



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 1KZY / pdb_00001kzy
Title : Crystal Structure of the 53bp1 BRCT Region Complexed to Tumor Suppressor P53
Authors : Joo, W.S.; Jeffrey, P.D.; Cantor, S.B.; Finnin, M.S.; Livingston, D.M.; Pavletich, N.P.
Deposited on : 2002-02-08
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

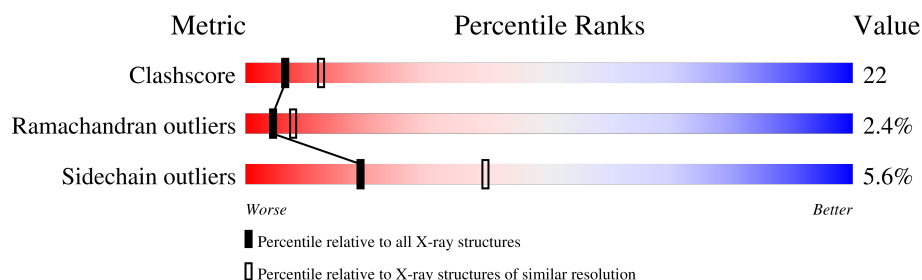
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	195	 64% 33% . .
1	B	195	 62% 33% 6%
2	C	259	 53% 31% 6% 10%
2	D	259	 50% 33% 7% 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6986 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 CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1530	942	282	290	16			
1	B	195	Total	C	N	O	S	0	0	0
			1530	942	282	290	16			

- Molecule 2 is a protein called TUMOR SUPPRESSOR P53-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	232	Total	C	N	O	S	0	0	0
			1854	1184	320	339	11			
2	D	232	Total	C	N	O	S	0	0	0
			1854	1184	320	339	11			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	58	Total	O	0	0
			58	58		
4	C	50	Total	O	0	0
			50	50		
4	D	51	Total	O	0	0
			51	51		

	A1714	L1715	E1716	Q1717	R1718	G1719	P1720	L1721	P1722	P1723	L1724	N1725		G1731		L1735	L1736	T1737		T1740	THR	SER	ASP	LYS	LEU	ALA	SER	ARG	SER	LYS	LEU	PRO	ASP	GLY	PRO	THR	GLY	SER	SER	GLU	GLU	GLU	GLU	PHE	LEU	GLU	I1768	P1769	P1770	F1771	N1772	K1773	Q1774	Y1775	T1776	E1777	S1778	Q1779	L1780
R1781		G1785	Y1786	L1787	L1788	E1789		N1792	E1793	A1794	Q1795	C1796		A1799	Y1800	Q1801	C1802	L1803	L1804	I1805	A1806	D1807	Q1808	H1809		K1814		H1828		H1832		C1835	H1836	A1837	N1838		L1848		S1853	L1854	E1855	E1856	Q1857	R1858	I1859		N1871		V1874	L1875		Q1881	Q1882	M1883	F1884	L1885	E1886		E1890
	T1894		A1898		K1901	Q1902	H1903	H1904	S1905	S1906	A1907	H1908	H1909	K1910	D1911	I1912	A1913	L1914	G1915	V1916		V1919	V1920	V1921	T1922	D1923	P1924		P1927		V1930		L1937	Q1938		V1941	V1942	S1943		Q1949		V1953	G1954	E1955	R1956	I1957		Q1961	H1962	P1963	K1964	Y1965	K1966	H1967	D1968	Y1969	V1970	S1971	H1972

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.13Å 94.98Å 133.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.77	0/1565	1.14	10/2121 (0.5%)
1	B	0.76	0/1565	1.14	15/2121 (0.7%)
2	C	0.74	0/1901	1.13	8/2584 (0.3%)
2	D	0.79	0/1901	1.15	13/2584 (0.5%)
All	All	0.77	0/6932	1.14	46/9410 (0.5%)

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	1

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1722	LEU	N-CA-C	-9.74	96.84	110.29
