



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:30 PM GMT

PDB ID : 1TWI
Title : Crystal structure of Diaminopimelate Decarboxylase from *M. jannaschii* in co-complex with L-lysine
Authors : Rajashankar, K.R.; Ray, S.S.; Bonanno, J.B.; Pinho, M.G.; He, G.; De Lencastre, H.; Tomasz, A.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-07-01
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

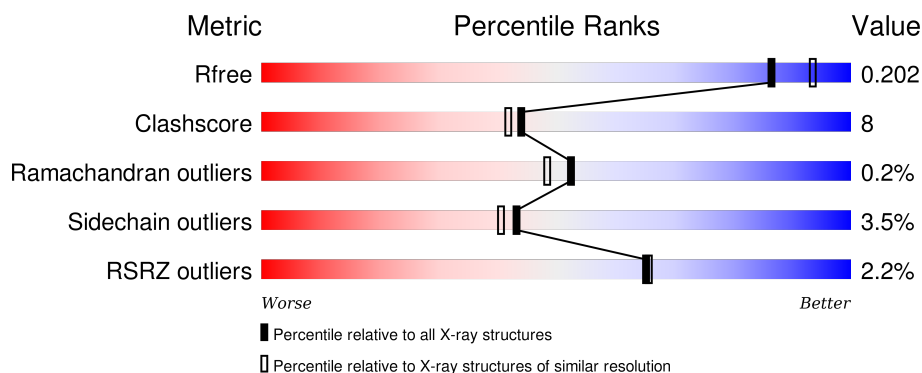
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	434	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	B	434	<div> <div>4%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	C	434	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	D	434	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LYS	D	1601	-	-	-	X
3	LYS	D	1602	-	-	-	X
3	LYS	D	1605	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15128 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 Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			
1	B	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			
1	C	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			
1	D	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			

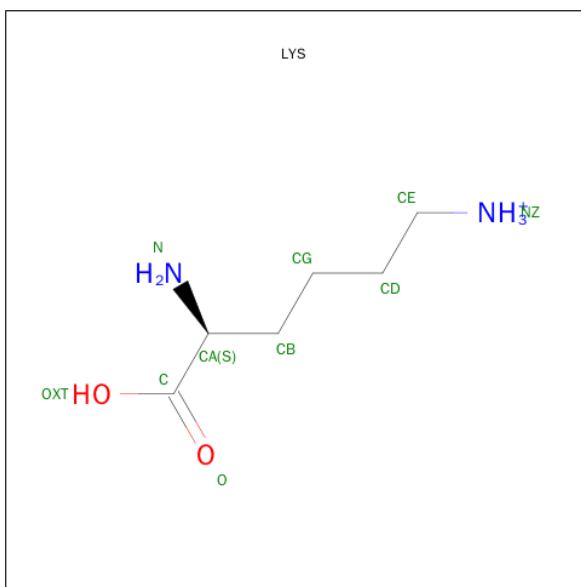
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	INITIATING METHIONINE	UNP Q58497
B	15	MET	-	INITIATING METHIONINE	UNP Q58497
C	15	MET	-	INITIATING METHIONINE	UNP Q58497
D	15	MET	-	INITIATING METHIONINE	UNP Q58497

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

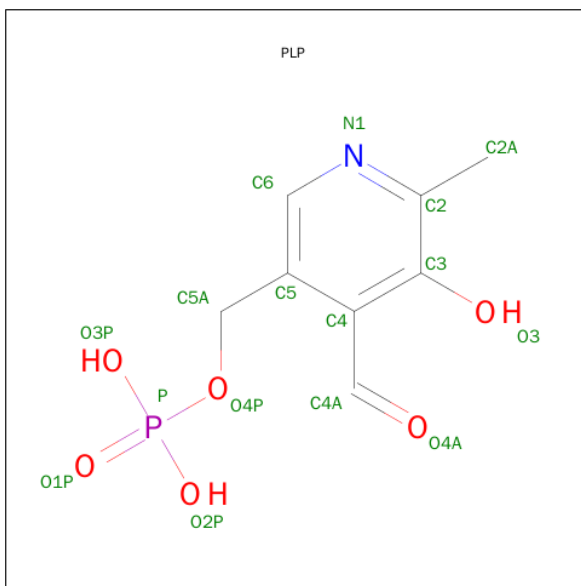
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	6	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
4	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
4	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

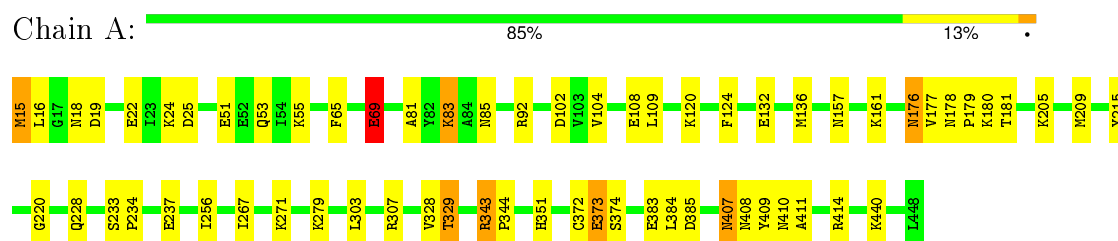
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total	O	0	0
			369	369		
5	B	301	Total	O	0	0
			301	301		
5	C	370	Total	O	0	0
			370	370		
5	D	383	Total	O	0	0
			383	383		

