



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:03 AM UTC

PDB ID : 1OD4 / pdb_00001od4
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

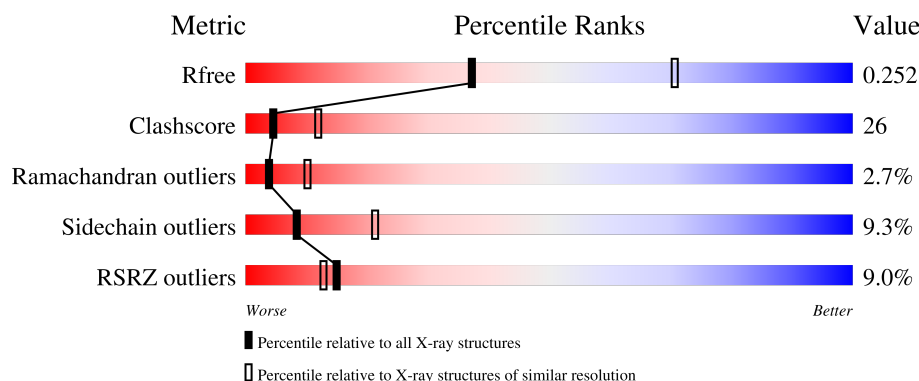
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	805	6% 46% 32% 6% 15%
1	B	805	8% 44% 34% 7% 15%
1	C	805	8% 44% 32% 6% 17%

2 Entry composition [i](#)

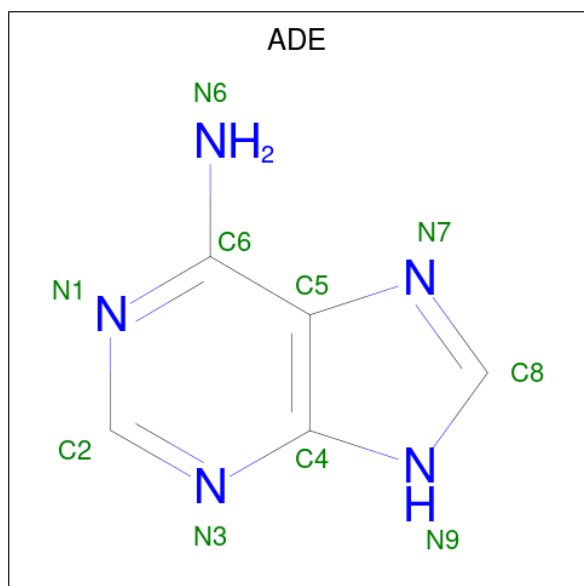
There are 3 unique types of molecules in this entry. The entry contains 16461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ADE) (formula: C₅H₅N₅).



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

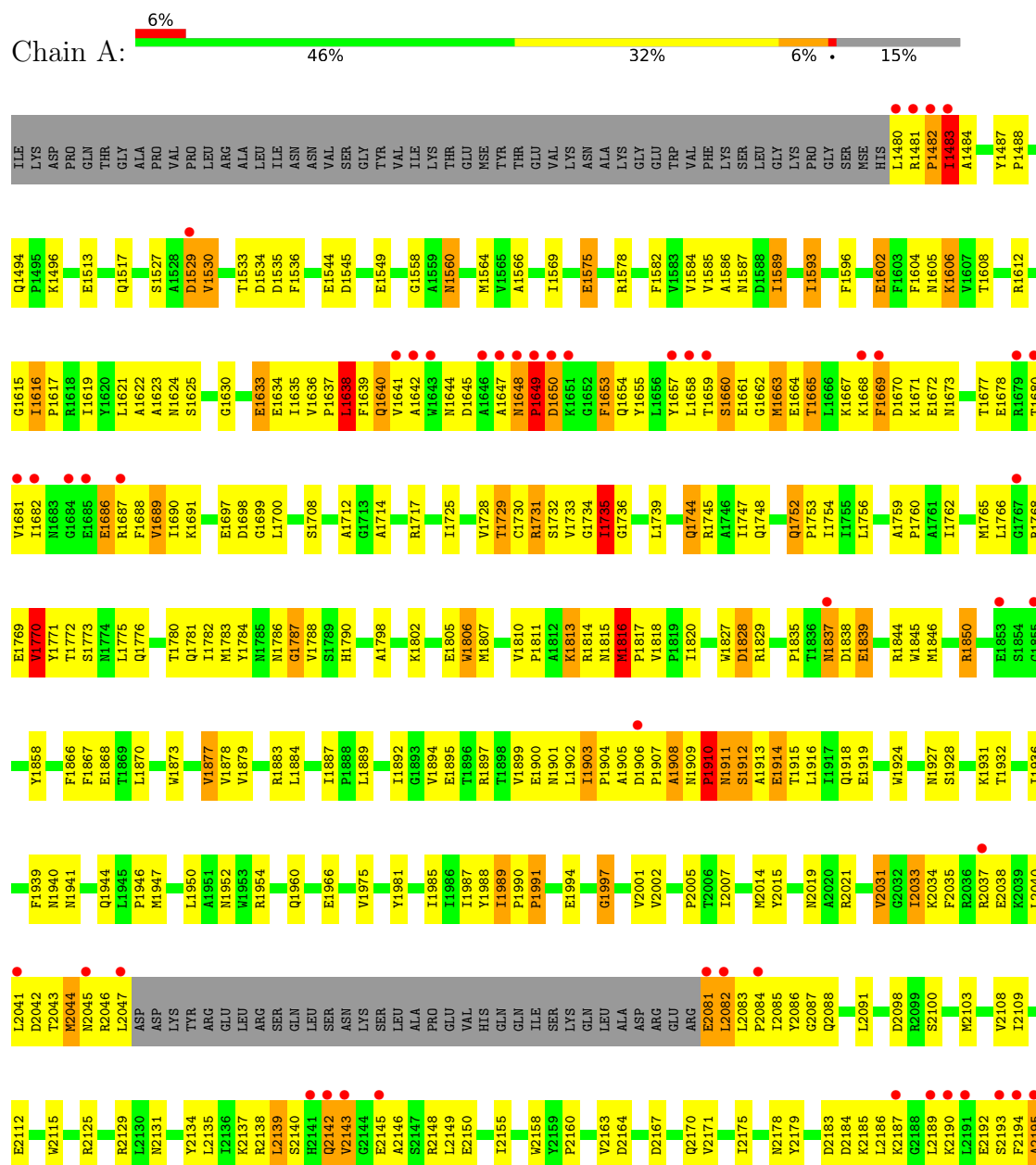
- Molecule 3 is water.

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

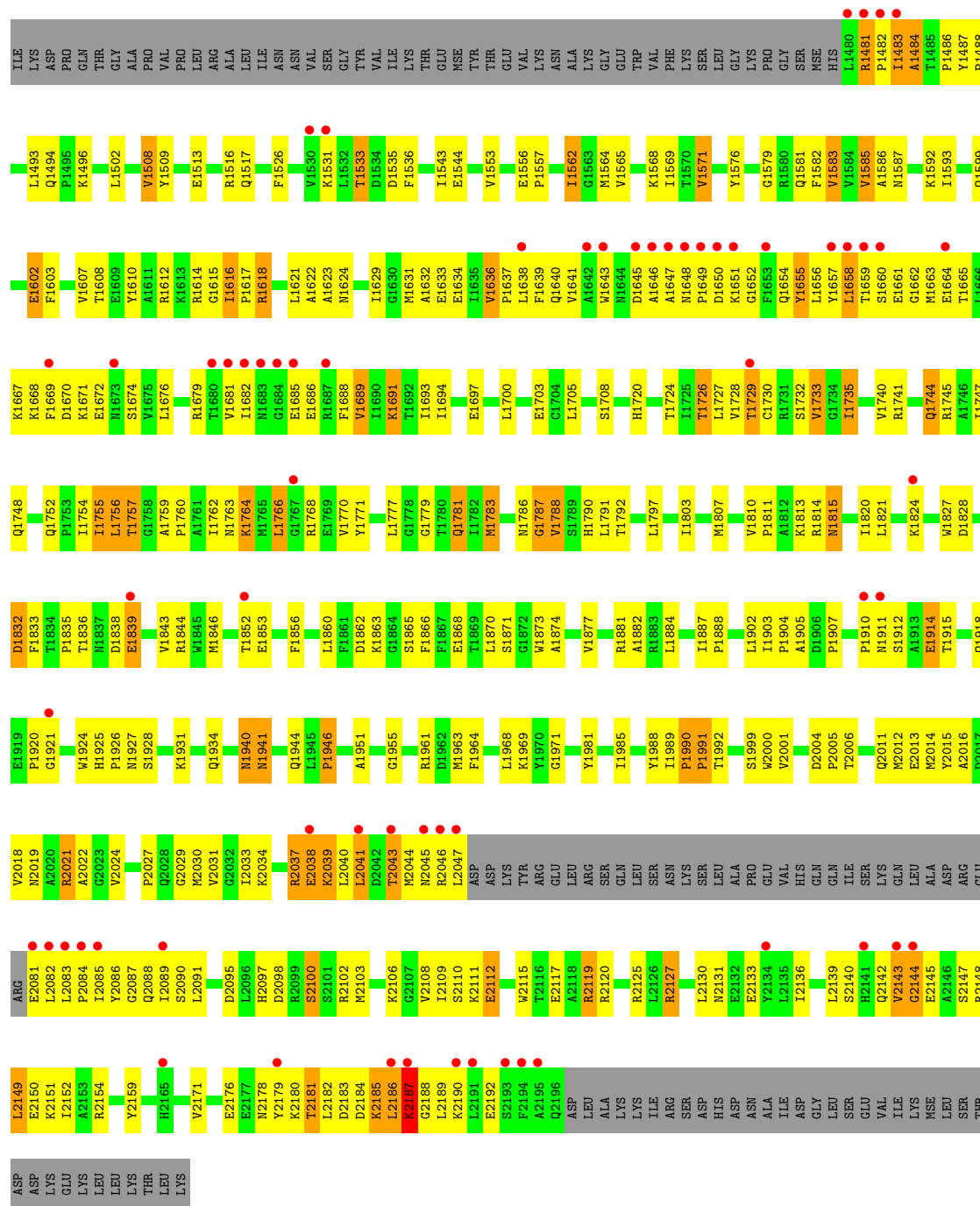
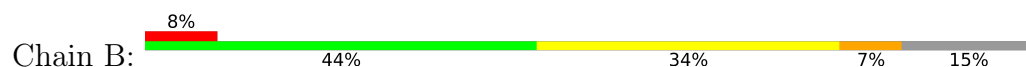
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-COENZYME A CARBOXYLASE



