



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 02:20 PM BST

PDB ID : 1BMV
Title : PROTEIN-RNA INTERACTIONS IN AN ICOSAHERAL VIRUS AT 3.0
ANGSTROMS RESOLUTION
Authors : Chen, Z.; Stauffacher, C.; Li, Y.; Schmidt, T.; Bomu, W.; Kamer, G.; Shanks,
M.; Lomonossoff, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

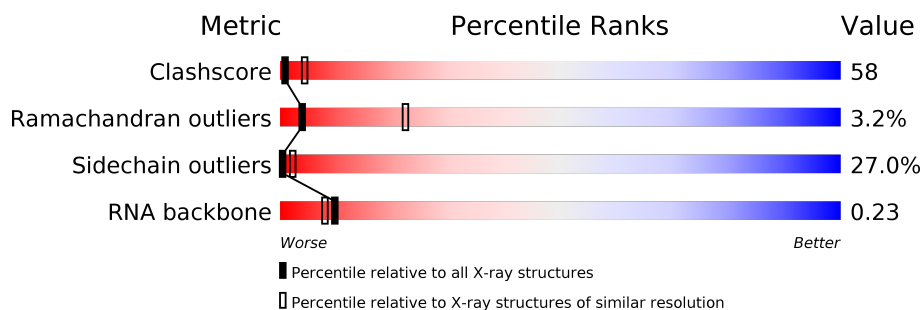
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	100%
2	1	198	31% 43% 18% • 7%
3	2	374	27% 50% 19% •

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.

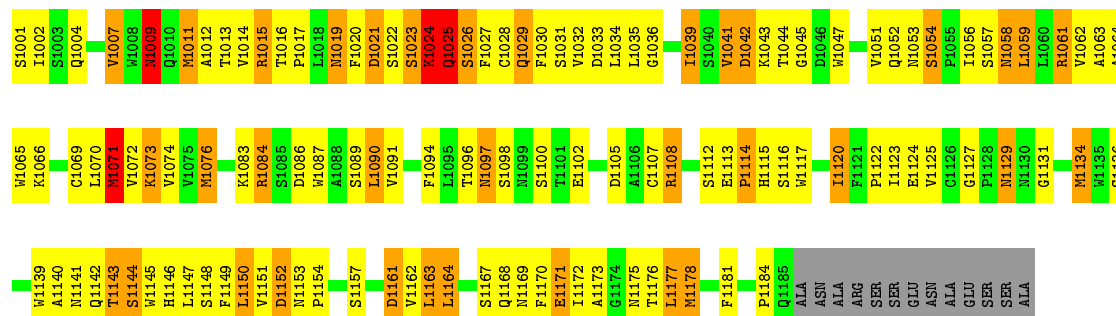
- Molecule 1: RNA (5'-R(*GP*GP*UP*CP*AP*AP*AP*AP*UP*GP*C)-3')

Chain M: 

G1 G2 U3 C4 A5 A6 A7 A8 U9 G10 C11

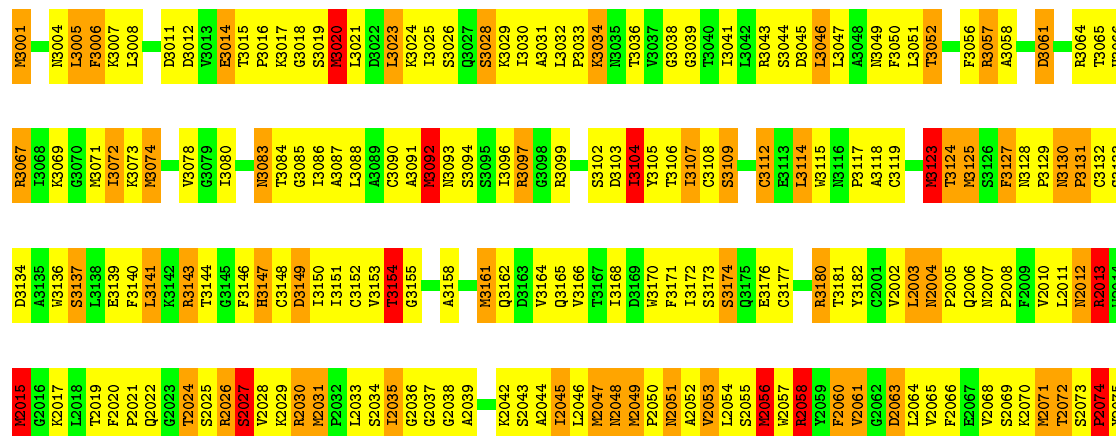
- Molecule 2: PROTEIN (ICOSAHEDRAL VIRUS - A DOMAIN)

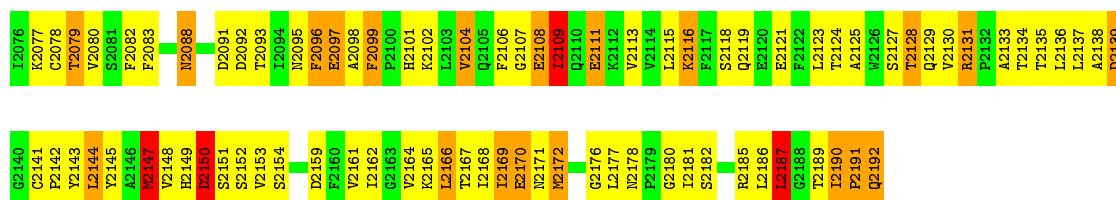
Chain 1: 



- Molecule 3: PROTEIN (ICOSAHEDRAL VIRUS - B AND C DOMAIN)

Chain 2: 





