



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:01 PM UTC

PDB ID : 6Q72 / pdb_00006q72
Title : Crystal structure of the alanine racemase from *Bacillus subtilis* in the presence of only PEG 4000 and Magnesium chloride in the crystallization condition
Authors : Bernardo-Garcia, N.; Gago, F.; Hermoso, J.A.
Deposited on : 2018-12-12
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

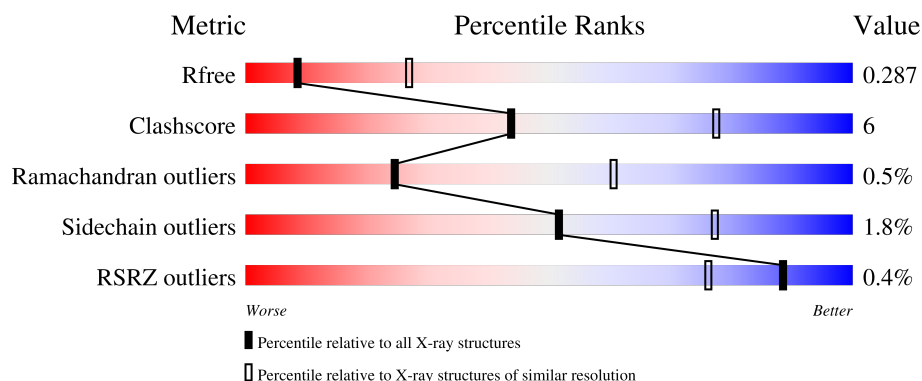
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	
1	B	394	
1	D	394	
1	E	394	

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	PLP	D	401	-	-	X	-
2	PLP	E	401	-	-	X	-

2 Entry composition [i](#)

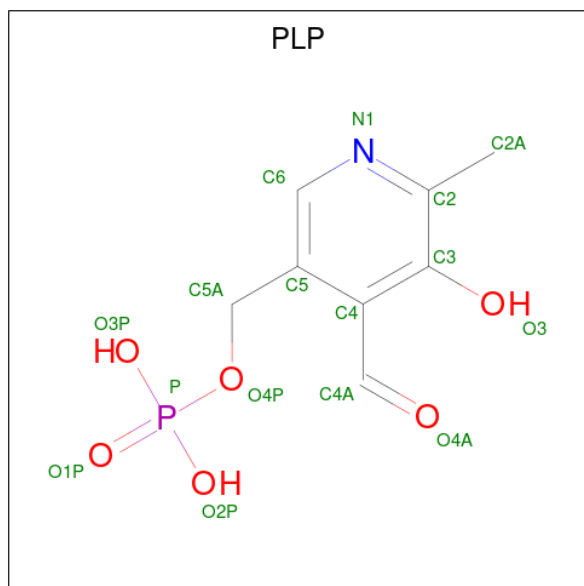
There are 4 unique types of molecules in this entry. The entry contains 12107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alanine racemase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3009	1924	527	544	14			
1	B	386	Total	C	N	O	S	0	0	0
			3009	1924	527	544	14			
1	D	386	Total	C	N	O	S	0	0	0
			3009	1924	527	544	14			
1	E	386	Total	C	N	O	S	0	0	0
			3009	1924	527	544	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

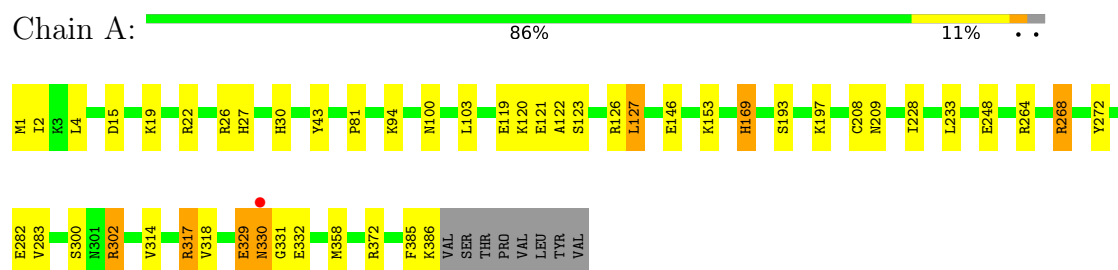
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	1	Total	O	0	0
			1	1		

