



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID : 1OD4
Title : ACETYL-COA CARBOXYLASE CARBOXYLTRANSFERASE DOMAIN
Authors : Zhang, H.; Yang, Z.; Shen, Y.; Tong, L.
Deposited on : 2003-02-12
Resolution : 2.70 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

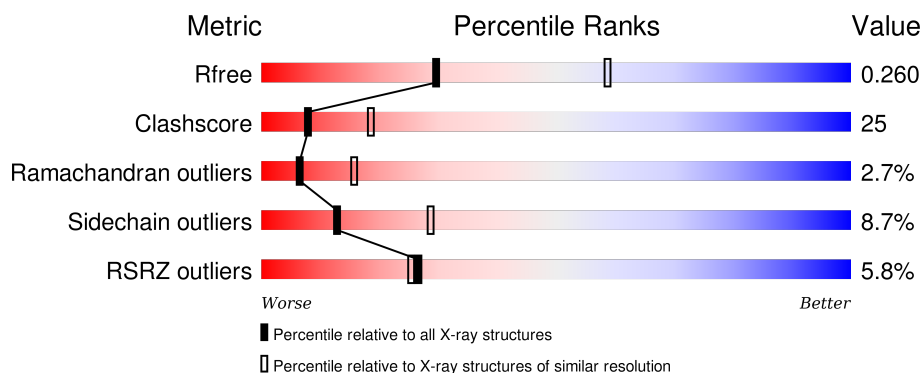
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	805	<div> <div>4%</div> <div>49% 31% 5% 15%</div> </div>
1	B	805	<div> <div>6%</div> <div>46% 34% 5% 15%</div> </div>
1	C	805	<div> <div>4%</div> <div>47% 30% 5% 17%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADE	C	3196	-	-	-	X

2 Entry composition [i](#)

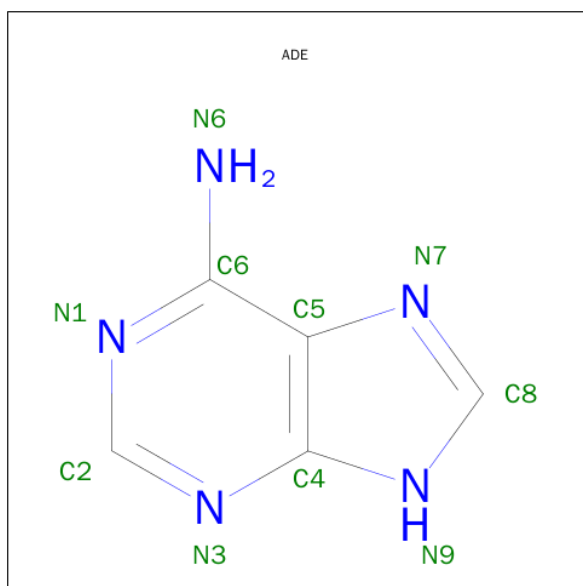
There are 3 unique types of molecules in this entry. The entry contains 16461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-COENZYME A CARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	Se	0	0	1
			5444	3471	936	1018	2	17			
1	B	684	Total	C	N	O	S	Se	0	0	1
			5444	3471	936	1018	2	17			
1	C	672	Total	C	N	O	S	Se	0	0	1
			5347	3406	920	1002	2	17			

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: C₅H₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			10	5	5		

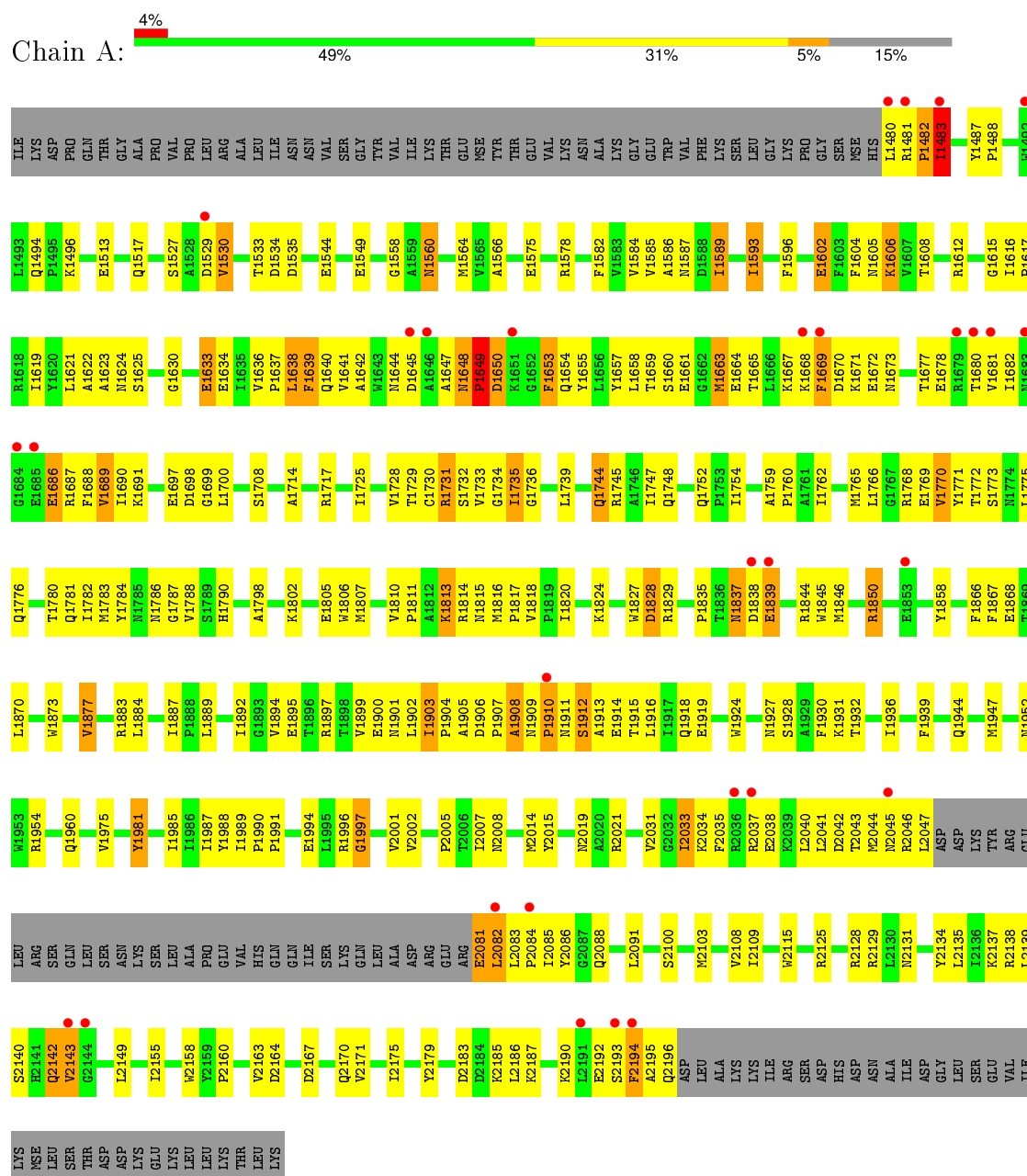
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total 86	O 86	0	0
3	B	70	Total 70	O 70	0	0
3	C	60	Total 60	O 60	0	0

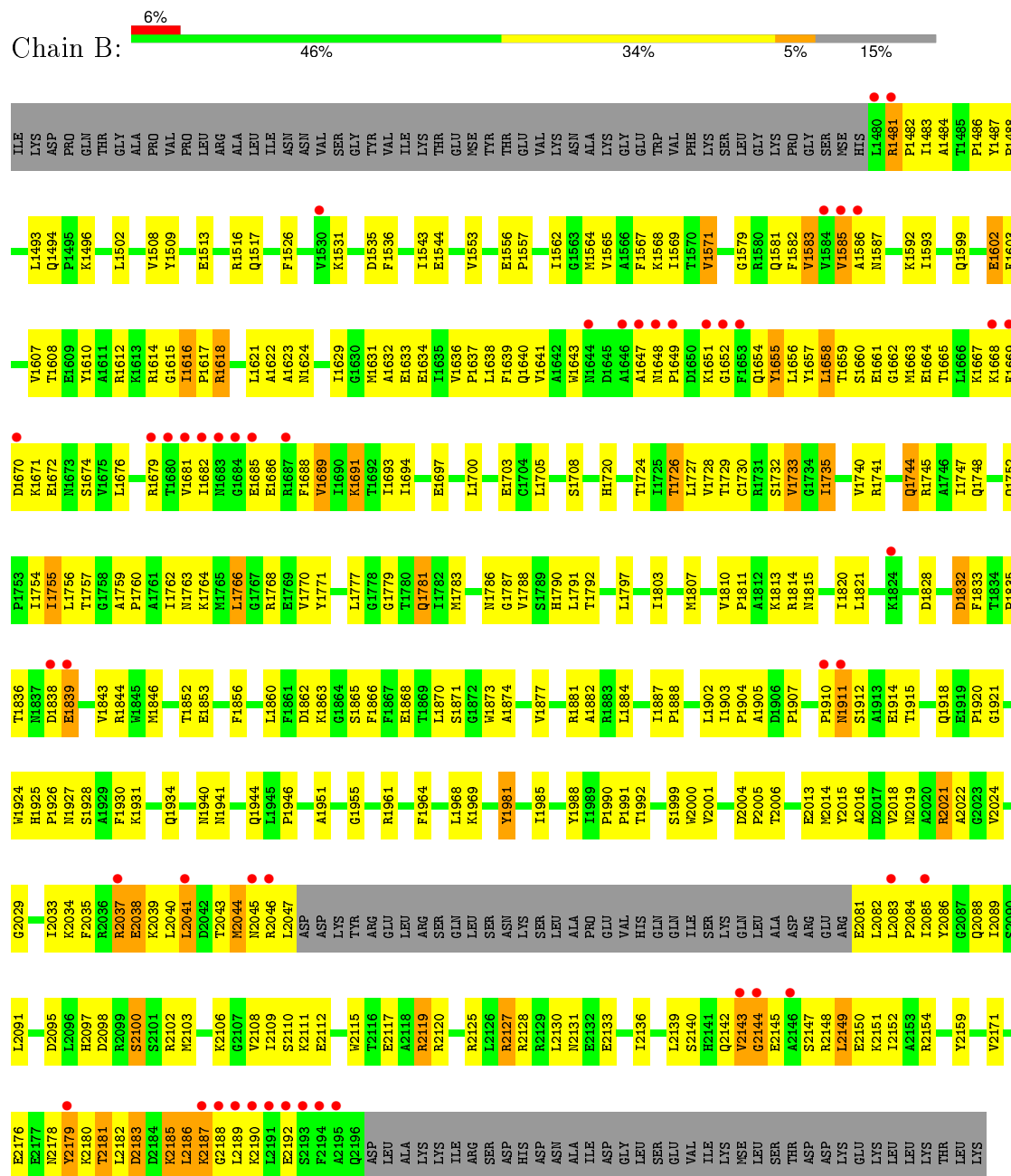
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

