Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:29 am BST

PDB ID	:	4C0E
Title	:	Structure of the NOT1 superfamily homology domain from Chaetomium thermophilum
Authors	:	Chen, Y.; Boland, A.; Raisch, T.; Jonas, S.; Izaurralde, E.; Weichenrieder, O.
Deposited on	:	2013-08-01
Resolution	:	3.20 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 ①) were used in the production of this report:

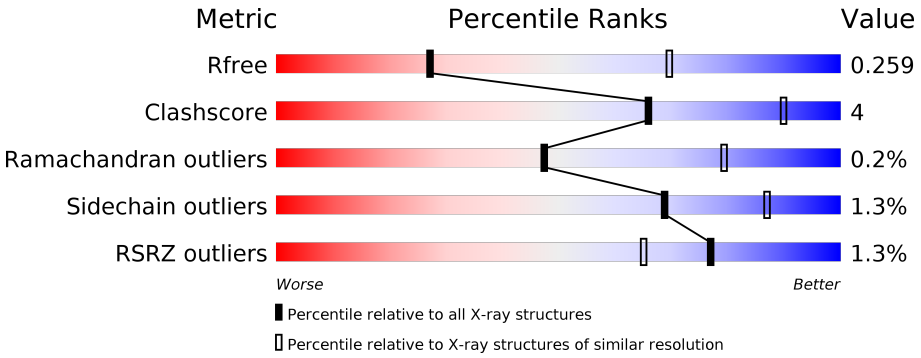
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	528	2% 84% 12% ·
1	B	528	% 83% 12% ·
1	C	528	% 87% 11% ·
1	D	528	% 88% 10% ·

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15737 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 NOT1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	Se	0	0	0
			3931	2548	671	697	5	10			
1	B	505	Total	C	N	O	S	Se	0	0	0
			3891	2530	665	681	5	10			
1	C	517	Total	C	N	O	S	Se	0	0	0
			3979	2588	675	700	5	11			
1	D	517	Total	C	N	O	S	Se	0	0	0
			3936	2558	672	691	5	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1666	ASN	-	expression tag	UNP G0SAL9
A	1667	LEU	-	expression tag	UNP G0SAL9
A	1668	TYR	-	expression tag	UNP G0SAL9
A	1669	PHE	-	expression tag	UNP G0SAL9
A	1670	GLN	-	expression tag	UNP G0SAL9
A	1671	GLY	-	expression tag	UNP G0SAL9
A	1672	HIS	-	expression tag	UNP G0SAL9
A	1673	MSE	-	expression tag	UNP G0SAL9
A	1674	LEU	-	expression tag	UNP G0SAL9
A	1675	GLU	-	expression tag	UNP G0SAL9
B	1666	ASN	-	expression tag	UNP G0SAL9
B	1667	LEU	-	expression tag	UNP G0SAL9
B	1668	TYR	-	expression tag	UNP G0SAL9
B	1669	PHE	-	expression tag	UNP G0SAL9
B	1670	GLN	-	expression tag	UNP G0SAL9
B	1671	GLY	-	expression tag	UNP G0SAL9
B	1672	HIS	-	expression tag	UNP G0SAL9
B	1673	MSE	-	expression tag	UNP G0SAL9
B	1674	LEU	-	expression tag	UNP G0SAL9
B	1675	GLU	-	expression tag	UNP G0SAL9
C	1666	ASN	-	expression tag	UNP G0SAL9

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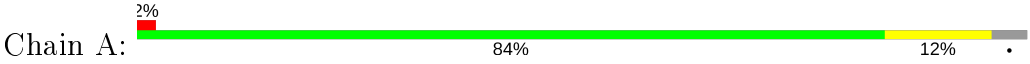
Chain	Residue	Modelled	Actual	Comment	Reference
C	1667	LEU	-	expression tag	UNP G0SAL9
C	1668	TYR	-	expression tag	UNP G0SAL9
C	1669	PHE	-	expression tag	UNP G0SAL9
C	1670	GLN	-	expression tag	UNP G0SAL9
C	1671	GLY	-	expression tag	UNP G0SAL9
C	1672	HIS	-	expression tag	UNP G0SAL9
C	1673	MSE	-	expression tag	UNP G0SAL9
C	1674	LEU	-	expression tag	UNP G0SAL9
C	1675	GLU	-	expression tag	UNP G0SAL9
D	1666	ASN	-	expression tag	UNP G0SAL9
D	1667	LEU	-	expression tag	UNP G0SAL9
D	1668	TYR	-	expression tag	UNP G0SAL9
D	1669	PHE	-	expression tag	UNP G0SAL9
D	1670	GLN	-	expression tag	UNP G0SAL9
D	1671	GLY	-	expression tag	UNP G0SAL9
D	1672	HIS	-	expression tag	UNP G0SAL9
D	1673	MSE	-	expression tag	UNP G0SAL9
D	1674	LEU	-	expression tag	UNP G0SAL9
D	1675	GLU	-	expression tag	UNP G0SAL9

