



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:17 AM UTC

PDB ID : 1TTQ / pdb_00001ttq
Title : TRYPTOPHAN SYNTHASE (E.C.4.2.1.20) IN THE PRESENCE OF POTASSIUM AT ROOM TEMPERATURE
Authors : Rhee, S.; Parris, K.; Ahmed, S.; Miles, E.W.; Davies, D.R.
Deposited on : 1995-10-11
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

<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

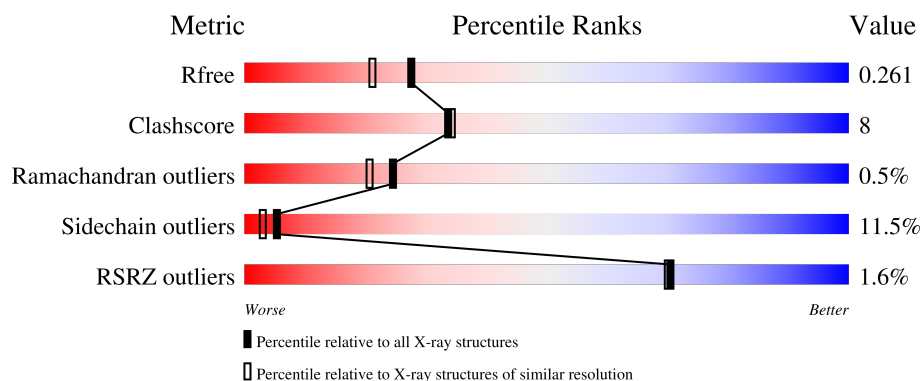
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	268	3% 71% 19% 6% .
2	B	397	67% 25% 6% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4978 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 TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1937	1236	333	360	8			

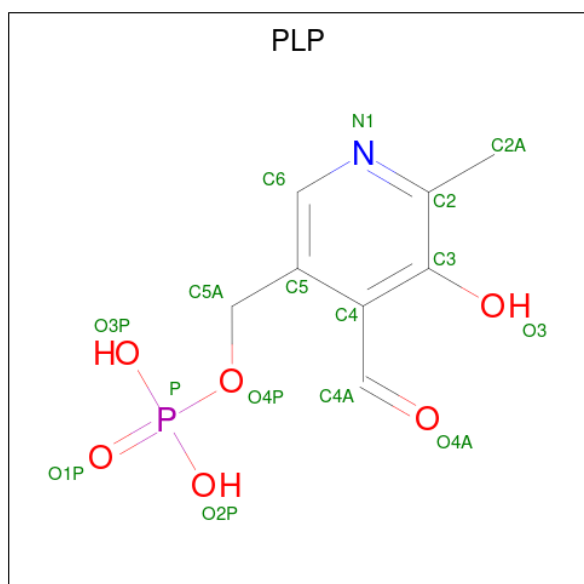
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	0	0
			2950	1855	518	558	19			

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

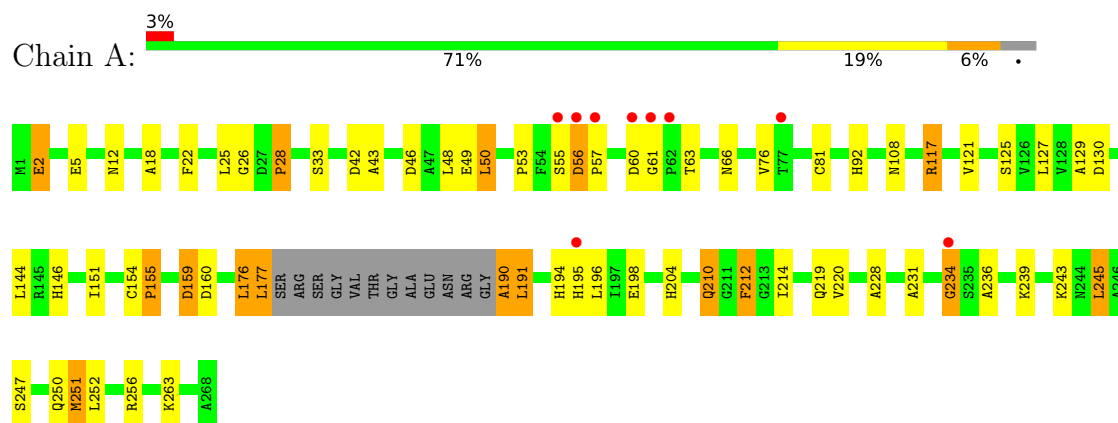
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	54	Total	O	0	0
			54	54		

