



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:06 AM UTC

PDB ID : 3H94 / pdb_00003h94
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli
Authors : Su, C.-C.; Yang, F.; Long, F.; Reyon, D.; Routh, M.D.; Kuo, D.W.; Mokhtari, A.K.; Van Ornam, J.D.; Rabe, K.L.; Hoy, J.A.; Lee, Y.J.; Rajashankar, K.R.; Yu, E.W.
Deposited on : 2009-04-30
Resolution : 3.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	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

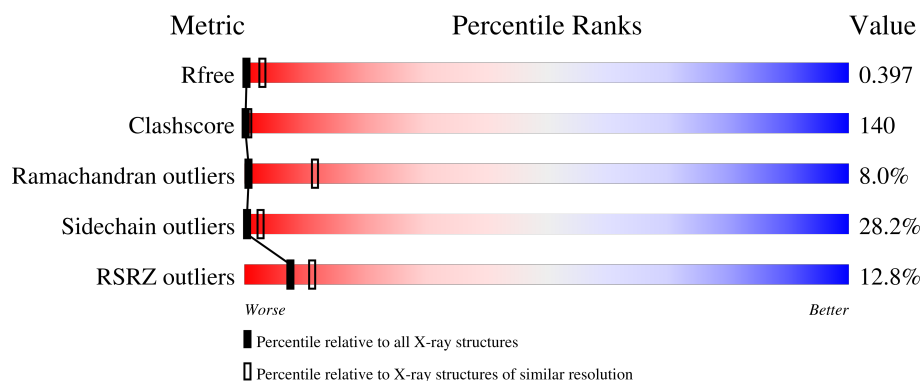
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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	407	9% 10% 33% 25% 5% 27%
1	B	407	10% 11% 32% 23% 7% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AG	A	408	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4550 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

- Molecule 2 is SILVER ION (CCD ID: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ag	0	0
			1	1		
2	B	1	Total	Ag	0	0
			1	1		

A366	L367	R368	S369	G370	L371	A372	E373	G374	E375	K376	V377	V378	S379	S380	G381	L382	F383	L384	I385	ASP	SER	GLU	ALA	ASN	ILE	SER	GLY	ALA	LEU	GLU	ARG	MET	ARG	SER	GLU	SER	ALA	THR	HIS	ALA	HIS																		
V244	W245	V246	T247	G248	A249	L250	P251	E252	S253	L254	A255	W256	L257	V258	K259	D260	A261	T265	L266	T267	V268	P269	A270	R271	P272	L273	D274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	V287	D288	A289	A290	T291	R292	T293	L294	Q295	L296	R297	L298	E299	V300	D301	N302	A303	D304	E305	
A306	L307	K308	P309	G310	M311	N312	A313	W314	L315	Q316	L317	N318	T319	A320	S321	E322	P323	M324	L325	L326	I327	P328	S329	Q330	A331	L332	I333	D334	T335	G336	S337	E338	Q339	R340	V341	I342	T343	V344	D345	A346	D347	G348	R349	F350	V351	P352	K353	R354	V355	A356	V357	F358	Q359	A360	S361	Q362	G363	V364	T365
R184	L185	R186	L187	A188	G189	W190	P191	E192	A193	D194	I195	R196	L197	L198	I199	A200	T201	Q202	K203	T204	Q205	T206	R207	F208	T209	L210	K211	A212	P213	I214	D215	G216	W217	I218	T219	A220	F221	D222	L223	R224	A225	Q226	W227	N228	I229	A230	K231	D232	W233	V234	V235	A236	K237	I238	Q239	G240	R241	D242	P243
I123	V124	Q125	A126	R127	A128	A129	G130	F131	I132	D133	K134	V135	I136	P137	L138	T139	V140	G141	D142	F143	V144	Q145	K146	G147	I148	P149	L150	L151	D152	L153	T154	I155	P156	D157	W158	V159	E160	A161	Q162	S163	E164	Y165	L166	L167	L168	T171	G172	G173	T174	A175	T176	Q177	T178	E179	G180	I181	L182	E183	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.00Å 114.42Å 259.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 3.84 47.20 – 3.84	Depositor EDS
% Data completeness (in resolution range)	87.3 (47.20-3.84) 99.6 (47.20-3.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.300 0.397 , 0.397	Depositor DCC
R_{free} test set	675 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	153.0	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 251.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4550	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AG

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	1.27	19/2313 (0.8%)	1.91	86/3152 (2.7%)
1	B	1.24	24/2313 (1.0%)	1.96	96/3152 (3.0%)
All	All	1.26	43/4626 (0.9%)	1.94	182/6304 (2.9%)

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	0	1
1	B	0	2
All	All	0	3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	VAL	C-N	15.75	1.52	1.33
1	A	97	ALA	C-O	-15.51	1.04	1.23
1	A	89	THR	C-N	12.86	1.51	1.33
1	A	149	PRO	C-N	12.33	1.50	1.33
1	A	377	VAL	C-O	-10.85	1.10	1.23
1	B	259	LYS	N-CA	8.78	1.57	1.46
1	A	320	ALA	CA-C	8.64	1.63	1.52
1	B	300	VAL	CA-CB	-8.16	1.44	1.54
1	B	213	PRO	C-N	-8.13	1.24	1.33
1	B	341	VAL	CA-CB	-7.85	1.43	1.54
1	B	245	TRP	C-O	-7.84	1.15	1.24
1	B	233	ASN	CA-C	-7.67	1.43	1.52
1	A	320	ALA	N-CA	7.58	1.55	1.46
1	B	259	LYS	CA-C	7.46	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	GLN	C-N	-7.38	1.22	1.33
1	B	333	ILE	C-O	-7.31	1.16	1.23
1	B	246	VAL	CA-CB	-7.24	1.45	1.54
1	B	137	PRO	CA-C	7.09	1.59	1.53
1	B	309	PRO	CA-C	-6.85	1.44	1.52
1	B	351	VAL	CA-CB	6.69	1.62	1.54
1	B	324	MET	C-N	-6.66	1.24	1.33
1	A	218	ILE	C-O	-6.56	1.16	1.24
1	B	323	PRO	C-N	-6.47	1.24	1.33
1	B	218	ILE	C-O	-6.40	1.17	1.24
1	B	279	ARG	C-O	-6.32	1.15	1.24
1	B	240	GLY	CA-C	-6.20	1.46	1.52
1	A	305	GLU	N-CA	6.18	1.53	1.46
1	B	220	ALA	CA-C	6.04	1.60	1.52
1	A	377	VAL	CA-CB	-5.95	1.46	1.55
1	B	340	ARG	CD-NE	5.78	1.54	1.46
1	B	339	GLN	CA-C	-5.64	1.45	1.52
1	A	341	VAL	CA-CB	-5.62	1.46	1.54
1	A	317	LEU	CA-C	-5.61	1.45	1.52
1	B	280	LYS	CA-C	-5.58	1.46	1.52
1	B	102	GLY	C-O	-5.50	1.16	1.24
1	A	303	ALA	CA-C	5.44	1.60	1.52
1	A	97	ALA	C-N	-5.41	1.26	1.33
1	A	340	ARG	CD-NE	5.26	1.53	1.46
1	B	357	VAL	CA-CB	-5.25	1.47	1.54
1	A	339	GLN	CA-C	-5.14	1.45	1.52
1	B	333	ILE	CA-CB	-5.11	1.47	1.54
1	A	367	LEU	C-N	5.08	1.41	1.33
1	A	357	VAL	CA-CB	-5.04	1.47	1.54

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	VAL	O-C-N	19.56	147.02	122.57
1	B	119	TYR	N-CA-CB	-18.91	80.77	110.46
1	A	274	LYS	N-CA-C	-18.16	91.48	111.28
1	A	235	VAL	N-CA-C	-16.87	96.13	112.83
1	B	258	VAL	N-CA-C	16.81	128.01	110.36
1	A	155	ILE	N-CA-C	16.35	125.71	107.89
1	B	225	ALA	N-CA-C	16.14	134.12	111.52
1	A	94	VAL	CA-C-N	-15.93	94.20	121.75
1	A	94	VAL	C-N-CA	-15.93	94.20	121.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	PRO	O-C-N	-15.85	103.51	122.85
1	B	213	PRO	CA-C-N	14.07	138.38	122.48
1	B	213	PRO	C-N-CA	14.07	138.38	122.48
1	B	259	LYS	N-CA-C	13.33	139.19	110.80
1	B	123	ILE	N-CA-C	-13.13	89.59	108.36
1	B	215	ASP	N-CA-C	-12.88	88.08	109.46
1	B	118	GLU	N-CA-C	12.03	127.06	112.38
1	A	304	ASP	N-CA-C	-12.00	93.79	110.35
1	B	213	PRO	O-C-N	-11.86	109.38	122.18
1	A	278	ILE	N-CA-C	-11.70	90.67	107.75
1	B	219	THR	N-CA-C	-11.67	89.49	108.52
1	B	373	GLU	N-CA-C	11.42	127.09	110.42
1	B	341	VAL	CB-CA-C	-11.36	92.66	111.29
1	A	225	ALA	N-CA-C	11.06	127.01	111.52
1	A	215	ASP	N-CA-C	-10.92	92.39	109.76
1	A	290	ALA	N-CA-C	-10.83	89.60	108.23
1	B	129	ALA	N-CA-C	-10.44	91.12	108.76
1	A	320	ALA	N-CA-C	10.41	123.10	108.74
1	A	341	VAL	CB-CA-C	-10.22	94.53	111.29
1	B	146	LYS	N-CA-C	-9.72	100.42	112.47
1	A	148	THR	CA-C-N	-9.54	107.91	119.84
1	A	148	THR	C-N-CA	-9.54	107.91	119.84
1	B	311	MET	N-CA-C	-9.43	94.95	109.85
1	B	96	THR	N-CA-C	9.06	122.92	109.24
1	A	342	ILE	N-CA-C	8.92	121.11	108.36
1	A	289	ALA	N-CA-C	-8.75	102.37	112.87
1	B	309	PRO	N-CA-C	-8.74	97.31	111.21
1	B	259	LYS	CB-CA-C	-8.68	93.16	110.42
1	A	379	SER	N-CA-C	8.64	124.01	113.38
1	B	323	PRO	CA-C-N	8.56	138.34	123.03
1	B	323	PRO	C-N-CA	8.56	138.34	123.03
1	B	102	GLY	CA-C-N	8.52	130.48	119.84
1	B	102	GLY	C-N-CA	8.52	130.48	119.84
1	A	287	VAL	N-CA-C	8.48	120.78	107.98
1	A	156	PRO	N-CA-C	8.40	129.78	112.47
1	B	155	ILE	N-CA-C	8.35	117.55	107.61
1	B	288	ASP	N-CA-C	-8.29	97.52	109.96
1	B	258	VAL	CB-CA-C	-8.18	101.41	111.88
1	B	350	PHE	N-CA-C	8.15	121.04	110.53
1	A	302	ASN	N-CA-C	8.11	122.29	109.39
1	B	150	LEU	N-CA-C	8.10	126.14	114.39
1	A	222	ASP	N-CA-C	7.93	125.14	114.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	THR	N-CA-C	-7.86	96.09	108.90
1	B	240	GLY	O-C-N	7.84	130.42	123.60
1	A	301	ASP	N-CA-C	7.83	121.37	109.62
1	B	219	THR	CA-C-N	-7.78	106.68	121.54
1	B	219	THR	C-N-CA	-7.78	106.68	121.54
1	A	381	GLY	O-C-N	7.75	131.63	122.64
1	B	222	ASP	N-CA-C	7.75	127.31	110.80
1	A	172	GLY	N-CA-C	-7.64	98.09	111.46
1	A	118	GLU	N-CA-C	7.63	119.60	111.28
1	A	96	THR	N-CA-C	7.52	120.59	109.24
1	B	300	VAL	N-CA-C	7.52	119.41	108.58
1	B	333	ILE	N-CA-C	7.50	118.55	108.27
1	B	139	THR	N-CA-C	-7.50	98.24	109.86
1	B	260	ASP	CB-CA-C	-7.48	97.87	110.43
1	A	95	LYS	N-CA-C	-7.39	97.83	109.07
1	B	342	ILE	N-CA-C	7.37	118.44	106.72
1	A	213	PRO	N-CA-C	7.35	123.98	113.47
1	A	89	THR	CA-C-N	7.35	135.58	121.54
1	A	89	THR	C-N-CA	7.35	135.58	121.54
1	A	381	GLY	CA-C-N	7.30	134.93	122.37
1	A	381	GLY	C-N-CA	7.30	134.93	122.37
1	A	260	ASP	CA-C-N	7.20	130.64	120.28
1	A	260	ASP	C-N-CA	7.20	130.64	120.28
1	A	333	ILE	N-CA-C	7.19	118.47	108.12
1	A	89	THR	O-C-N	-7.12	111.61	123.00
1	B	305	GLU	N-CA-C	7.08	121.63	112.92
1	A	360	ALA	N-CA-C	-7.07	98.57	109.24
1	A	250	ILE	N-CA-CB	-7.06	106.96	111.83
1	A	260	ASP	N-CA-C	7.04	125.79	110.80
1	B	240	GLY	N-CA-C	-7.04	100.86	111.14
1	B	92	LEU	N-CA-C	7.04	119.39	110.24
1	A	92	LEU	N-CA-C	7.03	119.37	110.24
1	B	257	LEU	N-CA-C	7.01	118.93	111.28
1	A	155	ILE	O-C-N	-6.94	115.16	121.41
1	B	217	VAL	N-CA-C	-6.92	98.20	108.99
1	A	126	ALA	N-CA-C	6.89	120.17	109.07
1	A	217	VAL	N-CA-C	-6.88	98.26	108.99
1	B	243	PRO	N-CA-C	-6.86	100.32	111.77
1	B	303	ALA	N-CA-C	-6.85	102.18	112.04
1	A	242	ASP	N-CA-C	-6.84	103.45	113.16
1	B	306	ALA	O-C-N	6.82	130.26	122.55
1	A	307	LEU	N-CA-C	6.68	120.29	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ILE	N-CA-C	6.64	115.21	107.84
1	B	379	SER	CA-C-N	-6.63	113.72	123.93
1	B	379	SER	C-N-CA	-6.63	113.72	123.93
1	A	350	PHE	N-CA-C	6.62	120.19	110.59
1	A	209	THR	N-CA-C	-6.57	97.81	108.52
1	A	322	GLU	N-CA-C	-6.49	102.14	109.60
1	A	232	ASP	N-CA-C	-6.49	96.47	108.02
1	B	103	PRO	N-CA-C	-6.49	99.10	112.47
1	A	258	VAL	N-CA-C	6.45	122.76	109.34
1	B	333	ILE	CA-C-N	6.43	132.69	122.59
1	B	333	ILE	C-N-CA	6.43	132.69	122.59
1	B	261	ALA	N-CA-C	6.42	119.10	111.71
1	B	244	VAL	CA-C-N	-6.41	113.97	123.00
1	B	244	VAL	C-N-CA	-6.41	113.97	123.00
1	B	127	ARG	N-CA-C	-6.36	98.37	108.73
1	A	378	VAL	N-CA-C	6.35	117.06	108.17
1	B	95	LYS	N-CA-C	-6.31	99.08	108.99
1	A	171	THR	N-CA-C	-6.28	97.42	110.80
1	B	136	TYR	N-CA-C	6.24	123.59	109.81
1	B	117	ASN	N-CA-C	6.20	119.62	109.76
1	A	97	ALA	O-C-N	-6.19	115.67	123.17
1	B	219	THR	O-C-N	-6.14	116.03	123.27
1	A	216	GLY	N-CA-C	6.08	119.37	110.80
1	B	280	LYS	N-CA-C	-6.06	100.20	108.38
1	A	340	ARG	CG-CD-NE	6.06	125.33	112.00
1	B	148	THR	CB-CA-C	6.05	122.09	110.17
1	B	260	ASP	CA-C-N	6.05	128.99	120.28
1	B	260	ASP	C-N-CA	6.05	128.99	120.28
1	A	230	ALA	N-CA-C	6.04	118.14	109.14
1	A	154	THR	CA-C-N	-6.02	116.81	123.43
1	A	154	THR	C-N-CA	-6.02	116.81	123.43
1	A	291	THR	N-CA-C	-6.00	98.01	110.80
1	B	278	ILE	N-CA-C	-5.96	99.11	108.23
1	A	229	ILE	N-CA-C	-5.92	99.18	108.95
1	B	154	THR	CA-C-N	-5.92	118.18	123.33
1	B	154	THR	C-N-CA	-5.92	118.18	123.33
1	A	173	GLY	N-CA-C	5.87	119.88	110.90
1	A	135	VAL	N-CA-C	5.85	121.51	109.34
1	A	239	GLN	CB-CA-C	5.85	119.51	109.51
1	B	252	GLU	N-CA-C	5.84	118.40	111.33
1	B	155	ILE	CA-C-N	5.84	125.21	118.85
1	B	155	ILE	C-N-CA	5.84	125.21	118.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	LEU	N-CA-C	-5.81	100.24	109.59
1	B	241	MET	CA-C-N	-5.74	107.78	121.80
1	B	241	MET	C-N-CA	-5.74	107.78	121.80
1	B	244	VAL	N-CA-C	-5.71	99.55	108.86
1	B	380	SER	N-CA-C	5.69	121.76	113.40
1	B	302	ASN	N-CA-C	5.68	118.45	108.56
1	A	321	SER	N-CA-C	5.67	117.80	109.24
1	B	216	GLY	N-CA-C	5.66	119.40	111.19
1	B	214	ILE	N-CA-C	5.64	117.31	109.29
1	B	311	MET	CA-C-N	-5.61	114.29	122.65
1	B	311	MET	C-N-CA	-5.61	114.29	122.65
1	A	214	ILE	N-CA-C	5.61	117.81	109.17
1	A	268	VAL	N-CA-C	5.60	120.98	108.88
1	B	236	ALA	N-CA-C	5.60	116.97	108.07
1	A	271	ARG	N-CA-C	5.60	122.18	109.81
1	A	142	ASP	N-CA-C	5.54	117.61	109.24
1	A	243	PRO	CA-C-N	5.54	130.56	122.69
1	A	243	PRO	C-N-CA	5.54	130.56	122.69
1	A	206	THR	N-CA-C	5.48	120.87	114.62
1	A	150	LEU	N-CA-C	5.45	122.41	110.80
1	A	102	GLY	O-C-N	5.41	127.18	121.77
1	B	340	ARG	CG-CD-NE	5.41	123.90	112.00
1	B	308	LYS	CA-C-N	5.41	125.35	119.78
1	B	308	LYS	C-N-CA	5.41	125.35	119.78
1	B	220	ALA	N-CA-C	5.36	122.21	110.80
1	A	383	PHE	N-CA-C	5.35	116.41	108.60
1	A	322	GLU	CA-C-N	5.33	125.26	119.78
1	A	322	GLU	C-N-CA	5.33	125.26	119.78
1	B	232	ASP	N-CA-C	-5.32	98.54	108.02
1	B	142	ASP	N-CA-C	5.31	117.75	109.52
1	A	320	ALA	CA-C-O	-5.29	115.75	121.36
1	B	291	THR	CB-CA-C	-5.26	110.53	116.63
1	A	304	ASP	CA-C-N	-5.26	115.40	123.07
1	A	304	ASP	C-N-CA	-5.26	115.40	123.07
1	A	303	ALA	N-CA-C	5.25	119.75	112.45
1	A	155	ILE	CB-CA-C	-5.24	104.77	110.37
1	B	322	GLU	N-CA-C	-5.22	103.60	109.60
1	B	358	PHE	N-CA-C	-5.21	105.14	112.12
1	B	206	THR	N-CA-C	5.18	121.83	110.80
1	B	125	GLN	N-CA-C	5.16	115.10	108.34
1	A	357	VAL	N-CA-C	-5.14	98.66	109.34
1	B	310	GLY	N-CA-C	5.04	122.83	113.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLY	CA-C-N	5.03	125.03	120.21
1	A	102	GLY	C-N-CA	5.03	125.03	120.21
1	B	242	ASP	N-CA-CB	5.01	119.28	110.37
1	B	259	LYS	CA-C-N	-5.00	111.76	121.91
1	B	259	LYS	C-N-CA	-5.00	111.76	121.91

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	PRO	Mainchain
1	B	323	PRO	Mainchain
1	B	341	VAL	Peptide

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	2274	0	2342	670	0
1	B	2274	0	2343	658	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4550	0	4685	1295	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 140.

