Worldwide PDB — PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:01 pm BST

PDB ID	:	1GZH
Title	:	Crystal structure of the BRCT domains of human 53BP1 bound to the p53 tumor supressor
Authors	:	Derbyshire, D.J.; Doherty, A.J.
Deposited on	:	2002-05-22
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		15
Ramachandran outliers		0.8%
Sidechain outliers		4.8%
RSRZ outliers		1.8%

Worse ← → Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
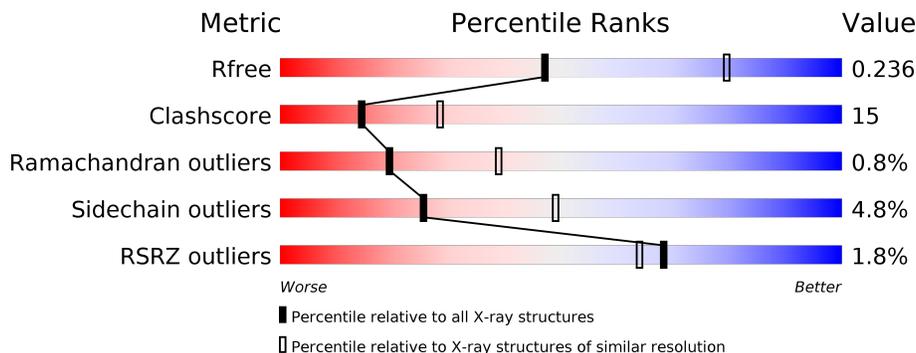
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	198	62% 29% · 6%
2	B	249	65% 23% · 10%
2	D	249	59% 24% · 14%
3	C	198	71% 27% ··

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6630 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	187	Total	C	N	O	S	0	0	0
			1486	920	278	272	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	GLU	ASP	conflict	UNP P04637

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	1
			1788	1142	309	327	10			
2	D	213	Total	C	N	O	S	0	0	1
			1704	1089	294	311	10			

- Molecule 3 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	1
			1530	942	283	289	16			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
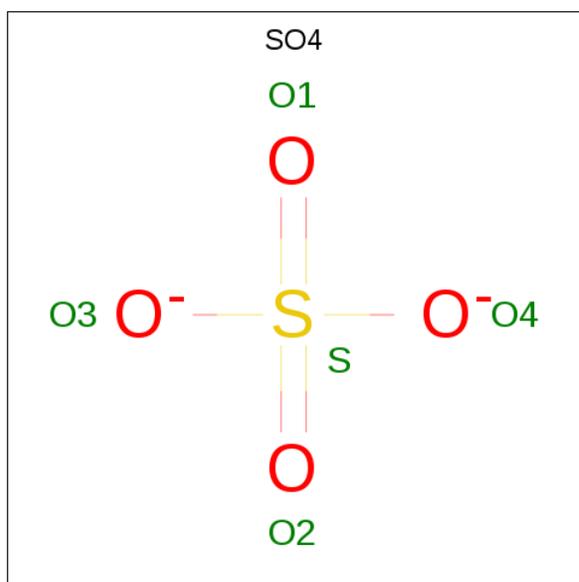
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total 44	O 44	0	0
6	B	43	Total 43	O 43	0	0
6	C	10	Total 10	O 10	0	0
6	D	13	Total 13	O 13	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CELLULAR TUMOR ANTIGEN P53
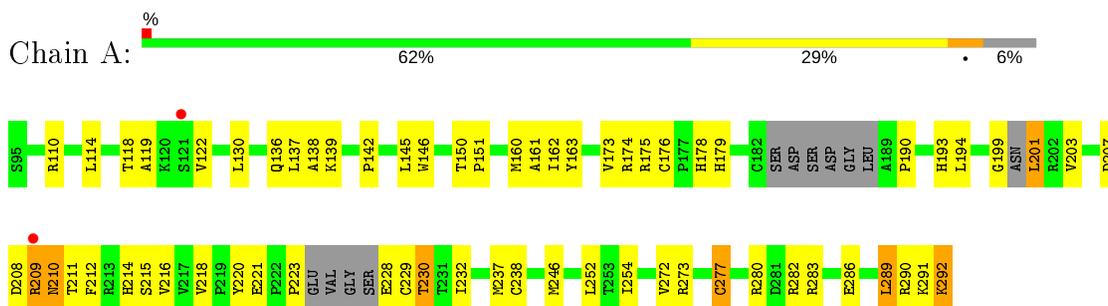
• Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1

• Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1

A1913 L1914 G1915 V1916 T1922 D1923 P1924 P1927 V1930 C1933 L1939 P1940 V1947 Q1961 K1964 V1970 SER HIS
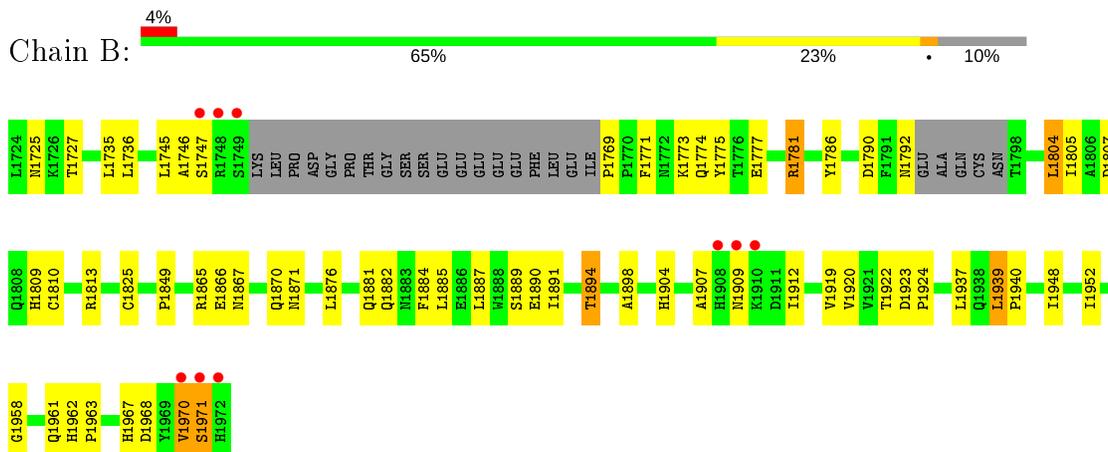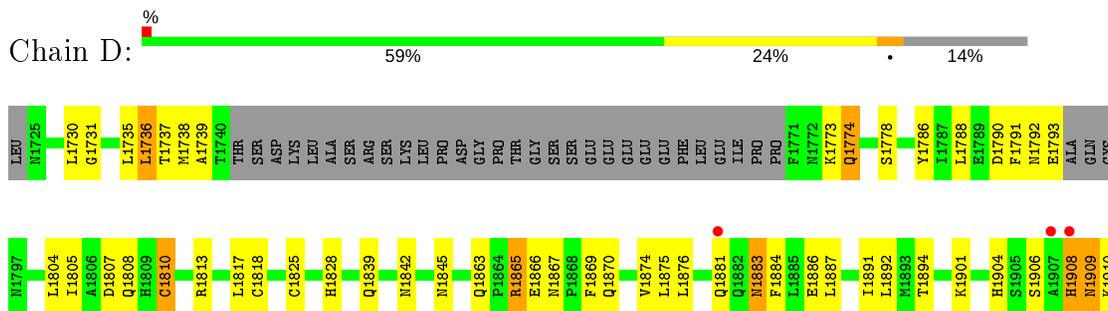
• Molecule 3: CELLULAR TUMOR ANTIGEN P53

Chain C:

S95 S96 V97 P98 S106 Y107 G108 F109 R110 V122 T125 K132 M133 F134 C135 Q136 L137 A138 K139 L145 P151 R158 I162 Y163 M169 R175 C176 P177 R181 C182 S183 A189 P190 P191 Q192 H193 L194 E198 G199 N200 Y205 V218 P219 Y220 E221

E224 Y234 N235 C238 M246 N247 R248 I251 L252 T253 I254 I255 T256 D259 S260 S261 G262 N263 E271 V272 R273 D281 R282 R283 T284 E285 E286 E287 R290 LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.52Å 94.57Å 136.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 2.60	Depositor
	38.84 – 2.60	EDS
% Data completeness	98.5 (38.84-2.60)	Depositor
(in resolution range)	99.1 (38.84-2.60)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.288	Depositor
	0.243 , 0.236	DCC
R_{free} test set	2724 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.8	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6630	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	0.43	0/1518	0.66	0/2049
2	B	0.41	0/1831	0.61	0/2486
2	D	0.44	0/1745	0.61	0/2369
3	C	0.41	0/1565	0.67	0/2123
All	All	0.43	0/6659	0.64	0/9027

There are no bond length outliers.

There are no bond angle outliers.

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	1486	0	1462	62	0
2	B	1788	0	1757	45	0
2	D	1704	0	1661	58	0
3	C	1530	0	1485	35	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	1	0
6	A	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	43	0	0	2	0
6	C	10	0	0	0	0
6	D	13	0	0	0	0
All	All	6630	0	6365	199	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 15.

