



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:35 PM GMT

PDB ID : 1KZY  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

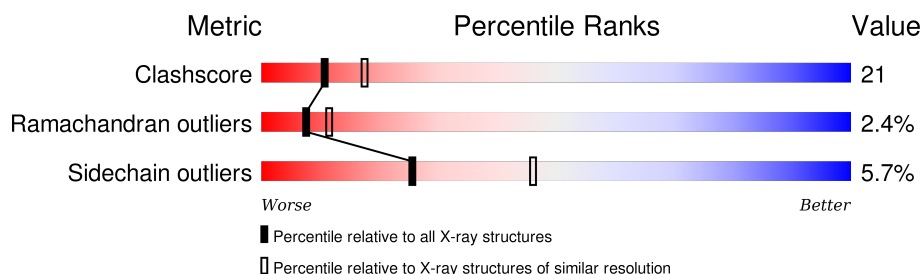
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	195	 67% 31% 2% 2%
1	B	195	 66% 29% 5% 0% 0%
2	C	259	 56% 30% 10% 4% 0%
2	D	259	 52% 31% 6% 10% 0%

## 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

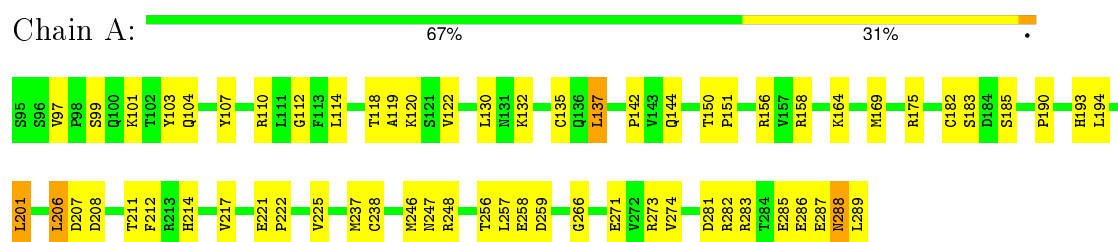
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	58	Total	O	0	0
			58	58		
4	C	50	Total	O	0	0
			50	50		
4	D	51	Total	O	0	0
			51	51		

### 3 Residue-property plots

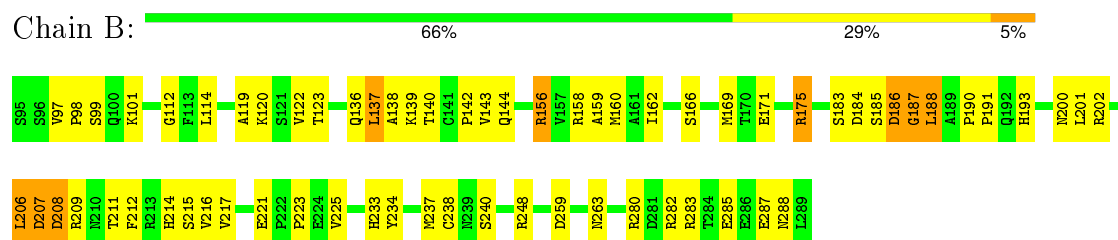
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

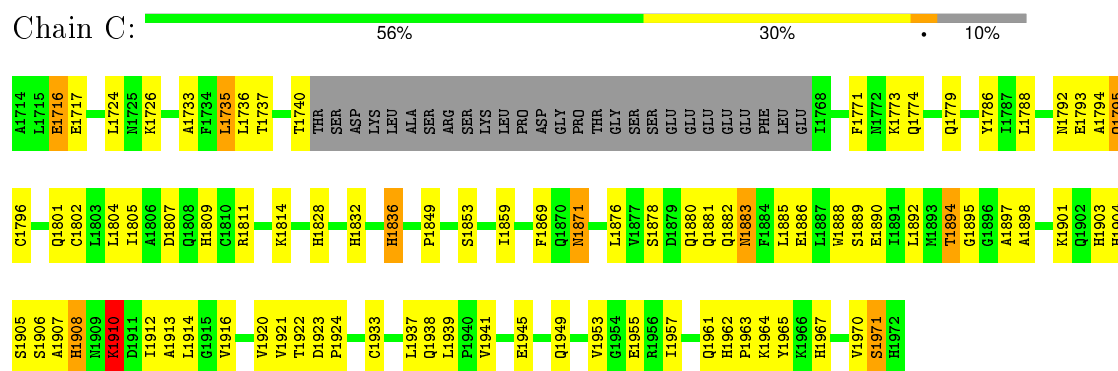
#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### • Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1



#### • Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1



A1714	L1715	E1716	E1717	Q1718	R1719	G1720	P1721	L1722	P1723	L1724	M1725		G1731		L1736	T1737		T1740	THR	SER	ASP	LYS	LEU	ALA	SER	ARG	SER	LYS	LEU	PRO	ASP	GLY	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			
	Y1786	I1787	L1788	E1789		M1792	E1793	A1794	Q1795	C1796			C1802	L1803	L1804	I1805	A1806	D1807	Q1808	H1809	C1810	R1811		K1814		H1828		H1832		C1835	H1836	A1837	M1838		S1853	L1854	E1855	E1856	Q1857	R1858	I1859		R1865		M1871		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 will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.63	0/1565	0.79	0/2121
1	B	0.61	0/1565	0.81	2/2121 (0.1%)
2	C	0.63	0/1901	0.79	0/2584
2	D	0.65	0/1901	0.81	3/2584 (0.1%)
All	All	0.63	0/6932	0.80	5/9410 (0.1%)

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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LEU	CA-CB-CG	6.94	131.27	115.30
2	D	1723	PRO	N-CA-C	5.58	126.62	112.10
2	D	1722	LEU	N-CA-C	-5.24	96.84	111.00
2	D	1811	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	282	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	53	0
1	B	1530	0	1485	62	0
2	C	1854	0	1814	79	0
2	D	1854	0	1814	92	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	10	0
All	All	6986	0	6598	281	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 21.

