



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:30 AM UTC

PDB ID : 5RUB / pdb_00005rub
Title : CRYSTALLOGRAPHIC REFINEMENT AND STRUCTURE OF RIBULO
SE-1,5-BISPHOSPHATE CARBOXYLASE FROM RHODOSPIRILLUM
RUBRUM AT 1.7 ANGSTROMS RESOLUTION
Authors : Schneider, G.; Lindqvist, Y.; Lundqvist, T.
Deposited on : 1990-05-29
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

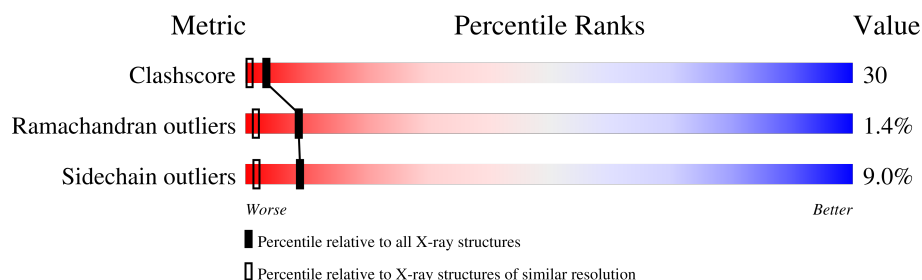
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

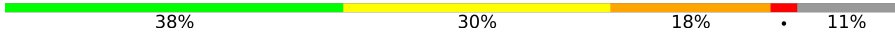
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	490	 38% 30% 18% • 11%
1	B	490	 40% 33% 12% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7377 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 RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	18	0	0
			3330	2110	588	617	15			
1	B	433	Total	C	N	O	S	9	0	0
			3311	2100	585	611	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	342	Total	O	0	0
			342	342		
2	B	394	Total	O	0	0
			394	394		

L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	F437	G442	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	R452	K453	A454	L455	G456	V457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA																
T344	E347	F352	Y353	R354	Q355	S356	K361	A362	C363	T364	S368	N371	N372	A373	L374	R375	M376	P377	G378	F379	F380	E381	N382	N385	A386	N387	T391	A392	G393	G394	G395	A396	F397	G398	H399	I400	D401	G402	P403	V404	A405	K411	Q412	Q415	D419	G420	V421	P422	V423			
R277	R278	F279	N282	F283	L284	H285	Y286	H287	R288	A289	G290	H291	G292	A293	V294	T295	Q298	S299	K300	R301	G302	Y303	T304	V307	H308	C309	K310	M311	Q315	G316	A317	S318	G319	I320	H321	T322	G323	THR	MET	GLY	PHE	GLY	GLY	LYS	MET	GLU	GLY	SER	D336	R337	A338	Y341
G197	N198	Q199	A202	P203	L204	R205	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	Y222	G223	E224	A225	K226	S229	A230	N231	L232	T233	A234	D235	D236	V247	T250	N254	H257	V258	A259	L260	L261	V262	D263	G264	Y265	G268	A269	A270	A271	T274	A275	R276			
F126	E130	R133	F136	D137	G138	P139	S140	V141	M142	I143	S144	A145	L146	W147	K148	V149	L150	G151	R152	P153	E154	G157	G158	L159	V160	W161	G162	T163	I164	I165	K166	P167	K168	L169	R172	P173	K174	P175	F176	A177	E178	A179	C180	H181	D188	F189	I190	D193	E194	P195	Q196	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	5.50 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (5.50-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.38	12/3410 (0.4%)	2.59	291/4620 (6.3%)
1	B	1.38	8/3391 (0.2%)	2.48	232/4594 (5.1%)
All	All	1.38	20/6801 (0.3%)	2.54	523/9214 (5.7%)

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	B	0	1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	LYS	N-CA	7.66	1.52	1.46
1	A	317	ALA	CA-C	6.63	1.61	1.52
1	A	279	PHE	N-CA	6.62	1.54	1.46
1	B	259	ALA	CA-C	6.40	1.60	1.52
1	B	102	ALA	N-CA	6.21	1.53	1.46

The worst 5 of 523 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	CD-NE-CZ	16.85	147.99	124.40
1	A	2	ASP	CA-CB-CG	14.30	126.90	112.60
1	B	316	GLY	CA-C-O	-13.23	106.33	118.77
1	B	172	ARG	CD-NE-CZ	12.66	142.13	124.40
1	A	425	ASP	CA-CB-CG	-11.59	101.01	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	277	ARG	Sidechain

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	3330	0	3233	194	1
1	B	3311	0	3216	217	0
2	A	342	0	0	30	0
2	B	394	0	0	30	0
All	All	7377	0	6449	392	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 30.

The worst 5 of 392 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:ASP:O	1:A:3:GLN:HG3	1.36	1.24
1:B:337:ARG:HD2	1:B:341:TYR:CZ	1.79	1.18
1:A:194:GLU:HG3	1:A:195:PRO:HD3	1.31	1.11
1:A:371:MET:HE2	1:A:375:ARG:HD3	1.29	1.08
1:B:456:GLY:O	1:B:457:VAL:HG23	1.54	1.07

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)
1:A:359:GLY:O	1:A:431:LYS:NZ[2_646]	1.94	0.26

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	430/490 (88%)	404 (94%)	20 (5%)	6 (1%)	9	2
1	B	427/490 (87%)	404 (95%)	17 (4%)	6 (1%)	9	2
All	All	857/980 (87%)	808 (94%)	37 (4%)	12 (1%)	9	2

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	B	3	GLN
1	B	112	ASN
1	A	33	LYS
1	A	34	ALA

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	329/376 (88%)	302 (92%)	27 (8%)	10	2
1	B	326/376 (87%)	294 (90%)	32 (10%)	7	1
All	All	655/752 (87%)	596 (91%)	59 (9%)	9	2

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	SER

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Mol	Chain	Res	Type
1	B	429	GLU
1	B	76	GLU
1	B	428	ARG
1	B	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	112	ASN
1	B	372	ASN
1	B	111	ASN
1	B	113	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.