All (1295) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:CD2	1:B:294:LEU:HD12	1.43	1.49
1:B:147:GLY:CA	1:B:212:ALA:HB3	1.45	1.45
1:B:370:GLY:C	1:B:371:LEU:HD23	1.44	1.42
1:A:92:LEU:HD13	1:A:93:GLY:N	1.32	1.41
1:B:187:LEU:HD12	1:B:188:ALA:N	1.38	1.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:HG21	1:B:307:LEU:CD1	1.53	1.38
1:B:92:LEU:HD13	1:B:93:GLY:N	1.32	1.37
1:B:167:LEU:HD12	1:B:168:LEU:N	1.38	1.36
1:A:132:ILE:CD1	1:A:229:ILE:HD11	1.54	1.36
1:B:151:LEU:HD23	1:B:152:ASP:N	1.36	1.36
1:B:147:GLY:HA3	1:B:212:ALA:CB	1.57	1.33
1:B:256:TRP:CH2	1:B:257:LEU:HD22	1.62	1.32
1:A:167:LEU:HD12	1:A:168:LEU:N	1.41	1.32
1:A:317:LEU:HD12	1:A:318:ASN:N	1.44	1.32
1:A:256:TRP:CH2	1:A:257:LEU:HD22	1.65	1.30
1:B:123:ILE:HD13	1:B:125:GLN:NE2	1.44	1.30
1:B:132:ILE:HD11	1:B:229:ILE:CD1	1.60	1.30
1:B:244:VAL:CG2	1:B:307:LEU:HD11	1.61	1.28
1:B:151:LEU:HD23	1:B:151:LEU:C	1.52	1.28
1:A:358:PHE:CD2	1:A:368:ARG:HG2	1.68	1.28
1:B:244:VAL:CG1	1:B:300:VAL:HB	1.64	1.28
1:A:167:LEU:HD12	1:A:167:LEU:C	1.55	1.27
1:A:122:ALA:HB2	1:A:214:ILE:CD1	1.65	1.27
1:B:193:ALA:HA	1:B:196:ARG:CZ	1.65	1.27
1:A:358:PHE:HD2	1:A:368:ARG:CG	1.47	1.25
1:B:291:THR:O	1:B:292:ARG:HD2	1.37	1.24
1:B:198:LEU:HD12	1:B:198:LEU:C	1.54	1.24
1:A:187:LEU:HD12	1:A:188:ALA:N	1.53	1.23
1:A:187:LEU:HD12	1:A:187:LEU:C	1.58	1.23
1:B:167:LEU:HD12	1:B:167:LEU:C	1.62	1.23
1:B:384:LEU:C	1:B:384:LEU:HD23	1.61	1.23
1:A:317:LEU:HD12	1:A:317:LEU:C	1.58	1.22
1:A:327:ILE:C	1:A:327:ILE:HD12	1.55	1.21
1:A:152:ASP:CG	1:A:209:THR:HG22	1.65	1.21
1:A:332:LEU:C	1:A:332:LEU:HD23	1.66	1.21
1:B:187:LEU:HD12	1:B:187:LEU:C	1.60	1.21
1:B:370:GLY:O	1:B:371:LEU:HD23	1.38	1.21
1:A:256:TRP:CZ3	1:A:257:LEU:HD22	1.77	1.20
1:A:165:TYR:CE2	1:A:182:LEU:HD11	1.73	1.20
1:A:132:ILE:HD11	1:A:229:ILE:CD1	1.72	1.19
1:A:283:LEU:HD21	1:A:294:LEU:CD1	1.71	1.19
1:A:122:ALA:CB	1:A:214:ILE:HD11	1.74	1.18
1:B:181:ILE:CB	1:B:184:ARG:HH21	1.57	1.18
1:A:94:VAL:CG1	1:A:95:LYS:N	2.03	1.17
1:B:158:TRP:O	1:B:162:GLN:HG3	1.40	1.17
1:B:123:ILE:O	1:B:123:ILE:HD12	1.40	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:CD2	1:B:294:LEU:CD1	2.22	1.17
1:A:283:LEU:CD2	1:A:294:LEU:HD13	1.74	1.17
1:B:246:VAL:CG2	1:B:298:LEU:HB2	1.76	1.16
1:A:347:ASP:HB2	1:A:349:ARG:HG2	1.21	1.15
1:A:106:PHE:CE2	1:B:253:SER:HA	1.82	1.15
1:A:178:THR:O	1:A:181:ILE:HG22	1.47	1.15
1:B:269:PRO:HD2	1:B:312:ASN:O	1.44	1.15
1:B:283:LEU:HD21	1:B:294:LEU:CD1	1.75	1.15
1:A:193:ALA:HA	1:A:196:ARG:HH11	0.98	1.15
1:A:327:ILE:HD12	1:A:328:PRO:N	1.61	1.15
1:B:256:TRP:CZ3	1:B:257:LEU:HD22	1.81	1.15
1:A:256:TRP:CH2	1:A:257:LEU:CD2	2.30	1.14
1:A:193:ALA:HA	1:A:196:ARG:NH1	1.62	1.14
1:A:250:ILE:HG22	1:A:254:ILE:HG23	1.22	1.14
1:A:256:TRP:CZ2	1:A:257:LEU:CD2	2.30	1.13
1:B:256:TRP:CZ2	1:B:257:LEU:CD2	2.30	1.13
1:A:274:LYS:O	1:A:275:THR:HG23	1.44	1.13
1:B:339:GLN:C	1:B:340:ARG:HG3	1.74	1.13
1:A:95:LYS:HB3	1:A:380:SER:HB3	1.29	1.13
1:B:276:LEU:N	1:B:276:LEU:HD23	1.62	1.12
1:A:186:ARG:HG2	1:A:195:ILE:HD12	1.18	1.12
1:B:193:ALA:CB	1:B:196:ARG:HH22	1.60	1.12
1:A:123:ILE:HD12	1:A:123:ILE:O	1.44	1.12
1:A:251:PRO:HD2	1:A:254:ILE:CG2	1.77	1.12
1:B:150:LEU:HD23	1:B:150:LEU:O	1.47	1.12
1:B:256:TRP:CH2	1:B:257:LEU:CD2	2.30	1.12
1:B:123:ILE:CD1	1:B:125:GLN:HE21	1.62	1.11
1:B:244:VAL:CG2	1:B:307:LEU:HD21	1.80	1.11
1:B:347:ASP:HB2	1:B:349:ARG:HG2	1.18	1.11
1:B:132:ILE:HD11	1:B:229:ILE:HD11	1.16	1.10
1:B:158:TRP:C	1:B:162:GLN:HE21	1.58	1.10
1:B:382:LEU:HD23	1:B:382:LEU:N	1.66	1.09
1:A:284:LEU:N	1:A:284:LEU:HD23	1.65	1.09
1:B:219:THR:O	1:B:220:ALA:HB3	1.48	1.08
1:B:181:ILE:HA	1:B:184:ARG:NE	1.67	1.08
1:B:153:LEU:N	1:B:153:LEU:HD23	1.63	1.08
1:B:193:ALA:HB2	1:B:196:ARG:HH22	1.17	1.08
1:B:181:ILE:HA	1:B:184:ARG:HE	1.06	1.07
1:A:153:LEU:H	1:A:153:LEU:CD2	1.63	1.07
1:A:384:LEU:HD23	1:A:384:LEU:N	1.65	1.07
1:A:332:LEU:HD23	1:A:332:LEU:O	1.52	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLN:C	1:A:340:ARG:HG3	1.75	1.06
1:A:218:ILE:HG21	1:A:221:PHE:HB2	1.31	1.06
1:A:90:GLN:HA	1:A:383:PHE:HB2	1.34	1.05
1:A:90:GLN:HA	1:A:383:PHE:CB	1.87	1.04
1:B:153:LEU:HD23	1:B:153:LEU:H	1.09	1.04
1:B:193:ALA:N	1:B:196:ARG:HH12	1.55	1.04
1:B:244:VAL:HG23	1:B:307:LEU:HD21	1.35	1.04
1:B:181:ILE:HG13	1:B:184:ARG:NH2	1.73	1.04
1:B:193:ALA:HA	1:B:196:ARG:NH2	1.70	1.04
1:A:132:ILE:CD1	1:A:229:ILE:CD1	2.32	1.03
1:A:162:GLN:HE22	1:A:205:GLN:HB2	1.19	1.03
1:A:94:VAL:HG12	1:A:95:LYS:N	1.71	1.03
1:A:177:GLN:OE1	1:A:177:GLN:HA	1.54	1.03
1:A:90:GLN:HG3	1:A:383:PHE:CD1	1.93	1.03
1:A:94:VAL:HG13	1:A:95:LYS:H	1.22	1.03
1:A:150:LEU:C	1:A:151:LEU:HD23	1.84	1.03
1:A:167:LEU:C	1:A:167:LEU:CD1	2.30	1.03
1:A:251:PRO:CD	1:A:254:ILE:HG21	1.89	1.03
1:A:153:LEU:HD22	1:A:153:LEU:N	1.52	1.02
1:B:121:TYR:HD2	1:B:121:TYR:O	1.38	1.02
1:B:174:THR:OG1	1:B:177:GLN:HB2	1.59	1.02
1:A:187:LEU:C	1:A:187:LEU:CD1	2.30	1.02
1:B:198:LEU:HD12	1:B:198:LEU:O	1.57	1.02
1:A:384:LEU:H	1:A:384:LEU:CD2	1.73	1.02
1:B:193:ALA:HA	1:B:196:ARG:NH1	1.74	1.02
1:B:256:TRP:CE3	1:B:256:TRP:C	2.38	1.02
1:B:151:LEU:C	1:B:151:LEU:CD2	2.30	1.02
1:B:382:LEU:HD23	1:B:382:LEU:H	1.19	1.02
1:A:276:LEU:N	1:A:276:LEU:HD23	1.73	1.01
1:B:256:TRP:CZ2	1:B:257:LEU:HD22	1.94	1.01
1:A:327:ILE:C	1:A:327:ILE:CD1	2.30	1.01
1:A:351:VAL:HG23	1:A:352:PRO:HD2	1.42	1.01
1:A:384:LEU:HD23	1:A:384:LEU:H	0.88	1.01
1:A:186:ARG:HG2	1:A:195:ILE:CD1	1.90	1.01
1:A:231:LYS:HG3	1:A:232:ASP:H	1.24	1.01
1:A:162:GLN:NE2	1:A:205:GLN:HB2	1.75	1.00
1:A:283:LEU:HD21	1:A:294:LEU:HD12	1.38	1.00
1:A:334:ASP:HB3	1:A:339:GLN:HE21	1.24	1.00
1:B:334:ASP:HB3	1:B:339:GLN:HE21	1.23	1.00
1:A:150:LEU:O	1:A:151:LEU:HB3	1.61	1.00
1:A:122:ALA:HB2	1:A:214:ILE:HD13	1.39	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:CA	1:B:184:ARG:HH21	1.74	1.00
1:A:256:TRP:CE3	1:A:256:TRP:C	2.40	0.99
1:B:90:GLN:HG2	1:B:350:PHE:CD2	1.97	0.99
1:B:231:LYS:HG3	1:B:232:ASP:H	1.23	0.99
1:A:122:ALA:HB2	1:A:214:ILE:HD11	1.35	0.99
1:A:106:PHE:HE2	1:B:253:SER:HA	1.23	0.99
1:B:89:THR:C	1:B:90:GLN:CD	2.30	0.99
1:A:321:SER:HB3	1:B:256:TRP:CD1	1.96	0.99
1:B:244:VAL:HB	1:B:307:LEU:CD2	1.93	0.99
1:A:175:ALA:O	1:A:178:THR:HG23	1.61	0.98
1:A:317:LEU:C	1:A:317:LEU:CD1	2.29	0.98
1:A:327:ILE:CD1	1:A:329:SER:N	2.26	0.98
1:A:370:GLY:C	1:A:371:LEU:HD23	1.88	0.98
1:B:151:LEU:CD2	1:B:152:ASP:N	2.25	0.98
1:A:331:ALA:HB2	1:A:378:VAL:O	1.62	0.98
1:A:121:TYR:HD2	1:A:121:TYR:O	1.46	0.98
1:B:370:GLY:O	1:B:371:LEU:CD2	2.10	0.98
1:A:153:LEU:HD23	1:A:153:LEU:O	1.61	0.98
1:B:123:ILE:HD13	1:B:125:GLN:HE21	0.94	0.98
1:B:121:TYR:C	1:B:121:TYR:CD2	2.38	0.98
1:B:178:THR:O	1:B:182:LEU:HD13	1.62	0.98
1:B:187:LEU:C	1:B:187:LEU:CD1	2.30	0.98
1:A:156:PRO:O	1:A:159:VAL:HG22	1.62	0.97
1:A:94:VAL:CG1	1:A:95:LYS:H	1.72	0.97
1:A:256:TRP:CZ2	1:A:257:LEU:HD22	1.94	0.97
1:B:132:ILE:HD13	1:B:227:MET:HB2	1.45	0.97
1:B:198:LEU:C	1:B:198:LEU:CD1	2.30	0.97
1:A:250:ILE:HG22	1:A:254:ILE:CG2	1.94	0.97
1:B:92:LEU:HD13	1:B:93:GLY:H	1.30	0.97
1:B:92:LEU:CD1	1:B:93:GLY:N	2.26	0.97
1:A:231:LYS:CG	1:A:232:ASP:H	1.75	0.97
1:A:140:VAL:HG22	1:A:221:PHE:O	1.64	0.96
1:A:358:PHE:HD2	1:A:368:ARG:HG2	0.82	0.96
1:A:164:GLU:C	1:A:164:GLU:CD	2.30	0.96
1:A:92:LEU:CD1	1:A:93:GLY:N	2.26	0.96
1:A:317:LEU:HD12	1:A:318:ASN:CA	1.95	0.96
1:B:244:VAL:CB	1:B:307:LEU:HD21	1.96	0.96
1:A:136:TYR:HB3	1:A:137:PRO:HD2	1.48	0.96
1:A:228:ASN:C	1:A:229:ILE:HD12	1.90	0.96
1:B:167:LEU:C	1:B:167:LEU:CD1	2.35	0.96
1:A:266:LEU:HD13	1:A:267:THR:N	1.80	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:HD23	1:B:294:LEU:CD1	1.94	0.96
1:B:126:ALA:O	1:B:232:ASP:HA	1.66	0.96
1:B:183:GLU:HA	1:B:186:ARG:NH1	1.81	0.95
1:B:132:ILE:CD1	1:B:229:ILE:HD11	1.94	0.95
1:B:280:LYS:HG2	1:B:299:GLU:HB3	1.48	0.95
1:A:251:PRO:HD2	1:A:254:ILE:HG21	0.98	0.95
1:B:167:LEU:CD1	1:B:168:LEU:N	2.30	0.95
1:A:193:ALA:CA	1:A:196:ARG:HH11	1.78	0.95
1:A:266:LEU:CD1	1:A:267:THR:N	2.30	0.95
1:B:256:TRP:O	1:B:256:TRP:HE3	1.48	0.95
1:A:122:ALA:CB	1:A:214:ILE:CD1	2.37	0.95
1:B:181:ILE:CB	1:B:184:ARG:NH2	2.30	0.95
1:A:351:VAL:HG23	1:A:352:PRO:CD	1.94	0.94
1:B:192:GLU:C	1:B:196:ARG:HH12	1.75	0.94
1:B:165:TYR:CD2	1:B:182:LEU:HD11	2.02	0.94
1:B:181:ILE:CG1	1:B:184:ARG:NH2	2.30	0.94
1:B:278:ILE:N	1:B:278:ILE:HD12	1.83	0.94
1:B:194:ASP:OD2	1:B:208:PHE:CD2	2.21	0.94
1:A:250:ILE:CG2	1:A:254:ILE:HG23	1.96	0.94
1:A:283:LEU:CD2	1:A:294:LEU:CD1	2.37	0.94
1:A:358:PHE:HD1	1:A:359:GLN:HG2	1.31	0.94
1:B:132:ILE:CD1	1:B:229:ILE:CD1	2.45	0.94
1:B:153:LEU:N	1:B:153:LEU:CD2	2.29	0.94
1:B:193:ALA:CB	1:B:196:ARG:NH2	2.30	0.94
1:B:367:LEU:CD1	1:B:367:LEU:N	2.31	0.94
1:A:135:VAL:HG11	1:A:224:ARG:HB2	1.50	0.94
1:A:327:ILE:HD11	1:A:329:SER:N	1.82	0.94
1:A:152:ASP:OD2	1:A:209:THR:HG22	1.68	0.93
1:B:121:TYR:HD2	1:B:121:TYR:C	1.71	0.93