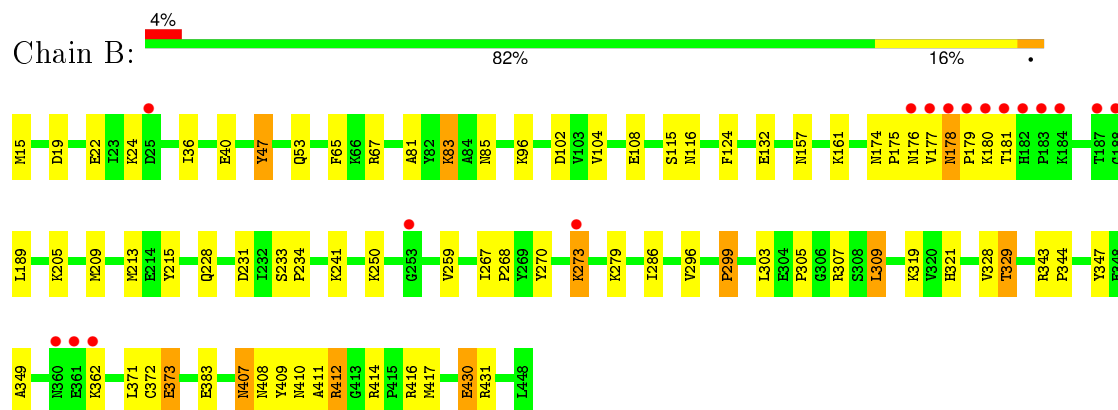
3 Residue-property plots

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

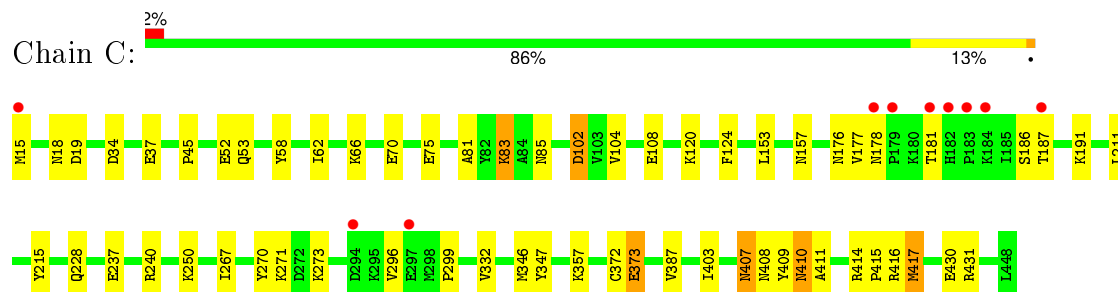
• Molecule 1: Diaminopimelate decarboxylase



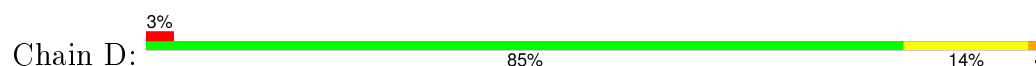
• Molecule 1: Diaminopimelate decarboxylase

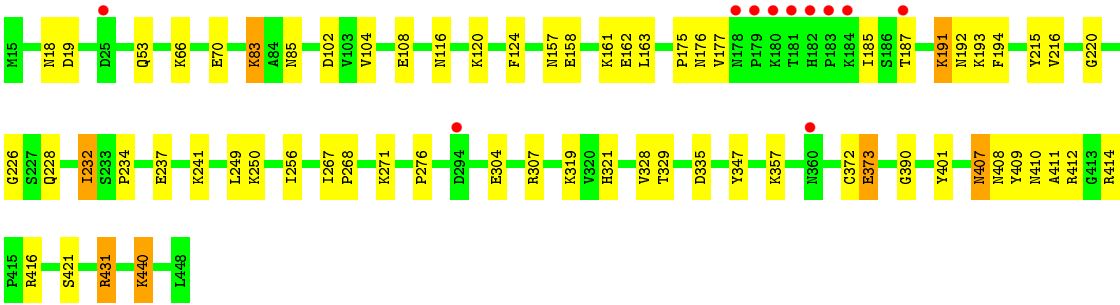


• Molecule 1: Diaminopimelate decarboxylase



• Molecule 1: Diaminopimelate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.24Å 147.07Å 89.39Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	29.25 – 2.00 29.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.25-2.00) 98.5 (29.25-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.56 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.157 , 0.202 0.157 , 0.202	Depositor DCC
R_{free} test set	6016 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 119717 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15128	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.95	2/3452 (0.1%)	0.91	4/4654 (0.1%)
1	B	0.90	4/3452 (0.1%)	0.88	2/4654 (0.0%)
1	C	0.95	0/3452	0.89	0/4654
1	D	0.96	2/3452 (0.1%)	0.92	4/4654 (0.1%)
All	All	0.94	8/13808 (0.1%)	0.90	10/18616 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	GLU	CG-CD	6.47	1.61	1.51
1	D	372	CYS	CB-SG	6.32	1.93	1.82
1	B	132	GLU	CD-OE1	5.40	1.31	1.25
1	A	132	GLU	CD-OE1	5.33	1.31	1.25
1	B	47	TYR	CD2-CE2	5.32	1.47	1.39
1	D	401	TYR	CE2-CZ	5.08	1.45	1.38
1	B	132	GLU	CG-CD	5.05	1.59	1.51
1	B	373	GLU	CB-CG	-5.04	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	92	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	307	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	92	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	D	307	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	343	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	412	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	412	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	412	ARG	NE-CZ-NH1	5.01	122.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	440	LYS	CD-CE-NZ	-5.00	100.19	111.70

There are no chirality outliers.

