



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:24 PM UTC

PDB ID : 1RUS / pdb_00001rus
Title : CRYSTAL STRUCTURE OF THE BINARY COMPLEX OF RIBULOSE-1, 5-BISPHOSPHATE CARBOXYLASE AND ITS PRODUCT, 3-PHOSPHO-D-GLYCERATE
Authors : Lundqvist, T.; Schneider, G.
Deposited on : 1991-10-10
Resolution : 2.90 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

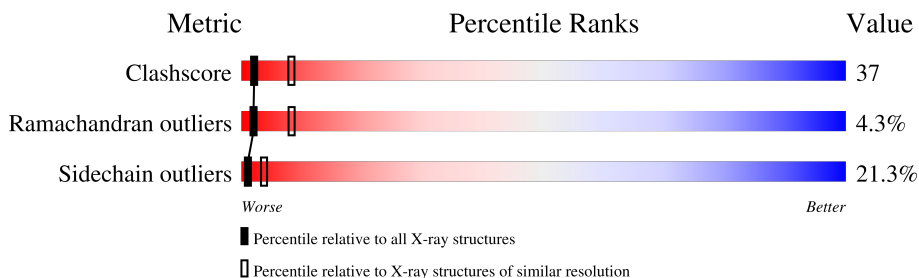
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	24% 34% 23% 8% 11%
1	B	490	24% 36% 23% 6% 11%

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
2	3PG	A	500	-	X	X	-
2	3PG	B	500	-	X	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6677 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.

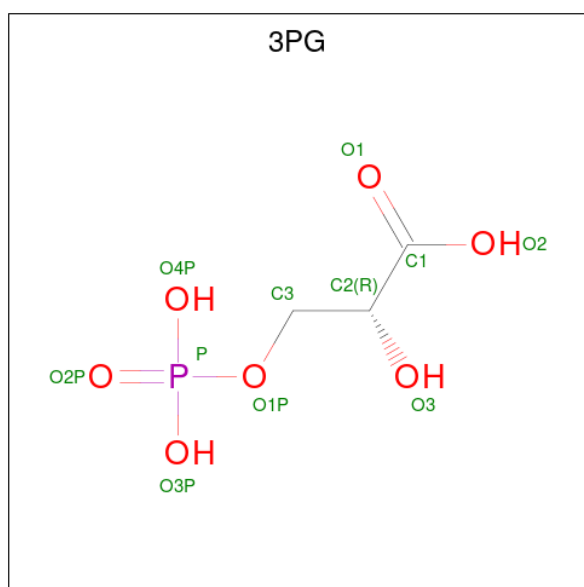
- Molecule 1 is a protein called RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	7	0	0
			3337	2115	589	617	16			
1	B	435	Total	C	N	O	S	10	0	0
			3318	2105	584	613	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 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	3	7	1		

