



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TTQ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

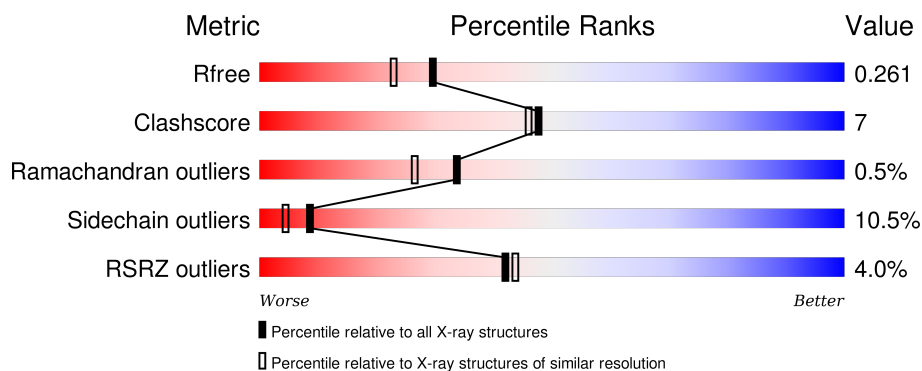
# 1 Overall quality at a glance

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
2	B	397	

## 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			

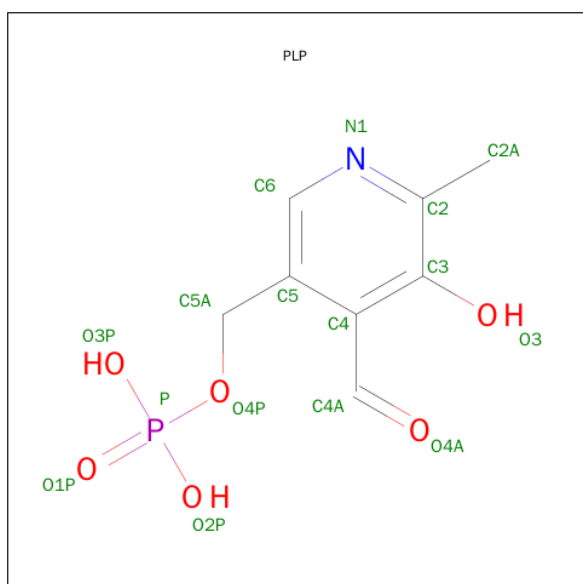
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

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 (three-letter code: K) (formula: K).

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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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		

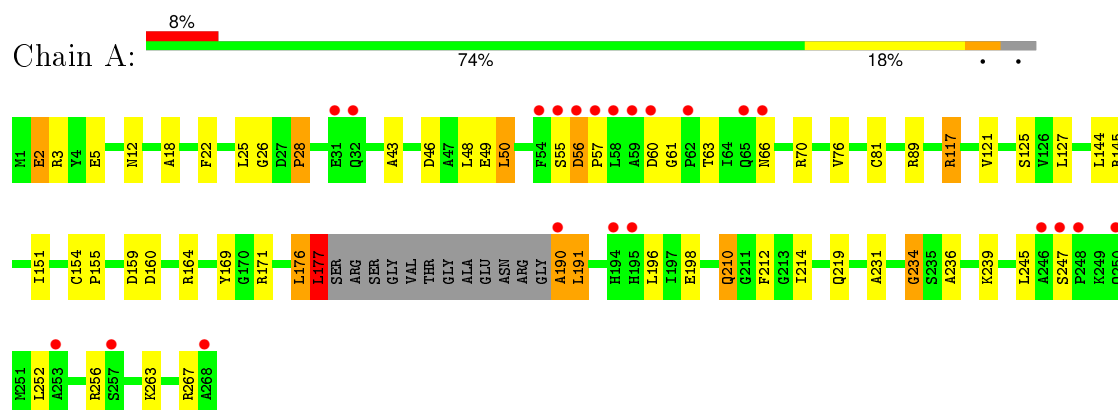
- Molecule 5 is water.

