



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:58 AM UTC

PDB ID : 3P01 / pdb_00003p01
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

<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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

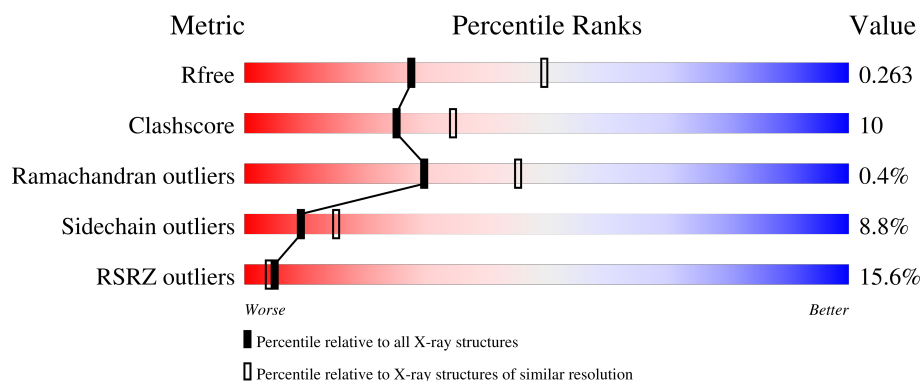
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 $\leq 5\%$. 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	4% 84% 11% • •
1	B	184	35% 62% 29% • 5%
1	C	184	4% 66% 22% • 8%

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

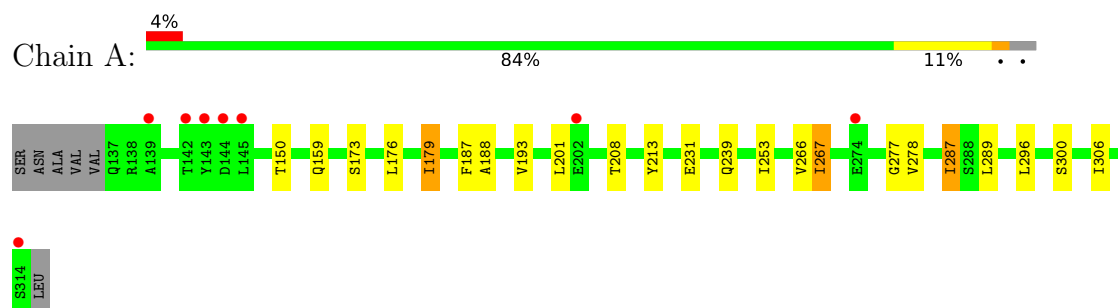
- Molecule 2 is water.

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		

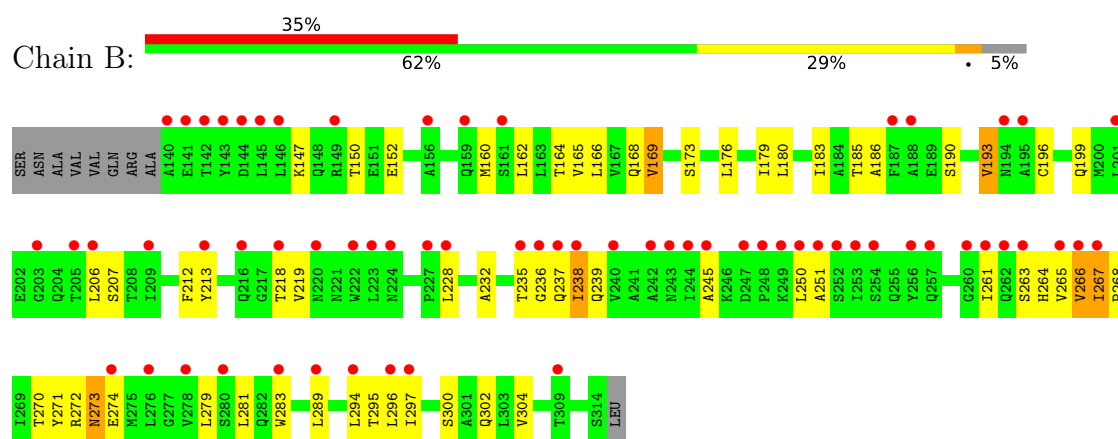
3 Residue-property plots [i](#)

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 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.

