



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2020 – 02:05 PM EST

PDB ID : 6X07
Title : Nic96 from *S. cerevisiae* bound by VHH-SAN12
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Deposited on : 2020-05-15
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

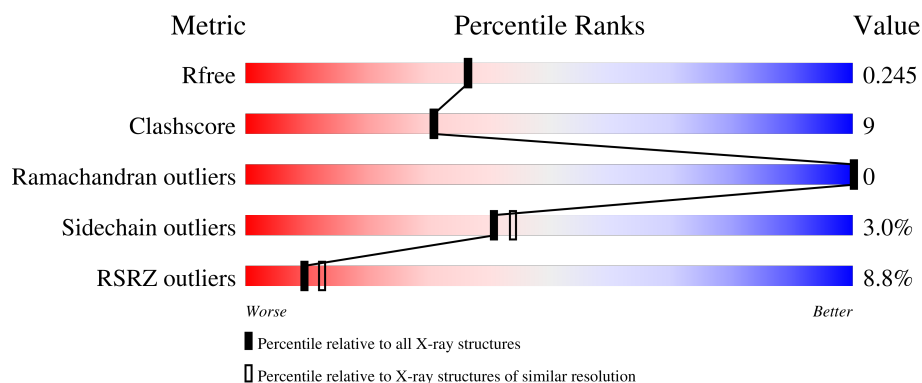
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	669	
2	B	133	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5802 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 Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	4	0
			4844	3099	810	919	16			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP P34077
A	172	PRO	-	expression tag	UNP P34077
A	173	GLY	-	expression tag	UNP P34077
A	174	SER	-	expression tag	UNP P34077
A	175	GLU	-	expression tag	UNP P34077
A	176	PHE	-	expression tag	UNP P34077
A	177	GLU	-	expression tag	UNP P34077
A	178	LEU	-	expression tag	UNP P34077
A	179	GLY	-	expression tag	UNP P34077
A	180	ALA	-	expression tag	UNP P34077
A	181	PRO	-	expression tag	UNP P34077
A	182	ALA	-	expression tag	UNP P34077
A	183	GLY	-	expression tag	UNP P34077
A	184	ARG	-	expression tag	UNP P34077
A	185	GLN	-	expression tag	UNP P34077

- Molecule 2 is a protein called VHH-SAN12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			830	510	147	169	4			

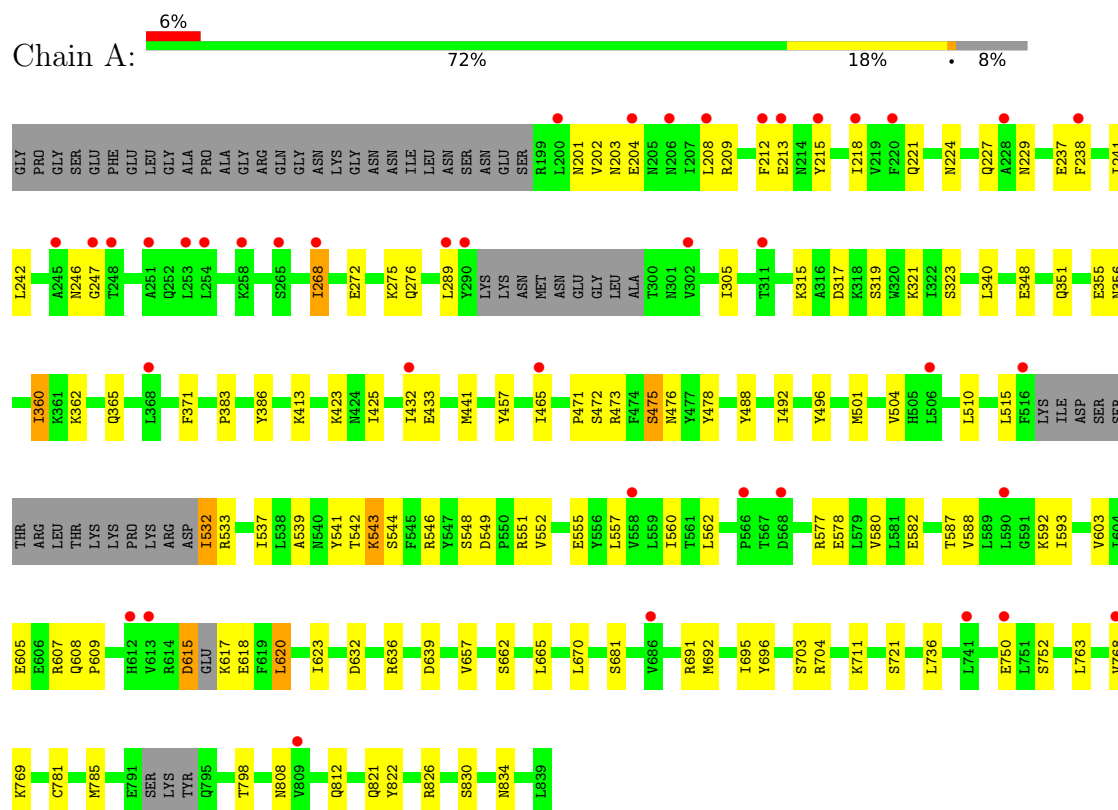
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	10	Total 10	O 10	0	0