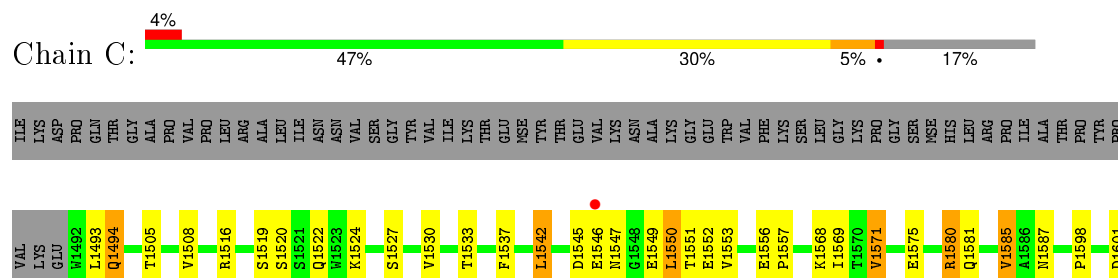
• Molecule 1: ACETYL-COENZYME A CARBOXYLASE



- Molecule 1: ACETYL-COENZYME A CARBOXYLASE



- Molecule 1: ACETYL-COENZYME A CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.91Å 123.91Å 145.07Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 28.94 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.70) 94.1 (28.94-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.262 0.225 , 0.260	Depositor DCC
R_{free} test set	11315 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 113445 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16461	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/5549	0.68	1/7491 (0.0%)
1	B	0.46	0/5549	0.68	1/7491 (0.0%)
1	C	0.45	0/5448	0.67	2/7351 (0.0%)
All	All	0.45	0/16546	0.68	4/22333 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1912	SER	N-CA-C	-6.10	94.53	111.00
1	C	1644	ASN	N-CA-C	-5.58	95.95	111.00
1	C	1656	LEU	N-CA-C	-5.33	96.59	111.00
1	B	1912	SER	N-CA-C	-5.02	97.44	111.00

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	5444	0	5388	269	1
1	B	5444	0	5388	292	0
1	C	5347	0	5283	280	0
2	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	86	0	0	4	0
3	B	70	0	0	4	0
3	C	60	0	0	4	0
All	All	16461	0	16063	804	1

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 25.

