



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:59 AM UTC

PDB ID : 5NW5 / pdb_00005nw5
Title : Crystal structure of the Rif1 N-terminal domain (RIF1-NTD) from *Saccharomyces cerevisiae* in complex with DNA
Authors : Bunker, R.D.; Reinert, J.K.; Shi, T.; Thoma, N.H.
Deposited on : 2017-05-05
Resolution : 6.50 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

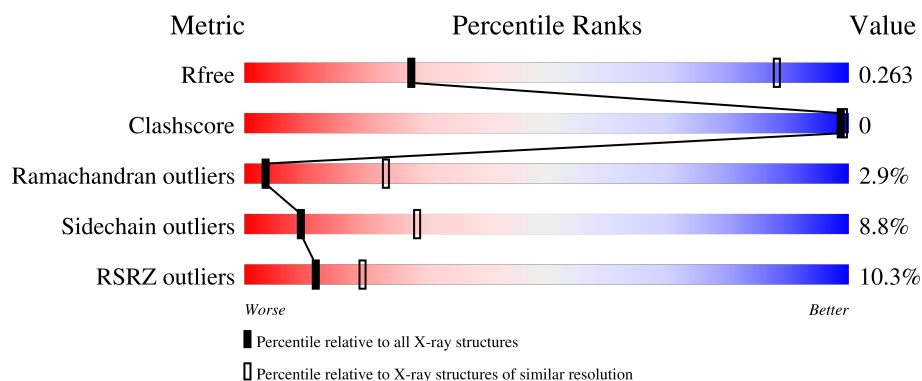
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	1226	10% 76% 11% • 12%
1	B	1226	8% 76% 11% • 12%
2	C	30	7% 67% 30% •
3	D	30	63% 30% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37748 atoms, of which 18886 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 Telomere length regulator protein RIF1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1085	Total	C	H	N	O	S	0	0	0
			17916	5717	9096	1455	1614	34			
1	B	1085	Total	C	H	N	O	S	0	0	0
			17914	5717	9096	1453	1614	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP P29539
A	97	GLY	-	expression tag	UNP P29539
A	98	GLY	-	expression tag	UNP P29539
A	99	ARG	-	expression tag	UNP P29539
B	96	GLY	-	expression tag	UNP P29539
B	97	GLY	-	expression tag	UNP P29539
B	98	GLY	-	expression tag	UNP P29539
B	99	ARG	-	expression tag	UNP P29539

