



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:22 PM UTC

PDB ID : 2Y9E / pdb_00002y9e
Title : Structural basis for the allosteric interference of myosin function by mutants G680A and G680V of Dictyostelium myosin-2
Authors : Preller, M.; Bauer, S.; Adamek, N.; Fujita-Becker, S.; Fedorov, R.; Geeves, M.A.; Manstein, D.J.
Deposited on : 2011-02-14
Resolution : 3.40 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

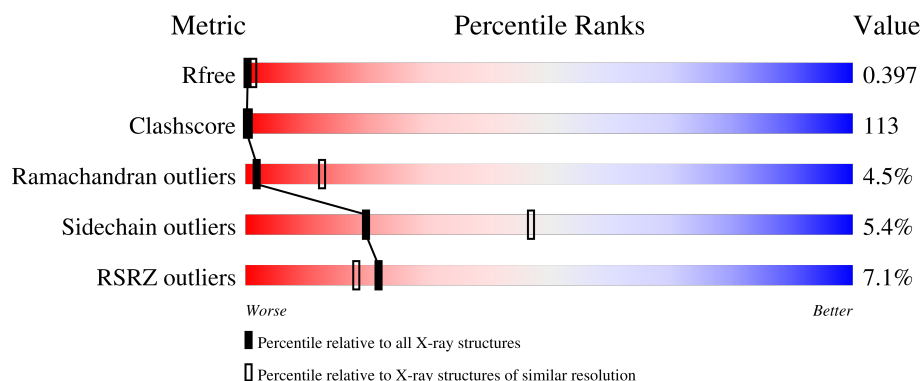
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	X	758	7% 16% 59% 23% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6348 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 MYOSIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	758	Total	C	N	O	S	0	0	0
			6092	3870	1053	1153	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	680	VAL	GLY	engineered mutation	UNP P08799

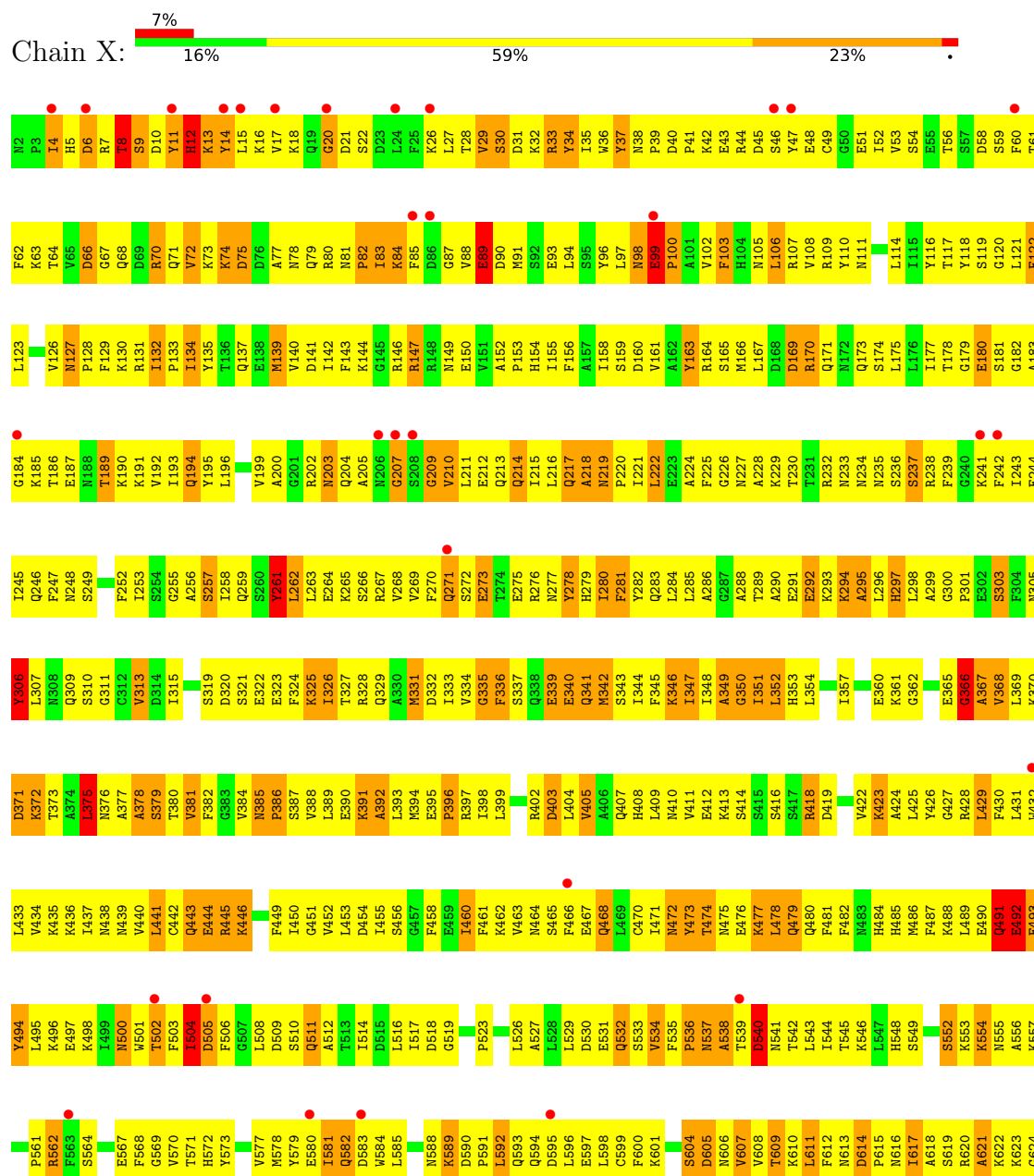
- Molecule 2 is water.

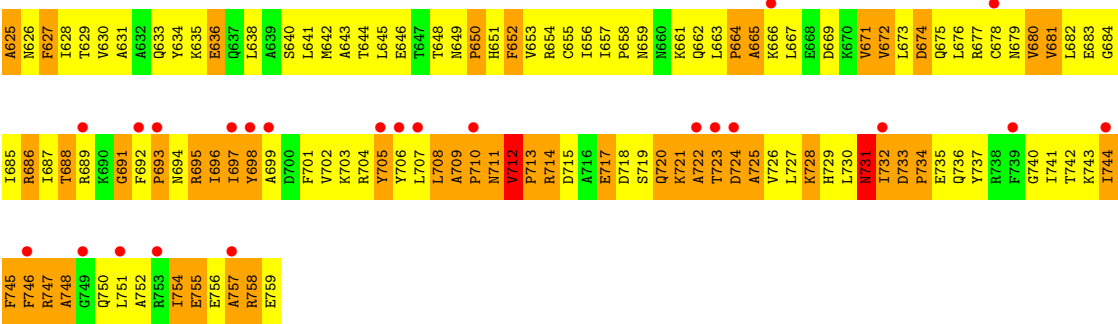
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	256	Total	O	0	0
			256	256		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYOSIN-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	55.00Å 105.80Å 180.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.40 19.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.40) 99.0 (19.96-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.36Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.282 , 0.372 0.292 , 0.397	Depositor DCC
R_{free} test set	760 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.66	0/6212	1.61	204/8382 (2.4%)

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	X	0	2

There are no bond length outliers.

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	X	502	THR	N-CA-C	-17.78	83.47	109.96
1	X	532	GLN	N-CA-CB	-15.32	89.38	110.67
1	X	98	ASN	N-CA-C	-14.95	88.91	108.19
1	X	204	GLN	N-CA-C	14.26	126.52	110.97
1	X	607	VAL	N-CA-C	14.03	123.27	111.90
1	X	720	GLN	N-CA-C	13.97	131.26	112.68
1	X	688	THR	N-CA-C	13.95	129.56	112.54
1	X	313	VAL	N-CA-C	-13.70	99.81	113.10
1	X	581	ILE	CB-CA-C	-13.55	89.07	111.29
1	X	758	ARG	N-CA-C	12.57	128.48	112.89
1	X	581	ILE	N-CA-C	12.45	135.24	109.34
1	X	748	ALA	N-CA-C	-12.38	96.63	112.23
1	X	446	LYS	N-CA-C	12.10	127.94	111.24
1	X	444	GLU	N-CA-C	11.21	127.59	112.68
1	X	445	ARG	N-CA-C	-11.18	99.14	113.12
1	X	403	ASP	N-CA-CB	-11.01	91.05	111.52
1	X	747	ARG	N-CA-C	-10.70	91.95	108.96
1	X	478	LEU	N-CA-C	10.56	125.54	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	697	ILE	N-CA-C	-10.45	95.26	109.37
1	X	13	LYS	N-CA-C	10.24	122.14	110.97
1	X	429	LEU	N-CA-C	-10.24	98.52	111.02
1	X	617	ILE	CB-CA-C	-10.15	101.09	110.63
1	X	681	VAL	N-CA-C	9.50	120.11	110.23
1	X	734	PRO	CB-CA-C	-9.48	97.42	112.21
1	X	746	PHE	CB-CA-C	9.23	121.15	109.80
1	X	249	SER	N-CA-C	9.11	123.41	111.75
1	X	418	ARG	N-CA-C	-9.04	102.24	113.18
1	X	740	GLY	N-CA-C	-9.01	99.76	112.37
1	X	385	ASN	CA-C-N	8.91	129.48	119.32
1	X	385	ASN	C-N-CA	8.91	129.48	119.32
1	X	281	PHE	N-CA-C	8.55	121.73	111.82
1	X	184	GLY	N-CA-C	-8.51	93.01	113.18
1	X	235	ASN	N-CA-CB	-8.50	95.89	111.36
1	X	511	GLN	N-CA-C	-8.39	102.06	111.71
1	X	431	LEU	N-CA-C	-8.31	102.18	111.07
1	X	714	ARG	N-CA-C	8.25	123.65	112.68
1	X	84	LYS	N-CA-C	-8.21	103.72	114.31
1	X	222	LEU	CB-CA-C	-8.20	97.70	110.81
1	X	11	TYR	N-CA-C	8.11	121.29	111.40
1	X	681	VAL	CB-CA-C	-8.07	101.37	111.70
1	X	491	GLN	N-CA-C	8.06	119.84	111.14
1	X	723	THR	N-CA-C	8.02	126.73	113.50
1	X	733	ASP	N-CA-C	8.00	127.49	109.81
1	X	237	SER	N-CA-C	-7.98	98.33	110.30
1	X	17	VAL	N-CA-C	-7.96	97.45	108.12
1	X	492	GLU	N-CA-C	-7.93	101.94	111.69
1	X	734	PRO	N-CA-C	7.92	124.35	113.65
1	X	505	ASP	N-CA-C	-7.91	102.93	112.58
1	X	509	ASP	N-CA-C	-7.88	103.56	113.02
1	X	12	HIS	N-CA-C	-7.75	102.83	111.82
1	X	82	PRO	N-CA-C	-7.74	98.65	111.26
1	X	218	ALA	N-CA-CB	-7.74	99.88	110.56
1	X	386	PRO	CB-CA-C	-7.73	99.20	112.64
1	X	718	ASP	N-CA-CB	7.71	123.42	111.24
1	X	705	TYR	CB-CA-C	-7.69	100.31	111.23
1	X	441	LEU	N-CA-C	-7.61	104.00	113.20
1	X	479	GLN	N-CA-C	-7.56	103.78	113.16
1	X	271	GLN	CB-CA-C	-7.55	94.21	110.45
1	X	366	GLY	N-CA-C	-7.55	95.30	113.18
1	X	83	ILE	N-CA-C	-7.50	93.75	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	429	LEU	N-CA-CB	-7.49	98.44	109.82
1	X	158	ILE	N-CA-C	-7.47	104.68	113.42
1	X	664	PRO	N-CA-C	-7.46	98.28	112.01
1	X	103	PHE	N-CA-C	-7.39	104.14	113.01
1	X	405	VAL	N-CA-CB	-7.39	104.17	112.45
1	X	391	LYS	N-CA-C	7.39	119.33	111.28
1	X	375	LEU	CB-CA-C	-7.36	98.34	110.85
1	X	278	TYR	N-CA-C	-7.35	98.59	110.20
1	X	341	GLN	N-CA-C	-7.26	104.39	113.18
1	X	538	ALA	N-CA-C	-7.19	95.48	110.80
1	X	644	THR	N-CA-C	7.15	119.69	111.11
1	X	387	SER	N-CA-C	-7.11	104.68	113.15
1	X	621	ALA	CB-CA-C	7.11	120.50	109.84
1	X	644	THR	CB-CA-C	-7.10	99.44	110.81
1	X	170	ARG	N-CA-C	-7.10	97.66	108.67
1	X	372	LYS	N-CA-CB	-7.06	98.95	110.59
1	X	444	GLU	CB-CA-C	-7.05	98.46	110.24
1	X	66	ASP	N-CA-C	-7.03	101.48	110.19
1	X	627	PHE	N-CA-CB	-7.02	98.62	110.49
1	X	592	LEU	N-CA-CB	-7.01	98.64	110.49
1	X	746	PHE	N-CA-C	-7.01	100.26	110.64
1	X	127	ASN	CA-C-N	6.96	128.54	119.84
1	X	127	ASN	C-N-CA	6.96	128.54	119.84
1	X	263	LEU	N-CA-C	-6.92	98.55	109.07
1	X	262	LEU	N-CA-CB	6.91	122.90	111.08
1	X	755	GLU	N-CA-C	6.90	120.14	107.73
1	X	278	TYR	CB-CA-C	6.89	121.17	109.53
1	X	349	ALA	N-CA-CB	-6.86	101.46	110.59
1	X	257	SER	N-CA-C	-6.86	97.07	108.32
1	X	405	VAL	N-CA-C	6.86	117.19	108.82
1	X	100	PRO	N-CA-C	-6.84	103.56	113.75
1	X	163	TYR	CB-CA-C	-6.83	99.32	110.79
1	X	681	VAL	N-CA-CB	-6.81	103.47	110.62
1	X	371	ASP	CB-CA-C	-6.75	96.92	111.11
1	X	207	GLY	N-CA-C	6.73	122.90	112.60
1	X	708	LEU	CB-CA-C	6.73	121.55	109.64
1	X	607	VAL	N-CA-CB	-6.72	100.60	111.82
1	X	340	GLU	CB-CA-C	-6.70	97.81	110.67
1	X	472	ASN	CB-CA-C	-6.70	95.99	109.99
1	X	342	MET	CB-CA-C	-6.60	99.83	110.79
1	X	733	ASP	N-CA-CB	-6.57	98.67	110.37
1	X	67	GLY	N-CA-C	6.51	120.05	112.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	347	ILE	N-CA-C	6.50	117.85	111.67
1	X	381	VAL	CB-CA-C	-6.48	104.56	110.91
1	X	712	VAL	N-CA-C	-6.47	94.91	108.88
1	X	222	LEU	N-CA-C	6.45	118.84	111.11
1	X	180	GLU	N-CA-C	-6.44	101.01	110.42
1	X	443	GLN	N-CA-C	6.44	120.03	109.85
1	X	4	ILE	N-CA-C	6.43	120.93	112.76
1	X	534	VAL	N-CA-C	6.40	121.77	113.07
1	X	710	PRO	CB-CA-C	-6.36	105.61	111.40
1	X	70	ARG	N-CA-C	-6.36	101.11	110.52
1	X	262	LEU	N-CA-C	-6.34	99.57	109.72
1	X	609	THR	CB-CA-C	-6.28	99.21	110.70
1	X	414	SER	N-CA-C	-6.28	104.54	111.82
1	X	477	LYS	CB-CA-C	6.27	122.62	110.46
1	X	725	ALA	N-CA-C	-6.26	97.67	108.56
1	X	720	GLN	CB-CA-C	-6.22	99.85	110.24
1	X	326	ILE	N-CA-C	6.22	117.23	111.45
1	X	349	ALA	N-CA-C	6.22	121.53	113.88
1	X	473	TYR	CB-CA-C	-6.18	98.80	110.67
1	X	257	SER	CB-CA-C	6.17	120.33	109.89
1	X	745	PHE	N-CA-C	6.14	118.43	107.80
1	X	537	ASN	N-CA-C	-6.13	97.86	108.52
1	X	185	LYS	N-CA-C	-6.11	105.62	114.12
1	X	752	ALA	N-CA-CB	-6.08	100.21	110.49
1	X	194	GLN	N-CA-C	6.02	117.51	111.07
1	X	89	GLU	N-CA-C	6.00	117.81	111.28
1	X	368	VAL	N-CA-CB	-5.99	102.25	111.05
1	X	403	ASP	N-CA-C	-5.98	99.60	108.99
1	X	391	LYS	CB-CA-C	-5.97	100.88	110.79
1	X	562	ARG	N-CA-C	5.96	117.58	111.14
1	X	466	PHE	CB-CA-C	-5.93	98.62	110.42
1	X	261	TYR	N-CA-C	5.90	123.37	110.80
1	X	350	GLY	N-CA-C	-5.88	105.54	113.24
1	X	517	ILE	CB-CA-C	-5.87	104.23	111.92
1	X	263	LEU	CB-CA-C	5.86	123.05	110.45
1	X	352	LEU	N-CA-C	5.83	118.11	111.11
1	X	200	ALA	N-CA-C	-5.83	106.41	112.93
1	X	29	VAL	N-CA-C	5.82	116.24	108.27
1	X	405	VAL	CB-CA-C	-5.81	103.20	111.34
1	X	589	LYS	CB-CA-C	5.80	118.33	109.34
1	X	311	GLY	N-CA-C	5.78	126.89	113.18
1	X	205	ALA	N-CA-CB	-5.78	102.72	111.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	423	LYS	N-CA-C	5.73	120.41	112.45
1	X	724	ASP	N-CA-C	5.72	119.07	111.75
1	X	504	ILE	N-CA-C	5.69	115.88	110.53
1	X	386	PRO	N-CA-C	5.67	122.20	113.75
1	X	478	LEU	CB-CA-C	-5.65	98.85	110.38
1	X	20	GLY	N-CA-C	5.64	120.60	112.82
1	X	754	ILE	N-CA-C	5.63	121.05	109.34
1	X	604	SER	N-CA-C	-5.62	100.02	108.96
1	X	416	SER	N-CA-C	5.60	120.11	113.16
1	X	554	LYS	CB-CA-C	5.59	117.84	109.13
1	X	680	VAL	CB-CA-C	-5.58	102.13	111.29
1	X	725	ALA	N-CA-CB	5.57	118.09	110.57
1	X	203	ASN	N-CA-C	-5.56	100.28	107.73
1	X	194	GLN	CB-CA-C	-5.53	102.20	110.88
1	X	757	ALA	CB-CA-C	-5.53	100.06	110.51
1	X	704	ARG	CB-CA-C	-5.52	100.60	110.70
1	X	170	ARG	N-CA-CB	5.51	118.76	109.94
1	X	494	TYR	CB-CA-C	5.50	120.02	110.72
1	X	446	LYS	CB-CA-C	-5.50	103.62	112.09
1	X	473	TYR	N-CA-CB	-5.49	101.77	110.28
1	X	189	THR	N-CA-C	-5.48	105.31	111.28
1	X	339	GLU	N-CA-C	5.47	119.92	112.04
1	X	705	TYR	N-CA-CB	5.46	120.39	110.95
1	X	295	ALA	N-CA-C	-5.46	105.25	112.34
1	X	30	SER	N-CA-C	5.43	118.66	109.76
1	X	331	MET	N-CA-C	5.42	117.00	111.14
1	X	758	ARG	N-CA-CB	-5.42	101.57	110.40
1	X	218	ALA	N-CA-C	5.41	118.99	112.93
1	X	99	GLU	N-CA-C	5.34	121.62	109.81
1	X	9	SER	N-CA-C	5.34	114.88	107.73
1	X	379	SER	N-CA-C	-5.33	106.83	113.38
1	X	500	ASN	N-CA-C	5.31	117.94	110.14
1	X	306	TYR	N-CA-C	-5.30	106.84	113.15
1	X	75	ASP	N-CA-C	5.29	118.89	112.23
1	X	384	VAL	N-CA-C	5.28	115.65	107.78
1	X	325	LYS	CB-CA-C	5.24	121.69	110.21
1	X	552	SER	N-CA-C	5.24	117.77	109.96
1	X	319	SER	N-CA-C	5.24	118.47	110.20
1	X	582	GLN	N-CA-CB	5.22	119.31	110.49
1	X	217	GLN	N-CA-C	5.21	119.39	113.19
1	X	392	ALA	N-CA-C	-5.20	106.20	112.54
1	X	744	ILE	CB-CA-C	-5.20	106.85	111.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	351	ILE	CB-CA-C	-5.19	105.17	111.87
1	X	691	GLY	N-CA-C	5.19	125.47	113.18
1	X	614	ASP	CA-C-N	5.18	125.64	120.04
1	X	614	ASP	C-N-CA	5.18	125.64	120.04
1	X	474	THR	N-CA-C	-5.18	105.32	111.69
1	X	367	ALA	N-CA-C	-5.16	101.30	109.76
1	X	33	ARG	N-CA-CB	-5.16	103.26	111.62
1	X	286	ALA	CB-CA-C	5.15	121.48	110.21
1	X	377	ALA	N-CA-C	-5.13	105.34	111.03
1	X	139	MET	N-CA-C	-5.12	106.87	113.01
1	X	502	THR	CB-CA-C	5.11	117.52	110.16
1	X	209	GLY	N-CA-C	-5.10	103.41	112.54
1	X	72	VAL	N-CA-C	5.08	115.23	108.27
1	X	714	ARG	N-CA-CB	-5.07	101.82	110.33
1	X	460	ILE	N-CA-CB	5.04	118.20	111.64
1	X	728	LYS	N-CA-C	-5.04	105.91	111.71
1	X	671	VAL	N-CA-C	5.04	116.21	111.48
1	X	504	ILE	N-CA-CB	-5.01	104.16	110.57

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	169	ASP	Peptide
1	X	696	ILE	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	X	6092	0	6051	1377	4
2	X	256	0	0	86	0
All	All	6348	0	6051	1377	4

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 113.

