



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:41 PM UTC

PDB ID : 1UYV / pdb_00001uyv
Title : Acetyl-CoA carboxylase carboxyltransferase domain L1705I/V1967I mutant
Authors : Zhang, H.; Tweel, B.; Tong, L.
Deposited on : 2004-03-02
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

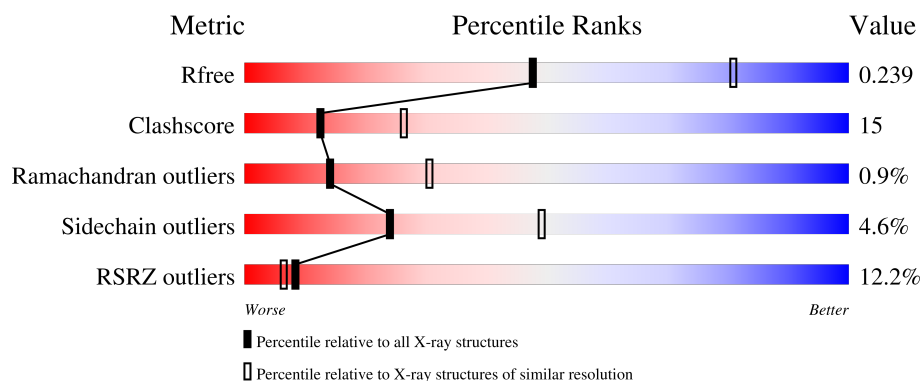
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	9% 53% 23% • 22%
1	B	737	9% 50% 23% • 25%
1	C	737	10% 52% 23% • 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13666 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	1
			4542	2895	786	845	16			
1	B	553	Total	C	N	O	S	0	0	1
			4399	2805	759	821	14			
1	C	571	Total	C	N	O	S	0	0	1
			4533	2884	786	847	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1705	ILE	LEU	engineered mutation	UNP Q00955
A	1967	ILE	VAL	engineered mutation	UNP Q00955
B	1705	ILE	LEU	engineered mutation	UNP Q00955
B	1967	ILE	VAL	engineered mutation	UNP Q00955
C	1705	ILE	LEU	engineered mutation	UNP Q00955
C	1967	ILE	VAL	engineered mutation	UNP Q00955

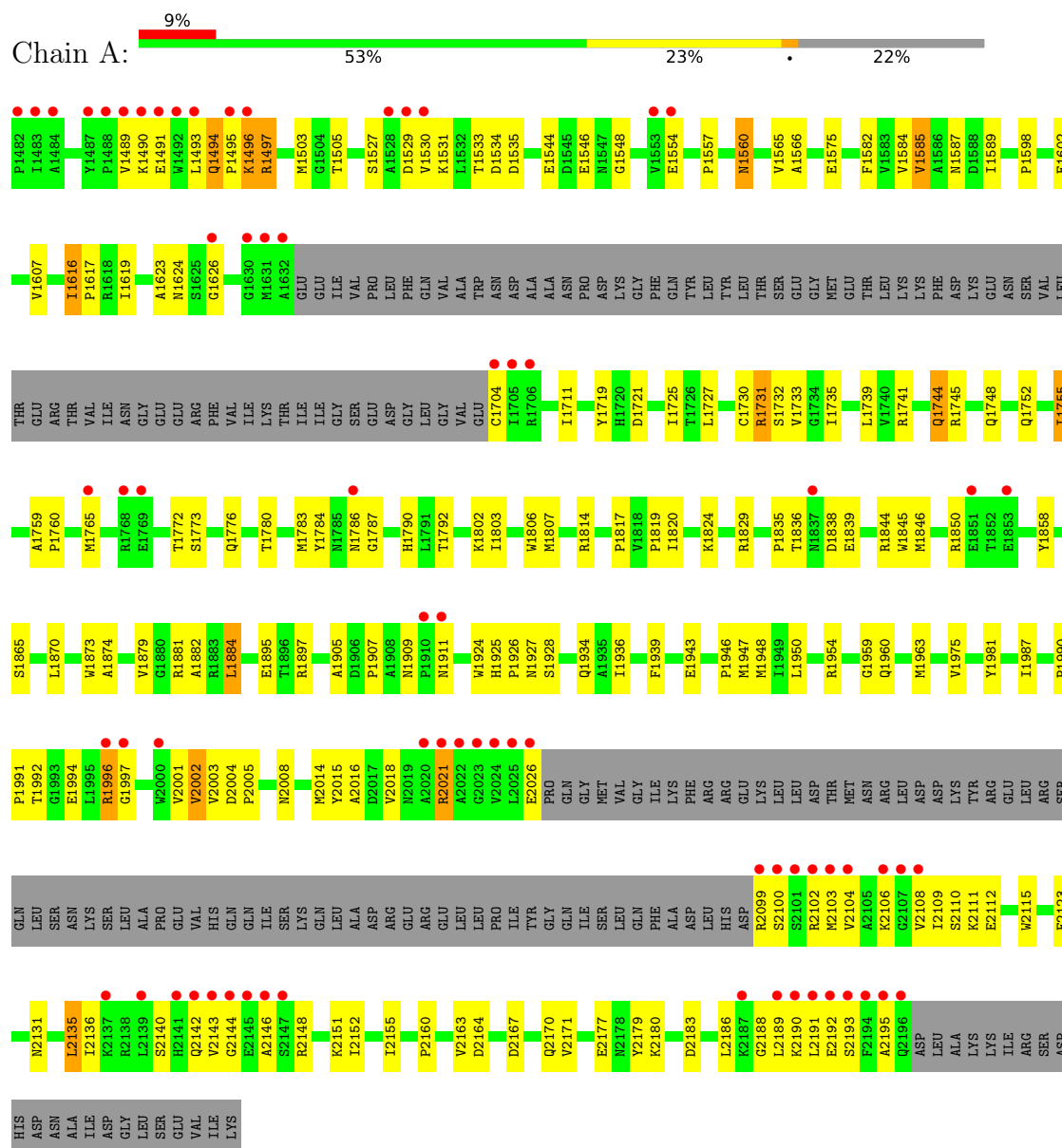
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	68	Total	O	0	0
			68	68		
2	C	49	Total	O	0	0
			49	49		

3 Residue-property plots

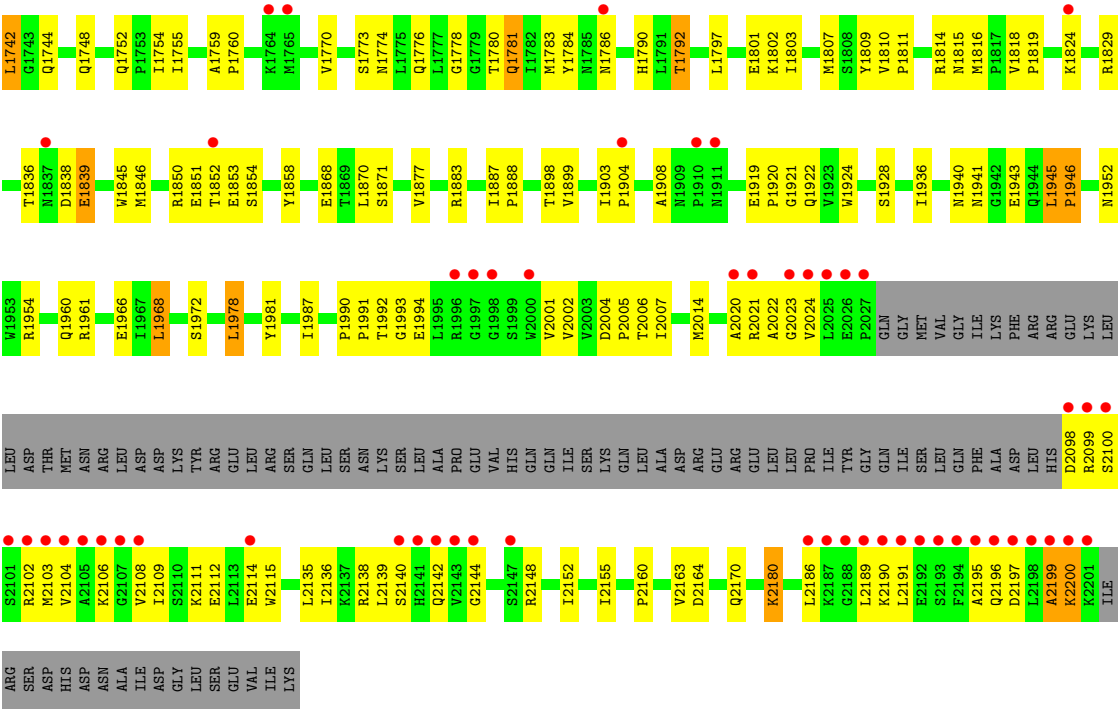
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ACETYL-COA CARBOXYLASE



• Molecule 1: ACETYL-COA CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.17Å 123.73Å 145.64Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	27.56 – 2.60 27.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.2 (27.56-2.60) 92.5 (27.56-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.237 0.213 , 0.239	Depositor DCC
