



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:09 PM UTC

PDB ID : 5CM9 / pdb_00005cm9
Title : Structural Basis for the Selectivity of Guanine Nucleotide Exchange Factors
for the small G-protein Ral
Authors : Popovic, M.; Schouten, A.; Rehmann, H.
Deposited on : 2015-07-16
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

<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
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

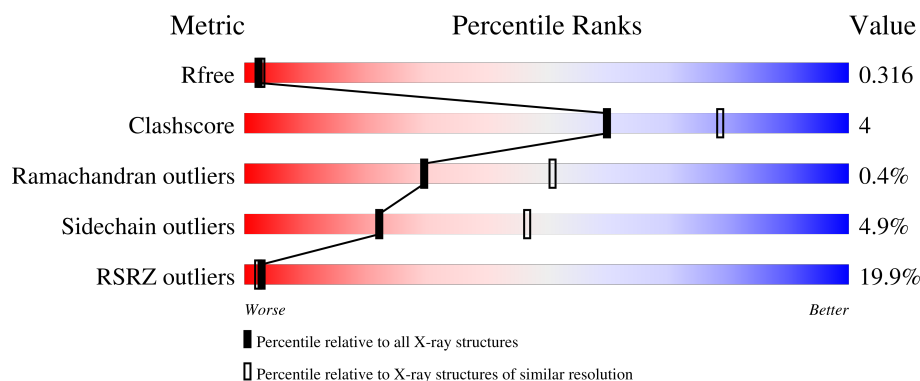
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	473	10% 71% 13% 14%
1	B	473	9% 72% 12% 16%
2	C	203	34% 60% 11% 28%
2	D	203	31% 67% 7% 26%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8619 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 Ral guanine nucleotide dissociation stimulator-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3162	1994	572	587	9			
1	B	396	Total	C	N	O	S	0	0	0
			3093	1951	557	576	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	expression tag	UNP Q61193
A	43	PRO	-	expression tag	UNP Q61193
A	44	LEU	-	expression tag	UNP Q61193
A	45	GLY	-	expression tag	UNP Q61193
A	46	SER	-	expression tag	UNP Q61193
A	47	PRO	-	expression tag	UNP Q61193
A	48	ASN	-	expression tag	UNP Q61193
A	49	SER	-	expression tag	UNP Q61193
A	147	TYR	HIS	conflict	UNP Q61193
A	402	THR	MET	conflict	UNP Q61193
B	42	GLY	-	expression tag	UNP Q61193
B	43	PRO	-	expression tag	UNP Q61193
B	44	LEU	-	expression tag	UNP Q61193
B	45	GLY	-	expression tag	UNP Q61193
B	46	SER	-	expression tag	UNP Q61193
B	47	PRO	-	expression tag	UNP Q61193
B	48	ASN	-	expression tag	UNP Q61193
B	49	SER	-	expression tag	UNP Q61193
B	147	TYR	HIS	conflict	UNP Q61193
B	402	THR	MET	conflict	UNP Q61193

- Molecule 2 is a protein called Ras-related protein Ral-a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	146	Total	C	N	O	S	0	0	0
			1144	725	196	217	6			
2	D	150	Total	C	N	O	S	0	0	0
			1184	747	201	230	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P48555
C	0	SER	-	expression tag	UNP P48555
D	-1	GLY	-	expression tag	UNP P48555
D	0	SER	-	expression tag	UNP P48555

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	16	Total	O	0	0
			16	16		
3	C	2	Total	O	0	0
			2	2		
3	D	4	Total	O	0	0
			4	4		