All (199) 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:B:1923:ASP:HB2	2:B:1924:PRO:HD2	1.46	0.96
1:A:210:ASN:HD22	1:A:211:THR:N	1.64	0.94
1:A:223:PRO:HB2	1:A:228:GLU:HG3	1.49	0.92
2:D:1736:LEU:HD13	2:D:1805:ILE:HB	1.58	0.85
2:D:1908:HIS:CD2	2:D:1908:HIS:H	1.95	0.84
1:A:292:LYS:HD3	1:A:292:LYS:H	1.43	0.83
2:B:1890:GLU:O	2:B:1894:THR:HG23	1.79	0.81
2:D:1774:GLN:NE2	2:D:1774:GLN:H	1.81	0.79
2:B:1867:ASN:HB2	2:B:1870:GLN:HE21	1.49	0.76
2:D:1904:HIS:HD2	2:D:1906:SER:H	1.34	0.74
3:C:189:ALA:HB2	3:C:205:TYR:CZ	2.23	0.73
1:A:209:ARG:HH12	3:C:183:SER:HB3	1.53	0.73
1:A:282:ARG:O	1:A:286:GLU:HG3	1.88	0.72
1:A:228:GLU:HA	1:A:228:GLU:OE1	1.92	0.70
3:C:259:ASP:OD2	3:C:263:ASN:HB2	1.91	0.69
2:B:1867:ASN:CB	2:B:1870:GLN:HE21	2.06	0.69
3:C:175:ARG:HD3	3:C:191:PRO:O	1.93	0.68
2:B:1736:LEU:HD13	2:B:1805:ILE:HB	1.75	0.68
3:C:163:TYR:OH	3:C:246:MET:HA	1.94	0.68
1:A:201:LEU:N	1:A:201:LEU:HD12	2.08	0.67
2:B:1781:ARG:HH21	2:B:1781:ARG:HG3	1.59	0.67
2:D:1867:ASN:HB2	2:D:1870:GLN:HE21	1.58	0.67
1:A:136:GLN:HB2	1:A:139:LYS:HG3	1.76	0.67
2:D:1867:ASN:HB2	2:D:1870:GLN:NE2	2.09	0.67
1:A:118:THR:HB	1:A:283:ARG:HG3	1.77	0.66
1:A:210:ASN:ND2	1:A:211:THR:HG23	2.11	0.66
2:D:1737:THR:HA	5:D:2970:SO4:O1	1.97	0.64
3:C:110:ARG:HH11	3:C:110:ARG:HG2	1.61	0.64
1:A:203:VAL:HA	1:A:218:VAL:HG12	1.80	0.63
2:D:1939:LEU:HD12	2:D:1940:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HD3	1:A:237:MET:HB2	1.81	0.62
3:C:98:PRO:HG2	3:C:162:ILE:HG21	1.82	0.61
2:D:1908:HIS:H	2:D:1908:HIS:HD2	1.43	0.61
2:D:1774:GLN:HE21	2:D:1774:GLN:H	1.49	0.61
2:D:1804:LEU:HD23	2:D:1805:ILE:N	2.15	0.61
1:A:210:ASN:C	1:A:210:ASN:HD22	2.03	0.60
1:A:146:TRP:CE2	1:A:229:CYS:HB3	2.37	0.60
2:D:1881:GLN:O	2:D:1886:GLU:HG3	2.00	0.60
1:A:210:ASN:HD22	1:A:211:THR:H	1.43	0.60
2:B:1781:ARG:NH2	2:B:1781:ARG:HG3	2.16	0.60
1:A:193:HIS:ND1	1:A:214:HIS:HB3	2.17	0.59
2:D:1804:LEU:HD12	2:D:1818:CYS:SG	2.43	0.59
2:D:1786:TYR:CE1	2:D:1788:LEU:HD23	2.37	0.58
2:D:1738:MET:HG2	2:D:1773:LYS:HD2	1.86	0.58
1:A:162:ILE:HG12	1:A:254:ILE:HD11	1.86	0.58
2:D:1927:PRO:HG2	2:D:1930:VAL:CG2	2.34	0.58
1:A:199:GLY:C	1:A:201:LEU:HD12	2.25	0.57
2:D:1813:ARG:HG3	2:D:1887:LEU:CD1	2.34	0.57
1:A:292:LYS:CD	1:A:292:LYS:H	2.16	0.57
2:D:1817:LEU:HD23	2:D:1891:ILE:HG12	1.86	0.57
1:A:291:LYS:HG3	1:A:292:LYS:HD3	1.86	0.56
