



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:09 PM UTC

PDB ID : 1BMV / pdb_00001bmv
Title : PROTEIN-RNA INTERACTIONS IN AN ICOSAHEDRAL VIRUS AT 3.0
ANGSTROMS RESOLUTION
Authors : Chen, Z.; Stauffacher, C.; Li, Y.; Schmidt, T.; Bomu, W.; Kamer, G.; Shanks,
M.; Lomonosoff, G.; Johnson, J.E.
Deposited on : 1989-10-09
Resolution : 3.00 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	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

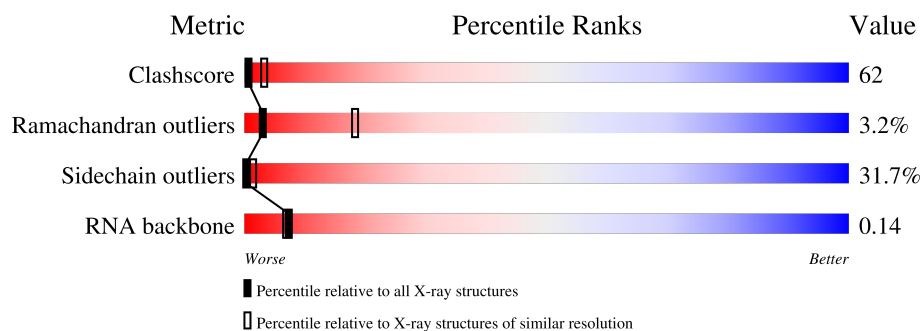
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	M	11	91% 9%
2	1	198	23% 45% 21% 7%
3	2	374	20% 49% 26% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4613 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 RNA chain called RNA (5'-R(*GP*GP*UP*CP*AP*AP*AP*AP*UP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	11	Total	C	N	O	P	0	0	0
			238	106	45	76	11			

- Molecule 2 is a protein called PROTEIN (ICOSAHEDRAL VIRUS - A DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	185	Total	C	N	O	S	0	0	0
			1451	924	244	274	9			

- Molecule 3 is a protein called PROTEIN (ICOSAHEDRAL VIRUS - B AND C DOMAIN).

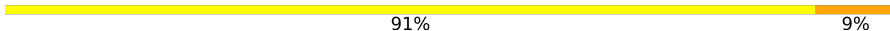
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	374	Total	C	N	O	S	0	6	0
			2924	1867	487	542	28			

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

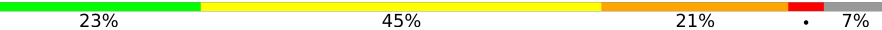
Note EDS failed to run properly.

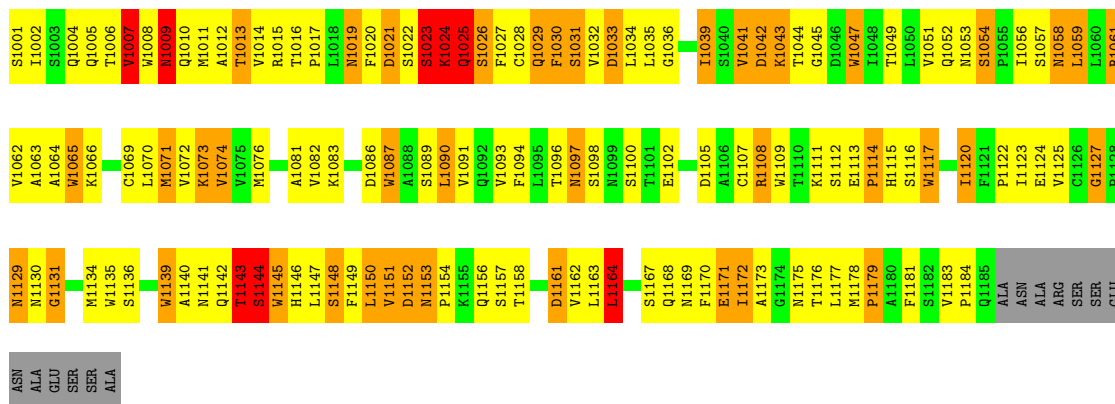
- Molecule 1: RNA (5'-R(*GP*GP*UP*CP*AP*AP*AP*AP*UP*GP*C)-3')

Chain M: 

G1 G2 U3 C4 U5 A5 A6 A7 U9 G10 C11

- Molecule 2: PROTEIN (ICOSAHEDRAL VIRUS - A DOMAIN)

Chain 1: 



Q2129	S2069	P2008
V2130	K2070	F2009
R2131	M2071	V2010
P2132	T2072	L2011
A2133	S2073	N2012
T2134	P2074	R2013
T2135	Y2075	N2014
L2136	I2076	M2015
L2137	K2077	G2016
A2138	C2078	K2017
D2139	T2079	L2018
G2140	V2080	T2019
C2141	S2081	F2020
P2142	F2082	P2021
Y2143	F2083	Q2022
L2144	I2084	G2023
Y2145	A2085	T2024
A2146	F2086	S2025
N2147	G2087	R2026
V2148	N2088	S2027
H2149	L2089	V2028
D2150	A2090	K2029
S2151	D2091	R2030
S2152	D2092	M2031
V2153	T2093	P2032
S2154	I2094	L2033
	N2095	S2034
G2158	F2096	I2035
D2159	E2097	G2036
F2160	A2098	G2037
V2161	F2099	G2038
I2162	P2100	A2039
G2163	H2101	
V2164	K2102	K2042
K2165	L2103	S2043
L2166	V2104	A2044
T2167	G2105	I2045
I2168	F2106	L2046
I2169	G2107	M2047
E2170	E2108	N2048
N2171	I2109	M2049
N2172	Q2110	P2050
	E2111	N2051
G2176	K2112	A2052
L2177	V2113	V2053
N2178	V2114	L2054
P2179	L2115	S2055
G2180	K2116	M2056
I2181	F2117	M2057
S2182	S2118	R2058
	Q2119	T2059
R2185	E2120	F2060
L2186	E2121	V2061
L2187	F2122	G2062
G2188	L2123	D2063
T2189	T2124	L2064
I2190	A2125	V2065
P2191	M2126	F2066
Q2192	S2127	E2067
	T2128	V2068

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	311.20Å 284.20Å 350.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	NONE	Depositor
R, R_{free}	0.330 , (Not available)	Depositor
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4613	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	M	0.79	1/266 (0.4%)	1.18	0/411
2	1	1.39	11/1490 (0.7%)	1.83	39/2031 (1.9%)
3	2	1.44	24/2988 (0.8%)	1.83	83/4056 (2.0%)
All	All	1.40	36/4744 (0.8%)	1.80	122/6498 (1.9%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2070	LYS	N-CA	12.10	1.60	1.46
3	2	2077	LYS	CA-C	-12.07	1.38	1.52
3	2	2074	PRO	C-N	11.04	1.50	1.33
3	2	3052	THR	C-N	10.16	1.48	1.33
3	2	2077	LYS	N-CA	8.94	1.56	1.46
3	2	2071	MET	C-N	-8.77	1.20	1.33
3	2	3026	SER	N-CA	7.14	1.54	1.46
3	2	3108	CYS	N-CA	6.47	1.54	1.46
3	2	3091	ALA	C-N	-6.34	1.23	1.33
3	2	2160	PHE	N-CA	5.99	1.53	1.46
2	1	1183	VAL	CA-C	-5.89	1.47	1.52
3	2	3156	TRP	NE1-CE2	-5.70	1.31	1.37
3	2	3115	TRP	NE1-CE2	-5.66	1.31	1.37
2	1	1087	TRP	NE1-CE2	-5.64	1.31	1.37
3	2	3136	TRP	NE1-CE2	-5.59	1.31	1.37
3	2	2126	TRP	NE1-CE2	-5.56	1.31	1.37
2	1	1117	TRP	NE1-CE2	-5.53	1.31	1.37
1	M	1	G	OP3-P	5.50	1.59	1.48
2	1	1139	TRP	NE1-CE2	-5.50	1.31	1.37
3	2	3040	THR	C-N	5.49	1.39	1.33
3	2	3170	TRP	NE1-CE2	-5.49	1.31	1.37
3	2	3030	ILE	C-N	5.43	1.40	1.33
2	1	1145	TRP	NE1-CE2	-5.43	1.31	1.37
3	2	2108	GLU	C-N	-5.40	1.28	1.34
2	1	1047	TRP	NE1-CE2	-5.37	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2014	TRP	NE1-CE2	-5.29	1.31	1.37
2	1	1065	TRP	NE1-CE2	-5.26	1.31	1.37
3	2	2133	ALA	C-N	-5.22	1.26	1.33
3	2	2075	TYR	C-N	-5.21	1.26	1.33
3	2	3169	ASP	C-N	-5.16	1.26	1.33
2	1	1109	TRP	NE1-CE2	-5.16	1.31	1.37
3	2	2057	TRP	NE1-CE2	-5.15	1.31	1.37
2	1	1164	LEU	C-N	-5.14	1.26	1.33
3	2	3155	GLY	C-N	5.12	1.40	1.33
2	1	1087	TRP	N-CA	5.09	1.52	1.46
2	1	1008	TRP	NE1-CE2	-5.09	1.31	1.37