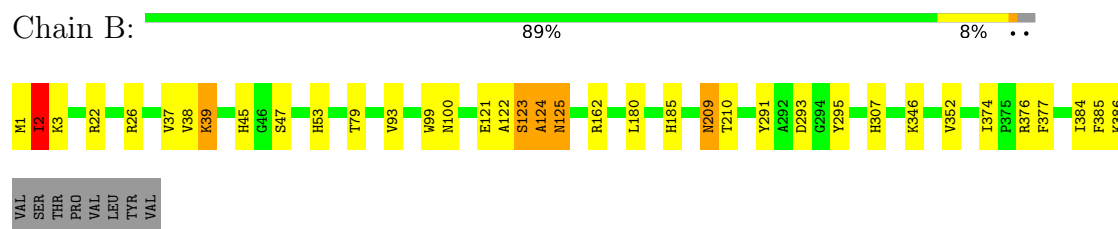
3 Residue-property plots

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.

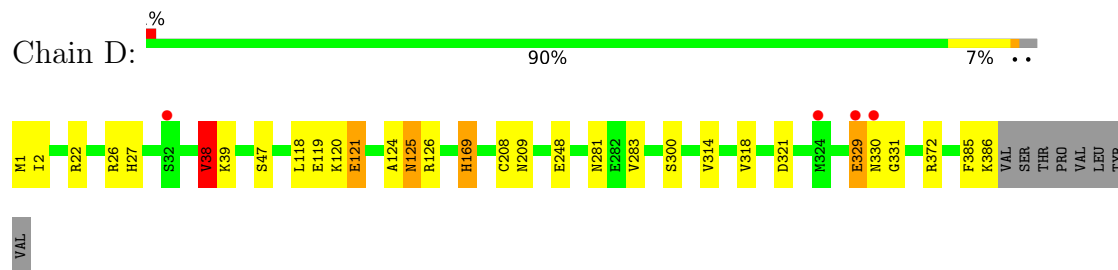
• Molecule 1: Alanine racemase 2



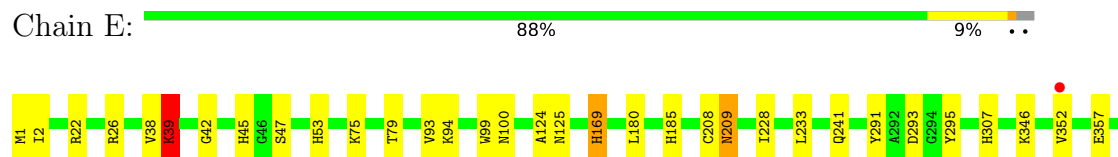
• Molecule 1: Alanine racemase 2



• Molecule 1: Alanine racemase 2



• Molecule 1: Alanine racemase 2



Y364		I374	P375	R376	F377		I384	F385	K386	VAL	SER	THR	PRO	VAL	LEU	TYR	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.43Å 110.53Å 88.51Å 90.00° 116.42° 90.00°	Depositor
Resolution (Å)	45.32 – 3.00 45.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.32-3.00) 99.0 (45.32-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.228 , 0.285 0.233 , 0.287	Depositor DCC
R_{free} test set	1527 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12107	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.98	12/3063 (0.4%)	1.00	9/4135 (0.2%)
1	B	0.92	7/3063 (0.2%)	0.94	10/4135 (0.2%)
1	D	0.90	7/3063 (0.2%)	0.97	11/4135 (0.3%)
1	E	0.91	6/3063 (0.2%)	0.94	12/4135 (0.3%)
All	All	0.93	32/12252 (0.3%)	0.96	42/16540 (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	B	0	1
1	D	1	0
1	E	0	1
All	All	1	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	209	ASN	CA-C	9.81	1.67	1.53
1	B	209	ASN	CA-C	9.76	1.66	1.53
1	E	209	ASN	N-CA	8.09	1.56	1.45
1	B	209	ASN	N-CA	8.00	1.56	1.45
1	D	125	ASN	CA-C	7.45	1.61	1.52
1	E	169	HIS	CA-C	6.97	1.60	1.52
1	A	302	ARG	CZ-NH2	6.86	1.42	1.33
1	A	268	ARG	CZ-NH1	6.48	1.41	1.32
1	D	126	ARG	CZ-NH2	6.44	1.41	1.33
1	D	126	ARG	CZ-NH1	6.41	1.41	1.32
1	A	302	ARG	CZ-NH1	6.38	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	ARG	CZ-NH2	6.32	1.41	1.33
1	A	126	ARG	CZ-NH1	6.26	1.41	1.32
1	A	126	ARG	CZ-NH2	6.26	1.41	1.33
1	A	317	ARG	CZ-NH1	6.25	1.41	1.32
1	A	268	ARG	CZ-NH2	5.90	1.41	1.33
1	A	169	HIS	CD2-NE2	-5.55	1.31	1.37
1	D	169	HIS	CD2-NE2	-5.53	1.31	1.37
1	D	209	ASN	C-O	-5.50	1.17	1.23
1	A	209	ASN	C-O	-5.49	1.17	1.23
1	A	27	HIS	CD2-NE2	-5.47	1.31	1.37
1	D	27	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	45	HIS	ND1-CE1	5.44	1.38	1.32
1	E	45	HIS	ND1-CE1	5.36	1.38	1.32
1	D	208	CYS	C-O	-5.31	1.17	1.24
1	B	307	HIS	ND1-CE1	5.19	1.37	1.32
1	A	208	CYS	C-O	-5.18	1.17	1.24
1	E	185	HIS	ND1-CE1	5.12	1.37	1.32
1	B	124	ALA	CA-C	5.12	1.59	1.52
1	E	307	HIS	ND1-CE1	5.10	1.37	1.32
1	B	185	HIS	ND1-CE1	5.01	1.37	1.32
