wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:56 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

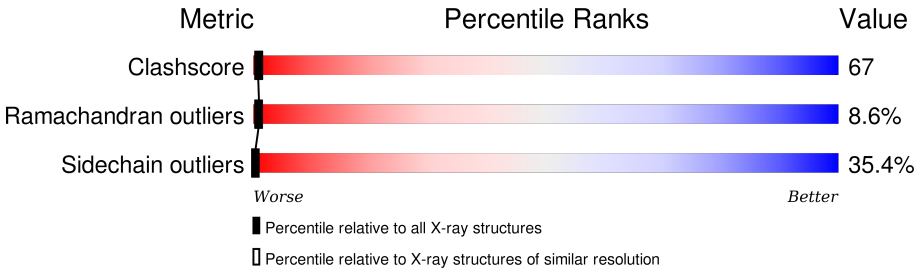
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 (i)

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		

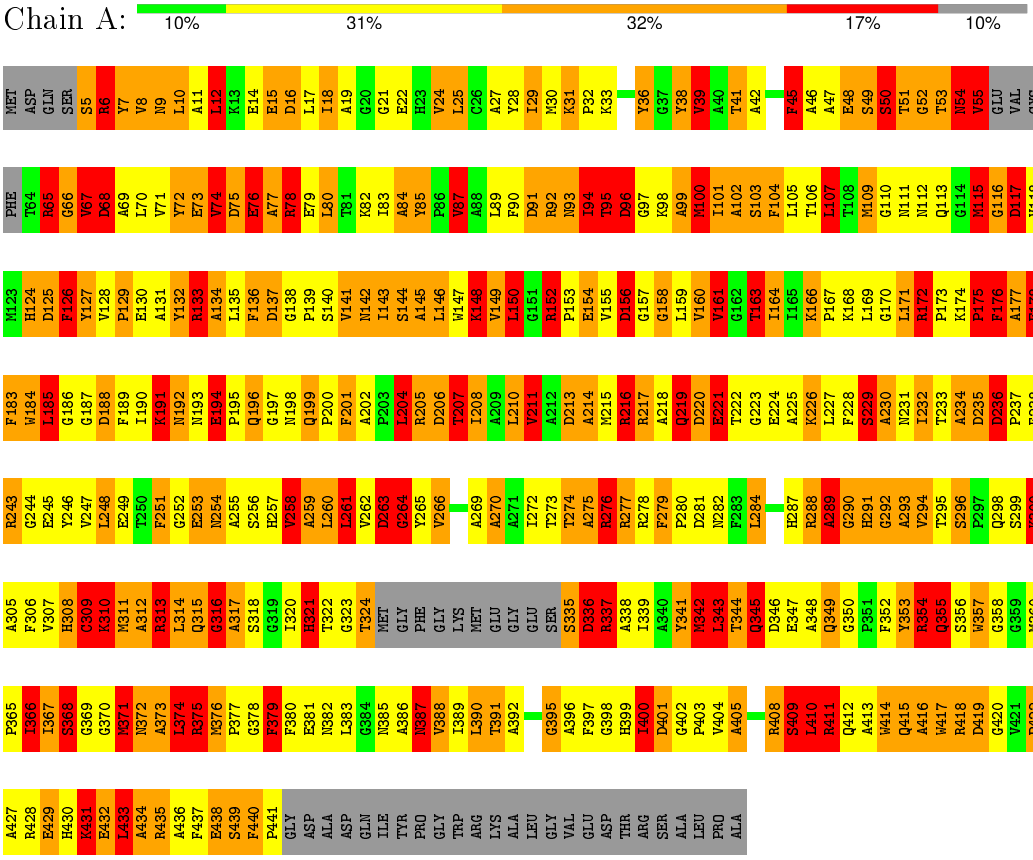
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

