



Full wwPDB X-ray Structure Validation Report

Jul 22, 2014 – 05:06 PM EDT

PDB ID : 3O10
Title : Crystal structure of the HEPN domain from human sarsin
Authors : Kozlov, G.; Gehring, K.
Deposited on : 2010-07-20
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

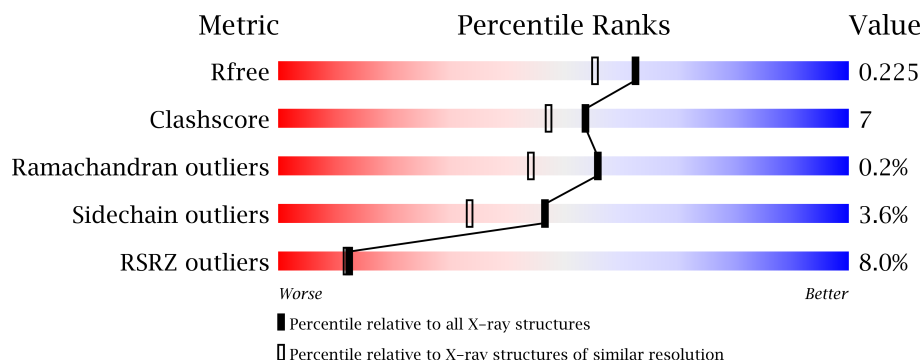
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	141	
1	B	141	
1	C	141	
1	D	141	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4829 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

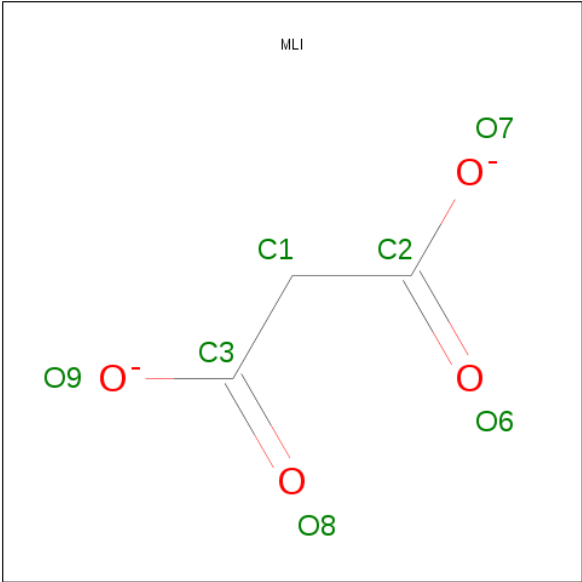
- Molecule 1 is a protein called Sacsin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	Se	0	3	0
			1125	709	201	208	4	3			
1	B	139	Total	C	N	O	S	Se	0	0	0
			1102	694	195	206	4	3			
1	C	136	Total	C	N	O	S	Se	0	0	0
			1085	684	192	202	4	3			
1	D	137	Total	C	N	O	S	Se	0	0	0
			1089	687	192	203	4	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4439	GLY	-	EXPRESSION TAG	UNP Q9NZJ4
B	4439	GLY	-	EXPRESSION TAG	UNP Q9NZJ4
C	4439	GLY	-	EXPRESSION TAG	UNP Q9NZJ4
D	4439	GLY	-	EXPRESSION TAG	UNP Q9NZJ4

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		
2	D	1	Total	C	O	0	0
			7	3	4		

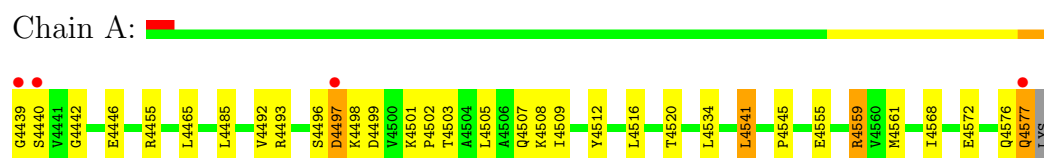
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	146	Total	O	0	0
			146	146		
3	C	51	Total	O	0	0
			51	51		
3	D	69	Total	O	0	0
			69	69		

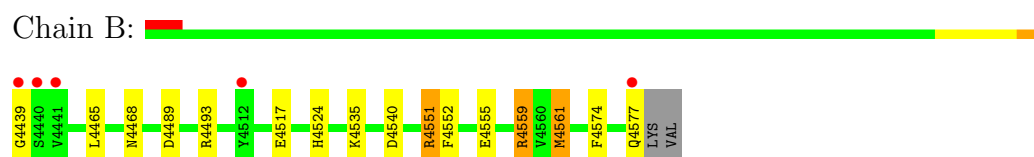
3 Residue-property plots

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.