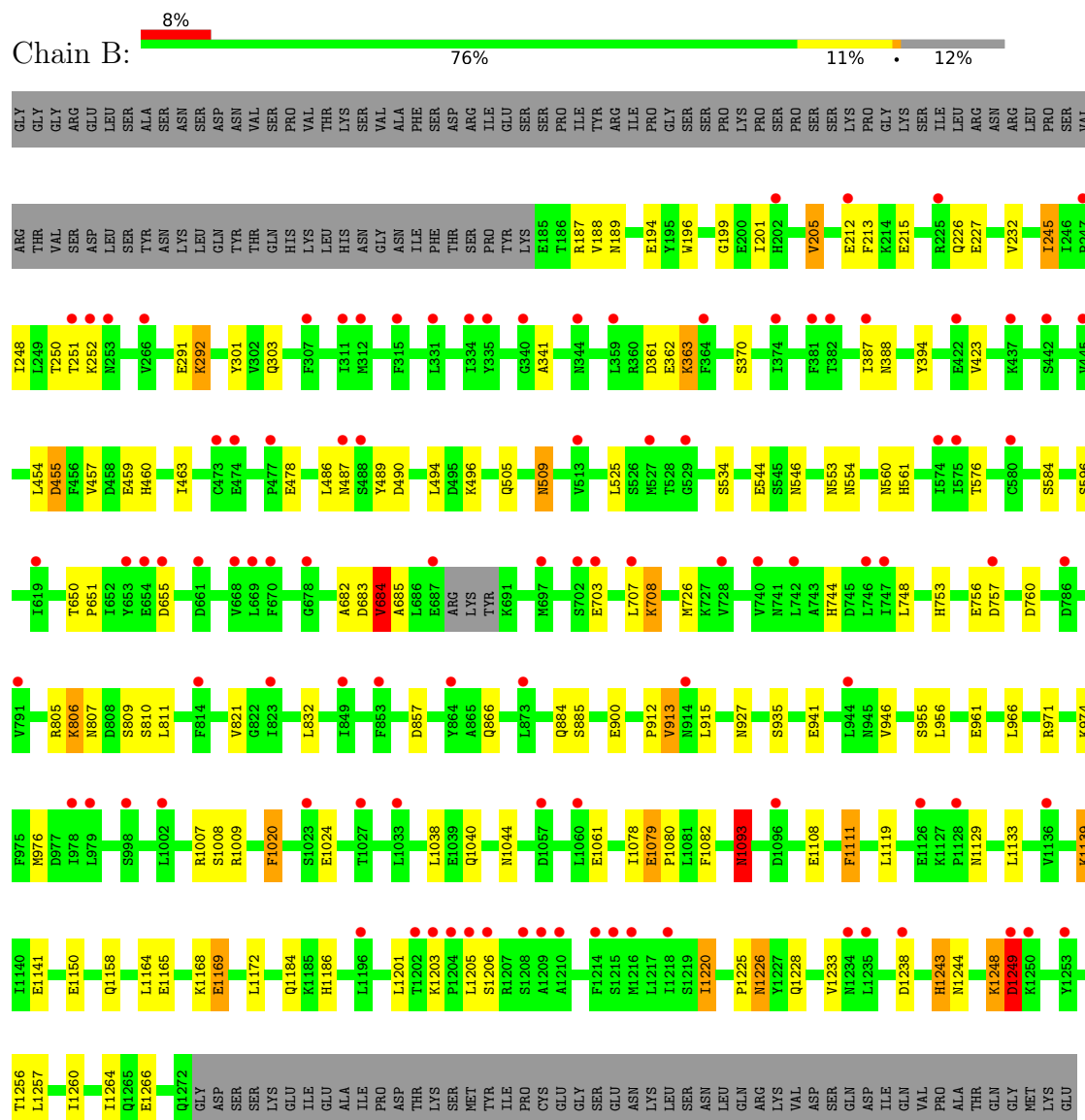
- Molecule 2 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	30	Total	C	H	N	O	P	0	0	0
			959	300	332	150	148	29			

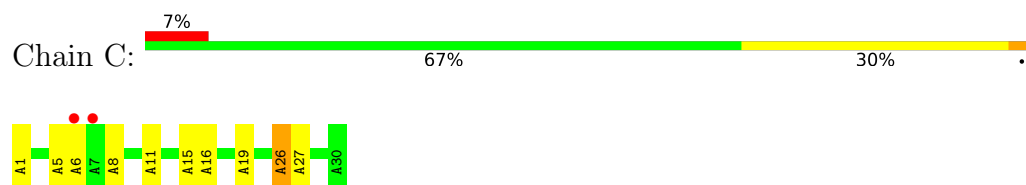
- Molecule 3 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	30	Total	C	H	N	O	P	0	0	0
			959	300	362	60	208	29			

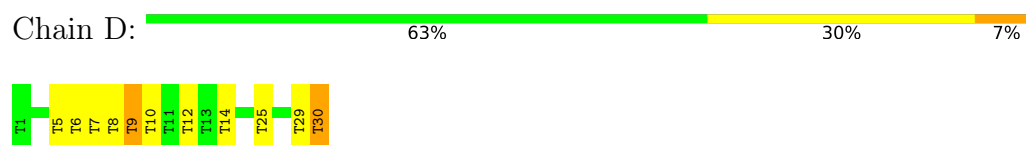
• Molecule 1: Telomere length regulator protein RIF1



• Molecule 2: DNA (60-MER)