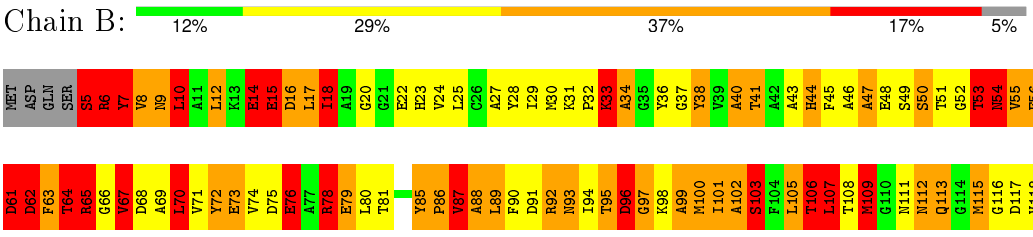
- Molecule 1: RUBISCO

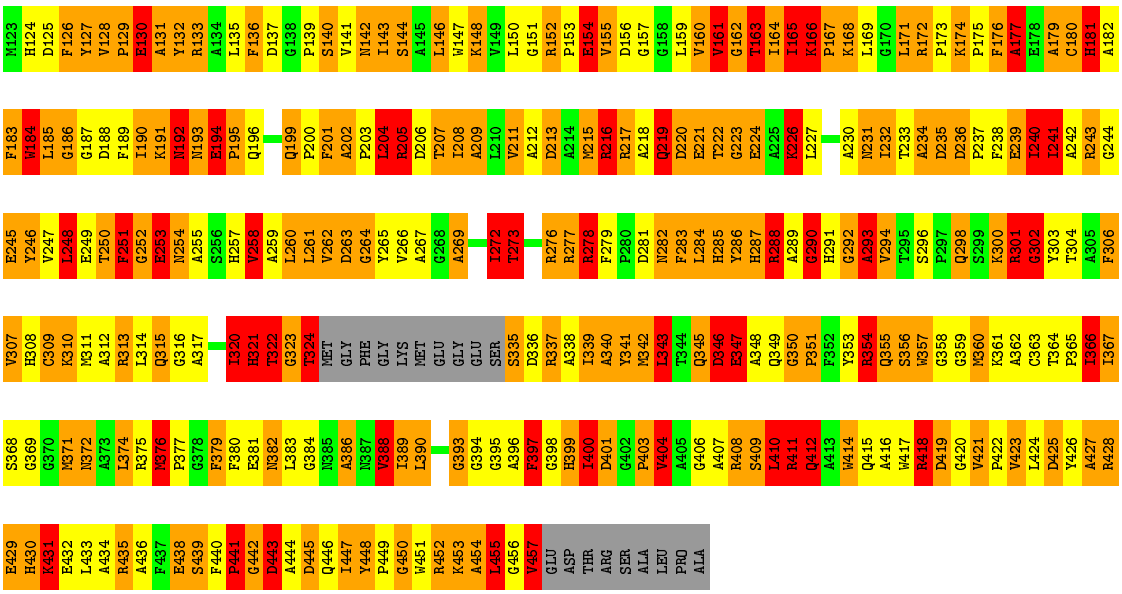
Chain A:



- Molecule 1: RUBISCO

Chain B:




M123 H124 D125 F126 Y127 V128 P129 E130 A131 Y132 R133 A134 L135 F136 D137 G138 P139 S140 V141 N142 I143 S144 A145 L146 W147 K148 Y149 L150 G151 R152 P153 E154 V155 D156 G157 G158 L159 V160 V161 G162 T163 I164 I165 K166 P167 K168 L169 G170 L171 R172 P173 K174 P175 F176 A177 E178 A179 C180 H181 A182
F183 W184 L185 G186 G187 D188 F189 I190 K191 N192 N193 E194 P195 Q196 Q199 P200 F201 A202 P203 L204 R205 D206 T207 I208 A209 L210 V211 A212 D213 A214 M215 R216 R217 A218 Q219 D220 E221 T222 G223 E224 A225 R226 L227 A230 N231 I232 T233 A234 D235 D236 P237 F238 E239 I240 I241 A242 R243 G244
E245 Y246 V247 L248 E249 T250 F251 G252 E253 N254 A255 S256 H257 V258 A259 L260 L261 V262 D263 G264 Y265 V266 A267 G268 A269 I272 T273 R276 R277 R278 F279 P280 D281 N282 F283 L284 H285 Y286 H287 R288 A289 G290 H291 G292 A293 V294 T295 S296 P297 Q298 S299 K300 R301 G302 Y303 T304 A305 F306
V307 H308 C309 K310 M311 A312 R313 L314 Q315 G316 A317 I320 H321 T322 G323 T324 MET GLY PHE GLY LYS MET GLU GLY GLU SER S335 D336 R337 A338 I339 A340 Y341 M342 L343 T344 Q345 D346 E347 A348 Q349 G350 P351 F352 Y353 R354 Q355 S356 W357 G358 G359 M360 K361 A362 C363 T364 P365 I366 I367
S368 G369 G370 M371 N372 A373 L374 R375 M376 P377 G378 F379 F380 E381 N382 L383 G384 N385 A386 N387 V388 I389 L390 G393 G394 G395 A396 F397 G398 H399 I400 D401 G402 P403 V404 A405 G406 A407 R408 S409 L410 R411 Q412 A413 W414 Q415 A416 W417 R418 D419 G420 V421 P422 V423 L424 D425 Y426 A427 R428
E429 H430 K431 E432 L433 A434 R435 A436 F437 E438 S439 F440 P441 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

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	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(^{o})	Ideal(^{o})
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:CA	1:B:41:THR:CB	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%)	1 1
1	B	439/466 (94%)	328 (75%)	75 (17%)	36 (8%)	1 1
All	All	850/932 (91%)	631 (74%)	146 (17%)	73 (9%)	1 1

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%)	0 0
1	B	335/354 (95%)	215 (64%)	120 (36%)	0 0

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

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

Mol	Chain	Res	Type
1	A	410	LEU
1	B	65	ARG
1	B	388	VAL
1	A	431	LYS
1	B	16	ASP

Some 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	315	GLN
1	A	355	GLN
1	B	349	GLN
1	A	321	HIS
1	A	415	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.