



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:12 PM UTC

PDB ID : 1TTP / pdb\_00001ttp  
Title : TRYPTOPHAN SYNTHASE (E.C.4.2.1.20) IN THE PRESENCE OF CESIUM, ROOM TEMPERATURE  
Authors : Rhee, S.; Parris, K.; Ahmed, S.; Miles, E.W.; Davies, D.R.  
Deposited on : 1995-10-11  
Resolution : 2.30 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](mailto: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>.

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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

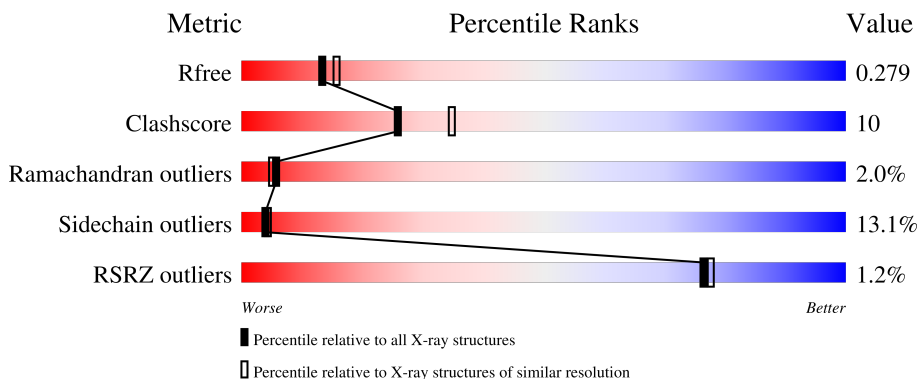
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">3%      65%      25%      6%      •</p>
2	B	397	<div style="display: flex; align-items: center;"> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">59%      29%      7%      ••</p>

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
4	PLP	B	402	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4918 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
			Total	C	N	O	S			
1	A	256	1937	1236	333	360	8	0	0	0

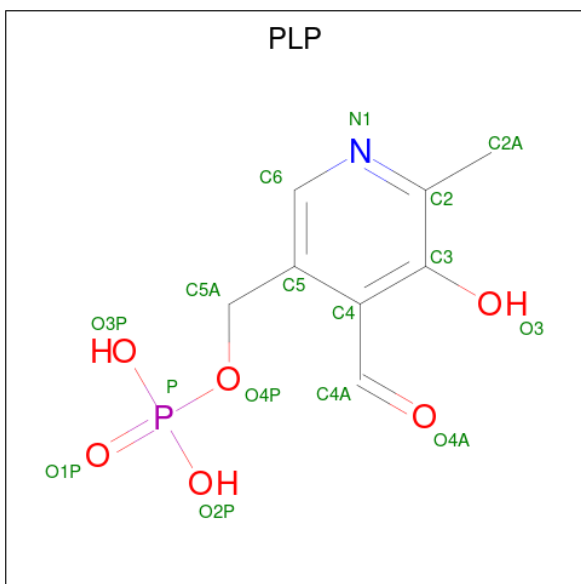
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

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

- Molecule 3 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cs		
3	B	2	2	2	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

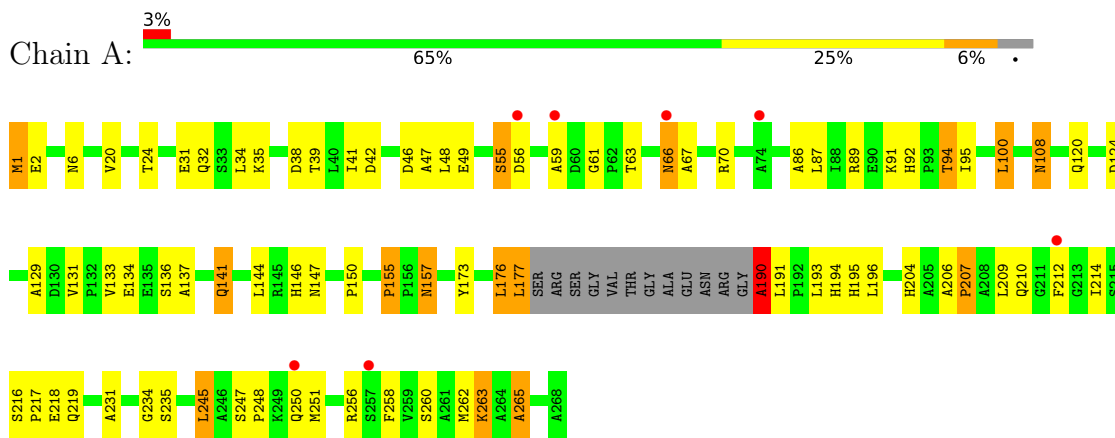
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	8	Total	O	0	0
			8	8		