• Molecule 3: DNA (30-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 169.80Å 390.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.23 – 6.50 43.23 – 6.50	Depositor EDS
% Data completeness (in resolution range)	70.2 (43.23-6.50) 69.9 (43.23-6.50)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 6.66Å)	Xtriage
Refinement program	PHENIX (dev_2205: AMBER)	Depositor
R, R_{free}	0.253 , 0.277 0.259 , 0.263	Depositor DCC
R_{free} test set	622 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	388.4	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 269.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	37748	wwPDB-VP
Average B, all atoms (Å ²)	327.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	0.88	0/8995	1.52	40/12178 (0.3%)
1	B	0.88	0/8993	1.52	51/12175 (0.4%)
2	C	0.73	0/716	1.53	1/1102 (0.1%)
3	D	0.80	0/656	1.62	3/1012 (0.3%)
All	All	0.87	0/19360	1.52	95/26467 (0.4%)

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	8
1	B	0	6
2	C	0	10
3	D	0	11
All	All	0	35

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ASP	CA-CB-CG	8.66	121.26	112.60
1	B	455	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	454	LEU	CA-C-N	7.50	131.08	120.28
1	A	454	LEU	C-N-CA	7.50	131.08	120.28
1	B	454	LEU	CA-C-N	7.00	130.36	120.28
1	B	454	LEU	C-N-CA	7.00	130.36	120.28
1	B	460	HIS	CA-CB-CG	6.97	120.77	113.80
3	D	30	DT	C2'-C3'-O3'	-6.93	101.11	111.50
1	A	460	HIS	CA-CB-CG	6.83	120.62	113.80
1	B	809	SER	CA-C-N	6.53	128.93	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	809	SER	C-N-CA	6.53	128.93	120.44
1	B	487	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	1093	ASN	CA-CB-CG	6.51	119.11	112.60
3	D	30	DT	C4'-C3'-O3'	6.49	119.73	110.00
1	A	945	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	A	363	LYS	CA-C-N	6.15	128.81	120.38
1	A	363	LYS	C-N-CA	6.15	128.81	120.38
1	A	1251	ARG	CD-NE-CZ	6.15	133.01	124.40
2	C	26	DA	N1-C6-N6	-6.12	109.82	119.00
1	A	494	LEU	CA-C-N	6.09	130.35	120.60
1	A	494	LEU	C-N-CA	6.09	130.35	120.60
1	B	1093	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	B	363	LYS	CA-C-N	6.04	128.70	120.54
1	B	363	LYS	C-N-CA	6.04	128.70	120.54
1	A	1093	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	B	976	MET	CA-C-N	5.97	128.88	120.28
1	B	976	MET	C-N-CA	5.97	128.88	120.28
1	B	1226	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	915	LEU	CA-C-N	5.84	128.90	120.38
1	A	915	LEU	C-N-CA	5.84	128.90	120.38
1	A	753	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	B	753	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	B	1244	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	1158	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	1158	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	B	1243	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	B	866	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	585	GLN	CA-C-N	5.64	129.29	120.82
1	A	585	GLN	C-N-CA	5.64	129.29	120.82
1	A	489	TYR	CA-C-N	5.62	128.08	120.38
1	A	489	TYR	C-N-CA	5.62	128.08	120.38
1	B	1082	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	1093	ASN	CA-C-N	5.52	128.68	120.17
1	B	1093	ASN	C-N-CA	5.52	128.68	120.17
1	B	509	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	584	SER	CB-CA-C	5.49	118.91	110.62
3	D	9	DT	O5'-C5'-C4'	5.49	119.03	110.80
1	A	1037	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	B	884	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	984	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	B	1044	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	546	ASN	OD1-CG-ND2	-5.38	117.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1226	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	1272	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	B	1111	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	1228	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	809	SER	CA-C-N	5.25	127.27	120.44
1	A	809	SER	C-N-CA	5.25	127.27	120.44
1	A	744	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	A	884	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	B	1203	LYS	CA-C-N	5.22	126.37	119.84
1	B	1203	LYS	C-N-CA	5.22	126.37	119.84
1	A	546	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	744	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	A	470	SER	CA-C-N	5.18	126.52	120.98
1	A	470	SER	C-N-CA	5.18	126.52	120.98
1	A	487	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	361	ASP	CA-C-N	5.16	127.50	120.54
1	B	361	ASP	C-N-CA	5.16	127.50	120.54
1	B	561	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	B	946	VAL	CA-C-N	5.14	127.17	120.28
1	B	946	VAL	C-N-CA	5.14	127.17	120.28
1	A	666	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	226	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	1129	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	B	1040	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	268	ILE	N-CA-C	5.12	115.84	110.62
1	B	1206	SER	CA-C-N	5.11	127.09	120.44
1	B	1206	SER	C-N-CA	5.11	127.09	120.44
1	B	226	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	1111	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	494	LEU	CA-C-N	5.08	129.20	120.72
1	B	494	LEU	C-N-CA	5.08	129.20	120.72
1	B	423	VAL	CA-C-N	5.07	126.43	120.09
1	B	423	VAL	C-N-CA	5.07	126.43	120.09
1	B	505	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	1186	HIS	CA-C-N	5.05	127.75	120.38
1	B	1186	HIS	C-N-CA	5.05	127.75	120.38
1	B	245	ILE	CA-CB-CG1	5.04	118.97	110.40
1	A	777	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	1044	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	B	971	ARG	CA-C-N	5.01	128.40	120.89
1	B	971	ARG	C-N-CA	5.01	128.40	120.89
1	B	362	GLU	N-CA-C	5.00	117.11	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	913	VAL	CA-CB-CG2	5.00	118.90	110.40

