



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:57 PM UTC

PDB ID : 6Q70 / pdb_00006q70
Title : Crystal structure of the alanine racemase Bsu17640 from *Bacillus subtilis* in the presence of HEPES
Authors : Bernardo-Garcia, N.; Gago, F.; Hermoso, J.A.
Deposited on : 2018-12-12
Resolution : 2.05 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

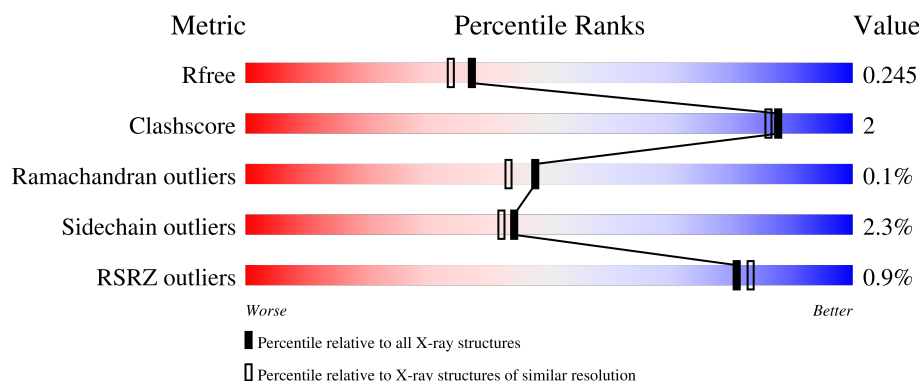
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	% 82% 15% ..
1	B	394	% 81% 16% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6406 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	1	0
			3018	1929	529	546	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

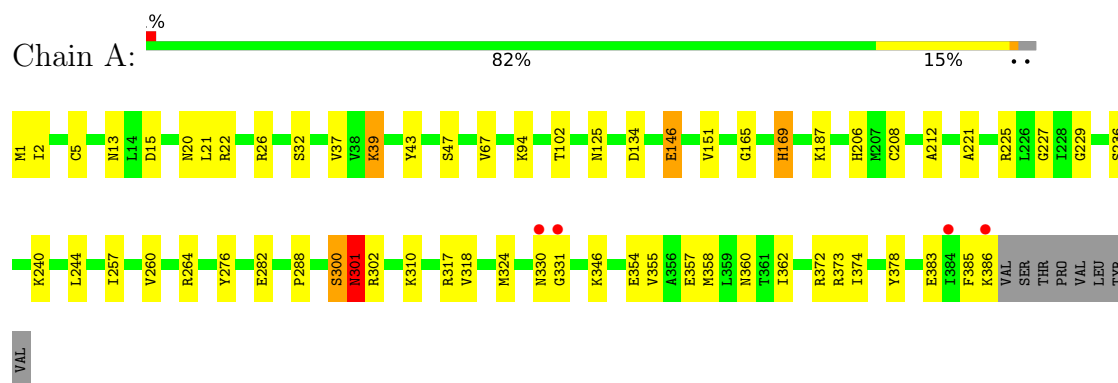
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	178	Total	O	0	0
			178	178		
5	B	167	Total	O	0	0
			167	167		