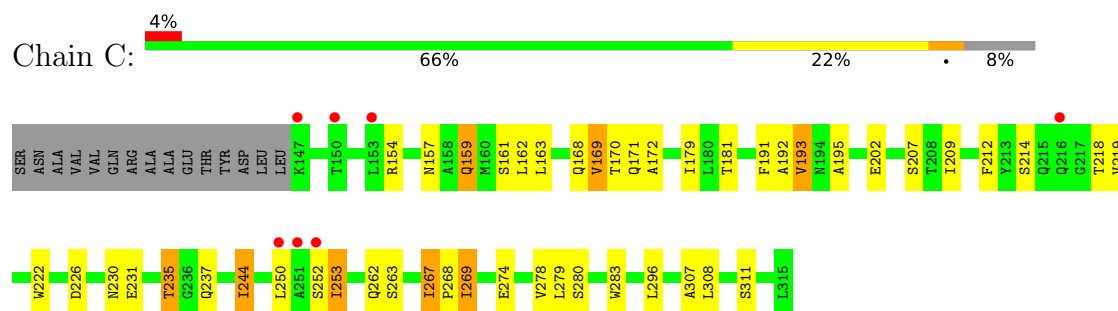
- Molecule 1: Two-component response regulator



- 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 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.65) 98.1 (50.00-2.65)	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 (4.99%)	wwPDB-VP
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 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.82	0/1335	0.98	4/1821 (0.2%)
1	B	0.76	2/1316 (0.2%)	0.99	1/1793 (0.1%)
1	C	0.83	0/1280	1.04	2/1746 (0.1%)
All	All	0.80	2/3931 (0.1%)	1.01	7/5360 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	ILE	CA-CB	5.63	1.58	1.54
1	B	261	ILE	CA-CB	5.45	1.60	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ILE	CB-CA-C	-6.50	102.85	111.70
1	A	267	ILE	CA-C-N	-5.38	114.70	120.03
1	A	267	ILE	C-N-CA	-5.38	114.70	120.03
1	C	181	THR	CA-C-N	-5.27	113.11	118.85
1	C	181	THR	C-N-CA	-5.27	113.11	118.85
1	A	306	ILE	N-CA-C	-5.11	105.40	110.62
1	B	186	ALA	N-CA-C	-5.10	104.99	111.11

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	34	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	75	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 (75) 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:265:VAL:HG21	1:B:289:LEU:HD11	1.82	0.61
1:B:267:ILE:HG23	1:B:279:LEU:HB3	1.80	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:C:250:LEU:C	1:C:252:SER:H	2.11	0.57
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:170:THR:C	1:C:171:GLN:O	2.46	0.53
1:C:263:SER:HB3	1:C:283:TRP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HG	1:A:277:GLY:HA2	1.91	0.52
1:A:188:ALA:HA	1:A:193:VAL:HG22	1.91	0.51
1:C:168:GLN:CD	2:C:25:HOH:O	2.53	0.51
1:C:235:THR:CG2	1:C:237:GLN:HG2	2.40	0.51
1:C:250:LEU:C	1:C:252:SER:N	2.69	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:C:169:VAL:C	1:C:171:GLN:O	2.55	0.50
1:A:159:GLN:HG2	1:A:296:LEU:HD22	1.93	0.49
1:A:213:TYR:CD2	1:A:213:TYR:C	2.91	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:212:PHE:CZ	1:C:219:VAL:HG22	2.48	0.48
1:B:164:THR:O	1:B:168:GLN:HG3	2.14	0.47
1:B:212:PHE:HB2	1:B:219:VAL:HG11	1.95	0.47
1:B:162:LEU:O	1:B:166:LEU:HG	2.13	0.47
1:B:218:THR:HG22	1:B:219:VAL:N	2.30	0.47
1:B:193:VAL:HG11	1:B:196:CYS:HB2	1.97	0.47
1:B:176:LEU:O	1:B:180:LEU:HG	2.14	0.47
1:A:187:PHE:CZ	1:A:300:SER:HB3	2.49	0.47
1:C:191:PHE:O	1:C:192:ALA:C	2.58	0.47
1:C:244:ILE:O	1:C:244:ILE:HG23	2.15	0.46
1:C:171:GLN:O	1:C:172:ALA:HB3	2.16	0.46
1:A:231:GLU:HG2	1:A:239:GLN:CD	2.40	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:C:161:SER:O	1:C:162:LEU:C	2.58	0.45
1:B:162:LEU:HD23	1:B:296:LEU:HD11	1.97	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: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:O	1:C:244:ILE:HG22	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:307:ALA:O	1:C:308:LEU:C	2.62	0.43
1:C:202:GLU:HG3	1:C:207:SER:HB3	2.00	0.42
1:B:294:LEU:O	1:B:295:THR:C	2.63	0.42
1:C:202:GLU:OE1	1:C:207:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:CD1	1:C:279:LEU:HB2	2.42	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:B:185:THR:HG23	1:B:213:TYR:CE1	2.55	0.41
1:B:238:ILE:HD11	1:B:265:VAL:CG1	2.51	0.41
1:C:193:VAL:HG13	1:C:195:ALA:N	2.36	0.40

There are no symmetry-related clashes.