2	C	1799	ALA	N-CA-C	9.72	121.95	111.36
2	C	1722	LEU	N-CA-C	-7.39	99.45	110.24
1	A	180	GLU	N-CA-C	-7.32	103.33	111.82
2	D	1768	ILE	CA-C-N	7.32	127.91	120.38
2	D	1768	ILE	C-N-CA	7.32	127.91	120.38
1	A	237	MET	N-CA-C	7.28	121.81	113.15
1	A	189	ALA	N-CA-C	6.94	118.39	109.72
1	B	154	GLY	N-CA-C	-6.90	105.95	114.92
1	B	189	ALA	N-CA-C	6.89	118.82	109.24
2	D	1723	PRO	N-CA-C	6.87	126.62	112.47
1	B	180	GLU	N-CA-C	-6.83	103.85	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLY	N-CA-C	-6.79	105.68	114.85
2	C	1768	ILE	CA-C-N	6.66	127.24	120.38
2	C	1768	ILE	C-N-CA	6.66	127.24	120.38
1	B	237	MET	N-CA-C	6.65	121.06	113.15
1	A	131	ASN	N-CA-C	-6.40	102.41	111.24
1	B	131	ASN	N-CA-C	-6.27	102.58	111.24
1	A	150	THR	CA-C-N	6.16	126.73	120.38
1	A	150	THR	C-N-CA	6.16	126.73	120.38
1	A	265	LEU	N-CA-C	-5.97	106.63	114.04
1	B	203	VAL	N-CA-C	5.94	116.68	108.84
2	D	1799	ALA	N-CA-C	5.81	120.38	113.12
1	B	259	ASP	N-CA-C	-5.81	101.36	110.36
2	C	1882	GLN	N-CA-C	-5.80	102.32	110.50
1	B	190	PRO	N-CA-C	-5.78	103.64	110.70
1	B	274	VAL	N-CA-C	-5.76	99.58	107.99
2	D	1801	GLN	N-CA-C	-5.67	99.28	108.41
1	B	150	THR	CA-C-N	5.61	123.70	119.66
1	B	150	THR	C-N-CA	5.61	123.70	119.66
1	A	173	VAL	CB-CA-C	-5.54	104.59	111.08
2	D	1785	GLY	N-CA-C	-5.45	105.11	112.14
1	B	164	LYS	N-CA-C	5.43	118.37	111.69
1	B	256	THR	N-CA-C	5.37	117.71	109.07
1	A	195	ILE	N-CA-C	5.30	116.22	108.58
2	D	1942	VAL	N-CA-C	5.21	116.21	108.65
2	C	1874	VAL	N-CA-C	5.20	116.79	108.89
2	D	1848	LEU	CA-C-N	-5.17	114.92	120.03
2	D	1848	LEU	C-N-CA	-5.17	114.92	120.03
2	C	1826	VAL	N-CA-C	5.17	116.02	108.53
2	D	1874	VAL	N-CA-C	5.13	116.92	108.97
2	D	1922	THR	N-CA-C	5.13	114.92	108.45
2	D	1800	TYR	N-CA-C	5.13	117.47	109.52
2	C	1794	ALA	N-CA-C	-5.12	104.64	111.24
1	B	143	VAL	N-CA-C	-5.09	100.98	108.11
1	B	251	ILE	CB-CA-C	-5.02	104.31	111.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TYR	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	1530	0	1485	56	0
1	B	1530	0	1485	63	0
2	C	1854	0	1814	80	0
2	D	1854	0	1814	96	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	57	0	0	4	0
4	B	58	0	0	7	0
4	C	50	0	0	9	0
4	D	51	0	0	11	0
All	All	6986	0	6598	290	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 22.

All (290) 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:D:1774:GLN:HA	4:D:51:HOH:O	1.54	1.06
2:D:1890:GLU:O	2:D:1894:THR:HG22	1.58	1.01
2:D:1923:ASP:HB2	2:D:1924:PRO:HD2	1.43	1.00