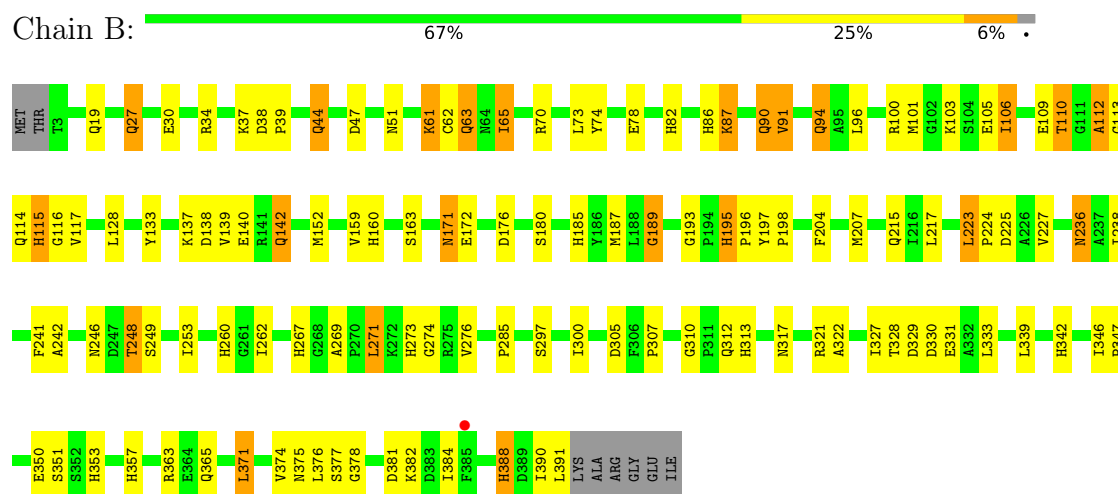
3 Residue-property plots

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: TRYPTOPHAN SYNTHASE



• Molecule 2: TRYPTOPHAN SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.00Å 61.30Å 67.70Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	71.7 (8.00-2.00) 70.2 (8.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.285 0.199 , 0.261	Depositor DCC
R_{free} test set	3595 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4978	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	2.11	18/1976 (0.9%)	1.94	41/2684 (1.5%)
2	B	1.05	19/3008 (0.6%)	1.80	67/4064 (1.6%)
All	All	1.56	37/4984 (0.7%)	1.86	108/6748 (1.6%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ALA	N-CA	62.16	2.64	1.46
1	A	190	ALA	C-O	36.24	1.96	1.23
1	A	177	LEU	N-CA	27.24	1.98	1.46
1	A	190	ALA	C-N	17.32	1.69	1.33
1	A	177	LEU	CG-CD2	17.00	2.08	1.52
1	A	177	LEU	CA-CB	15.75	1.84	1.53
1	A	177	LEU	CG-CD1	14.46	2.00	1.52
1	A	177	LEU	CB-CG	-9.89	1.33	1.53
1	A	190	ALA	CA-CB	9.71	1.84	1.52
1	A	176	LEU	C-N	-9.35	1.20	1.33
1	A	177	LEU	CA-C	-7.61	1.36	1.52
2	B	185	HIS	CD2-NE2	-7.35	1.29	1.37
2	B	87	LYS	CB-CG	7.25	1.74	1.52
2	B	357	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	146	HIS	CD2-NE2	-6.92	1.30	1.37
2	B	353	HIS	CD2-NE2	-6.85	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	267	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	190	ALA	CA-C	-6.79	1.38	1.52
2	B	342	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	194	HIS	CD2-NE2	-6.26	1.30	1.37
2	B	195	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	92	HIS	CD2-NE2	-6.13	1.31	1.37
2	B	388	HIS	CD2-NE2	-6.12	1.31	1.37
2	B	160	HIS	CD2-NE2	-6.09	1.31	1.37
2	B	260	HIS	CD2-NE2	-6.03	1.31	1.37
2	B	313	HIS	CD2-NE2	-6.03	1.31	1.37
2	B	273	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	204	HIS	CD2-NE2	-5.89	1.31	1.37
2	B	115	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	195	HIS	CD2-NE2	-5.83	1.31	1.37
2	B	86	HIS	CD2-NE2	-5.56	1.31	1.37
2	B	253	ILE	CA-CB	5.53	1.61	1.54
2	B	300	ILE	CA-CB	5.51	1.61	1.54
2	B	238	ILE	CA-CB	5.49	1.61	1.54
1	A	177	LEU	C-O	5.38	1.34	1.23
2	B	82	HIS	CD2-NE2	-5.25	1.32	1.37
2	B	195	HIS	CG-ND1	-5.14	1.32	1.38

