



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:29 PM UTC

PDB ID : 2RUS / pdb_00002rus
Title : CRYSTAL STRUCTURE OF THE TERNARY COMPLEX OF RIBULOSE
-1,5-BISPHOSPHATE CARBOXYLASE, MG(II), AND ACTIVATOR CO2
AT 2.3-ANGSTROMS RESOLUTION
Authors : Lundqvist, T.; Schneider, G.
Deposited on : 1991-10-11
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

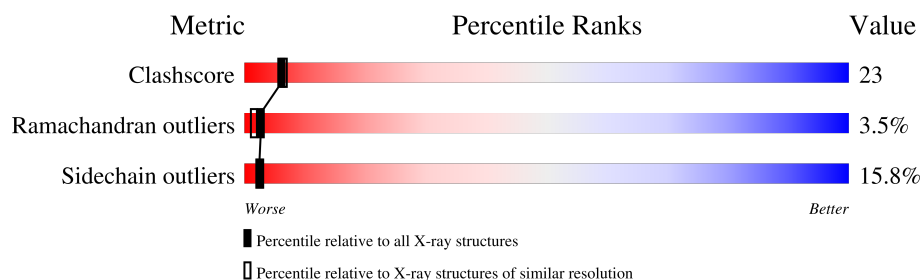
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 ≥ 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	
1	B	490	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7447 atoms, of which 2 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	437	Total	C	N	O	S	14	0	0
			3339	2115	590	619	15			
1	B	444	Total	C	N	O	S	28	0	0
			3386	2145	598	627	16			

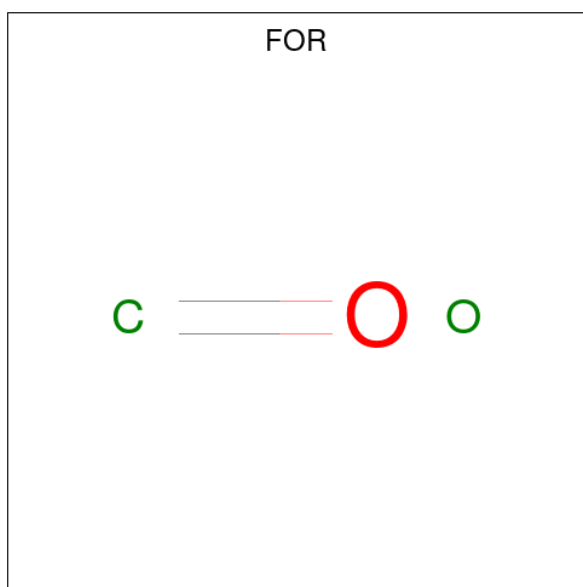
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FORMYL GROUP (CCD ID: FOR) (formula: CH₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			3	1	1	1		
3	B	1	Total	C	H	O	0	0
			3	1	1	1		

- Molecule 4 is water.