1:B:194:ASP:OD2	1:B:208:PHE:HD2	1.51	0.93
1:A:193:ALA:CA	1:A:196:ARG:NH1	2.30	0.93
1:B:384:LEU:C	1:B:384:LEU:CD2	2.38	0.93
1:B:244:VAL:HG12	1:B:300:VAL:O	1.69	0.93
1:B:246:VAL:HG22	1:B:298:LEU:HB2	1.47	0.93
1:A:167:LEU:CD1	1:A:168:LEU:N	2.31	0.93
1:B:193:ALA:CA	1:B:196:ARG:NH2	2.31	0.93
1:B:219:THR:O	1:B:220:ALA:CB	2.13	0.93
1:B:384:LEU:HD23	1:B:385:ILE:O	1.68	0.93
1:B:187:LEU:CD1	1:B:188:ALA:N	2.30	0.93
1:B:116:TYR:CE2	1:B:309:PRO:HG2	2.04	0.93
1:B:291:THR:O	1:B:292:ARG:CD	2.16	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLN:HA	1:B:205:GLN:OE1	1.65	0.92
1:A:138:LEU:HB2	1:A:221:PHE:CE1	2.05	0.92
1:A:132:ILE:HD11	1:A:229:ILE:HD11	0.94	0.92
1:A:358:PHE:CD2	1:A:368:ARG:CG	2.36	0.92
1:B:165:TYR:CD1	1:B:165:TYR:C	2.48	0.91
1:B:244:VAL:HG21	1:B:307:LEU:HD11	0.92	0.91
1:B:334:ASP:HB2	1:B:338:GLU:O	1.69	0.91
1:A:244:VAL:CG2	1:A:302:ASN:HB2	1.99	0.91
1:B:97:ALA:CB	1:B:328:PRO:HG2	2.00	0.91
1:A:186:ARG:CG	1:A:195:ILE:HD12	2.00	0.91
1:A:95:LYS:CB	1:A:380:SER:HB3	2.00	0.91
1:B:187:LEU:HD12	1:B:188:ALA:CA	2.00	0.91
1:A:256:TRP:HE3	1:A:256:TRP:O	1.53	0.91
1:B:256:TRP:C	1:B:256:TRP:HE3	1.76	0.91
1:B:220:ALA:HB3	1:B:237:LYS:HB2	1.53	0.90
1:B:167:LEU:HD12	1:B:168:LEU:CA	2.02	0.90
1:A:151:LEU:C	1:A:152:ASP:OD1	2.15	0.90
1:A:256:TRP:CZ2	1:A:257:LEU:HD21	2.04	0.90
1:B:174:THR:O	1:B:178:THR:HG23	1.71	0.90
1:A:319:THR:CG2	1:A:320:ALA:N	2.34	0.89
1:B:192:GLU:C	1:B:196:ARG:NH1	2.30	0.89
1:B:244:VAL:CG2	1:B:307:LEU:CD2	2.49	0.89
1:A:256:TRP:CD1	1:B:321:SER:HB3	2.07	0.89
1:A:321:SER:CB	1:B:256:TRP:CD1	2.55	0.89
1:A:317:LEU:CD1	1:A:318:ASN:N	2.33	0.89
1:B:181:ILE:HB	1:B:184:ARG:HH21	1.36	0.89
1:B:231:LYS:CG	1:B:232:ASP:H	1.84	0.89
1:A:384:LEU:N	1:A:384:LEU:CD2	2.31	0.89
1:A:327:ILE:CD1	1:A:328:PRO:C	2.46	0.89
1:A:334:ASP:HB2	1:A:338:GLU:O	1.72	0.89
1:B:370:GLY:C	1:B:371:LEU:CD2	2.41	0.89
1:B:244:VAL:HB	1:B:307:LEU:HD22	1.54	0.89
1:A:228:ASN:O	1:A:229:ILE:HD12	1.74	0.88
1:A:327:ILE:CD1	1:A:328:PRO:N	2.36	0.88
1:B:178:THR:O	1:B:181:ILE:HG22	1.72	0.88
1:A:121:TYR:C	1:A:121:TYR:CD2	2.47	0.88
1:B:159:VAL:HA	1:B:162:GLN:NE2	1.88	0.88
1:B:371:LEU:HD23	1:B:371:LEU:N	1.83	0.88
1:A:256:TRP:C	1:A:256:TRP:HE3	1.79	0.88
1:B:269:PRO:CD	1:B:312:ASN:O	2.21	0.88
1:B:276:LEU:N	1:B:276:LEU:CD2	2.35	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PHE:HD1	1:B:359:GLN:HG2	1.35	0.88
1:A:124:VAL:HG12	1:A:235:VAL:HB	1.54	0.88
1:B:183:GLU:HA	1:B:186:ARG:HH12	1.35	0.88
1:A:198:LEU:HB2	1:A:205:GLN:HG2	1.55	0.88
1:A:164:GLU:OE1	1:A:165:TYR:HA	1.74	0.87
1:A:186:ARG:CG	1:A:195:ILE:CD1	2.52	0.87
1:B:127:ARG:O	1:B:128:ALA:CB	2.20	0.87
1:A:92:LEU:HD13	1:A:93:GLY:H	1.30	0.87
1:B:181:ILE:CA	1:B:184:ARG:HE	1.88	0.87
1:A:167:LEU:HD12	1:A:168:LEU:CA	2.05	0.86
1:A:244:VAL:HG21	1:A:307:LEU:CD1	2.05	0.86
1:A:250:ILE:O	1:A:293:THR:CG2	2.23	0.86
1:A:256:TRP:CZ3	1:A:257:LEU:HA	2.09	0.86
1:A:128:ALA:HB2	1:A:158:TRP:HZ2	1.40	0.86
1:B:193:ALA:CA	1:B:196:ARG:NH1	2.39	0.86
1:B:280:LYS:HG3	1:B:281:TRP:N	1.88	0.86
1:B:132:ILE:HD12	1:B:227:MET:O	1.76	0.86
1:B:219:THR:OG1	1:B:237:LYS:HE2	1.75	0.86
1:B:342:ILE:O	1:B:342:ILE:HG22	1.75	0.86
1:A:234:VAL:HG22	1:A:236:ALA:CA	2.04	0.85
1:B:203:LYS:O	1:B:203:LYS:HE2	1.75	0.85
1:B:132:ILE:HD12	1:B:132:ILE:N	1.91	0.85
1:B:273:ASP:CG	1:B:274:LYS:H	1.84	0.85
1:A:140:VAL:HA	1:A:221:PHE:HB3	1.56	0.85
1:B:174:THR:OG1	1:B:177:GLN:CB	2.24	0.85
1:B:162:GLN:OE1	1:B:205:GLN:HB2	1.77	0.85
1:A:121:TYR:O	1:A:121:TYR:CD2	2.30	0.85
1:B:151:LEU:HD23	1:B:152:ASP:CA	2.07	0.85
1:A:106:PHE:CD2	1:B:253:SER:HA	2.11	0.85
1:A:287:VAL:HG23	1:A:287:VAL:O	1.74	0.84
1:B:92:LEU:HD13	1:B:92:LEU:C	2.01	0.84
1:A:165:TYR:CE2	1:A:182:LEU:CD1	2.58	0.84
1:B:340:ARG:HG2	1:B:354:ARG:HA	1.58	0.84
1:A:244:VAL:HG21	1:A:307:LEU:HD13	1.59	0.84
1:B:132:ILE:HD12	1:B:132:ILE:H	1.43	0.84
1:A:162:GLN:HE22	1:A:205:GLN:CB	1.89	0.84
1:B:317:LEU:HD12	1:B:318:ASN:H	1.40	0.84
1:A:92:LEU:HD13	1:A:92:LEU:C	2.01	0.84
1:A:106:PHE:CD2	1:B:253:SER:CA	2.61	0.84
1:A:331:ALA:CB	1:A:378:VAL:O	2.25	0.84
1:B:181:ILE:HG22	1:B:182:LEU:HD12	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ILE:HD12	1:B:278:ILE:H	1.43	0.84
1:B:347:ASP:CB	1:B:349:ARG:HG2	2.04	0.84
1:A:112:ALA:HA	1:A:247:THR:O	1.78	0.84
1:A:266:LEU:HD13	1:A:267:THR:H	1.39	0.84
1:A:266:LEU:CD1	1:A:266:LEU:C	2.51	0.84
1:B:367:LEU:N	1:B:367:LEU:HD12	1.91	0.84
1:A:150:LEU:HB3	1:A:151:LEU:HD23	1.57	0.83
1:A:167:LEU:O	1:A:171:THR:HG23	1.78	0.83
1:A:317:LEU:CD1	1:A:318:ASN:O	2.26	0.83
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.39	0.83
1:B:244:VAL:HG11	1:B:300:VAL:HB	1.56	0.83
1:B:379:SER:O	1:B:380:SER:HB3	1.77	0.83
1:A:319:THR:HG22	1:A:320:ALA:N	1.91	0.83
1:A:283:LEU:C	1:A:284:LEU:HD23	2.03	0.83
1:A:319:THR:HG23	1:A:320:ALA:H	1.41	0.83
1:A:256:TRP:CE3	1:A:257:LEU:HD22	2.14	0.83
1:A:327:ILE:HD12	1:A:328:PRO:CA	2.09	0.83
1:B:244:VAL:CG1	1:B:300:VAL:CB	2.55	0.83
1:A:284:LEU:N	1:A:284:LEU:CD2	2.42	0.82
1:A:327:ILE:HD12	1:A:328:PRO:C	2.04	0.82
1:A:358:PHE:CD1	1:A:359:GLN:HG2	2.13	0.82
1:B:121:TYR:O	1:B:121:TYR:CD2	2.29	0.82
1:B:384:LEU:HD23	1:B:385:ILE:N	1.93	0.82
1:A:135:VAL:HG12	1:A:135:VAL:O	1.80	0.82
1:B:256:TRP:CZ3	1:B:257:LEU:HA	2.14	0.82
1:A:140:VAL:HG22	1:A:221:PHE:C	2.04	0.82
1:B:164:GLU:OE1	1:B:165:TYR:HA	1.80	0.82
1:B:165:TYR:HD1	1:B:166:LEU:N	1.77	0.82
1:B:256:TRP:CZ2	1:B:257:LEU:HD21	2.14	0.82
1:A:256:TRP:CE3	1:A:257:LEU:HA	2.12	0.82
1:A:133:ASP:HB2	1:A:152:ASP:O	1.80	0.82
1:A:150:LEU:C	1:A:151:LEU:CD2	2.52	0.82
1:A:174:THR:OG1	1:A:177:GLN:HB2	1.80	0.82
1:B:117:ASN:HB3	1:B:245:TRP:NE1	1.95	0.82
1:B:256:TRP:CE3	1:B:257:LEU:HA	2.13	0.82
1:A:319:THR:CG2	1:A:320:ALA:H	1.91	0.81
1:B:345:ASP:C	1:B:347:ASP:H	1.88	0.81
1:A:106:PHE:CE2	1:B:253:SER:CA	2.63	0.81
1:A:153:LEU:H	1:A:153:LEU:HD22	0.72	0.81
1:B:283:LEU:O	1:B:285:PRO:HD3	1.79	0.81
1:A:122:ALA:HB3	1:A:214:ILE:HD11	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:CB	1:A:221:PHE:CE1	2.63	0.81
1:B:276:LEU:HD23	1:B:276:LEU:H	1.45	0.81
1:A:283:LEU:O	1:A:285:PRO:HD3	1.80	0.81
1:B:244:VAL:HG12	1:B:300:VAL:HB	1.62	0.81
1:A:192:GLU:O	1:A:196:ARG:HG3	1.80	0.81
1:B:181:ILE:CG2	1:B:182:LEU:HD12	2.10	0.81
1:B:165:TYR:CE2	1:B:182:LEU:HD11	2.16	0.81
1:A:278:ILE:HG23	1:A:298:LEU:HD22	1.62	0.81
1:B:89:THR:O	1:B:90:GLN:HG3	1.80	0.81
1:B:132:ILE:CD1	1:B:227:MET:O	2.28	0.81
1:B:283:LEU:HD21	1:B:294:LEU:HD12	0.83	0.81
1:B:246:VAL:HG23	1:B:246:VAL:O	1.78	0.81
1:B:123:ILE:CD1	1:B:125:GLN:NE2	2.30	0.80
1:A:198:LEU:HD12	1:A:203:LYS:O	1.81	0.80
1:B:94:VAL:HG12	1:B:95:LYS:N	1.96	0.80
1:B:382:LEU:N	1:B:382:LEU:CD2	2.41	0.80
1:B:89:THR:O	1:B:90:GLN:CG	2.30	0.80
1:B:193:ALA:CA	1:B:196:ARG:HH22	1.92	0.80
1:A:317:LEU:CD1	1:A:318:ASN:C	2.55	0.80
1:A:347:ASP:CB	1:A:349:ARG:HG2	2.09	0.80
1:B:384:LEU:CD2	1:B:385:ILE:O	2.30	0.80
1:A:253:SER:HB3	1:B:106:PHE:HD2	1.47	0.80
1:B:127:ARG:O	1:B:128:ALA:HB2	1.80	0.80
1:B:132:ILE:HD13	1:B:227:MET:CB	2.12	0.79
1:B:181:ILE:HA	1:B:184:ARG:CZ	2.12	0.79
1:A:150:LEU:O	1:A:151:LEU:CB	2.27	0.79
1:A:153:LEU:CD2	1:A:153:LEU:O	2.30	0.79
1:A:175:ALA:O	1:A:178:THR:CG2	2.30	0.79
1:B:193:ALA:N	1:B:196:ARG:NH1	2.30	0.79
1:A:140:VAL:CG2	1:A:221:PHE:O	2.30	0.79
1:A:258:VAL:O	1:A:259:LYS:HB2	1.79	0.79
1:B:244:VAL:CB	1:B:307:LEU:CD2	2.57	0.79
1:A:89:THR:C	1:A:90:GLN:CD	2.50	0.79
1:A:144:VAL:HG21	1:A:238:ILE:HD13	1.63	0.79
1:A:167:LEU:HD11	1:A:168:LEU:HD12	1.65	0.79
1:A:177:GLN:OE1	1:A:177:GLN:CA	2.30	0.79
1:B:343:THR:HB	1:B:351:VAL:HG13	1.65	0.79
1:A:253:SER:HA	1:B:106:PHE:HE2	1.47	0.79
1:B:178:THR:O	1:B:182:LEU:CD1	2.30	0.79
1:A:137:PRO:C	1:A:138:LEU:HD22	2.08	0.78
1:B:95:LYS:HB3	1:B:379:SER:O	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:CG2	1:B:246:VAL:O	2.31	0.78
1:B:116:TYR:CE2	1:B:309:PRO:CG	2.65	0.78
1:B:244:VAL:HG21	1:B:307:LEU:HD13	1.65	0.78
1:B:273:ASP:OD1	1:B:274:LYS:N	2.16	0.78
1:A:160:GLU:OE2	1:A:161:ALA:HA	1.83	0.78
1:A:210:LEU:O	1:A:210:LEU:HD12	1.84	0.78
1:A:327:ILE:HD12	1:A:329:SER:N	1.97	0.78
1:B:219:THR:O	1:B:237:LYS:HB2	1.83	0.78
1:A:128:ALA:HB2	1:A:158:TRP:CZ2	2.19	0.78
1:B:181:ILE:CA	1:B:184:ARG:NH2	2.46	0.78
1:A:234:VAL:HG22	1:A:236:ALA:N	1.99	0.78
1:A:287:VAL:O	1:A:287:VAL:CG2	2.30	0.78
1:B:250:ILE:HG22	1:B:251:PRO:N	1.99	0.78
1:A:92:LEU:HD13	1:A:93:GLY:CA	2.13	0.78
1:A:256:TRP:CE2	1:A:257:LEU:CD2	2.66	0.78
1:A:275:THR:C	1:A:276:LEU:HD23	2.08	0.78
1:A:251:PRO:CD	1:A:254:ILE:CG2	2.55	0.78
1:A:317:LEU:HD11	1:A:318:ASN:O	1.84	0.77
1:A:185:LEU:HD11	1:A:190:MET:HG3	1.65	0.77
1:A:234:VAL:HG22	1:A:236:ALA:H	1.48	0.77
1:A:174:THR:OG1	1:A:177:GLN:CB	2.33	0.77
1:A:187:LEU:HD12	1:A:188:ALA:CA	2.15	0.77
1:B:92:LEU:HD13	1:B:93:GLY:CA	2.13	0.77
1:A:351:VAL:CG2	1:A:352:PRO:CD	2.62	0.77