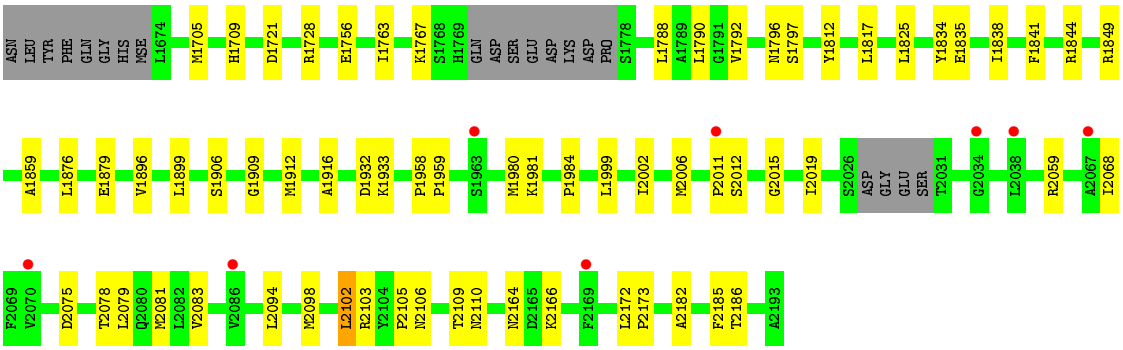
3 Residue-property plots (i)

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: NOT1

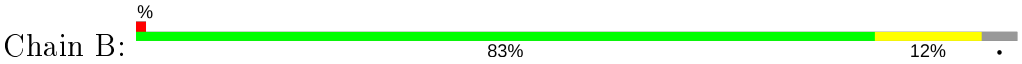
Chain A:

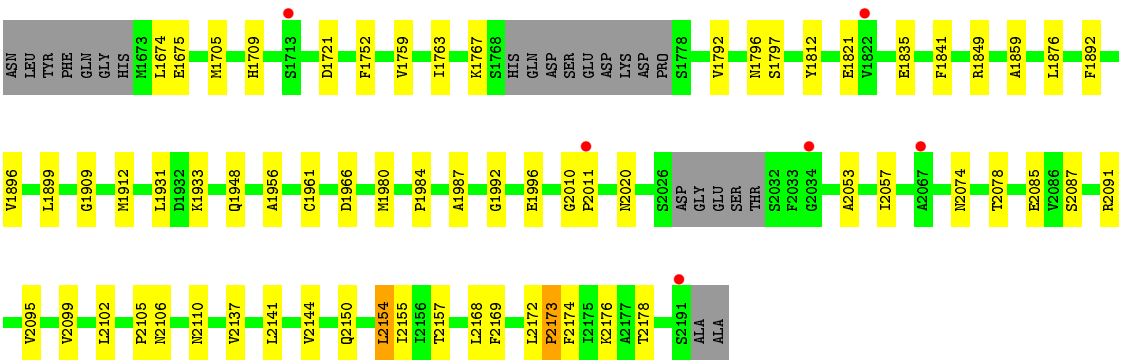




- Molecule 1: NOT1

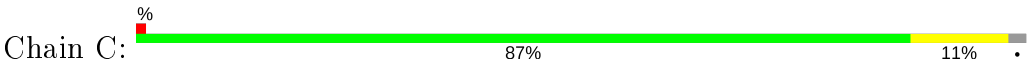
Chain B:

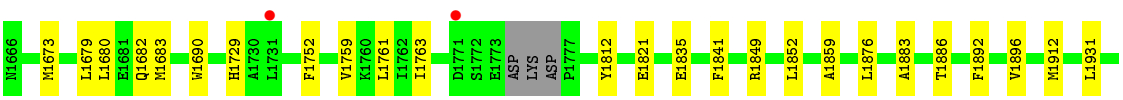


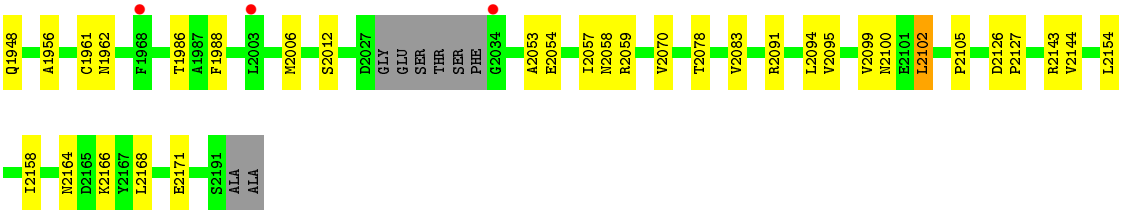


- Molecule 1: NOT1

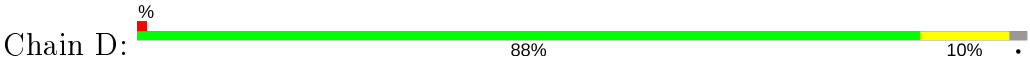
Chain C:

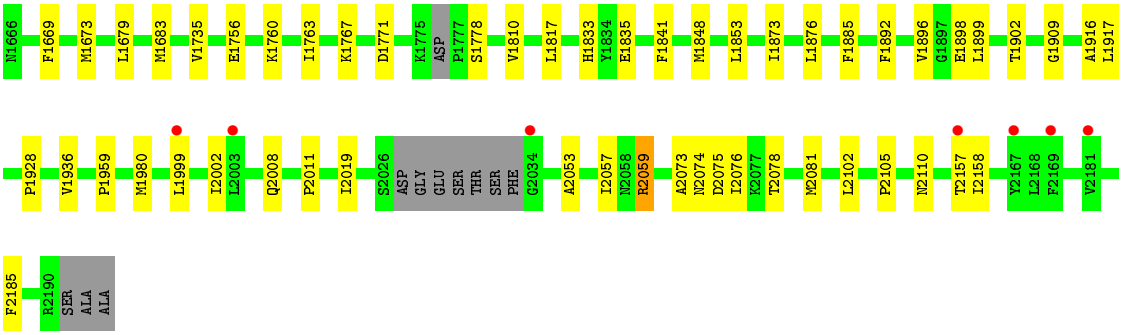






- Molecule 1: NOT1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.75Å 127.22Å 130.20Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	63.61 – 3.20 90.93 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.61-3.20) 99.9 (90.93-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.259 0.216 , 0.259	Depositor DCC
R_{free} test set	2112 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15737	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.21	0/4014	0.35	0/5443
1	B	0.22	0/3973	0.35	0/5393
1	C	0.21	0/4066	0.34	0/5518
1	D	0.20	0/4021	0.34	0/5463
All	All	0.21	0/16074	0.35	0/21817

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

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	3931	0	3869	39	0
1	B	3891	0	3815	33	0
1	C	3979	0	3872	31	0
1	D	3936	0	3798	27	0
All	All	15737	0	15354	125	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 4.

