Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:59 AM GMT

PDB ID	:	2Z1Z
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)

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 (1)) were used in the production of this report:

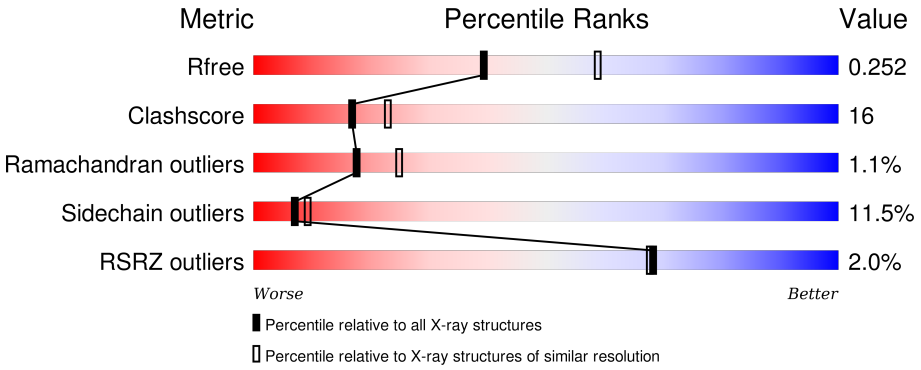
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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.

Mol	Chain	Length	Quality of chain
1	A	432	% 63% 25% 6% • 6%
1	B	432	3% 63% 24% 6% • 6%

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	-	-	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.

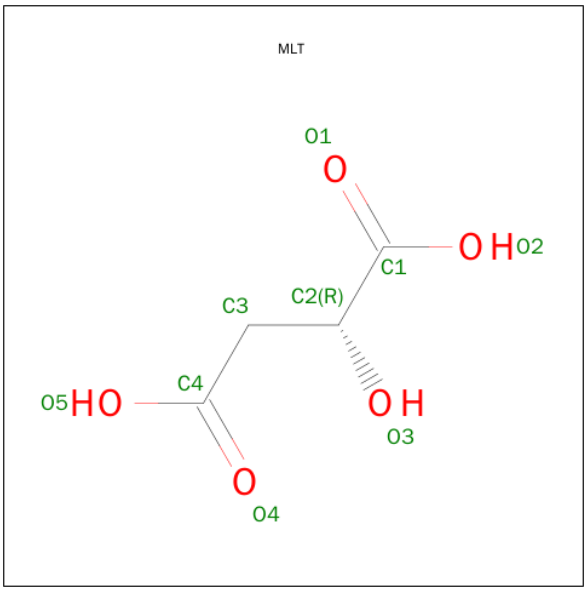
- Molecule 1 is a protein called LL-diaminopimelate aminotransferase.

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:

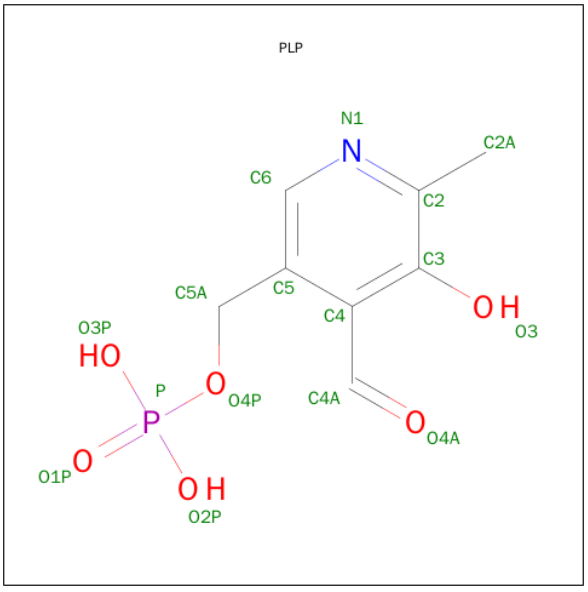
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	EXPRESSION TAG	UNP O81885
A	428	HIS	-	EXPRESSION TAG	UNP O81885
A	429	HIS	-	EXPRESSION TAG	UNP O81885
A	430	HIS	-	EXPRESSION TAG	UNP O81885
A	431	HIS	-	EXPRESSION TAG	UNP O81885
A	432	HIS	-	EXPRESSION TAG	UNP O81885
B	427	HIS	-	EXPRESSION TAG	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 MALATE ION (three-letter code: MLT) (formula: $C_4H_6O_5$).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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.

