



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:55 PM UTC

PDB ID : 8KA2 / pdb_00008ka2
Title : Crystal structure of the RID-dependent transforming NADase domain (RD TND)/calmodulin-binding domain of Rho inactivation domain (RID-CBD) from *Vibrio vulnificus*
Authors : Lee, Y.; Choi, S.; Hwang, J.; Kim, M.H.
Deposited on : 2023-08-02
Resolution : 3.38 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

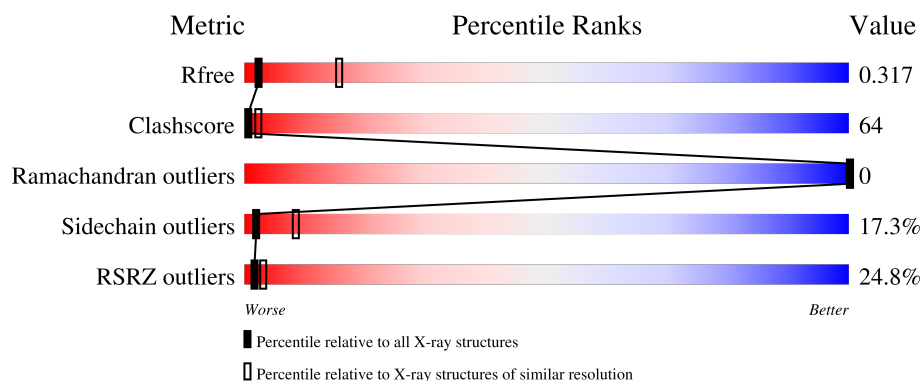
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	419	
1	B	419	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5848 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 RDTND-RID CBD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	Se	0	0	0
			3101	1955	530	611	5			
1	B	342	Total	C	N	O	Se	0	0	0
			2747	1738	467	537	5			

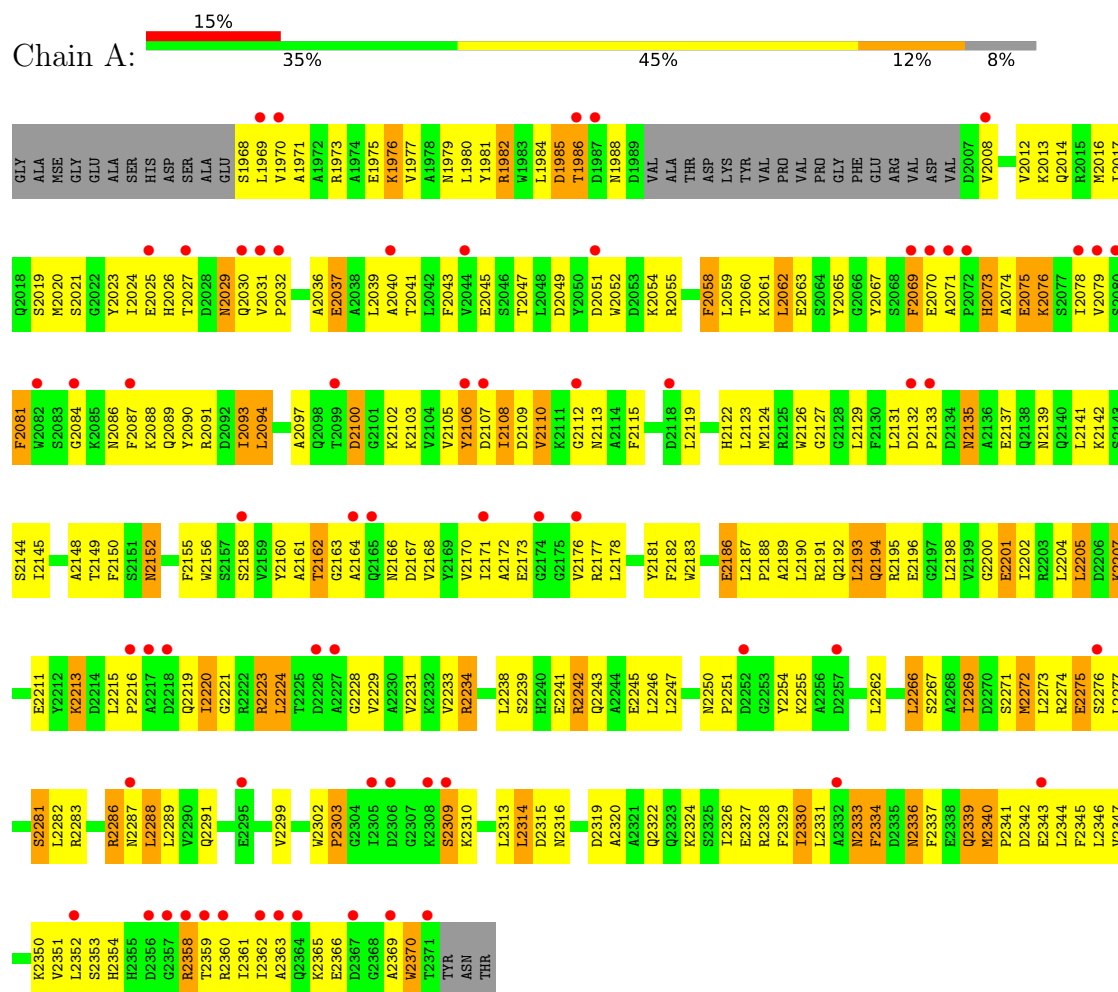
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1956	GLY	-	cloning artifact	UNP A0A2S3R7M0
A	1957	ALA	-	cloning artifact	UNP A0A2S3R7M0
A	1958	MSE	-	cloning artifact	UNP A0A2S3R7M0
B	1956	GLY	-	cloning artifact	UNP A0A2S3R7M0
B	1957	ALA	-	cloning artifact	UNP A0A2S3R7M0
B	1958	MSE	-	cloning artifact	UNP A0A2S3R7M0

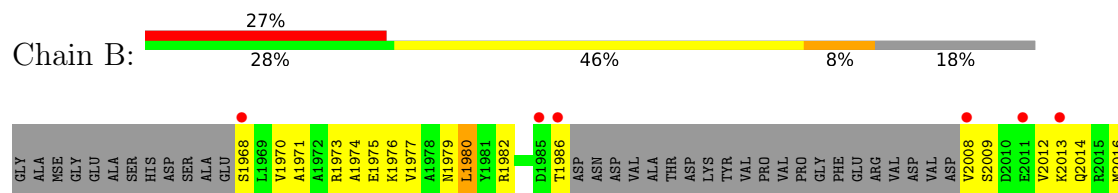
3 Residue-property plots

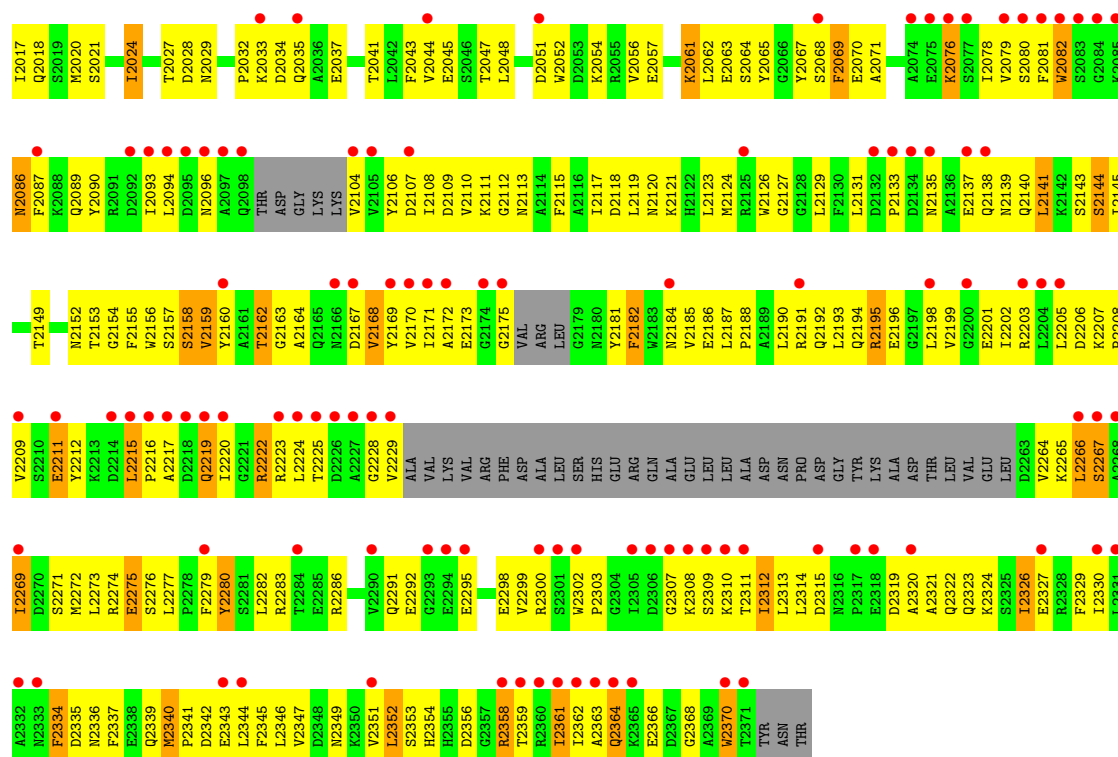
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: RDTND-RID CBD





4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	207.73Å 207.73Å 54.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.42 – 3.38 40.42 – 3.38	Depositor EDS
% Data completeness (in resolution range)	82.8 (40.42-3.38) 82.8 (40.42-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.286 , 0.322 0.284 , 0.317	Depositor DCC
R_{free} test set	830 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	2/3157 (0.1%)	1.47	7/4265 (0.2%)
1	B	1.02	2/2796 (0.1%)	1.44	5/3772 (0.1%)
All	All	1.02	4/5953 (0.1%)	1.46	12/8037 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	2
1	B	2	0
All	All	4	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2333	ASN	CA-C	6.70	1.55	1.52
1	A	2250	ASN	N-CA	5.94	1.50	1.46
1	B	2266	LEU	N-CA	5.08	1.52	1.46
1	B	2361	ILE	N-CA	5.01	1.50	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2356	ASP	N-CA-C	-6.03	107.75	114.62
1	A	2176	VAL	CB-CA-C	5.97	121.09	111.29
1	A	2303	PRO	N-CA-C	-5.93	101.19	110.50
1	A	2272	MSE	CG-SE-CE	5.83	111.75	98.92
1	B	2086	ASN	N-CA-C	-5.73	101.82	110.70
1	A	2176	VAL	N-CA-C	-5.50	97.89	109.34
1	B	2356	ASP	CA-C-N	5.32	126.83	121.35
1	B	2356	ASP	C-N-CA	5.32	126.83	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2251	PRO	N-CA-C	5.30	120.73	113.84
1	A	2019	SER	N-CA-C	-5.12	105.70	111.28
1	A	2100	ASP	N-CA-C	-5.06	106.45	113.18
1	B	2211	GLU	O-C-N	5.03	128.11	122.22

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2020	MSE	CA
1	A	2124	MSE	CA
1	B	2020	MSE	CA
1	B	2124	MSE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2081	PHE	Mainchain
1	A	2370	TRP	Mainchain

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	3101	0	2997	394	0
1	B	2747	0	2649	351	0
All	All	5848	0	5646	732	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 64.