Q2196
ASP
LEU
ALA
LYS
GLN
LYS
ILE
ARG
PRO
ASP
HIS
VAL
PRO
ASN
ALA
ILE
ASP
GLY
LEU
ASN
SER
GLU
VAL
ILE
TYR
LYS
VAL
ASN
LEU
SER
THR
ASP
ASP
LYS
GLU
LYS
LEU
LEU
LYS
LEU
LEU
LYS

• 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 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.70) 94.5 (30.00-2.70)	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 0.217 , 0.252	Depositor DCC
R_{free} test set	11315 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.53	1/5549 (0.0%)	1.04	33/7491 (0.4%)
1	B	0.54	0/5549	1.03	30/7491 (0.4%)
1	C	0.52	0/5448	1.03	32/7351 (0.4%)
All	All	0.53	1/16546 (0.0%)	1.03	95/22333 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2195	ALA	C-N	-5.11	1.26	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2039	LYS	N-CA-C	-11.56	98.68	111.28
1	A	1941	ASN	N-CA-C	11.13	123.50	111.36
1	B	1941	ASN	N-CA-C	10.49	122.41	110.97
1	A	2189	LEU	N-CA-C	-9.57	102.17	114.04
1	C	1536	PHE	N-CA-C	-9.41	101.80	113.28
1	C	1941	ASN	N-CA-C	9.04	122.43	111.40
1	A	1912	SER	N-CA-C	-8.41	94.53	108.32
1	C	1644	ASN	N-CA-C	-8.19	95.95	108.96
1	C	2102	ARG	N-CA-C	-8.12	102.39	111.07
1	B	1650	ASP	N-CA-C	-8.04	104.34	114.56
1	A	2139	LEU	N-CA-C	-7.99	102.79	112.54
1	A	1752	GLN	CA-C-N	7.84	127.77	119.85
1	A	1752	GLN	C-N-CA	7.84	127.77	119.85
1	B	1990	PRO	CA-C-N	7.81	129.60	119.84
1	B	1990	PRO	C-N-CA	7.81	129.60	119.84
1	B	1729	THR	N-CA-C	7.16	123.04	112.94
1	B	1533	THR	N-CA-C	-7.01	100.09	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1788	VAL	N-CA-C	-6.97	104.19	111.58
1	C	1787	GLY	N-CA-C	-6.96	105.45	114.85
1	A	1787	GLY	N-CA-C	-6.96	105.49	115.64
1	A	1735	ILE	N-CA-C	-6.88	101.99	111.89
1	A	1989	ILE	CA-C-N	6.81	127.39	120.38
1	A	1989	ILE	C-N-CA	6.81	127.39	120.38
1	C	1946	PRO	N-CA-C	-6.80	100.99	111.13
1	B	1912	SER	N-CA-C	-6.73	97.44	108.41
1	C	2148	ARG	N-CA-C	-6.72	103.96	111.28
1	C	1656	LEU	N-CA-C	-6.67	96.59	110.80
1	A	1635	ILE	N-CA-C	-6.65	107.39	113.71
1	A	1729	THR	N-CA-C	6.64	122.46	113.97
1	B	1636	VAL	CB-CA-C	-6.63	107.32	114.35
1	A	2148	ARG	N-CA-C	-6.63	104.08	111.71
1	B	1484	ALA	N-CA-C	6.63	117.89	108.54
1	C	1940	ASN	N-CA-C	6.63	119.84	111.69
1	C	1736	GLY	N-CA-C	-6.62	104.30	112.77
1	A	1660	SER	N-CA-C	-6.60	105.20	113.18
1	C	2044	MSE	N-CA-C	-6.51	103.41	112.45
1	A	1911	ASN	N-CA-C	6.50	118.80	107.49
1	B	1989	ILE	CA-C-N	6.49	127.06	120.38
1	B	1989	ILE	C-N-CA	6.49	127.06	120.38
1	C	2012	MSE	N-CA-C	6.45	120.34	109.76
1	B	2112	GLU	N-CA-C	-6.12	99.73	109.76
1	A	1966	GLU	N-CA-C	6.11	120.03	112.58
1	A	1770	VAL	N-CA-C	6.06	118.66	111.09
1	B	1783	MSE	N-CA-C	6.03	117.85	111.28
1	B	1483	ILE	N-CA-C	6.00	121.81	109.34
1	B	2012	MSE	N-CA-C	5.96	119.79	110.32
1	C	1572	LYS	N-CA-C	-5.92	99.55	108.96
1	A	1816	MSE	N-CA-C	-5.92	102.43	110.36
1	A	2044	MSE	N-CA-C	-5.86	104.80	111.07
1	C	1712	ALA	N-CA-C	-5.86	104.81	111.14
1	C	1576	TYR	CA-C-N	5.82	125.68	119.28
1	C	1576	TYR	C-N-CA	5.82	125.68	119.28
1	C	1903	ILE	N-CA-C	5.78	113.59	107.76
1	C	1682	ILE	N-CA-C	5.76	118.87	109.78
1	A	1484	ALA	N-CA-C	5.74	116.81	107.23
1	B	1787	GLY	N-CA-C	-5.73	107.27	115.64
1	B	1914	GLU	N-CA-C	-5.69	101.42	109.96
1	A	2112	GLU	N-CA-C	-5.64	101.35	110.32
1	A	1536	PHE	N-CA-C	-5.50	106.52	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1946	PRO	N-CA-C	-5.50	101.54	110.40
1	B	1576	TYR	CA-C-N	5.43	124.88	119.24
1	B	1576	TYR	C-N-CA	5.43	124.88	119.24
1	C	1966	GLU	N-CA-C	5.38	118.85	111.54
1	C	1733	VAL	N-CA-C	5.36	117.27	108.97
1	B	1940	ASN	N-CA-C	5.34	117.92	111.40
1	A	1483	ILE	N-CA-C	5.33	120.43	109.34
1	A	1638	LEU	N-CA-C	5.33	117.33	107.73
1	C	1909	ASN	CA-C-N	5.33	126.50	119.84
1	C	1909	ASN	C-N-CA	5.33	126.50	119.84
1	A	1753	PRO	N-CA-C	5.30	119.80	111.38
1	A	1665	THR	N-CA-C	-5.27	105.53	111.28
1	B	1971	GLY	N-CA-C	-5.26	106.03	112.77
1	A	1712	ALA	N-CA-C	-5.26	105.63	111.36
1	B	2011	GLN	N-CA-C	5.25	120.34	113.88
1	A	1940	ASN	N-CA-C	5.23	118.13	111.69
1	B	1990	PRO	N-CA-C	5.22	117.07	110.70
1	B	1508	VAL	N-CA-C	5.21	115.83	110.36
1	C	1783	MSE	N-CA-C	5.19	117.68	111.71
1	C	1847	ILE	N-CA-C	5.18	115.46	110.74
1	C	1568	LYS	N-CA-C	-5.16	100.83	109.24
1	A	1806	TRP	N-CA-C	-5.13	105.60	111.14
1	C	1673	ASN	N-CA-C	-5.13	106.77	112.57
1	C	1945	LEU	N-CA-C	5.13	117.06	110.39
1	A	1529	ASP	N-CA-C	5.13	116.72	111.03
1	B	1963	MSE	N-CA-C	-5.11	105.79	111.36
1	A	1569	ILE	N-CA-C	5.10	115.19	107.80
1	A	2184	ASP	N-CA-C	-5.08	105.66	111.14
1	C	2194	PHE	N-CA-C	-5.07	104.70	111.24
1	B	1827	TRP	N-CA-C	5.05	117.68	111.82
1	C	1502	LEU	N-CA-C	-5.04	106.39	112.54
1	A	1946	PRO	N-CA-C	-5.04	102.28	110.40
1	C	2112	GLU	N-CA-C	-5.03	101.10	109.46
1	B	1815	ASN	N-CA-C	5.01	120.52	113.56
1	C	1785	ASN	CA-C-N	5.01	126.95	120.44
1	C	1785	ASN	C-N-CA	5.01	126.95	120.44

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	5444	0	5388	277	1
1	B	5444	0	5388	305	0
1	C	5347	0	5283	298	0
2	C	10	0	4	0	0
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	843	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 26.