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	176/184 (96%)	172 (98%)	4 (2%)	0	100	100
1	B	173/184 (94%)	157 (91%)	15 (9%)	1 (1%)	21	34
1	C	167/184 (91%)	154 (92%)	12 (7%)	1 (1%)	21	34
All	All	516/552 (94%)	483 (94%)	31 (6%)	2 (0%)	30	45

All (2) Ramachandran outliers are listed below:

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

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	137/154 (89%)	129 (94%)	8 (6%)	18	31
1	B	135/154 (88%)	124 (92%)	11 (8%)	11	18
1	C	135/154 (88%)	118 (87%)	17 (13%)	4	6
All	All	407/462 (88%)	371 (91%)	36 (9%)	9	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	THR
1	A	173	SER
1	A	179	ILE
1	A	208	THR
1	A	253	ILE
1	A	266	VAL
1	A	267	ILE
1	A	278	VAL
1	B	152	GLU
1	B	169	VAL
1	B	173	SER
1	B	190	SER
1	B	193	VAL
1	B	206	LEU
1	B	238	ILE
1	B	266	VAL
1	B	272	ARG
1	B	274	GLU
1	B	297	ILE
1	C	159	GLN
1	C	163	LEU
1	C	169	VAL
1	C	193	VAL
1	C	209	ILE
1	C	218	THR
1	C	230	ASN
1	C	235	THR
1	C	244	ILE
1	C	253	ILE
1	C	262	GLN
1	C	267	ILE
1	C	269	ILE
1	C	274	GLU
1	C	278	VAL

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Mol	Chain	Res	Type
1	C	280	SER
1	C	311	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	257	GLN
1	A	259	ASN
1	B	199	GLN
1	B	220	ASN
1	B	221	ASN
1	B	239	GLN
1	B	255	GLN
1	B	259	ASN
1	C	159	GLN
1	C	210	GLN
1	C	224	ASN
1	C	237	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 oligosaccharides 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%)	-0.02	8 (4%) 37 29	32, 56, 110, 151	0
1	B	172/184 (93%)	1.70	65 (37%) 1 0	55, 109, 177, 228	0
1	C	166/184 (90%)	0.25	7 (4%) 40 32	40, 64, 113, 135	0
All	All	513/552 (92%)	0.65	80 (15%) 5 4	32, 70, 147, 228	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	LEU	5.4
1	B	140	ALA	5.4
1	C	147	LYS	5.3
1	B	254	SER	5.3
1	A	143	TYR	5.3
1	B	146	LEU	5.1
1	B	256	TYR	5.1
1	B	240	VAL	4.3
1	B	244	ILE	4.2
1	B	245	ALA	4.2
1	B	142	THR	4.1
1	B	265	VAL	4.0
1	B	296	LEU	3.9
1	B	250	LEU	3.9
1	B	252	SER	3.9
1	B	238	ILE	3.9
1	B	156	ALA	3.9
1	B	203	GLY	3.8
1	C	251	ALA	3.7
1	B	149	ARG	3.7
1	B	247	ASP	3.6
1	B	205	THR	3.4
1	B	143	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	283	TRP	3.3
1	B	251	ALA	3.3
1	B	144	ASP	3.3
1	B	235	THR	3.2
1	B	262	GLN	3.2
1	B	248	PRO	3.2
1	B	145	LEU	3.1
1	B	141	GLU	3.1
1	B	187	PHE	3.1
1	B	206	LEU	3.0
1	B	261	ILE	3.0
1	B	195	ALA	3.0
1	B	294	LEU	3.0
1	A	144	ASP	3.0
1	B	222	TRP	3.0
1	B	266	VAL	3.0
1	B	228	LEU	2.9
1	B	223	LEU	2.9
1	B	263	SER	2.9
1	B	249	LYS	2.9
1	C	153	LEU	2.8
1	B	216	GLN	2.8
1	C	216	GLN	2.8
1	B	243	ASN	2.8
1	B	280	SER	2.7
1	C	250	LEU	2.7
1	B	188	ALA	2.7
1	A	314	SER	2.7
1	A	139	ALA	2.6
1	C	252	SER	2.5
1	B	242	ALA	2.5
1	B	218	THR	2.5
1	B	267	ILE	2.5
1	B	276	LEU	2.4
1	A	202	GLU	2.4
1	A	274	GLU	2.4
1	B	159	GLN	2.4
1	B	257	GLN	2.4
1	C	150	THR	2.4
1	B	209	ILE	2.3
1	B	260	GLY	2.3
1	A	142	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLY	2.3
1	B	201	LEU	2.3
1	B	297	ILE	2.2
1	B	161	SER	2.2
1	B	274	GLU	2.2
1	B	213	TYR	2.1
1	B	309	THR	2.1
1	B	289	LEU	2.1
1	B	220	ASN	2.1
1	B	194	ASN	2.1
1	B	224	ASN	2.1
1	B	253	ILE	2.1
1	B	278	VAL	2.1
1	B	237	GLN	2.0
1	B	227	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.