All (732) 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:A:2020:MSE:SE	1:A:2119:LEU:HD12	1.69	1.43
1:B:2329:PHE:CE2	1:B:2362:ILE:HD13	1.61	1.35
1:A:2024:ILE:CG2	1:A:2031:VAL:HG11	1.56	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2334:PHE:CE2	1:A:2341:PRO:HD3	1.63	1.32
1:A:2020:MSE:SE	1:A:2119:LEU:CD1	2.40	1.20
1:B:2274:ARG:HA	1:B:2280:TYR:CD2	1.78	1.19
1:A:2024:ILE:HG23	1:A:2031:VAL:CG1	1.74	1.16
1:B:2279:PHE:HB3	1:B:2282:LEU:CD1	1.78	1.14
1:B:2171:ILE:HG12	1:B:2205:LEU:HD22	1.28	1.13
1:A:2024:ILE:CG2	1:A:2031:VAL:CG1	2.27	1.12
1:B:2208:PRO:HG2	1:B:2211:GLU:OE2	1.47	1.10
1:B:1976:LYS:HE3	1:B:2198:LEU:HD11	1.33	1.10
1:A:2078:ILE:HD11	1:A:2161:ALA:HB2	1.34	1.09
1:A:2078:ILE:CD1	1:A:2161:ALA:HB2	1.82	1.09
1:A:2131:LEU:HD21	1:A:2141:LEU:HD23	1.28	1.09
1:A:2334:PHE:HE2	1:A:2341:PRO:CD	1.65	1.09
1:B:2009:SER:HB3	1:B:2012:VAL:HG22	1.32	1.08
1:B:2215:LEU:HD13	1:B:2219:GLN:CB	1.82	1.08
1:B:2310:LYS:HE3	1:B:2340:MSE:HB3	1.10	1.08
1:B:2279:PHE:HB3	1:B:2282:LEU:HD12	1.15	1.08
1:B:2215:LEU:HD13	1:B:2219:GLN:HB3	1.10	1.08
1:A:2314:LEU:HD21	1:A:2326:ILE:HD12	1.19	1.07
1:B:2341:PRO:HG2	1:B:2344:LEU:HD21	1.29	1.07
1:B:2133:PRO:HA	1:B:2139:ASN:HB2	1.14	1.07
1:B:1976:LYS:CE	1:B:2198:LEU:HD11	1.84	1.06
1:A:2314:LEU:HD21	1:A:2326:ILE:CD1	1.86	1.06
1:B:2351:VAL:HB	1:B:2362:ILE:HG12	1.35	1.05
1:B:2222:ARG:NH2	1:B:2229:VAL:HG11	1.72	1.04
1:A:2076:LYS:CE	1:A:2164:ALA:HB3	1.87	1.04
1:B:2310:LYS:CE	1:B:2340:MSE:HB3	1.87	1.04
1:B:2135:ASN:HB3	1:B:2138:GLN:CG	1.88	1.04
1:A:2361:ILE:HG22	1:A:2361:ILE:O	1.58	1.03
1:B:2359:THR:O	1:B:2361:ILE:HG23	1.59	1.03
1:A:2171:ILE:HG12	1:A:2205:LEU:CD2	1.89	1.02
1:A:2288:LEU:HD22	1:A:2299:VAL:CG2	1.89	1.02
1:A:2239:SER:O	1:A:2243:GLN:HG3	1.58	1.02
1:A:2087:PHE:HE1	1:A:2173:GLU:HG2	1.25	1.02
1:B:2310:LYS:HE3	1:B:2340:MSE:CB	1.92	1.00
1:B:2188:PRO:HB3	1:B:2273:LEU:HD21	1.43	0.99
1:A:2171:ILE:HG12	1:A:2205:LEU:HD22	1.42	0.99
1:B:2329:PHE:HE2	1:B:2362:ILE:HD13	1.20	0.98
1:A:2215:LEU:HD13	1:A:2219:GLN:OE1	1.63	0.98
1:B:2329:PHE:CE2	1:B:2362:ILE:HG21	1.99	0.98
1:A:2076:LYS:HE2	1:A:2164:ALA:HB3	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2016:MSE:HE3	1:A:2126:TRP:CZ3	1.99	0.96
1:A:2215:LEU:HB3	1:A:2216:PRO:HD2	1.48	0.96
1:A:2016:MSE:CE	1:A:2126:TRP:CZ3	2.49	0.96
1:B:2274:ARG:HA	1:B:2280:TYR:HD2	1.17	0.95
1:A:2271:SER:HA	1:A:2274:ARG:NH1	1.82	0.95
1:B:2086:ASN:O	1:B:2090:TYR:HE1	1.48	0.95
1:A:2358:ARG:O	1:A:2358:ARG:NH1	1.99	0.95
1:A:1971:ALA:HB2	1:A:2060:THR:HG21	1.46	0.94
1:A:2171:ILE:CG1	1:A:2205:LEU:HD22	1.97	0.94
1:B:2207:LYS:HB3	1:B:2208:PRO:HD2	1.48	0.94
1:A:2233:VAL:HG21	1:B:2033:LYS:HG3	1.51	0.93
1:A:2106:TYR:HB2	1:A:2109:ASP:OD2	1.68	0.93
1:B:2341:PRO:HG2	1:B:2344:LEU:CD2	1.97	0.93
1:A:1973:ARG:HB3	1:A:2162:THR:HG21	1.49	0.93
1:A:1979:ASN:CG	1:A:2283:ARG:HH12	1.77	0.93
1:B:2351:VAL:CG2	1:B:2362:ILE:HD11	1.98	0.93
1:B:2135:ASN:HB3	1:B:2138:GLN:HG2	1.50	0.92
1:B:2351:VAL:HB	1:B:2362:ILE:CG1	1.99	0.92
1:A:2076:LYS:HE2	1:A:2164:ALA:CB	2.01	0.91
1:A:2310:LYS:HD2	1:A:2337:PHE:CE1	2.06	0.91
1:A:2314:LEU:CD2	1:A:2326:ILE:HD12	2.00	0.91
1:B:2329:PHE:HE2	1:B:2362:ILE:HG21	1.32	0.91
1:A:2178:LEU:HD11	1:A:2231:VAL:HG11	1.53	0.91
1:B:2186:GLU:O	1:B:2190:LEU:HG	1.71	0.91
1:B:2041:THR:O	1:B:2045:GLU:HG3	1.71	0.91
1:A:2075:GLU:OE1	1:A:2166:ASN:HB3	1.69	0.90
1:A:2361:ILE:O	1:A:2361:ILE:CG2	2.18	0.90
1:A:2314:LEU:CD2	1:A:2326:ILE:CD1	2.48	0.90
1:B:2222:ARG:HH21	1:B:2229:VAL:HG11	1.35	0.89
1:B:2135:ASN:HD22	1:B:2138:GLN:HG2	1.36	0.89
1:A:2286:ARG:HB3	1:A:2288:LEU:HD12	1.52	0.89
1:B:2279:PHE:CB	1:B:2282:LEU:HD12	2.01	0.89
1:A:2288:LEU:HD22	1:A:2299:VAL:HG21	1.56	0.87
1:A:2242:ARG:O	1:A:2242:ARG:HD3	1.75	0.86
1:A:2126:TRP:HZ3	1:A:2131:LEU:HD11	1.40	0.86
1:A:2345:PHE:HB3	1:A:2352:LEU:HB2	1.58	0.86
1:A:2076:LYS:HD3	1:A:2166:ASN:O	1.75	0.86
1:A:2087:PHE:CE1	1:A:2173:GLU:HG2	2.10	0.85
1:A:2182:PHE:HA	1:A:2186:GLU:HB2	1.57	0.85
1:B:2274:ARG:HG2	1:B:2280:TYR:CE2	2.11	0.85
1:A:2087:PHE:HE1	1:A:2173:GLU:CG	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2312:ILE:HG22	1:B:2312:ILE:O	1.77	0.85
1:A:2126:TRP:CZ3	1:A:2131:LEU:HD11	2.12	0.84
1:A:2062:LEU:HD21	1:A:2115:PHE:HD2	1.41	0.83
1:A:2288:LEU:HD22	1:A:2299:VAL:HG22	1.56	0.83
1:B:2329:PHE:CE2	1:B:2362:ILE:CD1	2.56	0.83
1:A:2047:THR:HG22	1:A:2148:ALA:HB1	1.60	0.83
1:A:2062:LEU:O	1:A:2067:TYR:HB2	1.77	0.83
1:B:2123:LEU:HD23	1:B:2149:THR:CG2	2.07	0.83
1:A:1970:VAL:HG21	1:A:2069:PHE:CD1	2.14	0.82
1:A:2329:PHE:CZ	1:A:2362:ILE:HD11	2.14	0.82
1:B:2133:PRO:CA	1:B:2139:ASN:HB2	2.06	0.82
1:A:2037:GLU:O	1:A:2041:THR:HG23	1.79	0.82
1:A:2361:ILE:O	1:A:2362:ILE:HD13	1.79	0.82
1:B:2052:TRP:O	1:B:2056:VAL:HG23	1.79	0.82
1:A:2076:LYS:HE3	1:A:2164:ALA:HB3	1.60	0.81
1:B:2222:ARG:NH2	1:B:2229:VAL:CG1	2.43	0.81
1:A:2194:GLN:NE2	1:A:2202:ILE:HD12	1.95	0.81
1:B:2224:LEU:HB3	1:B:2266:LEU:HD22	1.62	0.81
1:B:1976:LYS:HE2	1:B:2198:LEU:HD21	1.62	0.81
1:B:2274:ARG:HA	1:B:2280:TYR:CE2	2.16	0.81
1:B:2082:TRP:HB3	1:B:2173:GLU:HB2	1.63	0.80
1:A:2024:ILE:CG2	1:A:2031:VAL:CB	2.60	0.80
1:B:2076:LYS:HE2	1:B:2164:ALA:O	1.82	0.80
1:A:2362:ILE:HD12	1:A:2370:TRP:CZ3	2.16	0.80
1:B:2016:MSE:CE	1:B:2126:TRP:CZ3	2.65	0.80
1:B:2320:ALA:O	1:B:2324:LYS:HG3	1.81	0.80
1:B:2208:PRO:CG	1:B:2211:GLU:OE2	2.30	0.79
1:A:2233:VAL:CG2	1:B:2033:LYS:HG3	2.12	0.79
1:A:2024:ILE:HG23	1:A:2031:VAL:HG11	0.82	0.79
1:A:1982:ARG:O	1:A:1986:THR:HB	1.82	0.79
1:A:2084:GLY:HA3	1:A:2173:GLU:HG3	1.64	0.79
1:A:2020:MSE:HE1	1:A:2119:LEU:O	1.83	0.79
1:B:2086:ASN:O	1:B:2090:TYR:CE1	2.34	0.78
1:A:2055:ARG:O	1:A:2059:LEU:HG	1.83	0.78
1:B:2079:VAL:CG2	1:B:2087:PHE:HZ	1.97	0.78
