



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2016 – 09:32 AM EDT

PDB ID : 5I6H
Title : Crystal structure of CD-CT domains of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on : 2016-02-16
Resolution : 7.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027257

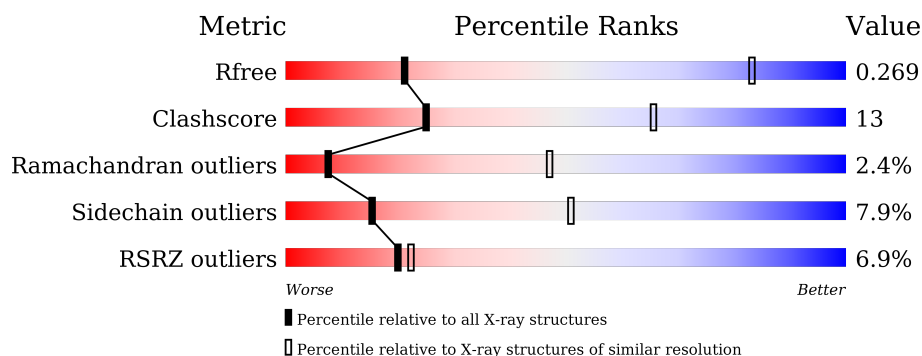
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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. 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	1487	<div> <div>7%</div> <div>63%</div> <div>28%</div> <div>• 6%</div> </div>
1	B	1487	<div> <div>6%</div> <div>64%</div> <div>27%</div> <div>• 5%</div> </div>

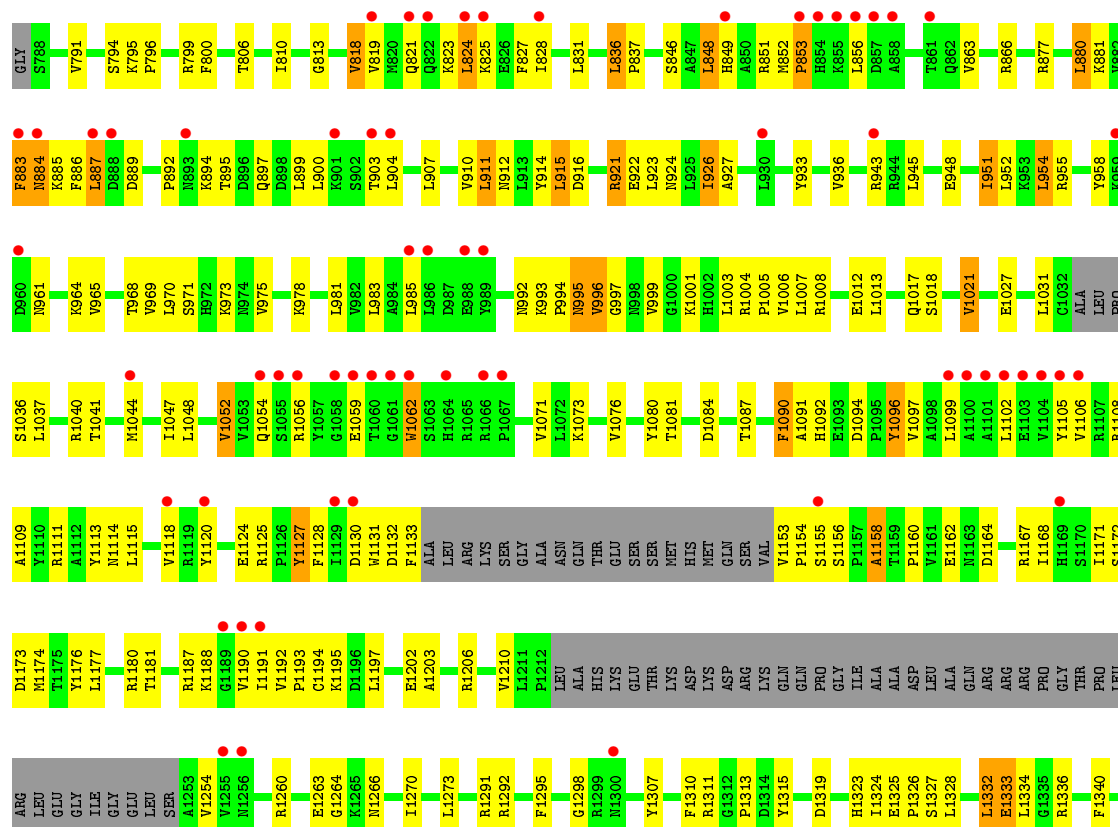
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22543 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	1404	Total	C	N	O	S	0	0	0
			11262	7144	1983	2096	39			
1	B	1406	Total	C	N	O	S	0	0	0
			11281	7156	1988	2098	39			





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	295.02Å 295.02Å 189.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 7.20 49.85 – 7.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.85-7.20) 100.0 (49.85-7.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 7.37Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.232 , 0.248 0.260 , 0.269	Depositor DCC
R_{free} test set	696 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	662.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 411.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22543	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/11439	0.72	3/15486 (0.0%)
1	B	0.50	0/11458	0.71	0/15511
All	All	0.49	0/22897	0.72	3/30997 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1988	LEU	CB-CG-CD2	5.41	120.20	111.00
1	A	1988	LEU	CB-CG-CD1	5.17	119.78	111.00
1	A	1090	PHE	C-N-CA	5.09	134.41	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11262	0	11181	289	0
1	B	11281	0	11205	295	0
All	All	22543	0	22386	571	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 13.