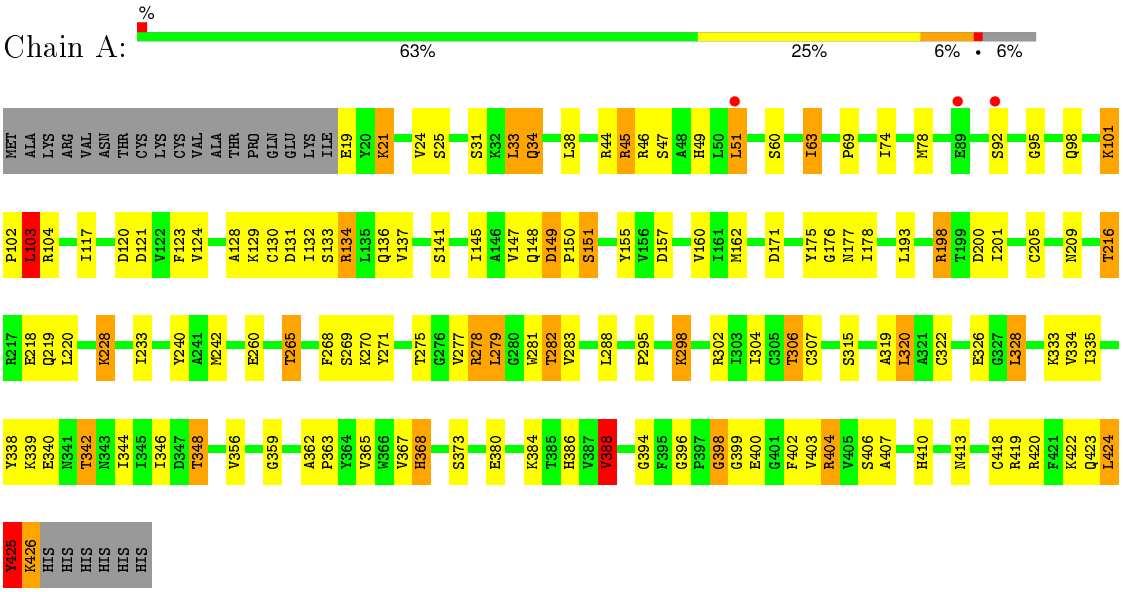
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0
4	B	118	Total O 118 118	0	0

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 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.

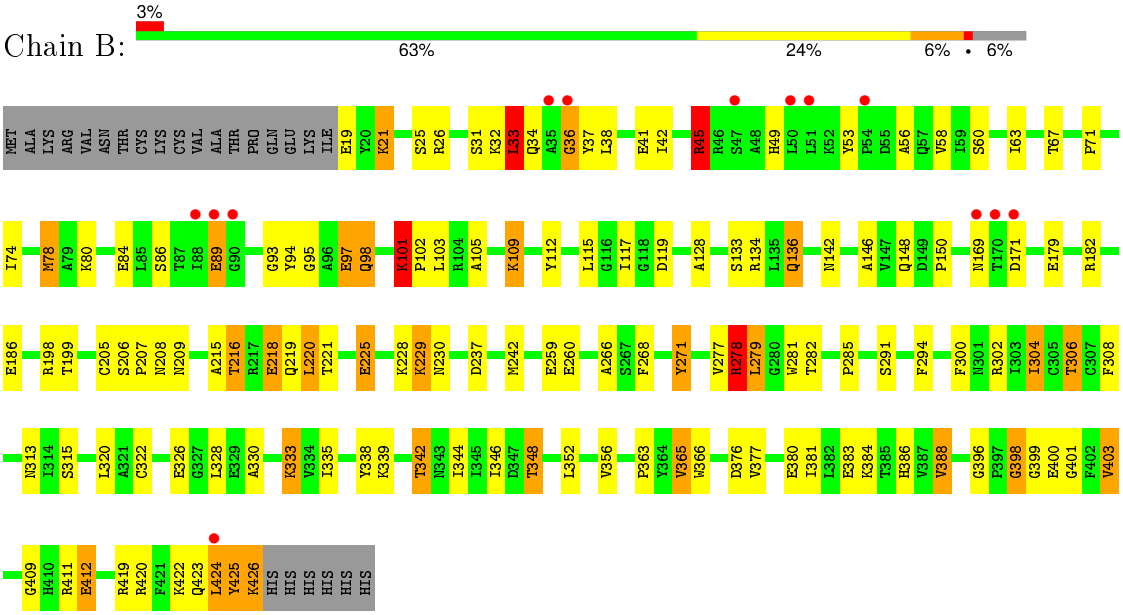
- Molecule 1: LL-diaminopimelate aminotransferase