1:A:2076:LYS:NZ	1:A:2076:LYS:HB3	1.99	0.78
1:A:2171:ILE:CG1	1:A:2205:LEU:CD2	2.57	0.78
1:A:2241:GLU:O	1:A:2245:GLU:HG3	1.84	0.78
1:A:2288:LEU:CD2	1:A:2299:VAL:HG22	2.14	0.77
1:A:2334:PHE:HD1	1:A:2334:PHE:H	1.32	0.77
1:B:2215:LEU:CD1	1:B:2219:GLN:CB	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2363:ALA:O	1:B:2368:GLY:HA3	1.84	0.77
1:B:2094:LEU:CB	1:B:2104:VAL:HG11	2.15	0.77
1:B:2337:PHE:HA	1:B:2340:MSE:HE3	1.67	0.77
1:B:2094:LEU:HB3	1:B:2104:VAL:HG11	1.66	0.76
1:A:2016:MSE:HE3	1:A:2126:TRP:CH2	2.19	0.76
1:A:2171:ILE:HG12	1:A:2205:LEU:HB2	1.65	0.76
1:A:2233:VAL:HG12	1:A:2234:ARG:N	2.00	0.76
1:A:2071:ALA:HB1	1:A:2105:VAL:HG11	1.68	0.76
1:A:2362:ILE:HG22	1:A:2363:ALA:H	1.51	0.76
1:A:2181:TYR:CD1	1:A:2186:GLU:OE2	2.38	0.76
1:A:2233:VAL:HG21	1:B:2033:LYS:CG	2.15	0.76
1:A:2326:ILE:HD11	1:A:2346:LEU:HB3	1.67	0.76
1:B:2171:ILE:CG1	1:B:2205:LEU:HD22	2.14	0.75
1:A:2271:SER:O	1:A:2275:GLU:CG	2.34	0.75
1:B:2016:MSE:HE2	1:B:2126:TRP:CZ3	2.22	0.75
1:B:2051:ASP:CB	1:B:2054:LYS:HB2	2.16	0.75
1:A:2310:LYS:CD	1:A:2337:PHE:CE1	2.70	0.74
1:A:2020:MSE:SE	1:A:2119:LEU:HD11	2.36	0.74
1:A:2233:VAL:HG22	1:B:2033:LYS:HZ2	1.51	0.74
1:A:2286:ARG:NH1	1:A:2331:LEU:HD22	2.02	0.74
1:A:1970:VAL:HG21	1:A:2069:PHE:HD1	1.50	0.74
1:A:2037:GLU:O	1:A:2037:GLU:HG3	1.86	0.74
1:B:2351:VAL:HG21	1:B:2362:ILE:HD11	1.69	0.74
1:A:1981:TYR:O	1:A:1985:ASP:HB3	1.88	0.74
1:A:2181:TYR:CE1	1:A:2186:GLU:OE2	2.39	0.74
1:A:2314:LEU:CD2	1:A:2326:ILE:HD11	2.17	0.74
1:B:2123:LEU:HD23	1:B:2149:THR:HG23	1.69	0.74
1:A:2233:VAL:HG11	1:B:2033:LYS:HG3	1.70	0.73
1:A:2302:TRP:HB3	1:A:2303:PRO:HD3	1.68	0.73
1:B:2140:GLN:O	1:B:2140:GLN:NE2	2.18	0.72
1:B:2224:LEU:HD22	1:B:2228:GLY:HA2	1.70	0.72
1:B:2271:SER:O	1:B:2275:GLU:HG2	1.88	0.72
1:A:2320:ALA:HB1	1:B:2129:LEU:HD13	1.70	0.72
1:B:2013:LYS:O	1:B:2017:ILE:HG13	1.89	0.72
1:B:2209:VAL:HA	1:B:2212:TYR:HB2	1.70	0.72
1:A:1979:ASN:HB3	1:A:2283:ARG:HH22	1.55	0.71
1:B:2187:LEU:HB3	1:B:2188:PRO:HD3	1.72	0.71
1:A:2110:VAL:CG1	1:A:2113:ASN:HB2	2.20	0.71
1:A:2329:PHE:CE1	1:A:2362:ILE:HD11	2.25	0.71
1:B:2135:ASN:HB3	1:B:2138:GLN:HG3	1.72	0.71
1:A:2282:LEU:HD11	1:A:2330:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2223:ARG:HH11	1:A:2223:ARG:HB2	1.56	0.70
1:A:2051:ASP:OD2	1:A:2054:LYS:HD2	1.91	0.70
1:A:2271:SER:CA	1:A:2274:ARG:NH1	2.54	0.70
1:A:2271:SER:O	1:A:2275:GLU:HG3	1.92	0.70
1:A:1973:ARG:HB3	1:A:2162:THR:CG2	2.20	0.70
1:A:2262:LEU:HD12	1:A:2262:LEU:O	1.92	0.70
1:A:1971:ALA:O	1:A:1975:GLU:HG3	1.92	0.70
1:A:2334:PHE:HE2	1:A:2341:PRO:HD3	0.71	0.70
1:B:2336:ASN:HB2	1:B:2339:GLN:HG2	1.74	0.70
1:A:2171:ILE:CD1	1:A:2205:LEU:HD23	2.21	0.70
1:B:2120:ASN:OD1	1:B:2149:THR:HG22	1.91	0.70
1:A:2024:ILE:HG22	1:A:2031:VAL:CB	2.20	0.69
1:A:2110:VAL:HG12	1:A:2113:ASN:HB2	1.75	0.69
1:A:2316:ASN:ND2	1:A:2319:ASP:HB2	2.06	0.69
1:A:2362:ILE:HG22	1:A:2363:ALA:N	2.06	0.69
1:B:2051:ASP:HB2	1:B:2054:LYS:HB2	1.73	0.69
1:B:2207:LYS:HB3	1:B:2208:PRO:CD	2.21	0.69
1:A:2286:ARG:HH11	1:A:2331:LEU:CD2	2.05	0.69
1:A:2363:ALA:HB1	1:A:2365:LYS:HG3	1.75	0.69
1:B:1971:ALA:O	1:B:1975:GLU:HG3	1.92	0.69
1:B:2135:ASN:ND2	1:B:2138:GLN:HG2	2.07	0.69
1:B:2329:PHE:HE2	1:B:2362:ILE:CD1	2.00	0.69
1:A:2024:ILE:O	1:A:2031:VAL:HG21	1.92	0.69
1:A:2286:ARG:NH1	1:A:2331:LEU:CD2	2.56	0.69
1:B:2037:GLU:O	1:B:2041:THR:HG23	1.91	0.69
1:B:2079:VAL:HG22	1:B:2087:PHE:HZ	1.58	0.69
1:A:2178:LEU:HD11	1:A:2231:VAL:CG1	2.23	0.69
1:A:2108:ILE:HG22	1:A:2108:ILE:O	1.93	0.68
1:B:2310:LYS:HD3	1:B:2341:PRO:O	1.93	0.68
1:A:2043:PHE:CG	1:A:2119:LEU:HD21	2.28	0.68
1:A:2233:VAL:HG22	1:B:2033:LYS:NZ	2.08	0.68
1:A:1968:SER:HA	1:A:2063:GLU:OE2	1.93	0.68
1:A:2069:PHE:HB3	1:A:2113:ASN:OD1	1.93	0.68
1:A:2093:ILE:HD13	1:A:2213:LYS:HD2	1.75	0.68
1:A:2106:TYR:HB2	1:A:2109:ASP:CG	2.19	0.68
1:B:2329:PHE:CD2	1:B:2362:ILE:HD13	2.25	0.68
1:B:2215:LEU:CD1	1:B:2219:GLN:HB3	2.05	0.67
1:A:1980:LEU:CD2	1:A:2277:LEU:HD11	2.23	0.67
1:A:2233:VAL:HG12	1:A:2234:ARG:H	1.58	0.67
1:A:2345:PHE:HE1	1:A:2347:VAL:HG22	1.59	0.67
1:B:1976:LYS:HE2	1:B:2198:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2359:THR:HG22	1:B:2361:ILE:CG2	2.24	0.67
1:B:2352:LEU:N	1:B:2352:LEU:HD12	2.10	0.67
1:A:1980:LEU:HD12	1:A:2193:LEU:CD1	2.24	0.67
1:B:2016:MSE:HE3	1:B:2126:TRP:CH2	2.29	0.67
1:B:2300:ARG:HE	1:B:2309:SER:HB3	1.58	0.67
1:B:2008:VAL:HG23	1:B:2008:VAL:O	1.94	0.67
1:B:2313:LEU:HD12	1:B:2313:LEU:H	1.58	0.67
1:B:2222:ARG:HH21	1:B:2229:VAL:CG1	2.04	0.66
1:A:2192:GLN:O	1:A:2192:GLN:NE2	2.19	0.66
1:A:2345:PHE:CE1	1:A:2347:VAL:CG2	2.78	0.66
1:A:2362:ILE:CD1	1:A:2370:TRP:CE3	2.78	0.66
1:B:2195:ARG:HH22	1:B:2274:ARG:NH2	1.94	0.66
1:B:2020:MSE:SE	1:B:2119:LEU:CD1	2.94	0.66
1:B:2080:SER:HB2	1:B:2171:ILE:O	1.96	0.66
1:A:2013:LYS:HE3	1:A:2017:ILE:HD11	1.78	0.66
1:A:2023:TYR:HB2	1:A:2122:HIS:CD2	2.31	0.66
1:B:2319:ASP:OD2	1:B:2322:GLN:HG2	1.96	0.66
1:A:2062:LEU:HD21	1:A:2115:PHE:CD2	2.26	0.66
1:B:2167:ASP:CG	1:B:2168:VAL:H	2.04	0.66
1:A:2233:VAL:CG1	1:B:2033:LYS:HG3	2.26	0.66
1:A:2326:ILE:HD11	1:A:2346:LEU:CB	2.25	0.66
1:A:2345:PHE:CD1	1:A:2347:VAL:HG23	2.31	0.66
1:B:2071:ALA:HB2	1:B:2160:TYR:OH	1.95	0.66
1:A:2238:LEU:HG	1:A:2239:SER:N	2.10	0.66
1:B:2079:VAL:N	1:B:2107:ASP:OD2	2.25	0.66
1:B:2188:PRO:HB3	1:B:2273:LEU:CD2	2.23	0.65
1:B:2024:ILE:HG23	1:B:2029:ASN:ND2	2.10	0.65
1:A:2093:ILE:HD11	1:A:2213:LYS:CD	2.27	0.65
1:A:2078:ILE:HD12	1:A:2168:VAL:HG11	1.77	0.65
1:A:2266:LEU:O	1:A:2266:LEU:HD22	1.97	0.65
1:B:2009:SER:HB3	1:B:2012:VAL:CG2	2.20	0.65
1:B:2310:LYS:CD	1:B:2340:MSE:HB3	2.26	0.65
1:A:2047:THR:CG2	1:A:2148:ALA:HB1	2.28	0.64
1:A:2078:ILE:HD12	1:A:2168:VAL:CG1	2.27	0.64
1:A:2093:ILE:CD1	1:A:2213:LYS:HD2	2.27	0.64