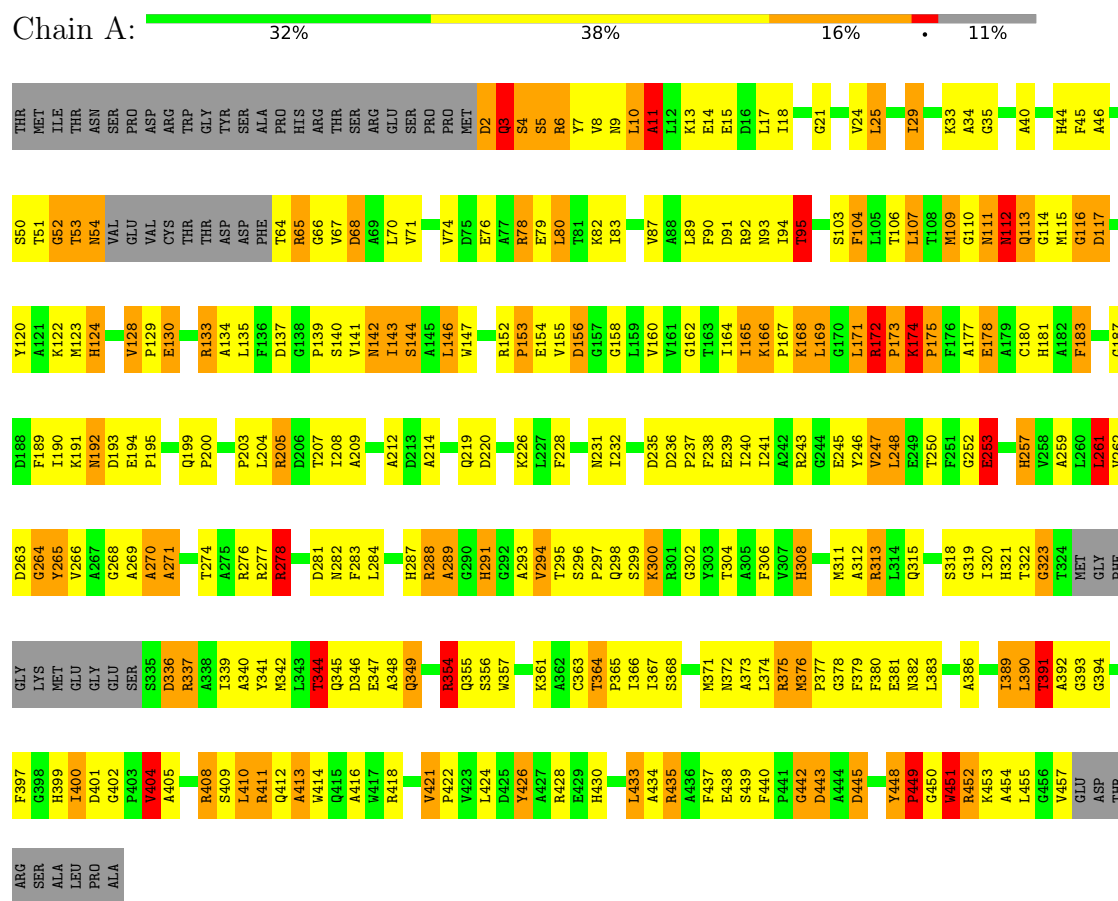
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	340	Total	O	0	0
			340	340		
4	B	374	Total	O	0	0
			374	374		

3 Residue-property plots

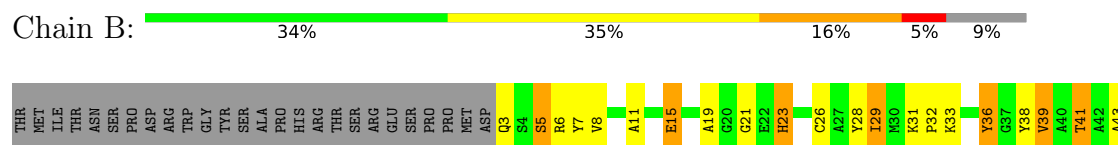
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)



- Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)



H44	F45	A46	A47	E48	S49	S50	T51	G52	T53	N54	VAL	GLU	VAL	CYS	THR	THR	ASP	ASP	PHE	T64	V67	D68	A69	V74	D75	E76	A77	R78	E79	L80	I83	L89	K98	A99	M100	I101	A102	L105	T106	L107	T108	M109	G110	N111	M112	Q113	G114	M115	G116	D117	V118	E119	Y120		
M123	H124	D125	F126	Y127	R133	F136	L204	R205	G138	T207	P139	S140	V141	N142	I143	L146	W147	R148	F149	L150	G151	R152	P153	E154	G158	L159	A225	V160	V161	G162	T163	I164	I165	K166	P167	K168	L169	R172	P173	K174	P175	F176	A179	G180	H181	A182	F183	W184	D188	F189	I190	K191	N192	D193	
E194	P195	Q196	G197	N198	F201	A202	P203	L204	R205	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	R152	P153	E221	G223	E224	A225	K226	L227	F228	S229	A230	N231	A234	D235	D236	P237	F238	E239	I240	R243	G244	E245	Y246	V247	L248	E249	G252	E253	H257	V258	A259	
L260	L261	V262	D263	G264	Y265	V266	A267	G268	A269	A270	A271	I272	T273	T274	A275	R276	R277	D281	N282	F283	L284	H285	Y286	H287	R288	A289	G290	H291	G292	A293	V294	T295	S296	P297	K300	R301	G302	Y303	T304	A305	F306	V307	H308	M311	G312	R313	L314	Q315	G316	H321	T322	G323	T324	M325	G326
R327	G328	K329	NET	GLU	G332	R333	S334	S335	D336	R337	A338	I339	A340	L343	T344	Q345	D346	E347	F352	Y353	R354	K361	A362	C363	T364	P365	I366	I367	S368	G369	N372	R375	M376	P377	G378	F379	F380	E381	A382	L383	A386	N387	V388	I389	L390	T391	A392	G393	F397	G398	P403				
Y404	A405	G406	A407	R408	S409	L410	R411	Q412	A413	W414	Q415	A416	V421	P422	V423	L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	A454	L455	G456	Y457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA							