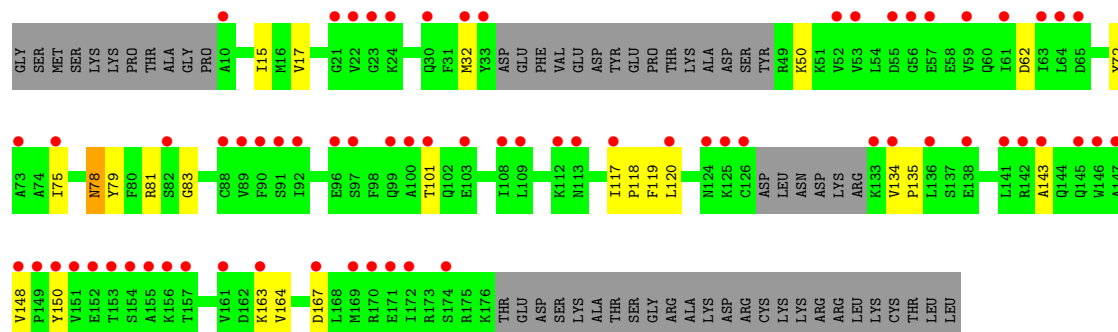
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- Molecule 1: Ral guanine nucleotide dissociation stimulator-like 2

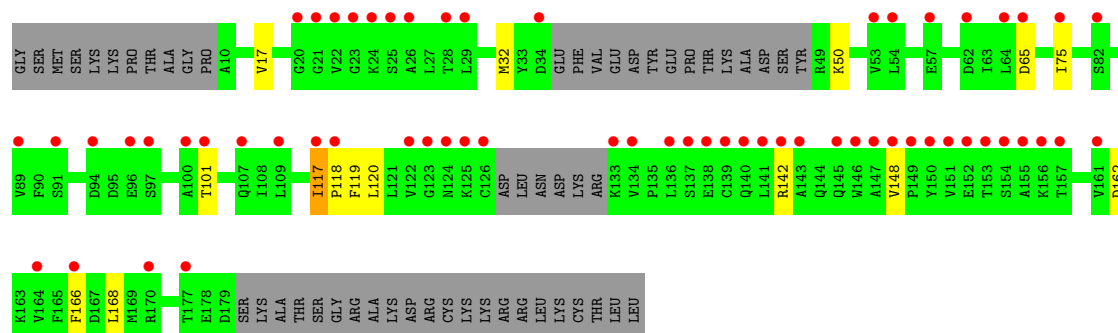




• Molecule 2: Ras-related protein Ral-a



• Molecule 2: Ras-related protein Ral-a



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.88Å 99.83Å 111.49Å 90.00° 127.00° 90.00°	Depositor
Resolution (Å)	46.63 – 2.60 46.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-2.60) 88.8 (46.63-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.273 , 0.320 0.269 , 0.316	Depositor DCC
R_{free} test set	2038 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8619	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7419e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.46	0/3229	0.85	4/4384 (0.1%)
1	B	0.44	0/3157	0.84	3/4288 (0.1%)
2	C	0.44	0/1160	0.79	0/1561
2	D	0.44	0/1200	0.77	0/1614
All	All	0.45	0/8746	0.83	7/11847 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLU	CA-C-N	7.38	125.05	119.66
1	A	511	GLU	C-N-CA	7.38	125.05	119.66
1	B	233	PRO	N-CA-CB	6.56	110.22	103.00
1	A	277	ARG	CA-C-N	6.43	127.88	119.84
1	A	277	ARG	C-N-CA	6.43	127.88	119.84
1	B	277	ARG	CA-C-N	5.61	126.85	119.84
1	B	277	ARG	C-N-CA	5.61	126.85	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3162	0	3164	33	0
1	B	3093	0	3094	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1144	0	1120	16	0
2	D	1184	0	1156	8	0
3	A	14	0	0	0	0
3	B	16	0	0	0	0
3	C	2	0	0	0	0
3	D	4	0	0	0	0
All	All	8619	0	8534	73	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 4.