1:A:2131:LEU:CD2	1:A:2141:LEU:HD23	2.18	0.64
1:A:2024:ILE:HG22	1:A:2031:VAL:HB	1.78	0.64
1:A:2078:ILE:HD11	1:A:2161:ALA:CB	2.21	0.64
1:A:2171:ILE:CD1	1:A:2205:LEU:CD2	2.74	0.64
1:A:2071:ALA:HB2	1:A:2160:TYR:HE1	1.62	0.64
1:A:2078:ILE:O	1:A:2170:VAL:HA	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2215:LEU:HB2	1:B:2216:PRO:CD	2.27	0.64
1:A:2076:LYS:HB3	1:A:2076:LYS:HZ2	1.62	0.64
1:B:2044:VAL:HG12	1:B:2048:LEU:HD12	1.79	0.64
1:B:2016:MSE:HE3	1:B:2126:TRP:CZ3	2.32	0.64
1:B:2171:ILE:HG12	1:B:2205:LEU:CD2	2.18	0.64
1:A:2024:ILE:HG21	1:A:2031:VAL:CG1	2.28	0.64
1:A:2193:LEU:HG	1:A:2198:LEU:HD12	1.77	0.64
1:A:2271:SER:HA	1:A:2274:ARG:CZ	2.27	0.64
1:A:2345:PHE:HD1	1:A:2347:VAL:HG23	1.62	0.64
1:B:1980:LEU:HD21	1:B:2192:GLN:HG2	1.80	0.64
1:B:2113:ASN:O	1:B:2117:ILE:HD12	1.96	0.64
1:A:2093:ILE:CD1	1:A:2213:LYS:CD	2.76	0.63
1:A:2187:LEU:HB3	1:A:2188:PRO:HD3	1.80	0.63
1:A:2238:LEU:HG	1:A:2239:SER:H	1.62	0.63
1:B:2081:PHE:HZ	1:B:2154:GLY:HA2	1.63	0.63
1:A:2362:ILE:CG2	1:A:2363:ALA:H	2.11	0.63
1:A:1980:LEU:HD23	1:A:2277:LEU:HD11	1.80	0.63
1:A:2032:PRO:O	1:A:2036:ALA:HB2	1.99	0.63
1:A:2017:ILE:CG2	1:A:2041:THR:HG22	2.29	0.63
1:A:1977:VAL:HG22	1:A:2193:LEU:HD21	1.81	0.63
1:A:2366:GLU:OE1	1:A:2366:GLU:N	2.30	0.62
1:B:2135:ASN:CB	1:B:2138:GLN:HG2	2.26	0.62
1:A:2302:TRP:CD1	1:A:2302:TRP:C	2.77	0.62
1:A:2329:PHE:CE1	1:A:2362:ILE:CD1	2.81	0.62
1:A:2362:ILE:HD12	1:A:2370:TRP:CE3	2.33	0.62
1:B:2051:ASP:HB3	1:B:2054:LYS:HB2	1.80	0.62
1:B:2167:ASP:OD1	1:B:2201:GLU:HB2	1.99	0.62
1:A:2334:PHE:CD2	1:A:2340:MSE:HA	2.34	0.62
1:B:2051:ASP:O	1:B:2054:LYS:N	2.31	0.62
1:B:2020:MSE:HE1	1:B:2119:LEU:O	1.99	0.62
1:B:2186:GLU:HG3	1:B:2190:LEU:HD11	1.80	0.62
1:A:2025:GLU:HG3	1:A:2036:ALA:HB3	1.82	0.62
1:A:2266:LEU:O	1:A:2266:LEU:HD13	1.99	0.62
1:A:2342:ASP:HB2	1:A:2354:HIS:HB3	1.80	0.62
1:B:2079:VAL:CG2	1:B:2087:PHE:CZ	2.82	0.62
1:B:2351:VAL:HB	1:B:2362:ILE:CD1	2.29	0.62
1:A:2346:LEU:C	1:A:2346:LEU:HD13	2.25	0.62
1:A:1980:LEU:CD1	1:A:2193:LEU:HD12	2.30	0.61
1:A:2310:LYS:HB2	1:A:2337:PHE:HE1	1.64	0.61
1:B:2017:ILE:HG21	1:B:2041:THR:HG22	1.82	0.61
1:B:2135:ASN:CB	1:B:2138:GLN:CG	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2020:MSE:SE	1:B:2119:LEU:HD12	2.50	0.61
1:A:2334:PHE:HD1	1:A:2334:PHE:N	1.97	0.61
1:A:2334:PHE:N	1:A:2334:PHE:CD1	2.68	0.61
1:B:2082:TRP:CZ3	1:B:2175:GLY:HA3	2.36	0.61
1:B:2133:PRO:HA	1:B:2139:ASN:CB	2.09	0.61
1:B:2184:ASN:OD1	1:B:2185:VAL:HG23	2.00	0.61
1:A:2309:SER:O	1:A:2309:SER:OG	2.12	0.61
1:A:2171:ILE:HD11	1:A:2205:LEU:CD2	2.31	0.61
1:A:2193:LEU:HG	1:A:2198:LEU:CD1	2.30	0.61
1:A:2194:GLN:HE21	1:A:2202:ILE:HD12	1.65	0.61
1:B:2167:ASP:OD1	1:B:2201:GLU:CB	2.49	0.60
1:A:2145:ILE:O	1:A:2149:THR:HG23	2.01	0.60
1:B:2215:LEU:HD11	1:B:2220:ILE:HG23	1.82	0.60
1:B:2216:PRO:HD2	1:B:2219:GLN:HB2	1.82	0.60
1:A:2067:TYR:CD1	1:A:2112:GLY:HA2	2.37	0.60
1:B:2020:MSE:HE3	1:B:2043:PHE:CD2	2.35	0.60
1:A:2024:ILE:CG2	1:A:2031:VAL:HB	2.30	0.60
1:A:2076:LYS:CD	1:A:2166:ASN:O	2.47	0.60
1:A:2086:ASN:O	1:A:2090:TYR:CE2	2.54	0.60
1:A:2233:VAL:CG1	1:A:2234:ARG:N	2.64	0.60
1:A:2205:LEU:HD12	1:A:2221:GLY:HA2	1.83	0.60
1:A:2037:GLU:O	1:A:2041:THR:CG2	2.48	0.60
1:B:1980:LEU:HD13	1:B:2193:LEU:CD1	2.31	0.60
1:B:2311:THR:OG1	1:B:2343:GLU:HB2	2.00	0.60
1:A:2059:LEU:HD11	1:A:2155:PHE:CE2	2.36	0.60
1:A:2041:THR:O	1:A:2045:GLU:HB2	2.01	0.60
1:A:2266:LEU:HD13	1:A:2266:LEU:C	2.27	0.60
1:A:2287:ASN:ND2	1:A:2302:TRP:HE3	1.99	0.60
1:A:2324:LYS:O	1:A:2328:ARG:HG3	2.01	0.60
1:A:2041:THR:O	1:A:2045:GLU:HG3	2.01	0.59
1:A:2016:MSE:HE2	1:A:2126:TRP:CZ3	2.36	0.59
1:B:2194:GLN:NE2	1:B:2202:ILE:HD13	2.17	0.59
1:B:2313:LEU:HD12	1:B:2313:LEU:N	2.16	0.59
1:A:2242:ARG:HG3	1:B:2034:ASP:OD2	2.02	0.59
1:A:2334:PHE:CE2	1:A:2341:PRO:CD	2.56	0.59
1:B:2269:ILE:O	1:B:2273:LEU:HG	2.02	0.59
1:B:2194:GLN:NE2	1:B:2202:ILE:CD1	2.65	0.59
1:B:2079:VAL:HG21	1:B:2108:ILE:HD11	1.85	0.58
1:A:2123:LEU:O	1:A:2127:GLY:N	2.36	0.58
1:A:2016:MSE:HE1	1:A:2145:ILE:HD11	1.85	0.58
1:A:2287:ASN:ND2	1:A:2302:TRP:CE3	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2051:ASP:O	1:A:2055:ARG:HG3	2.03	0.58
1:A:2233:VAL:CG1	1:A:2234:ARG:H	2.15	0.58
1:A:1971:ALA:CB	1:A:2060:THR:HG21	2.26	0.58
1:A:2337:PHE:O	1:A:2340:MSE:HB2	2.04	0.58
1:A:2363:ALA:HB3	1:A:2369:ALA:H	1.67	0.58
1:B:2196:GLU:OE2	1:B:2283:ARG:HD3	2.04	0.58
1:A:2191:ARG:O	1:A:2191:ARG:HG3	2.03	0.58
1:B:2358:ARG:HG2	1:B:2358:ARG:HH11	1.67	0.58
1:A:1976:LYS:O	1:A:2283:ARG:NH2	2.36	0.58
1:B:2272:MSE:O	1:B:2276:SER:N	2.37	0.57
1:B:2170:VAL:HG11	1:B:2182:PHE:HE2	1.68	0.57
1:B:2319:ASP:HB3	1:B:2322:GLN:HG3	1.85	0.57
1:B:2336:ASN:O	1:B:2340:MSE:HE2	2.04	0.57
1:A:2016:MSE:HE2	1:A:2126:TRP:CE3	2.40	0.57
1:B:2310:LYS:CE	1:B:2337:PHE:O	2.53	0.57
1:B:2311:THR:OG1	1:B:2343:GLU:CB	2.53	0.57
1:B:2329:PHE:CZ	1:B:2362:ILE:HG21	2.38	0.57
1:A:1980:LEU:CD1	1:A:2193:LEU:CD1	2.83	0.57
1:B:2032:PRO:HD3	1:B:2065:TYR:CD1	2.39	0.57
1:B:2188:PRO:CB	1:B:2273:LEU:HD21	2.27	0.57
1:B:2211:GLU:OE2	1:B:2211:GLU:N	2.30	0.57
1:A:2233:VAL:CG2	1:B:2033:LYS:HZ2	2.18	0.57
1:B:1970:VAL:HG21	1:B:2069:PHE:CD1	2.40	0.57
1:A:2073:HIS:N	1:A:2073:HIS:CD2	2.72	0.56
1:A:2171:ILE:HG12	1:A:2205:LEU:HD23	1.84	0.56
1:A:2314:LEU:CG	1:A:2326:ILE:CD1	2.83	0.56
1:A:2336:ASN:C	1:A:2336:ASN:OD1	2.48	0.56
1:A:2345:PHE:HE1	1:A:2347:VAL:CG2	2.17	0.56
1:A:2345:PHE:CE1	1:A:2347:VAL:HG22	2.40	0.56
1:B:2215:LEU:CD1	1:B:2220:ILE:HG23	2.35	0.56
1:B:2310:LYS:HD2	1:B:2340:MSE:HB3	1.87	0.56
1:B:2314:LEU:HD22	1:B:2346:LEU:HB3	1.87	0.56
1:B:2315:ASP:OD1	1:B:2322:GLN:NE2	2.38	0.56
1:B:2334:PHE:HB3	1:B:2339:GLN:CB	2.36	0.56
1:A:2086:ASN:O	1:A:2090:TYR:CD2	2.58	0.56
1:A:2171:ILE:HG12	1:A:2205:LEU:CB	2.35	0.56