All (843) 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:HD13	1:B:1735:ILE:H	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:HD13	1:B:1735:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1483:ILE:H	1:B:1483:ILE:HD12	1.48	0.79
1:B:2178:ASN:HD22	1:B:2181:THR:HG21	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:1587:ASN:HD22	1:A:1623:ALA:H	1.31	0.78
1:A:1630:GLY:HA3	1:A:1700:LEU:HD22	1.66	0.78
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.48	0.77
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.30	0.77
1:B:2147:SER:OG	1:B:2150:GLU:HG3	1.84	0.77
1:B:2022:ALA:HB3	1:B:2103:MSE:HE2	1.65	0.77
1:C:1665:THR:O	1:C:1668:LYS:HB3	1.85	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:B:2046:ARG:C	1:B:2047:LEU:HD22	2.09	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:N	1:A:1560:ASN:HD22	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:HD22	1:A:1560:ASN:H	1.34	0.74
1:B:1757:THR:HG22	1:B:1762:ILE:HG13	1.68	0.73
1:C:1642:ALA:H	1:C:1657:TYR:HE1	1.35	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:HG3	1:B:1768:ARG:HH11	1.53	0.72
1:B:1638:LEU:HD12	1:B:1638:LEU:O	1.89	0.72
1:C:2142:GLN:HB2	1:C:2190:LYS:HZ1	1.51	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2149:LEU:C	1:A:2149:LEU:HD23	2.15	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:1527:SER:O	1:C:1530:VAL:HG22	1.91	0.71
1:C:1645:ASP:OD2	1:C:1648:ASN:HB2	1.90	0.71
1:B:1667:LYS:HE3	1:B:1672:GLU:HG2	1.74	0.70
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:B:2097:HIS:HE1	1:C:1632:ALA:H	1.41	0.69
1:C:2145:GLU:OE1	1:C:2145:GLU:HA	1.92	0.69
1:A:1533:THR:HG22	1:A:1535:ASP:H	1.56	0.69
1:B:1671:LYS:HB3	1:B:1674:SER:OG	1.93	0.69
1:B:1755:ILE:HD13	1:B:1755:ILE:H	1.56	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:A:1494:GLN:OE1	1:A:1496:LYS:HG2	1.93	0.68
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.92	0.68
1:B:2085:ILE:HG21	1:C:1650:ASP:HA	1.75	0.68
1:A:1593:ILE:HG22	1:A:1593:ILE:O	1.92	0.68
1:B:1881:ARG:HH11	1:B:1881:ARG:HG2	1.59	0.68
1:B:2046:ARG:O	1:B:2047:LEU:HD13	1.93	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:C:1641:VAL:O	1:C:1642:ALA:C	2.38	0.67
1:B:1488:PRO:HB3	1:B:1493:LEU:HD11	1.77	0.67
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.76	0.67
1:B:1728:VAL:HG21	1:B:1754:ILE:HD11	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.78	0.65
1:B:1762:ILE:HD12	1:B:1777:LEU:HD21	1.77	0.65
1:C:1852:THR:HG22	1:C:1854:SER:H	1.61	0.65
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.11	0.65
1:C:1737:ALA:O	1:C:1740:VAL:HG22	1.96	0.65
1:C:2181:THR:O	1:C:2184:ASP:HB2	1.96	0.65
1:C:1545:ASP:OD2	1:C:1549:GLU:HB3	1.96	0.65
1:C:1797:LEU:O	1:C:1801:GLU:HG3	1.96	0.65
1:A:1748:GLN:HE22	1:A:1783:MSE:HB2	1.62	0.65
1:A:1892:ILE:CD1	1:A:1947:MSE:HE2	2.26	0.65
1:C:2044:MSE:HA	1:C:2086:TYR:CE2	2.32	0.65
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:1575:GLU:CD	1:C:1575:GLU:H	2.05	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:C:1909:ASN:C	1:C:1909:ASN:HD22	2.06	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:A:1636:VAL:N	1:A:1637:PRO:HD2	2.15	0.62
1:A:1728:VAL:HG21	1:A:1754:ILE:HD11	1.80	0.62
1:B:1964:PHE:O	1:C:1786:ASN:ND2	2.32	0.62
1:C:1762:ILE:HG21	1:C:1771:TYR:HE1	1.64	0.62
1:C:1846:MSE:HE1	1:C:1990:PRO:HB2	1.81	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:N	1:A:1634:GLU:OE2	2.30	0.61
1:A:2044:MSE:HE2	1:A:2082:LEU:HB2	1.81	0.61
1:C:1520:SER:O	1:C:1524:LYS:HG2	1.99	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:A:1900:GLU:OE1	1:A:1916:LEU:HD21	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1736:GLY:O	1:C:1740:VAL:HG13	2.01	0.61
1:C:2190:LYS:C	1:C:2192:GLU:H	2.09	0.61
1:C:1783:MSE:HA	1:C:1786:ASN:HB2	1.82	0.61
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.15	0.61
1:B:2180:LYS:HA	1:B:2183:ASP:OD1	2.01	0.61
1:C:1655:TYR:CE2	1:C:1689:VAL:HG22	2.36	0.61
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.83	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: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:C:2001:VAL:HG23	1:C:2002:VAL:HG13	1.83	0.60
1:B:1881:ARG:HG2	1:B:1881:ARG:NH1	2.16	0.60
1:A:1680:THR:HG22	1:A:1680:THR:O	2.00	0.60
1:B:1691:LYS:HE2	1:B:1691:LYS:HA	1.84	0.59
1:B:1755:ILE:HD13	1:B:1755:ILE:N	2.17	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:B:2180:LYS:C	1:B:2182:LEU:H	2.09	0.59
1:C:2036:ARG:HG3	1:C:2036:ARG:HH11	1.66	0.59
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.16	0.59
1:C:1644:ASN:HD21	1:C:1654:GLN:NE2	2.00	0.59
1:B:1733:VAL:HG13	1:B:1755:ILE:HG12	1.83	0.59
1:B:2041:LEU:HD22	1:B:2044:MSE:CE	2.32	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:1606:LYS:HD3	3:C:5004:HOH:O	2.03	0.59
1:C:1782:ILE:O	1:C:1786:ASN:HB2	2.03	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:1697:GLU:O	1:B:1700:LEU:HD13	2.02	0.59
1:B:1786:ASN:HB3	1:B:1788:VAL:HG23	1.85	0.59
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.32	0.59
1:B:2082:LEU:C	1:B:2082:LEU:HD12	2.27	0.59
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.20	0.59
1:B:2106:LYS:HE2	1:B:2106:LYS:HA	1.84	0.59
1:A:1759:ALA:O	1:A:1760:PRO:C	2.46	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1655:TYR:HE1	1:B:1657:TYR:HB3	1.67	0.58
1:B:1856:PHE:CZ	1:B:1863:LYS:HG3	2.38	0.58
1:B:1860:LEU:O	1:B:2119:ARG:HG3	2.04	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:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.85	0.58
1:B:2186:LEU:O	1:B:2188:GLY:N	2.36	0.58
1:C:2187:LYS:C	1:C:2189:LEU:H	2.09	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
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.34	0.57
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.52	0.57
1:C:2083:LEU:HB2	1:C:2084:PRO:HD3	1.86	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:1728:VAL:HG21	1:C:1754:ILE:HD11	1.87	0.57
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.03	0.57
1:C:1505:THR:HB	1:C:1729:THR:O	2.05	0.57
1:C:1903:ILE:N	1:C:1903:ILE:HD12	2.20	0.57
1:C:2148:ARG:CZ	1:C:2152:ILE:HD11	2.35	0.57
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.86	0.57
1:B:1708:SER:HB3	1:C:2001:VAL:HG12	1.86	0.57
1:B:1907:PRO:HD2	1:C:1960:GLN:HG2	1.87	0.57
1:B:2043:THR:HG22	1:B:2086:TYR:HE2	1.69	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:1568:LYS:HE2	1:B:1581:GLN:OE1	2.05	0.56
1:B:2185:LYS:O	1:B:2189:LEU:HD23	2.05	0.56
1:B:1766:LEU:HD12	1:B:1770:VAL:HG21	1.87	0.56
1:C:1519:SER:O	1:C:1522:GLN:HB3	2.04	0.56
1:A:1987:ILE:HB	1:A:2014:MSE:HG3	1.85	0.56
1:B:1781:GLN:CD	1:B:1781:GLN:H	2.13	0.56
1:B:2040:LEU:HD11	1:B:2086:TYR:HB3	1.86	0.56
1:B:2148:ARG:HG3	1:B:2148:ARG:HH11	1.69	0.56
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	1.87	0.56
1:A:1530:VAL:O	1:A:1530:VAL:HG13	2.03	0.56
1:A:1708:SER:CB	1:A:1735:ILE:HG12	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1911:ASN:C	1:B:1911:ASN:HD22	2.12	0.56
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.39	0.56
1:C:1729:THR:O	1:C:1730:CYS:HB2	2.05	0.56
1:C:2110:SER:O	1:C:2111:LYS:HG3	2.05	0.56
1:C:2148:ARG:NE	1:C:2152:ILE:HD11	2.20	0.56
1:A:1668:LYS:C	1:A:1670:ASP:H	2.14	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:C:1653:PHE:C	1:C:1653:PHE:CD2	2.83	0.56
1:A:2081:GLU:OE1	1:A:2081:GLU:N	2.39	0.56
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	1.87	0.56
1:B:2044:MSE:SE	1:B:2082:LEU:HD11	2.55	0.56
1:B:2110:SER:O	1:B:2111:LYS: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
1:C:2097:HIS:O	1:C:2102:ARG:HG3	2.05	0.56
1:B:2148:ARG:HG3	1:B:2148:ARG:NH1	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:1669:PHE:O	1:B:1670:ASP:HB3	2.06	0.56
1:B:1781:GLN:H	1:B:1781:GLN:NE2	2.04	0.56
1:C:1602:GLU:HG3	1:C:1603:PHE:N	2.21	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:B:1616:ILE:HD12	1:B:1813:LYS:HG2	1.88	0.55
1:C:2001:VAL:HG23	1:C:2002:VAL:N	2.22	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:OE1	1:B:1654:GLN:HA	2.06	0.55
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.07	0.55
1:B:1708:SER:CB	1:C:2001:VAL:HG12	2.36	0.55
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.88	0.55
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.36	0.55
1:B:2186:LEU:C	1:B:2188:GLY:H	2.15	0.55
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.55	0.55
1:C:1735:ILE:O	1:C:1739:LEU:HG	2.06	0.55
1:C:2142:GLN:CD	1:C:2190:LYS:HE2	2.32	0.55
1:C:2192:GLU:CD	1:C:2192:GLU:O	2.50	0.55
1:A:1991:PRO:O	1:A:2019:ASN:O	2.24	0.55
1:A:2140:SER:C	1:A:2142:GLN:H	2.14	0.55
1:B:1564:MSE:CE	1:B:1585:VAL:HG12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.89	0.54
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.23	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:1645:ASP:C	1:A:1647:ALA:H	2.15	0.54
1:A:2037:ARG:O	1:A:2038:GLU:C	2.50	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:C:1747:ILE:HD13	1:C:1802:LYS:HB3	1.89	0.54
1:C:2173:THR:O	1:C:2177:GLU:HB2	2.08	0.54
1:A:2137:LYS:O	1:A:2138:ARG:HD2	2.07	0.54
1:C:1585:VAL:HG13	1:C:1607:VAL:HG11	1.90	0.54
