



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:22 PM UTC

PDB ID : 6TM1 / pdb_00006tm1
Title : Crystal structure of the DHR2 domain of DOCK10 in complex with RAC3
Authors : Barford, D.; Fan, D.; Cronin, N.; Yang, J.
Deposited on : 2019-12-03
Resolution : 3.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

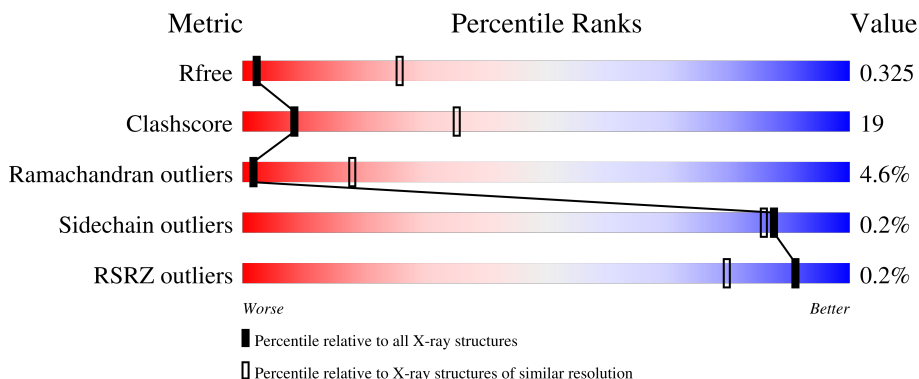
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	457	63%26%10%
2	A	192	% 51%39%8%
3	C	458	58%25%15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6775 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 Deducator of cytokinesis protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	412	Total	C	N	O	S	0	0	0
			2969	1890	505	561	13			

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	177	Total	C	N	O	S	0	0	0
			1243	796	209	231	7			

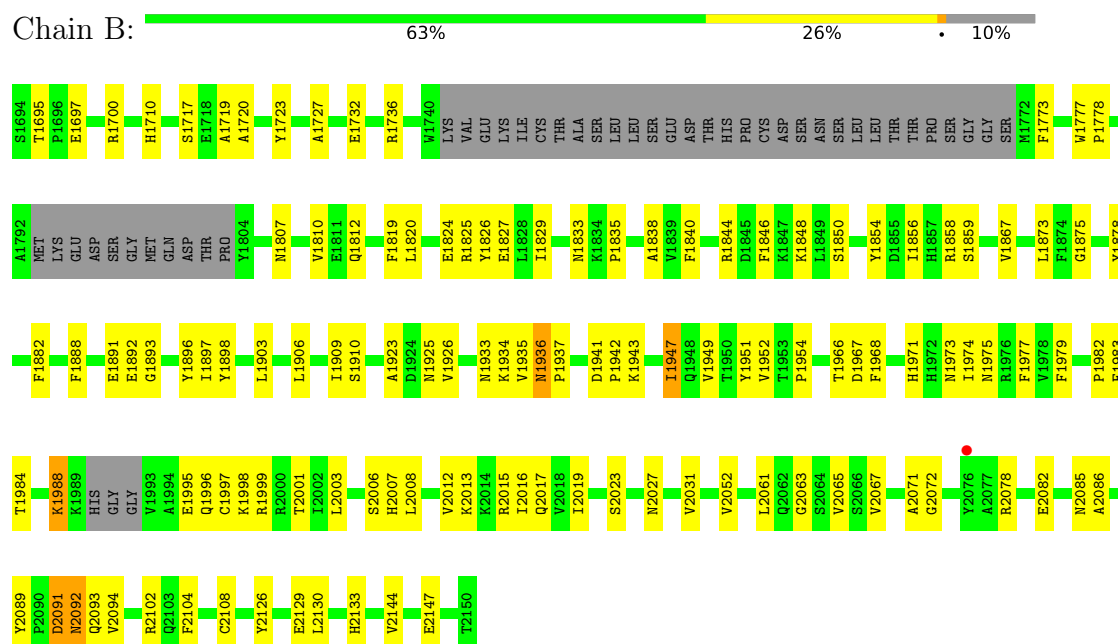
- Molecule 3 is a protein called Deducator of cytokinesis protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	388	Total	C	N	O	S	0	0	0
			2563	1620	446	490	7			

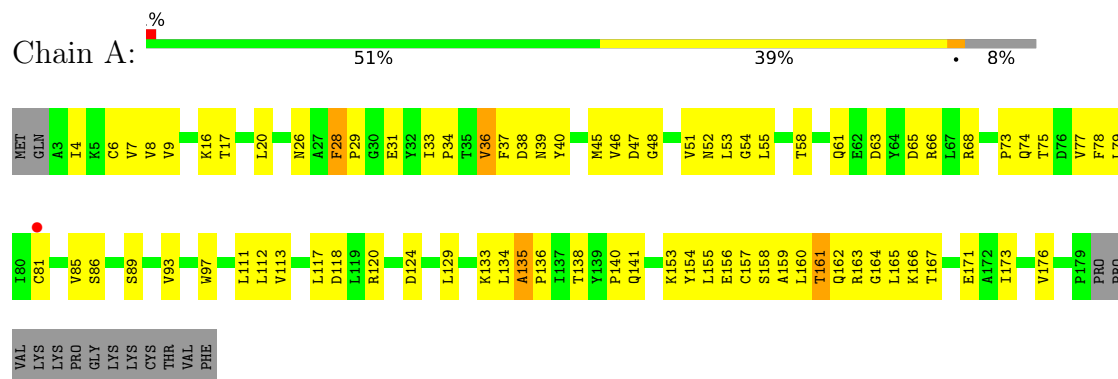
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Dedicator of cytokinesis protein 10



• Molecule 2: Ras-related C3 botulinum toxin substrate 3



• Molecule 3: Dedicator of cytokinesis protein 10



VAL	LYS	V2069	G2072	P2073	M2074	A2075	Y2076	A2079	F2080	L2081	E2082	GLU	THR	ASN	LYS	LYS	LYS	TYR	PRO	D2091	V2094	K2095	G2109	Q2110	A2111	L2138	I2149	THR	GLY																									
E1960	I1974	N1975	R1976	F1977	F1983	T1984	L1985	S1986	G1987	LYS	LYS	HIS	GLY	GLY	VAL	ALA	GLU	GLN	C1997	K1998	R1999	E2000	T2001	L2002	G2003	T2004	T2005	S2006	E2007	L2008	F2009	P2010	Y2011	V2012	I2016	Q2017	V2018	I2019	S2023	T2024	E2025	T2048	M2049	E2050	D2053	M2054	Q2058	G2063	S2064	V2065	SER			
V1863	S1869	E1870	K1871	R1872	R1876	Y1877	Y1878	R1879	V1880	A1881	F1882	F1887	F1888	E1891	Y1896	I1897	Y1898	K1899	L1903	T1904	G1905	L1906	S1907	F1908	I1909	F1921	V1926	I1929	N1933	K1934	V1935	N1936	P1937	K1938	D1939	A1945	Y1946	I1947	Q1948	Y1951	V1952	T1953	P1954	F1955	F1956	E1957								