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2072	THR	N-CA-CB	-19.27	81.78	110.87
3	2	2068	VAL	N-CA-CB	-13.73	95.15	111.21
3	2	2070	LYS	N-CA-C	-12.40	89.63	109.59
3	2	2070	LYS	CB-CA-C	11.82	130.65	109.38
3	2	2077	LYS	CB-CA-C	11.46	130.01	109.38
3	2	2079	THR	N-CA-CB	-10.42	94.19	110.55
2	1	1184	PRO	O-C-N	9.88	134.57	122.71
3	2	2070	LYS	CA-C-O	9.55	130.83	120.71
3	2	3180	ARG	O-C-N	9.41	132.15	123.50
3	2	2068	VAL	CB-CA-C	9.08	123.42	110.98
3	2	3171	PHE	CA-CB-CG	8.93	122.73	113.80
3	2	2096	PHE	CB-CA-C	-8.56	97.43	110.88
3	2	2072	THR	CB-CA-C	8.29	127.96	111.22
3	2	2071	MET	O-C-N	-8.07	111.21	122.26
2	1	1089	SER	O-C-N	7.98	133.21	122.59
2	1	1114	PRO	O-C-N	7.86	132.55	123.03
2	1	1024	LYS	O-C-N	7.82	133.00	122.59
2	1	1025	GLN	O-C-N	7.69	132.82	122.59
3	2	2109	ILE	CB-CA-C	7.56	124.08	111.37
3	2	3154	THR	O-C-N	7.42	131.78	123.40
3	2	3104	ILE	CB-CA-C	7.25	123.19	111.29
3	2	3105	TYR	O-C-N	7.20	129.48	122.07
2	1	1158	THR	N-CA-C	7.08	118.88	111.03
3	2	2099	PHE	O-C-N	-7.04	114.75	121.57
2	1	1045	GLY	O-C-N	6.78	131.82	123.61
3	2	2060	PHE	CA-CB-CG	6.73	120.53	113.80
3	2	3039	GLY	N-CA-C	-6.71	105.63	115.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	1093	VAL	O-C-N	6.63	129.90	123.14
2	1	1157	SER	O-C-N	6.62	131.23	122.56
3	2	3171	PHE	O-C-N	-6.56	115.55	123.10
3	2	2118	SER	O-C-N	6.56	130.41	123.06
2	1	1009	ASN	O-C-N	6.55	131.26	123.33
3	2	2061	VAL	CB-CA-C	-6.54	100.56	111.29
3	2	3100	ALA	O-C-N	6.54	130.43	122.84
3	2	2096	PHE	N-CA-CB	6.44	119.36	110.01
3	2	2185	ARG	O-C-N	6.44	130.22	122.68
2	1	1171	GLU	CB-CA-C	6.43	121.33	109.70
2	1	1127	GLY	CA-C-N	6.24	125.86	119.56
2	1	1127	GLY	C-N-CA	6.24	125.86	119.56
3	2	3173	SER	O-C-N	6.22	130.06	123.03
2	1	1179	PRO	O-C-N	6.22	130.17	122.71
3	2	2096	PHE	CA-CB-CG	6.14	119.94	113.80
3	2	2151	SER	O-C-N	6.10	129.50	123.46
3	2	2073	SER	CA-C-N	6.07	127.42	119.84
3	2	2073	SER	C-N-CA	6.07	127.42	119.84
3	2	2159	ASP	O-C-N	-6.04	116.24	123.31
3	2	2089	LEU	O-C-N	6.04	130.17	123.16
2	1	1130	ASN	N-CA-C	-6.03	104.37	113.89
3	2	3066	HIS	CB-CA-C	-6.01	97.36	109.55
2	1	1144	SER	O-C-N	5.98	130.55	122.59
3	2	2034	SER	O-C-N	-5.94	116.09	123.04
2	1	1122	PRO	CB-CA-C	-5.93	102.49	110.85
2	1	1043	LYS	O-C-N	5.89	130.33	122.26
3	2	2171	ASN	O-C-N	5.89	129.32	122.67
2	1	1081	ALA	N-CA-C	-5.84	105.99	113.23
3	2	2109	ILE	N-CA-CB	-5.80	102.34	112.08
3	2	2073	SER	O-C-N	-5.79	115.28	121.42
3	2	2150	ASP	CB-CA-C	-5.77	98.93	110.42
3	2	2004	ASN	O-C-N	5.77	125.40	121.19
3	2	2047	MET	N-CA-C	5.77	118.04	108.99
2	1	1171	GLU	N-CA-CB	-5.76	100.83	110.80
3	2	2079	THR	CA-C-O	5.75	126.65	120.32
2	1	1131	GLY	O-C-N	5.75	130.17	122.70
3	2	2140	GLY	O-C-N	5.67	127.36	121.97
2	1	1023	SER	O-C-N	5.64	128.69	123.50
2	1	1025	GLN	CA-C-N	5.63	128.88	120.31
2	1	1025	GLN	C-N-CA	5.63	128.88	120.31
2	1	1130	ASN	CB-CA-C	5.60	119.38	109.75
2	1	1157	SER	CA-C-N	5.60	128.24	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	1157	SER	C-N-CA	5.60	128.24	120.63
3	2	3145	GLY	O-C-N	-5.57	116.29	122.47
3	2	2170	GLU	CB-CA-C	-5.56	100.10	109.72
3	2	3180	ARG	NE-CZ-NH2	5.55	124.19	119.20
2	1	1049	THR	O-C-N	5.49	130.08	123.16
3	2	3064	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	1	1143	THR	N-CA-CB	-5.45	101.11	110.86
3	2	2098	ALA	O-C-N	5.44	129.16	122.20
3	2	3146	PHE	O-C-N	5.40	129.58	122.93
2	1	1030	PHE	O-C-N	5.38	129.17	123.42
2	1	1005	GLN	O-C-N	5.36	129.37	123.16
2	1	1158	THR	CB-CA-C	-5.35	102.65	110.95
2	1	1033	ASP	O-C-N	5.34	129.37	122.43
3	2	2027	SER	CA-C-N	5.33	128.55	120.77
3	2	2027	SER	C-N-CA	5.33	128.55	120.77
3	2	3071	MET	N-CA-C	5.32	118.07	109.40
2	1	1061	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	2	3097	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	2	2186	LEU	O-C-N	5.31	128.90	122.85
3	2	3057	ARG	NE-CZ-NH2	5.29	123.97	119.20
3	2	3033	PRO	O-C-N	5.29	129.09	123.01
3	2	3043	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	2	3067	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	2	3014	GLU	N-CA-C	5.27	118.33	109.95
3	2	2167	THR	CB-CA-C	5.27	119.56	110.86
3	2	2013	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	2	2150	ASP	O-C-N	5.24	129.56	122.59
3	2	3155	GLY	CA-C-N	5.24	128.29	120.90
3	2	3155	GLY	C-N-CA	5.24	128.29	120.90
3	2	2034	SER	N-CA-C	-5.22	101.46	109.76
3	2	3157	THR	O-C-N	5.20	129.92	122.28
3	2	3028	SER	O-C-N	5.19	129.26	123.19
3	2	3039	GLY	O-C-N	5.18	128.39	122.38
2	1	1108	ARG	NE-CZ-NH2	5.18	123.86	119.20
3	2	3180	ARG	CB-CA-C	5.16	118.63	111.51
3	2	3099	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	1	1153	ASN	CA-C-N	5.12	125.19	119.87
2	1	1153	ASN	C-N-CA	5.12	125.19	119.87
3	2	2074	PRO	CA-N-CD	5.12	119.16	112.00
3	2	3124	THR	CB-CA-C	-5.11	103.16	110.62
3	2	3145	GLY	CA-C-N	-5.11	113.80	120.95
3	2	3145	GLY	C-N-CA	-5.11	113.80	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	1153	ASN	O-C-N	5.09	127.17	121.32
3	2	2095	ASN	N-CA-C	5.09	119.24	113.19
3	2	2109	ILE	O-C-N	5.05	127.04	122.14
3	2	2076	ILE	CA-C-N	5.04	130.24	122.93
3	2	2076	ILE	C-N-CA	5.04	130.24	122.93
3	2	3159	THR	O-C-N	5.03	125.98	121.35
3	2	2140	GLY	N-CA-C	-5.03	107.05	115.80
3	2	3077	THR	N-CA-C	5.02	116.22	107.93
3	2	2069	SER	CA-C-N	-5.02	115.65	122.93
3	2	2069	SER	C-N-CA	-5.02	115.65	122.93
2	1	1007	VAL	O-C-N	5.02	129.64	122.62

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	M	238	0	120	15	0
2	1	1451	0	1402	151	0
3	2	2924	0	2939	422	0
All	All	4613	0	4461	561	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 62.