All (571) 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:1389:LEU:HD11	1:B:1425:PHE:HB3	1.33	1.08
1:A:994:PRO:HA	1:A:1037:LEU:HB3	1.35	1.07
1:B:994:PRO:HA	1:B:1037:LEU:HB3	1.40	1.01
1:A:1090:PHE:HB2	1:A:1193:PRO:HB3	1.39	0.99
1:B:1176:TYR:HE2	1:B:1291:ARG:HD3	1.23	0.98
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.49	0.93
1:A:1125:ARG:HH11	1:A:1203:ALA:HB2	1.31	0.92
1:B:1168:ILE:HB	1:B:1181:THR:HG21	1.51	0.92
1:A:827:PHE:O	1:A:831:LEU:HD23	1.70	0.91
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.51	0.91
1:B:827:PHE:O	1:B:831:LEU:HD23	1.70	0.91
1:A:1192:VAL:HG21	1:A:1203:ALA:HB1	1.53	0.89
1:A:848:LEU:HD23	1:A:851:ARG:HG3	1.55	0.88
1:A:1168:ILE:HB	1:A:1181:THR:HG21	1.57	0.86
1:B:1131:TRP:O	1:B:1188:LYS:HA	1.75	0.85
1:B:848:LEU:HD23	1:B:851:ARG:HG3	1.54	0.85
1:A:852:MET:HB3	1:A:853:PRO:HD2	1.59	0.84
1:A:1376:PRO:HG2	1:A:1423:HIS:HB2	1.57	0.84
1:B:926:ILE:HD12	1:B:985:LEU:HD11	1.59	0.84
1:B:1059:GLU:HB3	1:B:1062:TRP:HZ3	1.43	0.84
1:B:1176:TYR:CE2	1:B:1291:ARG:HD3	2.11	0.84
1:A:926:ILE:HD12	1:A:985:LEU:HD11	1.60	0.83
1:B:852:MET:HB3	1:B:853:PRO:HD2	1.59	0.83
1:B:1192:VAL:HG11	1:B:1203:ALA:HB1	1.61	0.83
1:A:1980:PHE:HD2	1:A:1988:LEU:HD11	1.43	0.82
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.62	0.81
1:B:1192:VAL:CG1	1:B:1203:ALA:HB1	2.10	0.81
1:A:1059:GLU:HB3	1:A:1062:TRP:HZ3	1.47	0.80
1:B:1127:TYR:HB2	1:B:1193:PRO:HD2	1.64	0.80
1:B:1415:ASN:HB2	1:B:1452:VAL:HA	1.61	0.80
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.64	0.80
1:B:1324:ILE:HG23	1:B:1353:HIS:HE1	1.46	0.79
1:A:1125:ARG:NH1	1:A:1203:ALA:HB2	1.97	0.79
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.63	0.79
1:B:1125:ARG:HD2	1:B:1203:ALA:HB2	1.64	0.79
1:B:1091:ALA:HB2	1:B:1260:ARG:HG2	1.64	0.78
1:B:994:PRO:CA	1:B:1037:LEU:HB3	2.15	0.77
1:B:2249:LYS:HA	1:B:2252:ILE:HD12	1.68	0.76
1:A:1389:LEU:HD13	1:A:1459:ILE:HD11	1.68	0.74
1:A:895:THR:HB	1:A:900:LEU:HD12	1.70	0.74
1:B:1108:ARG:HH21	1:B:1375:ARG:NH2	1.85	0.74
1:A:1083:PHE:HE2	1:A:1375:ARG:HH12	1.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:THR:HB	1:B:900:LEU:HD12	1.70	0.74
1:B:961:ASN:O	1:B:965:VAL:HG23	1.87	0.74
1:A:961:ASN:O	1:A:965:VAL:HG23	1.88	0.72
1:B:2037:ARG:HE	1:B:2067:GLU:HA	1.54	0.72
1:B:1516:MET:HG3	1:B:1519:LEU:HD12	1.69	0.72
1:A:1133:PHE:CZ	1:A:1187:ARG:HB2	2.24	0.72
1:B:1090:PHE:HB2	1:B:1193:PRO:HB3	1.72	0.72
1:A:1056:ARG:HD2	1:A:1062:TRP:CZ2	2.25	0.71
1:B:1106:VAL:HG22	1:B:1191:ILE:HD11	1.71	0.70
1:B:1056:ARG:HD2	1:B:1062:TRP:CZ2	2.27	0.70
1:B:1059:GLU:HB3	1:B:1062:TRP:CZ3	2.27	0.70
1:A:1254:VAL:HG11	1:A:1292:ARG:NH2	2.07	0.70
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.72	0.69
1:A:2065:VAL:HG23	1:B:1741:GLY:HA2	1.73	0.69
1:A:1081:THR:HA	1:A:1375:ARG:HH21	1.56	0.68
1:B:1517:HIS:HB3	1:B:1598:VAL:HG23	1.75	0.68
1:B:1336:ARG:HB2	1:B:1371:ARG:NH2	2.07	0.68
1:A:2123:LEU:HD21	1:B:1694:PRO:HG2	1.76	0.68
1:B:1105:TYR:HD2	1:B:1191:ILE:HD13	1.58	0.68
1:A:1127:TYR:HE2	1:A:1190:VAL:HG13	1.59	0.68
1:A:806:THR:HB	1:A:818:VAL:HG11	1.76	0.68
1:B:1336:ARG:HB2	1:B:1371:ARG:HH22	1.59	0.68
1:B:1040:ARG:HH11	1:B:1378:ARG:HG3	1.59	0.67
1:A:1173:ASP:OD1	1:A:1311:ARG:HD3	1.95	0.67
1:B:1609:MET:CE	1:B:1630:VAL:HG13	2.25	0.67
1:B:2241:ASN:HA	1:B:2244:LEU:HD12	1.77	0.67
1:A:1059:GLU:HB3	1:A:1062:TRP:CZ3	2.29	0.66
1:A:1985:GLN:HB3	1:A:2024:LYS:HE3	1.76	0.66
1:A:1515:SER:HA	1:A:1599:SER:O	1.95	0.66
1:A:2123:LEU:CD2	1:B:1694:PRO:HG2	2.25	0.66
1:A:1448:TRP:CE3	1:A:1448:TRP:HA	2.30	0.66
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.78	0.66
1:B:958:TYR:HB2	1:B:961:ASN:HB2	1.77	0.66
1:B:1173:ASP:OD1	1:B:1311:ARG:HD3	1.97	0.65
1:B:1325:GLU:HB2	1:B:1328:LEU:HB2	1.78	0.65
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.77	0.65
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.77	0.65
1:B:994:PRO:HA	1:B:1037:LEU:CB	2.21	0.65
1:B:1448:TRP:CE3	1:B:1448:TRP:HA	2.32	0.65
1:B:1490:GLU:OE2	1:B:1514:GLY:HA3	1.96	0.65
1:B:1263:GLU:HG3	1:B:1264:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1324:ILE:HG23	1:B:1353:HIS:CE1	2.31	0.64
1:B:806:THR:HB	1:B:818:VAL:HG11	1.79	0.64
1:A:958:TYR:HB2	1:A:961:ASN:HB2	1.79	0.64
1:B:1080:TYR:CB	1:B:1378:ARG:HG2	2.28	0.64
1:A:1090:PHE:CB	1:A:1193:PRO:HB3	2.22	0.63
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.81	0.63
1:A:1259:VAL:HG12	1:A:1260:ARG:N	2.14	0.63
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.81	0.63
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.81	0.63
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.81	0.63
1:A:936:VAL:HG23	1:A:968:THR:HG23	1.79	0.63
1:A:853:PRO:HB2	1:A:894:LYS:HD2	1.81	0.63
1:B:856:LEU:HB2	1:B:894:LYS:HE2	1.81	0.63
1:B:853:PRO:HB2	1:B:894:LYS:HD2	1.81	0.62
1:A:936:VAL:HG21	1:A:971:SER:HB3	1.81	0.62
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	1.80	0.62
1:B:1985:GLN:HB3	1:B:2024:LYS:HE3	1.79	0.62
1:B:936:VAL:HG23	1:B:968:THR:HG23	1.81	0.62
1:A:1258:ALA:HA	1:A:1296:ILE:HG23	1.81	0.62
1:A:1486:VAL:C	1:A:1488:GLN:H	2.02	0.62
1:A:1054:GLN:HB3	1:A:1062:TRP:CD1	2.35	0.61
1:A:1127:TYR:HB2	1:A:1193:PRO:HD3	1.81	0.61
1:A:1514:GLY:O	1:A:1599:SER:HB3	1.99	0.61
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.82	0.61
1:A:1001:LYS:HA	1:A:1004:ARG:HG3	1.83	0.61
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.40	0.61
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.82	0.61
1:A:856:LEU:HB2	1:A:894:LYS:HE2	1.82	0.61
1:A:1091:ALA:CB	1:A:1260:ARG:HG2	2.31	0.61
1:A:927:ALA:HA	1:A:1006:VAL:HG21	1.83	0.61
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.83	0.61
1:A:993:LYS:HB2	1:A:994:PRO:HD3	1.82	0.61
1:B:936:VAL:HG21	1:B:971:SER:HB3	1.83	0.61
1:B:1001:LYS:HA	1:B:1004:ARG:HG3	1.82	0.61
1:B:1195:LYS:HA	1:B:1260:ARG:HD2	1.83	0.61
1:B:1739:GLY:HA2	1:B:1744:CYS:SG	2.40	0.61
1:B:961:ASN:HA	1:B:964:LYS:HB2	1.83	0.60
1:A:1853:GLN:HG2	1:A:1854:ARG:H	1.65	0.60
1:A:1367:ARG:HH21	1:A:1528:LYS:HG3	1.66	0.60
1:B:975:VAL:HG11	1:B:1017:GLN:HG2	1.82	0.60
1:B:1210:VAL:HG12	1:B:1210:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ALA:HA	1:B:1006:VAL:HG21	1.84	0.60
1:B:1530:TRP:O	1:B:1533:PRO:HD2	2.00	0.60
1:A:1099:LEU:HG	1:A:1120:TYR:CD1	2.37	0.60
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.83	0.60
1:A:961:ASN:HA	1:A:964:LYS:HB2	1.83	0.60
1:A:975:VAL:HG11	1:A:1017:GLN:HG2	1.83	0.60
1:A:1741:GLY:HA2	1:B:2065:VAL:HG23	1.83	0.59
1:B:1054:GLN:HB3	1:B:1062:TRP:CD1	2.37	0.59
1:B:1187:ARG:HG2	1:B:1291:ARG:HH12	1.66	0.59
1:B:1853:GLN:HG2	1:B:1854:ARG:H	1.66	0.59
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.84	0.59
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.22	0.59
1:B:1059:GLU:CB	1:B:1062:TRP:HZ3	2.13	0.59
1:B:1389:LEU:HD11	1:B:1425:PHE:CB	2.21	0.59
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.85	0.59
