



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:25 PM UTC

PDB ID : 4C0E / pdb_00004c0e
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

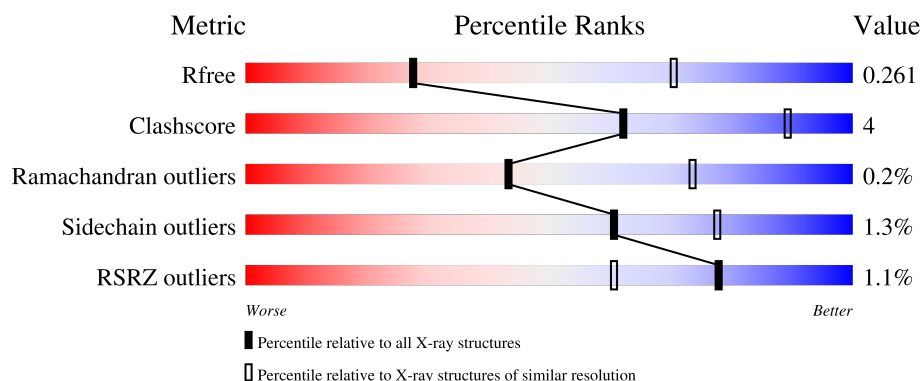
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	A	528	% 83% 13% .
1	B	528	2% 83% 12% .
1	C	528	% 87% 10% .
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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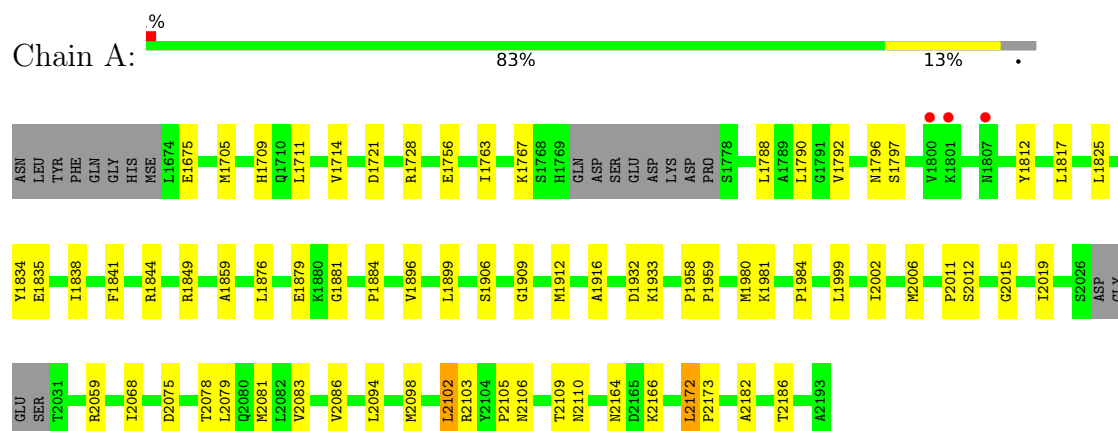
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1667	LEU	-	expression tag	UNP G0SAL9
C	1668	TYR	-	expression tag	UNP G0SAL9
C	1669	PHE	-	expression tag	UNP G0SAL9
C	1670	GLN	-	expression tag	UNP G0SAL9
C	1671	GLY	-	expression tag	UNP G0SAL9
C	1672	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