All (561) 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)
3:2:2190[A]:ILE:HG12	3:2:2191[A]:PRO:CD	1.51	1.39
3:2:2066:PHE:CE2	3:2:2166:LEU:HD12	1.63	1.32
3:2:2186:LEU:C	3:2:2187[B]:LEU:HA	1.56	1.28
3:2:2033:LEU:HB2	3:2:2142:PRO:O	1.40	1.18
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:HD2	1.72	1.17
3:2:2189[A]:THR:O	3:2:2190[A]:ILE:CB	1.91	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2057:TRP:CZ3	3:2:2172:MET:HE1	1.80	1.15
2:1:1134:MET:HE1	3:2:3144:THR:HG23	1.28	1.15
3:2:2190[B]:ILE:HB	3:2:2191[B]:PRO:CD	1.78	1.13
3:2:2190[B]:ILE:HB	3:2:2191[B]:PRO:HD3	1.29	1.13
3:2:2057:TRP:HZ3	3:2:2172:MET:CE	1.61	1.12
3:2:3025:ILE:HD11	3:2:3051:LEU:HD22	1.31	1.11
3:2:2057:TRP:HZ3	3:2:2172:MET:HE1	1.08	1.10
3:2:2066:PHE:CZ	3:2:2166:LEU:HD12	1.90	1.05
3:2:2057:TRP:CZ3	3:2:2172:MET:CE	2.39	1.05
3:2:3182:TYR:CD1	3:2:2049:MET:HE2	1.93	1.04
3:2:3092:MET:HE1	3:2:3170:TRP:HH2	1.22	1.04
3:2:2035:ILE:HD11	3:2:2060:PHE:CZ	1.93	1.02
2:1:1012:ALA:HB3	2:1:1162:VAL:HB	1.07	1.02
2:1:1134:MET:HE1	3:2:3144:THR:CG2	1.90	1.02
3:2:2048:ASN:C	3:2:2048:ASN:HD22	1.66	1.01
3:2:2066:PHE:CZ	3:2:2166:LEU:CD1	2.43	1.01
3:2:3123:MET:HE2	3:2:3125:MET:HB2	1.40	1.01
3:2:3128:ASN:ND2	3:2:3177:CYS:HB3	1.76	1.01
2:1:1011:MET:HE1	2:1:1034:LEU:HA	1.37	1.00
3:2:2066:PHE:CE2	3:2:2166:LEU:CD1	2.43	1.00
1:M:3:U:C2'	1:M:4:C:H5'	1.91	0.99
3:2:2106:PHE:CE1	3:2:2113:VAL:HG23	1.96	0.99
3:2:2135:THR:O	3:2:2137:LEU:N	1.95	0.99
3:2:3026:SER:HG	3:2:3170:TRP:CD1	1.81	0.99
2:1:1134:MET:CE	3:2:3144:THR:HG23	1.91	0.98
2:1:1012:ALA:CB	2:1:1162:VAL:HB	1.94	0.97
2:1:1012:ALA:HB3	2:1:1162:VAL:CB	1.95	0.96
2:1:1129:ASN:OD1	3:2:3130:ASN:ND2	1.97	0.96
3:2:2047:MET:HE2	3:2:2052:ALA:HA	1.46	0.96
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:CD	2.37	0.94
3:2:2190[B]:ILE:CG1	3:2:2191[B]:PRO:HD2	1.96	0.94
2:1:1020:PHE:CE1	2:1:1044:THR:HG21	2.02	0.94
3:2:3130:ASN:O	3:2:3132:CYS:N	2.02	0.93
3:2:2048:ASN:O	3:2:2048:ASN:ND2	2.02	0.93
3:2:2190[B]:ILE:CB	3:2:2191[B]:PRO:CD	2.48	0.92
3:2:2047:MET:CE	3:2:2052:ALA:HA	1.99	0.92
3:2:2135:THR:C	3:2:2137:LEU:H	1.77	0.92
3:2:2192[B]:GLN:NE2	3:2:2192[B]:GLN:HA	1.84	0.91
2:1:1069:CYS:O	2:1:1167:SER:CB	2.18	0.91
3:2:3114:LEU:HD11	3:2:3153:VAL:HG21	1.53	0.90
2:1:1091:VAL:HG11	2:1:1117:TRP:HZ2	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2079:THR:HB	3:2:2150:ASP:OD2	1.72	0.89
3:2:2030:ARG:HD3	3:2:2145:TYR:CE1	2.08	0.89
3:2:3084:THR:HB	3:2:3158:ALA:HB3	1.52	0.89
3:2:2190[B]:ILE:HG13	3:2:2191[B]:PRO:HD2	1.55	0.89
2:1:1105:ASP:OD1	2:1:1108:ARG:NH1	2.07	0.88
2:1:1054:SER:O	2:1:1058:ASN:HB2	1.72	0.88
3:2:3083:ASN:H	3:2:3083:ASN:HD22	1.20	0.88
3:2:2189[A]:THR:O	3:2:2190[A]:ILE:HB	1.02	0.88
3:2:3052:THR:HG22	3:2:3052:THR:O	1.72	0.88
3:2:2104:VAL:HG13	3:2:2113:VAL:HG11	1.56	0.88
2:1:1020:PHE:CE1	2:1:1044:THR:CG2	2.56	0.88
3:2:3030:ILE:CD1	3:2:3150:ILE:HD13	2.05	0.87
3:2:3092:MET:HE1	3:2:3170:TRP:CH2	2.09	0.87
1:M:3:U:O2'	1:M:4:C:H5'	1.73	0.87
2:1:1032:VAL:HG12	2:1:1034:LEU:HD12	1.55	0.87
2:1:1091:VAL:HG11	2:1:1117:TRP:CZ2	2.10	0.86
3:2:3105:TYR:HE1	3:2:2046:LEU:O	1.56	0.86
3:2:2048:ASN:ND2	3:2:2050:PRO:HD2	1.89	0.86
2:1:1021:ASP:C	2:1:1023:SER:H	1.82	0.86
3:2:3091:ALA:CB	3:2:3107:ILE:HG13	2.05	0.86
3:2:2031:MET:HE1	3:2:2164:VAL:HG21	1.58	0.85
2:1:1069:CYS:O	2:1:1167:SER:HB2	1.73	0.85
3:2:3074:MET:CE	3:2:3123:MET:HE1	2.06	0.84
3:2:2073:SER:O	3:2:2075:TYR:N	2.09	0.84
2:1:1025:GLN:HG3	2:1:1026:SER:H	1.41	0.84
2:1:1020:PHE:HE1	2:1:1044:THR:HG21	1.39	0.84
2:1:1065:TRP:HB2	2:1:1173:ALA:O	1.78	0.84
2:1:1021:ASP:O	2:1:1023:SER:N	2.10	0.84
3:2:3018:GLY:N	3:2:3023:LEU:HD11	1.93	0.83
3:2:2022:GLN:HA	3:2:2152:SER:HB3	1.59	0.83
3:2:2104:VAL:CG1	3:2:2113:VAL:HG11	2.09	0.82
3:2:2030:ARG:HD3	3:2:2145:TYR:CZ	2.15	0.82
3:2:3047:LEU:HD13	3:2:3092:MET:HE3	1.59	0.82
3:2:2096:PHE:O	3:2:2099:PHE:HB2	1.78	0.82
3:2:3025:ILE:CD1	3:2:3051:LEU:HD22	2.09	0.82
3:2:2030:ARG:NH2	3:2:2091:ASP:OD2	2.12	0.82
3:2:3074:MET:HE1	3:2:3090:CYS:HB3	1.60	0.82
2:1:1016:THR:CG2	2:1:1017:PRO:HD2	2.10	0.82
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:CG2	2.10	0.82
3:2:2106:PHE:HE1	3:2:2113:VAL:HG23	1.41	0.81
2:1:1057:SER:O	2:1:1061:ARG:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:3020:MET:HE3	3:2:3073:LYS:HZ2	1.44	0.81
3:2:3104:ILE:O	3:2:3108:CYS:SG	2.39	0.81
3:2:3047:LEU:HG	3:2:3051:LEU:HD11	1.61	0.81
3:2:2129:GLN:HB3	3:2:2181:ILE:HD12	1.61	0.81
2:1:1053:ASN:OD1	2:1:1061:ARG:NH2	2.13	0.80
3:2:3030:ILE:HD11	3:2:3150:ILE:HD13	1.64	0.79
3:2:2048:ASN:HD22	3:2:2050:PRO:HD2	1.45	0.79
3:2:2039:ALA:HB3	3:2:2046:LEU:HB2	1.64	0.79
2:1:1020:PHE:HE1	2:1:1044:THR:CG2	1.93	0.79
3:2:3182:TYR:CD1	3:2:2049:MET:CE	2.65	0.79
3:2:3091:ALA:HB2	3:2:3107:ILE:HG13	1.64	0.78
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:HG23	1.64	0.78
1:M:5:A:O2'	1:M:6:A:H5'	1.82	0.78
1:M:5:A:C2'	1:M:6:A:H5'	2.14	0.77
2:1:1073:LYS:CG	2:1:1120:ILE:HD13	2.14	0.77
1:M:3:U:H2'	1:M:4:C:H5'	1.66	0.77
3:2:3007:LYS:O	3:2:3007:LYS:HG3	1.84	0.77
3:2:3052:THR:O	3:2:3052:THR:CG2	2.30	0.77
3:2:3114:LEU:HD21	3:2:2071:MET:HE2	1.64	0.77
2:1:1069:CYS:O	2:1:1167:SER:HB3	1.84	0.76
3:2:3074:MET:HE1	3:2:3090:CYS:CB	2.14	0.76
3:2:2006:GLN:CG	3:2:2007:ASN:H	1.96	0.76
3:2:3130:ASN:C	3:2:3132:CYS:H	1.93	0.76
3:2:3026:SER:HB3	3:2:3051:LEU:O	1.84	0.76
3:2:2058:ARG:O	3:2:2128:THR:HB	1.85	0.76
2:1:1016:THR:HG22	2:1:1017:PRO:HD2	1.67	0.75
3:2:2048:ASN:ND2	3:2:2050:PRO:CD	2.49	0.75
3:2:2190[A]:ILE:HG12	3:2:2191[A]:PRO:HD2	0.79	0.75
3:2:2078:CYS:SG	3:2:2148:VAL:HG13	2.26	0.75
3:2:2064:LEU:CD2	3:2:2169:ILE:HG23	2.17	0.75
3:2:2053:VAL:O	3:2:2056:MET:HB2	1.87	0.75
2:1:1056:ILE:HG23	2:1:1057:SER:N	2.00	0.74
3:2:3020:MET:HE3	3:2:3073:LYS:NZ	2.02	0.74
3:2:3047:LEU:HD13	3:2:3092:MET:CE	2.16	0.74
3:2:3080:ILE:HG22	3:2:3117:PRO:HB2	1.69	0.74
3:2:3086:ILE:HG23	3:2:3088:LEU:HD12	1.68	0.74
3:2:2106:PHE:CE1	3:2:2113:VAL:CG2	2.71	0.74
2:1:1026:SER:OG	2:1:1152:ASP:OD2	2.05	0.73
2:1:1181:PHE:O	3:2:2044:ALA:HB1	1.89	0.73
3:2:2073:SER:C	3:2:2075:TYR:H	1.96	0.73
3:2:2139:ASP:OD1	3:2:2143:TYR:CE2	2.42	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1007:VAL:HG21	3:2:2177:LEU:HB3	1.70	0.72
3:2:2096:PHE:C	3:2:2098:ALA:H	1.96	0.72
3:2:3114:LEU:HD21	3:2:2071:MET:CE	2.18	0.72
2:1:1007:VAL:HG22	2:1:1007:VAL:O	1.88	0.72
2:1:1020:PHE:CD1	2:1:1044:THR:CG2	2.73	0.72
3:2:2057:TRP:CZ3	3:2:2172:MET:HE2	2.22	0.72
3:2:3018:GLY:N	3:2:3023:LEU:CD1	2.52	0.72
2:1:1173:ALA:HA	3:2:2049:MET:HE1	1.72	0.72
3:2:3074:MET:HE3	3:2:3123:MET:SD	2.30	0.72
3:2:2186:LEU:O	3:2:2187[B]:LEU:HA	1.87	0.72
3:2:2190[A]:ILE:HG12	3:2:2191[A]:PRO:HD3	1.64	0.71
2:1:1091:VAL:CG1	2:1:1117:TRP:CZ2	2.74	0.71
