W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 03:32 am GMT

PDB ID	:	1HKV
Title	:	mycobacterium diaminopimelate dicarboxylase (lysa)
Authors	:	Gokulan, K.; Rupp, B.; Pavelka Jr, M.S.; Jacobs Jr, W.R.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2003-03-11
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36
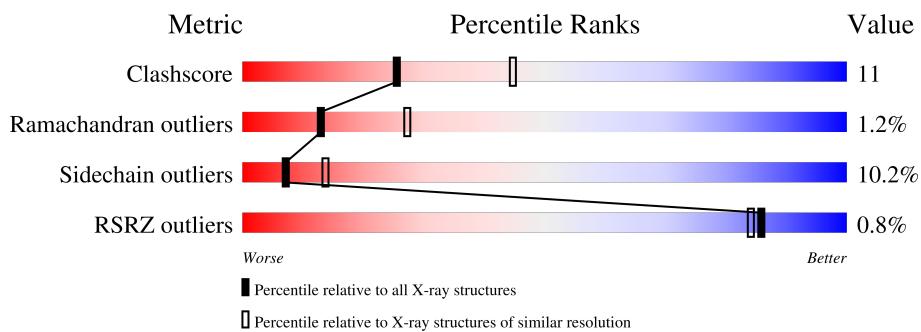
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
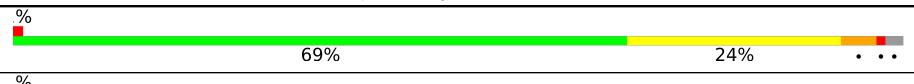
The reported resolution of this entry is 2.60 Å.

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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	453	69% 24% · · ··
1	B	453	66% 26% 6% ·

2 Entry composition ⓘ
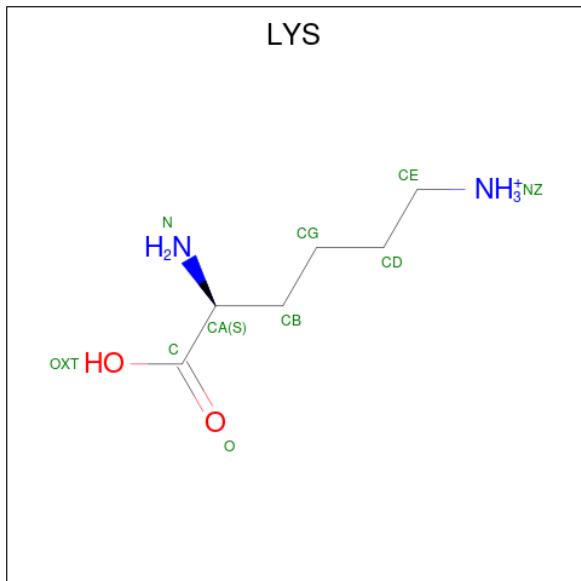
There are 4 unique types of molecules in this entry. The entry contains 6946 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.
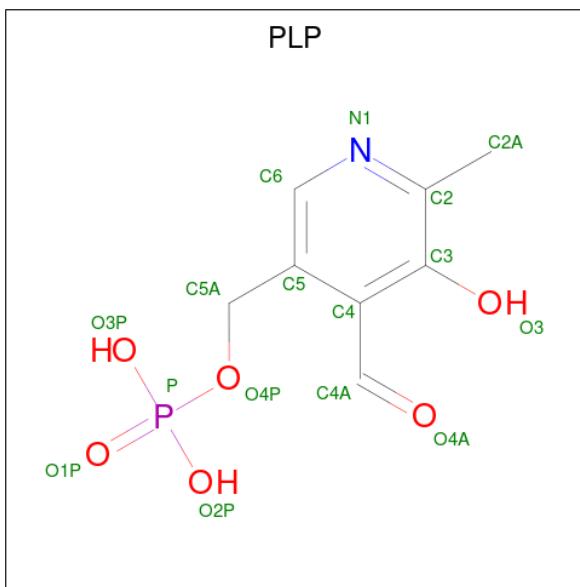
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3330	2089	591	639	11			
1	B	446	Total	C	N	O	S	0	0	0
			3330	2089	591	639	11			

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).

