



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:15 pm GMT

PDB ID : 3M3W
Title : Crystal structure of mouse PACSIN3 BAR domain mutant
Authors : Meng, G.; Bai, X.Y.
Deposited on : 2010-03-10
Resolution : 2.60 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

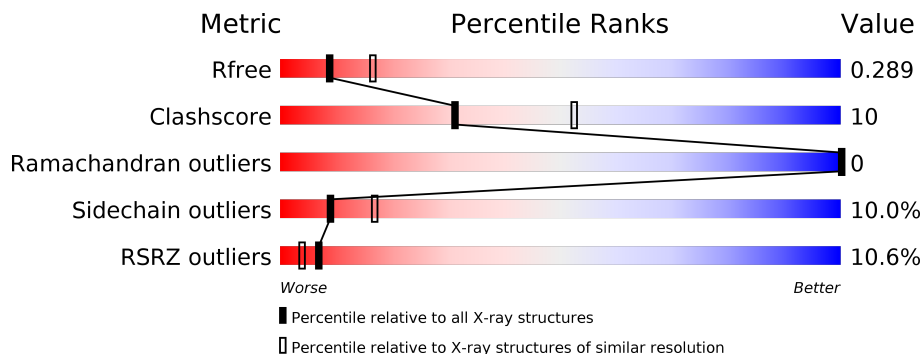
1 Overall quality at a glance

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))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 $\leq 5\%$. 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	320	
1	B	320	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4560 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 Protein kinase C and casein kinase II substrate protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2262	1402	429	422	9			
1	B	286	Total	C	N	O	S	0	0	0
			2288	1424	436	419	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	GLU	ENGINEERED MUTATION	UNP Q99JB8
B	128	ALA	GLU	ENGINEERED MUTATION	UNP Q99JB8

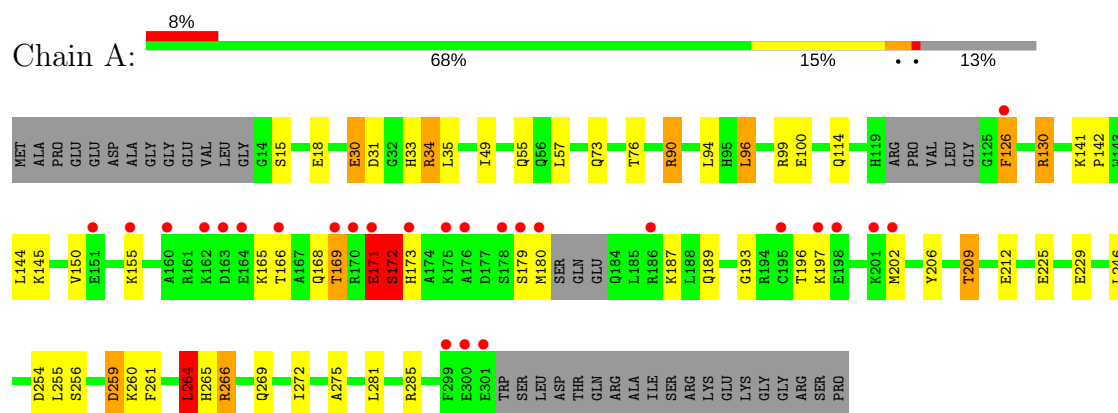
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	1	Total	O	0	0
			1	1		

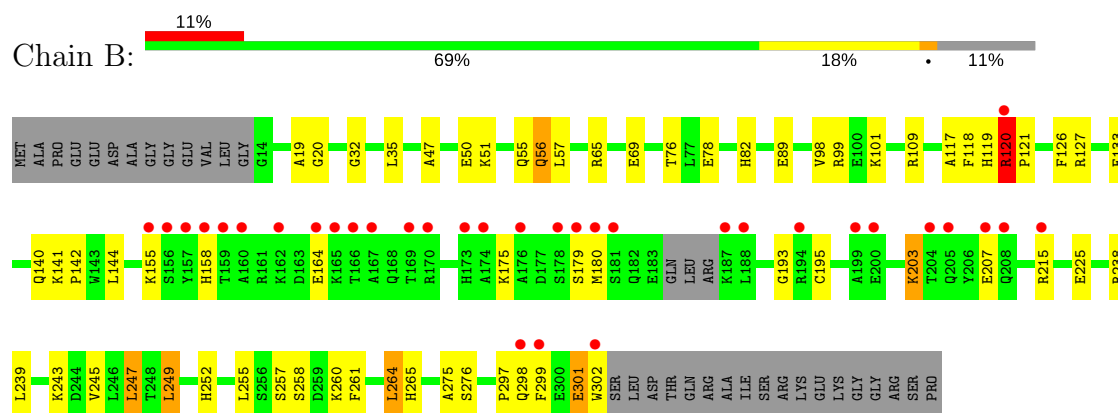
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Protein kinase C and casein kinase II substrate protein 3