Chain A:



- Molecule 1: LL-diaminopimelate aminotransferase

Chain B:



4 Data and refinement statistics (i)

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 29.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.40) 90.2 (29.61-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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	1913 reflections (5.34%)	DCC
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 , 47.9	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 37812 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MLT, 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	1.32	6/3219 (0.2%)	1.16	21/4362 (0.5%)
1	B	1.34	12/3219 (0.4%)	1.18	14/4362 (0.3%)
All	All	1.33	18/6438 (0.3%)	1.17	35/8724 (0.4%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	GLU	CB-CG	8.01	1.67	1.52
1	B	218	GLU	CG-CD	7.20	1.62	1.51
1	A	271	TYR	CE1-CZ	7.19	1.47	1.38
1	B	225	GLU	CG-CD	7.07	1.62	1.51
1	A	218	GLU	CG-CD	6.54	1.61	1.51
1	A	130	CYS	CB-SG	6.42	1.93	1.82
1	B	412	GLU	CG-CD	5.99	1.60	1.51
1	B	186	GLU	CG-CD	5.95	1.60	1.51
1	B	271	TYR	CE1-CZ	5.77	1.46	1.38
1	A	326	GLU	CG-CD	5.77	1.60	1.51
1	B	333	LYS	CD-CE	5.67	1.65	1.51
1	A	425	TYR	CD2-CE2	5.47	1.47	1.39
1	B	101	LYS	CE-NZ	5.43	1.62	1.49
1	B	326	GLU	CG-CD	5.40	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	GLU	CG-CD	5.31	1.59	1.51
1	A	340	GLU	CG-CD	5.27	1.59	1.51
1	B	313	ASN	CB-CG	5.11	1.62	1.51
1	B	294	PHE	CE1-CZ	5.08	1.47	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	420	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	278	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	36	GLY	N-CA-C	-7.57	94.19	113.10
1	A	398	GLY	N-CA-C	7.40	131.60	113.10
1	A	149	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	193	LEU	CB-CG-CD1	-7.03	99.04	111.00
1	B	420	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	404	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	237	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	365	VAL	CB-CA-C	6.39	123.54	111.40
1	A	45	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	398	GLY	N-CA-C	6.27	128.78	113.10
1	A	149	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	271	TYR	CA-CB-CG	6.15	125.09	113.40
1	B	45	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	420	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	388	VAL	CG1-CB-CG2	5.96	120.44	110.90
1	B	352	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	120	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	398	GLY	CA-C-N	5.63	127.47	116.20
1	A	242	MET	CG-SD-CE	5.63	109.21	100.20
1	A	103	LEU	CB-CG-CD2	5.61	120.53	111.00
1	A	328	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	171	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	404	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	134	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	157	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	401	GLY	N-CA-C	-5.26	99.94	113.10
1	B	271	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	B	420	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	171	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	78	MET	CG-SD-CE	-5.09	92.06	100.20
1	B	271	TYR	CB-CG-CD1	5.07	124.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	398	GLY	CA-C-N	5.02	126.23	116.20

