	0.40
1:A:134:ARG:CD	1:A:304:ILE:HD11	2.44	0.40
1:B:138:MET:HE2	1:B:138:MET:HB3	1.98	0.40
1:A:307:CYS:HB3	1:B:133:SER:OG	2.22	0.40
1:B:80:LYS:O	1:B:84:GLU:HG3	2.22	0.40
1:A:133:SER:O	1:A:137:VAL:HG23	2.20	0.40
1:A:145:ILE:HG22	1:A:201:ILE:HB	2.02	0.40
1:B:169:ASN:OD1	1:B:171:ASP:HB2	2.21	0.40
1:A:38:LEU:CD1	1:A:394:GLY:HA3	2.51	0.40
1:A:396:GLY:O	1:A:399:GLY:HA3	2.21	0.40
1:B:198:ARG:HG2	1:B:199:THR:N	2.36	0.40
1:B:259:GLU:HA	1:B:285:PRO:HG3	2.03	0.40
1:B:302:ARG:HD2	1:B:306:THR:CG2	2.51	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	406/432 (94%)	391 (96%)	13 (3%)	2 (0%)	24	37
1	B	406/432 (94%)	375 (92%)	24 (6%)	7 (2%)	7	10
All	All	812/864 (94%)	766 (94%)	37 (5%)	9 (1%)	11	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	TYR
1	A	95	GLY
1	B	33	LEU
1	A	278	ARG
1	B	36	GLY

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Mol	Chain	Res	Type
1	B	278	ARG
1	B	89	GLU
1	B	423	GLN
1	B	63	ILE

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	334/356 (94%)	286 (86%)	48 (14%)	3	4
1	B	334/356 (94%)	293 (88%)	41 (12%)	4	6
All	All	668/712 (94%)	579 (87%)	89 (13%)	4	5

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	24	VAL
1	A	25	SER
1	A	31	SER
1	A	33	LEU
1	A	34	GLN
1	A	45	ARG
1	A	46	ARG
1	A	51	LEU
1	A	63	ILE
1	A	92	SER
1	A	97	GLU
1	A	98	GLN
1	A	101	LYS
1	A	103	LEU
1	A	117	ILE
1	A	145	ILE
1	A	151	SER
1	A	216	THR

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	225	GLU
1	A	228	LYS
1	A	265	THR
1	A	278	ARG
1	A	279	LEU
1	A	282	THR
1	A	298	LYS
1	A	303	ILE
1	A	304	ILE
1	A	306	THR
1	A	320	LEU
1	A	326	GLU
1	A	328	LEU
1	A	333	LYS
1	A	334	VAL
1	A	342	THR
1	A	348	THR
1	A	356	VAL
1	A	365	VAL
1	A	368	HIS
1	A	373	SER
1	A	388	VAL
1	A	403	VAL
1	A	419	ARG
1	A	420	ARG
1	A	423	GLN
1	A	424	LEU
1	A	426	LYS
1	B	21	LYS
1	B	23	LYS
1	B	24	VAL
1	B	25	SER
1	B	28	SER
1	B	31	SER
1	B	33	LEU
1	B	38	LEU
1	B	41	GLU
1	B	45	ARG
1	B	97	GLU
1	B	98	GLN
1	B	101	LYS

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Mol	Chain	Res	Type
1	B	103	LEU
1	B	109	LYS
1	B	117	ILE
1	B	216	THR
1	B	220	LEU
1	B	229	LYS
1	B	271	TYR
1	B	278	ARG
1	B	279	LEU
1	B	304	ILE
1	B	306	THR
1	B	320	LEU
1	B	326	GLU
1	B	328	LEU
1	B	333	LYS
1	B	334	VAL
1	B	342	THR
1	B	348	THR
1	B	350	THR
1	B	356	VAL
1	B	365	VAL
1	B	388	VAL
1	B	400	GLU
1	B	403	VAL
1	B	412	GLU
1	B	419	ARG
1	B	424	LEU
1	B	426	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	34	GLN
1	A	83	HIS
1	A	98	GLN
1	A	136	GLN
1	A	148	GLN
1	A	301	ASN
1	A	371	ASN
1	A	386	HIS
1	A	413	ASN