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	1.11	0/266	1.44	0/411
2	1	1.13	0/1490	1.57	21/2031 (1.0%)
3	2	1.11	6/2988 (0.2%)	1.58	54/4056 (1.3%)
All	All	1.12	6/4744 (0.1%)	1.57	75/6498 (1.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2070	LYS	N-CA	7.12	1.60	1.46
3	2	2074	PRO	C-N	6.92	1.50	1.34
3	2	3052	THR	C-N	6.03	1.48	1.34
3	2	2071	MET	C-N	-5.98	1.20	1.34
3	2	2077	LYS	CA-C	-5.60	1.38	1.52
3	2	2077	LYS	N-CA	5.18	1.56	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2072	THR	N-CA-CB	-15.00	81.79	110.30
3	2	2070	LYS	CB-CA-C	10.12	130.63	110.40
3	2	2077	LYS	CB-CA-C	9.80	130.00	110.40
3	2	2079	THR	N-CA-CB	-8.46	94.22	110.30
3	2	2070	LYS	N-CA-C	-7.92	89.63	111.00
3	2	3180	ARG	NE-CZ-NH2	7.81	124.21	120.30
3	2	3064	ARG	NE-CZ-NH2	7.66	124.13	120.30
3	2	2068	VAL	N-CA-CB	-7.45	95.11	111.50
2	1	1061	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	1	1184	PRO	O-C-N	7.42	134.57	122.70
3	2	3067	ARG	NE-CZ-NH2	7.35	123.98	120.30
3	2	3097	ARG	NE-CZ-NH2	7.34	123.97	120.30
3	2	3057	ARG	NE-CZ-NH2	7.30	123.95	120.30
3	2	3043	ARG	NE-CZ-NH2	7.28	123.94	120.30
3	2	2013	ARG	NE-CZ-NH2	7.25	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2071	MET	O-C-N	-7.18	111.21	122.70
2	1	1108	ARG	NE-CZ-NH2	7.12	123.86	120.30
3	2	3099	ARG	NE-CZ-NH2	7.09	123.84	120.30
3	2	3143	ARG	NE-CZ-NH2	6.64	123.62	120.30
2	1	1089	SER	O-C-N	6.59	133.24	122.70
3	2	3066	HIS	CB-CA-C	-6.54	97.33	110.40
2	1	1011	MET	CG-SD-CE	6.53	110.65	100.20
3	2	3071	MET	CG-SD-CE	6.53	110.64	100.20
3	2	2049	MET	CG-SD-CE	6.48	110.56	100.20
3	2	2096	PHE	CB-CA-C	-6.47	97.46	110.40
2	1	1024	LYS	O-C-N	6.47	133.05	122.70
3	2	3074	MET	CG-SD-CE	6.35	110.36	100.20
3	2	2058	ARG	NE-CZ-NH2	6.35	123.47	120.30
2	1	1025	GLN	O-C-N	6.34	132.85	122.70
3	2	2068	VAL	CB-CA-C	6.33	123.42	111.40
2	1	1076	MET	CG-SD-CE	6.32	110.31	100.20
3	2	2172	MET	CG-SD-CE	6.27	110.24	100.20
3	2	2109	ILE	CB-CA-C	6.24	124.08	111.60
3	2	2147	MET	CG-SD-CE	6.21	110.13	100.20
3	2	2031	MET	CG-SD-CE	6.20	110.13	100.20
3	2	2015	MET	CG-SD-CE	6.19	110.10	100.20
3	2	2056	MET	CG-SD-CE	6.17	110.08	100.20
3	2	3123	MET	CG-SD-CE	6.17	110.07	100.20
3	2	3001	MET	CG-SD-CE	6.17	110.06	100.20
2	1	1114	PRO	O-C-N	6.16	132.55	122.70
3	2	3092	MET	CG-SD-CE	6.13	110.02	100.20
3	2	3125	MET	CG-SD-CE	6.13	110.00	100.20
2	1	1134	MET	CG-SD-CE	6.11	109.98	100.20
3	2	2131	ARG	NE-CZ-NH2	6.11	123.35	120.30
3	2	2030	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	1	1071	MET	CG-SD-CE	6.08	109.92	100.20
3	2	2072	THR	CB-CA-C	6.06	127.96	111.60
3	2	2047	MET	CG-SD-CE	6.04	109.86	100.20
3	2	2026	ARG	NE-CZ-NH2	6.02	123.31	120.30
2	1	1178	MET	CG-SD-CE	5.98	109.77	100.20
3	2	3180	ARG	O-C-N	5.92	132.18	122.70
3	2	3020	MET	CG-SD-CE	5.90	109.64	100.20
3	2	3161	MET	CG-SD-CE	5.89	109.63	100.20
3	2	2071	MET	CG-SD-CE	5.89	109.63	100.20
3	2	2187[A]	LEU	N-CA-CB	-5.84	98.71	110.40
3	2	2187[B]	LEU	N-CA-CB	-5.84	98.71	110.40
2	1	1084	ARG	NE-CZ-NH2	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	3104	ILE	CB-CA-C	5.80	123.19	111.60
3	2	2150	ASP	CB-CA-C	-5.74	98.92	110.40
2	1	1015	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	1	1045	GLY	O-C-N	5.69	131.81	122.70
3	2	2061	VAL	CB-CA-C	-5.69	100.59	111.40
2	1	1171	GLU	CB-CA-C	5.49	121.37	110.40
2	1	1171	GLU	N-CA-CB	-5.45	100.80	110.60
3	2	2070	LYS	CA-C-N	-5.43	105.25	117.20
3	2	2074	PRO	CA-N-CD	5.35	119.18	111.70
2	1	1157	SER	O-C-N	5.34	131.24	122.70
2	1	1009	ASN	O-C-N	5.33	131.24	122.70
3	2	2185	ARG	NE-CZ-NH1	5.31	122.96	120.30
3	2	3171	PHE	CB-CA-C	-5.27	99.85	110.40
2	1	1025	GLN	CA-C-N	-5.21	105.74	117.20
3	2	2170	GLU	CB-CA-C	-5.16	100.08	110.40
3	2	2070	LYS	CA-C-O	5.10	130.82	120.10
3	2	3154	THR	O-C-N	5.08	131.83	123.20
2	1	1024	LYS	CA-C-N	-5.04	106.11	117.20

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	16	0
2	1	1451	0	1402	148	0
3	2	2924	0	2938	389	0
All	All	4613	0	4460	530	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 58.

