



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:57 PM UTC

PDB ID : 1Z5Z / pdb_00001z5z
Title : Sulfolobus solfataricus SWI2/SNF2 ATPase C-terminal domain
Authors : Duerr, H.; Koerner, C.; Mueller, M.; Hickmann, V.; Hopfner, K.P.
Deposited on : 2005-03-21
Resolution : 2.00 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

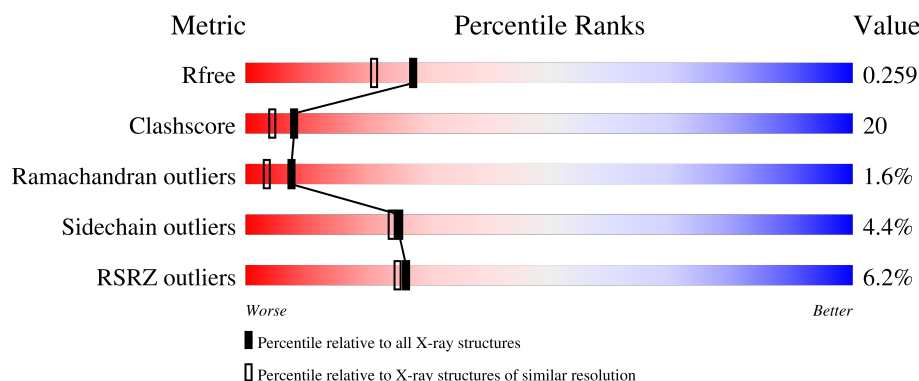
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	271	4% 61% 21% • 15%
1	B	271	7% 52% 27% 5% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3910 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 Helicase of the snf2/rad54 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	36	0	0
			1832	1172	309	345	6			
1	B	228	Total	C	N	O	S	40	0	0
			1819	1163	307	343	6			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	636	MET	-	expression tag	UNP Q97XQ5
A	637	GLY	-	expression tag	UNP Q97XQ5
A	638	SER	-	expression tag	UNP Q97XQ5
A	639	SER	-	expression tag	UNP Q97XQ5
A	640	HIS	-	expression tag	UNP Q97XQ5
A	641	HIS	-	expression tag	UNP Q97XQ5
A	642	HIS	-	expression tag	UNP Q97XQ5
A	643	HIS	-	expression tag	UNP Q97XQ5
A	644	HIS	-	expression tag	UNP Q97XQ5
A	645	HIS	-	expression tag	UNP Q97XQ5
A	646	SER	-	expression tag	UNP Q97XQ5
A	647	SER	-	expression tag	UNP Q97XQ5
A	648	GLY	-	expression tag	UNP Q97XQ5
A	649	LEU	-	expression tag	UNP Q97XQ5
A	650	VAL	-	expression tag	UNP Q97XQ5
A	651	PRO	-	expression tag	UNP Q97XQ5
A	652	ARG	-	expression tag	UNP Q97XQ5
A	653	GLY	-	expression tag	UNP Q97XQ5
A	654	SER	-	expression tag	UNP Q97XQ5
A	655	HIS	-	expression tag	UNP Q97XQ5
A	656	MET	-	expression tag	UNP Q97XQ5
A	657	ALA	-	expression tag	UNP Q97XQ5
A	658	SER	-	expression tag	UNP Q97XQ5
B	636	MET	-	expression tag	UNP Q97XQ5
B	637	GLY	-	expression tag	UNP Q97XQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	638	SER	-	expression tag	UNP Q97XQ5
B	639	SER	-	expression tag	UNP Q97XQ5
B	640	HIS	-	expression tag	UNP Q97XQ5
B	641	HIS	-	expression tag	UNP Q97XQ5
B	642	HIS	-	expression tag	UNP Q97XQ5
B	643	HIS	-	expression tag	UNP Q97XQ5
B	644	HIS	-	expression tag	UNP Q97XQ5
B	645	HIS	-	expression tag	UNP Q97XQ5
B	646	SER	-	expression tag	UNP Q97XQ5
B	647	SER	-	expression tag	UNP Q97XQ5
B	648	GLY	-	expression tag	UNP Q97XQ5
B	649	LEU	-	expression tag	UNP Q97XQ5
B	650	VAL	-	expression tag	UNP Q97XQ5
B	651	PRO	-	expression tag	UNP Q97XQ5
B	652	ARG	-	expression tag	UNP Q97XQ5
B	653	GLY	-	expression tag	UNP Q97XQ5
B	654	SER	-	expression tag	UNP Q97XQ5
B	655	HIS	-	expression tag	UNP Q97XQ5
B	656	MET	-	expression tag	UNP Q97XQ5
B	657	ALA	-	expression tag	UNP Q97XQ5
B	658	SER	-	expression tag	UNP Q97XQ5