1:A:1127:TYR:CE2	1:A:1190:VAL:HG13	2.36	0.59
1:A:1980:PHE:CD2	1:A:1988:LEU:HD11	2.31	0.59
1:B:1132:ASP:HA	1:B:1187:ARG:O	2.02	0.59
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.84	0.59
1:A:994:PRO:CA	1:A:1037:LEU:HB3	2.22	0.59
1:A:1846:TRP:HZ2	1:A:1910:THR:HG21	1.68	0.59
1:B:856:LEU:CB	1:B:894:LYS:HE2	2.33	0.59
1:A:994:PRO:HA	1:A:1037:LEU:CB	2.24	0.59
1:B:1080:TYR:HB3	1:B:1378:ARG:HG2	1.84	0.58
1:A:1123:GLU:HB2	1:A:1128:PHE:CE1	2.38	0.58
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.84	0.58
1:B:993:LYS:HB2	1:B:994:PRO:HD3	1.85	0.58
1:A:1759:TYR:HB2	1:A:1764:THR:HG21	1.84	0.58
1:A:1195:LYS:HA	1:A:1260:ARG:HD2	1.85	0.58
1:A:1040:ARG:HH22	1:A:1084:ASP:HB3	1.69	0.58
1:B:1292:ARG:NH1	1:B:1326:PRO:HB3	2.19	0.58
1:B:1426:GLN:HG2	1:B:1462:MET:HB3	1.85	0.58
1:A:2020:THR:HG21	1:B:1757:ARG:HG2	1.85	0.58
1:A:1266:ASN:HB3	1:A:1270:ILE:HB	1.86	0.58
1:A:856:LEU:CB	1:A:894:LYS:HE2	2.34	0.58
1:B:1108:ARG:HH21	1:B:1375:ARG:HH22	1.50	0.58
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.86	0.57
1:A:1059:GLU:CB	1:A:1062:TRP:HZ3	2.15	0.57
1:A:836:LEU:HD12	1:A:914:TYR:OH	2.04	0.57
1:A:1091:ALA:HB1	1:A:1260:ARG:HD3	1.87	0.57
1:A:1980:PHE:HD2	1:A:1988:LEU:CD1	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2243:LYS:HA	1:B:2246:LYS:HD2	1.87	0.57
1:A:1171:ILE:HD13	1:A:1327:SER:O	2.05	0.57
1:B:852:MET:SD	1:B:903:THR:HG21	2.45	0.57
1:A:1496:LEU:HD12	1:A:1498:GLU:H	1.70	0.56
1:B:877:ARG:HE	1:B:915:LEU:HG	1.69	0.56
1:A:813:GLY:HA3	1:A:971:SER:HA	1.86	0.56
1:A:2253:ALA:HB1	1:A:2257:ARG:HH21	1.70	0.56
1:B:2177:LEU:HA	1:B:2180:ILE:HD12	1.85	0.56
1:A:1340:PHE:CZ	1:A:1527:THR:HG22	2.41	0.56
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.05	0.56
1:A:1497:SER:O	1:A:1498:GLU:HB3	2.05	0.56
1:A:852:MET:SD	1:A:903:THR:HG21	2.46	0.56
1:A:883:PHE:CE2	1:A:911:LEU:HD21	2.41	0.56
1:B:1073:LYS:HA	1:B:1076:VAL:HG22	1.88	0.56
1:B:1844:VAL:HA	1:B:1847:LEU:HD12	1.87	0.56
1:A:948:GLU:O	1:A:952:LEU:HD12	2.06	0.56
1:B:836:LEU:HD12	1:B:914:TYR:OH	2.05	0.55
1:B:1087:THR:HG21	1:B:1298:GLY:HA3	1.88	0.55
1:A:2181:GLU:OE1	1:A:2181:GLU:HA	2.07	0.55
1:A:1259:VAL:HG12	1:A:1260:ARG:H	1.71	0.55
1:A:1448:TRP:HE3	1:A:1448:TRP:HA	1.70	0.55
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.71	0.55
1:A:1781:ARG:HH12	1:A:1975:GLN:HE22	1.53	0.55
1:B:1630:VAL:HG11	1:B:1649:PHE:CD2	2.42	0.55
1:B:1448:TRP:HA	1:B:1448:TRP:HE3	1.71	0.55
1:B:883:PHE:CE2	1:B:911:LEU:HD21	2.41	0.55
1:A:1844:VAL:HA	1:A:1847:LEU:HD12	1.89	0.55
1:A:795:LYS:HB2	1:A:796:PRO:HD3	1.88	0.55
1:A:1087:THR:HA	1:A:1090:PHE:CE2	2.42	0.54
1:B:1813:SER:HB3	1:B:1816:GLN:HB2	1.88	0.54
1:B:1195:LYS:CA	1:B:1260:ARG:HD2	2.37	0.54
1:B:880:LEU:HD13	1:B:915:LEU:HD12	1.90	0.54
1:B:948:GLU:O	1:B:952:LEU:HD12	2.06	0.54
1:A:1073:LYS:HA	1:A:1076:VAL:HG22	1.89	0.54
1:A:1168:ILE:HB	1:A:1181:THR:CG2	2.35	0.54
1:B:1291:ARG:HG3	1:B:1292:ARG:N	2.23	0.54
1:B:795:LYS:HB2	1:B:796:PRO:HD3	1.88	0.54
1:B:1001:LYS:HG3	1:B:1004:ARG:HH21	1.73	0.54
1:A:1127:TYR:CD2	1:A:1192:VAL:HB	2.43	0.53
1:A:1191:ILE:HG12	1:A:1256:ASN:HB2	1.90	0.53
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1846:TRP:CZ2	1:A:1910:THR:HG21	2.43	0.53
1:B:1609:MET:HE1	1:B:1630:VAL:HG13	1.89	0.53
1:B:1087:THR:HA	1:B:1090:PHE:CE2	2.43	0.53
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.74	0.53
1:A:1517:HIS:HB3	1:A:1598:VAL:HG23	1.91	0.53
1:A:1813:SER:HB3	1:A:1816:GLN:HB2	1.90	0.53
1:B:887:LEU:HD21	1:B:904:LEU:HD12	1.91	0.53
1:B:1099:LEU:HG	1:B:1120:TYR:CD1	2.44	0.52
1:B:945:LEU:HD11	1:B:954:LEU:HD13	1.92	0.52
1:B:1609:MET:HE3	1:B:1630:VAL:HG13	1.90	0.52
1:B:1534:LYS:NZ	1:B:1604:MET:H	2.08	0.52
1:A:1040:ARG:NH2	1:A:1084:ASP:HB3	2.23	0.52
1:A:1091:ALA:HB1	1:A:1260:ARG:CD	2.40	0.52
1:A:1886:TRP:HB3	1:A:1891:LYS:HB2	1.92	0.52
1:A:895:THR:O	1:A:895:THR:HG23	2.09	0.52
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.75	0.52
1:A:1190:VAL:HG12	1:A:1255:VAL:HG23	1.91	0.52
1:A:1001:LYS:HG3	1:A:1004:ARG:HH21	1.75	0.52
1:A:1192:VAL:HG13	1:A:1257:VAL:HG13	1.92	0.52
1:A:1750:LEU:HD13	1:B:2047:THR:HB	1.91	0.52
1:B:1018:SER:O	1:B:1021:VAL:HG12	2.10	0.52
1:B:1106:VAL:CG2	1:B:1191:ILE:CD1	2.88	0.52
1:A:1885:ARG:HD2	1:A:1919:VAL:HG11	1.90	0.51
1:B:1333:GLU:HG2	1:B:1336:ARG:HG3	1.92	0.51
1:A:1018:SER:O	1:A:1021:VAL:HG12	2.10	0.51
1:A:1088:LEU:O	1:A:1091:ALA:HB3	2.10	0.51
1:A:948:GLU:OE1	1:A:969:VAL:HG13	2.11	0.51
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	1.92	0.51
1:B:813:GLY:HA3	1:B:971:SER:HA	1.90	0.51
1:B:1109:ALA:O	1:B:1327:SER:HB2	2.10	0.51
1:B:852:MET:HB2	1:B:900:LEU:HD21	1.92	0.51
1:B:1609:MET:HE1	1:B:1649:PHE:HD2	1.75	0.51
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.92	0.51
1:A:1638:ILE:HD12	1:A:1640:SER:HB3	1.91	0.51
1:B:1106:VAL:CG2	1:B:1191:ILE:HD11	2.37	0.51
1:B:831:LEU:HD12	1:B:922:GLU:HA	1.92	0.51
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.90	0.51
1:A:887:LEU:HD21	1:A:904:LEU:HD12	1.92	0.51
1:B:1125:ARG:HH21	1:B:1202:GLU:HB2	1.76	0.51
1:B:895:THR:O	1:B:895:THR:HG23	2.10	0.51
1:B:948:GLU:OE1	1:B:969:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:VAL:HG22	1:B:1036:SER:N	2.25	0.51
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.93	0.51
1:A:1048:LEU:O	1:A:1052:VAL:HG23	2.11	0.51
1:A:1127:TYR:HB2	1:A:1193:PRO:CD	2.40	0.51
1:B:1168:ILE:HD12	1:B:1181:THR:OG1	2.10	0.51
1:A:1928:ILE:HD11	1:A:2168:ARG:HG3	1.93	0.51
1:A:831:LEU:HD12	1:A:922:GLU:HA	1.93	0.51
1:B:1154:PRO:HB2	1:B:1158:ALA:HB2	1.92	0.51
1:B:2037:ARG:HH11	1:B:2068:PRO:HD3	1.75	0.51
1:A:1811:TYR:CE1	1:B:2001:GLN:HB2	2.46	0.51
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.76	0.51
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.93	0.51
1:B:2022:PHE:HE2	1:B:2024:LYS:HB2	1.75	0.51
1:B:2143:ARG:HH12	1:B:2147:LYS:HE2	1.74	0.51
1:B:1047:ILE:HG23	1:B:1071:VAL:HG12	1.93	0.50
1:A:1403:ALA:O	1:A:1406:ILE:HG13	2.12	0.50
1:B:1332:LEU:HG	1:B:1371:ARG:HB3	1.92	0.50
1:A:1389:LEU:HD13	1:A:1459:ILE:CD1	2.40	0.50
1:A:852:MET:HB2	1:A:900:LEU:HD21	1.93	0.50
1:B:1048:LEU:O	1:B:1052:VAL:HG23	2.11	0.50
1:B:1187:ARG:HG2	1:B:1291:ARG:HH22	1.77	0.50
1:A:1091:ALA:HB1	1:A:1260:ARG:HG2	1.94	0.50
1:A:1102:LEU:O	1:A:1106:VAL:HG23	2.12	0.50
1:B:1027:GLU:O	1:B:1031:LEU:HG	2.12	0.50
1:A:1304:TYR:HB3	1:A:1350:LYS:HB2	1.94	0.50
1:A:2137:LEU:HA	1:A:2140:ARG:HD3	1.94	0.50
1:B:1081:THR:HG23	1:B:1375:ARG:HE	1.77	0.50
1:B:886:PHE:HB3	1:B:894:LYS:HG2	1.94	0.50
1:A:2022:PHE:HE2	1:A:2024:LYS:HB2	1.75	0.50
1:B:1340:PHE:CZ	1:B:1527:THR:HG22	2.47	0.50
1:A:1103:GLU:OE1	1:A:1118:VAL:HG21	2.12	0.50
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.16	0.50
1:B:1885:ARG:HD2	1:B:1919:VAL:HG11	1.93	0.50
1:A:1534:LYS:NZ	1:A:1604:MET:H	2.09	0.49
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.94	0.49
1:A:1047:ILE:HG23	1:A:1071:VAL:HG12	1.95	0.49