LYS

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

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

PLP

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		
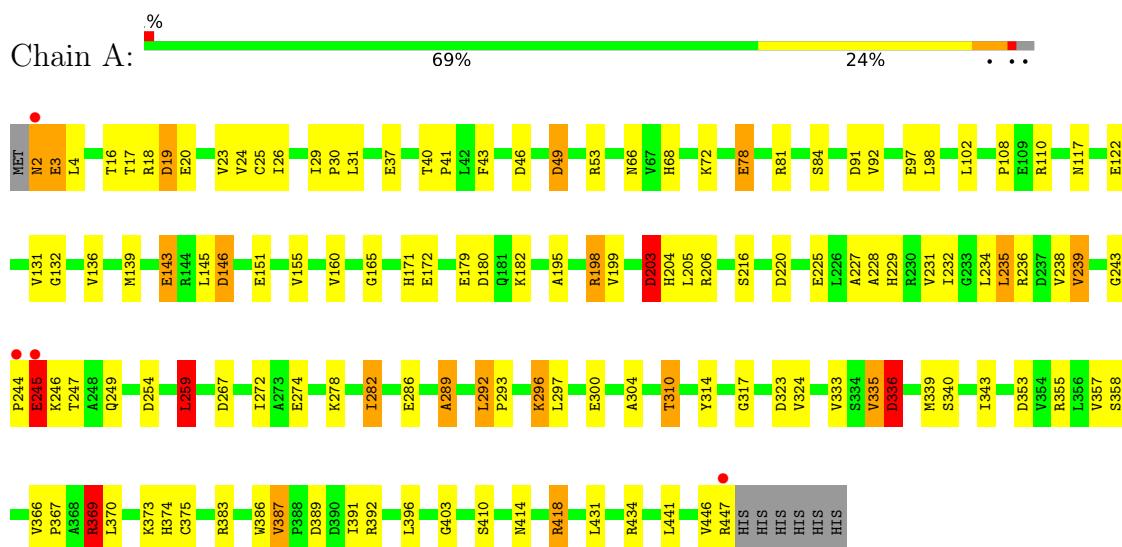
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	127	Total	O	0	0
			127	127		
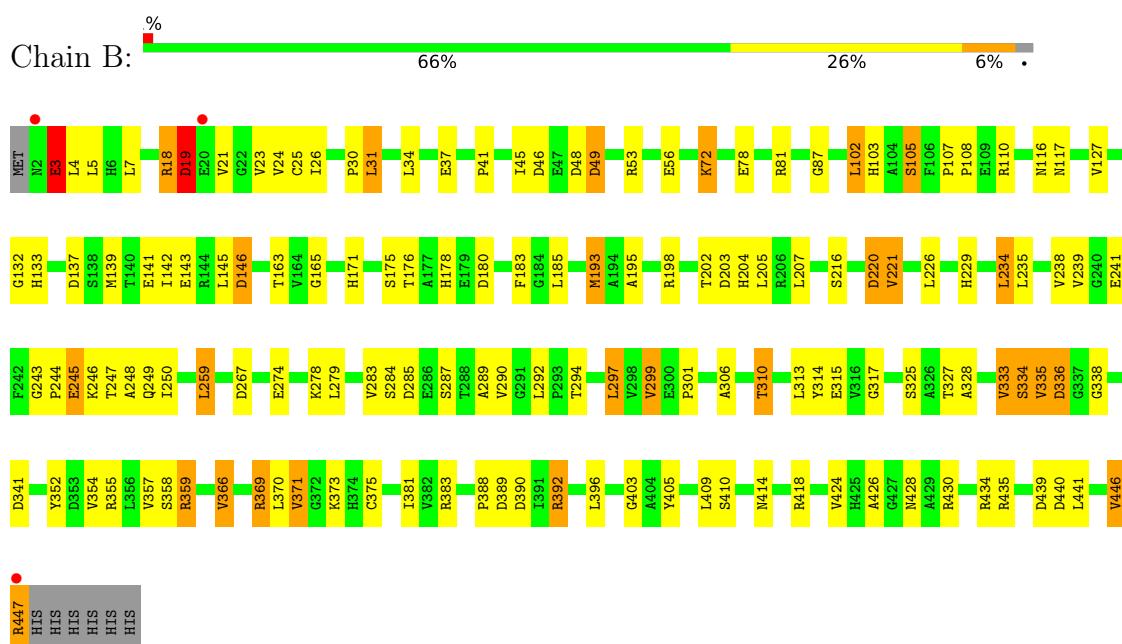
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DIAMINOPIMELATE DECARBOXYLASE

