



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:43 AM UTC

PDB ID : 1S4F / pdb_00001s4f
Title : Crystal Structure of RNA-dependent RNA polymerase construct 2 from bovine viral diarrhea virus (BVDV)
Authors : Choi, K.H.; Groarke, J.M.; Young, D.C.; Kuhn, R.J.; Smith, J.L.; Pevear, D.C.; Rossmann, M.G.
Deposited on : 2004-01-16
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

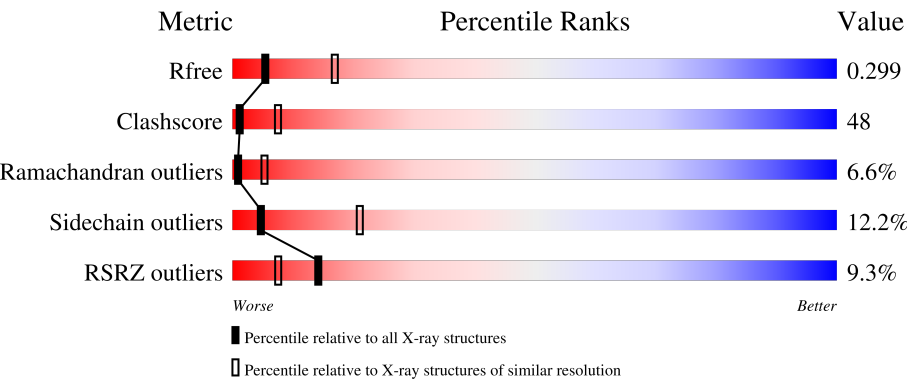
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	601	4% 37% 48% 11% ..
1	B	601	4% 41% 45% 10% ..
1	C	601	15% 28% 49% 16% ..
1	D	601	12% 26% 51% 15% ..

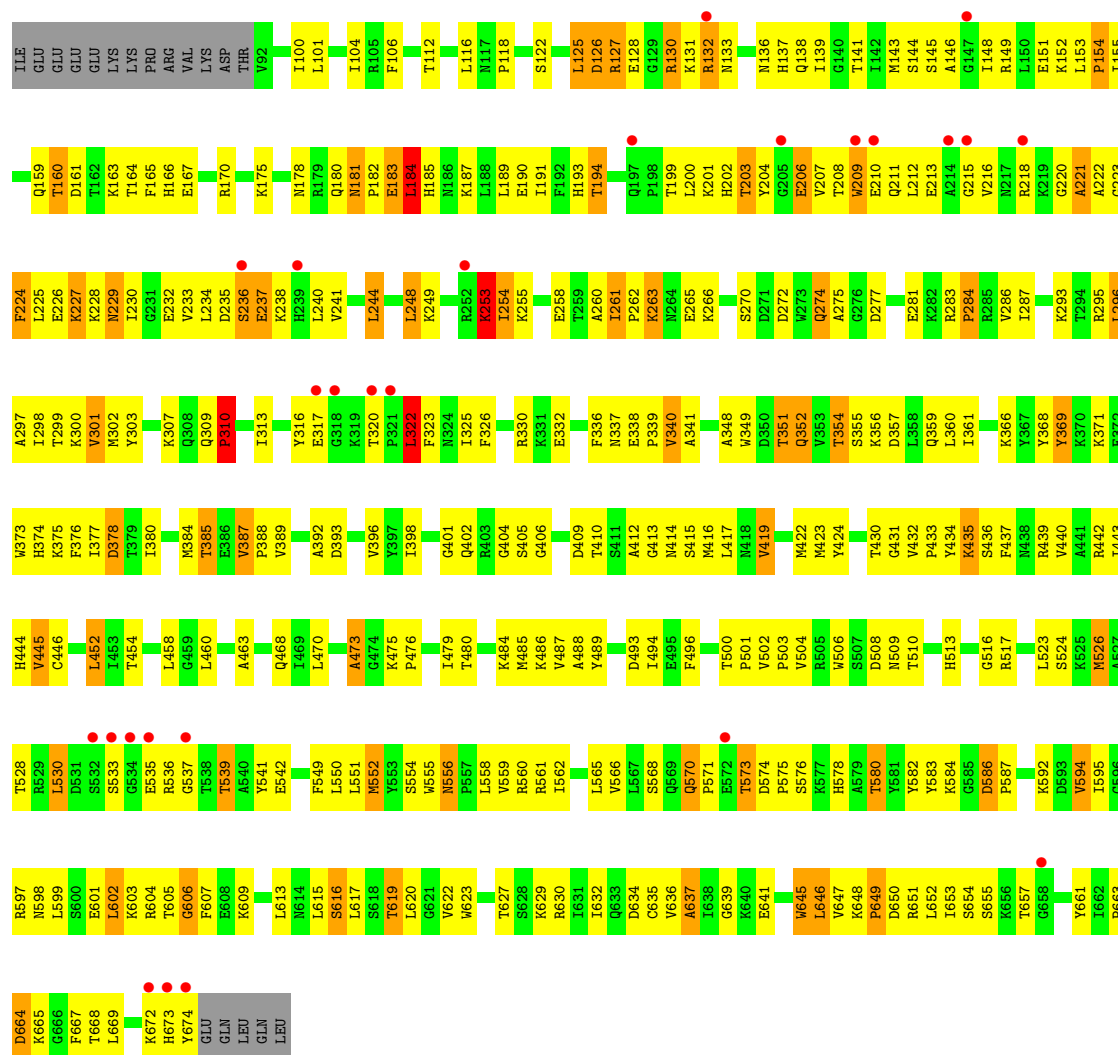
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18714 atoms, of which 0 are hydrogens and 0 are deuteriums.