- Molecule 1: Protein kinase C and casein kinase II substrate protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.49Å 52.27Å 196.46Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 46.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.60) 99.6 (46.10-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.89 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.281 0.242 , 0.289	Depositor DCC
R_{free} test set	1497 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4560	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.95% 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

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	0.63	0/2311	0.72	4/3105 (0.1%)
1	B	0.62	0/2340	0.76	6/3150 (0.2%)
All	All	0.62	0/4651	0.74	10/6255 (0.2%)

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	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	LEU	CA-CB-CG	9.30	136.69	115.30
1	B	175	LYS	CB-CA-C	-8.21	93.97	110.40
1	A	173	HIS	N-CA-C	-7.90	89.67	111.00
1	A	264	LEU	CA-CB-CG	6.68	130.67	115.30
1	B	301	GLU	N-CA-C	6.64	128.94	111.00
1	B	120	ARG	C-N-CD	-6.60	106.09	120.60
1	B	301	GLU	CB-CA-C	-6.43	97.54	110.40
1	A	171	GLU	N-CA-C	-5.97	94.87	111.00
1	A	172	SER	CB-CA-C	-5.47	99.70	110.10
1	B	299	PHE	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PHE	Peptide
1	B	120	ARG	Peptide

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	2262	0	2123	37	0
1	B	2288	0	2140	59	0
2	A	9	0	0	0	0
2	B	1	0	0	0	0
All	All	4560	0	4263	91	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 (91) 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:120:ARG:HB2	1:B:127:ARG:H	1.01	1.14
1:B:120:ARG:CB	1:B:127:ARG:H	1.61	1.12
1:B:76:THR:HG21	1:B:276:SER:H	1.08	1.10
1:A:171:GLU:O	1:A:172:SER:HB3	1.50	1.07
1:B:120:ARG:HB2	1:B:127:ARG:N	1.80	0.95
1:B:120:ARG:CD	1:B:126:PHE:HB3	1.96	0.95
1:B:120:ARG:HD3	1:B:126:PHE:HB3	1.45	0.93
1:B:120:ARG:HB3	1:B:127:ARG:HB2	1.51	0.91
1:A:76:THR:HG22	1:A:275:ALA:HA	1.59	0.84
1:B:117:ALA:O	1:B:120:ARG:NH1	2.10	0.84
1:A:76:THR:CG2	1:A:275:ALA:HA	2.08	0.84
1:B:76:THR:HG21	1:B:276:SER:N	1.91	0.84
1:B:101:LYS:HD2	1:B:252:HIS:CD2	2.13	0.83
1:B:297:PRO:O	1:B:298:GLN:HG3	1.81	0.81
1:B:76:THR:CG2	1:B:276:SER:H	1.92	0.81
1:A:126:PHE:O	1:A:130:ARG:HB2	1.81	0.79
1:B:203:LYS:O	1:B:207:GLU:HG2	1.86	0.75
1:B:65:ARG:NH2	1:B:89:GLU:OE2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:HG3	1:B:126:PHE:HA	1.70	0.74
1:A:171:GLU:C	1:A:171:GLU:OE1	2.30	0.70
1:A:254:ASP:OD1	1:A:256:SER:OG	2.11	0.69
1:B:120:ARG:CB	1:B:127:ARG:N	2.46	0.67
1:B:179:SER:CB	1:B:180:MET:CB	2.74	0.66
1:A:172:SER:O	1:A:172:SER:OG	2.10	0.66
1:B:260:LYS:N	1:B:260:LYS:HD2	2.13	0.64
1:A:266:ARG:HA	1:A:266:ARG:NE	2.12	0.64
1:B:120:ARG:CB	1:B:127:ARG:HB2	2.28	0.63
1:B:261:PHE:O	1:B:265:HIS:HD2	1.82	0.62
1:A:33:HIS:CE1	1:A:114:GLN:HE21	2.18	0.61
1:B:245:VAL:HG12	1:B:249:LEU:HD22	1.82	0.61