Chain A:

• Molecule 1: DIAMINOPIMELATE DECARBOXYLASE

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.45Å 111.45Å 238.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60 29.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (18.00-2.60) 98.3 (29.92-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.268 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 24.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6946	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.41	21/3392 (0.6%)	0.95	15/4626 (0.3%)
1	B	1.39	17/3392 (0.5%)	0.93	15/4626 (0.3%)
All	All	1.40	38/6784 (0.6%)	0.94	30/9252 (0.3%)

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

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	ASP	CB-CG	-7.64	1.35	1.51
1	B	245	GLU	CG-CD	7.58	1.63	1.51
1	B	143	GLU	CD-OE1	6.93	1.33	1.25
1	A	386	TRP	CG-CD1	6.79	1.46	1.36
1	A	203	ASP	CB-CG	6.76	1.66	1.51
1	B	274	GLU	CD-OE2	6.63	1.32	1.25
1	B	336	ASP	CB-CG	-6.54	1.38	1.51
1	B	245	GLU	CB-CG	6.44	1.64	1.52
1	A	20	GLU	CD-OE1	6.34	1.32	1.25
1	B	241	GLU	CD-OE1	-6.14	1.18	1.25
1	A	324	VAL	CB-CG1	-6.01	1.40	1.52
1	B	245	GLU	CD-OE1	5.92	1.32	1.25
1	A	387	VAL	CB-CG1	-5.90	1.40	1.52
1	B	3	GLU	CG-CD	5.82	1.60	1.51
1	A	274	GLU	CD-OE1	5.79	1.32	1.25
1	A	199	VAL	CA-CB	5.78	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLU	CG-CD	5.76	1.60	1.51
1	A	245	GLU	CD-OE2	5.74	1.31	1.25
1	A	304	ALA	CA-CB	-5.69	1.40	1.52
1	A	19	ASP	CB-CG	-5.66	1.39	1.51
1	B	37	GLU	CD-OE1	5.63	1.31	1.25
1	A	20	GLU	CG-CD	5.54	1.60	1.51
1	B	21	VAL	CB-CG1	5.52	1.64	1.52
1	A	259	LEU	CA-CB	-5.51	1.41	1.53
1	B	141	GLU	CD-OE1	5.51	1.31	1.25
1	A	43	PHE	CB-CG	-5.51	1.42	1.51
1	A	3	GLU	CG-CD	5.47	1.60	1.51
1	B	426	ALA	CA-CB	5.46	1.64	1.52
1	B	56	GLU	CD-OE2	5.35	1.31	1.25
1	A	182	LYS	CD-CE	5.29	1.64	1.51
1	A	78	GLU	CD-OE1	-5.25	1.19	1.25
1	B	245	GLU	CD-OE2	5.19	1.31	1.25
1	A	172	GLU	CD-OE1	5.18	1.31	1.25
1	B	352	TYR	CD2-CE2	-5.18	1.31	1.39
1	B	375	CYS	CB-SG	-5.14	1.73	1.81
1	A	92	VAL	CB-CG1	-5.12	1.42	1.52
1	B	274	GLU	CD-OE1	5.11	1.31	1.25
1	A	151	GLU	CD-OE2	5.03	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	LEU	O-C-N	-9.14	107.66	123.20
1	A	203	ASP	CB-CG-OD2	8.16	125.65	118.30
1	B	440	ASP	CB-CG-OD2	7.38	124.94	118.30
1	B	46	ASP	CB-CG-OD2	7.34	124.91	118.30
1	B	137	ASP	CB-CG-OD2	6.88	124.50	118.30
1	A	369	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	180	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	146	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	389	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	389	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	220	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	19	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	323	ASP	CB-CG-OD2	5.91	123.61	118.30
1	A	267	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	267	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	46	ASP	CB-CG-OD2	5.77	123.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	341	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	259	LEU	CB-CA-C	5.52	120.69	110.20
1	B	390	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	49	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	353	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	439	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	146	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	2	ASN	CB-CA-C	5.32	121.04	110.40
1	B	203	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	336	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	180	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	418	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	B	285	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLY	Peptide
1	A	259	LEU	Mainchain
1	A	289	ALA	Mainchain

