



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:26 AM GMT

PDB ID : 3P01
Title : Crystal structure of two-component response regulator from Nostoc sp. PCC 7120
Authors : Chang, C.; Mack, J.; Feldman, B.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-09-27
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

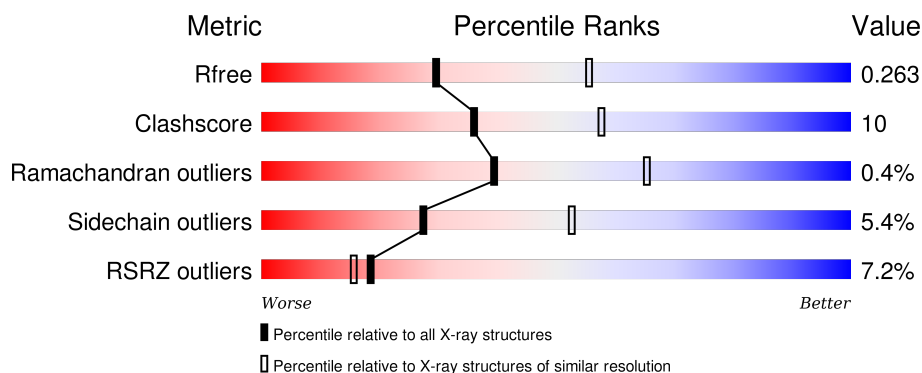
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	184	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
1	B	184	<div> <div>14%</div> <div>65%</div> <div>27%</div> <div>• 5%</div> </div>
1	C	184	<div> <div>3%</div> <div>67%</div> <div>23%</div> <div>• 8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3934 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 Two-component response regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	Se	0	0	0
			1322	828	231	258	2	3			
1	B	175	Total	C	N	O	S	Se	0	0	0
			1303	822	228	248	2	3			
1	C	169	Total	C	N	O	S	Se	0	0	0
			1267	796	219	247	2	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	SER	-	EXPRESSION TAG	UNP Q8YLP5
A	133	ASN	-	EXPRESSION TAG	UNP Q8YLP5
B	132	SER	-	EXPRESSION TAG	UNP Q8YLP5
B	133	ASN	-	EXPRESSION TAG	UNP Q8YLP5
C	132	SER	-	EXPRESSION TAG	UNP Q8YLP5
C	133	ASN	-	EXPRESSION TAG	UNP Q8YLP5

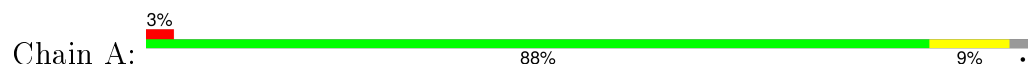
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	7	Total	O	0	0
			7	7		
2	C	16	Total	O	0	0
			16	16		

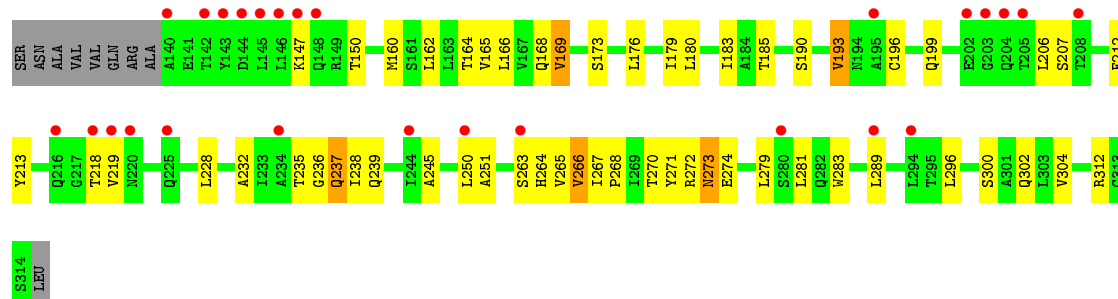
3 Residue-property plots

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.

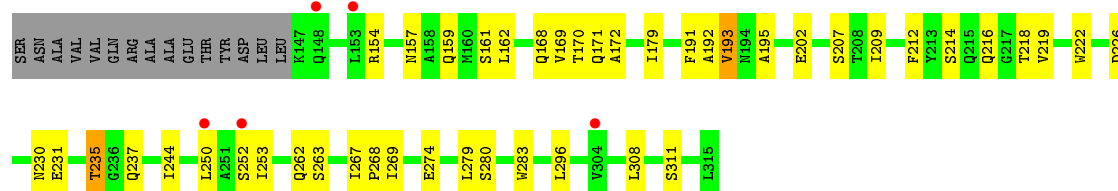
- Molecule 1: Two-component response regulator



- Molecule 1: Two-component response regulator



- Molecule 1: Two-component response regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.88Å 111.88Å 112.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.65 36.62 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.65) 98.2 (36.62-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.268 0.227 , 0.263	Depositor DCC
R_{free} test set	1206 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23627 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3934	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.63	0/1335	0.71	0/1821
1	B	0.55	0/1316	0.65	0/1793
1	C	0.63	0/1280	0.73	0/1746
All	All	0.60	0/3931	0.70	0/5360

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1322	0	1294	8	0
1	B	1303	0	1293	33	0
1	C	1267	0	1251	34	0
2	A	19	0	0	0	0
2	B	7	0	0	1	0
2	C	16	0	0	1	0
All	All	3934	0	3838	74	0

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 10.