SER	MET	PHE	SER	MET	GLY	W1777	P1778	A1779	F1780	I1783	T1784	F1785	N1786	I1787	E1790	GLY	ALA	MET	LYS	GLU	ASP	T1802	P1803	C1816	R1825	Y1826	E1827	A1830	D1831	V1832	N1833	K1834	P1835	R1844	D1845	F1846	K1847	K1848	L1849	S1850	D1851	L1852	Y1853	I1856	Y1860									
S1694	T1695	P1696	E1697	L1698	R1699	W1702	L1703	M1706	A1707	K1708	I1709	H1710	S1717	E1718	A1719	M1720	M1721	C1722	Y1723	I1724	H1725	A1728	T1739	TRP	LYS	VAL	GLU	LYS	ILE	CYS	THR	ALA	SER	LEU	LEU	SER	GLU	ASP	THR	HIS	PRO	CYS	ASP	SER	ASN	SER	LEU	LEU	THR	THR	PRO	SER	GLY	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.08Å 128.46Å 215.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 3.71 29.60 – 3.71	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.60-3.71) 96.1 (29.60-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.260 , 0.321 0.261 , 0.325	Depositor DCC
R_{free} test set	818 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	152.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 147.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6775	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.21	0/3028	0.49	0/4133
2	A	0.21	0/1273	0.49	0/1753
3	C	0.20	0/2606	0.51	0/3586
All	All	0.20	0/6907	0.50	0/9472

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
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1695	THR	Peptide

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	B	2969	0	2562	100	0
2	A	1243	0	1117	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2563	0	1997	83	0
All	All	6775	0	5676	237	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 19.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1973:ASN:HB3	1:B:2008:LEU:HD23	1.26	1.17
1:B:1973:ASN:HB3	1:B:2008:LEU:CD2	1.99	0.91
3:C:2054:MET:O	3:C:2058:GLN:OE1	1.93	0.86
2:A:93:VAL:HA	2:A:97:TRP:HD1	1.39	0.85
1:B:2091:ASP:O	1:B:2093:GLN:N	2.11	0.83