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1204	PRO	Peptide
1	A	196	TRP	Peptide
1	A	301	TYR	Sidechain
1	A	394	TYR	Sidechain
1	A	561	HIS	Sidechain
1	A	573	ARG	Sidechain
1	A	807	ASN	Peptide
1	A	914	ASN	Peptide
1	B	1243	HIS	Sidechain
1	B	196	TRP	Peptide
1	B	301	TYR	Sidechain
1	B	394	TYR	Sidechain
1	B	684	VAL	Peptide
1	B	807	ASN	Peptide
2	C	1	DA	Sidechain
2	C	11	DA	Sidechain
2	C	15	DA	Sidechain
2	C	16	DA	Sidechain
2	C	19	DA	Sidechain
2	C	26	DA	Sidechain
2	C	27	DA	Sidechain
2	C	5	DA	Sidechain
2	C	6	DA	Sidechain
2	C	8	DA	Sidechain
3	D	10	DT	Sidechain
3	D	12	DT	Sidechain
3	D	14	DT	Sidechain
3	D	25	DT	Sidechain
3	D	29	DT	Sidechain
3	D	30	DT	Sidechain
3	D	5	DT	Sidechain
3	D	6	DT	Sidechain
3	D	7	DT	Sidechain
3	D	8	DT	Sidechain
3	D	9	DT	Sidechain

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	8820	9096	9094	13	0
1	B	8818	9096	9094	5	0
2	C	627	332	332	0	0
3	D	597	362	362	0	0
All	All	18862	18886	18882	18	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 0.

All (18) 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:A:1224:ASN:H	1:A:1225:PRO:HD3	1.80	0.47
1:A:703:GLU:OE1	1:A:706:LYS:HE3	2.15	0.47
1:A:1111:PHE:CG	1:A:1139:LYS:HE3	2.50	0.46
1:A:584:SER:OG	1:A:586:LYS:HE2	2.17	0.44
1:A:650:THR:HB	1:A:651:PRO:HD3	2.00	0.44
1:B:1111:PHE:CG	1:B:1139:LYS:HE3	2.54	0.43
1:B:650:THR:HB	1:B:651:PRO:HD3	1.99	0.43
1:A:980:GLU:CD	1:A:1007:ARG:HH21	2.26	0.43
1:B:1248:LYS:HE2	1:B:1249:ASP:OD1	2.18	0.43
1:A:289:SER:O	1:A:292:LYS:HE2	2.19	0.43
1:B:1079:GLU:H	1:B:1080:PRO:CD	2.31	0.42
1:A:1079:GLU:H	1:A:1080:PRO:CD	2.32	0.42
1:B:250:THR:HB	1:B:252:LYS:HE3	2.02	0.42
1:A:1262:LYS:HE2	1:A:1266:GLU:OE2	2.20	0.42
1:A:470:SER:HA	1:A:471:PRO:HD3	1.93	0.41
1:A:632:SER:O	1:A:634:LYS:HE3	2.20	0.41
1:A:1005:LEU:H	1:A:1005:LEU:HD12	1.86	0.41
1:A:1092:ASN:C	1:A:1094:MET:H	2.30	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	1081/1226 (88%)	930 (86%)	120 (11%)	31 (3%)	3	23
1	B	1081/1226 (88%)	924 (86%)	125 (12%)	32 (3%)	3	22
All	All	2162/2452 (88%)	1854 (86%)	245 (11%)	63 (3%)	3	23

