



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:31 PM UTC

PDB ID : 5I6G / pdb_00005i6g
Title : Crystal structure of C-terminal variant 2 of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on : 2016-02-16
Resolution : 4.50 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

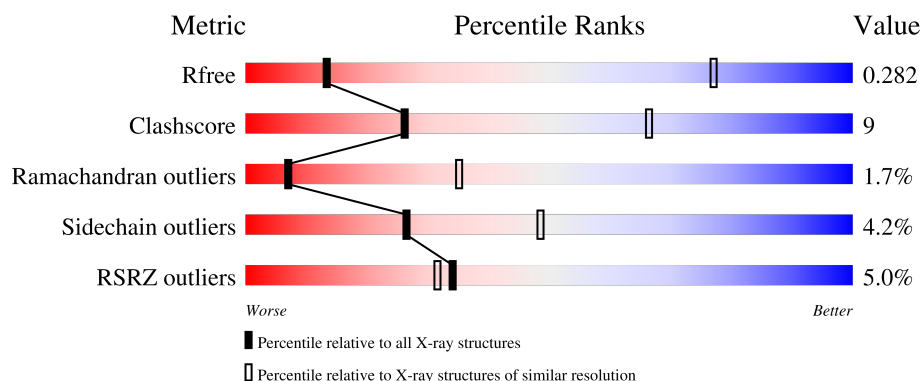
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	1161	
1	B	1161	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16405 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, Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	0	0	0
			8193	5204	1434	1526	29			
1	B	1030	Total	C	N	O	S	0	0	0
			8212	5216	1439	1528	29			

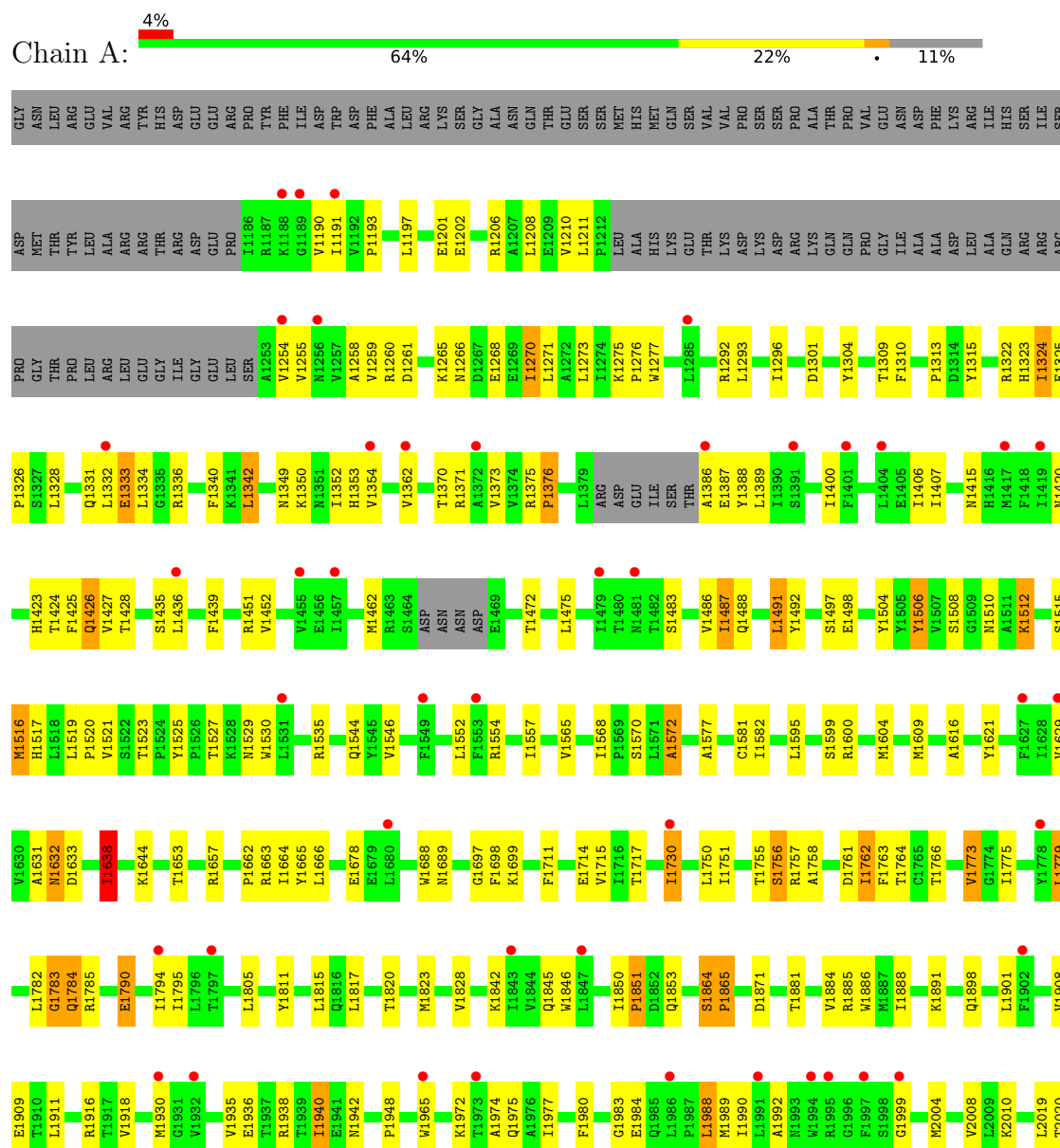
There are 2 discrepancies between the modelled and reference sequences:

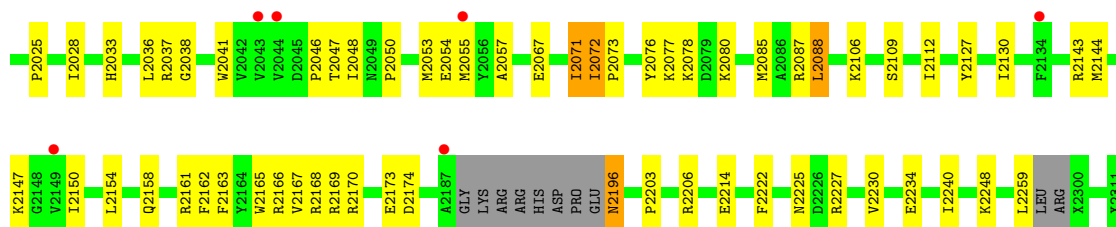
Chain	Residue	Modelled	Actual	Comment	Reference
A	1113	GLY	-	expression tag	UNP G0S3L5
B	1113	GLY	-	expression tag	UNP G0S3L5