All (1377) 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:X:242:PHE:CE2	1:X:244:GLU:HG3	1.39	1.54
1:X:163:TYR:CE1	1:X:167:LEU:HD11	1.44	1.49
1:X:242:PHE:CE2	1:X:244:GLU:CG	1.97	1.46
1:X:247:PHE:CD1	1:X:253:ILE:HA	1.48	1.46
1:X:242:PHE:CE2	1:X:244:GLU:CB	2.00	1.44
1:X:689:ARG:CB	1:X:695:ARG:HH21	1.31	1.42
1:X:78:ASN:HB3	1:X:98:ASN:ND2	1.14	1.41
1:X:685:ILE:HG21	1:X:689:ARG:NH2	1.23	1.40
1:X:503:PHE:CE1	1:X:504:ILE:CD1	2.06	1.37
1:X:685:ILE:HG21	1:X:689:ARG:CZ	1.55	1.37
1:X:78:ASN:CB	1:X:98:ASN:ND2	1.86	1.36
1:X:230:THR:CG2	1:X:238:ARG:HH22	1.36	1.36
1:X:626:ASN:OD1	1:X:627:PHE:CD2	1.79	1.34
1:X:242:PHE:CZ	1:X:451:GLY:HA3	1.62	1.33
1:X:503:PHE:CE1	1:X:504:ILE:HD12	1.63	1.33
1:X:682:LEU:HD12	1:X:683:GLU:N	1.43	1.33
1:X:689:ARG:CB	1:X:695:ARG:NH2	1.88	1.32
1:X:296:LEU:C	1:X:297:HIS:ND1	1.84	1.32
1:X:614:ASP:OD1	1:X:615:PRO:CD	1.79	1.31
1:X:242:PHE:CZ	1:X:244:GLU:HG3	1.66	1.30
1:X:539:THR:O	1:X:541:ASN:N	1.62	1.29
1:X:695:ARG:HG2	2:X:2226:HOH:O	1.21	1.29
1:X:464:ASN:CB	1:X:468:GLN:HG2	1.62	1.29
1:X:709:ALA:HB1	1:X:710:PRO:CD	1.61	1.28
1:X:609:THR:O	1:X:613:ASN:HB2	1.23	1.28
1:X:503:PHE:CD1	1:X:504:ILE:HD12	1.67	1.28
1:X:242:PHE:CE2	1:X:244:GLU:HB2	1.64	1.28
1:X:698:TYR:CE2	1:X:699:ALA:HB3	1.69	1.28
1:X:477:LYS:O	1:X:480:GLN:CD	1.78	1.27
1:X:135:TYR:CD2	1:X:191:LYS:HE3	1.71	1.26
1:X:477:LYS:O	1:X:480:GLN:NE2	1.69	1.25
1:X:98:ASN:OD1	1:X:100:PRO:HD2	1.30	1.24
1:X:137:GLN:O	1:X:140:VAL:HG22	1.30	1.24
1:X:725:ALA:HB1	1:X:729:HIS:NE2	1.53	1.23
1:X:692:PHE:CD1	1:X:745:PHE:HB2	1.73	1.22
1:X:29:VAL:CG1	1:X:758:ARG:HB3	1.66	1.22
1:X:464:ASN:HB2	1:X:468:GLN:CG	1.70	1.22
1:X:325:LYS:O	1:X:329:GLN:HB2	1.32	1.21
1:X:641:LEU:O	1:X:645:LEU:HD13	1.41	1.20
1:X:210:VAL:CG2	1:X:214:GLN:OE1	1.88	1.20
1:X:477:LYS:O	1:X:480:GLN:OE1	1.55	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:242:PHE:HE2	1:X:244:GLU:CG	1.40	1.20
1:X:685:ILE:CG2	1:X:689:ARG:CZ	2.20	1.19
1:X:725:ALA:HB1	1:X:729:HIS:CD2	1.78	1.19
1:X:137:GLN:O	1:X:140:VAL:CG2	1.90	1.19
1:X:692:PHE:HD1	1:X:745:PHE:CB	1.57	1.17
1:X:64:THR:HG21	1:X:68:GLN:O	1.45	1.16
1:X:375:LEU:HD13	1:X:375:LEU:O	1.45	1.16
1:X:709:ALA:HB1	1:X:710:PRO:HD2	1.17	1.15
1:X:510:SER:O	1:X:514:ILE:HD12	1.46	1.15
1:X:29:VAL:CG1	1:X:758:ARG:CB	2.24	1.14
1:X:64:THR:CG2	1:X:68:GLN:O	1.95	1.14
1:X:362:GLY:HA3	1:X:366:GLY:O	1.46	1.14
1:X:689:ARG:HE	1:X:695:ARG:CZ	1.59	1.14
1:X:751:LEU:O	1:X:751:LEU:HD12	1.46	1.14
1:X:626:ASN:OD1	1:X:627:PHE:N	1.79	1.13
1:X:689:ARG:HB3	1:X:695:ARG:NH2	1.50	1.13
1:X:64:THR:HG23	1:X:66:ASP:O	1.50	1.12
1:X:247:PHE:CD1	1:X:253:ILE:CA	2.30	1.12
1:X:48:GLU:HG3	1:X:49:CYS:H	1.11	1.11
1:X:238:ARG:CZ	1:X:267:ARG:NH2	2.13	1.11
1:X:681:VAL:HG23	1:X:682:LEU:H	1.05	1.10
1:X:581:ILE:O	1:X:584:TRP:CD1	2.05	1.10
1:X:230:THR:HG23	1:X:238:ARG:NH2	1.66	1.09
1:X:29:VAL:HG11	1:X:758:ARG:CB	1.82	1.09
1:X:85:PHE:HD1	1:X:88:VAL:HG21	1.15	1.09
1:X:210:VAL:HG13	1:X:211:LEU:H	1.13	1.09
1:X:592:LEU:O	1:X:592:LEU:HD12	1.49	1.09
1:X:135:TYR:CE2	1:X:191:LYS:HE3	1.88	1.09
1:X:365:GLU:HG3	1:X:366:GLY:H	1.11	1.09
1:X:98:ASN:OD1	1:X:100:PRO:CD	2.00	1.08
1:X:137:GLN:NE2	1:X:140:VAL:HG21	1.66	1.08
1:X:230:THR:CG2	1:X:238:ARG:NH2	2.16	1.08
1:X:689:ARG:HB2	1:X:695:ARG:NH2	1.69	1.08
1:X:163:TYR:HE1	1:X:167:LEU:CD1	1.66	1.08
1:X:246:GLN:HE21	1:X:443:GLN:HB2	0.98	1.07
1:X:691:GLY:HA2	1:X:747:ARG:NH1	1.68	1.07
1:X:163:TYR:CE1	1:X:167:LEU:CD1	2.37	1.07
1:X:298:LEU:HD12	1:X:299:ALA:N	1.69	1.07
1:X:230:THR:HG23	1:X:238:ARG:HH22	1.06	1.07
1:X:291:GLU:HB2	2:X:2099:HOH:O	1.52	1.06
1:X:424:ALA:O	1:X:428:ARG:CG	2.02	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:685:ILE:HG22	1:X:689:ARG:NH1	1.69	1.06
1:X:210:VAL:HG21	1:X:214:GLN:OE1	1.56	1.06
1:X:503:PHE:CZ	1:X:504:ILE:HD11	1.89	1.05
1:X:614:ASP:OD1	1:X:615:PRO:HD2	0.90	1.05
1:X:238:ARG:NH1	1:X:267:ARG:HH21	1.51	1.05
1:X:685:ILE:CG2	1:X:689:ARG:NH1	2.18	1.05
1:X:8:THR:HG22	1:X:8:THR:O	1.52	1.05
1:X:701:PHE:CZ	1:X:713:PRO:O	2.09	1.05
1:X:464:ASN:HB2	1:X:468:GLN:HG2	1.06	1.04
1:X:526:LEU:HD22	1:X:631:ALA:HB1	1.40	1.04
1:X:709:ALA:CB	1:X:710:PRO:CD	2.32	1.04
1:X:230:THR:HG21	1:X:238:ARG:HH22	1.20	1.03
1:X:675:GLN:HA	1:X:678:CYS:HB2	1.40	1.03
1:X:741:ILE:HG23	1:X:742:THR:CG2	1.87	1.03
1:X:741:ILE:CG2	1:X:742:THR:HG23	1.87	1.03
1:X:692:PHE:CE1	1:X:745:PHE:HB2	1.92	1.03
1:X:698:TYR:CE2	1:X:699:ALA:CB	2.41	1.03
1:X:705:TYR:CD1	1:X:705:TYR:O	2.11	1.03
1:X:60:PHE:HB3	1:X:72:VAL:O	1.59	1.02
1:X:709:ALA:O	2:X:2234:HOH:O	1.75	1.02
1:X:458:PHE:HE1	1:X:475:ASN:HB3	1.21	1.02
1:X:365:GLU:CG	1:X:366:GLY:H	1.72	1.02
1:X:503:PHE:CE1	1:X:504:ILE:HD11	1.92	1.02
1:X:203:ASN:HB2	1:X:207:GLY:O	1.58	1.02
1:X:296:LEU:O	1:X:297:HIS:ND1	1.91	1.02
1:X:698:TYR:CG	1:X:699:ALA:N	2.26	1.02
1:X:56:THR:HB	1:X:59:SER:O	1.60	1.01
1:X:210:VAL:HG22	1:X:214:GLN:OE1	1.57	1.01
1:X:681:VAL:HG23	1:X:682:LEU:N	1.70	1.01
1:X:78:ASN:CB	1:X:98:ASN:HD22	1.59	1.01
1:X:238:ARG:NH1	1:X:267:ARG:NH2	2.06	1.01
1:X:685:ILE:CG2	1:X:689:ARG:NH2	2.19	1.01
1:X:689:ARG:HB3	1:X:695:ARG:HH21	0.85	1.01
1:X:247:PHE:HD1	1:X:253:ILE:HA	1.18	1.01
1:X:726:VAL:HG23	1:X:730:LEU:HD21	1.41	1.00
1:X:243:ILE:HG23	1:X:258:ILE:HG13	1.41	1.00
1:X:692:PHE:CD1	1:X:745:PHE:CB	2.37	1.00
1:X:741:ILE:HG23	1:X:742:THR:HG23	1.00	0.99
1:X:424:ALA:O	1:X:428:ARG:HG3	1.62	0.99
1:X:726:VAL:O	1:X:730:LEU:HG	1.62	0.99
1:X:242:PHE:CD2	1:X:244:GLU:HB2	1.98	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:693:PRO:HG2	1:X:748:ALA:H	1.22	0.98
1:X:87:GLY:HA2	1:X:109:ARG:HD3	1.43	0.98
1:X:11:TYR:O	1:X:15:LEU:HB2	1.62	0.98
1:X:682:LEU:O	2:X:2217:HOH:O	1.80	0.98
1:X:424:ALA:O	1:X:428:ARG:CD	2.12	0.98
1:X:85:PHE:CD1	1:X:88:VAL:HG21	1.99	0.98
1:X:474:THR:O	1:X:478:LEU:HD13	1.64	0.97
1:X:490:GLU:O	1:X:494:TYR:HD2	1.47	0.97
1:X:13:LYS:HA	1:X:18:LYS:HD2	1.43	0.97
1:X:682:LEU:CD1	1:X:683:GLU:N	2.27	0.96
1:X:480:GLN:HB2	1:X:508:LEU:CD2	1.94	0.96
1:X:685:ILE:HG21	1:X:689:ARG:HH22	1.19	0.96
1:X:736:GLN:O	1:X:747:ARG:CG	2.14	0.96
1:X:247:PHE:HD1	1:X:253:ILE:CA	1.75	0.96
1:X:98:ASN:OD1	1:X:99:GLU:N	1.99	0.95
1:X:75:ASP:OD1	2:X:2041:HOH:O	1.83	0.95
1:X:98:ASN:CG	1:X:100:PRO:HD2	1.90	0.95
1:X:242:PHE:CZ	1:X:451:GLY:CA	2.49	0.95
1:X:698:TYR:CZ	1:X:699:ALA:HB2	2.00	0.95
1:X:724:ASP:OD2	2:X:2243:HOH:O	1.84	0.95
1:X:736:GLN:O	1:X:747:ARG:HG3	1.64	0.95
1:X:121:LEU:HD13	1:X:652:PHE:CE2	2.02	0.95
1:X:609:THR:O	1:X:613:ASN:CB	2.15	0.95
1:X:350:GLY:O	1:X:354:LEU:HG	1.67	0.95
1:X:641:LEU:O	1:X:645:LEU:CD1	2.14	0.95
1:X:424:ALA:O	1:X:428:ARG:HD2	1.66	0.94
1:X:242:PHE:HZ	1:X:451:GLY:HA3	1.19	0.94
1:X:504:ILE:HD12	1:X:505:ASP:H	1.32	0.94
1:X:626:ASN:OD1	1:X:627:PHE:HD2	1.26	0.94
1:X:689:ARG:NE	1:X:695:ARG:CZ	2.29	0.94
1:X:709:ALA:CB	1:X:710:PRO:HD2	1.94	0.94
1:X:183:ALA:HB1	1:X:655:CYS:HB3	1.47	0.93
1:X:682:LEU:HD12	1:X:683:GLU:CA	1.98	0.93
1:X:485:HIS:HE1	1:X:650:PRO:HD2	1.33	0.93
1:X:748:ALA:O	1:X:751:LEU:HG	1.66	0.93
1:X:337:SER:HB3	1:X:340:GLU:HG2	1.50	0.93
1:X:581:ILE:O	1:X:584:TRP:HD1	1.51	0.93
1:X:689:ARG:NE	1:X:695:ARG:NH2	2.15	0.93
1:X:78:ASN:CA	1:X:98:ASN:HD22	1.81	0.92
1:X:689:ARG:CD	1:X:695:ARG:NH2	2.33	0.92
1:X:698:TYR:CZ	1:X:699:ALA:CB	2.53	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:37:TYR:HE1	1:X:39:PRO:HA	1.33	0.92
1:X:246:GLN:NE2	1:X:443:GLN:HB2	1.84	0.92
1:X:87:GLY:HA2	1:X:109:ARG:CD	1.99	0.92
1:X:229:LYS:HB2	1:X:234:ASN:O	1.71	0.91
1:X:294:LYS:HD2	1:X:297:HIS:HA	1.50	0.91
1:X:7:ARG:HE	1:X:18:LYS:HB3	1.35	0.91
1:X:242:PHE:CZ	1:X:244:GLU:CG	2.37	0.91
1:X:166:MET:O	1:X:170:ARG:HA	1.71	0.91
1:X:238:ARG:CZ	1:X:267:ARG:HH21	1.78	0.90
1:X:362:GLY:CA	1:X:366:GLY:O	2.19	0.90
1:X:48:GLU:HG3	1:X:49:CYS:N	1.85	0.90
1:X:135:TYR:CD2	1:X:191:LYS:CE	2.53	0.90
1:X:29:VAL:HG13	1:X:758:ARG:CB	2.00	0.90
1:X:539:THR:O	1:X:539:THR:HG23	1.70	0.90
1:X:137:GLN:C	1:X:140:VAL:HG22	1.96	0.90
1:X:56:THR:HG22	1:X:59:SER:H	1.37	0.89
1:X:393:LEU:HD12	1:X:596:LEU:HD21	1.55	0.89
1:X:548:HIS:O	1:X:552:SER:OG	1.89	0.89
1:X:474:THR:O	1:X:478:LEU:CD1	2.20	0.89
1:X:681:VAL:CG2	1:X:682:LEU:H	1.86	0.89
1:X:210:VAL:HG13	1:X:211:LEU:N	1.88	0.89
1:X:458:PHE:CE1	1:X:475:ASN:HB3	2.07	0.88
1:X:588:ASN:O	1:X:630:VAL:HG22	1.73	0.88
1:X:398:ILE:HD13	1:X:407:GLN:HG3	1.56	0.88
1:X:532:GLN:OE1	1:X:543:LEU:HD13	1.74	0.88
1:X:725:ALA:CB	1:X:729:HIS:CD2	2.56	0.88
1:X:689:ARG:HB2	1:X:695:ARG:HH22	1.36	0.88
1:X:698:TYR:CD1	2:X:2227:HOH:O	2.26	0.88
1:X:241:LYS:CE	1:X:243:ILE:HD11	2.05	0.87
1:X:709:ALA:HB1	1:X:710:PRO:HD3	1.55	0.87
1:X:725:ALA:C	1:X:729:HIS:HD2	1.82	0.87
1:X:117:THR:O	1:X:123:LEU:HD12	1.74	0.87
1:X:29:VAL:HG13	1:X:758:ARG:HB3	1.57	0.87
1:X:379:SER:OG	1:X:389:LEU:HD22	1.75	0.87
1:X:710:PRO:O	1:X:711:ASN:HB2	1.73	0.87
1:X:379:SER:OG	1:X:389:LEU:CD2	2.22	0.87
1:X:247:PHE:CE1	1:X:253:ILE:HA	2.09	0.87
1:X:255:GLY:HA3	1:X:443:GLN:HG3	1.54	0.87
1:X:685:ILE:HD13	1:X:689:ARG:NH2	1.90	0.87
1:X:689:ARG:HE	1:X:695:ARG:NH2	1.71	0.86
