Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:44 AM EDT

PDB ID	:	5I6F
Title	:	Crystal structure of C-terminal variant 1 of Chaetomium thermophilum acetyl-CoA carboxylase
Authors	:	Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on	:	2016-02-16
Resolution	:	3.60 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 (i) 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 (1)) were used in the production of this report:

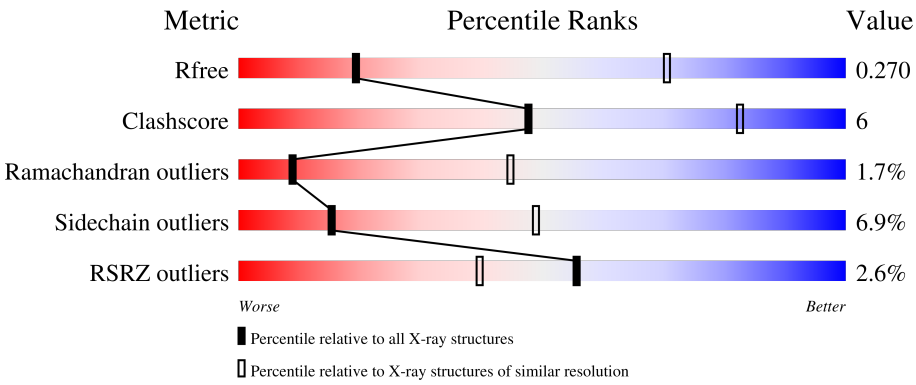
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	1179	3% 69% 18% • 11%
1	B	1179	2% 69% 19% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16592 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 Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1044	8286	5260	1453	1544	29	0	0	0
1	B	1048	8306	5272	1457	1548	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

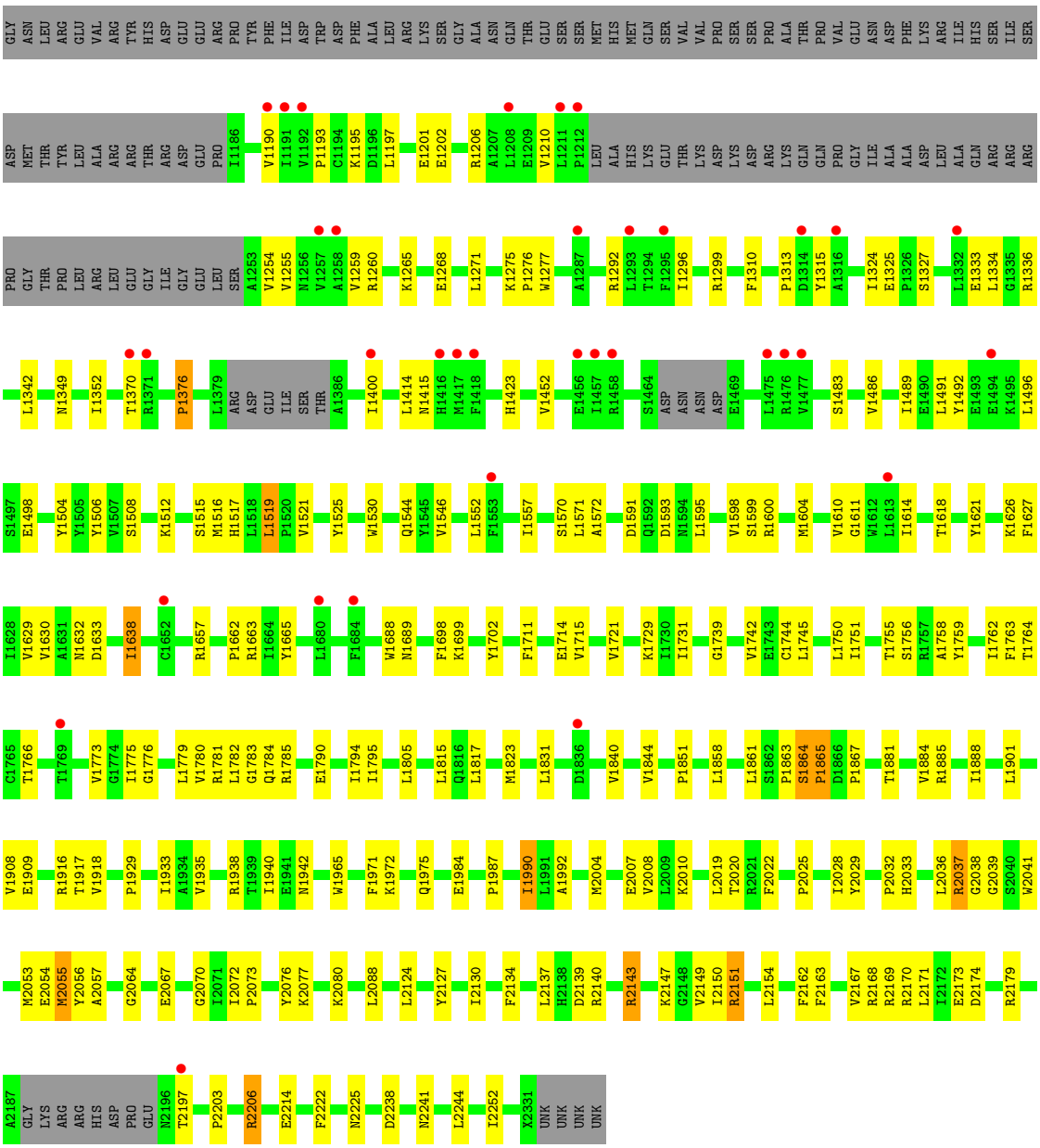
Chain	Residue	Modelled	Actual	Comment	Reference
A	1113	GLY	-	expression tag	UNP G0S3L5
B	1113	GLY	-	expression tag	UNP G0S3L5