1:B:171:GLU:HG3	4:B:318:HOH:O	1.60	1.00
2:D:1776:THR:HA	2:D:1779:GLN:HE21	1.25	1.00
2:C:1923:ASP:HB2	2:C:1924:PRO:HD2	1.49	0.94
2:D:1966:LYS:HG2	4:D:64:HOH:O	1.68	0.94
2:D:1719:ARG:HH21	2:D:1772:ASN:HD21	0.98	0.92
1:A:97:VAL:HG21	1:A:169:MET:HB3	1.49	0.92
2:D:1719:ARG:HH21	2:D:1772:ASN:ND2	1.66	0.91
2:D:1913:ALA:O	2:D:1916:VAL:HG12	1.69	0.91
2:D:1725:ASN:HB2	2:D:1838:ASN:HD21	1.36	0.91
1:B:283:ARG:O	1:B:287:GLU:HG2	1.74	0.86
2:C:1913:ALA:O	2:C:1916:VAL:HG12	1.77	0.84
2:C:1779:GLN:HE22	2:C:1832:HIS:HD2	1.27	0.83
2:D:1776:THR:HA	2:D:1779:GLN:NE2	1.92	0.83
1:A:104:GLN:NE2	1:A:110:ARG:HG2	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:O	1:A:287:GLU:HG2	1.82	0.80
2:C:1962:HIS:HD2	2:C:1964:LYS:H	1.30	0.80
2:D:1772:ASN:HA	4:D:58:HOH:O	1.82	0.80
2:D:1736:LEU:HD22	2:D:1805:ILE:HB	1.62	0.79
2:C:1736:LEU:HD22	2:C:1805:ILE:HB	1.65	0.79
2:C:1794:ALA:N	4:C:207:HOH:O	2.14	0.79
2:C:1904:HIS:O	2:C:1908:HIS:HB2	1.84	0.78
2:D:1771:PHE:HB2	2:D:1807:ASP:HB3	1.66	0.78
2:C:1716:GLU:HG3	2:C:1717:GLU:N	1.98	0.78
2:C:1903:HIS:CD2	2:C:1912:ILE:HD11	2.19	0.77
2:C:1726:LYS:HG2	4:C:216:HOH:O	1.85	0.76
2:C:1779:GLN:HE22	2:C:1832:HIS:CD2	2.03	0.76
1:B:97:VAL:HG21	1:B:169:MET:HB3	1.68	0.76
2:C:1949:GLN:HB3	2:C:1957:ILE:HD11	1.69	0.75
2:D:1736:LEU:CD2	2:D:1805:ILE:HB	2.17	0.75
2:D:1962:HIS:HD2	2:D:1964:LYS:H	1.35	0.75
1:B:202:ARG:NE	4:B:337:HOH:O	2.19	0.74
2:C:1828:HIS:HD2	2:C:1832:HIS:CE1	2.05	0.74
1:A:201:LEU:N	1:A:201:LEU:HD12	2.03	0.74
1:A:175:ARG:HG3	1:A:238:CYS:SG	2.28	0.73
1:A:182:CYS:HB3	1:B:209:ARG:NH2	2.03	0.73
2:D:1904:HIS:O	2:D:1908:HIS:HB2	1.89	0.72
1:B:120:LYS:N	1:B:120:LYS:HD2	2.04	0.72
2:C:1796:CYS:HA	2:C:1802:CYS:SG	2.30	0.72
2:C:1871:ASN:HD22	2:C:1898:ALA:HB2	1.55	0.72
1:A:201:LEU:HD12	1:A:201:LEU:H	1.53	0.72
2:C:1914:LEU:HD12	2:C:1933:CYS:HB3	1.72	0.71
1:B:99:SER:OG	1:B:101:LYS:HD2	1.90	0.71
2:D:1773:LYS:O	2:D:1773:LYS:HG2	1.90	0.71
2:D:1903:HIS:CD2	2:D:1912:ILE:HD11	2.25	0.71
1:A:190:PRO:HB2	1:A:193:HIS:HD2	1.54	0.71
2:C:1774:GLN:HG3	2:D:1731:GLY:HA2	1.73	0.70
1:B:200:ASN:C	1:B:201:LEU:HD12	2.17	0.70
1:A:130:LEU:HB3	4:A:346:HOH:O	1.92	0.69
2:C:1792:ASN:OD1	2:C:1795:GLN:HG3	1.92	0.69
1:B:158:ARG:HH12	1:B:206:LEU:HD13	1.58	0.69
2:D:1923:ASP:HB2	2:D:1924:PRO:CD	2.19	0.68
1:A:193:HIS:CE1	1:A:214:HIS:HB3	2.29	0.67
1:B:211:THR:O	1:B:212:PHE:HB2	1.94	0.67
2:C:1774:GLN:CG	2:D:1731:GLY:HA2	2.23	0.67
2:D:1725:ASN:HB2	2:D:1838:ASN:ND2	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1910:LYS:H	2:D:1910:LYS:HD3	1.60	0.67