1	B	185	HIS	CD2-NE2	-5.00	1.32	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	VAL	N-CA-C	10.98	121.68	111.91
1	B	45	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	E	45	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	E	185	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	B	185	HIS	CB-CG-CD2	-6.54	122.69	131.20
1	E	53	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	B	53	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	E	307	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	B	307	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	D	27	HIS	CB-CG-CD2	-6.34	122.95	131.20
1	A	27	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	A	208	CYS	N-CA-C	6.16	119.55	109.76
1	D	208	CYS	N-CA-C	6.13	119.51	109.76
1	E	39	LYS	CB-CA-C	-6.12	98.24	110.42
1	A	169	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	D	169	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	E	169	HIS	N-CA-C	5.99	118.66	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	VAL	N-CA-CB	5.84	119.23	112.39
1	B	2	ILE	N-CA-C	5.84	121.49	109.34
1	E	53	HIS	CB-CG-ND1	5.71	131.27	122.70
1	B	124	ALA	N-CA-C	-5.69	104.77	110.97
1	E	169	HIS	CA-C-O	5.68	126.50	120.36
1	B	53	HIS	CB-CG-ND1	5.67	131.21	122.70
1	B	185	HIS	CB-CG-ND1	5.61	131.11	122.70
1	E	185	HIS	CB-CG-ND1	5.58	131.07	122.70
1	B	307	HIS	CB-CG-ND1	5.55	131.02	122.70
1	E	307	HIS	CB-CG-ND1	5.51	130.96	122.70
1	D	27	HIS	CB-CG-ND1	5.46	130.90	122.70
1	A	169	HIS	CB-CG-ND1	5.46	130.89	122.70
1	D	169	HIS	CB-CG-ND1	5.45	130.87	122.70
1	E	45	HIS	CB-CG-ND1	5.44	130.86	122.70
1	B	45	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	27	HIS	CB-CG-ND1	5.42	130.83	122.70
1	D	38	VAL	CB-CA-C	5.39	118.39	112.19
1	A	330	ASN	CB-CA-C	5.24	120.85	110.42
1	D	39	LYS	N-CA-C	5.22	117.27	110.43
1	D	169	HIS	CA-C-N	5.18	128.91	121.50
1	D	169	HIS	C-N-CA	5.18	128.91	121.50
1	A	264	ARG	N-CA-C	5.15	116.58	111.07
1	A	169	HIS	CA-C-N	5.12	128.81	121.50
1	A	169	HIS	C-N-CA	5.12	128.81	121.50
1	E	208	CYS	N-CA-C	5.04	116.96	109.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	38	VAL	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	209	ASN	Mainchain
1	E	209	ASN	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	3009	0	3110	35	4
1	B	3009	0	3110	53	0
1	D	3009	0	3111	35	0
1	E	3009	0	3110	63	4
2	A	15	0	6	4	0
2	B	15	0	4	1	0
2	D	15	0	6	12	0
2	E	15	0	6	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	6	0	0	0	0
4	B	1	0	0	3	0
All	All	12107	0	12463	150	4