1:X:485:HIS:CE1	1:X:650:PRO:HD2	2.10	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:539:THR:HG23	1:X:541:ASN:HB3	1.55	0.86
1:X:693:PRO:HG2	1:X:748:ALA:N	1.91	0.86
1:X:11:TYR:CE2	1:X:16:LYS:HB2	2.10	0.86
1:X:666:LYS:O	2:X:2213:HOH:O	1.92	0.86
1:X:84:LYS:CE	1:X:85:PHE:CE2	2.59	0.86
1:X:604:SER:O	1:X:605:ASP:CG	2.19	0.86
1:X:7:ARG:NH2	2:X:2002:HOH:O	2.09	0.85
1:X:7:ARG:O	1:X:8:THR:HB	1.74	0.85
1:X:121:LEU:HD11	1:X:482:PHE:CE2	2.10	0.85
1:X:474:THR:HG23	1:X:638:LEU:HD13	1.58	0.85
1:X:33:ARG:HD2	1:X:52:ILE:CG2	2.06	0.85
1:X:365:GLU:HG3	1:X:366:GLY:N	1.91	0.85
1:X:298:LEU:CD1	1:X:299:ALA:O	2.24	0.85
1:X:691:GLY:HA2	1:X:747:ARG:HH12	1.32	0.85
1:X:16:LYS:HD2	1:X:152:ALA:HB2	1.57	0.85
1:X:29:VAL:CG1	1:X:758:ARG:HB2	2.03	0.85
1:X:510:SER:O	1:X:514:ILE:CD1	2.22	0.85
1:X:428:ARG:HH12	1:X:618:ALA:HA	1.40	0.85
1:X:8:THR:O	1:X:8:THR:CG2	2.24	0.85
1:X:121:LEU:HD21	1:X:486:MET:SD	2.17	0.84
1:X:313:VAL:O	1:X:315:ILE:HG13	1.77	0.84
1:X:534:VAL:HG23	1:X:535:PHE:CE2	2.11	0.84
1:X:35:ILE:HB	1:X:52:ILE:HD11	1.56	0.84
1:X:293:LYS:HE2	1:X:298:LEU:HD11	1.58	0.84
1:X:285:LEU:HD13	1:X:301:PRO:HB3	1.57	0.84
1:X:134:ILE:HG13	1:X:134:ILE:O	1.78	0.83
1:X:294:LYS:HB3	1:X:294:LYS:HZ2	1.43	0.83
1:X:29:VAL:HG11	1:X:758:ARG:HB2	1.60	0.83
1:X:244:GLU:HG2	1:X:451:GLY:CA	2.09	0.83
1:X:485:HIS:CE1	1:X:650:PRO:CD	2.62	0.83
1:X:539:THR:C	1:X:541:ASN:H	1.86	0.83
1:X:84:LYS:HE3	1:X:85:PHE:CE2	2.14	0.83
1:X:689:ARG:CG	1:X:695:ARG:HH21	1.90	0.83
1:X:465:SER:N	1:X:468:GLN:OE1	2.09	0.83
1:X:11:TYR:OH	1:X:152:ALA:HB3	1.77	0.83
1:X:726:VAL:HG23	1:X:730:LEU:CD2	2.09	0.83
1:X:219:ASN:H	1:X:220:PRO:HD2	1.42	0.83
1:X:203:ASN:ND2	1:X:207:GLY:HA3	1.95	0.82
1:X:651:HIS:HE1	2:X:2207:HOH:O	1.62	0.82
1:X:705:TYR:O	1:X:705:TYR:CG	2.31	0.82
1:X:689:ARG:HD2	1:X:695:ARG:NE	1.94	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:470:CYS:HB3	1:X:634:TYR:CZ	2.14	0.82
1:X:539:THR:C	1:X:541:ASN:N	2.34	0.82
1:X:147:ARG:N	1:X:150:GLU:OE2	2.12	0.82
1:X:243:ILE:HG23	1:X:258:ILE:CG1	2.10	0.82
1:X:693:PRO:CG	1:X:748:ALA:H	1.92	0.81
1:X:203:ASN:HB2	1:X:207:GLY:C	2.04	0.81
1:X:239:PHE:CE2	1:X:241:LYS:HD3	2.16	0.81
1:X:325:LYS:O	1:X:329:GLN:CB	2.24	0.81
1:X:464:ASN:HB3	1:X:468:GLN:HG2	1.59	0.81
1:X:490:GLU:O	1:X:494:TYR:CD2	2.32	0.81
1:X:689:ARG:HD2	1:X:695:ARG:HE	1.43	0.81
1:X:246:GLN:HE21	1:X:443:GLN:CB	1.89	0.81
1:X:475:ASN:O	1:X:478:LEU:HB2	1.80	0.81
1:X:607:VAL:HA	1:X:610:LYS:HB3	1.63	0.81
1:X:46:SER:OG	1:X:669:ASP:OD2	1.99	0.81
1:X:572:HIS:CD2	1:X:577:VAL:HG21	2.16	0.81
1:X:492:GLU:O	1:X:495:LEU:HG	1.80	0.80
1:X:464:ASN:HB2	1:X:468:GLN:CB	2.11	0.80
1:X:102:VAL:O	1:X:106:LEU:HB2	1.82	0.80
1:X:369:LEU:HD11	1:X:372:LYS:HE3	1.62	0.80
1:X:486:MET:HE1	1:X:689:ARG:NH1	1.97	0.80
1:X:682:LEU:HD12	1:X:683:GLU:H	1.43	0.80
1:X:211:LEU:HB3	2:X:2087:HOH:O	1.82	0.80
1:X:331:MET:O	1:X:336:PHE:HB2	1.82	0.80
1:X:13:LYS:HD3	1:X:18:LYS:NZ	1.97	0.80
1:X:121:LEU:HD13	1:X:652:PHE:HE2	1.47	0.80
1:X:609:THR:HG23	1:X:613:ASN:ND2	1.97	0.80
1:X:677:ARG:HA	2:X:2218:HOH:O	1.80	0.80
1:X:78:ASN:CG	1:X:98:ASN:ND2	2.39	0.79
1:X:541:ASN:O	1:X:545:THR:HG23	1.81	0.79
1:X:38:ASN:HB2	1:X:47:TYR:CE1	2.16	0.79
1:X:279:HIS:O	1:X:283:GLN:HG2	1.83	0.79
1:X:285:LEU:HD23	1:X:298:LEU:HD22	1.65	0.79
1:X:597:GLU:C	1:X:601:LYS:HG3	2.08	0.79
1:X:754:ILE:HG23	1:X:755:GLU:N	1.97	0.79
1:X:126:VAL:HG23	1:X:656:ILE:O	1.83	0.79
1:X:582:GLN:HB2	2:X:2186:HOH:O	1.82	0.79
1:X:7:ARG:HH21	1:X:18:LYS:HE2	1.47	0.79
1:X:84:LYS:HE2	1:X:85:PHE:CE2	2.18	0.79
1:X:242:PHE:HE2	1:X:244:GLU:CB	1.67	0.79
1:X:64:THR:HG22	1:X:68:GLN:O	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:375:LEU:O	1:X:375:LEU:CD1	2.29	0.79
1:X:518:ASP:HB2	1:X:635:LYS:NZ	1.97	0.79
1:X:679:ASN:HB2	1:X:681:VAL:HG13	1.62	0.79
1:X:230:THR:HB	1:X:275:GLU:OE2	1.83	0.78
1:X:736:GLN:O	1:X:747:ARG:CD	2.31	0.78
1:X:488:LYS:O	1:X:491:GLN:HB3	1.84	0.78
1:X:226:GLY:O	1:X:238:ARG:HB3	1.84	0.78
1:X:375:LEU:HD13	1:X:375:LEU:C	2.09	0.78
1:X:733:ASP:HB2	1:X:734:PRO:HD2	1.65	0.78
1:X:689:ARG:CD	1:X:695:ARG:HH21	1.95	0.78
1:X:494:TYR:HB3	1:X:500:ASN:CG	2.09	0.78
1:X:33:ARG:HD2	1:X:52:ILE:HG21	1.64	0.78
1:X:20:GLY:HA3	2:X:2011:HOH:O	1.84	0.78
1:X:132:ILE:O	1:X:134:ILE:HG23	1.83	0.78
1:X:247:PHE:HD1	1:X:253:ILE:N	1.81	0.78
1:X:701:PHE:HZ	1:X:713:PRO:O	1.66	0.78
1:X:121:LEU:HD11	1:X:482:PHE:HE2	1.46	0.77
1:X:365:GLU:CG	1:X:366:GLY:N	2.45	0.77
1:X:202:ARG:HG2	1:X:252:PHE:HD2	1.49	0.77
1:X:219:ASN:H	1:X:220:PRO:CD	1.97	0.77
1:X:477:LYS:HD3	1:X:638:LEU:HD21	1.64	0.77
1:X:680:VAL:HG22	1:X:684:GLY:HA2	1.65	0.77
1:X:121:LEU:HD13	1:X:652:PHE:CD2	2.19	0.77
1:X:152:ALA:HB1	1:X:153:PRO:HD2	1.66	0.77
1:X:36:TRP:HE3	1:X:48:GLU:O	1.65	0.77
1:X:241:LYS:HE2	1:X:243:ILE:HD11	1.65	0.77
1:X:626:ASN:CG	1:X:627:PHE:HD2	1.91	0.77
1:X:282:TYR:HB3	2:X:2098:HOH:O	1.84	0.77
1:X:562:ARG:NH1	2:X:2178:HOH:O	2.17	0.77
1:X:717:GLU:O	1:X:717:GLU:HG2	1.85	0.77
1:X:751:LEU:O	1:X:751:LEU:CD1	2.31	0.77
1:X:81:ASN:HB3	1:X:82:PRO:HD2	1.65	0.77
1:X:343:SER:HA	1:X:346:LYS:HB2	1.65	0.77
1:X:503:PHE:CD1	1:X:504:ILE:CD1	2.51	0.77
1:X:391:LYS:O	1:X:395:GLU:O	2.02	0.77
1:X:484:HIS:O	1:X:487:PHE:HB3	1.83	0.77
1:X:56:THR:HB	1:X:59:SER:C	2.09	0.77
1:X:187:GLU:HA	1:X:190:LYS:HB2	1.67	0.76
1:X:272:SER:OG	1:X:273:GLU:N	2.19	0.76
1:X:146:ARG:HA	1:X:150:GLU:OE2	1.86	0.76
1:X:7:ARG:O	1:X:8:THR:CB	2.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:12:HIS:HB3	1:X:18:LYS:HG2	1.66	0.76
1:X:247:PHE:HE1	1:X:253:ILE:HB	1.50	0.76
1:X:664:PRO:O	1:X:665:ALA:CB	2.33	0.76
1:X:701:PHE:HD2	2:X:2229:HOH:O	1.68	0.76
1:X:5:HIS:O	1:X:6:ASP:HB2	1.84	0.75
1:X:698:TYR:CE1	1:X:699:ALA:HB2	2.20	0.75
1:X:210:VAL:CG1	1:X:211:LEU:H	1.97	0.75
1:X:386:PRO:O	1:X:390:GLU:HG2	1.86	0.75
1:X:491:GLN:O	2:X:2155:HOH:O	2.04	0.75
1:X:626:ASN:OD1	1:X:627:PHE:CG	2.38	0.75
1:X:56:THR:CG2	1:X:59:SER:H	2.00	0.75
1:X:85:PHE:HD1	1:X:88:VAL:CG2	1.99	0.75
1:X:641:LEU:C	1:X:645:LEU:HD13	2.11	0.75
1:X:651:HIS:CE1	2:X:2207:HOH:O	2.37	0.75
1:X:331:MET:C	1:X:336:PHE:HB2	2.11	0.75
1:X:12:HIS:O	1:X:18:LYS:HG3	1.85	0.75
1:X:432:TRP:CZ2	1:X:610:LYS:HD3	2.22	0.75
1:X:5:HIS:O	1:X:6:ASP:CB	2.34	0.75
1:X:675:GLN:HA	1:X:678:CYS:CB	2.17	0.75
1:X:296:LEU:C	1:X:297:HIS:CG	2.65	0.74
1:X:490:GLU:HA	1:X:493:GLU:HB2	1.69	0.74
1:X:540:ASP:OD1	1:X:585:LEU:HD12	1.87	0.74
1:X:546:LYS:HB3	2:X:2172:HOH:O	1.86	0.74
1:X:33:ARG:HG3	1:X:52:ILE:HB	1.69	0.74
1:X:247:PHE:CE1	1:X:253:ILE:CA	2.70	0.74
1:X:344:ILE:O	1:X:348:ILE:HG12	1.87	0.74
1:X:375:LEU:CD1	1:X:375:LEU:C	2.61	0.74
1:X:480:GLN:HB2	1:X:508:LEU:HD21	1.70	0.74
1:X:87:GLY:CA	1:X:109:ARG:HD3	2.18	0.74
1:X:698:TYR:CD2	1:X:699:ALA:HB3	2.22	0.74
1:X:464:ASN:CB	1:X:468:GLN:CG	2.46	0.73
1:X:685:ILE:O	1:X:688:THR:N	2.20	0.73
1:X:369:LEU:HD12	1:X:369:LEU:O	1.86	0.73
1:X:15:LEU:HD21	1:X:139:MET:SD	2.29	0.73
1:X:244:GLU:HG2	1:X:451:GLY:HA2	1.70	0.73
1:X:242:PHE:CD2	1:X:244:GLU:CB	2.62	0.73
1:X:539:THR:O	1:X:541:ASN:CA	2.37	0.73
1:X:685:ILE:HG21	1:X:689:ARG:NH1	1.94	0.73
1:X:129:PHE:HE2	1:X:658:PRO:HG2	1.52	0.73
1:X:228:ALA:HA	1:X:279:HIS:CE1	2.23	0.73
1:X:428:ARG:NH1	1:X:618:ALA:HA	2.04	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:98:ASN:OD1	1:X:98:ASN:C	2.31	0.73
1:X:582:GLN:HA	1:X:582:GLN:NE2	2.04	0.73
1:X:728:LYS:HA	1:X:734:PRO:HD3	1.69	0.73
1:X:78:ASN:HB3	1:X:98:ASN:HD21	0.92	0.73
1:X:163:TYR:CD1	1:X:167:LEU:HD11	2.18	0.72
1:X:132:ILE:HD12	1:X:132:ILE:N	2.04	0.72
1:X:702:VAL:HA	1:X:714:ARG:O	1.89	0.72
1:X:215:ILE:HG12	1:X:441:LEU:HD22	1.72	0.72
1:X:743:LYS:HD3	2:X:2248:HOH:O	1.89	0.72
1:X:298:LEU:HD12	1:X:299:ALA:O	1.87	0.72
1:X:90:ASP:HA	1:X:118:TYR:HB2	1.71	0.72
1:X:342:MET:O	1:X:342:MET:SD	2.48	0.72
1:X:479:GLN:NE2	1:X:573:TYR:CD2	2.58	0.72
1:X:597:GLU:O	1:X:601:LYS:HG3	1.90	0.72
1:X:99:GLU:O	1:X:102:VAL:HG12	1.90	0.72
1:X:332:ASP:HB3	1:X:336:PHE:O	1.89	0.72
1:X:213:GLN:HA	1:X:216:LEU:HD13	1.70	0.72
1:X:224:ALA:O	1:X:280:ILE:HG23	1.90	0.71
1:X:306:TYR:HE2	1:X:422:VAL:HG11	1.53	0.71
1:X:84:LYS:HE3	1:X:85:PHE:CZ	2.25	0.71
1:X:122:PHE:CE1	1:X:652:PHE:HB2	2.25	0.71
1:X:156:PHE:HA	1:X:159:SER:OG	1.90	0.71
1:X:294:LYS:HE2	1:X:297:HIS:HB3	1.71	0.71
1:X:572:HIS:HD2	1:X:577:VAL:HG21	1.55	0.71
1:X:642:MET:SD	1:X:645:LEU:HD22	2.30	0.71
1:X:347:ILE:HA	1:X:382:PHE:HE1	1.54	0.71
1:X:389:LEU:HD13	1:X:600:PHE:CZ	2.25	0.71
1:X:242:PHE:CE1	1:X:451:GLY:HA3	2.23	0.71
1:X:298:LEU:HD13	1:X:299:ALA:O	1.90	0.71
1:X:458:PHE:HE1	1:X:475:ASN:CB	2.02	0.71
1:X:728:LYS:HG2	1:X:734:PRO:HG3	1.72	0.71
1:X:534:VAL:HG23	1:X:535:PHE:CD2	2.25	0.71
1:X:7:ARG:NE	1:X:18:LYS:HB3	2.05	0.71
1:X:210:VAL:CG2	1:X:214:GLN:CD	2.64	0.71
1:X:245:ILE:HD11	1:X:450:ILE:HB	1.72	0.71
1:X:245:ILE:O	1:X:245:ILE:HD12	1.91	0.70
1:X:692:PHE:HD1	1:X:745:PHE:CG	2.08	0.70
1:X:698:TYR:CD2	1:X:699:ALA:N	2.52	0.70
1:X:247:PHE:CE1	1:X:253:ILE:HB	2.27	0.70
1:X:29:VAL:HG11	1:X:758:ARG:HD2	1.73	0.70
