



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:43 pm BST

PDB ID : 4ADB  
Title : Structural and functional study of succinyl-ornithine transaminase from E. coli  
Authors : Newman, J.; Peat, T.S.  
Deposited on : 2011-12-23  
Resolution : 2.20 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](mailto: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.

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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

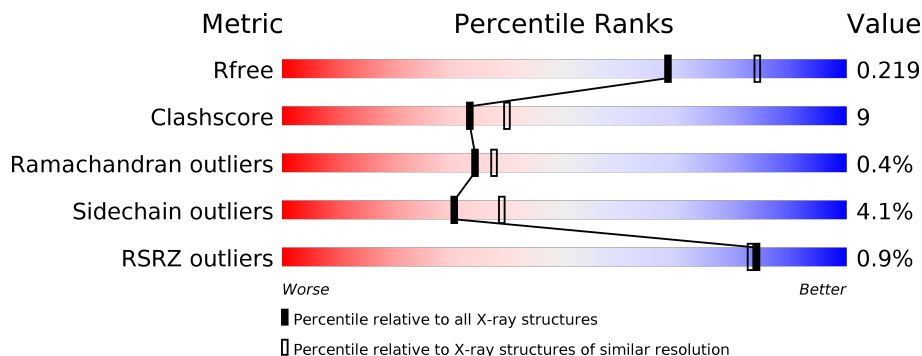
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	406	 2% 83% 14% ..
1	B	406	 80% 17% ..
1	C	406	 81% 15% ..
1	D	406	 2% 78% 18% ..

## 2 Entry composition [i](#)

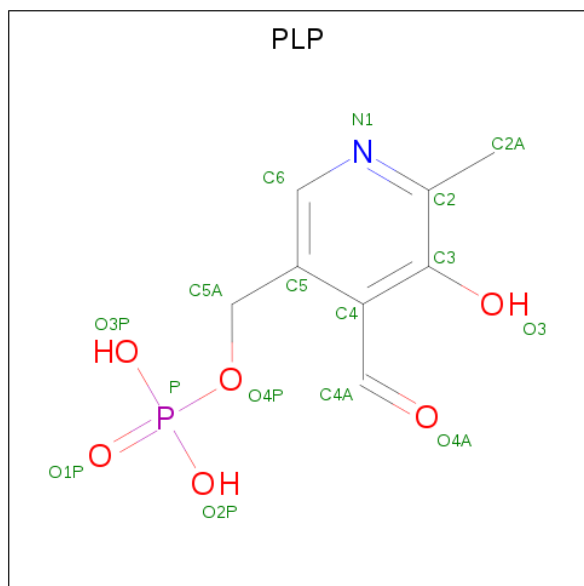
There are 5 unique types of molecules in this entry. The entry contains 13095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUCCINYLORNITHINE TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	Total 3111	C 1968	N 552	O 580	S 11	0	10	0
1	B	401	Total 3095	C 1958	N 549	O 577	S 11	0	7	0
1	C	399	Total 3080	C 1951	N 540	O 577	S 12	0	8	0
1	D	400	Total 3099	C 1963	N 547	O 578	S 11	0	9	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

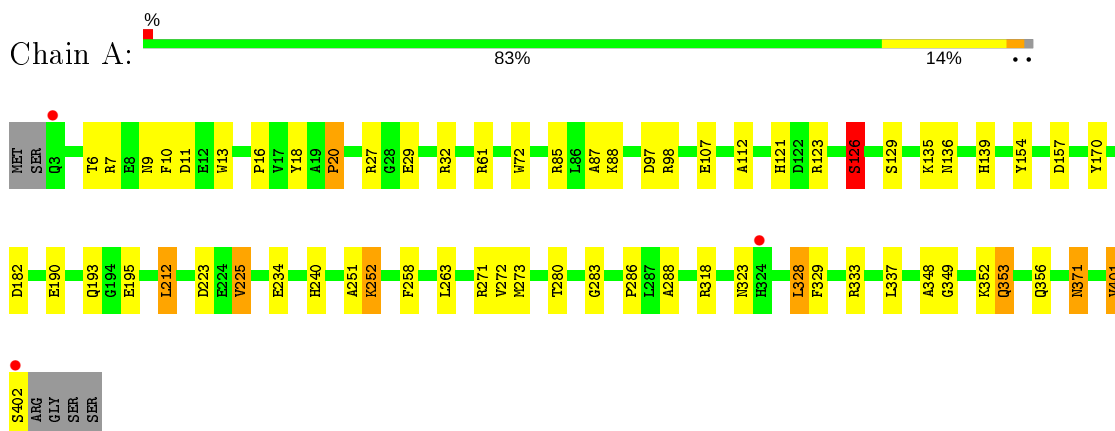
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	181	Total	O	0	0
			181	181		
5	C	155	Total	O	0	0
			155	155		
5	D	85	Total	O	0	0
			85	85		