1:B:334:ASP:C	1:B:334:ASP:OD1	2.27	0.77
1:B:159:VAL:N	1:B:162:GLN:HE21	1.81	0.77
1:B:244:VAL:HG13	1:B:300:VAL:HB	1.62	0.77
1:A:201:THR:O	1:A:202:GLN:C	2.28	0.77
1:A:277:THR:OG1	1:A:301:ASP:HB2	1.84	0.77
1:A:321:SER:O	1:A:322:GLU:C	2.27	0.77
1:B:193:ALA:CA	1:B:196:ARG:CZ	2.55	0.77
1:A:138:LEU:HB2	1:A:221:PHE:HE1	1.49	0.77
1:B:244:VAL:CG2	1:B:307:LEU:CD1	2.35	0.77
1:A:228:ASN:C	1:A:229:ILE:CD1	2.58	0.77
1:A:256:TRP:CE3	1:A:257:LEU:N	2.53	0.77
1:A:265:THR:HB	1:A:316:GLN:HG2	1.65	0.76
1:B:244:VAL:HB	1:B:307:LEU:HD21	1.63	0.76
1:B:372:ALA:O	1:B:375:GLU:HB2	1.86	0.76
1:B:132:ILE:CD1	1:B:227:MET:C	2.59	0.76
1:A:90:GLN:CA	1:A:383:PHE:HB2	2.15	0.76
1:A:123:ILE:O	1:A:123:ILE:CD1	2.30	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LEU:HD12	1:B:318:ASN:N	2.00	0.76
1:A:147:GLY:HA3	1:A:212:ALA:N	2.00	0.76
1:A:147:GLY:HA3	1:A:212:ALA:O	1.84	0.76
1:A:332:LEU:O	1:A:332:LEU:CD2	2.33	0.76
1:B:147:GLY:HA2	1:B:212:ALA:HB3	1.65	0.76
1:A:274:LYS:O	1:A:275:THR:CG2	2.30	0.76
1:B:256:TRP:CE3	1:B:257:LEU:N	2.54	0.76
1:A:250:ILE:O	1:A:293:THR:HG22	1.85	0.75
1:B:147:GLY:HA3	1:B:212:ALA:HB3	0.76	0.75
1:B:150:LEU:O	1:B:151:LEU:CB	2.32	0.75
1:A:164:GLU:O	1:A:167:LEU:HG	1.85	0.75
1:B:165:TYR:HD2	1:B:182:LEU:HD11	1.51	0.75
1:A:90:GLN:HG2	1:A:350:PHE:CD2	2.21	0.75
1:A:171:THR:OG1	1:A:172:GLY:N	2.11	0.75
1:B:198:LEU:O	1:B:198:LEU:CD1	2.30	0.75
1:A:218:ILE:CG2	1:A:221:PHE:HB2	2.14	0.75
1:A:332:LEU:C	1:A:332:LEU:CD2	2.42	0.75
1:A:334:ASP:CB	1:A:339:GLN:HE21	1.98	0.75
1:B:245:TRP:CZ3	1:B:297:ARG:CZ	2.70	0.75
1:B:246:VAL:HG21	1:B:298:LEU:HB2	1.66	0.75
1:A:136:TYR:HB3	1:A:137:PRO:CD	2.16	0.75
1:A:164:GLU:C	1:A:164:GLU:OE1	2.30	0.75
1:A:165:TYR:HB2	1:A:181:ILE:HD13	1.67	0.75
1:A:370:GLY:O	1:A:371:LEU:HD23	1.85	0.75
1:A:132:ILE:O	1:A:226:GLY:HA2	1.86	0.75
1:A:231:LYS:CG	1:A:232:ASP:N	2.49	0.75
1:A:258:VAL:HG12	1:A:259:LYS:N	2.02	0.75
1:A:345:ASP:C	1:A:347:ASP:H	1.93	0.75
1:B:135:VAL:O	1:B:136:TYR:HB2	1.87	0.75
1:A:121:TYR:HD2	1:A:121:TYR:C	1.88	0.75
1:A:261:ALA:O	1:A:264:PHE:HB2	1.87	0.75
1:A:185:LEU:HD21	1:A:190:MET:SD	2.26	0.75
1:B:217:VAL:O	1:B:238:ILE:HG23	1.87	0.75
1:A:160:GLU:OE2	1:A:160:GLU:C	2.30	0.74
1:B:158:TRP:O	1:B:162:GLN:CG	2.30	0.74
1:A:277:THR:OG1	1:A:301:ASP:CB	2.35	0.74
1:B:132:ILE:CD1	1:B:227:MET:HB2	2.17	0.74
1:A:91:ASN:OD1	1:A:92:LEU:N	2.21	0.74
1:A:327:ILE:HD12	1:A:327:ILE:O	1.87	0.74
1:A:317:LEU:HD12	1:A:318:ASN:C	2.11	0.74
1:B:123:ILE:O	1:B:123:ILE:CD1	2.30	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HD13	1:B:351:VAL:O	1.87	0.74
1:A:146:LYS:C	1:A:212:ALA:O	2.31	0.74
1:A:256:TRP:CE2	1:A:257:LEU:HD22	2.22	0.74
1:A:217:VAL:O	1:A:238:ILE:HG23	1.87	0.74
1:A:234:VAL:HG22	1:A:236:ALA:HA	1.68	0.74
1:A:244:VAL:HG21	1:A:302:ASN:HB2	1.69	0.74
1:A:253:SER:HA	1:B:106:PHE:CE2	2.23	0.74
1:A:334:ASP:OD1	1:A:334:ASP:C	2.31	0.74
1:B:132:ILE:HD13	1:B:227:MET:C	2.12	0.74
1:B:184:ARG:O	1:B:187:LEU:HG	1.88	0.74
1:A:280:LYS:CE	1:A:281:TRP:H	2.01	0.73
1:B:147:GLY:CA	1:B:212:ALA:CB	2.39	0.73
1:B:192:GLU:CD	1:B:196:ARG:HH11	1.96	0.73
1:A:106:PHE:HD2	1:B:253:SER:HB3	1.53	0.73
1:B:89:THR:O	1:B:90:GLN:CD	2.30	0.73
1:A:153:LEU:CD2	1:A:153:LEU:N	2.31	0.73
1:A:149:PRO:HG2	1:A:150:LEU:H	1.53	0.73
1:A:266:LEU:C	1:A:266:LEU:HD12	2.14	0.73
1:A:282:THR:HG23	1:A:297:ARG:HB3	1.68	0.73
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.02	0.73
1:B:256:TRP:CE2	1:B:257:LEU:CD2	2.72	0.73
1:B:132:ILE:HD11	1:B:229:ILE:HD13	1.67	0.73
1:A:351:VAL:CG2	1:A:352:PRO:HD2	2.19	0.73
1:B:321:SER:O	1:B:322:GLU:C	2.26	0.73
1:A:266:LEU:HD12	1:A:267:THR:N	2.02	0.73
1:A:276:LEU:N	1:A:276:LEU:CD2	2.42	0.73
1:A:164:GLU:OE1	1:A:165:TYR:CA	2.38	0.72
1:A:263:GLN:O	1:A:263:GLN:HG3	1.89	0.72
1:B:164:GLU:C	1:B:164:GLU:CD	2.56	0.72
1:A:139:THR:O	1:A:140:VAL:HB	1.90	0.72
1:A:290:ALA:O	1:A:291:THR:CB	2.37	0.72
1:A:145:GLN:HA	1:A:215:ASP:HA	1.72	0.72
1:A:165:TYR:CD2	1:A:182:LEU:HD11	2.24	0.72
1:A:90:GLN:CG	1:A:383:PHE:CD1	2.70	0.72
1:B:132:ILE:HD13	1:B:227:MET:CA	2.20	0.72
1:B:164:GLU:OE1	1:B:164:GLU:C	2.33	0.72
1:B:164:GLU:O	1:B:167:LEU:HG	1.90	0.71
1:A:90:GLN:HA	1:A:383:PHE:HB3	1.69	0.71
1:A:219:THR:CG2	1:A:239:GLN:HG2	2.20	0.71
1:A:302:ASN:HB2	1:A:307:LEU:HD12	1.73	0.71
1:B:95:LYS:HB3	1:B:380:SER:HB3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MET:CE	1:B:194:ASP:HB2	2.21	0.71
1:A:250:ILE:O	1:A:293:THR:HG23	1.89	0.71
1:B:319:THR:HG22	1:B:320:ALA:N	2.04	0.71
1:A:106:PHE:HD2	1:B:253:SER:CB	2.04	0.71
1:A:256:TRP:CH2	1:A:257:LEU:HD21	2.19	0.71
1:A:269:PRO:HD2	1:A:312:ASN:O	1.91	0.71
1:A:280:LYS:HE2	1:A:281:TRP:H	1.53	0.71
1:B:147:GLY:HA3	1:B:212:ALA:CA	2.20	0.71
1:B:331:ALA:HB2	1:B:378:VAL:O	1.90	0.71
1:B:165:TYR:CD1	1:B:166:LEU:N	2.58	0.71
1:B:319:THR:CG2	1:B:320:ALA:N	2.53	0.71
1:A:166:LEU:HD22	1:A:202:GLN:HG2	1.72	0.70
1:A:198:LEU:CD1	1:A:203:LYS:O	2.39	0.70
1:B:384:LEU:HD23	1:B:384:LEU:O	1.90	0.70
1:B:228:ASN:C	1:B:229:ILE:HD12	2.16	0.70
1:B:273:ASP:CG	1:B:274:LYS:N	2.48	0.70
1:B:350:PHE:CD1	1:B:350:PHE:N	2.57	0.70
1:B:358:PHE:CD1	1:B:359:GLN:HG2	2.22	0.70
1:B:90:GLN:HG2	1:B:350:PHE:CE2	2.26	0.70
1:B:231:LYS:CG	1:B:232:ASP:N	2.54	0.70
1:B:366:ALA:C	1:B:367:LEU:HD12	2.17	0.70
1:A:150:LEU:O	1:A:151:LEU:CD2	2.40	0.70
1:A:166:LEU:CD2	1:A:202:GLN:HG2	2.21	0.70
1:A:367:LEU:CD1	1:A:367:LEU:N	2.55	0.69
1:B:256:TRP:CH2	1:B:257:LEU:HD21	2.23	0.69
1:B:124:VAL:HG12	1:B:235:VAL:CG2	2.22	0.69
1:B:256:TRP:CE3	1:B:257:LEU:HD22	2.26	0.69
1:B:151:LEU:O	1:B:152:ASP:OD1	2.11	0.69
1:A:250:ILE:C	1:A:293:THR:HG23	2.17	0.69
1:A:283:LEU:HD21	1:A:294:LEU:HD13	1.43	0.69
1:A:90:GLN:CA	1:A:383:PHE:CB	2.69	0.69
1:A:164:GLU:HG3	1:A:181:ILE:HD11	1.75	0.69
1:A:191:PRO:HG2	1:A:194:ASP:OD2	1.93	0.69
1:A:218:ILE:HG21	1:A:221:PHE:CB	2.18	0.69
1:A:321:SER:HA	1:B:256:TRP:NE1	2.07	0.69
1:B:89:THR:C	1:B:90:GLN:OE1	2.34	0.69
1:B:97:ALA:O	1:B:377:VAL:HG12	1.92	0.69
1:A:136:TYR:CB	1:A:137:PRO:HD2	2.22	0.69
1:B:117:ASN:HB3	1:B:245:TRP:CE2	2.27	0.69
1:B:151:LEU:C	1:B:152:ASP:OD1	2.35	0.69
1:B:193:ALA:CA	1:B:196:ARG:HH12	2.01	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ILE:CD1	1:B:229:ILE:N	2.55	0.69
1:B:90:GLN:CB	1:B:350:PHE:CE2	2.76	0.69
1:B:206:THR:HG23	1:B:207:ARG:H	1.58	0.69
1:B:235:VAL:O	1:B:236:ALA:HB2	1.93	0.69
1:B:171:THR:O	1:B:172:GLY:C	2.35	0.68
1:B:275:THR:C	1:B:276:LEU:HD23	2.17	0.68
1:B:338:GLU:HB2	1:B:340:ARG:NH1	2.08	0.68
1:A:357:VAL:HG23	1:B:285:PRO:HG2	1.76	0.68
1:B:340:ARG:C	1:B:341:VAL:HG13	2.19	0.68
1:B:368:ARG:O	1:B:368:ARG:HD3	1.94	0.68
1:B:116:TYR:CZ	1:B:309:PRO:CG	2.76	0.68
1:B:239:GLN:HE21	1:B:240:GLY:H	1.39	0.68
1:A:136:TYR:HB3	1:A:138:LEU:CD2	2.24	0.68
1:B:158:TRP:CE3	1:B:208:PHE:CZ	2.82	0.68
1:A:106:PHE:HD2	1:B:253:SER:CA	2.07	0.68
1:A:185:LEU:CD1	1:A:190:MET:HG3	2.24	0.68
1:B:279:ARG:HG2	1:B:299:GLU:HG2	1.75	0.68
1:B:116:TYR:CZ	1:B:309:PRO:HG2	2.28	0.68
1:B:136:TYR:HB3	1:B:137:PRO:CD	2.24	0.68
1:B:159:VAL:CA	1:B:162:GLN:NE2	2.56	0.68
1:B:278:ILE:H	1:B:278:ILE:CD1	2.05	0.68
1:A:178:THR:O	1:A:181:ILE:CG2	2.36	0.68
1:B:181:ILE:HG13	1:B:184:ARG:CZ	2.23	0.68
1:B:229:ILE:HG23	1:B:233:ASN:HB2	1.76	0.68
1:A:256:TRP:CE3	1:A:257:LEU:CA	2.77	0.67
1:B:145:GLN:C	1:B:147:GLY:N	2.45	0.67
1:B:198:LEU:HD12	1:B:199:ILE:N	2.09	0.67
1:B:90:GLN:HB3	1:B:350:PHE:HE2	1.59	0.67
1:B:181:ILE:HA	1:B:184:ARG:NH2	2.09	0.67
1:B:130:GLY:O	1:B:228:ASN:HA	1.95	0.67
1:B:150:LEU:O	1:B:150:LEU:CD2	2.36	0.67
1:B:331:ALA:CB	1:B:378:VAL:O	2.43	0.67
1:A:201:THR:O	1:A:203:LYS:N	2.28	0.67
1:B:94:VAL:CG1	1:B:95:LYS:N	2.58	0.67
1:B:329:SER:HA	1:B:365:THR:HG23	1.75	0.67
1:B:190:MET:CE	1:B:194:ASP:CB	2.72	0.67
1:B:367:LEU:N	1:B:367:LEU:HD13	2.09	0.67
1:B:105:THR:HA	1:B:319:THR:O	1.94	0.67
1:B:244:VAL:HG23	1:B:307:LEU:CD2	2.16	0.67
1:A:227:MET:O	1:A:229:ILE:HD13	1.95	0.66
1:B:104:LEU:HD11	1:B:364:VAL:HG23	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ILE:CD1	1:B:208:PHE:HE1	2.08	0.66
1:B:250:ILE:CG2	1:B:251:PRO:N	2.58	0.66
1:A:90:GLN:CB	1:A:350:PHE:HE2	2.08	0.66
1:A:97:ALA:CB	1:A:328:PRO:HG2	2.25	0.66
1:A:329:SER:OG	1:A:365:THR:HG23	1.96	0.66
1:B:338:GLU:HB2	1:B:340:ARG:HH11	1.61	0.66
1:B:384:LEU:CG	1:B:385:ILE:N	2.58	0.66
1:A:261:ALA:HA	1:A:264:PHE:CD1	2.30	0.66
1:A:271:ARG:O	1:A:271:ARG:HG3	1.96	0.66
1:A:327:ILE:HG13	1:A:365:THR:OG1	1.96	0.66
1:B:164:GLU:OE1	1:B:165:TYR:CA	2.43	0.66
1:A:255:ALA:HB1	1:A:283:LEU:HD11	1.76	0.66
1:B:229:ILE:HD12	1:B:229:ILE:N	2.11	0.66
1:A:89:THR:C	1:A:90:GLN:NE2	2.54	0.66
1:A:124:VAL:HG12	1:A:235:VAL:CB	2.25	0.66
1:A:327:ILE:HD11	1:A:329:SER:CA	2.25	0.66
1:A:358:PHE:O	1:B:285:PRO:HG3	1.96	0.66
1:A:367:LEU:N	1:A:367:LEU:HD12	2.11	0.66
1:B:278:ILE:N	1:B:278:ILE:CD1	2.54	0.66
1:A:90:GLN:HG2	1:A:350:PHE:CE2	2.31	0.65
1:A:123:ILE:HD12	1:A:123:ILE:C	2.21	0.65