All (73) 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)
2:C:119:PHE:HB3	2:C:148:VAL:HG11	1.67	0.75
1:A:425:GLY:HA3	1:A:481:ASP:H	1.53	0.72
1:B:104:LEU:HD11	1:B:162:VAL:HG11	1.73	0.70
1:B:97:LEU:HD22	1:B:128:THR:HG21	1.73	0.68
1:A:264:PRO:HB3	1:A:470:LEU:HD11	1.75	0.67
1:B:235:ASP:OD1	1:B:237:THR:HG22	1.95	0.67
1:A:128:THR:HG22	1:A:129:SER:H	1.63	0.62
1:B:254:LEU:HD11	1:B:489:GLN:HE22	1.64	0.62
2:C:117:ILE:HG13	2:C:118:PRO:HD2	1.82	0.62
1:B:264:PRO:HB3	1:B:470:LEU:HD11	1.83	0.61
1:A:264:PRO:HB3	1:A:470:LEU:CD1	2.31	0.60
2:D:117:ILE:HG13	2:D:118:PRO:HD2	1.83	0.59
1:A:235:ASP:OD1	1:A:237:THR:HG22	2.03	0.58
1:A:176:SER:HB2	1:A:179:LYS:HE2	1.85	0.57
2:D:101:THR:HB	2:D:142:ARG:HH21	1.70	0.57
1:B:97:LEU:CD2	1:B:128:THR:HG21	2.35	0.56
1:B:306:LEU:O	1:B:308:ALA:N	2.39	0.55
2:C:163:LYS:O	2:C:167:ASP:HB2	2.06	0.55
2:D:32:MET:HE3	2:D:50:LYS:HB2	1.88	0.55
1:A:294:PHE:CZ	2:C:75:ILE:HD11	2.43	0.54
1:A:352:TYR:CE2	2:C:75:ILE:HD12	2.44	0.53
2:C:78:ASN:HD22	2:C:78:ASN:N	2.07	0.52
1:A:359:GLN:O	2:C:81:ARG:NH2	2.41	0.52
1:B:154:ARG:O	1:B:158:VAL:HG23	2.10	0.52
2:C:15:ILE:HD11	2:C:83:GLY:HA3	1.92	0.52
2:C:72:TYR:HB3	2:C:75:ILE:HG12	1.90	0.52
1:A:437:LYS:O	1:A:441:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:HG11	1:A:363:ILE:HD12	1.92	0.51
1:A:309:THR:O	1:A:318:VAL:HG23	2.10	0.51
1:B:300:ALA:O	1:B:304:SER:HB2	2.10	0.51
1:B:118:PRO:HB2	1:B:464:PHE:CZ	2.46	0.51
1:A:255:ASP:HB3	1:A:429:VAL:HG11	1.94	0.49
1:A:425:GLY:CA	1:A:481:ASP:H	2.23	0.48
1:A:294:PHE:HZ	2:C:75:ILE:HD11	1.77	0.48
1:A:358:LEU:HD23	1:A:363:ILE:HD11	1.95	0.48
1:B:255:ASP:HB3	1:B:429:VAL:HG11	1.95	0.48
1:B:240:LEU:HA	1:B:334:LYS:HE2	1.95	0.47
2:D:162:ASP:O	2:D:166:PHE:HD1	1.98	0.47
1:A:69:VAL:HG22	1:A:90:ARG:HG3	1.97	0.47
1:A:352:TYR:CZ	2:C:75:ILE:HD12	2.50	0.47
1:A:76:PRO:HB3	1:A:84:PRO:HD3	1.97	0.46
1:A:118:PRO:HB2	1:A:464:PHE:CZ	2.50	0.46
2:C:15:ILE:CD1	2:C:83:GLY:HA3	2.45	0.46
1:A:284:CYS:N	1:A:285:PRO:HD3	2.30	0.46
2:C:32:MET:HE3	2:C:50:LYS:HB2	1.98	0.46
1:B:352:TYR:CE2	2:D:75:ILE:HD12	2.51	0.45
1:A:325:PRO:HB2	1:A:326:PRO:HD3	1.98	0.45
1:B:357:ALA:O	1:B:360:SER:HB3	2.16	0.45
1:A:360:SER:OG	1:A:362:PRO:HD2	2.17	0.45
1:B:325:PRO:HB2	1:B:326:PRO:HD3	1.97	0.45
2:D:119:PHE:HD2	2:D:148:VAL:HG11	1.82	0.45
1:A:365:ARG:O	1:A:367:ARG:N	2.50	0.44
1:A:293:GLN:O	1:A:297:VAL:HG23	2.18	0.44
1:A:156:THR:O	1:A:160:ILE:HG12	2.17	0.44
1:B:69:VAL:HG22	1:B:90:ARG:HG3	2.00	0.43
1:B:255:ASP:OD2	1:B:350:SER:OG	2.31	0.43
1:A:277:ARG:HB2	1:A:280:HIS:HD2	1.83	0.43
1:A:308:ALA:HB3	1:A:498:LEU:HD11	2.01	0.43
2:C:134:VAL:HA	2:C:135:PRO:HD3	1.83	0.43
1:A:144:LEU:HA	1:A:147:TYR:CD1	2.54	0.43
1:A:330:ARG:HA	1:A:330:ARG:HD3	1.92	0.43
1:A:361:SER:N	1:A:362:PRO:HD2	2.33	0.43
1:B:76:PRO:HB3	1:B:84:PRO:HD3	2.00	0.42
2:C:75:ILE:HG22	2:C:79:TYR:HE1	1.84	0.42
1:B:136:LEU:HA	1:B:139:ASP:HB2	2.01	0.42
1:A:255:ASP:OD2	1:A:350:SER:OG	2.34	0.41
1:B:274:HIS:HB3	1:B:277:ARG:HD2	2.03	0.41
1:B:360:SER:OG	1:B:362:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLN:O	1:B:297:VAL:HG23	2.20	0.41
1:B:294:PHE:HZ	2:D:75:ILE:HD11	1.85	0.41
2:C:143:ALA:HB2	2:C:150:TYR:HB2	2.03	0.40
1:A:154:ARG:O	1:A:158:VAL:HG23	2.20	0.40
1:B:352:TYR:CZ	2:D:75:ILE:HD12	2.55	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	397/473 (84%)	386 (97%)	8 (2%)	3 (1%)	16	34
1	B	388/473 (82%)	378 (97%)	9 (2%)	1 (0%)	36	58
2	C	140/203 (69%)	135 (96%)	5 (4%)	0	100	100
2	D	144/203 (71%)	140 (97%)	4 (3%)	0	100	100
All	All	1069/1352 (79%)	1039 (97%)	26 (2%)	4 (0%)	30	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	GLY
1	A	366	LEU
1	A	425	GLY
1	A	278	PRO