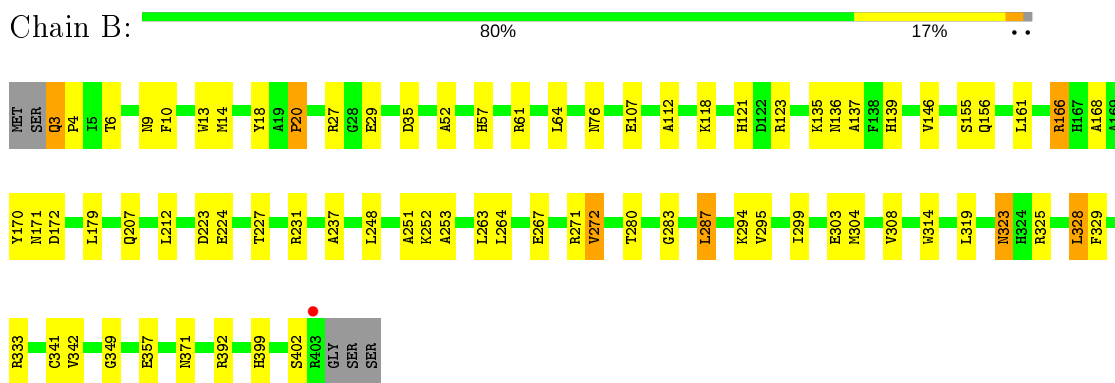
### 3 Residue-property plots [i](#)

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.

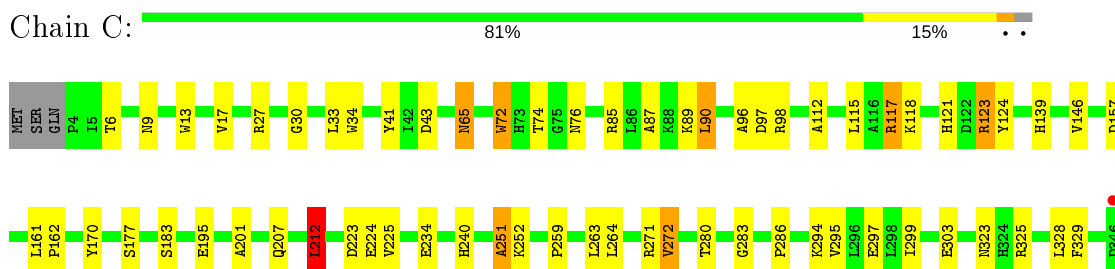
- Molecule 1: SUCCINYLORNITHINE TRANSAMINASE

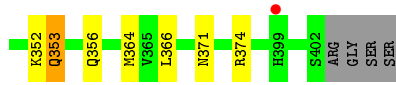


- Molecule 1: SUCCINYLORNITHINE TRANSAMINASE

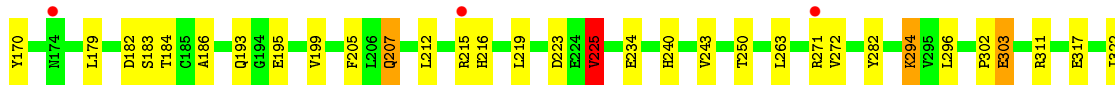
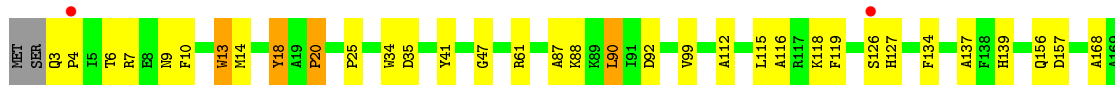
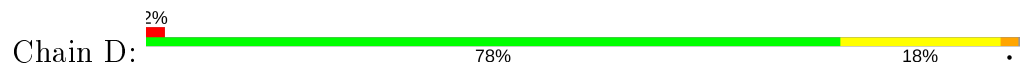