3:2:2026:ARG:HG2	3:2:2147:MET:HG2	1.73	0.70
3:2:2079:THR:HB	3:2:2150:ASP:CG	2.15	0.70
3:2:3080:ILE:HG23	3:2:3118:ALA:HA	1.73	0.70
3:2:3107:ILE:HG13	3:2:3107:ILE:O	1.92	0.70
3:2:2130:VAL:CG1	3:2:2134:THR:HG21	2.22	0.70
3:2:2011:LEU:HD12	3:2:2050:PRO:O	1.92	0.70
2:1:1039:ILE:HD11	2:1:1051:VAL:HG23	1.74	0.69
3:2:3029:LYS:HE2	3:2:3165:GLN:OE1	1.92	0.69
3:2:2192[B]:GLN:HA	3:2:2192[B]:GLN:HE21	1.53	0.69
2:1:1091:VAL:CG1	2:1:1117:TRP:HZ2	2.04	0.69
3:2:2063:ASP:OD2	3:2:2119:GLN:HB2	1.91	0.69
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:CA	2.23	0.69
2:1:1039:ILE:HD11	2:1:1051:VAL:CG2	2.23	0.69
3:2:3084:THR:CB	3:2:3158:ALA:HB3	2.22	0.69
3:2:2035:ILE:HD11	3:2:2060:PHE:HZ	1.53	0.69
3:2:3113:GLU:HB3	3:2:3123:MET:HE3	1.73	0.69
3:2:3115:TRP:HA	3:2:2111:GLU:OE1	1.92	0.69
3:2:2006:GLN:HG2	3:2:2007:ASN:H	1.56	0.69
3:2:2025:SER:C	3:2:2027:SER:H	2.00	0.69
2:1:1014:VAL:HG21	2:1:1030:PHE:CE1	2.28	0.68
2:1:1043:LYS:O	2:1:1043:LYS:HG2	1.92	0.68
3:2:2048:ASN:C	3:2:2048:ASN:ND2	2.36	0.68
3:2:2187[B]:LEU:HD11	3:2:2190[B]:ILE:HA	1.75	0.68
3:2:2028:VAL:HG22	3:2:2147:MET:HG3	1.74	0.67
3:2:3061:ASP:O	3:2:3065:THR:HB	1.94	0.67
3:2:2190[B]:ILE:CB	3:2:2191[B]:PRO:HD2	2.22	0.67
3:2:2057:TRP:CH2	3:2:2172:MET:HE1	2.29	0.67
3:2:2187[B]:LEU:CD2	3:2:2190[B]:ILE:HG23	2.24	0.67
2:1:1073:LYS:HG2	2:1:1120:ILE:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2015:MET:HE2	3:2:2035:ILE:HG21	1.76	0.67
3:2:2024:THR:O	3:2:2024:THR:OG1	2.00	0.67
3:2:3017:LYS:C	3:2:3023:LEU:HD11	2.19	0.67
2:1:1143:THR:HG23	2:1:1144:SER:N	2.09	0.67
3:2:3025:ILE:HG22	3:2:3172:ILE:HD12	1.77	0.66
3:2:3080:ILE:HG23	3:2:3118:ALA:CA	2.24	0.66
2:1:1153:ASN:N	2:1:1154:PRO:HD3	2.09	0.66
2:1:1127:GLY:O	2:1:1131:GLY:HA2	1.95	0.66
3:2:2049:MET:HB3	3:2:2050:PRO:HD3	1.78	0.66
3:2:3007:LYS:O	3:2:3007:LYS:CG	2.42	0.66
3:2:2018:LEU:HD21	3:2:2031:MET:HE2	1.77	0.66
2:1:1020:PHE:CE2	2:1:1154:PRO:HG2	2.31	0.66
3:2:3086:ILE:HG23	3:2:3088:LEU:CD1	2.26	0.66
3:2:3182:TYR:CG	3:2:2049:MET:HE2	2.30	0.66
3:2:2064:LEU:HD22	3:2:2169:ILE:HG23	1.77	0.66
3:2:3025:ILE:CG2	3:2:3172:ILE:HD12	2.27	0.65
2:1:1172:ILE:HG13	3:2:2049:MET:HE3	1.79	0.65
3:2:3105:TYR:CE1	3:2:2046:LEU:O	2.46	0.65
3:2:2107:GLY:O	3:2:2108:GLU:C	2.39	0.65
3:2:3005:LEU:HD12	3:2:3008:LEU:HD22	1.78	0.65
1:M:2:G:C2'	1:M:3:U:H5'	2.26	0.65
3:2:2073:SER:C	3:2:2075:TYR:N	2.54	0.65
3:2:2192[B]:GLN:NE2	3:2:2192[B]:GLN:CA	2.59	0.65
3:2:2066:PHE:CD2	3:2:2166:LEU:HD12	2.27	0.65
3:2:3139:GLU:OE2	3:2:3143:ARG:HD2	1.97	0.65
2:1:1178:MET:SD	3:2:3097:ARG:HB3	2.37	0.64
3:2:2096:PHE:O	3:2:2098:ALA:N	2.31	0.64
2:1:1002:ILE:HB	3:2:2003:LEU:O	1.98	0.64
2:1:1074:VAL:HG11	2:1:1149:PHE:CZ	2.32	0.64
3:2:3023:LEU:HD23	3:2:3172:ILE:CG2	2.28	0.64
3:2:2189[B]:THR:O	3:2:2190[B]:ILE:C	2.39	0.64
2:1:1032:VAL:HG12	2:1:1034:LEU:CD1	2.25	0.64
3:2:3083:ASN:H	3:2:3083:ASN:ND2	1.95	0.64
2:1:1021:ASP:C	2:1:1023:SER:N	2.49	0.64
3:2:2189[B]:THR:O	3:2:2190[B]:ILE:HG12	1.97	0.64
2:1:1020:PHE:CD1	2:1:1044:THR:HG22	2.33	0.64
3:2:3080:ILE:CG2	3:2:3118:ALA:N	2.61	0.64
3:2:2080:VAL:CG1	3:2:2082:PHE:CE1	2.82	0.63
3:2:3072:ILE:HG12	3:2:3136:TRP:CZ2	2.32	0.63
2:1:1011:MET:HE1	2:1:1034:LEU:CA	2.21	0.63
2:1:1056:ILE:HG23	2:1:1057:SER:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1020:PHE:HD1	2:1:1044:THR:HG22	1.63	0.62
3:2:2189[B]:THR:O	3:2:2192[B]:GLN:HG2	1.99	0.62
2:1:1056:ILE:CG2	2:1:1057:SER:N	2.62	0.62
2:1:1134:MET:SD	3:2:3144:THR:HG23	2.39	0.62
3:2:2030:ARG:H	3:2:2191[B]:PRO:HD3	1.65	0.62
2:1:1019:ASN:H	2:1:1019:ASN:ND2	1.98	0.62
2:1:1071:MET:O	2:1:1164:LEU:HA	1.99	0.62
2:1:1029:GLN:HG3	2:1:1150:LEU:HD12	1.81	0.61
3:2:2057:TRP:O	3:2:2178:ASN:HB2	1.99	0.61
2:1:1073:LYS:HG3	2:1:1120:ILE:HD13	1.82	0.61
3:2:3069:LYS:CG	3:2:3069:LYS:O	2.48	0.61
3:2:3026:SER:OG	3:2:3170:TRP:CD1	2.52	0.61
3:2:3030:ILE:HD13	3:2:3150:ILE:HD13	1.82	0.61
3:2:3109:SER:HB3	3:2:2050:PRO:HG2	1.81	0.61
3:2:3020:MET:CE	3:2:3073:LYS:NZ	2.62	0.61
3:2:3091:ALA:HB1	3:2:3107:ILE:O	2.00	0.61
3:2:2093:THR:HB	3:2:2096:PHE:CE1	2.35	0.61
3:2:3080:ILE:CG2	3:2:3117:PRO:HB2	2.31	0.61
3:2:3105:TYR:HD1	3:2:2046:LEU:HB3	1.66	0.61
3:2:2080:VAL:HG12	3:2:2082:PHE:CE1	2.34	0.61
3:2:2135:THR:O	3:2:2138:ALA:N	2.27	0.61
3:2:3133:SER:OG	3:2:3134:ASP:N	2.15	0.60
3:2:3047:LEU:CD1	3:2:3092:MET:CE	2.79	0.60
2:1:1140:ALA:O	2:1:1141:ASN:C	2.45	0.60
3:2:2170:GLU:O	3:2:2171:ASN:HB2	2.01	0.60
3:2:3119:CYS:HB3	3:2:2109:ILE:O	2.02	0.60
3:2:3074:MET:HE3	3:2:3123:MET:HE1	1.82	0.60
3:2:3086:ILE:HG22	3:2:3117:PRO:HG2	1.84	0.60
3:2:3123:MET:CE	3:2:3125:MET:HB2	2.24	0.60
2:1:1135:TRP:CD1	2:1:1144:SER:HG	2.19	0.60
2:1:1056:ILE:CG2	2:1:1057:SER:H	2.14	0.59
2:1:1175:ASN:ND2	3:2:3093:ASN:OD1	2.35	0.59
3:2:3047:LEU:HG	3:2:3051:LEU:CD1	2.29	0.59
2:1:1139:TRP:HB3	2:1:1142:GLN:NE2	2.17	0.59
2:1:1042:ASP:HB2	2:1:1047:TRP:HE1	1.68	0.59
2:1:1181:PHE:O	3:2:2044:ALA:CB	2.51	0.59
3:2:3147:HIS:ND1	3:2:3149:ASP:OD2	2.36	0.59
3:2:2095:ASN:OD1	3:2:2095:ASN:O	2.21	0.58
2:1:1007:VAL:O	2:1:1007:VAL:CG2	2.50	0.58
3:2:3023:LEU:HD23	3:2:3172:ILE:HG22	1.85	0.58
3:2:3038:GLY:HA2	3:2:3152:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2096:PHE:HD2	3:2:2147:MET:HE1	1.68	0.58
3:2:2135:THR:C	3:2:2137:LEU:N	2.44	0.58
3:2:2018:LEU:CD2	3:2:2031:MET:HE2	2.34	0.58
3:2:2096:PHE:CE2	3:2:2147:MET:SD	2.97	0.58
3:2:3123:MET:HG2	3:2:3124:THR:N	2.18	0.57
3:2:3018:GLY:CA	3:2:3023:LEU:HD12	2.34	0.57
3:2:2139:ASP:OD1	3:2:2143:TYR:CZ	2.58	0.57
2:1:1054:SER:O	2:1:1058:ASN:CB	2.49	0.57
3:2:3128:ASN:HD22	3:2:3177:CYS:HB3	1.65	0.57
3:2:3129:PRO:O	3:2:3131:PRO:HD3	2.04	0.57
3:2:3032:LEU:HD11	3:2:3088:LEU:HD11	1.85	0.57
1:M:3:U:H2'	1:M:4:C:C5'	2.34	0.57
2:1:1083:LYS:O	2:1:1086:ASP:HB2	2.05	0.57
3:2:3078:VAL:HG11	3:2:3166:VAL:HG22	1.85	0.57
3:2:3023:LEU:CD2	3:2:3172:ILE:HG22	2.34	0.57
3:2:3154:THR:HG23	3:2:2192[A]:GLN:O	2.03	0.57
3:2:2026:ARG:NH2	3:2:2096:PHE:CE2	2.73	0.57
3:2:3025:ILE:HD11	3:2:3051:LEU:CD2	2.21	0.57
3:2:3024:LYS:O	3:2:3056:PHE:O	2.23	0.57
3:2:2079:THR:CB	3:2:2150:ASP:OD2	2.51	0.56
2:1:1042:ASP:CG	2:1:1044:THR:OG1	2.48	0.56
3:2:2021:PRO:HA	3:2:2159:ASP:OD2	2.05	0.56
3:2:2096:PHE:C	3:2:2098:ALA:N	2.64	0.56
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:HA	1.86	0.56
2:1:1096:THR:O	2:1:1146:HIS:HB2	2.06	0.56
3:2:3032:LEU:HD11	3:2:3088:LEU:HD21	1.88	0.56
3:2:3092:MET:CE	3:2:3148:CYS:SG	2.94	0.56
3:2:3114:LEU:CD1	3:2:3153:VAL:HG21	2.33	0.56
2:1:1043:LYS:O	2:1:1043:LYS:CG	2.54	0.55
3:2:3091:ALA:HA	3:2:3112:CYS:HB2	1.88	0.55
3:2:2002:VAL:HG12	3:2:2002:VAL:O	2.05	0.55
3:2:3047:LEU:O	3:2:3050:PHE:HB2	2.06	0.55
3:2:2083:PHE:CE1	3:2:2145:TYR:HB2	2.41	0.55