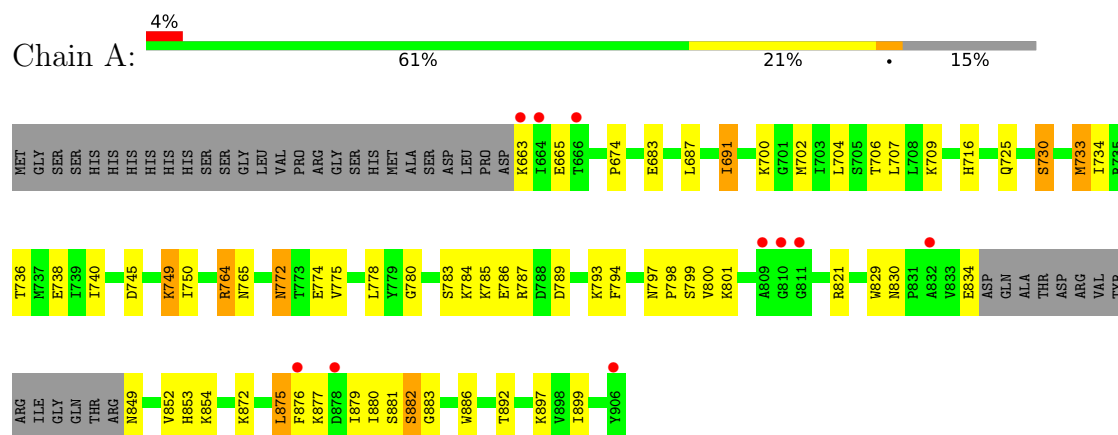
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		
2	B	120	Total	O	0	0
			120	120		

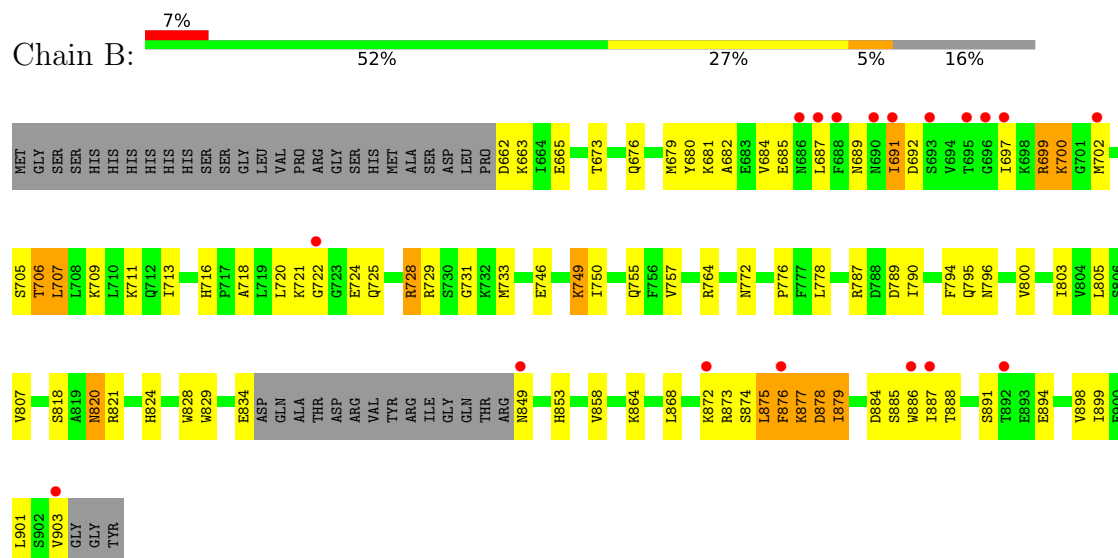
3 Residue-property plots

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: Helicase of the *snf2*/rad54 family