All (281) 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
2:D:1776:THR:HA	2:D:1779:GLN:HE21	1.25	1.00
1:B:171:GLU:HG3	4:B:318:HOH:O	1.60	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)
2:D:1772:ASN:HA	4:D:58:HOH:O	1.82	0.80
2:C:1962:HIS:HD2	2:C:1964:LYS:H	1.30	0.80
1:A:283:ARG:O	1:A:287:GLU:HG2	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:HD2	1:B:120:LYS:N	2.04	0.72
2:C:1796:CYS:HG	2:C:1802:CYS:HG	0.73	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:H	1:A:201:LEU:HD12	1.53	0.72
2:C:1914:LEU:HD12	2:C:1933:CYS:HB3	1.72	0.71
2:D:1773:LYS:HG2	2:D:1773:LYS:O	1.90	0.71
2:D:1903:HIS:CD2	2:D:1912:ILE:HD11	2.25	0.71
1:B:99:SER:OG	1:B:101:LYS:HD2	1.90	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: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:A:211:THR:O	1:A:212:PHE:HB2	1.94	0.67
2:C:1774:GLN:CG	2:D:1731:GLY:HA2	2.23	0.67
1:B:211:THR:O	1:B:212:PHE:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1725:ASN:HB2	2:D:1838:ASN:ND2	2.07	0.67
2:D:1910:LYS:H	2:D:1910:LYS:HD3	1.60	0.67
2:C:1962:HIS:CD2	2:C:1964:LYS:H	2.12	0.66
2:D:1771:PHE:CB	2:D:1807:ASP:HB3	2.25	0.66
2:C:1876:LEU:HD23	2:C:1921:VAL:HB	1.77	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:200:ASN:C	1:B:201:LEU:HD12	2.17	0.65
1:B:156:ARG:HH11	1:B:156:ARG:HG2	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:N	2:D:1910:LYS:HD3	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
2:C:1726:LYS:HE2	4:C:182:HOH:O	1.97	0.63
1:B:201:LEU:HD12	1:B:201:LEU:N	2.13	0.63
2:D:1953:VAL:HG12	2:D:1955:GLU:HG2	1.81	0.63
1:B:186:ASP:O	1:B:188:LEU:N	2.28	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:C:1735:LEU:C	2:C:1736:LEU:HD23	2.20	0.62
2:D:1853:SER:HA	2:D:1949:GLN:OE1	1.99	0.62
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:D:1962:HIS:CD2	2:D:1964:LYS:H	2.18	0.61
1:B:185:SER:C	1:B:187:GLY:H	2.02	0.61
1:B:285:GLU:HA	1:B:288:ASN:ND2	2.16	0.61
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
1:A:222:PRO:HG3	4:A:312:HOH:O	2.03	0.59
1:B:156:ARG:NH1	1:B:156:ARG:HG2	2.17	0.59
2:D:1772:ASN:CA	4:D:58:HOH:O	2.46	0.59
1:B:190:PRO:HB2	1:B:193:HIS:HD2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:1970:VAL:O	2:D:1971:SER:C	2.42	0.57
2:D:1910:LYS:H	2:D:1910:LYS:CD	2.18	0.56
2:C:1804:LEU:HD23	2:C:1804:LEU:C	2.25	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
1:B:137:LEU:HD21	1:B:237:MET:C	2.26	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:N	2:C:1736:LEU:HD23	2.21	0.56
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:N	2:C:1910:LYS:HD3	2.21	0.55
1:B:112:GLY:O	1:B:144:GLN:HG3	2.06	0.55
2:D:1809:HIS:HE1	2:D:1859:ILE:HD13	1.72	0.55
2:C:1740:THR:HG22	2:C:1740:THR:O	2.06	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: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:175:ARG:HG2	1:B:238:CYS:SG	2.48	0.54
1:B:136:GLN:HB2	1:B:139:LYS:HG3	1.89	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:C:1773:LYS:NZ	4:C:211:HOH:O	2.42	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
1:B:114:LEU:HD12	1:B:142:PRO:HG3	1.91	0.52
2:C:1923:ASP:HB2	2:C:1924:PRO:CD	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1890:GLU:O	2:D:1894:THR:CG2	2.46	0.52
2:D:1781:ARG:HH11	2:D:1781:ARG:HG3	1.76	0.51
2:D:1737:THR:HG21	2:D:1814:LYS:HB2	1.91	0.51
2:C:1949:GLN:HG2	2:C:1965:TYR:OH	2.11	0.51
1:B:159:ALA:HB3	1:B:216:VAL:HG13	1.92	0.51
2:D:1855:GLU:HB2	4:D:163:HOH:O	2.11	0.51
1:B:280:ARG:HG2	1:B:280:ARG:HH11	1.76	0.51
2:C:1881:GLN:HG3	2:C:1886:GLU:OE2	2.10	0.51
2:C:1853:SER:HA	2:C:1949:GLN:OE1	2.11	0.51
1:A:114:LEU:HD12	1:A:142:PRO:HG3	1.93	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:D:1804:LEU:HD23	2:D:1804:LEU:C	2.32	0.51
2:C:1922:THR:HG23	2:C:1967:HIS:HB2	1.92	0.50
2:C:1735:LEU:HD22	2:C:1814:LYS:HD3	1.93	0.50
2:C:1724:LEU:CB	4:C:184:HOH:O	2.57	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:183:SER:C	1:B:185:SER:H	2.14	0.50
1:B:223:PRO:HD3	4:B:330:HOH:O	2.11	0.49
1:B:120:LYS:CD	1:B:120:LYS:N	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:175:ARG:HD3	1:B:191:PRO:O	2.13	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