3 Residue-property plots

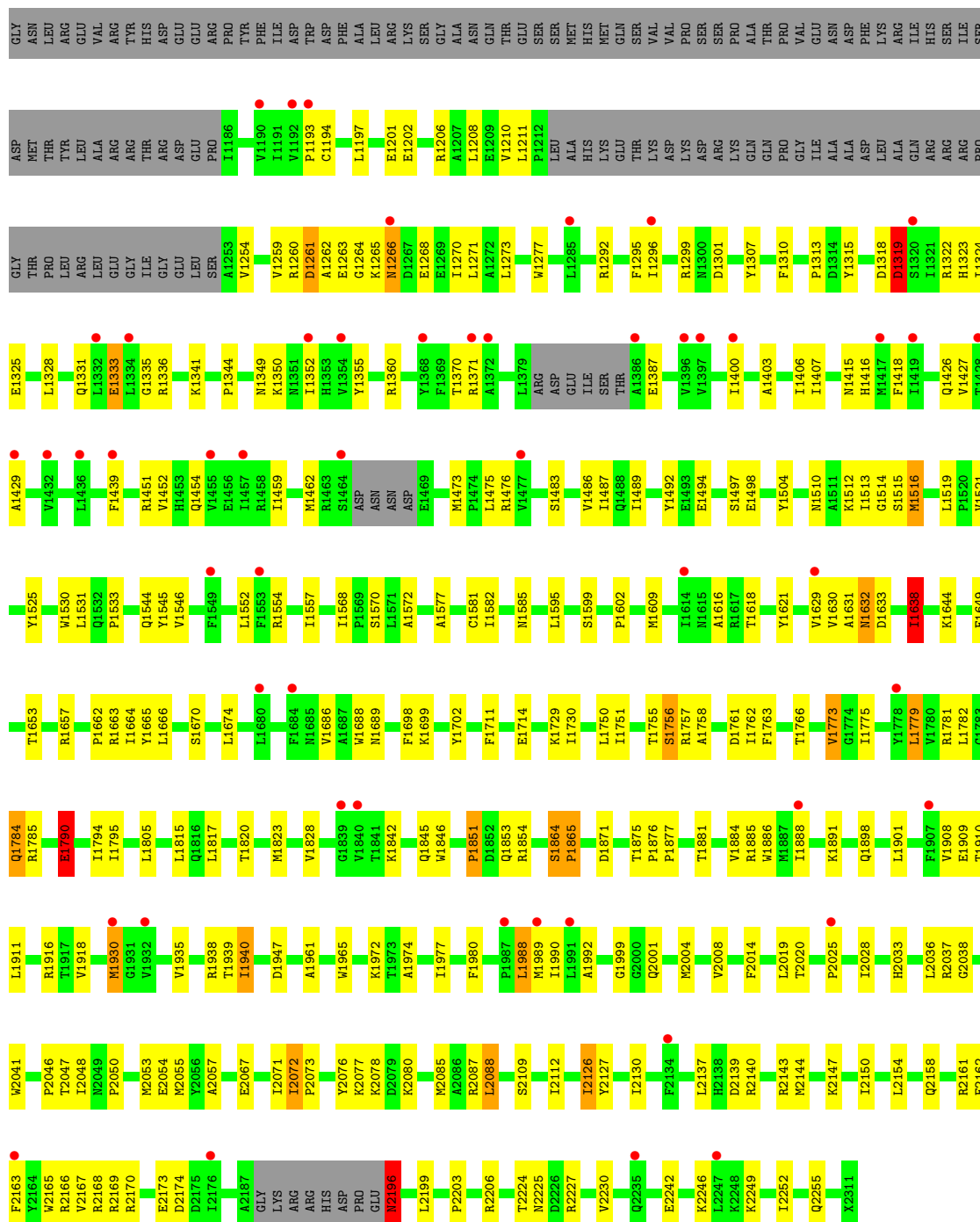
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, Acetyl-CoA carboxylase-like protein





● Molecule 1: Acetyl-CoA carboxylase-like protein, Acetyl-CoA carboxylase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.17Å 153.45Å 249.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 4.50 49.10 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.10-4.50) 99.3 (49.10-4.50)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 4.45Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.236 , 0.240 (Not available) , 0.282	Depositor DCC
R_{free} test set	1112 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	202.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 339.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16405	wwPDB-VP
Average B, all atoms (Å ²)	275.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 ⓘ