2:C:1735:LEU:C	2:C:1736:LEU:HD23	2.20	0.66
2:C:1962:HIS:CD2	2:C:1964:LYS:H	2.12	0.66
2:C:1876:LEU:HD23	2:C:1921:VAL:HB	1.77	0.66
2:D:1771:PHE:CB	2:D:1807:ASP:HB3	2.25	0.66
1:A:211:THR:O	1:A:212:PHE:HB2	1.94	0.66
1:B:185:SER:C	1:B:187:GLY:H	2.02	0.66
2:D:1949:GLN:HG2	2:D:1965:TYR:OH	1.95	0.65
1:B:166:SER:HA	1:B:169:MET:HG3	1.78	0.65
2:C:1890:GLU:O	2:C:1894:THR:HG22	1.94	0.65
1:B:156:ARG:HG2	1:B:156:ARG:HH11	1.62	0.65
2:D:1792:ASN:OD1	2:D:1794:ALA:HB3	1.97	0.64
1:A:158:ARG:HH12	1:A:206:LEU:HD13	1.63	0.64
2:D:1901:LYS:NZ	2:D:1912:ILE:HG23	2.13	0.63
2:D:1910:LYS:HD3	2:D:1910:LYS:N	2.13	0.63
1:A:256:THR:HG22	1:A:258:GLU:HG2	1.79	0.63
1:A:119:ALA:O	1:A:122:VAL:HG12	1.98	0.63
1:B:201:LEU:HD12	1:B:201:LEU:N	2.13	0.63
2:C:1726:LYS:HE2	4:C:182:HOH:O	1.97	0.63
1:B:186:ASP:O	1:B:188:LEU:N	2.28	0.63
2:D:1953:VAL:HG12	2:D:1955:GLU:HG2	1.81	0.63
2:C:1724:LEU:HB3	4:C:184:HOH:O	1.99	0.62
1:B:188:LEU:HG	4:B:320:HOH:O	1.98	0.62
2:C:1828:HIS:HD2	2:C:1832:HIS:HE1	1.47	0.62
1:B:259:ASP:OD1	1:B:263:ASN:HB2	1.99	0.62
2:C:1890:GLU:O	2:C:1894:THR:CG2	2.47	0.62
2:D:1853:SER:HA	2:D:1949:GLN:OE1	1.99	0.62
2:D:1970:VAL:O	2:D:1971:SER:C	2.42	0.61
2:D:1906:SER:O	2:D:1908:HIS:N	2.34	0.61
2:C:1771:PHE:HB2	2:C:1807:ASP:HB3	1.81	0.61
2:C:1804:LEU:HD23	2:C:1804:LEU:C	2.25	0.61
2:D:1962:HIS:CD2	2:D:1964:LYS:H	2.18	0.61
1:B:285:GLU:HA	1:B:288:ASN:ND2	2.16	0.61
1:B:137:LEU:HD21	1:B:237:MET:C	2.26	0.60
2:D:1716:GLU:HG3	2:D:1717:GLU:N	2.16	0.60
1:A:248:ARG:HD2	4:A:343:HOH:O	2.01	0.60
2:C:1901:LYS:NZ	2:C:1912:ILE:HG23	2.16	0.60
2:C:1796:CYS:CB	2:C:1802:CYS:HG	2.14	0.60
1:A:222:PRO:HG3	4:A:312:HOH:O	2.03	0.59
1:B:156:ARG:HG2	1:B:156:ARG:NH1	2.17	0.59
1:B:190:PRO:HB2	1:B:193:HIS:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1772:ASN:CA	4:D:58:HOH:O	2.46	0.59
2:D:1723:PRO:O	2:D:1725:ASN:N	2.36	0.58
2:D:1737:THR:HG23	2:D:1814:LYS:HD2	1.86	0.58
1:A:247:ASN:O	1:A:248:ARG:HB2	2.03	0.58
1:A:193:HIS:ND1	1:A:214:HIS:HB3	2.18	0.58
2:D:1881:GLN:OE1	2:D:1885:LEU:HD12	2.04	0.58
1:A:104:GLN:HE22	1:A:110:ARG:HG2	1.69	0.58
2:D:1809:HIS:CE1	2:D:1859:ILE:HD13	2.39	0.58
1:A:182:CYS:HB3	1:B:209:ARG:HH22	1.66	0.57
2:D:1796:CYS:HA	2:D:1802:CYS:SG	2.44	0.57
2:D:1719:ARG:NH2	2:D:1772:ASN:ND2	2.46	0.57
2:D:1966:LYS:CG	4:D:64:HOH:O	2.38	0.57
1:B:196:ARG:NH2	1:B:237:MET:HE2	2.20	0.57
2:D:1910:LYS:H	2:D:1910:LYS:CD	2.18	0.56
2:C:1801:GLN:HG2	4:C:208:HOH:O	2.05	0.56
2:C:1793:GLU:HA	2:C:1796:CYS:HB2	1.88	0.56