1:B:1973:ASN:CB	1:B:2008:LEU:HD23	2.08	0.81
1:B:1833:ASN:HD22	1:B:1856:ILE:HD11	1.50	0.77
3:C:1830:ALA:HB2	3:C:1860:TYR:HE1	1.53	0.74
3:C:1882:PHE:HB3	3:C:1947:ILE:HG22	1.68	0.73
2:A:8:VAL:HG21	2:A:20:LEU:HD21	1.68	0.73
2:A:58:THR:HB	2:A:68:ARG:HD2	1.71	0.73
2:A:7:VAL:HG13	2:A:75:THR:HG21	1.70	0.72
1:B:1936:ASN:H	1:B:1937:PRO:CD	2.03	0.71
1:B:1888:PHE:HB2	1:B:1892:GLU:HA	1.73	0.71
1:B:1941:ASP:O	1:B:1943:LYS:N	2.23	0.71
2:A:120:ARG:HH22	2:A:138:THR:HA	1.56	0.70
3:C:1876:ARG:NH1	3:C:1903:LEU:O	2.26	0.68
1:B:2086:ALA:HA	1:B:2089:TYR:HD2	1.58	0.68
3:C:1850:SER:OG	3:C:1851:ASP:N	2.27	0.67
2:A:93:VAL:HA	2:A:97:TRP:CD1	2.27	0.67
3:C:1999:ARG:HA	3:C:2025:GLU:HA	1.77	0.66
1:B:2102:ARG:NH2	1:B:2147:GLU:OE2	2.28	0.66
2:A:117:LEU:HD12	2:A:156:GLU:HB3	1.78	0.66
1:B:1829:ILE:HD11	1:B:1859:SER:CB	2.27	0.65
3:C:2005:THR:HA	3:C:2018:VAL:HA	1.77	0.65
2:A:86:SER:O	2:A:89:SER:OG	2.15	0.64
2:A:158:SER:OG	2:A:160:LEU:O	2.12	0.64
2:A:138:THR:HG23	2:A:141:GLN:H	1.62	0.64
3:C:1703:LEU:O	3:C:1707:ALA:N	2.31	0.63
1:B:2006:SER:OG	1:B:2007:HIS:N	2.30	0.62
3:C:1721:MET:HE1	3:C:1784:THR:HG21	1.82	0.62
1:B:1903:LEU:HB2	2:A:45:MET:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1936:ASN:H	1:B:1937:PRO:HD2	1.62	0.62
1:B:1988:LYS:O	1:B:1996:GLN:NE2	2.32	0.62
3:C:1777:TRP:O	3:C:1779:ALA:N	2.33	0.62
1:B:2129:GLU:O	1:B:2133:HIS:ND1	2.33	0.62
1:B:1971:HIS:HA	1:B:1974:ILE:HD11	1.82	0.62
1:B:1974:ILE:C	1:B:2008:LEU:HD11	2.25	0.61
2:A:29:PRO:HG2	2:A:160:LEU:HA	1.81	0.61
2:A:160:LEU:C	2:A:162:GLN:H	2.09	0.61
1:B:1973:ASN:CB	1:B:2008:LEU:CD2	2.75	0.61
3:C:1702:TRP:HE1	3:C:1706:MET:HE2	1.66	0.60
2:A:118:ASP:OD1	2:A:118:ASP:N	2.33	0.60
3:C:1896:TYR:HB2	3:C:2016:ILE:O	2.01	0.60
3:C:1896:TYR:HB2	3:C:2017:GLN:HA	1.82	0.60
1:B:1854:TYR:OH	1:B:1858:ARG:NH1	2.35	0.59
3:C:1926:VAL:HG12	3:C:1945:ALA:HB1	1.85	0.59
1:B:1697:GLU:HA	1:B:1700:ARG:HE	1.68	0.58
3:C:1896:TYR:CB	3:C:2017:GLN:HA	2.33	0.58
1:B:2091:ASP:HA	1:B:2094:VAL:HG22	1.84	0.57