- Molecule 1: SUCCINYLORNITHINE TRANSAMINASE





● Molecule 1: SUCCINYLORNITHINE TRANSAMINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.71Å 118.43Å 109.79Å 90.00° 96.69° 90.00°	Depositor
Resolution (Å)	109.05 – 2.20 19.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (109.05-2.20) 99.8 (19.80-2.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.171 , 0.219 0.171 , 0.219	Depositor DCC
$R_{free}$ test set	5936 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: NA, MG, 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	1.17	4/3197 (0.1%)	1.07	15/4341 (0.3%)
1	B	1.16	4/3179 (0.1%)	1.08	10/4316 (0.2%)
1	C	1.09	4/3170 (0.1%)	1.01	5/4303 (0.1%)
1	D	1.03	3/3188 (0.1%)	1.01	6/4330 (0.1%)
All	All	1.11	15/12734 (0.1%)	1.04	36/17290 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLU	CD-OE2	7.19	1.33	1.25
1	A	13	TRP	CD2-CE2	6.91	1.49	1.41
1	B	18	TYR	CE1-CZ	6.32	1.46	1.38
1	B	314	TRP	CD2-CE2	6.22	1.48	1.41
1	C	224	GLU	CD-OE1	6.11	1.32	1.25
1	C	34	TRP	CD2-CE2	5.96	1.48	1.41
1	C	30	GLY	N-CA	5.73	1.54	1.46
1	A	190	GLU	CD-OE1	5.61	1.31	1.25
1	D	34	TRP	CD2-CE2	5.51	1.48	1.41
1	D	13	TRP	CD2-CE2	5.47	1.48	1.41
1	C	72	TRP	CD2-CE2	5.34	1.47	1.41
1	A	126	SER	CB-OG	-5.23	1.35	1.42
1	D	18	TYR	CE1-CZ	5.15	1.45	1.38
1	B	107	GLU	CD-OE1	5.05	1.31	1.25
1	B	137	ALA	C-O	5.04	1.32	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	A	333	ARG	NE-CZ-NH1	-8.21	116.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	333	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	B	27	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	391	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	318	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	90	LEU	CA-CB-CG	7.01	131.42	115.30
1	B	231	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	11	ASP	CB-CG-OD1	6.70	124.33	118.30
1	D	225	VAL	CG1-CB-CG2	6.63	121.51	110.90
1	B	333	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	D	391	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	212	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	182	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	32	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	318	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	61	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	D	311	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	273	MET	CG-SD-CE	5.70	109.32	100.20
1	B	35	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	A	11	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	C	212	LEU	CA-CB-CG	5.67	128.35	115.30
1	C	325	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	D	92	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	61	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	392	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	166[A]	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	166[B]	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	392	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	123	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	85	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	328	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	225	VAL	CG1-CB-CG2	5.13	119.10	110.90
1	B	172	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	29	GLU	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

## 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	3111	0	3032	55	0
1	B	3095	0	3027	57	0
1	C	3080	0	3013	54	0
1	D	3099	0	3027	67	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	2	0
2	D	15	0	6	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	223	0	0	7	1
5	B	181	0	0	8	0
5	C	155	0	0	6	1
5	D	85	0	0	1	0
All	All	13095	0	12123	210	1

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 9.

