



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:37 PM UTC

PDB ID : 5I6F / pdb_00005i6f
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

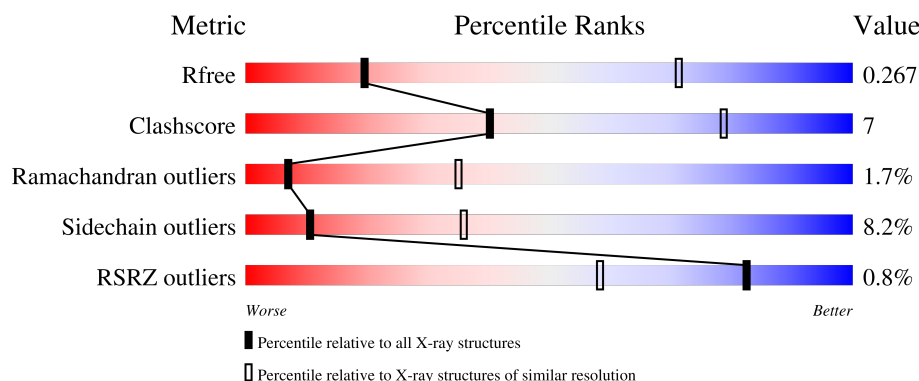
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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 $\leq 5\%$. 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	1179	65% 22% • 11%
1	B	1179	65% 22% • 11%

2 Entry composition

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
1	A	1044	Total	C	N	O	S	0	0	0
			8286	5260	1453	1544	29			
1	B	1048	Total	C	N	O	S	0	0	0
			8306	5272	1457	1548	29			

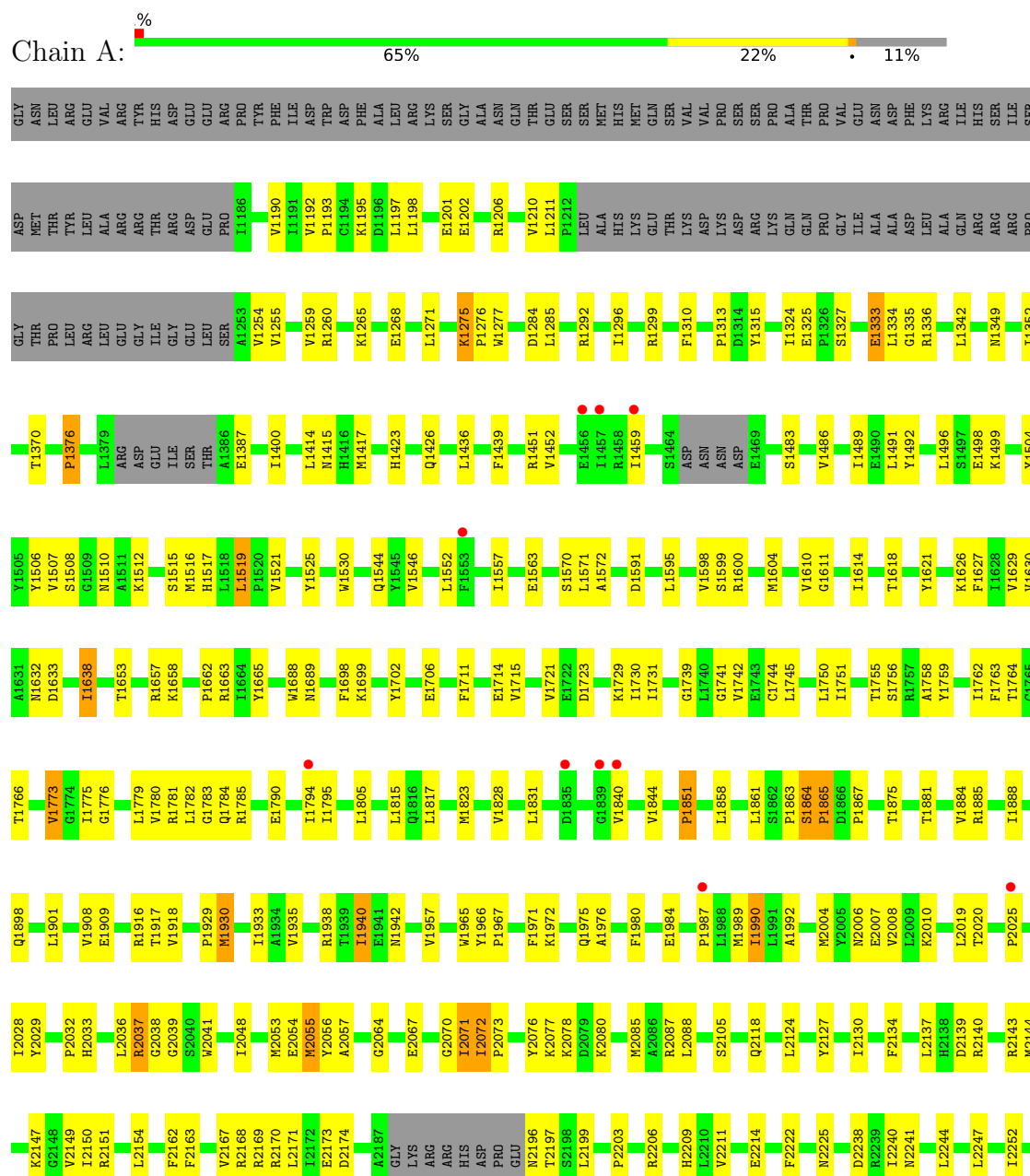
There are 2 discrepancies between the modelled and reference sequences:

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.203 , 0.243 0.230 , 0.267	Depositor DCC
R_{free} test set	2011 reflections (3.72%)	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)	0.28 , 165.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

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	0.81	2/8349 (0.0%)	1.33	39/11306 (0.3%)
1	B	0.81	3/8349 (0.0%)	1.35	50/11306 (0.4%)
All	All	0.81	5/16698 (0.0%)	1.34	89/22612 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2072	ILE	CA-CB	7.02	1.57	1.54
1	A	2072	ILE	CA-CB	6.60	1.57	1.54
1	B	2224	THR	CA-C	5.91	1.57	1.53
1	A	2072	ILE	CA-C	5.12	1.58	1.52
1	B	2072	ILE	CA-C	5.07	1.58	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2048	ILE	N-CA-C	-6.93	103.90	110.42
1	A	2048	ILE	N-CA-C	-6.82	104.01	110.42
1	A	1980	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	2196	ASN	CA-C-N	6.26	130.62	120.60
1	A	2196	ASN	C-N-CA	6.26	130.62	120.60
1	B	1980	PHE	CA-CB-CG	6.25	120.05	113.80
1	B	2196	ASN	CA-C-N	6.19	130.50	120.60
1	B	2196	ASN	C-N-CA	6.19	130.50	120.60
1	A	1439	PHE	CA-CB-CG	6.09	119.89	113.80
1	B	1266	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	1439	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	2249	LYS	CA-C-N	5.87	128.07	120.44
1	B	2249	LYS	C-N-CA	5.87	128.07	120.44
1	B	1851	PRO	CA-C-N	5.84	128.39	120.38
1	B	1851	PRO	C-N-CA	5.84	128.39	120.38
1	B	1331	GLN	CA-C-N	5.81	128.65	120.28
1	B	1331	GLN	C-N-CA	5.81	128.65	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1851	PRO	CA-C-N	5.81	128.34	120.38
1	A	1851	PRO	C-N-CA	5.81	128.34	120.38
1	B	1387	GLU	CA-C-N	5.73	128.23	120.44
1	B	1387	GLU	C-N-CA	5.73	128.23	120.44
1	A	2006	ASN	CA-C-N	5.72	130.25	122.07
1	A	2006	ASN	C-N-CA	5.72	130.25	122.07
1	A	1436	LEU	CA-C-N	5.66	128.14	120.38
1	A	1436	LEU	C-N-CA	5.66	128.14	120.38
1	B	1261	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	1194	CYS	CA-C-N	5.62	128.37	120.28
1	B	1194	CYS	C-N-CA	5.62	128.37	120.28
1	A	1828	VAL	N-CA-C	-5.50	105.00	111.00
1	B	1510	ASN	CA-CB-CG	5.47	118.07	112.60
1	B	1653	THR	N-CA-C	-5.44	105.25	111.07
1	A	1653	THR	N-CA-C	-5.42	105.27	111.07
1	B	2105	SER	CA-C-N	5.41	127.53	120.28
1	B	2105	SER	C-N-CA	5.41	127.53	120.28
1	B	2006	ASN	CA-C-N	5.40	129.80	122.07
1	B	2006	ASN	C-N-CA	5.40	129.80	122.07
1	A	1510	ASN	CA-C-N	5.40	130.24	122.35
1	A	1510	ASN	C-N-CA	5.40	130.24	122.35