3:C:1879:ARG:HD3	3:C:2003:LEU:CD2	2.34	0.57
3:C:2048:THR:O	3:C:2050:GLU:N	2.36	0.57
3:C:1786:ASN:HD22	3:C:2008:LEU:H	1.52	0.57
3:C:1899:LYS:HB2	3:C:2009:PHE:HE2	1.70	0.56
2:A:138:THR:O	2:A:141:GLN:HG2	2.06	0.56
2:A:46:VAL:O	2:A:48:GLY:N	2.39	0.56
2:A:153:LYS:HE2	2:A:171:GLU:HG3	1.87	0.56
1:B:1906:LEU:O	1:B:1910:SER:OG	2.16	0.56
2:A:79:LEU:HB3	2:A:111:LEU:HD12	1.88	0.56
3:C:1896:TYR:HA	3:C:2018:VAL:HG13	1.86	0.56
2:A:29:PRO:C	2:A:31:GLU:H	2.15	0.55
1:B:2104:PHE:O	1:B:2108:CYS:HB2	2.07	0.55
1:B:2061:LEU:HD11	1:B:2130:LEU:HD13	1.90	0.54
1:B:2078:ARG:O	1:B:2085:ASN:ND2	2.40	0.54
2:A:8:VAL:HG22	2:A:79:LEU:HD11	1.89	0.54
2:A:16:LYS:HG3	2:A:17:THR:H	1.73	0.54
3:C:1844:ARG:HB2	3:C:1846:PHE:CE1	2.42	0.54
1:B:1982:PRO:HA	1:B:1998:LYS:HA	1.89	0.54
3:C:1957:GLU:HG3	3:C:1976:ARG:NH2	2.23	0.54
3:C:1844:ARG:HB2	3:C:1846:PHE:HE1	1.72	0.53
2:A:6:CYS:HA	2:A:77:VAL:O	2.08	0.53
2:A:38:ASP:HA	2:A:40:TYR:CE1	2.43	0.53
1:B:1829:ILE:HD11	1:B:1859:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1933:ASN:O	1:B:1935:VAL:N	2.42	0.53
1:B:2067:VAL:HG21	1:B:2072:GLY:HA2	1.90	0.52
3:C:1710:HIS:NE2	3:C:2012:VAL:O	2.40	0.52
3:C:1974:ILE:HD12	3:C:1977:PHE:CE1	2.44	0.52
3:C:1830:ALA:HB2	3:C:1860:TYR:CE1	2.40	0.52
3:C:1876:ARG:HH21	3:C:1951:TYR:HE2	1.56	0.52
3:C:1695:THR:O	3:C:1697:GLU:N	2.43	0.52
3:C:1846:PHE:HA	3:C:1849:LEU:HB2	1.92	0.52
2:A:165:LEU:HG	2:A:166:LYS:H	1.75	0.52
1:B:1717:SER:OG	1:B:1825:ARG:NH1	2.42	0.52
2:A:8:VAL:HG13	2:A:81:CYS:SG	2.49	0.52
3:C:1695:THR:C	3:C:1697:GLU:H	2.16	0.52
3:C:1869:SER:C	3:C:1871:LYS:H	2.18	0.51
3:C:1880:VAL:HG22	3:C:1896:TYR:O	2.09	0.51
3:C:1897:ILE:HG21	3:C:1977:PHE:CD2	2.44	0.51
1:B:1896:TYR:HA	1:B:2017:GLN:HA	1.93	0.51
1:B:1949:VAL:HG23	2:A:28:PHE:HE2	1.74	0.51
1:B:1891:GLU:N	1:B:1891:GLU:OE1	2.44	0.51
3:C:1876:ARG:HD2	3:C:1951:TYR:OH	2.11	0.51
1:B:1954:PRO:HA	1:B:1977:PHE:HD1	1.75	0.51
1:B:1906:LEU:HD23	2:A:26:ASN:HB3	1.92	0.51
3:C:2076:TYR:HA	3:C:2079:ALA:HB3	1.93	0.51
1:B:1732:GLU:HB2	1:B:1777:TRP:HD1	1.74	0.50