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Mol	Chain	Res	Type
1	B	29	ASN
1	B	98	GLN
1	B	136	GLN
1	B	148	GLN
1	B	167	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
1	B	386	HIS
1	B	423	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	MLT	A	433	-	8,8,8	1.43	1 (12%)	10,10,10	1.85	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	B	501	1	15,15,16	1.34	1 (6%)	21,22,23	2.05	10 (47%)
3	PLP	A	500	-	15,15,16	1.92	5 (33%)	21,22,23	2.83	7 (33%)

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	MLT	A	433	-	1/1/3/3	2/8/8/8	-
3	PLP	B	501	1	-	5/6/6/8	0/1/1/1
3	PLP	A	500	-	-	3/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	O3-C3	-4.63	1.26	1.36
3	B	501	PLP	O3-C3	-4.00	1.27	1.36
3	A	500	PLP	C2-N1	2.71	1.38	1.33
3	A	500	PLP	C6-C5	2.70	1.43	1.37
3	A	500	PLP	C3-C2	2.30	1.43	1.41
3	A	500	PLP	P-O1P	2.08	1.56	1.50
2	A	433	MLT	O2-C1	-2.01	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLP	C5A-C5-C6	6.84	130.50	119.36
3	A	500	PLP	C5A-C5-C4	-6.35	110.10	122.64
3	A	500	PLP	O4P-C5A-C5	4.46	117.72	109.36
3	A	500	PLP	C4A-C4-C5	-4.29	116.52	120.94
3	A	500	PLP	O3-C3-C2	3.41	124.66	117.58
3	B	501	PLP	O4P-P-O1P	-3.41	97.22	106.44
3	B	501	PLP	C2A-C2-C3	3.37	124.74	120.80
2	A	433	MLT	O2-C1-O1	-3.01	117.26	124.08
2	A	433	MLT	O2-C1-C2	2.97	119.01	112.74
3	A	500	PLP	O4P-P-O1P	-2.93	98.51	106.44
3	B	501	PLP	C4A-C4-C5	-2.75	118.11	120.94
3	B	501	PLP	C5-C6-N1	-2.71	119.42	123.83
3	B	501	PLP	C6-N1-C2	2.69	124.07	119.20
3	B	501	PLP	C6-C5-C4	2.58	120.21	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	PLP	O2P-P-O4P	2.57	113.37	106.67
3	B	501	PLP	C5A-C5-C4	-2.51	117.69	122.64
3	B	501	PLP	O3-C3-C2	2.28	122.31	117.58
3	B	501	PLP	C3-C2-N1	-2.20	118.18	120.96
3	A	500	PLP	C5-C6-N1	-2.08	120.44	123.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	433	MLT	C2

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	433	MLT	C1-C2-C3-C4
2	A	433	MLT	O3-C2-C3-C4
3	A	500	PLP	C5A-O4P-P-O1P
3	A	500	PLP	C5A-O4P-P-O2P
3	A	500	PLP	C5A-O4P-P-O3P
3	B	501	PLP	C5A-O4P-P-O1P
3	B	501	PLP	C5A-O4P-P-O2P
3	B	501	PLP	C5A-O4P-P-O3P
3	B	501	PLP	C4-C5-C5A-O4P
3	B	501	PLP	C6-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	PLP	2	0
3	A	500	PLP	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	408/432 (94%)	-0.47	2 (0%) 87 85	19, 34, 51, 63	0
1	B	408/432 (94%)	-0.35	5 (1%) 76 73	21, 35, 60, 72	0
All	All	816/864 (94%)	-0.41	7 (0%) 81 78	19, 34, 56, 72	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	ALA	3.4
1	B	64	GLY	2.7
1	B	91	TYR	2.5
1	A	348	THR	2.3
1	A	95	GLY	2.3
1	B	63	ILE	2.2
1	B	424	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	PLP	B	501	15/16	0.87	0.12	50,57,61,62	0
3	PLP	A	500	15/16	0.91	0.10	46,51,53,54	0
2	MLT	A	433	9/9	0.93	0.09	51,58,62,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.