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LEU	O-C-N	20.81	146.78	123.27
1	A	176	LEU	CA-C-N	-19.26	87.03	121.70
1	A	176	LEU	C-N-CA	-19.26	87.03	121.70
1	A	177	LEU	CD1-CG-CD2	-18.61	69.86	110.80
1	A	2	GLU	N-CA-C	16.47	128.92	110.97
1	A	177	LEU	CB-CG-CD2	14.54	154.31	110.70
1	A	190	ALA	O-C-N	-14.25	100.20	123.00
2	B	274	GLY	O-C-N	-12.97	113.96	123.95
1	A	56	ASP	CA-CB-CG	12.83	125.43	112.60
1	A	177	LEU	CA-C-O	-12.80	99.04	120.80
1	A	177	LEU	CA-CB-CG	-12.70	71.84	116.30
1	A	190	ALA	CA-C-O	-10.80	102.44	120.80
2	B	236	ASN	CA-CB-CG	10.36	122.96	112.60
1	A	190	ALA	N-CA-C	9.54	137.72	111.00
2	B	171	ASN	CA-CB-CG	-8.60	104.00	112.60
2	B	38	ASP	CA-CB-CG	8.48	121.08	112.60
2	B	19	GLN	OE1-CD-NE2	-8.24	114.36	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ALA	CB-CA-C	-8.19	98.22	110.50
2	B	63	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	A	190	ALA	CA-C-N	8.01	141.35	121.80
1	A	190	ALA	C-N-CA	8.01	141.35	121.80
2	B	353	HIS	CB-CG-CD2	-7.68	121.21	131.20
2	B	342	HIS	CB-CG-CD2	-7.64	121.27	131.20
2	B	176	ASP	CA-CB-CG	7.56	120.16	112.60
2	B	227	VAL	N-CA-C	-7.55	97.54	108.11
2	B	225	ASP	N-CA-C	-7.52	104.24	113.41
2	B	189	GLY	N-CA-C	7.34	123.04	114.16
1	A	212	PHE	CA-CB-CG	-7.33	106.47	113.80
2	B	63	GLN	CG-CD-NE2	7.29	127.34	116.40
1	A	194	HIS	CB-CG-CD2	-7.19	121.85	131.20
1	A	177	LEU	CB-CA-C	-7.12	96.58	110.10
2	B	112	ALA	N-CA-C	-6.86	98.86	109.76
2	B	115	HIS	CB-CG-CD2	-6.82	122.33	131.20
1	A	130	ASP	CA-CB-CG	6.77	119.37	112.60
2	B	241	PHE	N-CA-C	6.61	118.56	111.36
1	A	194	HIS	CA-CB-CG	6.53	120.33	113.80
2	B	86	HIS	CA-CB-CG	-6.52	107.28	113.80
2	B	317	ASN	OD1-CG-ND2	-6.52	116.08	122.60
2	B	305	ASP	N-CA-C	6.37	119.98	112.72
2	B	51	ASN	OD1-CG-ND2	-6.34	116.25	122.60
2	B	300	ILE	N-CA-C	-6.34	104.32	110.72
1	A	195	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	A	56	ASP	N-CA-CB	6.26	122.30	110.65
1	A	245	LEU	N-CA-C	6.26	119.76	111.75
2	B	193	GLY	CA-C-N	6.21	126.13	119.85
2	B	193	GLY	C-N-CA	6.21	126.13	119.85
2	B	353	HIS	CB-CG-ND1	6.17	131.95	122.70
1	A	42	ASP	CA-CB-CG	6.15	118.75	112.60
2	B	160	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	A	159	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	108	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	92	HIS	CB-CG-CD2	-6.02	123.38	131.20
2	B	346	ILE	N-CA-C	-6.02	102.08	107.56
1	A	129	ALA	N-CA-C	5.98	119.41	111.75
2	B	357	HIS	CA-CB-CG	-5.95	107.85	113.80
2	B	171	ASN	N-CA-C	5.94	117.42	111.07