3:C:1717:SER:HB3	3:C:1825:ARG:HH11	1.75	0.50
1:B:1723:TYR:HE2	1:B:1819:PHE:CE2	2.29	0.50
1:B:2063:GLY:HA2	2:A:37:PHE:O	2.11	0.50
2:A:165:LEU:O	2:A:167:THR:N	2.42	0.50
3:C:2094:VAL:HG13	3:C:2095:LYS:H	1.76	0.50
2:A:33:ILE:HD12	2:A:34:PRO:HD2	1.93	0.50
2:A:135:ALA:HB3	2:A:136:PRO:HD3	1.94	0.50
1:B:2082:GLU:HA	1:B:2144:VAL:O	2.12	0.50
3:C:1725:HIS:NE2	3:C:1787:ILE:HA	2.27	0.50
1:B:1732:GLU:O	1:B:1736:ARG:N	2.42	0.50
2:A:4:ILE:HG22	2:A:52:ASN:O	2.12	0.49
3:C:1832:VAL:C	3:C:1834:LYS:H	2.20	0.49
2:A:157:CYS:SG	2:A:158:SER:N	2.85	0.49
1:B:1973:ASN:C	1:B:2008:LEU:HD21	2.37	0.49
2:A:8:VAL:O	2:A:58:THR:OG1	2.25	0.49
3:C:1723:TYR:HB3	3:C:1816:CYS:HB2	1.95	0.49
1:B:1906:LEU:HA	1:B:1909:ILE:HG22	1.93	0.49
1:B:1949:VAL:HG23	2:A:28:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1898:TYR:CE1	1:B:2015:ARG:HB3	2.49	0.48
3:C:1974:ILE:HG13	3:C:2009:PHE:HB2	1.95	0.48
2:A:20:LEU:HG	2:A:55:LEU:HD13	1.96	0.48
1:B:1720:ALA:HB1	1:B:1820:LEU:HD12	1.95	0.48
3:C:1905:GLY:O	3:C:1907:SER:N	2.46	0.48
1:B:2063:GLY:O	2:A:37:PHE:HA	2.14	0.48
3:C:1957:GLU:HG3	3:C:1976:ARG:HH22	1.79	0.48
2:A:112:LEU:O	2:A:154:TYR:HA	2.14	0.48
3:C:1845:ASP:O	3:C:1847:LYS:N	2.47	0.48
1:B:1973:ASN:CA	1:B:2008:LEU:CD2	2.91	0.48
1:B:2126:TYR:CZ	1:B:2130:LEU:HD11	2.48	0.48
2:A:4:ILE:HD11	2:A:176:VAL:HG21	1.95	0.48
2:A:6:CYS:HB3	2:A:54:GLY:O	2.12	0.48
1:B:1710:HIS:HB3	1:B:1719:ALA:HB2	1.96	0.48
1:B:1933:ASN:O	1:B:1935:VAL:HG23	2.14	0.47
1:B:2016:ILE:HD12	1:B:2017:GLN:H	1.77	0.47
2:A:89:SER:O	2:A:93:VAL:HG13	2.14	0.47
2:A:129:LEU:CB	2:A:135:ALA:HB2	2.43	0.47
2:A:93:VAL:HG12	2:A:97:TRP:CD1	2.50	0.47
3:C:2054:MET:HE3	3:C:2058:GLN:NE2	2.28	0.47
1:B:1951:TYR:CD2	2:A:26:ASN:HB2	2.50	0.47
1:B:1867:VAL:HG13	1:B:1966:THR:OG1	2.14	0.47
1:B:1878:TYR:HD1	1:B:1951:TYR:HA	1.79	0.47
1:B:1710:HIS:NE2	1:B:2012:VAL:O	2.47	0.47
1:B:2003:LEU:HD12	1:B:2003:LEU:O	2.15	0.47
3:C:1937:PRO:C	3:C:1939:ASP:H	2.23	0.47
2:A:61:GLN:O	2:A:63:ASP:N	2.45	0.47
3:C:1899:LYS:HB2	3:C:2009:PHE:CE2	2.49	0.47
