Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:27 am BST

PDB ID	:	5I6I
Title	:	Crystal structure of a dBCCP-variant of Chaetomium thermophilum acetyl-CoA carboxylase
Authors	:	Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on	:	2016-02-16
Resolution	:	8.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

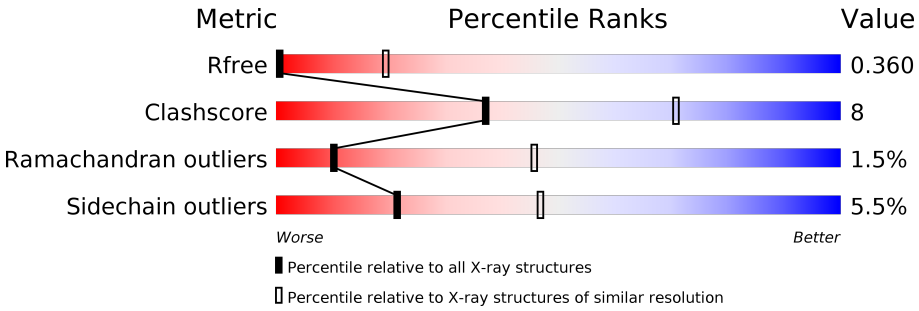
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 8.40 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	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2211	48% 13% • 37%
1	B	2211	49% 13% • 37%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22445 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,Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1399	Total	C	N	O	S	0	0	0
			11224	7122	1978	2086	38			
1	B	1394	Total	C	N	O	S	0	0	0
			11221	7120	1976	2086	39			

There are 8 discrepancies between the modelled and reference sequences:

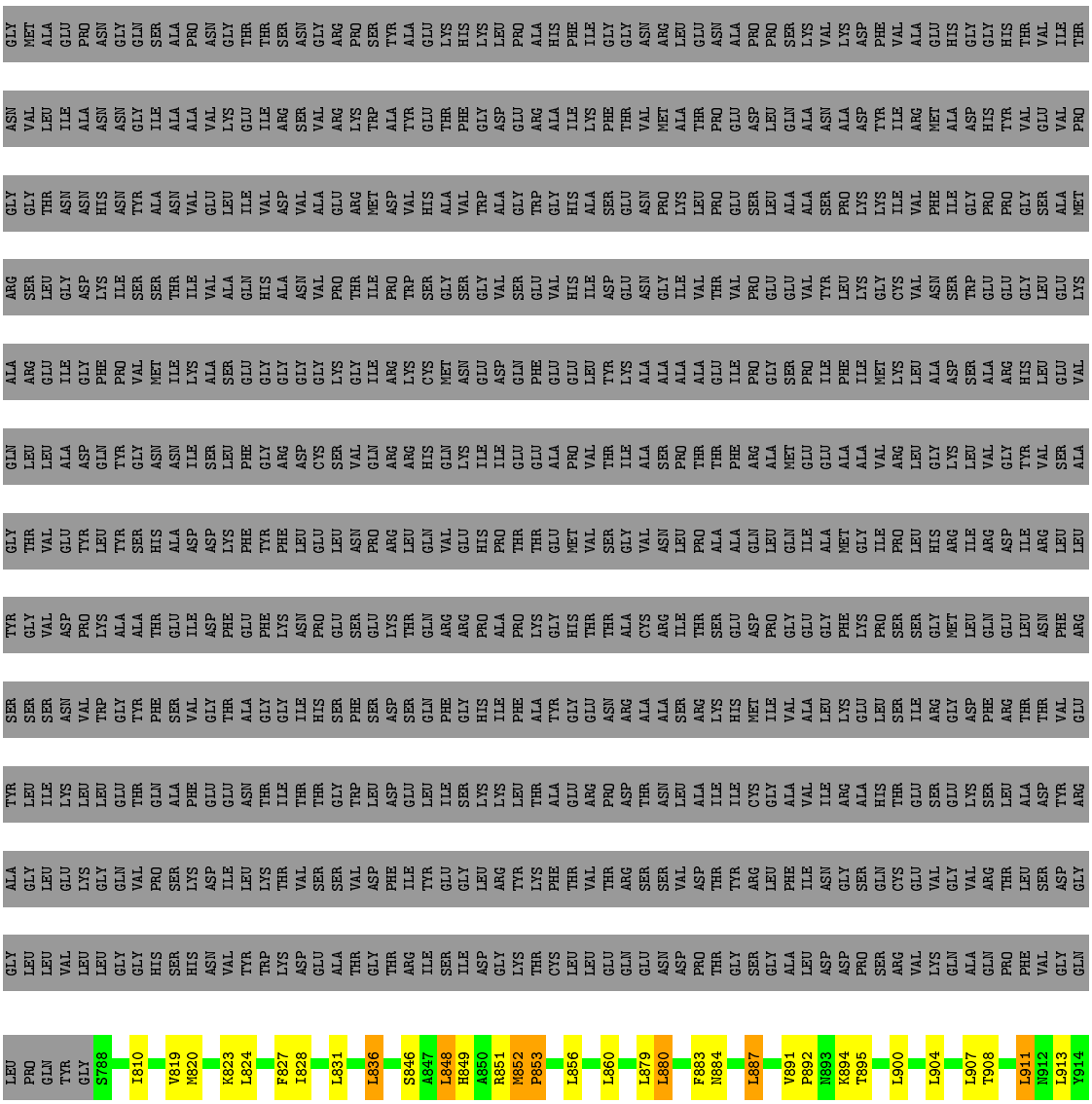
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP G0S3L5
A	763	GLY	-	linker	UNP G0S3L5
A	764	SER	-	linker	UNP G0S3L5
A	765	GLY	-	linker	UNP G0S3L5
B	63	GLY	-	expression tag	UNP G0S3L5
B	763	GLY	-	linker	UNP G0S3L5
B	764	SER	-	linker	UNP G0S3L5
B	765	GLY	-	linker	UNP G0S3L5