All (530) 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	1.40
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	1.26
3:2:2033:LEU:HB2	3:2:2142:PRO:O	1.40	1.19
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:HD2	1.72	1.18
3:2:3025:ILE:HD11	3:2:3051:LEU:HD22	1.31	1.12
3:2:2190[B]:ILE:HB	3:2:2191[B]:PRO:HD3	1.29	1.12
3:2:2057:TRP:HZ3	3:2:2172:MET:CE	1.61	1.12
3:2:2190[B]:ILE:HB	3:2:2191[B]:PRO:CD	1.78	1.11
3:2:2189[A]:THR:O	3:2:2190[A]:ILE:CB	1.91	1.10
3:2:2057:TRP:CZ3	3:2:2172:MET:CE	2.39	1.06
2:1:1012:ALA:HB3	2:1:1162:VAL:HB	1.07	1.04
3:2:2066:PHE:CZ	3:2:2166:LEU:HD12	1.90	1.04
3:2:2035:ILE:HD11	3:2:2060:PHE:CZ	1.93	1.02
3:2:2066:PHE:CZ	3:2:2166:LEU:CD1	2.43	1.01
3:2:2066:PHE:CE2	3:2:2166:LEU:CD1	2.43	1.01
1:M:3:U:C2'	1:M:4:C:H5'	1.91	1.01
3:2:2057:TRP:HZ3	3:2:2172:MET:HE1	1.22	1.00
3:2:2135:THR:O	3:2:2137:LEU:N	1.95	1.00
2:1:1134:MET:CE	3:2:3144:THR:HG23	1.91	1.00
3:2:2057:TRP:CZ3	3:2:2172:MET:HE1	1.96	1.00
3:2:3047:LEU:HD13	3:2:3092:MET:HE3	1.43	1.00
3:2:2047:MET:HE2	3:2:2052:ALA:HA	1.42	0.99
3:2:2106:PHE:CE1	3:2:2113:VAL:HG23	1.96	0.99
3:2:2048:ASN:HD22	3:2:2048:ASN:C	1.66	0.99
3:2:3128:ASN:ND2	3:2:3177:CYS:HB3	1.76	0.99
3:2:3182:TYR:CD1	3:2:2049:MET:HE1	1.99	0.98
2:1:1129:ASN:OD1	3:2:3130:ASN:ND2	1.97	0.97
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
3:2:2190[B]:ILE:CG1	3:2:2191[B]:PRO:HD2	1.96	0.95
2:1:1020:PHE:CE1	2:1:1044:THR:HG21	2.02	0.95
3:2:2189[A]:THR:O	3:2:2190[A]:ILE:HB	1.02	0.94
3:2:3092:MET:HE1	3:2:3170:TRP:HH2	1.31	0.94
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:CD	2.37	0.93
2:1:1134:MET:HE1	3:2:3144:THR:HG23	1.49	0.93
3:2:3130:ASN:O	3:2:3132:CYS:N	2.02	0.92
2:1:1069:CYS:O	2:1:1167:SER:CB	2.18	0.92
3:2:2047:MET:CE	3:2:2052:ALA:HA	1.99	0.92
3:2:2048:ASN:ND2	3:2:2048:ASN:O	2.02	0.92
3:2:2190[B]:ILE:CB	3:2:2191[B]:PRO:CD	2.48	0.91
3:2:3084:THR:HB	3:2:3158:ALA:HB3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1054:SER:O	2:1:1058:ASN:HB2	1.72	0.90
3:2:2192[B]:GLN:NE2	3:2:2192[B]:GLN:HA	1.84	0.90
3:2:2057:TRP:CZ3	3:2:2172:MET:HE2	2.05	0.90
3:2:3114:LEU:HD21	3:2:2071:MET:HE2	1.52	0.89
3:2:3052:THR:O	3:2:3052:THR:HG22	1.72	0.89
3:2:2079:THR:HB	3:2:2150:ASP:OD2	1.71	0.89
2:1:1091:VAL:HG11	2:1:1117:TRP:HZ2	1.36	0.89
2:1:1020:PHE:CE1	2:1:1044:THR:CG2	2.56	0.88
3:2:2135:THR:C	3:2:2137:LEU:H	1.77	0.88
3:2:3105:TYR:HE1	3:2:2046:LEU:O	1.56	0.88
2:1:1032:VAL:HG12	2:1:1034:LEU:HD12	1.55	0.88
3:2:2030:ARG:HD3	3:2:2145:TYR:CE1	2.08	0.88
3:2:2190[B]:ILE:HG13	3:2:2191[B]:PRO:HD2	1.55	0.88
2:1:1105:ASP:OD1	2:1:1108:ARG:NH1	2.07	0.88
1:M:3:U:O2'	1:M:4:C:H5'	1.73	0.87
2:1:1069:CYS:O	2:1:1167:SER:HB2	1.73	0.87
3:2:3114:LEU:HD11	3:2:3153:VAL:HG21	1.53	0.87
2:1:1020:PHE:HE1	2:1:1044:THR:HG21	1.39	0.87
3:2:2104:VAL:HG13	3:2:2113:VAL:HG11	1.56	0.87
3:2:3030:ILE:CD1	3:2:3150:ILE:HD13	2.05	0.86
3:2:3091:ALA:CB	3:2:3107:ILE:HG13	2.05	0.86
3:2:2048:ASN:ND2	3:2:2050:PRO:HD2	1.89	0.86
2:1:1091:VAL:HG11	2:1:1117:TRP:CZ2	2.10	0.85
3:2:2022:GLN:HA	3:2:2152:SER:HB3	1.59	0.84
3:2:3083:ASN:HD22	3:2:3083:ASN:H	1.21	0.84
3:2:2073:SER:O	3:2:2075:TYR:N	2.09	0.83
3:2:2096:PHE:O	3:2:2099:PHE:HB2	1.78	0.83
3:2:2104:VAL:CG1	3:2:2113:VAL:HG11	2.09	0.83
3:2:3047:LEU:HG	3:2:3051:LEU:HD11	1.61	0.83
2:1:1021:ASP:O	2:1:1023:SER:N	2.10	0.83
3:2:3018:GLY:N	3:2:3023:LEU:HD11	1.93	0.83
2:1:1021:ASP:C	2:1:1023:SER:H	1.82	0.83
2:1:1057:SER:O	2:1:1061:ARG:HG3	1.79	0.82
3:2:2129:GLN:HB3	3:2:2181:ILE:HD12	1.61	0.82
2:1:1016:THR:CG2	2:1:1017:PRO:HD2	2.10	0.82
3:2:2106:PHE:HE1	3:2:2113:VAL:HG23	1.41	0.82
3:2:3025:ILE:CD1	3:2:3051:LEU:HD22	2.09	0.82
2:1:1065:TRP:HB2	2:1:1173:ALA:O	1.78	0.82
2:1:1025:GLN:HG3	2:1:1026:SER:H	1.41	0.82
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:CG2	2.10	0.82
3:2:2030:ARG:HD3	3:2:2145:TYR:CZ	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1020:PHE:HE1	2:1:1044:THR:CG2	1.93	0.81
3:2:2030:ARG:NH2	3:2:2091:ASP:OD2	2.12	0.81
3:2:2048:ASN:HD22	3:2:2050:PRO:HD2	1.45	0.81
2:1:1053:ASN:OD1	2:1:1061:ARG:NH2	2.13	0.81
3:2:3123:MET:HE1	3:2:3125:MET:HB2	1.63	0.81
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:HG23	1.64	0.80
3:2:3104:ILE:O	3:2:3108:CYS:SG	2.39	0.80
3:2:3133:SER:OG	3:2:3134:ASP:N	2.15	0.80
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	0.79
1:M:5:A:O2'	1:M:6:A:H5'	1.82	0.79
3:2:2190[A]:ILE:HG12	3:2:2191[A]:PRO:HD3	1.64	0.79
3:2:2006:GLN:CG	3:2:2007:ASN:H	1.96	0.79
3:2:3052:THR:O	3:2:3052:THR:CG2	2.30	0.78
3:2:3030:ILE:HD11	3:2:3150:ILE:HD13	1.64	0.78
2:1:1073:LYS:CG	2:1:1120:ILE:HD13	2.14	0.78
3:2:2039:ALA:HB3	3:2:2046:LEU:HB2	1.64	0.78
1:M:3:U:H2'	1:M:4:C:H5'	1.66	0.77
1:M:5:A:C2'	1:M:6:A:H5'	2.14	0.77
3:2:2024:THR:OG1	3:2:2024:THR:O	2.00	0.77
3:2:2190[A]:ILE:HG12	3:2:2191[A]:PRO:HD2	0.79	0.77
3:2:2058:ARG:O	3:2:2128:THR:HB	1.84	0.77
3:2:3007:LYS:HG3	3:2:3007:LYS:O	1.84	0.77