2:D:1883:ASN:HD22	2:D:1883:ASN:N	2.04	0.56
2:D:1791:PHE:HE1	2:D:1894:THR:HG21	1.71	0.55
3:C:125:THR:HG23	3:C:282:ARG:HD2	1.88	0.55
2:B:1725:ASN:OD1	2:B:1727:THR:HG22	2.07	0.55
3:C:192:GLN:HG2	3:C:193:HIS:HD2	1.72	0.55
1:A:291:LYS:HE3	1:A:292:LYS:NZ	2.22	0.55
1:A:210:ASN:HD21	1:A:211:THR:HG23	1.70	0.55
2:D:1927:PRO:HG2	2:D:1930:VAL:HG23	1.88	0.55
1:A:163:TYR:OH	1:A:246:MET:HA	2.07	0.54
1:A:291:LYS:HE3	1:A:292:LYS:HE2	1.89	0.54
3:C:193:HIS:CE1	3:C:205:TYR:HB3	2.42	0.54
3:C:108:GLY:O	3:C:110:ARG:NH1	2.40	0.54
2:B:1809:HIS:HB3	2:B:1849:PRO:HG2	1.89	0.54
2:B:1871:ASN:HA	2:B:1898:ALA:HB2	1.89	0.54
3:C:247:ASN:O	3:C:248:ARG:HB2	2.08	0.54
2:B:1962:HIS:CG	2:B:1963:PRO:HD2	2.43	0.54
1:A:291:LYS:CG	1:A:292:LYS:HD3	2.38	0.54
3:C:137:LEU:HD23	3:C:138:ALA:N	2.23	0.53
2:B:1922:THR:HG23	2:B:1967:HIS:HB2	1.91	0.53
2:B:1881:GLN:HG3	2:B:1881:GLN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:LEU:HD12	3:C:271:GLU:HA	1.90	0.53
2:B:1867:ASN:HB2	2:B:1870:GLN:HG2	1.90	0.52
1:A:211:THR:O	1:A:212:PHE:HB2	2.08	0.52
1:A:163:TYR:CE1	1:A:173:VAL:HG22	2.44	0.52
2:D:1786:TYR:HE1	2:D:1788:LEU:HD23	1.75	0.52
1:A:277:CYS:HB3	1:A:280:ARG:HB3	1.92	0.52
3:C:110:ARG:NH1	3:C:110:ARG:HG2	2.24	0.52
3:C:200:ASN:HD22	3:C:218:VAL:CG1	2.23	0.52
1:A:291:LYS:HE3	1:A:292:LYS:CE	2.40	0.52
2:D:1774:GLN:N	2:D:1774:GLN:NE2	2.53	0.52
2:D:1737:THR:HG22	2:D:1804:LEU:HD21	1.93	0.51
2:D:1735:LEU:C	2:D:1736:LEU:HD22	2.31	0.51
2:D:1807:ASP:OD1	2:D:1808:GLN:HG2	2.11	0.50
2:B:1773:LYS:HB3	2:B:1774:GLN:OE1	2.11	0.50
2:B:1909:ASN:CB	2:B:1912:ILE:HD11	2.41	0.50
2:D:1908:HIS:CD2	2:D:1908:HIS:N	2.69	0.50
3:C:132:LYS:CE	3:C:273:ARG:HB2	2.41	0.50
3:C:194:LEU:CD1	3:C:238:CYS:HB2	2.41	0.50
1:A:162:ILE:HG12	1:A:254:ILE:CD1	2.41	0.50
2:B:1792:ASN:O	2:B:1792:ASN:OD1	2.30	0.50
2:B:1881:GLN:HA	2:B:1885:LEU:HD12	1.93	0.49
2:B:1923:ASP:HB2	2:B:1924:PRO:CD	2.29	0.49
1:A:176:CYS:SG	1:A:178:HIS:HB3	2.51	0.49
2:D:1791:PHE:O	2:D:1793:GLU:N	2.38	0.49
2:D:1904:HIS:CD2	2:D:1906:SER:H	2.24	0.49
2:D:1916:VAL:HG22	2:D:1916:VAL:O	2.11	0.49
1:A:291:LYS:HG2	1:A:292:LYS:N	2.27	0.49
2:B:1939:LEU:HD12	2:B:1939:LEU:C	2.33	0.49
3:C:151:PRO:HG2	3:C:220:TYR:CE1	2.47	0.49
1:A:145:LEU:HD11	1:A:232:ILE:HD11	1.95	0.49
3:C:132:LYS:HE2	3:C:134:PHE:CE2	2.48	0.49
2:D:1875:LEU:HD12	2:D:1901:LYS:O	2.13	0.48
1:A:292:LYS:N	1:A:292:LYS:HD3	2.21	0.48