R_{free} test set	12751 reflections (9.38%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13666	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	1/4647 (0.0%)	0.87	7/6299 (0.1%)
1	B	0.47	1/4503 (0.0%)	0.88	8/6109 (0.1%)
1	C	0.45	1/4635 (0.0%)	0.82	4/6280 (0.1%)
All	All	0.46	3/13785 (0.0%)	0.86	19/18688 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2195	ALA	C-N	-5.56	1.25	1.33
1	C	2200	LYS	C-N	-5.45	1.25	1.33
1	B	2189	LEU	C-N	-5.34	1.25	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1946	PRO	N-CA-C	-7.18	100.43	111.13
1	A	1494	GLN	CA-C-N	6.79	126.48	119.56
1	A	1494	GLN	C-N-CA	6.79	126.48	119.56
1	C	1946	PRO	N-CA-C	-6.75	101.78	111.22
1	B	1946	PRO	N-CA-C	-6.16	102.60	111.22
1	B	1787	GLY	N-CA-C	-5.74	107.46	114.92
1	B	1966	GLU	N-CA-C	5.62	119.43	112.24
1	A	1787	GLY	N-CA-C	-5.55	106.87	114.64
1	C	1579	GLY	N-CA-C	5.52	118.95	111.72
1	A	1755	ILE	N-CA-C	5.49	117.30	108.85
1	B	2012	MET	N-CA-C	5.47	118.57	110.48
1	C	1733	VAL	N-CA-C	5.43	117.21	108.85
1	B	1847	ILE	N-CA-C	5.40	115.49	110.42
1	A	2004	ASP	CA-C-N	5.34	125.15	119.28
1	A	2004	ASP	C-N-CA	5.34	125.15	119.28
1	B	1494	GLN	CA-C-N	5.32	124.98	119.56
1	B	1494	GLN	C-N-CA	5.32	124.98	119.56
1	B	1712	ALA	N-CA-C	-5.21	105.49	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1966	GLU	N-CA-C	5.10	118.80	112.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4542	0	4484	137	0
1	B	4399	0	4326	144	0
1	C	4533	0	4467	142	0
2	A	75	0	0	0	0
2	B	68	0	0	1	0
2	C	49	0	0	3	0
All	All	13666	0	13277	408	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 15.