3:2:3074:MET:HE2	3:2:3123:MET:HE1	1.65	0.77
3:2:3026:SER:HB3	3:2:3051:LEU:O	1.84	0.76
2:1:1069:CYS:O	2:1:1167:SER:HB3	1.84	0.76
3:2:2048:ASN:ND2	3:2:2050:PRO:CD	2.49	0.76
2:1:1016:THR:HG22	2:1:1017:PRO:HD2	1.67	0.76
3:2:2078:CYS:SG	3:2:2148:VAL:HG13	2.26	0.75
2:1:1056:ILE:HG23	2:1:1057:SER:N	2.00	0.75
3:2:3086:ILE:HG23	3:2:3088:LEU:HD12	1.68	0.75
2:1:1026:SER:OG	2:1:1152:ASP:OD2	2.05	0.75
3:2:2064:LEU:CD2	3:2:2169:ILE:HG23	2.17	0.75
3:2:3047:LEU:HD13	3:2:3092:MET:CE	2.16	0.75
3:2:3080:ILE:HG22	3:2:3117:PRO:HB2	1.69	0.74
3:2:2057:TRP:HZ3	3:2:2172:MET:HE2	1.41	0.74
3:2:3114:LEU:HD21	3:2:2071:MET:CE	2.18	0.74
3:2:2106:PHE:CE1	3:2:2113:VAL:CG2	2.71	0.73
3:2:2139:ASP:OD1	3:2:2143:TYR:CE2	2.42	0.73
3:2:2186:LEU:O	3:2:2187[B]:LEU:HA	1.87	0.73
3:2:2053:VAL:O	3:2:2056:MET:HB2	1.87	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
3:2:2192[B]:GLN:HE21	3:2:2192[B]:GLN:HA	1.53	0.72
3:2:3018:GLY:N	3:2:3023:LEU:CD1	2.52	0.72
2:1:1020:PHE:CD1	2:1:1044:THR:CG2	2.73	0.72
2:1:1181:PHE:O	3:2:2044:ALA:HB1	1.89	0.72
3:2:2035:ILE:HD11	3:2:2060:PHE:HZ	1.53	0.71
3:2:3130:ASN:C	3:2:3132:CYS:H	1.93	0.71
2:1:1007:VAL:HG22	2:1:1007:VAL:O	1.88	0.71
3:2:2026:ARG:HG2	3:2:2147:MET:HG2	1.73	0.70
3:2:2006:GLN:HG2	3:2:2007:ASN:H	1.56	0.70
3:2:2130:VAL:CG1	3:2:2134:THR:HG21	2.22	0.70
2:1:1091:VAL:CG1	2:1:1117:TRP:CZ2	2.74	0.70
3:2:3080:ILE:HG23	3:2:3118:ALA:HA	1.73	0.70
3:2:3084:THR:CB	3:2:3158:ALA:HB3	2.22	0.70
3:2:2063:ASP:OD2	3:2:2119:GLN:HB2	1.91	0.70
2:1:1043:LYS:O	2:1:1043:LYS:HG2	1.92	0.69
3:2:2011:LEU:HD12	3:2:2050:PRO:O	1.92	0.69
3:2:2028:VAL:HG22	3:2:2147:MET:HG3	1.74	0.69
3:2:3115:TRP:HA	3:2:2111:GLU:OE1	1.92	0.69
3:2:2135:THR:C	3:2:2137:LEU:N	2.44	0.69
3:2:2187[B]:LEU:HD11	3:2:2190[B]:ILE:HA	1.75	0.69
2:1:1014:VAL:HG21	2:1:1030:PHE:CE1	2.28	0.69
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:CA	2.23	0.69
3:2:3107:ILE:O	3:2:3107:ILE:HG13	1.92	0.69
2:1:1172:ILE:HG13	3:2:2049:MET:HE3	1.75	0.68
3:2:2073:SER:C	3:2:2075:TYR:H	1.96	0.68
2:1:1143:THR:HG23	2:1:1144:SER:N	2.09	0.68
3:2:3092:MET:HE1	3:2:3170:TRP:CH2	2.20	0.68
2:1:1039:ILE:HD11	2:1:1051:VAL:CG2	2.23	0.68
2:1:1039:ILE:HD11	2:1:1051:VAL:HG23	1.75	0.68
3:2:3029:LYS:HE2	3:2:3165:GLN:OE1	1.92	0.68
3:2:2187[B]:LEU:CD2	3:2:2190[B]:ILE:HG23	2.24	0.67
3:2:2066:PHE:CD2	3:2:2166:LEU:HD12	2.28	0.67
3:2:3007:LYS:O	3:2:3007:LYS:CG	2.42	0.67
3:2:3080:ILE:HG23	3:2:3118:ALA:CA	2.24	0.67
3:2:3061:ASP:O	3:2:3065:THR:HB	1.94	0.67
3:2:3123:MET:CE	3:2:3125:MET:HB2	2.24	0.67
2:1:1091:VAL:CG1	2:1:1117:TRP:HZ2	2.04	0.67
2:1:1073:LYS:HG2	2:1:1120:ILE:HD13	1.75	0.67
3:2:2064:LEU:HD22	3:2:2169:ILE:HG23	1.77	0.67
3:2:3083:ASN:HD22	3:2:3083:ASN:N	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:3123:MET:HE1	3:2:3125:MET:CB	2.24	0.67
3:2:2048:ASN:C	3:2:2048:ASN:ND2	2.36	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
2:1:1127:GLY:O	2:1:1131:GLY:HA2	1.95	0.66
3:2:2096:PHE:C	3:2:2098:ALA:H	1.96	0.66
3:2:3074:MET:HE2	3:2:3123:MET:CE	2.26	0.66
2:1:1153:ASN:N	2:1:1154:PRO:HD3	2.09	0.66
3:2:2049:MET:HB3	3:2:2050:PRO:HD3	1.78	0.66
3:2:3025:ILE:HG22	3:2:3172:ILE:HD12	1.77	0.66
2:1:1011:MET:HE1	2:1:1034:LEU:HA	1.78	0.65
3:2:2079:THR:HB	3:2:2150:ASP:CG	2.15	0.65
2:1:1134:MET:CE	3:2:3144:THR:CG2	2.73	0.65
3:2:3025:ILE:CG2	3:2:3172:ILE:HD12	2.27	0.65
3:2:3105:TYR:CE1	3:2:2046:LEU:O	2.46	0.64
3:2:2096:PHE:O	3:2:2098:ALA:N	2.30	0.64
3:2:2189[B]:THR:O	3:2:2190[B]:ILE:HG12	1.97	0.64
2:1:1074:VAL:HG11	2:1:1149:PHE:CZ	2.32	0.64
1:M:2:G:C2'	1:M:3:U:H5'	2.26	0.64
3:2:3005:LEU:HD12	3:2:3008:LEU:HD22	1.78	0.64
3:2:3072:ILE:HG12	3:2:3136:TRP:CZ2	2.32	0.64
3:2:2025:SER:C	3:2:2027:SER:H	2.00	0.64
2:1:1032:VAL:HG12	2:1:1034:LEU:CD1	2.25	0.64
3:2:2135:THR:O	3:2:2138:ALA:N	2.27	0.64
2:1:1178:MET:SD	3:2:3097:ARG:HB3	2.37	0.64
3:2:3139:GLU:OE2	3:2:3143:ARG:HD2	1.97	0.64
3:2:3080:ILE:CG2	3:2:3118:ALA:N	2.61	0.64
3:2:3023:LEU:HD23	3:2:3172:ILE:CG2	2.28	0.63
3:2:2189[B]:THR:O	3:2:2192[B]:GLN:HG2	1.99	0.63
3:2:2080:VAL:CG1	3:2:2082:PHE:CE1	2.82	0.63
2:1:1002:ILE:HB	3:2:2003:LEU:O	1.98	0.63
2:1:1020:PHE:CD1	2:1:1044:THR:HG22	2.33	0.63
2:1:1056:ILE:HG23	2:1:1057:SER:H	1.62	0.63
3:2:3017:LYS:C	3:2:3023:LEU:HD11	2.19	0.63
3:2:3020:MET:CE	3:2:3073:LYS:NZ	2.62	0.63
3:2:2057:TRP:O	3:2:2178:ASN:HB2	1.99	0.63
2:1:1029:GLN:HG3	2:1:1150:LEU:HD12	1.81	0.62
3:2:3109:SER:HB3	3:2:2050:PRO:HG2	1.81	0.62
2:1:1134:MET:SD	3:2:3144:THR:HG23	2.39	0.62
2:1:1071:MET:O	2:1:1164:LEU:HA	1.99	0.62
3:2:2080:VAL:HG12	3:2:2082:PHE:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1056:ILE:CG2	2:1:1057:SER:N	2.62	0.62
2:1:1011:MET:CE	2:1:1034:LEU:HA	2.29	0.61
3:2:3069:LYS:O	3:2:3069:LYS:CG	2.48	0.61
3:2:3091:ALA:HB1	3:2:3107:ILE:O	2.00	0.61
3:2:2030:ARG:H	3:2:2191[B]:PRO:HD3	1.65	0.61
3:2:2170:GLU:O	3:2:2171:ASN:HB2	2.01	0.61
3:2:2189[B]:THR:O	3:2:2190[B]:ILE:C	2.39	0.61