3 Residue-property plots (i)

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.

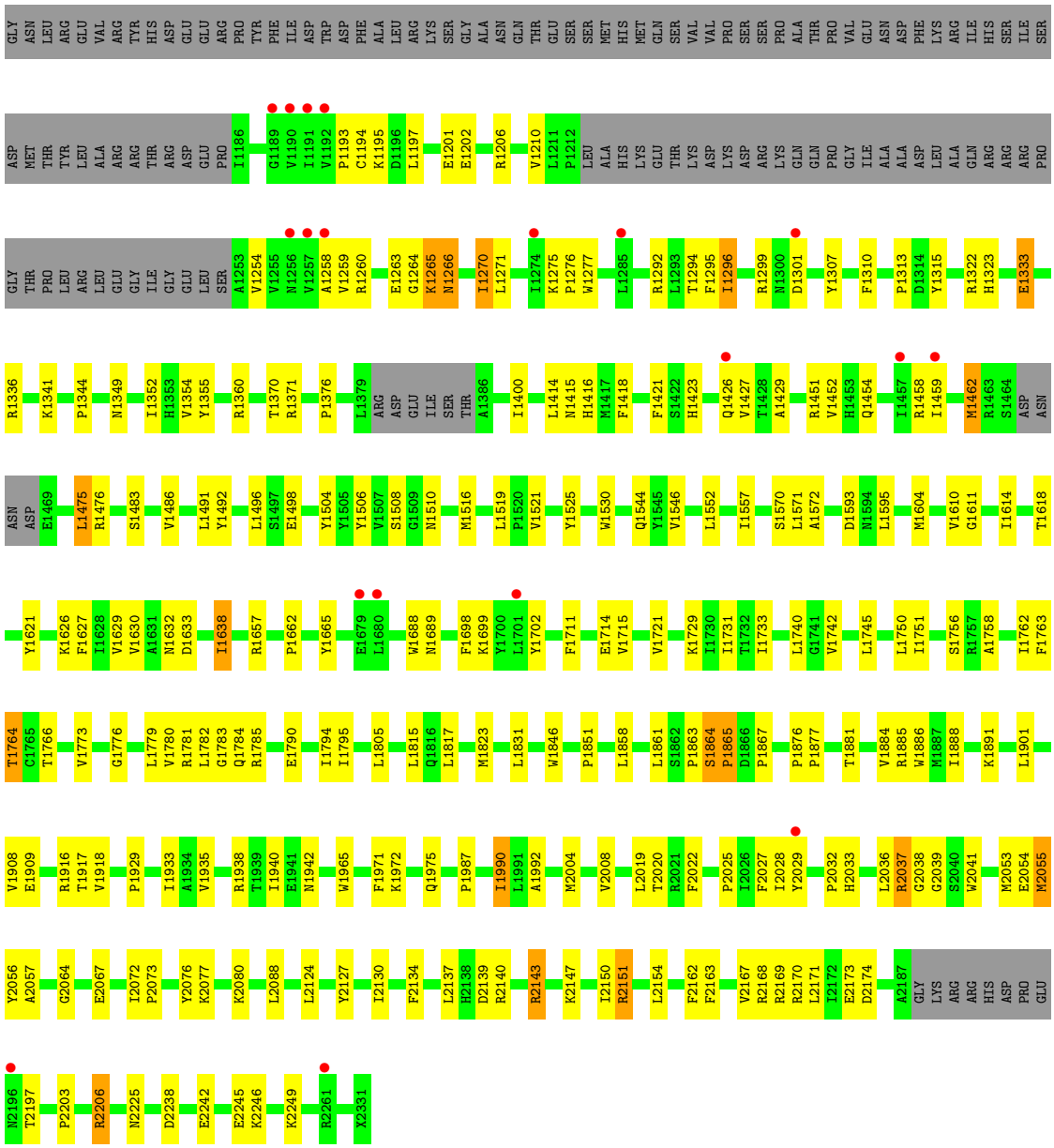
- Molecule 1: Acetyl-CoA carboxylase-like protein