All (804) 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:1735:ILE:H	1:B:1735:ILE:HD13	1.06	1.21
1:B:1631:MSE:HE2	1:C:2034:LYS:HB3	1.35	1.09
1:C:2014:MSE:HE3	1:C:2109:ILE:HG22	1.36	1.08
1:A:1658:LEU:HD12	1:A:1663:MSE:HE1	1.40	1.03
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.42	0.99
1:A:1936:ILE:HG12	1:A:1947:MSE:HE1	1.45	0.98
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.12	0.96
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.50	0.90
1:B:2086:TYR:HA	1:B:2089:ILE:HD13	1.52	0.89
1:A:1658:LEU:HD12	1:A:1663:MSE:CE	2.05	0.87
1:C:2142:GLN:HB2	1:C:2190:LYS:NZ	1.92	0.85
1:A:1641:VAL:HG12	1:A:1642:ALA:H	1.42	0.84
1:B:2186:LEU:HD23	1:B:2190:LYS:HE2	1.57	0.84
1:C:2189:LEU:O	1:C:2192:GLU:HG3	1.77	0.84
1:C:1852:THR:HB	1:C:1855:GLY:O	1.76	0.83
1:B:1735:ILE:N	1:B:1735:ILE:HD13	1.90	0.81
1:A:1903:ILE:HB	1:A:1915:THR:HG23	1.63	0.81
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.61	0.81
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.63	0.80
1:A:1593:ILE:HG22	1:A:1625:SER:OG	1.82	0.80
1:A:1798:ALA:O	1:A:1802:LYS:HD3	1.82	0.80
1:A:1813:LYS:HG3	1:A:1816:MSE:HG3	1.63	0.79
1:A:1939:PHE:CD1	1:A:1947:MSE:HE3	2.17	0.79
1:B:2178:ASN:HD22	1:B:2181:THR:HG21	1.48	0.79
1:B:1483:ILE:HD12	1:B:1483:ILE:H	1.48	0.79
1:B:1735:ILE:H	1:B:1735:ILE:CD1	1.91	0.79
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.64	0.79
1:A:1630:GLY:HA3	1:A:1700:LEU:HD22	1.66	0.78
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.31	0.78
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2147:SER:OG	1:B:2150:GLU:HG3	1.84	0.77
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.30	0.77
1:C:1665:THR:O	1:C:1668:LYS:HB3	1.85	0.77
1:B:2022:ALA:HB3	1:B:2103:MSE:HE2	1.65	0.77
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.50	0.77
1:A:1663:MSE:O	1:A:1667:LYS:HG2	1.85	0.76
1:B:2041:LEU:HA	1:B:2044:MSE:HE2	1.68	0.76
1:C:1805:GLU:O	1:C:1808:SER:HB3	1.86	0.76
1:A:2139:LEU:O	1:A:2142:GLN:HB2	1.84	0.76
1:C:1657:TYR:HA	1:C:1690:ILE:HG12	1.67	0.76
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.33	0.76
1:C:1647:ALA:O	1:C:1649:PRO:HD3	1.85	0.76
1:A:1708:SER:HB2	1:A:1735:ILE:HG12	1.67	0.75
1:B:2154:ARG:NH2	1:B:2189:LEU:HD13	2.00	0.75
1:B:2038:GLU:HA	1:B:2041:LEU:HB2	1.67	0.75
1:A:1560:ASN:HD22	1:A:1560:ASN:N	1.84	0.75
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.67	0.75
1:C:2039:LYS:O	1:C:2043:THR:HG22	1.87	0.75
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	1.67	0.74
1:B:2001:VAL:HG21	1:C:1735:ILE:HG23	1.69	0.74
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.34	0.74
1:C:1642:ALA:H	1:C:1657:TYR:HE1	1.35	0.73
1:B:1757:THR:HG22	1:B:1762:ILE:HG13	1.68	0.73
1:C:2046:ARG:HG3	1:C:2047:LEU:HD22	1.69	0.73
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.71	0.73
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.87	0.72
1:A:1644:ASN:ND2	1:A:1654:GLN:HG2	2.04	0.72
1:B:1768:ARG:HH11	1:B:1768:ARG:HG3	1.53	0.72
1:B:1638:LEU:O	1:B:1638:LEU:HD12	1.89	0.72
1:B:2046:ARG:C	1:B:2047:LEU:HD22	2.09	0.72
1:C:2142:GLN:HB2	1:C:2190:LYS:HZ1	1.51	0.72
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.36	0.71
1:A:1644:ASN:HD21	1:A:1654:GLN:HG2	1.54	0.71
1:A:1782:ILE:O	1:A:1786:ASN:HB2	1.90	0.71
1:A:1606:LYS:HE2	1:A:1606:LYS:HA	1.71	0.71
1:B:1779:GLY:HA3	1:B:1781:GLN:HE22	1.55	0.71
1:A:1939:PHE:HD1	1:A:1947:MSE:HE3	1.52	0.71
1:A:1813:LYS:HG3	1:A:1816:MSE:CG	2.20	0.71
1:C:1645:ASP:OD2	1:C:1648:ASN:HB2	1.90	0.71
1:C:1527:SER:O	1:C:1530:VAL:HG22	1.91	0.71
1:B:1667:LYS:HE3	1:B:1672:GLU:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1681:VAL:HA	1:C:1686:GLU:HA	1.72	0.70
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.26	0.70
1:A:1630:GLY:HA3	1:A:1700:LEU:CD2	2.20	0.69
1:A:2037:ARG:HB3	1:A:2037:ARG:NH1	2.07	0.69
1:C:2145:GLU:HA	1:C:2145:GLU:OE1	1.92	0.69
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.41	0.69
1:A:1533:THR:HG22	1:A:1535:ASP:H	1.56	0.69
1:B:1755:ILE:HD13	1:B:1755:ILE:H	1.56	0.69
1:B:1671:LYS:HB3	1:B:1674:SER:OG	1.93	0.69
1:B:2004:ASP:OD2	1:B:2006:THR:HG22	1.93	0.69
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.88	0.68
1:A:1645:ASP:OD2	1:A:1648:ASN:HB2	1.93	0.68
1:A:1657:TYR:CZ	1:A:1687:ARG:HD2	2.27	0.68
1:B:2085:ILE:HG21	1:C:1650:ASP:HA	1.75	0.68
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.92	0.68
1:A:1494:GLN:OE1	1:A:1496:LYS:HG2	1.93	0.68
1:A:1593:ILE:O	1:A:1593:ILE:HG22	1.92	0.68
1:B:2046:ARG:O	1:B:2047:LEU:HD13	1.93	0.68
1:B:1881:ARG:HH11	1:B:1881:ARG:HG2	1.59	0.68
1:A:1660:SER:O	1:A:1664:GLU:HG2	1.94	0.68
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.92	0.68
1:B:2148:ARG:O	1:B:2152:ILE:HG13	1.94	0.67
1:A:1681:VAL:HA	1:A:1686:GLU:HA	1.77	0.67
1:B:1838:ASP:O	1:B:1839:GLU:HG3	1.95	0.67
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.76	0.67
1:B:1488:PRO:HB3	1:B:1493:LEU:HD11	1.77	0.67
1:B:1728:VAL:HG21	1:B:1754:ILE:HD11	1.75	0.67
1:A:2149:LEU:C	1:A:2149:LEU:HD23	2.15	0.67
1:A:2085:ILE:HG23	1:A:2086:TYR:N	2.09	0.66
1:A:2134:TYR:O	1:A:2138:ARG:HG2	1.95	0.66
1:B:1661:GLU:O	1:B:1664:GLU:HB2	1.95	0.66
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.42	0.66
1:A:2164:ASP:H	1:A:2170:GLN:NE2	1.94	0.65
1:C:2046:ARG:O	1:C:2047:LEU:HD13	1.96	0.65
1:C:1852:THR:HG22	1:C:1854:SER:H	1.61	0.65
1:B:1762:ILE:HD12	1:B:1777:LEU:HD21	1.77	0.65
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.78	0.65
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.11	0.65
1:C:2181:THR:O	1:C:2184:ASP:HB2	1.96	0.65
1:C:1737:ALA:O	1:C:1740:VAL:HG22	1.96	0.65
1:C:1797:LEU:O	1:C:1801:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1545:ASP:OD2	1:C:1549:GLU:HB3	1.96	0.65
1:A:1892:ILE:CD1	1:A:1947:MSE:HE2	2.26	0.65
1:A:1748:GLN:HE22	1:A:1783:MSE:HB2	1.62	0.65
1:C:2044:MSE:HA	1:C:2086:TYR:CE2	2.32	0.65
1:A:1593:ILE:HG22	1:A:1625:SER:HG	1.63	0.64
1:A:1673:ASN:N	1:A:1673:ASN:HD22	1.95	0.64
1:A:1975:VAL:HG23	1:A:2002:VAL:HG23	1.80	0.64
1:B:1654:GLN:O	1:B:1655:TYR:HB3	1.98	0.64
1:B:2178:ASN:HB3	1:B:2181:THR:HG23	1.79	0.64
1:A:1936:ILE:CG1	1:A:1947:MSE:HE1	2.24	0.63
1:C:1654:GLN:O	1:C:1655:TYR:HB2	1.96	0.63
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.81	0.63
1:A:1762:ILE:HA	1:A:1765:MSE:HE2	1.81	0.63
1:C:2142:GLN:NE2	1:C:2190:LYS:HE2	2.14	0.63
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.96	0.62
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.12	0.62
1:C:1641:VAL:O	1:C:1642:ALA:C	2.38	0.62
1:B:1964:PHE:O	1:C:1786:ASN:ND2	2.32	0.62
1:A:1728:VAL:HG21	1:A:1754:ILE:HD11	1.80	0.62
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.15	0.62
1:C:1846:MSE:HE1	1:C:1990:PRO:HB2	1.81	0.62
1:C:1762:ILE:HG21	1:C:1771:TYR:HE1	1.64	0.62
1:A:1639:PHE:HA	1:A:1658:LEU:CD2	2.30	0.62
1:B:2038:GLU:CA	1:B:2041:LEU:HB2	2.29	0.61
1:A:1634:GLU:OE2	1:A:1634:GLU:N	2.30	0.61
1:C:1520:SER:O	1:C:1524:LYS:HG2	1.99	0.61
1:A:2044:MSE:HE2	1:A:2082:LEU:HB2	1.81	0.61
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.47	0.61
1:B:1846:MSE:HE1	1:B:1990:PRO:HB2	1.82	0.61
1:C:1736:GLY:O	1:C:1740:VAL:HG13	2.01	0.61
1:A:1900:GLU:OE1	1:A:1916:LEU:HD21	2.01	0.61
1:C:1783:MSE:HA	1:C:1786:ASN:HB2	1.82	0.61
1:C:1655:TYR:CE2	1:C:1689:VAL:HG22	2.36	0.61
1:B:2180:LYS:HA	1:B:2183:ASP:OD1	2.01	0.61
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.15	0.61
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.83	0.60
1:C:2145:GLU:HG3	1:C:2151:LYS:HZ1	1.66	0.60
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.46	0.60
1:A:2167:ASP:O	1:A:2171:VAL:HG23	2.00	0.60
1:B:2081:GLU:HG2	1:B:2082:LEU:H	1.66	0.60
1:C:2001:VAL:HG23	1:C:2002:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1745:ARG:NH2	3:A:5036:HOH:O	2.31	0.60
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.83	0.60
1:B:1881:ARG:NH1	1:B:1881:ARG:HG2	2.16	0.60
1:A:1680:THR:O	1:A:1680:THR:HG22	2.00	0.60
1:B:1755:ILE:HD13	1:B:1755:ILE:N	2.17	0.59
1:B:1691:LYS:HA	1:B:1691:LYS:HE2	1.84	0.59
1:C:1642:ALA:HB2	1:C:1657:TYR:CE1	2.37	0.59
1:A:1838:ASP:O	1:A:1839:GLU:HB2	2.02	0.59
1:C:2036:ARG:HG3	1:C:2036:ARG:HH11	1.66	0.59
1:C:1644:ASN:HD21	1:C:1654:GLN:NE2	2.00	0.59
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.16	0.59
1:B:2041:LEU:HD22	1:B:2044:MSE:CE	2.32	0.59
1:B:1733:VAL:HG13	1:B:1755:ILE:HG12	1.83	0.59
1:B:1768:ARG:HH11	1:B:1768:ARG:CG	2.16	0.59
1:B:1756:LEU:HD23	1:C:1963:MSE:SE	2.53	0.59
1:C:1782:ILE:O	1:C:1786:ASN:HB2	2.03	0.59
1:C:1606:LYS:HD3	3:C:5004:HOH:O	2.03	0.59
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.32	0.59
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.02	0.59
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.01	0.59
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.03	0.59
1:B:1786:ASN:HB3	1:B:1788:VAL:HG23	1.85	0.59
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.20	0.59
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.05	0.59
1:B:2106:LYS:HA	1:B:2106:LYS:HE2	1.84	0.59
1:A:1708:SER:HB2	1:A:1735:ILE:CG1	2.33	0.58
1:C:1954:ARG:O	1:C:1996:ARG:HB2	2.03	0.58
1:C:1808:SER:OG	1:C:1883:ARG:NH2	2.36	0.58
1:B:1655:TYR:HE1	1:B:1657:TYR:HB3	1.67	0.58
1:B:1860:LEU:O	1:B:2119:ARG:HG3	2.04	0.58
1:B:1856:PHE:CZ	1:B:1863:LYS:HG3	2.38	0.58
1:C:1960:GLN:HG3	1:C:1961:ARG:N	2.17	0.58
1:C:2038:GLU:O	1:C:2041:LEU:N	2.36	0.58
1:B:1582:PHE:CD2	1:B:1807:MSE:HE1	2.39	0.58
1:A:1564:MSE:HE3	1:A:1604:PHE:HB2	1.86	0.58
1:C:1909:ASN:HD22	1:C:1909:ASN:C	2.06	0.58
1:B:2186:LEU:O	1:B:2188:GLY:N	2.36	0.58
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.85	0.58
1:A:2005:PRO:CG	1:A:2014:MSE:HB2	2.34	0.57
1:A:2005:PRO:HG3	1:A:2014:MSE:HB2	1.85	0.57
1:B:1724:THR:H	1:B:1745:ARG:HH21	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.34	0.57
1:C:2083:LEU:HB2	1:C:2084:PRO:HD3	1.86	0.57