All (210) 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:353[A]:GLN:NE2	5:A:2199:HOH:O	1.56	1.32
1:A:7:ARG:NH2	1:A:20[A]:PRO:HD2	1.56	1.16
1:B:267:GLU:OE2	1:B:271[B]:ARG:NH1	1.78	1.14
1:D:271[B]:ARG:CG	1:D:271[B]:ARG:HH11	1.64	1.08
1:D:7:ARG:NH2	1:D:20[A]:PRO:HD2	1.70	1.04
1:C:65:ASN:OD1	5:C:2042:HOH:O	1.76	1.03
1:D:271[B]:ARG:HG2	1:D:271[B]:ARG:HH11	1.25	1.00
1:C:207:GLN:OE1	5:C:2114:HOH:O	1.77	0.99
1:C:87:ALA:HB2	1:D:14:MET:HE1	1.47	0.96
1:A:349:GLY:H	1:A:371:ASN:ND2	1.68	0.91
1:C:87:ALA:CB	1:D:14:MET:HE1	1.99	0.91
1:B:227[A]:THR:HG21	1:B:237:ALA:HB2	1.53	0.90
1:B:227[A]:THR:CG2	1:B:237:ALA:HB2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PHE:CE1	1:A:20[A]:PRO:HD3	2.11	0.85
1:C:252:LYS:HZ3	2:C:1404:PLP:C4A	1.55	0.84
1:D:7:ARG:HH21	1:D:20[A]:PRO:HD2	1.43	0.83
1:B:227[A]:THR:HG21	1:B:237:ALA:CB	2.09	0.82
1:D:271[B]:ARG:CG	1:D:271[B]:ARG:NH1	2.38	0.81
1:D:18:TYR:HB3	1:D:20[B]:PRO:HD3	1.65	0.78
1:B:3:GLN:HE21	1:B:3:GLN:HA	1.50	0.76
1:A:10:PHE:CE1	1:A:20[B]:PRO:HD2	2.21	0.75
1:D:127:HIS:HD2	1:D:183:SER:HB3	1.51	0.75
1:B:166[B]:ARG:HG3	5:B:2089:HOH:O	1.86	0.74
1:D:271[B]:ARG:HG3	1:D:271[B]:ARG:HH11	1.51	0.73
1:A:87:ALA:CB	1:B:14:MET:HE3	2.18	0.73
1:D:323:ASN:HD21	1:D:329:PHE:H	1.36	0.73
1:A:271[A]:ARG:HD3	1:C:271[A]:ARG:HD3	1.72	0.71
1:C:87:ALA:CB	1:D:14:MET:CE	2.68	0.71
1:A:223:ASP:OD1	1:A:225:VAL:HG13	1.91	0.71
1:C:352:LYS:O	1:C:356:GLN:HG3	1.91	0.70
1:C:323:ASN:HD21	1:C:329:PHE:H	1.38	0.70
1:A:154:TYR:CD2	5:A:2129:HOH:O	2.43	0.70
1:B:139:HIS:HD2	1:B:223:ASP:OD2	1.77	0.68
1:A:10:PHE:CZ	1:A:20[B]:PRO:HD2	2.29	0.68
1:B:267:GLU:HG3	1:B:271[B]:ARG:HD2	1.75	0.67
1:A:139:HIS:HD2	1:A:223:ASP:OD2	1.77	0.67
1:D:41:TYR:HB2	1:D:364:MET:CE	2.25	0.67
1:A:323:ASN:HD21	1:A:329:PHE:H	1.43	0.66
1:A:7:ARG:HH21	1:A:20[A]:PRO:HD2	1.52	0.66
1:D:271[B]:ARG:NH1	1:D:271[B]:ARG:HG2	2.04	0.66
1:D:303[A]:GLU:CD	1:D:303[A]:GLU:H	1.99	0.66
1:D:182:ASP:OD1	1:D:216:HIS:HD2	1.79	0.65
1:B:135:LYS:O	1:B:136:ASN:HB2	1.96	0.65
1:B:349:GLY:H	1:B:371:ASN:ND2	1.96	0.64
1:B:13:TRP:HB2	1:B:14:MET:HE2	1.81	0.63
1:A:349:GLY:N	1:A:371:ASN:ND2	2.44	0.63
1:D:401:VAL:O	1:D:402:SER:CB	2.47	0.63
1:A:349:GLY:H	1:A:371:ASN:HD22	1.47	0.62
1:C:177:SER:HB3	1:C:212:LEU:HD21	1.81	0.62
1:C:6:THR:H	1:C:9:ASN:ND2	1.98	0.61
1:B:10:PHE:CZ	1:B:20:PRO:HD3	2.36	0.61
1:A:87:ALA:CB	1:B:14:MET:CE	2.78	0.61
1:B:123[A]:ARG:NH1	5:B:2077:HOH:O	1.72	0.61
1:B:227[A]:THR:CG2	1:B:227[A]:THR:O	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:NE2	1:B:4:PRO:HD2	2.15	0.60
1:C:139:HIS:HD2	1:C:223:ASP:OD2	1.84	0.59
1:D:127:HIS:CD2	1:D:183:SER:HB3	2.35	0.59
1:A:352:LYS:O	1:A:356:GLN:HG3	2.03	0.58
1:B:64:LEU:HD12	1:B:287:LEU:HD22	1.85	0.58
1:A:280:THR:HG21	1:A:283:GLY:HA3	1.85	0.58
1:C:252:LYS:NZ	2:C:1404:PLP:C4	2.60	0.58
1:C:96:ALA:HB2	1:C:264:LEU:HB3	1.86	0.58
1:A:234:GLU:HG3	1:A:240:HIS:HB2	1.86	0.58
1:C:280:THR:HG21	1:C:283:GLY:HA3	1.86	0.58
1:A:157:ASP:OD2	1:B:118:LYS:HE2	2.04	0.58
1:A:72:TRP:O	1:A:286:PRO:HD2	2.04	0.57
1:D:401:VAL:O	1:D:402:SER:HB3	2.05	0.57
1:C:41:TYR:HB2	1:C:364[A]:MET:HE2	1.86	0.57
1:D:18:TYR:C	1:D:20[B]:PRO:HD3	2.25	0.57