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	3330	0	3312	69	0
1	B	3330	0	3312	81	0
2	A	10	0	12	1	0
2	B	10	0	12	0	0
3	A	15	0	7	1	0
3	B	15	0	7	0	0
4	A	109	0	0	4	0
4	B	127	0	0	4	0
All	All	6946	0	6662	142	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 11.

All (142) 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:259:LEU:H	1:B:259:LEU:HD12	1.22	1.01
1:B:259:LEU:H	1:B:259:LEU:CD1	1.78	0.96
1:A:239:VAL:HG12	1:A:247:THR:HG21	1.54	0.89
1:B:259:LEU:HD12	1:B:259:LEU:N	1.87	0.87
1:B:239:VAL:HG12	1:B:247:THR:HG21	1.61	0.83
1:B:283:VAL:O	1:B:287:SER:HB2	1.83	0.79
1:A:369:ARG:HG2	1:A:383:ARG:O	1.84	0.78
1:B:369:ARG:HG2	1:B:383:ARG:O	1.85	0.77
1:A:245:GLU:HG2	1:A:246:LYS:H	1.53	0.73
1:B:359:ARG:HH11	1:B:359:ARG:HG3	1.57	0.70
1:A:245:GLU:HG2	1:A:246:LYS:N	2.07	0.70
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.58	0.68
1:A:171:HIS:HA	1:A:220:ASP:OD1	1.94	0.67
1:A:16:THR:HG22	1:A:26:ILE:HG12	1.78	0.65
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.61	0.64
1:B:4:LEU:HD23	1:B:388:PRO:HD3	1.79	0.64
1:A:41:PRO:HG3	1:A:336:ASP:HB3	1.80	0.63
1:B:31:LEU:HD23	1:B:357:VAL:HG21	1.80	0.63
1:B:139:MET:HE2	1:B:195:ALA:HB2	1.80	0.62
1:B:284:SER:HA	1:B:294:THR:HG22	1.80	0.62
1:A:314:TYR:HB3	1:A:335:VAL:HG22	1.81	0.62
1:B:314:TYR:HB3	1:B:335:VAL:HG22	1.80	0.62
1:B:244:PRO:HA	1:B:247:THR:OG1	1.99	0.62
1:A:146:ASP:OD2	1:A:204:HIS:HB2	2.01	0.61
1:A:310:THR:HG23	1:A:403:GLY:HA3	1.83	0.60
1:A:278:LYS:O	1:A:282:ILE:HG23	2.01	0.60
1:B:306:ALA:O	1:B:403:GLY:HA3	2.02	0.60
1:A:286:GLU:HG3	4:A:2072:HOH:O	2.03	0.59
1:A:236:ARG:HG2	1:A:236:ARG:HH21	1.68	0.59
1:A:143:GLU:HG3	1:A:198:ARG:NH2	2.18	0.59
1:B:103:HIS:HD2	4:B:2033:HOH:O	1.85	0.59
1:A:374:HIS:CD2	1:A:414:ASN:HD22	2.21	0.58
1:B:78:GLU:OE2	1:B:81:ARG:NH2	2.37	0.58
1:B:290:VAL:HG23	1:B:292:LEU:HD23	1.85	0.58
1:B:18:ARG:HH11	1:B:18:ARG:CG	2.16	0.58
1:A:117:ASN:HD21	1:B:317:GLY:HA3	1.67	0.58
1:A:122:GLU:OE1	1:B:373:LYS:NZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASP:HB2	1:B:23:VAL:H	1.69	0.57
1:A:282:ILE:O	1:A:286:GLU:HB2	2.05	0.57
1:A:418:ARG:NH1	1:B:418:ARG:HH22	2.04	0.56
1:A:66:ASN:ND2	4:A:2030:HOH:O	2.39	0.56
1:B:127:VAL:HG23	4:B:2045:HOH:O	2.06	0.56
1:B:405:TYR:O	1:B:409:LEU:HD12	2.07	0.55
1:A:19:ASP:HB2	1:A:23:VAL:H	1.72	0.55
1:A:317:GLY:HA3	1:B:117:ASN:HD21	1.71	0.55