All (125) 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:C:1763:ILE:HG13	1:C:1821:GLU:HG2	1.73	0.71
1:D:1760:LYS:HA	1:D:1763:ILE:HD12	1.73	0.70
1:A:1932:ASP:OD1	1:A:2103:ARG:NH2	2.24	0.70
1:C:1673:MSE:HE1	1:C:1682:GLN:HA	1.75	0.68
1:D:1999:LEU:HD23	1:D:2002:ILE:HD12	1.76	0.68
1:B:1763:ILE:HG13	1:B:1821:GLU:HG2	1.78	0.66
1:B:1896:VAL:HG12	1:B:1912:MSE:HB3	1.77	0.65
1:A:2006:MSE:HE3	1:A:2012:SER:H	1.61	0.65
1:A:2059:ARG:NH1	1:A:2075:ASP:OD1	2.29	0.65
1:A:1705:MSE:O	1:A:1709:HIS:ND1	2.30	0.64
1:D:2102:LEU:HD13	1:D:2157:THR:HG21	1.80	0.64
1:C:1961:CYS:SG	1:C:1962:ASN:N	2.71	0.64
1:B:1948:GLN:OE1	1:C:1948:GLN:NE2	2.28	0.63
1:D:1835:GLU:HG2	1:D:1876:LEU:HD22	1.81	0.63
1:B:2144:VAL:HG22	1:B:2154:LEU:HD21	1.80	0.62
1:A:1999:LEU:HD21	1:A:2019:ILE:HG12	1.81	0.62
1:C:2059:ARG:HH12	1:C:2070:VAL:HB	1.65	0.62
1:A:1981:LYS:HA	1:A:2068:ILE:HD11	1.83	0.61
1:D:2011:PRO:HB2	1:D:2081:MSE:HE2	1.83	0.60
1:C:1986:THR:HG22	1:C:1988:PHE:H	1.66	0.60
1:C:1679:LEU:HD11	1:C:1683:MSE:HE3	1.83	0.60
1:C:1835:GLU:HG2	1:C:1876:LEU:HD22	1.85	0.59
1:B:1705:MSE:O	1:B:1709:HIS:ND1	2.32	0.59
1:C:2006:MSE:HE3	1:C:2012:SER:H	1.68	0.59
1:D:2011:PRO:HB3	1:D:2078:THR:HA	1.84	0.58
1:A:1999:LEU:HD11	1:A:2019:ILE:HA	1.84	0.58
1:C:2006:MSE:HE2	1:C:2078:THR:HG23	1.86	0.58
1:D:1896:VAL:HG21	1:D:1916:ALA:HB2	1.86	0.57
1:B:2011:PRO:HB3	1:B:2078:THR:HA	1.87	0.57
1:B:1763:ILE:HG22	1:B:1767:LYS:HE2	1.87	0.57
1:D:2073:ALA:HB3	1:D:2076:ILE:HD13	1.86	0.57
1:D:2059:ARG:NH2	1:D:2075:ASP:OD1	2.33	0.56
1:A:2006:MSE:HE2	1:A:2078:THR:HG23	1.86	0.56
1:C:2083:VAL:O	1:C:2091:ARG:NH1	2.38	0.55
1:D:2008:GLN:O	1:D:2074:ASN:ND2	2.38	0.55
1:B:1835:GLU:HG2	1:B:1876:LEU:HD22	1.88	0.54
1:A:1896:VAL:HG22	1:A:1912:MSE:HG3	1.90	0.54
1:C:2054:GLU:O	1:C:2058:ASN:ND2	2.40	0.53
1:A:2182:ALA:O	1:A:2186:THR:OG1	2.23	0.53
1:D:1899:LEU:HD13	1:D:1909:GLY:HA2	1.90	0.53
1:A:2172:LEU:HD22	1:A:2173:PRO:HD2	1.90	0.53
1:C:1896:VAL:HG12	1:C:1912:MSE:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1849:ARG:NH1	1:B:1721:ASP:OD2	2.42	0.52
1:C:1849:ARG:HH21	1:C:1852:LEU:HD11	1.74	0.52
1:A:1906:SER:OG	1:B:1675:GLU:OE2	2.25	0.52
1:D:2158:ILE:HD11	1:D:2185:PHE:HE1	1.73	0.52
1:A:1980:MSE:HG3	1:A:2110:ASN:HB2	1.91	0.51
1:A:1721:ASP:OD2	1:B:1849:ARG:NH1	2.43	0.51
1:C:2164:ASN:HD22	1:C:2166:LYS:HE2	1.75	0.51
1:D:1928:PRO:HG2	1:D:1959:PRO:HD3	1.93	0.51
1:A:1788:LEU:HB3	1:A:1844:ARG:HG3	1.92	0.50
1:D:1999:LEU:HD13	1:D:2019:ILE:HA	1.92	0.50
1:C:2168:LEU:HB3	1:C:2171:GLU:HG3	1.93	0.50
1:A:1728:ARG:HG2	1:A:1790:LEU:HD13	1.94	0.50
1:A:1812:TYR:HB2	1:A:1859:ALA:HB1	1.93	0.49
1:B:2102:LEU:HD13	1:B:2157:THR:HG21	1.94	0.49