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 6.

All (150) 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:99:TRP:CH2	1:E:75:LYS:HG2	1.68	1.27
1:B:125:ASN:CB	1:E:100:ASN:ND2	2.05	1.20
1:D:169:HIS:CE1	2:D:401:PLP:N1	2.18	1.12
1:B:125:ASN:HB3	1:E:100:ASN:ND2	1.69	1.05
1:B:125:ASN:HB3	1:E:100:ASN:CG	1.82	1.02
1:B:125:ASN:ND2	1:E:100:ASN:HD22	1.58	1.01
1:B:100:ASN:HD21	1:E:99:TRP:HA	1.23	0.97
1:D:169:HIS:CE1	2:D:401:PLP:C2	2.47	0.97
1:A:100:ASN:CG	1:D:125:ASN:HB3	1.89	0.96
1:B:125:ASN:HB2	1:E:100:ASN:ND2	1.83	0.94
1:B:100:ASN:ND2	1:E:99:TRP:HA	1.84	0.92
1:B:125:ASN:HD22	1:E:100:ASN:HD22	1.04	0.91
1:B:99:TRP:CZ3	1:E:99:TRP:HH2	1.91	0.88
1:B:3:LYS:CE	4:B:501:HOH:O	2.22	0.88
1:A:94:LYS:NZ	1:A:121:GLU:OE2	2.05	0.88
1:B:3:LYS:HE3	4:B:501:HOH:O	1.74	0.86
1:B:99:TRP:CH2	1:E:75:LYS:CG	2.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASN:CB	1:E:100:ASN:HD22	1.84	0.86
1:E:2:ILE:HD13	1:E:377:PHE:CZ	2.10	0.85
1:D:169:HIS:HE1	2:D:401:PLP:N1	1.73	0.84
1:B:99:TRP:CE3	1:E:99:TRP:HH2	1.95	0.83
1:E:2:ILE:HG21	1:E:377:PHE:CZ	2.14	0.82
1:B:99:TRP:CZ3	1:E:75:LYS:HG2	2.14	0.81
1:E:169:HIS:CE1	2:E:401:PLP:N1	2.48	0.81
1:E:169:HIS:CE1	2:E:401:PLP:C2	2.65	0.80
1:D:283:VAL:HG21	1:D:331:GLY:CA	2.09	0.80
1:B:99:TRP:CE3	1:E:99:TRP:CH2	2.71	0.79
1:B:125:ASN:CG	1:E:100:ASN:HD22	1.93	0.77
1:E:2:ILE:HD13	1:E:377:PHE:CE2	2.19	0.77
1:B:125:ASN:HD22	1:E:100:ASN:ND2	1.81	0.76
1:D:169:HIS:ND1	2:D:401:PLP:C2A	2.50	0.75
1:A:81:PRO:HG3	1:D:124:ALA:HB2	1.69	0.74
1:B:100:ASN:HD21	1:E:99:TRP:CA	2.00	0.72
1:A:302:ARG:HH21	1:A:358:MET:HG3	1.55	0.72
1:D:283:VAL:HG21	1:D:331:GLY:HA3	1.72	0.72
1:B:162:ARG:NH1	1:E:124:ALA:O	2.25	0.70
1:D:169:HIS:CG	2:D:401:PLP:H2A2	2.28	0.69
1:D:169:HIS:HE1	2:D:401:PLP:C6	2.06	0.69
1:D:283:VAL:HG21	1:D:331:GLY:HA2	1.74	0.68
1:A:2:ILE:HG22	1:A:4:LEU:HG	1.75	0.68
1:D:38:VAL:CG2	1:D:47:SER:HB2	2.24	0.68
1:A:2:ILE:CG2	1:A:4:LEU:HG	2.26	0.65
1:B:79:THR:OG1	1:E:94:LYS:HE3	1.97	0.65
1:B:38:VAL:HG12	1:B:47:SER:HB2	1.79	0.64
1:A:100:ASN:ND2	1:D:125:ASN:HB3	2.13	0.63
1:E:169:HIS:HE1	2:E:401:PLP:N1	1.96	0.63
1:D:169:HIS:ND1	2:D:401:PLP:N1	2.46	0.63
1:E:38:VAL:CG1	1:E:47:SER:HA	2.29	0.62