1:B:116:ASN:HB3	1:B:183:PHE:CE1	2.42	0.55
1:A:374:HIS:HD2	1:A:414:ASN:HD22	1.55	0.54
1:B:239:VAL:HG12	1:B:247:THR:CG2	2.37	0.54
1:A:333:VAL:HG22	1:A:370:LEU:HD12	1.89	0.53
1:B:279:LEU:HB3	1:B:297:LEU:HD11	1.90	0.53
1:B:410:SER:OG	1:B:418:ARG:HD3	2.08	0.53
1:A:108:PRO:O	1:A:131:VAL:O	2.27	0.53
1:B:335:VAL:HG22	1:B:336:ASP:H	1.74	0.52
1:B:207:LEU:HD23	1:B:250:ILE:HD11	1.92	0.52
1:B:132:GLY:O	1:B:133:HIS:ND1	2.42	0.52
1:A:340:SER:HB3	1:A:374:HIS:NE2	2.24	0.52
1:B:3:GLU:C	1:B:5:LEU:H	2.14	0.51
1:B:165:GLY:O	1:B:175:SER:HA	2.10	0.51
1:B:176:THR:HG22	1:B:178:HIS:H	1.75	0.51
1:A:78:GLU:OE1	1:A:81:ARG:NH2	2.43	0.51
1:A:139:MET:HE2	1:A:195:ALA:HB2	1.93	0.51
1:A:24:VAL:O	1:A:31:LEU:HD13	2.10	0.51
1:A:40:THR:HB	1:A:41:PRO:HA	1.93	0.51
1:A:97:GLU:OE1	1:B:414:ASN:HA	2.11	0.51
1:A:84:SER:HA	1:A:110:ARG:NH1	2.27	0.50
1:A:375:CYS:O	1:B:72:LYS:HE3	2.12	0.49
1:A:235:LEU:O	1:A:238:VAL:HG22	2.12	0.49
1:A:229:HIS:ND1	1:A:286:GLU:OE2	2.29	0.49
1:B:185:LEU:HD13	1:B:195:ALA:HB2	1.95	0.49
1:A:19:ASP:HB2	1:A:23:VAL:N	2.28	0.48
1:A:259:LEU:N	1:A:259:LEU:HD23	2.28	0.48
1:A:418:ARG:HH12	1:B:418:ARG:HH22	1.59	0.48
1:B:424:VAL:HG23	1:B:424:VAL:O	2.13	0.48
1:B:392:ARG:HD3	4:B:2107:HOH:O	2.13	0.48
1:A:49:ASP:O	1:A:53:ARG:HG3	2.13	0.48
1:B:299:VAL:HG13	1:B:301:PRO:HD3	1.96	0.48
1:B:193:MET:HE1	1:B:238:VAL:HA	1.95	0.48
1:A:216:SER:OG	2:A:501:LYS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:MET:HB2	1:A:343:ILE:HD12	1.96	0.47
1:A:30:PRO:HG3	4:A:2009:HOH:O	2.15	0.47
1:A:108:PRO:O	1:A:131:VAL:HA	2.14	0.47
1:A:228:ALA:O	1:A:232:ILE:HG12	2.13	0.47
1:B:193:MET:CE	1:B:238:VAL:HG22	2.45	0.47
1:A:431:LEU:HD21	1:A:434:ARG:HB3	1.96	0.47
1:A:225:GLU:HA	1:A:282:ILE:HD12	1.97	0.46
1:B:359:ARG:HH11	1:B:359:ARG:CG	2.26	0.46
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.78	0.46
1:B:26:ILE:HG22	1:B:424:VAL:HG21	1.97	0.46
1:A:358:SER:HB3	1:A:396:LEU:HB2	1.98	0.45
1:A:254:ASP:OD2	1:A:300:GLU:OE1	2.33	0.45
1:B:234:LEU:O	1:B:238:VAL:HG23	2.16	0.45
1:A:68:HIS:HB3	1:A:91:ASP:OD1	2.17	0.45
1:B:315:GLU:H	1:B:336:ASP:HB2	1.82	0.45
1:A:335:VAL:HG13	1:A:336:ASP:N	2.32	0.44
1:B:41:PRO:O	1:B:435:ARG:NH1	2.51	0.44
1:B:146:ASP:HA	1:B:205:LEU:CD1	2.48	0.44
1:B:325:SER:HB3	1:B:328:ALA:HB3	1.99	0.44
1:B:333:VAL:HG22	1:B:370:LEU:HD12	2.00	0.44