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	0.86	4/8311 (0.0%)	1.36	44/11255 (0.4%)
1	B	0.84	5/8330 (0.1%)	1.34	44/11280 (0.4%)
All	All	0.85	9/16641 (0.1%)	1.35	88/22535 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2126	ILE	CG1-CD1	-6.15	1.27	1.51
1	A	2072	ILE	CA-CB	6.14	1.57	1.54
1	B	2224	THR	CA-C	6.08	1.57	1.53
1	A	1487	ILE	CA-C	5.86	1.60	1.52
1	A	1638	ILE	CA-C	5.42	1.59	1.52
1	B	1761	ASP	CA-C	5.25	1.56	1.52
1	B	2072	ILE	CA-C	5.17	1.58	1.52
1	B	1487	ILE	CA-C	5.14	1.59	1.52
1	A	2072	ILE	CA-C	5.10	1.58	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2196	ASN	CA-C-N	8.32	133.91	120.60
1	B	2196	ASN	C-N-CA	8.32	133.91	120.60
1	B	1871	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	1871	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	1387	GLU	CA-C-N	7.31	130.38	120.44
1	A	1387	GLU	C-N-CA	7.31	130.38	120.44
1	A	1909	GLU	CB-CG-CD	7.21	124.85	112.60
1	B	1318	ASP	CA-C-N	7.12	130.53	120.28
1	B	1318	ASP	C-N-CA	7.12	130.53	120.28
1	A	1439	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	1439	PHE	CA-CB-CG	6.70	120.50	113.80
1	B	2048	ILE	N-CA-C	-6.52	104.29	110.42
1	B	1909	GLU	CB-CG-CD	6.43	123.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1980	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	1980	PHE	CA-CB-CG	6.41	120.21	113.80
1	B	1999	GLY	CA-C-N	6.34	126.78	120.31
1	B	1999	GLY	C-N-CA	6.34	126.78	120.31
1	A	1376	PRO	N-CA-C	6.17	119.86	111.22
1	A	2048	ILE	N-CA-C	-6.14	104.65	110.42
1	A	1999	GLY	CA-C-N	6.11	126.54	120.31
1	A	1999	GLY	C-N-CA	6.11	126.54	120.31
1	B	1756	SER	CA-C-N	5.90	128.47	120.44
1	B	1756	SER	C-N-CA	5.90	128.47	120.44
1	A	2234	GLU	CB-CG-CD	5.63	122.17	112.60
1	A	1784	GLN	CA-C-N	5.59	131.58	122.07
1	A	1784	GLN	C-N-CA	5.59	131.58	122.07
1	A	2033	HIS	CA-C-N	5.58	125.28	119.92
1	A	2033	HIS	C-N-CA	5.58	125.28	119.92
1	B	1261	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	1510	ASN	CA-C-N	5.57	130.48	122.35
1	A	1510	ASN	C-N-CA	5.57	130.48	122.35
1	B	1632	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	1756	SER	CA-C-N	5.55	128.00	120.44
1	A	1756	SER	C-N-CA	5.55	128.00	120.44
1	A	1632	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	1828	VAL	N-CA-C	-5.47	105.03	111.00
1	B	1828	VAL	N-CA-C	-5.42	105.10	111.00
1	B	1319	ASP	CA-C-N	5.35	127.71	120.65
1	B	1319	ASP	C-N-CA	5.35	127.71	120.65
1	B	2033	HIS	CA-C-N	5.31	125.02	119.92
1	B	2033	HIS	C-N-CA	5.31	125.02	119.92
1	A	1678	GLU	CB-CG-CD	5.31	121.62	112.60
1	B	1930	MET	CA-C-N	5.31	125.72	120.31
1	B	1930	MET	C-N-CA	5.31	125.72	120.31
1	B	1644	LYS	CA-C-N	5.25	127.74	120.29
1	B	1644	LYS	C-N-CA	5.25	127.74	120.29
1	B	1790	GLU	CB-CG-CD	5.23	121.50	112.60
1	B	1266	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	1644	LYS	CA-C-N	5.22	127.70	120.29
1	A	1644	LYS	C-N-CA	5.22	127.70	120.29
1	B	1653	THR	CA-C-N	5.20	127.51	120.38
1	B	1653	THR	C-N-CA	5.20	127.51	120.38
1	A	1983	GLY	CA-C-N	5.20	127.20	120.44
1	A	1983	GLY	C-N-CA	5.20	127.20	120.44
1	A	1851	PRO	CA-C-N	5.20	127.50	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1851	PRO	C-N-CA	5.20	127.50	120.38
1	A	1426	GLN	CA-C-N	5.17	131.29	121.97
1	A	1426	GLN	C-N-CA	5.17	131.29	121.97
1	A	1783	GLY	CA-C-N	5.17	131.42	121.54
1	A	1783	GLY	C-N-CA	5.17	131.42	121.54
1	A	1506	TYR	CA-CB-CG	5.17	123.20	113.90
1	B	1387	GLU	CA-C-N	5.17	127.47	120.44
1	B	1387	GLU	C-N-CA	5.17	127.47	120.44
1	A	1261	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	1779	LEU	CA-C-N	5.14	127.14	120.56
1	A	1779	LEU	C-N-CA	5.14	127.14	120.56
1	B	2249	LYS	CA-C-N	5.14	127.12	120.44
1	B	2249	LYS	C-N-CA	5.14	127.12	120.44
1	B	1947	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	1436	LEU	CA-C-N	5.12	127.40	120.38
1	A	1436	LEU	C-N-CA	5.12	127.40	120.38
1	A	1653	THR	CA-C-N	5.11	127.38	120.38
1	A	1653	THR	C-N-CA	5.11	127.38	120.38
1	B	1779	LEU	CA-C-N	5.11	127.10	120.56
1	B	1779	LEU	C-N-CA	5.11	127.10	120.56
1	B	1335	GLY	N-CA-C	-5.10	107.71	115.66
1	A	1506	TYR	CA-C-N	5.09	131.14	121.97
1	A	1506	TYR	C-N-CA	5.09	131.14	121.97
1	B	1331	GLN	CA-C-N	5.09	128.04	120.31
1	B	1331	GLN	C-N-CA	5.09	128.04	120.31
1	B	2199	LEU	CA-C-N	5.08	128.03	120.31
1	B	2199	LEU	C-N-CA	5.08	128.03	120.31
1	B	1875	THR	CB-CA-C	5.07	116.26	109.42
1	A	1462	MET	CA-C-N	-5.05	115.49	122.30
1	A	1462	MET	C-N-CA	-5.05	115.49	122.30
1	B	1851	PRO	CA-C-N	5.04	127.28	120.38
1	B	1851	PRO	C-N-CA	5.04	127.28	120.38
1	B	2014	PHE	CA-CB-CG	5.01	118.81	113.80

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	8193	0	8096	158	0
1	B	8212	0	8120	163	0
All	All	16405	0	16216	307	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 9.