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

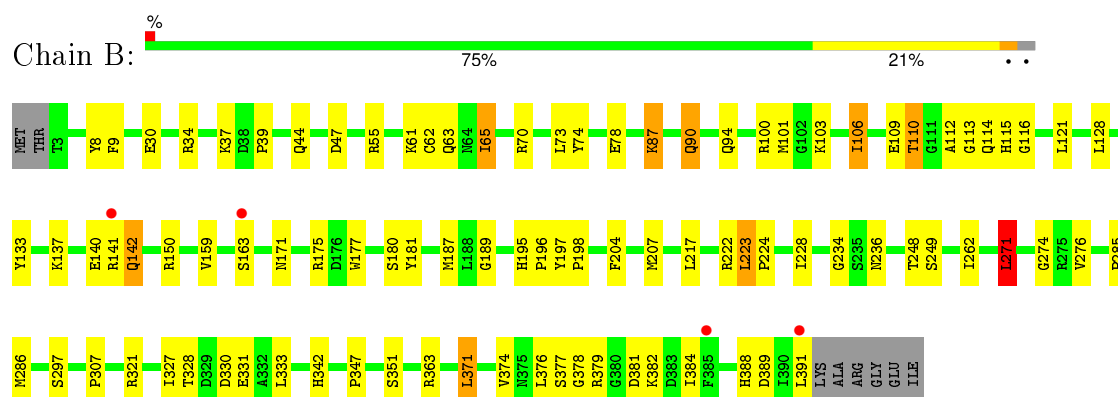
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	185.00 Å   61.30 Å   67.70 Å 90.00°   94.70°   90.00°	Depositor
Resolution (Å)	8.00 – 2.00 7.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	71.7 (8.00-2.00) 71.4 (7.99-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.00 Å)	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 84.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 35959 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1.98	13/1976 (0.7%)	1.60	28/2684 (1.0%)
2	B	0.80	1/3008 (0.0%)	1.42	23/4064 (0.6%)
All	All	1.39	14/4984 (0.3%)	1.49	51/6748 (0.8%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ALA	N-CA	59.00	2.64	1.46
1	A	190	ALA	C-O	38.25	1.96	1.23
1	A	177	LEU	N-CA	25.83	1.98	1.46
1	A	190	ALA	C-N	15.37	1.69	1.34
1	A	177	LEU	CG-CD2	15.35	2.08	1.51
1	A	190	ALA	CA-CB	15.31	1.84	1.52
1	A	177	LEU	CA-CB	13.57	1.84	1.53
1	A	177	LEU	CG-CD1	13.08	2.00	1.51
2	B	87	LYS	CB-CG	8.02	1.74	1.52
1	A	177	LEU	CB-CG	-6.51	1.33	1.52
1	A	177	LEU	CA-C	-6.15	1.36	1.52
1	A	176	LEU	C-N	-5.99	1.20	1.34
1	A	177	LEU	C-O	5.77	1.34	1.23
1	A	190	ALA	CA-C	-5.48	1.38	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	CB-CG-CD2	25.48	154.31	111.00
1	A	177	LEU	CA-CB-CG	-18.90	71.84	115.30
1	A	176	LEU	O-C-N	15.05	146.78	122.70
1	A	190	ALA	O-C-N	-14.06	100.20	122.70
1	A	176	LEU	C-N-CA	-13.87	87.03	121.70
1	A	177	LEU	CD1-CG-CD2	-13.55	69.86	110.50
1	A	176	LEU	CA-C-N	-11.20	92.57	117.20
1	A	190	ALA	CA-C-N	10.97	141.34	117.20
1	A	177	LEU	CA-C-O	-10.03	99.04	120.10
1	A	190	ALA	N-CA-C	9.89	137.72	111.00
1	A	3	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	A	190	ALA	CA-C-O	-8.41	102.44	120.10
1	A	190	ALA	CB-CA-C	-7.92	98.22	110.10
1	A	190	ALA	C-N-CA	7.86	141.35	121.70
1	A	177	LEU	CB-CG-CD1	-7.61	98.07	111.00
1	A	145	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	177	LEU	CB-CA-C	-7.17	96.58	110.20
2	B	177	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	A	70	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	145	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	2	GLU	N-CA-C	6.64	128.92	111.00
2	B	121	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	56	ASP	N-CA-CB	6.50	122.30	110.60
2	B	150	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	B	55	ARG	NE-CZ-NH1	6.37	123.48	120.30
2	B	271	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	267	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	B	177	TRP	CE2-CD2-CG	-5.91	102.57	107.30
2	B	379	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	222	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	B	181	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	169	TYR	CB-CG-CD2	-5.71	117.57	121.00
2	B	197	TYR	CB-CG-CD1	-5.70	117.58	121.00
2	B	8	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	A	164	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	B	222	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	56	ASP	CA-CB-CG	5.47	125.43	113.40
2	B	274	GLY	O-C-N	-5.46	113.96	122.70
1	A	171	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	B	379	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	B	389	ASP	CB-CG-OD1	5.31	123.08	118.30
2	B	286	MET	CA-CB-CG	5.28	122.28	113.30
2	B	141	ARG	NE-CZ-NH1	5.23	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	B	274	GLY	CA-C-N	5.19	128.62	117.20
2	B	9	PHE	N-CA-C	-5.17	97.04	111.00
2	B	175	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	228	ILE	CG1-CB-CG2	-5.09	100.21	111.40
2	B	234	GLY	CA-C-N	5.08	128.38	117.20
1	A	89	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	B	271	LEU	CB-CG-CD2	-5.01	102.48	111.00

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 [i](#)

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	33	0
3	B	1	0	0	0	0
4	B	15	0	6	1	0
5	A	21	0	0	0	0
5	B	54	0	0	2	0
All	All	4978	0	4879	72	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 7.