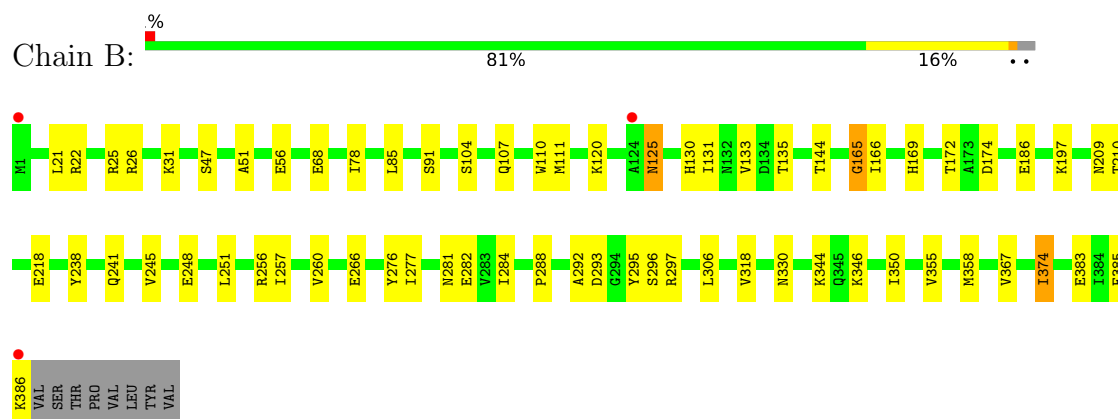
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.66Å 73.66Å 331.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.05 49.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.29-2.05) 99.9 (49.29-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.185 , 0.237 0.197 , 0.245	Depositor DCC
R_{free} test set	2927 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6406	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: MG, 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	1.66	32/3063 (1.0%)	1.44	24/4135 (0.6%)
1	B	1.68	36/3072 (1.2%)	1.36	14/4147 (0.3%)
All	All	1.67	68/6135 (1.1%)	1.40	38/8282 (0.5%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLY	C-O	9.41	1.35	1.23
1	B	238	TYR	C-O	8.92	1.34	1.24
1	B	131	ILE	C-O	-8.69	1.14	1.24
1	B	344	LYS	CA-C	-8.37	1.42	1.52
1	B	374	ILE	N-CA	-8.29	1.40	1.46
1	B	277	ILE	C-O	-8.04	1.15	1.24
1	B	318	VAL	C-O	-7.87	1.15	1.24
1	A	236	SER	C-O	7.77	1.33	1.23
1	A	221	ALA	CA-C	7.33	1.59	1.53
1	B	68	GLU	CG-CD	7.29	1.70	1.52
1	B	385	PHE	CA-C	7.23	1.61	1.52
1	A	43	TYR	C-O	7.13	1.33	1.23
1	A	67	VAL	C-O	-6.99	1.16	1.24
1	A	301	ASN	N-CA	6.88	1.56	1.46
1	A	385	PHE	CA-C	6.69	1.60	1.52
1	B	248	GLU	CA-C	6.68	1.59	1.52
1	B	358	MET	C-O	-6.63	1.16	1.24
1	A	212	ALA	C-O	-6.51	1.15	1.24
1	A	206	HIS	C-O	-6.50	1.16	1.24
1	A	169	HIS	N-CA	-6.33	1.38	1.46
1	B	165	GLY	C-O	-6.30	1.17	1.24
1	B	218	GLU	C-O	-6.19	1.16	1.24
1	A	5	CYS	N-CA	5.94	1.53	1.46
1	A	360	ASN	CA-CB	5.93	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	CYS	C-O	5.92	1.31	1.23
1	A	26	ARG	C-O	-5.88	1.16	1.24
1	A	20	ASN	CA-CB	5.83	1.62	1.53
1	B	210	THR	CA-C	5.82	1.60	1.52
1	A	354	GLU	C-O	-5.74	1.16	1.24
1	B	21	LEU	CA-C	5.72	1.60	1.52
1	B	47	SER	N-CA	-5.71	1.39	1.46
1	B	295	TYR	CA-CB	5.69	1.60	1.52
1	A	302	ARG	N-CA	5.68	1.53	1.46
1	B	251	LEU	CA-C	-5.67	1.45	1.52
1	B	125	ASN	CA-C	-5.66	1.45	1.52
1	B	25	ARG	NE-CZ	5.62	1.39	1.33
1	A	318	VAL	C-O	-5.62	1.17	1.24
1	B	209	ASN	C-O	5.61	1.30	1.23
1	A	102	THR	C-O	-5.60	1.17	1.24
1	A	244	LEU	N-CA	-5.58	1.39	1.46
1	A	21	LEU	CA-C	5.55	1.59	1.52
1	A	288	PRO	N-CA	-5.54	1.41	1.47
1	B	292	ALA	N-CA	5.48	1.53	1.46
1	A	22	ARG	N-CA	5.47	1.52	1.46
1	A	21	LEU	N-CA	-5.45	1.39	1.46
1	A	358	MET	SD-CE	5.44	1.93	1.79
1	B	166	ILE	N-CA	-5.42	1.39	1.46
1	B	256	ARG	CA-C	-5.39	1.46	1.52