1:A:1378:ARG:HB2	1:A:1388:TYR:CZ	2.46	0.49
1:B:1702:TYR:HA	1:B:1729:LYS:HA	1.94	0.49
1:B:907:LEU:O	1:B:911:LEU:HD13	2.12	0.49
1:A:1759:TYR:CE2	1:A:1784:GLN:HG3	2.47	0.49
1:A:2047:THR:HB	1:B:1750:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:MET:HB3	1:A:853:PRO:CD	2.38	0.49
1:B:823:LYS:NZ	1:B:981:LEU:HD11	2.27	0.49
1:A:1197:LEU:HD13	1:A:1273:LEU:HD23	1.94	0.49
1:B:1403:ALA:O	1:B:1406:ILE:HG13	2.11	0.49
1:B:897:GLN:HB3	1:B:899:LEU:CD2	2.42	0.49
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.12	0.49
1:A:995:ASN:HB2	1:A:999:VAL:HG22	1.94	0.49
1:B:824:LEU:O	1:B:828:ILE:HG12	2.12	0.49
1:B:994:PRO:HB3	1:B:1037:LEU:HD22	1.94	0.49
1:A:1702:TYR:HA	1:A:1729:LYS:HA	1.95	0.49
1:A:824:LEU:O	1:A:828:ILE:HG12	2.12	0.49
1:B:1609:MET:HE1	1:B:1630:VAL:CG1	2.42	0.49
1:A:1259:VAL:CG1	1:A:1260:ARG:H	2.25	0.49
1:A:1171:ILE:HG22	1:A:1329:ALA:HB3	1.95	0.49
1:A:1757:ARG:HG2	1:B:2020:THR:HG21	1.94	0.49
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.94	0.49
1:A:2143:ARG:HH12	1:A:2147:LYS:HE2	1.78	0.49
1:A:886:PHE:HB3	1:A:894:LYS:HG2	1.94	0.49
1:A:897:GLN:HB3	1:A:899:LEU:CD2	2.43	0.49
1:B:995:ASN:HB2	1:B:999:VAL:HG22	1.95	0.49
1:A:1171:ILE:HG23	1:A:1330:PHE:N	2.27	0.49
1:A:1259:VAL:CG1	1:A:1260:ARG:N	2.76	0.49
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.95	0.49
1:A:2169:ARG:O	1:A:2173:GLU:HB2	2.13	0.49
1:A:923:LEU:HD21	1:A:999:VAL:HG12	1.94	0.49
1:B:1127:TYR:HE2	1:B:1190:VAL:CG1	2.26	0.49
1:B:880:LEU:HG	1:B:911:LEU:HD23	1.95	0.49
1:A:1119:ARG:HB2	1:A:1130:ASP:HB3	1.94	0.49
1:B:1527:THR:O	1:B:1530:TRP:HD1	1.96	0.49
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.13	0.49
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.94	0.48
1:A:2028:ILE:HB	1:A:2055:MET:HG3	1.94	0.48
1:A:907:LEU:O	1:A:911:LEU:HD13	2.13	0.48
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	1.94	0.48
1:A:1056:ARG:HD2	1:A:1062:TRP:HZ2	1.76	0.48
1:B:2072:ILE:CG2	1:B:2073:PRO:HD3	2.42	0.48
1:A:1164:ASP:H	1:A:1167:ARG:NE	2.11	0.48
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.95	0.48
1:A:1154:PRO:HB2	1:A:1158:ALA:HB2	1.94	0.48
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.96	0.48
1:B:1164:ASP:H	1:B:1167:ARG:NE	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2028:ILE:HB	1:B:2055:MET:HG3	1.94	0.48
1:B:887:LEU:HD22	1:B:900:LEU:HB3	1.96	0.48
1:B:881:LYS:HA	1:B:884:ASN:OD1	2.14	0.48
1:A:887:LEU:HD22	1:A:900:LEU:HB3	1.95	0.48
1:B:1424:THR:HA	1:B:1460:ASN:HB2	1.95	0.48
1:B:933:TYR:HD1	1:B:978:LYS:HG2	1.79	0.48
1:B:2143:ARG:NH1	1:B:2147:LYS:HE2	2.27	0.48
1:A:837:PRO:HB3	1:A:914:TYR:CD1	2.49	0.48
1:B:1127:TYR:HE2	1:B:1190:VAL:HG13	1.76	0.48
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.79	0.48
1:B:1479:ILE:HA	1:B:1488:GLN:O	2.14	0.48
1:B:1638:ILE:HD12	1:B:1640:SER:HB3	1.95	0.48
1:A:994:PRO:HB3	1:A:1037:LEU:HD22	1.96	0.48
1:A:1358:VAL:HA	1:A:1365:ASP:O	2.13	0.48
1:B:1462:MET:SD	1:B:1469:GLU:HB3	2.54	0.48
1:A:823:LYS:NZ	1:A:981:LEU:HD11	2.29	0.47
1:B:1333:GLU:O	1:B:1334:LEU:HB2	2.14	0.47
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.96	0.47
1:A:1091:ALA:HB2	1:A:1260:ARG:HG2	1.95	0.47
1:B:1307:TYR:CZ	1:B:1325:GLU:HG3	2.49	0.47
1:A:800:PHE:HB2	1:A:836:LEU:HD21	1.97	0.47
1:B:887:LEU:HD22	1:B:900:LEU:HD13	1.96	0.47
1:A:881:LYS:HA	1:A:884:ASN:OD1	2.13	0.47
1:A:933:TYR:HD1	1:A:978:LYS:HG2	1.79	0.47
1:B:1091:ALA:CB	1:B:1260:ARG:HG2	2.39	0.47
1:B:1481:ASN:HA	1:B:1486:VAL:HA	1.95	0.47
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	1.97	0.47
1:A:2177:LEU:HA	1:A:2180:ILE:HD12	1.96	0.47
1:A:880:LEU:HG	1:A:911:LEU:HD23	1.95	0.47
1:B:1054:GLN:HB3	1:B:1062:TRP:NE1	2.30	0.47
1:B:1162:GLU:HG3	1:B:1522:SER:OG	2.14	0.47
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.97	0.47
1:A:1096:TYR:C	1:A:1096:TYR:CD1	2.88	0.47
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.97	0.47
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.95	0.47
1:B:1477:VAL:HG23	1:B:1490:GLU:O	2.13	0.47
1:B:837:PRO:HB3	1:B:914:TYR:CD1	2.49	0.47
1:B:1928:ILE:HD11	1:B:2168:ARG:HG3	1.95	0.47
1:A:1621:TYR:OH	1:A:1851:PRO:HA	2.15	0.47
1:A:952:LEU:HD11	1:A:969:VAL:HG21	1.96	0.47
1:B:952:LEU:HD11	1:B:969:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:ILE:HD11	1:A:1191:ILE:HB	1.97	0.47
1:A:887:LEU:HD22	1:A:900:LEU:HD13	1.97	0.47
1:A:936:VAL:HG23	1:A:968:THR:CG2	2.44	0.47
1:B:1492:TYR:HA	1:B:1506:TYR:HA	1.97	0.47
1:A:1336:ARG:HB3	1:A:1525:TYR:CE2	2.49	0.47
1:B:1292:ARG:CZ	1:B:1326:PRO:HB3	2.45	0.47
1:B:1790:GLU:HA	1:B:1820:THR:HG21	1.96	0.47
1:B:895:THR:CB	1:B:900:LEU:HD12	2.43	0.47
1:B:1114:ASN:O	1:B:1133:PHE:HD1	1.98	0.46
1:B:885:LYS:O	1:B:889:ASP:HB3	2.15	0.46
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.96	0.46
1:B:1102:LEU:O	1:B:1106:VAL:HG23	2.15	0.46
1:B:1344:PRO:HA	1:B:1355:TYR:HA	1.96	0.46
1:A:1054:GLN:HB3	1:A:1062:TRP:NE1	2.30	0.46
1:A:996:VAL:HG22	1:A:1036:SER:N	2.31	0.46
1:A:1160:PRO:HG2	1:A:1494:GLU:OE2	2.16	0.46
1:A:945:LEU:HD11	1:A:954:LEU:HD13	1.97	0.46
1:B:948:GLU:O	1:B:951:ILE:HG22	2.16	0.46
1:A:2143:ARG:NH1	1:A:2147:LYS:HE2	2.30	0.46
1:A:885:LYS:O	1:A:889:ASP:HB3	2.15	0.46
1:A:955:ARG:HH22	1:A:968:THR:HG21	1.81	0.46
1:B:2070:GLY:O	1:B:2073:PRO:HD2	2.15	0.46
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.97	0.46
1:A:2241:ASN:HA	1:A:2244:LEU:HD12	1.96	0.46
1:B:1040:ARG:NH2	1:B:1084:ASP:HB3	2.30	0.46
1:B:1091:ALA:HB1	1:B:1260:ARG:HD3	1.98	0.46
1:B:1096:TYR:CD1	1:B:1096:TYR:C	2.89	0.46
1:A:2249:LYS:HA	1:A:2252:ILE:HD12	1.97	0.46
1:A:863:VAL:O	1:A:866:ARG:HG2	2.16	0.46
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.97	0.46
1:B:2057:ALA:HB3	1:B:2150:ILE:HD13	1.98	0.46
1:A:1125:ARG:HD2	1:A:1203:ALA:HB2	1.98	0.46
1:B:1621:TYR:OH	1:B:1851:PRO:HA	2.16	0.46
1:A:1915:ALA:HB2	1:A:1968:ASN:HB2	1.98	0.45
1:A:1935:VAL:HB	1:A:1993:ASN:HB3	1.98	0.45
1:B:1863:PRO:HB2	1:B:1867:PRO:HA	1.98	0.45
1:B:863:VAL:O	1:B:866:ARG:HG2	2.16	0.45
1:A:1631:ALA:HB2	1:A:1666:LEU:HB2	1.99	0.45
1:A:948:GLU:O	1:A:951:ILE:HG22	2.16	0.45
1:B:1125:ARG:CD	1:B:1203:ALA:HB2	2.41	0.45
1:B:1668:ALA:HB2	1:B:1769:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.98	0.45
1:B:836:LEU:HG	1:B:921:ARG:HH12	1.81	0.45
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.18	0.45
1:B:1884:VAL:HG21	1:B:1935:VAL:O	2.16	0.45
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.97	0.45
1:B:910:VAL:O	1:B:914:TYR:HD2	1.99	0.45
1:A:1131:TRP:CE3	1:A:1189:GLY:HA3	2.51	0.45
1:A:1293:LEU:O	1:A:1309:THR:HA	2.15	0.45
1:B:1354:VAL:HG22	1:B:1370:THR:HG23	1.99	0.45
1:A:1367:ARG:NH2	1:A:1528:LYS:HG3	2.29	0.45
1:A:2057:ALA:HB3	1:A:2150:ILE:HD13	1.99	0.45
1:A:2256:MET:HA	1:A:2259:LEU:HD12	1.98	0.45
1:B:1935:VAL:HB	1:B:1993:ASN:HB3	1.98	0.45
1:A:2070:GLY:O	1:A:2073:PRO:HD2	2.16	0.45
1:B:923:LEU:HD21	1:B:999:VAL:HG12	1.98	0.45
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.98	0.45