All (72) 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	1.43
1:A:177:LEU:CG	1:A:177:LEU:CD1	2.00	1.37
1:A:177:LEU:CD2	1:A:177:LEU:CG	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:177:LEU:HD11	1:A:177:LEU:HD22	1.35	1.08
1:A:177:LEU:CD2	1:A:177:LEU:CD1	2.34	1.06
1:A:176:LEU:C	1:A:177:LEU:CA	2.26	1.04
1:A:190:ALA:O	1:A:190:ALA:C	1.96	1.02
1:A:177:LEU:HD11	1:A:177:LEU:CD2	1.99	0.89
1:A:177:LEU:C	1:A:177:LEU:CB	2.42	0.87
1:A:190:ALA:C	1:A:190:ALA:CB	2.46	0.84
1:A:177:LEU:CB	1:A:177:LEU:CD1	2.55	0.84
1:A:177:LEU:HD22	1:A:177:LEU:CD1	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	0.70
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:271:LEU:O	2:B:271:LEU:HD12	2.15	0.46
2:B:78:GLU:HB2	2:B:377:SER:HA	1.96	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:115:HIS:CE1	2:B:189:GLY:HA2	2.51	0.45
2:B:37:LYS:O	2:B:39:PRO:HD3	2.16	0.45
2:B:94:GLN:OE1	2:B:187:MET:HA	2.16	0.45
1:A:18:ALA:HA	1:A:46:ASP:OD2	2.17	0.45
2:B:61:LYS:HB2	2:B:74:TYR:CE1	2.52	0.44
1:A:190:ALA:O	1:A:190:ALA:CA	2.63	0.43
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.70	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%)	24	15
2	B	387/397 (98%)	372 (96%)	14 (4%)	1 (0%)	46	41
All	All	639/665 (96%)	612 (96%)	24 (4%)	3 (0%)	34	26

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%)	178 (89%)	22 (11%)	8	4
2	B	305/311 (98%)	274 (90%)	31 (10%)	9	5
All	All	505/519 (97%)	452 (90%)	53 (10%)	8	4

All (53) 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
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

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Mol	Chain	Res	Type
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	177	LEU
1	A	198	GLU
1	A	210	GLN
1	A	219	GLN
1	A	252	LEU
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	106	ILE
2	B	110	THR
2	B	140	GLU
2	B	142	GLN
2	B	159	VAL
2	B	171	ASN
2	B	180	SER
2	B	198	PRO
2	B	207	MET
2	B	223	LEU
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	342	HIS
2	B	347	PRO
2	B	351	SER
2	B	363	ARG
2	B	371	LEU
2	B	376	LEU
2	B	382	LYS

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Mol	Chain	Res	Type
2	B	391	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	146	HIS
1	A	210	GLN
2	B	90	GLN
2	B	195	HIS
2	B	342	HIS
2	B	365	GLN
2	B	370	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	3.19	8 (53%)	21,22,23	2.26	6 (28%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	PLP	P-O4P	-2.84	1.50	1.60
4	B	401	PLP	P-O3P	-2.72	1.44	1.54
4	B	401	PLP	C6-N1	2.02	1.38	1.34
4	B	401	PLP	C5-C4	2.79	1.43	1.40
4	B	401	PLP	C6-C5	3.21	1.44	1.37
4	B	401	PLP	C4A-C4	4.42	1.60	1.51
4	B	401	PLP	C3-C4	4.99	1.52	1.40
4	B	401	PLP	C3-C2	7.93	1.46	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	PLP	C3-C2-N1	-2.68	116.91	120.61
4	B	401	PLP	C5A-C5-C4	2.42	124.86	121.65
4	B	401	PLP	C6-N1-C2	3.06	125.52	119.28
4	B	401	PLP	O3P-P-O4P	4.52	119.58	106.56
4	B	401	PLP	C2A-C2-C3	4.88	126.92	121.04
4	B	401	PLP	O4P-C5A-C5	5.12	117.45	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.12	22 (8%) 13 14	11, 38, 82, 96	4 (1%)
2	B	389/397 (97%)	-0.65	4 (1%) 84 84	5, 20, 54, 78	3 (0%)
All	All	645/665 (96%)	-0.35	26 (4%) 42 44	5, 26, 70, 96	7 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	HIS	5.2
1	A	56	ASP	5.0
1	A	60	ASP	4.7
1	A	194	HIS	4.2
1	A	55	SER	3.6
1	A	247	SER	3.6
1	A	59	ALA	3.4
1	A	57	PRO	3.4
1	A	31	GLU	3.2
1	A	268	ALA	3.1
1	A	246	ALA	3.0
2	B	385	PHE	2.9
2	B	163	SER	2.9
1	A	248	PRO	2.8
1	A	257	SER	2.8
1	A	250	GLN	2.7
1	A	58	LEU	2.7
1	A	253	ALA	2.5
1	A	62	PRO	2.5
1	A	65	GLN	2.5
1	A	66	ASN	2.4
1	A	54	PHE	2.2
1	A	32	GLN	2.2
1	A	190	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	391	LEU	2.1
2	B	141	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PLP	B	401	15/16	0.98	0.08	0.37	13,28,38,44	0
3	K	B	400	1/1	0.98	0.06	-1.32	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.