There are no planarity outliers.

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	3395	0	3457	56	0
1	B	3395	0	3457	67	0
1	C	3395	0	3457	54	0
1	D	3395	0	3457	54	0
2	C	1	0	0	0	0
3	D	60	0	72	18	0
4	A	16	0	7	2	0
4	B	16	0	7	2	0
4	C	16	0	8	1	0
4	D	16	0	7	2	0
5	A	369	0	0	10	0
5	B	301	0	0	11	0
5	C	370	0	0	9	0
5	D	383	0	0	9	0
All	All	15128	0	13929	219	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 8.

All (219) 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:C:270:TYR:HB2	1:C:273:LYS:HE2	1.48	0.96
1:B:430:GLU:HG2	5:B:1559:HOH:O	1.76	0.86
1:A:407:ASN:HD22	1:A:409:TYR:H	1.24	0.85
1:C:414:ARG:HH12	1:D:408:ASN:HD22	1.25	0.85
1:B:47:TYR:HB2	1:B:417:MET:HG2	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ASN:HD22	1:B:409:TYR:H	1.25	0.84
1:A:83:LYS:HE2	5:A:1795:HOH:O	1.78	0.83
1:D:407:ASN:HD22	1:D:409:TYR:H	1.26	0.82
1:C:373:GLU:OE1	3:D:1605:LYS:HG2	1.80	0.81
1:C:187:THR:O	1:C:191:LYS:HG2	1.81	0.80
1:D:187:THR:HG22	1:D:191:LYS:HD3	1.64	0.80
1:A:414:ARG:HH12	1:B:408:ASN:HD22	1.30	0.80
1:C:414:ARG:HH12	1:D:408:ASN:ND2	1.80	0.79
1:A:81:ALA:HB1	1:A:83:LYS:HE3	1.63	0.79
1:A:228:GLN:HE22	1:A:267:ILE:H	1.32	0.77
1:B:228:GLN:HE22	1:B:267:ILE:H	1.31	0.77
1:D:373:GLU:OE2	3:D:1603:LYS:HG2	1.84	0.77
1:B:83:LYS:HE2	5:B:1504:HOH:O	1.84	0.76
1:C:408:ASN:ND2	1:D:414:ARG:HH12	1.83	0.76
1:A:328:VAL:HG13	1:A:329:THR:HG23	1.66	0.76
1:A:408:ASN:HD22	1:B:414:ARG:HH12	1.33	0.76
5:A:1554:HOH:O	1:B:321:HIS:HD2	1.69	0.75
1:A:440:LYS:HE3	5:B:1710:HOH:O	1.86	0.75
1:C:407:ASN:HD22	1:C:409:TYR:H	1.36	0.74
1:A:414:ARG:HH12	1:B:408:ASN:ND2	1.85	0.74
1:C:228:GLN:HE22	1:C:267:ILE:H	1.33	0.74
1:C:416:ARG:HG3	1:C:431:ARG:HB3	1.70	0.74
1:B:270:TYR:HB2	1:B:273:LYS:HE3	1.70	0.74
1:A:328:VAL:HG22	1:A:329:THR:HG22	1.70	0.73
1:D:187:THR:O	1:D:191:LYS:HG2	1.88	0.72
1:C:408:ASN:HD22	1:D:414:ARG:HH12	1.37	0.72
1:D:228:GLN:HE22	1:D:267:ILE:H	1.39	0.70
1:D:187:THR:CG2	1:D:191:LYS:HD3	2.20	0.70
3:D:1606:LYS:HE2	5:D:1955:HOH:O	1.91	0.70
1:A:120:LYS:HG2	5:A:1692:HOH:O	1.92	0.69
1:D:120:LYS:HG2	5:D:1818:HOH:O	1.93	0.69
1:A:25:ASP:HB3	5:A:1724:HOH:O	1.92	0.69
1:A:408:ASN:ND2	1:B:414:ARG:HH12	1.91	0.69
1:C:414:ARG:NH1	1:D:408:ASN:HD22	1.90	0.68
1:A:372:CYS:H	1:A:410:ASN:HD21	1.42	0.66
1:A:178:ASN:HB3	1:A:181:THR:OG1	1.95	0.66
1:C:357:LYS:HE2	5:C:1748:HOH:O	1.94	0.66
1:A:329:THR:HG21	5:B:1578:HOH:O	1.95	0.65
1:D:19:ASP:H	1:D:53:GLN:HE22	1.42	0.65
1:C:157:ASN:HD21	1:C:215:TYR:H	1.42	0.65
1:D:83:LYS:HE3	5:D:1608:HOH:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:VAL:HG13	1:D:237:GLU:HG2	1.79	0.64