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	342/399 (86%)	324 (95%)	18 (5%)	20	43
1	B	335/399 (84%)	319 (95%)	16 (5%)	23	47
2	C	122/178 (68%)	116 (95%)	6 (5%)	22	47
2	D	128/178 (72%)	123 (96%)	5 (4%)	28	55
All	All	927/1154 (80%)	882 (95%)	45 (5%)	22	47

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	104	LEU
1	A	120	LEU
1	A	128	THR
1	A	182	LEU
1	A	241	VAL
1	A	250	GLN
1	A	290	THR
1	A	293	GLN
1	A	303	SER
1	A	313	GLU
1	A	317	GLU
1	A	318	VAL
1	A	321	ARG
1	A	363	ILE
1	A	375	ARG
1	A	471	LEU
1	A	510	VAL
1	B	72	ARG
1	B	98	GLU
1	B	120	LEU
1	B	153	GLU
1	B	164	SER
1	B	190	LEU
1	B	241	VAL
1	B	290	THR
1	B	293	GLN
1	B	330	ARG
1	B	337	ARG
1	B	428	VAL

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Mol	Chain	Res	Type
1	B	441	MET
1	B	471	LEU
1	B	472	ARG
1	B	510	VAL
2	C	17	VAL
2	C	62	ASP
2	C	78	ASN
2	C	101	THR
2	C	120	LEU
2	C	164	VAL
2	D	17	VAL
2	D	65	ASP
2	D	117	ILE
2	D	120	LEU
2	D	168	LEU

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	73	GLN
1	A	280	HIS
1	A	293	GLN
1	A	386	GLN
1	A	496	GLN
1	A	504	HIS
1	B	246	HIS
1	B	489	GLN
1	B	504	HIS
2	C	60	GLN
2	C	124	ASN
2	D	60	GLN
2	D	113	ASN