Chain A: 3% 69% 18% 11%



- Molecule 1: Acetyl-CoA carboxylase-like protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.66Å 165.34Å 219.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.60 49.24 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-3.60) 99.7 (49.24-3.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.203 , 0.243 0.234 , 0.270	Depositor DCC
R_{free} test set	2011 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	158.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 161.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16592	wwPDB-VP
Average B, all atoms (Å^2)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 (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	0.45	0/8349	0.66	0/11306
1	B	0.45	0/8349	0.67	0/11306
All	All	0.45	0/16698	0.67	0/22612

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	8286	0	8150	97	0
1	B	8306	0	8153	110	0
All	All	16592	0	16303	200	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 6.

All (200) 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:1415:ASN:HB2	1:B:1452:VAL:HA	1.66	0.78
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.65	0.77
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.66	0.76
1:B:1427:VAL:HG11	1:B:1459:ILE:HD12	1.69	0.74
1:A:2163:PHE:O	1:A:2167:VAL:HG23	1.86	0.73
1:B:2163:PHE:O	1:B:2167:VAL:HG23	1.89	0.73
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.72	0.71
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.73	0.70
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.55	0.70
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.74	0.70
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.74	0.69
1:A:1519:LEU:HD11	1:A:1600:ARG:HD2	1.75	0.69
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.75	0.68
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.75	0.68
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.76	0.68
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.74	0.67
1:A:1933:ILE:HB	1:A:1990:ILE:HG23	1.77	0.67
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.77	0.67
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.77	0.67
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.77	0.66
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.77	0.66
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.77	0.66
1:B:1933:ILE:HB	1:B:1990:ILE:HG23	1.77	0.66
1:A:1785:ARG:NH1	1:A:1984:GLU:HG3	2.11	0.65
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.77	0.65
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.78	0.65
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.61	0.65
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.79	0.63
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.82	0.62
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.81	0.62