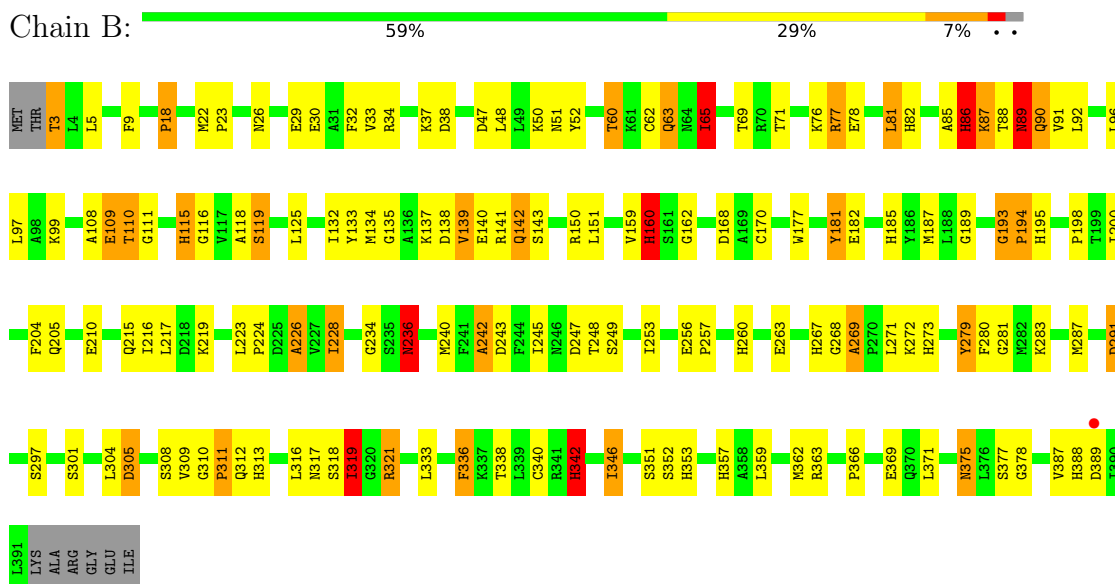
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	185.30Å 61.30Å 68.10Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 8.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	67.2 (8.00-2.30) 65.7 (8.00-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.30Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.217 , 0.302 0.199 , 0.279	Depositor DCC
$R_{free}$ test set	2230 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtrriage
Anisotropy	0.929	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 85.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CS, 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	2.31	15/1976 (0.8%)	2.10	52/2684 (1.9%)
2	B	1.25	25/3008 (0.8%)	1.88	71/4064 (1.7%)
All	All	1.75	40/4984 (0.8%)	1.97	123/6748 (1.8%)