1:B:2203:ARG:NH2	1:B:2223:ARG:HD3	2.21	0.56
1:B:2274:ARG:HG2	1:B:2280:TYR:HE2	1.67	0.56
1:A:2127:GLY:O	1:A:2131:LEU:HD12	2.05	0.56
1:B:2123:LEU:HG	1:B:2145:ILE:HG23	1.87	0.56
1:A:1969:LEU:O	1:A:1973:ARG:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2330:ILE:HG21	1:A:2344:LEU:HD13	1.88	0.56
1:B:2089:GLN:HE22	1:B:2209:VAL:HG21	1.70	0.56
1:B:2329:PHE:CD1	1:B:2329:PHE:C	2.84	0.56
1:A:2178:LEU:CD1	1:A:2231:VAL:HB	2.36	0.56
1:B:2173:GLU:O	1:B:2206:ASP:O	2.23	0.56
1:A:2013:LYS:HG3	1:A:2017:ILE:HD11	1.86	0.55
1:B:2215:LEU:HB2	1:B:2216:PRO:HD2	1.87	0.55
1:A:2020:MSE:C	1:A:2040:ALA:CB	2.79	0.55
1:B:2349:ASN:HB3	1:B:2364:GLN:CB	2.37	0.55
1:A:2167:ASP:HB3	1:A:2201:GLU:HB2	1.89	0.55
1:B:2351:VAL:HG23	1:B:2362:ILE:HD11	1.84	0.55
1:A:2074:ALA:HB3	1:A:2105:VAL:HG23	1.89	0.55
1:A:2223:ARG:HH11	1:A:2223:ARG:CB	2.19	0.55
1:B:2269:ILE:O	1:B:2272:MSE:HG3	2.07	0.55
1:B:2286:ARG:HG2	1:B:2335:ASP:O	2.07	0.55
1:A:2192:GLN:O	1:A:2196:GLU:HG3	2.07	0.55
1:A:2013:LYS:CG	1:A:2017:ILE:HD11	2.37	0.55
1:B:2020:MSE:O	1:B:2024:ILE:HG13	2.06	0.55
1:B:2326:ILE:HG12	1:B:2346:LEU:HD22	1.89	0.55
1:B:2215:LEU:CD1	1:B:2219:GLN:C	2.80	0.55
1:B:2279:PHE:HD2	1:B:2282:LEU:HD11	1.70	0.55
1:A:2043:PHE:CG	1:A:2119:LEU:CD2	2.90	0.55
1:B:2024:ILE:HG23	1:B:2029:ASN:HD21	1.71	0.55
1:A:2079:VAL:HB	1:A:2087:PHE:CE2	2.42	0.54
1:B:1973:ARG:NH2	1:B:2163:GLY:HA3	2.22	0.54
1:B:1980:LEU:CD1	1:B:2193:LEU:CD1	2.84	0.54
1:B:2187:LEU:HA	1:B:2190:LEU:HD12	1.88	0.54
1:B:2342:ASP:HB2	1:B:2354:HIS:O	2.07	0.54
1:B:2279:PHE:HB3	1:B:2282:LEU:HD13	1.84	0.54
1:B:2336:ASN:O	1:B:2340:MSE:CE	2.55	0.54
1:A:2167:ASP:HA	1:A:2200:GLY:O	2.07	0.54
1:A:2281:SER:CB	1:A:2327:GLU:OE2	2.55	0.54
1:B:2274:ARG:CG	1:B:2280:TYR:CE2	2.87	0.54
1:A:2059:LEU:HD11	1:A:2155:PHE:CZ	2.43	0.54
1:B:2220:ILE:HG13	1:B:2220:ILE:O	2.06	0.54
1:A:2345:PHE:CD1	1:A:2347:VAL:CG2	2.91	0.54
1:B:1986:THR:CG2	1:B:2052:TRP:HE1	2.19	0.54
1:A:2233:VAL:HG13	1:B:2033:LYS:HZ2	1.72	0.54
1:B:2319:ASP:OD2	1:B:2321:ALA:HB3	2.07	0.54
1:A:2192:GLN:HE21	1:A:2192:GLN:C	2.12	0.54
1:A:2362:ILE:CG2	1:A:2363:ALA:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1968:SER:N	1:B:2063:GLU:OE2	2.40	0.54
1:B:2274:ARG:CG	1:B:2280:TYR:HE2	2.21	0.54
1:B:2307:GLY:O	1:B:2308:LYS:CD	2.56	0.54
1:A:2024:ILE:HG22	1:A:2031:VAL:HG21	1.90	0.54
1:A:2093:ILE:HD13	1:A:2213:LYS:HA	1.90	0.54
1:B:2207:LYS:HB2	1:B:2212:TYR:CZ	2.43	0.54
1:B:2279:PHE:CB	1:B:2282:LEU:CD1	2.70	0.54
1:B:2353:SER:O	1:B:2359:THR:N	2.38	0.54
1:A:2207:LYS:HD3	1:A:2211:GLU:HG3	1.91	0.53
1:B:2079:VAL:HG22	1:B:2087:PHE:CZ	2.41	0.53
1:B:2168:VAL:HG12	1:B:2202:ILE:HA	1.89	0.53
1:B:2340:MSE:HG3	1:B:2341:PRO:CD	2.39	0.53
1:A:1971:ALA:HB2	1:A:2060:THR:CG2	2.30	0.53
1:B:2020:MSE:SE	1:B:2119:LEU:HG	2.59	0.53
1:A:2023:TYR:HB2	1:A:2122:HIS:HD2	1.70	0.53
1:B:2016:MSE:CE	1:B:2145:ILE:HD11	2.38	0.53
1:A:2045:GLU:O	1:A:2049:ASP:HB2	2.08	0.53
1:A:1973:ARG:HH21	1:A:2163:GLY:HA3	1.72	0.53
1:A:2020:MSE:HE1	1:A:2123:LEU:H	1.73	0.53
1:A:2024:ILE:HG22	1:A:2031:VAL:CG2	2.38	0.53
1:B:2167:ASP:CG	1:B:2168:VAL:N	2.66	0.53
1:B:2182:PHE:CD1	1:B:2182:PHE:C	2.87	0.53
1:A:1970:VAL:HG21	1:A:2069:PHE:CE1	2.43	0.53
1:A:2021:SER:O	1:A:2025:GLU:HB2	2.09	0.53
1:A:2329:PHE:CZ	1:A:2362:ILE:CD1	2.90	0.52
1:B:2217:ALA:O	1:B:2220:ILE:HG12	2.08	0.52
1:B:2272:MSE:O	1:B:2276:SER:CB	2.58	0.52
1:A:2058:PHE:C	1:A:2058:PHE:CD1	2.87	0.52
1:B:1980:LEU:CD1	1:B:2193:LEU:HD12	2.40	0.52
1:B:2205:LEU:N	1:B:2205:LEU:CD1	2.73	0.52
1:A:2127:GLY:O	1:A:2131:LEU:CD1	2.57	0.52
1:A:2329:PHE:HZ	1:A:2362:ILE:HD11	1.73	0.52
1:B:2193:LEU:O	1:B:2198:LEU:HB2	2.08	0.52
1:A:2351:VAL:HB	1:A:2362:ILE:CG1	2.40	0.52
1:B:2280:TYR:C	1:B:2280:TYR:HD1	2.18	0.52
1:B:1977:VAL:HG22	1:B:2193:LEU:HD21	1.90	0.52
1:B:2135:ASN:CB	1:B:2138:GLN:HG3	2.37	0.52
1:B:2349:ASN:HB3	1:B:2364:GLN:HB3	1.91	0.52
1:A:2061:LYS:O	1:A:2065:TYR:CD2	2.62	0.52
1:A:2076:LYS:HB3	1:A:2160:TYR:OH	2.09	0.52
1:A:2262:LEU:HD12	1:A:2262:LEU:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2334:PHE:HB3	1:B:2339:GLN:HB3	1.92	0.52
1:B:2361:ILE:C	1:B:2362:ILE:HG23	2.34	0.52
1:A:2310:LYS:HD3	1:A:2340:MSE:HB3	1.92	0.52
1:A:2334:PHE:CE2	1:A:2340:MSE:HA	2.44	0.52
1:B:2137:GLU:HA	1:B:2140:GLN:HB3	1.90	0.52
1:A:2078:ILE:HD13	1:A:2161:ALA:HB2	1.86	0.52
1:A:2020:MSE:C	1:A:2040:ALA:HB1	2.35	0.51
1:A:2361:ILE:O	1:A:2370:TRP:HA	2.10	0.51
1:B:1979:ASN:O	1:B:1982:ARG:HB2	2.10	0.51
1:B:2307:GLY:O	1:B:2308:LYS:HG2	2.09	0.51
1:A:2302:TRP:CB	1:A:2303:PRO:HD3	2.38	0.51
1:B:2172:ALA:O	1:B:2205:LEU:O	2.28	0.51
1:B:2205:LEU:N	1:B:2205:LEU:HD12	2.26	0.51
1:B:2326:ILE:HD11	1:B:2346:LEU:HB2	1.92	0.51
1:B:2324:LYS:O	1:B:2327:GLU:HB3	2.10	0.51
1:A:1980:LEU:HD12	1:A:2193:LEU:HD12	1.91	0.51
1:A:1982:ARG:CZ	1:A:2291:GLN:NE2	2.74	0.51
1:B:2140:GLN:HE21	1:B:2140:GLN:C	2.14	0.51
1:B:2162:THR:OG1	1:B:2193:LEU:HD23	2.10	0.51
1:B:2274:ARG:CA	1:B:2280:TYR:HD2	2.05	0.51
1:A:1973:ARG:HH21	1:A:2163:GLY:CA	2.23	0.51
1:B:2043:PHE:O	1:B:2047:THR:HG23	2.11	0.51
1:B:2168:VAL:HG11	1:B:2202:ILE:HG13	1.92	0.51
1:B:2229:VAL:HG12	1:B:2229:VAL:O	2.11	0.51
1:A:2314:LEU:HG	1:A:2326:ILE:CD1	2.40	0.51
1:B:2127:GLY:O	1:B:2131:LEU:HD13	2.11	0.51
1:B:2168:VAL:CG1	1:B:2202:ILE:HG13	2.41	0.51
1:B:2191:ARG:O	1:B:2195:ARG:HB2	2.10	0.51
1:A:2247:LEU:HD21	1:A:2254:TYR:HB2	1.92	0.50
1:B:2126:TRP:CZ3	1:B:2131:LEU:HD11	2.45	0.50
1:B:2352:LEU:N	1:B:2352:LEU:CD1	2.74	0.50
1:A:2016:MSE:CE	1:A:2145:ILE:HD11	2.41	0.50
1:A:2047:THR:HG22	1:A:2148:ALA:CB	2.36	0.50
1:A:2171:ILE:HD11	1:A:2205:LEU:HD23	1.92	0.50
1:A:2076:LYS:HB3	1:A:2076:LYS:HZ3	1.75	0.50
1:A:2070:GLU:HG3	1:A:2070:GLU:O	2.10	0.50