3:C:2001:THR:HA	3:C:2023:SER:HA	1.95	0.47
3:C:2006:SER:HB2	3:C:2019:ILE:HG23	1.97	0.47
1:B:1875:GLY:HA2	1:B:1971:HIS:HE1	1.79	0.47
3:C:1695:THR:C	3:C:1697:GLU:N	2.72	0.47
1:B:1975:ASN:N	1:B:2008:LEU:HD11	2.30	0.46
3:C:1879:ARG:HD3	3:C:2003:LEU:HD21	1.97	0.46
1:B:1873:LEU:HD12	1:B:1873:LEU:O	2.15	0.46
1:B:2092:ASN:OD1	1:B:2093:GLN:N	2.47	0.46
2:A:138:THR:OG1	2:A:140:PRO:HD2	2.15	0.46
1:B:1923:ALA:O	1:B:1925:ASN:N	2.37	0.46
1:B:2013:LYS:HE3	1:B:2015:ARG:HD3	1.96	0.46
1:B:1840:PHE:HE2	1:B:1848:LYS:HB3	1.80	0.46
2:A:129:LEU:O	2:A:133:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1829:ILE:HD11	1:B:1859:SER:HB3	1.98	0.46
3:C:1933:ASN:OD1	3:C:1933:ASN:N	2.42	0.46
3:C:1721:MET:HG3	3:C:2010:PRO:HG2	1.96	0.46
3:C:2054:MET:C	3:C:2058:GLN:OE1	2.58	0.46
1:B:1952:VAL:HG23	1:B:1979:PHE:HB3	1.97	0.46
3:C:1699:ARG:O	3:C:1702:TRP:HB3	2.16	0.46
1:B:1732:GLU:HB2	1:B:1777:TRP:CD1	2.50	0.45
3:C:1860:TYR:HA	3:C:1863:VAL:HG12	1.98	0.45
3:C:1897:ILE:HG21	3:C:1977:PHE:HD2	1.80	0.45
1:B:1807:ASN:HA	1:B:1810:VAL:HG12	1.97	0.45
1:B:1732:GLU:CB	1:B:1777:TRP:HD1	2.29	0.45
1:B:1846:PHE:O	1:B:1850:SER:N	2.45	0.45
1:B:1941:ASP:C	1:B:1943:LYS:H	2.24	0.45
2:A:157:CYS:HA	2:A:164:GLY:HA3	1.98	0.45
1:B:1840:PHE:O	1:B:1844:ARG:N	2.43	0.45
3:C:2063:GLY:O	3:C:2065:VAL:N	2.50	0.45
1:B:1966:THR:OG1	1:B:1967:ASP:N	2.50	0.45
3:C:1725:HIS:HA	3:C:1728:ALA:HB3	1.98	0.45
3:C:1960:GLU:OE1	3:C:1976:ARG:NH2	2.50	0.45
1:B:1720:ALA:HB2	1:B:1819:PHE:HB3	1.98	0.45
1:B:1878:TYR:CD2	1:B:1909:ILE:HG21	2.51	0.45
3:C:2005:THR:OG1	3:C:2016:ILE:HG13	2.17	0.45
2:A:124:ASP:OD1	2:A:124:ASP:N	2.48	0.44
3:C:1786:ASN:ND2	3:C:2008:LEU:O	2.50	0.44
3:C:1954:PRO:HA	3:C:1977:PHE:HA	1.98	0.44
3:C:1983:PHE:C	3:C:1985:LEU:H	2.25	0.44
1:B:1983:PHE:CD2	1:B:1999:ARG:HB2	2.52	0.44
1:B:1967:ASP:N	1:B:1967:ASP:OD1	2.51	0.44
1:B:1973:ASN:CA	1:B:2008:LEU:HD23	2.48	0.44
1:B:2001:THR:HG22	1:B:2023:SER:HB3	1.99	0.44
2:A:160:LEU:C	2:A:162:GLN:N	2.75	0.44