All (408) 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:C:2144:GLY:HA3	1:C:2197:ASP:HB3	1.46	0.94
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.07	0.92
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.97	0.92
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.36	0.90
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.16	0.90
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.54	0.87
1:B:1766:LEU:HD13	1:B:1770:VAL:HG21	1.57	0.87
1:A:1846:MET:HE1	1:A:1990:PRO:HB3	1.57	0.86
1:A:2164:ASP:H	1:A:2170:GLN:NE2	1.74	0.86
1:B:1705:ILE:HD13	1:B:1705:ILE:H	1.39	0.86
1:A:1496:LYS:H	1:A:1496:LYS:HD2	1.41	0.86
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.74	0.85
1:A:1909:ASN:HD21	1:A:1911:ASN:HB3	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.58	0.83
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.26	0.81
1:B:1843:VAL:HG11	1:B:1894:VAL:O	1.80	0.81
1:C:1987:ILE:HG21	1:C:2014:MET:HE2	1.61	0.80
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.27	0.80
1:A:1494:GLN:HE22	1:A:1557:PRO:HB2	1.46	0.80
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.30	0.80
1:A:1497:ARG:HH11	1:A:1497:ARG:HB2	1.47	0.79
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.29	0.79
1:B:2007:ILE:HB	1:B:2012:MET:HE1	1.65	0.78
1:B:1852:THR:HG23	1:B:1855:GLY:H	1.48	0.78
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.28	0.77
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.34	0.75
1:C:1493:LEU:HD21	1:C:1557:PRO:HB2	1.68	0.75
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.54	0.72
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	1.71	0.72
1:A:2100:SER:HA	1:A:2103:MET:HE3	1.71	0.72
1:B:1836:THR:HB	1:B:1839:GLU:HB2	1.70	0.72
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.73	0.71
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.73	0.71
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.72	0.70
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.73	0.69
1:C:2142:GLN:HB3	1:C:2190:LYS:HG2	1.73	0.69
1:C:2104:VAL:HG22	1:C:2109:ILE:HD11	1.74	0.69
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.82	0.69
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	1.74	0.69
1:B:1827:TRP:HA	1:B:2119:ARG:HH11	1.57	0.69
1:B:1776:GLN:O	1:C:1960:GLN:HG3	1.94	0.68
1:B:1533:THR:HB	1:B:1535:ASP:OD1	1.94	0.68
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.40	0.68
1:B:1511:PHE:HZ	1:B:1729:THR:HG21	1.60	0.67
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.77	0.67
1:B:1585:VAL:HG22	1:B:1607:VAL:HG11	1.75	0.67
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	1.76	0.67
1:C:1852:THR:HG22	1:C:1854:SER:H	1.60	0.67
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.82	0.66
1:C:1630:GLY:HA2	1:C:1701:GLY:HA2	1.78	0.66
1:B:2008:ASN:N	1:B:2012:MET:HE3	2.11	0.65
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.42	0.65
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.93	0.65
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.61	0.64
1:C:1846:MET:HE1	1:C:1990:PRO:HB2	1.79	0.64
1:C:1921:GLY:HA2	2:C:3029:HOH:O	1.97	0.64
1:A:1773:SER:H	1:A:1776:GLN:NE2	1.96	0.63
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.11	0.63
1:C:2164:ASP:H	1:C:2170:GLN:NE2	1.97	0.63
1:C:2020:ALA:O	1:C:2021:ARG:HG2	1.99	0.62
1:C:2138:ARG:HH11	1:C:2138:ARG:HB3	1.65	0.62
1:A:1491:GLU:O	1:A:1495:PRO:HA	2.00	0.62
1:B:1735:ILE:HD13	1:B:1735:ILE:O	2.00	0.62
1:A:1546:GLU:CD	1:A:1546:GLU:H	2.07	0.61
1:C:1824:LYS:H	1:C:1824:LYS:HE2	1.65	0.61
1:B:1511:PHE:CZ	1:B:1729:THR:HG21	2.35	0.61
1:C:2196:GLN:NE2	1:C:2200:LYS:HD3	2.15	0.61
1:A:1909:ASN:ND2	1:A:1911:ASN:HB3	2.14	0.61
1:C:1922:GLN:CD	1:C:1954:ARG:HH12	2.08	0.60
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.49	0.60
1:B:1705:ILE:H	1:B:1705:ILE:CD1	2.12	0.60
1:A:1939:PHE:HD1	1:A:1947:MET:HE2	1.66	0.60
1:A:2003:VAL:HG12	1:A:2003:VAL:O	2.00	0.60
1:A:1936:ILE:HG23	1:A:1947:MET:HE1	1.83	0.59
1:C:1877:VAL:HG23	1:C:1928:SER:HB2	1.84	0.59
1:C:2100:SER:HA	1:C:2103:MET:CE	2.32	0.59
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.02	0.59
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.95	0.59
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	1.84	0.59
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.83	0.59
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.84	0.59
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.83	0.59
1:C:2139:LEU:O	1:C:2142:GLN:HG2	2.03	0.59
1:A:2189:LEU:O	1:A:2192:GLU:HG2	2.03	0.58
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.36	0.58
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.33	0.58
