



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:35 PM EDT

PDB ID : 6X03 / pdb_00006x03
Title : Nup84-Nup133 (aa521-1157) from *S. cerevisiae* bound by VHH-SAN8 and VHH-SAN9
Authors : Nordeen, S.A.; Schwartz, T.U.
Deposited on : 2020-05-15
Resolution : 7.30 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

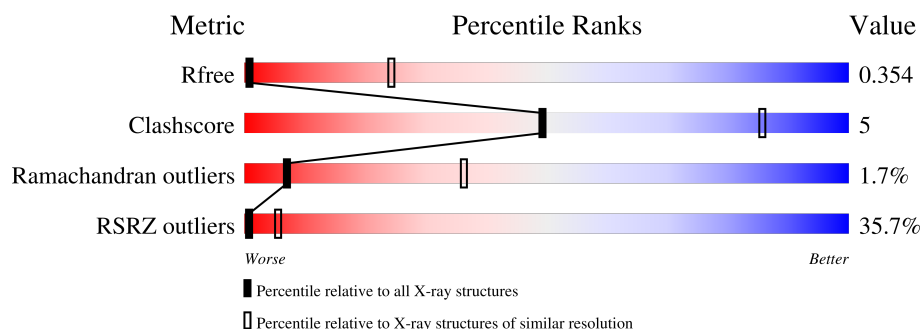
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.30 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	726	33% 84% 6% 10%
2	B	643	32% 84% 9% 6%
3	C	131	24% 62% 7% 31%
4	D	128	27% 64% • 32%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7091 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 NUP84.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	0	0	0
			3234	1934	650	650			

- Molecule 2 is a protein called Nucleoporin NUP133.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	602	Total	C	N	O	0	0	0
			2993	1789	602	602			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	515	MET	-	expression tag	UNP P36161
B	516	ALA	-	expression tag	UNP P36161
B	517	ASP	-	expression tag	UNP P36161
B	518	PRO	-	expression tag	UNP P36161
B	519	GLY	-	expression tag	UNP P36161
B	520	PHE	-	expression tag	UNP P36161

- Molecule 3 is a protein called VHH-SAN8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	90	Total	C	N	O	0	0	0
			440	260	90	90			

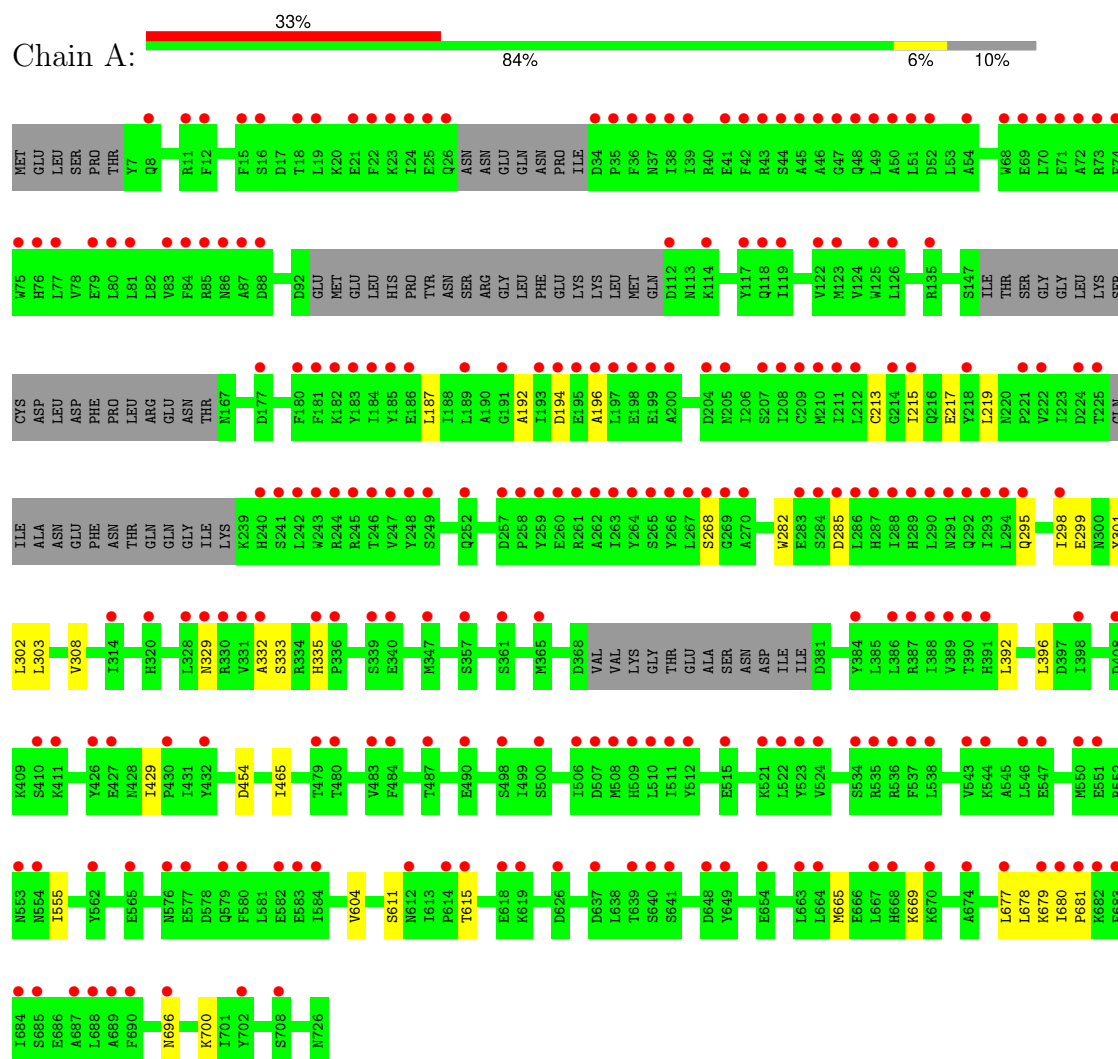
- Molecule 4 is a protein called VHH-SAN9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	87	Total	C	N	O	0	0	0
			424	250	87	87			