2	B	94	GLN	OE1-CD-NE2	-5.89	116.71	122.60
2	B	44	GLN	OE1-CD-NE2	-5.77	116.83	122.60
2	B	185	HIS	CB-CG-CD2	-5.76	123.71	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	ILE	N-CA-C	-5.76	104.90	110.72
2	B	322	ALA	N-CA-C	-5.75	100.56	109.24
1	A	33	SER	CA-CB-OG	5.71	122.51	111.10
2	B	82	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	56	ASP	O-C-N	5.66	126.25	121.84
1	A	251	MET	N-CA-C	-5.66	105.02	111.07
2	B	87	LYS	CA-CB-CG	-5.65	102.80	114.10
2	B	241	PHE	CB-CA-C	-5.63	101.28	110.85
2	B	339	LEU	N-CA-C	-5.63	105.23	111.36
2	B	273	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	146	HIS	CB-CG-CD2	-5.59	123.93	131.20
2	B	313	HIS	CB-CG-CD2	-5.56	123.97	131.20
2	B	38	ASP	CA-C-N	5.54	125.64	119.32
2	B	38	ASP	C-N-CA	5.54	125.64	119.32
1	A	220	VAL	N-CA-C	-5.53	105.33	110.53
2	B	91	VAL	N-CA-CB	-5.53	103.02	110.54
2	B	312	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	155	PRO	CB-CA-C	5.51	117.64	110.92
2	B	246	ASN	OD1-CG-ND2	-5.48	117.12	122.60
2	B	267	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	194	HIS	CB-CG-ND1	5.46	130.88	122.70
1	A	204	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	250	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	A	56	ASP	CB-CA-C	-5.39	101.71	109.63
2	B	242	ALA	N-CA-C	5.34	117.51	111.11
2	B	329	ASP	CA-CB-CG	5.33	117.93	112.60
2	B	138	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	310	GLY	CA-C-N	5.29	125.61	119.47
2	B	310	GLY	C-N-CA	5.29	125.61	119.47
2	B	357	HIS	CE1-NE2-CD2	5.29	114.29	109.00
1	A	53	PRO	N-CA-C	5.28	118.78	110.80
1	A	195	HIS	CB-CG-ND1	5.25	130.58	122.70
2	B	269	ALA	CA-C-N	5.24	124.56	118.85
2	B	269	ALA	C-N-CA	5.24	124.56	118.85
2	B	115	HIS	CB-CG-ND1	5.23	130.54	122.70
2	B	215	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	228	ALA	N-CA-C	-5.18	102.02	110.20
2	B	365	GLN	OE1-CD-NE2	-5.18	117.42	122.60
2	B	197	TYR	CA-C-O	-5.16	113.67	118.73
2	B	27	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	B	27	GLN	CA-CB-CG	5.12	124.34	114.10
2	B	61	LYS	CB-CG-CD	-5.12	99.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	260	HIS	CA-CB-CG	5.10	118.90	113.80
2	B	86	HIS	CB-CG-CD2	-5.10	124.57	131.20
2	B	248	THR	CA-C-N	5.08	127.59	120.28
2	B	248	THR	C-N-CA	5.08	127.59	120.28
2	B	375	ASN	OD1-CG-ND2	-5.07	117.53	122.60
2	B	51	ASN	CA-CB-CG	-5.03	107.57	112.60
2	B	350	GLU	N-CA-C	-5.02	105.27	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	SER	Peptide
1	A	55	SER	Peptide
1	A	61	GLY	Peptide