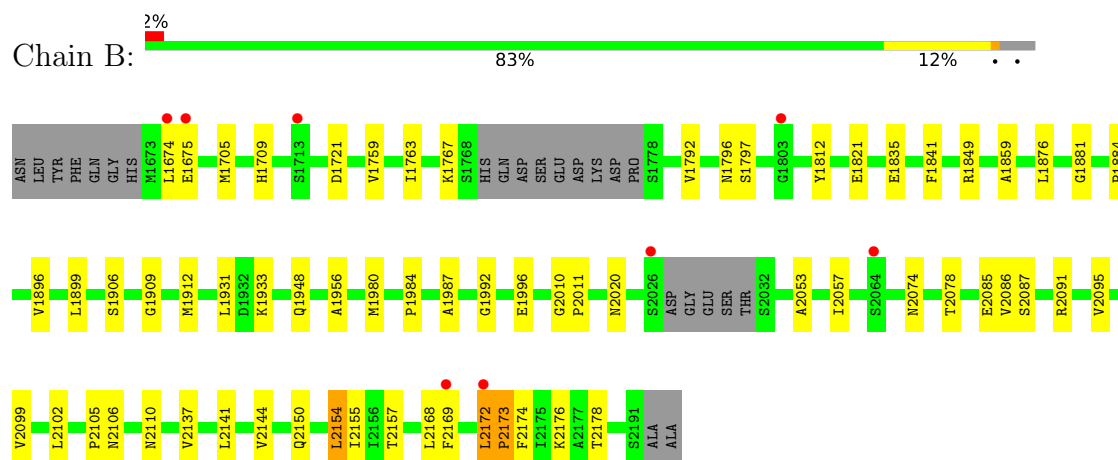
3 Residue-property plots

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.

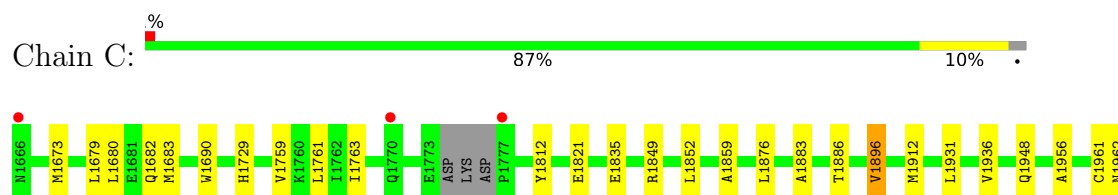
• Molecule 1: NOT1

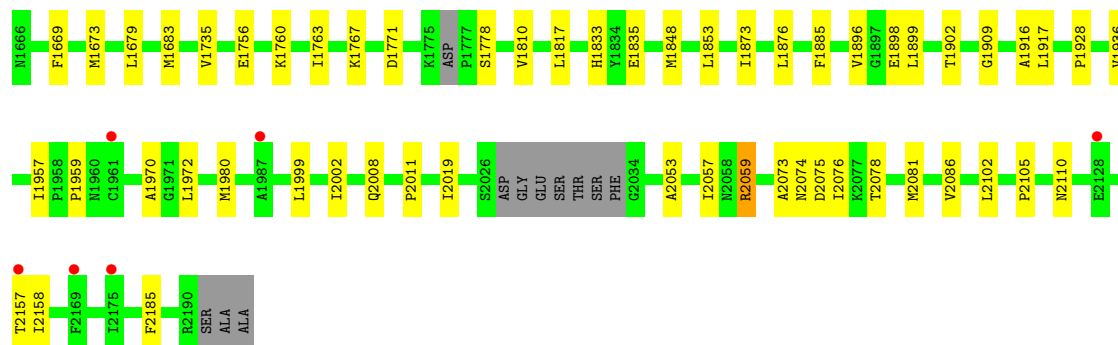


• Molecule 1: NOT1



• Molecule 1: NOT1





4 Data and refinement statistics

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 63.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.61-3.20) 99.9 (63.61-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.259 0.219 , 0.261	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 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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	A	0.28	0/4014	0.71	0/5443
1	B	0.28	0/3973	0.69	2/5393 (0.0%)
1	C	0.27	0/4066	0.69	0/5518
1	D	0.27	0/4021	0.70	3/5463 (0.1%)
All	All	0.28	0/16074	0.70	5/21817 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1957	ILE	CA-C-N	5.76	123.86	119.66
1	D	1957	ILE	C-N-CA	5.76	123.86	119.66
1	B	2172	LEU	CA-C-N	5.69	126.96	119.84
1	B	2172	LEU	C-N-CA	5.69	126.96	119.84
1	D	1970	ALA	CB-CA-C	-5.20	110.56	116.54