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	103	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	204	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 (204) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:78:MET:HE1	1:B:277:VAL:HG11	1.46	0.97
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:78:MET:CE	1:B:277:VAL:HG11	2.04	0.88
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:A:34:GLN:NE2	1:A:34:GLN:HA	1.94	0.82
1:B:49:HIS:NE2	1:B:386:HIS:CD2	2.46	0.81
1:A:302:ARG:HH11	1:A:306:THR:HG22	1.46	0.80
1:B:101:LYS:CD	1:B:101:LYS:H	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
1:A:78:MET:HE2	1:A:315:SER:HA	1.64	0.78
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:A:78:MET:HE3	1:A:277:VAL:HG11	1.69	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:MET:CE	1:A:277:VAL:HG11	2.25	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:B:101:LYS:HD2	1:B:101:LYS:N	2.08	0.64
1:A:384:LYS:HD3	1:A:424:LEU:HD21	1.80	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:209:ASN:HD22	3:B:501:PLP:H2A1	1.65	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:233:ILE:HG12	1:A:288:LEU:HD11	1.85	0.58
1:A:136:GLN:HA	1:A:136:GLN:HE21	1.69	0.58
1:A:117:ILE:HG12	1:A:283:VAL:HG11	1.85	0.58
1:A:78:MET:CE	1:A:277:VAL:CG1	2.82	0.58
1:B:78:MET:HE3	1:B:315:SER:HA	1.86	0.57
1:B:78:MET:CE	1:B:277:VAL:CG1	2.80	0.57
1:A:63:ILE:HG23	4:A:517:HOH:O	2.03	0.56
1:A:275:THR:OG1	1:B:93:GLY:HA2	2.05	0.56
1:B:277:VAL:C	1:B:278:ARG:HG2	2.26	0.55
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:HE21	1:B:136:GLN:HA	1.72	0.54
1:A:368:HIS:HD2	4:A:568:HOH:O	1.91	0.54
1:B:109:LYS:NZ	1:B:119:ASP:OD1	2.37	0.53
1:A:338:TYR:O	1:A:342:THR:HG23	2.08	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:A:78:MET:HE3	1:A:277:VAL:CG1	2.37	0.53
1:B:33:LEU:O	1:B:34:GLN:CG	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:338:TYR:O	1:B:342:THR:CG2	2.57	0.51
1:A:295:PRO:HG2	1:A:298:LYS:HD2	1.93	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: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:78:MET:CE	1:B:315:SER:HA	2.42	0.49
1:B:216:THR:HG22	1:B:218:GLU:H	1.76	0.49
1:B:146:ALA:HA	1:B:179:GLU:O	2.13	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
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:B:344:ILE:O	1:B:348:THR:CG2	2.61	0.48
1:A:339:LYS:HA	1:A:342:THR:HG23	1.95	0.48
1:B:426:LYS:HB2	4:B:609:HOH:O	2.13	0.48
1:A:176:GLY:O	1:A:177:ASN:HB3	2.14	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:B:78:MET:HE2	1:B:277:VAL:CG1	2.42	0.47
1:B:150:PRO:HG3	1:B:366:TRP:CZ2	2.50	0.47
1:B:142:ASN:O	1:B:142:ASN:CG	2.53	0.47
1:A:34:GLN:NE2	1:A:34:GLN:CA	2.64	0.47
1:A:78:MET:HE1	1:A:277:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:NZ	1:B:291:SER:O	2.47	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:B:128:ALA:HB3	3:B:501:PLP:H5A1	1.97	0.46