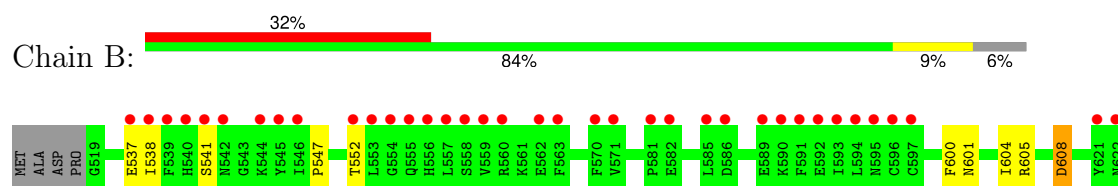
3 Residue-property plots [i](#)

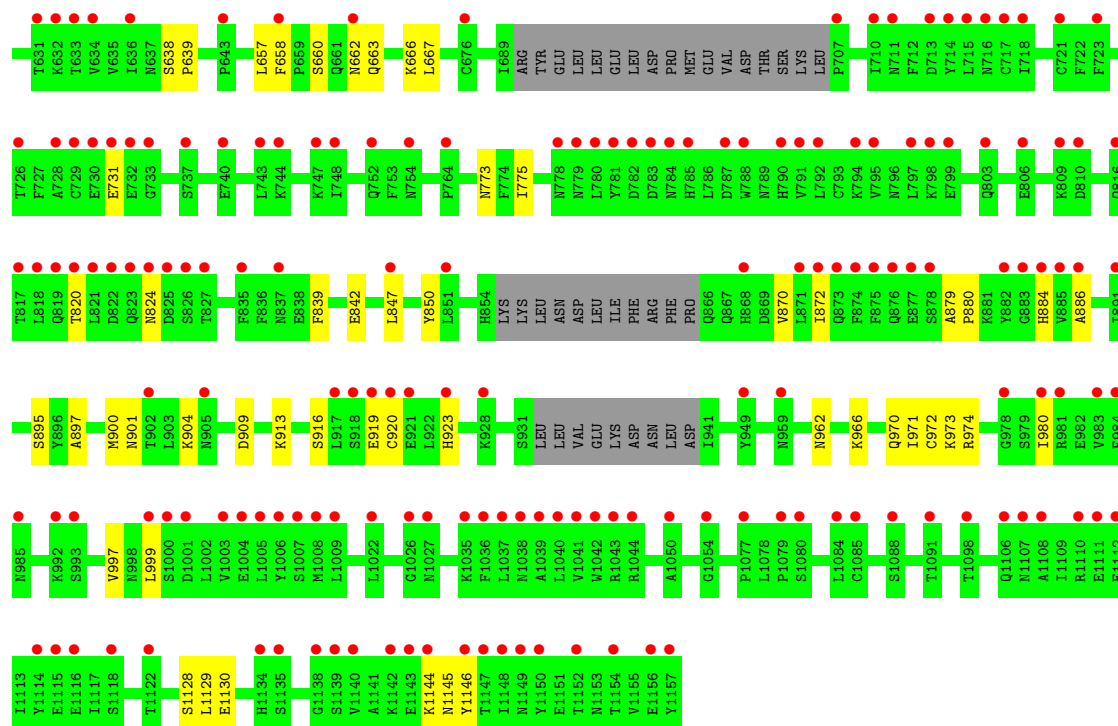
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 NUP84