1:B:123:SER:OG	1:B:123:SER:O	2.15	0.62
1:E:2:ILE:HD13	1:E:377:PHE:CE1	2.34	0.62
1:A:302:ARG:NH2	1:A:358:MET:O	2.34	0.61
1:B:99:TRP:CZ3	1:E:99:TRP:CH2	2.83	0.60
1:B:125:ASN:N	1:B:125:ASN:OD1	2.32	0.60
1:D:300:SER:HA	1:D:318:VAL:HG23	1.84	0.60
1:D:169:HIS:ND1	2:D:401:PLP:H2A2	2.17	0.60
1:A:300:SER:HA	1:A:318:VAL:HG23	1.84	0.59
1:A:121:GLU:O	1:A:123:SER:N	2.36	0.59
1:B:3:LYS:HE2	4:B:501:HOH:O	1.90	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:HG21	1:A:331:GLY:HA3	1.85	0.59
1:E:38:VAL:HG12	1:E:38:VAL:O	2.03	0.58
1:B:125:ASN:HB3	1:E:100:ASN:CB	2.34	0.58
1:A:193:SER:O	1:A:197:LYS:HG3	2.03	0.57
1:B:38:VAL:HG12	1:B:38:VAL:O	2.03	0.57
1:D:283:VAL:CG2	1:D:331:GLY:HA2	2.34	0.57
1:A:94:LYS:CE	1:A:121:GLU:OE2	2.53	0.56
1:D:169:HIS:CE1	2:D:401:PLP:C2A	2.88	0.56
1:A:94:LYS:HD2	1:A:121:GLU:OE2	2.06	0.55
1:B:38:VAL:CG1	1:B:47:SER:HB2	2.36	0.55
1:D:118:LEU:O	1:D:121:GLU:O	2.24	0.55
1:B:376:ARG:O	1:B:386:LYS:HD3	2.07	0.55
1:D:321:ASP:OD2	1:E:39:LYS:HD2	2.07	0.54
1:A:302:ARG:NH2	1:A:358:MET:HG3	2.22	0.54
1:E:376:ARG:O	1:E:386:LYS:HD3	2.07	0.54
1:A:169:HIS:CE1	2:A:401:PLP:C2	2.92	0.53
1:B:121:GLU:O	1:B:122:ALA:HB3	2.09	0.53
1:E:38:VAL:HG12	1:E:47:SER:HB2	1.91	0.53
1:E:364:TYR:HE2	2:E:401:PLP:O2P	1.92	0.52
1:E:38:VAL:CG1	1:E:47:SER:HB2	2.39	0.52
1:B:38:VAL:HG12	1:B:47:SER:CB	2.39	0.52
1:D:38:VAL:HG23	1:D:38:VAL:O	2.09	0.52
1:B:38:VAL:CG1	1:B:47:SER:HA	2.40	0.52
1:A:282:GLU:HA	1:A:329:GLU:HA	1.92	0.51
1:B:2:ILE:HD12	1:B:377:PHE:CZ	2.46	0.51
1:B:99:TRP:CZ2	1:E:75:LYS:HG2	2.38	0.51
1:B:124:ALA:H	1:E:79:THR:HB	1.75	0.51
1:E:38:VAL:CG1	1:E:47:SER:CB	2.89	0.50
1:E:38:VAL:HG12	1:E:47:SER:CB	2.40	0.50
1:E:169:HIS:CG	2:E:401:PLP:H2A2	2.47	0.50
1:E:169:HIS:ND1	2:E:401:PLP:H2A2	2.26	0.50
1:B:162:ARG:NH2	1:E:125:ASN:OD1	2.45	0.50
1:A:100:ASN:CB	1:D:125:ASN:HB3	2.42	0.49
1:B:99:TRP:CZ3	1:E:75:LYS:HE2	2.47	0.49
1:D:38:VAL:HG23	1:D:47:SER:CB	2.41	0.49
1:D:38:VAL:HG23	1:D:47:SER:HB2	1.93	0.49
1:A:385:PHE:O	1:A:386:LYS:HB2	2.13	0.49
1:D:281:ASN:OD1	1:D:329:GLU:HB2	2.13	0.49
1:E:38:VAL:HG13	1:E:42:GLY:HA2	1.93	0.49
1:A:268:ARG:HG3	1:A:268:ARG:NH1	2.28	0.49