1:A:38:LEU:HD13	1:A:394:GLY:CA	2.45	0.46
1:B:348:THR:HB	1:B:422:LYS:HE3	1.98	0.46
1:B:216:THR:HG22	1:B:218:GLU:N	2.30	0.46
1:A:367:VAL:O	1:A:402:PHE:HA	2.14	0.46
1:B:21:LYS:HB2	1:B:21:LYS:HZ2	1.81	0.46
1:B:33:LEU:O	1:B:34:GLN:HG3	2.16	0.46
1:A:19:GLU:HG3	1:A:19:GLU:O	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: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:123:PHE:O	1:A:281:TRP:HA	2.16	0.45
1:A:141:SER:HB2	1:A:162:MET:O	2.16	0.45
1:B:215:ALA:HB1	1:B:220:LEU:HD13	1.99	0.45
1:A:128:ALA:O	1:A:132:ILE:HG13	2.17	0.45
1:B:97:GLU:HG2	1:B:97:GLU:H	1.17	0.45
1:B:282:THR:HG21	1:B:300:PHE:CZ	2.52	0.45
1:B:105:ALA:C	1:B:109:LYS:HE3	2.30	0.44
1:B:33:LEU:C	1:B:34:GLN:HG3	2.38	0.44
1:A:228:LYS:HE2	1:A:228:LYS:HB2	1.72	0.44
1:A:175:TYR:HB2	1:A:178:ILE:HD12	2.00	0.44
1:B:60:SER:HA	1:B:388:VAL:HG13	1.99	0.44
1:B:101:LYS:HB2	1:B:102:PRO:HD3	1.99	0.44
1:A:424:LEU:HD13	1:A:425:TYR:CZ	2.52	0.44
1:B:49:HIS:CE1	1:B:386:HIS:CD2	3.05	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:B:377:VAL:CG1	1:B:403:VAL:HG11	2.48	0.43
1:A:124:VAL:HG13	1:A:279:LEU:HD21	1.99	0.43
1:A:362:ALA:HB1	1:A:363:PRO:HD2	2.01	0.43
1:B:346:ILE:HD13	1:B:346:ILE:HG21	1.79	0.43
1:B:58:VAL:HA	1:B:386:HIS:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LYS:O	1:B:33:LEU:O	2.37	0.43
1:A:270:LYS:HA	1:A:270:LYS:HD3	1.72	0.43
1:A:69:PRO:HB3	1:B:86:SER:C	2.39	0.42
1:B:78:MET:HE1	1:B:277:VAL:CG1	2.34	0.42
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: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:A:141:SER:CB	1:A:162:MET:O	2.68	0.42
1:A:304:ILE:HA	1:A:304:ILE:HD13	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:B:377:VAL:CG1	1:B:381:ILE:HD12	2.50	0.41
1:A:145:ILE:HD12	1:A:147:VAL:HG13	2.02	0.41
1:B:206:SER:HA	1:B:207:PRO:C	2.40	0.41
1:A:149:ASP:HA	1:A:150:PRO:HA	1.89	0.41
1:B:242:MET:HB3	1:B:335:ILE:HD13	2.02	0.41
1:B:45:ARG:HB3	1:B:45:ARG:HH11	1.86	0.41
1:A:117:ILE:HG12	1:A:283:VAL:CG1	2.50	0.41
1:A:131:ASP:CG	1:A:282:THR:CG2	2.89	0.41
1:A:270:LYS:NZ	3:A:500:PLP:C4A	2.84	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: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:80:LYS:O	1:B:84:GLU:HG3	2.22	0.40
1:A:307:CYS:HB3	1:B:133:SER:OG	2.22	0.40
1:A:145:ILE:HG22	1:A:201:ILE:HB	2.02	0.40
1:A:133:SER:O	1:A:137:VAL:HG23	2.20	0.40
1:B:169:ASN:OD1	1:B:171:ASP:HB2	2.21	0.40
1:B:302:ARG:HD2	1:B:306:THR:CG2	2.51	0.40
1:A:38:LEU:CD1	1:A:394:GLY:HA3	2.51	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:A:396:GLY:O	1:A:399:GLY:HA3	2.21	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	406/432 (94%)	391 (96%)	13 (3%)	2 (0%)	34 48
1	B	406/432 (94%)	375 (92%)	24 (6%)	7 (2%)	11 14
All	All	812/864 (94%)	766 (94%)	37 (5%)	9 (1%)	17 25

