



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:47 PM UTC

PDB ID : 1RBA / pdb_00001rba
Title : SUBSTITUTION OF ASP193 TO ASN AT THE ACTIVE SITE OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE RESULTS IN CONFORMATIONAL CHANGES
Authors : Schneider, G.; Soderlind, E.
Deposited on : 1991-11-18
Resolution : 2.60 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

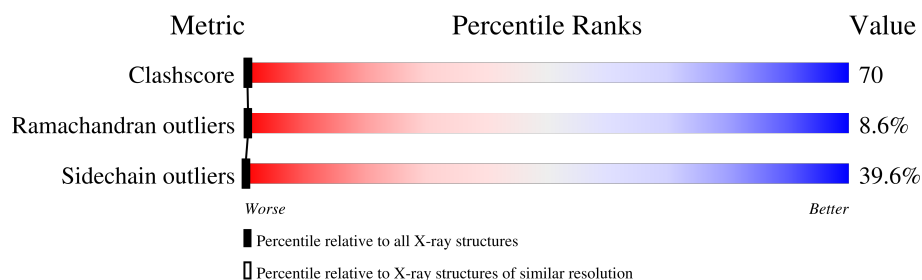
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	466	
1	B	466	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6695 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3200	2029	566	590	15			
1	B	443	Total	C	N	O	S	0	0	0
			3385	2146	596	627	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
A	193	ASN	ASP	engineered mutation	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718
B	193	ASN	ASP	engineered mutation	UNP P04718

- Molecule 2 is water.

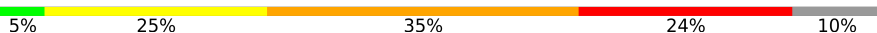
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total	O	0	0
			67	67		
2	B	43	Total	O	0	0
			43	43		

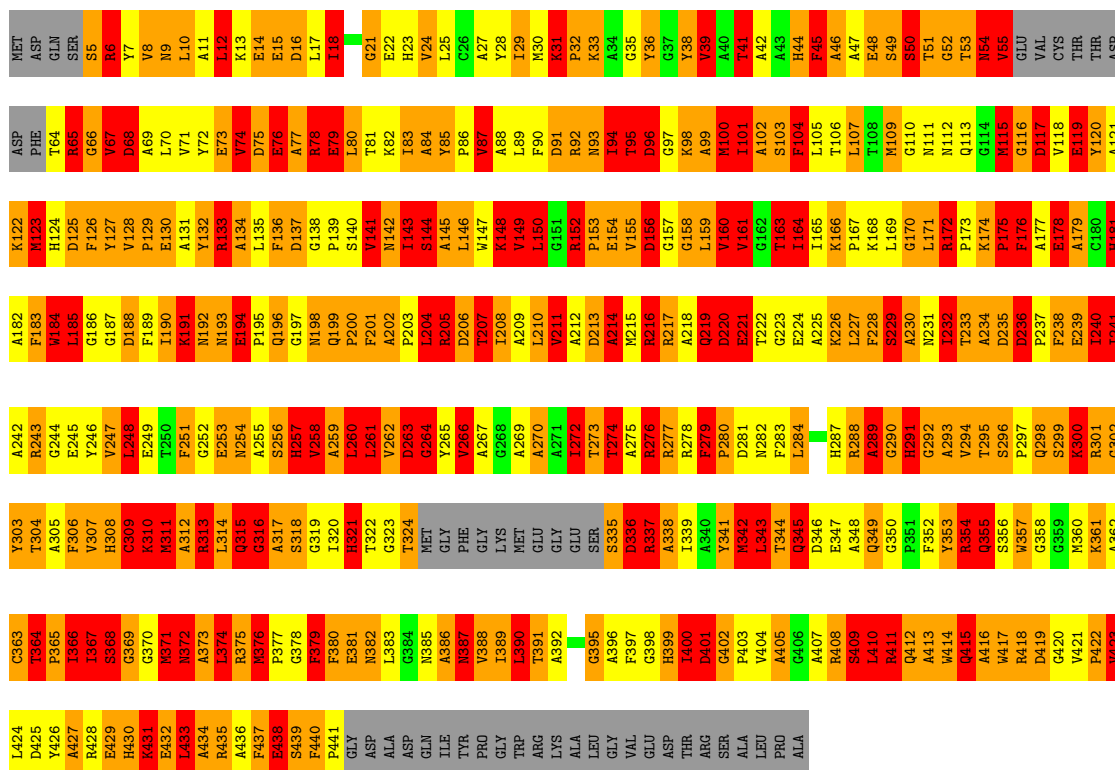
3 Residue-property plots

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

Chain A: 