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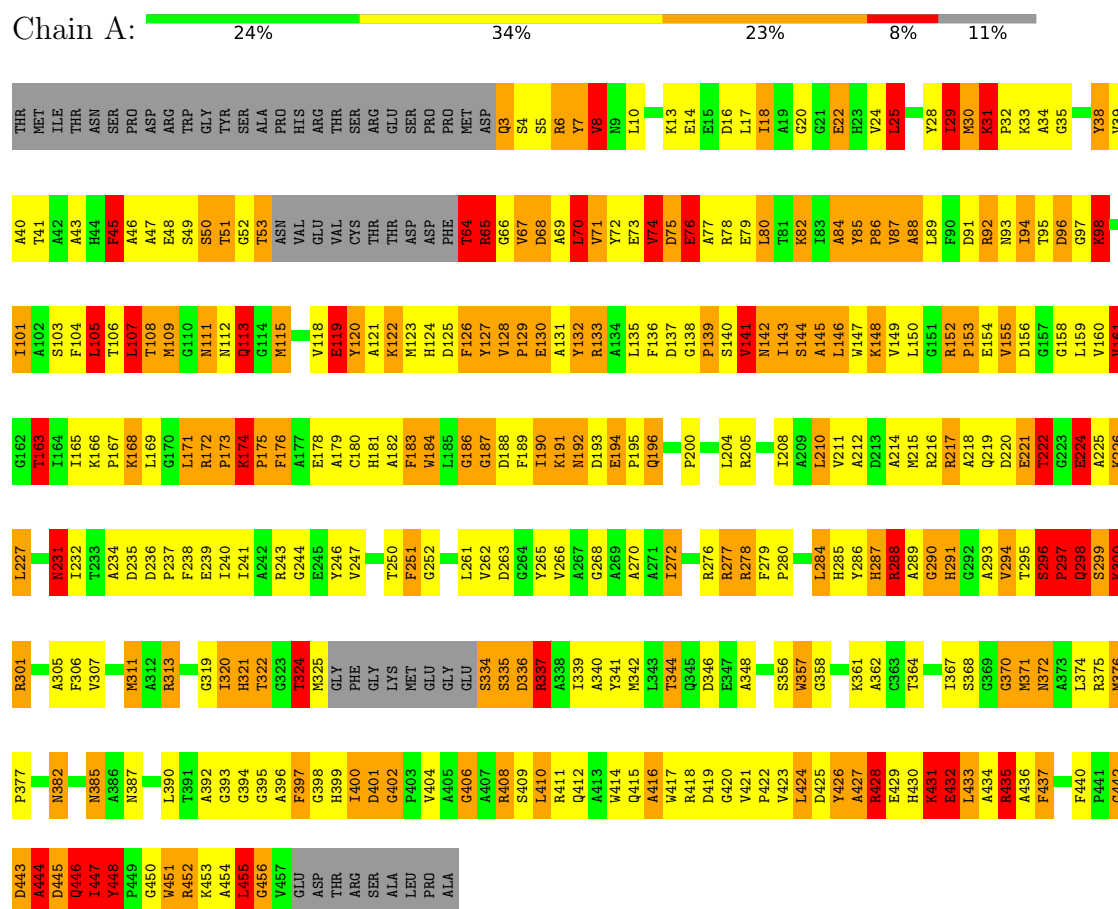
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			11	3	7	1		

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)



D445	Q446	F447	Y448	P449	G450	W451	R452	K453	A454	L455	G456	V457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA																																							
F379	F380	E381	N382	L383	G384	N385	A386	N387		T391	A392	G393	G394	G395	A396	F397	G398	H399	I400	D401	G402	P403	V404	A405		R408	S409	L410	R411	Q412	A413	W414	Q415	W417	R418	D419	G420	V421	P422	Y423	L424		R428	E429	H430	K431	E432	L433	A434	R435	A436	F437	E438	S439	F440		D443	A444		
F306	V307	H308		M311	A312	R313	L314	Q315	G316	A317		I320	H321	T322	G323	T324	M325	GLY	PHE	GLY	LYS	MET	GLU	GLY	S334	S335	D336	R337	A338	I339	A340	Y341	M342	L343	T344	Q345		A348	R354		W357		A362	C363	H364	P365	I366	I367		M371	N372	A373	L374	R375	M376	P377	G378			
D235		E239	I240	I241	A242	R243	G244	E245	Y246	V247		T250	F251		N254	A255	S256	H257	V258	A259	L260	L261		Y265	V266	A267	G268	A269	A270	A271	I272	T273	T274	A275	R276	R277	R278	F279		L284	H285	Y286	H287	R288	A289	G290	H291	G292	A293	V294	T295	S296	P297	G298	S299	K300	R301	G302		
I164	I165	K166	P167	K168	L169		R172	P173	K174	P175		E178		F183	W184	L185		F189	I190	A191	N192	D193	E194	E195	Q196		P200	F201	A202	A131	P203	L204	L205	D206	T207	I208	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	D220	E221	T222	G223	E224	A225	R226	L227		N231	I232	T233	A234
T101	A102	S103	F104	L105	T106	L107	T108	M109	G110	N111	N112	G113	G114	M115	G116	D117	V118	E119	Y120	A121	K122	M123		F126	Y127	V128	P129	E130	A131	Y132	R133	A134	L135	F136	D137	G138	P139	S140	V141	N142		L146	W147	K148	V149	L150	G151	R152	P153	E154	V155	D156	G157	G158	L159	V160	V161	G162	T163	
T41	A42	A43	H44	F45	A46	A47	E48	S49	S50	T51	G52	T53	ASN	VAL	GLU	VAL	CYS	THR	THR	ASP	ASP	PHE	THR	ARG	G66	V67	D68	A69	L70	V71	Y72	E73	V74	D75	E76	A77	R78	E79	L80	T81	K82	I83	A84	Y85	P86	V87	A88	L89	F90	D91	N92	N93	I94	T95	D96	G97	R98	A99	M100	