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 (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ALA	N-CA	64.08	2.68	1.46
1	A	190	ALA	C-O	40.65	2.04	1.23
1	A	177	LEU	N-CA	30.48	2.04	1.46
1	A	177	LEU	CA-CB	29.73	2.12	1.53
1	A	177	LEU	CG-CD2	23.68	2.30	1.52
1	A	177	LEU	CB-CG	-14.46	1.24	1.53
1	A	190	ALA	C-N	14.23	1.63	1.33
1	A	190	ALA	CA-CB	9.24	1.83	1.52
1	A	176	LEU	C-N	-7.38	1.23	1.33
2	B	185	HIS	CD2-NE2	-7.16	1.29	1.37
2	B	342	HIS	CD2-NE2	-6.89	1.30	1.37
2	B	353	HIS	CG-ND1	-6.77	1.30	1.38
1	A	177	LEU	C-O	-6.59	1.10	1.23
2	B	86	HIS	CD2-NE2	-6.40	1.30	1.37
2	B	388	HIS	CD2-NE2	-6.30	1.30	1.37
2	B	313	HIS	CD2-NE2	-6.26	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	357	HIS	CD2-NE2	-6.16	1.31	1.37
2	B	65	ILE	CA-CB	6.12	1.62	1.54
2	B	160	HIS	CD2-NE2	-6.08	1.31	1.37
2	B	267	HIS	CD2-NE2	-6.07	1.31	1.37
2	B	353	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	195	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	194	HIS	CD2-NE2	-6.03	1.31	1.37
2	B	87	LYS	CB-CG	6.03	1.70	1.52
1	A	92	HIS	CD2-NE2	-5.85	1.31	1.37
2	B	87	LYS	CA-CB	-5.84	1.43	1.53
1	A	146	HIS	CD2-NE2	-5.79	1.31	1.37
2	B	313	HIS	CG-ND1	-5.69	1.31	1.38
2	B	115	HIS	CD2-NE2	-5.69	1.31	1.37
2	B	185	HIS	CG-ND1	-5.62	1.32	1.38
2	B	194	PRO	CA-CB	-5.61	1.46	1.53
2	B	260	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	204	HIS	CD2-NE2	-5.55	1.31	1.37
2	B	388	HIS	CG-ND1	-5.50	1.32	1.38
2	B	319	ILE	CA-CB	5.49	1.61	1.54
2	B	87	LYS	N-CA	5.44	1.53	1.46
2	B	82	HIS	CD2-NE2	-5.42	1.31	1.37
2	B	18	PRO	CA-CB	-5.23	1.46	1.53
2	B	87	LYS	CA-C	5.22	1.59	1.52
2	B	273	HIS	CD2-NE2	-5.17	1.32	1.37