1:B:1785:ARG:HD2	1:B:1846:TRP:HZ3	1.65	0.60
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.83	0.60
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.66	0.59
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.83	0.59
1:A:1764:THR:HG23	1:A:1783:GLY:O	2.01	0.59
1:B:1764:THR:HG23	1:B:1783:GLY:O	2.03	0.58
1:B:1742:VAL:HA	1:B:1745:LEU:HD12	1.85	0.58
1:A:1864:SER:CB	1:A:1865:PRO:HD3	2.34	0.58
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.86	0.58
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.85	0.57
1:B:1864:SER:CB	1:B:1865:PRO:HD3	2.35	0.57
1:A:1742:VAL:HA	1:A:1745:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.86	0.57
1:A:1515:SER:HA	1:A:1599:SER:O	2.04	0.57
1:A:2028:ILE:HB	1:A:2055:MET:HG2	1.87	0.56
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.85	0.56
1:A:1621:TYR:OH	1:A:1851:PRO:HA	2.06	0.56
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.86	0.56
1:B:1265:LYS:HD2	1:B:1299:ARG:HE	1.70	0.56
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.89	0.55
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.87	0.55
1:B:1785:ARG:CD	1:B:1846:TRP:HZ3	2.19	0.55
1:B:1621:TYR:OH	1:B:1851:PRO:HA	2.05	0.55
1:B:1881:THR:HB	1:B:1938:ARG:HG2	1.89	0.54
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.89	0.54
1:B:2028:ILE:HB	1:B:2055:MET:HG2	1.88	0.54
1:A:1881:THR:HB	1:A:1938:ARG:HG2	1.89	0.54
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.90	0.54
1:B:1271:LEU:HD11	1:B:1322:ARG:HH22	1.73	0.54
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.90	0.54
1:B:1785:ARG:HB3	1:B:1846:TRP:CZ3	2.43	0.54
1:B:1333:GLU:HG2	1:B:1336:ARG:HG3	1.90	0.53
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.89	0.53
1:A:2214:GLU:HG2	1:A:2222:PHE:CD1	2.44	0.53
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.08	0.53
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.91	0.53
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	1.91	0.52
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	1.92	0.52
1:A:1190:VAL:HB	1:A:1255:VAL:HA	1.91	0.52
1:A:2019:LEU:HB3	1:A:2053:MET:CE	2.40	0.52
1:B:1371:ARG:HH22	1:B:1525:TYR:HE2	1.58	0.52
1:B:2019:LEU:HB3	1:B:2053:MET:CE	2.41	0.51
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.92	0.51
1:A:1376:PRO:HG2	1:A:1423:HIS:CD2	2.45	0.51
1:B:1341:LYS:HG3	1:B:1360:ARG:HG2	1.92	0.51
1:B:1884:VAL:HG21	1:B:1935:VAL:O	2.11	0.51
1:B:1504:TYR:CE1	1:B:1521:VAL:HA	2.45	0.51
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.93	0.50
1:B:1263:GLU:HG3	1:B:1264:GLY:H	1.75	0.50
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	1.93	0.50
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.93	0.50
1:A:1751:ILE:HD12	1:A:1779:LEU:HD11	1.93	0.49
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:GLU:HG3	1:A:1277:TRP:CE3	2.48	0.49