1	B	284	ILE	CA-C	-5.38	1.46	1.52
1	A	32	SER	CA-C	-5.32	1.45	1.52
1	A	134	ASP	C-O	-5.32	1.17	1.24
1	B	355	VAL	CA-CB	5.31	1.60	1.54
1	B	385	PHE	N-CA	5.30	1.52	1.46
1	B	296	SER	N-CA	5.29	1.52	1.46
1	B	251	LEU	N-CA	5.25	1.52	1.46
1	B	367	VAL	N-CA	5.24	1.52	1.46
1	A	378	TYR	CA-C	5.23	1.58	1.52
1	A	357	GLU	N-CA	5.22	1.52	1.46
1	A	362	ILE	C-O	5.18	1.29	1.23
1	B	68	GLU	CD-OE1	5.18	1.35	1.25
1	B	135	THR	N-CA	5.16	1.52	1.46
1	A	125	ASN	CA-C	5.13	1.59	1.52
1	B	144	THR	CA-C	-5.12	1.46	1.52
1	B	56	GLU	C-O	-5.07	1.17	1.24
1	B	51	ALA	N-CA	-5.06	1.40	1.46
1	A	221	ALA	C-O	-5.06	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	ILE	CA-C	5.06	1.58	1.52
1	B	133	VAL	CA-CB	5.06	1.60	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	SER	CA-C-N	-12.37	101.07	123.34
1	A	300	SER	C-N-CA	-12.37	101.07	123.34
1	A	300	SER	O-C-N	-7.62	113.35	122.11
1	B	125	ASN	CB-CA-C	-7.33	99.16	110.88
1	B	385	PHE	N-CA-C	7.26	118.76	108.74
1	A	310	LYS	N-CA-C	7.19	120.10	109.24
1	B	172	THR	N-CA-C	6.81	120.83	111.71
1	B	297	ARG	NE-CZ-NH2	6.36	124.92	119.20
1	A	151	VAL	N-CA-C	-6.35	104.32	110.42
1	A	346	LYS	CB-CA-C	-6.35	109.24	116.54
1	B	383	GLU	N-CA-C	6.30	119.28	109.52
1	A	373	ARG	CA-C-N	6.30	127.12	122.59
1	A	373	ARG	C-N-CA	6.30	127.12	122.59
1	A	373	ARG	N-CA-C	6.28	120.40	112.87
1	A	372	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	A	330	ASN	CA-C-N	6.18	133.52	121.41
1	A	330	ASN	C-N-CA	6.18	133.52	121.41
1	A	240	LYS	CD-CE-NZ	-5.99	92.72	111.90
1	A	383	GLU	N-CA-C	5.96	119.26	109.72
1	A	264	ARG	N-CA-C	5.78	117.66	111.36
1	A	385	PHE	N-CA-C	5.74	118.00	108.99
1	A	165	GLY	N-CA-C	5.70	119.07	110.18
1	B	110	TRP	CA-C-O	-5.58	114.92	120.90
1	B	91	SER	CB-CA-C	-5.44	99.60	110.42
1	B	111	MET	N-CA-CB	5.41	117.85	110.01
1	B	358	MET	CG-SD-CE	5.38	112.74	100.90
1	A	374	ILE	CB-CA-C	-5.35	104.98	110.71
1	A	373	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	B	111	MET	CB-CA-C	-5.28	102.59	110.88
1	A	94	LYS	N-CA-C	-5.19	105.54	111.14
1	B	85	LEU	N-CA-C	5.14	117.79	111.82
1	B	385	PHE	CA-C-N	5.14	130.96	121.70
1	B	385	PHE	C-N-CA	5.14	130.96	121.70
1	A	39	LYS	CG-CD-CE	5.12	123.07	111.30
1	A	47	SER	N-CA-C	5.09	116.83	111.28
1	B	297	ARG	NE-CZ-NH1	-5.05	116.45	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	VAL	N-CA-C	-5.05	105.78	110.53
1	A	21	LEU	N-CA-C	-5.01	105.81	111.28