3:2:2190[B]:ILE:CB	3:2:2191[B]:PRO:HD2	2.22	0.61
3:2:2192[B]:GLN:NE2	3:2:2192[B]:GLN:CA	2.59	0.61
3:2:3047:LEU:HG	3:2:3051:LEU:CD1	2.29	0.61
3:2:3128:ASN:ND2	3:2:3177:CYS:CB	2.60	0.61
2:1:1020:PHE:HD1	2:1:1044:THR:HG22	1.63	0.61
3:2:3080:ILE:CG2	3:2:3117:PRO:HB2	2.31	0.61
3:2:3092:MET:CE	3:2:3170:TRP:HH2	2.11	0.61
3:2:2093:THR:HB	3:2:2096:PHE:CE1	2.35	0.61
3:2:2107:GLY:O	3:2:2108:GLU:C	2.39	0.61
2:1:1056:ILE:CG2	2:1:1057:SER:H	2.14	0.61
3:2:2073:SER:C	3:2:2075:TYR:N	2.54	0.61
2:1:1134:MET:HE3	3:2:3144:THR:O	2.01	0.60
3:2:3047:LEU:CD1	3:2:3092:MET:CE	2.79	0.60
2:1:1054:SER:O	2:1:1058:ASN:CB	2.49	0.60
2:1:1019:ASN:H	2:1:1019:ASN:ND2	1.98	0.60
3:2:3030:ILE:HD13	3:2:3150:ILE:HD13	1.83	0.60
3:2:3083:ASN:ND2	3:2:3083:ASN:H	1.95	0.60
3:2:3105:TYR:HD1	3:2:2046:LEU:HB3	1.66	0.60
2:1:1175:ASN:ND2	3:2:3093:ASN:OD1	2.35	0.60
3:2:3119:CYS:HB3	3:2:2109:ILE:O	2.02	0.59
3:2:3032:LEU:HD11	3:2:3088:LEU:HD11	1.85	0.59
3:2:2048:ASN:HD22	3:2:2050:PRO:CD	2.12	0.59
2:1:1139:TRP:HB3	2:1:1142:GLN:NE2	2.17	0.59
3:2:3038:GLY:HA2	3:2:3152:CYS:SG	2.43	0.59
3:2:3154:THR:HG23	3:2:2192[A]:GLN:O	2.03	0.59
2:1:1073:LYS:HG3	2:1:1120:ILE:HD13	1.82	0.58
3:2:2095:ASN:O	3:2:2095:ASN:OD1	2.21	0.58
2:1:1007:VAL:O	2:1:1007:VAL:CG2	2.50	0.58
3:2:2006:GLN:CG	3:2:2007:ASN:N	2.64	0.58
3:2:3086:ILE:HG22	3:2:3117:PRO:HG2	1.84	0.58
3:2:3078:VAL:HG11	3:2:3166:VAL:HG22	1.85	0.58
3:2:2096:PHE:CE2	3:2:2147:MET:SD	2.97	0.58
3:2:3074:MET:CE	3:2:3123:MET:HE1	2.32	0.58
1:M:3:U:H2'	1:M:4:C:C5'	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1042:ASP:HB2	2:1:1047:TRP:HE1	1.68	0.58
3:2:3123:MET:HG2	3:2:3124:THR:N	2.18	0.58
2:1:1181:PHE:O	3:2:2044:ALA:CB	2.51	0.58
3:2:3147:HIS:ND1	3:2:3149:ASP:OD2	2.36	0.58
3:2:3128:ASN:HD22	3:2:3177:CYS:HB3	1.65	0.58
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:HD3	2.26	0.57
3:2:3023:LEU:CD2	3:2:3172:ILE:HG22	2.34	0.57
3:2:3023:LEU:HD23	3:2:3172:ILE:HG22	1.85	0.57
3:2:3020:MET:CE	3:2:3073:LYS:HZ2	2.15	0.57
3:2:3129:PRO:O	3:2:3131:PRO:HD3	2.04	0.57
3:2:3018:GLY:CA	3:2:3023:LEU:HD12	2.34	0.57
3:2:3024:LYS:O	3:2:3056:PHE:O	2.23	0.57
3:2:2139:ASP:OD1	3:2:2143:TYR:CZ	2.57	0.56
3:2:2026:ARG:NH2	3:2:2096:PHE:CE2	2.73	0.56
3:2:2096:PHE:HD2	3:2:2147:MET:HE1	1.69	0.56
3:2:3092:MET:CE	3:2:3148:CYS:SG	2.94	0.56
2:1:1083:LYS:O	2:1:1086:ASP:HB2	2.05	0.56
3:2:2047:MET:CE	3:2:2052:ALA:CA	2.80	0.56
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:HA	1.86	0.56
3:2:2021:PRO:HA	3:2:2159:ASP:OD2	2.05	0.56
3:2:2002:VAL:HG12	3:2:2002:VAL:O	2.05	0.56
2:1:1175:ASN:HB3	3:2:3093:ASN:OD1	2.06	0.56
2:1:1043:LYS:CG	2:1:1043:LYS:O	2.54	0.56
3:2:2057:TRP:CH2	3:2:2172:MET:HE1	2.41	0.55
3:2:3047:LEU:O	3:2:3050:PHE:HB2	2.06	0.55
3:2:3091:ALA:HA	3:2:3112:CYS:HB2	1.89	0.55
3:2:2178:ASN:OD1	3:2:2180:GLY:HA2	2.07	0.55
2:1:1032:VAL:CG1	2:1:1034:LEU:HD12	2.33	0.55
2:1:1172:ILE:HG13	3:2:2049:MET:CE	2.37	0.55
2:1:1041:VAL:HG23	2:1:1042:ASP:O	2.07	0.55
3:2:2083:PHE:CE1	3:2:2145:TYR:HB2	2.41	0.55
3:2:2159:ASP:O	3:2:2161:VAL:HG23	2.07	0.55
2:1:1096:THR:O	2:1:1146:HIS:HB2	2.06	0.54
2:1:1140:ALA:O	2:1:1141:ASN:C	2.45	0.54
2:1:1009:ASN:OD1	2:1:1056:ILE:HG22	2.07	0.54
3:2:3114:LEU:CD1	3:2:3153:VAL:HG21	2.33	0.54
3:2:3092:MET:CE	3:2:3170:TRP:CH2	2.89	0.54
3:2:3141:LEU:HD12	3:2:3146:PHE:HB2	1.90	0.54
2:1:1016:THR:HG23	2:1:1017:PRO:HD2	1.88	0.54
3:2:3050:PHE:CE2	3:2:3148:CYS:HB3	2.43	0.54
3:2:2039:ALA:HB3	3:2:2046:LEU:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2129:GLN:NE2	3:2:2181:ILE:O	2.40	0.54
3:2:3074:MET:CE	3:2:3123:MET:CE	2.85	0.54
3:2:2187[B]:LEU:CD2	3:2:2190[B]:ILE:CG2	2.85	0.54
2:1:1035:LEU:HD11	2:1:1125:VAL:HG22	1.89	0.53
3:2:2187[B]:LEU:HD11	3:2:2190[B]:ILE:CA	2.37	0.53
2:1:1021:ASP:C	2:1:1023:SER:N	2.49	0.53
3:2:3182:TYR:CG	3:2:2049:MET:HE2	2.43	0.53
3:2:2079:THR:CB	3:2:2150:ASP:OD2	2.51	0.53
3:2:3005:LEU:O	3:2:3008:LEU:HB2	2.07	0.53
3:2:3032:LEU:HD11	3:2:3088:LEU:HD21	1.88	0.53
1:M:5:A:H2'	1:M:6:A:H5'	1.91	0.53
3:2:2083:PHE:CE1	3:2:2145:TYR:CB	2.92	0.53
2:1:1145:TRP:CE3	2:1:1145:TRP:HA	2.43	0.53
2:1:1169:ASN:O	2:1:1169:ASN:ND2	2.40	0.53
3:2:3130:ASN:C	3:2:3132:CYS:N	2.56	0.53
3:2:2025:SER:C	3:2:2027:SER:N	2.62	0.53
3:2:2187[B]:LEU:CG	3:2:2190[B]:ILE:H	2.21	0.53
1:M:3:U:H2'	1:M:4:C:O4'	2.07	0.53
2:1:1091:VAL:HA	2:1:1150:LEU:O	2.09	0.53
2:1:1036:GLY:O	3:2:3097:ARG:NH1	2.38	0.52
3:2:2005:PRO:HG3	3:2:2057:TRP:CZ2	2.44	0.52
3:2:3018:GLY:CA	3:2:3023:LEU:CD1	2.86	0.52
2:1:1153:ASN:N	2:1:1154:PRO:CD	2.71	0.52
3:2:3025:ILE:CG2	3:2:3172:ILE:CD1	2.87	0.52
3:2:3026:SER:OG	3:2:3170:TRP:CD1	2.52	0.52
3:2:2030:ARG:CD	3:2:2145:TYR:CE1	2.90	0.52
3:2:3080:ILE:CD1	3:2:3085:GLY:HA2	2.40	0.52
3:2:3107:ILE:O	3:2:3107:ILE:CG1	2.58	0.52
2:1:1065:TRP:O	2:1:1172:ILE:HA	2.10	0.52
3:2:3105:TYR:OH	3:2:2038:GLY:HA3	2.10	0.52
3:2:3030:ILE:HD11	3:2:3150:ILE:CD1	2.36	0.52