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.94	0.49
1:B:1751:ILE:HD12	1:B:1779:LEU:HD11	1.94	0.49
1:B:2077:LYS:H	1:B:2080:LYS:HD2	1.78	0.49
1:A:2203:PRO:HA	1:A:2206:ARG:HB3	1.95	0.48
1:A:1884:VAL:HG21	1:A:1935:VAL:O	2.12	0.48
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.77	0.48
1:B:1201:GLU:HG3	1:B:1277:TRP:CE3	2.48	0.48
1:B:2143:ARG:HH12	1:B:2147:LYS:HE2	1.77	0.48
1:B:2242:GLU:HG2	1:B:2246:LYS:HE3	1.96	0.48
1:A:1987:PRO:HG3	1:A:2171:LEU:HD21	1.95	0.47
1:B:2203:PRO:HA	1:B:2206:ARG:HB3	1.95	0.47
1:A:1334:LEU:C	1:A:1336:ARG:H	2.17	0.47
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.96	0.47
1:A:1776:GLY:O	1:A:1780:VAL:HG23	2.15	0.47
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.97	0.47
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.97	0.47
1:A:1517:HIS:HB3	1:A:1598:VAL:HG23	1.97	0.47
1:B:1426:GLN:HG2	1:B:1462:MET:HB3	1.97	0.47
1:A:1530:TRP:HH2	1:A:1604:MET:HG3	1.81	0.46
1:B:1376:PRO:HB3	1:B:1423:HIS:HB2	1.97	0.46
1:B:2032:PRO:O	1:B:2033:HIS:HB3	2.16	0.46
1:A:2143:ARG:HH12	1:A:2147:LYS:HE2	1.79	0.46
1:B:1530:TRP:HH2	1:B:1604:MET:HG3	1.80	0.46
1:A:1759:TYR:HB2	1:A:1764:THR:HG21	1.96	0.46
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.81	0.46
1:A:1492:TYR:CD1	1:A:1504:TYR:HB3	2.51	0.46
1:A:1663:ARG:HH12	1:A:1755:THR:HG23	1.81	0.46
1:B:2019:LEU:HB3	1:B:2053:MET:HE1	1.98	0.46
1:A:2032:PRO:O	1:A:2033:HIS:HB3	2.15	0.46
1:B:1776:GLY:O	1:B:1780:VAL:HG23	2.15	0.46
1:A:1908:VAL:O	1:A:1908:VAL:HG23	2.15	0.46
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.98	0.46
1:B:1763:PHE:HZ	1:B:1846:TRP:HE3	1.65	0.46
1:A:1794:ILE:HD12	1:A:1823:MET:HG3	1.98	0.45
1:B:2057:ALA:HB3	1:B:2150:ILE:HD13	1.99	0.45
1:B:1987:PRO:HG3	1:B:2171:LEU:HD21	1.97	0.45
1:A:2007:GLU:HG2	1:A:2010:LYS:HE3	1.99	0.45
1:A:2019:LEU:HB3	1:A:2053:MET:HE1	1.99	0.45
1:B:1908:VAL:O	1:B:1908:VAL:HG23	2.17	0.45
1:B:1785:ARG:HD2	1:B:1846:TRP:CZ3	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.17	0.45
1:A:2169:ARG:O	1:A:2173:GLU:HB2	2.16	0.45
1:B:1794:ILE:HD12	1:B:1823:MET:HG3	1.99	0.45
1:B:1627:PHE:HB3	1:B:1662:PRO:HG2	1.99	0.44
1:A:1858:LEU:HD22	1:A:1929:PRO:HG2	2.00	0.44
1:B:1611:GLY:HA2	1:B:1629:VAL:O	2.16	0.44
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.81	0.44
1:A:1611:GLY:HA2	1:A:1629:VAL:O	2.18	0.44
1:B:2245:GLU:HG3	1:B:2249:LYS:HE3	1.99	0.44
1:B:1858:LEU:HD22	1:B:1929:PRO:HG2	2.00	0.44
1:A:1863:PRO:HB2	1:A:1867:PRO:HA	2.00	0.43
1:A:2134:PHE:HA	1:A:2137:LEU:HD12	2.00	0.43
1:B:2027:PHE:CE2	1:B:2167:VAL:HG22	2.53	0.43
1:B:2072:ILE:CG2	1:B:2073:PRO:HD3	2.48	0.43
1:B:1258:ALA:HA	1:B:1296:ILE:HG23	2.00	0.43
1:B:1354:VAL:HG22	1:B:1370:THR:HG23	1.99	0.43
1:A:2057:ALA:HB3	1:A:2150:ILE:HD13	1.99	0.43
1:B:1544:GLN:HG3	1:B:1552:LEU:HD11	2.00	0.43
1:A:1544:GLN:HG3	1:A:1552:LEU:HD11	2.00	0.43