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 [i](#)

There are no oligosaccharides 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	405/473 (85%)	0.79	46 (11%) 10 7	28, 48, 73, 79	0
1	B	396/473 (83%)	0.86	41 (10%) 11 9	30, 51, 71, 81	0
2	C	146/203 (71%)	2.03	69 (47%) 0 0	52, 80, 94, 96	0
2	D	150/203 (73%)	1.90	62 (41%) 0 0	49, 78, 97, 98	0
All	All	1097/1352 (81%)	1.13	218 (19%) 3 2	28, 55, 86, 98	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	152	GLU	6.9
2	D	139	CYS	6.5
1	A	425	GLY	5.6
2	D	136	LEU	5.1
1	B	183	ASP	5.1
2	C	21	GLY	5.0
2	D	28	THR	5.0
2	D	147	ALA	4.9
2	C	109	LEU	4.8
2	C	155	ALA	4.8
2	C	151	VAL	4.8
2	C	55	ASP	4.6
2	D	155	ALA	4.4
1	B	53	ALA	4.2
2	D	117	ILE	4.1
2	C	65	ASP	4.0
1	B	282	HIS	3.9
2	D	146	TRP	3.9
2	C	136	LEU	3.8
2	C	56	GLY	3.8
1	A	70	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	72	ARG	3.8
2	C	148	VAL	3.8
2	D	151	VAL	3.8
1	B	172	GLU	3.7
2	D	53	VAL	3.7
1	A	71	SER	3.7
2	C	161	VAL	3.6
1	B	70	THR	3.6
2	C	22	VAL	3.6
2	C	82	SER	3.6
2	C	120	LEU	3.5
2	D	65	ASP	3.5
2	D	149	PRO	3.5
2	C	149	PRO	3.5
2	D	122	VAL	3.5
2	D	142	ARG	3.5
1	A	66	THR	3.4
2	C	147	ALA	3.4
2	D	148	VAL	3.4
1	B	281	SER	3.4
2	C	23	GLY	3.4
2	D	141	LEU	3.3
1	B	383	SER	3.3
2	D	97	SER	3.3
1	A	424	ARG	3.3
1	A	81	ALA	3.3
2	C	133	LYS	3.3
2	D	133	LYS	3.3
2	C	134	VAL	3.3
1	A	279	GLY	3.3
2	C	100	ALA	3.2
1	A	423	PHE	3.2
1	B	190	LEU	3.2
1	B	481	ASP	3.1
2	C	92	ILE	3.1
2	C	64	LEU	3.1
2	C	113	ASN	3.1
2	D	177	THR	3.1
1	B	388	PHE	3.1
1	A	383	SER	3.1
1	A	74	TYR	3.0
2	C	59	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	143	ALA	3.0
2	D	22	VAL	3.0
1	A	58	TRP	3.0
2	D	157	THR	3.0
2	D	161	VAL	3.0
2	D	64	LEU	2.9
2	C	146	TRP	2.9
2	D	23	GLY	2.9
2	C	91	SER	2.9
1	A	376	ASP	2.9
2	C	150	TYR	2.9
1	B	185	LEU	2.9
2	D	96	GLU	2.9
1	B	176	SER	2.9
1	A	72	ARG	2.9
2	D	124	ASN	2.9
2	C	157	THR	2.9
1	A	470	LEU	2.9
2	C	154	SER	2.9
2	D	154	SER	2.9
2	C	61	ILE	2.9
1	B	182	LEU	2.9
2	C	125	LYS	2.9
2	D	21	GLY	2.8
2	D	34	ASP	2.8
2	D	156	LYS	2.8
2	C	142	ARG	2.8
2	D	82	SER	2.8
2	C	156	LYS	2.8
2	D	153	THR	2.8
2	C	169	MET	2.8
2	D	134	VAL	2.8
2	D	152	GLU	2.8
1	A	352	TYR	2.8