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.16	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: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
1:A:1560:ASN:N	1:A:1560:ASN:ND2	2.56	0.53
1:A:1657:TYR:O	1:A:1658:LEU:HD23	2.08	0.53
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.90	0.53
1:C:2000:TRP:CZ2	1:C:2014:MSE:HE1	2.43	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:HD23	1:A:2149:LEU:O	2.08	0.53
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.09	0.53
1:A:1905:ALA:HB2	1:A:1913:ALA:HA	1.90	0.53
1:B:1481:ARG:HB2	1:B:1482:PRO:CD	2.38	0.53
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.27	0.53
1:C:1674:SER:O	1:C:1675:VAL:HG13	2.09	0.53
1:C:2033:ILE:HG22	1:C:2034:LYS:HD2	1.89	0.53
1:A:1529:ASP:O	1:A:1530:VAL:C	2.51	0.53
1:A:1640:GLN:HB3	1:A:1657:TYR:CE1	2.43	0.53
1:A:2194:PHE:O	1:A:2196:GLN:N	2.42	0.53
1:C:2046:ARG:O	1:C:2046:ARG:HD2	2.09	0.53
1:A:1678:GLU:CD	1:A:1691:LYS:HE3	2.34	0.52
1:B:1586:ALA:CB	1:B:1621:LEU:HB2	2.39	0.52
1:C:1659:THR:OG1	1:C:1661:GLU:HB3	2.09	0.52
1:A:1677:THR:HG22	1:A:1689:VAL:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2031:VAL:C	1:A:2033:ILE:H	2.18	0.52
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.16	0.52
1:C:2148:ARG:HD3	1:C:2152:ILE:HD11	1.91	0.52
1:A:1927:ASN:OD1	1:A:1928:SER:N	2.43	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:1759:ALA:HB3	1:A:1760:PRO:HD3	1.90	0.52
1:B:1643:TRP:CE3	1:B:1649:PRO:HB2	2.44	0.52
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.94	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: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:C:1883:ARG:HA	1:C:1887:ILE:O	2.10	0.52
1:A:1901:ASN:ND2	1:A:1903:ILE:HD11	2.25	0.52
1:A:2134:TYR:CD2	1:A:2135:LEU:HD12	2.45	0.52
1:B:1564:MSE:HE2	1:B:1585:VAL:HG12	1.91	0.52
1:B:1660:SER:O	1:B:1664:GLU:HG2	2.09	0.52
1:B:2033:ILE:O	1:B:2034:LYS:HD2	2.10	0.52
1:B:2005:PRO:HG3	1:B:2014:MSE:HB2	1.91	0.51
1:B:2041:LEU:O	1:B:2044:MSE:HB3	2.10	0.51
1:C:2140:SER:O	1:C:2142:GLN:N	2.40	0.51
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.40	0.51
1:B:2180:LYS:C	1:B:2182:LEU:N	2.67	0.51
1:A:1589:ILE:HG12	1:A:1623:ALA:O	2.10	0.51
1:A:2085:ILE:HG23	1:A:2086:TYR:H	1.74	0.51
1:A:2085:ILE:CG2	1:A:2086:TYR:N	2.73	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:1646:ALA:O	1:C:1647:ALA:C	2.54	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:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.75	0.51
1:A:2005:PRO:HD3	1:A:2014:MSE:HE3	1.92	0.51
1:A:2084:PRO:O	1:A:2088:GLN:HG2	2.11	0.51
1:B:1667:LYS:CE	1:B:1672:GLU:HG2	2.39	0.51
1:B:2149:LEU:HD23	1:B:2149:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1775:LEU:N	1:C:1775:LEU:HD12	2.25	0.51
1:B:1720:HIS:ND1	1:B:1941:ASN:ND2	2.59	0.51
1:B:2148:ARG:HG2	1:B:2152:ILE:HD11	1.93	0.51
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.76	0.51
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.09	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:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.76	0.51
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.11	0.51
1:C:1641:VAL:O	1:C:1641:VAL:HG12	2.11	0.51
1:C:1759:ALA:O	1:C:1760:PRO:C	2.54	0.51
1:A:1827:TRP:CD2	1:A:1828:ASP:N	2.79	0.51
1:B:1481:ARG:HB2	1:B:1482:PRO:HD2	1.92	0.51
1:B:1565:VAL:HA	3:B:5010:HOH:O	2.10	0.51
1:B:1592:LYS:C	1:B:1593:ILE:HG12	2.36	0.51
1:B:1940:ASN:HB2	1:B:1981:TYR:CE1	2.46	0.51
1:C:1601:ASP:OD1	1:C:1707:GLY:HA3	2.11	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:A:1787:GLY:HA3	1:A:1873:TRP:CE3	2.46	0.50
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.11	0.50
1:C:2036:ARG:HG3	1:C:2036:ARG:NH1	2.27	0.50
1:C:2186:LEU:C	1:C:2188:GLY:N	2.68	0.50
1:A:2149:LEU:C	1:A:2149:LEU:CD2	2.83	0.50
1:B:1856:PHE:CE2	1:B:1863:LYS:HG3	2.46	0.50
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.76	0.50
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	1.93	0.50
1:B:1662:GLY:O	1:B:1665:THR:HB	2.12	0.50
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.09	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:1653:PHE:CD1	1:A:1653:PHE:N	2.80	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:C:1580:ARG:HH11	1:C:1580:ARG:HG3	1.76	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:C:2005:PRO:HG3	1:C:2014:MSE:HB2	1.94	0.50
1:C:2148:ARG:CD	1:C:2152:ILE:HD11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.76	0.50
1:A:1527:SER:O	1:A:1530:VAL:HG12	2.12	0.49
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:C:2192:GLU:CD	1:C:2192:GLU:C	2.80	0.49
1:A:1655:TYR:CD1	1:A:1689:VAL:HG13	2.46	0.49
1:A:1698:ASP:OD1	1:A:1699:GLY:N	2.45	0.49
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.94	0.49
1:A:1681:VAL:O	1:A:1682:ILE:HG12	2.11	0.49
1:B:1783:MSE:HA	1:B:1786:ASN:HB2	1.93	0.49
1:A:1805:GLU:HG2	1:A:1867:PHE:CE1	2.48	0.49
1:A:2002:VAL:O	1:A:2002:VAL:HG22	2.12	0.49
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.48	0.49
1:B:1526:PHE:CE2	1:B:1821:LEU:HD11	2.47	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:A:2082:LEU:HD12	1:A:2082:LEU:N	2.28	0.49
1:B:2142:GLN:O	1:B:2143:VAL:C	2.56	0.49
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.13	0.49
1:B:1556:GLU:O	1:B:1557:PRO:C	2.54	0.49
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.94	0.49
1:B:1991:PRO:HG2	1:B:2115:TRP:CG	2.47	0.49
1:C:1660:SER:HB2	1:C:1686:GLU:OE2	2.13	0.49
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.95	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:C:2190:LYS:C	1:C:2192:GLU:N	2.69	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:C:1639:PHE:CD1	1:C:1639:PHE:C	2.91	0.49
1:A:1624:ASN:HD21	1:A:1736:GLY:HA3	1.78	0.48
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.47	0.48
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.44	0.48
1:A:1513:GLU:HG3	1:A:1517:GLN:NE2	2.28	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:B:1951:ALA:O	1:B:1990:PRO:HD2	2.13	0.48
1:A:2042:ASP:O	1:A:2046:ARG:HG2	2.12	0.48
1:A:2085:ILE:HG23	1:A:2086:TYR:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1682:ILE:O	1:B:1682:ILE:HG22	2.14	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:C:1659:THR:C	1:C:1661:GLU:N	2.70	0.48
1:C:1680:THR:CG2	1:C:1681:VAL:N	2.76	0.48
1:C:2036:ARG:O	1:C:2037:ARG:C	2.55	0.48
1:B:1786:ASN:OD1	1:C:1964:PHE:O	2.31	0.48
1:C:1653:PHE:O	1:C:1655:TYR:N	2.46	0.48
1:C:1680:THR:HG22	1:C:1681:VAL:N	2.26	0.48
1:C:1781:GLN:CD	1:C:1781:GLN:H	2.21	0.48
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.95	0.48
1:C:2031:VAL:C	1:C:2033:ILE:H	2.22	0.48
1:A:1905:ALA:HB1	1:A:1912:SER:O	2.13	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:B:1852:THR:HG22	1:B:1853:GLU:H	1.79	0.48
1:C:2136:ILE:HD11	1:C:2152:ILE:HG12	1.96	0.48
1:C:2139:LEU:HD13	1:C:2186:LEU:HD21	1.95	0.48
1:B:1592:LYS:O	1:B:1593:ILE:HG12	2.13	0.48
1:B:1852:THR:HG22	1:B:1853:GLU:N	2.28	0.48
1:B:1925:HIS:O	1:B:1926:PRO:C	2.55	0.48
1:C:1634:GLU:OE1	1:C:1634:GLU:N	2.47	0.48
1:C:1653:PHE:O	1:C:1654:GLN:C	2.57	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:A:1905:ALA:HB2	1:A:1913:ALA:C	2.39	0.48
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.28	0.48
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:1764:LYS:HD3	1:C:2028:GLN:CD	2.39	0.47
1:B:1902:LEU:HD11	1:B:1914:GLU:HG2	1.95	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:A:1994:GLU:HA	1:A:2021:ARG:O	2.13	0.47
1:A:2190:LYS:C	1:A:2192:GLU:H	2.22	0.47
1:B:1846:MSE:HE1	1:B:1990:PRO:CB	2.44	0.47
1:B:1888:PRO:HG3	3:B:5044:HOH:O	2.14	0.47
1:C:1909:ASN:C	1:C:1909:ASN:ND2	2.70	0.47
1:C:1952:ASN:OD1	1:C:1993:GLY:HA2	2.14	0.47
1:A:1734:GLY:C	1:A:1736:GLY:N	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:2145:GLU:HG3	1:C:2151:LYS:NZ	2.29	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:1634:GLU:CD	1:C:1634:GLU:H	2.19	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:B:2181:THR:O	1:B:2185:LYS:HB2	2.15	0.47
1:C:1568:LYS:HE2	1:C:1581:GLN:NE2	2.29	0.47
1:C:1680:THR:CG2	1:C:1682:ILE:HG12	2.44	0.47
1:C:2044:MSE:HE2	1:C:2082:LEU:CB	2.44	0.47
1:C:2142:GLN:HB2	1:C:2190:LYS:CE	2.44	0.47
1:B:1726:THR:HG21	1:B:1740:VAL:HA	1.97	0.47
1:C:1550:LEU:HD12	1:C:1550:LEU:HA	1.76	0.47
1:C:1644:ASN:HD21	1:C:1654:GLN:CD	2.22	0.47
1:C:1755:ILE:HD12	1:C:1758:GLY:HA2	1.96	0.47
1:A:1866:PHE:CE1	1:A:1868:GLU:HB2	2.50	0.47
1:A:1991:PRO:CG	1:A:2115:TRP:HB2	2.44	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:C:1991:PRO:C	1:C:1993:GLY:H	2.22	0.47
1:A:1657:TYR:HB2	1:A:1688:PHE:O	2.15	0.47
1:A:1663:MSE:CE	1:A:1663:MSE:HA	2.45	0.47
1:A:1766:LEU:CD2	1:A:1770:VAL:HG11	2.45	0.47
1:A:1902:LEU:O	1:A:1904:PRO:HD3	2.15	0.47
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.15	0.47
1:B:1667:LYS:HZ2	1:B:1672:GLU:HA	1.79	0.47
1:B:1676:LEU:O	1:B:1691:LYS:HB2	2.15	0.47
1:B:2038:GLU:H	1:B:2041:LEU:H	1.63	0.47
1:B:2086:TYR:HA	1:B:2089:ILE:CD1	2.35	0.47
1:B:2119:ARG:HH11	1:B:2119:ARG:CG	2.28	0.47
1:C:1645:ASP:O	1:C:1646:ALA:C	2.57	0.47
