



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2024 – 09:43 AM EST

PDB ID : 1RBA  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

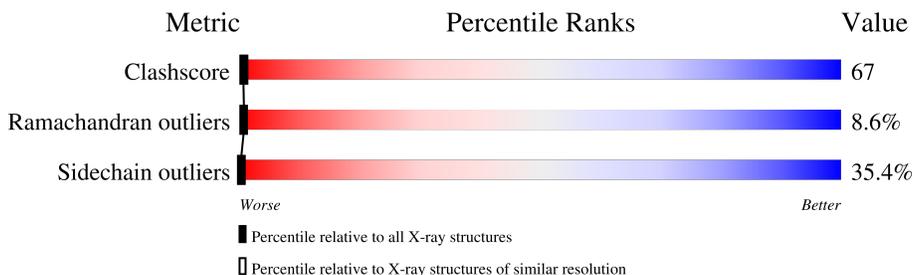
# 1 Overall quality at a glance

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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  $\geq 3$ , 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	 10% 31% 32% 17% 10%
1	B	466	 12% 29% 37% 17% 5%

## 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
			Total	C	N	O	S			
1	A	419	3200	2029	566	590	15	0	0	0
1	B	443	3385	2146	596	627	16	0	0	0

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		

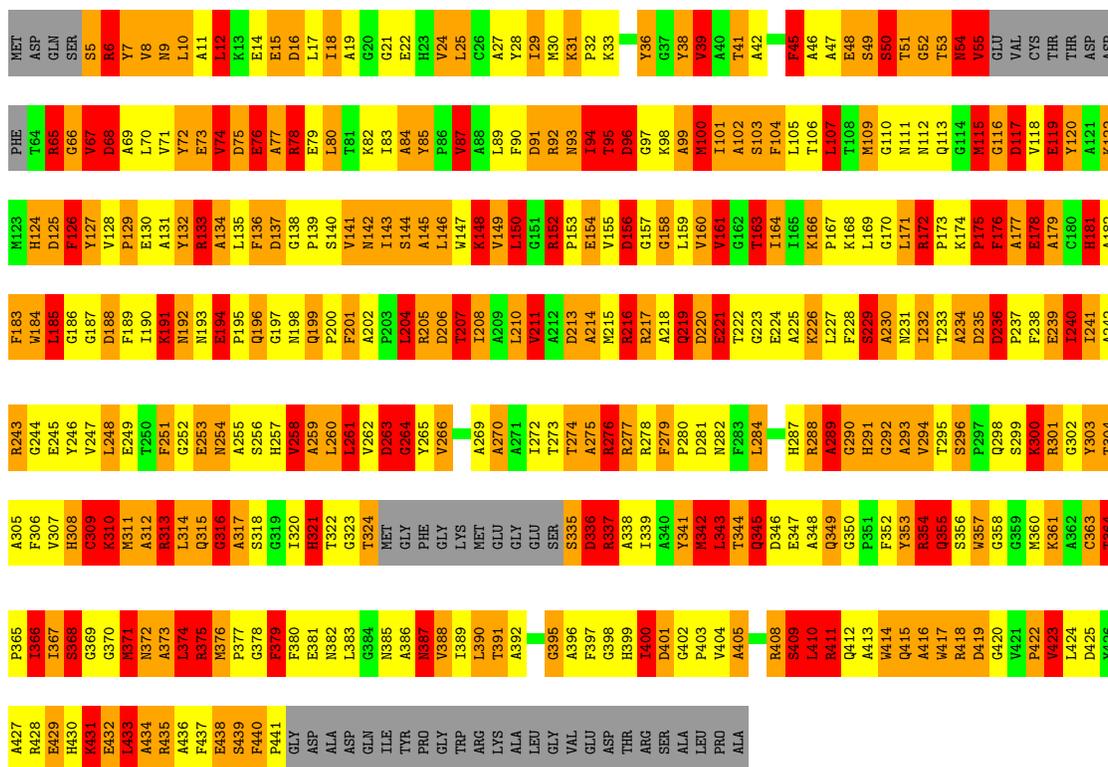
### 3 Residue-property plots

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.

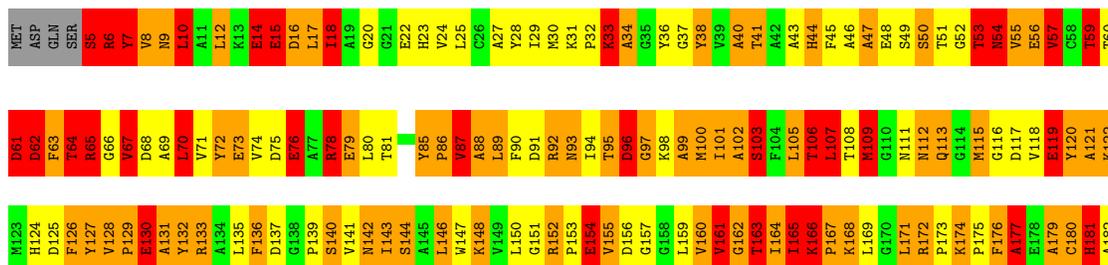
- Molecule 1: RUBISCO

Chain A: 



- Molecule 1: RUBISCO

Chain B: 