1:C:1773:SER:HB3	1:C:1776:GLN:HE21	1.69	0.58
1:C:1582:PHE:CD2	1:C:1807:MET:HE1	2.38	0.58
1:A:2190:LYS:C	1:A:2192:GLU:H	2.10	0.58
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.34	0.58
1:A:1497:ARG:HH11	1:A:1497:ARG:CB	2.17	0.58
1:B:1705:ILE:HD13	1:B:1705:ILE:N	2.16	0.58
1:A:1835:PRO:HB2	1:A:1992:THR:HG23	1.85	0.58
1:C:1759:ALA:N	1:C:1774:ASN:HD21	1.88	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1773:SER:N	1:C:1776:GLN:NE2	2.52	0.57
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.70	0.57
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.05	0.57
1:A:2021:ARG:NH1	1:A:2021:ARG:HB3	2.20	0.57
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.86	0.57
1:C:1513:GLU:O	1:C:1517:GLN:HG3	2.05	0.57
1:C:2138:ARG:O	1:C:2190:LYS:HD3	2.04	0.57
1:B:1494:GLN:NE2	1:B:1496:LYS:HG3	2.21	0.56
1:A:2183:ASP:OD1	1:B:1482:PRO:HD3	2.06	0.56
1:C:2195:ALA:O	1:C:2199:ALA:HB3	2.06	0.56
1:C:2100:SER:HB2	1:C:2112:GLU:OE2	2.06	0.56
1:A:1996:ARG:HD2	1:A:1996:ARG:N	2.21	0.56
1:C:1790:HIS:HD2	2:C:3027:HOH:O	1.89	0.56
1:A:1598:PRO:HG3	1:A:1704:CYS:HA	1.88	0.56
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.88	0.56
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.06	0.55
1:A:1503:MET:HG2	1:A:1589:ILE:HG12	1.87	0.55
1:A:2110:SER:O	1:A:2111:LYS:HG3	2.06	0.55
1:B:1494:GLN:HG3	1:B:1496:LYS:HB2	1.89	0.55
1:A:1975:VAL:HG23	1:A:2002:VAL:HG23	1.89	0.55
1:B:1582:PHE:HA	1:B:1616:ILE:CG2	2.32	0.55
1:C:1560:ASN:ND2	1:C:1560:ASN:H	2.05	0.55
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.07	0.55
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.42	0.55
1:A:1954:ARG:HG2	1:A:1994:GLU:OE2	2.07	0.55
1:C:1868:GLU:HG2	1:C:1871:SER:HB3	1.88	0.55
1:A:2021:ARG:HH12	1:A:2099:ARG:HH12	1.54	0.55
1:B:1494:GLN:CD	1:B:1496:LYS:HD2	2.32	0.55
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.87	0.54
1:B:1491:GLU:HG3	1:B:1497:ARG:HB3	1.88	0.54
1:B:2187:LYS:C	1:B:2189:LEU:H	2.16	0.54
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.07	0.54
1:B:2008:ASN:H	1:B:2012:MET:HE3	1.73	0.53
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.38	0.53
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.89	0.53
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.90	0.53
1:B:2013:GLU:OE1	1:B:2125:ARG:NH2	2.42	0.53
1:B:2156:ARG:HG2	1:B:2159:TYR:CE1	2.43	0.53
1:C:1936:ILE:HD13	1:C:1978:LEU:CD1	2.39	0.53
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.73	0.53
1:C:1568:LYS:HE2	1:C:1581:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1706:ARG:HB2	1:C:2108:VAL:HG12	1.90	0.52
1:B:2000:TRP:NE1	1:C:1705:ILE:HG23	2.24	0.52
1:C:1730:CYS:O	1:C:1731:ARG:C	2.51	0.52
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.10	0.52
1:A:1792:THR:O	1:A:1802:LYS:HE3	2.08	0.52
1:A:1927:ASN:OD1	1:A:1928:SER:N	2.43	0.52
1:C:1845:TRP:CE2	1:C:1850:ARG:HD3	2.44	0.52
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.18	0.52
1:B:1587:ASN:ND2	1:B:1623:ALA:H	2.03	0.52
1:C:1623:ALA:HB2	1:C:1729:THR:HG23	1.91	0.52
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.92	0.52
1:B:1998:GLY:O	1:B:2001:VAL:HG12	2.09	0.51
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.57	0.51
1:A:1987:ILE:HB	1:A:2014:MET:HG3	1.92	0.51
1:A:1711:ILE:HD11	1:A:1735:ILE:HG12	1.92	0.51
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.24	0.51
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.25	0.51
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.10	0.51
1:C:1952:ASN:OD1	1:C:1993:GLY:HA2	2.09	0.51
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.18	0.51
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.09	0.51
1:A:1560:ASN:H	1:A:1560:ASN:ND2	2.08	0.51
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.41	0.51
1:A:1497:ARG:HB2	1:A:1497:ARG:NH1	2.21	0.50
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.93	0.50
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.93	0.50
1:C:2148:ARG:HG2	1:C:2148:ARG:HH11	1.76	0.50
1:A:1909:ASN:ND2	1:A:1911:ASN:H	2.09	0.50
1:B:1489:VAL:HG23	1:B:1492:TRP:HB3	1.93	0.50
1:B:1954:ARG:HG2	1:B:1994:GLU:OE2	2.11	0.50
1:C:1845:TRP:CD2	1:C:1850:ARG:HD3	2.47	0.50
1:C:2100:SER:HA	1:C:2103:MET:HE3	1.94	0.50
1:C:2138:ARG:HB3	1:C:2138:ARG:NH1	2.27	0.50
1:A:2100:SER:O	1:A:2104:VAL:HG23	2.11	0.49
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.20	0.49
1:B:2015:TYR:HB3	1:B:2113:LEU:HD21	1.94	0.49
1:C:1528:ALA:O	1:C:1530:VAL:HG22	2.11	0.49
1:C:2111:LYS:HG2	1:C:2112:GLU:N	2.27	0.49
1:B:1582:PHE:CD2	1:B:1807:MET:HE1	2.47	0.49
1:C:1741:ARG:HD3	1:C:1741:ARG:C	2.37	0.49
1:A:1721:ASP:OD2	1:A:1814:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1873:TRP:O	1:B:1874:ALA:C	2.55	0.49