1:X:193:ILE:HD11	2:X:2072:HOH:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:474:THR:HG23	1:X:638:LEU:CD1	2.22	0.70
1:X:490:GLU:HB3	1:X:494:TYR:HE2	1.56	0.70
1:X:736:GLN:O	1:X:747:ARG:HD2	1.91	0.70
1:X:129:PHE:HB2	1:X:664:PRO:HB3	1.72	0.70
1:X:721:LYS:HE2	2:X:2241:HOH:O	1.91	0.70
1:X:48:GLU:CG	1:X:49:CYS:H	1.96	0.70
1:X:238:ARG:HG2	1:X:278:TYR:OH	1.91	0.70
1:X:590:ASP:N	1:X:591:PRO:HD3	2.05	0.70
1:X:532:GLN:OE1	1:X:543:LEU:CD1	2.39	0.70
1:X:685:ILE:HD13	1:X:689:ARG:HH21	1.56	0.70
1:X:36:TRP:CE3	1:X:48:GLU:O	2.44	0.70
1:X:105:ASN:O	1:X:109:ARG:HG2	1.92	0.70
1:X:326:ILE:HG23	2:X:2114:HOH:O	1.90	0.70
1:X:38:ASN:HB2	1:X:47:TYR:CD1	2.26	0.69
1:X:283:GLN:HB2	1:X:324:PHE:HD1	1.56	0.69
1:X:490:GLU:HB3	1:X:494:TYR:CE2	2.27	0.69
1:X:508:LEU:HA	2:X:2161:HOH:O	1.91	0.69
1:X:389:LEU:CD1	1:X:600:PHE:CZ	2.75	0.69
1:X:130:LYS:HG2	1:X:131:ARG:H	1.57	0.69
1:X:464:ASN:HA	1:X:468:GLN:CD	2.17	0.69
1:X:691:GLY:CA	1:X:747:ARG:NH1	2.53	0.69
1:X:109:ARG:O	1:X:114:LEU:HB2	1.91	0.69
1:X:13:LYS:HD3	1:X:18:LYS:HZ3	1.57	0.69
1:X:535:PHE:HB2	1:X:536:PRO:HD2	1.75	0.69
1:X:130:LYS:HB3	1:X:132:ILE:HD11	1.75	0.69
1:X:155:ILE:HG23	1:X:156:PHE:HD1	1.58	0.69
1:X:93:GLU:OE1	1:X:694:ASN:CG	2.36	0.68
1:X:7:ARG:HH21	1:X:18:LYS:CE	2.06	0.68
1:X:33:ARG:CD	1:X:52:ILE:HB	2.24	0.68
1:X:134:ILE:HG13	1:X:135:TYR:CD1	2.27	0.68
1:X:389:LEU:CD1	1:X:600:PHE:HZ	2.06	0.68
1:X:692:PHE:HD1	1:X:745:PHE:HB3	1.57	0.68
1:X:708:LEU:O	1:X:709:ALA:O	2.10	0.68
1:X:380:THR:HG22	1:X:380:THR:O	1.93	0.68
1:X:438:ASN:O	1:X:442:CYS:HB2	1.93	0.68
1:X:516:LEU:HD22	1:X:555:ASN:OD1	1.93	0.68
1:X:28:THR:HG22	1:X:29:VAL:N	2.07	0.68
1:X:137:GLN:NE2	1:X:140:VAL:CG2	2.51	0.68
1:X:238:ARG:CZ	1:X:267:ARG:CZ	2.70	0.68
1:X:393:LEU:HD12	1:X:596:LEU:CD2	2.23	0.68
1:X:461:PHE:HB2	2:X:2145:HOH:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:728:LYS:HG3	1:X:737:TYR:OH	1.94	0.68
1:X:202:ARG:HG2	1:X:252:PHE:CD2	2.28	0.68
1:X:477:LYS:C	1:X:480:GLN:OE1	2.34	0.68
1:X:174:SER:OG	1:X:650:PRO:HA	1.93	0.68
1:X:238:ARG:O	1:X:238:ARG:HG3	1.92	0.68
1:X:389:LEU:HD13	1:X:600:PHE:CE1	2.29	0.68
1:X:493:GLU:HA	1:X:493:GLU:OE1	1.92	0.68
1:X:730:LEU:C	1:X:730:LEU:HD12	2.18	0.68
1:X:165:SER:O	1:X:169:ASP:N	2.25	0.68
1:X:255:GLY:HA3	1:X:443:GLN:CG	2.24	0.68
1:X:480:GLN:HG3	2:X:2150:HOH:O	1.92	0.68
1:X:518:ASP:HB2	1:X:635:LYS:HZ2	1.55	0.68
1:X:455:ILE:HG22	1:X:456:SER:N	2.09	0.68
1:X:675:GLN:O	1:X:678:CYS:N	2.26	0.68
1:X:52:ILE:HG12	1:X:60:PHE:CZ	2.29	0.68
1:X:7:ARG:NH2	1:X:18:LYS:CE	2.58	0.67
1:X:37:TYR:CE1	1:X:39:PRO:HA	2.23	0.67
1:X:238:ARG:NH2	1:X:267:ARG:NH2	2.41	0.67
1:X:332:ASP:HA	1:X:336:PHE:H	1.58	0.67
1:X:357:ILE:N	1:X:418:ARG:HH12	1.93	0.67
1:X:711:ASN:C	1:X:713:PRO:HD3	2.19	0.67
1:X:322:GLU:HB2	2:X:2111:HOH:O	1.94	0.67
1:X:381:VAL:O	2:X:2126:HOH:O	2.13	0.67
1:X:494:TYR:HB3	1:X:500:ASN:ND2	2.09	0.67
1:X:526:LEU:CD2	1:X:631:ALA:HB1	2.22	0.67
1:X:225:PHE:CG	1:X:280:ILE:HG21	2.29	0.67
1:X:33:ARG:HD2	1:X:52:ILE:CB	2.23	0.67
1:X:283:GLN:HB2	1:X:324:PHE:CD1	2.29	0.67
1:X:604:SER:O	1:X:605:ASP:CB	2.41	0.67
1:X:146:ARG:CA	1:X:150:GLU:OE2	2.41	0.67
1:X:392:ALA:HB3	1:X:596:LEU:HD23	1.76	0.67
1:X:496:LYS:O	1:X:742:THR:OG1	2.13	0.67
1:X:22:SER:HB3	1:X:26:LYS:NZ	2.09	0.67
1:X:379:SER:OG	1:X:389:LEU:HD23	1.94	0.67
1:X:682:LEU:CD1	1:X:683:GLU:H	2.00	0.67
1:X:689:ARG:CD	1:X:695:ARG:CZ	2.69	0.67
1:X:110:TYR:HE2	1:X:126:VAL:HG13	1.60	0.67
1:X:135:TYR:CE2	1:X:191:LYS:CE	2.75	0.67
1:X:692:PHE:CD1	1:X:745:PHE:CG	2.83	0.67
1:X:119:SER:HB2	1:X:122:PHE:CB	2.24	0.66
1:X:385:ASN:O	1:X:388:VAL:HB	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:609:THR:CG2	1:X:613:ASN:HD22	2.07	0.66
1:X:43:GLU:HG3	1:X:45:ASP:H	1.60	0.66
1:X:97:LEU:HD12	1:X:97:LEU:O	1.94	0.66
1:X:186:THR:O	1:X:190:LYS:HG3	1.95	0.66
1:X:432:TRP:O	1:X:435:LYS:HB3	1.95	0.66
1:X:503:PHE:CD1	1:X:505:ASP:N	2.63	0.66
1:X:52:ILE:CG1	1:X:60:PHE:CZ	2.78	0.66
1:X:296:LEU:CA	1:X:297:HIS:ND1	2.58	0.66
1:X:385:ASN:HB3	1:X:388:VAL:HG21	1.77	0.66
1:X:503:PHE:HD1	1:X:505:ASP:H	1.42	0.66
1:X:592:LEU:O	1:X:592:LEU:CD1	2.36	0.66
1:X:736:GLN:HG2	1:X:747:ARG:HB2	1.78	0.66
1:X:121:LEU:CD1	1:X:482:PHE:HE2	2.08	0.66
1:X:389:LEU:O	1:X:393:LEU:HD13	1.95	0.66
1:X:33:ARG:HD2	1:X:52:ILE:HB	1.78	0.66
1:X:33:ARG:CG	1:X:52:ILE:HB	2.25	0.66
1:X:532:GLN:C	1:X:534:VAL:H	2.03	0.66
1:X:84:LYS:HE2	1:X:85:PHE:HE2	1.59	0.66
1:X:664:PRO:O	1:X:665:ALA:HB3	1.96	0.66
1:X:229:LYS:HD3	1:X:276:ARG:HD3	1.76	0.66
1:X:247:PHE:CE1	1:X:253:ILE:CB	2.78	0.66
1:X:353:HIS:CB	1:X:378:ALA:HB2	2.26	0.66
1:X:399:LEU:HD12	1:X:403:ASP:O	1.96	0.66
1:X:698:TYR:HE2	1:X:720:GLN:HE22	1.43	0.66
1:X:56:THR:CG2	1:X:58:ASP:OD1	2.43	0.65
1:X:183:ALA:HB1	1:X:655:CYS:CB	2.23	0.65
1:X:539:THR:O	1:X:539:THR:CG2	2.42	0.65
1:X:532:GLN:HE22	1:X:543:LEU:HB2	1.61	0.65
1:X:685:ILE:CG2	1:X:689:ARG:HH12	2.06	0.65
1:X:691:GLY:HA2	1:X:747:ARG:HH11	1.60	0.65
1:X:473:TYR:HE2	1:X:638:LEU:HD23	1.62	0.65
1:X:691:GLY:CA	1:X:747:ARG:HH12	2.08	0.65
1:X:701:PHE:CD2	2:X:2229:HOH:O	2.47	0.65
1:X:726:VAL:O	1:X:730:LEU:N	2.27	0.65
1:X:143:PHE:O	1:X:146:ARG:HG2	1.97	0.65
1:X:241:LYS:HE2	1:X:243:ILE:CD1	2.26	0.65
1:X:710:PRO:HB2	2:X:2235:HOH:O	1.97	0.65
1:X:239:PHE:HE2	1:X:241:LYS:HD3	1.59	0.65
1:X:182:GLY:HA3	1:X:657:ILE:HD12	1.80	0.64
1:X:609:THR:HG23	1:X:613:ASN:HD22	1.61	0.64
1:X:572:HIS:HD2	1:X:577:VAL:CG2	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:485:HIS:CE1	1:X:650:PRO:CG	2.80	0.64
1:X:533:SER:O	1:X:589:LYS:HE2	1.96	0.64
1:X:29:VAL:HG13	1:X:758:ARG:HB2	1.74	0.64
1:X:98:ASN:HD21	1:X:100:PRO:HG2	1.62	0.64
1:X:155:ILE:HG23	1:X:156:PHE:CD1	2.31	0.64
1:X:504:ILE:HD12	1:X:505:ASP:N	2.10	0.64
1:X:623:LYS:HG3	1:X:624:GLY:H	1.62	0.64
1:X:37:TYR:O	1:X:48:GLU:N	2.31	0.64
1:X:298:LEU:HD12	1:X:299:ALA:CA	2.28	0.64
1:X:623:LYS:O	1:X:626:ASN:O	2.16	0.64
1:X:725:ALA:CA	1:X:729:HIS:HD2	2.10	0.64
1:X:289:THR:C	1:X:291:GLU:N	2.55	0.64
1:X:33:ARG:HG2	2:X:2016:HOH:O	1.98	0.63
1:X:160:ASP:O	1:X:163:TYR:HB3	1.99	0.63
1:X:246:GLN:HG2	1:X:255:GLY:HA3	1.79	0.63
1:X:519:GLY:O	1:X:523:PRO:HA	1.99	0.63
1:X:70:ARG:HB2	2:X:2037:HOH:O	1.98	0.63
1:X:146:ARG:HD3	2:X:2061:HOH:O	1.97	0.63
1:X:30:SER:O	1:X:756:GLU:O	2.16	0.63
1:X:689:ARG:HD2	1:X:695:ARG:CZ	2.29	0.63
1:X:701:PHE:CD2	1:X:701:PHE:O	2.52	0.63
1:X:432:TRP:CZ2	1:X:436:LYS:HE2	2.34	0.63
1:X:90:ASP:OD1	1:X:120:GLY:N	2.28	0.62
1:X:552:SER:O	1:X:553:LYS:HB2	1.99	0.62
1:X:163:TYR:CD1	1:X:163:TYR:C	2.77	0.62
1:X:347:ILE:C	1:X:349:ALA:H	2.07	0.62
1:X:354:LEU:O	1:X:418:ARG:HD2	1.98	0.62
1:X:477:LYS:HD3	1:X:638:LEU:CD2	2.29	0.62
1:X:477:LYS:C	1:X:480:GLN:HE22	2.06	0.62
1:X:539:THR:HG22	1:X:542:THR:CG2	2.28	0.62
1:X:11:TYR:HA	1:X:15:LEU:HD13	1.81	0.62
1:X:222:LEU:O	1:X:226:GLY:N	2.33	0.62
1:X:593:GLN:OE1	1:X:593:GLN:HA	1.99	0.62
1:X:701:PHE:CD1	2:X:2231:HOH:O	2.51	0.62
1:X:538:ALA:HA	2:X:2171:HOH:O	1.98	0.62
1:X:624:GLY:O	1:X:625:ALA:HB3	1.99	0.62
1:X:685:ILE:HG13	1:X:686:ARG:N	2.14	0.62
1:X:492:GLU:HA	1:X:495:LEU:CD2	2.30	0.62
1:X:723:THR:O	1:X:723:THR:OG1	2.15	0.62
1:X:93:GLU:OE1	1:X:694:ASN:OD1	2.16	0.62
1:X:503:PHE:HD1	1:X:505:ASP:N	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:230:THR:HG21	1:X:238:ARG:NH2	1.96	0.62
1:X:544:ILE:HD11	1:X:548:HIS:CE1	2.35	0.62
1:X:217:GLN:C	1:X:220:PRO:HD2	2.24	0.62
1:X:698:TYR:CD2	1:X:699:ALA:CB	2.81	0.62
1:X:117:THR:HG22	1:X:118:TYR:H	1.65	0.61
1:X:620:ARG:HH22	1:X:630:VAL:HG13	1.65	0.61
1:X:671:VAL:HG23	1:X:672:VAL:H	1.65	0.61
1:X:93:GLU:OE1	1:X:694:ASN:ND2	2.33	0.61
1:X:147:ARG:H	1:X:150:GLU:CD	2.07	0.61
1:X:171:GLN:NE2	2:X:2069:HOH:O	2.33	0.61
1:X:436:LYS:O	1:X:439:ASN:OD1	2.18	0.61
1:X:682:LEU:HD12	1:X:682:LEU:C	2.23	0.61
1:X:272:SER:O	1:X:310:SER:HB2	2.00	0.61
1:X:289:THR:C	1:X:291:GLU:H	2.08	0.61
1:X:680:VAL:O	1:X:684:GLY:HA3	2.00	0.61
1:X:689:ARG:CG	1:X:695:ARG:NH2	2.54	0.61
1:X:342:MET:HG3	1:X:346:LYS:HG3	1.83	0.61
1:X:54:SER:HB2	1:X:61:THR:O	2.00	0.61
1:X:103:PHE:O	1:X:107:ARG:HG3	1.99	0.61
1:X:242:PHE:CE2	1:X:244:GLU:HB3	2.22	0.61
1:X:473:TYR:CE2	1:X:638:LEU:HD23	2.36	0.61
1:X:35:ILE:HG13	1:X:36:TRP:O	2.01	0.61
1:X:491:GLN:HA	1:X:491:GLN:OE1	2.00	0.61
1:X:11:TYR:OH	1:X:152:ALA:CB	2.46	0.61
1:X:12:HIS:O	1:X:18:LYS:CG	2.49	0.61
1:X:78:ASN:HA	1:X:98:ASN:HD22	1.63	0.61
1:X:219:ASN:HA	1:X:222:LEU:HG	1.83	0.61
1:X:736:GLN:HG3	1:X:750:GLN:HB2	1.82	0.61
1:X:293:LYS:CE	1:X:298:LEU:HD11	2.31	0.61
1:X:504:ILE:CD1	1:X:505:ASP:H	2.12	0.61
1:X:134:ILE:O	1:X:135:TYR:HD1	1.83	0.61
1:X:300:GLY:O	1:X:303:SER:HB3	2.00	0.61
1:X:332:ASP:HA	1:X:336:PHE:N	2.16	0.61
1:X:367:ALA:HB2	1:X:411:VAL:N	2.16	0.61
1:X:626:ASN:CG	1:X:627:PHE:CD2	2.70	0.61
1:X:339:GLU:O	1:X:342:MET:HB3	2.00	0.61
1:X:480:GLN:HB2	1:X:508:LEU:HD22	1.81	0.61
1:X:14:TYR:CE1	1:X:133:PRO:HG2	2.35	0.60
1:X:297:HIS:ND1	1:X:297:HIS:N	2.47	0.60
1:X:730:LEU:HD12	1:X:731:ASN:HB2	1.82	0.60
1:X:91:MET:O	1:X:94:LEU:HG	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:294:LYS:HB3	1:X:294:LYS:NZ	2.14	0.60