2:1:1036:GLY:O	3:2:3097:ARG:NH1	2.38	0.55
3:2:3092:MET:HE3	3:2:3148:CYS:SG	2.46	0.55
2:1:1172:ILE:HG13	3:2:2049:MET:CE	2.37	0.55
2:1:1016:THR:HG23	2:1:1017:PRO:HD2	1.88	0.55
3:2:3074:MET:HE2	3:2:3123:MET:HE1	1.87	0.55
3:2:2047:MET:CE	3:2:2052:ALA:CA	2.80	0.55
3:2:2129:GLN:NE2	3:2:2181:ILE:O	2.40	0.55
2:1:1009:ASN:OD1	2:1:1056:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1175:ASN:HB3	3:2:3093:ASN:OD1	2.06	0.54
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:HD3	2.26	0.54
3:2:3030:ILE:HD11	3:2:3150:ILE:CD1	2.36	0.54
3:2:2178:ASN:OD1	3:2:2180:GLY:HA2	2.07	0.54
3:2:2187[B]:LEU:HD11	3:2:2190[B]:ILE:CA	2.37	0.54
3:2:3020:MET:CE	3:2:3073:LYS:HZ3	2.20	0.54
3:2:3105:TYR:HE1	3:2:2046:LEU:C	2.16	0.54
3:2:3114:LEU:CD2	3:2:2071:MET:HE3	2.37	0.54
2:1:1035:LEU:HD11	2:1:1125:VAL:HG22	1.89	0.54
2:1:1041:VAL:HG23	2:1:1042:ASP:O	2.07	0.54
2:1:1169:ASN:O	2:1:1169:ASN:ND2	2.40	0.54
3:2:3005:LEU:O	3:2:3008:LEU:HB2	2.07	0.54
3:2:3050:PHE:CE2	3:2:3148:CYS:HB3	2.43	0.54
1:M:3:U:H2'	1:M:4:C:O4'	2.07	0.54
3:2:3083:ASN:HD22	3:2:3083:ASN:N	1.93	0.54
3:2:2066:PHE:CZ	3:2:2166:LEU:HD11	2.41	0.53
3:2:3074:MET:HE3	3:2:3123:MET:CE	2.37	0.53
2:1:1145:TRP:HA	2:1:1145:TRP:CE3	2.43	0.53
3:2:3080:ILE:CG2	3:2:3117:PRO:C	2.81	0.53
3:2:2025:SER:C	3:2:2027:SER:N	2.62	0.53
3:2:2159:ASP:O	3:2:2161:VAL:HG23	2.07	0.53
2:1:1153:ASN:N	2:1:1154:PRO:CD	2.71	0.53
3:2:3018:GLY:CA	3:2:3023:LEU:CD1	2.86	0.53
3:2:2187[B]:LEU:CD2	3:2:2190[B]:ILE:CG2	2.85	0.53
3:2:3074:MET:CE	3:2:3123:MET:CE	2.85	0.53
3:2:3141:LEU:HD12	3:2:3146:PHE:HB2	1.90	0.53
3:2:2048:ASN:HD22	3:2:2050:PRO:CD	2.12	0.53
3:2:3025:ILE:CG2	3:2:3172:ILE:CD1	2.87	0.52
3:2:2083:PHE:CE1	3:2:2145:TYR:CB	2.92	0.52
3:2:2187[B]:LEU:CG	3:2:2190[B]:ILE:H	2.21	0.52
1:M:2:G:H2'	1:M:3:U:H5'	1.91	0.52
3:2:3080:ILE:CD1	3:2:3085:GLY:HA2	2.40	0.52
3:2:2039:ALA:HB3	3:2:2046:LEU:CB	2.37	0.52
3:2:2047:MET:HE3	3:2:2052:ALA:N	2.24	0.52
3:2:3026:SER:OG	3:2:3170:TRP:HB2	2.10	0.52
2:1:1091:VAL:HA	2:1:1150:LEU:O	2.09	0.52
3:2:3078:VAL:HG21	3:2:3164:VAL:CG1	2.40	0.52
3:2:3128:ASN:ND2	3:2:3177:CYS:CB	2.60	0.52
3:2:2005:PRO:HG3	3:2:2057:TRP:CZ2	2.44	0.52
3:2:2017:LYS:NZ	3:2:2190[A]:ILE:HG22	2.25	0.52
3:2:2189[B]:THR:C	3:2:2190[B]:ILE:HG12	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:3080:ILE:HG22	3:2:3117:PRO:C	2.35	0.52
1:M:2:G:O2'	1:M:3:U:H5'	2.10	0.51
2:1:1065:TRP:O	2:1:1172:ILE:HA	2.10	0.51
2:1:1072:VAL:CG1	2:1:1073:LYS:N	2.73	0.51
3:2:2080:VAL:HG11	3:2:2082:PHE:CE1	2.44	0.51
2:1:1020:PHE:CD1	2:1:1044:THR:HG21	2.42	0.51
3:2:3012:ASP:OD2	3:2:3014:GLU:HB2	2.10	0.51
3:2:3154:THR:HA	3:2:2192[A]:GLN:C	2.34	0.51
3:2:3031:ALA:C	3:2:3033:PRO:HD3	2.34	0.51
3:2:3129:PRO:C	3:2:3131:PRO:HD3	2.35	0.51
3:2:2026:ARG:HH22	3:2:2093:THR:C	2.18	0.51
3:2:2133:ALA:O	3:2:2134:THR:C	2.53	0.51
3:2:2190[B]:ILE:CG1	3:2:2191[B]:PRO:CD	2.74	0.51
3:2:3105:TYR:OH	3:2:2038:GLY:HA3	2.10	0.51
3:2:3164:VAL:CG1	3:2:3165:GLN:N	2.74	0.51
3:2:2031:MET:HG3	3:2:2144:LEU:O	2.11	0.51
1:M:5:A:H2'	1:M:6:A:H5'	1.91	0.51
2:1:1042:ASP:CB	2:1:1047:TRP:HE1	2.23	0.51
2:1:1032:VAL:CG1	2:1:1034:LEU:HD12	2.33	0.51
3:2:2047:MET:HE3	3:2:2052:ALA:HA	1.91	0.51
3:2:2083:PHE:HE2	3:2:2147:MET:HE2	1.76	0.51
3:2:3046:LEU:O	3:2:3047:LEU:C	2.53	0.51
2:1:1172:ILE:CG1	3:2:2049:MET:HE3	2.39	0.51
3:2:3011:ASP:O	3:2:3011:ASP:CG	2.52	0.51
3:2:3137:SER:O	3:2:3140:PHE:HB3	2.11	0.51
2:1:1033:ASP:OD2	2:1:1036:GLY:N	2.44	0.50
2:1:1097:ASN:HB2	2:1:1143:THR:OG1	2.12	0.50
3:2:3004:ASN:OD1	3:2:3006:PHE:HB2	2.11	0.50
3:2:3154:THR:O	3:2:3154:THR:HG22	2.11	0.50
3:2:3114:LEU:CD2	3:2:2071:MET:CE	2.88	0.50
2:1:1134:MET:HE1	3:2:3144:THR:O	2.12	0.50
3:2:2049:MET:O	3:2:2053:VAL:CG1	2.59	0.50
3:2:2058:ARG:HB3	3:2:2176:GLY:HA3	1.93	0.50
3:2:3056:PHE:O	3:2:3058:ALA:N	2.45	0.50
2:1:1014:VAL:HG11	2:1:1030:PHE:CE1	2.47	0.50
2:1:1071:MET:O	2:1:1164:LEU:CA	2.60	0.50
2:1:1097:ASN:ND2	2:1:1097:ASN:H	2.10	0.50
3:2:3047:LEU:CD1	3:2:3092:MET:HE2	2.42	0.50
3:2:2095:ASN:O	3:2:2095:ASN:CG	2.55	0.49
3:2:3133:SER:HG	3:2:3134:ASP:H	1.53	0.49
3:2:3105:TYR:CD1	3:2:2046:LEU:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2042:LYS:O	3:2:2043:SER:HB2	2.12	0.49
3:2:3127:PHE:CD1	3:2:3127:PHE:N	2.80	0.49
3:2:2189[B]:THR:OG1	3:2:2192[B]:GLN:HB2	2.12	0.49
3:2:2030:ARG:CD	3:2:2145:TYR:CE1	2.90	0.49
2:1:1004:GLN:HB3	2:1:1007:VAL:HG11	1.95	0.49
2:1:1007:VAL:HG22	3:2:2177:LEU:HD23	1.94	0.49
2:1:1056:ILE:O	2:1:1059:LEU:N	2.45	0.49
3:2:2035:ILE:O	3:2:2051:ASN:ND2	2.33	0.49
3:2:2073:SER:OG	3:2:2074:PRO:HD2	2.13	0.49
3:2:2097:GLU:O	3:2:2101:HIS:CE1	2.65	0.49
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:N	2.27	0.49
3:2:3086:ILE:O	3:2:3117:PRO:HD2	2.13	0.48
3:2:2017:LYS:NZ	3:2:2191[A]:PRO:O	2.46	0.48
3:2:2027:SER:O	3:2:2029:LYS:HD3	2.13	0.48
2:1:1090:LEU:HD12	2:1:1091:VAL:N	2.27	0.48
3:2:2054:LEU:HD12	3:2:2057:TRP:CZ3	2.49	0.48
2:1:1056:ILE:O	2:1:1057:SER:C	2.56	0.48
2:1:1062:VAL:O	2:1:1176:THR:N	2.38	0.48
3:2:3086:ILE:CG2	3:2:3088:LEU:CD1	2.92	0.48
3:2:2065:VAL:HG22	3:2:2116:LYS:HD2	1.96	0.48
3:2:2020:PHE:HD2	3:2:2148:VAL:CG2	2.26	0.48
3:2:2053:VAL:HG22	3:2:2054:LEU:N	2.28	0.48
2:1:1054:SER:HB2	2:1:1057:SER:HB3	1.96	0.48
3:2:2003:LEU:HD12	3:2:2003:LEU:HA	1.77	0.48
3:2:2020:PHE:CD2	3:2:2148:VAL:CG2	2.97	0.48
3:2:2057:TRP:HZ3	3:2:2172:MET:HE2	1.56	0.48
3:2:2150:ASP:OD2	3:2:2150:ASP:N	2.47	0.48
1:M:3:U:C2'	1:M:4:C:C5'	2.79	0.47
2:1:1181:PHE:HB2	3:2:2045:ILE:HG12	1.96	0.47
3:2:3072:ILE:HD11	3:2:3136:TRP:CH2	2.49	0.47
3:2:2017:LYS:HZ2	3:2:2190[A]:ILE:HG22	1.79	0.47
3:2:2027:SER:O	3:2:2029:LYS:CD	2.63	0.47
2:1:1074:VAL:HG11	2:1:1149:PHE:CE2	2.50	0.47
3:2:3080:ILE:HD11	3:2:3084:THR:HG23	1.95	0.47
3:2:3078:VAL:CG1	3:2:3166:VAL:HG22	2.44	0.47
3:2:2069:SER:O	3:2:2162:ILE:HA	2.15	0.47
3:2:3074:MET:HE2	3:2:3125:MET:HB3	1.96	0.47
3:2:3080:ILE:HG23	3:2:3118:ALA:N	2.29	0.47
3:2:2047:MET:HE3	3:2:2052:ALA:CA	2.44	0.47
3:2:2192[A]:GLN:O	3:2:2192[A]:GLN:HG2	2.14	0.47
3:2:3083:ASN:ND2	3:2:3083:ASN:N	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2082:PHE:CE1	3:2:2104:VAL:HG21	2.50	0.47
2:1:1070:LEU:HG	2:1:1170:PHE:CE1	2.50	0.47
2:1:1139:TRP:HB3	2:1:1142:GLN:HE21	1.78	0.47
3:2:2187[B]:LEU:HG	3:2:2190[B]:ILE:H	1.79	0.47
2:1:1143:THR:HG23	2:1:1144:SER:H	1.79	0.46
3:2:2030:ARG:HE	3:2:2191[B]:PRO:HB3	1.80	0.46
2:1:1034:LEU:HD23	2:1:1123:ILE:HD13	1.96	0.46
3:2:3107:ILE:O	3:2:3107:ILE:CG1	2.58	0.46
3:2:3182:TYR:CG	3:2:2049:MET:CE	2.96	0.46
3:2:2088:ASN:OD1	3:2:2088:ASN:N	2.47	0.46
2:1:1143:THR:CG2	2:1:1144:SER:N	2.76	0.46
3:2:3050:PHE:CZ	3:2:3150:ILE:CD1	2.98	0.46
3:2:3069:LYS:O	3:2:3069:LYS:HG3	2.16	0.46
3:2:2049:MET:O	3:2:2051:ASN:N	2.47	0.46