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LEU	O-C-N	26.11	153.73	123.19
1	A	176	LEU	CA-C-N	-25.77	75.31	121.70
1	A	176	LEU	C-N-CA	-25.77	75.31	121.70
1	A	177	LEU	CD1-CG-CD2	-22.93	60.37	110.80
1	A	190	ALA	CA-C-O	-13.65	97.59	120.80
1	A	177	LEU	CA-C-O	-13.32	98.16	120.80
1	A	177	LEU	CA-CB-CG	-12.71	71.81	116.30
1	A	177	LEU	CB-CG-CD2	12.67	148.72	110.70
2	B	389	ASP	CA-CB-CG	12.67	125.27	112.60
1	A	190	ALA	O-C-N	-11.36	104.82	123.00
1	A	190	ALA	N-CA-C	10.46	140.29	111.00
1	A	136	SER	N-CA-C	10.33	122.62	111.36
2	B	236	ASN	CA-CB-CG	10.27	122.86	112.60
1	A	190	ALA	N-CA-CB	-9.60	96.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	ASN	OD1-CG-ND2	-9.54	113.06	122.60
1	A	42	ASP	CA-CB-CG	8.54	121.14	112.60
2	B	305	ASP	CA-CB-CG	8.31	120.91	112.60
2	B	291	ASP	CA-CB-CG	8.08	120.68	112.60
1	A	177	LEU	CB-CA-C	-7.90	95.09	110.10
2	B	142	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	A	190	ALA	CA-C-N	7.83	140.91	121.80
1	A	190	ALA	C-N-CA	7.83	140.91	121.80
2	B	357	HIS	CA-CB-CG	-7.71	106.09	113.80
1	A	150	PRO	O-C-N	-7.61	117.33	122.73
2	B	3	THR	CA-CB-OG1	-7.56	98.26	109.60
2	B	89	ASN	CB-CG-ND2	7.45	127.58	116.40
2	B	193	GLY	CA-C-N	7.36	127.41	119.90
2	B	193	GLY	C-N-CA	7.36	127.41	119.90
1	A	66	ASN	CA-CB-CG	7.33	119.93	112.60
2	B	89	ASN	CA-CB-CG	7.22	119.82	112.60
1	A	137	ALA	CA-C-O	-7.08	110.46	120.16
2	B	219	LYS	N-CA-C	7.07	118.78	111.14
2	B	181	TYR	N-CA-C	6.89	121.14	112.87
2	B	318	SER	CA-C-O	-6.88	113.20	120.63
2	B	205	GLN	OE1-CD-NE2	-6.85	115.75	122.60
2	B	86	HIS	CA-CB-CG	-6.83	106.97	113.80
1	A	2	GLU	N-CA-C	6.70	122.42	111.37
2	B	51	ASN	N-CA-C	6.70	121.54	113.23
2	B	63	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	A	190	ALA	CB-CA-C	-6.50	100.75	110.50
2	B	387	VAL	N-CA-C	-6.49	102.98	111.09
2	B	88	THR	O-C-N	-6.48	115.36	122.09
2	B	346	ILE	N-CA-C	-6.46	101.15	107.55
2	B	226	ALA	CA-C-O	-6.41	113.61	121.11
1	A	147	ASN	CA-CB-CG	-6.36	106.24	112.60
2	B	3	THR	CA-CB-CG2	6.36	121.31	110.50
2	B	234	GLY	CA-C-O	-6.32	111.82	119.03
2	B	312	GLN	OE1-CD-NE2	-6.26	116.34	122.60
2	B	88	THR	CA-C-O	-6.24	114.22	120.90
1	A	92	HIS	CB-CG-CD2	-6.15	123.20	131.20
2	B	389	ASP	N-CA-C	-6.13	105.63	113.23
2	B	352	SER	N-CA-C	-6.12	104.73	111.82
1	A	219	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	A	195	HIS	CB-CG-CD2	-6.08	123.29	131.20
2	B	82	HIS	CB-CG-CD2	-6.08	123.30	131.20
2	B	247	ASP	CA-CB-CG	6.06	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	HIS	CB-CG-CD2	-6.04	123.35	131.20
2	B	342	HIS	CB-CG-CD2	-6.03	123.36	131.20
2	B	150	ARG	CA-CB-CG	6.02	126.14	114.10
2	B	215	GLN	OE1-CD-NE2	-6.02	116.58	122.60
2	B	318	SER	CA-CB-OG	-6.02	99.07	111.10
2	B	375	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	38	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	157	ASN	OD1-CG-ND2	-5.91	116.69	122.60