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.12	0.49
1:A:1873:TRP:O	1:A:1874:ALA:C	2.56	0.49
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.94	0.49
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.13	0.49
1:C:2004:ASP:OD2	1:C:2005:PRO:HD2	2.13	0.49
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.94	0.49
1:A:1881:ARG:CZ	1:A:1939:PHE:HE2	2.26	0.48
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.48	0.48
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.94	0.48
1:A:2190:LYS:C	1:A:2192:GLU:N	2.71	0.48
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.48	0.48
1:B:1991:PRO:HG3	1:B:2017:ASP:CG	2.38	0.48
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.48	0.48
1:A:2021:ARG:HB3	1:A:2021:ARG:CZ	2.43	0.48
1:C:1773:SER:N	1:C:1776:GLN:HE22	2.11	0.48
1:C:2196:GLN:HE22	1:C:2200:LYS:HD3	1.78	0.48
1:B:1987:ILE:HG21	1:B:2014:MET:HE2	1.94	0.48
1:A:1544:GLU:HB3	1:A:1548:GLY:HA2	1.96	0.48
1:A:2146:ALA:O	1:A:2151:LYS:HE3	2.12	0.48
1:C:1754:ILE:O	1:C:1778:GLY:HA3	2.14	0.48
1:C:2100:SER:HA	1:C:2103:MET:HE2	1.94	0.48
1:C:2195:ALA:C	1:C:2199:ALA:HB3	2.39	0.47
1:A:1489:VAL:O	1:A:1493:LEU:HG	2.14	0.47
1:A:1527:SER:OG	1:A:1530:VAL:HG13	2.14	0.47
1:B:1991:PRO:O	1:B:1992:THR:OG1	2.31	0.47
1:C:1943:GLU:O	1:C:1945:LEU:HD13	2.14	0.47
1:C:2111:LYS:HG2	1:C:2112:GLU:O	2.13	0.47
1:B:1491:GLU:HG2	1:B:1498:TYR:HB2	1.95	0.47
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.13	0.47
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.14	0.47
1:C:1626:GLY:N	1:C:1733:VAL:HB	2.29	0.47
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.44	0.47
1:A:1824:LYS:HE2	1:A:1824:LYS:H	1.78	0.47
1:B:1820:ILE:HD13	1:B:1887:ILE:HA	1.97	0.47
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.48	0.47
1:B:2000:TRP:CE2	1:C:1705:ILE:HG23	2.49	0.47
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.44	0.47
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.45	0.47
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.12	0.47
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1768:ARG:HG2	1:B:1768:ARG:HH11	1.79	0.47
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.14	0.47
1:C:2148:ARG:HG2	1:C:2148:ARG:NH1	2.30	0.47
1:C:1509:TYR:HE1	1:C:1560:ASN:ND2	2.12	0.47
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.29	0.47
1:C:1838:ASP:O	1:C:1839:GLU:HB2	2.14	0.47
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.96	0.47
1:B:2129:ARG:HG3	1:B:2129:ARG:HH11	1.79	0.47
1:A:1582:PHE:CD2	1:A:1807:MET:HE1	2.49	0.46
1:C:2022:ALA:HB3	1:C:2103:MET:SD	2.55	0.46
1:A:1836:THR:HB	1:A:1839:GLU:HB2	1.97	0.46
1:C:2021:ARG:NH2	1:C:2099:ARG:HE	2.14	0.46
1:B:2008:ASN:HB3	1:B:2012:MET:HE3	1.97	0.46
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.97	0.46
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.23	0.46
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.97	0.46
1:A:1730:CYS:O	1:A:1731:ARG:HB2	2.16	0.46
1:C:1713:GLY:O	1:C:1717:ARG:HG3	2.15	0.46
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.97	0.46
1:C:1809:TYR:O	1:C:1945:LEU:HD11	2.15	0.46
1:B:1756:LEU:HD21	1:C:1968:LEU:HD11	1.96	0.46
1:B:2113:LEU:HD23	1:B:2113:LEU:N	2.31	0.46
1:C:1603:PHE:O	1:C:1607:VAL:HG23	2.16	0.46
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.15	0.46
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	1.96	0.46
1:B:1983:GLN:HB3	1:B:1984:PRO:HD2	1.98	0.46
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.15	0.46
1:A:2186:LEU:C	1:A:2188:GLY:H	2.23	0.46
1:B:1491:GLU:O	1:B:1495:PRO:HA	2.16	0.46
1:C:1569:ILE:HG22	1:C:1571:VAL:HG23	1.97	0.46
1:B:1490:LYS:HE2	1:B:1497:ARG:CZ	2.45	0.45
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.16	0.45
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.98	0.45
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.49	0.45
1:C:2180:LYS:HE2	1:C:2180:LYS:HA	1.98	0.45
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.97	0.45
1:A:2140:SER:O	1:A:2144:GLY:HA2	2.17	0.45
1:A:2177:GLU:O	1:B:1501:HIS:HE1	1.99	0.45
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.16	0.45
1:C:1797:LEU:O	1:C:1801:GLU:HG3	2.17	0.45
1:A:1745:ARG:NH1	1:A:1943:GLU:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.17	0.45
1:C:1792:THR:O	1:C:1802:LYS:HE3	2.16	0.45
1:C:2190:LYS:C	1:C:2191:LEU:HD12	2.41	0.45
1:A:1845:TRP:CE2	1:A:1850:ARG:HD3	2.51	0.45
1:C:1898:THR:HG22	1:C:1920:PRO:HA	1.99	0.45
1:C:1903:ILE:N	1:C:1903:ILE:HD12	2.31	0.45
1:B:1550:LEU:HD12	1:B:1610:TYR:HB2	1.99	0.45
1:B:1792:THR:O	1:B:1802:LYS:HE3	2.17	0.45
1:B:2134:TYR:O	1:B:2138:ARG:HG3	2.17	0.45