L242	T364	A242	A182
D425	P365	R243	F183
Y426	I366	G244	W184
A427	I367	E245	L185
R428	S368	Y246	G186
P429	G369	V247	G187
H430	G370	L248	D188
K431	M371	E249	F189
E432	N372	T250	I190
L433	R373	F251	K191
A434	L374	G252	M192
R435	R375	E253	M193
A436	M376	N254	E194
F437	P377	A255	P195
E438	G378	S256	Q196
S439	F379	H257	Q197
F440	F380	V258	N198
P441	E381	A259	Q199
G442	N382	L260	P200
D443	L383	L261	F201
A444	G384	V262	A202
D445	N385	D263	P203
Q446	A386	G264	L204
I447	N387	Y265	R205
Y448	Y388	V266	D206
P449	I389		T207
G450	L390	A269	T208
W451	T391		A209
R452	A392	T272	L210
K453	G393	T273	V211
A454	G394	T274	A212
L455	G395	A275	D213
G456	A396	R276	A214
Y457	F397	R277	M215
GLU	G398	R278	R216
THR	H399	F279	R217
ASP	I400	P280	A218
ARG	D401	D281	Q219
SER	Q402	M282	D220
ALA	P403	F283	E221
LEU	V404	L284	T222
PRO	A405	H285	G223
ALA	Q406	Y286	E224
	A407	H287	A225
	R408	R288	K226
	S409	A289	L227
	L410	G290	F228
	R411	H291	S229
	Q412	G292	A230
	A413	A293	M231
	W414	V294	T232
	Q415	T295	T233
	A416	S296	A234
	W417	P297	D235
	R418	Q298	D236
	D419	S299	P237
	G420	M300	F238
	V421	R301	E239
	P422	G302	I240
	Y423	Y303	I241

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 69.30Å 103.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	2.06	56/3275 (1.7%)	4.27	800/4436 (18.0%)
1	B	2.01	59/3467 (1.7%)	4.26	871/4702 (18.5%)
All	All	2.03	115/6742 (1.7%)	4.27	1671/9138 (18.3%)

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	1	3
1	B	0	2
All	All	1	5

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	ILE	C-N	34.30	1.82	1.33
1	A	78	ARG	CA-CB	-33.88	0.98	1.53
1	A	361	LYS	CD-CE	23.53	2.23	1.52
1	B	278	ARG	CA-CB	-18.62	1.20	1.53
1	A	349	GLN	CA-CB	-18.34	1.22	1.53

The worst 5 of 1671 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ASP	CA-CB-CG	32.93	145.53	112.60
1	A	401	ASP	CA-CB-CG	31.16	143.76	112.60
1	B	354	ARG	CD-NE-CZ	29.86	166.20	124.40
1	B	441	PRO	CA-C-N	29.73	179.67	121.41
1	B	441	PRO	C-N-CA	29.73	179.67	121.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	349	GLN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	GLU	Mainchain
1	A	354	ARG	Sidechain
1	A	433	LEU	Mainchain
1	B	288	ARG	Sidechain
1	B	301	ARG	Sidechain

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	3200	0	3110	485	2
1	B	3385	0	3278	478	2
2	A	67	0	0	3	0
2	B	43	0	0	1	0
All	All	6695	0	6388	903	3

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 70.

The worst 5 of 903 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:B:41:THR:CB	1:B:41:THR:CA	1.75	1.61
1:A:164:ILE:CA	1:A:164:ILE:CB	1.74	1.60
1:A:335:SER:HB3	1:A:338:ALA:CB	1.21	1.56
1:A:191:LYS:CD	1:A:191:LYS:CE	1.78	1.56
1:B:190:ILE:C	1:B:191:LYS:N	1.82	1.37

All (3) 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:419:ASP:OD1	1:B:60:THR:O[2_646]	1.73	0.47
1:A:358:GLY:O	1:A:431:LYS:CB[2_646]	1.97	0.23
1:B:172:ARG:NH1	1:B:419:ASP:OD1[2_745]	2.17	0.03

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	411/466 (88%)	303 (74%)	71 (17%)	37 (9%)	0	0
1	B	439/466 (94%)	328 (75%)	75 (17%)	36 (8%)	0	0
All	All	850/932 (91%)	631 (74%)	146 (17%)	73 (9%)	0	0

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	95	THR
1	A	130	GLU
1	A	155	VAL
1	A	188	ASP

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	317/354 (90%)	188 (59%)	129 (41%)	0	0
1	B	335/354 (95%)	206 (62%)	129 (38%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	652/708 (92%)	394 (60%)	258 (40%)	0 0

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	366	ILE
1	B	382	ASN
1	A	321	HIS
1	A	313	ARG
1	B	404	VAL

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	A	415	GLN
1	B	54	ASN
1	B	287	HIS
1	B	44	HIS
1	B	112	ASN

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 ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	439:SER	C	440:PHE	N	2.16
1	B	190:ILE	C	191:LYS	N	1.82
1	B	323:GLY	C	324:THR	N	1.17

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.