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	3009	0	3110	12	0
1	B	3018	0	3118	14	0
2	A	15	0	6	2	0
2	B	15	0	7	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	178	0	0	2	0
5	B	167	0	0	0	1
All	All	6406	0	6241	25	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 2.

All (25) 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:301:ASN:O	5:A:501:HOH:O	2.11	0.68
1:B:281:ASN:HB2	1:B:330:ASN:HD21	1.57	0.68
1:B:22:ARG:HG2	1:B:26:ARG:HD3	1.77	0.65
1:B:169:HIS:CG	2:B:401:PLP:H2A2	2.39	0.58
1:A:257:ILE:HG21	1:A:260:VAL:HG23	1.86	0.57
1:B:281:ASN:HB2	1:B:330:ASN:ND2	2.22	0.52
1:B:293:ASP:HB3	1:B:374:ILE:HD11	1.92	0.52
1:A:187:LYS:NZ	1:B:266:GLU:O	2.43	0.52
1:A:300:SER:HB3	1:A:317:ARG:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107[A]:GLN:NE2	1:B:107[A]:GLN:HA	2.28	0.49
1:A:169:HIS:CE1	2:A:401:PLP:N1	2.81	0.48
1:B:130:HIS:CE1	1:B:165:GLY:HA3	2.50	0.46
1:A:225:ARG:HE	2:A:401:PLP:C6	2.28	0.46
1:B:276:TYR:OH	1:B:282:GLU:OE2	2.27	0.45
1:A:146:GLU:HB3	5:A:518:HOH:O	2.17	0.45
1:A:1:MET:HE3	1:A:2:ILE:H	1.83	0.44
1:A:13:ASN:OD1	1:A:15:ASP:HB2	2.17	0.44
1:A:276:TYR:OH	1:A:282:GLU:OE2	2.31	0.42
1:B:257:ILE:HG21	1:B:260:VAL:CG2	2.50	0.41
1:B:306:LEU:HD21	1:B:350:ILE:HG13	2.02	0.41
1:B:104:SER:HA	1:B:130:HIS:O	2.21	0.41
1:A:37:VAL:HB	1:A:227:GLY:HA2	2.02	0.40
1:B:257:ILE:HG21	1:B:260:VAL:HG23	2.02	0.40
1:A:300:SER:CB	1:A:317:ARG:HA	2.52	0.40
1:B:174:ASP:OD1	1:B:174:ASP:N	2.55	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:B:662:HOH:O	5:B:662:HOH:O[5_657]	0.60	1.60

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	384/394 (98%)	370 (96%)	13 (3%)	1 (0%)	36	30
1	B	385/394 (98%)	374 (97%)	11 (3%)	0	100	100
All	All	769/788 (98%)	744 (97%)	24 (3%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	GLY

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%)	315 (98%)	5 (2%)	55	56
1	B	321/328 (98%)	311 (97%)	10 (3%)	35	30
All	All	641/656 (98%)	626 (98%)	15 (2%)	44	42