1:B:1876:PRO:HA	1:B:1877:PRO:HD3	1.91	0.43
1:B:2134:PHE:HA	1:B:2137:LEU:HD12	2.00	0.43
1:A:1627:PHE:HB3	1:A:1662:PRO:HG2	2.00	0.43
1:B:1863:PRO:HB2	1:B:1867:PRO:HA	2.00	0.43
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	2.00	0.43
1:B:1195:LYS:HA	1:B:1260:ARG:HD2	2.01	0.43
1:A:2041:TRP:HB3	1:B:1745:LEU:HD22	2.01	0.43
1:B:1546:VAL:CG2	1:B:1633:ASP:HA	2.43	0.43
1:A:2041:TRP:CD1	1:B:1745:LEU:HB3	2.54	0.43
1:B:1344:PRO:HA	1:B:1355:TYR:HA	2.01	0.42
1:B:1429:ALA:HB2	1:B:1475:LEU:HD13	2.01	0.42
1:A:1689:ASN:HA	1:A:1699:LYS:HE3	2.01	0.42
1:A:2029:TYR:HA	1:A:2056:TYR:O	2.20	0.42
1:A:2143:ARG:HH21	1:B:1740:LEU:HB2	1.85	0.42
1:B:1491:LEU:HB2	1:B:1508:SER:HA	2.01	0.42
1:B:1933:ILE:HB	1:B:1990:ILE:CG2	2.48	0.42
1:B:2029:TYR:HA	1:B:2056:TYR:O	2.19	0.42
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	2.02	0.42
1:A:1265:LYS:HA	1:A:1299:ARG:HH22	1.85	0.42
1:A:1702:TYR:HA	1:A:1729:LYS:HA	2.01	0.42
1:A:1504:TYR:HE1	1:A:1521:VAL:HA	1.85	0.41
1:A:1614:ILE:O	1:A:1626:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2056:TYR:CE2	1:B:2151:ARG:HB2	2.55	0.41
1:A:1370:THR:HG21	1:A:1400:ILE:HG23	2.03	0.41
1:B:1275:LYS:HG3	1:B:1276:PRO:HD3	2.02	0.41
1:B:1614:ILE:O	1:B:1626:LYS:HA	2.20	0.41
1:A:1275:LYS:HG3	1:A:1276:PRO:HD3	2.02	0.41
1:A:2056:TYR:CE2	1:A:2151:ARG:HB2	2.55	0.41
1:A:2072:ILE:CG2	1:A:2073:PRO:HD3	2.48	0.41
1:B:1702:TYR:HA	1:B:1729:LYS:HA	2.01	0.41
1:B:2037:ARG:HA	1:B:2064:GLY:O	2.20	0.41
1:A:2241:ASN:HA	1:A:2244:LEU:HD12	2.02	0.41
1:B:2143:ARG:NH1	1:B:2147:LYS:HE2	2.35	0.41
1:A:1325:GLU:HG3	1:A:1327:SER:H	1.84	0.41
1:B:1421:PHE:HB2	1:B:1458:ARG:O	2.20	0.41
1:B:1371:ARG:HD3	1:B:1418:PHE:HB3	2.02	0.41
1:B:1492:TYR:CD1	1:B:1506:TYR:HB3	2.56	0.41
1:A:2037:ARG:HA	1:A:2064:GLY:O	2.21	0.41
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.24	0.41
1:A:1195:LYS:HA	1:A:1260:ARG:HB2	2.03	0.41
1:A:1745:LEU:HD22	1:B:2041:TRP:HB3	2.03	0.41
1:A:1933:ILE:HB	1:A:1990:ILE:CG2	2.49	0.41
1:A:2149:VAL:HG11	1:B:1742:VAL:HB	2.03	0.41
1:B:1370:THR:HG21	1:B:1400:ILE:HG23	2.03	0.41
1:B:1689:ASN:HA	1:B:1699:LYS:HE3	2.03	0.41
1:B:2154:LEU:HD21	1:B:2162:PHE:CD2	2.56	0.41
1:A:2137:LEU:HB2	1:B:1733:ILE:HD12	2.02	0.41
1:A:2154:LEU:HD21	1:A:2162:PHE:CD2	2.55	0.41
1:B:1416:HIS:HD2	1:B:1454:GLN:HG3	1.86	0.40
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.61	0.40
1:A:1840:VAL:O	1:A:1844:VAL:HG23	2.22	0.40
1:A:2070:GLY:O	1:A:2073:PRO:HD2	2.22	0.40
1:A:2143:ARG:NH1	1:A:2147:LYS:HE2	2.36	0.40
1:A:2137:LEU:HA	1:A:2140:ARG:HD3	2.02	0.40
1:A:2143:ARG:NH2	1:B:1740:LEU:HB2	2.37	0.40
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	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	1011/1179 (86%)	902 (89%)	90 (9%)	19 (2%)	8 42
1	B	1011/1179 (86%)	905 (90%)	90 (9%)	16 (2%)	9 46
All	All	2022/2358 (86%)	1807 (89%)	180 (9%)	35 (2%)	9 45