1:C:1766:LEU:O	1:C:1768:ARG:HG2	2.15	0.47
1:C:2044:MSE:HA	1:C:2086:TYR:HE2	1.78	0.47
1:A:1673:ASN:N	1:A:1673:ASN:ND2	2.62	0.47
1:A:2190:LYS:C	1:A:2192:GLU:N	2.71	0.47
1:B:1617:PRO:HG2	1:B:1807:MSE:HE3	1.97	0.47
1:B:1681:VAL:HG13	1:B:1685:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2022:ALA:HB3	1:B:2103:MSE:CE	2.40	0.47
1:B:2087:GLY:O	1:B:2090:SER:OG	2.30	0.47
1:B:2127:ARG:HD2	1:B:2176:GLU:OE1	2.15	0.47
1:C:1644:ASN:ND2	1:C:1654:GLN:HE22	2.13	0.47
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.83	0.47
1:C:1552:GLU:O	1:C:1553:VAL:HG13	2.14	0.47
1:C:1766:LEU:CD1	1:C:1770:VAL:HG11	2.45	0.47
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.50	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:A:2100:SER:HA	1:A:2103:MSE:HE3	1.97	0.46
1:C:1660:SER:O	1:C:1664:GLU:HB2	2.15	0.46
1:C:2171:VAL:O	1:C:2175:ILE:HG13	2.16	0.46
1:A:2085:ILE:O	1:A:2088:GLN:HB2	2.16	0.46
1:C:1580:ARG:NH2	1:C:1810:VAL:O	2.47	0.46
1:C:2110:SER:O	1:C:2111:LYS:CG	2.64	0.46
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.51	0.46
1:C:1636:VAL:O	1:C:1639:PHE:HD2	1.99	0.46
1:C:1657:TYR:CE2	1:C:1687:ARG:HG2	2.51	0.46
1:C:1659:THR:O	1:C:1660:SER:C	2.58	0.46
1:A:1790:HIS:HD2	3:A:5051:HOH:O	1.98	0.46
1:B:1832:ASP:O	1:B:1833:PHE:C	2.59	0.46
1:C:1636:VAL:HB	1:C:1637:PRO:CD	2.46	0.46
1:B:1652:GLY:HA2	1:C:2085:ILE:CD1	2.46	0.46
1:B:2102:ARG:NH2	1:C:1700:LEU:HB2	2.31	0.46
1:C:1921:GLY:O	1:C:1923:VAL:HG23	2.15	0.46
1:A:1844:ARG:HG3	1:A:1844:ARG:NH1	2.31	0.46
1:C:1642:ALA:N	1:C:1657:TYR:HE1	2.10	0.46
1:A:1593:ILE:O	1:A:1593:ILE:CG2	2.63	0.46
1:A:2083:LEU:O	1:A:2084:PRO:C	2.59	0.46
1:B:2140:SER:O	1:B:2142:GLN:N	2.48	0.46
1:A:2183:ASP:O	1:A:2187:LYS:HD3	2.16	0.46
1:B:1643:TRP:HZ2	1:C:2047:LEU:HB3	1.81	0.46
1:B:2181:THR:O	1:B:2185:LYS:HE2	2.15	0.46
1:A:1587:ASN:ND2	1:A:1622:ALA:HA	2.30	0.46
1:A:1895:GLU:OE2	1:A:1897:ARG:NH1	2.49	0.46
1:B:1667:LYS:NZ	1:B:1672:GLU:HA	2.30	0.46
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.98	0.46
1:B:1991:PRO:HG2	1:B:2115:TRP:CD2	2.51	0.45
1:B:2159:TYR:CE1	1:B:2171:VAL:HG13	2.51	0.45
1:A:1903:ILE:CD1	1:A:1903:ILE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1659:THR:OG1	1:B:1661:GLU:HB3	2.17	0.45
1:C:2046:ARG:HG3	1:C:2047:LEU:CD2	2.44	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:1790:HIS:HA	1:B:1870:LEU:HD23	1.98	0.45
1:C:1645:ASP:OD2	1:C:1648:ASN:CB	2.63	0.45
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.46	0.45
1:B:1509:TYR:CB	1:B:1557:PRO:HB3	2.47	0.45
1:B:1865:SER:O	1:B:1882:ALA:HA	2.16	0.45
1:B:1988:TYR:HA	1:B:2015:TYR:O	2.17	0.45
1:B:2029:GLY:O	1:B:2033:ILE:HG13	2.16	0.45
1:B:2045:ASN:OD1	1:B:2045:ASN:C	2.59	0.45
1:B:2178:ASN:C	1:B:2180:LYS:H	2.25	0.45
1:A:1827:TRP:CG	1:A:1828:ASP:N	2.84	0.45
1:A:2037:ARG:NH1	1:A:2037:ARG:CB	2.78	0.45
1:B:2187:LYS:O	1:B:2187:LYS:HG2	2.16	0.45
1:C:1664:GLU:O	1:C:1665:THR:C	2.60	0.45
1:C:2154:ARG:HG3	1:C:2154:ARG:NH1	2.32	0.45
1:A:1578:ARG:HB2	3:A:5014:HOH:O	2.16	0.45
1:B:1481:ARG:C	1:B:1481:ARG:HD2	2.41	0.45
1:B:2119:ARG:HH11	1:B:2119:ARG:HG2	1.82	0.45
1:C:1516:ARG:NH1	3:C:5003:HOH:O	2.49	0.45
1:C:1775:LEU:N	1:C:1775:LEU:CD1	2.80	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:A:1811:PRO:HG3	1:A:1818:VAL:HA	1.98	0.45
1:A:2186:LEU:O	1:A:2187:LYS:C	2.60	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:2085:ILE:O	1:C:2089:ILE:HG13	2.16	0.45
1:C:2160:PRO:HD3	1:C:2174:TRP:CE2	2.51	0.45
1:A:1615:GLY:O	1:A:1813:LYS:HA	2.16	0.45
1:A:1762:ILE:HG21	1:A:1771:TYR:HE1	1.82	0.45
1:B:1768:ARG:CG	1:B:1768:ARG:NH1	2.78	0.45
1:B:2082:LEU:C	1:B:2082:LEU:CD1	2.90	0.45
1:B:2086:TYR:O	1:B:2089:ILE:HB	2.17	0.45
1:A:1747:ILE:HD13	1:A:1802:LYS:HB3	1.99	0.45
1:A:1909:ASN:O	1:A:1911:ASN:N	2.50	0.45
1:B:1757:THR:CG2	1:B:1762:ILE:HG13	2.42	0.45
1:C:1668:LYS:HG2	1:C:1669:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1686:GLU:O	1:C:1687:ARG:HG3	2.17	0.45
1:A:1649:PRO:O	1:A:1650:ASP:C	2.60	0.44
1:A:1954:ARG:HG3	1:A:1954:ARG:HH11	1.82	0.44
1:B:1836:THR:C	1:B:1838:ASP:N	2.73	0.44
1:C:2131:ASN:HB3	1:C:2175:ILE:HG21	1.98	0.44
1:B:1632:ALA:HB1	1:B:1634:GLU:OE2	2.17	0.44
1:C:1793:ALA:HB1	1:C:1798:ALA:HB3	2.00	0.44
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.18	0.44
1:A:1932:THR:O	1:A:1936:ILE:HG13	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:C:2040:LEU:O	1:C:2043:THR:HG23	2.17	0.44
1:C:2114:GLU:O	1:C:2115:TRP:C	2.60	0.44
1:C:2183:ASP:O	1:C:2186:LEU:HB2	2.18	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: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:B:2024:VAL:HG23	1:C:1701:GLY:HA2	1.98	0.44
1:C:1632:ALA:HB1	1:C:1634:GLU:OE1	2.17	0.44
1:C:1633:GLU:OE2	1:C:1633:GLU:HA	2.16	0.44
1:C:1900:GLU:CD	1:C:1918:GLN:HE22	2.24	0.44
1:A:1688:PHE:N	1:A:1688:PHE:CD1	2.85	0.44
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.15	0.44
1:B:1790:HIS:HD2	3:B:5041:HOH:O	2.00	0.44
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.48	0.44
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.17	0.44
1:A:1909:ASN:O	1:A:1910:PRO:C	2.60	0.44
1:C:1763:ASN:OD1	1:C:1770:VAL:N	2.49	0.44
1:C:2178:ASN:O	1:C:2179:TYR:C	2.60	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: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: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:A:1735:ILE:HD12	1:A:1735:ILE:H	1.82	0.44
1:B:1787:GLY:HA3	1:B:1873:TRP:CE3	2.53	0.44
1:C:1824:LYS:HB2	1:C:1824:LYS:NZ	2.33	0.44
1:C:2038:GLU:O	1:C:2039:LYS:C	2.61	0.44
1:A:1835:PRO:HG2	1:A:1846:MSE:SE	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2146:ALA:HB1	1:A:2150:GLU:CD	2.43	0.44
1:B:1651:LYS:O	1:B:1651:LYS:HG2	2.17	0.44
1:B:1911:ASN:C	1:B:1911:ASN:ND2	2.76	0.44
1:A:1892:ILE:HD11	1:A:1947:MSE:HE2	1.99	0.43
1:C:1580:ARG:HG3	1:C:1580:ARG:NH1	2.33	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:2137:LYS:C	1:C:2139:LEU:N	2.75	0.43
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	2.01	0.43
1:B:2082:LEU:HD12	1:B:2083:LEU:N	2.33	0.43
1:A:1728:VAL:HG21	1:A:1754:ILE:CD1	2.46	0.43
1:B:1755:ILE:HA	1:C:1963:MSE:CE	2.48	0.43
1:C:1675:VAL:O	1:C:1676:LEU:C	2.60	0.43
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.36	0.43
1:A:1662:GLY:O	1:A:1663:MSE:C	2.61	0.43
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.50	0.43
1:B:1747:ILE:HD12	1:B:1803:ILE:HG13	2.01	0.43
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	2.00	0.43
1:B:2030:MSE:O	1:B:2031:VAL:C	2.61	0.43
1:C:1875:LYS:HB3	3:C:5032:HOH:O	2.17	0.43
1:A:1664:GLU:O	1:A:1667:LYS:N	2.49	0.43
1:B:2088:GLN:O	1:B:2091:LEU:HB2	2.18	0.43
1:C:1493:LEU:O	1:C:1494:GLN:C	2.61	0.43
1:C:1494:GLN:HB2	3:C:5001:HOH:O	2.18	0.43
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.65	0.43
1:C:1811:PRO:HG3	1:C:1818:VAL:HA	2.01	0.43
1:A:1533:THR:CG2	1:A:1535:ASP:OD2	2.67	0.43
1:A:1735:ILE:O	1:A:1739:LEU:N	2.48	0.43
1:A:2131:ASN:HB3	1:A:2175:ILE:HG21	2.01	0.43
1:B:1587:ASN:ND2	1:B:1622:ALA:HA	2.33	0.43
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.64	0.43
1:B:2013:GLU:OE1	1:B:2125:ARG:NH2	2.41	0.43
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.18	0.43
1:B:1703:GLU:OE2	1:C:2102:ARG:NH2	2.52	0.43
1:B:2085:ILE:CG2	1:C:1650:ASP:HA	2.45	0.43
1:C:1697:GLU:HB2	1:C:1700:LEU:HD11	2.00	0.43
1:C:1770:VAL:HG21	1:C:1908:ALA:HA	1.99	0.43
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.01	0.43
1:A:1606:LYS:HE2	1:A:1606:LYS:CA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2143:VAL:O	1:B:2145:GLU:N	2.45	0.43
1:C:1654:GLN:O	1:C:1655:TYR:CB	2.65	0.43
1:C:1768:ARG:HH12	1:C:1770:VAL:HG23	1.84	0.43
1:C:1841:TYR:CZ	1:C:1896:THR:HG21	2.52	0.43
1:C:1869:THR:O	1:C:1870:LEU:HB2	2.19	0.43
1:A:1681:VAL:O	1:A:1682:ILE:HD13	2.19	0.43
1:A:1905:ALA:CB	1:A:1913:ALA:HA	2.48	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:1646:ALA:O	1:C:1648:ASN:N	2.51	0.43
1:C:1940:ASN:HB2	1:C:1981:TYR:CE1	2.54	0.43
1:C:2148:ARG:HD3	1:C:2152:ILE:CD1	2.48	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.19	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:1836:THR:O	1:C:1838:ASP:N	2.51	0.43
1:C:2135:LEU:HB3	1:C:2155:ILE:HD13	2.01	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:2186:LEU:C	1:C:2188:GLY:H	2.27	0.42
1:A:1633:GLU:OE1	1:A:1633:GLU:HA	2.18	0.42
1:A:2033:ILE:HG22	1:A:2034:LYS:CD	2.49	0.42
1:A:2086:TYR:O	1:A:2087:GLY:C	2.62	0.42
1:B:1659:THR:C	1:B:1661:GLU:N	2.76	0.42
1:B:2088:GLN:HA	1:B:2091:LEU:HD12	2.00	0.42
1:C:1735:ILE:N	1:C:1735:ILE:HD12	2.35	0.42
1:C:1827:TRP:CD2	1:C:1828:ASP:N	2.87	0.42
1:B:1759:ALA:O	1:B:1760:PRO:C	2.62	0.42
1:B:1844:ARG:HG3	1:B:1844:ARG:HH11	1.85	0.42
1:A:2042:ASP:O	1:A:2045:ASN:HB3	2.20	0.42
1:B:1946:PRO:CG	1:B:2130:LEU:HD21	2.45	0.42
1:B:2100:SER:HB2	1:B:2112:GLU:OE1	2.19	0.42
1:B:2110:SER:O	1:B:2111:LYS:CG	2.67	0.42
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.58	0.42
1:C:1927:ASN:OD1	1:C:1928:SER:N	2.52	0.42
1:C:2028:GLN:O	1:C:2029:GLY:C	2.61	0.42
1:C:2142:GLN:HE21	1:C:2190:LYS:HD3	1.84	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

