



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:52 pm BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

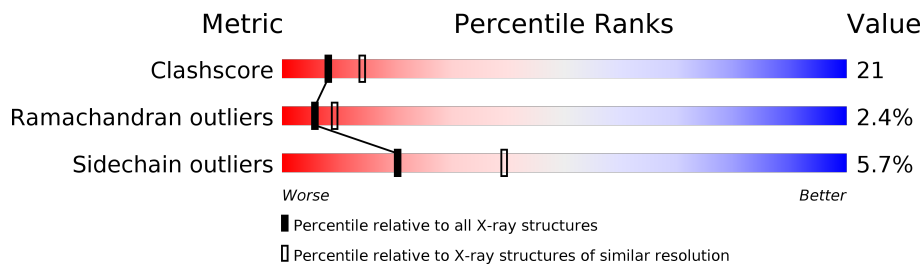
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 ≥ 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	
1	B	195	
2	C	259	
2	D	259	

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
			Total	C	N	O	S			
1	A	195	1530	942	282	290	16	0	0	0
1	B	195	1530	942	282	290	16	0	0	0

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

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

- 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.

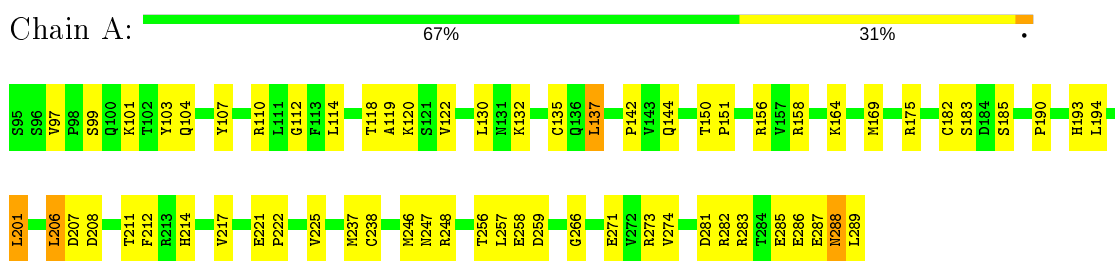
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	58	Total	O	0	0
			58	58		
4	C	50	Total	O	0	0
			50	50		
4	D	51	Total	O	0	0
			51	51		

3 Residue-property plots

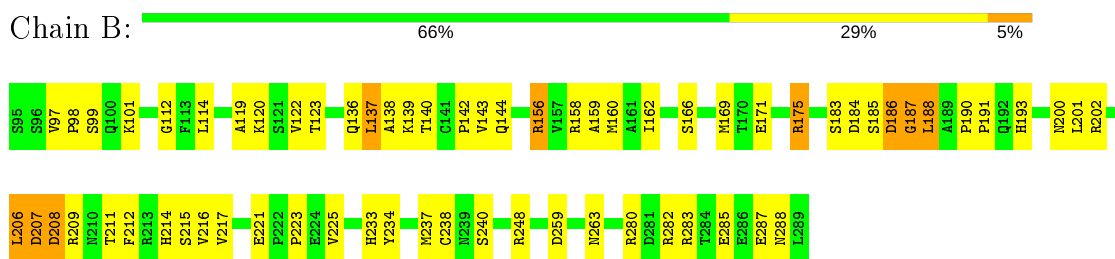
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

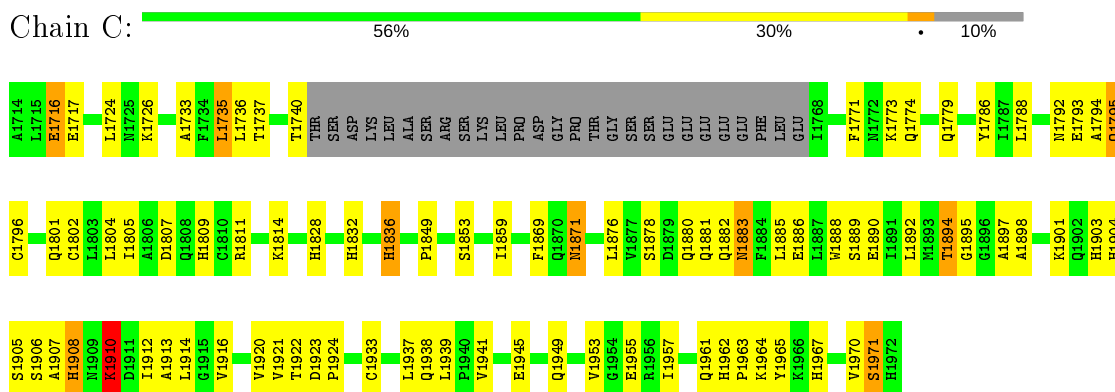
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1



- Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1



A1714	Y1786	A1898
L1715	I1787	K1901
E1716	Q1902	Q1902
E1717	L1788	H1903
Q1718	E1789	H1904
R1719	M1792	S1905
G1720	E1793	S1906
P1721	A1794	A1907
L1722	Q1795	H1908
P1723	C1796	N1909
L1724	C1802	K1910
M1725	L1803	D1911
G1731	L1804	I1912
L1736	L1805	A1913
T1737	A1806	L1914
T1740	D1807	G1915
THR	Q1808	V1916
SER	H1809	V1919
ASP	C1810	V1920
LYS	R1811	Y1921
LEU	K1814	T1922
ALA	H1828	D1923
SER	H1832	P1924
ARG	H1835	P1927
SER	H1836	V1930
LYS	H1837	L1937
LEU	M1838	Q1938
PRO	S1853	Y1941
ASP	L1854	Y1942
GLY	E1855	S1943
GLY	E1856	Q1949
THR	Q1857	Y1953
THR	R1858	G1954
GLY	I1859	E1955
SER	R1865	R1956
SER	M1871	I1957
GLU	V1874	Q1961
GLU	L1875	H1962
GLU	L1881	P1963
GLU	Q1882	K1964
GLU	Q1883	Y1965
GLU	M1883	K1966
GLU	F1884	H1967
GLU	L1885	D1968
PHE	E1886	Y1969
LEU	E1890	V1970
LEU	T1894	S1971
GLU		H1972
I1768		
P1769		
P1770		
F1771		
M1772		
K1773		
Q1774		
Y1775		
T1776		
E1777		
S1778		
Q1779		
L1780		
R1781		

4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å ²)	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
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: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
1:B:99:SER:OG	1:B:101:LYS:HD2	1.90	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: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:211:THR:O	1:A:212:PHE:HB2	1.94	0.67
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

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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: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
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
1:B:200:ASN:C	1:B:201:LEU:HD12	2.17	0.65
2:C:1890:GLU:O	2:C:1894:THR:HG22	1.94	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:1910:LYS:N	2:D:1910:LYS:HD3	2.13	0.63
2:D:1901:LYS:NZ	2:D:1912:ILE:HG23	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: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
1:B:185:SER:C	1:B:187:GLY:H	2.02	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
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
1:B:190:PRO:HB2	1:B:193:HIS:HD2	1.67	0.59
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

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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: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: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:1773:LYS:NZ	4:C:211:HOH:O	2.42	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
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
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:HG2	1:B:280:ARG:HH11	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:1920:VAL:HB	2:C:1941:VAL:HG22	1.93	0.51
2:C:1853:SER:HA	2:C:1949:GLN:OE1	2.11	0.51
2:D:1804:LEU:HD23	2:D:1804:LEU:C	2.32	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: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
1:A:137:LEU:HD21	1:A:237:MET:C	2.34	0.47
2:C:1878:SER:OG	2:C:1923:ASP:OD1	2.29	0.47
2:D:1740:THR:O	2:D:1740:THR:HG22	2.14	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: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
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: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
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: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:CD	2:C:1910:LYS:H	2.31	0.44
2:C:1888:TRP:O	2:C:1892:LEU:HG	2.18	0.44
1:A:97:VAL:CG1	1:A:97:VAL:O	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:C:1970:VAL:O	2:C:1971:SER:C	2.57	0.43
2:D:1910:LYS:O	2:D:1910:LYS:HG2	2.18	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:201:LEU:CD1	1:B:201:LEU:N	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: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: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
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
1:A:183:SER:C	1:A:185:SER:H	2.24	0.41
2:C:1809:HIS:CE1	2:C:1859:ILE:HD13	2.55	0.41
2:D:1718:GLN:HG3	2:D:1718:GLN:H	1.73	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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:1904:HIS:O	2:D:1905:SER:C	2.60	0.41
1:A:132:LYS:HD2	1:A:271:GLU:CD	2.41	0.40
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
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
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
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
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

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%)	15 28
1	B	193/195 (99%)	175 (91%)	13 (7%)	5 (3%)	5 8
2	C	228/259 (88%)	206 (90%)	17 (8%)	5 (2%)	6 10
2	D	228/259 (88%)	204 (90%)	16 (7%)	8 (4%)	3 4
All	All	842/908 (93%)	765 (91%)	57 (7%)	20 (2%)	6 9

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 [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	175/175 (100%)	167 (95%)	8 (5%)	27	50
1	B	175/175 (100%)	166 (95%)	9 (5%)	24	45
2	C	203/227 (89%)	190 (94%)	13 (6%)	17	33
2	D	203/227 (89%)	190 (94%)	13 (6%)	17	33
All	All	756/804 (94%)	713 (94%)	43 (6%)	20	39

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 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.