1:B:297:PRO:O	1:B:298:GLN:CG	2.48	0.61
1:B:301:GLU:O	1:B:302:TRP:CB	2.48	0.60
1:B:120:ARG:HG3	1:B:126:PHE:CA	2.31	0.60
1:A:206:TYR:O	1:A:209:THR:HG22	2.01	0.60
1:B:260:LYS:N	1:B:260:LYS:CD	2.64	0.60
1:B:20:GLY:H	1:B:140:GLN:HE22	1.50	0.60
1:B:120:ARG:CG	1:B:127:ARG:H	2.15	0.59
1:A:150:VAL:HG22	1:A:209:THR:HG23	1.83	0.59
1:A:179:SER:O	1:A:180:MET:C	2.40	0.59
1:A:30:GLU:OE1	1:A:31:ASP:OD1	2.21	0.58
1:B:78:GLU:HG2	1:B:82:HIS:CD2	2.41	0.56
1:A:76:THR:HG21	1:A:275:ALA:HA	1.89	0.55
1:A:171:GLU:OE1	1:A:172:SER:CB	2.55	0.54
1:B:76:THR:HG23	1:B:275:ALA:HA	1.89	0.54
1:A:261:PHE:O	1:A:265:HIS:HD2	1.92	0.53
1:A:171:GLU:OE1	1:A:172:SER:HB3	2.09	0.53
1:B:141:LYS:N	1:B:142:PRO:HD2	2.23	0.52
1:A:49:ILE:HG12	1:B:56:GLN:HG2	1.92	0.52
1:B:65:ARG:O	1:B:69:GLU:HB2	2.10	0.51
1:A:187:LYS:O	1:A:189:GLN:N	2.43	0.51
1:A:259:ASP:OD1	1:A:259:ASP:N	2.45	0.50
1:B:78:GLU:HG2	1:B:82:HIS:HD2	1.74	0.50
1:A:179:SER:O	1:A:180:MET:O	2.30	0.50
1:A:171:GLU:O	1:A:171:GLU:OE1	2.30	0.50
1:A:96:LEU:O	1:A:100:GLU:HG2	2.11	0.50
1:B:260:LYS:H	1:B:260:LYS:CD	2.25	0.49
1:A:193:GLY:O	1:A:196:THR:HG22	2.13	0.49
1:B:120:ARG:HG3	1:B:126:PHE:CB	2.43	0.49
1:B:215:ARG:HA	1:B:215:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HB1	1:B:99:ARG:HG2	1.94	0.49
1:B:118:PHE:C	1:B:120:ARG:H	2.14	0.49
1:B:120:ARG:CB	1:B:127:ARG:CB	2.90	0.49
1:A:165:LYS:HA	1:A:168:GLN:HG2	1.95	0.48
1:A:166:THR:O	1:A:169:THR:HG22	2.13	0.48
1:A:171:GLU:O	1:A:172:SER:CB	2.32	0.48
1:B:120:ARG:CG	1:B:126:PHE:HB3	2.44	0.47
1:B:120:ARG:HB3	1:B:127:ARG:CB	2.33	0.47
1:B:117:ALA:O	1:B:120:ARG:CZ	2.61	0.47
1:B:50:GLU:HG3	1:B:98:VAL:CG1	2.45	0.47
1:B:193:GLY:C	1:B:195:CYS:H	2.18	0.46
1:A:15:SER:HB3	1:A:18:GLU:HG3	1.96	0.46
1:B:119:HIS:O	1:B:121:PRO:HD3	2.14	0.46
1:B:32:GLY:HA3	1:B:238:ARG:HD2	1.96	0.46
1:B:155:LYS:HA	1:B:158:HIS:CD2	2.51	0.46
1:A:73:GLN:HE22	1:B:238:ARG:HH21	1.64	0.46
1:A:90:ARG:HA	1:A:90:ARG:HD3	1.72	0.45
1:A:141:LYS:HB3	1:A:142:PRO:HD3	1.98	0.44
1:B:120:ARG:HG2	1:B:120:ARG:H	1.61	0.43
1:B:19:ALA:HB2	1:B:144:LEU:HD21	2.00	0.43
1:A:285:ARG:NH2	1:B:225:GLU:OE1	2.48	0.42
1:A:261:PHE:HA	1:A:264:LEU:HD13	2.02	0.42
1:A:31:ASP:O	1:A:34:ARG:HG3	2.20	0.42
1:A:94:LEU:HD21	1:A:260:LYS:HB2	2.00	0.42
1:B:120:ARG:HE	1:B:120:ARG:HB3	1.73	0.42
1:B:179:SER:CB	1:B:180:MET:CA	2.98	0.41
1:A:272:ILE:HG22	1:B:247:LEU:HD22	2.02	0.41
1:A:275:ALA:HB3	1:B:243:LYS:HG3	2.03	0.41
1:B:76:THR:CG2	1:B:275:ALA:HA	2.51	0.40
1:B:50:GLU:HG3	1:B:98:VAL:HG12	2.03	0.40
1:B:297:PRO:C	1:B:298:GLN:HG3	2.39	0.40
1:B:51:LYS:HB2	1:B:99:ARG:HG3	2.04	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	274/320 (86%)	265 (97%)	9 (3%)	0	100	100
1	B	282/320 (88%)	270 (96%)	12 (4%)	0	100	100
All	All	556/640 (87%)	535 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	221/268 (82%)	193 (87%)	28 (13%)	5	9
1	B	219/268 (82%)	203 (93%)	16 (7%)	16	33
All	All	440/536 (82%)	396 (90%)	44 (10%)	9	17