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.52	0.57
1:A:2044:MSE:CE	1:A:2082:LEU:HB2	2.35	0.57
1:B:2046:ARG:O	1:B:2047:LEU:HD22	2.05	0.57
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.03	0.57
1:C:1728:VAL:HG21	1:C:1754:ILE:HD11	1.87	0.57
1:C:1505:THR:HB	1:C:1729:THR:O	2.05	0.57
1:C:2148:ARG:CZ	1:C:2152:ILE:HD11	2.35	0.57
1:C:1903:ILE:HD12	1:C:1903:ILE:N	2.20	0.57
1:B:1708:SER:HB3	1:C:2001:VAL:HG12	1.86	0.57
1:B:2043:THR:HG22	1:B:2086:TYR:HE2	1.69	0.57
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.86	0.57
1:B:1907:PRO:HD2	1:C:1960:GLN:HG2	1.87	0.57
1:B:2143:VAL:HG23	1:B:2144:GLY:H	1.70	0.57
1:C:2100:SER:HA	1:C:2103:MSE:HE3	1.87	0.57
1:A:1681:VAL:HG12	1:A:1686:GLU:H	1.70	0.56
1:B:2185:LYS:O	1:B:2189:LEU:HD23	2.05	0.56
1:B:1568:LYS:HE2	1:B:1581:GLN:OE1	2.05	0.56
1:C:1519:SER:O	1:C:1522:GLN:HB3	2.04	0.56
1:B:1766:LEU:HD12	1:B:1770:VAL:HG21	1.87	0.56
1:B:2040:LEU:HD11	1:B:2086:TYR:HB3	1.86	0.56
1:B:2148:ARG:HH11	1:B:2148:ARG:HG3	1.69	0.56
1:A:1987:ILE:HB	1:A:2014:MSE:HG3	1.85	0.56
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	1.87	0.56
1:A:1708:SER:CB	1:A:1735:ILE:HG12	2.34	0.56
1:C:1729:THR:O	1:C:1730:CYS:HB2	2.05	0.56
1:C:2148:ARG:NE	1:C:2152:ILE:HD11	2.20	0.56
1:A:1530:VAL:O	1:A:1530:VAL:HG13	2.03	0.56
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.39	0.56
1:C:2110:SER:O	1:C:2111:LYS:HG3	2.05	0.56
1:C:2190:LYS:C	1:C:2192:GLU:H	2.09	0.56
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.06	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:HD2	1.87	0.56
1:B:2044:MSE:SE	1:B:2082:LEU:HD11	2.55	0.56
1:A:2081:GLU:OE1	1:A:2081:GLU:N	2.39	0.56
1:B:2110:SER:O	1:B:2111:LYS:HG3	2.05	0.56
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	1.87	0.56
1:C:2097:HIS:O	1:C:2102:ARG:HG3	2.05	0.56
1:A:1770:VAL:HG21	1:A:1908:ALA:HA	1.87	0.56
1:A:2040:LEU:O	1:A:2043:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2148:ARG:NH1	1:B:2148:ARG:HG3	2.19	0.56
1:C:2044:MSE:HE2	1:C:2082:LEU:HB2	1.87	0.56
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	1.88	0.56
1:B:1781:GLN:NE2	1:B:1781:GLN:H	2.04	0.56
1:C:1602:GLU:HG3	1:C:1603:PHE:N	2.21	0.56
1:B:1669:PHE:O	1:B:1670:ASP:HB3	2.06	0.56
1:B:2043:THR:HG22	1:B:2086:TYR:CE2	2.40	0.56
1:A:1480:LEU:HG	1:A:1481:ARG:H	1.70	0.55
1:C:2001:VAL:HG23	1:C:2002:VAL:N	2.22	0.55
1:B:1616:ILE:HD12	1:B:1813:LYS:HG2	1.88	0.55
1:C:2033:ILE:HG22	1:C:2034:LYS:CD	2.37	0.55
1:C:1616:ILE:HD12	1:C:1813:LYS:HB3	1.88	0.55
1:B:1654:GLN:HA	1:B:1654:GLN:OE1	2.06	0.55
1:B:1708:SER:CB	1:C:2001:VAL:HG12	2.36	0.55
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.07	0.55
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.36	0.55
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.88	0.55
1:C:1735:ILE:O	1:C:1739:LEU:HG	2.06	0.55
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.55	0.55
1:A:1991:PRO:O	1:A:2019:ASN:O	2.24	0.55
1:B:1564:MSE:CE	1:B:1585:VAL:HG12	2.37	0.55
1:B:2180:LYS:C	1:B:2182:LEU:H	2.09	0.54
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.23	0.54
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.89	0.54
1:B:2037:ARG:HA	1:B:2040:LEU:HB3	1.89	0.54
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.08	0.54
1:A:2081:GLU:HB2	1:A:2082:LEU:HD12	1.89	0.54
1:A:2158:TRP:CD1	1:A:2185:LYS:HE2	2.42	0.54
1:B:2082:LEU:HD12	1:B:2082:LEU:C	2.27	0.54
1:C:2173:THR:O	1:C:2177:GLU:HB2	2.08	0.54
1:C:1747:ILE:HD13	1:C:1802:LYS:HB3	1.89	0.54
1:A:2137:LYS:O	1:A:2138:ARG:HD2	2.07	0.54
1:A:1759:ALA:O	1:A:1760:PRO:C	2.46	0.54
1:C:1585:VAL:HG13	1:C:1607:VAL:HG11	1.90	0.54
1:A:1661:GLU:O	1:A:1664:GLU:HB2	2.08	0.54
1:B:1955:GLY:HA2	1:B:1999:SER:HB3	1.90	0.54
1:C:1701:GLY:O	1:C:1704:CYS:HB2	2.08	0.53
1:C:1908:ALA:O	1:C:1910:PRO:HD3	2.07	0.53
1:C:2187:LYS:C	1:C:2189:LEU:H	2.09	0.53
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	1.89	0.53
1:B:2139:LEU:HD23	1:B:2151:LYS:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2000:TRP:CZ2	1:C:2014:MSE:HE1	2.43	0.53
1:A:1657:TYR:O	1:A:1658:LEU:HD23	2.08	0.53
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.56	0.53
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.90	0.53
1:A:1667:LYS:HD3	1:A:1672:GLU:CG	2.38	0.53
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.90	0.53
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.07	0.53
1:A:2149:LEU:O	1:A:2149:LEU:HD23	2.08	0.53
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.09	0.53
1:B:1481:ARG:HB2	1:B:1482:PRO:CD	2.38	0.53
1:A:1905:ALA:HB2	1:A:1913:ALA:HA	1.90	0.53
1:C:2033:ILE:HG22	1:C:2034:LYS:HD2	1.89	0.53
1:C:1674:SER:O	1:C:1675:VAL:HG13	2.09	0.53
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.27	0.53
1:A:1640:GLN:HB3	1:A:1657:TYR:CE1	2.43	0.53
1:C:2046:ARG:O	1:C:2046:ARG:HD2	2.09	0.53
1:A:2194:PHE:O	1:A:2196:GLN:N	2.42	0.53
1:C:1659:THR:OG1	1:C:1661:GLU:HB3	2.09	0.52
1:B:1781:GLN:H	1:B:1781:GLN:CD	2.13	0.52
1:B:1586:ALA:CB	1:B:1621:LEU:HB2	2.39	0.52
1:A:1677:THR:HG22	1:A:1689:VAL:O	2.08	0.52
1:C:2148:ARG:HD3	1:C:2152:ILE:HD11	1.91	0.52
1:B:1748:GLN:HE22	1:B:1783:MSE:HB2	1.74	0.52
1:C:1519:SER:HA	1:C:1522:GLN:HE21	1.74	0.52
1:A:1927:ASN:OD1	1:A:1928:SER:N	2.43	0.52
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.94	0.52
1:B:1643:TRP:CE3	1:B:1649:PRO:HB2	2.44	0.52
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.90	0.52
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	1.90	0.52
1:A:1641:VAL:HG12	1:A:1642:ALA:N	2.19	0.52
1:B:1562:ILE:HG22	1:B:1564:MSE:H	1.74	0.52
1:A:1681:VAL:HG12	1:A:1686:GLU:N	2.24	0.52
1:B:1615:GLY:O	1:B:1813:LYS:HA	2.09	0.52
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.10	0.52
1:A:1636:VAL:HB	1:A:1637:PRO:CD	2.40	0.52
1:A:1669:PHE:O	1:A:1671:LYS:HG3	2.10	0.52
1:A:1894:VAL:HG11	1:A:1952:ASN:O	2.09	0.52
1:A:2134:TYR:CD2	1:A:2135:LEU:HD12	2.45	0.52
1:A:1901:ASN:ND2	1:A:1903:ILE:HD11	2.25	0.52
1:B:1660:SER:O	1:B:1664:GLU:HG2	2.09	0.52
1:B:1564:MSE:HE2	1:B:1585:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2033:ILE:O	1:B:2034:LYS:HD2	2.10	0.52
1:B:1911:ASN:C	1:B:1911:ASN:HD22	2.12	0.52
1:C:2140:SER:O	1:C:2142:GLN:N	2.40	0.51
1:B:2041:LEU:O	1:B:2044:MSE:HB3	2.10	0.51
1:B:2005:PRO:HG3	1:B:2014:MSE:HB2	1.91	0.51
1:C:1653:PHE:CD2	1:C:1653:PHE:C	2.83	0.51
1:A:1668:LYS:C	1:A:1670:ASP:H	2.14	0.51
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.40	0.51
1:A:1589:ILE:HG12	1:A:1623:ALA:O	2.10	0.51
1:A:2085:ILE:CG2	1:A:2086:TYR:N	2.73	0.51
1:A:2085:ILE:HG23	1:A:2086:TYR:H	1.74	0.51
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.08	0.51
1:A:1686:GLU:HG3	1:A:1688:PHE:HE1	1.74	0.51
1:C:2179:TYR:O	1:C:2183:ASP:HB2	2.10	0.51
1:A:1936:ILE:HG12	1:A:1947:MSE:CE	2.31	0.51
1:B:1667:LYS:CE	1:B:1672:GLU:HG2	2.39	0.51
1:A:2084:PRO:O	1:A:2088:GLN:HG2	2.11	0.51
1:A:2005:PRO:HD3	1:A:2014:MSE:HE3	1.92	0.51
1:B:2149:LEU:HD23	1:B:2149:LEU:O	2.11	0.51
1:C:1775:LEU:N	1:C:1775:LEU:HD12	2.25	0.51
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.75	0.51
1:B:2148:ARG:HG2	1:B:2152:ILE:HD11	1.93	0.51
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.09	0.51
1:B:1720:HIS:ND1	1:B:1941:ASN:ND2	2.59	0.51
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.76	0.51
1:C:1641:VAL:O	1:C:1641:VAL:HG12	2.11	0.51
1:A:1644:ASN:HD21	1:A:1654:GLN:CG	2.23	0.51
1:A:1820:ILE:HD12	1:B:1486:PRO:O	2.11	0.51
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.11	0.51
1:A:1844:ARG:HH11	1:A:1844:ARG:HG3	1.76	0.51
1:B:1940:ASN:HB2	1:B:1981:TYR:CE1	2.46	0.51
1:B:1481:ARG:HB2	1:B:1482:PRO:HD2	1.92	0.51
1:C:1601:ASP:OD1	1:C:1707:GLY:HA3	2.11	0.51
1:A:1827:TRP:CD2	1:A:1828:ASP:N	2.79	0.51
1:B:1565:VAL:HA	3:B:5010:HOH:O	2.10	0.51
1:A:1638:LEU:HD12	1:A:1638:LEU:O	2.10	0.50
1:B:1663:MSE:HE2	1:B:1688:PHE:HB3	1.92	0.50
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.11	0.50
1:C:2036:ARG:NH1	1:C:2036:ARG:HG3	2.27	0.50
1:A:1787:GLY:HA3	1:A:1873:TRP:CE3	2.46	0.50
1:B:1856:PHE:CE2	1:B:1863:LYS:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2154:ARG:HH11	1:C:2154:ARG:HG3	1.76	0.50
1:B:2186:LEU:C	1:B:2188:GLY:H	2.15	0.50
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.09	0.50
1:B:1662:GLY:O	1:B:1665:THR:HB	2.12	0.50
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	1.93	0.50
1:C:2142:GLN:CD	1:C:2190:LYS:HE2	2.32	0.50
1:C:2192:GLU:CD	1:C:2192:GLU:O	2.50	0.50
1:A:1494:GLN:NE2	1:A:1558:GLY:HA3	2.27	0.50
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.93	0.50
1:B:1636:VAL:N	1:B:1637:PRO:CD	2.75	0.50
1:B:1961:ARG:NH2	3:B:5059:HOH:O	2.43	0.50
1:A:1900:GLU:OE2	1:A:1918:GLN:OE1	2.29	0.50
1:B:1766:LEU:CD1	1:B:1770:VAL:HG21	2.41	0.50
1:A:1653:PHE:N	1:A:1653:PHE:CD1	2.80	0.50
1:C:1580:ARG:HH11	1:C:1580:ARG:HG3	1.76	0.50
1:C:2005:PRO:HG3	1:C:2014:MSE:HB2	1.94	0.50
1:A:2140:SER:C	1:A:2142:GLN:H	2.14	0.50
1:C:2148:ARG:CD	1:C:2152:ILE:HD11	2.42	0.50
1:C:1697:GLU:O	1:C:1700:LEU:HD13	2.11	0.50
1:C:1943:GLU:O	1:C:1945:LEU:HD13	2.12	0.50
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.76	0.50
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.47	0.49
1:B:1697:GLU:O	1:B:1700:LEU:CD1	2.60	0.49
1:A:1527:SER:O	1:A:1530:VAL:HG12	2.12	0.49
1:A:1655:TYR:CD1	1:A:1689:VAL:HG13	2.46	0.49
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.94	0.49
1:A:1698:ASP:OD1	1:A:1699:GLY:N	2.45	0.49
1:A:1681:VAL:O	1:A:1682:ILE:HG12	2.11	0.49
1:A:2037:ARG:O	1:A:2038:GLU:C	2.50	0.49
1:A:1645:ASP:C	1:A:1647:ALA:H	2.15	0.49
1:B:1783:MSE:HA	1:B:1786:ASN:HB2	1.93	0.49
1:A:2002:VAL:HG22	1:A:2002:VAL:O	2.12	0.49
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.48	0.49
1:A:1805:GLU:HG2	1:A:1867:PHE:CE1	2.48	0.49
1:C:1644:ASN:HD21	1:C:1654:GLN:HE22	1.61	0.49
1:C:1702:VAL:HA	1:C:1705:LEU:HD22	1.95	0.49
1:B:1526:PHE:CE2	1:B:1821:LEU:HD11	2.47	0.49