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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:C:1653:PHE:C	1:C:1653:PHE:HD2	2.26	0.42
1:A:1659:THR:OG1	1:A:1661:GLU:HB3	2.20	0.42
1:A:1775:LEU:N	1:A:1775:LEU:HD12	2.34	0.42
1:A:1780:THR:O	1:A:1784:TYR: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:1681:VAL:O	1:A:1682:ILE:CG1	2.67	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:C:2140:SER:OG	1:C:2151:LYS:HE3	2.20	0.42
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.50	0.42
1:A:2134:TYR:OH	1:A:2138:ARG:NH1	2.53	0.42
1:B:1640:GLN:HB3	1:B:1657:TYR:CE1	2.55	0.42
1:B:1693:ILE:HG21	1:C:2097:HIS:NE2	2.35	0.42
1:B:1828:ASP:OD2	1:B:2120:ARG:NE	2.53	0.42
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.89	0.42
1:C:1545:ASP:OD1	1:C:1547:ASN:N	2.44	0.42
1:C:1587:ASN:HD21	1:C:1624:ASN:HD22	1.68	0.42
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.54	0.42
1:C:1903:ILE:N	1:C:1903:ILE:CD1	2.82	0.42
1:B:2097:HIS:CD2	1:C:1693:ILE:HB	2.55	0.42
1:B:2184:ASP:O	1:B:2185:LYS:C	2.63	0.42
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	2.02	0.42
1:C:1655:TYR:O	1:C:1656:LEU:HD13	2.20	0.42
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:A:1845:TRP:CD1	1:A:1850:ARG:HG3	2.55	0.41
1:B:1755:ILE:N	1:B:1755:ILE:CD1	2.83	0.41
1:B:1755:ILE:HA	1:C:1963:MSE:HE1	2.01	0.41
1:C:1677:THR:HG22	1:C:1690:ILE:HA	2.01	0.41
1:C:2124:TRP:O	1:C:2168:ASP:HB3	2.19	0.41
1:A:1494:GLN:HE21	1:A:1558:GLY:HA3	1.84	0.41
1:A:1680:THR:HG22	1:A:1682:ILE:HG12	2.01	0.41
1:A:2043:THR:O	1:A:2046:ARG:HG3	2.19	0.41
1:A:2134:TYR:HD2	1:A:2135:LEU:HD12	1.83	0.41
1:B:1610:TYR:CE1	1:B:1614:ARG:CZ	3.04	0.41
1:B:1665:THR:O	1:B:1668:LYS:HB3	2.19	0.41
1:B:1968:LEU:HD23	1:C:1783:MSE:HE1	2.01	0.41
1:A:1744:GLN:NE2	3:A:5035:HOH:O	2.53	0.41
1:B:1608:THR:O	1:B:1612:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1645:ASP:O	1:B:1646:ALA:C	2.62	0.41
1:B:1764:LYS:HB2	1:B:1764:LYS:NZ	2.35	0.41
1:B:2142:GLN:HB2	1:B:2190:LYS:NZ	2.36	0.41
1:A:1770:VAL:HG21	1:A:1908:ALA:CA	2.51	0.41
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	2.02	0.41
1:A:2140:SER:C	1:A:2142:GLN:N	2.77	0.41
1:B:1569:ILE:CG2	1:B:1571:VAL:HG22	2.49	0.41
1:B:1587:ASN:ND2	1:B:1623:ALA:H	2.09	0.41
1:C:1530:VAL:O	1:C:1530:VAL:HG23	2.20	0.41
1:C:1549:GLU:HG2	1:C:1550:LEU:O	2.20	0.41
1:C:1786:ASN:HB3	1:C:1788:VAL:H	1.85	0.41
1:B:2021:ARG:HD3	1:B:2095:ASP:OD2	2.20	0.41
1:C:1731:ARG:HA	1:C:1753:PRO:O	2.20	0.41
1:A:1545:ASP:OD2	1:A:1545:ASP:C	2.62	0.41
1:A:1645:ASP:O	1:A:1647:ALA:N	2.53	0.41
1:A:1783:MSE:HA	1:A:1786:ASN:HB2	2.01	0.41
1:A:2143:VAL:HB	1:A:2193:SER:HB3	2.03	0.41
1:B:1641:VAL:O	1:B:1657:TYR:HE1	2.03	0.41
1:A:1587:ASN:HD22	1:A:1622:ALA:HA	1.85	0.41
1:A:1906:ASP:HA	1:A:1907:PRO:HD3	1.80	0.41
1:B:1544:GLU:OE1	1:B:1602:GLU:OE1	2.39	0.41
1:B:1562:ILE:HD11	1:B:1599:GLN:OE1	2.20	0.41
1:B:1991:PRO:O	1:B:2019:ASN:O	2.38	0.41
1:B:2004:ASP:OD2	1:B:2006:THR:CG2	2.63	0.41
1:C:2187:LYS:C	1:C:2189:LEU:N	2.75	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:1814:ARG:O	1:B:1815:ASN:HB2	2.20	0.41
1:B:1835:PRO:HB2	1:B:1992:THR:HG23	2.03	0.41
1:B:2186:LEU:CD2	1:B:2190:LYS:HE2	2.39	0.41
1:A:1616:ILE:HD12	1:A:1813:LYS:HB3	2.02	0.41
1:A:2081:GLU:HB2	1:A:2082:LEU:CD1	2.51	0.41
1:A:2140:SER:O	1:A:2145:GLU:CD	2.64	0.41
1:B:2046:ARG:O	1:B:2046:ARG:HG3	2.20	0.41
1:B:2081:GLU:HG2	1:B:2082:LEU:N	2.35	0.41
1:B:2089:ILE:HG13	1:C:1653:PHE:CD1	2.55	0.41
1:B:2102:ARG:HA	1:C:1694:ILE:HD12	2.02	0.41
1:B:2133:GLU:OE1	1:B:2148:ARG:NH2	2.54	0.41
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	2.03	0.41
1:B:2154:ARG:HH21	1:B:2189:LEU:HD13	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1633:GLU:O	1:C:1636:VAL:HB	2.21	0.41
1:A:1487:TYR:HB3	1:A:1488:PRO:CD	2.51	0.41
1:B:1533:THR:HG1	1:B:1535:ASP:CG	2.29	0.41
1:B:2178:ASN:HB3	1:B:2181:THR:CG2	2.48	0.41
1:C:2001:VAL:HG23	1:C:2002:VAL:H	1.85	0.41
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.49	0.40
1:A:1766:LEU:HD12	1:A:1766:LEU:N	2.36	0.40
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.68	0.40
1:B:1583:VAL:HG12	1:B:1618:ARG:HA	2.03	0.40
1:B:1705:LEU:HB3	1:C:2000:TRP:CG	2.57	0.40
1:B:1708:SER:HB3	1:B:1735:ILE:CG2	2.51	0.40
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.20	0.40
1:B:2039:LYS:HE3	1:B:2039:LYS:HB2	1.93	0.40
1:B:2147:SER:O	1:B:2148:ARG:C	2.63	0.40
1:B:2186:LEU:C	1:B:2188:GLY:N	2.79	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:A:1829:ARG:NH2	1:A:1858:TYR:HB3	2.36	0.40
1:B:1508:VAL:HG23	1:B:1509:TYR:N	2.36	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:2142:GLN:HE22	1:B:2189:LEU:CD1	2.35	0.40
1:B:2188:GLY:C	1:B:2190:LYS:H	2.29	0.40
1:C:1542:LEU:HD12	1:C:1542:LEU:HA	1.76	0.40
1:C:1616:ILE:CD1	1:C:1813:LYS:HB3	2.52	0.40
1:C:1836:THR:O	1:C:1837:ASN:C	2.64	0.40
1:C:2135:LEU:CB	1:C:2155:ILE:HD13	2.51	0.40
1:B:1708:SER:HB3	1:B:1735:ILE:HG23	2.03	0.40
1:B:1862:ASP:HB2	1:B:1865:SER:HB3	2.02	0.40
1:C:1762:ILE:HG21	1:C:1771:TYR:CE1	2.51	0.40
1:C:1877:VAL:HG23	1:C:1928:SER:OG	2.21	0.40
1:C:1991:PRO:C	1:C:1993:GLY:N	2.80	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:A:1913:ALA:O	1:A:1914:GLU:C	2.63	0.40
1:A:2178:ASN:O	1:A:2179:TYR:C	2.64	0.40
1:B:1483:ILE:H	1:B:1483:ILE:CD1	2.18	0.40
1:B:1629:ILE:HG22	1:C:2024:VAL:HG11	2.03	0.40
1:C:1575:GLU:CD	1:C:1575:GLU:N	2.77	0.40
1:C:1592:LYS:C	1:C:1593:ILE:HG12	2.46	0.40
1:C:1730:CYS:O	1:C:1731:ARG:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1734:GLY:C	1:C:1736:GLY:N	2.78	0.40
1:C:1996:ARG:O	1:C:1997:GLY:C	2.64	0.40
1:C:2184:ASP:O	1:C:2185:LYS:C	2.64	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%)	3	8
1	B	680/805 (84%)	602 (88%)	64 (9%)	14 (2%)	5	15
1	C	668/805 (83%)	582 (87%)	66 (10%)	20 (3%)	3	8
All	All	2028/2415 (84%)	1773 (87%)	200 (10%)	55 (3%)	4	10