1:C:2004:ASP:O	1:C:2007:ILE:HG13	2.17	0.45
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.17	0.45
1:B:1494:GLN:HB3	1:B:1497:ARG:HH21	1.81	0.45
1:B:1578:ARG:HH11	1:B:1578:ARG:HG2	1.81	0.45
1:B:1996:ARG:HA	1:B:1996:ARG:HD3	1.82	0.45
1:A:1987:ILE:HG21	1:A:2014:MET:HE2	1.99	0.45
1:B:1530:VAL:O	1:B:1530:VAL:HG13	2.16	0.45
1:C:1507:TYR:HB3	1:C:1510:ASP:OD2	2.17	0.45
1:C:1940:ASN:HB2	1:C:1981:TYR:CE1	2.52	0.45
1:A:1936:ILE:HA	1:A:1947:MET:CE	2.47	0.45
1:B:1494:GLN:HB3	1:B:1497:ARG:NH2	2.32	0.45
1:A:1505:THR:HB	1:A:1730:CYS:HB2	1.99	0.44
1:A:1865:SER:O	1:A:1882:ALA:HA	2.18	0.44
1:B:2151:LYS:O	1:B:2155:ILE:HG13	2.17	0.44
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.47	0.44
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	2.00	0.44
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.99	0.44
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.46	0.44
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.18	0.44
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.10	0.44
1:C:2140:SER:C	1:C:2142:GLN:H	2.26	0.44
1:B:1843:VAL:CG1	1:B:1894:VAL:O	2.57	0.44
1:B:2013:GLU:CD	1:B:2125:ARG:HH21	2.25	0.44
1:C:1824:LYS:H	1:C:1824:LYS:CE	2.29	0.44
1:A:2143:VAL:HB	1:A:2192:GLU:OE1	2.17	0.44
1:C:2148:ARG:O	1:C:2152:ILE:HG12	2.18	0.44
1:A:2014:MET:HG2	1:A:2015:TYR:N	2.33	0.44
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.82	0.44
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.99	0.44
1:B:1762:ILE:HD12	1:B:1777:LEU:HD21	1.99	0.44
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	2.00	0.44
1:C:1816:MET:HE2	2:C:3021:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1607:VAL:O	1:B:1610:TYR:HB3	2.18	0.43
1:C:1592:LYS:C	1:C:1593:ILE:HG12	2.43	0.43
1:C:1954:ARG:HG3	1:C:1954:ARG:HH11	1.82	0.43
1:A:2186:LEU:C	1:A:2188:GLY:N	2.77	0.43
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.48	0.43
1:A:1490:LYS:HE3	1:A:1497:ARG:NH2	2.33	0.43
1:B:1578:ARG:HG2	1:B:1578:ARG:NH1	2.33	0.43
1:B:1894:VAL:HG11	1:B:1922:GLN:HA	1.99	0.43
1:B:2128:ARG:HE	1:B:2132:GLU:CD	2.26	0.43
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	2.01	0.43
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.19	0.43
1:A:2102:ARG:O	1:A:2106:LYS:HG2	2.19	0.43
1:B:1582:PHE:CD1	1:B:1619:ILE:HD13	2.53	0.43
1:C:1836:THR:HB	1:C:1839:GLU:HB3	2.01	0.43
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.15	0.43
1:B:2004:ASP:OD1	1:B:2005:PRO:HD2	2.19	0.43
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.82	0.43
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.48	0.43
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	1.99	0.43
1:C:1741:ARG:HD3	1:C:1741:ARG:O	2.19	0.43
1:C:2135:LEU:HD13	1:C:2155:ILE:HG23	1.99	0.43
1:B:1821:LEU:O	1:B:1886:GLY:HA2	2.19	0.43
1:B:2143:VAL:C	1:B:2145:GLU:H	2.26	0.43
1:B:1766:LEU:HD23	1:B:1766:LEU:O	2.19	0.43
1:B:1951:ALA:HB1	1:B:1995:LEU:HD13	2.01	0.43
1:C:1704:CYS:SG	1:C:1705:ILE:N	2.91	0.43
1:C:2142:GLN:CB	1:C:2190:LYS:HG2	2.46	0.43
1:B:1511:PHE:CD2	1:B:1514:LEU:HD12	2.53	0.43
1:B:2002:VAL:HG23	1:B:2003:VAL:HG13	2.01	0.43
1:A:1947:MET:HE3	1:A:1981:TYR:CE1	2.54	0.42
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.31	0.42
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.66	0.42
1:B:1730:CYS:O	1:B:1731:ARG:HB3	2.19	0.42
1:B:1742:LEU:HD23	1:C:1972:SER:HB3	2.01	0.42
1:B:1925:HIS:O	1:B:1926:PRO:C	2.61	0.42
1:B:1964:PHE:O	1:C:1786:ASN:ND2	2.52	0.42
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.34	0.42
1:C:2102:ARG:NH1	1:C:2106:LYS:HE2	2.35	0.42
1:A:2135:LEU:HB3	1:A:2155:ILE:CD1	2.39	0.42
1:B:2004:ASP:HB3	1:C:1709:GLY:HA3	2.00	0.42
1:C:2023:GLY:HA3	1:C:2098:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.35	0.42
1:B:1592:LYS:O	1:B:1593:ILE:CG1	2.67	0.42
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.34	0.42
1:C:2104:VAL:CG2	1:C:2109:ILE:HD11	2.47	0.42
1:A:1626:GLY:N	1:A:1733:VAL:HB	2.34	0.42
1:B:1508:VAL:HG23	1:B:1509:TYR:H	1.83	0.42
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.53	0.42
1:C:1719:TYR:O	1:C:1941:ASN:HB3	2.19	0.42
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.54	0.42
1:A:1996:ARG:NH2	1:A:2026:GLU:HG2	2.35	0.42
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.20	0.42
1:B:1776:GLN:O	1:B:1782:ILE:HD11	2.20	0.42
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.85	0.42
1:C:2021:ARG:NH2	1:C:2099:ARG:HH21	2.18	0.42
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	2.01	0.42
1:B:1837:ASN:HA	1:B:2021:ARG:HH21	1.83	0.41
1:C:1991:PRO:C	1:C:1992:THR:HG23	2.45	0.41
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.02	0.41