1:C:121:HIS:HB3	5:C:2082:HOH:O	2.05	0.57
1:A:18:TYR:C	1:A:20[B]:PRO:HD3	2.26	0.56
1:B:3:GLN:HE21	1:B:3:GLN:CA	2.17	0.56
1:B:227[A]:THR:HG22	1:B:227[A]:THR:O	2.04	0.55
1:D:10:PHE:CZ	1:D:20[B]:PRO:HD2	2.42	0.55
1:A:121:HIS:HE1	1:A:129:SER:OG	1.90	0.55
1:D:14:MET:HE2	1:D:14:MET:HA	1.88	0.55
1:D:41:TYR:CB	1:D:364:MET:HE3	2.37	0.55
1:A:139:HIS:HE1	5:A:2123:HOH:O	1.89	0.55
1:D:223:ASP:OD1	1:D:225:VAL:HG13	2.07	0.55
1:D:18:TYR:CB	1:D:20[B]:PRO:HD3	2.37	0.54
1:B:13:TRP:CB	1:B:14:MET:HE2	2.38	0.54
1:D:90:LEU:HD13	1:D:296:LEU:HD11	1.90	0.53
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:NH1	2.22	0.53
1:A:6:THR:H	1:A:9:ASN:ND2	2.07	0.53
1:C:323:ASN:ND2	1:C:328:LEU:H	2.07	0.53
1:B:323:ASN:ND2	1:B:328:LEU:H	2.07	0.53
1:C:76:ASN:O	1:D:20[B]:PRO:HG3	2.08	0.53
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:HH11	1.74	0.53
1:D:6:THR:H	1:D:9:ASN:ND2	2.06	0.53
1:A:126:SER:HB3	5:A:2119:HOH:O	2.08	0.52
1:B:224:GLU:OE1	1:B:227[A]:THR:HG22	2.10	0.52
1:D:41:TYR:HB2	1:D:364:MET:HE2	1.91	0.52
1:B:323:ASN:HD21	1:B:329:PHE:H	1.57	0.52
1:A:10:PHE:CZ	1:A:20[B]:PRO:CD	2.94	0.51
1:B:156:GLN:HE22	1:D:156:GLN:HE22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ALA:HA	1:D:219:LEU:HD12	1.92	0.51
1:B:272:VAL:HG22	5:B:2076:HOH:O	2.10	0.51
1:C:353:GLN:H	1:C:353:GLN:HE21	1.59	0.50
1:B:248:LEU:HD22	1:B:264:LEU:HD22	1.94	0.50
1:C:115:LEU:C	1:C:115:LEU:HD23	2.32	0.50
1:C:157:ASP:OD2	1:D:118:LYS:HE2	2.11	0.50
1:C:123:ARG:HD3	1:C:124:TYR:CE2	2.46	0.50
1:A:7:ARG:NH2	1:A:20[A]:PRO:CD	2.50	0.50
1:B:139:HIS:HE1	5:B:2090:HOH:O	1.93	0.50
1:C:87:ALA:HB1	1:D:14:MET:HE1	1.89	0.50
1:D:13:TRP:O	1:D:14:MET:HE2	2.11	0.50
1:C:74:THR:O	1:D:47:GLY:HA2	2.12	0.50
1:A:348:ALA:HA	1:A:371:ASN:HD21	1.77	0.49
1:D:168:ALA:HB2	1:D:179:LEU:HD12	1.93	0.49
1:B:280:THR:HG21	1:B:283:GLY:HA3	1.95	0.49
1:B:399:HIS:CD2	5:B:2180:HOH:O	2.64	0.49
1:C:87:ALA:HB1	1:D:14:MET:CE	2.43	0.49
1:B:121:HIS:HB3	5:B:2074:HOH:O	2.12	0.48
1:A:195[B]:GLU:HG3	5:A:2153:HOH:O	2.13	0.48
1:B:295:VAL:CG1	1:B:299:ILE:HD12	2.44	0.48
1:C:170:TYR:OH	1:C:201:ALA:HB2	2.13	0.48
1:D:139:HIS:HD2	1:D:223:ASP:OD2	1.95	0.48
1:D:170:TYR:CE2	1:D:193:GLN:HG3	2.47	0.48
1:C:112:ALA:HB2	1:C:263:LEU:HD13	1.96	0.48
1:A:121:HIS:CE1	1:A:129:SER:OG	2.65	0.48
1:C:89:LYS:NZ	1:C:297[A]:GLU:HG3	2.29	0.48
1:D:271[B]:ARG:HG3	1:D:271[B]:ARG:NH1	2.15	0.48
1:B:319:LEU:HD13	1:B:341:CYS:SG	2.53	0.48
1:C:295:VAL:HG13	1:C:299:ILE:HD12	1.95	0.47
1:A:16:PRO:HB2	5:A:2013:HOH:O	2.14	0.47
1:A:258:PHE:CE1	1:A:288:ALA:HB2	2.49	0.47
1:A:87:ALA:HB1	1:B:14:MET:CE	2.44	0.47
1:A:328:LEU:HD21	1:A:401:VAL:HG23	1.96	0.47
1:B:329:PHE:HA	1:B:342:VAL:O	2.15	0.47
1:B:6:THR:H	1:B:9:ASN:ND2	2.12	0.47
1:A:87:ALA:HB1	1:B:14:MET:HE1	1.96	0.47
1:B:112:ALA:HB2	1:B:263:LEU:HD13	1.97	0.47
1:B:227[A]:THR:CG2	1:B:237:ALA:CB	2.78	0.47
5:B:2163:HOH:O	1:C:183:SER:HB3	2.14	0.46
1:D:87:ALA:HA	1:D:99[A]:VAL:HG11	1.98	0.46
1:D:41:TYR:CB	1:D:364:MET:CE	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:CA	1:A:371:ASN:HD21	2.29	0.46
1:D:343:LEU:HD21	1:D:354:ILE:CD1	2.45	0.46
1:A:20[B]:PRO:HG3	1:B:76:ASN:O	2.16	0.46
1:B:168:ALA:HB2	1:B:179:LEU:HD12	1.98	0.46