All (307) 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:1515:SER:HA	1:B:1599:SER:O	1.25	1.28
1:B:1609:MET:HE1	1:B:1630:VAL:CG1	1.70	1.22
1:B:1319:ASP:HB2	1:B:1344:PRO:HG2	1.39	1.02
1:B:1515:SER:CA	1:B:1599:SER:O	2.19	0.89
1:A:1336:ARG:HB3	1:A:1525:TYR:CD2	2.09	0.88
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.56	0.86
1:B:1324:ILE:HG13	1:B:1328:LEU:HB3	1.59	0.84
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.58	0.82
1:B:1296:ILE:HG12	1:B:1307:TYR:CE1	2.16	0.81
1:B:1609:MET:HE1	1:B:1630:VAL:HG13	1.61	0.81
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.06	0.80
1:B:1609:MET:HE1	1:B:1630:VAL:HG12	1.62	0.80
1:B:1530:TRP:CH2	1:B:1602:PRO:O	2.35	0.80
1:B:1609:MET:CE	1:B:1630:VAL:CG1	2.57	0.80
1:B:1473:MET:HE3	1:B:1475:LEU:HD21	1.65	0.78
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.66	0.76
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.67	0.75
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.67	0.75
1:A:1336:ARG:HB3	1:A:1525:TYR:CE2	2.23	0.74
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.67	0.74
1:B:1853:GLN:HG2	1:B:1854:ARG:H	1.53	0.74
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.71	0.72
1:B:1609:MET:CE	1:B:1630:VAL:HG13	2.20	0.71
1:B:2163:PHE:O	1:B:2167:VAL:HG23	1.91	0.71
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.73	0.71
1:A:2163:PHE:O	1:A:2167:VAL:HG23	1.90	0.71
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.72	0.71
1:B:1415:ASN:HB2	1:B:1452:VAL:HA	1.72	0.70
1:B:1884:VAL:HG21	1:B:1935:VAL:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1884:VAL:HG21	1:A:1935:VAL:O	1.92	0.69
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.75	0.68
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.74	0.68
1:B:1476:ARG:HG3	1:B:1494:GLU:OE1	1.94	0.67
1:B:1609:MET:HE1	1:B:1630:VAL:HG11	1.72	0.67
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.74	0.67
1:A:1519:LEU:HD11	1:A:1600:ARG:HD2	1.75	0.67
1:B:2168:ARG:HD3	1:B:2230:VAL:HG11	1.77	0.67
1:B:1427:VAL:HG11	1:B:1459:ILE:HD12	1.75	0.67
1:A:1323:HIS:O	1:A:1324:ILE:HG12	1.95	0.67
1:B:1514:GLY:C	1:B:1599:SER:HB3	2.20	0.66
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.77	0.66
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.77	0.65
1:B:1531:LEU:HD11	1:B:1545:TYR:CD2	2.33	0.64
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.79	0.64
1:B:1785:ARG:HB3	1:B:1846:TRP:CZ3	2.32	0.64
1:A:1259:VAL:HG12	1:A:1260:ARG:N	2.13	0.64
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.78	0.64
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.77	0.64
1:B:1371:ARG:HH22	1:B:1525:TYR:HE2	1.46	0.64
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.80	0.64
1:A:2037:ARG:HE	1:A:2067:GLU:HA	1.64	0.63
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.80	0.63
1:A:2010:LYS:HG2	1:B:1781:ARG:HE	1.63	0.63
1:A:1497:SER:O	1:A:1498:GLU:HB2	1.99	0.62
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.80	0.62
1:A:1715:VAL:HG13	1:A:1730:ILE:HG23	1.82	0.62
1:B:1296:ILE:HG12	1:B:1307:TYR:HE1	1.64	0.62
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.82	0.62
1:B:1197:LEU:HD13	1:B:1273:LEU:HD23	1.81	0.62
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.80	0.62
1:A:1785:ARG:NH1	1:A:1984:GLU:HG3	2.16	0.61
1:B:1323:HIS:CE1	1:B:1350:LYS:HD2	2.35	0.61
1:A:2168:ARG:CD	1:A:2230:VAL:HG11	2.31	0.61
1:A:1519:LEU:HD11	1:A:1600:ARG:CD	2.31	0.61
1:B:1557:ILE:HD13	1:B:1616:ALA:HB1	1.82	0.60
1:B:2037:ARG:HE	1:B:2067:GLU:HA	1.65	0.60
1:B:1988:LEU:HD13	1:B:1990:ILE:HD11	1.82	0.60
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.84	0.60
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	1.83	0.60
1:B:1513:ILE:HG23	1:B:1585:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.84	0.60
1:A:1557:ILE:HD13	1:A:1616:ALA:HB1	1.82	0.60
1:A:1715:VAL:CG1	1:A:1730:ILE:HG23	2.32	0.59
1:B:1531:LEU:HD11	1:B:1545:TYR:CE2	2.37	0.59
1:A:1325:GLU:H	1:A:1328:LEU:HD12	1.65	0.59
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.67	0.59
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.83	0.59
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.68	0.59
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.84	0.59
1:B:1265:LYS:HE3	1:B:1299:ARG:HG3	1.84	0.58
1:B:1333:GLU:HG2	1:B:1336:ARG:HG3	1.86	0.58
1:A:1515:SER:HA	1:A:1599:SER:O	2.04	0.58
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.86	0.58
1:A:2088:LEU:HG	1:B:1686:VAL:HG23	1.86	0.57
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.85	0.57
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.85	0.57
1:A:1324:ILE:HG23	1:A:1328:LEU:HB2	1.87	0.57
1:A:2020:THR:HG21	1:B:1757:ARG:HG2	1.85	0.57
1:B:1530:TRP:HH2	1:B:1602:PRO:O	1.81	0.57
1:A:1504:TYR:HE1	1:A:1521:VAL:HA	1.69	0.57
1:A:1516:MET:HG3	1:A:1519:LEU:HD22	1.86	0.56
1:A:1811:TYR:CE1	1:B:2001:GLN:HB2	2.40	0.56
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.86	0.56
1:A:1557:ILE:HD12	1:A:1582:ILE:CG2	2.35	0.56
1:B:1557:ILE:HD12	1:B:1582:ILE:CG2	2.35	0.56
1:A:2168:ARG:HD3	1:A:2230:VAL:HG11	1.88	0.56
1:A:1621:TYR:OH	1:A:1851:PRO:HA	2.06	0.55