1:A:1790:GLU:HA	1:A:1820:THR:HG21	1.98	0.45
1:B:800:PHE:HB2	1:B:836:LEU:HD21	1.98	0.45
1:B:1480:THR:H	1:B:1488:GLN:HB3	1.82	0.45
1:B:1631:ALA:HB2	1:B:1666:LEU:HB2	1.99	0.45
1:B:1965:TRP:HB3	1:B:1997:PHE:CE2	2.52	0.45
1:B:955:ARG:HH22	1:B:968:THR:HG21	1.82	0.45
1:A:1516:MET:HG3	1:A:1519:LEU:HD22	1.98	0.45
1:A:1162:GLU:HG3	1:A:1522:SER:HB3	1.98	0.45
1:B:1080:TYR:HB2	1:B:1378:ARG:HG2	1.99	0.45
1:A:846:SER:HA	1:A:849:HIS:ND1	2.32	0.44
1:A:1161:VAL:HG22	1:A:1162:GLU:H	1.82	0.44
1:A:910:VAL:O	1:A:914:TYR:HD2	2.00	0.44
1:B:1630:VAL:HG12	1:B:1665:TYR:HD1	1.83	0.44
1:B:846:SER:HA	1:B:849:HIS:ND1	2.32	0.44
1:B:1094:ASP:HB3	1:B:1097:VAL:HG23	1.99	0.44
1:B:1108:ARG:O	1:B:1111:ARG:HG3	2.17	0.44
1:B:1640:SER:OG	1:B:1673:ARG:HG2	2.17	0.44
1:A:2072:ILE:CG2	1:A:2073:PRO:HD3	2.43	0.44
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.99	0.44
1:A:1161:VAL:HG22	1:A:1162:GLU:N	2.33	0.44
1:A:1191:ILE:HA	1:A:1256:ASN:O	2.18	0.44
1:A:836:LEU:HG	1:A:921:ARG:HH12	1.82	0.44
1:B:1477:VAL:HG22	1:B:1479:ILE:HD11	1.99	0.44
1:A:1908:VAL:HG23	1:A:1908:VAL:O	2.17	0.44
1:A:1096:TYR:O	1:A:1099:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ARG:O	1:A:1111:ARG:HG3	2.17	0.44
1:B:1194:CYS:SG	1:B:1203:ALA:CB	3.06	0.44
1:A:1676:LEU:HG	1:B:2138:HIS:CE1	2.53	0.44
1:A:1052:VAL:HG22	1:A:1096:TYR:CE1	2.53	0.44
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	2.00	0.44
1:B:1333:GLU:HB2	1:B:1371:ARG:NH1	2.33	0.44
1:A:1005:PRO:HA	1:A:1008:ARG:HG2	2.00	0.43
1:A:1195:LYS:HA	1:A:1260:ARG:CD	2.48	0.43
1:A:1965:TRP:HB3	1:A:1997:PHE:CE2	2.53	0.43
1:B:1416:HIS:HD2	1:B:1454:GLN:HG3	1.83	0.43
1:A:1390:ILE:HB	1:A:1439:PHE:HE2	1.83	0.43
1:A:1884:VAL:HG21	1:A:1935:VAL:O	2.17	0.43
1:A:951:ILE:O	1:A:955:ARG:HG3	2.18	0.43
1:B:1423:HIS:HE1	1:B:1425:PHE:HD1	1.66	0.43
1:B:2047:THR:HA	1:B:2050:PRO:HG3	2.00	0.43
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	2.01	0.43
1:A:2046:PRO:HA	1:A:2053:MET:SD	2.59	0.43
1:B:1915:ALA:HB2	1:B:1968:ASN:HB2	1.99	0.43
1:B:1324:ILE:CG2	1:B:1353:HIS:HE1	2.24	0.43
1:B:1369:PHE:CD2	1:B:1416:HIS:HB3	2.54	0.43
1:A:1668:ALA:HB2	1:A:1769:THR:HG23	2.00	0.43
1:B:1527:THR:O	1:B:1530:TRP:CD1	2.72	0.43
1:A:1741:GLY:CA	1:B:2065:VAL:HG23	2.47	0.43
1:A:1640:SER:OG	1:A:1673:ARG:HG2	2.18	0.43
1:B:1742:VAL:HA	1:B:1745:LEU:HD12	2.01	0.43
1:A:1094:ASP:HB3	1:A:1097:VAL:HG23	2.00	0.43
1:A:1371:ARG:HH22	1:A:1525:TYR:HE2	1.65	0.43
1:A:895:THR:CB	1:A:900:LEU:HD12	2.43	0.43
1:B:1005:PRO:HA	1:B:1008:ARG:HG2	2.00	0.43
1:A:1325:GLU:C	1:A:1327:SER:H	2.22	0.43
1:B:1737:GLU:HG2	1:B:1740:LEU:HD21	2.00	0.43
1:A:1170:SER:HB2	1:A:1173:ASP:HB2	2.01	0.43
1:B:1588:VAL:HG21	1:B:1600:ARG:NH1	2.34	0.43
1:A:1336:ARG:HB3	1:A:1525:TYR:CD2	2.54	0.43
1:A:1663:ARG:HH21	1:A:1765:CYS:H	1.66	0.43
1:A:883:PHE:HE2	1:A:911:LEU:HD21	1.83	0.43
1:B:969:VAL:HG12	1:B:973:LYS:HE3	2.01	0.43
1:A:1863:PRO:HB2	1:A:1867:PRO:HA	2.01	0.42
1:B:2077:LYS:H	1:B:2080:LYS:HD2	1.84	0.42
1:B:1052:VAL:HG22	1:B:1096:TYR:CE1	2.54	0.42
1:B:936:VAL:HG23	1:B:968:THR:CG2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:THR:HA	1:A:2050:PRO:HG3	2.00	0.42
1:A:2065:VAL:HG23	1:B:1741:GLY:CA	2.44	0.42
1:B:1106:VAL:HG11	1:B:1131:TRP:CD1	2.53	0.42
1:A:1776:GLY:O	1:A:1780:VAL:HG23	2.19	0.42
1:A:1781:ARG:NH1	1:A:1975:GLN:HE22	2.15	0.42
1:A:2134:PHE:HA	1:A:2137:LEU:HD12	2.02	0.42
1:B:1506:TYR:CE1	1:B:1517:HIS:HB2	2.54	0.42
1:A:2029:TYR:HA	1:A:2056:TYR:O	2.20	0.42
1:A:2032:PRO:O	1:A:2033:HIS:HB3	2.19	0.42
1:B:1461:CYS:O	1:B:1461:CYS:SG	2.78	0.42
1:B:1480:THR:O	1:B:1486:VAL:HG13	2.18	0.42
1:A:991:PRO:C	1:A:994:PRO:HD2	2.40	0.42
1:B:1096:TYR:O	1:B:1099:LEU:HB3	2.19	0.42
1:B:1106:VAL:HG23	1:B:1191:ILE:HD12	2.02	0.42
1:B:2032:PRO:O	1:B:2033:HIS:HB3	2.19	0.42
1:B:883:PHE:HE2	1:B:911:LEU:HD21	1.83	0.42
1:B:951:ILE:O	1:B:955:ARG:HG3	2.19	0.42
1:B:810:ILE:HG21	1:B:981:LEU:HD23	2.01	0.42
1:A:1389:LEU:HD11	1:A:1425:PHE:CB	2.50	0.42
1:A:791:VAL:HB	1:A:794:SER:HB3	2.01	0.42
1:B:837:PRO:HB3	1:B:914:TYR:CE1	2.55	0.42
1:B:994:PRO:HA	1:B:1037:LEU:H	1.83	0.42
1:A:1123:GLU:HB3	1:A:1124:GLU:H	1.73	0.42
1:A:1358:VAL:CG1	1:A:1363:GLU:HA	2.50	0.42
1:A:1717:THR:HB	1:A:1728:HIS:HB3	2.02	0.42
1:A:1742:VAL:HA	1:A:1745:LEU:HD12	2.01	0.42
1:B:1319:ASP:O	1:B:1344:PRO:HG2	2.20	0.42
1:A:852:MET:CB	1:A:853:PRO:HD2	2.42	0.41
1:A:1909:GLU:HG2	1:A:1910:THR:N	2.34	0.41
1:A:837:PRO:HB3	1:A:914:TYR:CE1	2.55	0.41
1:B:1390:ILE:HB	1:B:1439:PHE:HE2	1.84	0.41
1:B:1842:LYS:O	1:B:1845:GLN:HB3	2.20	0.41
1:B:2134:PHE:HA	1:B:2137:LEU:HD12	2.01	0.41
1:B:1099:LEU:O	1:B:1099:LEU:HD23	2.20	0.41
1:B:1776:GLY:O	1:B:1780:VAL:HG23	2.19	0.41
1:A:2116:MET:C	1:A:2118:GLN:H	2.24	0.41
1:A:1087:THR:CB	1:A:1298:GLY:HA3	2.50	0.41
1:B:1113:TYR:HA	1:B:1153:VAL:HG22	2.02	0.41
1:A:1087:THR:HB	1:A:1298:GLY:HA3	2.02	0.41
1:A:1535:ARG:HA	1:A:1545:TYR:HB2	2.03	0.41
1:A:2214:GLU:HG2	1:A:2222:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1784:GLN:HE22	1:B:1975:GLN:NE2	2.19	0.41
1:B:2046:PRO:HA	1:B:2053:MET:SD	2.60	0.41
1:B:1106:VAL:HG22	1:B:1191:ILE:CD1	2.43	0.41
1:B:1535:ARG:HA	1:B:1545:TYR:HB2	2.03	0.41
1:B:821:GLN:O	1:B:825:LYS:HG2	2.20	0.41
1:A:821:GLN:O	1:A:825:LYS:HG2	2.21	0.41
1:B:1659:MET:HB2	1:B:1661:ILE:HG12	2.03	0.41
1:A:1125:ARG:HD2	1:A:1203:ALA:HA	2.02	0.41
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.84	0.41
1:B:2256:MET:HE2	1:B:2256:MET:HB3	2.00	0.41
1:A:2138:HIS:CE1	1:B:1676:LEU:HG	2.57	0.40
1:B:1717:THR:HB	1:B:1728:HIS:HB3	2.02	0.40
1:B:2029:TYR:HA	1:B:2056:TYR:O	2.20	0.40
1:B:1858:LEU:HD12	1:B:2171:LEU:HD21	2.03	0.40
1:A:1208:LEU:HD23	1:A:1211:LEU:HD12	2.02	0.40
1:A:1588:VAL:HG21	1:A:1600:ARG:NH1	2.36	0.40
1:A:1842:LYS:O	1:A:1845:GLN:HB3	2.21	0.40
1:A:2019:LEU:HB3	1:A:2053:MET:CE	2.52	0.40
1:A:2109:SER:HA	1:A:2112:ILE:HD12	2.03	0.40
1:A:800:PHE:CB	1:A:836:LEU:HD21	2.51	0.40
1:B:1988:LEU:HD22	1:B:1990:ILE:CD1	2.50	0.40
1:B:791:VAL:HB	1:B:794:SER:HB3	2.02	0.40
1:A:1629:VAL:HG22	1:A:1664:ILE:HB	2.04	0.40
1:A:1737:GLU:HG2	1:A:1740:LEU:HD21	2.03	0.40
1:A:2184:ILE:HD12	1:A:2209:HIS:CE1	2.56	0.40
1:B:1056:ARG:HD2	1:B:1062:TRP:HZ2	1.78	0.40
1:B:1197:LEU:HD13	1:B:1273:LEU:HD23	2.03	0.40
1:B:1908:VAL:O	1:B:1908:VAL:HG23	2.20	0.40
1:B:2109:SER:HA	1:B:2112:ILE:HD12	2.02	0.40
1:B:2217:VAL:HG12	1:B:2219:ILE:H	1.87	0.40
1:A:1156:SER:HB2	1:A:1157:PRO:HD3	2.03	0.40
1:A:1294:THR:OG1	1:A:1326:PRO:HG3	2.21	0.40
1:A:930:LEU:HD13	1:A:985:LEU:HD23	2.03	0.40
1:B:1160:PRO:HA	1:B:1502:TRP:CD1	2.57	0.40
1:B:1898:GLN:HG2	1:B:1898:GLN:H	1.80	0.40
1:A:1794:ILE:HD12	1:A:1823:MET:HG3	2.04	0.40
1:B:921:ARG:HE	1:B:921:ARG:HB3	1.78	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	1378/1487 (93%)	1221 (89%)	121 (9%)	36 (3%)	7	45
1	B	1380/1487 (93%)	1221 (88%)	130 (9%)	29 (2%)	9	50
All	All	2758/2974 (93%)	2442 (88%)	251 (9%)	65 (2%)	7	47