2:D:1871:ASN:HA	2:D:1898:ALA:HB2	1.88	0.56
1:A:99:SER:OG	1:A:101:LYS:HD2	2.06	0.56
1:A:120:LYS:HD2	1:A:120:LYS:N	2.21	0.56
2:C:1736:LEU:HD23	2:C:1736:LEU:N	2.21	0.56
2:D:1804:LEU:C	2:D:1804:LEU:HD23	2.32	0.55
2:D:1881:GLN:O	2:D:1886:GLU:HG2	2.06	0.55
2:C:1717:GLU:O	2:C:1836:HIS:HE1	1.89	0.55
2:C:1910:LYS:HD3	2:C:1910:LYS:N	2.21	0.55
1:B:112:GLY:O	1:B:144:GLN:HG3	2.06	0.55
2:C:1740:THR:HG22	2:C:1740:THR:O	2.06	0.55
2:D:1809:HIS:HE1	2:D:1859:ILE:HD13	1.72	0.55
1:A:112:GLY:O	1:A:144:GLN:HG3	2.07	0.55
2:D:1718:GLN:OE1	2:D:1770:PRO:HD2	2.07	0.54
1:B:183:SER:C	1:B:185:SER:H	2.14	0.54
1:A:97:VAL:CG2	1:A:169:MET:HB3	2.31	0.54
2:D:1882:GLN:HA	4:D:32:HOH:O	2.06	0.54
1:B:136:GLN:HB2	1:B:139:LYS:HG3	1.89	0.54
1:B:175:ARG:HG2	1:B:238:CYS:SG	2.48	0.54
2:C:1953:VAL:HG12	2:C:1955:GLU:HG2	1.90	0.54
2:C:1885:LEU:O	2:C:1889:SER:HB2	2.08	0.54
2:D:1718:GLN:HB3	2:D:1769:PRO:HB3	1.90	0.53
2:C:1828:HIS:CD2	2:C:1832:HIS:CE1	2.93	0.53
2:D:1786:TYR:HE2	2:D:1788:LEU:HD23	1.74	0.53
1:A:273:ARG:NH1	1:A:281:ASP:OD1	2.41	0.53
2:D:1723:PRO:O	2:D:1724:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD12	1:B:142:PRO:HG3	1.91	0.52
1:A:137:LEU:HD21	1:A:237:MET:C	2.34	0.52
2:C:1923:ASP:HB2	2:C:1924:PRO:CD	2.31	0.52
2:D:1890:GLU:O	2:D:1894:THR:CG2	2.46	0.52
2:D:1781:ARG:HG3	2:D:1781:ARG:HH11	1.76	0.51
2:D:1737:THR:HG21	2:D:1814:LYS:HB2	1.91	0.51
1:B:159:ALA:HB3	1:B:216:VAL:HG13	1.92	0.51
2:C:1949:GLN:HG2	2:C:1965:TYR:OH	2.11	0.51
2:D:1855:GLU:HB2	4:D:163:HOH:O	2.11	0.51
1:B:280:ARG:HH11	1:B:280:ARG:HG2	1.76	0.51
2:C:1881:GLN:HG3	2:C:1886:GLU:OE2	2.10	0.51
1:A:114:LEU:HD12	1:A:142:PRO:HG3	1.93	0.51
2:C:1853:SER:HA	2:C:1949:GLN:OE1	2.11	0.51
2:C:1920:VAL:HB	2:C:1941:VAL:HG22	1.93	0.51
2:D:1871:ASN:HD22	2:D:1898:ALA:HB2	1.75	0.51
2:C:1922:THR:HG23	2:C:1967:HIS:HB2	1.92	0.50
2:C:1724:LEU:CB	4:C:184:HOH:O	2.57	0.50
2:C:1735:LEU:HD22	2:C:1814:LYS:HD3	1.93	0.50
1:B:211:THR:HG21	4:B:346:HOH:O	2.12	0.50
2:D:1968:ASP:O	2:D:1970:VAL:HG23	2.12	0.50
1:B:160:MET:HG3	1:B:214:HIS:O	2.12	0.50
1:B:223:PRO:HD3	4:B:330:HOH:O	2.11	0.49
2:C:1881:GLN:C	2:C:1886:GLU:HG2	2.37	0.49
1:B:120:LYS:N	1:B:120:LYS:CD	2.75	0.49
1:A:164:LYS:HE3	1:A:271:GLU:OE2	2.12	0.49
2:C:1916:VAL:HG22	2:C:1916:VAL:O	2.12	0.49
2:D:1914:LEU:HB2	2:D:1937:LEU:CD1	2.42	0.49
1:B:185:SER:C	1:B:187:GLY:N	2.68	0.49
1:B:175:ARG:HD3	1:B:191:PRO:O	2.13	0.49
2:D:1769:PRO:O	2:D:1770:PRO:C	2.56	0.49
1:A:282:ARG:O	1:A:286:GLU:HG3	2.13	0.48