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	1937	0	1949	39	0
2	B	2950	0	2924	36	0
3	B	1	0	0	0	0
4	B	15	0	6	2	0
5	A	21	0	0	0	0
5	B	54	0	0	2	0
All	All	4978	0	4879	75	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 (75) 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:177:LEU:HG	1:A:177:LEU:CA	1.21	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:CA	1:A:190:ALA:CB	1.84	1.49
1:A:177:LEU:CA	1:A:177:LEU:CG	1.91	1.48
1:A:177:LEU:CA	1:A:177:LEU:CB	1.85	1.47
1:A:190:ALA:C	1:A:191:LEU:N	1.69	1.47
1:A:177:LEU:CG	1:A:177:LEU:CD1	2.00	1.37
1:A:177:LEU:CG	1:A:177:LEU:CD2	2.08	1.32
1:A:177:LEU:CA	1:A:177:LEU:N	1.98	1.25
1:A:177:LEU:HG	1:A:177:LEU:HA	1.19	1.15
1:A:176:LEU:C	1:A:177:LEU:CA	2.26	1.09
1:A:177:LEU:HD22	1:A:177:LEU:HD11	1.35	1.08
1:A:190:ALA:C	1:A:190:ALA:O	1.96	1.07
1:A:177:LEU:CD1	1:A:177:LEU:CD2	2.34	1.06
1:A:177:LEU:CB	1:A:177:LEU:C	2.42	0.91
1:A:190:ALA:CB	1:A:190:ALA:C	2.46	0.89
1:A:177:LEU:CD2	1:A:177:LEU:HD11	1.99	0.89
1:A:177:LEU:CB	1:A:177:LEU:CD1	2.55	0.84
1:A:177:LEU:CD1	1:A:177:LEU:HD22	1.97	0.84
1:A:176:LEU:O	1:A:177:LEU:HA	1.86	0.76
1:A:176:LEU:C	1:A:177:LEU:HA	2.11	0.75
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.77	0.67
2:B:62:CYS:SG	2:B:65:ILE:HD11	2.39	0.63
1:A:190:ALA:CA	1:A:190:ALA:N	2.64	0.61
1:A:236:ALA:HA	1:A:239:LYS:HD2	1.83	0.60
1:A:210:GLN:HE21	1:A:214:ILE:HD11	1.68	0.56
2:B:112:ALA:HA	2:B:142:GLN:HG2	1.87	0.56
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.89	0.55
2:B:378:GLY:HA3	4:B:401:PLP:H2A3	1.89	0.54
2:B:34:ARG:HG2	2:B:100:ARG:HH22	1.72	0.53
2:B:262:ILE:HG12	5:B:429:HOH:O	2.09	0.52
2:B:381:ASP:O	2:B:384:ILE:HG12	2.10	0.52
2:B:110:THR:HG21	2:B:116:GLY:H	1.75	0.51
1:A:191:LEU:HD13	1:A:196:LEU:HD13	1.92	0.51
1:A:177:LEU:CG	1:A:177:LEU:HA	1.99	0.51
1:A:25:LEU:HD13	1:A:50:LEU:HG	1.92	0.50
1:A:154:CYS:HB3	1:A:176:LEU:HD12	1.92	0.50
2:B:90:GLN:HE22	2:B:94:GLN:HE21	1.59	0.49
2:B:276:VAL:HA	2:B:285:PRO:HA	1.94	0.49
2:B:117:VAL:HG13	2:B:152:MET:HE1	1.94	0.49
2:B:378:GLY:HA3	4:B:401:PLP:C2A	2.43	0.48