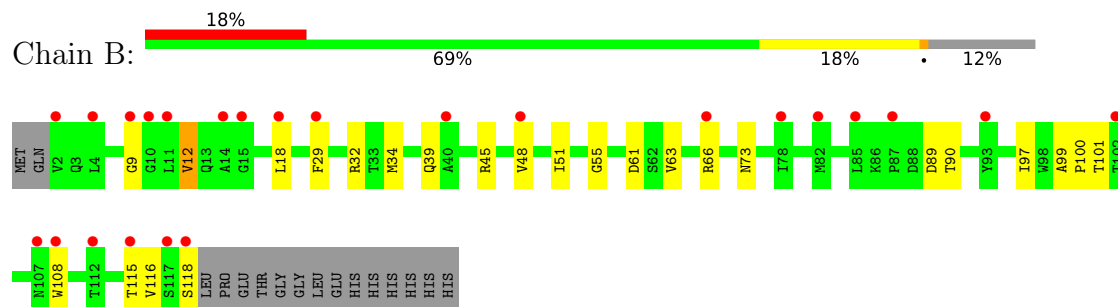
3 Residue-property plots [i](#)

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: Nucleoporin NIC96



• Molecule 2: VHH-SAN12



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.13Å 79.65Å 283.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.91 – 2.10 60.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (60.91-2.10) 99.4 (60.91-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.227 , 0.245 0.227 , 0.245	Depositor DCC
R_{free} test set	1997 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5802	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.54	0/4928	0.59	1/6692 (0.0%)
2	B	0.64	0/845	0.67	0/1153
All	All	0.56	0/5773	0.60	1/7845 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ILE	N-CA-C	5.64	126.22	111.00

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	4844	0	4729	85	0
2	B	830	0	738	17	0
3	A	118	0	0	4	0
3	B	10	0	0	1	0
All	All	5802	0	5467	101	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 9.