1:A:285:GLU:HA	1:A:288:ASN:ND2	2.28	0.48
2:C:1912:ILE:HG22	2:C:1913:ALA:H	1.78	0.48
1:B:207:ASP:O	1:B:208:ASP:C	2.57	0.48
2:C:1795:GLN:HA	4:C:137:HOH:O	2.14	0.48
2:D:1776:THR:CA	2:D:1779:GLN:HE21	2.12	0.48
2:C:1910:LYS:HD3	2:C:1910:LYS:H	1.79	0.48
1:B:119:ALA:O	1:B:122:VAL:HG12	2.14	0.48
1:B:101:LYS:HD2	1:B:101:LYS:H	1.79	0.47
2:C:1878:SER:OG	2:C:1923:ASP:OD1	2.29	0.47
2:C:1970:VAL:O	2:C:1971:SER:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1721:PRO:HA	2:D:1775:TYR:HH	1.79	0.47
1:A:132:LYS:NZ	1:A:285:GLU:OE1	2.39	0.47
2:C:1773:LYS:NZ	4:C:211:HOH:O	2.42	0.47
2:C:1912:ILE:HG22	2:C:1913:ALA:N	2.30	0.47
2:D:1723:PRO:O	2:D:1838:ASN:OD1	2.32	0.47
2:D:1740:THR:HG22	2:D:1740:THR:O	2.14	0.47
2:D:1856:GLU:O	2:D:1857:GLN:HB2	2.14	0.47
2:C:1913:ALA:O	2:C:1916:VAL:CG1	2.57	0.47
1:B:193:HIS:CE1	1:B:214:HIS:HB3	2.50	0.47
1:A:287:GLU:C	1:A:289:LEU:H	2.23	0.46
2:C:1881:GLN:O	2:C:1886:GLU:HG2	2.15	0.46
1:A:183:SER:C	1:A:185:SER:H	2.24	0.46
1:B:207:ASP:O	1:B:208:ASP:O	2.33	0.46
1:A:118:THR:HG21	1:A:283:ARG:CG	2.46	0.46
2:C:1869:PHE:HD1	2:C:1895:GLY:HA3	1.81	0.46
2:D:1777:GLU:HB3	4:D:51:HOH:O	2.16	0.46
1:A:135:CYS:O	1:A:274:VAL:HA	2.15	0.46
2:D:1874:VAL:HG12	2:D:1875:LEU:N	2.32	0.46
1:A:247:ASN:O	1:A:248:ARG:CB	2.64	0.45
2:D:1723:PRO:HD3	2:D:1835:CYS:SG	2.56	0.45
2:D:1871:ASN:ND2	2:D:1898:ALA:HB2	2.31	0.45
2:D:1927:PRO:HG2	2:D:1930:VAL:CG2	2.46	0.45
1:B:159:ALA:HB3	1:B:216:VAL:CG1	2.46	0.45
1:B:200:ASN:OD1	1:B:201:LEU:N	2.48	0.45
1:A:211:THR:O	1:A:212:PHE:CB	2.61	0.45
1:A:132:LYS:HD2	1:A:271:GLU:CD	2.41	0.45
1:A:259:ASP:C	1:A:259:ASP:OD2	2.59	0.45
1:B:99:SER:OG	1:B:101:LYS:CD	2.62	0.45
1:B:202:ARG:CZ	4:B:337:HOH:O	2.62	0.45
1:B:183:SER:C	1:B:185:SER:N	2.74	0.45
2:D:1735:LEU:C	2:D:1736:LEU:HD23	2.42	0.45
1:A:190:PRO:HB2	1:A:193:HIS:CD2	2.43	0.45
1:A:246:MET:N	4:A:302:HOH:O	2.43	0.45
2:D:1949:GLN:HB3	2:D:1957:ILE:HD11	1.97	0.45
2:C:1737:THR:HG23	2:C:1814:LYS:HD2	1.99	0.45
2:D:1904:HIS:O	2:D:1905:SER:C	2.60	0.45
2:C:1962:HIS:HD2	2:C:1964:LYS:N	2.07	0.45
1:B:283:ARG:HB2	1:B:283:ARG:NH1	2.32	0.44
1:B:285:GLU:HA	1:B:288:ASN:HD22	1.80	0.44
2:C:1882:GLN:O	2:C:1883:ASN:CB	2.65	0.44
2:D:1922:THR:HG23	2:D:1967:HIS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:HH11	1:B:156:ARG:CG	2.28	0.44
2:D:1789:GLU:OE2	2:D:1789:GLU:HA	2.18	0.44
2:C:1916:VAL:O	2:C:1916:VAL:CG2	2.66	0.44
2:D:1721:PRO:HA	2:D:1775:TYR:OH	2.16	0.44
2:D:1961:GLN:HG3	4:D:163:HOH:O	2.18	0.44
1:A:201:LEU:H	1:A:201:LEU:CD1	2.28	0.44