- Molecule 1: Helicase of the *snf2*/rad54 family



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.80Å 61.13Å 74.97Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 95.7 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.260 0.218 , 0.259	Depositor DCC
R_{free} test set	1705 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.80% 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	0.75	0/1858	1.10	10/2498 (0.4%)
1	B	0.73	0/1844	1.05	13/2481 (0.5%)
All	All	0.74	0/3702	1.08	23/4979 (0.5%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	699	ARG	N-CA-C	-7.14	102.03	111.24
1	A	749	LYS	N-CA-C	-6.63	98.43	109.24
1	A	899	ILE	N-CA-C	6.53	122.99	113.39
1	B	820	ASN	N-CA-C	-6.46	105.70	113.97
1	A	829	TRP	N-CA-C	6.19	118.91	110.55
1	B	899	ILE	N-CA-C	6.08	122.33	113.39
1	B	796	ASN	N-CA-C	6.04	121.71	113.97
1	B	829	TRP	N-CA-C	6.03	119.91	110.32
1	A	880	ILE	N-CA-C	5.97	119.41	111.17
1	A	830	ASN	CA-C-N	5.95	125.43	119.24
1	A	830	ASN	C-N-CA	5.95	125.43	119.24
1	B	750	ILE	N-CA-C	5.87	116.33	108.11
1	B	691	ILE	N-CA-C	5.84	116.02	110.53
1	A	750	ILE	N-CA-C	5.58	115.98	108.17
1	A	730	SER	N-CA-C	5.56	117.45	108.34
1	B	878	ASP	N-CA-C	5.47	119.81	113.20
1	B	749	LYS	N-CA-C	-5.45	100.41	109.46
1	A	881	SER	N-CA-C	5.39	116.96	111.14
1	B	689	ASN	N-CA-C	-5.39	105.97	112.54
1	B	728	ARG	N-CA-C	5.39	118.64	111.75
1	A	780	GLY	N-CA-C	5.36	119.36	112.83
1	B	891	SER	N-CA-C	-5.15	103.73	110.53
1	B	894	GLU	N-CA-C	-5.02	105.50	110.97

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	1832	0	1892	56	0
1	B	1819	0	1881	86	0
2	A	139	0	0	20	0
2	B	120	0	0	32	0
All	All	3910	0	3773	142	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 20.