1:B:2137:VAL:HG21	1:B:2169:PHE:HE1	1.77	0.49
1:B:2172:LEU:HG	1:B:2173:PRO:HD2	1.93	0.49
1:A:2164:ASN:HD21	1:A:2166:LYS:HE2	1.77	0.49
1:A:1879:GLU:OE1	1:A:1933:LYS:NZ	2.40	0.48
1:B:2137:VAL:HG22	1:B:2141:LEU:HD13	1.96	0.48
1:A:2102:LEU:HA	1:A:2109:THR:HA	1.96	0.47
1:C:2168:LEU:HD22	1:C:2171:GLU:HG3	1.95	0.47
1:B:1980:MSE:HG3	1:B:2110:ASN:HB2	1.97	0.47
1:A:1835:GLU:HG2	1:A:1876:LEU:HD22	1.97	0.47
1:A:2011:PRO:HB3	1:A:2078:THR:HA	1.96	0.47
1:C:2144:VAL:HG21	1:C:2158:ILE:HD12	1.95	0.47
1:A:1792:VAL:O	1:A:1796:ASN:ND2	2.34	0.46
1:B:1984:PRO:HB3	1:B:2106:ASN:HD22	1.80	0.46
1:A:1763:ILE:HG22	1:A:1767:LYS:HE2	1.97	0.46
1:A:2011:PRO:HB2	1:A:2081:MSE:SE	2.65	0.46
1:B:2172:LEU:O	1:B:2174:PHE:N	2.49	0.46
1:D:1873:ILE:HD13	1:D:1885:PHE:HB2	1.96	0.46
1:A:1797:SER:HA	1:B:1797:SER:HB2	1.99	0.45
1:C:2102:LEU:HD13	1:C:2154:LEU:HA	1.99	0.45
1:D:1756:GLU:HG2	1:D:1817:LEU:HD11	1.99	0.45
1:D:1763:ILE:HG22	1:D:1767:LYS:HE3	1.99	0.44
1:A:1756:GLU:HG2	1:A:1817:LEU:HD11	1.99	0.44
1:C:1812:TYR:HB2	1:C:1859:ALA:HB1	2.00	0.44
1:B:1759:VAL:O	1:B:1763:ILE:HG12	2.17	0.44
1:B:1792:VAL:O	1:B:1796:ASN:ND2	2.40	0.44
1:B:2150:GLN:HB2	1:B:2155:ILE:HD11	1.99	0.44
1:C:1680:LEU:HD11	1:C:1729:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1899:LEU:HD13	1:A:1909:GLY:HA2	2.00	0.44
1:B:1899:LEU:HD13	1:B:1909:GLY:HA2	2.00	0.43
1:D:1679:LEU:HD11	1:D:1683:MSE:HE3	1.99	0.43
1:D:1898:GLU:O	1:D:1902:THR:OG1	2.35	0.43
1:C:2053:ALA:O	1:C:2057:ILE:HG12	2.18	0.43
1:C:2095:VAL:O	1:C:2099:VAL:HG23	2.19	0.43
1:B:2010:GLY:HA2	1:B:2074:ASN:HB3	2.00	0.43
1:C:2083:VAL:HG12	1:C:2094:LEU:HD22	2.00	0.43
1:D:1669:PHE:HD2	1:D:1673:MSE:HG3	1.83	0.43
1:C:1931:LEU:HD23	1:C:1956:ALA:HB2	2.00	0.43
1:C:1759:VAL:O	1:C:1763:ILE:HG12	2.19	0.42
1:C:2100:ASN:OD1	1:C:2143:ARG:NH2	2.52	0.42
1:B:1966:ASP:N	1:B:1966:ASP:OD1	2.52	0.42
1:B:2053:ALA:O	1:B:2057:ILE:HG12	2.19	0.42
1:B:2095:VAL:O	1:B:2099:VAL:HG23	2.18	0.42
1:D:1980:MSE:HG3	1:D:2110:ASN:HB2	2.01	0.42
1:A:1728:ARG:HG2	1:A:1790:LEU:CD1	2.50	0.42
1:C:2126:ASP:HA	1:C:2127:PRO:HD3	1.85	0.42
1:A:1896:VAL:HG21	1:A:1916:ALA:HB2	2.00	0.42
1:A:1984:PRO:HD3	1:A:2106:ASN:HB2	2.01	0.41
1:C:1883:ALA:O	1:C:1886:THR:HG22	2.20	0.41
1:B:1931:LEU:HD23	1:B:1956:ALA:HB2	2.03	0.41
1:B:2020:ASN:ND2	1:B:2085:GLU:O	2.53	0.41
1:C:1690:TRP:NE1	1:C:1761:LEU:HB2	2.35	0.41
1:A:1767:LYS:HD3	1:A:1825:LEU:HD21	2.03	0.41
1:A:2002:ILE:HD11	1:A:2015:GLY:HA2	2.02	0.41
1:B:2087:SER:O	1:B:2091:ARG:N	2.49	0.41
1:A:1958:PRO:HA	1:A:1959:PRO:HD3	1.88	0.41
1:C:2102:LEU:H	1:C:2102:LEU:HG	1.75	0.41
1:D:1735:VAL:HG22	1:D:1810:VAL:HG11	2.03	0.41
1:D:2053:ALA:O	1:D:2057:ILE:HG12	2.21	0.41