1:B:2280:TYR:C	1:B:2280:TYR:CD1	2.88	0.50
1:A:2233:VAL:HG12	1:A:2234:ARG:O	2.11	0.50
1:A:2347:VAL:O	1:A:2350:LYS:HB2	2.11	0.50
1:B:2302:TRP:N	1:B:2303:PRO:HD2	2.27	0.50
1:A:2339:GLN:HG3	1:A:2339:GLN:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2280:TYR:HD1	1:B:2280:TYR:O	1.94	0.49
1:A:2100:ASP:HB3	1:A:2102:LYS:H	1.77	0.49
1:A:2228:GLY:HA2	1:A:2266:LEU:HB2	1.95	0.49
1:A:2031:VAL:HG23	1:A:2031:VAL:O	2.13	0.49
1:A:2043:PHE:CD1	1:A:2119:LEU:HD23	2.47	0.49
1:A:2353:SER:O	1:A:2358:ARG:HA	2.12	0.49
1:A:2091:ARG:CZ	1:A:2106:TYR:CD1	2.96	0.49
1:A:2178:LEU:HG	1:A:2183:TRP:CE2	2.48	0.49
1:A:2178:LEU:CD1	1:A:2231:VAL:CB	2.91	0.49
1:A:2299:VAL:HG12	1:A:2310:LYS:O	2.12	0.49
1:B:2169:TYR:CE1	1:B:2203:ARG:HD2	2.47	0.49
1:B:2172:ALA:N	1:B:2205:LEU:O	2.46	0.49
1:A:2013:LYS:CE	1:A:2017:ILE:HD11	2.42	0.49
1:B:2032:PRO:CD	1:B:2065:TYR:CE1	2.96	0.49
1:B:2152:ASN:HB3	1:B:2156:TRP:CZ2	2.48	0.49
1:B:2310:LYS:CD	1:B:2341:PRO:O	2.61	0.49
1:A:2281:SER:OG	1:A:2327:GLU:OE2	2.27	0.49
1:A:2313:LEU:HB2	1:A:2345:PHE:CD2	2.48	0.48
1:A:2351:VAL:HB	1:A:2362:ILE:HG12	1.95	0.48
1:A:1977:VAL:HG11	1:A:2158:SER:HB3	1.95	0.48
1:B:2069:PHE:CD1	1:B:2069:PHE:N	2.81	0.48
1:B:2081:PHE:CZ	1:B:2154:GLY:HA2	2.45	0.48
1:A:1979:ASN:OD1	1:A:2283:ARG:NH1	2.46	0.48
1:A:2106:TYR:CB	1:A:2109:ASP:CG	2.85	0.48
1:A:2272:MSE:O	1:A:2276:SER:HB2	2.14	0.48
1:B:2057:GLU:O	1:B:2061:LYS:HB2	2.14	0.48
1:A:2013:LYS:HG3	1:A:2017:ILE:CD1	2.44	0.48
1:B:2140:GLN:O	1:B:2143:SER:OG	2.31	0.48
1:B:2279:PHE:HD2	1:B:2282:LEU:CD1	2.26	0.48
1:B:2312:ILE:O	1:B:2312:ILE:CG2	2.49	0.48
1:B:2359:THR:HG22	1:B:2361:ILE:HG23	1.93	0.48
1:B:2361:ILE:O	1:B:2362:ILE:CG2	2.62	0.48
1:B:2277:LEU:O	1:B:2280:TYR:HB2	2.12	0.48
1:A:2016:MSE:HE1	1:A:2141:LEU:HD21	1.94	0.48
1:B:2009:SER:CB	1:B:2012:VAL:HG22	2.22	0.48
1:B:2228:GLY:CA	1:B:2266:LEU:HB2	2.44	0.48
1:B:2351:VAL:CB	1:B:2362:ILE:HD11	2.42	0.48
1:B:2370:TRP:HA	1:B:2370:TRP:CE3	2.49	0.48
1:B:1986:THR:HG21	1:B:2052:TRP:HE1	1.79	0.48
1:B:2044:VAL:CG1	1:B:2048:LEU:CD1	2.91	0.48
1:A:2047:THR:HA	1:A:2055:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1977:VAL:HG11	1:B:2158:SER:HB2	1.96	0.47
1:B:2186:GLU:OE2	1:B:2186:GLU:HA	2.13	0.47
1:B:2115:PHE:O	1:B:2115:PHE:CD1	2.68	0.47
1:B:2307:GLY:O	1:B:2308:LYS:CG	2.62	0.47
1:B:2310:LYS:HE3	1:B:2337:PHE:O	2.15	0.47
1:A:2052:TRP:HA	1:A:2055:ARG:HG3	1.97	0.47
1:A:2070:GLU:O	1:A:2070:GLU:CG	2.62	0.47
1:A:2076:LYS:CG	1:A:2166:ASN:O	2.63	0.47
1:A:2081:PHE:O	1:A:2150:PHE:CE2	2.67	0.47
1:B:2017:ILE:CG2	1:B:2041:THR:HG22	2.44	0.47
1:A:2078:ILE:HG13	1:A:2160:TYR:CE2	2.50	0.47
1:B:2094:LEU:HB2	1:B:2104:VAL:HG11	1.95	0.47
1:B:2265:LYS:HG3	1:B:2267:SER:OG	2.15	0.47
1:A:1977:VAL:CG2	1:A:2193:LEU:HD21	2.44	0.47
1:A:2017:ILE:HG23	1:A:2041:THR:HG22	1.97	0.47
1:A:2108:ILE:O	1:A:2108:ILE:CG2	2.61	0.47
1:A:2178:LEU:HD11	1:A:2231:VAL:CB	2.44	0.47
1:B:2020:MSE:HE3	1:B:2043:PHE:CE2	2.50	0.47
1:A:2271:SER:O	1:A:2275:GLU:HG2	2.13	0.47
1:B:2131:LEU:HD12	1:B:2131:LEU:N	2.30	0.47
1:B:2299:VAL:HG12	1:B:2310:LYS:HB2	1.97	0.47
1:A:2076:LYS:HG2	1:A:2166:ASN:O	2.16	0.46
1:A:2223:ARG:CB	1:A:2223:ARG:NH1	2.77	0.46
1:A:2281:SER:HB2	1:A:2327:GLU:OE2	2.15	0.46
1:A:2078:ILE:HG13	1:A:2160:TYR:HE2	1.80	0.46
1:A:2139:ASN:OD1	1:A:2139:ASN:O	2.33	0.46
1:A:2167:ASP:HB2	1:A:2201:GLU:O	2.15	0.46
1:A:2331:LEU:HD23	1:A:2331:LEU:HA	1.80	0.46
1:A:2192:GLN:HB2	1:A:2273:LEU:CD1	2.45	0.46
1:A:2314:LEU:HD23	1:A:2326:ILE:HD11	1.96	0.46
1:B:1970:VAL:O	1:B:1974:ALA:HB2	2.15	0.46
1:B:2155:PHE:O	1:B:2159:VAL:CG1	2.63	0.46
1:B:2370:TRP:HA	1:B:2370:TRP:HE3	1.80	0.46
1:A:2087:PHE:CE1	1:A:2173:GLU:CG	2.82	0.46
1:B:2155:PHE:CD1	1:B:2155:PHE:C	2.93	0.46
1:B:2016:MSE:HE2	1:B:2145:ILE:HD11	1.97	0.46
1:B:2299:VAL:CG1	1:B:2310:LYS:HB2	2.46	0.46
1:A:2020:MSE:HE1	1:A:2123:LEU:N	2.31	0.46
1:A:2172:ALA:O	1:A:2205:LEU:O	2.34	0.46
1:A:2326:ILE:HG12	1:A:2346:LEU:HB2	1.97	0.46
1:B:2117:ILE:O	1:B:2121:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2059:LEU:HD21	1:A:2156:TRP:CD1	2.50	0.46
1:B:2155:PHE:O	1:B:2159:VAL:HG13	2.15	0.46
1:B:2334:PHE:HB3	1:B:2339:GLN:HB2	1.97	0.46
1:B:2067:TYR:CD1	1:B:2112:GLY:HA2	2.51	0.46
1:B:2307:GLY:O	1:B:2308:LYS:HD2	2.16	0.46
1:A:2213:LYS:HD2	1:A:2213:LYS:HA	1.63	0.45
1:A:2334:PHE:HD2	1:A:2340:MSE:HA	1.82	0.45
1:B:2063:GLU:O	1:B:2063:GLU:HG2	2.15	0.45
1:B:2186:GLU:C	1:B:2190:LEU:HG	2.40	0.45
1:B:2323:GLN:O	1:B:2327:GLU:HB2	2.16	0.45
1:B:2326:ILE:CG1	1:B:2346:LEU:HD22	2.46	0.45
1:A:2342:ASP:C	1:A:2343:GLU:HG3	2.42	0.45
1:B:2266:LEU:O	1:B:2266:LEU:HG	2.16	0.45
1:A:2074:ALA:HB3	1:A:2105:VAL:CG2	2.46	0.45
1:A:2238:LEU:CG	1:A:2239:SER:H	2.26	0.45
1:B:2014:GLN:O	1:B:2018:GLN:HG2	2.16	0.45
1:B:2024:ILE:CG2	1:B:2029:ASN:HD21	2.29	0.45
1:A:2030:GLN:HG3	1:A:2030:GLN:O	2.17	0.45
1:A:2192:GLN:HB2	1:A:2273:LEU:HD13	1.97	0.45
1:B:1973:ARG:HB3	1:B:2162:THR:HG22	1.98	0.45
1:A:2020:MSE:HA	1:A:2040:ALA:HB1	1.99	0.45
1:A:2287:ASN:HD22	1:A:2302:TRP:HE3	1.63	0.45
1:A:2346:LEU:C	1:A:2346:LEU:CD1	2.90	0.44
1:A:1980:LEU:HD21	1:A:2192:GLN:CG	2.47	0.44
1:A:2113:ASN:HD21	1:A:2160:TYR:HB2	1.82	0.44
1:A:2238:LEU:CG	1:A:2239:SER:N	2.79	0.44
1:B:2135:ASN:HD22	1:B:2138:GLN:CG	2.20	0.44
1:B:2282:LEU:CD2	1:B:2330:ILE:HD11	2.47	0.44
1:A:1982:ARG:CZ	1:A:2291:GLN:HE21	2.30	0.44
1:A:2192:GLN:NE2	1:A:2192:GLN:HA	2.33	0.44
1:B:2345:PHE:CD1	1:B:2347:VAL:HG23	2.53	0.44
1:B:2351:VAL:CB	1:B:2362:ILE:CD1	2.95	0.44
1:A:2041:THR:O	1:A:2045:GLU:CB	2.66	0.44
1:B:2047:THR:HG22	1:B:2152:ASN:HD21	1.81	0.44
1:B:2118:ASP:OD1	1:B:2119:LEU:N	2.50	0.44
1:A:2229:VAL:HG21	1:A:2269:ILE:CD1	2.48	0.44
1:B:2168:VAL:HG12	1:B:2168:VAL:O	2.17	0.44
1:B:2181:TYR:O	1:B:2185:VAL:HB	2.18	0.44