1	B	1741	GLY	CA-C-N	5.40	128.14	120.53
1	B	1741	GLY	C-N-CA	5.40	128.14	120.53
1	A	1387	GLU	CA-C-N	5.39	127.77	120.44
1	A	1387	GLU	C-N-CA	5.39	127.77	120.44
1	A	2105	SER	CA-C-N	5.35	127.44	120.28
1	A	2105	SER	C-N-CA	5.35	127.44	120.28
1	B	2199	LEU	CA-C-N	5.34	127.97	120.28
1	B	2199	LEU	C-N-CA	5.34	127.97	120.28
1	A	1741	GLY	CA-C-N	5.33	128.04	120.53
1	A	1741	GLY	C-N-CA	5.33	128.04	120.53
1	A	2118	GLN	N-CA-C	-5.29	106.77	113.43
1	B	1284	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	2196	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	1653	THR	CA-C-N	5.26	127.59	120.38
1	A	1653	THR	C-N-CA	5.26	127.59	120.38
1	B	1875	THR	CB-CA-C	5.26	116.52	109.42
1	B	1723	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	2071	ILE	CA-C-N	5.25	125.47	120.43
1	B	2071	ILE	C-N-CA	5.25	125.47	120.43
1	B	1828	VAL	N-CA-C	-5.25	105.28	111.00
1	B	2118	GLN	N-CA-C	-5.24	106.83	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1875	THR	CB-CA-C	5.22	116.47	109.42
1	A	1971	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	1653	THR	CA-C-N	5.18	127.48	120.38
1	B	1653	THR	C-N-CA	5.18	127.48	120.38
1	A	1285	LEU	CA-C-N	5.17	127.48	120.44
1	A	1285	LEU	C-N-CA	5.17	127.48	120.44
1	B	2072	ILE	N-CA-CB	5.17	113.98	110.52
1	B	1783	GLY	CA-C-N	5.16	131.40	121.54
1	B	1783	GLY	C-N-CA	5.16	131.40	121.54
1	A	2199	LEU	CA-C-N	5.16	128.15	120.31
1	A	2199	LEU	C-N-CA	5.16	128.15	120.31
1	B	1285	LEU	CA-C-N	5.15	127.44	120.44
1	B	1285	LEU	C-N-CA	5.15	127.44	120.44
1	A	2071	ILE	CA-C-N	5.15	125.37	120.43
1	A	2071	ILE	C-N-CA	5.15	125.37	120.43
1	A	1723	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	1284	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	2224	THR	CA-C-N	5.09	131.26	121.54
1	B	2224	THR	C-N-CA	5.09	131.26	121.54
1	B	1871	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	1930	MET	CA-C-N	5.08	125.49	120.31
1	A	1930	MET	C-N-CA	5.08	125.49	120.31
1	A	1976	ALA	CA-C-N	5.07	126.95	120.56
1	A	1976	ALA	C-N-CA	5.07	126.95	120.56
1	B	2196	ASN	CA-CB-CG	5.05	117.65	112.60
1	B	1503	VAL	CA-C-N	5.03	130.38	122.34
1	B	1503	VAL	C-N-CA	5.03	130.38	122.34
1	B	1784	GLN	CA-C-N	5.01	128.46	121.24
1	B	1784	GLN	C-N-CA	5.01	128.46	121.24
1	B	1971	PHE	CA-CB-CG	5.00	118.80	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	8286	0	8150	104	0
1	B	8306	0	8153	119	0
All	All	16592	0	16303	216	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 7.