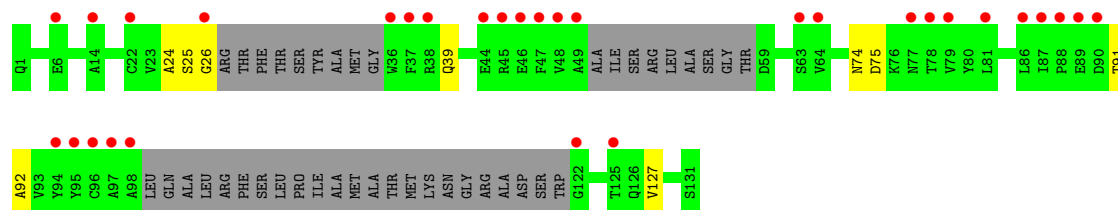


• Molecule 2: Nucleoporin NUP133

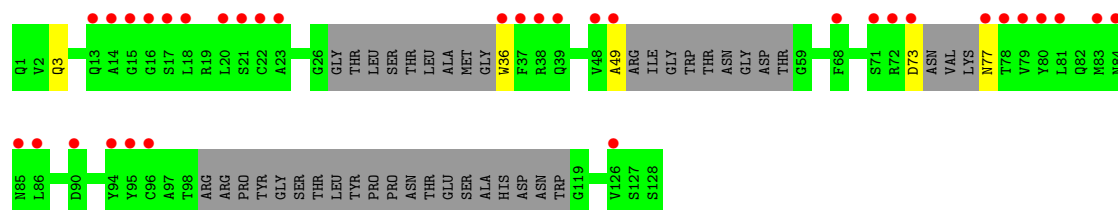




● Molecule 3: VHH-SAN8



● Molecule 4: VHH-SAN9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.25Å 295.20Å 295.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.80 – 7.30 147.80 – 7.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (147.80-7.30) 99.7 (147.80-7.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 7.44Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.335 , 0.353 0.335 , 0.354	Depositor DCC
R_{free} test set	1306 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	763.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 720.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7091	wwPDB-VP
Average B, all atoms (Å ²)	668.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	0.16	0/3228	0.43	2/4500 (0.0%)
2	B	0.25	0/2989	1.00	12/4168 (0.3%)
3	C	0.14	0/436	0.34	0/598
4	D	0.36	0/419	0.52	0/572
All	All	0.22	0/7072	0.73	14/9838 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	658	PHE	CA-C-N	34.30	154.20	119.56
2	B	658	PHE	C-N-CA	34.30	154.20	119.56
2	B	971	ILE	CB-CA-C	-8.73	103.54	111.74
2	B	971	ILE	N-CA-C	8.43	117.99	107.70
2	B	970	GLN	N-CA-C	8.35	120.16	111.14
2	B	973	LYS	N-CA-C	7.85	119.84	111.28
2	B	972	CYS	N-CA-C	-6.62	97.75	108.41
2	B	974	ARG	N-CA-C	5.94	117.75	111.28
2	B	839	PHE	CA-C-N	5.86	125.72	119.28
2	B	839	PHE	C-N-CA	5.86	125.72	119.28
1	A	301	TYR	N-CA-C	-5.45	104.99	111.69
1	A	194	ASP	N-CA-C	-5.45	105.44	111.71
2	B	547	PRO	CA-C-N	5.20	124.82	119.05
2	B	547	PRO	C-N-CA	5.20	124.82	119.05

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	3234	0	1392	18	0
2	B	2993	0	1244	32	0
3	C	440	0	211	4	0
4	D	424	0	202	4	0
All	All	7091	0	3049	55	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 5.