1:C:13:TRP:CE2	1:D:88:LYS:HD3	2.51	0.46
1:C:118:LYS:HD3	1:C:272:VAL:HG13	1.97	0.46
1:C:41:TYR:CD1	1:C:41:TYR:N	2.84	0.46
1:D:41:TYR:HB3	1:D:364:MET:HE3	1.98	0.46
1:B:155:SER:HB2	1:B:161:LEU:HD11	1.98	0.45
1:D:139:HIS:HE1	5:D:2048:HOH:O	2.00	0.45
1:A:271[B]:ARG:CG	1:A:271[B]:ARG:HH11	2.29	0.45
1:D:335:LEU:O	1:D:336:GLY:C	2.53	0.45
1:D:6:THR:H	1:D:9:ASN:HD22	1.65	0.45
1:C:280:THR:CG2	1:C:283:GLY:HA3	2.47	0.44
1:C:43:ASP:HB2	1:C:364[A]:MET:HE1	1.99	0.44
1:D:215:ARG:HB2	1:D:215:ARG:HE	1.49	0.44
1:A:280:THR:CG2	1:A:283:GLY:HA3	2.47	0.44
1:B:267:GLU:CD	1:B:271[B]:ARG:NH1	2.64	0.44
1:C:294:LYS:HB2	1:C:294:LYS:HE2	1.56	0.44
1:A:170:TYR:CZ	1:A:193:GLN:HG3	2.53	0.44
1:D:10:PHE:CE1	1:D:20[A]:PRO:HD3	2.52	0.44
1:C:303[A]:GLU:H	1:C:303[A]:GLU:CD	2.21	0.44
1:B:57:HIS:O	1:B:61:ARG:HG3	2.18	0.44
1:C:33:LEU:HB3	1:C:364[A]:MET:HE2	2.00	0.44
1:C:161:LEU:O	1:C:162:PRO:C	2.53	0.43
1:B:295:VAL:HG13	1:B:299:ILE:HD12	2.00	0.43
1:A:225:VAL:HG23	1:A:252:LYS:HG3	2.00	0.43
1:C:89:LYS:CE	1:C:297[A]:GLU:HG3	2.48	0.43
1:D:294:LYS:HD3	1:D:294:LYS:HA	1.69	0.43
1:C:118:LYS:HG3	1:D:157:ASP:HB3	1.99	0.43
1:B:29:GLU:HG2	5:B:2020:HOH:O	2.17	0.43
1:B:52:ALA:HB2	1:B:253:ALA:HB1	1.99	0.43
1:C:115:LEU:O	1:C:115:LEU:HD23	2.19	0.43
1:A:85[A]:ARG:HE	1:B:3:GLN:HG3	1.84	0.42
1:C:225:VAL:HG13	1:C:251:ALA:HB3	2.01	0.42
1:A:112:ALA:HB2	1:A:263:LEU:HD13	2.00	0.42
1:C:27:ARG:O	1:C:33:LEU:HD12	2.19	0.42
1:C:195[A]:GLU:HG2	5:C:2111:HOH:O	2.18	0.42
1:A:87:ALA:HB3	1:B:14:MET:HE3	1.99	0.42
1:B:170:TYR:O	1:B:171:ASN:HB2	2.19	0.42
1:D:115:LEU:C	1:D:115:LEU:HD23	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85[A]:ARG:HE	1:B:3:GLN:CG	2.33	0.41
1:A:88:LYS:HD3	1:B:13:TRP:CE2	2.55	0.41
5:A:2008:HOH:O	1:B:267:GLU:OE1	2.21	0.41
1:C:366:LEU:HB2	1:C:374:ARG:HB3	2.02	0.41
1:A:223:ASP:OD1	1:A:223:ASP:C	2.58	0.41
1:C:72:TRP:O	1:C:286:PRO:HD2	2.19	0.41
1:C:97:ASP:O	1:C:98:ARG:HG2	2.20	0.41
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.80	0.41
1:B:135:LYS:O	1:B:136:ASN:CB	2.65	0.41
1:C:117:ARG:HD2	1:C:117:ARG:HH11	1.67	0.41
1:C:121:HIS:CB	5:C:2082:HOH:O	2.66	0.41
1:A:135:LYS:O	1:A:136:ASN:HB2	2.21	0.41
1:C:234:GLU:HG3	1:C:240:HIS:HB2	2.03	0.41
1:D:3:GLN:HB3	1:D:4:PRO:HD3	2.02	0.41
1:B:6:THR:H	1:B:9:ASN:HD22	1.69	0.41
1:D:234:GLU:HG3	1:D:240:HIS:HB2	2.03	0.41
1:D:322:ILE:HG12	1:D:394:ALA:HB2	2.03	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.95	0.41
1:A:6:THR:H	1:A:9:ASN:HD22	1.69	0.40
1:C:259:PRO:HA	1:D:282:TYR:CE2	2.55	0.40
1:D:225:VAL:HG22	2:D:1404:PLP:C3	2.50	0.40
1:D:207:GLN:HE21	1:D:243:VAL:HG22	1.86	0.40
1:D:25:PRO:HA	1:D:35:ASP:HA	2.04	0.40
1:D:112:ALA:HB2	1:D:263:LEU:HD13	2.03	0.40
1:D:119:PHE:C	1:D:119:PHE:CD1	2.95	0.40
1:D:137:ALA:HB1	1:D:139:HIS:CE1	2.56	0.40
1:D:184:THR:HG22	1:D:186:ALA:H	1.86	0.40
1:D:347:TYR:O	1:D:348:ALA:C	2.59	0.40
1:D:219:LEU:HA	1:D:219:LEU:HD23	1.78	0.40
1:B:304:MET:O	1:B:308:VAL:HG23	2.22	0.40
1:C:139:HIS:HE1	5:C:2091:HOH:O	2.05	0.40
1:A:97:ASP:O	1:A:98:ARG:HG2	2.21	0.40
1:D:134:PHE:CE2	1:D:205:PHE:HZ	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2037:HOH:O	5:C:2022:HOH:O[3_445]	2.09	0.11