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	531 (92%)	48 (8%)	10	26
1	B	579/668 (87%)	529 (91%)	50 (9%)	10	25
1	C	568/668 (85%)	506 (89%)	62 (11%)	6	16
All	All	1726/2004 (86%)	1566 (91%)	160 (9%)	8	21

All (160) 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	1575	GLU
1	A	1585	VAL
1	A	1589	ILE
1	A	1602	GLU
1	A	1606	LYS
1	A	1616	ILE
1	A	1633	GLU
1	A	1638	LEU
1	A	1640	GLN
1	A	1648	ASN
1	A	1649	PRO
1	A	1653	PHE
1	A	1663	MSE

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Mol	Chain	Res	Type
1	A	1665	THR
1	A	1689	VAL
1	A	1697	GLU
1	A	1732	SER
1	A	1735	ILE
1	A	1756	LEU
1	A	1770	VAL
1	A	1781	GLN
1	A	1813	LYS
1	A	1816	MSE
1	A	1837	ASN
1	A	1850	ARG
1	A	1877	VAL
1	A	1878	VAL
1	A	1879	VAL
1	A	1884	LEU
1	A	1889	LEU
1	A	1903	ILE
1	A	1910	PRO
1	A	1924	TRP
1	A	1950	LEU
1	A	1960	GLN
1	A	1991	PRO
1	A	2031	VAL
1	A	2035	PHE
1	A	2041	LEU
1	A	2081	GLU
1	A	2082	LEU
1	A	2091	LEU
1	A	2098	ASP
1	B	1481	ARG
1	B	1502	LEU
1	B	1531	LYS
1	B	1536	PHE
1	B	1562	ILE
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