All (55) 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:662:ASN:O	2:B:666:LYS:CB	1.83	1.25
1:A:298:ILE:O	1:A:302:LEU:CB	1.99	1.10
2:B:662:ASN:O	2:B:666:LYS:N	1.97	0.96
1:A:329:ASN:CB	4:D:77:ASN:N	2.35	0.89
2:B:537:GLU:O	2:B:541:SER:O	1.94	0.86
2:B:663:GLN:O	2:B:667:LEU:N	2.08	0.85
1:A:282:TRP:CB	1:A:335:HIS:CB	2.57	0.82
1:A:332:ALA:O	4:D:73:ASP:C	2.23	0.81
1:A:696:ASN:HA	1:A:700:LYS:HA	1.61	0.80
2:B:662:ASN:O	2:B:666:LYS:CA	2.30	0.78
2:B:601:ASN:O	2:B:605:ARG:N	2.18	0.75
1:A:333:SER:CB	4:D:73:ASP:CB	2.64	0.75
1:A:268:SER:O	1:A:295:GLN:CB	2.34	0.75
1:A:192:ALA:O	1:A:196:ALA:N	2.20	0.73
1:A:299:GLU:O	1:A:303:LEU:CB	2.42	0.67
2:B:962:ASN:O	2:B:966:LYS:CB	2.45	0.65
2:B:847:LEU:O	2:B:850:TYR:N	2.31	0.64
2:B:657:LEU:O	2:B:660:SER:O	2.18	0.61
2:B:662:ASN:CB	2:B:731:GLU:CB	2.79	0.61
2:B:919:GLU:O	2:B:923:HIS:N	2.32	0.61
1:A:298:ILE:O	1:A:302:LEU:N	2.36	0.59
1:A:213:CYS:O	1:A:217:GLU:N	2.34	0.59
2:B:604:ILE:O	2:B:608:ASP:N	2.27	0.58
2:B:847:LEU:O	2:B:850:TYR:CB	2.52	0.57
2:B:900:MET:O	2:B:904:LYS:N	2.30	0.56
3:C:24:ALA:O	3:C:26:GLY:N	2.39	0.56
1:A:392:LEU:O	1:A:396:LEU:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:LEU:C	2:B:660:SER:H	2.13	0.55
2:B:897:ALA:O	2:B:901:ASN:N	2.39	0.55
2:B:886:ALA:HB1	2:B:901:ASN:CB	2.37	0.55
3:C:74:ASN:O	3:C:75:ASP:CB	2.55	0.54
2:B:916:SER:O	2:B:920:CYS:N	2.28	0.53
1:A:215:ILE:O	1:A:219:LEU:N	2.44	0.51
2:B:820:THR:O	2:B:824:ASN:N	2.44	0.51
2:B:1144:LYS:O	2:B:1146:TYR:N	2.43	0.51
2:B:600:PHE:O	2:B:604:ILE:N	2.37	0.49
2:B:663:GLN:O	2:B:667:LEU:CB	2.61	0.49
2:B:884:HIS:C	2:B:886:ALA:H	2.21	0.48
1:A:665:MET:O	1:A:669:LYS:N	2.46	0.48
2:B:538:ILE:HA	2:B:541:SER:O	2.14	0.48
2:B:847:LEU:C	2:B:850:TYR:H	2.21	0.47
2:B:909:ASP:HA	2:B:913:LYS:CB	2.46	0.46
1:A:677:LEU:O	1:A:679:LYS:N	2.45	0.45
3:C:91:THR:HA	3:C:127:VAL:O	2.16	0.45
1:A:611:SER:O	1:A:615:THR:N	2.44	0.44
2:B:1128:SER:O	2:B:1129:LEU:C	2.61	0.44
2:B:997:VAL:C	2:B:999:LEU:H	2.25	0.43
2:B:657:LEU:O	2:B:660:SER:N	2.43	0.43
2:B:870:VAL:C	2:B:872:ILE:H	2.26	0.43
4:D:36:TRP:N	4:D:49:ALA:O	2.51	0.43
1:A:187:LEU:O	1:A:192:ALA:HB3	2.19	0.42
2:B:1129:LEU:O	2:B:1130:GLU:C	2.60	0.42
2:B:884:HIS:C	2:B:886:ALA:N	2.77	0.41
3:C:39:GLN:O	3:C:92:ALA:HB1	2.21	0.41
1:A:298:ILE:O	1:A:302:LEU:CA	2.65	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	638/726 (88%)	576 (90%)	52 (8%)	10 (2%)	7	38
2	B	594/643 (92%)	520 (88%)	62 (10%)	12 (2%)	6	31
3	C	82/131 (63%)	76 (93%)	5 (6%)	1 (1%)	10	44
4	D	77/128 (60%)	74 (96%)	2 (3%)	1 (1%)	9	42
All	All	1391/1628 (85%)	1246 (90%)	121 (9%)	24 (2%)	7	36

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	638	SER
2	B	639	PRO
2	B	773	ASN
2	B	879	ALA
2	B	880	PRO
1	A	285	ASP
1	A	308	VAL
1	A	604	VAL
2	B	552	THR
2	B	980	ILE
2	B	1145	ASN
3	C	25	SER
4	D	3	GLN
2	B	775	ILE
2	B	895	SER
1	A	429	ILE
1	A	678	LEU
2	B	608	ASP
2	B	842	GLU
1	A	465	ILE
1	A	555	ILE
1	A	454	ASP
1	A	681	PRO
1	A	680	ILE