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	146	GLU
1	A	301	ASN
1	A	324	MET
1	A	386	LYS
1	B	31	LYS
1	B	120	LYS
1	B	125	ASN
1	B	186	GLU
1	B	197	LYS
1	B	241	GLN
1	B	245	VAL
1	B	288	PRO
1	B	346	LYS
1	B	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	330	ASN
1	B	335	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	B	401	1	15,15,16	5.62	8 (53%)	21,22,23	2.14	8 (38%)
2	PLP	A	401	1	15,15,16	5.21	6 (40%)	21,22,23	2.93	11 (52%)

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	B	401	1	-	1/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	401	1	-	0/6/6/8	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	14.50	1.56	1.41
2	A	401	PLP	C3-C2	13.27	1.54	1.41
2	B	401	PLP	C5-C4	12.52	1.54	1.40
2	A	401	PLP	C5-C4	12.30	1.54	1.40
2	B	401	PLP	C3-C4	5.83	1.51	1.40
2	A	401	PLP	C3-C4	5.62	1.50	1.40
2	B	401	PLP	C2A-C2	4.47	1.57	1.50
2	A	401	PLP	C2A-C2	4.32	1.57	1.50
2	B	401	PLP	C2-N1	3.99	1.40	1.33
2	B	401	PLP	P-O1P	3.24	1.60	1.50
2	A	401	PLP	P-O1P	3.07	1.60	1.50
2	B	401	PLP	C5A-C5	2.80	1.58	1.50
2	A	401	PLP	P-O2P	-2.19	1.46	1.54
2	B	401	PLP	C6-C5	2.14	1.42	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C2A-C2-C3	5.81	127.60	120.80
2	A	401	PLP	C3-C2-N1	-5.52	114.00	120.96
2	B	401	PLP	C3-C2-N1	-5.09	114.54	120.96
2	A	401	PLP	C6-N1-C2	4.82	127.94	119.20
2	A	401	PLP	C4A-C4-C3	4.72	128.40	120.52
2	B	401	PLP	C6-N1-C2	4.25	126.90	119.20
2	A	401	PLP	C4A-C4-C5	-4.25	116.56	120.94
2	A	401	PLP	C5A-C5-C6	-3.54	113.58	119.36
2	B	401	PLP	C2A-C2-C3	3.22	124.56	120.80
2	A	401	PLP	C3-C4-C5	-3.19	114.76	118.59
2	B	401	PLP	O4P-C5A-C5	-3.05	103.63	109.36
2	A	401	PLP	C5A-C5-C4	2.80	128.16	122.64
2	A	401	PLP	O2P-P-O4P	-2.51	100.13	106.67
2	B	401	PLP	O2P-P-O4P	-2.40	100.41	106.67
2	B	401	PLP	C5A-C5-C6	-2.33	115.57	119.36
2	B	401	PLP	C4A-C4-C5	2.28	123.28	120.94
2	A	401	PLP	O3P-P-O1P	2.12	119.09	110.83
2	B	401	PLP	C5A-C5-C4	2.09	126.77	122.64
2	A	401	PLP	O3-C3-C4	2.00	123.33	118.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	PLP	C6-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PLP	1	0
2	A	401	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, 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%)	-0.12	4 (1%) 79 81	26, 40, 67, 82	0
1	B	386/394 (97%)	-0.11	3 (0%) 82 84	22, 41, 68, 90	1 (0%)
All	All	772/788 (97%)	-0.12	7 (0%) 81 83	22, 41, 68, 90	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	ASN	3.5
1	A	386	LYS	2.8
1	B	1	MET	2.6
1	B	386	LYS	2.2
1	A	331	GLY	2.2
1	B	124	ALA	2.2
1	A	384	ILE	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($\text{\AA}^2$)	Q<0.9
4	MG	A	404	1/1	0.87	0.28	69,69,69,69	0
2	PLP	B	401	15/16	0.93	0.12	30,47,56,57	0
2	PLP	A	401	15/16	0.94	0.10	28,43,53,56	0
3	CL	B	402	1/1	0.97	0.06	51,51,51,51	0
3	CL	A	402	1/1	0.97	0.06	46,46,46,46	0
3	CL	A	403	1/1	0.99	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.