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	GLU
1	A	391	ASN
1	A	457	VAL
1	A	806	LYS
1	A	913	VAL
1	A	1093	ASN
1	B	227	GLU
1	B	457	VAL
1	B	682	ALA
1	B	685	ALA
1	B	806	LYS
1	B	1093	ASN
1	A	205	VAL
1	A	292	LYS
1	A	388	ASN
1	A	805	ARG
1	A	946	VAL
1	A	1011	SER
1	A	1078	ILE
1	A	1181	SER
1	A	1182	ASN
1	A	1246	LYS
1	B	205	VAL
1	B	388	ASN
1	B	912	PRO

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Mol	Chain	Res	Type
1	B	1009	ARG
1	B	1078	ILE
1	A	363	LYS
1	A	1249	ASP
1	B	292	LYS
1	B	684	VAL
1	B	708	LYS
1	B	805	ARG
1	B	1007	ARG
1	B	1020	PHE
1	B	1079	GLU
1	B	1249	ASP
1	A	1007	ARG
1	A	1079	GLU
1	A	1223	PRO
1	A	1224	ASN
1	B	341	ALA
1	B	363	LYS
1	B	486	LEU
1	B	560	ASN
1	B	913	VAL
1	B	1169	GLU
1	A	189	ASN
1	A	201	ILE
1	A	341	ALA
1	A	1169	GLU
1	B	189	ASN
1	B	201	ILE
1	B	387	ILE
1	B	1008	SER
1	A	387	ILE
1	A	1128	PRO
1	B	1225	PRO
1	A	878	ILE
1	A	199	GLY
1	B	1220	ILE
1	A	1221	LEU
1	B	199	GLY

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	1020/1148 (89%)	931 (91%)	89 (9%)	9	29
1	B	1020/1148 (89%)	929 (91%)	91 (9%)	9	28
All	All	2040/2296 (89%)	1860 (91%)	180 (9%)	9	28

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	188	VAL
1	A	194	GLU
1	A	205	VAL
1	A	208	GLU
1	A	212	GLU
1	A	213	PHE
1	A	215	GLU
1	A	232	VAL
1	A	245	ILE
1	A	248	ILE
1	A	251	THR
1	A	256	GLU
1	A	291	GLU
1	A	292	LYS
1	A	303	GLN
1	A	319	LYS
1	A	387	ILE
1	A	395	GLU
1	A	405	SER
1	A	455	ASP
1	A	459	GLU
1	A	463	ILE
1	A	474	GLU
1	A	478	GLU
1	A	487	ASN
1	A	489	TYR

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Mol	Chain	Res	Type
1	A	490	ASP
1	A	496	LYS
1	A	509	ASN
1	A	525	LEU
1	A	534	SER
1	A	544	GLU
1	A	553	ASN
1	A	563	LYS
1	A	576	THR
1	A	584	SER
1	A	684	VAL
1	A	687	GLU
1	A	703	GLU
1	A	707	LEU
1	A	708	LYS
1	A	711	SER
1	A	726	MET
1	A	748	LEU
1	A	756	GLU
1	A	757	ASP
1	A	760	ASP
1	A	785	ARG
1	A	806	LYS
1	A	810	SER
1	A	811	LEU
1	A	821	VAL
1	A	832	LEU
1	A	857	ASP
1	A	926	ASN
1	A	945	ASN
1	A	950	THR
1	A	973	ASN
1	A	984	HIS
1	A	998	SER
1	A	1038	LEU
1	A	1061	GLU
1	A	1074	MET
1	A	1093	ASN
1	A	1098	LEU
1	A	1119	LEU
1	A	1133	LEU
1	A	1141	GLU