1:B:2217:ALA:O	1:B:2220:ILE:CG1	2.66	0.44
1:A:2132:ASP:OD2	1:A:2135:ASN:HB2	2.18	0.44
1:B:2216:PRO:HD2	1:B:2219:GLN:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1977:VAL:HG22	1:A:2193:LEU:HD11	1.99	0.44
1:A:2013:LYS:O	1:A:2017:ILE:HG13	2.18	0.44
1:A:2047:THR:O	1:A:2055:ARG:NH2	2.50	0.44
1:A:2329:PHE:CE1	1:A:2333:ASN:OD1	2.71	0.44
1:B:2215:LEU:HD11	1:B:2219:GLN:C	2.42	0.44
1:B:2265:LYS:HG3	1:B:2267:SER:H	1.83	0.44
1:B:2274:ARG:CA	1:B:2280:TYR:CE2	2.94	0.44
1:B:2279:PHE:CD2	1:B:2282:LEU:CD1	3.00	0.44
1:B:1970:VAL:O	1:B:1974:ALA:CB	2.65	0.44
1:B:2090:TYR:CD1	1:B:2090:TYR:N	2.86	0.44
1:A:2090:TYR:CG	1:A:2171:ILE:HD13	2.53	0.44
1:B:2090:TYR:O	1:B:2094:LEU:HG	2.18	0.44
1:B:2298:GLU:HB3	1:B:2309:SER:HB2	1.99	0.44
1:B:2044:VAL:HG12	1:B:2048:LEU:CD1	2.47	0.43
1:B:2068:SER:O	1:B:2110:VAL:CG1	2.66	0.43
1:B:2203:ARG:HA	1:B:2222:ARG:O	2.18	0.43
1:A:2043:PHE:CB	1:A:2119:LEU:HD21	2.48	0.43
1:A:2327:GLU:O	1:A:2331:LEU:HB2	2.18	0.43
1:B:2135:ASN:HD22	1:B:2138:GLN:HE21	1.66	0.43
1:B:2340:MSE:HG3	1:B:2341:PRO:HD3	1.99	0.43
1:A:2076:LYS:HD2	1:A:2076:LYS:N	2.32	0.43
1:A:2358:ARG:H	1:A:2358:ARG:HG3	1.62	0.43
1:B:2359:THR:HG22	1:B:2361:ILE:HG22	1.99	0.43
1:A:2081:PHE:O	1:A:2150:PHE:CZ	2.71	0.43
1:A:2093:ILE:HD11	1:A:2213:LYS:HE3	2.00	0.43
1:B:2194:GLN:NE2	1:B:2202:ILE:HD12	2.32	0.43
1:A:2132:ASP:HA	1:A:2133:PRO:HD3	1.87	0.43
1:A:2310:LYS:HA	1:A:2342:ASP:O	2.19	0.43
1:A:2013:LYS:O	1:A:2016:MSE:HB3	2.19	0.43
1:B:2082:TRP:O	1:B:2173:GLU:OE1	2.35	0.43
1:B:2141:LEU:HD12	1:B:2141:LEU:O	2.19	0.43
1:B:2282:LEU:HD22	1:B:2330:ILE:HD11	2.01	0.43
1:A:2189:ALA:O	1:A:2193:LEU:HB2	2.19	0.43
1:A:2330:ILE:CG2	1:A:2344:LEU:HD13	2.47	0.43
1:B:1976:LYS:CE	1:B:2198:LEU:CD1	2.76	0.43
1:A:2084:GLY:CA	1:A:2173:GLU:HG3	2.43	0.43
1:A:2192:GLN:NE2	1:A:2192:GLN:CA	2.81	0.43
1:A:2204:LEU:HD11	1:A:2224:LEU:HG	2.00	0.43
1:A:2362:ILE:HD13	1:A:2370:TRP:CE3	2.52	0.43
1:B:2115:PHE:O	1:B:2119:LEU:HB2	2.19	0.43
1:A:2334:PHE:CD2	1:A:2340:MSE:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2016:MSE:HE2	1:B:2126:TRP:CE3	2.53	0.42
1:A:2107:ASP:HB3	1:A:2160:TYR:CD2	2.55	0.42
1:A:2023:TYR:O	1:A:2027:THR:OG1	2.32	0.42
1:B:2051:ASP:OD2	1:B:2054:LYS:HD2	2.20	0.42
1:B:2351:VAL:HB	1:B:2362:ILE:HD11	2.00	0.42
1:B:2152:ASN:HB3	1:B:2156:TRP:CE2	2.54	0.42
1:B:2370:TRP:CE3	1:B:2370:TRP:CA	3.02	0.42
1:A:2093:ILE:HD13	1:A:2213:LYS:CD	2.44	0.42
1:B:2034:ASP:OD1	1:B:2035:GLN:N	2.53	0.42
1:B:2141:LEU:O	1:B:2144:SER:N	2.50	0.42
1:B:2215:LEU:HD11	1:B:2220:ILE:CG2	2.46	0.42
1:B:2330:ILE:HB	1:B:2334:PHE:HE1	1.84	0.42
1:B:2359:THR:O	1:B:2359:THR:HG22	2.17	0.42
1:B:2090:TYR:OH	1:B:2173:GLU:OE2	2.30	0.42
1:A:2094:LEU:O	1:A:2097:ALA:HB3	2.19	0.42
1:A:2314:LEU:HD22	1:A:2322:GLN:HB3	2.01	0.42
1:B:2351:VAL:CG2	1:B:2362:ILE:CD1	2.85	0.42
1:B:2351:VAL:HG21	1:B:2362:ILE:CD1	2.45	0.42
1:A:2029:ASN:HD22	1:A:2029:ASN:HA	1.59	0.42
1:A:2078:ILE:HD12	1:A:2168:VAL:HG13	2.01	0.42
1:A:2315:ASP:OD1	1:A:2316:ASN:N	2.53	0.42
1:A:2324:LYS:HD2	1:A:2324:LYS:HA	1.79	0.42
1:B:1973:ARG:CZ	1:B:2163:GLY:CA	2.98	0.42
1:B:2299:VAL:HG13	1:B:2337:PHE:HE1	1.85	0.42
1:A:2145:ILE:O	1:A:2149:THR:CG2	2.67	0.41
1:A:2233:VAL:HG21	1:B:2033:LYS:CB	2.49	0.41
1:A:2233:VAL:CG1	1:B:2033:LYS:HZ2	2.33	0.41
1:B:2061:LYS:O	1:B:2064:SER:OG	2.36	0.41
1:B:2153:THR:O	1:B:2157:SER:OG	2.37	0.41
1:B:2194:GLN:HB2	1:B:2199:VAL:HG12	2.01	0.41
1:A:1979:ASN:ND2	1:A:2289:LEU:HD22	2.35	0.41
1:A:2043:PHE:CD1	1:A:2119:LEU:CD2	3.04	0.41
1:A:2273:LEU:HD23	1:A:2273:LEU:HA	1.91	0.41
1:B:1986:THR:HG22	1:B:2052:TRP:HE1	1.85	0.41
1:B:2182:PHE:O	1:B:2182:PHE:CG	2.73	0.41
1:B:2228:GLY:HA3	1:B:2264:VAL:HG13	2.02	0.41
1:B:2194:GLN:CA	1:B:2199:VAL:HG12	2.50	0.41
1:B:2362:ILE:HG22	1:B:2370:TRP:CE3	2.55	0.41
1:A:1984:LEU:HD23	1:A:2276:SER:OG	2.20	0.41
1:A:2069:PHE:CD1	1:A:2069:PHE:N	2.87	0.41
1:A:2079:VAL:HG12	1:A:2171:ILE:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2220:ILE:O	1:A:2220:ILE:HG22	2.19	0.41
1:B:2155:PHE:CE1	1:B:2159:VAL:HG11	2.56	0.41
1:A:2014:GLN:HA	1:A:2017:ILE:HD12	2.03	0.41
1:A:2239:SER:HB3	1:A:2242:ARG:CB	2.51	0.41
1:A:2282:LEU:HG	1:A:2327:GLU:HG3	2.02	0.41
1:A:2078:ILE:CD1	1:A:2161:ALA:CB	2.75	0.41
1:A:2089:GLN:O	1:A:2093:ILE:HG13	2.21	0.41
1:A:2310:LYS:CD	1:A:2337:PHE:HE1	2.30	0.41
1:B:2021:SER:OG	1:B:2037:GLU:HA	2.21	0.41
1:B:2272:MSE:O	1:B:2276:SER:HB3	2.21	0.41
1:A:2089:GLN:HE21	1:A:2089:GLN:HB3	1.68	0.41
1:A:2215:LEU:CD1	1:A:2219:GLN:OE1	2.52	0.41
1:B:1973:ARG:NE	1:B:2163:GLY:HA2	2.35	0.41
1:B:2089:GLN:HG2	1:B:2093:ILE:HD11	2.03	0.41
1:B:2274:ARG:CA	1:B:2280:TYR:CD2	2.73	0.41
1:A:1970:VAL:HA	1:A:1973:ARG:NH1	2.36	0.41
1:A:2302:TRP:CD1	1:A:2302:TRP:O	2.74	0.41
1:A:2315:ASP:OD1	1:A:2322:GLN:NE2	2.53	0.41
1:A:1980:LEU:HD21	1:A:2192:GLN:HG2	2.01	0.40
1:A:2363:ALA:C	1:A:2365:LYS:H	2.29	0.40
1:B:1973:ARG:CZ	1:B:2163:GLY:HA2	2.51	0.40
1:B:2286:ARG:CG	1:B:2335:ASP:O	2.69	0.40
1:A:2093:ILE:CD1	1:A:2213:LYS:HD3	2.50	0.40
1:A:2152:ASN:O	1:A:2155:PHE:HB3	2.21	0.40
1:B:1970:VAL:HG22	1:B:2069:PHE:HB2	2.03	0.40
1:A:2024:ILE:CG2	1:A:2031:VAL:HG21	2.52	0.40
1:A:2069:PHE:HA	1:A:2110:VAL:HG11	2.02	0.40
1:A:2345:PHE:CD1	1:A:2352:LEU:HD12	2.57	0.40
1:B:1976:LYS:HE2	1:B:2198:LEU:CD2	2.41	0.40
1:B:2032:PRO:CD	1:B:2065:TYR:CD1	3.05	0.40
1:B:2106:TYR:HB2	1:B:2109:ASP:CG	2.46	0.40
1:B:2286:ARG:HG2	1:B:2335:ASP:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/419 (91%)	354 (92%)	29 (8%)	0	100	100
1	B	332/419 (79%)	311 (94%)	21 (6%)	0	100	100
All	All	715/838 (85%)	665 (93%)	50 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	332/351 (95%)	266 (80%)	66 (20%)	1	5
1	B	294/351 (84%)	252 (86%)	42 (14%)	3	13