All (142) 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:872:LYS:HD3	1:A:875:LEU:HD21	1.33	1.10
1:B:795:GLN:HE22	1:B:818:SER:H	1.03	0.93
1:A:783:SER:OG	1:A:786:GLU:HG3	1.67	0.92
1:A:749:LYS:HE2	1:A:800:VAL:O	1.72	0.90
1:B:884:ASP:HB3	1:B:887:ILE:HD12	1.54	0.89
1:B:874:SER:O	1:B:877:LYS:HG3	1.75	0.84
1:A:872:LYS:HA	2:A:181:HOH:O	1.77	0.84
1:A:821:ARG:HH11	1:A:853:HIS:HE1	1.24	0.82
1:A:774:GLU:HA	2:A:209:HOH:O	1.81	0.81
1:A:872:LYS:HB3	1:A:875:LEU:HG	1.61	0.81
1:B:821:ARG:HH11	1:B:853:HIS:HE1	1.26	0.80
1:B:873:ARG:O	1:B:877:LYS:HG2	1.86	0.76
1:A:663:LYS:HG2	2:A:189:HOH:O	1.86	0.76
1:B:898:VAL:HG23	2:B:199:HOH:O	1.86	0.76
1:A:702:MET:HA	2:A:66:HOH:O	1.87	0.74
1:B:673:THR:H	1:B:676:GLN:HE21	1.36	0.73
1:A:749:LYS:HE3	1:A:798:PRO:HA	1.70	0.72
1:B:834:GLU:HB2	2:B:96:HOH:O	1.89	0.72
1:A:764:ARG:NH1	1:A:765:ASN:OD1	2.22	0.71
1:B:795:GLN:NE2	1:B:818:SER:H	1.85	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:HG12	1:A:886:TRP:HB3	1.74	0.69
1:A:772:ASN:HB3	2:A:88:HOH:O	1.93	0.69
1:B:824:HIS:HD2	1:B:828:TRP:HE1	1.37	0.68
1:A:691:ILE:HG12	2:A:223:HOH:O	1.92	0.68
1:B:821:ARG:HH11	1:B:853:HIS:CE1	2.08	0.68
1:B:824:HIS:CD2	1:B:828:TRP:HE1	2.11	0.67
1:B:713:ILE:HG13	1:B:720:LEU:CD1	2.24	0.67
1:B:794:PHE:HB2	2:B:198:HOH:O	1.95	0.67
1:A:821:ARG:HH11	1:A:853:HIS:CE1	2.11	0.66
1:B:725:GLN:HB2	2:B:153:HOH:O	1.96	0.66
1:B:790:ILE:HB	2:B:255:HOH:O	1.96	0.66
1:B:680:TYR:O	1:B:684:VAL:HG23	1.96	0.66
1:A:725:GLN:HA	2:A:105:HOH:O	1.96	0.64
1:B:884:ASP:CB	1:B:887:ILE:HD12	2.26	0.64
1:A:663:LYS:N	1:A:849:ASN:OD1	2.31	0.64
1:B:858:VAL:HG13	2:B:251:HOH:O	1.98	0.63
1:A:749:LYS:NZ	1:A:794:PHE:O	2.32	0.63
1:B:749:LYS:H	1:B:820:ASN:HD22	1.47	0.63
1:B:681:LYS:HE3	1:B:901:LEU:HD23	1.81	0.62
1:B:803:ILE:HB	2:B:198:HOH:O	1.99	0.61
1:B:879:ILE:HG22	2:B:210:HOH:O	1.99	0.61
1:B:778:LEU:HG	2:B:255:HOH:O	2.00	0.61
1:B:776:PRO:HB2	1:B:790:ILE:HG23	1.83	0.60
1:B:876:PHE:O	1:B:878:ASP:N	2.34	0.60
1:B:778:LEU:HD23	2:B:228:HOH:O	2.02	0.60
1:B:776:PRO:HG2	2:B:198:HOH:O	2.01	0.59
1:B:681:LYS:HD2	2:B:226:HOH:O	2.01	0.59
1:B:879:ILE:HB	2:B:180:HOH:O	2.02	0.59
1:B:724:GLU:OE1	1:B:728:ARG:NH2	2.35	0.59
1:B:876:PHE:HB2	2:B:257:HOH:O	2.02	0.59
1:B:903:VAL:HG12	1:B:903:VAL:O	2.03	0.58
1:B:873:ARG:O	1:B:877:LYS:CG	2.51	0.57
1:A:797:ASN:OD1	1:A:799:SER:HB2	2.04	0.57
1:A:725:GLN:HE22	1:A:765:ASN:HD22	1.52	0.57
1:B:662:ASP:CG	1:B:849:ASN:N	2.63	0.56
1:B:757:VAL:HG23	2:B:107:HOH:O	2.05	0.56
1:A:691:ILE:CG2	2:A:223:HOH:O	2.53	0.56
1:B:875:LEU:O	1:B:877:LYS:N	2.37	0.55
1:B:687:LEU:HD22	1:B:706:THR:HG21	1.88	0.55
1:A:716:HIS:CE1	2:A:105:HOH:O	2.59	0.55
1:B:705:SER:OG	1:B:709:LYS:NZ	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:GLU:HG2	2:B:141:HOH:O	2.06	0.54
1:A:709:LYS:HE3	2:A:21:HOH:O	2.07	0.54
1:B:676:GLN:HE22	1:B:731:GLY:H	1.55	0.53
1:A:783:SER:HG	1:A:786:GLU:HG3	1.72	0.53
1:B:699:ARG:O	1:B:702:MET:N	2.40	0.53
1:A:799:SER:O	1:A:801:LYS:HG2	2.10	0.52
1:B:874:SER:O	1:B:875:LEU:O	2.26	0.52
1:B:787:ARG:HD3	2:B:228:HOH:O	2.09	0.52
1:B:879:ILE:HD11	1:B:886:TRP:CE2	2.45	0.52
1:A:784:LYS:HE2	2:A:213:HOH:O	2.09	0.52
1:B:873:ARG:O	1:B:877:LYS:HE2	2.09	0.52
1:B:879:ILE:HG23	1:B:879:ILE:O	2.10	0.52
1:A:872:LYS:HB3	1:A:875:LEU:CG	2.36	0.51