1:B:178:ASN:HD21	1:B:180:LYS:HB2	1.63	0.64
1:A:19:ASP:H	1:A:53:GLN:HE22	1.43	0.64
1:D:177:VAL:HG13	1:D:237:GLU:CG	2.28	0.64
1:A:307:ARG:HH22	3:D:1601:LYS:HB2	1.64	0.63
3:D:1605:LYS:HE3	5:D:1850:HOH:O	1.99	0.62
1:B:416:ARG:HG3	1:B:431:ARG:HB3	1.82	0.62
1:A:157:ASN:HD21	1:A:215:TYR:H	1.46	0.62
1:B:15:MET:HB2	5:B:1685:HOH:O	1.99	0.62
1:B:81:ALA:HB1	1:B:83:LYS:HE3	1.81	0.61
1:C:177:VAL:HG23	1:C:237:GLU:HG2	1.82	0.61
1:D:157:ASN:HD21	1:D:215:TYR:H	1.49	0.61
1:C:34:ASP:OD1	1:C:37:GLU:HG3	2.01	0.61
1:B:157:ASN:HD21	1:B:215:TYR:H	1.49	0.61
1:A:407:ASN:ND2	1:A:409:TYR:H	1.99	0.59
1:D:232:ILE:HD13	1:D:276:PRO:HB3	1.84	0.59
1:B:19:ASP:H	1:B:53:GLN:HE22	1.50	0.59
1:C:108:GLU:HG3	1:D:411:ALA:HB3	1.85	0.59
1:A:307:ARG:NH2	3:D:1601:LYS:HB2	2.18	0.58
1:D:407:ASN:ND2	1:D:409:TYR:H	1.99	0.58
1:B:362:LYS:HD2	1:B:383:GLU:CD	2.24	0.58
1:C:346:MET:HG2	1:C:347:TYR:CZ	2.39	0.58
1:A:108:GLU:HG3	1:B:411:ALA:HB3	1.86	0.58
1:D:185:ILE:HG13	1:D:234:PRO:HB3	1.86	0.58
1:D:431:ARG:C	1:D:431:ARG:HD2	2.24	0.58
1:B:329:THR:CG2	5:B:1544:HOH:O	2.51	0.57
1:B:343:ARG:NH2	1:B:349:ALA:HB1	2.18	0.57
1:D:321:HIS:HE1	1:D:335:ASP:OD2	1.87	0.57
5:C:1924:HOH:O	1:D:440:LYS:HE3	2.03	0.57
1:A:176:ASN:ND2	5:A:1756:HOH:O	2.37	0.57
1:B:319:LYS:NZ	5:B:1794:HOH:O	2.37	0.56
1:A:328:VAL:HG13	1:A:329:THR:CG2	2.35	0.56
1:C:177:VAL:HG11	1:C:186:SER:HA	1.87	0.56
5:C:1656:HOH:O	1:D:321:HIS:HD2	1.86	0.56
1:A:307:ARG:HH22	3:D:1601:LYS:CB	2.18	0.56
1:B:96:LYS:NZ	5:B:1673:HOH:O	2.39	0.56
1:A:177:VAL:HG13	1:A:237:GLU:HG2	1.88	0.55
1:A:411:ALA:HB3	1:B:108:GLU:HG3	1.89	0.55
1:B:279:LYS:HG2	5:B:1569:HOH:O	2.06	0.55
1:B:250:LYS:HG3	1:B:296:VAL:HG12	1.89	0.55
1:C:409:TYR:O	1:C:410:ASN:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:O	1:C:70:GLU:HG3	2.08	0.54
1:B:178:ASN:HD22	1:B:180:LYS:H	1.56	0.54
3:D:1604:LYS:N	5:D:1984:HOH:O	2.40	0.54
1:C:157:ASN:ND2	1:C:215:TYR:H	2.06	0.54
1:A:19:ASP:N	1:A:53:GLN:HE22	2.07	0.53
1:B:407:ASN:ND2	1:B:409:TYR:H	2.02	0.53
1:A:22:GLU:HG3	1:A:24:LYS:HG3	1.91	0.53
1:B:250:LYS:CG	1:B:296:VAL:HG12	2.38	0.53
1:B:36:ILE:O	1:B:40:GLU:HG3	2.09	0.53
1:B:267:ILE:HB	1:B:268:PRO:HD2	1.91	0.53
1:B:371:LEU:HD12	1:B:371:LEU:N	2.24	0.53
1:B:231:ASP:O	1:B:234:PRO:HD2	2.10	0.52
1:C:83:LYS:HZ3	1:C:104:VAL:HG13	1.75	0.52
1:B:178:ASN:ND2	1:B:180:LYS:H	2.08	0.52
1:A:19:ASP:H	1:A:53:GLN:NE2	2.08	0.52
1:A:109:LEU:HD23	1:A:136:MET:HG2	1.92	0.52
1:C:81:ALA:HB1	1:C:83:LYS:HE3	1.91	0.51
1:B:115:SER:O	1:B:116:ASN:HB2	2.10	0.51
1:D:249:LEU:HD13	1:D:256:ILE:HD11	1.93	0.51
4:B:1502:PLP:O4A	3:D:1602:LYS:NZ	2.42	0.51
1:D:19:ASP:N	1:D:53:GLN:HE22	2.06	0.50