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	VAL
1	A	943	ARG
1	A	1092	HIS
1	A	1117	GLU
1	A	1128	PHE
1	A	1156	SER
1	A	1487	ILE
1	A	1784	GLN
1	A	1864	SER
1	B	819	VAL
1	B	943	ARG
1	B	1128	PHE
1	B	1156	SER
1	B	1864	SER
1	A	853	PRO
1	A	1486	VAL
1	A	2038	GLY
1	A	2201	ALA
1	A	2225	ASN
1	B	853	PRO
1	B	997	GLY
1	B	1486	VAL
1	B	2038	GLY
1	B	2201	ALA
1	B	2225	ASN

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Mol	Chain	Res	Type
1	A	892	PRO
1	A	997	GLY
1	A	1158	ALA
1	A	1572	ALA
1	B	892	PRO
1	B	1092	HIS
1	B	1155	SER
1	B	1180	ARG
1	A	887	LEU
1	A	1116	ARG
1	A	1155	SER
1	A	1180	ARG
1	A	1333	GLU
1	A	1516	MET
1	A	1570	SER
1	A	1638	ILE
1	B	887	LEU
1	B	1570	SER
1	B	1572	ALA
1	B	1638	ILE
1	B	1784	GLN
1	B	1790	GLU
1	A	1313	PRO
1	A	1498	GLU
1	A	1508	SER
1	A	1512	LYS
1	A	1527	THR
1	A	1576	PRO
1	A	1790	GLU
1	B	1158	ALA
1	B	1313	PRO
1	B	1487	ILE
1	B	1576	PRO
1	B	1516	MET
1	A	1052	VAL
1	B	1052	VAL
1	A	926	ILE
1	B	926	ILE
1	B	996	VAL
1	A	996	VAL