All (101) 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:B:9:GLY:HA2	2:B:18:LEU:CD2	1.69	1.20
2:B:9:GLY:CA	2:B:18:LEU:HD21	1.70	1.19
1:A:432:ILE:HD12	1:A:433:GLU:H	1.28	0.99
1:A:532:ILE:HG22	1:A:537:ILE:CD1	1.94	0.96
1:A:532:ILE:HG22	1:A:537:ILE:HD11	1.46	0.96
1:A:432:ILE:HD12	1:A:433:GLU:N	1.83	0.93
1:A:615:ASP:HB2	1:A:617:LYS:N	1.89	0.87
1:A:615:ASP:CB	1:A:617:LYS:N	2.46	0.79
1:A:539:ALA:O	1:A:542:THR:HG22	1.86	0.76
1:A:549:ASP:HB3	1:A:552:VAL:HG12	1.74	0.69
1:A:475:SER:OG	1:A:476:ASN:N	2.27	0.68
1:A:615:ASP:HB3	1:A:618:GLU:H	1.58	0.67
1:A:532:ILE:HG22	1:A:537:ILE:HD13	1.77	0.66
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.28	0.65
1:A:543:LYS:HD2	1:A:546:ARG:HD2	1.77	0.65
1:A:272:GLU:O	1:A:276:GLN:HG3	1.98	0.64
1:A:605:GLU:HA	1:A:608:GLN:HG3	1.82	0.62
2:B:32:ARG:HA	3:B:202:HOH:O	2.02	0.60
1:A:362:LYS:HA	1:A:365:GLN:HB2	1.84	0.59
1:A:580:VAL:HB	1:A:623:ILE:HD11	1.83	0.59
1:A:215:TYR:HA	1:A:218:ILE:HD12	1.86	0.58
1:A:551:ARG:HG3	1:A:603:VAL:HG11	1.85	0.58
1:A:423:LYS:HE2	1:A:457:TYR:CD1	2.38	0.58
1:A:492:ILE:HD11	1:A:510:LEU:HD12	1.86	0.58
1:A:413:LYS:HD2	1:A:425:ILE:HD11	1.86	0.58
1:A:665:LEU:HD21	1:A:721[A]:SER:OG	2.04	0.57
1:A:808[A]:ASN:O	1:A:812[A]:GLN:HG2	2.04	0.57
2:B:90:THR:HG23	2:B:115:THR:HA	1.89	0.55
1:A:315:LYS:HG3	1:A:321:LYS:HG2	1.89	0.55
1:A:555:GLU:OE2	1:A:607:ARG:NH2	2.39	0.55
1:A:549:ASP:HB3	1:A:552:VAL:CG1	2.37	0.55
1:A:201:ASN:ND2	1:A:204:GLU:HB3	2.22	0.54
1:A:213:GLU:HG3	3:A:918:HOH:O	2.08	0.54
1:A:703:SER:OG	1:A:711:LYS:NZ	2.22	0.54
2:B:9:GLY:HA2	2:B:18:LEU:HD21	0.76	0.54
1:A:615:ASP:HB3	1:A:617:LYS:N	2.22	0.54
1:A:504:VAL:HG21	1:A:541:TYR:HB2	1.90	0.53
1:A:557:LEU:O	1:A:560:ILE:HG13	2.09	0.53
1:A:704:ARG:HH12	2:B:101:THR:CG2	2.21	0.53
1:A:488:TYR:CZ	1:A:515:LEU:HD13	2.43	0.53
2:B:39:GLN:HB2	2:B:45:ARG:HG3	1.90	0.53
2:B:12:VAL:O	2:B:116:VAL:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:HA	3:A:911:HOH:O	2.09	0.52
1:A:202:VAL:HG11	1:A:212:PHE:CG	2.45	0.52
1:A:548:SER:HB3	3:A:925:HOH:O	2.10	0.51
1:A:227:GLN:HE21	1:A:609:PRO:HG2	1.74	0.51
1:A:218:ILE:HD11	1:A:241:ILE:HD13	1.92	0.51
1:A:539:ALA:O	1:A:543:LYS:HD3	2.11	0.50
2:B:34:MET:SD	2:B:97:ILE:HD13	2.51	0.50
1:A:781:CYS:O	1:A:785:MET:HE2	2.10	0.50
2:B:29:PHE:HE2	2:B:73:ASN:OD1	1.95	0.50
1:A:432:ILE:CD1	1:A:433:GLU:N	2.65	0.49
1:A:317:ASP:HB2	1:A:319:SER:HB3	1.93	0.49
1:A:351:GLN:O	1:A:355:GLU:HG3	2.11	0.49
2:B:45:ARG:HD3	2:B:108:TRP:CZ3	2.46	0.49
1:A:830:SER:O	1:A:834:ASN:ND2	2.45	0.49
1:A:657:VAL:HG21	1:A:692:MET:HG3	1.94	0.48
1:A:203:ASN:OD1	1:A:209:ARG:NH1	2.39	0.48
1:A:317:ASP:HB2	1:A:319:SER:H	1.79	0.47
1:A:268:ILE:O	1:A:268:ILE:HG22	2.15	0.47
2:B:32:ARG:HD3	2:B:97:ILE:HD12	1.97	0.47
1:A:533:ARG:O	1:A:537:ILE:HG12	2.14	0.47
1:A:496:TYR:OH	1:A:537:ILE:HD12	2.15	0.47
1:A:471:PRO:HB3	1:A:478:TYR:CD2	2.50	0.46
1:A:501:MET:HG2	1:A:541:TYR:HE1	1.81	0.45
1:A:763:LEU:HB2	1:A:768:VAL:HG13	1.99	0.45
1:A:588:VAL:HG12	3:A:904:HOH:O	2.17	0.45
1:A:305:ILE:HD13	1:A:340:LEU:HD23	2.00	0.44
1:A:620:LEU:HA	1:A:620:LEU:HD23	1.52	0.44
1:A:356:ASN:O	1:A:360:ILE:HG23	2.18	0.44
1:A:562:LEU:HA	1:A:562:LEU:HD23	1.57	0.44
1:A:592:LYS:HG2	1:A:593:ILE:H	1.82	0.44
1:A:578:GLU:O	1:A:582:GLU:HB2	2.17	0.44
1:A:681:SER:HB2	1:A:691:ARG:HD3	1.99	0.44
2:B:99:ALA:HB1	2:B:100:PRO:HD2	1.99	0.44
1:A:246:ASN:HB3	1:A:247:GLY:H	1.63	0.43