2:D:1961:GLN:O	2:D:1961:GLN:HG2	2.13	0.48
2:D:1730:LEU:HD12	2:D:1731:GLY:H	1.79	0.48
2:D:1874:VAL:HG21	2:D:1892:LEU:HD13	1.96	0.48
2:D:1913:ALA:O	2:D:1916:VAL:HG12	2.13	0.48
2:D:1842:ASN:HB3	2:D:1845:ASN:ND2	2.29	0.48
3:C:200:ASN:ND2	3:C:218:VAL:HB	2.29	0.47
2:B:1876:LEU:HD22	2:B:1884:PHE:CE2	2.48	0.47
1:A:190:PRO:HB2	1:A:193:HIS:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:N	1:A:201:LEU:CD1	2.76	0.47
2:B:1790:ASP:OD1	2:B:1813:ARG:NH2	2.45	0.47
2:B:1967:HIS:CE1	2:B:1968:ASP:HB3	2.49	0.47
2:B:1970:VAL:HG12	2:B:1971:SER:N	2.29	0.47
3:C:136:GLN:HB2	3:C:139:LYS:HG3	1.97	0.47
3:C:281:ASP:O	3:C:285:GLU:HG3	2.15	0.47
2:D:1791:PHE:CE1	2:D:1894:THR:HG21	2.50	0.47
2:D:1804:LEU:HD12	2:D:1818:CYS:CB	2.45	0.47
1:A:194:LEU:CD1	1:A:238:CYS:HB2	2.44	0.46
2:B:1769:PRO:N	6:B:2009:HOH:O	2.48	0.46
2:D:1876:LEU:HD22	2:D:1884:PHE:CE2	2.51	0.46
2:B:1735:LEU:C	2:B:1736:LEU:HD22	2.36	0.46
1:A:119:ALA:O	1:A:122:VAL:HG12	2.16	0.46
2:B:1885:LEU:O	2:B:1889:SER:HB2	2.16	0.46
2:B:1909:ASN:HB3	2:B:1912:ILE:HD11	1.98	0.46
3:C:158:ARG:HB3	3:C:256:THR:OG1	2.16	0.46
2:D:1866:GLU:O	2:D:1867:ASN:C	2.55	0.46
1:A:201:LEU:HD23	6:A:2028:HOH:O	2.15	0.45
2:D:1736:LEU:CD2	2:D:1736:LEU:N	2.79	0.45
2:D:1909:ASN:HD22	2:D:1910:LYS:H	1.64	0.45
2:B:1922:THR:OG1	2:B:1923:ASP:N	2.48	0.45
2:B:1771:PHE:CB	2:B:1807:ASP:HB3	2.47	0.45
2:D:1736:LEU:HD22	2:D:1736:LEU:N	2.30	0.45
2:B:1958:GLY:HA3	2:B:1961:GLN:HB2	1.99	0.45
2:D:1817:LEU:CD2	2:D:1891:ILE:HG12	2.46	0.45
2:D:1922:THR:OG1	2:D:1923:ASP:N	2.48	0.45
2:D:1739:ALA:CB	2:D:1810:CYS:HB3	2.46	0.45
3:C:97:VAL:HG21	3:C:169:MET:HE1	1.99	0.45
2:D:1804:LEU:HD13	2:D:1825:CYS:SG	2.57	0.45
1:A:114:LEU:HD12	1:A:142:PRO:HG3	1.98	0.45
1:A:199:GLY:HA3	1:A:201:LEU:CD1	2.47	0.45
2:D:1730:LEU:HD12	2:D:1731:GLY:N	2.32	0.45
3:C:177:PRO:O	3:C:181:ARG:HG3	2.16	0.44
1:A:145:LEU:HB2	1:A:230:THR:HG23	1.99	0.44
1:A:162:ILE:CD1	1:A:254:ILE:HD11	2.47	0.44
1:A:254:ILE:HD12	1:A:254:ILE:N	2.33	0.44
2:B:1866:GLU:O	2:B:1867:ASN:C	2.56	0.44
1:A:146:TRP:CD2	1:A:229:CYS:HB3	2.53	0.44
3:C:284:THR:O	3:C:287:GLU:HG3	2.18	0.44
1:A:110:ARG:HH11	1:A:110:ARG:HG3	1.82	0.43
2:B:1745:LEU:O	2:B:1747:SER:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1804:LEU:HD22	2:B:1825:CYS:SG	2.58	0.43
1:A:210:ASN:C	1:A:210:ASN:ND2	2.71	0.43
2:B:1904:HIS:HB3	2:B:1907:ALA:HB2	1.99	0.43