2	B	77	ARG	N-CA-C	5.81	117.97	110.65
2	B	71	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	91	LYS	N-CA-C	-5.75	106.26	113.28
1	A	100	LEU	N-CA-C	-5.70	100.39	109.96
2	B	369	GLU	CB-CG-CD	5.70	122.28	112.60
1	A	204	HIS	CB-CG-CD2	-5.66	123.84	131.20
2	B	160	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	95	ILE	N-CA-C	5.62	114.46	108.95
2	B	142	GLN	CG-CD-NE2	5.62	124.82	116.40
1	A	131	VAL	N-CA-C	-5.58	102.62	108.15
2	B	269	ALA	CA-C-N	5.58	125.04	119.24
2	B	269	ALA	C-N-CA	5.58	125.04	119.24
2	B	119	SER	N-CA-C	-5.57	104.06	111.24
2	B	273	HIS	CB-CG-CD2	-5.53	124.01	131.20
2	B	234	GLY	N-CA-C	5.53	122.38	114.64
2	B	63	GLN	CG-CD-NE2	5.52	124.67	116.40
2	B	366	PRO	N-CA-C	5.51	123.83	112.47
2	B	87	LYS	CA-CB-CG	-5.51	103.09	114.10
1	A	150	PRO	CB-CA-C	5.50	116.49	111.87
1	A	120	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	195	HIS	CA-CB-CG	5.48	119.28	113.80
2	B	359	LEU	CA-C-N	5.48	127.57	120.44
2	B	359	LEU	C-N-CA	5.48	127.57	120.44
2	B	336	PHE	N-CA-C	-5.48	104.95	111.03
1	A	147	ASN	N-CA-C	5.46	118.87	111.17
1	A	6	ASN	OD1-CG-ND2	-5.45	117.15	122.60
2	B	81	LEU	N-CA-C	-5.42	101.45	110.17
2	B	357	HIS	CA-C-O	-5.38	114.72	120.42
2	B	51	ASN	CA-CB-CG	-5.34	107.25	112.60
2	B	287	MET	CA-CB-CG	-5.33	103.44	114.10
2	B	359	LEU	N-CA-C	-5.33	105.14	111.69
1	A	94	THR	N-CA-C	5.31	119.86	112.90
2	B	86	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	235	SER	N-CA-C	5.30	118.54	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ALA	CA-C-N	5.30	126.46	119.84
1	A	206	ALA	C-N-CA	5.30	126.46	119.84
2	B	76	LYS	N-CA-C	-5.29	100.55	108.96
2	B	185	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	61	GLY	CA-C-N	5.28	124.91	119.05
1	A	61	GLY	C-N-CA	5.28	124.91	119.05
1	A	155	PRO	CB-CA-C	5.27	117.35	110.92
2	B	60	THR	N-CA-C	5.24	117.27	109.25
1	A	108	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	141	GLN	CB-CA-C	-5.18	102.52	110.81
1	A	155	PRO	CA-C-N	5.18	124.63	119.24
1	A	155	PRO	C-N-CA	5.18	124.63	119.24
1	A	124	ASP	N-CA-C	5.15	118.02	111.69
2	B	317	ASN	N-CA-C	-5.13	105.38	110.97
2	B	38	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	47	ASP	CA-CB-CG	-5.12	107.48	112.60
2	B	260	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	86	ALA	O-C-N	-5.09	116.72	122.12
2	B	38	ASP	CA-C-N	5.09	125.12	119.32
2	B	38	ASP	C-N-CA	5.09	125.12	119.32
2	B	228	ILE	CB-CG1-CD1	5.05	124.41	113.80
1	A	141	GLN	CG-CD-NE2	5.05	123.98	116.40
1	A	49	GLU	N-CA-C	-5.03	100.21	108.41
2	B	9	PHE	CA-CB-CG	-5.02	108.78	113.80
2	B	195	HIS	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Mainchain
1	A	190	ALA	Mainchain
1	A	247	SER	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	36	0
2	B	2950	0	2924	62	0
3	B	2	0	0	0	1
4	B	15	0	7	3	0
5	A	6	0	0	0	0
5	B	8	0	0	1	0
All	All	4918	0	4880	93	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 10.