3:2:2073:SER:O	3:2:2074:PRO:C	2.55	0.46
2:1:1129:ASN:HD22	2:1:1129:ASN:HA	1.61	0.46
3:2:3026:SER:HG	3:2:3170:TRP:CG	2.30	0.46
3:2:3039:GLY:N	3:2:3152:CYS:O	2.46	0.46
3:2:2004:ASN:N	3:2:2005:PRO:HD3	2.31	0.46
1:M:1:G:N7	3:2:2168:ILE:HD13	2.30	0.46
2:1:1064:ALA:O	2:1:1134:MET:HG3	2.16	0.46
2:1:1134:MET:HE1	3:2:3144:THR:HG22	1.91	0.46
3:2:3164:VAL:HG12	3:2:3165:GLN:N	2.30	0.46
3:2:3028:SER:OG	3:2:3170:TRP:NE1	2.48	0.46
3:2:3130:ASN:O	3:2:3131:PRO:C	2.58	0.46
2:1:1094:PHE:O	2:1:1147:LEU:HD12	2.15	0.46
3:2:2011:LEU:HD23	3:2:2013:ARG:HB2	1.98	0.46
2:1:1039:ILE:HD11	2:1:1051:VAL:HG22	1.95	0.45
3:2:3154:THR:HG21	3:2:2071:MET:HB2	1.97	0.45
2:1:1023:SER:C	2:1:1024:LYS:HG3	2.41	0.45
3:2:3141:LEU:HD12	3:2:3146:PHE:CB	2.45	0.45
3:2:3090:CYS:O	3:2:3112:CYS:HA	2.16	0.45
3:2:3128:ASN:HD22	3:2:3177:CYS:CB	2.24	0.45
3:2:2006:GLN:CG	3:2:2007:ASN:N	2.64	0.45
3:2:2011:LEU:CD2	3:2:2013:ARG:HB2	2.46	0.45
3:2:3091:ALA:CB	3:2:3107:ILE:CG1	2.88	0.45
2:1:1087:TRP:CE2	2:1:1114:PRO:HA	2.52	0.45
3:2:2063:ASP:C	3:2:2064:LEU:HD23	2.42	0.45
3:2:3114:LEU:HD22	3:2:2071:MET:HE3	1.99	0.45
3:2:2030:ARG:HG2	3:2:2145:TYR:CD1	2.52	0.45
2:1:1076:MET:O	2:1:1116:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2186:LEU:HA	3:2:2186:LEU:HD23	1.81	0.45
3:2:2047:MET:HG3	3:2:2048:ASN:N	2.32	0.45
3:2:2048:ASN:C	3:2:2050:PRO:HD2	2.42	0.45
3:2:3092:MET:CE	3:2:3170:TRP:CH2	2.89	0.45
3:2:2011:LEU:O	3:2:2050:PRO:HB2	2.16	0.45
3:2:3113:GLU:CB	3:2:3123:MET:HE3	2.46	0.44
3:2:3155:GLY:N	3:2:2192[A]:GLN:C	2.75	0.44
3:2:2096:PHE:HE2	3:2:2147:MET:SD	2.39	0.44
3:2:2049:MET:C	3:2:2051:ASN:H	2.25	0.44
3:2:2033:LEU:HA	3:2:2033:LEU:HD23	1.73	0.44
3:2:2048:ASN:ND2	3:2:2050:PRO:CG	2.79	0.44
2:1:1059:LEU:HA	3:2:2052:ALA:HB1	1.99	0.44
3:2:2020:PHE:CD2	3:2:2148:VAL:HG22	2.51	0.44
3:2:2049:MET:C	3:2:2051:ASN:N	2.73	0.44
1:M:4:C:H4'	3:2:3124:THR:O	2.17	0.44
2:1:1096:THR:O	2:1:1146:HIS:N	2.47	0.44
3:2:3045:ASP:O	3:2:3147:HIS:CD2	2.70	0.44
2:1:1004:GLN:HB3	2:1:1007:VAL:CG1	2.46	0.44
2:1:1074:VAL:HG11	2:1:1149:PHE:HZ	1.78	0.44
2:1:1096:THR:HG22	2:1:1098:SER:H	1.80	0.44
3:2:3016:PRO:O	3:2:3023:LEU:HD21	2.17	0.44
3:2:3154:THR:O	3:2:3154:THR:CG2	2.65	0.44
3:2:2036:GLY:CA	3:2:2055:SER:OG	2.66	0.44
3:2:2025:SER:O	3:2:2027:SER:N	2.50	0.44
2:1:1069:CYS:SG	2:1:1124:GLU:HG3	2.58	0.44
3:2:2026:ARG:HG2	3:2:2147:MET:CG	2.44	0.43
3:2:2187[B]:LEU:CD2	3:2:2190[B]:ILE:H	2.31	0.43
3:2:3087:ALA:HB2	3:2:2071:MET:HB3	2.00	0.43
3:2:2029:LYS:HG3	3:2:2190[B]:ILE:HG21	2.00	0.43
3:2:2065:VAL:CG2	3:2:2116:LYS:HD2	2.48	0.43
3:2:2118:SER:C	3:2:2120:GLU:H	2.26	0.43
2:1:1027:PHE:HA	2:1:1151:VAL:O	2.19	0.43
2:1:1041:VAL:HG23	2:1:1042:ASP:N	2.34	0.43
3:2:3078:VAL:HG21	3:2:3164:VAL:HG11	2.00	0.43
3:2:3173:SER:OG	3:2:3174:SER:N	2.50	0.43
3:2:2002:VAL:O	3:2:2002:VAL:CG1	2.66	0.43
2:1:1025:GLN:HG3	2:1:1026:SER:N	2.22	0.43
3:2:3145:GLY:O	3:2:3146:PHE:C	2.60	0.43
3:2:2049:MET:O	3:2:2053:VAL:HG13	2.19	0.43
3:2:2096:PHE:CD2	3:2:2147:MET:SD	3.11	0.43
3:2:3030:ILE:CD1	3:2:3150:ILE:CD1	2.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1042:ASP:CG	2:1:1044:THR:HG1	2.27	0.43
3:2:2115:LEU:HD12	3:2:2115:LEU:HA	1.81	0.43
2:1:1039:ILE:CD1	2:1:1051:VAL:HG23	2.46	0.43
2:1:1072:VAL:HG22	2:1:1164:LEU:HD23	2.01	0.43
3:2:3080:ILE:HD13	3:2:3085:GLY:HA2	2.00	0.43
3:2:2058:ARG:HB3	3:2:2177:LEU:N	2.34	0.43
2:1:1059:LEU:HD11	2:1:1172:ILE:CD1	2.49	0.43
3:2:3045:ASP:CG	3:2:3046:LEU:H	2.27	0.43
3:2:3047:LEU:C	3:2:3049:ASN:N	2.78	0.42
3:2:3154:THR:C	3:2:2192[A]:GLN:O	2.61	0.42
3:2:2192[A]:GLN:O	3:2:2192[A]:GLN:CG	2.67	0.42
3:2:3107:ILE:HD13	3:2:3107:ILE:HG21	1.82	0.42
3:2:2049:MET:CB	3:2:2050:PRO:HD3	2.46	0.42
2:1:1070:LEU:HD11	2:1:1170:PHE:CZ	2.55	0.42
2:1:1167:SER:C	2:1:1169:ASN:N	2.75	0.42
2:1:1171:GLU:HA	3:2:3182:TYR:O	2.18	0.42
2:1:1013:THR:OG1	2:1:1161:ASP:OD2	2.38	0.42
2:1:1063:ALA:O	2:1:1066:LYS:NZ	2.49	0.42
3:2:2026:ARG:O	3:2:2028:VAL:N	2.53	0.42
2:1:1042:ASP:HB2	2:1:1047:TRP:NE1	2.31	0.42
3:2:3074:MET:O	3:2:3124:THR:HA	2.19	0.42
3:2:2049:MET:O	3:2:2053:VAL:HG12	2.20	0.42
3:2:2123:LEU:HD23	3:2:2124:THR:OG1	2.19	0.42
2:1:1023:SER:O	2:1:1024:LYS:CG	2.67	0.42
2:1:1030:PHE:CD2	2:1:1149:PHE:HB2	2.55	0.42
3:2:2150:ASP:HB2	3:2:2151:SER:H	1.27	0.41
2:1:1001:SER:OG	2:1:1002:ILE:N	2.46	0.41
3:2:3018:GLY:C	3:2:3023:LEU:HD12	2.45	0.41
3:2:3129:PRO:O	3:2:3131:PRO:CD	2.67	0.41
2:1:1019:ASN:ND2	2:1:1019:ASN:N	2.64	0.41
3:2:3012:ASP:OD2	3:2:3012:ASP:C	2.63	0.41
3:2:2037:GLY:O	3:2:2047:MET:SD	2.78	0.41
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:H	1.83	0.41
2:1:1030:PHE:O	2:1:1149:PHE:N	2.38	0.41
3:2:2124:THR:HG22	3:2:2125:ALA:O	2.20	0.41
3:2:3005:LEU:HD12	3:2:3005:LEU:HA	1.76	0.41
3:2:2099:PHE:O	3:2:2100:PRO:C	2.59	0.41
3:2:2010:VAL:CG1	3:2:2012:ASN:ND2	2.83	0.41
3:2:2049:MET:HB3	3:2:2050:PRO:CD	2.49	0.41
3:2:3025:ILE:HG21	3:2:3025:ILE:HD13	1.80	0.41
3:2:3123:MET:HE2	3:2:3125:MET:CB	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:3130:ASN:C	3:2:3130:ASN:HD22	2.29	0.41
2:1:1062:VAL:HG11	3:2:2049:MET:N	2.36	0.41
2:1:1082:VAL:HG11	2:1:1156:GLN:HE21	1.86	0.41
2:1:1178:MET:HE3	2:1:1179:PRO:HD2	2.03	0.41
3:2:3050:PHE:CZ	3:2:3150:ILE:HD11	2.56	0.41
3:2:2006:GLN:HG2	3:2:2007:ASN:N	2.30	0.41
1:M:1:G:C8	3:2:2008:PRO:HG2	2.55	0.41
2:1:1011:MET:SD	2:1:1164:LEU:HD21	2.61	0.41
2:1:1016:THR:HA	2:1:1017:PRO:HD3	1.89	0.41
3:2:2035:ILE:HD11	3:2:2060:PHE:CE1	2.52	0.41
3:2:3086:ILE:CG2	3:2:3117:PRO:HG2	2.49	0.40
3:2:3168:ILE:HD13	3:2:3168:ILE:HG21	1.86	0.40
3:2:2017:LYS:NZ	3:2:2190[A]:ILE:CG2	2.83	0.40
3:2:3140:PHE:O	3:2:3144:THR:HB	2.20	0.40
3:2:2013:ARG:O	3:2:2165:LYS:HA	2.21	0.40
3:2:2022:GLN:NE2	3:2:2158:GLY:O	2.53	0.40
3:2:2064:LEU:HD23	3:2:2064:LEU:N	2.36	0.40
3:2:3077:THR:O	3:2:3077:THR:HG22	2.22	0.40
3:2:2131:ARG:H	3:2:2131:ARG:HG2	1.67	0.40
3:2:2170:GLU:O	3:2:2171:ASN:CB	2.69	0.40
2:1:1031:SER:HA	2:1:1148:SER:HA	2.03	0.40
3:2:2085:ALA:HB1	3:2:2086:PHE:H	1.66	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	
2	1	183/198 (92%)	158 (86%)	20 (11%)	5 (3%)	4	22
3	2	377/374 (101%)	316 (84%)	46 (12%)	15 (4%)	2	14
All	All	560/572 (98%)	474 (85%)	66 (12%)	20 (4%)	3	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	1022	SER
2	1	1024	LYS
2	1	1025	GLN
2	1	1136	SER
3	2	3057	ARG
3	2	2027	SER
3	2	2074	PRO
3	2	2097	GLU
3	2	2136	LEU
3	2	2190[A]	ILE
3	2	2190[B]	ILE
3	2	2191[A]	PRO
3	2	2191[B]	PRO
3	2	3155	GLY
3	2	3034	LYS
3	2	3131	PRO
3	2	2012	ASN
2	1	1115	HIS
3	2	3103	ASP
3	2	3104	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	
2	1	165/174 (95%)	118 (72%)	47 (28%)	0	2
3	2	329/324 (102%)	219 (67%)	110 (33%)	0	1
All	All	494/498 (99%)	337 (68%)	157 (32%)	0	1