1:D:385:PHE:O	1:D:386:LYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HG2	1:B:26:ARG:HD3	1.95	0.48
1:E:22:ARG:HG2	1:E:26:ARG:HD3	1.95	0.48
1:A:268:ARG:HG3	1:A:268:ARG:HH11	1.79	0.48
1:B:99:TRP:HZ3	1:E:75:LYS:HE2	1.78	0.48
1:B:37:VAL:HG12	1:B:39:LYS:HG2	1.97	0.47
1:B:2:ILE:CD1	1:B:377:PHE:CE2	2.98	0.46
1:E:2:ILE:HD13	1:E:377:PHE:CD2	2.51	0.46
1:E:169:HIS:ND1	2:E:401:PLP:C2A	2.79	0.46
1:D:38:VAL:CG2	1:D:47:SER:CB	2.93	0.46
1:B:125:ASN:ND2	1:E:100:ASN:HB2	2.31	0.46
1:B:162:ARG:CZ	1:E:124:ALA:O	2.63	0.46
1:E:38:VAL:CG1	1:E:47:SER:CA	2.93	0.46
1:B:38:VAL:CG1	1:B:47:SER:CB	2.94	0.46
1:B:38:VAL:HG13	1:B:47:SER:HA	1.98	0.46
1:A:43:TYR:OH	2:A:401:PLP:H5A1	2.16	0.45
1:A:123:SER:O	1:A:123:SER:OG	2.25	0.45
1:E:293:ASP:HB3	1:E:374:ILE:HD11	1.98	0.45
1:A:81:PRO:HG3	1:D:124:ALA:CB	2.41	0.45
1:A:272:TYR:O	1:A:317:ARG:HD2	2.17	0.44
1:B:210:THR:OG1	2:B:401:PLP:O3P	2.28	0.44
1:A:169:HIS:ND1	2:A:401:PLP:H2A2	2.33	0.44
1:E:169:HIS:CE1	2:E:401:PLP:C2A	3.01	0.44
1:B:125:ASN:ND2	1:E:100:ASN:ND2	2.43	0.44
1:B:293:ASP:HB3	1:B:374:ILE:HD11	1.98	0.44
1:B:291:TYR:HA	1:B:295:TYR:O	2.18	0.44
1:A:22:ARG:HG2	1:A:26:ARG:HD3	2.00	0.43
1:A:146:GLU:OE1	1:A:146:GLU:N	2.46	0.43
1:D:119:GLU:O	1:D:120:LYS:C	2.61	0.43
1:E:2:ILE:CG2	1:E:377:PHE:CZ	2.95	0.43
1:E:291:TYR:HA	1:E:295:TYR:O	2.18	0.43
1:D:169:HIS:CE1	2:D:401:PLP:H2A2	2.54	0.43
1:E:38:VAL:HG13	1:E:42:GLY:CA	2.49	0.43
1:E:169:HIS:HE1	2:E:401:PLP:C6	2.31	0.43
1:D:169:HIS:CG	2:D:401:PLP:C2A	2.99	0.42
1:A:15:ASP:O	1:A:19:LYS:HG3	2.19	0.42
1:D:1:MET:HE3	1:D:2:ILE:H	1.85	0.42
1:D:300:SER:O	1:D:314:VAL:HG12	2.20	0.42
1:A:103:LEU:HG	1:A:127:LEU:HD11	2.01	0.42
1:D:22:ARG:HG2	1:D:26:ARG:HD3	2.00	0.42
1:A:119:GLU:O	1:A:120:LYS:C	2.62	0.42
1:A:169:HIS:CE1	2:A:401:PLP:N1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:ILE:CG2	1:E:385:PHE:N	2.82	0.42
1:D:169:HIS:ND1	2:D:401:PLP:C2	2.71	0.42
1:B:384:ILE:CG2	1:B:385:PHE:N	2.83	0.42
1:E:38:VAL:HG13	1:E:47:SER:HA	2.02	0.41
1:A:228:ILE:HG13	1:A:233:LEU:HB2	2.02	0.41
1:A:300:SER:O	1:A:314:VAL:HG12	2.20	0.41
1:A:94:LYS:CD	1:A:121:GLU:OE2	2.68	0.40
1:E:2:ILE:HG21	1:E:377:PHE:HZ	1.81	0.40
1:B:38:VAL:CG1	1:B:47:SER:CA	2.99	0.40
1:E:228:ILE:HG13	1:E:233:LEU:HB2	2.03	0.40