1:A:1340:PHE:CZ	1:A:1527:THR:HG22	2.42	0.55
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.87	0.55
1:A:2047:THR:HB	1:B:1750:LEU:HD13	1.89	0.55
1:B:1265:LYS:HG3	1:B:1299:ARG:HE	1.71	0.55
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.88	0.54
1:A:1324:ILE:HG13	1:A:1353:HIS:NE2	2.22	0.54
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.88	0.54
1:B:2143:ARG:HH12	1:B:2147:LYS:HE2	1.73	0.54
1:B:1259:VAL:CG1	1:B:1261:ASP:CG	2.81	0.53
1:A:1864:SER:CB	1:A:1865:PRO:HD3	2.38	0.53
1:B:1621:TYR:OH	1:B:1851:PRO:HA	2.08	0.53
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.89	0.53
1:B:1530:TRP:O	1:B:1533:PRO:HD2	2.09	0.53
1:B:1265:LYS:HE3	1:B:1299:ARG:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	1.91	0.53
1:B:1864:SER:CB	1:B:1865:PRO:HD3	2.38	0.53
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.74	0.52
1:A:1324:ILE:HG23	1:A:1328:LEU:CB	2.39	0.52
1:A:1362:VAL:HG11	1:A:1529:ASN:HB2	1.90	0.52
1:B:2168:ARG:CD	1:B:2230:VAL:HG11	2.39	0.52
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	1.91	0.52
1:A:2214:GLU:HG2	1:A:2222:PHE:CD1	2.44	0.52
1:A:2143:ARG:HH12	1:A:2147:LYS:HE2	1.74	0.52
1:B:1429:ALA:HB2	1:B:1475:LEU:HD13	1.91	0.52
1:A:1336:ARG:HB3	1:A:1525:TYR:HD2	1.70	0.52
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.74	0.52
1:B:1426:GLN:HG2	1:B:1462:MET:HB3	1.90	0.52
1:A:1197:LEU:HD13	1:A:1273:LEU:HD23	1.92	0.51
1:A:1504:TYR:CE1	1:A:1521:VAL:HA	2.45	0.51
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.75	0.51
1:B:1325:GLU:HB2	1:B:1328:LEU:HB2	1.90	0.51
1:B:1341:LYS:HG3	1:B:1360:ARG:HG2	1.93	0.51
1:A:1517:HIS:H	1:A:1519:LEU:HD13	1.76	0.51
1:B:2019:LEU:HB3	1:B:2053:MET:CE	2.40	0.51
1:A:1340:PHE:CE1	1:A:1527:THR:HG22	2.45	0.51
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.92	0.51
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.93	0.51
1:B:2085:MET:C	1:B:2087:ARG:H	2.19	0.51
1:B:2143:ARG:NH1	1:B:2147:LYS:HE2	2.25	0.51
1:A:1259:VAL:HG12	1:A:1260:ARG:H	1.75	0.50
1:A:1386:ALA:C	1:A:1388:TYR:H	2.17	0.50
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.92	0.50
1:A:2085:MET:C	1:A:2087:ARG:H	2.20	0.50
1:B:1663:ARG:HH12	1:B:1755:THR:HG23	1.77	0.50
1:B:1784:GLN:NE2	1:B:1784:GLN:HA	2.27	0.49
1:B:1794:ILE:HD12	1:B:1823:MET:HG3	1.93	0.49
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.77	0.49
1:A:2143:ARG:NH1	1:A:2147:LYS:HE2	2.26	0.49
1:A:1757:ARG:HG2	1:B:2020:THR:HG21	1.95	0.49
1:B:1197:LEU:HD13	1:B:1273:LEU:CD2	2.43	0.49
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.95	0.49
1:A:2259:LEU:HD21	1:B:2255:GLN:OE1	2.13	0.49
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.95	0.48
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.95	0.48
1:A:1370:THR:HG21	1:A:1400:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1930:MET:HE2	1:A:1989:MET:HB2	1.95	0.48
1:A:1475:LEU:CD1	1:A:1492:TYR:O	2.62	0.48
1:A:1190:VAL:HB	1:A:1255:VAL:HA	1.94	0.48
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.94	0.48
1:A:1663:ARG:HH12	1:A:1755:THR:HG23	1.77	0.48
1:B:1259:VAL:CG1	1:B:1261:ASP:OD1	2.61	0.48
1:A:2019:LEU:HB3	1:A:2053:MET:CE	2.44	0.48
1:A:1271:LEU:HD11	1:A:1322:ARG:HH22	1.79	0.48
1:B:2050:PRO:HG2	1:B:2196:ASN:HA	1.95	0.48
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.95	0.48
1:A:1715:VAL:HG12	1:A:1717:THR:HG23	1.96	0.47
1:A:1948:PRO:HD3	1:B:2001:GLN:NE2	2.29	0.47
1:B:1208:LEU:HD23	1:B:1211:LEU:HD12	1.97	0.47
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.13	0.47
1:B:1638:ILE:HD12	1:B:1670:SER:CB	2.45	0.47
1:A:1333:GLU:HB3	1:A:1371:ARG:NH1	2.30	0.47
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.96	0.47
1:A:1258:ALA:HA	1:A:1296:ILE:HG23	1.95	0.47
1:A:1259:VAL:CG1	1:A:1260:ARG:N	2.76	0.47
1:B:1631:ALA:HB2	1:B:1666:LEU:HB2	1.97	0.47
1:B:1908:VAL:HG23	1:B:1908:VAL:O	2.15	0.47
1:B:1930:MET:HE2	1:B:1989:MET:HB2	1.96	0.47
1:A:1689:ASN:HA	1:A:1699:LYS:HE3	1.96	0.47
1:A:2169:ARG:O	1:A:2173:GLU:HB2	2.15	0.47
1:B:1271:LEU:HD11	1:B:1322:ARG:HH22	1.80	0.47
1:B:1370:THR:HG21	1:B:1400:ILE:HG23	1.97	0.47
1:A:1974:ALA:HA	1:A:1977:ILE:HD12	1.97	0.46
1:B:1263:GLU:HG3	1:B:1264:GLY:H	1.80	0.46
1:B:1344:PRO:HA	1:B:1355:TYR:HA	1.97	0.46
1:B:1785:ARG:CD	1:B:1846:TRP:HZ3	2.28	0.46
1:A:1688:TRP:HH2	1:B:2088:LEU:HD12	1.80	0.46
1:B:1504:TYR:CE1	1:B:1521:VAL:HA	2.48	0.46
1:B:1323:HIS:CG	1:B:1350:LYS:HB3	2.50	0.46
1:B:1497:SER:O	1:B:1498:GLU:HB2	2.15	0.46
1:A:1259:VAL:CG1	1:A:1260:ARG:H	2.27	0.46
1:A:1266:ASN:HB3	1:A:1270:ILE:HB	1.98	0.46
1:B:1259:VAL:HG12	1:B:1261:ASP:CG	2.41	0.46
1:B:1531:LEU:CD1	1:B:1545:TYR:CE2	2.98	0.46
1:B:1201:GLU:HG3	1:B:1277:TRP:CE3	2.50	0.46
1:A:1342:LEU:HD22	1:A:1342:LEU:O	2.15	0.46
1:A:1631:ALA:HB2	1:A:1666:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:ILE:HD12	1:A:1823:MET:HG3	1.97	0.46
1:A:1334:LEU:C	1:A:1336:ARG:H	2.23	0.46
1:A:1324:ILE:CG2	1:A:1328:LEU:HB2	2.46	0.46
1:A:1328:LEU:O	1:A:1331:GLN:HB2	2.16	0.46
1:A:1988:LEU:HD22	1:A:1990:ILE:HG13	1.98	0.46
1:B:2203:PRO:HA	1:B:2206:ARG:HB3	1.98	0.46
1:A:1325:GLU:N	1:A:1328:LEU:HD12	2.31	0.46
1:A:1842:LYS:O	1:A:1845:GLN:HB3	2.16	0.46