1:C:403:ILE:HB	1:C:417:MET:HE1	1.92	0.50
1:A:373:GLU:OE1	3:D:1602:LYS:HD3	2.12	0.50
3:D:1606:LYS:N	5:D:1965:HOH:O	2.43	0.50
1:C:177:VAL:CG1	1:C:186:SER:HA	2.39	0.50
1:B:177:VAL:O	1:B:179:PRO:HD3	2.11	0.50
1:A:83:LYS:HD2	4:A:1501:PLP:C4A	2.41	0.50
1:C:120:LYS:CE	5:C:1890:HOH:O	2.59	0.50
1:C:177:VAL:HG23	1:C:237:GLU:CG	2.41	0.50
1:A:157:ASN:ND2	1:A:215:TYR:H	2.10	0.50
1:D:421:SER:HA	5:D:1709:HOH:O	2.11	0.50
1:C:19:ASP:H	1:C:53:GLN:HE22	1.60	0.49
1:D:19:ASP:H	1:D:53:GLN:NE2	2.10	0.49
1:C:120:LYS:HE2	5:C:1890:HOH:O	2.12	0.49
1:B:19:ASP:N	1:B:53:GLN:HE22	2.10	0.49
1:A:414:ARG:NH1	1:B:408:ASN:HD22	2.06	0.49
1:C:414:ARG:NH1	1:D:408:ASN:ND2	2.52	0.48
1:B:178:ASN:HB3	1:B:181:THR:OG1	2.13	0.48
1:C:81:ALA:HB1	1:C:83:LYS:CE	2.42	0.48
1:C:411:ALA:HB3	1:D:108:GLU:HG3	1.94	0.48
1:D:319:LYS:HE3	1:D:390:GLY:HA2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:HG3	5:A:1526:HOH:O	2.14	0.48
1:A:220:GLY:HA2	1:A:256:ILE:HG23	1.96	0.48
1:D:175:PRO:HB2	1:D:241:LYS:CB	2.44	0.48
1:D:226:GLY:HA2	3:D:1606:LYS:HE3	1.96	0.48
1:A:161:LYS:HE3	5:A:1863:HOH:O	2.14	0.48
1:C:332:VAL:HG11	1:C:387:VAL:HG11	1.96	0.48
1:C:178:ASN:HB3	1:C:181:THR:OG1	2.14	0.47
1:B:259:VAL:HG23	1:B:299:PRO:HG3	1.96	0.47
1:B:307:ARG:HH22	3:D:1602:LYS:HB3	1.79	0.47
1:B:174:ASN:HA	1:B:189:LEU:HD22	1.96	0.47
1:C:177:VAL:HG13	1:C:186:SER:HB2	1.97	0.47
1:A:18:ASN:HD21	1:A:271:LYS:NZ	2.12	0.47
1:D:157:ASN:HD22	1:D:216:VAL:HG13	1.80	0.47
1:C:18:ASN:HD21	1:C:271:LYS:NZ	2.12	0.46
1:C:250:LYS:CG	1:C:296:VAL:HG12	2.45	0.46
1:C:250:LYS:HG3	1:C:296:VAL:HG12	1.96	0.46
1:C:83:LYS:HZ3	1:C:104:VAL:CG1	2.28	0.46
1:C:15:MET:N	1:C:18:ASN:HD22	2.14	0.46
1:B:279:LYS:HE2	5:B:1555:HOH:O	2.15	0.46
1:C:407:ASN:HB3	1:D:407:ASN:HB3	1.97	0.46
1:D:347:TYR:HH	3:D:1605:LYS:N	2.13	0.46
1:B:83:LYS:HD2	4:B:1502:PLP:C4A	2.46	0.46
1:D:161:LYS:HG3	1:D:215:TYR:CZ	2.51	0.46
1:B:176:ASN:OD1	1:B:241:LYS:HD2	2.16	0.46
1:C:403:ILE:CB	1:C:417:MET:HE1	2.46	0.46
1:D:193:LYS:HE3	1:D:194:PHE:CE1	2.51	0.45
1:C:240:ARG:NE	5:C:1791:HOH:O	2.49	0.45
1:A:407:ASN:HB3	1:B:407:ASN:HB3	1.99	0.45
1:D:175:PRO:HB2	1:D:241:LYS:HB3	1.97	0.45
1:D:18:ASN:HD21	1:D:271:LYS:NZ	2.14	0.45
1:A:51:GLU:HG2	1:A:55:LYS:HE2	1.98	0.45
1:D:158:GLU:O	1:D:162:GLU:HG3	2.17	0.45
1:C:240:ARG:HD2	5:C:1791:HOH:O	2.16	0.45
1:C:83:LYS:HD2	4:C:1503:PLP:C4A	2.46	0.45
1:A:83:LYS:HD2	4:A:1501:PLP:O4A	2.16	0.45
1:D:304:GLU:O	4:D:1504:PLP:H6	2.16	0.45
1:B:412:ARG:NE	5:B:1546:HOH:O	2.33	0.45
1:B:22:GLU:HG3	1:B:24:LYS:HG3	1.99	0.45
1:B:307:ARG:NH2	3:D:1602:LYS:HB3	2.32	0.44
1:B:270:TYR:CB	1:B:273:LYS:HE3	2.45	0.44