2:B:90:GLN:HA	2:B:204:PHE:HB3	1.96	0.48
2:B:109:GLU:HA	2:B:133:TYR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ILE:HD13	2:B:128:LEU:HD13	1.96	0.47
2:B:224:PRO:HA	2:B:371:LEU:HD13	1.97	0.47
2:B:195:HIS:HD2	5:B:438:HOH:O	1.96	0.47
1:A:125:SER:HB2	1:A:151:ILE:HG12	1.97	0.46
2:B:78:GLU:HB2	2:B:377:SER:HA	1.96	0.46
2:B:271:LEU:HD12	2:B:271:LEU:O	2.15	0.46
2:B:217:LEU:HD21	2:B:223:LEU:HD13	1.97	0.46
2:B:90:GLN:NE2	2:B:94:GLN:HE21	2.13	0.46
1:A:177:LEU:HD23	1:A:212:PHE:HD1	1.80	0.46
2:B:37:LYS:O	2:B:39:PRO:HD3	2.16	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.51	0.45
1:A:18:ALA:HA	1:A:46:ASP:OD2	2.17	0.45
2:B:94:GLN:OE1	2:B:187:MET:HA	2.16	0.45
2:B:61:LYS:HB2	2:B:74:TYR:CE1	2.52	0.44
1:A:190:ALA:CA	1:A:190:ALA:O	2.63	0.43
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.70	0.43
2:B:207:MET:HE3	2:B:207:MET:HB3	1.75	0.43
1:A:28:PRO:HB3	1:A:245:LEU:HD11	2.00	0.43
2:B:328:THR:HG22	2:B:330:ASP:H	1.83	0.43
1:A:117:ARG:O	1:A:121:VAL:HG22	2.19	0.43
1:A:214:ILE:HG21	1:A:231:ALA:HB1	1.99	0.43
2:B:87:LYS:HD2	2:B:114:GLN:HG3	2.01	0.42
2:B:297:SER:OG	2:B:307:PRO:HA	2.19	0.42
2:B:101:MET:HB2	2:B:103:LYS:HD3	2.02	0.42
1:A:43:ALA:HB2	1:A:256:ARG:HG3	2.01	0.41
2:B:137:LYS:HD3	2:B:163:SER:O	2.20	0.41
2:B:388:HIS:O	2:B:388:HIS:CG	2.74	0.41
2:B:110:THR:HG23	2:B:115:HIS:HB3	2.02	0.41
1:A:57:PRO:HB2	1:A:60:ASP:O	2.21	0.41
1:A:22:PHE:HB3	1:A:234:GLY:HA2	2.02	0.41
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.56	0.40
2:B:73:LEU:HD11	2:B:374:VAL:HG23	2.03	0.40
2:B:62:CYS:HB3	2:B:65:ILE:HG12	2.02	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	252/268 (94%)	240 (95%)	10 (4%)	2 (1%)	16	11
2	B	387/397 (98%)	372 (96%)	14 (4%)	1 (0%)	36	35
All	All	639/665 (96%)	612 (96%)	24 (4%)	3 (0%)	24	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	113	GLY
1	A	191	LEU
1	A	234	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	200/208 (96%)	177 (88%)	23 (12%)	5	3
2	B	305/311 (98%)	270 (88%)	35 (12%)	5	3
All	All	505/519 (97%)	447 (88%)	58 (12%)	5	3