1:B:728:ARG:NH2	2:B:211:HOH:O	2.44	0.50
1:B:876:PHE:HB3	2:B:180:HOH:O	2.11	0.50
1:A:785:LYS:HE2	1:A:789:ASP:OD1	2.11	0.50
1:B:886:TRP:HD1	2:B:179:HOH:O	1.95	0.50
1:A:834:GLU:HA	2:A:242:HOH:O	2.11	0.50
1:B:713:ILE:HG13	1:B:720:LEU:HD13	1.93	0.49
1:A:879:ILE:CG1	1:A:886:TRP:HB3	2.43	0.48
1:B:681:LYS:O	1:B:685:GLU:HG3	2.12	0.48
1:B:877:LYS:HA	2:B:210:HOH:O	2.13	0.48
1:A:683:GLU:HG3	1:A:706:THR:HG23	1.96	0.48
1:A:704:LEU:HD23	1:A:704:LEU:HA	1.70	0.48
1:A:730:SER:HB3	1:A:733:MET:HB2	1.95	0.47
1:B:868:LEU:HD23	1:B:876:PHE:CE2	2.49	0.47
1:B:879:ILE:O	1:B:879:ILE:HG12	2.13	0.47
1:B:821:ARG:HD2	1:B:853:HIS:HE1	1.79	0.47
1:B:886:TRP:HB2	2:B:166:HOH:O	2.14	0.47
1:A:674:PRO:HB3	2:A:253:HOH:O	2.14	0.47
1:B:687:LEU:CD1	1:B:702:MET:HG2	2.44	0.47
1:B:729:ARG:HD3	2:B:200:HOH:O	2.16	0.46
1:A:883:GLY:HA2	2:A:122:HOH:O	2.14	0.46
1:B:755:GLN:HA	1:B:807:VAL:O	2.16	0.46
1:A:778:LEU:HD22	1:A:787:ARG:HG3	1.98	0.46
1:A:665:GLU:HA	1:A:852:VAL:HB	1.97	0.45
1:A:691:ILE:O	1:A:691:ILE:HG13	2.15	0.45
1:A:764:ARG:HG2	1:A:775:VAL:CG1	2.46	0.45
1:A:821:ARG:HD2	1:A:853:HIS:CE1	2.51	0.45
1:B:682:ALA:HA	1:B:685:GLU:OE1	2.16	0.45
1:B:729:ARG:HB2	2:B:200:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:LYS:HE2	1:B:800:VAL:O	2.17	0.45
1:B:872:LYS:HA	2:B:257:HOH:O	2.16	0.45
1:A:892:THR:CG2	2:A:223:HOH:O	2.65	0.45
1:B:876:PHE:O	1:B:877:LYS:C	2.59	0.45
1:A:764:ARG:HG2	1:A:775:VAL:HG12	1.99	0.44
1:B:821:ARG:HD2	1:B:853:HIS:CE1	2.53	0.44
1:B:876:PHE:C	1:B:878:ASP:N	2.75	0.44
1:B:711:LYS:NZ	2:B:78:HOH:O	2.44	0.44
1:A:687:LEU:CD1	1:A:702:MET:HG2	2.48	0.44
1:B:679:MET:HE2	1:B:713:ILE:HG12	1.99	0.44
1:B:721:LYS:O	1:B:722:GLY:C	2.58	0.44
1:B:885:SER:HA	2:B:108:HOH:O	2.17	0.44
1:B:716:HIS:CE1	2:B:200:HOH:O	2.71	0.43
1:A:821:ARG:HD2	1:A:853:HIS:HE1	1.83	0.43
1:A:772:ASN:ND2	2:A:88:HOH:O	2.51	0.43
1:B:700:LYS:HG2	1:B:888:THR:HB	2.00	0.43
1:A:793:LYS:HG2	1:A:800:VAL:HG21	2.01	0.43
1:A:876:PHE:CD1	1:A:876:PHE:N	2.86	0.43
1:B:709:LYS:O	1:B:713:ILE:HD12	2.19	0.43
1:B:662:ASP:OD2	1:B:849:ASN:N	2.51	0.43
1:B:691:ILE:HG23	1:B:692:ASP:N	2.33	0.43
1:B:821:ARG:HE	1:B:821:ARG:HB2	1.75	0.43
1:B:772:ASN:HB2	2:B:231:HOH:O	2.19	0.43
1:A:691:ILE:HG21	2:A:223:HOH:O	2.18	0.42
1:A:734:ILE:O	1:A:738:GLU:HG3	2.18	0.42
1:B:713:ILE:HG13	1:B:720:LEU:HD11	1.99	0.42
1:A:665:GLU:N	2:A:189:HOH:O	2.53	0.42
1:B:873:ARG:HB2	2:B:112:HOH:O	2.19	0.42
1:B:718:ALA:HB1	2:B:202:HOH:O	2.20	0.42
1:A:854:LYS:HB3	1:A:854:LYS:HE2	1.84	0.42
1:B:707:LEU:HD12	1:B:707:LEU:HA	1.83	0.42
1:B:665:GLU:HG2	2:B:113:HOH:O	2.20	0.41
1:A:691:ILE:HG23	2:A:223:HOH:O	2.19	0.41
1:B:681:LYS:HE3	1:B:901:LEU:CD2	2.49	0.41
1:B:795:GLN:NE2	1:B:818:SER:HB2	2.36	0.41
1:A:883:GLY:HA3	2:A:150:HOH:O	2.20	0.41
1:B:778:LEU:HD13	1:B:805:LEU:HD23	2.03	0.41
1:A:797:ASN:OD1	1:A:797:ASN:C	2.64	0.40
1:A:663:LYS:HA	1:A:849:ASN:HB3	2.03	0.40
1:A:736:THR:O	1:A:740:ILE:HG13	2.21	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	226/271 (83%)	215 (95%)	9 (4%)	2 (1%)	14	9
1	B	224/271 (83%)	204 (91%)	15 (7%)	5 (2%)	5	2
All	All	450/542 (83%)	419 (93%)	24 (5%)	7 (2%)	7	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	875	LEU
1	B	876	PHE
1	A	877	LYS
1	B	877	LYS
1	A	882	SER
1	B	879	ILE
1	B	697	ILE