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

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 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	650/726 (89%)	1.91	239 (36%) 1 5	178, 684, 1012, 1336	0
2	B	602/643 (93%)	1.75	206 (34%) 1 6	260, 516, 789, 970	0
3	C	90/131 (68%)	1.60	31 (34%) 1 6	562, 1027, 1295, 1338	0
4	D	87/128 (67%)	2.54	34 (39%) 1 5	838, 1014, 1188, 1276	0
All	All	1429/1628 (87%)	1.86	510 (35%) 1 5	178, 631, 1112, 1338	0

All (510) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	79	VAL	19.6
1	A	84	PHE	14.6
4	D	72	ARG	14.3
2	B	791	VAL	14.1
2	B	1139	SER	12.0
2	B	1111	GLU	11.9
2	B	817	THR	11.9
2	B	1147	THR	11.7
1	A	47	GLY	11.2
1	A	287	HIS	10.9
2	B	1007	SER	10.7
3	C	96	CYS	10.0
4	D	22	CYS	10.0
4	D	78	THR	10.0
1	A	267	LEU	10.0
1	A	83	VAL	9.7
2	B	1038	ASN	9.7
2	B	826	SER	9.5
2	B	554	GLY	9.5
4	D	77	ASN	9.4
1	A	69	GLU	9.2

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Mol	Chain	Res	Type	RSRZ
2	B	730	GLU	9.0
1	A	211	ILE	8.9
2	B	1040	LEU	8.8
1	A	243	TRP	8.8
1	A	34	ASP	8.6
2	B	790	HIS	8.6
2	B	555	GLN	8.5
2	B	582	GLU	8.3
1	A	22	PHE	8.2
2	B	788	TRP	8.2
1	A	35	PRO	8.1
1	A	387	ARG	7.9
1	A	189	LEU	7.8
1	A	37	ASN	7.7
1	A	332	ALA	7.6
4	D	16	GLY	7.6
1	A	509	HIS	7.6
4	D	86	LEU	7.3
1	A	268	SER	7.3
2	B	1148	ILE	7.3
1	A	208	ILE	7.3
1	A	291	ASN	7.2
1	A	483	VAL	7.1
4	D	73	ASP	7.1
2	B	874	PHE	7.1
2	B	824	ASN	7.1
2	B	729	CYS	7.1
2	B	795	VAL	7.0
3	C	46	GLU	7.0
1	A	266	TYR	7.0
2	B	798	LYS	7.0
2	B	784	ASN	7.0
2	B	1039	ALA	6.9
1	A	391	HIS	6.9
2	B	717	CYS	6.8
3	C	95	TYR	6.8
1	A	576	ASN	6.7
1	A	289	HIS	6.7
1	A	244	ARG	6.6
1	A	87	ALA	6.6
2	B	713	ASP	6.6
2	B	558	SER	6.5