1:A:165:GLY:HA2	1:A:179:GLU:HB2	2.00	0.44
1:B:25:CYS:SG	1:B:30:PRO:HA	2.58	0.44
1:B:107:PRO:HA	1:B:108:PRO:HD3	1.78	0.44
1:A:136:VAL:CG2	1:A:160:VAL:HG12	2.48	0.43
1:B:171:HIS:HA	1:B:220:ASP:OD1	2.19	0.43
1:A:239:VAL:HG11	1:A:292:LEU:HD11	1.99	0.43
1:A:24:VAL:HG21	1:A:357:VAL:HG12	2.00	0.43
1:A:236:ARG:HG2	1:A:236:ARG:NH2	2.34	0.43
1:A:292:LEU:HD12	1:A:293:PRO:HD2	2.01	0.43
1:B:246:LYS:O	1:B:249:GLN:HG2	2.18	0.43
1:B:299:VAL:CG1	1:B:301:PRO:HD3	2.48	0.43
1:A:447:ARG:CZ	1:A:447:ARG:HA	2.49	0.43
1:A:155:VAL:O	1:A:155:VAL:HG23	2.19	0.42
1:A:227:ALA:O	1:A:231:VAL:HG23	2.19	0.42
1:B:284:SER:HA	1:B:294:THR:CG2	2.47	0.42
1:A:29:ILE:HA	1:A:30:PRO:HD3	1.90	0.42
1:A:203:ASP:OD2	1:A:203:ASP:N	2.49	0.42
1:B:354:VAL:O	1:B:354:VAL:HG13	2.19	0.42
1:A:366:VAL:HG13	1:A:367:PRO:HD2	2.02	0.42
1:B:146:ASP:OD2	1:B:204:HIS:HB2	2.20	0.41
1:B:146:ASP:OD2	1:B:202:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASN:HD21	1:B:317:GLY:CA	2.33	0.41
1:A:296:LYS:CD	4:A:2030:HOH:O	2.68	0.41
1:B:45:ILE:HA	1:B:310:THR:HB	2.01	0.41
1:B:193:MET:HE1	1:B:238:VAL:HG22	2.02	0.41
1:B:221:VAL:CG2	1:B:279:LEU:CD1	2.98	0.41
1:B:235:LEU:HD21	1:B:250:ILE:CG2	2.50	0.41
1:B:366:VAL:HG13	4:B:2090:HOH:O	2.21	0.41
1:A:410:SER:OG	1:A:418:ARG:HD3	2.20	0.41
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.79	0.41
1:B:102:LEU:O	1:B:105:SER:N	2.53	0.41
1:B:334:SER:HA	1:B:371:VAL:HG12	2.01	0.41
1:A:300:GLU:O	3:A:500:PLP:H6	2.20	0.41
1:B:24:VAL:HG21	1:B:357:VAL:HG12	2.02	0.41
1:B:226:LEU:O	1:B:229:HIS:HB3	2.21	0.41
1:B:446:VAL:O	1:B:447:ARG:HB2	2.20	0.41
1:B:358:SER:HB3	1:B:396:LEU:HB2	2.02	0.41
1:B:49:ASP:OD1	1:B:53:ARG:NH2	2.53	0.40
1:B:87:GLY:HA2	1:B:110:ARG:NH1	2.36	0.40
1:B:234:LEU:O	1:B:234:LEU:HD22	2.22	0.40
1:A:225:GLU:HA	1:A:282:ILE:CD1	2.51	0.40
1:B:338:GLY:HA2	1:B:381:ILE:HD11	2.03	0.40
1:A:17:THR:OG1	1:A:25:CYS:HB2	2.21	0.40
1:B:235:LEU:HD21	1:B:250:ILE:HG21	2.03	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	444/453 (98%)	415 (94%)	25 (6%)	4 (1%)	17	35
1	B	444/453 (98%)	412 (93%)	25 (6%)	7 (2%)	9	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	888/906 (98%)	827 (93%)	50 (6%)	11 (1%)	13 27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ALA
1	B	245	GLU
1	A	243	GLY
1	B	19	ASP
1	B	289	ALA
1	A	245	GLU
1	B	105	SER
1	B	243	GLY
1	B	248	ALA
1	B	446	VAL
1	A	244	PRO