1:A:2082:LEU:N	1:A:2082:LEU:HD12	2.28	0.49
1:C:1680:THR:HG22	1:C:1681:VAL:N	2.26	0.49
1:C:1660:SER:HB2	1:C:1686:GLU:OE2	2.13	0.49
1:B:1991:PRO:HG2	1:B:2115:TRP:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.13	0.49
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.94	0.49
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.95	0.49
1:A:1575:GLU:H	1:A:1575:GLU:CD	2.16	0.49
1:A:1481:ARG:O	1:A:1483:ILE:N	2.45	0.49
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.12	0.49
1:B:1689:VAL:HG22	1:B:1691:LYS:HE3	1.94	0.49
1:C:1901:ASN:ND2	1:C:1903:ILE:HD11	2.28	0.49
1:A:1657:TYR:CE1	1:A:1687:ARG:HD2	2.48	0.49
1:A:1877:VAL:HG22	1:A:1928:SER:HB2	1.95	0.49
1:A:1624:ASN:HD21	1:A:1736:GLY:HA3	1.78	0.48
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.44	0.48
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.47	0.48
1:B:1951:ALA:O	1:B:1990:PRO:HD2	2.13	0.48
1:A:1768:ARG:HG2	1:A:1769:GLU:N	2.28	0.48
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.47	0.48
1:A:1513:GLU:HG3	1:A:1517:GLN:NE2	2.28	0.48
1:B:2187:LYS:HA	1:B:2190:LYS:HD3	1.95	0.48
1:C:1759:ALA:H	1:C:1774:ASN:HD22	1.60	0.48
1:A:2085:ILE:HG23	1:A:2086:TYR:HD1	1.78	0.48
1:A:2042:ASP:O	1:A:2046:ARG:HG2	2.12	0.48
1:B:1682:ILE:HG22	1:B:1682:ILE:O	2.14	0.48
1:C:1680:THR:CG2	1:C:1681:VAL:N	2.76	0.48
1:C:1653:PHE:O	1:C:1655:TYR:N	2.46	0.48
1:B:1786:ASN:OD1	1:C:1964:PHE:O	2.31	0.48
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.95	0.48
1:B:2180:LYS:C	1:B:2182:LEU:N	2.67	0.48
1:A:1905:ALA:HB1	1:A:1912:SER:O	2.13	0.48
1:C:2139:LEU:HD13	1:C:2186:LEU:HD21	1.95	0.48
1:A:1903:ILE:HB	1:A:1915:THR:CG2	2.41	0.48
1:A:2085:ILE:HG23	1:A:2086:TYR:CD1	2.48	0.48
1:C:2136:ILE:HD11	1:C:2152:ILE:HG12	1.96	0.48
1:A:1529:ASP:O	1:A:1530:VAL:C	2.51	0.48
1:B:1852:THR:HG22	1:B:1853:GLU:H	1.79	0.48
1:C:1634:GLU:N	1:C:1634:GLU:OE1	2.47	0.48
1:B:1852:THR:HG22	1:B:1853:GLU:N	2.28	0.48
1:B:1592:LYS:O	1:B:1593:ILE:HG12	2.13	0.48
1:B:1720:HIS:HA	1:B:1941:ASN:HD22	1.78	0.48
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.29	0.48
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.28	0.48
1:A:1678:GLU:CD	1:A:1691:LYS:HE3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1582:PHE:CD2	1:A:1807:MSE:HE1	2.49	0.47
1:A:1677:THR:HG22	1:A:1690:ILE:CA	2.43	0.47
1:B:1902:LEU:HD11	1:B:1914:GLU:HG2	1.95	0.47
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.16	0.47
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.14	0.47
1:A:1664:GLU:O	1:A:1667:LYS:HB2	2.14	0.47
1:A:1813:LYS:HD2	1:A:1816:MSE:SE	2.64	0.47
1:B:1846:MSE:HE1	1:B:1990:PRO:CB	2.44	0.47
1:C:1952:ASN:OD1	1:C:1993:GLY:HA2	2.14	0.47
1:B:1888:PRO:HG3	3:B:5044:HOH:O	2.14	0.47
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.13	0.47
1:A:2037:ARG:HB3	1:A:2037:ARG:CZ	2.45	0.47
1:C:1625:SER:HB3	1:C:1731:ARG:NH2	2.29	0.47
1:C:1905:ALA:HB1	1:C:1912:SER:OG	2.13	0.47
1:A:1730:CYS:O	1:A:1731:ARG:HB3	2.13	0.47
1:B:1660:SER:HB3	1:B:1686:GLU:HG3	1.97	0.47
1:C:1680:THR:CG2	1:C:1682:ILE:HG12	2.44	0.47
1:C:2142:GLN:HB2	1:C:2190:LYS:CE	2.44	0.47
1:B:2181:THR:O	1:B:2185:LYS:HB2	2.15	0.47
1:C:2044:MSE:HE2	1:C:2082:LEU:CB	2.44	0.47
1:B:1655:TYR:CE1	1:B:1657:TYR:HB3	2.48	0.47
1:B:1727:LEU:HG	1:B:1729:THR:HG23	1.94	0.47
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.48	0.47
1:C:1568:LYS:HE2	1:C:1581:GLN:NE2	2.29	0.47
1:C:1550:LEU:HA	1:C:1550:LEU:HD12	1.76	0.47
1:B:1726:THR:HG21	1:B:1740:VAL:HA	1.97	0.47
1:C:1755:ILE:HD12	1:C:1758:GLY:HA2	1.96	0.47
1:A:2037:ARG:CB	1:A:2037:ARG:HH11	2.28	0.47
1:B:1728:VAL:HG21	1:B:1754:ILE:CD1	2.44	0.47
1:A:1991:PRO:CG	1:A:2115:TRP:HB2	2.44	0.47
1:A:1866:PHE:CE1	1:A:1868:GLU:HB2	2.50	0.47
1:A:1663:MSE:CE	1:A:1663:MSE:HA	2.45	0.47
1:A:1657:TYR:HB2	1:A:1688:PHE:O	2.15	0.47
1:B:2086:TYR:HA	1:B:2089:ILE:CD1	2.35	0.47
1:B:2038:GLU:H	1:B:2041:LEU:H	1.63	0.47
1:C:2044:MSE:HA	1:C:2086:TYR:HE2	1.78	0.47
1:A:1766:LEU:CD2	1:A:1770:VAL:HG11	2.45	0.47
1:B:1676:LEU:O	1:B:1691:LYS:HB2	2.15	0.47
1:B:2119:ARG:HH11	1:B:2119:ARG:CG	2.28	0.47
1:C:1766:LEU:O	1:C:1768:ARG:HG2	2.15	0.47
1:A:1902:LEU:O	1:A:1904:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.15	0.47
1:C:1644:ASN:ND2	1:C:1654:GLN:HE22	2.13	0.47
1:B:1617:PRO:HG2	1:B:1807:MSE:HE3	1.97	0.47
1:B:2022:ALA:HB3	1:B:2103:MSE:CE	2.40	0.47
1:A:1673:ASN:N	1:A:1673:ASN:ND2	2.62	0.47
1:B:2127:ARG:HD2	1:B:2176:GLU:OE1	2.15	0.47
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.83	0.47
1:B:1681:VAL:HG13	1:B:1685:GLU:O	2.15	0.47
1:C:1646:ALA:O	1:C:1647:ALA:C	2.54	0.47
1:C:1766:LEU:CD1	1:C:1770:VAL:HG11	2.45	0.47
1:C:1552:GLU:O	1:C:1553:VAL:HG13	2.14	0.47
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.50	0.46
1:C:1660:SER:O	1:C:1664:GLU:HB2	2.15	0.46
1:A:1634:GLU:HG3	1:A:1671:LYS:HD3	1.97	0.46
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.51	0.46
1:C:2171:VAL:O	1:C:2175:ILE:HG13	2.16	0.46
1:A:2100:SER:HA	1:A:2103:MSE:HE3	1.97	0.46
1:A:2085:ILE:O	1:A:2088:GLN:HB2	2.16	0.46
1:C:2110:SER:O	1:C:2111:LYS:CG	2.64	0.46
1:C:1580:ARG:NH2	1:C:1810:VAL:O	2.47	0.46
1:A:2031:VAL:C	1:A:2033:ILE:H	2.18	0.46
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.51	0.46
1:C:1657:TYR:CE2	1:C:1687:ARG:HG2	2.51	0.46
1:C:1636:VAL:O	1:C:1639:PHE:HD2	1.99	0.46
1:C:1636:VAL:HB	1:C:1637:PRO:CD	2.46	0.46
1:A:1790:HIS:HD2	3:A:5051:HOH:O	1.98	0.46
1:B:2102:ARG:NH2	1:C:1700:LEU:HB2	2.31	0.46
1:B:1652:GLY:HA2	1:C:2085:ILE:CD1	2.46	0.46
1:C:1921:GLY:O	1:C:1923:VAL:HG23	2.15	0.46
1:C:1642:ALA:N	1:C:1657:TYR:HE1	2.10	0.46
1:C:1759:ALA:O	1:C:1760:PRO:C	2.54	0.46
1:A:1844:ARG:NH1	1:A:1844:ARG:HG3	2.31	0.46
1:B:1592:LYS:C	1:B:1593:ILE:HG12	2.36	0.46
1:B:2140:SER:O	1:B:2142:GLN:N	2.48	0.46
1:A:1593:ILE:O	1:A:1593:ILE:CG2	2.63	0.46
1:C:2186:LEU:C	1:C:2188:GLY:N	2.68	0.46
1:B:2181:THR:O	1:B:2185:LYS:HE2	2.15	0.46
1:B:1643:TRP:HZ2	1:C:2047:LEU:HB3	1.81	0.46
1:A:2183:ASP:O	1:A:2187:LYS:HD3	2.16	0.46
1:C:2190:LYS:C	1:C:2192:GLU:N	2.69	0.46
1:A:1587:ASN:ND2	1:A:1622:ALA:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1667:LYS:NZ	1:B:1672:GLU:HA	2.30	0.46
1:C:1633:GLU:HA	1:C:1633:GLU:OE2	2.16	0.46
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.98	0.46
1:A:1895:GLU:OE2	1:A:1897:ARG:NH1	2.49	0.46
1:B:1991:PRO:HG2	1:B:2115:TRP:CD2	2.51	0.45
1:B:1667:LYS:HZ2	1:B:1672:GLU:HA	1.80	0.45
1:A:2149:LEU:C	1:A:2149:LEU:CD2	2.83	0.45
1:B:2159:TYR:CE1	1:B:2171:VAL:HG13	2.51	0.45
1:A:1903:ILE:N	1:A:1903:ILE:CD1	2.79	0.45
1:C:2046:ARG:HG3	1:C:2047:LEU:CD2	2.44	0.45
1:B:1659:THR:OG1	1:B:1661:GLU:HB3	2.17	0.45
1:C:1645:ASP:OD2	1:C:1648:ASN:CB	2.63	0.45
1:A:1533:THR:HG22	1:A:1535:ASP:OD2	2.16	0.45
1:A:2046:ARG:O	1:A:2047:LEU:HB3	2.16	0.45
1:B:1663:MSE:HG3	1:B:1688:PHE:CD2	2.51	0.45
1:B:1556:GLU:O	1:B:1557:PRO:C	2.54	0.45
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.98	0.45
1:B:2029:GLY:O	1:B:2033:ILE:HG13	2.16	0.45
1:B:1509:TYR:CB	1:B:1557:PRO:HB3	2.47	0.45
1:B:1988:TYR:HA	1:B:2015:TYR:O	2.17	0.45
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.46	0.45
1:B:1865:SER:O	1:B:1882:ALA:HA	2.16	0.45
1:B:2187:LYS:O	1:B:2187:LYS:HG2	2.16	0.45
1:A:2037:ARG:CB	1:A:2037:ARG:NH1	2.78	0.45
1:A:1734:GLY:C	1:A:1736:GLY:N	2.69	0.45
1:A:1827:TRP:CG	1:A:1828:ASP:N	2.84	0.45
1:C:2154:ARG:NH1	1:C:2154:ARG:HG3	2.32	0.45
1:B:2119:ARG:HG2	1:B:2119:ARG:HH11	1.82	0.45
1:C:1775:LEU:N	1:C:1775:LEU:CD1	2.80	0.45
1:C:1516:ARG:NH1	3:C:5003:HOH:O	2.49	0.45
1:A:1578:ARG:HB2	3:A:5014:HOH:O	2.16	0.45
1:C:1926:PRO:HG3	1:C:1967:VAL:HB	1.96	0.45
1:C:1906:ASP:OD2	1:C:1908:ALA:HB3	2.16	0.45
1:B:1633:GLU:O	1:B:1637:PRO:HD3	2.17	0.45
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.99	0.45
1:C:2160:PRO:HD3	1:C:2174:TRP:CE2	2.51	0.45
1:C:2085:ILE:O	1:C:2089:ILE:HG13	2.16	0.45
1:A:1811:PRO:HG3	1:A:1818:VAL:HA	1.98	0.45
1:B:2086:TYR:O	1:B:2089:ILE:HB	2.17	0.45
1:A:1615:GLY:O	1:A:1813:LYS:HA	2.16	0.45
1:B:1768:ARG:NH1	1:B:1768:ARG:CG	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1762:ILE:HG21	1:A:1771:TYR:HE1	1.82	0.45
1:C:1668:LYS:HG2	1:C:1669:PHE:CD2	2.52	0.45
1:C:1686:GLU:O	1:C:1687:ARG:HG3	2.17	0.45
1:C:2145:GLU:HG3	1:C:2151:LYS:NZ	2.29	0.45
1:A:1747:ILE:HD13	1:A:1802:LYS:HB3	1.99	0.45
1:B:1757:THR:CG2	1:B:1762:ILE:HG13	2.42	0.45
1:C:1909:ASN:C	1:C:1909:ASN:ND2	2.70	0.45
1:A:1909:ASN:O	1:A:1911:ASN:N	2.50	0.45
1:C:2131:ASN:HB3	1:C:2175:ILE:HG21	1.98	0.44
1:A:1954:ARG:HH11	1:A:1954:ARG:HG3	1.82	0.44
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.18	0.44
1:C:1793:ALA:HB1	1:C:1798:ALA:HB3	2.00	0.44
1:B:1632:ALA:HB1	1:B:1634:GLU:OE2	2.17	0.44
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.17	0.44
1:C:2183:ASP:O	1:C:2186:LEU:HB2	2.18	0.44
1:B:2142:GLN:O	1:B:2143:VAL:C	2.56	0.44
1:C:2040:LEU:O	1:C:2043:THR:HG23	2.17	0.44
1:A:2085:ILE:CG2	1:A:2086:TYR:H	2.30	0.44
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.17	0.44
1:A:1663:MSE:HA	1:A:1663:MSE:HE3	2.00	0.44
1:A:1667:LYS:HD3	1:A:1672:GLU:HG2	1.99	0.44
1:C:1632:ALA:HB1	1:C:1634:GLU:OE1	2.17	0.44
1:B:2024:VAL:HG23	1:C:1701:GLY:HA2	1.98	0.44
1:B:1543:ILE:HD13	1:B:1553:VAL:HG21	1.99	0.44
1:B:1647:ALA:O	1:B:1648:ASN:ND2	2.51	0.44
1:A:1688:PHE:CD1	1:A:1688:PHE:N	2.85	0.44
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.48	0.44
1:B:1790:HIS:HD2	3:B:5041:HOH:O	2.00	0.44
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.15	0.44
1:C:1639:PHE:CD1	1:C:1639:PHE:C	2.91	0.44
1:C:1763:ASN:OD1	1:C:1770:VAL:N	2.49	0.44
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.17	0.44
1:C:1987:ILE:O	1:C:2014:MSE:HA	2.17	0.44
1:C:2186:LEU:O	1:C:2189:LEU:N	2.49	0.44
1:B:2024:VAL:HB	1:C:1629:ILE:HG22	1.99	0.44
1:C:1598:PRO:HG2	1:C:1698:ASP:OD2	2.18	0.44
1:B:1607:VAL:O	1:B:1610:TYR:HB3	2.17	0.44
1:B:1820:ILE:HD13	1:B:1887:ILE:HA	2.00	0.44