All (4) 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)
1:A:153:LYS:CD	1:E:26:ARG:NH1[1_655]	1.86	0.34
1:A:26:ARG:NH1	1:E:241:GLN:NE2[2_5412]	2.01	0.19
1:A:22:ARG:NH1	1:E:357:GLU:OE1[2_5412]	2.02	0.18
1:A:26:ARG:CZ	1:E:241:GLN:NE2[2_5412]	2.05	0.15

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	384/394 (98%)	363 (94%)	16 (4%)	5 (1%)	9	38
1	B	384/394 (98%)	369 (96%)	14 (4%)	1 (0%)	36	70
1	D	384/394 (98%)	368 (96%)	16 (4%)	0	100	100
1	E	384/394 (98%)	370 (96%)	13 (3%)	1 (0%)	36	70
All	All	1536/1576 (98%)	1470 (96%)	59 (4%)	7 (0%)	24	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA
1	A	329	GLU
1	B	2	ILE
1	A	127	LEU
1	A	330	ASN
1	A	332	GLU
1	E	39	LYS

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	320/328 (98%)	316 (99%)	4 (1%)	61	81
1	B	320/328 (98%)	312 (98%)	8 (2%)	42	72
1	D	320/328 (98%)	314 (98%)	6 (2%)	50	76
1	E	320/328 (98%)	315 (98%)	5 (2%)	55	79
All	All	1280/1312 (98%)	1257 (98%)	23 (2%)	51	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	HIS
1	A	248	GLU
1	A	372	ARG
1	B	1	MET
1	B	39	LYS
1	B	93	VAL
1	B	123	SER
1	B	125	ASN
1	B	180	LEU
1	B	346	LYS
1	B	352	VAL
1	D	38	VAL
1	D	121	GLU
1	D	248	GLU

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Mol	Chain	Res	Type
1	D	329	GLU
1	D	330	ASN
1	D	372	ARG
1	E	1	MET
1	E	93	VAL
1	E	180	LEU
1	E	346	LYS
1	E	352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	107	GLN
1	B	100	ASN
1	B	209	ASN
1	B	241	GLN
1	B	335	GLN
1	D	107	GLN
1	E	100	ASN
1	E	209	ASN
1	E	335	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	A	401	1	15,15,16	2.57	3 (20%)	21,22,23	1.60	5 (23%)
2	PLP	D	401	1	15,15,16	3.02	4 (26%)	21,22,23	1.62	4 (19%)
2	PLP	E	401	1	15,15,16	3.01	4 (26%)	21,22,23	1.91	7 (33%)
2	PLP	B	401	1	15,15,16	3.22	3 (20%)	21,22,23	1.56	4 (19%)