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	353/360 (98%)	319 (90%)	34 (10%)	8 16
1	B	353/360 (98%)	316 (90%)	37 (10%)	7 13
All	All	706/720 (98%)	635 (90%)	71 (10%)	7 14

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	GLU
1	A	4	LEU
1	A	18	ARG
1	A	72	LYS
1	A	98	LEU
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	143	GLU
1	A	145	LEU
1	A	198	ARG
1	A	203	ASP
1	A	205	LEU
1	A	206	ARG
1	A	234	LEU
1	A	235	LEU
1	A	239	VAL
1	A	249	GLN
1	A	259	LEU
1	A	272	ILE
1	A	282	ILE
1	A	292	LEU
1	A	296	LYS
1	A	297	LEU
1	A	310	THR
1	A	335	VAL
1	A	336	ASP
1	A	355	ARG
1	A	369	ARG
1	A	373	LYS
1	A	387	VAL
1	A	391	ILE
1	A	392	ARG
1	A	441	LEU
1	A	446	VAL
1	B	3	GLU
1	B	7	LEU
1	B	18	ARG
1	B	19	ASP
1	B	31	LEU
1	B	34	LEU
1	B	48	ASP
1	B	72	LYS
1	B	102	LEU
1	B	142	ILE
1	B	145	LEU
1	B	163	THR
1	B	193	MET
1	B	198	ARG
1	B	216	SER

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Mol	Chain	Res	Type
1	B	221	VAL
1	B	234	LEU
1	B	259	LEU
1	B	278	LYS
1	B	297	LEU
1	B	299	VAL
1	B	310	THR
1	B	313	LEU
1	B	327	THR
1	B	333	VAL
1	B	334	SER
1	B	335	VAL
1	B	355	ARG
1	B	359	ARG
1	B	366	VAL
1	B	369	ARG
1	B	371	VAL
1	B	392	ARG
1	B	428	ASN
1	B	434	ARG
1	B	441	LEU
1	B	447	ARG