2:1:1042:ASP:CG	2:1:1044:THR:OG1	2.48	0.52
2:1:1062:VAL:O	2:1:1176:THR:N	2.38	0.52
3:2:3012:ASP:OD2	3:2:3014:GLU:HB2	2.10	0.52
3:2:2017:LYS:NZ	3:2:2190[A]:ILE:HG22	2.25	0.51
2:1:1072:VAL:CG1	2:1:1073:LYS:N	2.73	0.51
2:1:1042:ASP:CB	2:1:1047:TRP:HE1	2.23	0.51
1:M:3:U:HO2'	1:M:4:C:H5'	1.72	0.51
3:2:2080:VAL:HG11	3:2:2082:PHE:CE1	2.44	0.51
3:2:3026:SER:OG	3:2:3170:TRP:HB2	2.10	0.51
1:M:2:G:O2'	1:M:3:U:H5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:3004:ASN:OD1	3:2:3006:PHE:HB2	2.11	0.51
3:2:3078:VAL:HG21	3:2:3164:VAL:CG1	2.40	0.51
3:2:2035:ILE:O	3:2:2051:ASN:ND2	2.33	0.51
3:2:3020:MET:HE1	3:2:3073:LYS:NZ	2.25	0.51
3:2:3154:THR:HG22	3:2:3154:THR:O	2.11	0.51
2:1:1033:ASP:OD2	2:1:1036:GLY:N	2.44	0.50
3:2:3137:SER:O	3:2:3140:PHE:HB3	2.11	0.50
3:2:3028:SER:HG	3:2:3170:TRP:HE1	1.60	0.50
2:1:1020:PHE:CD1	2:1:1044:THR:HG21	2.42	0.50
3:2:2031:MET:HE1	3:2:2164:VAL:HG21	1.93	0.50
3:2:2049:MET:O	3:2:2053:VAL:CG1	2.59	0.50
3:2:3127:PHE:N	3:2:3127:PHE:CD1	2.80	0.50
3:2:2042:LYS:O	3:2:2043:SER:HB2	2.12	0.50
3:2:3020:MET:HE3	3:2:3073:LYS:HZ2	1.76	0.50
3:2:3164:VAL:CG1	3:2:3165:GLN:N	2.74	0.50
1:M:2:G:H2'	1:M:3:U:H5'	1.91	0.50
2:1:1097:ASN:H	2:1:1097:ASN:ND2	2.10	0.50
3:2:3025:ILE:HD11	3:2:3051:LEU:CD2	2.21	0.50
2:1:1007:VAL:HG22	3:2:2177:LEU:HD23	1.94	0.50
2:1:1014:VAL:HG11	2:1:1030:PHE:CE1	2.47	0.50
3:2:2066:PHE:CZ	3:2:2166:LEU:HD11	2.41	0.50
2:1:1097:ASN:HB2	2:1:1143:THR:OG1	2.12	0.50
2:1:1056:ILE:O	2:1:1059:LEU:N	2.45	0.50
3:2:2058:ARG:HB3	3:2:2176:GLY:HA3	1.93	0.49
3:2:3056:PHE:O	3:2:3058:ALA:N	2.45	0.49
3:2:3128:ASN:HD22	3:2:3177:CYS:CB	2.24	0.49
3:2:2047:MET:HE3	3:2:2052:ALA:N	2.28	0.49
2:1:1001:SER:OG	2:1:1002:ILE:N	2.46	0.49
3:2:2031:MET:HG3	3:2:2144:LEU:O	2.11	0.49
3:2:2189[B]:THR:OG1	3:2:2192[B]:GLN:HB2	2.12	0.49
2:1:1071:MET:O	2:1:1164:LEU:CA	2.60	0.49
3:2:3080:ILE:CG2	3:2:3117:PRO:C	2.81	0.49
2:1:1004:GLN:HB3	2:1:1007:VAL:HG11	1.95	0.49
2:1:1090:LEU:HD12	2:1:1091:VAL:N	2.27	0.49
3:2:2017:LYS:NZ	3:2:2191[A]:PRO:O	2.46	0.49
3:2:3114:LEU:CD2	3:2:2071:MET:CE	2.88	0.49
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:N	2.27	0.49
3:2:2020:PHE:HD2	3:2:2148:VAL:CG2	2.26	0.49
3:2:2027:SER:O	3:2:2029:LYS:HD3	2.13	0.49
3:2:3086:ILE:O	3:2:3117:PRO:HD2	2.13	0.48
3:2:3182:TYR:CG	3:2:2049:MET:CE	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3:U:C2'	1:M:4:C:C5'	2.79	0.48
3:2:2097:GLU:O	3:2:2101:HIS:CE1	2.65	0.48
3:2:2073:SER:OG	3:2:2074:PRO:HD2	2.13	0.48
2:1:1074:VAL:HG11	2:1:1149:PHE:HZ	1.78	0.48
3:2:3031:ALA:C	3:2:3033:PRO:HD3	2.34	0.48
3:2:2020:PHE:CD2	3:2:2148:VAL:CG2	2.97	0.48
3:2:3154:THR:HA	3:2:2192[A]:GLN:C	2.34	0.48
2:1:1143:THR:CG2	2:1:1144:SER:N	2.76	0.48
3:2:3080:ILE:HD11	3:2:3084:THR:HG23	1.95	0.48
2:1:1139:TRP:HB3	2:1:1142:GLN:HE21	1.78	0.48
3:2:3030:ILE:CD1	3:2:3150:ILE:CD1	2.88	0.48
3:2:3086:ILE:CG2	3:2:3088:LEU:CD1	2.92	0.48
3:2:2053:VAL:HG22	3:2:2054:LEU:N	2.29	0.48
3:2:2192[A]:GLN:O	3:2:2192[A]:GLN:HG2	2.14	0.48
3:2:3072:ILE:HD11	3:2:3136:TRP:CH2	2.49	0.48
3:2:2150:ASP:OD2	3:2:2150:ASP:N	2.47	0.47
3:2:2088:ASN:N	3:2:2088:ASN:OD1	2.47	0.47
3:2:2069:SER:O	3:2:2162:ILE:HA	2.15	0.47
3:2:2049:MET:O	3:2:2051:ASN:N	2.47	0.47
3:2:2054:LEU:HD12	3:2:2057:TRP:CZ3	2.49	0.47
3:2:3078:VAL:CG1	3:2:3166:VAL:HG22	2.44	0.47
2:1:1039:ILE:HD11	2:1:1051:VAL:HG22	1.95	0.47
3:2:2189[B]:THR:C	3:2:2190[B]:ILE:HG12	2.35	0.47
3:2:3105:TYR:HE1	3:2:2046:LEU:C	2.16	0.47
3:2:3154:THR:HG21	3:2:2071:MET:HB2	1.97	0.47
1:M:1:G:N7	3:2:2168:ILE:HD13	2.30	0.47
2:1:1054:SER:HB2	2:1:1057:SER:HB3	1.96	0.47
2:1:1094:PHE:O	2:1:1147:LEU:HD12	2.15	0.47
3:2:2017:LYS:HZ3	3:2:2190[A]:ILE:CG2	2.27	0.47
3:2:2027:SER:O	3:2:2029:LYS:CD	2.63	0.47
2:1:1070:LEU:HG	2:1:1170:PHE:CE1	2.50	0.47
3:2:3141:LEU:HD12	3:2:3146:PHE:CB	2.45	0.47
3:2:2030:ARG:HE	3:2:2191[B]:PRO:HB3	1.80	0.47
3:2:3083:ASN:N	3:2:3083:ASN:ND2	2.57	0.47
3:2:3080:ILE:HG22	3:2:3117:PRO:C	2.35	0.47
3:2:3164:VAL:HG12	3:2:3165:GLN:N	2.30	0.47
2:1:1143:THR:HG23	2:1:1144:SER:H	1.79	0.46
3:2:2133:ALA:O	3:2:2134:THR:C	2.53	0.46
3:2:3074:MET:HE2	3:2:3123:MET:SD	2.54	0.46
2:1:1034:LEU:HD23	2:1:1123:ILE:HD13	1.96	0.46
2:1:1181:PHE:HB2	3:2:2045:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1019:ASN:N	2:1:1019:ASN:ND2	2.64	0.46
3:2:3105:TYR:CD1	3:2:2046:LEU:HB3	2.47	0.46
3:2:2187[B]:LEU:HG	3:2:2190[B]:ILE:H	1.79	0.46
3:2:3020:MET:HE3	3:2:3073:LYS:NZ	2.30	0.46
3:2:3050:PHE:CZ	3:2:3150:ILE:CD1	2.98	0.46
3:2:3080:ILE:HG23	3:2:3118:ALA:N	2.29	0.46
2:1:1074:VAL:HG11	2:1:1149:PHE:CE2	2.49	0.46
3:2:2065:VAL:HG22	3:2:2116:LYS:HD2	1.96	0.46
3:2:2004:ASN:N	3:2:2005:PRO:HD3	2.31	0.46
3:2:2015:MET:HE2	3:2:2035:ILE:HG21	1.97	0.46
3:2:2033:LEU:HD23	3:2:2033:LEU:HA	1.73	0.46
3:2:2082:PHE:CE1	3:2:2104:VAL:HG21	2.50	0.46
2:1:1064:ALA:O	2:1:1134:MET:HG3	2.16	0.46
3:2:2048:ASN:ND2	3:2:2050:PRO:CG	2.79	0.46
3:2:2020:PHE:CD2	3:2:2148:VAL:HG22	2.51	0.46