All (74) 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:C:235:THR:HG22	1:C:237:GLN:H	1.31	0.94
1:B:300:SER:O	1:B:304:VAL:HG23	1.79	0.83
1:C:231:GLU:O	1:C:235:THR:HB	1.84	0.77
1:B:263:SER:HB2	1:B:283:TRP:HB2	1.65	0.77
1:C:269:ILE:HD11	1:C:279:LEU:HB2	1.64	0.77
1:C:235:THR:HG22	1:C:237:GLN:N	2.00	0.76
1:B:199:GLN:NE2	1:B:207:SER:O	2.21	0.74
1:B:238:ILE:HD13	1:B:267:ILE:HD13	1.70	0.72
1:C:179:ILE:HD11	1:C:308:LEU:HD23	1.73	0.71
1:B:237:GLN:O	1:B:239:GLN:NE2	2.24	0.71
1:B:302:GLN:NE2	2:B:10:HOH:O	2.23	0.70
1:C:244:ILE:CG2	1:C:244:ILE:O	2.46	0.64
1:B:235:THR:HG22	1:B:237:GLN:H	1.64	0.62
1:B:267:ILE:HG23	1:B:279:LEU:HB3	1.80	0.61
1:B:265:VAL:HG21	1:B:289:LEU:HD11	1.82	0.61
1:B:165:VAL:O	1:B:169:VAL:HB	2.02	0.59
1:B:160:MSE:HE3	1:C:159:GLN:HB3	1.84	0.59
1:B:228:LEU:HD13	1:B:250:LEU:HD11	1.85	0.59
1:C:154:ARG:O	1:C:157:ASN:HB2	2.04	0.58
1:B:267:ILE:HD12	1:B:268:PRO:HD2	1.86	0.56
1:B:179:ILE:O	1:B:183:ILE:HG13	2.05	0.55
1:B:232:ALA:HA	1:B:239:GLN:HE21	1.71	0.55
1:B:218:THR:HG22	1:B:219:VAL:H	1.71	0.55
1:C:235:THR:HG23	1:C:237:GLN:HG2	1.89	0.54
1:B:264:HIS:HD2	1:B:281:LEU:O	1.90	0.54
1:C:263:SER:HB3	1:C:283:TRP:HB2	1.91	0.53
1:C:250:LEU:C	1:C:252:SER:H	2.11	0.53
1:A:201:LEU:HG	1:A:277:GLY:HA2	1.91	0.52
1:C:235:THR:CG2	1:C:237:GLN:HG2	2.40	0.51
1:A:188:ALA:HA	1:A:193:VAL:HG22	1.91	0.51
1:A:176:LEU:O	1:A:179:ILE:HG22	2.12	0.50
1:B:236:GLY:O	1:B:268:PRO:HG2	2.12	0.50
1:A:159:GLN:HG2	1:A:296:LEU:HD22	1.93	0.49
1:B:264:HIS:CE1	1:B:266:VAL:HG22	2.48	0.49
1:C:159:GLN:HG2	1:C:296:LEU:HD13	1.93	0.49
1:C:170:THR:C	1:C:171:GLN:O	2.46	0.48
1:C:212:PHE:CZ	1:C:219:VAL:HG22	2.48	0.48
1:B:212:PHE:HB2	1:B:219:VAL:HG11	1.95	0.47
1:B:164:THR:O	1:B:168:GLN:HG3	2.14	0.47
1:B:218:THR:HG22	1:B:219:VAL:N	2.30	0.47
1:B:162:LEU:O	1:B:166:LEU:HG	2.13	0.47
1:B:193:VAL:HG11	1:B:196:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:O	1:B:180:LEU:HG	2.14	0.47
1:C:168:GLN:CD	2:C:25:HOH:O	2.53	0.47
1:A:187:PHE:CZ	1:A:300:SER:HB3	2.49	0.47
1:C:250:LEU:C	1:C:252:SER:N	2.69	0.46
1:C:244:ILE:HG23	1:C:244:ILE:O	2.15	0.46
1:C:171:GLN:O	1:C:172:ALA:HB3	2.16	0.46
1:C:267:ILE:HG13	1:C:268:PRO:HD2	1.96	0.46
1:B:147:LYS:O	1:B:150:THR:HG22	2.16	0.46
1:B:185:THR:HG23	1:B:213:TYR:CD1	2.51	0.46
1:B:162:LEU:HD23	1:B:296:LEU:HD11	1.97	0.45
1:C:169:VAL:C	1:C:171:GLN:O	2.55	0.45
1:C:214:SER:OG	1:C:219:VAL:HG13	2.17	0.45
1:B:245:ALA:HA	1:B:251:ALA:HB2	1.98	0.44
1:A:213:TYR:C	1:A:213:TYR:CD2	2.91	0.44
1:C:159:GLN:CG	1:C:296:LEU:HD13	2.48	0.44
1:C:222:TRP:CZ3	1:C:226:ASP:HB2	2.53	0.44
1:C:244:ILE:HG22	1:C:244:ILE:O	2.18	0.43
1:C:169:VAL:O	1:C:171:GLN:O	2.35	0.43
1:A:287:ILE:HD12	1:A:289:LEU:HG	2.00	0.43
1:B:270:THR:CG2	1:B:273:ASN:HA	2.49	0.43
1:C:202:GLU:HG3	1:C:207:SER:HB3	2.00	0.42
1:C:269:ILE:CD1	1:C:279:LEU:HB2	2.42	0.42
1:C:202:GLU:OE1	1:C:207:SER:HB2	2.19	0.42
1:C:191:PHE:O	1:C:192:ALA:C	2.58	0.42
1:B:271:TYR:O	1:B:273:ASN:N	2.52	0.42
1:C:235:THR:CG2	1:C:237:GLN:HB2	2.50	0.41
1:A:231:GLU:HG2	1:A:239:GLN:CD	2.40	0.41
1:B:185:THR:HG23	1:B:213:TYR:CE1	2.55	0.41
1:C:161:SER:O	1:C:162:LEU:C	2.58	0.41
1:B:238:ILE:HD11	1:B:265:VAL:CG1	2.51	0.41
1:C:214:SER:HG	1:C:219:VAL:HG13	1.87	0.40
1:C:193:VAL:HG13	1:C:195:ALA:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	176/184 (96%)	172 (98%)	4 (2%)	0	100	100
1	B	173/184 (94%)	157 (91%)	15 (9%)	1 (1%)	30	54
1	C	167/184 (91%)	154 (92%)	12 (7%)	1 (1%)	30	54
All	All	516/552 (94%)	483 (94%)	31 (6%)	2 (0%)	39	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	ASN
1	C	253	ILE