2:B:1948:ILE:O	2:B:1952:ILE:HD13	2.18	0.43
2:D:1790:ASP:CG	2:D:1813:ARG:HH22	2.18	0.43
3:C:138:ALA:O	3:C:139:LYS:HG2	2.19	0.43
1:A:130:LEU:HD21	1:A:289:LEU:HD23	2.00	0.43
3:C:259:ASP:OD1	3:C:261:SER:N	2.52	0.43
1:A:210:ASN:ND2	1:A:211:THR:N	2.48	0.43
2:D:1923:ASP:HB2	2:D:1924:PRO:CD	2.49	0.43
3:C:97:VAL:HG21	3:C:169:MET:CE	2.49	0.42
3:C:162:ILE:CD1	3:C:254:ILE:HD11	2.49	0.42
3:C:109:PHE:CE1	3:C:145:LEU:HD22	2.55	0.42
1:A:193:HIS:CE1	1:A:214:HIS:HB3	2.53	0.42
2:B:1736:LEU:HD22	2:B:1736:LEU:N	2.34	0.42
2:B:1939:LEU:HD12	2:B:1940:PRO:N	2.35	0.42
2:D:1738:MET:HG2	2:D:1773:LYS:CD	2.48	0.42
2:B:1937:LEU:N	2:B:1937:LEU:HD12	2.35	0.42
2:D:1869:PHE:CZ	2:D:1947:VAL:HG13	2.54	0.42
2:B:1775:TYR:HB3	6:B:2011:HOH:O	2.20	0.42
3:C:132:LYS:HE3	3:C:273:ARG:HB2	2.01	0.42
3:C:234:TYR:O	3:C:235:ASN:ND2	2.53	0.42
2:D:1804:LEU:HD12	2:D:1818:CYS:HB2	2.01	0.42
1:A:291:LYS:HE3	1:A:292:LYS:HZ1	1.84	0.42
2:B:1792:ASN:C	2:B:1792:ASN:OD1	2.59	0.41
1:A:151:PRO:HD2	1:A:220:TYR:CE1	2.56	0.41
2:D:1914:LEU:HD12	2:D:1933:CYS:HB3	2.02	0.41
2:D:1964:LYS:HE3	2:D:1964:LYS:HB2	1.88	0.41
1:A:118:THR:HG22	1:A:282:ARG:HD3	2.03	0.41
2:D:1863:GLN:O	2:D:1865:ARG:HD2	2.20	0.41
1:A:137:LEU:HD23	1:A:138:ALA:N	2.35	0.41
1:A:161:ALA:HA	1:A:252:LEU:O	2.21	0.41
1:A:272:VAL:HG12	1:A:273:ARG:N	2.35	0.41
2:B:1876:LEU:HD22	2:B:1884:PHE:HE2	1.84	0.41
1:A:208:ASP:OD1	1:A:210:ASN:ND2	2.54	0.41
3:C:246:MET:SD	3:C:251:ILE:HD13	2.61	0.41
2:D:1790:ASP:OD1	2:D:1813:ARG:NH2	2.40	0.41
2:D:1909:ASN:HD22	2:D:1910:LYS:N	2.19	0.41
2:B:1919:VAL:HG22	2:B:1920:VAL:N	2.36	0.41
1:A:175:ARG:NH1	1:A:179:HIS:HB3	2.36	0.40
1:A:223:PRO:HB3	1:A:229:CYS:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1773:LYS:O	2:B:1777:GLU:HG3	2.21	0.40
2:B:1887:LEU:HD23	2:B:1891:ILE:HD12	2.03	0.40
1:A:150:THR:HA	1:A:151:PRO:HD3	1.95	0.40
1:A:160:MET:HE3	1:A:215:SER:HB3	2.03	0.40
1:A:162:ILE:CG1	1:A:254:ILE:HD11	2.51	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	179/198 (90%)	170 (95%)	8 (4%)	1 (1%)	25	47
2	B	219/249 (88%)	201 (92%)	15 (7%)	3 (1%)	11	22
2	D	207/249 (83%)	194 (94%)	12 (6%)	1 (0%)	29	52
3	C	194/198 (98%)	186 (96%)	7 (4%)	1 (0%)	29	52
All	All	799/894 (89%)	751 (94%)	42 (5%)	6 (1%)	19	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1792	ASN
1	A	290	ARG
3	C	122	VAL
2	B	1971	SER
2	B	1746	ALA
2	B	1970	VAL

