



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:37 AM UTC

PDB ID : 3E66 / pdb_00003e66
Title : Crystal structure of the beta-finger domain of yeast Prp8
Authors : Yang, K.; Zhang, L.; Xu, T.; Heroux, A.; Zhao, R.
Deposited on : 2008-08-14
Resolution : 2.05 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

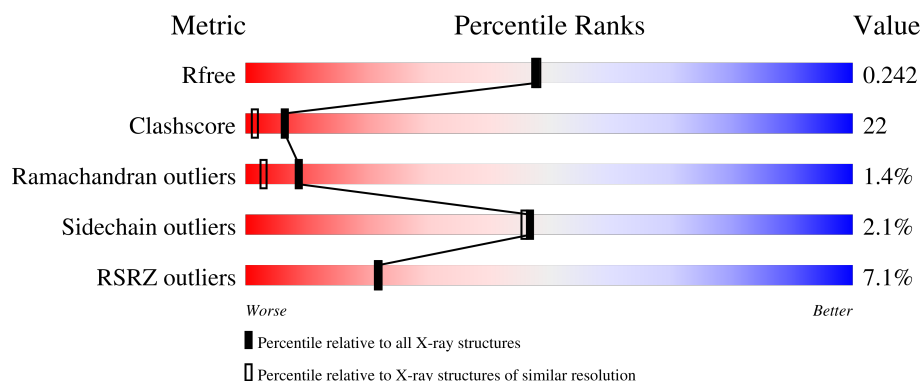
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	282	
1	B	282	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4367 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 PRP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2060	1326	344	382	8			
1	B	255	Total	C	N	O	S	0	0	0
			2060	1326	344	382	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1814	GLY	-	expression tag	UNP P33334
A	1815	PRO	-	expression tag	UNP P33334
A	1816	LEU	-	expression tag	UNP P33334
A	1817	GLY	-	expression tag	UNP P33334
A	1818	SER	-	expression tag	UNP P33334
A	1819	PRO	-	expression tag	UNP P33334
A	1820	GLU	-	expression tag	UNP P33334
A	1821	PHE	-	expression tag	UNP P33334
B	1814	GLY	-	expression tag	UNP P33334
B	1815	PRO	-	expression tag	UNP P33334
B	1816	LEU	-	expression tag	UNP P33334
B	1817	GLY	-	expression tag	UNP P33334
B	1818	SER	-	expression tag	UNP P33334
B	1819	PRO	-	expression tag	UNP P33334
B	1820	GLU	-	expression tag	UNP P33334
B	1821	PHE	-	expression tag	UNP P33334

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	130	Total	O	0	0
			130	130		
2	B	117	Total	O	0	0
			117	117		

- Molecule 1: PRP8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.17Å 84.81Å 94.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 50.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.0 (50.00-2.05) 91.2 (50.00-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.236 0.221 , 0.242	Depositor DCC
R_{free} test set	6922 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4367	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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	0.44	0/2103	0.90	3/2854 (0.1%)
1	B	0.43	0/2103	0.88	3/2854 (0.1%)
All	All	0.44	0/4206	0.89	6/5708 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1931	LYS	N-CA-C	-5.57	106.53	113.38
1	A	1931	LYS	N-CA-C	-5.47	105.33	112.23
1	A	1993	ASP	CB-CA-C	-5.34	110.40	116.54
1	B	1845	ASN	N-CA-C	-5.29	103.90	110.41
1	B	1882	LEU	N-CA-C	5.28	117.68	108.76
1	A	1882	LEU	N-CA-C	5.24	117.94	109.40

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	2060	0	2104	79	0
1	B	2060	0	2104	108	0
2	A	130	0	0	37	1
2	B	117	0	0	50	1
All	All	4367	0	4208	182	1

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 22.