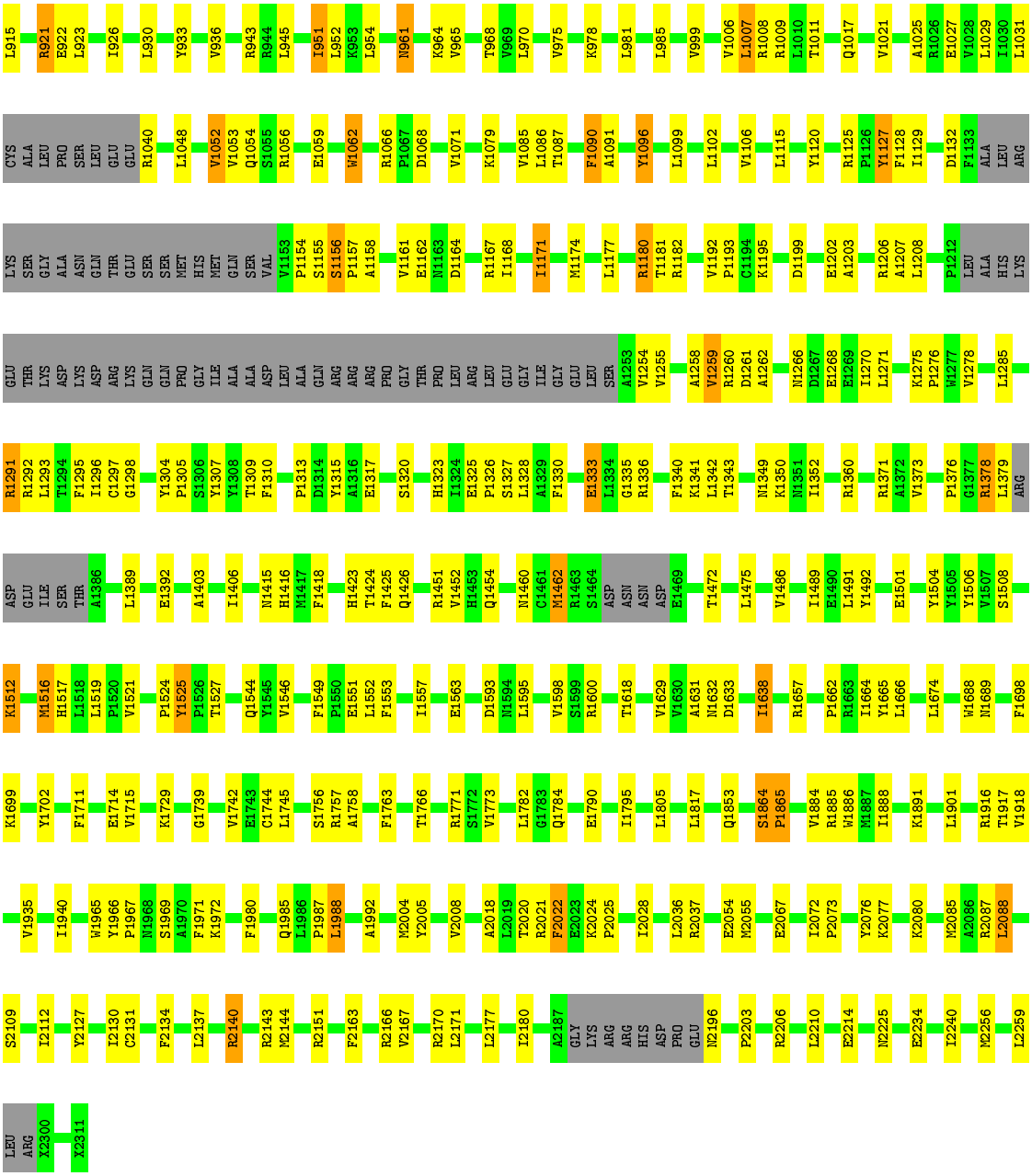
3 Residue-property plots (i)

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

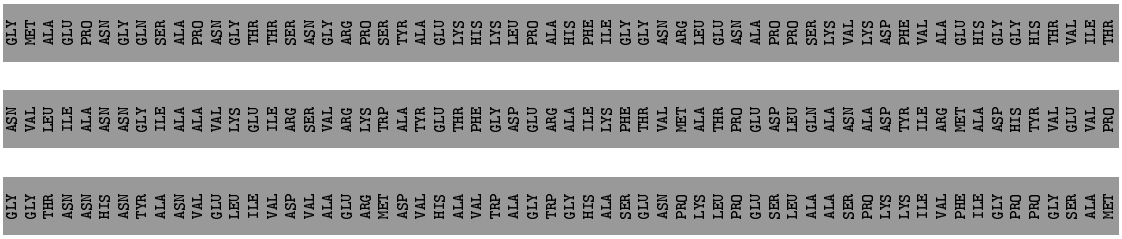
Chain A:

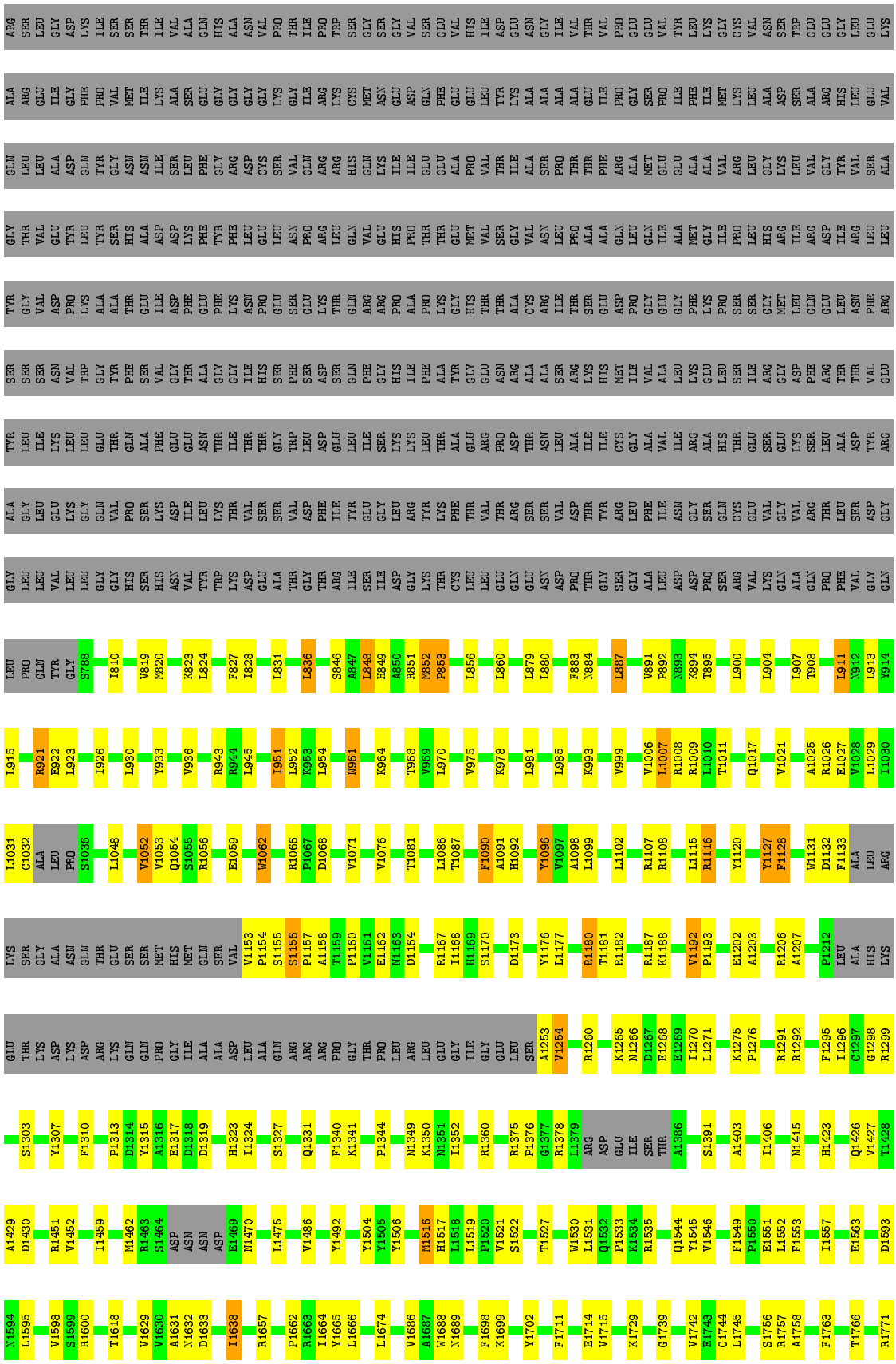


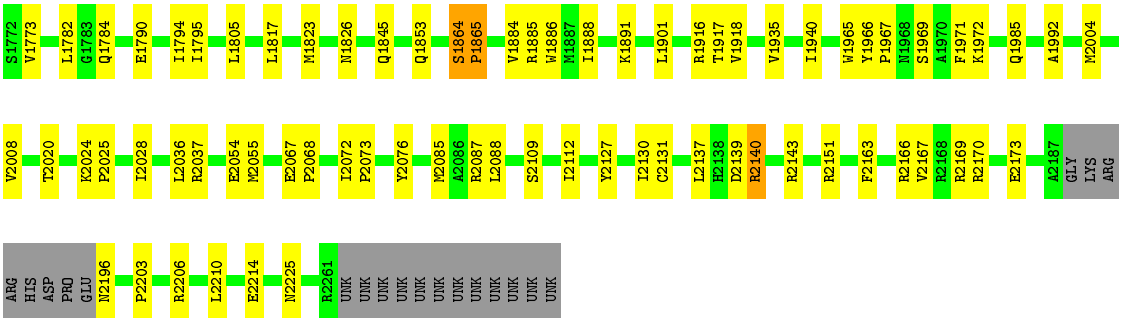


• Molecule 1: Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein

Chain B:






S1772 V1773 L1782 G1783 Q1784 E1790 I1794 I1795 L1805 L1817 M1823 N1826 Q1845 Q1853 S1864 P1865 V1884 R1885 W1886 M1887 I1888 K1891 L1901 R1916 T1917 V1918 V1935 I1940 W1965 Y1966 P1967 N1968 S1969 A1970 F1971 K1972 Q1985 A1992 M2004
V2008 T2020 K2024 P2025 I2028 L2036 R2037 E2054 M2055 E2067 P2068 I2072 P2073 Y2076 M2085 A2086 R2087 L2088 S2109 I2112 Y2127 I2130 C2131 L2137 H2138 D2139 R2140 R2143 R2151 F2163 R2166 V2167 R2168 R2169 R2170 E2173 A2187 GLY LYS ARG
ARG HIS ASP PRO GLU N2196 P2203 R2206 L2210 E2214 N2225 R2261 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	462.20Å 462.20Å 204.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.95 – 8.40 49.95 – 8.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.95-8.40) 99.8 (49.95-8.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 8.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.297 , 0.324 0.340 , 0.360	Depositor DCC
R_{free} test set	549 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å^2)	572.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 899.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	22445	wwPDB-VP
Average B, all atoms (Å^2)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/11401	0.64	0/15435
1	B	0.41	0/11458	0.63	0/15511
All	All	0.41	0/22859	0.63	0/30946

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11224	0	11148	178	0
1	B	11221	0	11191	174	0
All	All	22445	0	22339	347	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 8.