## 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	408/406 (100%)	390 (96%)	16 (4%)	2 (0%)	29	31
1	B	406/406 (100%)	387 (95%)	17 (4%)	2 (0%)	29	31
1	C	405/406 (100%)	387 (96%)	17 (4%)	1 (0%)	47	55
1	D	407/406 (100%)	384 (94%)	22 (5%)	1 (0%)	47	55
All	All	1626/1624 (100%)	1548 (95%)	72 (4%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	LYS
1	A	251	ALA
1	B	251	ALA
1	A	252	LYS
1	C	251	ALA
1	D	401	VAL

### 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	316/312 (101%)	305 (96%)	11 (4%)	36	46
1	B	314/312 (101%)	299 (95%)	15 (5%)	25	32
1	C	314/312 (101%)	305 (97%)	9 (3%)	42	54
1	D	316/312 (101%)	295 (93%)	21 (7%)	16	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1260/1248 (101%)	1204 (96%)	56 (4%)	30 35

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20[A]	PRO
1	A	20[B]	PRO
1	A	123	ARG
1	A	126	SER
1	A	212	LEU
1	A	272	VAL
1	A	353[A]	GLN
1	A	353[B]	GLN
1	A	371	ASN
1	A	401	VAL
1	A	402	SER
1	B	3	GLN
1	B	20	PRO
1	B	146	VAL
1	B	207	GLN
1	B	212	LEU
1	B	272	VAL
1	B	287	LEU
1	B	294	LYS
1	B	303[A]	GLU
1	B	303[B]	GLU
1	B	323	ASN
1	B	325	ARG
1	B	328	LEU
1	B	357	GLU
1	B	402	SER
1	C	17	VAL
1	C	65	ASN
1	C	90	LEU
1	C	117	ARG
1	C	146	VAL
1	C	212	LEU
1	C	272	VAL
1	C	353	GLN
1	C	371	ASN
1	D	20[A]	PRO
1	D	20[B]	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	90	LEU
1	D	126	SER
1	D	195[A]	GLU
1	D	195[B]	GLU
1	D	199	VAL
1	D	207	GLN
1	D	212	LEU
1	D	225	VAL
1	D	250	THR
1	D	272	VAL
1	D	294	LYS
1	D	302	PRO
1	D	303[A]	GLU
1	D	303[B]	GLU
1	D	317	GLU
1	D	323	ASN
1	D	342	VAL
1	D	346	ASP
1	D	371	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	9	ASN
1	A	121	HIS
1	A	139	HIS
1	A	151	GLN
1	A	203	ASN
1	A	216	HIS
1	A	323	ASN
1	A	356	GLN
1	A	371	ASN
1	A	399	HIS
1	B	3	GLN
1	B	9	ASN
1	B	139	HIS
1	B	156	GLN
1	B	240	HIS
1	B	310	GLN
1	B	323	ASN
1	B	371	ASN
1	C	9	ASN

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Mol	Chain	Res	Type
1	C	139	HIS
1	C	207	GLN
1	C	216	HIS
1	C	310	GLN
1	C	323	ASN
1	C	350	GLN
1	C	353	GLN
1	C	356	GLN
1	C	371	ASN
1	D	9	ASN
1	D	65	ASN
1	D	121	HIS
1	D	127	HIS
1	D	139	HIS
1	D	207	GLN
1	D	216	HIS
1	D	310	GLN
1	D	323	ASN
1	D	350	GLN
1	D	371	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	PLP	D	1404	1	15,15,16	2.78	4 (26%)	20,22,23	1.52	4 (20%)
2	PLP	C	1404	1	15,15,16	3.08	3 (20%)	20,22,23	1.68	6 (30%)
2	PLP	B	1404	1	15,15,16	2.50	5 (33%)	20,22,23	2.15	7 (35%)
2	PLP	A	1404	1	15,15,16	2.56	5 (33%)	20,22,23	1.66	3 (15%)