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	5	GLU
1	A	12	ASN

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Mol	Chain	Res	Type
1	A	28	PRO
1	A	48	LEU
1	A	49	GLU
1	A	50	LEU
1	A	56	ASP
1	A	63	THR
1	A	66	ASN
1	A	81	CYS
1	A	117	ARG
1	A	127	LEU
1	A	144	LEU
1	A	155	PRO
1	A	159	ASP
1	A	160	ASP
1	A	198	GLU
1	A	210	GLN
1	A	219	GLN
1	A	243	LYS
1	A	251	MET
1	A	252	LEU
2	B	27	GLN
2	B	30	GLU
2	B	44	GLN
2	B	47	ASP
2	B	63	GLN
2	B	65	ILE
2	B	70	ARG
2	B	90	GLN
2	B	91	VAL
2	B	96	LEU
2	B	105	GLU
2	B	106	ILE
2	B	110	THR
2	B	139	VAL
2	B	140	GLU
2	B	142	GLN
2	B	159	VAL
2	B	171	ASN
2	B	172	GLU
2	B	180	SER
2	B	198	PRO
2	B	223	LEU

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Mol	Chain	Res	Type
2	B	236	ASN
2	B	248	THR
2	B	249	SER
2	B	271	LEU
2	B	321	ARG
2	B	333	LEU
2	B	347	PRO
2	B	351	SER
2	B	363	ARG
2	B	371	LEU
2	B	376	LEU
2	B	382	LYS
2	B	391	LEU

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	120	GLN
1	A	146	HIS
1	A	210	GLN
2	B	36	GLN
2	B	64	ASN
2	B	86	HIS
2	B	90	GLN
2	B	195	HIS
2	B	260	HIS
2	B	342	HIS

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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	B	401	2	15,15,16	3.06	9 (60%)	21,22,23	2.28	5 (23%)

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	B	401	2	-	0/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	PLP	C3-C4	6.51	1.52	1.40
4	B	401	PLP	C3-C2	5.10	1.46	1.41
4	B	401	PLP	C4A-C4	4.56	1.60	1.51
4	B	401	PLP	C6-C5	3.56	1.44	1.37
4	B	401	PLP	P-O4P	-3.03	1.50	1.60
4	B	401	PLP	C5-C4	2.86	1.43	1.40
4	B	401	PLP	P-O3P	-2.66	1.44	1.54
4	B	401	PLP	C6-N1	2.15	1.38	1.34
4	B	401	PLP	C2-N1	2.12	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	PLP	C2A-C2-C3	5.23	126.92	120.80
4	B	401	PLP	O3P-P-O4P	4.95	119.58	106.67
4	B	401	PLP	O4P-C5A-C5	4.32	117.45	109.36
4	B	401	PLP	C6-N1-C2	3.49	125.52	119.20
4	B	401	PLP	C3-C2-N1	-3.21	116.91	120.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	PLP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	190:ALA	C	191:LEU	N	1.69
1	A	176:LEU	C	177:LEU	N	1.20

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	256/268 (95%)	-0.07	9 (3%)	47 46	9, 38, 82, 96	4 (1%)
2	B	389/397 (97%)	-0.68	1 (0%)	90 89	5, 20, 54, 78	3 (0%)
All	All	645/665 (96%)	-0.44	10 (1%)	70 70	5, 26, 70, 96	7 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ASP	3.4
1	A	55	SER	2.8
1	A	195	HIS	2.8
2	B	385	PHE	2.7
1	A	62	PRO	2.6
1	A	57	PRO	2.5
1	A	61	GLY	2.4
1	A	77	THR	2.1
1	A	234	GLY	2.1
1	A	60	ASP	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 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	K	B	400	1/1	0.97	0.06	32,32,32,32	0
4	PLP	B	401	15/16	0.97	0.06	13,28,38,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.