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Mol	Chain	Res	Type	RSRZ
2	B	721	CYS	6.5
2	B	1138	GLY	6.5
1	A	290	LEU	6.4
2	B	1115	GLU	6.4
2	B	919	GLU	6.3
1	A	46	ALA	6.3
2	B	737	SER	6.3
2	B	827	THR	6.2
2	B	794	LYS	6.2
1	A	183	TYR	6.2
2	B	1112	GLU	6.2
2	B	710	ILE	6.1
1	A	479	THR	6.1
1	A	262	ALA	6.1
1	A	221	PRO	6.1
1	A	72	ALA	6.0
4	D	83	MET	6.0
1	A	196	ALA	6.0
2	B	595	ASN	6.0
1	A	225	THR	5.9
1	A	15	PHE	5.9
1	A	199	GLU	5.9
2	B	552	THR	5.9
2	B	553	LEU	5.8
3	C	47	PHE	5.8
2	B	981	ARG	5.7
1	A	480	THR	5.7
2	B	1122	THR	5.7
1	A	45	ALA	5.7
2	B	711	ASN	5.6
4	D	84	ASN	5.6
2	B	636	ILE	5.6
2	B	1004	GLU	5.6
2	B	1135	SER	5.6
4	D	15	GLY	5.6
2	B	714	TYR	5.5
1	A	260	GLU	5.5
2	B	821	LEU	5.5
1	A	521	LYS	5.5
1	A	546	LEU	5.5
1	A	44	SER	5.4
1	A	50	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	680	ILE	5.4
1	A	547	GLU	5.4
1	A	537	PHE	5.4
1	A	612	ASN	5.3
2	B	818	LEU	5.3
2	B	1041	VAL	5.2
1	A	580	PHE	5.2
1	A	535	ARG	5.1
2	B	799	GLU	5.1
2	B	732	GLU	5.1
2	B	825	ASP	5.1
2	B	984	PHE	5.1
1	A	49	LEU	5.1
1	A	215	ILE	5.1
1	A	249	SER	5.0
1	A	23	LYS	5.0
1	A	288	ILE	5.0
1	A	641	SER	4.9
1	A	508	MET	4.9
2	B	819	GLN	4.9
2	B	586	ASP	4.9
2	B	875	PHE	4.8
2	B	1008	MET	4.8
2	B	823	GLN	4.8
1	A	118	GLN	4.8
1	A	212	LEU	4.8
1	A	550	MET	4.8
3	C	90	ASP	4.8
4	D	81	LEU	4.8
1	A	562	TYR	4.7
2	B	559	VAL	4.7
1	A	48	GLN	4.7
1	A	123	MET	4.7
2	B	1003	VAL	4.7
2	B	593	ILE	4.7
2	B	570	PHE	4.7
1	A	21	GLU	4.7
1	A	195	GLU	4.7
2	B	782	ASP	4.7
1	A	71	GLU	4.6
1	A	126	LEU	4.6
1	A	209	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	38	ILE	4.6
1	A	12	PHE	4.6
2	B	1142	LYS	4.6
1	A	18	THR	4.6
2	B	1001	ASP	4.6
4	D	85	ASN	4.6
3	C	97	ALA	4.6
2	B	731	GLU	4.5
1	A	75	TRP	4.5
2	B	633	THR	4.5
1	A	214	GLY	4.5
3	C	22	CYS	4.5
1	A	73	ARG	4.5
1	A	194	ASP	4.5
1	A	180	PHE	4.4
1	A	515	GLU	4.4
1	A	117	TYR	4.4
1	A	538	LEU	4.4
2	B	785	HIS	4.4
1	A	284	SER	4.4
1	A	294	LEU	4.4
2	B	1037	LEU	4.4
1	A	295	GLN	4.3
2	B	744	LYS	4.3
1	A	522	LEU	4.3
2	B	542	ASN	4.3
2	B	980	ILE	4.3
1	A	579	GLN	4.3
2	B	1000	SER	4.3
2	B	820	THR	4.3
1	A	339	SER	4.2
1	A	702	TYR	4.2
1	A	184	ILE	4.2
2	B	983	VAL	4.2
2	B	541	SER	4.2
4	D	80	TYR	4.2
1	A	614	PRO	4.2
1	A	200	ALA	4.2
1	A	77	LEU	4.1
1	A	114	LYS	4.1
1	A	26	GLN	4.1
1	A	390	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	1108	ALA	4.1
3	C	86	LEU	4.1
1	A	683	PHE	4.1
2	B	1088	SER	4.1
1	A	263	ILE	4.1
1	A	565	GLU	4.1
2	B	1036	PHE	4.1
1	A	197	LEU	4.1
1	A	264	TYR	4.1
2	B	540	HIS	4.0
2	B	917	LEU	4.0
4	D	96	CYS	4.0
2	B	1107	ASN	4.0
2	B	851	LEU	4.0
2	B	1110	ARG	4.0
1	A	681	PRO	4.0
2	B	585	LEU	4.0
1	A	510	LEU	3.9
2	B	1143	GLU	3.9
4	D	13	GLN	3.9
2	B	715	LEU	3.9