All (347) 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:A:1192:VAL:HG21	1:A:1203:ALA:HB1	1.48	0.94
1:B:1108:ARG:HH21	1:B:1375:ARG:HH22	1.21	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.65	0.79
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.65	0.79
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.65	0.78
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.69	0.75
1:B:1091:ALA:HB2	1:B:1260:ARG:HG2	1.66	0.75
1:B:1131:TRP:O	1:B:1188:LYS:HA	1.87	0.74
1:B:1462:MET:HG2	1:B:1470:ASN:HB2	1.69	0.74
1:B:1415:ASN:HB2	1:B:1452:VAL:HA	1.71	0.73
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.72	0.72
1:B:1516:MET:HG3	1:B:1519:LEU:HD12	1.71	0.71
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.71	0.70
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.71	0.70
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.75	0.68
1:A:961:ASN:HA	1:A:964:LYS:HB2	1.74	0.68
1:B:961:ASN:HA	1:B:964:LYS:HB2	1.74	0.68
1:A:1007:LEU:HD12	1:A:1029:LEU:HG	1.76	0.67
1:B:1007:LEU:HD12	1:B:1029:LEU:HG	1.77	0.67
1:B:2037:ARG:HE	1:B:2067:GLU:HA	1.59	0.67
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.75	0.67
1:B:926:ILE:HD12	1:B:985:LEU:HD11	1.78	0.66
1:B:1376:PRO:HB3	1:B:1423:HIS:HB2	1.77	0.66
1:B:1127:TYR:HB2	1:B:1193:PRO:HD2	1.78	0.65
1:B:1299:ARG:HD2	1:B:1303:SER:HB2	1.78	0.65
1:B:1180:ARG:HD2	1:B:1182:ARG:HD3	1.79	0.64
1:A:926:ILE:HD12	1:A:985:LEU:HD11	1.78	0.64
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.80	0.63
1:A:1171:ILE:HG23	1:A:1330:PHE:HB2	1.80	0.63
1:A:1180:ARG:HD2	1:A:1182:ARG:HD3	1.79	0.63
1:A:1195:LYS:HA	1:A:1260:ARG:HD2	1.81	0.63
1:A:848:LEU:HD23	1:A:851:ARG:HG3	1.81	0.63
1:B:1427:VAL:HG11	1:B:1459:ILE:HD12	1.80	0.63
1:A:1087:THR:HG21	1:A:1305:PRO:HG2	1.80	0.62
1:B:1007:LEU:HD11	1:B:1025:ALA:O	2.00	0.62
1:B:848:LEU:HD23	1:B:851:ARG:HG3	1.81	0.62
1:A:1007:LEU:HD11	1:A:1025:ALA:O	2.00	0.62
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.82	0.61
1:A:880:LEU:HD13	1:A:915:LEU:HD13	1.80	0.61
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.82	0.61
1:A:1161:VAL:HB	1:A:1330:PHE:HZ	1.66	0.60
1:B:1176:TYR:CE2	1:B:1291:ARG:HD3	2.36	0.60
1:A:1168:ILE:HB	1:A:1181:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.83	0.60
1:A:1376:PRO:HG2	1:A:1423:HIS:HB2	1.82	0.60
1:B:1108:ARG:HH21	1:B:1375:ARG:NH2	1.96	0.60
1:A:1517:HIS:HB3	1:A:1598:VAL:HG23	1.84	0.60
1:A:852:MET:HB3	1:A:853:PRO:HD2	1.83	0.60
1:B:1341:LYS:HG3	1:B:1360:ARG:HG2	1.84	0.60
1:B:852:MET:HB3	1:B:853:PRO:HD2	1.83	0.60
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.85	0.59
1:A:1091:ALA:CB	1:A:1260:ARG:HG2	2.33	0.59
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.66	0.59
1:B:1090:PHE:HB2	1:B:1193:PRO:HB3	1.85	0.59
1:A:2163:PHE:O	1:A:2167:VAL:HG23	2.03	0.59
1:B:1116:ARG:HE	1:B:1132:ASP:HB2	1.66	0.58
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.85	0.58
1:B:2163:PHE:O	1:B:2167:VAL:HG23	2.04	0.58
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.86	0.58
1:B:1549:PHE:O	1:B:1553:PHE:HD1	1.87	0.58
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.85	0.58
1:A:1304:TYR:HB3	1:A:1350:LYS:HB2	1.86	0.58
1:B:1156:SER:HB2	1:B:1157:PRO:HD3	1.85	0.58
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.86	0.58
1:A:1068:ASP:HB3	1:A:1071:VAL:HG23	1.86	0.57
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.70	0.57
1:B:887:LEU:HD22	1:B:900:LEU:HB3	1.86	0.57
1:A:1162:GLU:HG3	1:A:1501:GLU:HG2	1.86	0.57
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.87	0.57
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.86	0.57
1:A:1087:THR:CB	1:A:1298:GLY:HA3	2.34	0.57
1:A:1549:PHE:O	1:A:1553:PHE:HD1	1.86	0.57
1:B:1884:VAL:HG21	1:B:1935:VAL:O	2.04	0.57
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.87	0.57
1:B:1081:THR:HG23	1:B:1375:ARG:HE	1.70	0.57
1:B:1517:HIS:HB3	1:B:1598:VAL:HG23	1.86	0.57
1:A:1884:VAL:HG21	1:A:1935:VAL:O	2.04	0.57
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.86	0.56
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.87	0.56
1:B:1059:GLU:HB3	1:B:1062:TRP:HZ3	1.70	0.56
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.86	0.56
1:A:1307:TYR:H	1:A:1323:HIS:HA	1.71	0.56
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.86	0.56