All (216) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1473:MET:HE3	1:B:1475:LEU:HD21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:LEU:C	1:A:1336:ARG:H	2.17	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
1:B:1930:MET:HE2	1:B:1989:MET:HB2	1.94	0.49
1:A:1201:GLU:HG3	1:A:1277:TRP:CE3	2.48	0.49
1:A:1930:MET:HE2	1:A:1989:MET:HB2	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:ARG:HH12	1:A:1755:THR:HG23	1.81	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:HG23	1:A:1908:VAL:O	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:1415:ASN:HD22	1:B:1451:ARG:C	2.24	0.45
1:B:2085:MET:C	1:B:2087:ARG:H	2.25	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:B:1908:VAL:HG23	1:B:1908:VAL:O	2.17	0.45
1:B:1785:ARG:HD2	1:B:1846:TRP:CZ3	2.49	0.45
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:A:1333:GLU:C	1:A:1335:GLY:H	2.25	0.44
1:B:1627:PHE:HB3	1:B:1662:PRO:HG2	1.99	0.44
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.24	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:2085:MET:C	1:A:2087:ARG:H	2.25	0.44
1:B:2209:HIS:C	1:B:2211:VAL:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1417:MET:HE3	1:A:1452:VAL:HG11	2.01	0.42
1:B:2041:TRP:CH2	1:B:2144:MET:HE3	2.54	0.42
1:A:2209:HIS:C	1:A:2211:VAL:H	2.26	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:2041:TRP:CH2	1:A:2144:MET:HE3	2.54	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
1:B:1267:ASP:C	1:B:1269:GLU:H	2.28	0.41
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:1966:TYR:O	1:A:1967:PRO:C	2.63	0.41
1:A:2241:ASN:HA	1:A:2244:LEU:HD12	2.02	0.41
1:B:1417:MET:HE3	1:B:1452:VAL:HG11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1637:LYS:C	1:B:1638:ILE:HG13	2.46	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:B:1966:TYR:O	1:B:1967:PRO:C	2.65	0.40
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.61	0.40
1:B:1483:SER:C	1:B:1485:PHE:H	2.29	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%)	6	33
1	B	1011/1179 (86%)	905 (90%)	90 (9%)	16 (2%)	7	36
All	All	2022/2358 (86%)	1807 (89%)	180 (9%)	35 (2%)	7	35

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
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 ⓘ

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%)	804 (92%)	71 (8%)	11	36
1	B	875/991 (88%)	803 (92%)	72 (8%)	10	36
All	All	1750/1982 (88%)	1607 (92%)	143 (8%)	10	36

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1192	VAL
1	A	1197	LEU
1	A	1198	LEU
1	A	1210	VAL
1	A	1211	LEU
1	A	1259	VAL
1	A	1275	LYS
1	A	1296	ILE
1	A	1324	ILE
1	A	1342	LEU
1	A	1414	LEU
1	A	1426	GLN
1	A	1459	ILE
1	A	1489	ILE
1	A	1496	LEU
1	A	1498	GLU
1	A	1499	LYS
1	A	1507	VAL
1	A	1519	LEU
1	A	1557	ILE
1	A	1563	GLU
1	A	1591	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	1658	LYS
1	A	1706	GLU
1	A	1715	VAL
1	A	1721	VAL
1	A	1730	ILE
1	A	1731	ILE
1	A	1750	LEU