1:C:2031:VAL:C	1:C:2033:ILE:H	2.22	0.44
1:A:1735:ILE:H	1:A:1735:ILE:HD12	1.82	0.44
1:C:1824:LYS:NZ	1:C:1824:LYS:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1787:GLY:HA3	1:B:1873:TRP:CE3	2.53	0.44
1:A:1873:TRP:O	1:A:1931:LYS:HE3	2.17	0.44
1:A:1989:ILE:HA	1:A:1990:PRO:HD3	1.78	0.44
1:A:1835:PRO:HG2	1:A:1846:MSE:SE	2.68	0.44
1:B:1651:LYS:O	1:B:1651:LYS:HG2	2.17	0.44
1:A:1892:ILE:HD11	1:A:1947:MSE:HE2	1.99	0.43
1:C:1648:ASN:ND2	1:C:1650:ASP:OD1	2.51	0.43
1:C:1708:SER:OG	1:C:1735:ILE:HG12	2.18	0.43
1:C:2036:ARG:O	1:C:2037:ARG:C	2.55	0.43
1:C:1580:ARG:NH1	1:C:1580:ARG:HG3	2.33	0.43
1:B:2082:LEU:HD12	1:B:2083:LEU:N	2.33	0.43
1:C:1991:PRO:C	1:C:1993:GLY:H	2.22	0.43
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	2.01	0.43
1:B:1755:ILE:HA	1:C:1963:MSE:CE	2.48	0.43
1:A:1728:VAL:HG21	1:A:1754:ILE:CD1	2.46	0.43
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.36	0.43
1:C:1781:GLN:CD	1:C:1781:GLN:H	2.21	0.43
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	2.00	0.43
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.50	0.43
1:C:1875:LYS:HB3	3:C:5032:HOH:O	2.17	0.43
1:B:1747:ILE:HD12	1:B:1803:ILE:HG13	2.01	0.43
1:A:1664:GLU:O	1:A:1667:LYS:N	2.49	0.43
1:C:1659:THR:C	1:C:1661:GLU:N	2.70	0.43
1:C:1653:PHE:O	1:C:1654:GLN:C	2.57	0.43
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.65	0.43
1:B:2088:GLN:O	1:B:2091:LEU:HB2	2.18	0.43
1:C:1811:PRO:HG3	1:C:1818:VAL:HA	2.01	0.43
1:B:1925:HIS:O	1:B:1926:PRO:C	2.55	0.43
1:C:1494:GLN:HB2	3:C:5001:HOH:O	2.18	0.43
1:A:1735:ILE:O	1:A:1739:LEU:N	2.48	0.43
1:B:1587:ASN:ND2	1:B:1622:ALA:HA	2.33	0.43
1:A:1533:THR:CG2	1:A:1535:ASP:OD2	2.67	0.43
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.64	0.43
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.18	0.43
1:A:2131:ASN:HB3	1:A:2175:ILE:HG21	2.01	0.43
1:B:2013:GLU:OE1	1:B:2125:ARG:NH2	2.41	0.43
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.01	0.43
1:B:2085:ILE:CG2	1:C:1650:ASP:HA	2.45	0.43
1:B:1703:GLU:OE2	1:C:2102:ARG:NH2	2.52	0.43
1:C:1770:VAL:HG21	1:C:1908:ALA:HA	1.99	0.43
1:A:1905:ALA:HB2	1:A:1913:ALA:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1697:GLU:HB2	1:C:1700:LEU:HD11	2.00	0.43
1:C:1654:GLN:O	1:C:1655:TYR:CB	2.65	0.43
1:B:2143:VAL:O	1:B:2145:GLU:N	2.45	0.43
1:C:1645:ASP:O	1:C:1646:ALA:C	2.57	0.43
1:A:1606:LYS:CA	1:A:1606:LYS:HE2	2.44	0.43
1:C:1768:ARG:HH12	1:C:1770:VAL:HG23	1.84	0.43
1:C:1869:THR:O	1:C:1870:LEU:HB2	2.19	0.43
1:B:1764:LYS:HD3	1:C:2028:GLN:CD	2.39	0.43
1:C:1841:TYR:CZ	1:C:1896:THR:HG21	2.52	0.43
1:A:1681:VAL:O	1:A:1682:ILE:HD13	2.19	0.43
1:C:1646:ALA:O	1:C:1648:ASN:N	2.51	0.43
1:C:2148:ARG:HD3	1:C:2152:ILE:CD1	2.48	0.43
1:A:1905:ALA:CB	1:A:1913:ALA:HA	2.48	0.43
1:A:2190:LYS:C	1:A:2192:GLU:H	2.22	0.43
1:B:1810:VAL:HA	1:B:1811:PRO:HD3	1.91	0.43
1:B:1835:PRO:HB2	1:B:1992:THR:CG2	2.49	0.43
1:C:1940:ASN:HB2	1:C:1981:TYR:CE1	2.54	0.43
1:B:1679:ARG:CZ	1:B:1686:GLU:OE1	2.66	0.43
1:C:1636:VAL:O	1:C:1639:PHE:CD2	2.72	0.43
1:C:2135:LEU:HB3	1:C:2155:ILE:HD13	2.01	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.19	0.43
1:C:1836:THR:O	1:C:1838:ASP:N	2.51	0.43
1:A:1616:ILE:HA	1:A:1617:PRO:HD3	1.94	0.42
1:A:1766:LEU:HD23	1:A:1770:VAL:HG11	2.01	0.42
1:B:1902:LEU:HD11	1:B:1914:GLU:CG	2.48	0.42
1:A:2033:ILE:HG22	1:A:2034:LYS:HD3	2.00	0.42
1:C:1644:ASN:HD21	1:C:1654:GLN:CD	2.22	0.42
1:C:1735:ILE:HD12	1:C:1735:ILE:N	2.35	0.42
1:C:1827:TRP:CD2	1:C:1828:ASP:N	2.87	0.42
1:A:2033:ILE:HG22	1:A:2034:LYS:CD	2.49	0.42
1:B:2088:GLN:HA	1:B:2091:LEU:HD12	2.00	0.42
1:A:1633:GLU:OE1	1:A:1633:GLU:HA	2.18	0.42
1:A:2190:LYS:C	1:A:2192:GLU:N	2.71	0.42
1:B:1844:ARG:HG3	1:B:1844:ARG:HH11	1.85	0.42
1:C:2142:GLN:HE21	1:C:2190:LYS:HD3	1.84	0.42
1:B:1946:PRO:CG	1:B:2130:LEU:HD21	2.45	0.42
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.58	0.42
1:B:2110:SER:O	1:B:2111:LYS:CG	2.67	0.42
1:A:2042:ASP:O	1:A:2045:ASN:HB3	2.20	0.42
1:B:2100:SER:HB2	1:B:2112:GLU:OE1	2.19	0.42
1:C:1927:ASN:OD1	1:C:1928:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1657:TYR:O	1:B:1658:LEU:HD12	2.19	0.42
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	2.00	0.42
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.01	0.42
1:A:1659:THR:OG1	1:A:1661:GLU:HB3	2.20	0.42
1:A:2134:TYR:HD2	1:A:2135:LEU:CD1	2.32	0.42
1:C:1556:GLU:HA	1:C:1557:PRO:HD3	1.87	0.42
1:A:1775:LEU:HD12	1:A:1775:LEU:N	2.34	0.42
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.20	0.42
1:A:1681:VAL:O	1:A:1682:ILE:CG1	2.67	0.42
1:C:2140:SER:OG	1:C:2151:LYS:HE3	2.20	0.42
1:B:1641:VAL:HG22	1:B:1656:LEU:HD22	2.01	0.42
1:B:2033:ILE:O	1:B:2033:ILE:HG22	2.20	0.42
1:A:2134:TYR:OH	1:A:2138:ARG:NH1	2.53	0.42
1:C:1587:ASN:HD21	1:C:1624:ASN:HD22	1.68	0.42
1:B:1693:ILE:HG21	1:C:2097:HIS:NE2	2.35	0.42
1:C:1545:ASP:OD1	1:C:1547:ASN:N	2.44	0.42
1:B:1640:GLN:HB3	1:B:1657:TYR:CE1	2.55	0.42
1:C:1903:ILE:CD1	1:C:1903:ILE:N	2.82	0.42
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.50	0.42
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.89	0.42
1:B:1828:ASP:OD2	1:B:2120:ARG:NE	2.53	0.42
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.54	0.42
1:C:1655:TYR:O	1:C:1656:LEU:HD13	2.20	0.42
1:B:2097:HIS:CD2	1:C:1693:ILE:HB	2.55	0.42
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	2.02	0.42
1:C:1677:THR:HG22	1:C:1690:ILE:HA	2.01	0.41
1:B:1755:ILE:CD1	1:B:1755:ILE:N	2.83	0.41
1:B:1755:ILE:HA	1:C:1963:MSE:HE1	2.01	0.41
1:A:1564:MSE:HE1	1:A:1596:PHE:CE2	2.55	0.41
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.34	0.41
1:C:2124:TRP:O	1:C:2168:ASP:HB3	2.19	0.41
1:A:1845:TRP:CD1	1:A:1850:ARG:HG3	2.55	0.41
1:A:1680:THR:HG22	1:A:1682:ILE:HG12	2.01	0.41
1:C:1659:THR:O	1:C:1660:SER:C	2.58	0.41
1:A:2134:TYR:HD2	1:A:2135:LEU:HD12	1.83	0.41
1:A:1494:GLN:HE21	1:A:1558:GLY:HA3	1.84	0.41
1:B:1968:LEU:HD23	1:C:1783:MSE:HE1	2.01	0.41
1:A:2043:THR:O	1:A:2046:ARG:HG3	2.19	0.41
1:B:1665:THR:O	1:B:1668:LYS:HB3	2.19	0.41
1:B:1610:TYR:CE1	1:B:1614:ARG:CZ	3.04	0.41
1:B:2142:GLN:HB2	1:B:2190:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1764:LYS:HB2	1:B:1764:LYS:NZ	2.35	0.41
1:B:1608:THR:O	1:B:1612:ARG:HG3	2.20	0.41
1:A:1744:GLN:NE2	3:A:5035:HOH:O	2.53	0.41
1:B:1832:ASP:O	1:B:1833:PHE:C	2.59	0.41
1:B:1587:ASN:ND2	1:B:1623:ALA:H	2.09	0.41
1:C:1530:VAL:HG23	1:C:1530:VAL:O	2.20	0.41
1:B:1569:ILE:CG2	1:B:1571:VAL:HG22	2.49	0.41
1:C:1549:GLU:HG2	1:C:1550:LEU:O	2.20	0.41
1:A:1770:VAL:HG21	1:A:1908:ALA:CA	2.51	0.41
1:C:1786:ASN:HB3	1:C:1788:VAL:H	1.85	0.41
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	2.02	0.41
1:C:1731:ARG:HA	1:C:1753:PRO:O	2.20	0.41
1:B:2021:ARG:HD3	1:B:2095:ASP:OD2	2.20	0.41
1:A:1783:MSE:HA	1:A:1786:ASN:HB2	2.01	0.41
1:A:1645:ASP:O	1:A:1647:ALA:N	2.53	0.41
1:A:2083:LEU:O	1:A:2084:PRO:C	2.59	0.41
1:B:1641:VAL:O	1:B:1657:TYR:HE1	2.03	0.41
1:A:2143:VAL:HB	1:A:2193:SER:HB3	2.03	0.41
1:B:1991:PRO:O	1:B:2019:ASN:O	2.38	0.41
1:A:1587:ASN:HD22	1:A:1622:ALA:HA	1.85	0.41
1:B:2004:ASP:OD2	1:B:2006:THR:CG2	2.63	0.41
1:B:1562:ILE:HD11	1:B:1599:GLN:OE1	2.20	0.41
1:B:1544:GLU:OE1	1:B:1602:GLU:OE1	2.39	0.41
1:A:1906:ASP:HA	1:A:1907:PRO:HD3	1.80	0.41
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.20	0.41
1:B:2186:LEU:CD2	1:B:2190:LYS:HE2	2.39	0.41
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.69	0.41
1:A:1900:GLU:HB3	1:A:1916:LEU:HD11	2.03	0.41
1:A:1907:PRO:O	1:A:1909:ASN:N	2.53	0.41
1:B:1835:PRO:HB2	1:B:1992:THR:HG23	2.03	0.41
1:B:2089:ILE:HG13	1:C:1653:PHE:CD1	2.55	0.41
1:B:2154:ARG:HH21	1:B:2189:LEU:HD13	1.82	0.41
1:A:1616:ILE:HD12	1:A:1813:LYS:HB3	2.02	0.41
1:B:2081:GLU:HG2	1:B:2082:LEU:N	2.35	0.41
1:B:2046:ARG:O	1:B:2046:ARG:HG3	2.20	0.41
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	2.03	0.41
1:B:2133:GLU:OE1	1:B:2148:ARG:NH2	2.54	0.41
1:A:2081:GLU:HB2	1:A:2082:LEU:CD1	2.51	0.41
1:C:1633:GLU:O	1:C:1636:VAL:HB	2.21	0.41
1:B:2102:ARG:HA	1:C:1694:ILE:HD12	2.02	0.41
1:C:2001:VAL:HG23	1:C:2002:VAL:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2178:ASN:HB3	1:B:2181:THR:CG2	2.48	0.41
1:A:1487:TYR:HB3	1:A:1488:PRO:CD	2.51	0.41
1:B:1708:SER:HB3	1:B:1735:ILE:CG2	2.51	0.40
1:B:1705:LEU:HB3	1:C:2000:TRP:CG	2.57	0.40
1:B:2178:ASN:C	1:B:2180:LYS:H	2.25	0.40
1:A:1766:LEU:HD12	1:A:1766:LEU:N	2.36	0.40
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.49	0.40
1:B:1481:ARG:C	1:B:1481:ARG:HD2	2.41	0.40
1:C:1753:PRO:HA	1:C:1778:GLY:O	2.21	0.40
1:C:1792:THR:CG2	1:C:1793:ALA:N	2.84	0.40
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.20	0.40
1:B:1583:VAL:HG12	1:B:1618:ARG:HA	2.03	0.40
1:B:2045:ASN:OD1	1:B:2045:ASN:C	2.59	0.40
1:B:2039:LYS:HB2	1:B:2039:LYS:HE3	1.93	0.40
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.68	0.40
1:C:1664:GLU:O	1:C:1665:THR:C	2.60	0.40
1:C:1634:GLU:CD	1:C:1634:GLU:H	2.19	0.40
1:C:1757:THR:HB	1:C:1762:ILE:HD11	2.04	0.40
1:C:2083:LEU:N	1:C:2084:PRO:CD	2.85	0.40
1:B:1508:VAL:HG23	1:B:1509:TYR:N	2.36	0.40
1:A:1829:ARG:NH2	1:A:1858:TYR:HB3	2.36	0.40
1:B:2142:GLN:HE22	1:B:2189:LEU:CD1	2.35	0.40
1:C:1616:ILE:CD1	1:C:1813:LYS:HB3	2.52	0.40
1:C:2135:LEU:CB	1:C:2155:ILE:HD13	2.51	0.40
1:C:1542:LEU:HD12	1:C:1542:LEU:HA	1.76	0.40
1:B:1708:SER:HB3	1:B:1735:ILE:HG23	2.03	0.40
1:C:2192:GLU:CD	1:C:2192:GLU:C	2.80	0.40
1:C:1762:ILE:HG21	1:C:1771:TYR:CE1	2.51	0.40
1:B:1862:ASP:HB2	1:B:1865:SER:HB3	2.02	0.40
1:C:1877:VAL:HG23	1:C:1928:SER:OG	2.21	0.40
1:C:2093:PHE:HA	1:C:2096:LEU:HD12	2.04	0.40
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.57	0.40
1:B:1483:ILE:H	1:B:1483:ILE:CD1	2.18	0.40
1:A:2186:LEU:O	1:A:2187:LYS:C	2.60	0.40
1:A:1649:PRO:O	1:A:1650:ASP:C	2.60	0.40
1:B:1629:ILE:HG22	1:C:2024:VAL:HG11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1717:ARG:NH2	1:A:2007:ILE:O[2_555]	2.16	0.04