2:A:161:THR:C	2:A:163:ARG:H	2.26	0.44
3:C:1780:PHE:HD2	3:C:1783:ILE:HD12	1.83	0.44
2:A:133:LYS:O	2:A:134:LEU:HD22	2.18	0.43
1:B:1897:ILE:HG21	1:B:1977:PHE:CE2	2.53	0.43
1:B:2061:LEU:O	1:B:2065:VAL:HG22	2.19	0.43
3:C:1879:ARG:NH1	3:C:1948:GLN:OE1	2.52	0.43
1:B:1875:GLY:HA2	1:B:1971:HIS:CE1	2.52	0.43
2:A:51:VAL:HG11	2:A:173:ILE:HD12	2.01	0.43
2:A:160:LEU:O	2:A:161:THR:HG22	2.19	0.43
3:C:1832:VAL:O	3:C:1835:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2072:GLY:C	3:C:2074:MET:H	2.26	0.43
3:C:2073:PRO:C	3:C:2075:ALA:H	2.26	0.43
1:B:1697:GLU:HA	1:B:1700:ARG:NE	2.32	0.43
3:C:1887:PHE:HZ	3:C:1921:PHE:HA	1.83	0.43
2:A:65:ASP:O	2:A:66:ARG:HB3	2.17	0.43
1:B:1984:THR:HA	1:B:1997:CYS:SG	2.59	0.42
1:B:1973:ASN:HA	1:B:2008:LEU:HG	2.02	0.42
3:C:1953:THR:O	3:C:1955:PHE:N	2.52	0.42
1:B:2091:ASP:HB3	1:B:2092:ASN:H	1.73	0.42
3:C:1853:TYR:HA	3:C:1856:ILE:HG22	2.00	0.42
3:C:2109:GLY:C	3:C:2111:ALA:N	2.77	0.42
1:B:2015:ARG:H	1:B:2015:ARG:HG2	1.46	0.42
2:A:160:LEU:O	2:A:162:GLN:N	2.53	0.42
3:C:1724:ILE:HG13	3:C:1816:CYS:SG	2.59	0.42
1:B:1951:TYR:CD1	1:B:1952:VAL:N	2.88	0.42
1:B:1827:GLU:HG3	1:B:1968:PHE:CD2	2.55	0.42
1:B:2067:VAL:HG21	1:B:2072:GLY:CA	2.50	0.42
1:B:2078:ARG:HG2	1:B:2144:VAL:HG21	2.01	0.42
2:A:73:PRO:O	2:A:74:GLN:HB2	2.20	0.41
2:A:36:VAL:O	2:A:38:ASP:N	2.49	0.41
2:A:75:THR:HB	2:A:78:PHE:CE1	2.56	0.41
1:B:1835:PRO:HA	1:B:1838:ALA:HB3	2.02	0.41
1:B:1951:TYR:HD1	1:B:1952:VAL:H	1.67	0.41
2:A:113:VAL:HG23	2:A:155:LEU:O	2.20	0.41
3:C:1710:HIS:HB3	3:C:1719:ALA:HB2	2.01	0.41
3:C:1877:TYR:HD2	3:C:1954:PRO:HD3	1.86	0.41
3:C:1827:GLU:OE1	3:C:1872:ARG:NH2	2.49	0.41
3:C:2109:GLY:C	3:C:2111:ALA:H	2.29	0.41
1:B:1727:ALA:HB2	1:B:1812:GLN:HB3	2.02	0.41
1:B:2027:ASN:O	1:B:2031:VAL:HG12	2.21	0.41
2:A:4:ILE:CG2	2:A:53:LEU:HA	2.50	0.41
3:C:1706:MET:O	3:C:1709:ILE:HG12	2.21	0.41
3:C:1976:ARG:O	3:C:1977:PHE:HD1	2.04	0.41
1:B:1988:LYS:C	1:B:1996:GLN:HE22	2.23	0.41
3:C:1951:TYR:CD1	3:C:1952:VAL:N	2.89	0.40
3:C:1906:LEU:N	3:C:1909:ILE:HG22	2.36	0.40