1:A:1087:THR:HG21	1:A:1305:PRO:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:LEU:HD22	1:A:900:LEU:HB3	1.87	0.56
1:B:1068:ASP:HB3	1:B:1071:VAL:HG23	1.88	0.56
1:A:1059:GLU:HB3	1:A:1062:TRP:HZ3	1.71	0.55
1:A:1156:SER:HB2	1:A:1157:PRO:HD3	1.87	0.55
1:A:1087:THR:OG1	1:A:1298:GLY:HA3	2.05	0.55
1:A:2072:ILE:HD12	1:A:2131:CYS:HB2	1.89	0.55
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.06	0.55
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.89	0.55
1:A:936:VAL:HG23	1:A:968:THR:HG23	1.89	0.55
1:B:1492:TYR:HA	1:B:1506:TYR:HA	1.87	0.55
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.88	0.55
1:B:936:VAL:HG23	1:B:968:THR:HG23	1.88	0.54
1:B:2072:ILE:HD12	1:B:2131:CYS:HB2	1.89	0.54
1:A:1333:GLU:HG2	1:A:1336:ARG:HG3	1.90	0.54
1:B:1516:MET:H	1:B:1600:ARG:HA	1.73	0.54
1:B:1176:TYR:HE2	1:B:1291:ARG:HD3	1.72	0.53
1:A:1371:ARG:HD3	1:A:1418:PHE:HB3	1.90	0.53
1:A:1295:PHE:O	1:A:1307:TYR:HA	2.07	0.53
1:A:1087:THR:HB	1:A:1298:GLY:HA3	1.91	0.53
1:B:1132:ASP:HA	1:B:1187:ARG:O	2.08	0.53
1:A:2037:ARG:HE	1:A:2067:GLU:HA	1.74	0.52
1:B:1116:ARG:HE	1:B:1132:ASP:CB	2.23	0.52
1:B:922:GLU:O	1:B:926:ILE:HG12	2.09	0.52
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.92	0.52
1:A:2256:MET:HA	1:A:2259:LEU:HD12	1.92	0.52
1:A:922:GLU:O	1:A:926:ILE:HG12	2.10	0.52
1:B:1059:GLU:HB3	1:B:1062:TRP:CZ3	2.45	0.52
1:B:1985:GLN:HB3	1:B:2024:LYS:HE3	1.92	0.52
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.92	0.51
1:A:1008:ARG:O	1:A:1011:THR:HG22	2.10	0.51
1:B:1133:PHE:HB2	1:B:1187:ARG:HB2	1.92	0.51
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.92	0.51
1:A:1702:TYR:HA	1:A:1729:LYS:HA	1.92	0.51
1:B:1702:TYR:HA	1:B:1729:LYS:HA	1.93	0.51
1:B:1026:ARG:HG2	1:B:1391:SER:OG	2.11	0.51
1:A:1333:GLU:CG	1:A:1336:ARG:HG3	2.41	0.51
1:A:1054:GLN:HB3	1:A:1062:TRP:CD1	2.46	0.51
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	1.92	0.51
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.92	0.51
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.93	0.51
1:B:1006:VAL:O	1:B:1009:ARG:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:ARG:O	1:B:1011:THR:HG22	2.10	0.50
1:B:1506:TYR:H	1:B:1517:HIS:CE1	2.30	0.50
1:A:1340:PHE:CZ	1:A:1527:THR:HG22	2.47	0.50
1:B:1054:GLN:HB3	1:B:1062:TRP:CD1	2.47	0.50
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.93	0.50
1:A:1492:TYR:CD1	1:A:1506:TYR:HB3	2.46	0.50
1:B:1091:ALA:HB2	1:B:1260:ARG:CG	2.39	0.50
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.93	0.50
1:A:1006:VAL:O	1:A:1009:ARG:HG2	2.11	0.50
1:A:907:LEU:O	1:A:911:LEU:HD13	2.12	0.50
1:A:1059:GLU:HB3	1:A:1062:TRP:CZ3	2.46	0.50
1:A:1091:ALA:HB1	1:A:1260:ARG:HG2	1.94	0.50
1:A:856:LEU:HB2	1:A:894:LYS:HE2	1.94	0.50
1:B:2210:LEU:O	1:B:2214:GLU:HB2	2.12	0.49
1:B:1535:ARG:HA	1:B:1545:TYR:HB2	1.94	0.49
1:A:1120:TYR:HD1	1:A:1129:ILE:HG22	1.78	0.49
1:A:1154:PRO:HB2	1:A:1158:ALA:HB2	1.93	0.49
1:B:907:LEU:O	1:B:911:LEU:HD13	2.12	0.49
1:A:1516:MET:H	1:A:1600:ARG:HA	1.77	0.49
1:A:1985:GLN:HB3	1:A:2024:LYS:HE3	1.93	0.49
1:B:1265:LYS:HE3	1:B:1299:ARG:HG3	1.93	0.49
1:B:1429:ALA:HB2	1:B:1475:LEU:HD13	1.94	0.49
1:A:827:PHE:O	1:A:831:LEU:HD23	2.13	0.49
1:B:1168:ILE:HB	1:B:1181:THR:HG21	1.95	0.49
1:A:1099:LEU:HA	1:A:1102:LEU:HD12	1.95	0.49
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.77	0.49
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.94	0.49
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.78	0.49
1:B:827:PHE:O	1:B:831:LEU:HD23	2.13	0.49
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.78	0.48
1:A:1328:LEU:HD22	1:A:1373:VAL:HG21	1.94	0.48
1:A:1980:PHE:CB	1:A:1988:LEU:HD21	2.43	0.48
1:A:2028:ILE:HB	1:A:2055:MET:HG3	1.94	0.48
1:A:2210:LEU:O	1:A:2214:GLU:HB2	2.12	0.48
1:A:860:LEU:HG	1:A:879:LEU:HD22	1.95	0.48
1:B:860:LEU:HG	1:B:879:LEU:HD22	1.95	0.48
1:B:1053:VAL:HG23	1:B:1062:TRP:HB3	1.95	0.48
1:A:1091:ALA:HB2	1:A:1260:ARG:HG2	1.94	0.48
1:B:1192:VAL:HG11	1:B:1203:ALA:O	2.13	0.48
1:B:2028:ILE:HB	1:B:2055:MET:HG3	1.94	0.48
1:B:856:LEU:HB2	1:B:894:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:VAL:HG23	1:A:1062:TRP:HB3	1.96	0.47
1:A:1293:LEU:O	1:A:1309:THR:HA	2.15	0.47
1:B:895:THR:O	1:B:895:THR:HG23	2.15	0.47
1:B:895:THR:HB	1:B:900:LEU:HD12	1.95	0.47
1:A:895:THR:HB	1:A:900:LEU:HD12	1.95	0.47