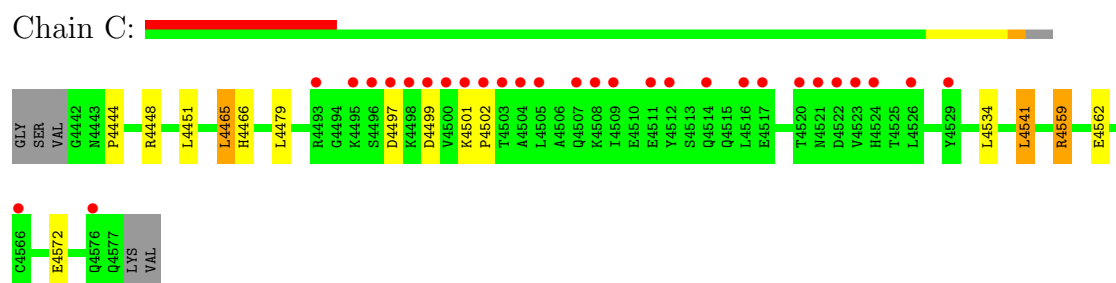
• Molecule 1: Sacsin



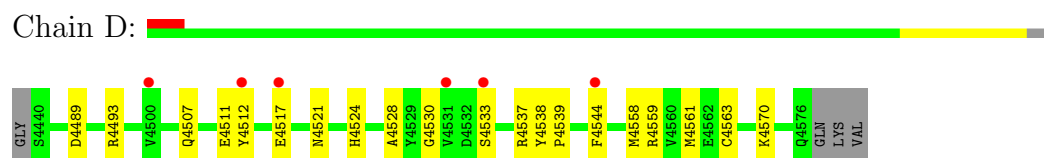
• Molecule 1: Sacsin



• Molecule 1: Sacsin



• Molecule 1: Sacsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.58Å 72.58Å 201.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.86 – 1.90 45.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.86-1.90) 98.1 (45.86-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.41 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.225 0.186 , 0.225	Depositor DCC
R_{free} test set	2441 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.6	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48258 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4829	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLI

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	0.74	0/1152	0.82	1/1553 (0.1%)
1	B	0.82	1/1120 (0.1%)	0.78	1/1511 (0.1%)
1	C	0.56	0/1103	0.65	0/1488
1	D	0.62	0/1107	0.65	0/1494
All	All	0.70	1/4482 (0.0%)	0.73	2/6046 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4561	MSE	SE-CE	-5.66	1.62	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4559	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	4559	ARG	NE-CZ-NH2	-5.79	117.40	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1125	0	1132	23	0
1	B	1102	0	1094	16	0
1	C	1085	0	1077	9	0
1	D	1089	0	1083	18	0
2	A	7	0	2	0	0
2	B	7	0	2	0	0
2	D	7	0	2	0	0
3	A	141	0	0	6	0
3	B	146	0	0	4	0
3	C	51	0	0	0	0
3	D	69	0	0	5	0
All	All	4829	0	4392	61	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:4559:ARG:NH1	1:C:4562:GLU:OE1	1.89	1.06
1:B:4555:GLU:OE1	3:B:92:HOH:O	1.81	0.98
1:A:4555:GLU:OE1	3:A:91:HOH:O	1.91	0.88
1:A:4501[B]:LYS:HD2	1:A:4502:PRO:HD2	1.59	0.85
3:A:96:HOH:O	1:D:4521:ASN:HB3	1.77	0.84
1:A:4559:ARG:NH2	3:A:49:HOH:O	2.12	0.83
1:C:4479:LEU:HD21	1:D:4537:ARG:HD2	1.64	0.80
1:B:4551:ARG:NH1	3:B:137:HOH:O	2.14	0.76
1:B:4439:GLY:HA3	1:B:4493:ARG:HB3	1.68	0.74
1:D:4517:GLU:OE2	3:D:66:HOH:O	2.06	0.73
1:A:4534:LEU:HB3	1:A:4541:LEU:HD23	1.71	0.72
1:B:4465:LEU:HD11	1:B:4561:MSE:CE	2.21	0.71
1:D:4563:CYS:HB2	3:D:26:HOH:O	1.91	0.70
1:A:4577:GLN:C	3:A:138:HOH:O	2.32	0.68
1:A:4501[B]:LYS:HD2	1:A:4502:PRO:CD	2.24	0.66
1:C:4501:LYS:HD2	1:C:4502:PRO:HD2	1.77	0.66
1:A:4501[B]:LYS:CD	1:A:4502:PRO:HD2	2.26	0.65
1:D:4563:CYS:CB	3:D:26:HOH:O	2.46	0.64
1:C:4444:PRO:O	1:C:4448:ARG:HG2	2.00	0.61
1:A:4497:ASP:N	1:A:4497:ASP:OD1	2.34	0.61
1:A:4455:ARG:NH1	1:A:4572:GLU:OE2	2.33	0.61
1:D:4493:ARG:HD3	1:D:4512:TYR:OH	2.03	0.58
1:A:4442:GLY:O	1:D:4521:ASN:ND2	2.36	0.57
1:B:4535:LYS:HD3	1:B:4551:ARG:HH21	1.71	0.56
3:A:72:HOH:O	1:D:4524:HIS:HE1	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:4468:ASN:ND2	3:B:145:HOH:O	2.39	0.55
1:B:4551:ARG:HH11	1:B:4551:ARG:CG	2.21	0.54
1:B:4465:LEU:HD21	1:B:4561:MSE:HE2	1.90	0.52
1:A:4503:THR:O	1:A:4507:GLN:HG3	2.09	0.52
1:B:4465:LEU:HD11	1:B:4561:MSE:HE1	1.91	0.52
1:A:4465:LEU:HD21	1:A:4561:MSE:SE	2.62	0.50
1:D:4570:LYS:HD2	3:D:69:HOH:O	2.13	0.48
1:D:4507:GLN:O	1:D:4511:GLU:HG3	2.14	0.47
1:B:4551:ARG:HD3	1:B:4552:PHE:CZ	2.50	0.47
1:D:4493:ARG:CD	1:D:4512:TYR:OH	2.63	0.47
1:A:4439:GLY:HA3	1:A:4493:ARG:HG2	1.95	0.46
1:B:4517:GLU:HG2	3:B:74:HOH:O	2.14	0.46
1:C:4479:LEU:HD21	1:D:4537:ARG:CD	2.40	0.46
1:A:4485:LEU:HB3	1:A:4505:LEU:HD23	1.97	0.46
1:C:4465:LEU:HD13	1:C:4466:HIS:NE2	2.30	0.46
1:C:4534:LEU:HB3	1:C:4541:LEU:HD23	1.98	0.46
1:A:4508:LYS:HE3	3:A:93:HOH:O	2.15	0.45
1:A:4568:ILE:O	1:A:4572:GLU:HG3	2.15	0.45
1:C:4501:LYS:CD	1:C:4502:PRO:HD2	2.45	0.45
1:B:4574:PHE:O	1:B:4577:GLN:HG3	2.16	0.45
1:D:4489:ASP:OD1	1:D:4493:ARG:HD3	2.17	0.45
1:A:4507:GLN:HG2	1:A:4520:THR:HG21	1.99	0.44
1:D:4493:ARG:HD3	1:D:4512:TYR:HH	1.82	0.44
1:A:4492:VAL:HG21	1:A:4512:TYR:CD2	2.52	0.44
1:B:4551:ARG:HD3	1:B:4552:PHE:CE2	2.53	0.43
1:A:4498:LYS:HE2	1:B:4540:ASP:OD2	2.20	0.42
1:D:4528:ALA:C	1:D:4530:GLY:N	2.72	0.42
1:B:4489:ASP:OD1	1:B:4493:ARG:HD3	2.19	0.42
1:A:4496:SER:C	1:A:4497:ASP:OD1	2.59	0.41
1:C:4451:LEU:HD21	1:C:4572:GLU:HG3	2.02	0.41
1:A:4576:GLN:O	1:A:4577:GLN:C	2.58	0.41
1:A:4509:ILE:HG22	1:A:4516:LEU:HD13	2.03	0.41
1:B:4524:HIS:NE2	1:D:4544:PHE:HB3	2.36	0.40
1:A:4501[B]:LYS:HZ3	1:A:4503:THR:H	1.68	0.40
1:D:4563:CYS:SG	3:D:14:HOH:O	2.62	0.40
1:D:4538:TYR:HA	1:D:4539:PRO:HD3	1.98	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	140/141 (99%)	139 (99%)	1 (1%)	0	100	100
1	B	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
1	C	134/141 (95%)	132 (98%)	2 (2%)	0	100	100
1	D	135/141 (96%)	132 (98%)	2 (2%)	1 (1%)	30	15
All	All	546/564 (97%)	537 (98%)	8 (2%)	1 (0%)	56	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4533	SER