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	205/240 (85%)	195 (95%)	10 (5%)	22	20
1	B	205/240 (85%)	197 (96%)	8 (4%)	28	28
All	All	410/480 (85%)	392 (96%)	18 (4%)	25	24

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

Mol	Chain	Res	Type
1	A	691	ILE
1	A	700	LYS
1	A	707	LEU
1	A	733	MET
1	A	745	ASP
1	A	764	ARG
1	A	772	ASN
1	A	875	LEU
1	A	882	SER
1	A	897	LYS
1	B	663	LYS
1	B	700	LYS
1	B	706	THR
1	B	707	LEU
1	B	733	MET
1	B	764	ARG
1	B	789	ASP
1	B	864	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	A	725	GLN
1	A	796	ASN
1	A	849	ASN
1	A	853	HIS
1	A	867	GLN
1	B	676	GLN
1	B	689	ASN
1	B	725	GLN
1	B	795	GLN
1	B	815	ASN
1	B	820	ASN
1	B	824	HIS
1	B	853	HIS

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	228/271 (84%)	0.14	10 (4%) 39 38	24, 41, 67, 78	9 (3%)
1	B	225/271 (83%)	0.25	18 (8%) 18 17	26, 43, 74, 82	10 (4%)
All	All	453/542 (83%)	0.19	28 (6%) 26 25	24, 42, 73, 82	19 (4%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	903	VAL	4.6
1	A	666	THR	4.3
1	B	849	ASN	3.5
1	B	702	MET	3.2
1	A	664	ILE	3.1
1	A	809	ALA	3.1
1	A	878	ASP	3.0
1	B	886	TRP	2.8
1	B	697	ILE	2.8
1	A	810	GLY	2.7
1	A	906	TYR	2.7
1	A	811	GLY	2.7
1	B	872	LYS	2.5
1	B	691	ILE	2.5
1	B	695	THR	2.5
1	B	892	THR	2.4
1	B	690	ASN	2.3
1	B	876	PHE	2.3
1	B	693	SER	2.3
1	B	887	ILE	2.3
1	B	687	LEU	2.3
1	A	832	ALA	2.2
1	B	696	GLY	2.2
1	B	722	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	686	ASN	2.1
1	A	876	PHE	2.1
1	B	688	PHE	2.0
1	A	663	LYS	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.