

Full wwPDB X-ray Structure Validation Report (i)

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 Title : Crystal structure of the RID-dependent transforming NADase domain (RE 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) 	PDB ID	:	8KA2
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	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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635(3.46-3.30)

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 <=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	А	419	37%	47%		8%	8%
1	В	419	29%	48%	•	18%	



2 Entry composition (i)

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	А	387	Total 3101	$\begin{array}{c} \mathrm{C} \\ 1955 \end{array}$	N 530	0 611	${ m Se} 5$	0	0	0
1	В	342	Total 2747	C 1738	N 467	0 537	$\frac{\mathrm{Se}}{5}$	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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



3 Residue-property plots (i)

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







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants	207.73Å 207.73Å 54.65Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	40.42 - 3.38	Depositor
Resolution (A)	40.39 - 3.38	EDS
% Data completeness	82.8 (40.42-3.38)	Depositor
(in resolution range)	82.9 (40.39-3.38)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.95 (at 3.40 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.286 , 0.322	Depositor
Λ, Λ_{free}	0.284 , 0.317	DCC
R_{free} test set	830 reflections $(5.20%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.3	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 33.1	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.69	0/3157	0.79	2/4265~(0.0%)	
1	В	0.70	0/2796	0.74	0/3772	
All	All	0.70	0/5953	0.77	2/8037~(0.0%)	

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	А	2	2
1	В	2	0
All	All	4	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	2272	MSE	CG-SE-CE	5.84	111.75	98.90
1	А	2176	VAL	CB-CA-C	5.10	121.09	111.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	А	2020	MSE	CA
1	А	2124	MSE	CA
1	В	2020	MSE	CA
1	В	2124	MSE	CA

All (2) planarity outliers are listed below:



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

5.2 Too-close contacts (i)

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	А	3101	0	2997	392	0
1	В	2747	0	2649	346	0
All	All	5848	0	5646	725	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 63.

All (725) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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: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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:1979:ASN:CG	1:A:2283:ARG:HH12	1.77	0.88
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
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



A + 1	A 4 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:2108:ILE:HG22	1:A:2108:ILE:O	1.93	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: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: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
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



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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:2106:TYR:HB2	1:A:2109:ASP:CG	2.19	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



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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: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
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:2167:ASP:CG	1:B:2168:VAL:H	2.04	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



A + 1	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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: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
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:A:2302:TRP:CD1	1:A:2302:TRP:C	2.77	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:A:2346:LEU:C	1:A:2346:LEU:HD13	2.25	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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
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: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: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:A:2266:LEU:HD13	1:A:2266:LEU:C	2.27	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:2279:PHE:HD2	1:B:2282:LEU:HD11	1.70	0.55



<u> </u>	A + 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:2362:ILE:CG2	1:A:2363:ALA:N	2.70	0.54
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: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



	A L O	Interatomic	Clash	
Atom-1 Atom-2		distance (\AA)	overlap (Å)	
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: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: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:B:1981:TYR:OH	1:B:2158:SER:OG	2.25	0.52	
1:B:2334:PHE:HB3	1:B:2339:GLN:HB3	1.92	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:2336:ASN:C	1:A:2336:ASN:OD1	2.48	0.52	
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:2329:PHE:CD1	1:B:2329:PHE:C	2.84	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:2020:MSE:C	1:A:2040:ALA:CB	2.79	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	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:2215:LEU:CD1	1:B:2219:GLN:C	2.80	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
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:2192:GLN:HE21	1:A:2192:GLN:C	2.12	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: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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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:2167:ASP:CG	1:B:2168:VAL:N	2.66	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:2182:PHE:CD1	1:B:2182:PHE:C	2.87	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
1:A:2058:PHE:C	1:A:2058:PHE:CD1	2.87	0.47
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:2280:TYR:HD1	1:B:2280:TYR:C	2.18	0.47
1:B:2280:TYR:C	1:B:2280:TYR:CD1	2.88	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:2361:ILE:C	1:B:2362:ILE:HG23	2.34	0.47
1:A:2262:LEU:HD12	1:A:2262:LEU:C	2.34	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:A:2020:MSE:C	1:A:2040:ALA:HB1	2.35	0.47
1:B:2020:MSE:HE3	1:B:2043:PHE:CE2	2.50	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:2140:GLN:HE21	1:B:2140:GLN:C	2.14	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
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: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: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



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:B:2359:THR:O	1:B:2359:THR:HG22	2.17	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
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: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:A:2106:TYR:CB	1:A:2109:ASP:CG	2.85	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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:2076:LYS:HD2	1:A:2076:LYS:HD2 1:A:2076:LYS:N		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
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: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:A:2023:TYR:O	1:A:2027:THR:OG1	2.32	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:A:2220:ILE:HG22	1:A:2220:ILE:O	2.19	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: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



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
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: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:2155:PHE:CD1	1:B:2155:PHE:C	2.93	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	
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:2342:ASP:C	1:A:2343:GLU:HG3	2.42	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	