1:B:256:TRP:CE2	1:B:257:LEU:HD22	2.31	0.65
1:A:152:ASP:CG	1:A:209:THR:CG2	2.57	0.65
1:B:157:ASP:OD2	1:B:157:ASP:N	2.30	0.65
1:A:132:ILE:HD11	1:A:229:ILE:CG1	2.26	0.65
1:A:344:VAL:HG12	1:A:345:ASP:N	2.12	0.65
1:B:327:ILE:HD12	1:B:328:PRO:N	2.10	0.65
1:A:160:GLU:OE2	1:A:161:ALA:CA	2.44	0.65
1:A:316:GLN:CG	1:A:316:GLN:O	2.42	0.65
1:A:371:LEU:HD23	1:A:371:LEU:N	2.09	0.65
1:A:118:GLU:N	1:A:118:GLU:OE1	2.30	0.65
1:A:160:GLU:OE2	1:A:161:ALA:N	2.30	0.65
1:A:160:GLU:C	1:A:160:GLU:CD	2.64	0.65
1:A:251:PRO:HB2	1:A:254:ILE:HG22	1.79	0.65
1:A:340:ARG:HG2	1:A:354:ARG:HA	1.79	0.65
1:B:192:GLU:OE2	1:B:196:ARG:NH1	2.30	0.65
1:A:229:ILE:CD1	1:A:229:ILE:N	2.59	0.65
1:B:167:LEU:O	1:B:171:THR:HG23	1.97	0.65
1:B:334:ASP:CB	1:B:339:GLN:HE21	2.05	0.65
1:A:193:ALA:O	1:A:196:ARG:NH1	2.30	0.65
1:A:256:TRP:CD1	1:B:321:SER:CB	2.80	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:THR:HB	1:B:316:GLN:HB3	1.79	0.65
1:B:283:LEU:HD23	1:B:294:LEU:HD12	1.51	0.65
1:B:304:ASP:OD1	1:B:305:GLU:N	2.30	0.65
1:A:120:GLN:OE1	1:A:120:GLN:HA	1.97	0.64
1:A:135:VAL:O	1:A:135:VAL:CG1	2.45	0.64
1:B:158:TRP:HE3	1:B:208:PHE:CZ	2.15	0.64
1:A:244:VAL:HG21	1:A:307:LEU:HD12	1.80	0.64
1:A:317:LEU:HD11	1:A:318:ASN:C	2.22	0.64
1:B:325:LEU:HD13	1:B:371:LEU:O	1.97	0.64
1:A:260:ASP:OD1	1:A:261:ALA:N	2.30	0.64
1:B:198:LEU:HB2	1:B:205:GLN:HG2	1.80	0.64
1:A:174:THR:OG1	1:A:177:GLN:N	2.29	0.64
1:A:198:LEU:HB2	1:A:205:GLN:CG	2.27	0.64
1:B:241:MET:O	1:B:302:ASN:HB3	1.97	0.64
1:B:361:SER:OG	1:B:362:GLN:N	2.30	0.64
1:B:164:GLU:OE1	1:B:165:TYR:N	2.30	0.64
1:B:271:ARG:O	1:B:273:ASP:N	2.31	0.64
1:A:149:PRO:O	1:A:150:LEU:HB2	1.96	0.64
1:A:235:VAL:O	1:A:236:ALA:HB3	1.98	0.64
1:A:300:VAL:CG1	1:A:301:ASP:N	2.60	0.64
1:B:145:GLN:HA	1:B:215:ASP:HA	1.78	0.64
1:B:244:VAL:HG12	1:B:300:VAL:C	2.23	0.64
1:A:116:TYR:HE2	1:A:241:MET:HG2	1.62	0.63
1:A:138:LEU:CB	1:A:221:PHE:HE1	2.09	0.63
1:A:152:ASP:OD1	1:A:152:ASP:N	2.30	0.63
1:A:157:ASP:OD2	1:A:157:ASP:N	2.30	0.63
1:A:283:LEU:HD22	1:A:294:LEU:HD13	1.78	0.63
1:A:382:LEU:HD22	1:A:382:LEU:O	1.98	0.63
1:B:256:TRP:CE3	1:B:257:LEU:CA	2.80	0.63
1:A:164:GLU:OE1	1:A:165:TYR:N	2.30	0.63
1:A:136:TYR:CB	1:A:137:PRO:CD	2.76	0.63
1:A:235:VAL:O	1:A:236:ALA:CB	2.46	0.63
1:A:174:THR:O	1:A:178:THR:HG22	1.99	0.63
1:A:144:VAL:HG21	1:A:238:ILE:CD1	2.29	0.63
1:A:285:PRO:HG3	1:B:358:PHE:O	1.98	0.63
1:B:218:ILE:HA	1:B:238:ILE:HA	1.81	0.63
1:B:159:VAL:N	1:B:162:GLN:NE2	2.47	0.62
1:A:338:GLU:HB2	1:A:340:ARG:NH1	2.13	0.62
1:B:124:VAL:HG12	1:B:235:VAL:HG22	1.79	0.62
1:A:256:TRP:CD2	1:A:257:LEU:HD22	2.34	0.62
1:B:181:ILE:HB	1:B:184:ARG:NH2	2.04	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:CD2	1:A:182:LEU:CD1	2.81	0.62
1:A:342:ILE:CD1	1:A:383:PHE:HZ	2.12	0.62
1:B:327:ILE:HD12	1:B:327:ILE:C	2.25	0.62
1:A:164:GLU:OE2	1:A:168:LEU:HD13	1.99	0.62
1:B:103:PRO:O	1:B:103:PRO:CD	2.47	0.62
1:A:147:GLY:O	1:A:149:PRO:N	2.33	0.62
1:A:258:VAL:O	1:A:259:LYS:O	2.16	0.62
1:B:125:GLN:HB3	1:B:233:ASN:O	2.00	0.62
1:B:217:VAL:O	1:B:239:GLN:N	2.31	0.62
1:A:147:GLY:CA	1:A:212:ALA:O	2.48	0.62
1:A:246:VAL:HG13	1:A:300:VAL:HG23	1.81	0.62
1:A:358:PHE:CE2	1:A:368:ARG:NE	2.68	0.62
1:B:117:ASN:ND2	1:B:243:PRO:HB2	2.15	0.62
1:B:135:VAL:HG21	1:B:224:ARG:HB2	1.82	0.62
1:B:155:ILE:HD12	1:B:208:PHE:HE1	1.65	0.62
1:A:276:LEU:HD23	1:A:276:LEU:H	1.63	0.62
1:B:130:GLY:O	1:B:229:ILE:N	2.27	0.62
1:B:351:VAL:HG23	1:B:352:PRO:HD2	1.81	0.61
1:A:219:THR:CG2	1:A:239:GLN:CG	2.78	0.61
1:B:156:PRO:O	1:B:159:VAL:HG22	2.00	0.61
1:A:258:VAL:C	1:A:259:LYS:O	2.39	0.61
1:A:300:VAL:HG12	1:A:301:ASP:N	2.13	0.61
1:B:192:GLU:O	1:B:196:ARG:NH1	2.34	0.61
1:A:339:GLN:C	1:A:340:ARG:CG	2.53	0.61
1:A:372:ALA:HB3	1:A:375:GLU:OE1	2.00	0.61
1:B:328:PRO:O	1:B:330:GLN:N	2.34	0.61
1:B:131:PHE:HA	1:B:227:MET:O	2.00	0.61
1:B:132:ILE:CD1	1:B:229:ILE:HD13	2.24	0.61
1:B:267:THR:HG23	1:B:314:TRP:HB2	1.82	0.61
1:A:91:ASN:OD1	1:A:91:ASN:C	2.43	0.61
1:A:250:ILE:C	1:A:293:THR:CG2	2.74	0.61
1:B:382:LEU:H	1:B:382:LEU:CD2	2.00	0.61
1:B:160:GLU:HG3	1:B:161:ALA:N	2.15	0.61
1:A:186:ARG:HG3	1:A:195:ILE:CD1	2.30	0.61
1:A:351:VAL:CG2	1:A:352:PRO:N	2.63	0.61
1:B:145:GLN:O	1:B:146:LYS:C	2.44	0.60
1:A:174:THR:HG1	1:A:177:GLN:H	1.49	0.60
1:B:187:LEU:HD12	1:B:188:ALA:HA	1.83	0.60
1:A:273:ASP:OD1	1:A:274:LYS:N	2.30	0.60
1:A:288:ASP:C	1:A:290:ALA:N	2.54	0.60
1:B:113:ASN:OD1	1:B:113:ASN:C	2.44	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:THR:HG22	1:B:207:ARG:HD2	1.82	0.60
1:B:171:THR:O	1:B:172:GLY:O	2.19	0.60
1:A:244:VAL:CG2	1:A:302:ASN:CB	2.78	0.60
1:A:241:MET:HB3	1:A:302:ASN:HD22	1.67	0.60
1:A:290:ALA:O	1:A:291:THR:HB	2.01	0.60
1:A:328:PRO:O	1:A:330:GLN:N	2.34	0.60
1:B:97:ALA:HB1	1:B:328:PRO:CG	2.32	0.60
1:B:180:GLY:O	1:B:184:ARG:HG3	2.02	0.60
1:A:203:LYS:O	1:A:204:ILE:C	2.41	0.60
1:A:247:THR:HG21	1:A:295:GLN:OE1	2.02	0.60
1:B:158:TRP:C	1:B:162:GLN:NE2	2.43	0.60
1:A:90:GLN:HG2	1:A:350:PHE:HD2	1.66	0.60
1:B:151:LEU:HD21	1:B:153:LEU:HD22	1.83	0.60
1:B:244:VAL:O	1:B:245:TRP:HD1	1.85	0.60
1:B:155:ILE:O	1:B:159:VAL:HG13	2.02	0.60
1:A:279:ARG:HG2	1:A:299:GLU:O	2.02	0.59
1:B:271:ARG:HG3	1:B:273:ASP:HB2	1.83	0.59
1:A:144:VAL:CG1	1:A:218:ILE:HD11	2.32	0.59
1:A:273:ASP:CG	1:A:274:LYS:H	2.10	0.59
1:B:266:LEU:CD2	1:B:298:LEU:HD13	2.32	0.59
1:A:121:TYR:HD1	1:A:237:LYS:NZ	2.01	0.59
1:A:138:LEU:HB3	1:A:221:PHE:CE1	2.36	0.59
1:B:90:GLN:HG2	1:B:350:PHE:HD2	1.60	0.59
1:B:97:ALA:CB	1:B:328:PRO:CG	2.78	0.59
1:B:219:THR:HG21	1:B:239:GLN:HG2	1.84	0.59
1:B:280:LYS:HE3	1:B:282:THR:HG22	1.83	0.59
1:B:304:ASP:CG	1:B:305:GLU:N	2.60	0.59
1:A:132:ILE:HD12	1:A:227:MET:O	2.02	0.59
1:A:139:THR:O	1:A:140:VAL:CB	2.50	0.59
1:B:219:THR:OG1	1:B:237:LYS:CE	2.48	0.59
1:A:256:TRP:CE3	1:A:256:TRP:O	2.43	0.59
1:B:97:ALA:HB1	1:B:328:PRO:HG2	1.84	0.59
1:B:207:ARG:CG	1:B:207:ARG:NH1	2.63	0.59
1:B:280:LYS:HE3	1:B:282:THR:CG2	2.33	0.59
1:B:154:THR:HG22	1:B:207:ARG:HB3	1.83	0.59
1:B:384:LEU:CD2	1:B:385:ILE:N	2.59	0.59
1:B:94:VAL:CG1	1:B:95:LYS:H	2.16	0.59
1:A:127:ARG:O	1:A:128:ALA:HB3	2.02	0.59
1:A:164:GLU:CD	1:A:164:GLU:O	2.45	0.59
1:A:187:LEU:CD1	1:A:188:ALA:N	2.46	0.59
1:A:278:ILE:HG23	1:A:298:LEU:CD2	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLN:HB3	1:B:350:PHE:CE2	2.38	0.59
1:B:132:ILE:CG1	1:B:229:ILE:HD11	2.33	0.59
1:A:92:LEU:CD1	1:A:93:GLY:H	2.07	0.59
1:B:132:ILE:CD1	1:B:132:ILE:H	2.14	0.59
1:B:339:GLN:O	1:B:340:ARG:HG3	2.00	0.59
1:A:132:ILE:CD1	1:A:227:MET:O	2.50	0.58
1:A:220:ALA:O	1:A:236:ALA:HB1	2.03	0.58
1:A:196:ARG:HB2	1:A:196:ARG:CZ	2.32	0.58
1:A:219:THR:HG22	1:A:239:GLN:CG	2.33	0.58
1:A:284:LEU:O	1:A:286:GLY:N	2.35	0.58
1:A:150:LEU:CB	1:A:151:LEU:HD23	2.30	0.58
1:A:227:MET:O	1:A:229:ILE:CD1	2.52	0.58
1:B:90:GLN:OE1	1:B:90:GLN:N	2.36	0.58
1:B:92:LEU:CD1	1:B:92:LEU:C	2.72	0.58
1:B:342:ILE:HG22	1:B:378:VAL:HG12	1.85	0.58
1:A:132:ILE:HD12	1:A:229:ILE:CD1	2.32	0.58
1:A:149:PRO:CG	1:A:150:LEU:H	2.13	0.58
1:A:345:ASP:C	1:A:347:ASP:N	2.62	0.58
1:B:192:GLU:OE2	1:B:196:ARG:HD3	2.03	0.58
1:B:358:PHE:HE1	1:B:359:GLN:HE21	1.51	0.58
1:A:126:ALA:O	1:A:232:ASP:HA	2.03	0.58
1:A:128:ALA:CB	1:A:158:TRP:CZ2	2.87	0.58
1:B:219:THR:O	1:B:237:LYS:CB	2.50	0.58
1:B:267:THR:CG2	1:B:314:TRP:HB2	2.34	0.58
1:A:167:LEU:HD12	1:A:168:LEU:HA	1.84	0.58
1:A:246:VAL:HG23	1:A:246:VAL:O	2.03	0.58
1:B:135:VAL:O	1:B:136:TYR:HD2	1.86	0.58
1:A:138:LEU:HD22	1:A:138:LEU:N	2.18	0.58
1:B:132:ILE:HG22	1:B:133:ASP:N	2.18	0.58
1:B:140:VAL:HG23	1:B:140:VAL:O	2.03	0.58
1:B:244:VAL:HG12	1:B:300:VAL:CB	2.27	0.58
1:B:239:GLN:HE21	1:B:240:GLY:N	2.02	0.57
1:B:239:GLN:NE2	1:B:240:GLY:H	2.01	0.57
1:B:279:ARG:CG	1:B:299:GLU:HG2	2.34	0.57
1:B:89:THR:C	1:B:90:GLN:CG	2.74	0.57
1:B:135:VAL:O	1:B:136:TYR:CB	2.51	0.57
1:B:150:LEU:O	1:B:151:LEU:HB3	2.04	0.57
1:B:193:ALA:HB2	1:B:196:ARG:NH2	2.00	0.57
1:A:144:VAL:CG2	1:A:238:ILE:HD13	2.34	0.57
1:B:319:THR:CG2	1:B:320:ALA:H	2.18	0.57
1:B:329:SER:HA	1:B:365:THR:CG2	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG22	1:A:352:PRO:N	2.19	0.57
1:A:92:LEU:CD1	1:A:92:LEU:C	2.72	0.57
1:B:106:PHE:O	1:B:318:ASN:HA	2.04	0.57
1:B:136:TYR:CD1	1:B:149:PRO:HB2	2.40	0.57
1:A:121:TYR:HD1	1:A:237:LYS:HZ1	1.53	0.57
1:B:104:LEU:O	1:B:320:ALA:HA	2.04	0.57
1:A:132:ILE:HD13	1:A:229:ILE:HD11	1.76	0.57
1:B:384:LEU:HG	1:B:385:ILE:N	2.20	0.57
1:A:106:PHE:CD2	1:B:253:SER:N	2.73	0.57
1:B:195:ILE:O	1:B:199:ILE:HG12	2.05	0.57
1:A:182:LEU:CD2	1:A:199:ILE:HD11	2.35	0.56
1:B:146:LYS:C	1:B:212:ALA:O	2.48	0.56
1:A:140:VAL:HG12	1:A:140:VAL:O	2.04	0.56
1:A:146:LYS:O	1:A:212:ALA:O	2.24	0.56
1:A:253:SER:HB3	1:B:106:PHE:CD2	2.35	0.56
1:B:150:LEU:O	1:B:151:LEU:HB2	2.06	0.56
1:B:334:ASP:CB	1:B:338:GLU:O	2.50	0.56
1:B:355:VAL:HG12	1:B:371:LEU:CD2	2.35	0.56