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Mol	Chain	Res	Type
1	A	1150	GLU
1	A	1164	LEU
1	A	1165	GLU
1	A	1168	LYS
1	A	1169	GLU
1	A	1177	ASN
1	A	1184	GLN
1	A	1187	LYS
1	A	1201	LEU
1	A	1220	ILE
1	A	1221	LEU
1	A	1227	TYR
1	A	1228	GLN
1	A	1229	THR
1	A	1233	VAL
1	A	1238	ASP
1	A	1244	ASN
1	A	1248	LYS
1	A	1249	ASP
1	A	1266	GLU
1	B	187	ARG
1	B	188	VAL
1	B	194	GLU
1	B	205	VAL
1	B	212	GLU
1	B	213	PHE
1	B	215	GLU
1	B	232	VAL
1	B	245	ILE
1	B	248	ILE
1	B	251	THR
1	B	291	GLU
1	B	292	LYS
1	B	303	GLN
1	B	370	SER
1	B	455	ASP
1	B	459	GLU
1	B	463	ILE
1	B	478	GLU
1	B	489	TYR
1	B	490	ASP
1	B	496	LYS

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Mol	Chain	Res	Type
1	B	509	ASN
1	B	525	LEU
1	B	534	SER
1	B	544	GLU
1	B	553	ASN
1	B	554	ASN
1	B	576	THR
1	B	584	SER
1	B	596	SER
1	B	655	ASP
1	B	683	ASP
1	B	684	VAL
1	B	703	GLU
1	B	707	LEU
1	B	708	LYS
1	B	726	MET
1	B	748	LEU
1	B	756	GLU
1	B	757	ASP
1	B	760	ASP
1	B	806	LYS
1	B	810	SER
1	B	811	LEU
1	B	821	VAL
1	B	832	LEU
1	B	857	ASP
1	B	885	SER
1	B	900	GLU
1	B	915	LEU
1	B	927	ASN
1	B	935	SER
1	B	941	GLU
1	B	955	SER
1	B	956	LEU
1	B	961	GLU
1	B	966	LEU
1	B	974	LYS
1	B	1020	PHE
1	B	1024	GLU
1	B	1038	LEU
1	B	1061	GLU
1	B	1093	ASN

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Mol	Chain	Res	Type
1	B	1108	GLU
1	B	1119	LEU
1	B	1129	ASN
1	B	1133	LEU
1	B	1139	LYS
1	B	1141	GLU
1	B	1150	GLU
1	B	1164	LEU
1	B	1165	GLU
1	B	1168	LYS
1	B	1169	GLU
1	B	1172	LEU
1	B	1184	GLN
1	B	1201	LEU
1	B	1205	LEU
1	B	1220	ILE
1	B	1226	ASN
1	B	1228	GLN
1	B	1233	VAL
1	B	1238	ASP
1	B	1248	LYS
1	B	1249	ASP
1	B	1256	THR
1	B	1257	LEU
1	B	1260	ILE
1	B	1264	ILE
1	B	1266	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	267	ASN
1	A	280	GLN
1	A	329	ASN
1	A	487	ASN
1	A	515	ASN
1	A	517	ASN
1	A	585	GLN
1	A	664	HIS
1	A	716	GLN
1	A	741	ASN

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Mol	Chain	Res	Type
1	A	753	HIS
1	A	807	ASN
1	A	895	ASN
1	A	940	ASN
1	A	945	ASN
1	A	973	ASN
1	A	1224	ASN
1	B	255	ASN
1	B	267	ASN
1	B	280	GLN
1	B	329	ASN
1	B	371	ASN
1	B	509	ASN
1	B	560	ASN
1	B	603	GLN
1	B	664	HIS
1	B	667	ASN
1	B	716	GLN
1	B	741	ASN
1	B	776	GLN
1	B	807	ASN
1	B	817	GLN
1	B	866	GLN
1	B	926	ASN
1	B	945	ASN
1	B	1036	GLN
1	B	1037	GLN
1	B	1129	ASN
1	B	1224	ASN
1	B	1226	ASN
1	B	1228	GLN
1	B	1272	GLN