3:2:2011:LEU:O	3:2:2050:PRO:HB2	2.16	0.45
3:2:2026:ARG:HH22	3:2:2093:THR:C	2.18	0.45
3:2:3011:ASP:CG	3:2:3011:ASP:O	2.52	0.45
2:1:1004:GLN:HB3	2:1:1007:VAL:CG1	2.46	0.45
3:2:3129:PRO:C	3:2:3131:PRO:HD3	2.35	0.45
2:1:1039:ILE:CD1	2:1:1051:VAL:HG23	2.46	0.45
3:2:2047:MET:HG3	3:2:2048:ASN:N	2.32	0.45
2:1:1059:LEU:HA	3:2:2052:ALA:HB1	1.99	0.45
3:2:3091:ALA:HB1	3:2:3107:ILE:HG13	1.94	0.45
2:1:1096:THR:HG22	2:1:1098:SER:H	1.80	0.45
3:2:3069:LYS:O	3:2:3069:LYS:HG3	2.16	0.45
3:2:3090:CYS:O	3:2:3112:CYS:HA	2.16	0.45
2:1:1096:THR:O	2:1:1146:HIS:N	2.47	0.45
2:1:1144:SER:HB3	2:1:1145:TRP:H	1.35	0.45
3:2:2049:MET:CB	3:2:2050:PRO:HD3	2.46	0.45
3:2:2011:LEU:CD2	3:2:2013:ARG:HB2	2.46	0.45
3:2:3045:ASP:O	3:2:3147:HIS:CD2	2.70	0.45
3:2:3016:PRO:O	3:2:3023:LEU:HD21	2.17	0.44
1:M:4:C:H4'	3:2:3124:THR:O	2.17	0.44
3:2:2025:SER:O	3:2:2027:SER:N	2.50	0.44
2:1:1087:TRP:CE2	2:1:1114:PRO:HA	2.52	0.44
3:2:2096:PHE:HE2	3:2:2147:MET:SD	2.39	0.44
2:1:1030:PHE:O	2:1:1149:PHE:N	2.38	0.44
3:2:2030:ARG:HG2	3:2:2145:TYR:CD1	2.52	0.44
3:2:3046:LEU:O	3:2:3047:LEU:C	2.53	0.44
3:2:3173:SER:OG	3:2:3174:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2095:ASN:O	3:2:2095:ASN:CG	2.55	0.44
3:2:2141:CYS:HA	3:2:2142:PRO:HD3	1.92	0.44
3:2:2187[B]:LEU:CD2	3:2:2190[B]:ILE:H	2.31	0.44
3:2:2036:GLY:CA	3:2:2055:SER:OG	2.66	0.44
3:2:2065:VAL:CG2	3:2:2116:LYS:HD2	2.48	0.44
2:1:1076:MET:O	2:1:1116:SER:HA	2.17	0.44
3:2:2187[B]:LEU:HD21	3:2:2190[B]:ILE:H	1.83	0.44
3:2:2029:LYS:HG3	3:2:2190[B]:ILE:HG21	2.00	0.43
3:2:3154:THR:CG2	3:2:3154:THR:O	2.65	0.43
2:1:1069:CYS:SG	2:1:1124:GLU:HG3	2.58	0.43
2:1:1171:GLU:HA	3:2:3182:TYR:O	2.18	0.43
2:1:1042:ASP:HB2	2:1:1047:TRP:NE1	2.31	0.43
2:1:1127:GLY:O	2:1:1131:GLY:CA	2.65	0.43
2:1:1153:ASN:H	2:1:1154:PRO:HD3	1.83	0.43
2:1:1056:ILE:O	2:1:1057:SER:C	2.56	0.43
3:2:2096:PHE:CD2	3:2:2147:MET:SD	3.11	0.43
2:1:1072:VAL:HG22	2:1:1164:LEU:HD23	2.01	0.43
3:2:2058:ARG:HB3	3:2:2177:LEU:N	2.34	0.43
3:2:3080:ILE:HD13	3:2:3085:GLY:HA2	2.00	0.43
3:2:3086:ILE:CG2	3:2:3117:PRO:HG2	2.49	0.43
3:2:2011:LEU:HD23	3:2:2013:ARG:HB2	1.98	0.43
3:2:2049:MET:O	3:2:2053:VAL:HG13	2.19	0.43
3:2:3005:LEU:HD12	3:2:3005:LEU:HA	1.76	0.42
3:2:3074:MET:O	3:2:3124:THR:HA	2.19	0.42
2:1:1023:SER:O	2:1:1024:LYS:CG	2.67	0.42
2:1:1027:PHE:HA	2:1:1151:VAL:O	2.19	0.42
3:2:3020:MET:CE	3:2:3073:LYS:HZ3	2.32	0.42
3:2:3078:VAL:HG21	3:2:3164:VAL:HG11	2.00	0.42
3:2:3039:GLY:N	3:2:3152:CYS:O	2.46	0.42
3:2:2017:LYS:NZ	3:2:2190[A]:ILE:CG2	2.83	0.42
3:2:3129:PRO:O	3:2:3131:PRO:CD	2.67	0.42
2:1:1059:LEU:HD11	2:1:1172:ILE:CD1	2.49	0.42
3:2:2026:ARG:O	3:2:2028:VAL:N	2.53	0.42
3:2:2096:PHE:C	3:2:2098:ALA:N	2.64	0.42
3:2:2096:PHE:CD2	3:2:2147:MET:HE1	2.53	0.42
2:1:1070:LEU:HD11	2:1:1170:PHE:CZ	2.55	0.42
3:2:3087:ALA:HB2	3:2:2071:MET:HB3	2.00	0.42
2:1:1025:GLN:HG3	2:1:1026:SER:N	2.22	0.42
3:2:2049:MET:O	3:2:2053:VAL:HG12	2.20	0.42
3:2:3114:LEU:CD2	3:2:2071:MET:HE3	2.49	0.42
3:2:2037:GLY:O	3:2:2047:MET:SD	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:2049:MET:C	3:2:2051:ASN:N	2.73	0.42
3:2:2047:MET:HE3	3:2:2052:ALA:CA	2.49	0.42
3:2:2123:LEU:HD23	3:2:2124:THR:OG1	2.19	0.42
2:1:1041:VAL:HG23	2:1:1042:ASP:N	2.34	0.42
2:1:1177:LEU:HD23	2:1:1177:LEU:HA	1.84	0.41
3:2:2002:VAL:CG1	3:2:2002:VAL:O	2.66	0.41
3:2:2010:VAL:CG1	3:2:2012:ASN:ND2	2.83	0.41
3:2:2083:PHE:HE2	3:2:2147:MET:HE2	1.84	0.41
2:1:1002:ILE:HD13	2:1:1002:ILE:HG21	1.84	0.41
3:2:3025:ILE:HD13	3:2:3025:ILE:HG21	1.80	0.41
2:1:1030:PHE:CD2	2:1:1149:PHE:HB2	2.55	0.41
3:2:2124:THR:HG22	3:2:2125:ALA:O	2.21	0.41
2:1:1129:ASN:HD22	2:1:1129:ASN:HA	1.61	0.41
3:2:2192[A]:GLN:O	3:2:2192[A]:GLN:CG	2.67	0.41
3:2:3140:PHE:O	3:2:3144:THR:HB	2.20	0.41
2:1:1013:THR:OG1	2:1:1161:ASP:OD2	2.38	0.41
2:1:1073:LYS:N	2:1:1163:LEU:O	2.54	0.41
3:2:2028:VAL:CG2	3:2:2147:MET:HG3	2.48	0.41
3:2:3015:THR:HA	3:2:3016:PRO:HD3	1.91	0.41
2:1:1063:ALA:O	2:1:1066:LYS:NZ	2.49	0.41
3:2:2083:PHE:CE1	3:2:2145:TYR:CG	3.09	0.41
3:2:2118:SER:OG	3:2:2119:GLN:N	2.54	0.41
3:2:2013:ARG:HD3	3:2:2013:ARG:HH11	1.76	0.41
3:2:2097:GLU:OE2	3:2:2149:HIS:ND1	2.53	0.41
3:2:3107:ILE:HG21	3:2:3107:ILE:HD13	1.82	0.41
1:M:1:G:C8	3:2:2008:PRO:HG2	2.55	0.41
3:2:3050:PHE:CZ	3:2:3150:ILE:HD11	2.56	0.41
2:1:1084:ARG:HG2	2:1:1084:ARG:O	2.21	0.40
2:1:1029:GLN:CG	2:1:1150:LEU:HD12	2.50	0.40
3:2:2013:ARG:O	3:2:2165:LYS:HA	2.21	0.40
3:2:2064:LEU:HD23	3:2:2064:LEU:N	2.37	0.40
2:1:1123:ILE:HD13	2:1:1123:ILE:HG21	1.93	0.40
2:1:1091:VAL:O	2:1:1091:VAL:HG13	2.22	0.40
3:2:2026:ARG:HG2	3:2:2147:MET:CG	2.44	0.40
3:2:2049:MET:CB	3:2:2050:PRO:CD	3.00	0.40
3:2:3020:MET:HE1	3:2:3073:LYS:HZ2	1.81	0.40
3:2:3168:ILE:HG21	3:2:3168:ILE:HD13	1.86	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%)	5	26
3	2	377/374 (101%)	316 (84%)	46 (12%)	15 (4%)	3	17
All	All	560/572 (98%)	474 (85%)	66 (12%)	20 (4%)	4	19