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	1213/1282 (95%)	1116 (92%)	97 (8%)	15	50
1	B	1215/1282 (95%)	1119 (92%)	96 (8%)	15	51
All	All	2428/2564 (95%)	2235 (92%)	193 (8%)	15	51

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	799	ARG
1	A	818	VAL
1	A	824	LEU
1	A	836	LEU
1	A	848	LEU
1	A	880	LEU
1	A	883	PHE
1	A	884	ASN
1	A	911	LEU
1	A	912	ASN
1	A	915	LEU
1	A	916	ASP
1	A	921	ARG
1	A	924	ASN
1	A	951	ILE
1	A	954	LEU
1	A	962	ILE
1	A	970	LEU
1	A	983	LEU
1	A	992	ASN
1	A	995	ASN
1	A	1003	LEU
1	A	1007	LEU
1	A	1012	GLU
1	A	1013	LEU
1	A	1021	VAL
1	A	1041	THR

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Mol	Chain	Res	Type
1	A	1044	MET
1	A	1062	TRP
1	A	1090	PHE
1	A	1096	TYR
1	A	1116	ARG
1	A	1124	GLU
1	A	1127	TYR
1	A	1129	ILE
1	A	1131	TRP
1	A	1172	SER
1	A	1174	MET
1	A	1177	LEU
1	A	1199	ASP
1	A	1324	ILE
1	A	1328	LEU
1	A	1342	LEU
1	A	1402	ASP
1	A	1448	TRP
1	A	1463	ARG
1	A	1470	ASN
1	A	1471	ASP
1	A	1473	MET
1	A	1475	LEU
1	A	1483	SER
1	A	1531	LEU
1	A	1557	ILE
1	A	1563	GLU
1	A	1570	SER
1	A	1571	LEU
1	A	1574	LYS
1	A	1593	ASP
1	A	1599	SER
1	A	1604	MET
1	A	1632	ASN
1	A	1638	ILE
1	A	1652	CYS
1	A	1659	MET
1	A	1663	ARG
1	A	1674	LEU
1	A	1715	VAL
1	A	1729	LYS
1	A	1759	TYR

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Mol	Chain	Res	Type
1	A	1760	ASN
1	A	1771	ARG
1	A	1815	LEU
1	A	1817	LEU
1	A	1885	ARG
1	A	1901	LEU
1	A	1917	THR
1	A	1941	GLU
1	A	1942	ASN
1	A	1958	THR
1	A	1965	TRP
1	A	1971	PHE
1	A	1988	LEU
1	A	2007	GLU
1	A	2022	PHE
1	A	2023	GLU
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	2168	ARG
1	A	2171	LEU
1	A	2175	ASP
1	A	2181	GLU
1	A	2197	THR
1	A	2240	ILE
1	B	799	ARG
1	B	818	VAL
1	B	824	LEU
1	B	836	LEU
1	B	848	LEU
1	B	880	LEU
1	B	883	PHE
1	B	884	ASN
1	B	911	LEU
1	B	912	ASN
1	B	915	LEU
1	B	916	ASP
1	B	921	ARG
1	B	924	ASN

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Mol	Chain	Res	Type
1	B	951	ILE
1	B	954	LEU
1	B	970	LEU
1	B	983	LEU
1	B	992	ASN
1	B	995	ASN
1	B	1003	LEU
1	B	1007	LEU
1	B	1012	GLU
1	B	1013	LEU
1	B	1021	VAL
1	B	1041	THR
1	B	1044	MET
1	B	1062	TRP
1	B	1090	PHE
1	B	1096	TYR
1	B	1115	LEU
1	B	1118	VAL
1	B	1124	GLU
1	B	1127	TYR
1	B	1130	ASP
1	B	1171	ILE
1	B	1172	SER
1	B	1174	MET
1	B	1177	LEU
1	B	1332	LEU
1	B	1333	GLU
1	B	1379	LEU
1	B	1402	ASP
1	B	1422	SER
1	B	1448	TRP
1	B	1469	GLU
1	B	1483	SER
1	B	1485	PHE
1	B	1496	LEU
1	B	1557	ILE
1	B	1563	GLU
1	B	1570	SER
1	B	1571	LEU
1	B	1574	LYS
1	B	1593	ASP
1	B	1599	SER