All (182) 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:1836:ASN:HA	2:A:202:HOH:O	1.38	1.24
1:B:1842:GLU:HA	2:B:226:HOH:O	1.39	1.18
1:B:2049:ILE:HA	2:B:149:HOH:O	1.46	1.14
1:B:1852:VAL:HG22	2:B:228:HOH:O	1.44	1.13
1:B:1896:THR:HG22	2:B:224:HOH:O	1.45	1.13
1:A:1876:ASN:HB3	2:A:118:HOH:O	1.51	1.11
1:B:1869:ASN:HA	2:B:35:HOH:O	1.53	1.09
1:B:1844:PHE:HA	2:B:174:HOH:O	1.52	1.06
1:B:1980:LYS:HE3	2:B:206:HOH:O	1.52	1.06
1:A:1895:HIS:HD2	2:A:240:HOH:O	1.41	1.02
1:A:1962:ARG:HH12	1:B:1949:LEU:HB3	1.23	1.01
1:A:2032:ILE:HG22	2:A:203:HOH:O	1.62	0.99
1:B:2032:ILE:HD11	1:B:2047:GLN:HE22	1.31	0.95
1:B:1885:LYS:HE2	2:B:204:HOH:O	1.67	0.94
1:B:1863:HIS:HE1	2:B:198:HOH:O	1.50	0.92
1:B:1836:ASN:H	1:B:1839:ASN:HD21	1.21	0.89
1:A:2015:LEU:HD22	2:A:141:HOH:O	1.72	0.88
1:B:1957:ARG:HD2	2:B:197:HOH:O	1.74	0.87
1:B:2037:TYR:CE2	2:B:245:HOH:O	2.28	0.85
1:B:1863:HIS:CE1	2:B:198:HOH:O	2.26	0.84
1:A:1861:THR:HA	2:A:209:HOH:O	1.77	0.83
1:B:1904:ARG:HG3	1:B:1907:GLN:HB3	1.60	0.82
1:A:1983:GLU:HB2	2:A:177:HOH:O	1.79	0.82
1:B:1867:GLU:HG3	1:B:1868:GLY:H	1.45	0.81
1:A:1962:ARG:NH1	1:B:1949:LEU:HB3	1.96	0.81
1:B:1864:LYS:HD2	1:B:1869:ASN:HB3	1.64	0.79
1:B:2035:LYS:HD3	2:B:245:HOH:O	1.82	0.78
1:B:1979:MET:HE2	1:B:1979:MET:HA	1.66	0.78
1:B:2052:GLU:OE1	2:B:149:HOH:O	2.02	0.78
1:A:1895:HIS:CD2	2:A:240:HOH:O	2.26	0.77
1:A:1837:SER:H	1:A:2086:GLN:NE2	1.82	0.76
1:B:1953:ASN:HB2	2:B:3:HOH:O	1.85	0.76
1:A:1970:SER:HB3	2:A:141:HOH:O	1.85	0.76
1:B:1864:LYS:HE2	2:B:72:HOH:O	1.85	0.75
1:B:1868:GLY:HA3	2:B:53:HOH:O	1.86	0.74
1:B:1976:ASP:HB3	2:B:206:HOH:O	1.86	0.74
1:A:1837:SER:H	1:A:2086:GLN:HE21	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1961:LEU:HG	2:A:202:HOH:O	1.87	0.73
1:A:1969:MET:SD	2:A:158:HOH:O	2.46	0.73
1:A:2027:LEU:HB3	2:A:169:HOH:O	1.88	0.73
1:A:2048:TRP:O	1:A:2052:GLU:HG3	1.89	0.73
1:B:2041:PRO:HG2	1:B:2043:PHE:CE1	2.24	0.72
1:B:1885:LYS:CE	2:B:204:HOH:O	2.33	0.71
1:B:1957:ARG:CD	2:B:197:HOH:O	2.35	0.70
1:B:1976:ASP:CB	2:B:206:HOH:O	2.37	0.70
1:A:2042:SER:N	2:A:203:HOH:O	2.22	0.69
1:A:1983:GLU:N	2:A:240:HOH:O	2.25	0.69
1:B:1836:ASN:H	1:B:1839:ASN:ND2	1.91	0.69
1:B:2035:LYS:CD	2:B:245:HOH:O	2.40	0.68
2:A:209:HOH:O	1:B:1925:PRO:HB3	1.91	0.68
1:B:2032:ILE:HD11	1:B:2047:GLN:NE2	2.08	0.68
1:A:2041:PRO:HG2	1:A:2043:PHE:CE1	2.28	0.68
1:B:1864:LYS:CE	2:B:72:HOH:O	2.42	0.68
1:A:2027:LEU:C	2:A:169:HOH:O	2.37	0.67
1:A:1867:GLU:OE2	2:A:120:HOH:O	2.12	0.67
1:A:1970:SER:CB	2:A:141:HOH:O	2.42	0.67
1:B:2048:TRP:O	1:B:2052:GLU:HG3	1.95	0.66
1:A:1861:THR:CB	2:A:209:HOH:O	2.44	0.66
1:B:1874:ALA:C	2:B:224:HOH:O	2.38	0.66
1:A:1984:PRO:HD2	2:A:177:HOH:O	1.96	0.65
1:B:2087:ASN:ND2	2:B:130:HOH:O	2.14	0.65
1:A:1849:LYS:HG2	1:A:1932:GLN:HG3	1.79	0.64