1:A:2028:ILE:HB	1:A:2055:MET:HG3	1.99	0.45
1:B:1324:ILE:CG1	1:B:1328:LEU:HB3	2.40	0.45
1:A:1304:TYR:HB3	1:A:1350:LYS:HB2	1.98	0.45
1:A:1846:TRP:O	1:A:1850:ILE:HG12	2.17	0.45
1:B:1785:ARG:HD2	1:B:1846:TRP:HZ3	1.82	0.45
1:A:1492:TYR:CD1	1:A:1506:TYR:HB3	2.50	0.45
1:A:2259:LEU:HD22	1:B:2252:ILE:HG23	1.98	0.45
1:B:1689:ASN:HA	1:B:1699:LYS:HE3	1.98	0.45
1:B:1785:ARG:HB3	1:B:1846:TRP:HZ3	1.78	0.45
1:B:1629:VAL:HG22	1:B:1664:ILE:HB	1.99	0.45
1:B:1544:GLN:HG3	1:B:1552:LEU:HD11	1.98	0.45
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.16	0.45
1:A:1201:GLU:HG3	1:A:1277:TRP:CE3	2.51	0.45
1:A:1544:GLN:HG3	1:A:1552:LEU:HD11	1.98	0.45
1:B:2041:TRP:CH2	1:B:2144:MET:HE3	2.52	0.45
1:A:1517:HIS:O	1:A:1519:LEU:CD1	2.66	0.44
1:B:1763:PHE:HZ	1:B:1846:TRP:HE3	1.65	0.44
1:A:1208:LEU:HD23	1:A:1211:LEU:HD12	1.98	0.44
1:A:1750:LEU:HD13	1:B:2047:THR:HB	1.99	0.44
1:A:1785:ARG:CD	1:A:1846:TRP:HZ3	2.30	0.44
1:A:1406:ILE:HD12	1:A:1407:ILE:HG13	2.00	0.44
1:B:1416:HIS:HD2	1:B:1454:GLN:HG3	1.81	0.44
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.83	0.44
1:A:1565:VAL:HG12	1:A:1572:ALA:CB	2.48	0.44
1:B:1842:LYS:O	1:B:1845:GLN:HB3	2.16	0.44
1:A:2158:GLN:CD	1:A:2161:ARG:HH11	2.26	0.44
1:A:2203:PRO:HA	1:A:2206:ARG:HB3	1.99	0.44
1:A:1697:GLY:HA2	1:B:2126:ILE:HD11	2.00	0.43
1:A:1886:TRP:HB3	1:A:1891:LYS:HB2	2.00	0.43
1:A:1908:VAL:HG23	1:A:1908:VAL:O	2.18	0.43
1:A:1375:ARG:HA	1:A:1376:PRO:HD3	1.83	0.43
1:B:1846:TRP:HZ2	1:B:1910:THR:HG21	1.83	0.43
1:B:1557:ILE:CD1	1:B:1616:ALA:HB1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	2.00	0.43
1:A:1293:LEU:O	1:A:1309:THR:HA	2.18	0.43
1:A:1911:LEU:HB2	1:A:1972:LYS:HE3	2.00	0.43
1:B:1663:ARG:NH1	1:B:1755:THR:HG23	2.34	0.43
1:B:1546:VAL:CG2	1:B:1633:ASP:HA	2.39	0.43
1:A:1197:LEU:HD13	1:A:1273:LEU:CD2	2.49	0.43
1:A:1530:TRP:HH2	1:A:1604:MET:HG3	1.83	0.43
1:A:1609:MET:HE3	1:A:1609:MET:HB3	1.93	0.43
1:B:1371:ARG:HD3	1:B:1418:PHE:HB3	2.00	0.43
1:B:2077:LYS:H	1:B:2080:LYS:HD2	1.84	0.43
1:A:2041:TRP:CH2	1:A:2144:MET:HE3	2.53	0.43
1:A:2071:ILE:HG23	1:B:1674:LEU:HD23	2.01	0.42
1:A:2165:TRP:CE3	1:A:2227:ARG:HA	2.54	0.42
1:B:1262:ALA:HA	1:B:1265:LYS:HE2	2.02	0.42
1:B:1492:TYR:CD1	1:B:1504:TYR:HB3	2.55	0.42
1:A:1629:VAL:HG22	1:A:1664:ILE:HB	2.00	0.42
1:B:2028:ILE:HB	1:B:2055:MET:HG3	2.01	0.42
1:B:1629:VAL:HG13	1:B:1666:LEU:HD13	2.01	0.42
1:B:1911:LEU:HB2	1:B:1972:LYS:HE3	2.02	0.42
1:B:2109:SER:HA	1:B:2112:ILE:HD12	2.02	0.42
1:A:1373:VAL:HG23	1:A:1420:ASN:HB3	2.01	0.42
1:A:1554:ARG:HG3	1:A:1581:CYS:HB2	2.01	0.42
1:A:1629:VAL:HG13	1:A:1666:LEU:HD13	2.02	0.42
1:B:1268:GLU:HA	1:B:1271:LEU:HD12	2.02	0.42
1:B:2046:PRO:HA	1:B:2053:MET:SD	2.60	0.42
1:B:2165:TRP:CE3	1:B:2227:ARG:HA	2.55	0.42
1:A:1389:LEU:HD11	1:A:1425:PHE:CG	2.55	0.42
1:A:2050:PRO:HG2	1:A:2196:ASN:HA	2.01	0.42
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	2.01	0.42
1:A:1790:GLU:HA	1:A:1820:THR:HG21	2.01	0.42
1:B:1630:VAL:HG11	1:B:1649:PHE:CD2	2.54	0.42
1:B:1881:THR:HB	1:B:1938:ARG:HG2	2.02	0.42
1:A:2154:LEU:HD21	1:A:2162:PHE:CD2	2.55	0.41
1:B:1554:ARG:HG3	1:B:1581:CYS:HB2	2.02	0.41
1:A:1764:THR:HG23	1:A:1783:GLY:O	2.20	0.41
1:A:1336:ARG:CB	1:A:1525:TYR:CE2	2.98	0.41
1:B:1974:ALA:HA	1:B:1977:ILE:HD12	2.01	0.41
1:A:1751:ILE:HD12	1:A:1779:LEU:HD11	2.02	0.41
1:A:2046:PRO:HA	1:A:2053:MET:SD	2.60	0.41
1:A:2158:GLN:OE1	1:A:2161:ARG:HD2	2.19	0.41
1:B:1516:MET:HG3	1:B:1519:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.29	0.41
1:B:2158:GLN:OE1	1:B:2161:ARG:HD2	2.20	0.41
1:A:1520:PRO:O	1:A:1523:THR:HG23	2.20	0.41
1:B:1406:ILE:HD12	1:B:1407:ILE:HG13	2.03	0.41
1:B:1568:ILE:HG12	1:B:1864:SER:HB3	2.02	0.41
1:B:1876:PRO:HA	1:B:1877:PRO:HD3	1.95	0.41
1:A:1324:ILE:HG23	1:A:1328:LEU:CD1	2.51	0.41
1:A:1761:ASP:OD2	1:A:1762:ILE:HG23	2.20	0.41
1:A:1332:LEU:O	1:A:1333:GLU:CB	2.68	0.41
1:A:1948:PRO:HD3	1:B:2001:GLN:CD	2.46	0.41
1:A:2057:ALA:HB3	1:A:2150:ILE:HD13	2.02	0.41
1:B:1510:ASN:C	1:B:1512:LYS:H	2.29	0.41
1:B:1751:ILE:HD12	1:B:1779:LEU:HD11	2.02	0.41
1:B:1790:GLU:HA	1:B:1820:THR:HG21	2.02	0.41
1:B:1939:THR:HG22	1:B:1961:ALA:HA	2.03	0.41
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	2.03	0.41
1:B:2158:GLN:CD	1:B:2161:ARG:HH11	2.27	0.41
1:A:1881:THR:HB	1:A:1938:ARG:HG2	2.03	0.41
1:A:1304:TYR:OH	1:A:1324:ILE:HD13	2.20	0.40
1:B:2242:GLU:HG2	1:B:2246:LYS:HE3	2.02	0.40
1:A:1492:TYR:OH	1:A:1516:MET:HB3	2.20	0.40
1:B:1403:ALA:O	1:B:1406:ILE:HG13	2.21	0.40
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.29	0.40
1:A:1884:VAL:HG21	1:A:1936:GLU:HA	2.03	0.40
1:B:1702:TYR:HA	1:B:1729:LYS:HA	2.03	0.40
1:A:1275:LYS:N	1:A:1276:PRO:HD2	2.37	0.40
1:A:2109:SER:HA	1:A:2112:ILE:HD12	2.02	0.40
1:B:2057:ALA:HB3	1:B:2150:ILE:HD13	2.03	0.40
1:B:2154:LEU:HD21	1:B:2162:PHE:CD2	2.56	0.40
1:A:1342:LEU:H	1:A:1342:LEU:HD13	1.86	0.40
1:A:1565:VAL:HG12	1:A:1572:ALA:HB1	2.02	0.40
1:A:1568:ILE:HG12	1:A:1864:SER:HB3	2.04	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	1006/1161 (87%)	898 (89%)	89 (9%)	19 (2%)	6	32
1	B	1008/1161 (87%)	897 (89%)	96 (10%)	15 (2%)	8	38
All	All	2014/2322 (87%)	1795 (89%)	185 (9%)	34 (2%)	7	35