2	B	1077	PRO	3.9
1	A	668	HIS	3.9
2	B	1140	VAL	3.9
1	A	242	LEU	3.9
2	B	787	ASP	3.9
1	A	285	ASP	3.9
1	A	336	PRO	3.9
2	B	1054	GLY	3.9
2	B	779	ASN	3.9
4	D	94	TYR	3.9
3	C	37	PHE	3.9
1	A	43	ARG	3.9
2	B	1026	GLY	3.8
2	B	780	LEU	3.8
1	A	685	SER	3.8
2	B	885	VAL	3.8
3	C	94	TYR	3.8
1	A	42	PHE	3.8
1	A	205	ASN	3.8
2	B	589	GLU	3.8
2	B	877	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
4	D	71	SER	3.8
2	B	1118	SER	3.8
1	A	298	ILE	3.8
2	B	806	GLU	3.8
1	A	293	ILE	3.7
1	A	240	HIS	3.7
2	B	1042	TRP	3.7
2	B	816	GLN	3.7
1	A	224	ASP	3.7
1	A	125	TRP	3.7
1	A	207	SER	3.7
2	B	920	CYS	3.7
1	A	398	ILE	3.7
1	A	292	GLN	3.7
2	B	716	ASN	3.6
2	B	556	HIS	3.6
2	B	643	PRO	3.6
1	A	328	LEU	3.6
1	A	430	PRO	3.6
1	A	218	TYR	3.6
1	A	259	TYR	3.6
1	A	16	SER	3.6
1	A	512	TYR	3.6
1	A	25	GLU	3.6
1	A	286	LEU	3.6
2	B	545	TYR	3.6
2	B	781	TYR	3.5
1	A	506	ILE	3.5
2	B	1146	TYR	3.5
2	B	905	ASN	3.5
3	C	36	TRP	3.5
2	B	837	ASN	3.5
2	B	621	TYR	3.5
1	A	76	HIS	3.5
1	A	331	VAL	3.5
1	A	536	ARG	3.5
1	A	554	ASN	3.5
2	B	590	LYS	3.5
2	B	662	ASN	3.5
2	B	591	PHE	3.4
1	A	654	GLU	3.4
1	A	684	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	667	LEU	3.4
2	B	1006	TYR	3.4
2	B	1114	TYR	3.4
4	D	90	ASP	3.4
3	C	79	VAL	3.4
1	A	24	ILE	3.4
2	B	537	GLU	3.4
4	D	49	ALA	3.4
1	A	8	GLN	3.4
2	B	1152	THR	3.4
1	A	626	ASP	3.4
3	C	63	SER	3.4
1	A	51	LEU	3.4
1	A	74	PHE	3.4
3	C	48	VAL	3.4
1	A	122	VAL	3.3
1	A	347	MET	3.3
2	B	1098	THR	3.3
1	A	534	SER	3.3
2	B	1079	PRO	3.3
2	B	622	ASN	3.3
2	B	728	ALA	3.3
1	A	247	VAL	3.3
1	A	524	VAL	3.3
2	B	1091	THR	3.3
1	A	245	ARG	3.2
2	B	783	ASP	3.2
4	D	36	TRP	3.2
1	A	682	LYS	3.2
1	A	11	ARG	3.2
1	A	186	GLU	3.2
1	A	384	TYR	3.2
1	A	618	GLU	3.2
3	C	89	GLU	3.2
2	B	748	ILE	3.2
1	A	484	PHE	3.2
2	B	740	GLU	3.2
2	B	1149	ASN	3.2
1	A	688	LEU	3.2
1	A	246	THR	3.1
2	B	985	ASN	3.1
3	C	45	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	876	GLN	3.1
1	A	185	TYR	3.1
1	A	248	TYR	3.1
1	A	258	PRO	3.1
3	C	98	ALA	3.1
3	C	14	ALA	3.1
2	B	1154	THR	3.1
1	A	427	GLU	3.1
1	A	193	ILE	3.0
1	A	388	ILE	3.0
4	D	18	LEU	3.0
2	B	707	PRO	3.0
2	B	1156	GLU	3.0
3	C	44	GLU	3.0
1	A	112	ASP	3.0
3	C	78	THR	3.0
3	C	87	ILE	3.0
2	B	539	PHE	3.0
1	A	670	LYS	3.0
2	B	928	LYS	3.0
2	B	1044	ARG	3.0
1	A	584	ILE	3.0
2	B	847	LEU	3.0
4	D	20	LEU	3.0
1	A	639	THR	3.0
1	A	269	GLY	3.0
1	A	340	GLU	3.0
1	A	210	MET	2.9
2	B	538	ILE	2.9
2	B	718	ILE	2.9
1	A	708	SER	2.9
1	A	664	LEU	2.9
2	B	1085	CYS	2.9
2	B	822	ASP	2.9
4	D	17	SER	2.9
4	D	95	TYR	2.9
1	A	543	VAL	2.9
2	B	868	HIS	2.9
2	B	597	CYS	2.9
1	A	507	ASP	2.9
1	A	583	GLU	2.9
2	B	594	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLN	2.9
2	B	563	PHE	2.9
2	B	1022	LEU	2.9