1:B:2087:ASN:ND2	2:B:186:HOH:O	2.31	0.64
1:B:1867:GLU:CG	1:B:1868:GLY:H	2.11	0.63
1:B:1860:VAL:HB	1:B:1872:THR:HG23	1.81	0.62
1:A:2046:GLU:H	1:A:2046:GLU:CD	2.07	0.61
1:A:2064:GLY:CA	1:A:2071:ILE:HD11	2.30	0.61
1:A:2021:SER:HA	1:A:2024:MET:HE2	1.80	0.61
1:B:1875:ILE:N	2:B:224:HOH:O	2.33	0.61
1:B:1845:ASN:CG	2:B:226:HOH:O	2.43	0.60
1:A:2018:ASN:HB3	1:A:2058:LEU:HD21	1.82	0.60
1:A:1942:ASP:HB3	1:A:1943:PRO:HD3	1.82	0.60
1:B:2087:ASN:N	2:B:229:HOH:O	2.34	0.59
1:B:1839:ASN:C	1:B:1839:ASN:HD22	2.10	0.59
1:A:1836:ASN:HB2	1:A:2086:GLN:HE22	1.68	0.59
1:B:1833:PRO:N	2:B:185:HOH:O	2.35	0.58
1:B:1892:LYS:HE2	1:B:1916:GLU:OE1	2.04	0.58
1:B:1869:ASN:C	2:B:35:HOH:O	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:MET:CB	2:A:158:HOH:O	2.52	0.57
1:A:1981:ALA:C	2:A:240:HOH:O	2.47	0.57
1:A:1983:GLU:CB	2:A:177:HOH:O	2.45	0.57
1:B:1976:ASP:CG	2:B:206:HOH:O	2.46	0.57
1:B:1868:GLY:CA	2:B:53:HOH:O	2.48	0.57
1:A:2027:LEU:CA	2:A:169:HOH:O	2.54	0.56
1:A:2064:GLY:HA3	1:A:2071:ILE:HD11	1.86	0.56
1:B:1845:ASN:OD1	2:B:226:HOH:O	2.18	0.56
1:B:1957:ARG:HB2	2:B:197:HOH:O	2.06	0.56
1:B:2035:LYS:HD2	1:B:2038:HIS:CE1	2.40	0.56
1:B:1932:GLN:OE1	2:B:197:HOH:O	2.18	0.55
1:B:1837:SER:H	1:B:2086:GLN:NE2	2.05	0.54
1:B:1864:LYS:HD2	1:B:1869:ASN:CB	2.34	0.54
1:B:1836:ASN:HB2	1:B:2086:GLN:HE22	1.71	0.54
1:A:1922:ARG:HG3	1:A:1951:PHE:HZ	1.73	0.54
1:A:1895:HIS:O	1:A:1898:VAL:HG13	2.08	0.54
1:A:1984:PRO:N	2:A:177:HOH:O	2.41	0.54
1:A:1969:MET:HB3	2:A:158:HOH:O	2.07	0.53
1:A:1984:PRO:CD	2:A:177:HOH:O	2.53	0.53
1:B:1874:ALA:HB1	2:B:224:HOH:O	2.09	0.53
1:B:1868:GLY:C	2:B:53:HOH:O	2.52	0.53
1:A:2015:LEU:HD13	2:A:141:HOH:O	2.08	0.52
1:A:1969:MET:CA	2:A:158:HOH:O	2.57	0.52
1:B:1852:VAL:HG13	2:B:228:HOH:O	2.09	0.52
1:B:1860:VAL:CB	1:B:1872:THR:HG23	2.40	0.52
1:B:1843:LEU:O	2:B:174:HOH:O	2.19	0.52
1:B:1969:MET:HE2	1:B:1969:MET:HA	1.92	0.52
1:A:1903:LYS:O	1:A:1904:ARG:C	2.54	0.51
1:A:1969:MET:HA	1:A:1969:MET:HE2	1.92	0.51
1:B:1885:LYS:HD3	2:B:174:HOH:O	2.11	0.50
1:A:1848:ILE:H	1:A:1931:LYS:NZ	2.10	0.50
1:B:1859:ARG:NH2	1:B:1979:MET:HE3	2.27	0.50
1:A:1854:ASP:OD1	1:A:1937:ARG:HD3	2.12	0.50
1:B:1966:SER:OG	1:B:2016:LYS:HE3	2.12	0.50
1:B:1926:LYS:HG2	2:B:134:HOH:O	2.10	0.49
1:B:1933:ILE:HG21	1:B:1944:LEU:HD21	1.94	0.49
1:A:2086:GLN:O	1:A:2087:ASN:HB2	2.12	0.49
1:B:1895:HIS:O	1:B:1898:VAL:HG22	2.12	0.49
1:B:2029:ASP:OD2	1:B:2032:ILE:HG12	2.12	0.49
1:A:1904:ARG:HD3	1:A:1907:GLN:OE1	2.13	0.49
1:A:2020:GLU:H	1:A:2020:GLU:CD	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1922:ARG:NH2	2:A:98:HOH:O	2.45	0.48
1:B:1853:ASP:HB3	1:B:1880:PHE:HB3	1.94	0.48
1:B:1974:LEU:O	1:B:1977:VAL:HG12	2.13	0.48
1:B:1885:LYS:HB2	2:B:174:HOH:O	2.14	0.48