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)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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: 3PG

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	1.33	8/3417 (0.2%)	2.88	377/4629 (8.1%)
1	B	1.44	13/3398 (0.4%)	2.96	405/4604 (8.8%)
All	All	1.39	21/6815 (0.3%)	2.92	782/9233 (8.5%)

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 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	GLY	C-N	-7.48	1.24	1.33
1	B	288	ARG	CD-NE	7.27	1.56	1.46
1	B	288	ARG	NE-CZ	6.75	1.40	1.33
1	A	322	THR	N-CA	6.64	1.55	1.46
1	A	163	THR	CA-CB	6.57	1.63	1.53

The worst 5 of 782 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASP	CA-CB-CG	24.39	136.99	112.60
1	B	429	GLU	CA-CB-CG	24.17	162.44	114.10
1	B	418	ARG	CD-NE-CZ	22.51	155.92	124.40
1	A	188	ASP	CA-CB-CG	18.40	131.00	112.60
1	A	321	HIS	CB-CA-C	17.17	130.92	109.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	ASN	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	3337	0	3245	268	2
1	B	3318	0	3222	256	0
2	A	11	0	4	8	0
2	B	11	0	4	5	0
All	All	6677	0	6475	492	2

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 37.

The worst 5 of 492 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:196:GLN:O	1:A:231:ASN:ND2	1.67	1.28
1:A:288:ARG:HD3	1:A:291:HIS:NE2	1.52	1.23
1:B:3:GLN:NE2	1:B:44:HIS:HA	1.50	1.22
1:B:321:HIS:HB3	2:B:500:3PG:O4P	1.41	1.17
1:B:335:SER:O	1:B:339:ILE:CG1	1.93	1.14

All (2) 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:346:ASP:OD2	1:A:408:ARG:NH2[2_646]	1.89	0.31
1:A:358:GLY:O	1:A:431:LYS:CD[2_646]	2.07	0.13

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%)	374 (87%)	38 (9%)	19 (4%)	2	8
1	B	429/490 (88%)	365 (85%)	46 (11%)	18 (4%)	2	9
All	All	860/980 (88%)	739 (86%)	84 (10%)	37 (4%)	2	8

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	298	GLN
1	A	372	ASN
1	B	4	SER
1	B	5	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	330/376 (88%)	251 (76%)	79 (24%)	1	3
1	B	327/376 (87%)	266 (81%)	61 (19%)	1	5
All	All	657/752 (87%)	517 (79%)	140 (21%)	1	4

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	320	ILE

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Mol	Chain	Res	Type
1	B	337	ARG
1	B	422	PRO
1	A	291	HIS
1	A	288	ARG

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	372	ASN
1	B	345	GLN
1	B	9	ASN
1	B	315	GLN
1	B	3	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](#)

2 ligands are 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	3PG	B	500	-	9,10,10	1.97	3 (33%)	11,14,14	2.34	4 (36%)
2	3PG	A	500	-	9,10,10	3.70	6 (66%)	11,14,14	3.50	9 (81%)

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	3PG	B	500	-	-	7/10/10/10	-
2	3PG	A	500	-	-	7/10/10/10	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	3PG	P-O1P	8.30	1.86	1.60
2	A	500	3PG	P-O2P	3.88	1.62	1.50
2	A	500	3PG	O1P-C3	3.88	1.59	1.44
2	B	500	3PG	P-O2P	3.47	1.61	1.50
2	A	500	3PG	O1-C1	2.97	1.30	1.22

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	3PG	O2-C1-C2	5.68	124.74	112.74
2	B	500	3PG	O1P-C3-C2	5.28	122.81	107.96
2	A	500	3PG	O1P-C3-C2	4.76	121.36	107.96
2	A	500	3PG	O3-C2-C1	-4.13	99.88	110.36
2	A	500	3PG	O1P-P-O2P	4.07	117.44	106.44

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	3PG	O1-C1-C2-O3
2	A	500	3PG	O2-C1-C2-O3
2	A	500	3PG	C1-C2-C3-O1P
2	A	500	3PG	O3-C2-C3-O1P
2	B	500	3PG	C2-C3-O1P-P

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	3PG	5	0
2	A	500	3PG	8	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.