1:B:120:LYS:HD2	1:B:120:LYS:H	1.81	0.44
2:C:1910:LYS:H	2:C:1910:LYS:CD	2.31	0.44
2:C:1888:TRP:O	2:C:1892:LEU:HG	2.18	0.44
1:A:97:VAL:O	1:A:97:VAL:CG1	2.66	0.43
2:D:1910:LYS:HG2	2:D:1910:LYS:O	2.18	0.43
1:A:285:GLU:HA	1:A:288:ASN:HD22	1.84	0.43
2:C:1786:TYR:C	2:C:1786:TYR:CD2	2.96	0.43
2:C:1914:LEU:HB2	2:C:1937:LEU:CD1	2.47	0.43
2:C:1914:LEU:CD1	2:C:1933:CYS:HB3	2.44	0.43
1:B:201:LEU:N	1:B:201:LEU:CD1	2.81	0.43
1:B:206:LEU:HD23	1:B:208:ASP:H	1.83	0.43
2:C:1786:TYR:HE2	2:C:1788:LEU:HD23	1.84	0.43
1:B:211:THR:O	1:B:212:PHE:CB	2.64	0.43
1:B:280:ARG:HG2	1:B:280:ARG:NH1	2.34	0.43
1:B:283:ARG:O	1:B:287:GLU:CG	2.59	0.43
1:B:202:ARG:CD	4:B:337:HOH:O	2.65	0.42
2:D:1719:ARG:HE	2:D:1772:ASN:ND2	2.17	0.42
2:C:1811:ARG:NH2	2:C:1945:GLU:OE1	2.50	0.42
2:C:1869:PHE:O	2:C:1897:ALA:HA	2.20	0.42
2:D:1772:ASN:C	4:D:58:HOH:O	2.62	0.42
2:D:1720:GLY:O	2:D:1775:TYR:CE2	2.72	0.42
2:D:1737:THR:CG2	2:D:1814:LYS:HB2	2.49	0.42
2:D:1904:HIS:ND1	2:D:1907:ALA:HB3	2.34	0.42
2:D:1725:ASN:CB	2:D:1838:ASN:HD21	2.18	0.42
1:A:118:THR:HG21	1:A:283:ARG:HG3	2.00	0.42
2:C:1769:PRO:O	2:C:1770:PRO:C	2.62	0.42
1:A:201:LEU:N	1:A:201:LEU:CD1	2.74	0.42
1:A:194:LEU:HD11	1:A:246:MET:HE2	2.01	0.41
2:C:1809:HIS:CE1	2:C:1859:ILE:HD13	2.55	0.41
2:D:1718:GLN:H	2:D:1718:GLN:HG3	1.73	0.41
2:D:1725:ASN:OD1	2:D:1725:ASN:C	2.62	0.41
1:A:150:THR:HA	1:A:151:PRO:HD3	1.75	0.41
1:B:206:LEU:HB3	1:B:215:SER:OG	2.20	0.41
1:A:194:LEU:CD1	1:A:238:CYS:HB2	2.50	0.41
1:B:283:ARG:CB	1:B:283:ARG:HH11	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1901:LYS:HZ3	2:C:1912:ILE:HG23	1.83	0.41
1:B:143:VAL:CG2	1:B:234:TYR:HD2	2.33	0.41
1:A:103:TYR:HD2	1:A:266:GLY:HA2	1.86	0.41
1:B:140:THR:CG2	1:B:233:HIS:HD2	2.33	0.41
1:B:259:ASP:OD2	1:B:259:ASP:C	2.64	0.41
2:D:1779:GLN:HB3	2:D:1835:CYS:SG	2.60	0.41
1:B:240:SER:O	1:B:248:ARG:N	2.50	0.41
1:A:112:GLY:HA3	1:A:144:GLN:HB2	2.03	0.41
2:D:1725:ASN:CB	2:D:1838:ASN:ND2	2.82	0.41
2:D:1943:SER:HB3	2:D:1967:HIS:HA	2.02	0.41
1:A:183:SER:C	1:A:185:SER:N	2.79	0.41
2:D:1773:LYS:O	2:D:1773:LYS:CG	2.67	0.41
2:D:1828:HIS:HD2	2:D:1832:HIS:CE1	2.38	0.41
1:A:248:ARG:CZ	2:C:1849:PRO:HD3	2.51	0.41
1:A:287:GLU:O	1:A:289:LEU:N	2.54	0.41
2:C:1906:SER:O	2:C:1908:HIS:N	2.50	0.41
2:D:1779:GLN:HE22	2:D:1832:HIS:CD2	2.39	0.41
2:D:1882:GLN:O	2:D:1883:ASN:CB	2.69	0.41
1:B:123:THR:HG21	1:B:139:LYS:HD2	2.03	0.40
1:A:122:VAL:O	1:A:122:VAL:HG13	2.20	0.40
2:D:1961:GLN:CG	4:D:163:HOH:O	2.69	0.40
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.87	0.40