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

Mol	Chain	Res	Type
1	A	15	ASN
1	A	36	GLN
1	A	66	ASN
1	A	68	HIS
1	A	116	ASN
1	A	117	ASN
1	A	374	HIS
1	B	66	ASN
1	B	68	HIS
1	B	116	ASN
1	B	117	ASN
1	B	229	HIS
1	B	351	GLN
1	B	374	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	LYS	A	501	-	8,9,9	1.48	2 (25%)	9,10,10	1.15	2 (22%)
3	PLP	A	500	1	15,15,16	2.02	4 (26%)	20,22,23	1.53	5 (25%)
2	LYS	B	501	-	8,9,9	1.94	2 (25%)	9,10,10	2.78	3 (33%)
3	PLP	B	500	1	15,15,16	2.06	5 (33%)	20,22,23	1.42	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	LYS	A	501	-	-	7/9/9/9	-
3	PLP	A	500	1	-	0/6/6/8	0/1/1/1
2	LYS	B	501	-	-	5/9/9/9	-
3	PLP	B	500	1	-	5/6/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	C4A-C4	-5.11	1.41	1.51
3	B	500	PLP	C4A-C4	-5.10	1.41	1.51
3	A	500	PLP	C2-N1	3.65	1.40	1.33
2	B	501	LYS	CG-CB	3.57	1.67	1.52
3	A	500	PLP	C6-N1	2.91	1.40	1.34
3	A	500	PLP	C3-C2	-2.78	1.38	1.40
2	B	501	LYS	O-C	2.71	1.30	1.22
3	B	500	PLP	C3-C2	-2.71	1.38	1.40
3	B	500	PLP	P-O3P	-2.57	1.44	1.54
3	B	500	PLP	C5-C4	2.50	1.43	1.40
2	A	501	LYS	CB-CA	2.29	1.58	1.53
2	A	501	LYS	CD-CE	2.17	1.62	1.51
3	B	500	PLP	C2-N1	2.11	1.37	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LYS	OXT-C-O	-6.76	108.74	124.09
2	B	501	LYS	OXT-C-CA	4.14	127.49	113.38
3	A	500	PLP	O4P-C5A-C5	3.50	116.02	109.35
3	B	500	PLP	O4P-C5A-C5	3.37	115.78	109.35
3	A	500	PLP	C5-C6-N1	-2.71	119.30	123.82
3	A	500	PLP	O3P-P-O4P	2.66	113.80	106.73
2	B	501	LYS	CB-CA-C	2.42	116.07	110.30
2	A	501	LYS	OXT-C-O	-2.36	118.73	124.09
3	B	500	PLP	O3-C3-C4	2.28	124.11	118.10
2	A	501	LYS	OXT-C-CA	2.26	121.08	113.38
3	B	500	PLP	C5-C6-N1	-2.23	120.10	123.82
3	A	500	PLP	C6-C5-C4	2.14	119.84	118.16
3	A	500	PLP	O3P-P-O2P	2.02	115.34	107.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LYS	C-CA-CB-CG
3	B	500	PLP	C4-C5-C5A-O4P
3	B	500	PLP	C6-C5-C5A-O4P
3	B	500	PLP	C5A-O4P-P-O1P
2	A	501	LYS	OXT-C-CA-N
2	B	501	LYS	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	A	501	LYS	O-C-CA-CB
2	A	501	LYS	OXT-C-CA-CB
2	A	501	LYS	CG-CD-CE-NZ
2	B	501	LYS	O-C-CA-CB
2	A	501	LYS	O-C-CA-N
2	B	501	LYS	O-C-CA-N
2	B	501	LYS	OXT-C-CA-CB
3	B	500	PLP	C5A-O4P-P-O3P
2	B	501	LYS	CE-CD-CG-CB
2	A	501	LYS	N-CA-CB-CG
3	B	500	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LYS	1	0
3	A	500	PLP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	446/453 (98%)	-0.61	4 (0%)	84	82	34, 48, 70, 89	0
1	B	446/453 (98%)	-0.58	3 (0%)	87	86	35, 49, 69, 93	0
All	All	892/906 (98%)	-0.59	7 (0%)	86	84	34, 48, 70, 93	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASN	4.3
1	A	447	ARG	4.0
1	A	245	GLU	3.1
1	A	244	PRO	2.7
1	B	447	ARG	2.4
1	A	2	ASN	2.2
1	B	20	GLU	2.1

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 ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LYS	B	501	10/10	0.69	0.33	63,70,72,73	0
2	LYS	A	501	10/10	0.76	0.30	71,74,75,75	0
3	PLP	B	500	15/16	0.98	0.17	35,64,75,76	0
3	PLP	A	500	15/16	0.99	0.13	33,50,58,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.