1:X:607:VAL:O	1:X:611:LEU:N	2.34	0.60
1:X:306:TYR:CE2	1:X:422:VAL:HG11	2.35	0.60
1:X:244:GLU:OE2	1:X:449:PHE:HB2	2.01	0.60
1:X:322:GLU:O	1:X:326:ILE:HD13	2.02	0.60
1:X:432:TRP:CZ2	1:X:610:LYS:CD	2.85	0.60
1:X:139:MET:O	1:X:143:PHE:CD2	2.54	0.60
1:X:165:SER:HA	2:X:2067:HOH:O	2.01	0.60
1:X:238:ARG:NH2	1:X:267:ARG:CZ	2.65	0.60
1:X:278:TYR:O	1:X:281:PHE:HB2	2.02	0.60
1:X:107:ARG:O	1:X:111:ASN:N	2.34	0.60
1:X:346:LYS:HD3	2:X:2126:HOH:O	2.02	0.60
1:X:219:ASN:N	1:X:220:PRO:HD2	2.17	0.60
1:X:324:PHE:HE2	1:X:328:ARG:NH1	2.00	0.60
1:X:597:GLU:HB3	1:X:601:LYS:HD2	1.83	0.60
1:X:661:LYS:O	1:X:662:GLN:HB2	2.02	0.60
1:X:696:ILE:HB	1:X:697:ILE:O	2.02	0.60
1:X:246:GLN:HG2	1:X:255:GLY:CA	2.32	0.60
1:X:105:ASN:O	1:X:109:ARG:CG	2.50	0.59
1:X:698:TYR:HE2	1:X:720:GLN:NE2	1.98	0.59
1:X:37:TYR:C	1:X:47:TYR:HD1	2.09	0.59
1:X:347:ILE:C	1:X:349:ALA:N	2.56	0.59
1:X:366:GLY:HA2	1:X:408:HIS:CE1	2.37	0.59
1:X:392:ALA:CB	1:X:596:LEU:HD23	2.31	0.59
1:X:7:ARG:NE	1:X:18:LYS:HE3	2.17	0.59
1:X:8:THR:O	1:X:9:SER:OG	2.20	0.59
1:X:27:LEU:O	1:X:28:THR:OG1	2.19	0.59
1:X:97:LEU:HD11	1:X:686:ARG:HG3	1.85	0.59
1:X:385:ASN:HB3	1:X:388:VAL:CG2	2.31	0.59
1:X:492:GLU:HA	1:X:495:LEU:HD23	1.84	0.59
1:X:581:ILE:O	1:X:581:ILE:HG22	1.97	0.59
1:X:597:GLU:O	1:X:601:LYS:N	2.32	0.59
1:X:636:GLU:O	1:X:636:GLU:HG2	1.99	0.59
1:X:21:ASP:HA	2:X:2012:HOH:O	2.02	0.59
1:X:455:ILE:CG2	1:X:456:SER:N	2.65	0.59
1:X:495:LEU:HA	2:X:2158:HOH:O	2.02	0.59
1:X:680:VAL:O	1:X:684:GLY:CA	2.50	0.59
1:X:708:LEU:HD22	1:X:712:VAL:HG13	1.85	0.59
1:X:79:GLN:OE1	1:X:96:TYR:HD2	1.85	0.59
1:X:458:PHE:HZ	1:X:479:GLN:OE1	1.85	0.59
1:X:353:HIS:HB3	1:X:378:ALA:HB2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:429:LEU:HD23	1:X:430:PHE:N	2.18	0.59
1:X:481:PHE:HE1	1:X:646:GLU:HA	1.67	0.59
1:X:617:ILE:HG22	1:X:617:ILE:O	2.02	0.59
1:X:52:ILE:CG1	1:X:60:PHE:HZ	2.16	0.59
1:X:476:GLU:OE2	1:X:573:TYR:HB2	2.02	0.59
1:X:130:LYS:HG2	1:X:131:ARG:N	2.17	0.59
1:X:147:ARG:O	1:X:150:GLU:HG2	2.03	0.59
1:X:539:THR:HG22	1:X:542:THR:HG23	1.84	0.59
1:X:52:ILE:HG12	1:X:60:PHE:HZ	1.68	0.58
1:X:682:LEU:CG	1:X:683:GLU:H	2.16	0.58
1:X:210:VAL:HG22	1:X:214:GLN:CD	2.28	0.58
1:X:397:ARG:HA	1:X:405:VAL:O	2.03	0.58
1:X:37:TYR:HE1	1:X:39:PRO:CA	2.11	0.58
1:X:210:VAL:HG23	1:X:214:GLN:HG3	1.85	0.58
1:X:492:GLU:O	1:X:494:TYR:N	2.36	0.58
1:X:701:PHE:O	1:X:701:PHE:CG	2.54	0.58
1:X:353:HIS:HB2	1:X:378:ALA:HB2	1.85	0.58
1:X:409:LEU:HD22	1:X:413:LYS:HB2	1.85	0.58
1:X:685:ILE:C	1:X:687:ILE:N	2.57	0.58
1:X:127:ASN:O	1:X:658:PRO:HG3	2.03	0.58
1:X:44:ARG:HH11	1:X:44:ARG:HA	1.69	0.58
1:X:89:GLU:CD	1:X:89:GLU:H	2.09	0.58
1:X:210:VAL:CG2	1:X:214:GLN:HG3	2.34	0.58
1:X:667:LEU:HD23	1:X:667:LEU:C	2.28	0.58
1:X:680:VAL:HG22	1:X:684:GLY:CA	2.32	0.58
1:X:192:VAL:HG23	1:X:193:ILE:N	2.18	0.58
1:X:233:ASN:OD1	1:X:234:ASN:N	2.34	0.58
1:X:682:LEU:C	2:X:2217:HOH:O	2.38	0.58
1:X:725:ALA:CA	1:X:729:HIS:CD2	2.86	0.58
1:X:754:ILE:HG23	1:X:755:GLU:H	1.68	0.58
1:X:759:GLU:OXT	1:X:759:GLU:HG2	2.03	0.58
1:X:13:LYS:HD3	1:X:18:LYS:HZ2	1.69	0.58
1:X:71:GLN:N	1:X:71:GLN:OE1	2.37	0.58
1:X:398:ILE:HD13	1:X:407:GLN:CG	2.33	0.58
1:X:64:THR:CG2	1:X:66:ASP:O	2.40	0.57
1:X:164:ARG:HD3	1:X:167:LEU:HD12	1.84	0.57
1:X:682:LEU:CG	1:X:683:GLU:N	2.66	0.57
1:X:692:PHE:CB	2:X:2226:HOH:O	2.52	0.57
1:X:743:LYS:C	1:X:744:ILE:HG23	2.29	0.57
1:X:29:VAL:HG11	1:X:758:ARG:CD	2.34	0.57
1:X:247:PHE:CD1	1:X:253:ILE:N	2.65	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:425:LEU:CD2	1:X:612:PHE:HZ	2.17	0.57
1:X:501:TRP:HB3	2:X:2160:HOH:O	2.03	0.57
1:X:81:ASN:CB	1:X:82:PRO:HD2	2.31	0.57
1:X:373:THR:HA	1:X:376:ASN:HD22	1.69	0.57
1:X:453:LEU:HD12	1:X:454:ASP:N	2.19	0.57
1:X:672:VAL:O	1:X:675:GLN:HG2	2.04	0.57
1:X:685:ILE:CD1	1:X:689:ARG:NH2	2.67	0.57
1:X:41:PRO:HD3	1:X:70:ARG:HH12	1.70	0.57
1:X:309:GLN:HB2	2:X:2107:HOH:O	2.05	0.57
1:X:491:GLN:OE1	1:X:491:GLN:CA	2.52	0.57
1:X:689:ARG:HD2	1:X:695:ARG:NH2	2.20	0.57
1:X:4:ILE:O	1:X:4:ILE:CG2	2.52	0.57
1:X:99:GLU:HG2	1:X:673:LEU:HD11	1.86	0.57
1:X:484:HIS:NE2	1:X:488:LYS:NZ	2.51	0.57
1:X:527:ALA:O	1:X:531:GLU:CG	2.53	0.57
1:X:282:TYR:CD1	1:X:282:TYR:N	2.72	0.57
1:X:544:ILE:HD11	1:X:548:HIS:NE2	2.20	0.57
1:X:154:HIS:ND1	1:X:156:PHE:HB2	2.20	0.56
1:X:160:ASP:O	1:X:163:TYR:N	2.35	0.56
1:X:733:ASP:HB2	1:X:734:PRO:CD	2.35	0.56
1:X:28:THR:HG22	1:X:29:VAL:H	1.69	0.56
1:X:60:PHE:CE2	1:X:62:PHE:CD2	2.92	0.56
1:X:193:ILE:CG1	1:X:194:GLN:N	2.67	0.56
1:X:245:ILE:HD12	1:X:450:ILE:H	1.70	0.56
1:X:342:MET:O	1:X:345:PHE:HB2	2.05	0.56
1:X:680:VAL:HG22	1:X:680:VAL:O	2.06	0.56
1:X:754:ILE:CG2	1:X:755:GLU:N	2.68	0.56
1:X:195:TYR:O	1:X:196:LEU:C	2.47	0.56
1:X:213:GLN:C	1:X:215:ILE:N	2.62	0.56
1:X:362:GLY:N	1:X:366:GLY:O	2.39	0.56
1:X:375:LEU:HD11	1:X:389:LEU:HD23	1.87	0.56
1:X:702:VAL:HG13	1:X:715:ASP:HB2	1.87	0.56
1:X:143:PHE:HD1	2:X:2060:HOH:O	1.88	0.56
1:X:539:THR:O	1:X:541:ASN:CB	2.53	0.56
1:X:707:LEU:HD11	2:X:2046:HOH:O	2.05	0.56
1:X:461:PHE:HD1	1:X:462:LYS:N	2.03	0.56
1:X:15:LEU:CD2	1:X:139:MET:SD	2.94	0.56
1:X:577:VAL:HG11	1:X:579:TYR:CZ	2.41	0.56
1:X:599:CYS:C	1:X:600:PHE:HD1	2.14	0.56
1:X:61:THR:HG22	1:X:62:PHE:N	2.21	0.56
1:X:345:PHE:C	1:X:347:ILE:N	2.63	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:736:GLN:CG	1:X:747:ARG:HB2	2.35	0.56
1:X:285:LEU:HD23	1:X:298:LEU:CD2	2.35	0.56
1:X:736:GLN:HG2	1:X:747:ARG:H	1.71	0.56
1:X:4:ILE:O	1:X:4:ILE:HG22	2.04	0.56
1:X:81:ASN:OD1	1:X:96:TYR:HB2	2.06	0.56
1:X:285:LEU:HD23	1:X:298:LEU:HB2	1.88	0.55
1:X:164:ARG:HA	1:X:167:LEU:HD12	1.88	0.55
1:X:225:PHE:CD2	1:X:280:ILE:HG21	2.41	0.55
1:X:99:GLU:HG2	1:X:673:LEU:CD1	2.35	0.55
1:X:642:MET:HA	1:X:645:LEU:HD22	1.88	0.55
1:X:267:ARG:O	1:X:267:ARG:HG2	2.06	0.55
1:X:588:ASN:OD1	2:X:2188:HOH:O	2.18	0.55
1:X:7:ARG:HE	1:X:18:LYS:CB	2.15	0.55
1:X:37:TYR:O	1:X:47:TYR:HB3	2.05	0.55
1:X:745:PHE:HD1	2:X:2224:HOH:O	1.90	0.55
1:X:347:ILE:HG21	1:X:429:LEU:HD12	1.87	0.55
1:X:455:ILE:CG2	1:X:456:SER:H	2.20	0.55
1:X:535:PHE:HB2	1:X:536:PRO:CD	2.37	0.55
1:X:432:TRP:O	1:X:435:LYS:N	2.39	0.55
1:X:298:LEU:HD12	1:X:299:ALA:C	2.31	0.55
1:X:529:LEU:O	1:X:533:SER:OG	2.22	0.55
1:X:693:PRO:HD2	1:X:746:PHE:O	2.07	0.55
1:X:98:ASN:HD21	1:X:100:PRO:CG	2.20	0.55
1:X:219:ASN:N	1:X:220:PRO:CD	2.62	0.55
1:X:399:LEU:HD13	1:X:404:LEU:HB3	1.89	0.55
1:X:402:ARG:O	1:X:402:ARG:HG2	2.06	0.54
1:X:679:ASN:CB	1:X:681:VAL:HG13	2.33	0.54
1:X:203:ASN:CB	1:X:207:GLY:C	2.77	0.54
1:X:230:THR:HG22	1:X:275:GLU:OE1	2.07	0.54
1:X:244:GLU:CG	1:X:451:GLY:CA	2.83	0.54
1:X:527:ALA:O	1:X:531:GLU:HG2	2.07	0.54
1:X:609:THR:CG2	1:X:613:ASN:ND2	2.68	0.54
1:X:638:LEU:O	1:X:641:LEU:HB3	2.08	0.54
1:X:242:PHE:HZ	1:X:244:GLU:HG3	1.55	0.54
1:X:265:LYS:O	1:X:423:LYS:HG2	2.07	0.54
1:X:294:LYS:C	1:X:296:LEU:N	2.63	0.54
1:X:390:GLU:HG3	1:X:391:LYS:N	2.21	0.54
1:X:691:GLY:O	1:X:747:ARG:NH1	2.40	0.54
1:X:712:VAL:N	1:X:713:PRO:HD3	2.21	0.54
1:X:386:PRO:C	1:X:388:VAL:H	2.15	0.54
1:X:486:MET:CE	1:X:689:ARG:HH11	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:82:PRO:C	1:X:84:LYS:H	2.15	0.54
1:X:351:ILE:O	1:X:354:LEU:HB2	2.07	0.54
1:X:461:PHE:CD1	1:X:462:LYS:N	2.75	0.54
1:X:465:SER:H	1:X:468:GLN:CD	2.10	0.54
1:X:333:ILE:C	1:X:335:GLY:H	2.14	0.54
1:X:518:ASP:HB2	1:X:635:LYS:HZ1	1.72	0.54
1:X:616:ASN:O	1:X:617:ILE:HD13	2.07	0.54
1:X:5:HIS:O	1:X:6:ASP:CG	2.50	0.54
1:X:7:ARG:CZ	1:X:18:LYS:HE3	2.38	0.54
1:X:394:MET:C	1:X:396:PRO:HD3	2.32	0.54
1:X:398:ILE:CG2	1:X:399:LEU:N	2.70	0.54
1:X:497:GLU:OE2	1:X:744:ILE:HA	2.08	0.54
1:X:569:GLY:HA3	1:X:578:MET:SD	2.48	0.54
1:X:641:LEU:HG	1:X:645:LEU:HD11	1.88	0.54
1:X:726:VAL:O	1:X:730:LEU:CG	2.48	0.54
1:X:163:TYR:CD1	1:X:167:LEU:CD1	2.84	0.54
1:X:529:LEU:HD23	1:X:631:ALA:HB2	1.90	0.54
1:X:110:TYR:CE2	1:X:126:VAL:HG13	2.42	0.54
1:X:35:ILE:CB	1:X:52:ILE:HD11	2.34	0.54
1:X:61:THR:HG23	1:X:71:GLN:HG3	1.90	0.54
1:X:357:ILE:H	1:X:418:ARG:HH12	1.56	0.54
1:X:373:THR:HA	1:X:376:ASN:ND2	2.22	0.54
1:X:35:ILE:HD11	1:X:77:ALA:HB1	1.90	0.53
1:X:131:ARG:C	1:X:132:ILE:HD12	2.32	0.53
1:X:342:MET:SD	1:X:342:MET:C	2.88	0.53
1:X:692:PHE:HE1	1:X:745:PHE:HB2	1.68	0.53
1:X:699:ALA:HB3	1:X:720:GLN:OE1	2.08	0.53
1:X:56:THR:CB	1:X:59:SER:O	2.45	0.53
1:X:245:ILE:CD1	1:X:450:ILE:HB	2.38	0.53
1:X:345:PHE:O	1:X:347:ILE:N	2.41	0.53
1:X:689:ARG:NH1	2:X:2221:HOH:O	2.23	0.53
1:X:692:PHE:HB3	2:X:2226:HOH:O	2.06	0.53
1:X:144:LYS:HE2	1:X:199:VAL:HG12	1.90	0.53
1:X:189:THR:O	1:X:192:VAL:HG22	2.08	0.53
1:X:470:CYS:HB3	1:X:634:TYR:CE2	2.43	0.53
1:X:98:ASN:OD1	1:X:100:PRO:N	2.41	0.53
1:X:238:ARG:HG2	1:X:278:TYR:CE1	2.44	0.53
1:X:326:ILE:N	1:X:326:ILE:HD12	2.23	0.53
1:X:119:SER:N	1:X:122:PHE:O	2.41	0.53
1:X:212:GLU:O	1:X:216:LEU:CD1	2.57	0.53
1:X:119:SER:HB2	1:X:122:PHE:HB2	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:424:ALA:O	1:X:428:ARG:CB	2.57	0.53
1:X:582:GLN:HA	1:X:582:GLN:HE21	1.70	0.53