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Mol	Chain	Res	Type
1	B	1604	MET
1	B	1630	VAL
1	B	1638	ILE
1	B	1652	CYS
1	B	1659	MET
1	B	1674	LEU
1	B	1715	VAL
1	B	1729	LYS
1	B	1759	TYR
1	B	1760	ASN
1	B	1771	ARG
1	B	1815	LEU
1	B	1817	LEU
1	B	1885	ARG
1	B	1901	LEU
1	B	1909	GLU
1	B	1917	THR
1	B	1941	GLU
1	B	1942	ASN
1	B	1958	THR
1	B	1965	TRP
1	B	1971	PHE
1	B	1975	GLN
1	B	1988	LEU
1	B	2007	GLU
1	B	2022	PHE
1	B	2023	GLU
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	2168	ARG
1	B	2171	LEU
1	B	2175	ASP
1	B	2197	THR
1	B	2256	MET
1	B	2260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	995	ASN
1	B	1043	GLN
1	B	1460	ASN

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 carbohydrates 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	9.73

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1392/1487 (93%)	0.15	102 (7%)	18 21	33, 251, 497, 500	0
1	B	1394/1487 (93%)	0.09	89 (6%)	23 24	13, 262, 498, 500	0
All	All	2786/2974 (93%)	0.12	191 (6%)	20 22	13, 258, 497, 500	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1353	HIS	10.5
1	A	1347	THR	8.4
1	A	1301	ASP	8.3
1	B	1103	GLU	7.9
1	A	959	LYS	7.8
1	A	1352	ILE	7.8
1	A	960	ASP	7.3
1	A	1372	ALA	7.3
1	B	985	LEU	7.2
1	A	1371	ARG	7.1
1	A	1345	VAL	7.1
1	A	1354	VAL	6.3
1	B	1191	ILE	5.5
1	B	959	LYS	5.4
1	A	958	TYR	5.4
1	B	857	ASP	5.3
1	B	2213	LEU	5.3
1	B	960	ASP	5.1
1	B	854	HIS	5.1
1	A	957	GLN	4.9
1	B	1129	ILE	4.9
1	A	1675	GLY	4.9
1	A	1300	ASN	4.8
1	B	1067	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1370	THR	4.6
1	B	1386	ALA	4.5
1	B	825	LYS	4.4
1	A	1257	VAL	4.4
1	B	1102	LEU	4.3
1	A	789	PRO	4.1
1	B	930	LEU	4.0
1	A	1351	ASN	4.0
1	B	824	LEU	4.0
1	A	1355	TYR	3.9
1	B	904	LEU	3.8
1	A	788	SER	3.8
1	B	1055	SER	3.8
1	B	1059	GLU	3.8
1	A	1404	LEU	3.8
1	B	1101	ALA	3.8
1	B	1054	GLN	3.7
1	A	1332	LEU	3.7
1	B	2198	SER	3.7
1	B	887	LEU	3.7
1	B	1066	ARG	3.7
1	A	1407	ILE	3.6
1	A	1295	PHE	3.6
1	A	1789	VAL	3.6
1	A	1054	GLN	3.6
1	B	883	PHE	3.6
1	B	1100	ALA	3.5
1	A	1676	LEU	3.5
1	A	1211	LEU	3.5
1	A	1290	VAL	3.5
1	A	1062	TRP	3.5
1	B	1387	GLU	3.5
1	B	888	ASP	3.5
1	B	1189	GLY	3.4
1	B	1056	ARG	3.4
1	A	2187	ALA	3.4
1	B	856	LEU	3.4
1	B	855	LYS	3.4
1	B	988	GLU	3.4
1	A	1350	LYS	3.4
1	B	853	PRO	3.4
1	B	1058	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1212	PRO	3.4
1	A	2196	ASN	3.3
1	A	790	VAL	3.3
1	A	1788	GLN	3.3
1	B	858	ALA	3.3
1	B	1256	ASN	3.3
1	A	1334	LEU	3.3
1	B	989	TYR	3.2
1	A	1400	ILE	3.2
1	B	986	LEU	3.1
1	B	1062	TRP	3.1
1	B	1118	VAL	3.1
1	B	1169	HIS	3.1
1	A	1256	ASN	3.1
1	A	1191	ILE	3.1
1	B	1060	THR	3.1
1	A	1373	VAL	3.0
1	B	1190	VAL	3.0
1	A	1376	PRO	3.0
1	A	1059	GLU	3.0
1	A	1677	ALA	3.0
1	A	903	THR	3.0
1	B	2212	GLN	3.0
1	A	1735	GLY	2.9
1	A	1403	ALA	2.9
1	A	1679	GLU	2.9
1	B	2018	ALA	2.9
1	B	1106	VAL	2.9
1	B	822	GLN	2.9
1	A	2213	LEU	2.8
1	A	1589	LEU	2.8
1	A	1105	TYR	2.8
1	B	1064	HIS	2.8
1	A	1836	ASP	2.8
1	A	963	GLN	2.8
1	A	1061	GLY	2.8
1	A	2020	THR	2.8
1	B	2209	HIS	2.8
1	B	1105	TYR	2.8
1	B	1433	ALA	2.7
1	B	849	HIS	2.7
1	A	1378	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	962	ILE	2.7
1	B	1099	LEU	2.7
1	A	1296	ILE	2.7
1	A	1374	VAL	2.7
1	B	893	ASN	2.7
1	A	1101	ALA	2.6
1	A	1736	ALA	2.6
1	A	1833	ALA	2.6
1	B	1981	ASN	2.6
1	A	961	ASN	2.6
1	A	1419	ILE	2.6
1	B	1061	GLY	2.6
1	B	2196	ASN	2.6
1	B	2216	TRP	2.6
1	A	1104	VAL	2.6
1	B	884	ASN	2.5
1	B	1483	SER	2.5
1	B	1120	TYR	2.5
1	A	1420	ASN	2.5
1	B	903	THR	2.5
1	B	1979	ASP	2.5
1	B	2020	THR	2.5
1	B	2197	THR	2.5
1	A	1055	SER	2.5
1	A	956	ASP	2.5
1	A	1418	PHE	2.5
1	A	1086	LEU	2.5
1	A	2018	ALA	2.4
1	B	2210	LEU	2.4
1	A	792	VAL	2.4
1	B	2201	ALA	2.4
1	A	1595	LEU	2.4
1	A	1349	ASN	2.4
1	A	1289	ARG	2.4
1	A	904	LEU	2.4
1	A	2197	THR	2.4
1	A	1484	GLY	2.4
1	B	1255	VAL	2.4
1	B	943	ARG	2.4
1	B	901	LYS	2.3
1	A	1046	HIS	2.3
1	B	821	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2199	LEU	2.3
1	A	1835	ASP	2.3
1	B	1130	ASP	2.3
1	A	1258	ALA	2.3
1	B	1155	SER	2.3
1	B	1300	ASN	2.3
1	B	1921	GLY	2.3
1	B	2176	ILE	2.2
1	A	1263	GLU	2.2
1	A	1255	VAL	2.2
1	A	1264	GLY	2.2
1	A	1322	ARG	2.2
1	A	2064	GLY	2.2
1	B	861	THR	2.2
1	B	1104	VAL	2.2
1	A	1987	PRO	2.2
1	B	1787	VAL	2.2
1	A	1379	LEU	2.1
1	B	1484	GLY	2.1
1	B	828	ILE	2.1
1	A	1397	VAL	2.1
1	A	1050	SER	2.1
1	A	1056	ARG	2.1
1	A	1320	SER	2.1
1	A	2025	PRO	2.1
1	B	819	VAL	2.1
1	A	1197	LEU	2.1
1	B	1044	MET	2.1
1	A	1169	HIS	2.1
1	B	1742	VAL	2.1
1	A	907	LEU	2.1
1	A	1337	LEU	2.1
1	B	1761	ASP	2.1
1	B	1760	ASN	2.1
1	A	2210	LEU	2.1
1	A	1396	VAL	2.1
1	A	1038	GLU	2.0
1	B	1923	ALA	2.0
1	A	1544	GLN	2.0
1	A	1737	GLU	2.0
1	B	1930	MET	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 carbohydrates 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.