1:A:1705:MSE:HE3	1:A:1709:HIS:CE1	2.55	0.41
1:A:2079:LEU:O	1:A:2083:VAL:HG23	2.21	0.41
1:D:1917:LEU:HD12	1:D:1917:LEU:HA	1.93	0.41
1:D:1771:ASP:HB2	1:D:1833:HIS:CD2	2.57	0.40
1:A:1834:TYR:O	1:A:1838:ILE:HG12	2.21	0.40
1:B:1933:LYS:HG2	1:B:1987:ALA:HB2	2.03	0.40
1:B:1992:GLY:O	1:B:1996:GLU:HG2	2.21	0.40
1:D:1848:MSE:HA	1:D:1853:LEU:HD13	2.03	0.40
1:D:1778:SER:HB2	1:D:1833:HIS:NE2	2.36	0.40
1:A:2094:LEU:HG	1:A:2098:MSE:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1812:TYR:HB2	1:B:1859:ALA:HB1	2.03	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	502/528 (95%)	491 (98%)	10 (2%)	1 (0%)	47	79
1	B	499/528 (94%)	487 (98%)	10 (2%)	2 (0%)	34	69
1	C	511/528 (97%)	499 (98%)	11 (2%)	1 (0%)	47	79
1	D	511/528 (97%)	503 (98%)	7 (1%)	1 (0%)	47	79
All	All	2023/2112 (96%)	1980 (98%)	38 (2%)	5 (0%)	47	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2173	PRO
1	B	2105	PRO
1	D	2105	PRO
1	A	2105	PRO
1	C	2105	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	405/438 (92%)	402 (99%)	3 (1%)	84 94
1	B	394/438 (90%)	385 (98%)	9 (2%)	50 78
1	C	403/438 (92%)	399 (99%)	4 (1%)	76 90
1	D	391/438 (89%)	387 (99%)	4 (1%)	76 90
All	All	1593/1752 (91%)	1573 (99%)	20 (1%)	69 87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1841	PHE
1	A	2102	LEU
1	A	2185	PHE
1	B	1674	LEU
1	B	1752	PHE
1	B	1841	PHE
1	B	1892	PHE
1	B	1961	CYS
1	B	2154	LEU
1	B	2168	LEU
1	B	2176	LYS
1	B	2178	THR
1	C	1752	PHE
1	C	1841	PHE
1	C	1892	PHE
1	C	2102	LEU
1	D	1841	PHE
1	D	1892	PHE
1	D	1936	VAL
1	D	2059	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1695	ASN
1	A	1753	GLN
1	B	1948	GLN
1	B	2020	ASN
1	C	1753	GLN
1	C	1769	HIS
1	C	1948	GLN
1	C	2018	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	498/528 (94%)	0.18	8 (1%)	72	59	39, 86, 152, 186	0
1	B	494/528 (93%)	0.13	6 (1%)	79	67	40, 80, 139, 175	0
1	C	506/528 (95%)	0.01	5 (0%)	82	72	41, 79, 133, 174	0
1	D	506/528 (95%)	0.14	7 (1%)	75	63	45, 90, 153, 187	0
All	All	2004/2112 (94%)	0.12	26 (1%)	77	65	39, 83, 148, 187	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2167	TYR	3.8
1	A	1963	SER	3.7
1	A	2067	ALA	3.4
1	D	2003	LEU	3.2
1	A	2034	GLY	3.1
1	D	2169	PHE	3.0
1	D	2181	VAL	2.9
1	A	2038	LEU	2.6
1	B	2034	GLY	2.5
1	D	2157	THR	2.5
1	D	2034	GLY	2.5
1	B	2191	SER	2.4
1	C	1771	ASP	2.4
1	B	1713	SER	2.4
1	A	2086	VAL	2.3
1	C	2003	LEU	2.2
1	B	2011	PRO	2.2
1	B	1822	VAL	2.1
1	C	2034	GLY	2.1
1	A	2011	PRO	2.1
1	A	2169	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1968	PHE	2.0
1	B	2067	ALA	2.0
1	D	1999	LEU	2.0
1	A	2070	VAL	2.0
1	C	1731	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.