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.29	0.41
1:A:1905:ALA:O	1:A:1907:PRO:HD3	2.20	0.41
1:A:2018:VAL:HG12	1:A:2112:GLU:OE1	2.19	0.41
1:C:2001:VAL:HG13	1:C:2002:VAL:HG13	2.02	0.41
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	2.02	0.41
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.19	0.41
1:B:1924:TRP:HZ3	1:B:1999:SER:HB2	1.86	0.41
1:C:1545:ASP:HB2	1:C:1546:GLU:OE2	2.20	0.41
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.36	0.41
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	2.01	0.41
1:B:1843:VAL:HG13	2:B:3045:HOH:O	2.20	0.41
1:B:1948:MET:HA	1:B:1986:ILE:O	2.20	0.41
1:A:1824:LYS:H	1:A:1824:LYS:CE	2.33	0.41
1:C:1770:VAL:HG21	1:C:1908:ALA:HA	2.01	0.41
1:A:1925:HIS:O	1:A:1926:PRO:C	2.63	0.41
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	2.02	0.41
1:A:2008:ASN:C	1:A:2008:ASN:ND2	2.79	0.41
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	2.02	0.41
1:A:1616:ILE:HA	1:A:1617:PRO:HD3	1.94	0.41
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.69	0.41
1:A:1844:ARG:HG3	1:A:1844:ARG:NH1	2.34	0.41
1:B:2007:ILE:HB	1:B:2012:MET:CE	2.43	0.41
1:B:2132:GLU:O	1:B:2136:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.21	0.41
1:B:1705:ILE:HG23	1:C:2024:VAL:HG22	2.03	0.41
1:B:1768:ARG:HG2	1:B:1768:ARG:NH1	2.36	0.41
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	2.03	0.41
1:C:1731:ARG:CB	1:C:1731:ARG:HH11	2.34	0.41
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.57	0.40
1:A:1947:MET:HG2	1:A:1948:MET:N	2.34	0.40
1:A:2148:ARG:O	1:A:2152:ILE:HG22	2.21	0.40
1:A:2189:LEU:C	1:A:2191:LEU:N	2.77	0.40
1:B:1511:PHE:O	1:B:1512:PRO:C	2.64	0.40
1:C:1781:GLN:HE21	1:C:1781:GLN:N	2.09	0.40
1:A:1531:LYS:HA	1:A:1531:LYS:HE2	2.03	0.40
1:A:2180:LYS:O	1:A:2183:ASP:HB3	2.22	0.40
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.02	0.40
1:C:1810:VAL:HG13	1:C:1811:PRO:HD2	2.03	0.40
1:A:1939:PHE:CD1	1:A:1947:MET:HE2	2.52	0.40
1:A:2167:ASP:O	1:A:2171:VAL:HG23	2.20	0.40
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	2.03	0.40
1:B:2001:VAL:O	1:B:2007:ILE:HD11	2.21	0.40
1:C:1560:ASN:H	1:C:1560:ASN:HD22	1.69	0.40
1:A:1533:THR:HB	1:A:1535:ASP:OD1	2.22	0.40
1:B:1619:ILE:HD12	1:B:1619:ILE:N	2.37	0.40
1:A:1626:GLY:HA2	1:A:1733:VAL:O	2.20	0.40
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.86	0.40
1:A:1759:ALA:N	1:A:1760:PRO:CD	2.85	0.40
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/737 (77%)	527 (93%)	34 (6%)	5 (1%)	14	30
1	B	547/737 (74%)	507 (93%)	37 (7%)	3 (0%)	24	46
1	C	565/737 (77%)	521 (92%)	37 (6%)	7 (1%)	10	23
All	All	1678/2211 (76%)	1555 (93%)	108 (6%)	15 (1%)	14	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1529	ASP
1	A	1731	ARG
1	A	2142	GLN
1	B	2142	GLN
1	C	2199	ALA
1	C	1744	GLN
1	B	1731	ARG
1	B	1744	GLN
1	C	1839	GLU
1	A	1744	GLN
1	A	2193	SER
1	C	1528	ALA
1	C	1508	VAL
1	C	1705	ILE
1	C	1904	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/628 (76%)	461 (96%)	19 (4%)	28	55
1	B	465/628 (74%)	444 (96%)	21 (4%)	24	50
1	C	479/628 (76%)	453 (95%)	26 (5%)	20	42
All	All	1424/1884 (76%)	1358 (95%)	66 (5%)	24	49

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1496	LYS
1	A	1497	ARG
1	A	1534	ASP
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1616	ILE
1	A	1732	SER
1	A	1765	MET
1	A	1879	VAL
1	A	1884	LEU
1	A	1924	TRP
1	A	1950	LEU
1	A	1960	GLN
1	A	1996	ARG
1	A	2002	VAL
1	A	2021	ARG
1	A	2135	LEU
1	B	1489	VAL
1	B	1491	GLU
1	B	1502	LEU
1	B	1516	ARG
1	B	1571	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1616	ILE
1	B	1618	ARG
1	B	1705	ILE
1	B	1726	THR
1	B	1732	SER
1	B	1735	ILE
1	B	1777	LEU
1	B	1786	ASN
1	B	1791	LEU
1	B	1797	LEU
1	B	1884	LEU
1	B	1924	TRP
1	B	1961	ARG
1	B	2113	LEU
1	C	1508	VAL
1	C	1536	PHE
1	C	1546	GLU

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Mol	Chain	Res	Type
1	C	1556	GLU
1	C	1560	ASN
1	C	1602	GLU
1	C	1618	ARG
1	C	1703	GLU
1	C	1705	ILE
1	C	1706	ARG
1	C	1731	ARG
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1781	GLN
1	C	1792	THR
1	C	1924	TRP
1	C	1945	LEU
1	C	1961	ARG
1	C	1968	LEU
1	C	1978	LEU
1	C	2006	THR
1	C	2114	GLU
1	C	2180	LYS
1	C	2186	LEU
1	C	2189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1501	HIS
1	A	1522	GLN
1	A	1525	ASN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1790	HIS
1	A	1815	ASN

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Mol	Chain	Res	Type
1	A	1909	ASN
1	A	1911	ASN
1	A	1922	GLN
1	A	1934	GLN
1	A	2008	ASN
1	A	2131	ASN
1	A	2142	GLN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1547	ASN
1	B	1587	ASN
1	B	1599	GLN
1	B	1605	ASN