1:B:1777:TRP:N	1:B:1778:PRO:CD	2.84	0.40
1:B:1824:GLU:HA	1:B:1826:TYR:CE1	2.55	0.40
1:B:1882:PHE:HD1	1:B:1947:ILE:HG22	1.86	0.40
1:B:1878:TYR:CD1	1:B:1951:TYR:HA	2.57	0.40
3:C:1887:PHE:CD2	3:C:1888:PHE:N	2.90	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	B	404/457 (88%)	341 (84%)	49 (12%)	14 (4%)	3	24
2	A	175/192 (91%)	148 (85%)	18 (10%)	9 (5%)	1	17
3	C	376/458 (82%)	310 (82%)	45 (12%)	21 (6%)	1	16
All	All	955/1107 (86%)	799 (84%)	112 (12%)	44 (5%)	2	18

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1934	LYS
1	B	1936	ASN
1	B	2019	ILE
1	B	2092	ASN
2	A	36	VAL
2	A	161	THR
3	C	1695	THR
3	C	1696	PRO
3	C	1906	LEU
3	C	1945	ALA
3	C	2049	MET
1	B	1773	PHE
1	B	2091	ASP
2	A	47	ASP
3	C	2080	PHE
1	B	1893	GLY
1	B	1942	PRO
2	A	39	ASN
2	A	135	ALA
2	A	159	ALA
3	C	1778	PRO

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Mol	Chain	Res	Type
3	C	1846	PHE
1	B	1926	VAL
1	B	1988	LYS
3	C	1891	GLU
3	C	1946	TYR
3	C	1985	LEU
3	C	2054	MET
3	C	2138	LEU
1	B	2052	VAL
1	B	2071	ALA
3	C	1934	LYS
3	C	1935	VAL
3	C	2050	GLU
3	C	2053	ASP
2	A	28	PHE
3	C	1957	GLU
2	A	9	VAL
2	A	85	VAL
1	B	1947	ILE
1	B	1695	THR
3	C	1929	ILE
3	C	1803	PRO
3	C	1954	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	B	259/411 (63%)	258 (100%)	1 (0%)	84	81
2	A	114/167 (68%)	114 (100%)	0	100	100
3	C	184/411 (45%)	184 (100%)	0	100	100
All	All	557/989 (56%)	556 (100%)	1 (0%)	87	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1995	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1930	GLN
2	A	61	GLN
3	C	1786	ASN
3	C	2127	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	B	412/457 (90%)	-0.35	1 (0%) 91 80	98, 151, 204, 230	0
2	A	177/192 (92%)	-0.21	1 (0%) 85 66	110, 152, 189, 207	0
3	C	388/458 (84%)	-0.47	0 100 100	96, 143, 181, 225	0
All	All	977/1107 (88%)	-0.37	2 (0%) 91 80	96, 147, 197, 230	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2076	TYR	4.2
2	A	81	CYS	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.