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	122/118 (103%)	115 (94%)	7 (6%)	29	15
1	B	118/118 (100%)	116 (98%)	2 (2%)	73	68
1	C	116/118 (98%)	111 (96%)	5 (4%)	40	26
1	D	117/118 (99%)	114 (97%)	3 (3%)	59	49
All	All	473/472 (100%)	456 (96%)	17 (4%)	47	33

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4440	SER

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Mol	Chain	Res	Type
1	A	4446	GLU
1	A	4497	ASP
1	A	4499	ASP
1	A	4541	LEU
1	A	4545	PRO
1	A	4577	GLN
1	B	4551	ARG
1	B	4559	ARG
1	C	4465	LEU
1	C	4497	ASP
1	C	4499	ASP
1	C	4541	LEU
1	C	4559	ARG
1	D	4558	MSE
1	D	4559	ARG
1	D	4561	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4470	ASN
1	A	4524	HIS
1	B	4546	GLN
1	C	4470	ASN
1	C	4573	ASN
1	D	4524	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLI	A	1	-	2,6,6	6.25	2 (100%)	0,7,7	0.00	-
2	MLI	B	1	-	2,6,6	4.64	2 (100%)	0,7,7	0.00	-
2	MLI	D	1	-	2,6,6	3.36	2 (100%)	0,7,7	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	A	1	-	-	0/0/4/4	0/0/0/0
2	MLI	B	1	-	-	0/0/4/4	0/0/0/0
2	MLI	D	1	-	-	0/0/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MLI	C1-C2	6.42	1.53	1.49
2	A	1	MLI	C1-C3	6.07	1.53	1.49
2	B	1	MLI	C1-C3	5.30	1.52	1.49
2	D	1	MLI	C1-C2	4.15	1.52	1.49
2	B	1	MLI	C1-C2	3.86	1.52	1.49
2	D	1	MLI	C1-C3	2.32	1.51	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	139/141 (98%)	0.01	4 (2%) 49 50	9, 17, 37, 46	0
1	B	139/141 (98%)	-0.02	5 (3%) 41 42	9, 18, 34, 46	0
1	C	136/141 (96%)	0.97	29 (21%) 1 1	16, 37, 77, 105	0
1	D	137/141 (97%)	0.25	6 (4%) 33 33	14, 31, 52, 67	0
All	All	551/564 (97%)	0.30	44 (7%) 12 12	9, 25, 56, 105	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4512	TYR	6.5
1	C	4514	GLN	6.4
1	C	4497	ASP	6.0
1	C	4509	ILE	5.8
1	C	4508	LYS	5.6
1	C	4505	LEU	4.9
1	B	4440	SER	4.5
1	C	4523	VAL	3.7
1	B	4439	GLY	3.7
1	C	4517	GLU	3.6
1	C	4500	VAL	3.3
1	C	4511	GLU	3.3
1	C	4522	ASP	3.3
1	C	4499	ASP	3.2
1	B	4441	VAL	3.2
1	C	4503	THR	3.1
1	A	4497	ASP	3.1
1	C	4495	LYS	3.1
1	D	4512	TYR	3.1
1	C	4516	LEU	3.1
1	C	4524	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	4531	VAL	3.0
1	C	4504	ALA	3.0
1	C	4526	LEU	2.9
1	C	4507	GLN	2.9
1	C	4501	LYS	2.7
1	A	4440	SER	2.7
1	C	4566	CYS	2.7
1	C	4502	PRO	2.5
1	B	4577	GLN	2.5
1	A	4439	GLY	2.4
1	C	4520	THR	2.4
1	C	4496	SER	2.3
1	D	4544	PHE	2.3
1	C	4529	TYR	2.2
1	D	4517	GLU	2.2
1	D	4533	SER	2.2
1	C	4493	ARG	2.2
1	C	4576	GLN	2.2
1	A	4577	GLN	2.1
1	B	4512	TYR	2.1
1	C	4498	LYS	2.0
1	D	4500	VAL	2.0
1	C	4521	ASN	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MLI	D	1	7/7	0.14	1.05	34,35,36,37	0
2	MLI	A	1	7/7	0.14	0.52	23,24,25,26	0
2	MLI	B	1	7/7	0.08	-1.11	22,23,24,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.