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
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%)	293 (88%)	41 (12%)	6 7
1	B	334/356 (94%)	298 (89%)	36 (11%)	8 11
All	All	668/712 (94%)	591 (88%)	77 (12%)	7 9

All (77) 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	44	ARG
1	A	45	ARG
1	A	46	ARG
1	A	51	LEU
1	A	63	ILE
1	A	92	SER
1	A	98	GLN
1	A	101	LYS
1	A	103	LEU
1	A	151	SER
1	A	198	ARG
1	A	216	THR
1	A	220	LEU
1	A	228	LYS
1	A	265	THR
1	A	279	LEU
1	A	282	THR
1	A	298	LYS
1	A	306	THR
1	A	320	LEU
1	A	328	LEU
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	406	SER
1	A	419	ARG
1	A	423	GLN
1	A	424	LEU
1	A	426	LYS
1	B	21	LYS

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Mol	Chain	Res	Type
1	B	25	SER
1	B	26	ARG
1	B	31	SER
1	B	33	LEU
1	B	41	GLU
1	B	45	ARG
1	B	97	GLU
1	B	98	GLN
1	B	101	LYS
1	B	103	LEU
1	B	109	LYS
1	B	136	GLN
1	B	182	ARG
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	328	LEU
1	B	333	LYS
1	B	342	THR
1	B	348	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	34	GLN
1	A	136	GLN

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Mol	Chain	Res	Type
1	A	148	GLN
1	A	371	ASN
1	A	386	HIS
1	A	413	ASN
1	B	29	ASN
1	B	98	GLN
1	B	136	GLN
1	B	148	GLN
1	B	173	GLN
1	B	208	ASN
1	B	386	HIS

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

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	-	1,8,8	1.23	0	2,10,10	1.48	0
3	PLP	A	500	-	15,15,16	1.95	4 (26%)	21,22,23	3.13	7 (33%)
3	PLP	B	501	1	15,15,16	1.30	1 (6%)	21,22,23	2.07	10 (47%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	O3-C3	-4.58	1.26	1.37
3	B	501	PLP	O3-C3	-3.97	1.27	1.37
3	A	500	PLP	C2-N1	2.17	1.38	1.34
3	A	500	PLP	C6-C5	2.45	1.43	1.37
3	A	500	PLP	C3-C2	3.74	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	PLP	C5A-C5-C4	-8.72	110.10	121.65
3	A	500	PLP	C4A-C4-C5	-4.18	116.52	120.88
3	B	501	PLP	O4P-P-O1P	-3.90	97.22	107.14
3	A	500	PLP	O4P-P-O1P	-3.39	98.51	107.14
3	B	501	PLP	C5A-C5-C4	-2.99	117.69	121.65
3	B	501	PLP	C4A-C4-C5	-2.66	118.11	120.88
3	B	501	PLP	C5-C6-N1	-2.56	119.42	123.86
3	B	501	PLP	O4P-C5A-C5	2.11	112.48	108.99
3	A	500	PLP	O3P-P-O1P	2.13	117.43	110.58
3	B	501	PLP	C6-N1-C2	2.35	124.07	119.28
3	B	501	PLP	O2P-P-O4P	2.36	113.37	106.56
3	B	501	PLP	C6-C5-C4	2.43	120.21	118.15
3	B	501	PLP	O3-C3-C2	2.67	122.31	117.66
3	B	501	PLP	C2A-C2-C3	3.07	124.74	121.04
3	A	500	PLP	O3-C3-C2	4.03	124.66	117.66
3	A	500	PLP	O4P-C5A-C5	5.28	117.72	108.99
3	A	500	PLP	C5A-C5-C6	5.94	130.50	119.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	433	MLT	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PLP	2	0
3	B	501	PLP	2	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, 95^{th} 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%)	-0.43	3 (0%) 89 88	19, 34, 51, 63	0
1	B	408/432 (94%)	-0.35	13 (3%) 51 51	21, 35, 60, 72	0
All	All	816/864 (94%)	-0.39	16 (1%) 68 68	19, 34, 56, 72	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ILE	3.7
1	B	51	LEU	3.6
1	B	50	LEU	3.6
1	A	51	LEU	3.4
1	B	89	GLU	3.3
1	B	47	SER	3.0
1	B	90	GLY	3.0
1	B	54	PRO	2.9
1	B	171	ASP	2.9
1	A	89	GLU	2.9
1	A	92	SER	2.7
1	B	170	THR	2.4
1	B	169	ASN	2.4
1	B	35	ALA	2.1
1	B	36	GLY	2.1
1	B	424	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MLT	A	433	9/9	0.94	0.27	3.06	51,58,62,65	0
3	PLP	A	500	15/16	0.95	0.16	0.34	46,51,53,54	0
3	PLP	B	501	15/16	0.91	0.15	-0.04	50,57,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.