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1864	SER
1	A	2225	ASN
1	B	1864	SER
1	B	2225	ASN
1	A	1483	SER
1	A	1570	SER
1	A	2038	GLY
1	B	1483	SER
1	B	1784	GLN
1	B	2038	GLY
1	B	1333	GLU
1	B	1516	MET
1	B	1570	SER
1	A	1333	GLU
1	A	1516	MET
1	A	1571	LEU
1	B	1571	LEU
1	A	1525	TYR
1	A	1572	ALA
1	A	1638	ILE
1	A	1784	GLN
1	A	1790	GLU
1	A	1865	PRO
1	B	1572	ALA
1	B	1865	PRO

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Mol	Chain	Res	Type
1	A	1313	PRO
1	A	1486	VAL
1	B	1313	PRO
1	B	1486	VAL
1	B	1638	ILE
1	B	1790	GLU
1	A	1193	PRO
1	B	2039	GLY
1	A	2039	GLY
1	A	1376	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	875/991 (88%)	817 (93%)	58 (7%)	16	51
1	B	875/991 (88%)	813 (93%)	62 (7%)	14	48
All	All	1750/1982 (88%)	1630 (93%)	120 (7%)	15	49

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1197	LEU
1	A	1210	VAL
1	A	1259	VAL
1	A	1296	ILE
1	A	1324	ILE
1	A	1342	LEU
1	A	1414	LEU
1	A	1489	ILE
1	A	1496	LEU
1	A	1498	GLU
1	A	1519	LEU
1	A	1557	ILE
1	A	1591	ASP

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Mol	Chain	Res	Type
1	A	1593	ASP
1	A	1595	LEU
1	A	1610	VAL
1	A	1618	THR
1	A	1630	VAL
1	A	1632	ASN
1	A	1638	ILE
1	A	1715	VAL
1	A	1721	VAL
1	A	1731	ILE
1	A	1750	LEU
1	A	1762	ILE
1	A	1775	ILE
1	A	1781	ARG
1	A	1805	LEU
1	A	1815	LEU
1	A	1817	LEU
1	A	1831	LEU
1	A	1861	LEU
1	A	1901	LEU
1	A	1909	GLU
1	A	1917	THR
1	A	1942	ASN
1	A	1965	TRP
1	A	1971	PHE
1	A	1975	GLN
1	A	1990	ILE
1	A	2020	THR
1	A	2022	PHE
1	A	2037	ARG
1	A	2055	MET
1	A	2067	GLU
1	A	2076	TYR
1	A	2088	LEU
1	A	2124	LEU
1	A	2139	ASP
1	A	2143	ARG
1	A	2151	ARG
1	A	2168	ARG
1	A	2174	ASP
1	A	2179	ARG
1	A	2197	THR