1:A:1174:MET:SD	1:A:1335:GLY:HA3	2.55	0.47
1:A:1516:MET:HG3	1:A:1519:LEU:HD22	1.96	0.47
1:A:1056:ARG:HD2	1:A:1062:TRP:CZ2	2.50	0.47
1:A:1090:PHE:HB2	1:A:1193:PRO:HB3	1.97	0.47
1:B:1403:ALA:O	1:B:1406:ILE:HG13	2.15	0.47
1:A:1426:GLN:HG3	1:A:1462:MET:HB3	1.97	0.47
1:B:1966:TYR:H	1:B:1969:SER:HB2	1.80	0.47
1:A:895:THR:O	1:A:895:THR:HG23	2.15	0.47
1:A:1403:ALA:O	1:A:1406:ILE:HG13	2.14	0.46
1:A:1886:TRP:HB3	1:A:1891:LYS:HB2	1.98	0.46
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.97	0.46
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.97	0.46
1:A:1266:ASN:HB2	1:A:1270:ILE:HB	1.97	0.46
1:B:1056:ARG:HD2	1:B:1062:TRP:CZ2	2.50	0.46
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	1.98	0.46
1:A:1102:LEU:O	1:A:1106:VAL:HG23	2.15	0.46
1:B:1155:SER:HB2	1:B:1168:ILE:HG12	1.98	0.46
1:A:1492:TYR:CD1	1:A:1504:TYR:HB3	2.50	0.46
1:A:1966:TYR:H	1:A:1969:SER:HB2	1.81	0.46
1:A:894:LYS:HG3	1:A:900:LEU:CD1	2.46	0.46
1:B:1096:TYR:CD1	1:B:1096:TYR:C	2.89	0.46
1:B:1102:LEU:HD21	1:B:1193:PRO:HG3	1.97	0.46
1:B:1127:TYR:OH	1:B:1207:ALA:HB1	2.16	0.46
1:A:1416:HIS:HD2	1:A:1454:GLN:HG3	1.80	0.46
1:B:2203:PRO:HA	1:B:2206:ARG:HB3	1.97	0.46
1:B:2037:ARG:HH11	1:B:2068:PRO:HD3	1.81	0.46
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.98	0.46
1:B:945:LEU:HD13	1:B:951:ILE:HG13	1.98	0.46
1:A:1155:SER:HB2	1:A:1168:ILE:HG12	1.98	0.46
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	1.98	0.46
1:B:1531:LEU:HG	1:B:1535:ARG:HD2	1.98	0.46
1:B:1154:PRO:HB2	1:B:1158:ALA:HB2	1.97	0.45
1:B:933:TYR:HD1	1:B:978:LYS:HG2	1.81	0.45
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	1.98	0.45
1:B:1531:LEU:HD23	1:B:1535:ARG:NH1	2.31	0.45
1:A:1255:VAL:O	1:A:1293:LEU:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:LEU:HD11	1:A:1600:ARG:HD2	1.97	0.45
1:A:1096:TYR:C	1:A:1096:TYR:CD1	2.89	0.45
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.99	0.45
1:B:1253:ALA:O	1:B:1291:ARG:HG2	2.16	0.45
1:A:904:LEU:O	1:A:908:THR:HG23	2.17	0.45
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.98	0.45
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.99	0.45
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.99	0.45
1:B:1323:HIS:CE1	1:B:1350:LYS:HD2	2.51	0.45
1:A:2020:THR:HG21	1:B:1757:ARG:HG2	1.98	0.45
1:A:887:LEU:HD21	1:A:904:LEU:HD12	1.99	0.45
1:B:1268:GLU:HA	1:B:1271:LEU:HD12	1.97	0.45
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.99	0.45
1:B:894:LYS:HG3	1:B:900:LEU:CD1	2.46	0.45
1:B:810:ILE:HD13	1:B:981:LEU:HD21	1.98	0.45
1:A:810:ILE:HD13	1:A:981:LEU:HD21	1.98	0.45
1:B:1291:ARG:HG3	1:B:1292:ARG:N	2.32	0.45
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	2.00	0.44
1:A:846:SER:HA	1:A:849:HIS:ND1	2.32	0.44
1:A:2144:MET:HG2	1:B:1742:VAL:HG11	1.98	0.44
1:A:1087:THR:HG22	1:A:1296:ILE:HD11	1.99	0.44
1:B:1864:SER:HB2	1:B:1865:PRO:CD	2.43	0.44
1:A:1127:TYR:OH	1:A:1207:ALA:HB1	2.17	0.44
1:A:1689:ASN:HA	1:A:1699:LYS:HE3	2.00	0.44
1:A:923:LEU:HD21	1:A:999:VAL:HG12	2.00	0.44
1:A:1629:VAL:HG22	1:A:1664:ILE:HB	1.99	0.44
1:A:933:TYR:HD1	1:A:978:LYS:HG2	1.82	0.44
1:B:846:SER:HA	1:B:849:HIS:ND1	2.33	0.44
1:A:1378:ARG:HD3	1:A:1392:GLU:HG2	1.99	0.44
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.58	0.44
1:B:1192:VAL:CG1	1:B:1203:ALA:HB1	2.48	0.44
1:A:887:LEU:HD11	1:A:904:LEU:HB2	2.00	0.44
1:B:1153:VAL:N	1:B:1154:PRO:CD	2.81	0.44
1:B:824:LEU:O	1:B:828:ILE:HG12	2.18	0.44
1:A:1052:VAL:HG22	1:A:1096:TYR:CE1	2.53	0.44
1:A:824:LEU:O	1:A:828:ILE:HG12	2.18	0.44
1:B:2109:SER:HA	1:B:2112:ILE:HD12	2.00	0.44
1:B:1087:THR:OG1	1:B:1298:GLY:HA3	2.17	0.44
1:A:1757:ARG:HG2	1:B:2020:THR:HG21	2.00	0.43
1:A:2109:SER:HA	1:A:2112:ILE:HD12	1.99	0.43
1:B:1544:GLN:HG3	1:B:1552:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1742:VAL:HA	1:B:1745:LEU:HD12	1.99	0.43
1:B:904:LEU:O	1:B:908:THR:HG23	2.18	0.43
1:A:1096:TYR:O	1:A:1099:LEU:HB3	2.18	0.43
1:A:945:LEU:HD13	1:A:951:ILE:HG13	2.00	0.43
1:B:891:VAL:HA	1:B:895:THR:HG22	2.01	0.43
1:A:1048:LEU:O	1:A:1052:VAL:HG23	2.18	0.43
1:A:891:VAL:HA	1:A:895:THR:HG22	2.00	0.43
1:B:1081:THR:OG1	1:B:1375:ARG:HB3	2.19	0.43
1:B:1116:ARG:NE	1:B:1132:ASP:HB2	2.31	0.43
1:B:1689:ASN:HA	1:B:1699:LYS:HE3	1.99	0.43
1:B:887:LEU:HD21	1:B:904:LEU:HD12	1.99	0.43
1:A:1258:ALA:HA	1:A:1296:ILE:HG23	2.00	0.43