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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	169/178 (95%)	158 (94%)	11 (6%)	17	34
2	B	197/219 (90%)	189 (96%)	8 (4%)	30	56
2	D	186/219 (85%)	176 (95%)	10 (5%)	22	44
3	C	175/178 (98%)	169 (97%)	6 (3%)	37	63
All	All	727/794 (92%)	692 (95%)	35 (5%)	25	49

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	ARG
1	A	201	LEU
1	A	207	ASP
1	A	209	ARG
1	A	210	ASN
1	A	216	VAL
1	A	221	GLU
1	A	230	THR
1	A	277	CYS
1	A	289	LEU
1	A	292	LYS
2	B	1781	ARG
2	B	1786	TYR
2	B	1804	LEU
2	B	1810	CYS
2	B	1865	ARG
2	B	1882	GLN
2	B	1894	THR
2	B	1939	LEU
3	C	106	SER
3	C	125	THR
3	C	198	GLU
3	C	221	GLU
3	C	224	GLU

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Mol	Chain	Res	Type
3	C	238	CYS
2	D	1736	LEU
2	D	1774	GLN
2	D	1778	SER
2	D	1810	CYS
2	D	1828	HIS
2	D	1839	GLN
2	D	1865	ARG
2	D	1883	ASN
2	D	1908	HIS
2	D	1909	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	210	ASN
1	A	235	ASN
2	B	1779	GLN
2	B	1828	HIS
2	B	1867	ASN
2	B	1870	GLN
2	B	1902	GLN
3	C	200	ASN
3	C	235	ASN
3	C	247	ASN
2	D	1774	GLN
2	D	1808	GLN
2	D	1838	ASN
2	D	1867	ASN
2	D	1870	GLN
2	D	1883	ASN
2	D	1903	HIS
2	D	1904	HIS
2	D	1908	HIS
2	D	1909	ASN
2	D	1961	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	SO4	D	2970	-	4,4,4	0.29	0	6,6,6	0.21	0
5	SO4	B	2972	-	4,4,4	0.36	0	6,6,6	0.25	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2970	SO4	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	187/198 (94%)	-0.05	2 (1%)	80	78	21, 35, 58, 83	0
2	B	225/249 (90%)	0.06	9 (4%)	38	31	17, 33, 60, 91	0
2	D	213/249 (85%)	0.02	3 (1%)	75	71	23, 36, 54, 75	0
3	C	196/198 (98%)	-0.02	1 (0%)	91	89	22, 36, 55, 71	0
All	All	821/894 (91%)	0.01	15 (1%)	68	64	17, 35, 56, 91	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1749	SER	6.2
2	D	1908	HIS	5.1
2	B	1748	ARG	4.8
2	B	1972	HIS	4.2
2	B	1747	SER	3.8
2	B	1971	SER	3.4
3	C	95	SER	3.3
2	B	1970	VAL	2.5
1	A	121	SER	2.4
1	A	209	ARG	2.3
2	B	1910	LYS	2.3
2	B	1908	HIS	2.2
2	D	1907	ALA	2.1
2	D	1881	GLN	2.1
2	B	1909	ASN	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	D	2970	5/5	0.92	0.22	54,54,57,57	0
5	SO4	B	2972	5/5	0.97	0.15	36,40,41,46	0
4	ZN	A	1293	1/1	0.99	0.07	31,31,31,31	0
4	ZN	C	1290	1/1	0.99	0.10	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.