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1864	SER
1	A	2225	ASN
1	B	1864	SER
1	A	1333	GLU
1	A	1483	SER
1	A	1784	GLN
1	A	2038	GLY
1	B	1483	SER
1	B	2038	GLY
1	B	2225	ASN
1	A	1512	LYS
1	B	1333	GLU
1	B	1516	MET
1	B	1784	GLN
1	A	1486	VAL
1	A	1516	MET
1	A	1570	SER
1	A	1577	ALA
1	A	1790	GLU
1	B	1486	VAL
1	B	1570	SER
1	B	1790	GLU
1	A	1313	PRO
1	A	1572	ALA
1	B	1313	PRO
1	B	1572	ALA
1	B	1577	ALA
1	A	1638	ILE
1	B	1638	ILE
1	A	1427	VAL
1	A	1487	ILE

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Mol	Chain	Res	Type
1	A	1865	PRO
1	B	1865	PRO
1	A	1193	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	872/990 (88%)	827 (95%)	45 (5%)	21	43
1	B	874/990 (88%)	845 (97%)	29 (3%)	33	55
All	All	1746/1980 (88%)	1672 (96%)	74 (4%)	26	48

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1191	ILE
1	A	1210	VAL
1	A	1265	LYS
1	A	1270	ILE
1	A	1301	ASP
1	A	1324	ILE
1	A	1342	LEU
1	A	1354	VAL
1	A	1423	HIS
1	A	1424	THR
1	A	1426	GLN
1	A	1428	THR
1	A	1435	SER
1	A	1472	THR
1	A	1488	GLN
1	A	1491	LEU
1	A	1535	ARG
1	A	1595	LEU
1	A	1632	ASN
1	A	1638	ILE