1:A:473:ARG:NH1	1:A:473:ARG:HB3	2.34	0.43
1:A:577:ARG:HA	1:A:623:ILE:CD1	2.49	0.43
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.84	0.42
1:A:238:PHE:O	1:A:242:LEU:HB2	2.19	0.42
1:A:577:ARG:HA	1:A:623:ILE:HD12	2.02	0.42
1:A:615:ASP:N	1:A:615:ASP:OD1	2.48	0.42
1:A:636:ARG:HB3	1:A:639:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ILE:HG13	1:A:696:TYR:CD1	2.55	0.42
1:A:821:GLN:HG3	1:A:822:TYR:CD1	2.54	0.42
1:A:204:GLU:HG2	1:A:208:LEU:HD23	2.02	0.42
1:A:587:THR:HG22	1:A:592:LYS:HG3	2.02	0.42
1:A:360:ILE:O	1:A:360:ILE:HG13	2.20	0.41
1:A:662:SER:OG	1:A:769:LYS:HD2	2.20	0.41
1:A:750:GLU:HA	1:A:812[A]:GLN:OE1	2.20	0.41
1:A:237:GLU:O	1:A:241:ILE:HD12	2.20	0.41
1:A:383:PRO:HG2	1:A:386:TYR:CD2	2.55	0.41
1:A:736:LEU:HD22	1:A:785:MET:CE	2.51	0.41
2:B:108:TRP:N	2:B:108:TRP:CD1	2.89	0.41
1:A:543:LYS:HD2	1:A:543:LYS:HA	1.67	0.41
1:A:275:LYS:HE3	1:A:441:MET:SD	2.61	0.41
2:B:51:ILE:HD11	2:B:55:GLY:HA2	2.03	0.40
1:A:221:GLN:CD	1:A:224:ASN:HD22	2.24	0.40
1:A:348:GLU:O	1:A:351:GLN:HB3	2.22	0.40
1:A:465:ILE:HA	1:A:465:ILE:HD12	1.93	0.40
2:B:48:VAL:HG13	2:B:63:VAL:HG21	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	607/669 (91%)	593 (98%)	14 (2%)	0	100	100
2	B	115/133 (86%)	112 (97%)	3 (3%)	0	100	100
All	All	722/802 (90%)	705 (98%)	17 (2%)	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	517/601 (86%)	502 (97%)	15 (3%)	42	46
2	B	78/108 (72%)	75 (96%)	3 (4%)	33	34
All	All	595/709 (84%)	577 (97%)	18 (3%)	41	44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	360	ILE
1	A	371	PHE
1	A	472	SER
1	A	475	SER
1	A	532	ILE
1	A	543	LYS
1	A	544	SER
1	A	615	ASP
1	A	620	LEU
1	A	632	ASP
1	A	670	LEU
1	A	752	SER
1	A	798	THR
1	A	826	ARG
2	B	12	VAL
2	B	61	ASP
2	B	118	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	380	HIS
1	A	536	ASN
1	A	608	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 monosaccharides 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	613/669 (91%)	0.81	40 (6%) 18 23	31, 71, 114, 142	0
2	B	117/133 (87%)	1.14	24 (20%) 1 1	48, 87, 113, 144	0
All	All	730/802 (91%)	0.87	64 (8%) 10 12	31, 73, 114, 144	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	GLY	5.0
1	A	613	VAL	4.6
2	B	4	LEU	4.5
1	A	289	LEU	3.9
1	A	311	THR	3.7
1	A	612	HIS	3.6
2	B	10	GLY	3.4
1	A	204	GLU	3.2
2	B	85	LEU	3.2
1	A	218	ILE	3.1
2	B	107	ASN	3.1
1	A	302	VAL	3.0
2	B	112	THR	2.9
1	A	212	PHE	2.9
1	A	228	ALA	2.9
1	A	432	ILE	2.8
1	A	247	GLY	2.8
1	A	568	ASP	2.8
2	B	9	GLY	2.7
1	A	265	SER	2.7
1	A	254	LEU	2.7
2	B	82	MET	2.7
2	B	117	SER	2.6
1	A	750	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	118	SER	2.6
1	A	253	LEU	2.6
2	B	87	PRO	2.6
2	B	102	THR	2.5
2	B	78	ILE	2.5
2	B	11	LEU	2.5
1	A	245	ALA	2.5
2	B	14	ALA	2.5
1	A	215	TYR	2.5
1	A	238	PHE	2.4
1	A	208	LEU	2.4
1	A	258	LYS	2.3
1	A	200	LEU	2.3
2	B	66	ARG	2.3
1	A	206	ASN	2.3
1	A	506	LEU	2.3
1	A	268	ILE	2.3
1	A	566	PRO	2.3
1	A	741	LEU	2.3
1	A	220	PHE	2.3
1	A	590	LEU	2.2
1	A	368	LEU	2.2
2	B	29	PHE	2.2
1	A	465	ILE	2.2
1	A	558	VAL	2.2
1	A	213	GLU	2.2
1	A	248	THR	2.2
2	B	93	TYR	2.2
1	A	290	TYR	2.2
1	A	251	ALA	2.2
2	B	108	TRP	2.1
2	B	2	VAL	2.1
2	B	48	VAL	2.1
2	B	18	LEU	2.1
1	A	768	VAL	2.1
1	A	809	VAL	2.1
1	A	686	VAL	2.0
2	B	115	THR	2.0
1	A	516	PHE	2.0
2	B	40	ALA	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 monosaccharides 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.