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%)	124 (75%)	41 (25%)	0	3
3	2	329/324 (102%)	236 (72%)	93 (28%)	0	2
All	All	494/498 (99%)	360 (73%)	134 (27%)	0	2

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	1007	VAL
2	1	1009	ASN
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	1090	LEU
2	1	1097	ASN
2	1	1100	SER
2	1	1102	GLU
2	1	1107	CYS
2	1	1112	SER
2	1	1113	GLU
2	1	1120	ILE
2	1	1122	PRO
2	1	1129	ASN

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Mol	Chain	Res	Type
2	1	1143	THR
2	1	1144	SER
2	1	1148	SER
2	1	1150	LEU
2	1	1152	ASP
2	1	1161	ASP
2	1	1163	LEU
2	1	1164	LEU
2	1	1168	GLN
2	1	1177	LEU
3	2	3001	MET
3	2	3005	LEU
3	2	3006	PHE
3	2	3014	GLU
3	2	3019	SER
3	2	3020	MET
3	2	3021	LEU
3	2	3023	LEU
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	3061	ASP
3	2	3067	ARG
3	2	3072	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	3114	LEU
3	2	3123	MET
3	2	3124	THR
3	2	3127	PHE

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Mol	Chain	Res	Type
3	2	3130	ASN
3	2	3137	SER
3	2	3141	LEU
3	2	3147	HIS
3	2	3149	ASP
3	2	3151	ILE
3	2	3154	THR
3	2	3161	MET
3	2	3162	GLN
3	2	3174	SER
3	2	3176	GLU
3	2	3180	ARG
3	2	3181	THR
3	2	2003	LEU
3	2	2004	ASN
3	2	2013	ARG
3	2	2015	MET
3	2	2019	THR
3	2	2024	THR
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	2056	MET
3	2	2058	ARG
3	2	2060	PHE
3	2	2061	VAL
3	2	2063	ASP
3	2	2072	THR
3	2	2088	ASN
3	2	2092	ASP
3	2	2099	PHE
3	2	2102	LYS
3	2	2104	VAL
3	2	2108	GLU
3	2	2109	ILE
3	2	2111	GLU
3	2	2115	LEU
3	2	2116	LYS

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Mol	Chain	Res	Type
3	2	2121	GLU
3	2	2127	SER
3	2	2128	THR
3	2	2131	ARG
3	2	2139	ASP
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	2182	SER
3	2	2187[A]	LEU
3	2	2187[B]	LEU
3	2	2192[A]	GLN
3	2	2192[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	1010	GLN
2	1	1058	ASN
2	1	1097	ASN
2	1	1103	HIS
2	1	1141	ASN
3	2	3035	ASN
3	2	3083	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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.