1:A:2177:LEU:HA	1:A:2180:ILE:HD12	2.00	0.43
1:A:856:LEU:CB	1:A:894:LYS:HE2	2.48	0.43
1:B:975:VAL:HG11	1:B:1017:GLN:HG2	2.01	0.43
1:B:1052:VAL:HG22	1:B:1096:TYR:CE1	2.54	0.43
1:B:1739:GLY:HA2	1:B:1744:CYS:SG	2.58	0.43
1:A:1266:ASN:CB	1:A:1270:ILE:HB	2.49	0.43
1:A:1262:ALA:HB2	1:A:1298:GLY:O	2.19	0.43
1:B:831:LEU:HD12	1:B:922:GLU:HA	2.01	0.43
1:A:1066:ARG:HH12	1:A:1120:TYR:HB3	1.84	0.43
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.22	0.43
1:A:1742:VAL:HA	1:A:1745:LEU:HD12	1.99	0.43
1:B:1164:ASP:H	1:B:1167:ARG:NE	2.17	0.43
1:B:1108:ARG:NH2	1:B:1375:ARG:HH22	2.03	0.43
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	2.01	0.43
1:A:1164:ASP:H	1:A:1167:ARG:NE	2.17	0.43
1:B:1099:LEU:HA	1:B:1102:LEU:HD12	2.00	0.43
1:A:831:LEU:HD12	1:A:922:GLU:HA	2.01	0.42
1:B:1096:TYR:O	1:B:1099:LEU:HB3	2.19	0.42
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.83	0.42
1:B:1629:VAL:HG22	1:B:1664:ILE:HB	2.00	0.42
1:A:2137:LEU:HA	1:A:2140:ARG:HD3	2.00	0.42
1:A:1631:ALA:HB2	1:A:1666:LEU:HB2	2.01	0.42
1:A:2085:MET:C	1:A:2087:ARG:H	2.23	0.42
1:A:836:LEU:HG	1:A:921:ARG:HH12	1.84	0.42
1:A:831:LEU:HD13	1:A:921:ARG:CZ	2.49	0.42
1:A:1040:ARG:HH21	1:A:1085:VAL:HB	1.84	0.42
1:A:1389:LEU:HD11	1:A:1425:PHE:CG	2.53	0.42
1:B:1275:LYS:N	1:B:1276:PRO:HD2	2.34	0.42
1:B:831:LEU:HD13	1:B:921:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:LEU:CB	1:B:894:LYS:HE2	2.50	0.42
1:A:1325:GLU:HG3	1:A:1327:SER:H	1.83	0.42
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.22	0.42
1:B:2085:MET:C	1:B:2087:ARG:H	2.23	0.42
1:A:1275:LYS:N	1:A:1276:PRO:HD2	2.35	0.42
1:A:1291:ARG:HE	1:A:1291:ARG:HB2	1.73	0.42
1:A:975:VAL:HG11	1:A:1017:GLN:HG2	2.02	0.42
1:A:1259:VAL:HG23	1:A:1297:CYS:HA	2.02	0.41
1:B:1170:SER:HB2	1:B:1187:ARG:HH22	1.85	0.41
1:B:1170:SER:HB3	1:B:1173:ASP:HB3	2.02	0.41
1:B:1631:ALA:HB2	1:B:1666:LEU:HB2	2.02	0.41
1:B:887:LEU:HD11	1:B:904:LEU:HB2	2.01	0.41
1:B:1048:LEU:O	1:B:1052:VAL:HG23	2.19	0.41
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.20	0.41
1:A:2018:ALA:HA	1:A:2021:ARG:HD2	2.01	0.41
1:A:1052:VAL:HG22	1:A:1096:TYR:CD1	2.56	0.41
1:A:1504:TYR:HE1	1:A:1521:VAL:HA	1.86	0.41
1:A:2203:PRO:HA	1:A:2206:ARG:HB3	2.01	0.41
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.21	0.41
1:B:1052:VAL:HG22	1:B:1096:TYR:CD1	2.56	0.41
1:B:1504:TYR:CE1	1:B:1521:VAL:HA	2.56	0.41
1:A:1208:LEU:HD21	1:A:1285:LEU:HD23	2.03	0.41
1:A:1275:LYS:HA	1:A:1278:VAL:HG12	2.03	0.41
1:A:961:ASN:O	1:A:965:VAL:HG23	2.21	0.41
1:B:836:LEU:HG	1:B:921:ARG:HH12	1.84	0.41
1:A:1544:GLN:HG3	1:A:1552:LEU:HD11	2.02	0.41
1:B:1098:ALA:O	1:B:1102:LEU:HG	2.21	0.41
1:B:1127:TYR:CG	1:B:1128:PHE:N	2.88	0.41
1:B:1265:LYS:HG3	1:B:1299:ARG:HE	1.86	0.41
1:B:820:MET:HA	1:B:823:LYS:HE3	2.03	0.41
1:B:1027:GLU:O	1:B:1031:LEU:HG	2.20	0.41
1:B:1066:ARG:HH12	1:B:1120:TYR:HB3	1.86	0.41
1:B:1319:ASP:C	1:B:1344:PRO:HG2	2.41	0.41
1:A:2088:LEU:HG	1:B:1686:VAL:HG23	2.01	0.41
1:A:1460:ASN:HD22	1:A:1472:THR:HG21	1.86	0.41
1:A:1524:PRO:O	1:A:1525:TYR:C	2.60	0.41
1:B:1054:GLN:HB3	1:B:1062:TRP:NE1	2.36	0.41
1:A:1054:GLN:HB3	1:A:1062:TRP:NE1	2.36	0.41
1:A:1341:LYS:HG3	1:A:1360:ARG:HG2	2.02	0.41
1:A:2134:PHE:HA	1:A:2137:LEU:HD12	2.03	0.41
1:B:1076:VAL:HG11	1:B:1107:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:LEU:HD21	1:B:999:VAL:HG12	2.01	0.41
1:B:1007:LEU:HD11	1:B:1025:ALA:C	2.41	0.40
1:B:1530:TRP:O	1:B:1533:PRO:HD2	2.21	0.40
1:A:1864:SER:HB2	1:A:1865:PRO:CD	2.43	0.40
1:A:1988:LEU:HG	1:A:2022:PHE:CZ	2.57	0.40
1:A:1987:PRO:HG3	1:A:2171:LEU:HD21	2.03	0.40
1:B:1162:GLU:HG3	1:B:1522:SER:OG	2.20	0.40
1:B:1794:ILE:HD12	1:B:1823:MET:HG3	2.04	0.40
1:B:993:LYS:HG2	1:B:1031:LEU:HD22	2.03	0.40
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.42	0.40
1:A:2005:TYR:HA	1:B:1826:ASN:HD22	1.87	0.40
1:B:1340:PHE:CZ	1:B:1527:THR:HG22	2.56	0.40
1:A:1125:ARG:HH22	1:A:1199:ASP:CG	2.25	0.40
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.87	0.40
1:A:820:MET:HA	1:A:823:LYS:HE3	2.02	0.40
1:B:1052:VAL:HA	1:B:1096:TYR:CZ	2.57	0.40
1:B:1527:THR:O	1:B:1530:TRP:CD1	2.75	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	1373/2211 (62%)	1229 (90%)	123 (9%)	21 (2%)	10	46
1	B	1380/2211 (62%)	1249 (90%)	110 (8%)	21 (2%)	10	46
All	All	2753/4422 (62%)	2478 (90%)	233 (8%)	42 (2%)	10	46