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	3931	0	3869	41	0
1	B	3891	0	3815	34	0
1	C	3979	0	3872	31	0
1	D	3936	0	3798	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15737	0	15354	127	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 (127) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1675:GLU:OE2	1:B:1906:SER:OG	2.28	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:1881:GLY:C	1:B:1884:PRO:HD2	2.45	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:1881:GLY:C	1:A:1884:PRO:HD2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1812:TYR:HB2	1:B:1859:ALA:HB1	2.03	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	A	502/528 (95%)	491 (98%)	10 (2%)	1 (0%)	43	73
1	B	499/528 (94%)	487 (98%)	10 (2%)	2 (0%)	30	62
1	C	511/528 (97%)	499 (98%)	11 (2%)	1 (0%)	43	73
1	D	511/528 (97%)	503 (98%)	7 (1%)	1 (0%)	43	73
All	All	2023/2112 (96%)	1980 (98%)	38 (2%)	5 (0%)	43	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2173	PRO
1	B	2105	PRO
1	D	2105	PRO

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Mol	Chain	Res	Type
1	A	2105	PRO
1	C	2105	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/438 (92%)	399 (98%)	6 (2%)	57	76
1	B	394/438 (90%)	387 (98%)	7 (2%)	51	74
1	C	403/438 (92%)	399 (99%)	4 (1%)	68	80
1	D	391/438 (89%)	387 (99%)	4 (1%)	68	80
All	All	1593/1752 (91%)	1572 (99%)	21 (1%)	61	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1711	LEU
1	A	1714	VAL
1	A	1841	PHE
1	A	2086	VAL
1	A	2102	LEU
1	A	2172	LEU
1	B	1674	LEU
1	B	1841	PHE
1	B	2086	VAL
1	B	2154	LEU
1	B	2168	LEU
1	B	2176	LYS
1	B	2178	THR
1	C	1896	VAL
1	C	1936	VAL
1	C	2086	VAL
1	C	2102	LEU
1	D	1936	VAL
1	D	1972	LEU

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Mol	Chain	Res	Type
1	D	2059	ARG
1	D	2086	VAL

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

Mol	Chain	Res	Type
1	A	1695	ASN
1	A	1753	GLN
1	A	1851	ASN
1	A	2024	ASN
1	B	1820	HIS
1	B	1851	ASN
1	B	1948	GLN
1	B	2122	HIS
1	C	1753	GLN
1	C	1769	HIS
1	C	1891	GLN
1	C	1924	GLN
1	C	1948	GLN
1	C	2018	GLN
1	C	2020	ASN
1	C	2122	HIS
1	C	2135	GLN
1	D	1715	GLN
1	D	1820	HIS
1	D	2024	ASN
1	D	2041	ASN
1	D	2135	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 oligosaccharides 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, 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	498/528 (94%)	0.08	3 (0%) 85 73	39, 86, 152, 186	0
1	B	494/528 (93%)	0.07	8 (1%) 70 51	40, 80, 139, 175	0
1	C	506/528 (95%)	0.06	6 (1%) 76 58	41, 79, 133, 174	0
1	D	506/528 (95%)	0.21	6 (1%) 76 58	45, 90, 153, 187	0
All	All	2004/2112 (94%)	0.11	23 (1%) 78 61	39, 83, 148, 187	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1674	LEU	3.5
1	C	2027	ASP	2.7
1	C	2034	GLY	2.6
1	C	1666	ASN	2.5
1	D	2128	GLU	2.4
1	B	1675	GLU	2.4
1	C	2035	TYR	2.4
1	D	1961	CYS	2.4
1	A	1801	LYS	2.3
1	B	1803	GLY	2.3
1	B	2172	LEU	2.3
1	B	2026	SER	2.3
1	D	1987	ALA	2.2
1	B	2169	PHE	2.2
1	B	1713	SER	2.2
1	D	2169	PHE	2.2
1	D	2157	THR	2.1
1	B	2064	SER	2.1
1	A	1800	VAL	2.1
1	A	1807	ASN	2.1
1	C	1777	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	2175	ILE	2.0
1	C	1770	GLN	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 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.