1:A:289:ALA:C	1:A:291:THR:O	2.49	0.56
1:A:320:ALA:O	1:B:256:TRP:NE1	2.38	0.56
1:B:108:GLN:O	1:B:317:LEU:N	2.27	0.56
1:B:115:SER:N	1:B:245:TRP:O	2.36	0.56
1:B:145:GLN:C	1:B:147:GLY:H	2.12	0.56
1:B:159:VAL:HG23	1:B:160:GLU:N	2.21	0.56
1:A:114:VAL:O	1:A:309:PRO:HA	2.06	0.56
1:B:102:GLY:O	1:B:323:PRO:HA	2.06	0.56
1:B:131:PHE:O	1:B:153:LEU:CB	2.54	0.56
1:B:150:LEU:HD23	1:B:150:LEU:C	2.27	0.56
1:B:192:GLU:CD	1:B:196:ARG:NH1	2.64	0.56
1:B:244:VAL:CG2	1:B:307:LEU:CG	2.84	0.56
1:B:244:VAL:HG23	1:B:307:LEU:HD11	1.79	0.56
1:B:342:ILE:O	1:B:342:ILE:CG2	2.42	0.56
1:A:130:GLY:O	1:A:229:ILE:HD13	2.06	0.56
1:A:147:GLY:HA3	1:A:212:ALA:CA	2.34	0.56
1:A:280:LYS:HA	1:A:280:LYS:HE3	1.88	0.56
1:B:201:THR:O	1:B:202:GLN:HB3	2.06	0.56
1:A:321:SER:HB2	1:B:256:TRP:CG	2.41	0.56
1:B:167:LEU:HD12	1:B:168:LEU:HA	1.86	0.56
1:A:186:ARG:NE	1:A:192:GLU:OE1	2.38	0.56
1:A:331:ALA:O	1:A:341:VAL:HG12	2.05	0.56
1:B:165:TYR:HD2	1:B:182:LEU:CD1	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:HG22	1:A:90:GLN:H	1.71	0.56
1:B:250:ILE:O	1:B:293:THR:HA	2.06	0.55
1:B:345:ASP:C	1:B:347:ASP:N	2.56	0.55
1:B:154:THR:HG22	1:B:207:ARG:CB	2.36	0.55
1:B:174:THR:HG1	1:B:177:GLN:CB	2.18	0.55
1:B:230:ALA:H	1:B:233:ASN:ND2	2.05	0.55
1:B:334:ASP:HB3	1:B:339:GLN:HA	1.89	0.55
1:A:173:GLY:O	1:A:174:THR:C	2.47	0.55
1:A:201:THR:C	1:A:203:LYS:N	2.64	0.55
1:A:241:MET:HB3	1:A:302:ASN:ND2	2.21	0.55
1:A:279:ARG:HD3	1:A:299:GLU:HG2	1.88	0.55
1:B:278:ILE:HG21	1:B:298:LEU:HD22	1.88	0.55
1:A:287:VAL:O	1:A:289:ALA:N	2.39	0.55
1:A:358:PHE:CD2	1:A:368:ARG:HG3	2.35	0.55
1:B:127:ARG:O	1:B:128:ALA:HB3	2.05	0.55
1:B:181:ILE:CG2	1:B:182:LEU:N	2.69	0.55
1:B:302:ASN:HB2	1:B:307:LEU:HD22	1.88	0.55
1:A:246:VAL:O	1:A:246:VAL:CG2	2.54	0.55
1:A:340:ARG:C	1:A:341:VAL:HG13	2.32	0.55
1:A:114:VAL:CG1	1:A:308:LYS:O	2.55	0.55
1:A:153:LEU:CD2	1:A:153:LEU:C	2.79	0.55
1:A:90:GLN:HB2	1:A:350:PHE:HE2	1.70	0.55
1:A:193:ALA:C	1:A:196:ARG:NH1	2.64	0.55
1:A:219:THR:HG21	1:A:239:GLN:HG2	1.89	0.55
1:B:292:ARG:NE	1:B:292:ARG:HA	2.21	0.55
1:A:150:LEU:O	1:A:151:LEU:HD22	2.06	0.55
1:A:190:MET:CE	1:A:194:ASP:HB3	2.37	0.54
1:B:125:GLN:CB	1:B:233:ASN:O	2.55	0.54
1:B:231:LYS:HE2	1:B:233:ASN:OD1	2.07	0.54
1:A:124:VAL:O	1:A:235:VAL:HB	2.07	0.54
1:A:210:LEU:HD12	1:A:210:LEU:C	2.32	0.54
1:A:256:TRP:C	1:A:256:TRP:CD2	2.82	0.54
1:B:116:TYR:CZ	1:B:309:PRO:HG3	2.42	0.54
1:B:327:ILE:HD12	1:B:328:PRO:C	2.32	0.54
1:A:361:SER:O	1:A:363:GLY:N	2.36	0.54
1:B:164:GLU:CD	1:B:181:ILE:CD1	2.80	0.54
1:A:149:PRO:CG	1:A:150:LEU:N	2.69	0.54
1:A:167:LEU:CD1	1:A:168:LEU:HD12	2.36	0.54
1:B:97:ALA:HB2	1:B:328:PRO:HG2	1.88	0.54
1:B:136:TYR:HB3	1:B:137:PRO:HD2	1.89	0.54
1:A:288:ASP:C	1:A:290:ALA:H	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:O	1:B:136:TYR:CD2	2.61	0.54
1:A:104:LEU:HD21	1:A:364:VAL:HG23	1.88	0.54
1:A:151:LEU:HD23	1:A:151:LEU:N	2.22	0.54
1:A:339:GLN:CA	1:A:340:ARG:HG3	2.38	0.54
1:B:145:GLN:O	1:B:147:GLY:N	2.40	0.54
1:B:183:GLU:C	1:B:183:GLU:OE1	2.51	0.54
1:B:219:THR:CG2	1:B:239:GLN:HG2	2.38	0.54
1:A:334:ASP:OD2	1:A:339:GLN:NE2	2.41	0.54
1:B:340:ARG:HB2	1:B:353:LYS:O	2.08	0.54
1:A:332:LEU:HD23	1:A:333:ILE:N	2.19	0.54
1:B:90:GLN:CG	1:B:350:PHE:CE2	2.91	0.54
1:B:208:PHE:CD1	1:B:208:PHE:N	2.76	0.54
1:B:256:TRP:CE3	1:B:256:TRP:O	2.38	0.54
1:B:284:LEU:O	1:B:286:GLY:N	2.41	0.54
1:B:241:MET:HB2	1:B:302:ASN:HD22	1.72	0.53
1:A:147:GLY:N	1:A:212:ALA:O	2.40	0.53
1:A:332:LEU:HA	1:A:341:VAL:CG1	2.38	0.53
1:A:90:GLN:CG	1:A:350:PHE:CE2	2.92	0.53
1:A:164:GLU:OE1	1:A:181:ILE:CD1	2.57	0.53
1:A:155:ILE:HD12	1:A:158:TRP:CZ3	2.43	0.53
1:B:181:ILE:HG22	1:B:182:LEU:CD1	2.33	0.53
1:B:133:ASP:N	1:B:152:ASP:O	2.41	0.53
1:B:144:VAL:CG1	1:B:218:ILE:HD11	2.38	0.53
1:A:89:THR:CA	1:A:90:GLN:NE2	2.72	0.53
1:A:181:ILE:HG23	1:A:182:LEU:N	2.24	0.53
1:B:153:LEU:O	1:B:207:ARG:HB2	2.09	0.53
1:B:291:THR:C	1:B:292:ARG:HD2	2.28	0.53
1:A:138:LEU:HB2	1:A:221:PHE:CZ	2.43	0.53
1:B:342:ILE:CG2	1:B:378:VAL:HG12	2.39	0.53
1:A:94:VAL:HG12	1:A:95:LYS:CA	2.39	0.52
1:A:260:ASP:O	1:A:263:GLN:HG2	2.10	0.52
1:B:135:VAL:HG12	1:B:136:TYR:N	2.23	0.52
1:A:263:GLN:HB2	1:A:318:ASN:HB2	1.92	0.52
1:B:190:MET:CE	1:B:194:ASP:HB3	2.38	0.52
1:A:239:GLN:HE21	1:A:240:GLY:H	1.57	0.52
1:B:112:ALA:HB2	1:B:248:ALA:HB2	1.91	0.52
1:A:90:GLN:HG3	1:A:383:PHE:CG	2.41	0.52
1:A:159:VAL:HG23	1:A:160:GLU:N	2.23	0.52
1:A:278:ILE:HD12	1:A:278:ILE:N	2.24	0.52
1:A:321:SER:HA	1:B:256:TRP:CE2	2.45	0.52
1:A:253:SER:CA	1:B:106:PHE:CE2	2.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TYR:CE2	1:B:309:PRO:HG3	2.44	0.52
1:B:288:ASP:HB2	1:B:293:THR:OG1	2.09	0.52
1:A:250:ILE:CG2	1:A:254:ILE:CG2	2.72	0.52
1:B:92:LEU:CD1	1:B:93:GLY:H	2.07	0.52
1:A:90:GLN:CG	1:A:383:PHE:CG	2.93	0.52
1:B:302:ASN:OD1	1:B:304:ASP:O	2.27	0.52
1:A:261:ALA:HA	1:A:264:PHE:HD1	1.75	0.51
1:A:344:VAL:CG1	1:A:345:ASP:N	2.73	0.51
1:B:367:LEU:HD13	1:B:367:LEU:H	1.76	0.51
1:A:361:SER:C	1:A:363:GLY:H	2.17	0.51
1:B:307:LEU:O	1:B:308:LYS:HG2	2.11	0.51
1:A:124:VAL:CG2	1:A:213:PRO:HD3	2.40	0.51
1:A:155:ILE:HG13	1:A:208:PHE:HE1	1.74	0.51
1:B:104:LEU:HD13	1:B:326:LEU:HD11	1.91	0.51
1:B:117:ASN:OD1	1:B:117:ASN:N	2.30	0.51
1:B:159:VAL:CG2	1:B:160:GLU:N	2.74	0.51
1:A:89:THR:O	1:A:90:GLN:HG3	2.11	0.51
1:A:317:LEU:O	1:A:317:LEU:HG	2.10	0.51
1:A:273:ASP:O	1:A:274:LYS:C	2.52	0.51
1:B:123:ILE:HD12	1:B:123:ILE:C	2.25	0.51
1:B:340:ARG:CB	1:B:353:LYS:O	2.58	0.51
1:A:190:MET:HB3	1:A:195:ILE:HG13	1.92	0.51
1:B:133:ASP:O	1:B:135:VAL:N	2.44	0.51
1:B:267:THR:HG23	1:B:267:THR:O	2.10	0.51
1:B:287:VAL:HG12	1:B:294:LEU:CD2	2.40	0.51
1:A:164:GLU:CG	1:A:181:ILE:HD11	2.39	0.51
1:A:185:LEU:CG	1:A:190:MET:HG3	2.41	0.51
1:A:278:ILE:CG2	1:A:298:LEU:CD2	2.88	0.51
1:B:154:THR:HA	1:B:207:ARG:CB	2.41	0.51
1:B:164:GLU:CG	1:B:181:ILE:HD11	2.41	0.51
1:A:164:GLU:OE2	1:A:168:LEU:CD1	2.59	0.50
1:B:162:GLN:OE1	1:B:205:GLN:N	2.44	0.50
1:A:181:ILE:HG23	1:A:182:LEU:HD12	1.92	0.50
1:B:203:LYS:O	1:B:204:ILE:HB	2.10	0.50
1:B:368:ARG:HD3	1:B:368:ARG:C	2.21	0.50
1:A:183:GLU:OE1	1:A:183:GLU:O	2.30	0.50
1:A:273:ASP:CG	1:A:274:LYS:N	2.70	0.50
1:A:327:ILE:HD11	1:A:329:SER:HA	1.91	0.50
1:B:192:GLU:O	1:B:192:GLU:OE1	2.30	0.50
1:B:256:TRP:C	1:B:256:TRP:CD2	2.81	0.50
1:B:245:TRP:CH2	1:B:297:ARG:CZ	2.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:HD23	1:B:294:LEU:HD13	1.91	0.50
1:B:368:ARG:HA	1:B:368:ARG:HH11	1.77	0.50
1:A:317:LEU:O	1:A:317:LEU:CG	2.56	0.50
1:B:103:PRO:O	1:B:103:PRO:HD2	2.12	0.50
1:B:113:ASN:OD1	1:B:113:ASN:O	2.30	0.50
1:A:108:GLN:OE1	1:A:254:ILE:CD1	2.60	0.50
1:A:217:VAL:O	1:A:239:GLN:N	2.41	0.50
1:B:136:TYR:CE1	1:B:149:PRO:HB2	2.47	0.50
1:A:239:GLN:NE2	1:A:240:GLY:H	2.09	0.50
1:A:184:ARG:O	1:A:187:LEU:HG	2.12	0.49
1:A:263:GLN:O	1:A:263:GLN:CG	2.54	0.49
1:A:290:ALA:O	1:A:291:THR:OG1	2.30	0.49
1:A:343:THR:O	1:A:351:VAL:HG12	2.12	0.49
1:B:94:VAL:HG12	1:B:95:LYS:H	1.71	0.49
1:A:153:LEU:HD23	1:A:208:PHE:HD1	1.77	0.49
1:A:251:PRO:CB	1:A:254:ILE:HG22	2.40	0.49
1:A:334:ASP:HB3	1:A:339:GLN:HA	1.94	0.49
1:B:179:GLU:HA	1:B:179:GLU:OE2	2.11	0.49
1:B:270:ALA:C	1:B:272:PRO:HD3	2.37	0.49
1:A:350:PHE:CD1	1:A:350:PHE:N	2.78	0.49
1:B:244:VAL:HG12	1:B:300:VAL:CA	2.42	0.49
1:B:133:ASP:OD1	1:B:134:LYS:N	2.45	0.49
1:B:183:GLU:OE1	1:B:183:GLU:O	2.30	0.49
1:B:379:SER:O	1:B:380:SER:CB	2.45	0.49
1:A:147:GLY:HA3	1:A:212:ALA:C	2.37	0.49
1:B:165:TYR:HB2	1:B:181:ILE:HG21	1.93	0.49
1:B:190:MET:HE1	1:B:194:ASP:CB	2.42	0.49
1:B:190:MET:HE1	1:B:194:ASP:HB3	1.95	0.49
1:B:115:SER:O	1:B:245:TRP:HB2	2.12	0.49
1:B:166:LEU:HD21	1:B:202:GLN:O	2.12	0.49
1:A:190:MET:HE3	1:A:194:ASP:HB3	1.95	0.49
1:A:241:MET:O	1:A:302:ASN:HB3	2.12	0.49
1:A:275:THR:CA	1:A:276:LEU:HD23	2.42	0.49
1:B:104:LEU:HD11	1:B:364:VAL:CG2	2.40	0.49
1:B:256:TRP:CD2	1:B:257:LEU:HD22	2.48	0.49
1:B:290:ALA:O	1:B:291:THR:OG1	2.29	0.49
1:A:175:ALA:HA	1:A:178:THR:CG2	2.41	0.49
1:A:90:GLN:HB3	1:A:383:PHE:CG	2.47	0.49
1:A:178:THR:C	1:A:181:ILE:HG22	2.31	0.49
1:A:242:ASP:HB3	1:A:243:PRO:HD3	1.94	0.49
1:B:273:ASP:C	1:B:274:LYS:O	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:CG2	1:B:285:PRO:HG2	2.42	0.48
1:B:256:TRP:CE2	1:B:257:LEU:HD23	2.46	0.48
1:B:384:LEU:O	1:B:385:ILE:O	2.30	0.48
1:A:277:THR:OG1	1:A:301:ASP:HB3	2.10	0.48
1:B:158:TRP:HE3	1:B:208:PHE:HZ	1.57	0.48
1:B:258:VAL:HG12	1:B:259:LYS:N	2.26	0.48
1:A:321:SER:HB2	1:B:256:TRP:CD1	2.47	0.48
1:B:181:ILE:CA	1:B:184:ARG:NE	2.58	0.48
1:A:182:LEU:HD21	1:A:199:ILE:HD11	1.94	0.48
1:A:275:THR:C	1:A:276:LEU:CD2	2.81	0.48
1:B:136:TYR:CB	1:B:137:PRO:CD	2.91	0.48
1:B:218:ILE:CG2	1:B:220:ALA:O	2.61	0.48
1:A:114:VAL:HG11	1:A:308:LYS:O	2.13	0.48
1:A:201:THR:OG1	1:A:203:LYS:HB2	2.13	0.48
1:B:165:TYR:CD2	1:B:182:LEU:CD1	2.87	0.48