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	680/805 (84%)	589 (87%)	70 (10%)	21 (3%)	5	12
1	B	680/805 (84%)	602 (88%)	64 (9%)	14 (2%)	9	23
1	C	668/805 (83%)	582 (87%)	66 (10%)	20 (3%)	5	13
All	All	2028/2415 (84%)	1773 (87%)	200 (10%)	55 (3%)	6	16

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1483	ILE
1	A	1530	VAL
1	A	1650	ASP
1	A	1839	GLU
1	B	2037	ARG
1	B	2038	GLU
1	B	2143	VAL
1	B	2187	LYS
1	C	1655	TYR
1	C	2037	ARG
1	C	2038	GLU
1	A	1649	PRO
1	A	1686	GLU
1	A	1731	ARG
1	A	1828	ASP
1	A	1914	GLU
1	B	1766	LEU
1	B	1921	GLY
1	C	1647	ALA

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Mol	Chain	Res	Type
1	C	1653	PHE
1	C	1654	GLN
1	C	1837	ASN
1	C	1997	GLY
1	A	1837	ASN
1	A	1908	ALA
1	A	2195	ALA
1	B	1655	TYR
1	B	1910	PRO
1	B	2179	TYR
1	C	1642	ALA
1	C	1675	VAL
1	C	1686	GLU
1	C	2039	LYS
1	C	2141	HIS
1	A	1482	PRO
1	A	1669	PHE
1	A	1744	GLN
1	A	1910	PRO
1	A	2142	GLN
1	A	2143	VAL
1	B	2185	LYS
1	C	1646	ALA
1	C	1730	CYS
1	C	1768	ARG
1	C	1828	ASP
1	C	2186	LEU
1	A	1997	GLY
1	B	1832	ASP
1	C	1494	GLN
1	B	1744	GLN
1	B	2098	ASP
1	B	2144	GLY
1	C	1910	PRO
1	A	2033	ILE
1	A	1593	ILE