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Mol	Chain	Res	Type
1	A	2206	ARG
1	A	2238	ASP
1	A	2252	ILE
1	B	1194	CYS
1	B	1197	LEU
1	B	1210	VAL
1	B	1259	VAL
1	B	1265	LYS
1	B	1266	ASN
1	B	1270	ILE
1	B	1294	THR
1	B	1296	ILE
1	B	1301	ASP
1	B	1414	LEU
1	B	1462	MET
1	B	1475	LEU
1	B	1476	ARG
1	B	1496	LEU
1	B	1498	GLU
1	B	1510	ASN
1	B	1519	LEU
1	B	1557	ILE
1	B	1593	ASP
1	B	1595	LEU
1	B	1610	VAL
1	B	1618	THR
1	B	1630	VAL
1	B	1632	ASN
1	B	1638	ILE
1	B	1715	VAL
1	B	1721	VAL
1	B	1731	ILE
1	B	1750	LEU
1	B	1762	ILE
1	B	1764	THR
1	B	1781	ARG
1	B	1805	LEU
1	B	1815	LEU
1	B	1817	LEU
1	B	1831	LEU
1	B	1861	LEU
1	B	1901	LEU

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Mol	Chain	Res	Type
1	B	1909	GLU
1	B	1917	THR
1	B	1942	ASN
1	B	1965	TRP
1	B	1971	PHE
1	B	1975	GLN
1	B	1990	ILE
1	B	2020	THR
1	B	2022	PHE
1	B	2037	ARG
1	B	2055	MET
1	B	2067	GLU
1	B	2076	TYR
1	B	2088	LEU
1	B	2124	LEU
1	B	2139	ASP
1	B	2143	ARG
1	B	2151	ARG
1	B	2168	ARG
1	B	2174	ASP
1	B	2197	THR
1	B	2206	ARG
1	B	2238	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2309:UNK	C	2319:UNK	N	17.80
1	B	2311:UNK	C	2317:UNK	N	12.67
1	B	2264:GLU	C	2300:UNK	N	4.07
1	A	2264:GLU	C	2300:UNK	N	3.20

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	1021/1179 (86%)	-0.03	35 (3%)	45	30	132, 229, 290, 296	0
1	B	1021/1179 (86%)	0.03	19 (1%)	66	51	119, 223, 291, 297	0
All	All	2042/2358 (86%)	-0.00	54 (2%)	56	40	119, 225, 291, 297	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1456	GLU	7.7
1	A	1476	ARG	5.9
1	B	1459	ILE	5.4
1	B	1190	VAL	4.8
1	B	1189	GLY	4.6
1	B	1301	ASP	4.5
1	A	1457	ILE	4.4
1	B	1256	ASN	4.3
1	B	1191	ILE	4.1
1	A	1371	ARG	4.0
1	B	1680	LEU	3.9
1	B	1457	ILE	3.8
1	A	1680	LEU	3.7
1	A	1257	VAL	3.7
1	A	1192	VAL	3.7
1	A	1417	MET	3.6
1	A	2197	THR	3.6
1	B	1192	VAL	3.6
1	B	1258	ALA	3.5
1	A	1684	PHE	3.4
1	B	1257	VAL	3.4
1	A	1287	ALA	3.4
1	A	1211	LEU	3.3
1	A	1293	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	2196	ASN	3.3
1	B	1274	ILE	3.2
1	A	1208	LEU	3.2
1	A	1416	HIS	3.1
1	B	1285	LEU	3.1
1	A	1314	ASP	3.1
1	A	1494	GLU	2.9
1	A	1370	THR	2.9
1	B	1426	GLN	2.8
1	A	1836	ASP	2.8
1	A	1769	THR	2.7
1	A	1477	VAL	2.6
1	A	1458	ARG	2.6
1	A	1332	LEU	2.6
1	A	1316	ALA	2.4
1	A	1295	PHE	2.4
1	A	1553	PHE	2.2
1	A	1418	PHE	2.2
1	A	1475	LEU	2.2
1	A	1400	ILE	2.2
1	B	1679	GLU	2.2
1	A	1652	CYS	2.1
1	A	1191	ILE	2.1
1	B	1701	LEU	2.1
1	B	2261	ARG	2.1
1	A	1258	ALA	2.1
1	A	1190	VAL	2.1
1	B	2029	TYR	2.1
1	A	1212	PRO	2.0
1	A	1613	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 monosaccharides 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.