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	1006	THR
2	1	1007	VAL
2	1	1009	ASN

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Mol	Chain	Res	Type
2	1	1010	GLN
2	1	1013	THR
2	1	1015	ARG
2	1	1019	ASN
2	1	1021	ASP
2	1	1023	SER
2	1	1024	LYS
2	1	1025	GLN
2	1	1026	SER
2	1	1028	CYS
2	1	1029	GLN
2	1	1031	SER
2	1	1039	ILE
2	1	1041	VAL
2	1	1042	ASP
2	1	1052	GLN
2	1	1054	SER
2	1	1058	ASN
2	1	1059	LEU
2	1	1071	MET
2	1	1073	LYS
2	1	1074	VAL
2	1	1090	LEU
2	1	1097	ASN
2	1	1100	SER
2	1	1102	GLU
2	1	1107	CYS
2	1	1111	LYS
2	1	1112	SER
2	1	1113	GLU
2	1	1120	ILE
2	1	1129	ASN
2	1	1143	THR
2	1	1144	SER
2	1	1148	SER
2	1	1150	LEU
2	1	1151	VAL
2	1	1152	ASP
2	1	1161	ASP
2	1	1163	LEU
2	1	1164	LEU
2	1	1168	GLN

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Mol	Chain	Res	Type
2	1	1172	ILE
2	1	1177	LEU
3	2	3001	MET
3	2	3002	GLU
3	2	3005	LEU
3	2	3008	LEU
3	2	3014	GLU
3	2	3019	SER
3	2	3021	LEU
3	2	3023	LEU
3	2	3024	LYS
3	2	3028	SER
3	2	3034	LYS
3	2	3036	THR
3	2	3041	ILE
3	2	3044	SER
3	2	3046	LEU
3	2	3049	ASN
3	2	3052	THR
3	2	3053	GLU
3	2	3060	VAL
3	2	3061	ASP
3	2	3067	ARG
3	2	3068	ILE
3	2	3072	ILE
3	2	3074	MET
3	2	3077	THR
3	2	3080	ILE
3	2	3083	ASN
3	2	3092	MET
3	2	3094	SER
3	2	3096	ILE
3	2	3102	SER
3	2	3104	ILE
3	2	3106	THR
3	2	3107	ILE
3	2	3109	SER
3	2	3112	CYS
3	2	3113	GLU
3	2	3114	LEU
3	2	3123	MET
3	2	3124	THR