1:C:66:LYS:HA	5:C:1838:HOH:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLU:CG	1:B:409:TYR:HE2	2.30	0.44
1:A:328:VAL:O	1:A:328:VAL:HG22	2.16	0.44
1:D:228:GLN:HG3	1:D:228:GLN:O	2.17	0.44
1:D:416:ARG:HG3	1:D:431:ARG:HB3	1.99	0.44
1:C:75:GLU:OE1	1:C:120:LYS:NZ	2.50	0.44
1:C:332:VAL:CG1	1:C:387:VAL:HG11	2.47	0.44
1:A:233:SER:HB3	1:A:234:PRO:HD3	2.00	0.44
1:B:19:ASP:H	1:B:53:GLN:NE2	2.14	0.44
1:D:357:LYS:NZ	5:D:1748:HOH:O	2.42	0.43
1:D:192:ASN:HB2	5:D:1822:HOH:O	2.18	0.43
1:D:66:LYS:O	1:D:70:GLU:HG3	2.17	0.43
1:B:233:SER:HB3	1:B:234:PRO:HD3	2.00	0.43
1:B:373:GLU:OE1	3:D:1601:LYS:HG2	2.18	0.43
1:A:328:VAL:C	1:A:329:THR:HG22	2.38	0.43
1:A:383:GLU:O	1:A:384:LEU:HD23	2.19	0.43
1:B:305:PRO:HG2	1:B:309:LEU:HD22	2.00	0.43
1:C:45:PRO:HG2	1:C:415:PRO:HB3	2.01	0.43
1:B:205:LYS:O	1:B:209:MET:HG3	2.19	0.42
1:C:58:TYR:CZ	1:C:62:ILE:HD11	2.54	0.42
1:B:175:PRO:HB2	1:B:241:LYS:HB3	2.01	0.42
1:A:65:PHE:CZ	1:A:303:LEU:HD11	2.55	0.42
1:A:69:GLU:HB2	5:A:1640:HOH:O	2.19	0.42
1:B:83:LYS:HZ2	1:B:104:VAL:HG11	1.85	0.42
1:B:343:ARG:HB2	1:B:344:PRO:HD3	2.00	0.42
1:D:104:VAL:HG22	1:D:104:VAL:O	2.20	0.42
1:C:372:CYS:SG	1:D:83:LYS:HD3	2.60	0.42
1:B:65:PHE:CZ	1:B:303:LEU:HD11	2.55	0.42
1:A:120:LYS:HE3	5:A:1692:HOH:O	2.20	0.41
1:A:104:VAL:HG22	1:A:108:GLU:OE1	2.19	0.41
1:A:179:PRO:HG2	1:A:180:LYS:NZ	2.35	0.41
1:B:67:ARG:HG3	1:B:286:ILE:HD13	2.02	0.41
3:D:1605:LYS:HD2	4:D:1504:PLP:O4A	2.20	0.41
1:B:228:GLN:NE2	1:B:228:GLN:HA	2.35	0.41
1:B:347:TYR:HH	3:D:1602:LYS:N	2.18	0.41
1:D:267:ILE:HB	1:D:268:PRO:HD2	2.02	0.41
1:B:215:TYR:N	1:B:215:TYR:CD1	2.88	0.41
1:A:343:ARG:HB2	1:A:344:PRO:HD3	2.01	0.41
1:B:328:VAL:HG12	1:B:329:THR:OG1	2.21	0.41
1:D:220:GLY:HA2	1:D:256:ILE:HG23	2.02	0.41
1:A:328:VAL:O	1:A:329:THR:HG22	2.21	0.41
1:A:205:LYS:O	1:A:209:MET:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASP:C	1:C:102:ASP:OD1	2.59	0.41
1:A:15:MET:HB2	5:A:1685:HOH:O	2.20	0.41
1:D:232:ILE:HA	1:D:232:ILE:HD12	1.88	0.40
1:A:343:ARG:HD3	1:A:351:HIS:NE2	2.36	0.40
1:C:52:GLU:HG3	5:C:1790:HOH:O	2.22	0.40
1:D:328:VAL:HG12	1:D:329:THR:OG1	2.21	0.40
1:C:211:LEU:HA	1:C:211:LEU:HD23	1.92	0.40
1:B:161:LYS:HG3	1:B:215:TYR:CZ	2.57	0.40
1:B:157:ASN:ND2	1:B:213:MET:HB3	2.37	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	432/434 (100%)	425 (98%)	6 (1%)	1 (0%)	52	48
1	B	432/434 (100%)	422 (98%)	9 (2%)	1 (0%)	52	48
1	C	432/434 (100%)	425 (98%)	6 (1%)	1 (0%)	52	48
1	D	432/434 (100%)	423 (98%)	8 (2%)	1 (0%)	52	48
All	All	1728/1736 (100%)	1695 (98%)	29 (2%)	4 (0%)	52	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	D	85	ASN
1	C	85	ASN
1	B	85	ASN