2:D:1721:PRO:HA	2:D:1775:TYR:HH	1.78	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:H	2:C:1910:LYS:HD3	1.79	0.48
1:B:119:ALA:O	1:B:122:VAL:HG12	2.14	0.48
1:B:101:LYS:H	1:B:101:LYS:HD2	1.79	0.47
2:C:1878:SER:OG	2:C:1923:ASP:OD1	2.29	0.47
1:A:137:LEU:HD21	1:A:237:MET:C	2.34	0.47
2:D:1723:PRO:O	2:D:1838:ASN:OD1	2.32	0.47
2:C:1912:ILE:HG22	2:C:1913:ALA:N	2.30	0.47
2:D:1740:THR:O	2:D:1740:THR:HG22	2.14	0.47
2:D:1856:GLU:O	2:D:1857:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1913:ALA:O	2:C:1916:VAL:CG1	2.57	0.47
1:B:185:SER:C	1:B:187:GLY:N	2.68	0.47
1:B:193:HIS:CE1	1:B:214:HIS:HB3	2.50	0.47
2:C:1881:GLN:O	2:C:1886:GLU:HG2	2.15	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
2:D:1723:PRO:HD3	2:D:1835:CYS:SG	2.56	0.45
1:A:247:ASN:O	1:A:248:ARG:CB	2.64	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:200:ASN:OD1	1:B:201:LEU:N	2.48	0.45
1:B:159:ALA:HB3	1:B:216:VAL:CG1	2.46	0.45
1:A:211:THR:O	1:A:212:PHE:CB	2.61	0.45
1:B:202:ARG:CZ	4:B:337:HOH:O	2.62	0.45
1:B:99:SER:OG	1:B:101:LYS:CD	2.62	0.45
2:C:1881:GLN:C	2:C:1886:GLU:HG2	2.37	0.45
1:A:190:PRO:HB2	1:A:193:HIS:CD2	2.43	0.45
2:D:1949:GLN:HB3	2:D:1957:ILE:HD11	1.97	0.45
1:A:246:MET:N	4:A:302:HOH:O	2.43	0.45
2:C:1737:THR:HG23	2:C:1814:LYS:HD2	1.99	0.45
2:C:1962:HIS:HD2	2:C:1964:LYS:N	2.07	0.45
1:B:283:ARG:NH1	1:B:283:ARG:HB2	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
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:1796:CYS:CB	2:C:1802:CYS:HG	2.24	0.44
2:C:1916:VAL:CG2	2:C:1916:VAL:O	2.66	0.44
2:D:1769:PRO:O	2:D:1770:PRO:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ASP:O	1:B:208:ASP:C	2.57	0.43
2:D:1910:LYS:O	2:D:1910:LYS:HG2	2.18	0.43
2:C:1970:VAL:O	2:C:1971:SER:C	2.57	0.43
1:A:285:GLU:HA	1:A:288:ASN:HD22	1.84	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:206:LEU:HD23	1:B:208:ASP:H	1.83	0.43
1:B:201:LEU:CD1	1:B:201:LEU:N	2.81	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:NH1	1:B:280:ARG:HG2	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:1904:HIS:ND1	2:D:1907:ALA:HB3	2.34	0.42
2:D:1737:THR:CG2	2:D:1814:LYS:HB2	2.49	0.42
2:D:1720:GLY:O	2:D:1775:TYR:CE2	2.72	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
1:A:287:GLU:C	1:A:289:LEU:H	2.23	0.42
1:A:201:LEU:N	1:A:201:LEU:CD1	2.74	0.42
2:D:1718:GLN:HG3	2:D:1718:GLN:H	1.73	0.41
2:C:1809:HIS:CE1	2:C:1859:ILE:HD13	2.55	0.41
1:A:183:SER:C	1:A:185:SER:H	2.24	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:B:283:ARG:HH11	1:B:283:ARG:CB	2.33	0.41
2:C:1901:LYS:HZ3	2:C:1912:ILE:HG23	1.83	0.41
1:A:194:LEU:CD1	1:A:238:CYS:HB2	2.50	0.41
1:B:143:VAL:CG2	1:B:234:TYR:HD2	2.33	0.41
2:D:1779:GLN:HB3	2:D:1835:CYS:SG	2.60	0.41
1:B:140:THR:CG2	1:B:233:HIS:HD2	2.33	0.41
1:A:103:TYR:HD2	1:A:266:GLY:HA2	1.86	0.41
1:B:240:SER:O	1:B:248:ARG:N	2.50	0.41
2:D:1725:ASN:CB	2:D:1838:ASN:ND2	2.82	0.41
1:A:112:GLY:HA3	1:A:144:GLN:HB2	2.03	0.41
2:D:1943:SER:HB3	2:D:1967:HIS:HA	2.02	0.41
2:D:1828:HIS:HD2	2:D:1832:HIS:CE1	2.38	0.41
2:D:1773:LYS:O	2:D:1773:LYS:CG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1779:GLN:HE22	2:D:1832:HIS:CD2	2.39	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:1904:HIS:O	2:D:1905:SER:C	2.60	0.41
1:A:248:ARG:CZ	2:C:1849:PRO:HD3	2.51	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:132:LYS:HD2	1:A:271:GLU:CD	2.41	0.40
1:A:122:VAL:O	1:A:122:VAL:HG13	2.20	0.40
1:A:259:ASP:OD2	1:A:259:ASP:C	2.59	0.40
2:D:1961:GLN:CG	4:D:163:HOH:O	2.69	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
1:B:183:SER:C	1:B:185:SER:N	2.74	0.40
2:C:1733:ALA:HB1	2:C:1788:LEU:HG	2.03	0.40
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.87	0.40
1:B:162:ILE:O	1:B:162:ILE:HG13	2.20	0.40
2:D:1920:VAL:HB	2:D:1941:VAL:HG22	2.02	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	193/195 (99%)	180 (93%)	11 (6%)	2 (1%)	19	34
1	B	193/195 (99%)	175 (91%)	13 (7%)	5 (3%)	7	10
2	C	228/259 (88%)	206 (90%)	17 (8%)	5 (2%)	8	13
2	D	228/259 (88%)	204 (90%)	16 (7%)	8 (4%)	4	6
All	All	842/908 (93%)	765 (91%)	57 (7%)	20 (2%)	7	11