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Mol	Chain	Res	Type
1	A	1762	ILE
1	A	1773	VAL
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	1898	GLN
1	A	1901	LEU
1	A	1909	GLU
1	A	1917	THR
1	A	1940	ILE
1	A	1942	ASN
1	A	1957	VAL
1	A	1965	TRP
1	A	1975	GLN
1	A	1990	ILE
1	A	2020	THR
1	A	2037	ARG
1	A	2055	MET
1	A	2067	GLU
1	A	2071	ILE
1	A	2076	TYR
1	A	2078	LYS
1	A	2088	LEU
1	A	2124	LEU
1	A	2139	ASP
1	A	2168	ARG
1	A	2174	ASP
1	A	2197	THR
1	A	2238	ASP
1	A	2240	ILE
1	A	2247	LEU
1	A	2252	ILE
1	B	1194	CYS
1	B	1197	LEU
1	B	1198	LEU
1	B	1210	VAL
1	B	1211	LEU
1	B	1259	VAL

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Mol	Chain	Res	Type
1	B	1265	LYS
1	B	1266	ASN
1	B	1270	ILE
1	B	1275	LYS
1	B	1294	THR
1	B	1296	ILE
1	B	1301	ASP
1	B	1324	ILE
1	B	1414	LEU
1	B	1427	VAL
1	B	1462	MET
1	B	1475	LEU
1	B	1476	ARG
1	B	1496	LEU
1	B	1498	GLU
1	B	1499	LYS
1	B	1510	ASN
1	B	1519	LEU
1	B	1557	ILE
1	B	1563	GLU
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	1674	LEU
1	B	1706	GLU
1	B	1715	VAL
1	B	1721	VAL
1	B	1730	ILE
1	B	1731	ILE
1	B	1750	LEU
1	B	1762	ILE
1	B	1764	THR
1	B	1773	VAL
1	B	1775	ILE
1	B	1781	ARG
1	B	1805	LEU
1	B	1815	LEU
1	B	1817	LEU
1	B	1831	LEU

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Mol	Chain	Res	Type
1	B	1861	LEU
1	B	1898	GLN
1	B	1901	LEU
1	B	1909	GLU
1	B	1917	THR
1	B	1940	ILE
1	B	1942	ASN
1	B	1965	TRP
1	B	1975	GLN
1	B	1990	ILE
1	B	2020	THR
1	B	2037	ARG
1	B	2055	MET
1	B	2067	GLU
1	B	2071	ILE
1	B	2076	TYR
1	B	2078	LYS
1	B	2088	LEU
1	B	2124	LEU
1	B	2139	ASP
1	B	2168	ARG
1	B	2174	ASP
1	B	2197	THR
1	B	2238	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1410	ASN
1	A	1453	HIS
1	A	1481	ASN
1	A	1532	GLN
1	A	1898	GLN
1	A	2001	GLN
1	A	2129	GLN
1	A	2133	GLN
1	B	1331	GLN
1	B	1410	ASN
1	B	1453	HIS
1	B	1481	ASN
1	B	1532	GLN
1	B	1615	ASN

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Mol	Chain	Res	Type
1	B	1898	GLN
1	B	1978	ASN
1	B	2129	GLN
1	B	2133	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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%)	-0.51	10 (0%)	79 54	132, 229, 290, 296	0
1	B	1021/1179 (86%)	-0.47	7 (0%)	84 61	119, 223, 291, 297	0
All	All	2042/2358 (86%)	-0.49	17 (0%)	82 58	119, 225, 291, 297	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1457	ILE	5.7
1	B	1457	ILE	4.6
1	A	2025	PRO	3.9
1	B	1459	ILE	3.7
1	A	1794	ILE	3.6
1	B	1989	MET	3.1
1	A	1839	GLY	3.0
1	B	2029	TYR	3.0
1	A	1987	PRO	2.9
1	A	1456	GLU	2.9
1	A	1835	ASP	2.8
1	A	1553	PHE	2.7
1	A	1840	VAL	2.3
1	B	1417	MET	2.3
1	B	1991	LEU	2.1
1	B	1455	VAL	2.1
1	A	1459	ILE	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.