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Mol	Chain	Res	Type
1	A	1730	ILE
1	A	1762	ILE
1	A	1773	VAL
1	A	1775	ILE
1	A	1805	LEU
1	A	1815	LEU
1	A	1817	LEU
1	A	1853	GLN
1	A	1898	GLN
1	A	1901	LEU
1	A	1940	ILE
1	A	1942	ASN
1	A	1965	TRP
1	A	1975	GLN
1	A	1988	LEU
1	A	2071	ILE
1	A	2076	TYR
1	A	2078	LYS
1	A	2088	LEU
1	A	2106	LYS
1	A	2166	ARG
1	A	2174	ASP
1	A	2196	ASN
1	A	2240	ILE
1	A	2248	LYS
1	B	1194	CYS
1	B	1210	VAL
1	B	1301	ASP
1	B	1319	ASP
1	B	1489	ILE
1	B	1595	LEU
1	B	1618	THR
1	B	1632	ASN
1	B	1638	ILE
1	B	1730	ILE
1	B	1762	ILE
1	B	1773	VAL
1	B	1775	ILE
1	B	1805	LEU
1	B	1815	LEU
1	B	1817	LEU
1	B	1898	GLN

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Mol	Chain	Res	Type
1	B	1901	LEU
1	B	1940	ILE
1	B	1965	TRP
1	B	1988	LEU
1	B	2071	ILE
1	B	2076	TYR
1	B	2078	LYS
1	B	2088	LEU
1	B	2139	ASP
1	B	2166	ARG
1	B	2174	ASP
1	B	2196	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1351	ASN
1	A	1410	ASN
1	A	1453	HIS
1	A	1460	ASN
1	A	1481	ASN
1	A	1529	ASN
1	A	1713	ASN
1	A	1760	ASN
1	A	1814	ASN
1	A	2133	GLN
1	B	1331	GLN
1	B	1351	ASN
1	B	1410	ASN
1	B	1453	HIS
1	B	1481	ASN
1	B	1713	ASN
1	B	1760	ASN
1	B	1814	ASN
1	B	1942	ASN
1	B	2133	GLN
1	B	2212	GLN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2261:ARG	C	2300:UNK	N	11.76

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	1016/1161 (87%)	0.26	50 (4%) 35 32	129, 237, 392, 485	0
1	B	1018/1161 (87%)	0.30	51 (5%) 34 31	147, 289, 446, 500	0
All	All	2034/2322 (87%)	0.28	101 (4%) 34 31	129, 257, 429, 500	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1553	PHE	7.4
1	A	1553	PHE	6.7
1	B	1432	VAL	6.1
1	B	1457	ILE	5.8
1	B	1190	VAL	5.4
1	B	1684	PHE	5.0
1	B	1930	MET	4.8
1	A	1680	LEU	4.8
1	A	2043	VAL	4.8
1	B	1778	TYR	4.6
1	A	1481	ASN	4.4
1	A	1994	TRP	4.3
1	B	1352	ILE	4.1
1	B	1400	ILE	4.1
1	A	1372	ALA	4.0
1	B	1396	VAL	4.0
1	A	1417	MET	4.0
1	A	1843	ILE	3.8
1	B	1436	LEU	3.8
1	A	1404	LEU	3.7
1	B	1372	ALA	3.5
1	B	1455	VAL	3.5
1	B	1549	PHE	3.5
1	A	1778	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1987	PRO	3.4
1	B	2247	LEU	3.4
1	B	2025	PRO	3.4
1	B	1332	LEU	3.3
1	A	1997	PHE	3.3
1	B	1320	SER	3.3
1	B	1932	VAL	3.3
1	A	1455	VAL	3.2
1	A	1479	ILE	3.2
1	A	1386	ALA	3.1
1	B	1439	PHE	3.1
1	B	1285	LEU	3.1
1	B	1614	ILE	3.0
1	B	2163	PHE	3.0
1	A	2187	ALA	2.9
1	B	1839	GLY	2.9
1	B	2134	PHE	2.9
1	A	1354	VAL	2.9
1	B	1334	LEU	2.9
1	B	1477	VAL	2.9
1	B	1907	PHE	2.9
1	B	1371	ARG	2.9
1	B	1419	ILE	2.8
1	A	2134	PHE	2.8
1	A	1191	ILE	2.7
1	B	1192	VAL	2.7
1	B	1464	SER	2.6
1	A	1794	ILE	2.6
1	B	1368	TYR	2.6
1	B	2235	GLN	2.5
1	A	1332	LEU	2.5
1	A	1930	MET	2.5
1	A	1627	PHE	2.5
1	B	1991	LEU	2.5
1	B	1989	MET	2.5
1	B	1429	ALA	2.5
1	A	1457	ILE	2.5
1	A	1256	ASN	2.5
1	A	1401	PHE	2.4
1	A	1436	LEU	2.4
1	A	1973	THR	2.4
1	A	1847	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1999	GLY	2.4
1	B	1296	ILE	2.4
1	A	1362	VAL	2.4
1	A	1932	VAL	2.3
1	A	1531	LEU	2.3
1	A	1986	LEU	2.3
1	A	1902	PHE	2.3
1	B	1386	ALA	2.3
1	B	1629	VAL	2.3
1	A	1549	PHE	2.3
1	A	1991	LEU	2.2
1	B	1193	PRO	2.2
1	A	2055	MET	2.2
1	A	1254	VAL	2.2
1	B	1888	ILE	2.2
1	A	1188	LYS	2.2
1	A	2149	VAL	2.2
1	B	1354	VAL	2.2
1	A	1730	ILE	2.2
1	A	1965	TRP	2.2
1	B	1417	MET	2.2
1	A	2044	VAL	2.2
1	B	1840	VAL	2.2
1	A	1419	ILE	2.1
1	A	1285	LEU	2.1
1	A	1797	THR	2.1
1	B	1428	THR	2.1
1	A	1629	VAL	2.1
1	A	1189	GLY	2.1
1	B	1680	LEU	2.0
1	B	1397	VAL	2.0
1	B	2176	ILE	2.0
1	A	1995	ARG	2.0
1	B	1266	ASN	2.0
1	A	1391	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.