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%)	167 (95%)	8 (5%)	33	57
1	B	175/175 (100%)	166 (95%)	9 (5%)	29	52
2	C	203/227 (89%)	190 (94%)	13 (6%)	22	39
2	D	203/227 (89%)	190 (94%)	13 (6%)	22	39
All	All	756/804 (94%)	713 (94%)	43 (6%)	25	46

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	156	ARG

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	206	LEU
1	A	207	ASP
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	175	ARG
1	B	206	LEU
1	B	207	ASP
1	B	217	VAL
1	B	221	GLU
1	B	225	VAL
2	C	1716	GLU
2	C	1735	LEU
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	1910	LYS
2	C	1938	GLN
2	C	1939	LEU
2	C	1961	GLN
2	C	1963	PRO
2	D	1716	GLU
2	D	1781	ARG
2	D	1789	GLU
2	D	1836	HIS
2	D	1865	ARG
2	D	1881	GLN
2	D	1894	THR
2	D	1908	HIS
2	D	1910	LYS
2	D	1911	ASP
2	D	1919	VAL
2	D	1938	GLN
2	D	1961	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	131	ASN
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	193	HIS
1	B	233	HIS
1	B	235	ASN
1	B	263	ASN
1	B	288	ASN
2	C	1779	GLN
2	C	1828	HIS
2	C	1832	HIS
2	C	1836	HIS
2	C	1839	GLN
2	C	1871	ASN
2	C	1903	HIS
2	C	1908	HIS
2	C	1961	GLN
2	C	1962	HIS
2	D	1772	ASN
2	D	1779	GLN
2	D	1809	HIS
2	D	1832	HIS
2	D	1838	ASN
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 ⓘ

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 carbohydrates 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 [i](#)

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.