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 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (5.50-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7447	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FOR

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	1.08	3/3419 (0.1%)	2.56	254/4633 (5.5%)
1	B	1.08	4/3467 (0.1%)	2.58	275/4694 (5.9%)
All	All	1.08	7/6886 (0.1%)	2.57	529/9327 (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	A	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLY	C-N	-7.44	1.23	1.33
1	A	165	ILE	N-CA	6.26	1.53	1.46
1	A	295	THR	CA-CB	5.97	1.59	1.53
1	B	3	GLN	C-N	-5.65	1.25	1.33
1	B	165	ILE	CA-CB	5.52	1.60	1.54

The worst 5 of 529 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	CD-NE-CZ	34.89	173.25	124.40
1	B	375	ARG	CD-NE-CZ	21.89	155.04	124.40
1	B	165	ILE	N-CA-CB	-21.16	86.87	111.00
1	A	3	GLN	CA-C-O	14.14	136.96	120.70
1	B	382	ASN	CA-CB-CG	-13.11	99.49	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	GLY	Mainchain
1	A	64	THR	Mainchain

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	3339	0	3239	149	0
1	B	3386	0	3286	162	6
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	1	0	0	0
3	B	2	1	0	0	0
4	A	340	0	0	13	6
4	B	374	0	0	13	10
All	All	7445	2	6525	298	13

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 23.

The worst 5 of 298 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:53:THR:O	1:A:54:ASN:HB2	1.47	1.07
1:A:219:GLN:HE21	1:A:226:LYS:H	1.02	1.01
1:A:438:GLU:OE2	1:A:457:VAL:HG22	1.64	0.98
1:B:333:GLU:HG2	1:B:334:SER:H	1.29	0.96
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.50	0.94

The worst 5 of 13 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)
4:B:540:HOH:O	4:B:691:HOH:O[2_645]	0.46	1.74
4:A:661:HOH:O	4:A:779:HOH:O[2_656]	1.54	0.66
4:A:681:HOH:O	4:A:685:HOH:O[2_646]	1.80	0.40
4:A:738:HOH:O	4:B:839:HOH:O[1_545]	1.87	0.33
1:B:327:PHE:O	4:B:690:HOH:O[2_645]	1.89	0.31

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	431/490 (88%)	382 (89%)	34 (8%)	15 (4%)	3	1
1	B	438/490 (89%)	387 (88%)	36 (8%)	15 (3%)	3	2
All	All	869/980 (89%)	769 (88%)	70 (8%)	30 (4%)	3	1

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	53	THR
1	A	264	GLY
1	A	443	ASP
1	A	451	TRP

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	330/376 (88%)	274 (83%)	56 (17%)	2	2
1	B	334/376 (89%)	285 (85%)	49 (15%)	3	3
All	All	664/752 (88%)	559 (84%)	105 (16%)	2	2

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
1	B	169	LEU
1	B	424	LEU
1	B	74	VAL
1	B	112	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	349	GLN
1	B	315	GLN
1	B	124	HIS
1	B	308	HIS
1	B	23	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	FOR	B	501	1	0,1,1	-	-	-		
3	FOR	A	501	2,1	0,1,1	-	-	-		

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 [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.