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	1085/1226 (88%)	0.73	128 (11%) 9 17	316, 316, 316, 316	0
1	B	1085/1226 (88%)	0.70	100 (9%) 14 22	316, 316, 316, 316	0
2	C	30/30 (100%)	0.92	2 (6%) 24 29	547, 547, 547, 547	0
3	D	30/30 (100%)	0.61	0 100 100	547, 547, 547, 547	0
All	All	2230/2512 (88%)	0.72	230 (10%) 12 19	316, 316, 316, 547	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	LEU	8.3
1	B	1234	ASN	7.3
1	B	1215	SER	5.6
1	B	212	GLU	5.2
1	B	1205	LEU	5.0
1	A	513	VAL	5.0
1	A	1167	LEU	5.0
1	B	998	SER	4.9
1	A	630	PHE	4.8
1	A	687	GLU	4.7
1	A	315	PHE	4.6
1	A	710	ILE	4.5
1	A	442	SER	4.5
1	A	619	ILE	4.4
1	A	1168	LYS	4.4
1	B	853	PHE	4.3
1	B	1060	LEU	4.3
1	B	252	LYS	4.3
1	B	670	PHE	4.2
1	A	899	ILE	4.2
1	B	1204	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	869	VAL	4.2
1	A	873	LEU	4.1
1	A	449	LEU	4.1
1	B	1206	SER	4.0
1	B	331	LEU	4.0
1	A	445	VAL	4.0
1	B	978	ILE	4.0
1	A	1129	ASN	3.9
1	A	623	LEU	3.9
1	A	427	ILE	3.9
1	A	221	LEU	3.9
1	A	527	MET	3.8
1	B	473	CYS	3.8
1	B	312	MET	3.8
1	B	1235	LEU	3.8
1	A	932	PHE	3.8
1	B	1203	LYS	3.7
1	A	684	VAL	3.7
1	B	742	LEU	3.7
1	B	791	VAL	3.7
1	A	655	ASP	3.7
1	A	444	VAL	3.6
1	B	364	PHE	3.6
1	A	665	LEU	3.5
1	A	905	LEU	3.5
1	B	669	LEU	3.5
1	B	381	PHE	3.5
1	A	446	LEU	3.5
1	B	655	ASP	3.5
1	A	574	ILE	3.5
1	B	1202	THR	3.4
1	A	669	LEU	3.4
1	A	914	ASN	3.4
1	A	990	LEU	3.4
1	A	670	PHE	3.3
1	A	1221	LEU	3.2
1	A	653	TYR	3.2
1	B	487	ASN	3.2
1	B	864	TYR	3.2
1	A	902	PHE	3.2
1	B	437	LYS	3.2
1	A	423	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	672	VAL	3.2
1	A	550	PHE	3.1
1	A	686	LEU	3.1
1	A	376	PRO	3.1
1	A	371	ASN	3.1
1	B	619	ILE	3.1
1	B	1238	ASP	3.0
1	A	1220	ILE	3.0
1	B	334	ILE	3.0
1	A	1121	LEU	3.0
1	A	998	SER	3.0
1	A	883	PHE	3.0
1	B	251	THR	2.9
1	B	580	CYS	2.9
1	B	1250	LYS	2.9
1	A	209	SER	2.9
1	A	707	LEU	2.9
1	A	847	PHE	2.9
1	B	1057	ASP	2.9
1	B	697	MET	2.9
1	A	950	THR	2.8
1	B	873	LEU	2.8
1	A	526	SER	2.8
1	B	477	PRO	2.8
1	B	307	PHE	2.8
1	A	733	VAL	2.8
1	A	1059	GLU	2.8
1	A	426	ARG	2.7
1	A	212	GLU	2.7
1	A	671	THR	2.7
1	B	1214	PHE	2.7
1	A	1240	ILE	2.7
1	B	374	ILE	2.7
1	A	525	LEU	2.7
1	A	770	LEU	2.7
1	A	1133	LEU	2.7
1	A	507	ILE	2.7
1	A	535	GLY	2.7
1	A	473	CYS	2.7
1	A	1217	LEU	2.7
1	B	1033	LEU	2.7