1:X:680:VAL:HA	1:X:683:GLU:CD	2.33	0.53
1:X:276:ARG:NH2	1:X:282:TYR:CG	2.77	0.53
1:X:121:LEU:HD11	1:X:482:PHE:CZ	2.44	0.53
1:X:398:ILE:HG22	1:X:399:LEU:N	2.24	0.53
1:X:501:TRP:O	1:X:502:THR:C	2.49	0.53
1:X:215:ILE:O	1:X:218:ALA:HB3	2.09	0.53
1:X:285:LEU:HD23	1:X:298:LEU:HD13	1.90	0.53
1:X:369:LEU:HD12	1:X:369:LEU:C	2.33	0.53
1:X:432:TRP:CH2	1:X:436:LYS:HE2	2.43	0.53
1:X:82:PRO:C	1:X:84:LYS:N	2.66	0.53
1:X:175:LEU:HD23	1:X:651:HIS:HB2	1.91	0.53
1:X:623:LYS:HG3	1:X:624:GLY:N	2.24	0.53
1:X:626:ASN:OD1	1:X:627:PHE:CB	2.56	0.53
1:X:685:ILE:O	1:X:687:ILE:N	2.42	0.53
1:X:689:ARG:CD	1:X:695:ARG:NE	2.69	0.53
1:X:743:LYS:O	1:X:744:ILE:CG2	2.57	0.53
1:X:289:THR:O	1:X:291:GLU:N	2.42	0.52
1:X:428:ARG:O	1:X:429:LEU:C	2.49	0.52
1:X:461:PHE:CE1	1:X:462:LYS:HG2	2.44	0.52
1:X:31:ASP:OD1	1:X:757:ALA:HA	2.10	0.52
1:X:228:ALA:O	1:X:236:SER:N	2.35	0.52
1:X:244:GLU:CG	1:X:451:GLY:HA2	2.38	0.52
1:X:667:LEU:HD23	1:X:667:LEU:O	2.09	0.52
1:X:675:GLN:O	1:X:676:LEU:C	2.51	0.52
1:X:711:ASN:O	1:X:713:PRO:HD3	2.09	0.52
1:X:743:LYS:O	1:X:744:ILE:HG23	2.09	0.52
1:X:29:VAL:HG12	1:X:758:ARG:HB3	1.77	0.52
1:X:241:LYS:HE3	1:X:243:ILE:HD11	1.89	0.52
1:X:514:ILE:CG2	1:X:518:ASP:OD2	2.58	0.52
1:X:539:THR:O	1:X:540:ASP:C	2.43	0.52
1:X:129:PHE:CE2	1:X:658:PRO:HG2	2.41	0.52
1:X:134:ILE:CD1	1:X:154:HIS:HE2	2.23	0.52
1:X:508:LEU:HD13	2:X:2150:HOH:O	2.09	0.52
1:X:542:THR:OG1	1:X:543:LEU:N	2.40	0.52
1:X:63:LYS:HG2	1:X:64:THR:H	1.75	0.52
1:X:82:PRO:O	1:X:84:LYS:N	2.36	0.52
1:X:134:ILE:CG1	1:X:135:TYR:CE1	2.93	0.52
1:X:270:PHE:C	1:X:271:GLN:NE2	2.67	0.52
1:X:345:PHE:N	1:X:345:PHE:CD1	2.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:498:LYS:HA	2:X:2159:HOH:O	2.09	0.52
1:X:570:VAL:CG1	1:X:571:THR:N	2.72	0.52
1:X:633:GLN:C	1:X:635:LYS:N	2.66	0.52
1:X:119:SER:HB2	1:X:122:PHE:HB3	1.90	0.51
1:X:221:ILE:HG22	1:X:222:LEU:N	2.25	0.51
1:X:474:THR:O	1:X:478:LEU:HD12	2.06	0.51
1:X:60:PHE:CE2	1:X:62:PHE:HD2	2.29	0.51
1:X:577:VAL:HG11	1:X:579:TYR:OH	2.10	0.51
1:X:153:PRO:O	1:X:154:HIS:HB2	2.10	0.51
1:X:471:ILE:O	1:X:475:ASN:OD1	2.29	0.51
1:X:530:ASP:OD1	1:X:629:THR:OG1	2.28	0.51
1:X:193:ILE:HG12	1:X:194:GLN:H	1.75	0.51
1:X:322:GLU:C	1:X:324:PHE:N	2.67	0.51
1:X:428:ARG:HB3	1:X:611:LEU:HD22	1.91	0.51
1:X:38:ASN:ND2	1:X:43:GLU:O	2.43	0.51
1:X:224:ALA:C	1:X:280:ILE:HG23	2.35	0.51
1:X:298:LEU:HD12	1:X:299:ALA:H	1.67	0.51
1:X:526:LEU:O	1:X:530:ASP:OD2	2.29	0.51
1:X:675:GLN:C	1:X:678:CYS:H	2.18	0.51
1:X:193:ILE:CG1	1:X:194:GLN:H	2.24	0.51
1:X:708:LEU:HB3	1:X:712:VAL:HG22	1.93	0.51
1:X:727:LEU:HD13	1:X:736:GLN:OE1	2.11	0.51
1:X:742:THR:O	1:X:743:LYS:HD2	2.11	0.51
1:X:492:GLU:C	1:X:494:TYR:N	2.66	0.51
1:X:707:LEU:O	1:X:708:LEU:C	2.53	0.51
1:X:98:ASN:OD1	1:X:99:GLU:CA	2.58	0.51
1:X:230:THR:O	1:X:233:ASN:O	2.29	0.51
1:X:699:ALA:O	1:X:719:SER:O	2.28	0.51
1:X:267:ARG:O	1:X:267:ARG:CG	2.59	0.51
1:X:468:GLN:O	1:X:472:ASN:ND2	2.44	0.51
1:X:474:THR:C	1:X:478:LEU:HD13	2.34	0.51
1:X:557:LYS:HD2	1:X:571:THR:HB	1.93	0.51
1:X:37:TYR:CE1	1:X:39:PRO:CA	2.91	0.50
1:X:107:ARG:O	1:X:110:TYR:N	2.39	0.50
1:X:280:ILE:O	1:X:284:LEU:HB2	2.11	0.50
1:X:685:ILE:O	1:X:686:ARG:C	2.54	0.50
1:X:724:ASP:O	2:X:2244:HOH:O	2.20	0.50
1:X:134:ILE:HD12	1:X:154:HIS:HE2	1.76	0.50
1:X:229:LYS:HG3	1:X:234:ASN:HA	1.91	0.50
1:X:477:LYS:C	1:X:480:GLN:NE2	2.62	0.50
1:X:485:HIS:ND1	1:X:650:PRO:CG	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:516:LEU:HD13	1:X:555:ASN:ND2	2.26	0.50
1:X:606:ASN:O	1:X:610:LYS:HB2	2.11	0.50
1:X:741:ILE:HG23	1:X:742:THR:N	2.27	0.50
1:X:28:THR:CG2	1:X:29:VAL:N	2.73	0.50
1:X:91:MET:SD	1:X:106:LEU:CD1	2.99	0.50
1:X:98:ASN:CG	1:X:99:GLU:N	2.62	0.50
1:X:203:ASN:ND2	1:X:207:GLY:CA	2.73	0.50
1:X:213:GLN:O	1:X:215:ILE:N	2.44	0.50
1:X:277:ASN:N	1:X:282:TYR:OH	2.43	0.50
1:X:285:LEU:CD2	1:X:298:LEU:HB2	2.41	0.50
1:X:296:LEU:C	1:X:296:LEU:HD12	2.36	0.50
1:X:29:VAL:HG11	1:X:758:ARG:CG	2.40	0.50
1:X:296:LEU:O	1:X:297:HIS:CG	2.64	0.50
1:X:43:GLU:OE2	1:X:45:ASP:HB2	2.11	0.50
1:X:177:ILE:HD12	1:X:189:THR:HG22	1.93	0.50
1:X:372:LYS:O	1:X:376:ASN:ND2	2.45	0.50
1:X:22:SER:HB3	1:X:26:LYS:HZ3	1.76	0.50
1:X:93:GLU:HA	1:X:694:ASN:ND2	2.27	0.50
1:X:392:ALA:HA	1:X:595:ASP:OD2	2.11	0.50
1:X:486:MET:CE	1:X:689:ARG:NH1	2.72	0.50
1:X:228:ALA:HB2	1:X:278:TYR:CD1	2.46	0.50
1:X:453:LEU:HD12	1:X:454:ASP:H	1.75	0.50
1:X:675:GLN:O	1:X:678:CYS:HB3	2.12	0.50
1:X:179:GLY:O	1:X:180:GLU:C	2.55	0.49
1:X:293:LYS:HG3	1:X:298:LEU:HG	1.93	0.49
1:X:429:LEU:CD2	1:X:430:PHE:N	2.75	0.49
1:X:617:ILE:O	1:X:617:ILE:CG2	2.60	0.49
1:X:682:LEU:CD1	1:X:683:GLU:HB3	2.41	0.49
1:X:108:VAL:C	1:X:110:TYR:H	2.20	0.49
1:X:264:GLU:OE1	1:X:267:ARG:NH2	2.45	0.49
1:X:396:PRO:HA	1:X:595:ASP:OD2	2.12	0.49
1:X:470:CYS:O	1:X:473:TYR:HB3	2.12	0.49
1:X:641:LEU:HG	1:X:645:LEU:CD1	2.41	0.49
1:X:126:VAL:HG13	1:X:126:VAL:O	2.13	0.49
1:X:485:HIS:HE1	1:X:650:PRO:CD	2.05	0.49
1:X:336:PHE:HB3	1:X:341:GLN:NE2	2.27	0.49
1:X:706:TYR:O	1:X:706:TYR:CD1	2.65	0.49
1:X:429:LEU:HD21	1:X:433:LEU:HD12	1.95	0.49
1:X:35:ILE:HD12	1:X:78:ASN:O	2.12	0.49
1:X:40:ASP:HB3	1:X:42:LYS:CG	2.43	0.49
1:X:91:MET:HB3	2:X:2049:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:116:TYR:CE2	1:X:154:HIS:CD2	3.00	0.49
1:X:128:PRO:O	1:X:129:PHE:HB2	2.13	0.49
1:X:15:LEU:O	1:X:114:LEU:HD22	2.13	0.49
1:X:135:TYR:HD2	1:X:191:LYS:NZ	2.10	0.49
1:X:227:ASN:OD1	1:X:237:SER:HA	2.13	0.49
1:X:336:PHE:HB3	1:X:341:GLN:HE21	1.77	0.49
1:X:484:HIS:CD2	1:X:488:LYS:NZ	2.79	0.49
1:X:726:VAL:CG2	1:X:730:LEU:HD21	2.29	0.49
1:X:584:TRP:O	1:X:588:ASN:HB2	2.13	0.49
1:X:186:THR:CG2	1:X:187:GLU:N	2.75	0.49
1:X:296:LEU:HA	1:X:297:HIS:CE1	2.48	0.49
1:X:329:GLN:O	1:X:333:ILE:CG1	2.60	0.49
1:X:61:THR:HG22	1:X:62:PHE:H	1.78	0.49
1:X:187:GLU:CA	1:X:190:LYS:HB2	2.42	0.49
1:X:486:MET:HE1	1:X:689:ARG:HH12	1.74	0.49
1:X:219:ASN:HB2	1:X:220:PRO:HD3	1.93	0.48
1:X:679:ASN:C	1:X:681:VAL:H	2.21	0.48
1:X:736:GLN:CG	1:X:750:GLN:HB2	2.43	0.48
1:X:135:TYR:CD2	1:X:191:LYS:NZ	2.80	0.48
1:X:425:LEU:HD21	1:X:612:PHE:HZ	1.77	0.48
1:X:481:PHE:O	1:X:485:HIS:HB2	2.13	0.48
1:X:110:TYR:CE2	1:X:126:VAL:CG1	2.96	0.48
1:X:210:VAL:CG2	1:X:214:GLN:CG	2.91	0.48
1:X:353:HIS:HB2	1:X:378:ALA:CB	2.44	0.48
1:X:339:GLU:HB3	2:X:2117:HOH:O	2.13	0.48
1:X:345:PHE:C	1:X:347:ILE:H	2.21	0.48
1:X:428:ARG:HB3	1:X:611:LEU:CD2	2.43	0.48
1:X:544:ILE:CG1	1:X:548:HIS:CE1	2.97	0.48
1:X:134:ILE:C	1:X:139:MET:HG3	2.39	0.48
1:X:492:GLU:C	1:X:494:TYR:H	2.20	0.48
1:X:37:TYR:C	1:X:37:TYR:CD1	2.92	0.48
1:X:91:MET:SD	1:X:106:LEU:HD13	2.54	0.48
1:X:134:ILE:HG13	1:X:135:TYR:CE1	2.49	0.48
1:X:229:LYS:HD3	1:X:276:ARG:CD	2.42	0.48
1:X:294:LYS:NZ	1:X:294:LYS:CB	2.76	0.48
1:X:329:GLN:O	1:X:333:ILE:HG13	2.14	0.48
1:X:449:PHE:CZ	1:X:648:THR:HG21	2.49	0.48
1:X:568:PHE:O	1:X:578:MET:SD	2.71	0.48
1:X:701:PHE:HD1	1:X:705:TYR:CZ	2.32	0.48
1:X:35:ILE:CD1	1:X:77:ALA:HB1	2.44	0.48
1:X:87:GLY:CA	1:X:109:ARG:CD	2.84	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:298:LEU:CD1	1:X:299:ALA:N	2.59	0.48
1:X:332:ASP:CB	1:X:336:PHE:O	2.61	0.48
1:X:353:HIS:HD2	1:X:378:ALA:HA	1.78	0.48
1:X:367:ALA:N	1:X:408:HIS:HE1	2.12	0.48
1:X:590:ASP:N	1:X:591:PRO:CD	2.77	0.48
1:X:620:ARG:NH2	1:X:630:VAL:CG1	2.77	0.48
1:X:426:TYR:O	1:X:427:GLY:C	2.57	0.47
1:X:243:ILE:HG12	1:X:258:ILE:CG2	2.44	0.47
1:X:623:LYS:HB3	1:X:628:ILE:HG23	1.95	0.47
1:X:667:LEU:O	1:X:667:LEU:CD2	2.62	0.47
1:X:73:LYS:O	1:X:75:ASP:N	2.47	0.47
1:X:305:ASN:C	1:X:307:LEU:H	2.21	0.47
1:X:347:ILE:HA	1:X:382:PHE:CE1	2.43	0.47
1:X:508:LEU:C	1:X:510:SER:H	2.22	0.47
1:X:117:THR:HG22	1:X:118:TYR:N	2.29	0.47
1:X:135:TYR:N	1:X:139:MET:HG3	2.29	0.47
1:X:210:VAL:O	1:X:213:GLN:N	2.31	0.47
1:X:546:LYS:O	1:X:549:SER:HB2	2.15	0.47
1:X:398:ILE:CG2	1:X:399:LEU:H	2.27	0.47
1:X:495:LEU:HB3	2:X:2155:HOH:O	2.14	0.47
1:X:620:ARG:O	1:X:621:ALA:C	2.58	0.47
1:X:633:GLN:C	1:X:635:LYS:H	2.21	0.47
1:X:22:SER:CB	1:X:26:LYS:HZ3	2.28	0.47
1:X:271:GLN:HG2	1:X:276:ARG:O	2.15	0.47
1:X:294:LYS:HZ2	1:X:294:LYS:CB	2.23	0.47
1:X:343:SER:HA	1:X:346:LYS:CB	2.42	0.47
1:X:390:GLU:O	1:X:393:LEU:HB2	2.14	0.47
1:X:674:ASP:OD2	2:X:2215:HOH:O	2.20	0.47
1:X:682:LEU:HG	1:X:683:GLU:H	1.80	0.47
1:X:28:THR:CG2	1:X:29:VAL:H	2.26	0.47
1:X:40:ASP:C	1:X:42:LYS:H	2.23	0.47
1:X:245:ILE:HD11	1:X:450:ILE:CB	2.44	0.47
1:X:267:ARG:HB3	1:X:278:TYR:CE2	2.50	0.47
1:X:327:THR:OG1	1:X:328:ARG:N	2.46	0.47
1:X:365:GLU:OE1	1:X:366:GLY:N	2.47	0.47
1:X:465:SER:OG	1:X:467:GLU:OE1	2.32	0.47
1:X:629:THR:CB	2:X:2188:HOH:O	2.62	0.47
1:X:641:LEU:CD2	1:X:645:LEU:HD11	2.44	0.47
1:X:701:PHE:CE2	1:X:722:ALA:HB3	2.50	0.47
1:X:726:VAL:HG23	1:X:730:LEU:CG	2.43	0.47
1:X:71:GLN:HB2	2:X:2038:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:97:LEU:HD12	1:X:97:LEU:C	2.40	0.47
1:X:154:HIS:CE1	1:X:156:PHE:CD1	3.02	0.47
1:X:285:LEU:HD23	1:X:298:LEU:CG	2.45	0.47
1:X:614:ASP:OD1	1:X:615:PRO:N	2.44	0.47
1:X:642:MET:O	1:X:645:LEU:HB2	2.15	0.47