All (93) 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	1.32	1.54
1:A:190:ALA:CA	1:A:190:ALA:CB	1.83	1.52
1:A:177:LEU:CD2	1:A:177:LEU:HD11	1.47	1.41
1:A:177:LEU:CD2	1:A:177:LEU:CD1	2.06	1.31
1:A:177:LEU:CA	1:A:177:LEU:CG	2.10	1.28
1:A:177:LEU:CA	1:A:177:LEU:CB	2.12	1.27
1:A:176:LEU:C	1:A:177:LEU:CA	2.09	1.24
1:A:177:LEU:CA	1:A:177:LEU:N	2.04	1.19
1:A:177:LEU:CD2	1:A:177:LEU:CG	2.30	1.07
1:A:177:LEU:HG	1:A:177:LEU:HA	1.39	1.01
1:A:190:ALA:C	1:A:190:ALA:O	2.04	0.99
1:A:176:LEU:C	1:A:177:LEU:HA	1.85	0.98
1:A:177:LEU:HD11	1:A:177:LEU:HD22	1.02	0.98
1:A:176:LEU:O	1:A:177:LEU:HA	1.68	0.92
1:A:177:LEU:CD1	1:A:177:LEU:HD22	1.90	0.87
2:B:89:ASN:H	2:B:89:ASN:HD22	1.25	0.85
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.59	0.85
2:B:194:PRO:HG3	2:B:281:GLY:HA3	1.61	0.83
1:A:190:ALA:CB	1:A:190:ALA:C	2.61	0.72
1:A:214:ILE:HG12	1:A:231:ALA:HB1	1.77	0.67
1:A:177:LEU:CB	1:A:177:LEU:C	2.70	0.64
2:B:256:GLU:HG2	2:B:269:ALA:HA	1.78	0.64
2:B:236:ASN:HD22	4:B:402:PLP:H6	1.66	0.61
2:B:90:GLN:HA	2:B:204:PHE:HB3	1.82	0.60
2:B:108:ALA:HB3	2:B:132:ILE:HD13	1.83	0.60
1:A:39:THR:HG23	1:A:256:ARG:NH1	2.17	0.59
1:A:108:ASN:HD21	2:B:291:ASP:HA	1.67	0.59
2:B:89:ASN:H	2:B:89:ASN:ND2	1.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:THR:O	2:B:342:HIS:HB2	2.03	0.57
1:A:190:ALA:CA	1:A:190:ALA:N	2.68	0.57
2:B:62:CYS:SG	2:B:65:ILE:HD11	2.44	0.57
2:B:111:GLY:O	2:B:138:ASP:HB3	2.06	0.55
2:B:60:THR:OG1	2:B:77:ARG:HD2	2.06	0.55
2:B:271:LEU:HD12	2:B:309:VAL:HG11	1.88	0.55
2:B:48:LEU:HB3	2:B:92:LEU:HD13	1.88	0.55
2:B:340:CYS:SG	2:B:346:ILE:HG12	2.47	0.54
2:B:137:LYS:O	2:B:141:ARG:HG2	2.07	0.54
2:B:3:THR:HG22	2:B:5:LEU:O	2.08	0.53
2:B:116:GLY:HA2	2:B:132:ILE:HD12	1.90	0.53
1:A:67:ALA:HA	1:A:70:ARG:HD3	1.90	0.53
2:B:89:ASN:HD22	2:B:89:ASN:N	2.02	0.53
2:B:110:THR:HG23	2:B:115:HIS:HB3	1.91	0.53
1:A:39:THR:HG23	1:A:256:ARG:HH11	1.74	0.52
2:B:52:TYR:CE1	2:B:125:LEU:HD13	2.45	0.51
2:B:226:ALA:HB1	2:B:253:ILE:CD1	2.41	0.51
2:B:236:ASN:HB3	4:B:402:PLP:O3P	2.10	0.51
2:B:91:VAL:HG11	2:B:118:ALA:O	2.10	0.51