1:B:2086:GLN:O	1:B:2087:ASN:HB2	2.14	0.48
1:B:1995:TRP:HB3	1:B:1999:ILE:HD11	1.96	0.47
1:B:2080:LYS:HB3	2:B:137:HOH:O	2.14	0.47
1:B:2021:SER:O	1:B:2025:ILE:HG13	2.15	0.47
1:A:2075:THR:OG1	1:A:2078:GLU:HG3	2.15	0.46
1:A:1974:LEU:O	1:A:1977:VAL:HG12	2.15	0.46
1:B:1957:ARG:CB	2:B:197:HOH:O	2.62	0.46
1:A:1970:SER:C	2:A:141:HOH:O	2.58	0.46
1:A:1899:TRP:O	1:A:1900:ALA:C	2.59	0.46
1:B:1867:GLU:CG	1:B:1868:GLY:N	2.78	0.46
1:B:1834:PHE:CD1	1:B:1834:PHE:N	2.84	0.46
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.55	0.46
1:A:2044:THR:OG1	1:A:2047:GLN:HG3	2.15	0.46
1:A:2032:ILE:HD11	1:A:2047:GLN:NE2	2.31	0.45
2:A:209:HOH:O	1:B:1925:PRO:CB	2.58	0.45
1:A:1877:GLY:N	2:A:118:HOH:O	2.48	0.45
1:B:1904:ARG:CG	1:B:1907:GLN:HB3	2.41	0.45
1:B:2052:GLU:CD	2:B:149:HOH:O	2.52	0.45
1:A:1870:VAL:HG22	1:B:1988:LEU:CD2	2.47	0.45
1:B:1864:LYS:HD2	1:B:1869:ASN:CG	2.43	0.44
1:A:1865:THR:OG1	1:A:1867:GLU:HG2	2.18	0.44
1:B:1860:VAL:HG11	1:B:1872:THR:CG2	2.47	0.44
1:B:1995:TRP:O	1:B:1999:ILE:HG12	2.18	0.44
1:A:1870:VAL:HG22	1:B:1988:LEU:HD21	2.00	0.44
1:B:1984:PRO:O	1:B:1985:GLN:HB3	2.18	0.44
1:A:1894:ILE:O	2:A:118:HOH:O	2.21	0.43
1:B:1921:VAL:HG11	1:B:1948:MET:HE1	1.98	0.43
1:B:2034:ILE:HG13	1:B:2040:TRP:O	2.18	0.43
1:B:1942:ASP:HB3	1:B:1943:PRO:HD3	2.00	0.43
1:B:1839:ASN:ND2	1:B:1839:ASN:C	2.77	0.42
1:A:2056:ARG:NE	2:A:235:HOH:O	2.43	0.42
1:A:1983:GLU:CG	2:A:177:HOH:O	2.67	0.42
1:B:1899:TRP:O	1:B:1900:ALA:C	2.63	0.42
1:B:1922:ARG:NH2	2:B:58:HOH:O	2.51	0.42
1:A:2066:LYS:HA	2:A:159:HOH:O	2.20	0.42
1:B:2075:THR:OG1	1:B:2078:GLU:HG3	2.19	0.42
1:A:2087:ASN:HD22	1:A:2087:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2086:GLN:O	1:B:2087:ASN:CB	2.68	0.42
1:A:1879:ILE:HB	1:A:1892:LYS:HB3	2.02	0.42
1:A:1846:ASN:OD1	1:A:1885:LYS:NZ	2.53	0.41
1:A:1867:GLU:HG2	1:A:1867:GLU:H	1.72	0.41
1:A:1987:VAL:C	1:A:1988:LEU:HD23	2.46	0.41
1:A:1962:ARG:NH1	1:B:1949:LEU:CB	2.78	0.41
1:B:1904:ARG:HG3	1:B:1907:GLN:CB	2.40	0.41
1:B:1870:VAL:N	2:B:35:HOH:O	2.52	0.41
1:A:1988:LEU:HD23	1:A:1988:LEU:N	2.36	0.41
1:B:1849:LYS:HB3	1:B:1932:GLN:HG2	2.03	0.41
1:B:1864:LYS:CD	1:B:1869:ASN:HB3	2.44	0.41
1:B:1918:SER:O	1:B:1922:ARG:HG3	2.21	0.41
1:B:1927:GLU:OE1	2:B:193:HOH:O	2.22	0.41
1:A:1848:ILE:HG13	1:A:1931:LYS:HZ2	1.85	0.40
1:A:2046:GLU:CD	1:A:2046:GLU:N	2.78	0.40
1:A:1845:ASN:O	1:A:1885:LYS:HD2	2.21	0.40
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.46	0.40
1:B:1864:LYS:NZ	2:B:72:HOH:O	2.31	0.40
1:B:1904:ARG:HG3	1:B:1904:ARG:O	2.22	0.40
1:A:1853:ASP:HB3	1:A:1880:PHE:HB3	2.03	0.40
1:B:1933:ILE:HD12	1:B:1948:MET:HE2	2.03	0.40
1:B:2032:ILE:HG21	1:B:2043:PHE:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:123:HOH:O	2:B:184:HOH:O[4_556]	2.18	0.02

