



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8RSZ / pdb_00008rsz
Title : TRYPTOPHAN SYNTHASE measured via serial crystallography from a kapton HARE-chip (125 micron)
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Deposited on : 2024-01-25
Resolution : 2.20 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

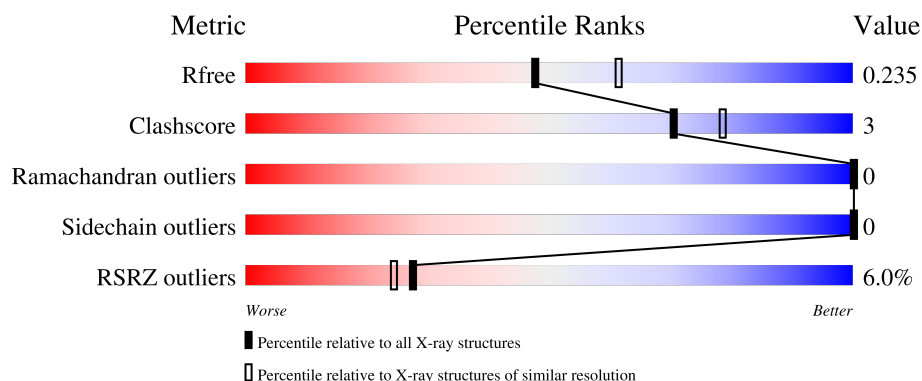
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	7% 86% 9% .
2	E	394	5% 93% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5139 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	2	0
			1955	1245	335	367	8			

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	394	Total	C	N	O	P S	0	3	0
			3017	1893	528	576	1 19			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cs	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Cl	0	0
			1	1		

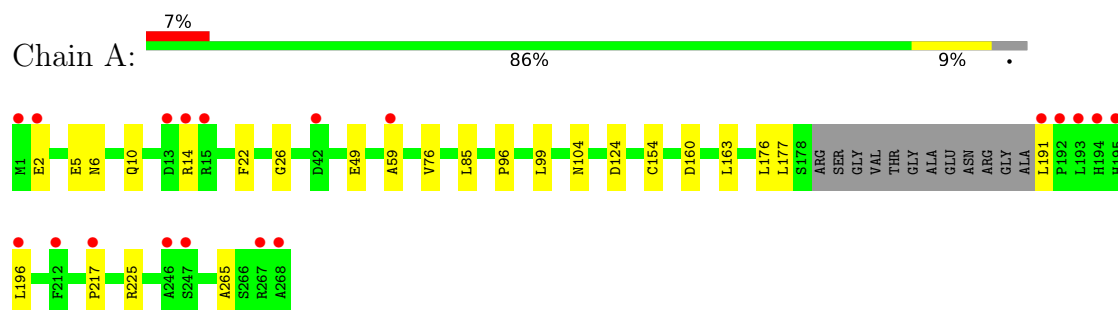
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	E	119	Total	O	0	0
			119	119		

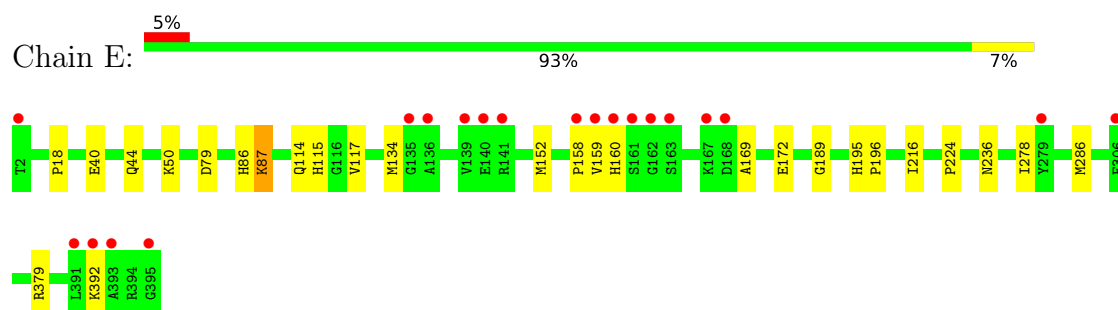
3 Residue-property plots [i](#)

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 alpha chain



- Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.60Å 61.50Å 67.60Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	91.51 – 2.20 91.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (91.51-2.20) 88.4 (91.51-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.201 , 0.232 0.202 , 0.235	Depositor DCC
R_{free} test set	2506 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5139	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: LLP, CS, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/1994	0.51	0/2708
2	E	0.39	0/3050	0.58	0/4119
All	All	0.37	0/5044	0.55	0/6827

There are no bond length outliers.

There are no bond angle outliers.

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	1955	0	1957	17	0
2	E	3017	0	2976	19	0
3	E	1	0	0	0	0
4	E	1	0	0	0	0
5	A	46	0	0	1	0
5	E	119	0	0	3	0
All	All	5139	0	4933	34	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 3.