1:B:250:ILE:HG23	1:B:251:PRO:HD2	1.95	0.48
1:B:350:PHE:N	1:B:350:PHE:HD1	2.05	0.48
1:A:321:SER:CA	1:B:256:TRP:NE1	2.75	0.48
1:B:300:VAL:HG12	1:B:301:ASP:N	2.29	0.48
1:A:234:VAL:CG2	1:A:236:ALA:HA	2.41	0.48
1:A:278:ILE:CG2	1:A:298:LEU:HD22	2.40	0.48
1:A:125:GLN:HA	1:A:233:ASN:O	2.14	0.48
1:A:189:GLY:O	1:A:190:MET:C	2.54	0.48
1:A:349:ARG:O	1:A:349:ARG:HG3	2.13	0.48
1:B:158:TRP:CE3	1:B:208:PHE:HZ	2.29	0.48
1:A:132:ILE:HG22	1:A:133:ASP:N	2.28	0.47
1:A:136:TYR:HD1	1:A:137:PRO:CD	2.26	0.47
1:A:90:GLN:CB	1:A:383:PHE:CB	2.92	0.47
1:A:162:GLN:OE1	1:A:205:GLN:N	2.46	0.47
1:A:291:THR:HG22	1:A:292:ARG:H	1.79	0.47
1:B:108:GLN:HG2	1:B:110:PHE:CE2	2.49	0.47
1:B:113:ASN:O	1:B:246:VAL:HA	2.14	0.47
1:B:219:THR:CG2	1:B:239:GLN:CG	2.92	0.47
1:B:345:ASP:O	1:B:347:ASP:N	2.46	0.47
1:A:89:THR:C	1:A:90:GLN:CG	2.87	0.47
1:A:358:PHE:CD2	1:A:368:ARG:NE	2.81	0.47
1:A:181:ILE:CG2	1:A:182:LEU:N	2.77	0.47
1:B:135:VAL:C	1:B:136:TYR:CD2	2.92	0.47
1:B:340:ARG:C	1:B:341:VAL:CG1	2.85	0.47
1:B:368:ARG:O	1:B:368:ARG:CD	2.61	0.47
1:A:132:ILE:CG2	1:A:133:ASP:N	2.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:THR:O	1:B:292:ARG:CG	2.62	0.47
1:A:127:ARG:O	1:A:128:ALA:CB	2.62	0.47
1:B:114:VAL:HG13	1:B:244:VAL:HG22	1.95	0.47
1:A:112:ALA:CA	1:A:247:THR:O	2.58	0.47
1:A:170:GLU:C	1:A:171:THR:O	2.54	0.47
1:A:321:SER:CB	1:B:256:TRP:CG	2.96	0.47
1:B:138:LEU:HB3	1:B:221:PHE:CE1	2.50	0.47
1:B:158:TRP:N	1:B:158:TRP:CD1	2.79	0.47
1:B:273:ASP:O	1:B:274:LYS:O	2.32	0.47
1:B:97:ALA:C	1:B:377:VAL:HG12	2.39	0.47
1:B:331:ALA:HB2	1:B:379:SER:HA	1.96	0.47
1:A:95:LYS:HB3	1:A:380:SER:CB	2.21	0.47
1:A:246:VAL:HG13	1:A:300:VAL:CG2	2.45	0.47
1:A:381:GLY:HA2	1:A:382:LEU:HD13	1.96	0.47
1:B:131:PHE:O	1:B:153:LEU:HA	2.13	0.47
1:B:159:VAL:CA	1:B:162:GLN:HE21	2.24	0.47
1:B:368:ARG:HD3	1:B:368:ARG:HA	1.56	0.47
1:A:273:ASP:C	1:A:275:THR:N	2.64	0.47
1:B:219:THR:HG21	1:B:239:GLN:CG	2.45	0.47
1:B:245:TRP:CH2	1:B:297:ARG:NH2	2.83	0.47
1:B:355:VAL:CG1	1:B:371:LEU:HG	2.45	0.47
1:B:368:ARG:C	1:B:368:ARG:CD	2.87	0.47
1:A:186:ARG:CZ	1:A:192:GLU:OE1	2.62	0.46
1:A:234:VAL:O	1:A:234:VAL:HG13	2.15	0.46
1:A:289:ALA:O	1:A:291:THR:O	2.34	0.46
1:B:355:VAL:HG11	1:B:371:LEU:HG	1.96	0.46
1:B:147:GLY:O	1:B:148:THR:O	2.33	0.46
1:B:148:THR:CB	1:B:149:PRO:CD	2.93	0.46
1:B:148:THR:HB	1:B:149:PRO:HD3	1.97	0.46
1:B:154:THR:HG22	1:B:207:ARG:CD	2.45	0.46
1:A:153:LEU:HD23	1:A:153:LEU:C	2.35	0.46
1:A:187:LEU:HD12	1:A:188:ALA:HA	1.92	0.46
1:A:358:PHE:HE1	1:A:359:GLN:HE21	1.62	0.46
1:B:228:ASN:OD1	1:B:228:ASN:N	2.48	0.46
1:A:164:GLU:OE1	1:A:164:GLU:O	2.34	0.46
1:A:183:GLU:OE1	1:A:183:GLU:C	2.59	0.46
1:A:274:LYS:C	1:A:275:THR:HG23	2.32	0.46
1:A:90:GLN:CB	1:A:383:PHE:CG	2.99	0.46
1:A:239:GLN:HE21	1:A:240:GLY:N	2.13	0.46
1:B:90:GLN:CB	1:B:350:PHE:HE2	2.19	0.46
1:B:230:ALA:O	1:B:231:LYS:C	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLN:C	1:B:340:ARG:CG	2.52	0.46
1:B:384:LEU:HD23	1:B:385:ILE:C	2.38	0.46
1:A:339:GLN:H	1:A:340:ARG:HG3	1.81	0.46
1:A:355:VAL:HG12	1:A:371:LEU:HD21	1.98	0.46
1:B:158:TRP:O	1:B:162:GLN:NE2	2.48	0.46
1:B:231:LYS:HG3	1:B:232:ASP:N	2.06	0.46
1:B:270:ALA:O	1:B:271:ARG:HB3	2.15	0.46
1:A:94:VAL:HG12	1:A:95:LYS:C	2.40	0.46
1:A:174:THR:HG1	1:A:177:GLN:HB2	1.80	0.46
1:A:230:ALA:O	1:A:231:LYS:HG2	2.16	0.46
1:B:198:LEU:O	1:B:202:GLN:N	2.40	0.46
1:B:266:LEU:HD21	1:B:298:LEU:HD13	1.96	0.46
1:B:340:ARG:HB3	1:B:355:VAL:HG22	1.96	0.46
1:A:250:ILE:N	1:A:293:THR:HG22	2.31	0.46
1:A:252:GLU:OE1	1:A:292:ARG:CG	2.64	0.46
1:A:120:GLN:HG2	1:A:243:PRO:HD2	1.98	0.45
1:A:241:MET:HE2	1:A:302:ASN:HD21	1.82	0.45
1:A:279:ARG:CD	1:A:299:GLU:HG2	2.45	0.45
1:B:114:VAL:CG1	1:B:307:LEU:HD11	2.46	0.45
1:A:90:GLN:CG	1:A:350:PHE:HE2	2.29	0.45
1:A:97:ALA:HB3	1:A:328:PRO:HG2	1.98	0.45
1:A:132:ILE:HD12	1:A:132:ILE:N	2.30	0.45
1:B:308:LYS:O	1:B:311:MET:HB2	2.17	0.45
1:A:144:VAL:HG11	1:A:218:ILE:HD11	1.98	0.45
1:A:150:LEU:HB3	1:A:151:LEU:CD2	2.37	0.45
1:A:288:ASP:O	1:A:290:ALA:O	2.33	0.45
1:B:342:ILE:CD1	1:B:351:VAL:O	2.59	0.45
1:B:384:LEU:HG	1:B:385:ILE:H	1.81	0.45
1:A:136:TYR:CD1	1:A:137:PRO:HD2	2.50	0.45
1:A:345:ASP:OD2	1:A:349:ARG:HD3	2.17	0.45
1:A:133:ASP:N	1:A:152:ASP:O	2.49	0.45
1:A:160:GLU:HG3	1:A:161:ALA:N	2.32	0.45
1:A:327:ILE:HD12	1:A:329:SER:H	1.80	0.45
1:B:159:VAL:HA	1:B:162:GLN:CD	2.42	0.45
1:A:234:VAL:C	1:A:236:ALA:H	2.13	0.45
1:A:245:TRP:HA	1:A:298:LEU:O	2.17	0.45
1:A:338:GLU:HB2	1:A:340:ARG:HH11	1.79	0.45
1:B:97:ALA:O	1:B:377:VAL:O	2.35	0.45
1:B:162:GLN:OE1	1:B:205:GLN:CB	2.58	0.45
1:B:256:TRP:CD2	1:B:257:LEU:N	2.85	0.45
1:A:97:ALA:CB	1:A:328:PRO:CG	2.94	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:CD1	1:A:125:GLN:HG2	2.47	0.45
1:A:132:ILE:O	1:A:226:GLY:CA	2.63	0.45
1:A:255:ALA:HA	1:A:258:VAL:HG23	1.98	0.45
1:A:331:ALA:HB1	1:A:378:VAL:O	2.13	0.45
1:B:150:LEU:HD12	1:B:212:ALA:HB2	1.99	0.45
1:B:160:GLU:C	1:B:160:GLU:OE2	2.60	0.45
1:B:237:LYS:HE2	1:B:237:LYS:HB3	1.78	0.45
1:B:384:LEU:O	1:B:385:ILE:C	2.60	0.45
1:A:106:PHE:CD2	1:B:253:SER:HB3	2.42	0.45
1:A:153:LEU:HD22	1:A:208:PHE:O	2.16	0.45
1:A:317:LEU:HD12	1:A:317:LEU:O	2.07	0.45
1:B:217:VAL:HG12	1:B:218:ILE:N	2.31	0.45
1:B:252:GLU:H	1:B:252:GLU:HG2	1.48	0.45
1:A:217:VAL:HG12	1:A:218:ILE:N	2.32	0.45
1:A:224:ARG:HG2	1:A:225:ALA:N	2.31	0.44
1:A:241:MET:HE2	1:A:302:ASN:ND2	2.32	0.44
1:B:135:VAL:C	1:B:136:TYR:HD2	2.25	0.44
1:B:319:THR:HG23	1:B:320:ALA:H	1.80	0.44
1:B:266:LEU:HD21	1:B:298:LEU:CD1	2.47	0.44
1:A:90:GLN:CD	1:A:90:GLN:N	2.75	0.44
1:A:131:PHE:HA	1:A:227:MET:O	2.16	0.44
1:A:327:ILE:CD1	1:A:329:SER:H	2.25	0.44
1:A:340:ARG:CB	1:A:353:LYS:O	2.65	0.44
1:B:342:ILE:HG21	1:B:378:VAL:CG1	2.48	0.44
1:A:136:TYR:CB	1:A:138:LEU:HD23	2.47	0.44
1:A:343:THR:CG2	1:A:375:GLU:HG2	2.48	0.44
1:B:274:LYS:HB3	1:B:275:THR:H	1.57	0.44
1:B:345:ASP:OD2	1:B:349:ARG:HG3	2.18	0.44
1:A:187:LEU:HD12	1:A:187:LEU:O	2.08	0.44
1:A:344:VAL:HG12	1:A:346:ALA:H	1.82	0.44
1:A:345:ASP:OD2	1:A:349:ARG:HG3	2.17	0.44
1:B:255:ALA:HB1	1:B:283:LEU:HD11	2.00	0.44
1:B:331:ALA:HB1	1:B:378:VAL:O	2.17	0.44
1:A:332:LEU:HD23	1:A:333:ILE:HA	1.99	0.44
1:A:358:PHE:CE2	1:A:368:ARG:CZ	3.00	0.44
1:B:183:GLU:CA	1:B:186:ARG:HH12	2.17	0.44
1:A:159:VAL:CG2	1:A:160:GLU:N	2.81	0.44
1:A:339:GLN:O	1:A:340:ARG:HG3	2.10	0.44
1:B:135:VAL:HG21	1:B:224:ARG:HA	1.99	0.44
1:A:98:THR:HG23	1:A:98:THR:O	2.17	0.44
1:A:367:LEU:HD13	1:A:367:LEU:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:O	1:A:382:LEU:CD2	2.65	0.44
1:B:204:ILE:CG2	1:B:205:GLN:N	2.80	0.44
1:A:120:GLN:HG3	1:A:120:GLN:O	2.17	0.44
1:B:134:LYS:O	1:B:135:VAL:HB	2.17	0.44
1:B:290:ALA:C	1:B:291:THR:OG1	2.61	0.44
1:A:136:TYR:CB	1:A:138:LEU:CD2	2.93	0.43
1:A:162:GLN:OE1	1:A:205:GLN:O	2.35	0.43
1:B:244:VAL:C	1:B:245:TRP:HD1	2.25	0.43
1:B:266:LEU:HD13	1:B:266:LEU:HA	1.66	0.43
1:A:187:LEU:CD1	1:A:187:LEU:O	2.65	0.43
1:A:342:ILE:HD13	1:A:383:PHE:HZ	1.84	0.43
1:B:171:THR:O	1:B:171:THR:OG1	2.30	0.43
1:A:271:ARG:O	1:A:272:PRO:C	2.60	0.43
1:B:177:GLN:OE1	1:B:177:GLN:HA	2.18	0.43
1:A:221:PHE:O	1:A:221:PHE:CG	2.71	0.43
1:A:246:VAL:CG1	1:A:300:VAL:CG2	2.97	0.43
1:A:256:TRP:CZ3	1:A:257:LEU:CD2	2.70	0.43
1:A:367:LEU:CD1	1:A:367:LEU:H	2.30	0.43
1:B:181:ILE:HG23	1:B:182:LEU:HD12	1.98	0.43
1:B:268:VAL:O	1:B:268:VAL:HG23	2.18	0.43
1:B:308:LYS:HA	1:B:309:PRO:HD3	1.55	0.43
1:B:342:ILE:HG21	1:B:378:VAL:HG11	2.00	0.43
1:A:106:PHE:CE2	1:B:252:GLU:C	2.97	0.43
1:A:117:ASN:OD1	1:A:117:ASN:O	2.36	0.43
1:A:190:MET:CE	1:A:194:ASP:CB	2.96	0.43
1:B:107:ALA:HA	1:B:318:ASN:OD1	2.18	0.43
1:B:339:GLN:CA	1:B:340:ARG:HG3	2.40	0.43
1:A:106:PHE:CE2	1:B:253:SER:N	2.85	0.43
1:A:175:ALA:C	1:A:178:THR:CG2	2.91	0.43
1:A:355:VAL:HG12	1:A:371:LEU:CD2	2.49	0.43
1:A:246:VAL:HG22	1:A:298:LEU:HB3	2.00	0.43
1:B:196:ARG:HH11	1:B:196:ARG:HG3	1.83	0.43
1:B:339:GLN:H	1:B:340:ARG:HD2	1.84	0.43
1:A:288:ASP:O	1:A:291:THR:O	2.37	0.43
1:B:227:MET:HE2	1:B:227:MET:HB3	1.90	0.43
1:B:250:ILE:CG2	1:B:251:PRO:CD	2.97	0.43
1:B:292:ARG:HA	1:B:292:ARG:HE	1.84	0.43
1:A:280:LYS:HE3	1:A:281:TRP:H	1.82	0.43
1:A:155:ILE:O	1:A:159:VAL:HG13	2.19	0.42
1:A:160:GLU:CG	1:A:161:ALA:N	2.82	0.42
1:B:144:VAL:HG11	1:B:218:ILE:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HG2	1:B:299:GLU:O	2.18	0.42
1:B:345:ASP:OD2	1:B:349:ARG:HD3	2.19	0.42
1:B:355:VAL:HG12	1:B:371:LEU:HD21	2.00	0.42
1:A:136:TYR:CD1	1:A:137:PRO:CD	3.02	0.42
1:A:280:LYS:CE	1:A:281:TRP:N	2.78	0.42
1:A:327:ILE:HG23	1:A:367:LEU:HD11	2.01	0.42
1:A:349:ARG:HE	1:A:349:ARG:HB2	1.56	0.42
1:B:160:GLU:OE2	1:B:160:GLU:O	2.37	0.42
1:B:244:VAL:O	1:B:245:TRP:CD1	2.70	0.42
1:B:250:ILE:HA	1:B:251:PRO:HD3	1.72	0.42
1:B:294:LEU:HA	1:B:294:LEU:HD22	1.67	0.42
1:B:349:ARG:HG3	1:B:349:ARG:O	2.19	0.42
1:A:124:VAL:CG1	1:A:235:VAL:HB	2.36	0.42