1	A	511	ILE	2.8
1	A	357	SER	2.8
2	B	726	THR	2.8
1	A	88	ASP	2.8
2	B	1116	GLU	2.8
2	B	923	HIS	2.8
1	A	80	LEU	2.8
1	A	487	THR	2.8
1	A	191	GLY	2.8
2	B	560	ARG	2.8
2	B	891	ILE	2.8
4	D	48	VAL	2.8
3	C	122	GLY	2.8
3	C	125	THR	2.8
2	B	752	GLN	2.8
1	A	619	LYS	2.8
2	B	596	CYS	2.8
2	B	571	VAL	2.8
1	A	177	ASP	2.8
3	C	77	ASN	2.8
1	A	182	LYS	2.8
1	A	68	TRP	2.8
2	B	557	LEU	2.8
2	B	546	ILE	2.7
1	A	261	ARG	2.7
2	B	676	CYS	2.7
2	B	959	ASN	2.7
1	A	52	ASP	2.7
1	A	335	HIS	2.7
1	A	330	ARG	2.7
2	B	803	GLN	2.7
1	A	41	GLU	2.7
2	B	999	LEU	2.7
3	C	49	ALA	2.7
1	A	119	ILE	2.7
1	A	270	ALA	2.6
1	A	679	LYS	2.6
1	A	663	LEU	2.6
2	B	581	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	2.6
1	A	329	ASN	2.6
2	B	562	GLU	2.6
2	B	871	LEU	2.6
1	A	411	LYS	2.5
2	B	878	SER	2.5
1	A	674	ALA	2.5
4	D	38	ARG	2.5
4	D	68	PHE	2.5
2	B	1084	LEU	2.5
1	A	86	ASN	2.5
2	B	902	THR	2.5
2	B	886	ALA	2.5
1	A	386	LEU	2.5
1	A	320	HIS	2.5
1	A	649	TYR	2.5
2	B	743	LEU	2.5
1	A	553	ASN	2.5
2	B	1050	ALA	2.5
1	A	498	SER	2.5
2	B	658	PHE	2.5
2	B	723	PHE	2.5
2	B	1009	LEU	2.5
1	A	582	GLU	2.4
1	A	85	ARG	2.4
2	B	1027	ASN	2.4
2	B	1035	LYS	2.4
2	B	1080	SER	2.4
4	D	126	VAL	2.4
1	A	361	SER	2.4
2	B	592	GLU	2.4
3	C	38	ARG	2.4
1	A	544	LYS	2.4
2	B	1144	LYS	2.4
1	A	648	ASP	2.4
1	A	36	PHE	2.4
1	A	39	ILE	2.4
2	B	631	THR	2.4
2	B	918	SER	2.4
1	A	222	VAL	2.4
1	A	410	SER	2.4
4	D	21	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	778	ASN	2.4
2	B	921	GLU	2.4
4	D	39	GLN	2.4
1	A	241	SER	2.4
2	B	634	VAL	2.4
2	B	882	TYR	2.4
1	A	677	LEU	2.4
2	B	792	LEU	2.3
1	A	577	GLU	2.3
3	C	81	LEU	2.3
1	A	637	ASP	2.3
1	A	551	GLU	2.3
2	B	992	LYS	2.3
1	A	198	GLU	2.3
2	B	1106	GLN	2.3
1	A	615	THR	2.3
1	A	432	TYR	2.3
2	B	835	PHE	2.3
2	B	632	LYS	2.3
2	B	747	LYS	2.3
2	B	733	GLY	2.3
1	A	687	ALA	2.3
3	C	64	VAL	2.3
1	A	54	ALA	2.2
4	D	14	ALA	2.2
1	A	204	ASP	2.2
1	A	257	ASP	2.2
2	B	872	ILE	2.2
1	A	19	LEU	2.2
1	A	81	LEU	2.2
1	A	265	SER	2.2
2	B	884	HIS	2.2
2	B	810	ASP	2.2
2	B	1150	TYR	2.2
4	D	23	ALA	2.2
2	B	754	ASN	2.2
2	B	797	LEU	2.2
2	B	1134	HIS	2.1
1	A	426	TYR	2.1
2	B	949	TYR	2.1
1	A	79	GLU	2.1
3	C	6	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	764	PRO	2.1
1	A	689	ALA	2.1
2	B	883	GLY	2.1
2	B	809	LYS	2.1
1	A	314	ILE	2.1
2	B	1043	ARG	2.1
2	B	978	GLY	2.1
1	A	690	PHE	2.1
1	A	696	ASN	2.1
3	C	26	GLY	2.1
1	A	490	GLU	2.1
2	B	1157	TYR	2.1
1	A	181	PHE	2.1
2	B	993	SER	2.1
1	A	135	ARG	2.0
2	B	544	LYS	2.0
1	A	408	ASP	2.0
3	C	88	PRO	2.0
1	A	389	VAL	2.0
1	A	365	MET	2.0
1	A	500	SER	2.0
1	A	640	SER	2.0
2	B	1005	LEU	2.0
1	A	523	TYR	2.0
2	B	873	GLN	2.0
1	A	283	GLU	2.0
4	D	37	PHE	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.