All (34) 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:2:GLU:HG3	1:A:5:GLU:HB2	1.53	0.91
2:E:169:ALA:O	5:E:501:HOH:O	2.00	0.79
2:E:117:VAL:HG13	2:E:152:MET:HE1	1.74	0.69
1:A:225:ARG:NH2	5:A:301:HOH:O	2.25	0.69
2:E:160:HIS:NE2	5:E:502:HOH:O	2.28	0.67
1:A:2:GLU:CG	1:A:5:GLU:HB2	2.27	0.63
2:E:40:GLU:O	2:E:44:GLN:HG3	1.99	0.63
2:E:172:GLU:HB3	5:E:501:HOH:O	2.01	0.61
1:A:10:GLN:O	1:A:14:ARG:HG3	2.01	0.60
1:A:6:ASN:O	1:A:10:GLN:HG2	2.02	0.59
2:E:86:HIS:CE1	2:E:236:ASN:HB3	2.38	0.58
2:E:87:LLP:NZ	2:E:87:LLP:O3	2.29	0.57
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.86	0.56
2:E:216:ILE:HG21	2:E:224:PRO:HD3	1.90	0.53
1:A:217:PRO:HB3	1:A:265:ALA:HB2	1.92	0.52
1:A:59:ALA:HB2	2:E:18:PRO:HG3	1.92	0.51
1:A:160:ASP:HA	1:A:163:LEU:HD12	1.93	0.51
2:E:87:LLP:HD3	2:E:114:GLN:HG3	1.93	0.51
2:E:392:LYS:HD2	2:E:392:LYS:N	2.26	0.50
2:E:50:LYS:HB2	2:E:50:LYS:NZ	2.27	0.48
2:E:79:ASP:HB2	2:E:379[A]:ARG:HB3	1.95	0.47
2:E:134:MET:O	2:E:159:VAL:N	2.46	0.46
1:A:154:CYS:HB3	1:A:176:LEU:HD12	1.98	0.46
2:E:286:MET:HB3	2:E:286:MET:HE2	1.83	0.45
2:E:134:MET:O	2:E:158:PRO:HA	2.18	0.44
1:A:191:LEU:HD23	1:A:196:LEU:HD13	2.01	0.43
1:A:96:PRO:HA	1:A:124:ASP:OD2	2.20	0.41
1:A:85:LEU:HD11	1:A:99:LEU:HD21	2.01	0.41
1:A:104:ASN:HB2	2:E:278:ILE:O	2.19	0.41
1:A:22:PHE:HA	1:A:49[A]:GLU:O	2.21	0.41
2:E:115:HIS:CE1	2:E:189:GLY:HA2	2.56	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.87	0.41
1:A:2:GLU:HA	1:A:2:GLU:OE2	2.21	0.40
2:E:195:HIS:CG	2:E:196:PRO:HA	2.56	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	254/268 (95%)	249 (98%)	5 (2%)	0	100	100
2	E	394/394 (100%)	384 (98%)	10 (2%)	0	100	100
All	All	648/662 (98%)	633 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	203/208 (98%)	203 (100%)	0	100	100
2	E	309/307 (101%)	309 (100%)	0	100	100
All	All	512/515 (99%)	512 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	65	GLN
1	A	68	ASN
1	A	250	GLN
2	E	44	GLN
2	E	273	HIS

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Mol	Chain	Res	Type
2	E	370	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	LLP	E	87	2	23,24,25	1.61	5 (21%)	25,32,34	1.36	5 (20%)

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	LLP	E	87	2	-	1/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	87	LLP	C4'-NZ	4.88	1.43	1.27
2	E	87	LLP	C3-C2	-2.36	1.38	1.41
2	E	87	LLP	C2-N1	2.32	1.38	1.33
2	E	87	LLP	C4-C5	-2.09	1.39	1.42
2	E	87	LLP	CE-NZ	2.06	1.51	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	87	LLP	CE-NZ-C4'	-2.94	109.30	118.72
2	E	87	LLP	C4-C4'-NZ	-2.68	111.66	124.04
2	E	87	LLP	OP4-C5'-C5	2.31	113.68	109.36
2	E	87	LLP	C3-C2-N1	-2.03	118.39	120.96
2	E	87	LLP	C4-C3-C2	2.02	121.28	120.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	87	LLP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	87	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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, 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%)	0.56	19 (7%)	20 18	17, 42, 75, 107	2 (0%)
2	E	393/394 (99%)	0.07	20 (5%)	33 30	12, 29, 58, 89	3 (0%)
All	All	649/662 (98%)	0.27	39 (6%)	27 24	12, 34, 64, 107	5 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	4.9
1	A	1	MET	4.3
1	A	194	HIS	4.2
2	E	159	VAL	4.2
2	E	395	GLY	4.1
2	E	163	SER	3.9
1	A	268	ALA	3.8
1	A	15	ARG	3.6
1	A	42	ASP	3.4
1	A	246	ALA	3.3
2	E	2	THR	3.2
1	A	212	PHE	3.2
2	E	160	HIS	3.1
1	A	13[A]	ASP	3.0
2	E	392	LYS	2.9
1	A	267	ARG	2.9
1	A	192	PRO	2.8
1	A	14	ARG	2.8
2	E	158	PRO	2.8
2	E	162	GLY	2.7
1	A	59	ALA	2.6
2	E	161	SER	2.6
1	A	193	LEU	2.5
1	A	217	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	135	GLY	2.4
2	E	168	ASP	2.4
2	E	139	VAL	2.3
1	A	195	HIS	2.3
2	E	141	ARG	2.3
2	E	140	GLU	2.3
1	A	2	GLU	2.3
2	E	393	ALA	2.2
2	E	306	PHE	2.2
2	E	167	LYS	2.2
2	E	279	TYR	2.1
1	A	247	SER	2.1
1	A	196	LEU	2.1
2	E	136	ALA	2.0
2	E	391	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	LLP	E	87	24/25	0.97	0.06	19,21,23,26	0

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
4	CL	E	402	1/1	0.91	0.23	59,59,59,59	1
3	CS	E	401	1/1	0.92	0.09	57,57,57,57	1

6.5 Other polymers [i](#)

There are no such residues in this entry.