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	943	ARG

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Mol	Chain	Res	Type
1	A	1156	SER
1	A	1516	MET
1	A	1784	GLN
1	A	1864	SER
1	B	943	ARG
1	B	1092	HIS
1	B	1156	SER
1	B	1864	SER
1	A	887	LEU
1	A	1128	PHE
1	A	1180	ARG
1	A	2225	ASN
1	B	887	LEU
1	B	1180	ARG
1	A	853	PRO
1	A	1486	VAL
1	A	1512	LYS
1	B	853	PRO
1	B	1160	PRO
1	B	1426	GLN
1	B	1516	MET
1	B	1638	ILE
1	B	1784	GLN
1	B	2225	ASN
1	A	892	PRO
1	A	1333	GLU
1	A	1638	ILE
1	A	1790	GLU
1	B	892	PRO
1	B	1128	PHE
1	B	1486	VAL
1	B	1790	GLU
1	A	1313	PRO
1	A	1317	GLU
1	A	1865	PRO
1	B	1313	PRO
1	B	1865	PRO
1	B	1317	GLU
1	A	1052	VAL
1	B	1052	VAL
1	A	1525	TYR

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	1208/1879 (64%)	1138 (94%)	70 (6%)	20 45
1	B	1215/1879 (65%)	1151 (95%)	64 (5%)	22 47
All	All	2423/3758 (64%)	2289 (94%)	134 (6%)	21 47

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	819	VAL
1	A	836	LEU
1	A	848	LEU
1	A	852	MET
1	A	880	LEU
1	A	883	PHE
1	A	884	ASN
1	A	911	LEU
1	A	913	LEU
1	A	921	ARG
1	A	930	LEU
1	A	951	ILE
1	A	952	LEU
1	A	954	LEU
1	A	961	ASN
1	A	970	LEU
1	A	1007	LEU
1	A	1021	VAL
1	A	1062	TRP
1	A	1079	LYS
1	A	1086	LEU
1	A	1090	PHE
1	A	1096	TYR
1	A	1115	LEU
1	A	1127	TYR
1	A	1132	ASP
1	A	1171	ILE

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Mol	Chain	Res	Type
1	A	1177	LEU
1	A	1259	VAL
1	A	1261	ASP
1	A	1291	ARG
1	A	1320	SER
1	A	1342	LEU
1	A	1343	THR
1	A	1378	ARG
1	A	1379	LEU
1	A	1424	THR
1	A	1462	MET
1	A	1475	LEU
1	A	1489	ILE
1	A	1551	GLU
1	A	1557	ILE
1	A	1563	GLU
1	A	1593	ASP
1	A	1595	LEU
1	A	1618	THR
1	A	1632	ASN
1	A	1638	ILE
1	A	1674	LEU
1	A	1715	VAL
1	A	1771	ARG
1	A	1805	LEU
1	A	1817	LEU
1	A	1853	GLN
1	A	1901	LEU
1	A	1917	THR
1	A	1965	TRP
1	A	1967	PRO
1	A	1971	PHE
1	A	1988	LEU
1	A	2022	PHE
1	A	2076	TYR
1	A	2088	LEU
1	A	2140	ARG
1	A	2143	ARG
1	A	2151	ARG
1	A	2166	ARG
1	A	2196	ASN
1	A	2234	GLU

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Mol	Chain	Res	Type
1	A	2240	ILE
1	B	819	VAL
1	B	836	LEU
1	B	848	LEU
1	B	852	MET
1	B	880	LEU
1	B	883	PHE
1	B	884	ASN
1	B	911	LEU
1	B	913	LEU
1	B	915	LEU
1	B	921	ARG
1	B	930	LEU
1	B	951	ILE
1	B	952	LEU
1	B	954	LEU
1	B	961	ASN
1	B	970	LEU
1	B	1007	LEU
1	B	1021	VAL
1	B	1032	CYS
1	B	1062	TRP
1	B	1086	LEU
1	B	1090	PHE
1	B	1096	TYR
1	B	1115	LEU
1	B	1116	ARG
1	B	1127	TYR
1	B	1177	LEU
1	B	1192	VAL
1	B	1254	VAL
1	B	1296	ILE
1	B	1324	ILE
1	B	1327	SER
1	B	1331	GLN
1	B	1378	ARG
1	B	1430	ASP
1	B	1551	GLU
1	B	1557	ILE
1	B	1563	GLU
1	B	1593	ASP
1	B	1595	LEU

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Mol	Chain	Res	Type
1	B	1618	THR
1	B	1632	ASN
1	B	1638	ILE
1	B	1674	LEU
1	B	1715	VAL
1	B	1771	ARG
1	B	1805	LEU
1	B	1817	LEU
1	B	1845	GLN
1	B	1853	GLN
1	B	1901	LEU
1	B	1917	THR
1	B	1965	TRP
1	B	1967	PRO
1	B	1971	PHE
1	B	2076	TYR
1	B	2088	LEU
1	B	2139	ASP
1	B	2140	ARG
1	B	2143	ARG
1	B	2151	ARG
1	B	2166	ARG
1	B	2196	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1415	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.