1:A:59:ALA:HB2	2:B:18:PRO:HG3	1.93	0.50
2:B:301:SER:HB2	2:B:304:LEU:HB2	1.92	0.50
2:B:242:ALA:HB3	5:B:412:HOH:O	2.12	0.50
2:B:134:MET:SD	2:B:139:VAL:HG23	2.51	0.50
2:B:240:MET:HE2	2:B:375:ASN:OD1	2.12	0.50
2:B:142:GLN:HE21	2:B:142:GLN:HA	1.78	0.49
1:A:56:ASP:HB2	2:B:279:TYR:OH	2.12	0.49
1:A:157:ASN:ND2	2:B:23:PRO:HG3	2.29	0.48
2:B:30:GLU:O	2:B:34:ARG:HG3	2.13	0.48
2:B:22:MET:HE3	2:B:26:ASN:HD21	1.79	0.48
2:B:177:TRP:O	2:B:181:TYR:HB3	2.13	0.48
2:B:63:GLN:HE21	2:B:63:GLN:HA	1.79	0.47
2:B:110:THR:HB	2:B:134:MET:HE3	1.96	0.47
2:B:193:GLY:HA2	2:B:280:PHE:O	2.14	0.47
2:B:109:GLU:HA	2:B:133:TYR:O	2.14	0.47
1:A:248:PRO:O	1:A:251:MET:HB3	2.15	0.46
2:B:91:VAL:HG13	2:B:187:MET:SD	2.56	0.46
2:B:125:LEU:O	2:B:125:LEU:HG	2.16	0.45
1:A:258:PHE:O	1:A:262:MET:HG2	2.17	0.45
2:B:69:THR:HG21	2:B:362:MET:HB2	1.98	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.45
2:B:29:GLU:O	2:B:33:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:GLY:HA2	2:B:159:VAL:HB	1.99	0.44
1:A:173:TYR:HB2	1:A:209:LEU:HD13	1.98	0.44
1:A:196:LEU:HA	1:A:196:LEU:HD23	1.85	0.44
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.53	0.44
2:B:321:ARG:O	2:B:321:ARG:HD3	2.18	0.43
2:B:162:GLY:HA3	2:B:168:ASP:OD1	2.18	0.43
2:B:78:GLU:HB2	2:B:377:SER:HA	1.99	0.43
2:B:316:LEU:HA	2:B:319:ILE:CD1	2.49	0.43
2:B:378:GLY:HA3	4:B:402:PLP:H2A3	2.01	0.42
1:A:41:ILE:HD11	1:A:48:LEU:HD11	2.01	0.42
2:B:81:LEU:HD22	2:B:86:HIS:HA	2.02	0.41
2:B:109:GLU:HG2	2:B:170:CYS:HA	2.03	0.41
2:B:257:PRO:HG2	2:B:268:GLY:O	2.20	0.41
2:B:272:LYS:HD3	2:B:272:LYS:HA	1.89	0.41
1:A:217:PRO:HB3	1:A:265:ALA:HB2	2.03	0.41
2:B:333:LEU:O	2:B:336:PHE:HB3	2.20	0.41
1:A:46:ASP:OD2	1:A:263:LYS:HE3	2.21	0.41
1:A:89:ARG:HH11	1:A:89:ARG:HD3	1.75	0.41
2:B:90:GLN:HE21	2:B:90:GLN:HB2	1.62	0.40
2:B:216:ILE:HD12	2:B:216:ILE:HA	1.73	0.40
2:B:310:GLY:HA2	2:B:311:PRO:HD2	1.78	0.40
1:A:20:VAL:HG22	1:A:47:ALA:HB3	2.04	0.40
1:A:108:ASN:ND2	2:B:291:ASP:HA	2.36	0.40
2:B:22:MET:N	2:B:23:PRO:HD2	2.37	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)
3:B:401:CS:CS	3:B:401:CS:CS[2_655]	1.88	0.32