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Mol	Chain	Res	Type
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	1756	LEU
1	B	1757	THR
1	B	1764	LYS
1	B	1781	GLN
1	B	1791	LEU
1	B	1792	THR
1	B	1797	LEU
1	B	1824	LYS
1	B	1839	GLU
1	B	1843	VAL
1	B	1884	LEU
1	B	1915	THR
1	B	1924	TRP
1	B	1991	PRO
1	B	2018	VAL
1	B	2021	ARG
1	B	2027	PRO
1	B	2041	LEU
1	B	2043	THR
1	B	2100	SER
1	B	2117	GLU
1	B	2119	ARG
1	B	2127	ARG
1	B	2131	ASN
1	B	2149	LEU
1	B	2181	THR
1	B	2186	LEU
1	B	2187	LYS
1	B	2192	GLU
1	C	1493	LEU
1	C	1499	LYS
1	C	1508	VAL
1	C	1514	LEU

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Mol	Chain	Res	Type
1	C	1533	THR
1	C	1542	LEU
1	C	1546	GLU
1	C	1550	LEU
1	C	1551	THR
1	C	1568	LYS
1	C	1571	VAL
1	C	1575	GLU
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
1	C	1653	PHE
1	C	1654	GLN
1	C	1655	TYR
1	C	1656	LEU
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	1824	LYS
1	C	1843	VAL
1	C	1851	GLU
1	C	1875	LYS
1	C	1879	VAL
1	C	1910	PRO
1	C	1911	ASN
1	C	1924	TRP

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Mol	Chain	Res	Type
1	C	1945	LEU
1	C	1960	GLN
1	C	2013	GLU
1	C	2027	PRO
1	C	2031	VAL
1	C	2035	PHE
1	C	2036	ARG
1	C	2037	ARG
1	C	2047	LEU
1	C	2081	GLU
1	C	2088	GLN
1	C	2106	LYS
1	C	2116	THR
1	C	2145	GLU
1	C	2189	LEU
1	C	2192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1517	GLN
1	A	1522	GLN
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	1673	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1815	ASN
1	A	1911	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

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Mol	Chain	Res	Type
1	A	2131	ASN
1	A	2142	GLN
1	A	2170	GLN
1	A	2178	ASN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	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
1	B	1918	GLN
1	B	1934	GLN
1	B	1937	ASN
1	B	1941	ASN
1	B	1944	GLN
1	B	2011	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2178	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1547	ASN
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	1683	ASN
1	C	1744	GLN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1815	ASN

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Mol	Chain	Res	Type
1	C	1909	ASN
1	C	1922	GLN
1	C	1941	ASN
1	C	1960	GLN
1	C	1983	GLN
1	C	2011	GLN
1	C	2088	GLN
1	C	2142	GLN
1	C	2170	GLN
1	C	2178	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	-	11,11,11	1.67	3 (27%)	15,15,15	0.74	0

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	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3196	ADE	C4-N3	2.62	1.39	1.35
2	C	3196	ADE	C8-N7	2.21	1.36	1.32
2	C	3196	ADE	C2-N1	2.04	1.37	1.33

There are no bond angle outliers.

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 [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	667/805 (82%)	0.27	49 (7%)	21 18	20, 36, 74, 88	0
1	B	667/805 (82%)	0.45	64 (9%)	13 11	21, 38, 77, 94	0
1	C	655/805 (81%)	0.42	66 (10%)	12 10	23, 39, 77, 92	0
All	All	1989/2415 (82%)	0.38	179 (8%)	15 13	20, 38, 76, 94	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2191	LEU	9.6
1	B	2144	GLY	7.9
1	C	2194	PHE	7.7
1	B	2143	VAL	6.9
1	C	2195	ALA	6.6
1	A	2191	LEU	6.3
1	B	2085	ILE	6.2
1	B	1480	LEU	6.1
1	B	2193	SER	6.1
1	B	2195	ALA	6.0
1	A	1646	ALA	6.0
1	C	2192	GLU	5.4
1	B	1481	ARG	5.2
1	C	1682	ILE	5.2
1	B	2194	PHE	5.2
1	B	1682	ILE	5.1
1	A	1482	PRO	4.9
1	A	1651	LYS	4.9
1	A	2143	VAL	4.7
1	B	1684	GLY	4.6
1	C	1655	TYR	4.6
1	A	1647	ALA	4.5
1	A	2193	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	2047	LEU	4.4
1	C	2143	VAL	4.4
1	A	1483	ILE	4.4
1	B	1646	ALA	4.4
1	B	2041	LEU	4.3
1	A	1682	ILE	4.3
1	B	1681	VAL	4.3
1	A	1680	THR	4.2
1	A	2194	PHE	4.2
1	C	2189	LEU	4.2
1	B	2179	TYR	4.2
1	B	2190	LYS	4.2
1	A	1649	PRO	4.1
1	B	2045	ASN	4.1
1	A	1480	LEU	4.1
1	C	1664	GLU	4.0
1	C	2191	LEU	3.9
1	A	1681	VAL	3.9
1	B	1648	ASN	3.8
1	C	1681	VAL	3.7
1	B	1685	GLU	3.7
1	C	2193	SER	3.7
1	B	1680	THR	3.7
1	C	2141	HIS	3.7
1	B	2083	LEU	3.6
1	B	2134	TYR	3.6
1	C	1685	GLU	3.6
1	C	2081	GLU	3.6
1	B	1483	ILE	3.6
1	A	1669	PHE	3.6
1	C	2149	LEU	3.6
1	B	1482	PRO	3.6
1	B	1530	VAL	3.6
1	B	1647	ALA	3.5
1	C	1647	ALA	3.5
1	B	2141	HIS	3.5
1	B	1921	GLY	3.5
1	C	1533	THR	3.5
1	C	2041	LEU	3.5
1	A	1906	ASP	3.4
1	B	1649	PRO	3.4
1	C	1679	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1651	LYS	3.3
1	C	1662	GLY	3.3
1	C	1686	GLU	3.2
1	C	1646	ALA	3.2
1	A	1648	ASN	3.2
1	A	1853	GLU	3.2
1	A	2082	LEU	3.2
1	C	1644	ASN	3.1
1	C	2190	LYS	3.1
1	A	2142	GLN	3.1
1	A	2190	LYS	3.1
1	B	1642	ALA	3.1
1	A	1481	ARG	3.1
1	C	2188	GLY	3.1
1	C	2047	LEU	3.0
1	B	1683	ASN	3.0
1	C	1680	THR	3.0
1	A	2195	ALA	2.9
1	B	1638	LEU	2.9
1	B	1852	THR	2.9
1	A	2084	PRO	2.9
1	B	2082	LEU	2.9
1	B	1659	THR	2.8
1	B	2186	LEU	2.8
1	C	2045	ASN	2.8
1	A	1668	LYS	2.8
1	A	1650	ASP	2.8
1	A	1684	GLY	2.8
1	C	1669	PHE	2.8
1	B	1910	PRO	2.8
1	A	1643	TRP	2.8
1	C	1501	HIS	2.8
1	A	2047	LEU	2.8
1	C	1688	PHE	2.8
1	C	2187	LYS	2.7
1	A	1837	ASN	2.7
1	B	1673	ASN	2.7
1	C	1683	ASN	2.7
1	C	2039	LYS	2.7
1	C	1652	GLY	2.7
1	B	2187	LYS	2.7
1	B	1911	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1648	ASN	2.7
1	C	1675	VAL	2.7
1	C	1911	ASN	2.7
1	B	1658	LEU	2.6
1	A	2141	HIS	2.6
1	A	1641	VAL	2.6
1	C	2046	ARG	2.6
1	C	1666	LEU	2.6
1	A	1657	TYR	2.6
1	A	1642	ALA	2.6
1	C	2083	LEU	2.5
1	B	1767	GLY	2.5
1	C	1645	ASP	2.5
1	B	1839	GLU	2.5
1	B	1824	LYS	2.5
1	B	1687	ARG	2.5
1	C	2037	ARG	2.5
1	A	2145	GLU	2.5
1	C	1667	LYS	2.4
1	C	2144	GLY	2.4
1	A	1658	LEU	2.4
1	B	1669	PHE	2.4
1	C	1659	THR	2.4
1	C	1673	ASN	2.4
1	C	1556	GLU	2.4
1	C	1657	TYR	2.3
1	C	1665	THR	2.3
1	B	2038	GLU	2.3
1	C	2036	ARG	2.3
1	C	2142	GLN	2.3
1	C	2082	LEU	2.3
1	A	1659	THR	2.3
1	B	1650	ASP	2.3
1	C	2043	THR	2.3
1	C	2145	GLU	2.3
1	B	1643	TRP	2.2
1	B	1653	PHE	2.2
1	C	2085	ILE	2.2
1	B	2043	THR	2.2
1	C	1838	ASP	2.2
1	C	1653	PHE	2.2
1	C	2089	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1685	GLU	2.2
1	A	2081	GLU	2.2
1	A	1529	ASP	2.2
1	A	2189	LEU	2.2
1	B	1660	SER	2.2
1	B	2089	ILE	2.2
1	B	2084	PRO	2.2
1	B	1531	LYS	2.2
1	B	2165	HIS	2.2
1	B	1729	THR	2.1
1	A	2045	ASN	2.1
1	C	1769	GLU	2.1
1	A	1687	ARG	2.1
1	B	2046	ARG	2.1
1	A	2041	LEU	2.1
1	B	1664	GLU	2.1
1	A	1679	ARG	2.1
1	A	1855	GLY	2.1
1	B	1645	ASP	2.1
1	A	2037	ARG	2.1
1	C	1492	TRP	2.1
1	A	2187	LYS	2.1
1	A	1767	GLY	2.1
1	C	1693	ILE	2.1
1	B	2081	GLU	2.0
1	C	1546	GLU	2.0
1	C	1531	LYS	2.0
1	B	1657	TYR	2.0
1	C	1651	LYS	2.0
1	C	2084	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ADE	C	3196	10/10	0.73	0.27	86,87,87,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.