5.3.2 Protein sidechains ⓘ

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	137/154 (89%)	135 (98%)	2 (2%)	72	90
1	B	135/154 (88%)	125 (93%)	10 (7%)	17	35
1	C	135/154 (88%)	125 (93%)	10 (7%)	17	35
All	All	407/462 (88%)	385 (95%)	22 (5%)	27	52

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	267	ILE
1	B	169	VAL
1	B	173	SER
1	B	190	SER
1	B	193	VAL
1	B	206	LEU

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Mol	Chain	Res	Type
1	B	237	GLN
1	B	266	VAL
1	B	272	ARG
1	B	274	GLU
1	B	312	ARG
1	C	193	VAL
1	C	209	ILE
1	C	216	GLN
1	C	218	THR
1	C	230	ASN
1	C	235	THR
1	C	262	GLN
1	C	274	GLU
1	C	280	SER
1	C	311	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	175/184 (95%)	-0.26	6 (3%) 49 47	32, 56, 110, 151	0
1	B	172/184 (93%)	0.74	26 (15%) 3 2	55, 109, 177, 228	0
1	C	166/184 (90%)	0.03	5 (3%) 54 52	40, 64, 113, 135	0
All	All	513/552 (92%)	0.17	37 (7%) 18 16	32, 70, 147, 228	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	LEU	5.4
1	B	216	GLN	5.3
1	B	146	LEU	4.8
1	B	203	GLY	4.5
1	B	219	VAL	4.4
1	A	314	SER	4.0
1	A	140	ALA	4.0
1	B	140	ALA	3.8
1	B	218	THR	3.7
1	B	144	ASP	3.6
1	B	195	ALA	3.5
1	B	143	TYR	3.4
1	B	220	ASN	3.4
1	B	202	GLU	3.3
1	B	250	LEU	3.2
1	A	313	CYS	3.0
1	A	139	ALA	2.9
1	B	208	THR	2.8
1	B	225	GLN	2.8
1	B	147	LYS	2.8
1	C	148	GLN	2.7
1	B	263	SER	2.6
1	A	138	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	294	LEU	2.5
1	C	250	LEU	2.5
1	B	148	GLN	2.4
1	C	252	SER	2.4
1	B	280	SER	2.4
1	B	142	THR	2.3
1	C	153	LEU	2.2
1	B	244	ILE	2.2
1	B	204	GLN	2.2
1	B	234	ALA	2.1
1	B	205	THR	2.1
1	C	304	VAL	2.0
1	B	289	LEU	2.0
1	A	202	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.