1:X:689:ARG:HD2	1:X:695:ARG:HH21	1.78	0.47
1:X:360:GLU:O	1:X:361:LYS:C	2.58	0.47
1:X:544:ILE:HG13	1:X:548:HIS:CE1	2.50	0.47
1:X:567:GLU:HB3	1:X:580:GLU:HA	1.97	0.47
1:X:620:ARG:NH2	1:X:630:VAL:HG13	2.30	0.47
1:X:28:THR:O	1:X:29:VAL:HG23	2.15	0.47
1:X:243:ILE:CG2	1:X:258:ILE:HG13	2.29	0.47
1:X:300:GLY:C	1:X:303:SER:HB3	2.39	0.47
1:X:306:TYR:O	1:X:307:LEU:HD23	2.14	0.47
1:X:367:ALA:HB1	1:X:411:VAL:CG2	2.45	0.47
1:X:473:TYR:O	1:X:477:LYS:HB2	2.15	0.47
1:X:514:ILE:HG23	1:X:518:ASP:OD2	2.15	0.47
1:X:121:LEU:CD2	1:X:486:MET:SD	2.98	0.46
1:X:322:GLU:C	1:X:324:PHE:H	2.23	0.46
1:X:323:GLU:O	1:X:326:ILE:HB	2.15	0.46
1:X:366:GLY:CA	1:X:408:HIS:CE1	2.97	0.46
1:X:419:ASP:O	1:X:423:LYS:HE2	2.14	0.46
1:X:623:LYS:HB3	1:X:628:ILE:CG2	2.45	0.46
1:X:730:LEU:HD12	1:X:730:LEU:O	2.15	0.46
1:X:122:PHE:CE1	1:X:654:ARG:HG2	2.50	0.46
1:X:140:VAL:HG23	1:X:141:ASP:N	2.29	0.46
1:X:180:GLU:O	1:X:181:SER:C	2.57	0.46
1:X:300:GLY:CA	1:X:303:SER:HB3	2.45	0.46
1:X:385:ASN:OD1	1:X:388:VAL:HG23	2.15	0.46
1:X:390:GLU:CG	1:X:391:LYS:N	2.78	0.46
1:X:508:LEU:CD1	2:X:2150:HOH:O	2.63	0.46
1:X:572:HIS:CD2	1:X:577:VAL:CG2	2.89	0.46
1:X:288:ALA:HB1	1:X:292:GLU:HG2	1.97	0.46
1:X:351:ILE:HG22	1:X:352:LEU:N	2.29	0.46
1:X:429:LEU:HD23	1:X:429:LEU:C	2.41	0.46
1:X:608:VAL:HG13	1:X:612:PHE:HE2	1.81	0.46
1:X:629:THR:HB	2:X:2188:HOH:O	2.14	0.46
1:X:14:TYR:CZ	2:X:2008:HOH:O	2.56	0.46
1:X:52:ILE:HA	1:X:62:PHE:HB3	1.96	0.46
1:X:73:LYS:C	1:X:75:ASP:N	2.74	0.46
1:X:134:ILE:HG13	1:X:135:TYR:HD1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:177:ILE:O	1:X:178:THR:HG23	2.15	0.46
1:X:294:LYS:CD	1:X:297:HIS:HA	2.35	0.46
1:X:371:ASP:OD1	1:X:372:LYS:N	2.42	0.46
1:X:391:LYS:HD3	1:X:391:LYS:HA	1.70	0.46
1:X:725:ALA:C	1:X:729:HIS:CD2	2.75	0.46
1:X:432:TRP:HA	1:X:435:LYS:HB3	1.97	0.46
1:X:485:HIS:CD2	2:X:2153:HOH:O	2.68	0.46
1:X:244:GLU:OE2	1:X:449:PHE:CD1	2.69	0.46
1:X:532:GLN:HE22	1:X:543:LEU:CB	2.26	0.46
1:X:588:ASN:ND2	1:X:630:VAL:HG23	2.31	0.46
1:X:703:LYS:HG3	1:X:714:ARG:NH2	2.30	0.46
1:X:721:LYS:HD3	2:X:2243:HOH:O	2.15	0.46
1:X:173:GLN:NE2	1:X:649:ASN:HB3	2.31	0.46
1:X:491:GLN:C	1:X:491:GLN:CD	2.83	0.46
1:X:730:LEU:C	1:X:730:LEU:CD1	2.88	0.46
1:X:735:GLU:O	1:X:736:GLN:C	2.57	0.46
1:X:186:THR:HG23	1:X:187:GLU:N	2.31	0.46
1:X:294:LYS:HA	1:X:297:HIS:H	1.80	0.46
1:X:327:THR:O	1:X:331:MET:HG3	2.15	0.46
1:X:418:ARG:O	1:X:422:VAL:HG23	2.16	0.46
1:X:439:ASN:OD1	1:X:439:ASN:C	2.59	0.46
1:X:593:GLN:OE1	1:X:593:GLN:CA	2.64	0.46
1:X:624:GLY:O	1:X:625:ALA:CB	2.63	0.46
1:X:52:ILE:HG13	1:X:60:PHE:CZ	2.51	0.46
1:X:63:LYS:HG2	1:X:64:THR:N	2.30	0.46
1:X:230:THR:CB	1:X:275:GLU:OE2	2.60	0.46
1:X:284:LEU:HD22	1:X:348:ILE:CG2	2.46	0.46
1:X:324:PHE:HE2	1:X:328:ARG:CZ	2.29	0.46
1:X:461:PHE:CD1	1:X:463:VAL:HG13	2.51	0.46
1:X:12:HIS:HA	1:X:16:LYS:HB3	1.98	0.46
1:X:476:GLU:OE2	1:X:573:TYR:N	2.49	0.46
1:X:682:LEU:HD11	1:X:683:GLU:HB3	1.97	0.46
1:X:116:TYR:CD2	1:X:154:HIS:CD2	3.03	0.45
1:X:149:ASN:ND2	1:X:697:ILE:HD11	2.31	0.45
1:X:166:MET:O	1:X:170:ARG:HD3	2.16	0.45
1:X:209:GLY:O	1:X:210:VAL:C	2.60	0.45
1:X:213:GLN:O	1:X:216:LEU:N	2.49	0.45
1:X:343:SER:O	1:X:347:ILE:N	2.48	0.45
1:X:508:LEU:HD23	2:X:2161:HOH:O	2.14	0.45
1:X:596:LEU:O	1:X:599:CYS:N	2.44	0.45
1:X:44:ARG:NH1	1:X:47:TYR:OH	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:108:VAL:C	1:X:110:TYR:N	2.74	0.45
1:X:127:ASN:OD1	1:X:127:ASN:C	2.59	0.45
1:X:243:ILE:HG12	1:X:258:ILE:HG23	1.98	0.45
1:X:682:LEU:HD12	1:X:683:GLU:CB	2.46	0.45
1:X:698:TYR:CE1	2:X:2227:HOH:O	2.60	0.45
1:X:21:ASP:HB3	2:X:2003:HOH:O	2.15	0.45
1:X:187:GLU:O	1:X:190:LYS:HB2	2.17	0.45
1:X:215:ILE:CG1	1:X:441:LEU:HD22	2.43	0.45
1:X:380:THR:O	1:X:380:THR:CG2	2.63	0.45
1:X:446:LYS:NZ	2:X:2143:HOH:O	2.48	0.45
1:X:473:TYR:OH	1:X:477:LYS:NZ	2.43	0.45
1:X:496:LYS:HB2	2:X:2248:HOH:O	2.17	0.45
1:X:692:PHE:HB2	2:X:2226:HOH:O	2.14	0.45
1:X:126:VAL:CG2	1:X:656:ILE:O	2.62	0.45
1:X:226:GLY:HA3	1:X:239:PHE:CE1	2.52	0.45
1:X:320:ASP:O	1:X:321:SER:C	2.58	0.45
1:X:464:ASN:CA	1:X:468:GLN:CD	2.88	0.45
1:X:532:GLN:C	1:X:534:VAL:N	2.66	0.45
1:X:570:VAL:HG12	1:X:571:THR:N	2.31	0.45
1:X:588:ASN:HD22	1:X:630:VAL:CG2	2.30	0.45
1:X:177:ILE:HD12	1:X:189:THR:CG2	2.46	0.45
1:X:324:PHE:CE2	1:X:328:ARG:CZ	2.99	0.45
1:X:346:LYS:HB3	2:X:2126:HOH:O	2.15	0.45
1:X:357:ILE:H	1:X:418:ARG:NH1	2.14	0.45
1:X:410:ASN:OD1	1:X:410:ASN:N	2.50	0.45
1:X:449:PHE:HZ	1:X:648:THR:HG21	1.81	0.45
1:X:487:PHE:C	1:X:489:LEU:N	2.73	0.45
1:X:588:ASN:HD22	1:X:630:VAL:HG23	1.82	0.45
1:X:54:SER:OG	1:X:61:THR:HB	2.16	0.45
1:X:594:GLN:NE2	2:X:2190:HOH:O	2.49	0.45
1:X:12:HIS:O	1:X:16:LYS:O	2.35	0.45
1:X:203:ASN:CG	1:X:207:GLY:C	2.84	0.45
1:X:429:LEU:HD21	1:X:433:LEU:CD1	2.46	0.45
1:X:285:LEU:HD23	1:X:298:LEU:CB	2.46	0.45
1:X:458:PHE:CE1	1:X:475:ASN:CB	2.88	0.45
1:X:477:LYS:CD	1:X:638:LEU:HD21	2.43	0.45
1:X:706:TYR:O	1:X:706:TYR:HD1	2.00	0.45
1:X:12:HIS:ND1	1:X:18:LYS:HA	2.31	0.45
1:X:38:ASN:N	1:X:47:TYR:HD1	2.14	0.45
1:X:98:ASN:OD1	1:X:99:GLU:C	2.60	0.45
1:X:219:ASN:O	1:X:220:PRO:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:423:LYS:HE3	1:X:423:LYS:HB2	1.78	0.45
1:X:470:CYS:O	1:X:634:TYR:OH	2.29	0.45
1:X:12:HIS:CB	1:X:18:LYS:HG2	2.43	0.45
1:X:34:TYR:HD1	1:X:51:GLU:HG2	1.82	0.45
1:X:83:ILE:HG22	1:X:83:ILE:O	2.17	0.45
1:X:270:PHE:C	1:X:270:PHE:CD1	2.95	0.45
1:X:409:LEU:HD23	1:X:409:LEU:HA	1.79	0.45
1:X:468:GLN:O	1:X:472:ASN:CG	2.59	0.45
1:X:529:LEU:HD21	1:X:588:ASN:ND2	2.32	0.45
1:X:730:LEU:O	1:X:731:ASN:HB2	2.17	0.45
1:X:134:ILE:C	1:X:135:TYR:CD1	2.95	0.44
1:X:257:SER:HA	1:X:438:ASN:ND2	2.32	0.44
1:X:238:ARG:HG2	1:X:278:TYR:CZ	2.52	0.44
1:X:276:ARG:NH2	1:X:282:TYR:CD1	2.85	0.44
1:X:347:ILE:O	1:X:349:ALA:N	2.50	0.44
1:X:354:LEU:HD12	1:X:422:VAL:HG22	1.99	0.44
1:X:597:GLU:HB3	1:X:601:LYS:CG	2.47	0.44
1:X:620:ARG:HH22	1:X:630:VAL:CG1	2.28	0.44
1:X:121:LEU:CD1	1:X:482:PHE:CE2	2.87	0.44
1:X:219:ASN:HA	1:X:222:LEU:CG	2.45	0.44
1:X:283:GLN:HB3	1:X:320:ASP:OD1	2.16	0.44
1:X:285:LEU:CD2	1:X:298:LEU:HD22	2.43	0.44
1:X:343:SER:O	1:X:344:ILE:C	2.59	0.44
1:X:367:ALA:HB1	1:X:411:VAL:HG22	1.99	0.44
1:X:461:PHE:CD1	1:X:462:LYS:HG2	2.53	0.44
1:X:8:THR:HA	1:X:13:LYS:NZ	2.32	0.44
1:X:134:ILE:C	1:X:135:TYR:HD1	2.25	0.44
1:X:192:VAL:HG23	1:X:193:ILE:H	1.81	0.44
1:X:552:SER:O	1:X:553:LYS:CB	2.61	0.44
1:X:712:VAL:O	1:X:712:VAL:CG2	2.64	0.44
1:X:116:TYR:CD2	1:X:154:HIS:HA	2.53	0.44
1:X:155:ILE:CG2	1:X:156:PHE:HD1	2.27	0.44
1:X:213:GLN:C	1:X:215:ILE:H	2.24	0.44
1:X:277:ASN:CG	1:X:278:TYR:H	2.26	0.44
1:X:335:GLY:HA2	2:X:2115:HOH:O	2.17	0.44
1:X:705:TYR:CD1	1:X:705:TYR:C	2.93	0.44
1:X:731:ASN:OD1	1:X:754:ILE:HB	2.17	0.44
1:X:270:PHE:C	1:X:271:GLN:HE21	2.24	0.44
1:X:292:GLU:HA	1:X:295:ALA:CB	2.48	0.44
1:X:360:GLU:HB2	1:X:370:LYS:HE2	2.00	0.44
1:X:368:VAL:HA	1:X:394:MET:SD	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:458:PHE:HZ	1:X:479:GLN:CD	2.25	0.44
1:X:561:PRO:HG2	1:X:564:SER:O	2.17	0.44
1:X:708:LEU:C	1:X:709:ALA:O	2.60	0.44
1:X:123:LEU:HD23	1:X:653:VAL:HG13	1.99	0.44
1:X:139:MET:HG2	2:X:2058:HOH:O	2.17	0.44
1:X:567:GLU:CB	1:X:580:GLU:HA	2.47	0.44
1:X:44:ARG:NH1	2:X:2025:HOH:O	2.50	0.44
1:X:49:CYS:SG	1:X:80:ARG:CD	3.06	0.44
1:X:163:TYR:CE1	1:X:167:LEU:CG	2.99	0.44
1:X:434:VAL:O	1:X:435:LYS:C	2.61	0.44
1:X:555:ASN:O	2:X:2175:HOH:O	2.21	0.44
1:X:583:ASP:O	1:X:584:TRP:C	2.61	0.44
1:X:745:PHE:CD1	2:X:2224:HOH:O	2.57	0.44
1:X:596:LEU:O	1:X:597:GLU:C	2.57	0.44
1:X:685:ILE:HG22	1:X:689:ARG:CZ	2.14	0.44
1:X:52:ILE:CG2	1:X:53:VAL:N	2.79	0.43
1:X:134:ILE:CG1	1:X:135:TYR:CD1	3.00	0.43
1:X:272:SER:O	1:X:275:GLU:HB2	2.18	0.43
1:X:135:TYR:HD2	2:X:2073:HOH:O	2.01	0.43
1:X:265:LYS:O	1:X:268:VAL:HG12	2.18	0.43
1:X:366:GLY:HA2	1:X:408:HIS:ND1	2.33	0.43
1:X:492:GLU:O	1:X:493:GLU:C	2.61	0.43
1:X:659:ASN:ND2	1:X:663:LEU:O	2.48	0.43
1:X:16:LYS:CD	1:X:152:ALA:HB2	2.39	0.43
1:X:33:ARG:CD	1:X:52:ILE:CB	2.91	0.43
1:X:129:PHE:CB	1:X:664:PRO:HB3	2.43	0.43
1:X:577:VAL:CG1	1:X:579:TYR:CZ	3.00	0.43
1:X:694:ASN:OD1	1:X:694:ASN:O	2.36	0.43
1:X:245:ILE:O	1:X:449:PHE:HA	2.18	0.43
1:X:256:ALA:HB3	1:X:441:LEU:HB3	2.01	0.43
1:X:375:LEU:HA	1:X:378:ALA:HB3	2.00	0.43
1:X:529:LEU:HG	1:X:588:ASN:OD1	2.18	0.43
1:X:577:VAL:HB	1:X:579:TYR:CE1	2.53	0.43
1:X:641:LEU:CD2	1:X:645:LEU:CD1	2.96	0.43
1:X:11:TYR:CE2	1:X:16:LYS:CB	2.93	0.43
1:X:177:ILE:C	1:X:178:THR:HG23	2.44	0.43
1:X:193:ILE:HD11	2:X:2080:HOH:O	2.18	0.43
1:X:300:GLY:HA3	1:X:303:SER:HB3	2.01	0.43
1:X:132:ILE:N	1:X:132:ILE:CD1	2.75	0.43
1:X:262:LEU:HD11	1:X:634:TYR:CE2	2.54	0.43
1:X:320:ASP:C	1:X:322:GLU:N	2.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:532:GLN:HE22	1:X:543:LEU:CA	2.32	0.43
1:X:732:ILE:HG13	1:X:733:ASP:N	2.33	0.43
1:X:213:GLN:O	1:X:214:GLN:C	2.61	0.43
1:X:365:GLU:CD	1:X:366:GLY:H	2.22	0.43
1:X:56:THR:HG22	1:X:58:ASP:OD1	2.15	0.43
1:X:143:PHE:O	1:X:144:LYS:C	2.62	0.43
1:X:326:ILE:N	1:X:326:ILE:CD1	2.81	0.43