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Mol	Chain	Res	Type
3	2	3127	PHE
3	2	3137	SER
3	2	3141	LEU
3	2	3147	HIS
3	2	3151	ILE
3	2	3153	VAL
3	2	3154	THR
3	2	3161	MET
3	2	3162	GLN
3	2	3167	THR
3	2	3172	ILE
3	2	3174	SER
3	2	3175	GLN
3	2	3176	GLU
3	2	3180	ARG
3	2	3181	THR
3	2	2003	LEU
3	2	2013	ARG
3	2	2015	MET
3	2	2019	THR
3	2	2024	THR
3	2	2026	ARG
3	2	2027	SER
3	2	2034	SER
3	2	2035	ILE
3	2	2045	ILE
3	2	2048	ASN
3	2	2051	ASN
3	2	2053	VAL
3	2	2054	LEU
3	2	2056	MET
3	2	2060	PHE
3	2	2061	VAL
3	2	2063	ASP
3	2	2072	THR
3	2	2084	ILE
3	2	2088	ASN
3	2	2092	ASP
3	2	2094	ILE
3	2	2099	PHE
3	2	2102	LYS
3	2	2104	VAL

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Mol	Chain	Res	Type
3	2	2108	GLU
3	2	2109	ILE
3	2	2111	GLU
3	2	2115	LEU
3	2	2116	LYS
3	2	2121	GLU
3	2	2124	THR
3	2	2127	SER
3	2	2128	THR
3	2	2131	ARG
3	2	2134	THR
3	2	2136	LEU
3	2	2137	LEU
3	2	2144	LEU
3	2	2147	MET
3	2	2150	ASP
3	2	2151	SER
3	2	2153	VAL
3	2	2154	SER
3	2	2166	LEU
3	2	2167	THR
3	2	2169	ILE
3	2	2177	LEU
3	2	2182	SER
3	2	2187[A]	LEU
3	2	2187[B]	LEU
3	2	2192[A]	GLN
3	2	2192[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	1010	GLN
2	1	1029	GLN
2	1	1058	ASN
2	1	1097	ASN
2	1	1103	HIS
2	1	1141	ASN
3	2	3035	ASN
3	2	3049	ASN
3	2	3083	ASN
3	2	3128	ASN

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Mol	Chain	Res	Type
3	2	2004	ASN
3	2	2006	GLN
3	2	2012	ASN
3	2	2048	ASN
3	2	2101	HIS
3	2	2119	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	10/11 (90%)	5 (50%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	7	A
1	M	8	A
1	M	9	U
1	M	10	G
1	M	11	C

There are no RNA pucker outliers to report.

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	2186:LEU	C	2187[B]:LEU	N	2.97
1	2	2071:MET	C	2072:THR	N	1.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.