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	253/282 (90%)	241 (95%)	11 (4%)	1 (0%)	30	22
1	B	253/282 (90%)	239 (94%)	8 (3%)	6 (2%)	4	1
All	All	506/564 (90%)	480 (95%)	19 (4%)	7 (1%)	9	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1900	ALA
1	B	2028	SER
1	B	1865	THR
1	B	1869	ASN
1	B	1900	ALA
1	B	1870	VAL
1	B	1901	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	233/256 (91%)	229 (98%)	4 (2%)	53	53
1	B	233/256 (91%)	227 (97%)	6 (3%)	40	37
All	All	466/512 (91%)	456 (98%)	10 (2%)	47	46

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1898	VAL
1	A	1988	LEU
1	A	2055	MET
1	A	2087	ASN
1	B	1839	ASN
1	B	1863	HIS
1	B	1866	PHE
1	B	1872	THR
1	B	1945	GLU

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Mol	Chain	Res	Type
1	B	2076	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1863	HIS
1	A	1895	HIS
1	A	1953	ASN
1	A	1985	GLN
1	A	2086	GLN
1	A	2087	ASN
1	B	1839	ASN
1	B	1863	HIS
1	B	1932	GLN
1	B	1985	GLN
1	B	2054	GLN
1	B	2068	ASN
1	B	2086	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	255/282 (90%)	0.26	16 (6%) 26 26	18, 33, 61, 78	0
1	B	255/282 (90%)	0.53	20 (7%) 19 19	23, 38, 66, 99	0
All	All	510/564 (90%)	0.39	36 (7%) 22 22	18, 35, 64, 99	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1866	PHE	5.9
1	B	1868	GLY	5.4
1	B	1833	PRO	4.0
1	B	1869	ASN	3.7
1	B	1904	ARG	3.6
1	B	2087	ASN	3.5
1	A	2030	PRO	3.5
1	B	2030	PRO	3.3
1	B	2073	ALA	3.2
1	A	2027	LEU	2.9
1	A	2031	THR	2.8
1	B	2076	GLN	2.8
1	A	1833	PRO	2.6
1	A	1900	ALA	2.6
1	A	2024	MET	2.5
1	B	1949	LEU	2.4
1	B	1834	PHE	2.4
1	A	1979	MET	2.4
1	A	2067	TYR	2.3
1	A	2057	ASP	2.3
1	B	2075	THR	2.3
1	B	1979	MET	2.3
1	A	1904	ARG	2.3
1	B	2024	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2027	LEU	2.3
1	B	1911	TRP	2.3
1	B	1867	GLU	2.2
1	A	1901	GLY	2.2
1	A	2028	SER	2.2
1	B	2071	ILE	2.2
1	A	1926	LYS	2.2
1	B	2057	ASP	2.2
1	A	2064	GLY	2.1
1	A	2071	ILE	2.1
1	A	2087	ASN	2.0
1	B	1864	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.