1	B	311	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1126	GLU	2.7
1	A	1086	LEU	2.7
1	B	1249	ASP	2.6
1	B	747	ILE	2.6
1	A	868	TRP	2.6
1	B	247	PRO	2.6
1	A	1171	LEU	2.6
1	B	814	PHE	2.6
1	A	661	ASP	2.6
1	B	1196	LEU	2.6
1	A	263	ILE	2.6
1	A	966	LEU	2.6
1	A	1151	LEU	2.6
1	B	661	ASP	2.6
1	B	702	SER	2.5
1	A	786	ASP	2.5
1	B	574	ILE	2.5
1	A	626	VAL	2.5
1	B	422	GLU	2.5
1	B	1210	ALA	2.5
1	A	361	ASP	2.5
1	A	261	PHE	2.5
1	A	1126	GLU	2.5
1	A	635	ASN	2.5
1	B	359	LEU	2.5
1	B	746	LEU	2.5
1	A	603	GLN	2.5
1	B	707	LEU	2.5
1	A	428	ILE	2.5
1	B	740	VAL	2.5
1	B	1136	VAL	2.5
1	A	1216	MET	2.5
1	A	307	PHE	2.5
1	A	797	TYR	2.5
1	B	944	LEU	2.4
1	B	654	GLU	2.4
1	B	1208	SER	2.4
1	A	889	ILE	2.4
1	B	757	ASP	2.4
1	A	322	THR	2.4
1	A	504	THR	2.4
1	A	602	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	703	GLU	2.4
1	A	306	ARG	2.4
1	B	445	VAL	2.4
2	C	6	DA	2.4
1	A	917	THR	2.4
1	B	527	MET	2.4
1	B	474	GLU	2.3
1	A	771	ILE	2.3
1	B	849	ILE	2.3
1	A	723	ASP	2.3
1	B	442	SER	2.3
1	A	947	ASP	2.3
1	A	1249	ASP	2.3
1	A	787	PHE	2.3
1	B	344	ASN	2.3
1	A	607	PRO	2.3
1	A	1172	LEU	2.3
1	B	315	PHE	2.3
1	A	838	ARG	2.3
1	A	622	LEU	2.3
1	A	903	LEU	2.3
1	A	523	LEU	2.3
1	A	946	VAL	2.3
1	B	1096	ASP	2.3
1	A	434	TYR	2.2
1	A	514	LYS	2.2
1	A	1250	LYS	2.2
1	A	198	SER	2.2
1	B	1128	PRO	2.2
1	A	702	SER	2.2
1	B	979	LEU	2.2
1	A	867	ASN	2.2
1	B	225	ARG	2.2
1	B	1023	SER	2.2
1	B	340	GLY	2.2
1	B	1027	THR	2.2
1	B	387	ILE	2.2
1	A	728	VAL	2.2
1	A	999	ASP	2.2
1	B	678	GLY	2.2
1	B	1216	MET	2.2
2	C	7	DA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	875	PRO	2.2
1	B	1218	ILE	2.2
1	B	1002	LEU	2.2
1	A	1050	ASN	2.1
1	B	202	HIS	2.1
1	A	1200	TYR	2.1
1	A	616	GLU	2.1
1	A	1057	ASP	2.1
1	A	367	PHE	2.1
1	B	575	ILE	2.1
1	A	907	LEU	2.1
1	B	653	TYR	2.1
1	B	488	SER	2.1
1	A	530	LEU	2.1
1	A	933	ILE	2.1
1	B	786	ASP	2.1
1	A	1196	LEU	2.1
1	B	382	THR	2.1
1	B	914	ASN	2.1
1	B	823	ILE	2.1
1	A	1170	PRO	2.1
1	B	728	VAL	2.1
1	A	349	LYS	2.1
1	A	267	ASN	2.1
1	B	253	ASN	2.1
1	B	529	GLY	2.1
1	B	1209	ALA	2.1
1	B	687	GLU	2.1
1	A	1197	VAL	2.1
1	B	266	VAL	2.1
1	B	1253	TYR	2.0
1	A	621	HIS	2.0
1	A	275	CYS	2.0
1	B	335	TYR	2.0
1	A	863	VAL	2.0
1	A	927	ASN	2.0
1	B	513	VAL	2.0
1	B	668	VAL	2.0
1	A	956	LEU	2.0
1	A	608	TYR	2.0
1	A	651	PRO	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.