1:A:140:VAL:O	1:A:140:VAL:CG1	2.67	0.42
1:A:246:VAL:HG22	1:A:298:LEU:CB	2.50	0.42
1:A:358:PHE:HB3	1:A:366:ALA:O	2.18	0.42
1:B:114:VAL:HG11	1:B:307:LEU:HD11	2.02	0.42
1:A:244:VAL:O	1:A:245:TRP:HD1	2.02	0.42
1:A:339:GLN:N	1:A:340:ARG:HG3	2.35	0.42
1:A:343:THR:HG23	1:A:375:GLU:HG2	2.00	0.42
1:B:142:ASP:O	1:B:218:ILE:HD12	2.19	0.42
1:B:151:LEU:HD22	1:B:210:LEU:HB2	2.00	0.42
1:B:350:PHE:C	1:B:351:VAL:HG12	2.44	0.42
1:A:234:VAL:O	1:A:234:VAL:CG1	2.66	0.42
1:A:302:ASN:CB	1:A:307:LEU:HD12	2.47	0.42
1:B:164:GLU:OE1	1:B:181:ILE:CD1	2.67	0.42
1:B:282:THR:HG23	1:B:297:ARG:HB3	2.01	0.42
1:A:283:LEU:HD23	1:A:294:LEU:HD13	1.86	0.42
1:A:342:ILE:HG21	1:A:350:PHE:HB3	2.02	0.42
1:B:148:THR:CB	1:B:149:PRO:HD3	2.50	0.42
1:B:243:PRO:HB3	1:B:299:GLU:HG3	2.01	0.42
1:B:331:ALA:O	1:B:341:VAL:HG11	2.19	0.42
1:A:133:ASP:O	1:A:135:VAL:N	2.47	0.42
1:A:341:VAL:HB	1:A:342:ILE:H	1.63	0.42
1:B:92:LEU:HD22	1:B:93:GLY:H	1.85	0.42
1:A:142:ASP:O	1:A:218:ILE:HD12	2.19	0.42
1:A:333:ILE:O	1:A:340:ARG:O	2.37	0.42
1:A:334:ASP:CB	1:A:339:GLN:HA	2.50	0.42
1:B:147:GLY:HA3	1:B:212:ALA:N	2.33	0.42
1:A:262:SER:C	1:A:264:PHE:H	2.27	0.42
1:A:92:LEU:HD22	1:A:93:GLY:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:VAL:HA	1:A:370:GLY:HA3	2.02	0.41
1:B:242:ASP:HA	1:B:302:ASN:O	2.20	0.41
1:B:342:ILE:HD13	1:B:342:ILE:HA	1.62	0.41
1:A:90:GLN:CA	1:A:383:PHE:HB3	2.41	0.41
1:A:289:ALA:O	1:A:291:THR:N	2.53	0.41
1:A:329:SER:OG	1:A:364:VAL:HA	2.20	0.41
1:B:160:GLU:O	1:B:163:SER:OG	2.32	0.41
1:B:250:ILE:HG23	1:B:251:PRO:CD	2.50	0.41
1:B:349:ARG:HE	1:B:349:ARG:HB2	1.50	0.41
1:A:122:ALA:N	1:A:214:ILE:HD11	2.35	0.41
1:A:359:GLN:HE22	1:B:256:TRP:N	2.18	0.41
1:B:151:LEU:CG	1:B:152:ASP:N	2.83	0.41
1:B:190:MET:HE3	1:B:194:ASP:CB	2.49	0.41
1:A:142:ASP:CG	1:A:143:LYS:N	2.78	0.41
1:A:242:ASP:CB	1:A:243:PRO:HD3	2.50	0.41
1:A:256:TRP:CD2	1:A:257:LEU:N	2.87	0.41
1:B:342:ILE:CG2	1:B:378:VAL:CG1	2.98	0.41
1:A:150:LEU:CA	1:A:151:LEU:HD23	2.50	0.41
1:A:174:THR:HG1	1:A:177:GLN:N	2.15	0.41
1:A:252:GLU:OE1	1:A:292:ARG:HG3	2.20	0.41
1:A:342:ILE:CG2	1:A:350:PHE:HB3	2.50	0.41
1:B:95:LYS:O	1:B:378:VAL:HG23	2.20	0.41
1:A:98:THR:HB	1:A:376:LYS:NZ	2.36	0.41
1:A:185:LEU:HG	1:A:190:MET:HG3	2.02	0.41
1:A:340:ARG:HB2	1:A:341:VAL:H	1.32	0.41
1:A:345:ASP:O	1:A:347:ASP:N	2.51	0.41
1:B:104:LEU:CD1	1:B:364:VAL:HG23	2.49	0.41
1:B:168:LEU:HA	1:B:168:LEU:HD12	1.88	0.41
1:A:94:VAL:CG1	1:A:95:LYS:O	2.68	0.41
1:A:145:GLN:C	1:A:147:GLY:H	2.27	0.41
1:A:153:LEU:N	1:A:153:LEU:HD13	2.36	0.41
1:B:127:ARG:N	1:B:127:ARG:CD	2.84	0.41
1:B:135:VAL:CG2	1:B:224:ARG:HA	2.51	0.41
1:B:206:THR:OG1	1:B:207:ARG:N	2.49	0.41
1:B:325:LEU:CD1	1:B:371:LEU:O	2.67	0.41
1:A:94:VAL:HG13	1:A:95:LYS:O	2.21	0.41
1:A:256:TRP:CE2	1:A:257:LEU:HD23	2.53	0.41
1:B:250:ILE:O	1:B:293:THR:CA	2.67	0.41
1:A:186:ARG:HD3	1:A:192:GLU:OE1	2.21	0.41
1:A:230:ALA:O	1:A:231:LYS:C	2.62	0.41
1:B:96:THR:HA	1:B:379:SER:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PHE:O	1:B:153:LEU:HB2	2.19	0.41
1:A:290:ALA:C	1:A:291:THR:OG1	2.63	0.41
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.86	0.41
1:B:247:THR:HA	1:B:296:LEU:O	2.21	0.41
1:B:333:ILE:HG13	1:B:334:ASP:N	2.34	0.41
1:A:246:VAL:HG11	1:A:300:VAL:HG21	2.04	0.40
1:A:280:LYS:HE3	1:A:281:TRP:N	2.36	0.40
1:B:114:VAL:HG13	1:B:244:VAL:CG2	2.51	0.40
1:B:154:THR:CG2	1:B:207:ARG:HD2	2.50	0.40
1:A:223:LEU:HD23	1:A:227:MET:CE	2.51	0.40
1:A:275:THR:HA	1:A:276:LEU:HD23	2.04	0.40
1:B:132:ILE:HG22	1:B:133:ASP:H	1.86	0.40
1:A:339:GLN:O	1:A:340:ARG:CG	2.68	0.40
1:B:183:GLU:C	1:B:183:GLU:CD	2.89	0.40
1:B:339:GLN:O	1:B:340:ARG:CG	2.66	0.40
1:A:288:ASP:O	1:A:290:ALA:N	2.53	0.40
1:B:174:THR:HG1	1:B:177:GLN:HB3	1.86	0.40
1:B:218:ILE:HG23	1:B:237:LYS:O	2.21	0.40
1:B:299:GLU:HG2	1:B:299:GLU:O	2.20	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	A	295/407 (72%)	242 (82%)	27 (9%)	26 (9%)	0	10
1	B	295/407 (72%)	248 (84%)	26 (9%)	21 (7%)	1	13
All	All	590/814 (72%)	490 (83%)	53 (9%)	47 (8%)	1	12

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	140	VAL
1	A	149	PRO
1	A	236	ALA
1	A	258	VAL
1	A	260	ASP
1	A	285	PRO
1	A	288	ASP
1	A	329	SER
1	A	340	ARG
1	B	128	ALA
1	B	136	TYR
1	B	148	THR
1	B	151	LEU
1	B	172	GLY
1	B	204	ILE
1	B	259	LYS
1	B	274	LYS
1	B	329	SER
1	B	340	ARG
1	B	341	VAL
1	B	362	GLN
1	A	90	GLN
1	A	128	ALA
1	A	151	LEU
1	A	202	GLN
1	A	341	VAL
1	A	171	THR
1	A	231	LYS
1	A	346	ALA
1	B	221	PHE
1	B	285	PRO
1	A	291	THR
1	B	231	LYS
1	B	346	ALA
1	A	148	THR
1	A	275	THR
1	A	363	GLY
1	B	301	ASP
1	A	111	PRO
1	A	136	TYR
1	A	189	GLY
1	A	259	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	220	ALA
1	B	272	PRO
1	B	352	PRO
1	B	251	PRO

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	243/332 (73%)	179 (74%)	64 (26%)	0	3
1	B	243/332 (73%)	170 (70%)	73 (30%)	0	2
All	All	486/664 (73%)	349 (72%)	137 (28%)	0	3

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	100	THR
1	A	121	TYR
1	A	144	VAL
1	A	145	GLN
1	A	150	LEU
1	A	152	ASP
1	A	153	LEU
1	A	157	ASP
1	A	160	GLU
1	A	164	GLU
1	A	167	LEU
1	A	168	LEU
1	A	171	THR
1	A	174	THR
1	A	177	GLN
1	A	178	THR
1	A	187	LEU
1	A	190	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	203	LYS
1	A	208	PHE
1	A	214	ILE
1	A	219	THR
1	A	222	ASP
1	A	224	ARG
1	A	227	MET
1	A	229	ILE
1	A	239	GLN
1	A	244	VAL
1	A	252	GLU
1	A	253	SER
1	A	256	TRP
1	A	259	LYS
1	A	266	LEU
1	A	276	LEU
1	A	280	LYS
1	A	282	THR
1	A	283	LEU
1	A	284	LEU
1	A	285	PRO
1	A	287	VAL
1	A	292	ARG
1	A	293	THR
1	A	296	LEU
1	A	316	GLN
1	A	317	LEU
1	A	319	THR
1	A	327	ILE
1	A	332	LEU
1	A	334	ASP
1	A	335	THR
1	A	337	SER
1	A	339	GLN
1	A	340	ARG
1	A	343	THR
1	A	351	VAL
1	A	357	VAL
1	A	361	SER
1	A	362	GLN
1	A	367	LEU
1	A	375	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	378	VAL
1	A	382	LEU
1	A	384	LEU
1	B	98	THR
1	B	117	ASN
1	B	121	TYR
1	B	123	ILE
1	B	125	GLN
1	B	132	ILE
1	B	138	LEU
1	B	140	VAL
1	B	144	VAL
1	B	145	GLN
1	B	148	THR
1	B	151	LEU
1	B	153	LEU
1	B	155	ILE
1	B	157	ASP
1	B	160	GLU
1	B	164	GLU
1	B	165	TYR
1	B	166	LEU
1	B	167	LEU
1	B	174	THR
1	B	176	THR
1	B	187	LEU
1	B	190	MET
1	B	192	GLU
1	B	198	LEU
1	B	202	GLN
1	B	203	LYS
1	B	204	ILE
1	B	206	THR
1	B	208	PHE
1	B	210	LEU
1	B	224	ARG
1	B	229	ILE
1	B	234	VAL
1	B	239	GLN
1	B	241	MET
1	B	252	GLU
1	B	253	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	256	TRP
1	B	257	LEU
1	B	266	LEU
1	B	273	ASP
1	B	276	LEU
1	B	277	THR
1	B	278	ILE
1	B	279	ARG
1	B	282	THR
1	B	283	LEU
1	B	291	THR
1	B	294	LEU
1	B	301	ASP
1	B	311	MET
1	B	316	GLN
1	B	324	MET
1	B	326	LEU
1	B	327	ILE
1	B	334	ASP
1	B	335	THR
1	B	337	SER
1	B	339	GLN
1	B	340	ARG
1	B	342	ILE
1	B	350	PHE
1	B	351	VAL
1	B	361	SER
1	B	365	THR
1	B	367	LEU
1	B	368	ARG
1	B	371	LEU
1	B	378	VAL
1	B	382	LEU
1	B	384	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	145	GLN
1	A	239	GLN
1	A	339	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	359	GLN
1	B	125	GLN
1	B	145	GLN
1	B	239	GLN
1	B	339	GLN
1	B	359	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/407 (72%)	0.82	36 (12%) 8 12	20, 161, 275, 353	0
1	B	297/407 (72%)	0.88	40 (13%) 7 10	20, 167, 274, 377	0
All	All	594/814 (72%)	0.85	76 (12%) 7 11	20, 164, 275, 377	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	MET	4.7
1	A	342	ILE	4.7
1	B	156	PRO	4.6
1	A	300	VAL	4.4
1	B	254	ILE	4.3
1	A	154	THR	4.2
1	A	144	VAL	4.2
1	B	294	LEU	4.0
1	A	157	ASP	3.9
1	B	89	THR	3.9
1	A	156	PRO	3.8
1	B	223	LEU	3.7
1	A	213	PRO	3.5
1	B	158	TRP	3.5
1	B	154	THR	3.3
1	B	206	THR	3.3
1	A	236	ALA	3.3
1	A	89	THR	3.3
1	A	150	LEU	3.2
1	A	358	PHE	3.2
1	B	342	ILE	3.2
1	A	307	LEU	3.2
1	B	129	ALA	3.1
1	B	255	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	229	ILE	3.1
1	B	159	VAL	3.0
1	A	212	ALA	3.0
1	B	328	PRO	2.9
1	A	130	GLY	2.9
1	B	385	ILE	2.8
1	A	359	GLN	2.8
1	A	129	ALA	2.8
1	B	260	ASP	2.8
1	A	206	THR	2.8
1	A	360	ALA	2.7
1	A	328	PRO	2.7
1	A	341	VAL	2.6
1	A	369	SER	2.6
1	B	157	ASP	2.6
1	A	254	ILE	2.6
1	B	359	GLN	2.6
1	B	355	VAL	2.5
1	A	153	LEU	2.5
1	B	325	LEU	2.5
1	A	132	ILE	2.5
1	A	202	GLN	2.5
1	B	93	GLY	2.5
1	B	221	PHE	2.5
1	B	273	ASP	2.4
1	B	341	VAL	2.4
1	A	368	ARG	2.4
1	B	235	VAL	2.4
1	B	289	ALA	2.4
1	A	381	GLY	2.3
1	B	372	ALA	2.3
1	B	358	PHE	2.3
1	B	322	GLU	2.3
1	A	123	ILE	2.2
1	A	155	ILE	2.2
1	B	306	ALA	2.2
1	A	234	VAL	2.2
1	A	170	GLU	2.2
1	B	185	LEU	2.2
1	B	368	ARG	2.1
1	B	123	ILE	2.1
1	B	320	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	LEU	2.1
1	B	332	LEU	2.1
1	B	224	ARG	2.1
1	B	225	ALA	2.1
1	B	290	ALA	2.1
1	A	294	LEU	2.0
1	A	241	MET	2.0
1	A	207	ARG	2.0
1	B	174	THR	2.0
1	A	311	MET	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AG	A	408	1/1	0.73	0.53	30,30,30,30	0
2	AG	B	408	1/1	0.88	0.51	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.