1:X:389:LEU:HD11	1:X:600:PHE:HZ	1.79	0.43
1:X:588:ASN:CG	2:X:2188:HOH:O	2.61	0.43
1:X:4:ILE:HD13	1:X:142:ILE:HA	2.00	0.43
1:X:49:CYS:SG	1:X:80:ARG:HD3	2.59	0.43
1:X:137:GLN:CD	1:X:140:VAL:HG21	2.40	0.43
1:X:193:ILE:HG13	1:X:194:GLN:N	2.32	0.43
1:X:259:GLN:HB2	2:X:2090:HOH:O	2.18	0.43
1:X:333:ILE:C	1:X:335:GLY:N	2.76	0.43
1:X:393:LEU:CD1	1:X:596:LEU:CD2	2.95	0.43
1:X:481:PHE:O	1:X:485:HIS:CB	2.67	0.43
1:X:230:THR:HG21	1:X:267:ARG:NH2	2.33	0.43
1:X:675:GLN:O	1:X:678:CYS:CB	2.67	0.43
1:X:679:ASN:HB2	1:X:681:VAL:CG1	2.39	0.43
1:X:73:LYS:O	1:X:74:LYS:C	2.62	0.42
1:X:155:ILE:O	1:X:159:SER:HB3	2.19	0.42
1:X:440:VAL:C	1:X:442:CYS:H	2.27	0.42
1:X:672:VAL:HA	1:X:675:GLN:HE21	1.83	0.42
1:X:689:ARG:HE	1:X:695:ARG:NH1	2.09	0.42
1:X:28:THR:O	1:X:29:VAL:CG2	2.67	0.42
1:X:340:GLU:HG3	1:X:341:GLN:N	2.33	0.42
1:X:353:HIS:CD2	1:X:378:ALA:HA	2.54	0.42
1:X:485:HIS:CE1	1:X:650:PRO:HG2	2.53	0.42
1:X:487:PHE:C	1:X:489:LEU:H	2.26	0.42
1:X:357:ILE:O	1:X:418:ARG:NH1	2.52	0.42
1:X:389:LEU:CD1	1:X:600:PHE:CE1	2.98	0.42
1:X:455:ILE:HG22	1:X:456:SER:H	1.79	0.42
1:X:470:CYS:C	1:X:634:TYR:OH	2.62	0.42
1:X:474:THR:HG22	1:X:478:LEU:HD11	2.00	0.42
1:X:532:GLN:NE2	1:X:543:LEU:HB2	2.29	0.42
1:X:597:GLU:O	1:X:600:PHE:N	2.51	0.42
1:X:640:SER:O	1:X:643:ALA:HB3	2.19	0.42
1:X:661:LYS:HB3	1:X:663:LEU:HG	2.01	0.42
1:X:36:TRP:HB2	1:X:78:ASN:O	2.19	0.42
1:X:554:LYS:C	2:X:2174:HOH:O	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:9:SER:O	1:X:13:LYS:HG2	2.20	0.42
1:X:222:LEU:O	1:X:226:GLY:CA	2.68	0.42
1:X:437:ILE:HG13	1:X:438:ASN:N	2.35	0.42
1:X:708:LEU:HB3	1:X:712:VAL:CG2	2.49	0.42
1:X:710:PRO:O	1:X:711:ASN:CB	2.54	0.42
1:X:289:THR:O	1:X:290:ALA:C	2.62	0.42
1:X:345:PHE:O	1:X:346:LYS:C	2.59	0.42
1:X:423:LYS:O	1:X:427:GLY:N	2.51	0.42
1:X:107:ARG:O	1:X:110:TYR:HB3	2.20	0.42
1:X:137:GLN:HE21	1:X:140:VAL:CG2	2.31	0.42
1:X:245:ILE:CD1	1:X:450:ILE:O	2.67	0.42
1:X:506:PHE:CD1	1:X:506:PHE:C	2.98	0.42
1:X:728:LYS:HA	1:X:734:PRO:CD	2.43	0.42
1:X:375:LEU:CD1	1:X:389:LEU:HD23	2.50	0.42
1:X:381:VAL:HG23	1:X:382:PHE:N	2.34	0.42
1:X:389:LEU:HD13	1:X:600:PHE:HE1	1.84	0.42
1:X:598:LEU:HD23	1:X:598:LEU:HA	1.76	0.42
1:X:698:TYR:HE1	1:X:744:ILE:O	2.01	0.42
1:X:701:PHE:HE2	1:X:722:ALA:HB3	1.85	0.42
1:X:726:VAL:HG22	1:X:730:LEU:HD11	2.01	0.42
1:X:36:TRP:N	1:X:78:ASN:O	2.50	0.42
1:X:266:SER:C	1:X:268:VAL:N	2.78	0.42
1:X:269:VAL:HA	1:X:306:TYR:CE1	2.55	0.42
1:X:305:ASN:C	1:X:307:LEU:N	2.78	0.42
1:X:544:ILE:CD1	1:X:548:HIS:CE1	3.02	0.42
1:X:71:GLN:N	1:X:71:GLN:CD	2.78	0.41
1:X:220:PRO:O	1:X:224:ALA:HB2	2.20	0.41
1:X:362:GLY:H	1:X:367:ALA:HA	1.84	0.41
1:X:22:SER:HB3	1:X:26:LYS:CE	2.49	0.41
1:X:203:ASN:CG	1:X:207:GLY:HA3	2.46	0.41
1:X:510:SER:C	1:X:512:ALA:N	2.73	0.41
1:X:597:GLU:HB3	1:X:601:LYS:CD	2.49	0.41
1:X:619:SER:OG	1:X:620:ARG:N	2.54	0.41
1:X:664:PRO:O	1:X:665:ALA:HB2	2.16	0.41
1:X:87:GLY:C	1:X:109:ARG:HD3	2.44	0.41
1:X:361:LYS:HA	1:X:361:LYS:HD3	1.85	0.41
1:X:743:LYS:C	1:X:744:ILE:CG2	2.92	0.41
1:X:78:ASN:CA	1:X:98:ASN:ND2	2.56	0.41
1:X:210:VAL:HG13	1:X:211:LEU:HG	2.02	0.41
1:X:261:TYR:CD1	1:X:261:TYR:N	2.87	0.41
1:X:292:GLU:HA	1:X:295:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:334:VAL:O	1:X:334:VAL:HG13	2.20	0.41
1:X:464:ASN:HA	1:X:468:GLN:NE2	2.35	0.41
1:X:501:TRP:O	1:X:503:PHE:N	2.52	0.41
1:X:604:SER:O	1:X:605:ASP:HB2	2.16	0.41
1:X:673:LEU:HA	1:X:676:LEU:HG	2.01	0.41
1:X:685:ILE:O	1:X:687:ILE:C	2.64	0.41
1:X:526:LEU:HD22	1:X:631:ALA:CB	2.29	0.41
1:X:219:ASN:O	1:X:222:LEU:N	2.53	0.41
1:X:243:ILE:O	1:X:452:VAL:HG22	2.20	0.41
1:X:273:GLU:OE2	2:X:2095:HOH:O	2.22	0.41
1:X:411:VAL:O	1:X:413:LYS:N	2.53	0.41
1:X:498:LYS:O	1:X:500:ASN:OD1	2.38	0.41
1:X:504:ILE:CD1	1:X:505:ASP:N	2.78	0.41
1:X:508:LEU:HB3	1:X:511:GLN:H	1.86	0.41
1:X:622:LYS:O	1:X:622:LYS:HG2	2.21	0.41
1:X:751:LEU:HD12	1:X:751:LEU:C	2.32	0.41
1:X:754:ILE:CG2	1:X:755:GLU:H	2.33	0.41
1:X:110:TYR:CD2	1:X:126:VAL:HG11	2.56	0.41
1:X:121:LEU:CD1	1:X:652:PHE:CD2	2.99	0.41
1:X:210:VAL:HG22	1:X:214:GLN:CG	2.51	0.41
1:X:266:SER:C	1:X:268:VAL:H	2.28	0.41
1:X:467:GLU:O	1:X:468:GLN:C	2.63	0.41
1:X:626:ASN:ND2	1:X:627:PHE:HD2	2.18	0.41
1:X:685:ILE:HG13	1:X:686:ARG:H	1.84	0.41
1:X:110:TYR:OH	1:X:128:PRO:HA	2.20	0.41
1:X:556:ALA:C	1:X:557:LYS:HD3	2.46	0.41
1:X:35:ILE:HD12	1:X:79:GLN:HA	2.03	0.41
1:X:134:ILE:HD12	1:X:154:HIS:NE2	2.36	0.41
1:X:147:ARG:HG2	1:X:150:GLU:OE2	2.21	0.41
1:X:178:THR:HA	1:X:455:ILE:O	2.21	0.41
1:X:192:VAL:CG2	1:X:193:ILE:N	2.84	0.41
1:X:294:LYS:C	1:X:296:LEU:H	2.27	0.41
1:X:305:ASN:HB3	1:X:309:GLN:HE21	1.86	0.41
1:X:365:GLU:O	1:X:366:GLY:O	2.39	0.41
1:X:588:ASN:ND2	2:X:2188:HOH:O	2.54	0.41
1:X:633:GLN:O	1:X:635:LYS:N	2.53	0.41
1:X:671:VAL:O	1:X:674:ASP:HB3	2.19	0.41
1:X:98:ASN:ND2	1:X:100:PRO:CG	2.83	0.41
1:X:99:GLU:O	1:X:100:PRO:C	2.63	0.41
1:X:103:PHE:CE2	1:X:669:ASP:HB3	2.56	0.41
1:X:103:PHE:CZ	1:X:669:ASP:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:163:TYR:O	1:X:167:LEU:HG	2.21	0.41
1:X:265:LYS:O	1:X:423:LYS:CG	2.69	0.41
1:X:588:ASN:ND2	1:X:630:VAL:CG2	2.83	0.41
1:X:91:MET:CB	2:X:2049:HOH:O	2.69	0.40
1:X:93:GLU:CA	1:X:694:ASN:ND2	2.84	0.40
1:X:329:GLN:O	1:X:333:ILE:HG12	2.22	0.40
1:X:212:GLU:O	1:X:216:LEU:HD13	2.21	0.40
1:X:685:ILE:HA	1:X:688:THR:OG1	2.21	0.40
1:X:248:ASN:HD21	1:X:252:PHE:HB2	1.86	0.40
1:X:411:VAL:O	1:X:412:GLU:C	2.64	0.40
1:X:491:GLN:O	1:X:491:GLN:CD	2.64	0.40
1:X:685:ILE:CG2	1:X:689:ARG:HH22	2.08	0.40
1:X:146:ARG:HA	1:X:146:ARG:HD2	1.96	0.40
1:X:155:ILE:O	1:X:159:SER:CB	2.69	0.40
1:X:163:TYR:HE1	1:X:167:LEU:HD11	0.70	0.40
1:X:210:VAL:O	1:X:211:LEU:C	2.65	0.40
1:X:221:ILE:O	1:X:225:PHE:HD1	2.05	0.40
1:X:224:ALA:C	1:X:280:ILE:CG2	2.95	0.40
1:X:280:ILE:CD1	1:X:348:ILE:HD12	2.51	0.40
1:X:294:LYS:HD2	1:X:294:LYS:HA	1.91	0.40
1:X:610:LYS:HB2	1:X:610:LYS:HE3	1.86	0.40
1:X:736:GLN:O	1:X:747:ARG:CB	2.68	0.40
1:X:37:TYR:CD1	1:X:38:ASN:N	2.89	0.40
1:X:337:SER:HB3	1:X:340:GLU:CG	2.36	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:22:SER:OG	1:X:541:ASN:ND2[3_655]	2.04	0.16
1:X:403:ASP:OD1	1:X:405:VAL:CA[2_556]	2.04	0.16
1:X:445:ARG:NH1	1:X:582:GLN:OE1[1_455]	2.10	0.10
1:X:29:VAL:CG2	1:X:537:ASN:OD1[3_655]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	756/758 (100%)	579 (77%)	143 (19%)	34 (4%)	2	12

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	6	ASP
1	X	8	THR
1	X	32	LYS
1	X	210	VAL
1	X	540	ASP
1	X	605	ASP
1	X	665	ALA
1	X	693	PRO
1	X	698	TYR
1	X	709	ALA
1	X	711	ASN
1	X	722	ALA
1	X	732	ILE
1	X	214	GLN
1	X	346	LYS
1	X	74	LYS
1	X	378	ALA
1	X	695	ARG
1	X	303	SER
1	X	493	GLU
1	X	674	ASP
1	X	686	ARG
1	X	468	GLN
1	X	536	PRO
1	X	625	ALA
1	X	731	ASN
1	X	396	PRO
1	X	672	VAL
1	X	219	ASN
1	X	335	GLY
1	X	650	PRO
1	X	134	ILE
1	X	366	GLY
1	X	713	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	X	663/663 (100%)	627 (95%)	36 (5%)	20 47

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	8	THR
1	X	10	ASP
1	X	12	HIS
1	X	14	TYR
1	X	34	TYR
1	X	37	TYR
1	X	89	GLU
1	X	99	GLU
1	X	106	LEU
1	X	122	PHE
1	X	132	ILE
1	X	147	ARG
1	X	161	VAL
1	X	232	ARG
1	X	261	TYR
1	X	273	GLU
1	X	280	ILE
1	X	292	GLU
1	X	294	LYS
1	X	297	HIS
1	X	306	TYR
1	X	336	PHE
1	X	375	LEU
1	X	444	GLU
1	X	460	ILE
1	X	491	GLN
1	X	492	GLU
1	X	504	ILE
1	X	540	ASP
1	X	611	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	636	GLU
1	X	652	PHE
1	X	712	VAL
1	X	717	GLU
1	X	721	LYS
1	X	731	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	112	GLN
1	X	137	GLN
1	X	149	ASN
1	X	173	GLN
1	X	203	ASN
1	X	217	GLN
1	X	234	ASN
1	X	271	GLN
1	X	305	ASN
1	X	309	GLN
1	X	341	GLN
1	X	353	HIS
1	X	376	ASN
1	X	407	GLN
1	X	408	HIS
1	X	443	GLN
1	X	475	ASN
1	X	485	HIS
1	X	537	ASN
1	X	548	HIS
1	X	582	GLN
1	X	588	ASN
1	X	613	ASN
1	X	637	GLN
1	X	649	ASN
1	X	694	ASN
1	X	711	ASN
1	X	729	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	X	758/758 (100%)	0.58	54 (7%)	22 18	0, 7, 48, 80	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	206	ASN	6.0
1	X	693	PRO	5.9
1	X	722	ALA	5.6
1	X	184	GLY	4.6
1	X	692	PHE	4.1
1	X	732	ILE	4.1
1	X	583	ASP	4.0
1	X	4	ILE	3.8
1	X	17	VAL	3.8
1	X	11	TYR	3.7
1	X	723	THR	3.6
1	X	689	ARG	3.6
1	X	60	PHE	3.4
1	X	14	TYR	3.4
1	X	724	ASP	3.4
1	X	746	PHE	3.4
1	X	705	TYR	3.3
1	X	432	TRP	3.3
1	X	20	GLY	3.3
1	X	749	GLY	3.2
1	X	751	LEU	3.2
1	X	24	LEU	3.2
1	X	698	TYR	3.2
1	X	207	GLY	3.0
1	X	739	PHE	3.0
1	X	757	ALA	2.9
1	X	706	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	502	THR	2.8
1	X	6	ASP	2.7
1	X	47	TYR	2.7
1	X	208	SER	2.6
1	X	710	PRO	2.6
1	X	15	LEU	2.6
1	X	242	PHE	2.5
1	X	697	ILE	2.5
1	X	505	ASP	2.5
1	X	539	THR	2.4
1	X	580	GLU	2.4
1	X	707	LEU	2.3
1	X	466	PHE	2.3
1	X	271	GLN	2.2
1	X	99	GLU	2.2
1	X	241	LYS	2.2
1	X	595	ASP	2.1
1	X	46	SER	2.1
1	X	86	ASP	2.1
1	X	699	ALA	2.1
1	X	563	PHE	2.1
1	X	26	LYS	2.0
1	X	744	ILE	2.0
1	X	753	ARG	2.0
1	X	85	PHE	2.0
1	X	666	LYS	2.0
1	X	678	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.