All	All	626/702 (89%)	518 (83%)	108 (17%)	2	8

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1976	LYS
1	A	1982	ARG
1	A	1985	ASP
1	A	1986	THR
1	A	1988	ASN
1	A	2008	VAL
1	A	2012	VAL
1	A	2026	HIS
1	A	2029	ASN
1	A	2037	GLU
1	A	2039	LEU
1	A	2058	PHE
1	A	2062	LEU
1	A	2069	PHE

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Mol	Chain	Res	Type
1	A	2073	HIS
1	A	2075	GLU
1	A	2076	LYS
1	A	2088	LYS
1	A	2093	ILE
1	A	2094	LEU
1	A	2103	LYS
1	A	2106	TYR
1	A	2108	ILE
1	A	2110	VAL
1	A	2124	MSE
1	A	2129	LEU
1	A	2135	ASN
1	A	2137	GLU
1	A	2142	LYS
1	A	2144	SER
1	A	2152	ASN
1	A	2162	THR
1	A	2177	ARG
1	A	2186	GLU
1	A	2190	LEU
1	A	2193	LEU
1	A	2194	GLN
1	A	2195	ARG
1	A	2201	GLU
1	A	2205	LEU
1	A	2207	LYS
1	A	2213	LYS
1	A	2220	ILE
1	A	2223	ARG
1	A	2224	LEU
1	A	2234	ARG
1	A	2242	ARG
1	A	2246	LEU
1	A	2255	LYS
1	A	2266	LEU
1	A	2267	SER
1	A	2269	ILE
1	A	2275	GLU
1	A	2281	SER
1	A	2286	ARG
1	A	2288	LEU

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Mol	Chain	Res	Type
1	A	2309	SER
1	A	2314	LEU
1	A	2330	ILE
1	A	2334	PHE
1	A	2336	ASN
1	A	2339	GLN
1	A	2340	MSE
1	A	2358	ARG
1	A	2359	THR
1	A	2360	ARG
1	B	1980	LEU
1	B	2024	ILE
1	B	2027	THR
1	B	2028	ASP
1	B	2061	LYS
1	B	2062	LEU
1	B	2069	PHE
1	B	2070	GLU
1	B	2076	LYS
1	B	2078	ILE
1	B	2082	TRP
1	B	2096	ASN
1	B	2111	LYS
1	B	2124	MSE
1	B	2141	LEU
1	B	2144	SER
1	B	2158	SER
1	B	2159	VAL
1	B	2162	THR
1	B	2168	VAL
1	B	2182	PHE
1	B	2195	ARG
1	B	2215	LEU
1	B	2219	GLN
1	B	2222	ARG
1	B	2225	THR
1	B	2267	SER
1	B	2269	ILE
1	B	2275	GLU
1	B	2280	TYR
1	B	2291	GLN
1	B	2292	GLU

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Mol	Chain	Res	Type
1	B	2295	GLU
1	B	2312	ILE
1	B	2326	ILE
1	B	2334	PHE
1	B	2340	MSE
1	B	2352	LEU
1	B	2358	ARG
1	B	2364	GLN
1	B	2366	GLU
1	B	2370	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1988	ASN
1	A	2035	GLN
1	A	2073	HIS
1	A	2089	GLN
1	A	2122	HIS
1	A	2140	GLN
1	A	2166	ASN
1	A	2184	ASN
1	A	2287	ASN
1	A	2291	GLN
1	A	2333	ASN
1	A	2339	GLN
1	B	2030	GLN
1	B	2086	ASN
1	B	2113	ASN
1	B	2135	ASN
1	B	2152	ASN
1	B	2364	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/419 (91%)	1.09	64 (16%) 4 5	8, 46, 95, 112	0
1	B	337/419 (80%)	1.55	114 (33%) 1 1	6, 73, 127, 148	0
All	All	719/838 (85%)	1.31	178 (24%) 2 3	6, 55, 121, 148	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2219	GLN	6.7
1	B	2228	GLY	6.6
1	B	2220	ILE	5.9
1	A	2358	ARG	5.7
1	B	2080	SER	5.1
1	A	2362	ILE	5.1
1	B	2134	ASP	5.0
1	A	2164	ALA	4.8
1	A	2079	VAL	4.8
1	B	2217	ALA	4.7
1	A	2080	SER	4.5
1	A	2118	ASP	4.4
1	A	2106	TYR	4.4
1	B	2216	PRO	4.2
1	A	1986	THR	4.2
1	B	2076	LYS	4.2
1	B	2096	ASN	4.2
1	A	2367	ASP	4.1
1	B	2331	LEU	4.0
1	A	2032	PRO	3.9
1	B	2077	SER	3.9
1	B	2362	ILE	3.9
1	A	2008	VAL	3.8
1	A	2031	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	2306	ASP	3.8
1	B	2309	SER	3.8
1	B	2079	VAL	3.8
1	B	2104	VAL	3.8
1	B	2305	ILE	3.8
1	B	2307	GLY	3.7
1	B	2171	ILE	3.6
1	B	2011	GLU	3.6
1	B	2095	ASP	3.6
1	A	2030	GLN	3.6
1	B	2092	ASP	3.6
1	A	2217	ALA	3.5
1	B	2358	ARG	3.5
1	B	2302	TRP	3.4
1	A	2343	GLU	3.4
1	A	2087	PHE	3.4
1	A	2078	ILE	3.4
1	B	1985	ASP	3.3
1	B	2051	ASP	3.3
1	A	2359	THR	3.3
1	B	2290	VAL	3.3
1	A	2072	PRO	3.3
1	B	2266	LEU	3.3
1	A	2357	GLY	3.3
1	A	1970	VAL	3.2
1	B	1968	SER	3.2
1	A	2252	ASP	3.1
1	B	2343	GLU	3.1
1	B	2093	ILE	3.1
1	B	2363	ALA	3.1
1	B	2008	VAL	3.1
1	A	2171	ILE	3.1
1	A	2071	ALA	3.1
1	B	2301	SER	3.1
1	A	2107	ASP	3.0
1	A	2363	ALA	3.0
1	A	2364	GLN	3.0
1	B	2359	THR	3.0
1	B	2167	ASP	3.0
1	A	1987	ASP	3.0
1	B	2135	ASN	3.0
1	A	1969	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	2229	VAL	2.9
1	B	2132	ASP	2.9
1	B	2191	ARG	2.9
1	B	2083	SER	2.8
1	B	2035	GLN	2.8
1	B	2227	ALA	2.8
1	A	2132	ASP	2.8
1	B	2209	VAL	2.8
1	A	2069	PHE	2.8
1	B	2330	ILE	2.8
1	B	2360	ARG	2.8
1	B	2033	LYS	2.8
1	A	2276	SER	2.7
1	B	2075	GLU	2.7
1	B	2320	ALA	2.7
1	A	2112	GLY	2.7
1	B	2218	ASP	2.7
1	B	2166	ASN	2.7
1	B	2365	LYS	2.6
1	A	2070	GLU	2.6
1	B	2344	LEU	2.6
1	A	2308	LYS	2.6
1	B	2175	GLY	2.6
1	B	2279	PHE	2.6
1	B	2013	LYS	2.6
1	B	2205	LEU	2.6
1	B	2138	GLN	2.6
1	B	2224	LEU	2.6
1	B	1986	THR	2.6
1	B	2311	THR	2.6
1	B	2361	ILE	2.5
1	B	2332	ALA	2.5
1	B	2068	SER	2.5
1	B	2084	GLY	2.5
1	B	2223	ARG	2.5
1	B	2308	LYS	2.5
1	A	2295	GLU	2.4
1	A	2218	ASP	2.4
1	A	2216	PRO	2.4
1	A	2360	ARG	2.4
1	B	2094	LEU	2.4
1	B	2133	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2317	PRO	2.4
1	B	2215	LEU	2.4
1	B	2200	GLY	2.4
1	B	2160	TYR	2.4
1	B	2306	ASP	2.4
1	B	2327	GLU	2.4
1	B	2098	GLN	2.3
1	A	2025	GLU	2.3
1	B	2318	GLU	2.3
1	A	2309	SER	2.3
1	A	2226	ASP	2.3
1	B	2107	ASP	2.3
1	B	2226	ASP	2.3
1	A	2257	ASP	2.3
1	A	2082	TRP	2.3
1	A	2084	GLY	2.3
1	A	2356	ASP	2.3
1	B	2295	GLU	2.3
1	A	2040	ALA	2.3
1	B	2074	ALA	2.3
1	B	2364	GLN	2.3
1	A	2027	THR	2.2
1	B	2184	ASN	2.2
1	A	2305	ILE	2.2
1	A	2369	ALA	2.2
1	B	2087	PHE	2.2
1	B	2125	ARG	2.2
1	B	2081	PHE	2.2
1	B	2082	TRP	2.2
1	B	2169	TYR	2.2
1	A	2158	SER	2.2
1	A	2165	GLN	2.2
1	A	2287	ASN	2.2
1	B	2085	LYS	2.2
1	B	2310	LYS	2.2
1	A	2371	THR	2.2
1	A	2176	VAL	2.2
1	B	2204	LEU	2.1
1	B	2268	ALA	2.1
1	B	2174	GLY	2.1
1	B	2300	ARG	2.1
1	A	2051	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2214	ASP	2.1
1	B	2198	LEU	2.1
1	A	2227	ALA	2.1
1	A	2133	PRO	2.1
1	A	2174	GLY	2.1
1	B	2137	GLU	2.1
1	B	2294	GLU	2.1
1	A	2352	LEU	2.1
1	B	2267	SER	2.1
1	B	2333	ASN	2.1
1	B	2105	VAL	2.1
1	B	2170	VAL	2.1
1	B	2097	ALA	2.1
1	B	2293	GLY	2.1
1	B	2044	VAL	2.1
1	B	2351	VAL	2.1
1	B	2370	TRP	2.1
1	B	2284	THR	2.1
1	A	2332	ALA	2.0
1	B	2172	ALA	2.0
1	B	2315	ASP	2.0
1	B	2211	GLU	2.0
1	B	2203	ARG	2.0
1	B	2269	ILE	2.0
1	A	2099	THR	2.0
1	B	2225	THR	2.0
1	B	2371	THR	2.0
1	A	2044	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.