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Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
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		

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	383/419~(91%)	354 (92%)	29~(8%)	0	100 100
1	В	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 (i)

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	А	332/351~(95%)	283~(85%)	49 (15%)	3 13	
Continued on next page						

Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	В	294/351~(84%)	263~(90%)	31 (10%)	7	26
All	All	626/702~(89%)	546 (87%)	80 (13%)	4	17

All (80) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	1976	LYS
1	А	1982	ARG
1	А	1985	ASP
1	А	1986	THR
1	А	1988	ASN
1	А	2012	VAL
1	А	2026	HIS
1	А	2029	ASN
1	А	2037	GLU
1	А	2039	LEU
1	А	2058	PHE
1	А	2069	PHE
1	А	2075	GLU
1	А	2076	LYS
1	А	2082	TRP
1	А	2093	ILE
1	А	2103	LYS
1	А	2106	TYR
1	А	2110	VAL
1	А	2124	MSE
1	А	2129	LEU
1	А	2135	ASN
1	А	2144	SER
1	А	2152	ASN
1	А	2162	THR
1	А	2177	ARG
1	А	2190	LEU
1	А	2193	LEU
1	А	2194	GLN
1	А	2195	ARG
1	А	2205	LEU
1	А	2214	ASP
1	А	2223	ARG
1	A	2224	LEU
1	А	2234	ARG
1	А	2242	ARG



Mol	ol Chain Res		Type		
1	А	2255	LYS		
1	А	2267	SER		
1	А	2275	GLU		
1	A	2281	SER		
1	А	2286	ARG		
1	А	2288	LEU		
1	А	2309	SER		
1	А	2313	LEU		
1	А	2334	PHE		
1	А	2336	ASN		
1	А	2358	ARG		
1	А	2360	ARG		
1	А	2370	TRP		
1	В	1973	ARG		
1	В	2027	THR		
1	В	2028	ASP		
1	В	2062	LEU		
1	В	2069	PHE		
1	В	2076	LYS		
1	В	2078	ILE		
1	1 B		TRP		
1	В	2087	PHE		
1	В	2124	MSE		
1	В	2141	LEU		
1	В	2150	PHE		
1	В	2158	SER		
1	В	2182	PHE		
1	В	2195	ARG		
1	В	2218	ASP		
1	В	2219	GLN		
1	В	2225	THR		
1	В	2270	ASP		
1	В	2275	GLU		
1	В	2280	TYR		
1	В	2291	GLN		
1	В	2292	GLU		
1	В	2295	GLU		
1	В	2334	PHE		
1	В	2340	MSE		
1	В	2345	PHE		
1	В	2358	ARG		
1	В	$2\overline{364}$	GLN		



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Mol	Chain	Res	Type
1	В	2366	GLU
1	В	2370	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	2073	HIS
1	А	2086	ASN
1	А	2122	HIS
1	А	2140	GLN
1	А	2184	ASN
1	А	2287	ASN
1	А	2291	GLN
1	А	2322	GLN
1	А	2333	ASN
1	А	2339	GLN
1	В	2030	GLN
1	В	2135	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	А	382/419~(91%)	0.17	16 (4%)	36	40	8, 46, 95, 112	0
1	В	337/419~(80%)	0.45	21 (6%)	20	24	6, 73, 127, 148	0
All	All	719/838~(85%)	0.30	37(5%)	28	31	6, 55, 121, 148	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	2219	GLN	5.9
1	В	2228	GLY	3.9
1	В	2134	ASP	3.5
1	А	2216	PRO	3.5
1	В	2216	PRO	3.5
1	А	2164	ALA	3.2
1	А	2218	ASP	3.1
1	В	2095	ASP	3.0
1	В	2096	ASN	2.9
1	В	2210	SER	2.9
1	А	2030	GLN	2.8
1	В	2080	SER	2.8
1	А	2364	GLN	2.8
1	А	1986	THR	2.7
1	В	2073	HIS	2.7
1	В	2083	SER	2.6
1	А	2358	ARG	2.6
1	А	2367	ASP	2.5
1	А	2096	ASN	2.5
1	В	2218	ASP	2.4
1	В	2295	GLU	2.4
1	А	2031	VAL	2.3
1	В	2085	LYS	2.3
1	А	2362	ILE	2.3



	5	1	1 5	
Mol	Chain	Res	Type	RSRZ
1	А	2035	GLN	2.3
1	В	2092	ASP	2.3
1	А	2025	GLU	2.3
1	В	2294	GLU	2.3
1	В	2098	GLN	2.2
1	В	2266	LEU	2.2
1	А	2099	THR	2.2
1	А	2219	GLN	2.2
1	В	2226	ASP	2.1
1	В	2331	LEU	2.1
1	А	2215	LEU	2.1
1	В	2362	ILE	2.0
1	В	2370	TRP	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 monosaccharides 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.