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	579/668 (87%)	534 (92%)	45 (8%)	16	35
1	B	579/668 (87%)	528 (91%)	51 (9%)	12	28
1	C	568/668 (85%)	513 (90%)	55 (10%)	10	23
All	All	1726/2004 (86%)	1575 (91%)	151 (9%)	13	29

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1482	PRO
1	A	1483	ILE
1	A	1534	ASP
1	A	1549	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1589	ILE
1	A	1602	GLU
1	A	1606	LYS
1	A	1633	GLU
1	A	1638	LEU
1	A	1639	PHE
1	A	1648	ASN
1	A	1649	PRO
1	A	1653	PHE
1	A	1663	MSE
1	A	1665	THR
1	A	1689	VAL
1	A	1697	GLU
1	A	1732	SER
1	A	1735	ILE
1	A	1770	VAL
1	A	1781	GLN
1	A	1813	LYS
1	A	1824	LYS
1	A	1837	ASN
1	A	1850	ARG
1	A	1877	VAL
1	A	1884	LEU
1	A	1889	LEU
1	A	1903	ILE

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Mol	Chain	Res	Type
1	A	1910	PRO
1	A	1924	TRP
1	A	1930	PHE
1	A	1960	GLN
1	A	1981	TYR
1	A	1996	ARG
1	A	2008	ASN
1	A	2035	PHE
1	A	2041	LEU
1	A	2081	GLU
1	A	2082	LEU
1	A	2091	LEU
1	A	2128	ARG
1	A	2194	PHE
1	B	1481	ARG
1	B	1502	LEU
1	B	1531	LYS
1	B	1535	ASP
1	B	1536	PHE
1	B	1567	PHE
1	B	1571	VAL
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1616	ILE
1	B	1618	ARG
1	B	1639	PHE
1	B	1658	LEU
1	B	1689	VAL
1	B	1691	LYS
1	B	1726	THR
1	B	1732	SER
1	B	1733	VAL
1	B	1735	ILE
1	B	1744	GLN
1	B	1755	ILE
1	B	1781	GLN
1	B	1791	LEU
1	B	1792	THR
1	B	1797	LEU
1	B	1839	GLU
1	B	1843	VAL

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Mol	Chain	Res	Type
1	B	1884	LEU
1	B	1911	ASN
1	B	1915	THR
1	B	1924	TRP
1	B	1930	PHE
1	B	1981	TYR
1	B	2018	VAL
1	B	2021	ARG
1	B	2035	PHE
1	B	2041	LEU
1	B	2044	MSE
1	B	2100	SER
1	B	2117	GLU
1	B	2119	ARG
1	B	2127	ARG
1	B	2128	ARG
1	B	2131	ASN
1	B	2149	LEU
1	B	2179	TYR
1	B	2181	THR
1	B	2183	ASP
1	B	2186	LEU
1	B	2192	GLU
1	C	1493	LEU
1	C	1508	VAL
1	C	1533	THR
1	C	1542	LEU
1	C	1546	GLU
1	C	1550	LEU
1	C	1551	THR
1	C	1571	VAL
1	C	1580	ARG
1	C	1585	VAL
1	C	1602	GLU
1	C	1616	ILE
1	C	1618	ARG
1	C	1634	GLU
1	C	1638	LEU
1	C	1639	PHE
1	C	1643	TRP
1	C	1644	ASN
1	C	1648	ASN

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Mol	Chain	Res	Type
1	C	1651	LYS
1	C	1653	PHE
1	C	1654	GLN
1	C	1655	TYR
1	C	1664	GLU
1	C	1675	VAL
1	C	1705	LEU
1	C	1731	ARG
1	C	1735	ILE
1	C	1741	ARG
1	C	1742	LEU
1	C	1770	VAL
1	C	1777	LEU
1	C	1781	GLN
1	C	1786	ASN
1	C	1802	LYS
1	C	1824	LYS
1	C	1843	VAL
1	C	1875	LYS
1	C	1909	ASN
1	C	1910	PRO
1	C	1924	TRP
1	C	1930	PHE
1	C	1945	LEU
1	C	1960	GLN
1	C	2031	VAL
1	C	2035	PHE
1	C	2036	ARG
1	C	2037	ARG
1	C	2081	GLU
1	C	2088	GLN
1	C	2106	LYS
1	C	2116	THR
1	C	2128	ARG
1	C	2145	GLU
1	C	2192	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1540	ASN

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Mol	Chain	Res	Type
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1648	ASN
1	A	1673	ASN
1	A	1683	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1786	ASN
1	A	1815	ASN
1	A	1918	GLN
1	A	1934	GLN
1	A	1965	ASN
1	A	2008	ASN
1	A	2028	GLN
1	A	2092	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	GLN
1	A	2170	GLN
1	A	2178	ASN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1781	GLN
1	B	1790	HIS
1	B	1815	ASN
1	B	1837	ASN
1	B	1911	ASN

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Mol	Chain	Res	Type
1	B	1918	GLN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2178	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN
1	C	1581	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1648	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1786	ASN
1	C	1815	ASN
1	C	1909	ASN
1	C	1918	GLN
1	C	1941	ASN
1	C	1960	GLN
1	C	2011	GLN
1	C	2088	GLN
1	C	2142	GLN
1	C	2170	GLN

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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADE	C	3196	-	8,11,11	1.55	2 (25%)	4,15,15	1.63	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADE	C	3196	-	-	0/0/0/0	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3196	ADE	C4-N9	2.27	1.39	1.34
2	C	3196	ADE	C2-N3	2.84	1.37	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3196	ADE	N3-C2-N1	-2.76	126.78	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	667/805 (82%)	-0.02	30 (4%)	37	36	20, 36, 74, 88	0
1	B	667/805 (82%)	0.08	49 (7%)	18	16	21, 38, 77, 94	0
1	C	655/805 (81%)	0.05	36 (5%)	29	27	23, 39, 77, 92	0
All	All	1989/2415 (82%)	0.04	115 (5%)	26	25	20, 38, 76, 94	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1480	LEU	6.8
1	B	2143	VAL	6.6
1	B	2194	PHE	6.5
1	B	2191	LEU	6.4
1	C	2194	PHE	6.3
1	B	2195	ALA	6.2
1	C	2195	ALA	5.8
1	B	2144	GLY	5.6
1	A	2194	PHE	5.6
1	B	2193	SER	5.0
1	C	2193	SER	5.0
1	A	1483	ILE	4.7
1	A	1681	VAL	4.6
1	B	2189	LEU	4.5
1	B	1646	ALA	4.3
1	C	1682	ILE	4.3
1	C	2143	VAL	4.3
1	B	1481	ARG	4.2
1	B	2083	LEU	4.2
1	B	1685	GLU	4.1
1	A	1481	ARG	4.1
1	A	1685	GLU	4.1
1	C	2144	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	2191	LEU	4.0
1	C	2037	ARG	4.0
1	C	1681	VAL	3.8
1	A	1646	ALA	3.8
1	A	1684	GLY	3.7
1	B	1480	LEU	3.7
1	B	1681	VAL	3.7
1	A	1669	PHE	3.7
1	B	1680	THR	3.7
1	A	2143	VAL	3.6
1	C	1647	ALA	3.6
1	A	1683	ASN	3.5
1	C	1680	THR	3.5
1	B	2037	ARG	3.5
1	C	2191	LEU	3.5
1	B	2041	LEU	3.4
1	B	1647	ALA	3.3
1	A	2193	SER	3.3
1	C	2192	GLU	3.2
1	C	2082	LEU	3.2
1	A	1910	PRO	3.1
1	A	2144	GLY	3.1
1	C	1669	PHE	3.1
1	C	1910	PRO	3.1
1	C	1685	GLU	3.0
1	B	2045	ASN	3.0
1	A	1668	LYS	3.0
1	C	1855	GLY	3.0
1	B	1839	GLU	2.9
1	B	1669	PHE	2.9
1	C	1648	ASN	2.9
1	B	2192	GLU	2.9
1	B	1838	ASP	2.9
1	C	1668	LYS	2.9
1	A	1853	GLU	2.8
1	A	1838	ASP	2.8
1	B	1584	VAL	2.8
1	B	1911	ASN	2.8
1	B	2046	ARG	2.7
1	B	1648	ASN	2.7
1	B	1683	ASN	2.7
1	A	2084	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1683	ASN	2.7
1	C	2045	ASN	2.7
1	B	1684	GLY	2.7
1	C	1679	ARG	2.6
1	B	1586	ALA	2.6
1	B	1682	ILE	2.6
1	B	1651	LYS	2.6
1	A	1492	TRP	2.6
1	C	1649	PRO	2.5
1	A	2037	ARG	2.5
1	B	1824	LYS	2.5
1	B	2085	ILE	2.5
1	C	2141	HIS	2.4
1	A	2036	ARG	2.4
1	C	1664	GLU	2.4
1	B	2190	LYS	2.4
1	C	1853	GLU	2.4
1	B	2188	GLY	2.4
1	B	1679	ARG	2.4
1	C	1655	TYR	2.4
1	C	2041	LEU	2.3
1	C	2083	LEU	2.3
1	A	1839	GLU	2.3
1	C	2036	ARG	2.3
1	A	2082	LEU	2.3
1	B	1670	ASP	2.3
1	C	1546	GLU	2.3
1	A	2045	ASN	2.3
1	C	2085	ILE	2.3
1	C	1645	ASP	2.2
1	B	1668	LYS	2.2
1	C	1911	ASN	2.2
1	B	1530	VAL	2.2
1	A	1679	ARG	2.2
1	B	2146	ALA	2.2
1	B	1644	ASN	2.2
1	B	2187	LYS	2.2
1	A	1680	THR	2.1
1	B	1585	VAL	2.1
1	B	1653	PHE	2.1
1	B	1687	ARG	2.1
1	C	1644	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1686	GLU	2.1
1	A	1529	ASP	2.1
1	A	1651	LYS	2.1
1	B	1652	GLY	2.1
1	B	2179	TYR	2.0
1	A	1645	ASP	2.0
1	B	1649	PRO	2.0
1	B	1910	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ADE	C	3196	10/10	0.69	0.36	5.24	86,87,87,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.