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	367/367 (100%)	355 (97%)	12 (3%)	45	43
1	B	367/367 (100%)	355 (97%)	12 (3%)	45	43
1	C	367/367 (100%)	356 (97%)	11 (3%)	48	47
1	D	367/367 (100%)	354 (96%)	13 (4%)	43	40
All	All	1468/1468 (100%)	1420 (97%)	48 (3%)	43	43

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	16	LEU
1	A	69	GLU
1	A	83	LYS
1	A	102	ASP
1	A	124	PHE
1	A	176	ASN
1	A	329	THR
1	A	373	GLU
1	A	374	SER
1	A	385	ASP
1	A	407	ASN
1	B	83	LYS
1	B	102	ASP
1	B	124	PHE
1	B	178	ASN
1	B	273	LYS
1	B	299	PRO
1	B	309	LEU
1	B	329	THR
1	B	372	CYS
1	B	407	ASN
1	B	410	ASN
1	B	430	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	83	LYS
1	C	102	ASP
1	C	124	PHE
1	C	153	LEU
1	C	176	ASN
1	C	299	PRO
1	C	373	GLU
1	C	407	ASN
1	C	410	ASN
1	C	417	MET
1	C	430	GLU
1	D	83	LYS
1	D	102	ASP
1	D	116	ASN
1	D	124	PHE
1	D	163	LEU
1	D	176	ASN
1	D	191	LYS
1	D	232	ILE
1	D	250	LYS
1	D	373	GLU
1	D	407	ASN
1	D	410	ASN
1	D	431	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	53	GLN
1	A	157	ASN
1	A	176	ASN
1	A	192	ASN
1	A	217	ASN
1	A	228	GLN
1	A	407	ASN
1	A	408	ASN
1	A	410	ASN
1	B	18	ASN
1	B	53	GLN
1	B	116	ASN
1	B	157	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	178	ASN
1	B	192	ASN
1	B	217	ASN
1	B	228	GLN
1	B	321	HIS
1	B	407	ASN
1	B	408	ASN
1	C	18	ASN
1	C	53	GLN
1	C	141	ASN
1	C	157	ASN
1	C	176	ASN
1	C	228	GLN
1	C	407	ASN
1	C	408	ASN
1	D	18	ASN
1	D	53	GLN
1	D	116	ASN
1	D	141	ASN
1	D	157	ASN
1	D	176	ASN
1	D	228	GLN
1	D	321	HIS
1	D	352	HIS
1	D	407	ASN
1	D	408	ASN