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	34	ARG
1	A	35	LEU
1	A	55	GLN
1	A	57	LEU
1	A	90	ARG
1	A	96	LEU
1	A	99	ARG
1	A	130	ARG
1	A	144	LEU
1	A	145	LYS
1	A	155	LYS
1	A	169	THR
1	A	171	GLU

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Mol	Chain	Res	Type
1	A	172	SER
1	A	197	LYS
1	A	202	MET
1	A	209	THR
1	A	212	GLU
1	A	225	GLU
1	A	229	GLU
1	A	246	LEU
1	A	255	LEU
1	A	259	ASP
1	A	264	LEU
1	A	266	ARG
1	A	269	GLN
1	A	281	LEU
1	B	35	LEU
1	B	55	GLN
1	B	56	GLN
1	B	57	LEU
1	B	109	ARG
1	B	120	ARG
1	B	133	GLU
1	B	164	GLU
1	B	203	LYS
1	B	239	LEU
1	B	247	LEU
1	B	249	LEU
1	B	255	LEU
1	B	257	SER
1	B	258	SER
1	B	264	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	73	GLN
1	A	205	GLN
1	A	208	GLN
1	A	265	HIS
1	A	269	GLN
1	A	270	GLN
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	73	GLN
1	B	140	GLN
1	B	158	HIS
1	B	237	GLN
1	B	250	HIS
1	B	251	GLN
1	B	265	HIS
1	B	298	GLN

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 carbohydrates 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](#)

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	280/320 (87%)	0.46	26 (9%) 9 6	3, 35, 124, 159	0
1	B	286/320 (89%)	0.63	34 (11%) 5 3	4, 41, 163, 211	0
All	All	566/640 (88%)	0.55	60 (10%) 7 4	3, 37, 154, 211	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	THR	10.1
1	B	158	HIS	8.9
1	B	204	THR	7.2
1	B	194	ARG	6.0
1	B	167	ALA	5.4
1	B	207	GLU	4.9
1	B	169	THR	4.6
1	B	188	LEU	4.5
1	B	178	SER	4.3
1	A	179	SER	4.0
1	B	166	THR	4.0
1	A	173	HIS	4.0
1	B	155	LYS	3.8
1	A	299	PHE	3.6
1	B	164	GLU	3.3
1	B	181	SER	3.2
1	A	198	GLU	3.1
1	B	120	ARG	3.1
1	A	170	ARG	3.1
1	A	195	CYS	3.0
1	A	180	MET	3.0
1	A	186	ARG	3.0
1	B	156	SER	3.0
1	B	179	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLN	3.0
1	B	173	HIS	3.0
1	B	298	GLN	2.9
1	B	174	ALA	2.9
1	A	176	ALA	2.9
1	B	199	ALA	2.8
1	A	126	PHE	2.7
1	B	187	LYS	2.7
1	A	155	LYS	2.7
1	B	302	TRP	2.7
1	A	164	GLU	2.6
1	A	171	GLU	2.6
1	B	215	ARG	2.6
1	B	162	LYS	2.5
1	B	205	GLN	2.5
1	A	163	ASP	2.5
1	A	162	LYS	2.5
1	A	300	GLU	2.5
1	A	160	ALA	2.4
1	B	200	GLU	2.4
1	B	160	ALA	2.4
1	B	170	ARG	2.4
1	A	301	GLU	2.3
1	A	202	MET	2.3
1	B	180	MET	2.3
1	B	176	ALA	2.3
1	A	201	LYS	2.2
1	B	157	TYR	2.2
1	A	178	SER	2.2
1	A	151	GLU	2.1
1	B	299	PHE	2.1
1	A	197	LYS	2.1
1	A	166	THR	2.0
1	A	175	LYS	2.0
1	A	169	THR	2.0
1	B	165	LYS	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 [i](#)

There are no carbohydrates 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.