2	D	150	TYR	2.8
2	D	75	ILE	2.7
2	C	97	SER	2.7
2	C	174	SER	2.7
1	B	257	GLU	2.7
1	B	66	THR	2.7
2	C	101	THR	2.7
1	A	82	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	213	ALA	2.7
2	C	89	VAL	2.7
1	B	375	ARG	2.6
1	A	217	PRO	2.6
2	D	166	PHE	2.6
1	B	55	VAL	2.6
1	B	71	SER	2.6
2	D	91	SER	2.6
1	A	78	ASP	2.6
1	A	154	ARG	2.6
2	C	153	THR	2.6
2	D	29	LEU	2.6
1	A	426	GLY	2.6
2	C	88	CYS	2.6
1	A	388	PHE	2.6
1	A	83	LEU	2.5
2	D	109	LEU	2.5
1	A	214	ARG	2.5
2	C	167	ASP	2.5
1	B	469	GLU	2.5
2	C	124	ASN	2.5
1	B	77	LEU	2.5
2	C	171	GLU	2.5
1	A	76	PRO	2.5
2	C	90	PHE	2.5
2	C	112	LYS	2.5
2	D	170	ARG	2.5
2	D	138	GLU	2.5
1	A	282	HIS	2.4
1	B	233	PRO	2.4
2	C	63	ILE	2.4
2	C	172	ILE	2.4
2	C	24	LYS	2.4
2	D	145	GLN	2.4
1	B	187	SER	2.4
2	D	25	SER	2.4
1	A	60	GLU	2.4
1	B	149	PRO	2.4
2	C	163	LYS	2.4
2	D	100	ALA	2.4
1	A	61	GLU	2.4
1	B	58	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	126	CYS	2.4
1	A	386	GLN	2.4
2	C	99	GLN	2.4
2	D	107	GLN	2.4
2	C	10	ALA	2.4
1	A	274	HIS	2.3
2	D	24	LYS	2.3
2	D	125	LYS	2.3
1	B	445	ALA	2.3
1	A	257	GLU	2.3
2	D	137	SER	2.3
2	D	26	ALA	2.3
1	B	61	GLU	2.3
1	A	382	SER	2.3
2	C	33	TYR	2.3
1	A	273	GLY	2.3
1	A	77	LEU	2.3
1	B	57	VAL	2.3
1	A	375	ARG	2.2
1	A	483	ARG	2.2
2	D	118	PRO	2.2
1	A	59	ASP	2.2
1	B	496	GLN	2.2
1	A	175	GLY	2.2
1	B	189	LEU	2.2
1	B	450	LEU	2.2
1	B	280	HIS	2.2
2	C	170	ARG	2.2
2	C	30	GLN	2.2
2	C	145	GLN	2.2
2	D	94	ASP	2.2
2	D	89	VAL	2.2
2	C	73	ALA	2.2
2	C	96	GLU	2.2
2	D	57	GLU	2.2
1	B	273	GLY	2.2
1	B	205	ALA	2.2
1	A	177	GLU	2.2
2	C	138	GLU	2.2
1	B	74	TYR	2.2
1	A	283	LEU	2.2
1	A	183	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	451	GLU	2.1
2	D	101	THR	2.1
2	C	126	CYS	2.1
1	B	210	ASN	2.1
2	C	32	MET	2.1
1	A	216	ASP	2.1
2	C	52	VAL	2.1
2	C	75	ILE	2.1
2	D	62	ASP	2.1
1	A	433	GLY	2.1
2	C	108	ILE	2.1
1	B	114	MET	2.1
2	C	53	VAL	2.1
1	B	91	ARG	2.1
2	C	103	GLU	2.1
2	D	140	GLN	2.1
2	C	141	LEU	2.1
2	D	164	VAL	2.1
1	B	188	PHE	2.1
1	A	176	SER	2.0
1	B	56	SER	2.0
2	C	143	ALA	2.0
2	D	54	LEU	2.0
1	A	422	GLY	2.0
2	C	117	ILE	2.0
2	D	20	GLY	2.0
2	C	57	GLU	2.0
1	A	84	PRO	2.0
2	D	123	GLY	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.