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	A	401	1	-	3/6/6/8	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	E	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	3/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C3-C2	8.92	1.50	1.41
2	E	401	PLP	C5-C4	7.47	1.49	1.40
2	D	401	PLP	C3-C2	7.37	1.48	1.41
2	D	401	PLP	C5-C4	7.32	1.48	1.40
2	A	401	PLP	C5-C4	7.07	1.48	1.40
2	B	401	PLP	C5-C4	7.05	1.48	1.40
2	E	401	PLP	C3-C2	6.73	1.48	1.41
2	A	401	PLP	C3-C2	4.97	1.46	1.41
2	E	401	PLP	C3-C4	3.96	1.47	1.40
2	B	401	PLP	C3-C4	3.80	1.47	1.40
2	D	401	PLP	C3-C4	3.53	1.46	1.40
2	A	401	PLP	C3-C4	3.43	1.46	1.40
2	E	401	PLP	P-O2P	-2.33	1.46	1.54
2	D	401	PLP	C4A-C4	-2.17	1.47	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C4A-C4-C5	4.03	125.10	120.94
2	E	401	PLP	O4P-C5A-C5	-3.66	102.50	109.36
2	D	401	PLP	O3P-P-O4P	-3.63	97.20	106.67
2	B	401	PLP	O3-C3-C2	3.33	124.48	117.58
2	E	401	PLP	C4A-C4-C5	3.28	124.32	120.94
2	D	401	PLP	C4A-C4-C5	3.16	124.20	120.94
2	E	401	PLP	C6-C5-C4	3.07	120.61	118.10
2	B	401	PLP	C2A-C2-C3	3.05	124.37	120.80
2	D	401	PLP	O3P-P-O2P	3.02	119.13	107.80
2	E	401	PLP	C5A-C5-C6	-2.97	114.52	119.36
2	B	401	PLP	C6-N1-C2	2.63	123.97	119.20
2	A	401	PLP	C3-C4-C5	-2.51	115.58	118.59
2	E	401	PLP	C6-N1-C2	2.39	123.53	119.20
2	E	401	PLP	C3-C4-C5	-2.34	115.78	118.59
2	D	401	PLP	C6-N1-C2	2.28	123.33	119.20
2	E	401	PLP	O4P-P-O1P	-2.28	100.28	106.44
2	A	401	PLP	C2A-C2-N1	2.18	121.75	117.64
2	A	401	PLP	C6-N1-C2	2.02	122.86	119.20
2	B	401	PLP	C4A-C4-C5	2.01	123.01	120.94
2	A	401	PLP	O3P-P-O4P	-2.00	101.45	106.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O3P
2	B	401	PLP	C5A-O4P-P-O1P
2	B	401	PLP	C5A-O4P-P-O2P
2	B	401	PLP	C5A-O4P-P-O3P
2	A	401	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	4	0
2	D	401	PLP	12	0
2	E	401	PLP	9	0
2	B	401	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/394 (97%)	-0.01	1 (0%) 90 79	40, 65, 98, 115	0
1	B	386/394 (97%)	0.03	0 100 100	45, 68, 94, 120	0
1	D	386/394 (97%)	0.05	4 (1%) 79 59	46, 71, 101, 126	0
1	E	386/394 (97%)	0.06	1 (0%) 90 79	43, 72, 107, 125	0
All	All	1544/1576 (97%)	0.03	6 (0%) 88 76	40, 69, 101, 126	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	330	ASN	2.9
1	E	352	VAL	2.8
1	D	324	MET	2.4
1	A	330	ASN	2.4
1	D	329	GLU	2.2
1	D	32	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	D	402	1/1	0.58	0.17	94,94,94,94	0
3	CL	B	402	1/1	0.65	0.17	83,83,83,83	0
2	PLP	D	401	15/16	0.81	0.12	62,72,92,102	0
2	PLP	A	401	15/16	0.88	0.10	52,71,82,83	0
2	PLP	E	401	15/16	0.89	0.11	50,66,85,89	0
3	CL	E	402	1/1	0.89	0.08	75,75,75,75	0
2	PLP	B	401	15/16	0.90	0.10	53,74,101,101	0
3	CL	A	402	1/1	0.94	0.08	76,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.