2:C:1733:ALA:HB1	2:C:1788:LEU:HG	2.03	0.40
2:C:1737:THR:CG2	2:C:1814:LYS:HD2	2.50	0.40
2:C:1774:GLN:HG2	4:C:105:HOH:O	2.21	0.40
2:D:1920:VAL:HB	2:D:1941:VAL:HG22	2.02	0.40
2:D:1718:GLN:O	2:D:1719:ARG:C	2.65	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	193/195 (99%)	180 (93%)	11 (6%)	2 (1%)	12	24
1	B	193/195 (99%)	175 (91%)	13 (7%)	5 (3%)	4	7
2	C	228/259 (88%)	206 (90%)	17 (8%)	5 (2%)	5	9
2	D	228/259 (88%)	204 (90%)	16 (7%)	8 (4%)	3	4
All	All	842/908 (93%)	765 (91%)	57 (7%)	20 (2%)	4	8

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	B	208	ASP
2	C	1905	SER
2	C	1910	LYS
2	C	1971	SER
2	D	1905	SER
2	D	1907	ALA
2	D	1971	SER
1	B	187	GLY
2	C	1883	ASN
2	C	1907	ALA
1	A	288	ASN
1	B	138	ALA
1	B	186	ASP
2	D	1770	PRO
2	D	1910	LYS
2	D	1883	ASN
1	B	184	ASP
2	D	1724	LEU
2	D	1769	PRO

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	175/175 (100%)	166 (95%)	9 (5%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	175/175 (100%)	167 (95%)	8 (5%)	24	48
2	C	203/227 (89%)	187 (92%)	16 (8%)	11	24
2	D	203/227 (89%)	194 (96%)	9 (4%)	25	50
All	All	756/804 (94%)	714 (94%)	42 (6%)	19	39

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	150	THR
1	A	156	ARG
1	A	201	LEU
1	A	203	VAL
1	A	206	LEU
1	A	217	VAL
1	A	221	GLU
1	A	225	VAL
1	B	98	PRO
1	B	137	LEU
1	B	156	ARG
1	B	203	VAL
1	B	206	LEU
1	B	217	VAL
1	B	221	GLU
1	B	225	VAL
2	C	1716	GLU
2	C	1735	LEU
2	C	1736	LEU
2	C	1789	GLU
2	C	1795	GLN
2	C	1836	HIS
2	C	1871	ASN
2	C	1880	GLN
2	C	1894	THR
2	C	1908	HIS
2	C	1912	ILE
2	C	1938	GLN
2	C	1939	LEU
2	C	1949	GLN
2	C	1961	GLN
2	C	1963	PRO

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Mol	Chain	Res	Type
2	D	1716	GLU
2	D	1789	GLU
2	D	1836	HIS
2	D	1881	GLN
2	D	1894	THR
2	D	1908	HIS
2	D	1912	ILE
2	D	1919	VAL
2	D	1938	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	131	ASN
1	A	178	HIS
1	A	233	HIS
1	A	235	ASN
1	A	288	ASN
1	B	104	GLN
1	B	115	HIS
1	B	131	ASN
1	B	165	GLN
1	B	193	HIS
1	B	233	HIS
1	B	235	ASN
1	B	263	ASN
1	B	288	ASN
2	C	1718	GLN
2	C	1779	GLN
2	C	1801	GLN
2	C	1828	HIS
2	C	1832	HIS
2	C	1836	HIS
2	C	1839	GLN
2	C	1871	ASN
2	C	1882	GLN
2	C	1883	ASN
2	C	1908	HIS
2	C	1961	GLN
2	C	1962	HIS
2	D	1772	ASN

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Mol	Chain	Res	Type
2	D	1779	GLN
2	D	1801	GLN
2	D	1809	HIS
2	D	1832	HIS
2	D	1839	GLN
2	D	1871	ASN
2	D	1903	HIS
2	D	1908	HIS
2	D	1961	GLN
2	D	1962	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.