## 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	252/268 (94%)	233 (92%)	12 (5%)	7 (3%)	4	2
2	B	387/397 (98%)	349 (90%)	32 (8%)	6 (2%)	7	7
All	All	639/665 (96%)	582 (91%)	44 (7%)	13 (2%)	6	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	SER
2	B	86	HIS
1	A	129	ALA
1	A	245	LEU
2	B	160	HIS
1	A	191	LEU
1	A	207	PRO
2	B	85	ALA
2	B	242	ALA
2	B	311	PRO
1	A	265	ALA
1	A	234	GLY
2	B	297	SER

### 5.3.2 Protein sidechains [i](#)

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%)	173 (86%)	27 (14%)	4	4
2	B	305/311 (98%)	266 (87%)	39 (13%)	4	4
All	All	505/519 (97%)	439 (87%)	66 (13%)	4	4

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	24	THR
1	A	31	GLU
1	A	32	GLN
1	A	34	LEU
1	A	35	LYS
1	A	55	SER
1	A	63	THR
1	A	66	ASN
1	A	87	LEU
1	A	94	THR
1	A	100	LEU
1	A	133	VAL
1	A	134	GLU
1	A	141	GLN
1	A	144	LEU
1	A	155	PRO
1	A	193	LEU
1	A	207	PRO
1	A	210	GLN
1	A	212	PHE
1	A	216	SER
1	A	218	GLU
1	A	245	LEU
1	A	250	GLN
1	A	260	SER
1	A	263	LYS
2	B	37	LYS
2	B	50	LYS
2	B	65	ILE
2	B	87	LYS
2	B	89	ASN
2	B	90	GLN
2	B	96	LEU
2	B	97	LEU
2	B	99	LYS
2	B	109	GLU
2	B	110	THR
2	B	119	SER
2	B	139	VAL
2	B	140	GLU
2	B	143	SER
2	B	151	LEU

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Mol	Chain	Res	Type
2	B	160	HIS
2	B	182	GLU
2	B	198	PRO
2	B	210	GLU
2	B	217	LEU
2	B	223	LEU
2	B	228	ILE
2	B	236	ASN
2	B	243	ASP
2	B	245	ILE
2	B	248	THR
2	B	249	SER
2	B	263	GLU
2	B	279	TYR
2	B	283	LYS
2	B	305	ASP
2	B	308	SER
2	B	319	ILE
2	B	321	ARG
2	B	342	HIS
2	B	351	SER
2	B	363	ARG
2	B	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	165	GLN
1	A	195	HIS
1	A	219	GLN
2	B	26	ASN
2	B	42	GLN
2	B	63	GLN
2	B	89	ASN
2	B	90	GLN
2	B	142	GLN
2	B	160	HIS
2	B	195	HIS
2	B	293	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 3 ligands modelled in this entry, 2 are 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	402	2	15,15,16	4.89	10 (66%)	21,22,23	2.49	7 (33%)

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	402	2	-	2/6/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	PLP	C3-C4	9.05	1.57	1.40
4	B	402	PLP	C5-C4	8.19	1.49	1.40
4	B	402	PLP	C4A-C4	7.49	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	PLP	C3-C2	6.55	1.47	1.41
4	B	402	PLP	C6-C5	5.68	1.48	1.37
4	B	402	PLP	P-O3P	-5.48	1.34	1.54
4	B	402	PLP	C6-N1	3.92	1.42	1.34
4	B	402	PLP	C2-N1	3.37	1.39	1.33
4	B	402	PLP	O4P-C5A	-3.13	1.33	1.44
4	B	402	PLP	P-O4P	-2.77	1.51	1.60

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	PLP	O3P-P-O4P	5.59	121.24	106.67
4	B	402	PLP	C2A-C2-C3	5.10	126.76	120.80
4	B	402	PLP	C6-N1-C2	4.23	126.86	119.20
4	B	402	PLP	O4P-C5A-C5	3.95	116.76	109.36
4	B	402	PLP	C3-C2-N1	-3.67	116.33	120.96
4	B	402	PLP	C6-C5-C4	-2.75	115.84	118.10
4	B	402	PLP	C5A-C5-C6	-2.19	115.79	119.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	PLP	C5-C5A-O4P-P
4	B	402	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	PLP	3	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	1

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	1.63

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	256/268 (95%)	-0.07	7 (2%) 56 58	8, 38, 79, 86	4 (1%)
2	B	389/397 (97%)	-0.53	1 (0%) 90 90	3, 19, 56, 75	3 (0%)
All	All	645/665 (96%)	-0.34	8 (1%) 76 77	3, 26, 68, 86	7 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	389	ASP	3.4
1	A	56	ASP	3.1
1	A	250	GLN	2.6
1	A	212	PHE	2.4
1	A	59	ALA	2.2
1	A	257	SER	2.1
1	A	66	ASN	2.1
1	A	74	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PLP	B	402	15/16	0.96	0.07	17,27,34,36	0
3	CS	B	401	1/1	0.97	0.15	116,116,116,116	0
3	CS	B	400	1/1	0.98	0.03	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.