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	PLP	D	1404	1	-	2/6/6/8	0/1/1/1
2	PLP	C	1404	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1404	1	-	3/6/6/8	0/1/1/1
2	PLP	A	1404	1	-	0/6/6/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1404	PLP	C3-C2	7.76	1.48	1.40
2	B	1404	PLP	C5-C4	7.69	1.49	1.40
2	C	1404	PLP	C5-C4	7.52	1.48	1.40
2	D	1404	PLP	C5-C4	6.70	1.47	1.40
2	A	1404	PLP	C3-C2	6.37	1.47	1.40
2	D	1404	PLP	C3-C2	5.95	1.46	1.40
2	A	1404	PLP	C5-C4	5.51	1.46	1.40
2	D	1404	PLP	C3-C4	4.72	1.49	1.40
2	C	1404	PLP	C3-C4	4.29	1.49	1.40
2	B	1404	PLP	C3-C4	3.87	1.48	1.40
2	A	1404	PLP	C3-C4	2.79	1.45	1.40
2	A	1404	PLP	C4A-C4	-2.67	1.46	1.51
2	B	1404	PLP	C3-C2	2.42	1.43	1.40
2	A	1404	PLP	C6-C5	2.23	1.42	1.37
2	D	1404	PLP	C2A-C2	-2.15	1.46	1.50
2	B	1404	PLP	P-O3P	-2.14	1.46	1.54
2	B	1404	PLP	C4A-C4	-2.02	1.47	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1404	PLP	C6-N1-C2	4.67	127.82	119.17
2	A	1404	PLP	C6-N1-C2	3.95	126.48	119.17
2	B	1404	PLP	C6-C5-C4	-3.55	115.36	118.16
2	A	1404	PLP	C3-C2-N1	-3.35	116.44	120.77
2	D	1404	PLP	C6-N1-C2	3.24	125.17	119.17
2	C	1404	PLP	O2P-P-O4P	-3.18	98.26	106.73
2	A	1404	PLP	C2A-C2-N1	3.14	123.80	117.67
2	C	1404	PLP	C2A-C2-C3	3.12	124.74	120.89
2	B	1404	PLP	O2P-P-O4P	-2.93	98.94	106.73
2	B	1404	PLP	C3-C2-N1	-2.79	117.16	120.77
2	C	1404	PLP	C6-N1-C2	2.74	124.25	119.17
2	B	1404	PLP	C2A-C2-N1	2.60	122.75	117.67
2	B	1404	PLP	O3P-P-O2P	2.47	117.08	107.64
2	C	1404	PLP	O3P-P-O2P	2.46	117.04	107.64
2	C	1404	PLP	C3-C4-C5	-2.35	116.20	118.74
2	B	1404	PLP	O2P-P-O1P	2.35	119.88	110.68
2	D	1404	PLP	O2P-P-O4P	-2.30	100.62	106.73
2	C	1404	PLP	C3-C2-N1	-2.23	117.89	120.77
2	D	1404	PLP	O3P-P-O2P	2.14	115.80	107.64
2	D	1404	PLP	O3-C3-C2	2.06	121.98	117.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1404	PLP	C5A-O4P-P-O1P
2	B	1404	PLP	C5A-O4P-P-O1P
2	B	1404	PLP	C5A-O4P-P-O2P
2	B	1404	PLP	C5A-O4P-P-O3P
2	D	1404	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1404	PLP	1	0
2	C	1404	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/406 (98%)	-0.60	3 (0%) 86 85	13, 22, 34, 72	15 (3%)
1	B	401/406 (98%)	-0.65	1 (0%) 95 94	13, 21, 33, 56	16 (3%)
1	C	399/406 (98%)	-0.51	2 (0%) 91 90	17, 26, 39, 61	18 (4%)
1	D	400/406 (98%)	-0.33	8 (2%) 65 63	18, 32, 48, 78	19 (4%)
All	All	1600/1624 (98%)	-0.52	14 (0%) 84 83	13, 25, 42, 78	68 (4%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	402	SER	3.6
1	A	402	SER	3.5
1	D	324	HIS	3.4
1	D	399[A]	HIS	3.3
1	D	174	ASN	3.0
1	A	324[A]	HIS	2.7
1	B	403	ARG	2.7
1	C	399	HIS	2.5
1	D	215	ARG	2.5
1	D	4	PRO	2.4
1	D	271[A]	ARG	2.3
1	A	3	GLN	2.2
1	C	346	ASP	2.1
1	D	126	SER	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, 95<sup>th</sup> 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
4	MG	A	1999	1/1	0.93	0.08	27,27,27,27	1
3	NA	D	1405	1/1	0.93	0.10	36,36,36,36	0
3	NA	C	1405	1/1	0.95	0.06	27,27,27,27	0
4	MG	B	1999	1/1	0.96	0.05	38,38,38,38	1
3	NA	A	1405	1/1	0.98	0.10	23,23,23,23	0
2	PLP	D	1404	15/16	0.98	0.07	20,24,26,26	0
2	PLP	C	1404	15/16	0.99	0.08	23,27,31,32	0
2	PLP	B	1404	15/16	0.99	0.07	13,15,19,20	0
2	PLP	A	1404	15/16	0.99	0.07	13,17,20,22	0
3	NA	B	1405	1/1	0.99	0.09	21,21,21,21	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.