E429	S368	V807	E245	H008	H321	I3200	F183
H430	G369	H308	Y246	T322	H321	H321	W184
K431	G370	C309	V247	G323	T324	T324	L185
E432	M371	K310	L248	T324	GLY	GLY	G186
L433	N372	M311	E249	GLY	PHE	PHE	G187
A434	A373	A312	T250	GLY	GLY	GLY	D188
R435	L374	R313	F251	GLY	GLY	GLY	F189
A436	R375	L314	G252	GLY	GLY	GLY	I190
F437	M376	Q315	E253	GLY	GLY	GLY	K191
E438	P377	G316	A254	GLY	GLY	GLY	M192
S439	G378	A317	A255	GLY	GLY	GLY	N193
F440	F379	I3200	S256	GLY	GLY	GLY	E194
R441	F380	H321	H257	GLY	GLY	GLY	P195
G442	E381	T322	V258	GLU	GLU	GLU	Q196
D443	N382	G323	A259	SER	SER	SER	Q199
A444	L383	G323	L260	S335	S335	S335	P200
D445	G384	T324	L261	D336	D336	D336	F201
Q446	N385	GLY	V262	A338	A338	A338	P202
I447	A386	PHE	G263	I339	I339	I339	P203
Y448	N387	GLY	G264	A340	A340	A340	L204
P449	V388	GLY	Y265	M342	M342	M342	R205
G450	I389	LYS	V266	M342	M342	M342	D206
W451	L390	GLU	A267	I343	I343	I343	T207
R452	G393	GLU	G268	T344	T344	T344	T207
K453	G394	GLU	A269	Q345	Q345	Q345	I208
A454	G395	SER	I272	D346	D346	D346	A209
L455	A396	S335	T273	E347	E347	E347	L210
V457	F397	D336	R276	A348	A348	A348	V211
ASP	G398	R337	R277	Q349	Q349	Q349	A212
THR	H399	A338	R278	R288	R288	R288	D213
ARG	I400	I339	F279	A289	A289	A289	A214
SER	D401	A340	P280	G290	G290	G290	M215
ALA	P403	M342	D281	H291	H291	H291	R216
LEU	V404	I343	N282	G292	G292	G292	R217
LEU	A405	T344	F283	R292	R292	R292	A218
PRO	G406	Q345	L284	A293	A293	A293	Q219
ALA	A407	D346	H285	V294	V294	V294	D220
	R408	E347	H286	T295	T295	T295	E221
	S409	A348	H287	S296	S296	S296	T222
	L410	Q349	Y286	F297	F297	F297	E224
	R411	R288	H287	Q298	Q298	Q298	G223
	Q412	A289	H288	S298	S298	S298	E224
	A413	G350	G290	Q298	Q298	Q298	A226
	W414	P351	H291	Q298	Q298	Q298	K226
	Q415	F352	G292	R291	R291	R291	L227
	A416	R354	A293	A293	A293	A293	A230
	W417	Q355	V294	R292	R292	R292	N231
	R418	S356	T295	V294	V294	V294	I232
	D419	W357	S296	T295	T295	T295	T233
	G420	G358	F297	S296	S296	S296	A234
	V421	G359	Q298	Q298	Q298	Q298	D235
	P422	M360	Q298	Q298	Q298	Q298	D236
	V423	K361	S299	S299	S299	S299	P237
	L424	A362	K300	K300	K300	K300	F238
	D425	C363	R301	R301	R301	R301	E239
	Y426	T364	G302	G302	G302	G302	I240
	A427	P366	I241	I241	I241	I241	I241
	R428	I367	A242	A242	A242	A242	A242
			R243	R243	R243	R243	R243
			G244	G244	G244	G244	G244
			F306	F306	F306	F306	F306

## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	1.60	21/3275 (0.6%)	3.37	475/4436 (10.7%)
1	B	1.51	21/3467 (0.6%)	3.32	453/4702 (9.6%)
All	All	1.55	42/6742 (0.6%)	3.35	928/9138 (10.2%)

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 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	LYS	CD-CE	28.72	2.23	1.51
1	A	78	ARG	CA-CB	-25.14	0.98	1.53
1	B	190	ILE	C-N	21.16	1.82	1.34
1	B	278	ARG	CA-CB	-15.28	1.20	1.53
1	A	349	GLN	CA-CB	-14.30	1.22	1.53

The worst 5 of 928 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ARG	CD-NE-CZ	30.43	166.20	123.60
1	A	435	ARG	CD-NE-CZ	28.34	163.27	123.60
1	B	133	ARG	NE-CZ-NH2	-27.72	106.44	120.30
1	B	92	ARG	CD-NE-CZ	27.45	162.03	123.60
1	B	441	PRO	C-N-CA	27.32	179.67	122.30

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	3097	469	2
1	B	3385	0	3266	459	2
2	A	67	0	0	3	0
2	B	43	0	0	1	0
All	All	6695	0	6363	871	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 67.

The worst 5 of 871 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	1.32

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%)	<b>1</b> <b>0</b>
1	B	439/466 (94%)	328 (75%)	75 (17%)	36 (8%)	<b>1</b> <b>1</b>
All	All	850/932 (91%)	631 (74%)	146 (17%)	73 (9%)	<b>1</b> <b>0</b>

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%)	206 (65%)	111 (35%)	<b>0</b> <b>0</b>
1	B	335/354 (95%)	215 (64%)	120 (36%)	<b>0</b> <b>0</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	652/708 (92%)	421 (65%)	231 (35%)	<b>0</b> <b>0</b>

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	GLU
1	B	414	TRP
1	B	107	LEU
1	B	411	ARG
1	B	345	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	GLN
1	B	192	ASN
1	B	355	GLN
1	B	112	ASN
1	B	231	ASN

### 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 monosaccharides 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](#)

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 [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.