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

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
4	PLP	A	1501	-	16,16,16	1.86	6 (37%)	21,23,23	1.75	4 (19%)
4	PLP	B	1502	-	16,16,16	1.65	2 (12%)	21,23,23	2.04	5 (23%)
4	PLP	C	1503	3	16,16,16	2.65	6 (37%)	21,23,23	1.60	4 (19%)
4	PLP	D	1504	-	16,16,16	2.95	6 (37%)	21,23,23	1.70	4 (19%)
3	LYS	D	1601	-	6,9,9	0.60	0	4,10,10	1.01	0
3	LYS	D	1602	-	6,9,9	0.62	0	4,10,10	0.73	0
3	LYS	D	1603	4	6,9,9	0.50	0	4,10,10	0.56	0
3	LYS	D	1604	-	6,9,9	0.45	0	4,10,10	0.32	0
3	LYS	D	1605	-	6,9,9	0.48	0	4,10,10	0.48	0
3	LYS	D	1606	-	6,9,9	0.63	0	4,10,10	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	A	1501	-	-	0/8/8/8	0/1/1/1
4	PLP	B	1502	-	-	0/8/8/8	0/1/1/1
4	PLP	C	1503	3	-	0/8/8/8	0/1/1/1
4	PLP	D	1504	-	-	0/8/8/8	0/1/1/1
3	LYS	D	1601	-	-	0/5/9/9	0/0/0/0
3	LYS	D	1602	-	-	0/5/9/9	0/0/0/0
3	LYS	D	1603	4	-	0/5/9/9	0/0/0/0
3	LYS	D	1604	-	-	0/5/9/9	0/0/0/0
3	LYS	D	1605	-	-	0/5/9/9	0/0/0/0
3	LYS	D	1606	-	-	0/5/9/9	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1504	PLP	O4A-C4A	-7.92	0.96	1.21
4	C	1503	PLP	C3-C2	-5.87	1.36	1.40
4	C	1503	PLP	O4A-C4A	-4.92	1.06	1.21
4	D	1504	PLP	C4-C3	-3.72	1.36	1.40
4	A	1501	PLP	C4-C3	-2.62	1.37	1.40
4	B	1502	PLP	C3-C2	-2.40	1.39	1.40
4	D	1504	PLP	P-O1P	-2.38	1.43	1.51
4	A	1501	PLP	P-O3P	-2.25	1.46	1.54
4	C	1503	PLP	C4-C3	-2.24	1.37	1.40
4	C	1503	PLP	C6-N1	2.09	1.38	1.34
4	A	1501	PLP	C2-N1	2.23	1.38	1.34
4	A	1501	PLP	C6-N1	2.41	1.39	1.34
4	A	1501	PLP	C2A-C2	2.45	1.55	1.50
4	D	1504	PLP	C6-N1	3.07	1.41	1.34
4	C	1503	PLP	C2-N1	3.32	1.41	1.34
4	D	1504	PLP	C2A-C2	3.42	1.57	1.50
4	A	1501	PLP	C4-C4A	4.52	1.57	1.46
4	B	1502	PLP	C4-C4A	4.54	1.57	1.46
4	D	1504	PLP	C4-C4A	4.67	1.57	1.46
4	C	1503	PLP	C4-C4A	4.69	1.57	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1501	PLP	O4A-C4A-C4	-4.38	116.27	125.11
4	B	1502	PLP	O4A-C4A-C4	-3.97	117.09	125.11
4	B	1502	PLP	C3-C2-N1	-2.40	117.29	120.61
4	A	1501	PLP	C3-C2-N1	-2.14	117.66	120.61
4	C	1503	PLP	C2A-C2-C3	2.81	124.42	121.04
4	D	1504	PLP	O4P-C5A-C5	2.90	113.78	108.99
4	B	1502	PLP	O4P-C5A-C5	3.04	114.01	108.99
4	C	1503	PLP	O4P-C5A-C5	3.04	114.03	108.99
4	A	1501	PLP	C5A-C5-C4	3.08	126.65	121.47
4	C	1503	PLP	C5A-C5-C4	3.11	126.69	121.47
4	D	1504	PLP	C5A-C5-C4	3.13	126.74	121.47
4	D	1504	PLP	O4A-C4A-C4	3.27	131.73	125.11
4	B	1502	PLP	C5A-C5-C4	3.38	127.15	121.47
4	C	1503	PLP	O4A-C4A-C4	3.73	132.66	125.11
4	D	1504	PLP	C2A-C2-C3	3.90	125.74	121.04
4	A	1501	PLP	C2A-C2-C3	4.00	125.86	121.04
4	B	1502	PLP	C2A-C2-C3	5.74	127.96	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	PLP	2	0
4	B	1502	PLP	2	0
4	C	1503	PLP	1	0
4	D	1504	PLP	2	0
3	D	1601	LYS	4	0
3	D	1602	LYS	5	0
3	D	1603	LYS	1	0
3	D	1604	LYS	1	0
3	D	1605	LYS	4	0
3	D	1606	LYS	3	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	434/434 (100%)	-0.60	0 100 100	9, 15, 27, 33	0
1	B	434/434 (100%)	-0.29	17 (3%) 43 45	9, 18, 36, 42	0
1	C	434/434 (100%)	-0.55	10 (2%) 64 64	8, 15, 30, 40	0
1	D	434/434 (100%)	-0.50	11 (2%) 61 61	8, 15, 31, 39	0
All	All	1736/1736 (100%)	-0.48	38 (2%) 65 66	8, 15, 32, 42	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	ASN	4.1
1	B	180	LYS	3.9
1	C	181	THR	3.7
1	B	181	THR	3.5
1	B	360	ASN	3.5
1	B	183	PRO	3.4
1	B	187	THR	3.4
1	B	179	PRO	3.4
1	D	181	THR	3.3
1	D	187	THR	3.3
1	C	187	THR	3.3
1	C	184	LYS	3.3
1	D	180	LYS	3.2
1	D	184	LYS	3.2
1	C	183	PRO	3.1
1	D	178	ASN	3.0
1	B	184	LYS	3.0
1	B	176	ASN	2.9
1	D	360	ASN	2.8
1	C	178	ASN	2.7
1	B	273	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	GLY	2.5
1	C	179	PRO	2.5
1	D	182	HIS	2.5
1	B	25	ASP	2.4
1	C	15	MET	2.4
1	D	179	PRO	2.4
1	D	294	ASP	2.4
1	B	188	GLY	2.3
1	B	182	HIS	2.2
1	C	182	HIS	2.2
1	D	183	PRO	2.2
1	C	294	ASP	2.1
1	D	25	ASP	2.1
1	B	362	LYS	2.1
1	B	361	GLU	2.1
1	C	297	GLU	2.0
1	B	177	VAL	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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	LYS	D	1602	10/10	0.84	0.20	4.25	33,34,35,36	0
3	LYS	D	1601	10/10	0.85	0.20	3.48	34,35,37,42	0
3	LYS	D	1605	10/10	0.90	0.15	2.40	25,28,38,39	0
3	LYS	D	1606	10/10	0.83	0.16	1.58	33,34,35,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LYS	D	1603	10/10	0.92	0.13	1.30	24,27,35,36	0
3	LYS	D	1604	10/10	0.86	0.13	1.01	42,47,49,49	0
4	PLP	B	1502	16/16	0.97	0.11	-0.01	15,17,20,30	0
4	PLP	A	1501	16/16	0.97	0.10	-0.05	9,12,15,31	0
4	PLP	C	1503	16/16	0.97	0.09	-0.37	11,12,17,26	0
4	PLP	D	1504	16/16	0.98	0.08	-0.76	9,11,16,27	0
2	MG	C	1607	1/1	0.98	0.02	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.