1	B	1624	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1918	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	1960	GLN
1	B	1983	GLN
1	B	2131	ASN
1	B	2178	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1581	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1786	ASN
1	C	1790	HIS

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Mol	Chain	Res	Type
1	C	1815	ASN
1	C	1911	ASN
1	C	1934	GLN
1	C	1941	ASN
1	C	2011	GLN
1	C	2142	GLN
1	C	2170	GLN
1	C	2196	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	572/737 (77%)	0.38	70 (12%) 8 6	21, 41, 93, 100	0
1	B	553/737 (75%)	0.37	65 (11%) 9 7	22, 42, 84, 100	0
1	C	571/737 (77%)	0.48	72 (12%) 8 6	23, 45, 97, 100	0
All	All	1696/2211 (76%)	0.41	207 (12%) 8 6	21, 43, 90, 100	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2024	VAL	8.6
1	C	2197	ASP	7.7
1	A	2024	VAL	7.5
1	B	1483	ILE	7.2
1	B	2108	VAL	7.1
1	A	1483	ILE	7.1
1	C	2025	LEU	6.6
1	B	2190	LYS	6.6
1	A	2195	ALA	6.5
1	A	1489	VAL	6.5
1	B	1997	GLY	6.3
1	C	1701	GLY	6.2
1	C	2027	PRO	6.1
1	A	2143	VAL	6.0
1	A	2191	LEU	6.0
1	C	2143	VAL	5.9
1	B	1492	TRP	5.8
1	C	2191	LEU	5.6
1	A	2194	PHE	5.6
1	B	2188	GLY	5.6
1	A	1632	ALA	5.5
1	A	2023	GLY	5.5
1	B	2144	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	2134	TYR	5.5
1	C	1706	ARG	5.4
1	C	2101	SER	5.4
1	B	1490	LYS	5.4
1	B	1488	PRO	5.4
1	A	1490	LYS	5.3
1	B	1482	PRO	5.3
1	C	2107	GLY	5.3
1	B	1493	LEU	5.3
1	A	2190	LYS	5.2
1	C	1629	ILE	5.2
1	A	2144	GLY	5.2
1	A	2104	VAL	5.2
1	A	2020	ALA	5.1
1	A	1492	TRP	5.0
1	A	1493	LEU	5.0
1	C	2023	GLY	5.0
1	B	2143	VAL	5.0
1	C	2194	PHE	4.9
1	B	1489	VAL	4.9
1	C	1531	LYS	4.9
1	A	1488	PRO	4.9
1	A	2100	SER	4.8
1	C	2190	LYS	4.8
1	C	2199	ALA	4.8
1	C	1704	CYS	4.7
1	C	1631	MET	4.6
1	B	2023	GLY	4.6
1	B	2022	ALA	4.5
1	A	2142	GLN	4.5
1	C	2106	LYS	4.4
1	C	2198	LEU	4.4
1	B	2145	GLU	4.3
1	C	2000	TRP	4.3
1	A	2103	MET	4.3
1	C	2141	HIS	4.3
1	B	1996	ARG	4.3
1	A	2196	GLN	4.3
1	C	2196	GLN	4.3
1	C	1702	VAL	4.2
1	B	1554	GLU	4.2
1	A	2107	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	2025	LEU	4.1
1	B	1491	GLU	4.1
1	A	1491	GLU	4.0
1	A	2022	ALA	4.0
1	C	2099	ARG	4.0
1	B	1494	GLN	3.9
1	C	2102	ARG	3.9
1	B	2189	LEU	3.9
1	B	1556	GLU	3.8
1	A	1705	ILE	3.8
1	A	2141	HIS	3.8
1	C	2189	LEU	3.7
1	B	1705	ILE	3.7
1	A	2106	LYS	3.7
1	C	2192	GLU	3.6
1	A	1554	GLU	3.5
1	C	1852	THR	3.4
1	A	1495	PRO	3.4
1	B	1497	ARG	3.4
1	C	2021	ARG	3.4
1	A	2026	GLU	3.4
1	C	1703	GLU	3.4
1	A	2145	GLU	3.4
1	A	2099	ARG	3.4
1	B	2141	HIS	3.4
1	A	2101	SER	3.3
1	A	2147	SER	3.3
1	C	2026	GLU	3.3
1	B	1998	GLY	3.3
1	B	2187	LYS	3.3
1	C	2200	LYS	3.3
1	A	2146	ALA	3.3
1	B	1911	ASN	3.3
1	C	1630	GLY	3.2
1	A	1528	ALA	3.2
1	B	1484	ALA	3.2
1	A	2102	ARG	3.1
1	C	1533	THR	3.1
1	B	1704	CYS	3.1
1	C	1525	ASN	3.1
1	A	2192	GLU	3.1
1	C	2142	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	2108	VAL	3.1
1	B	1703	GLU	3.0
1	A	2021	ARG	3.0
1	C	2104	VAL	3.0
1	C	2098	ASP	3.0
1	A	1706	ARG	3.0
1	C	2193	SER	2.9
1	A	1911	ASN	2.9
1	A	1704	CYS	2.9
1	A	1529	ASP	2.9
1	C	2195	ALA	2.9
1	A	1626	GLY	2.9
1	A	1765	MET	2.8
1	A	1910	PRO	2.8
1	A	2108	VAL	2.8
1	B	2021	ARG	2.8
1	A	2000	TRP	2.8
1	C	2201	LYS	2.8
1	C	2144	GLY	2.8
1	C	2100	SER	2.8
1	B	2149	LEU	2.8
1	B	1766	LEU	2.7
1	C	1626	GLY	2.7
1	C	1786	ASN	2.7
1	C	2020	ALA	2.7
1	B	2179	TYR	2.7
1	A	1484	ALA	2.7
1	C	1530	VAL	2.7
1	C	2105	ALA	2.7
1	A	1487	TYR	2.7
1	A	1630	GLY	2.6
1	B	1530	VAL	2.6
1	C	1765	MET	2.6
1	C	2188	GLY	2.6
1	A	2193	SER	2.6
1	B	1824	LYS	2.6
1	B	2185	LYS	2.6
1	B	1838	ASP	2.5
1	A	2189	LEU	2.5
1	B	1630	GLY	2.5
1	A	2139	LEU	2.5
1	B	2113	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	2152	ILE	2.5
1	C	1705	ILE	2.5
1	C	2114	GLU	2.5
1	C	1997	GLY	2.5
1	A	1631	MET	2.5
1	C	1911	ASN	2.4
1	A	1482	PRO	2.4
1	B	1855	GLY	2.4
1	B	1629	ILE	2.4
1	B	1826	THR	2.4
1	B	2181	THR	2.4
1	B	2137	LYS	2.4
1	C	2186	LEU	2.4
1	B	1840	THR	2.4
1	C	1554	GLU	2.4
1	C	2187	LYS	2.4
1	C	1998	GLY	2.4
1	A	1851	GLU	2.3
1	B	2142	GLN	2.3
1	C	1910	PRO	2.3
1	C	1492	TRP	2.3
1	B	1767	GLY	2.3
1	A	1496	LYS	2.2
1	B	2180	LYS	2.2
1	B	1533	THR	2.2
1	B	1768	ARG	2.2
1	A	1997	GLY	2.2
1	C	1627	ALA	2.2
1	A	1769	GLU	2.2
1	C	1824	LYS	2.2
1	C	2103	MET	2.2
1	B	1954	ARG	2.2
1	A	2137	LYS	2.2
1	A	1996	ARG	2.2
1	A	1530	VAL	2.2
1	B	2000	TRP	2.1
1	B	1529	ASP	2.1
1	B	1853	GLU	2.1
1	C	1731	ARG	2.1
1	A	2187	LYS	2.1
1	B	1531	LYS	2.1
1	A	1786	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1837	ASN	2.1
1	A	1853	GLU	2.1
1	B	1839	GLU	2.1
1	C	1904	PRO	2.1
1	A	1553	VAL	2.1
1	A	1768	ARG	2.0
1	C	2140	SER	2.0
1	B	1495	PRO	2.0
1	A	1837	ASN	2.0
1	B	1850	ARG	2.0
1	C	1996	ARG	2.0
1	B	1546	GLU	2.0
1	C	1764	LYS	2.0
1	C	2147	SER	2.0
1	B	1557	PRO	2.0
1	B	1558	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.