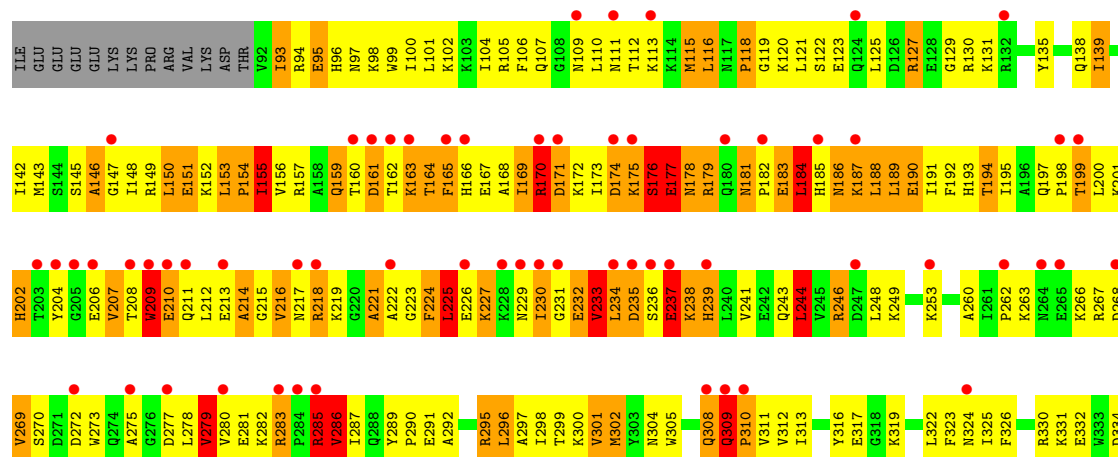
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

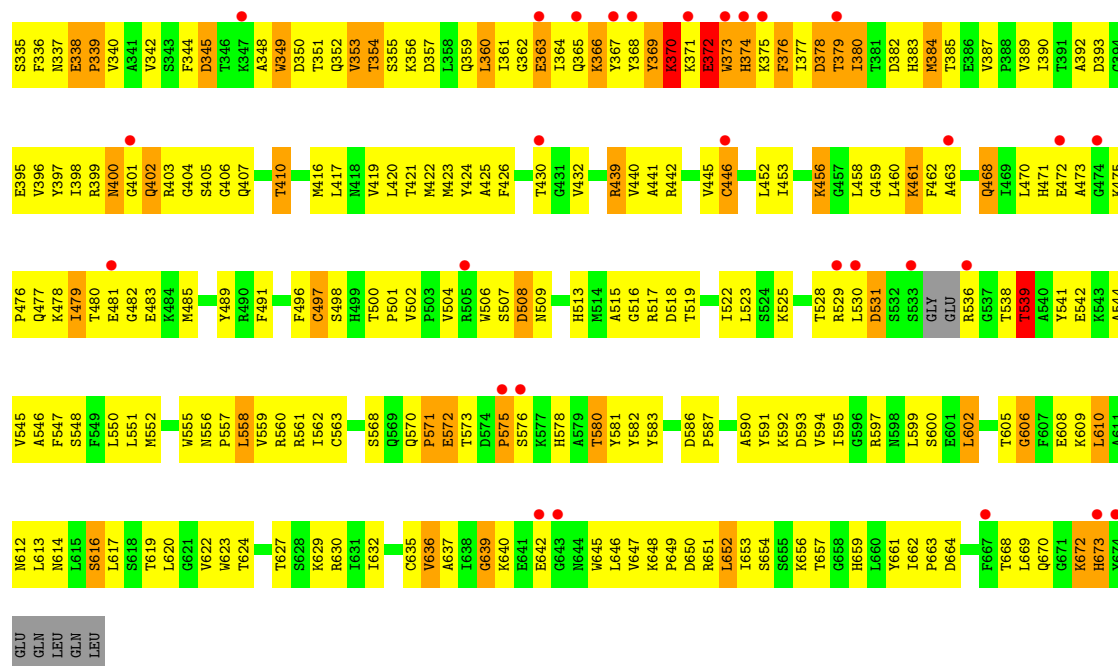
- Molecule 1 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4697	2984	830	866	17			
1	B	583	Total	C	N	O	S	0	0	0
			4697	2984	830	866	17			
1	C	581	Total	C	N	O	S	0	0	0
			4684	2977	828	862	17			
1	D	575	Total	C	N	O	S	0	0	0
			4636	2945	821	853	17			

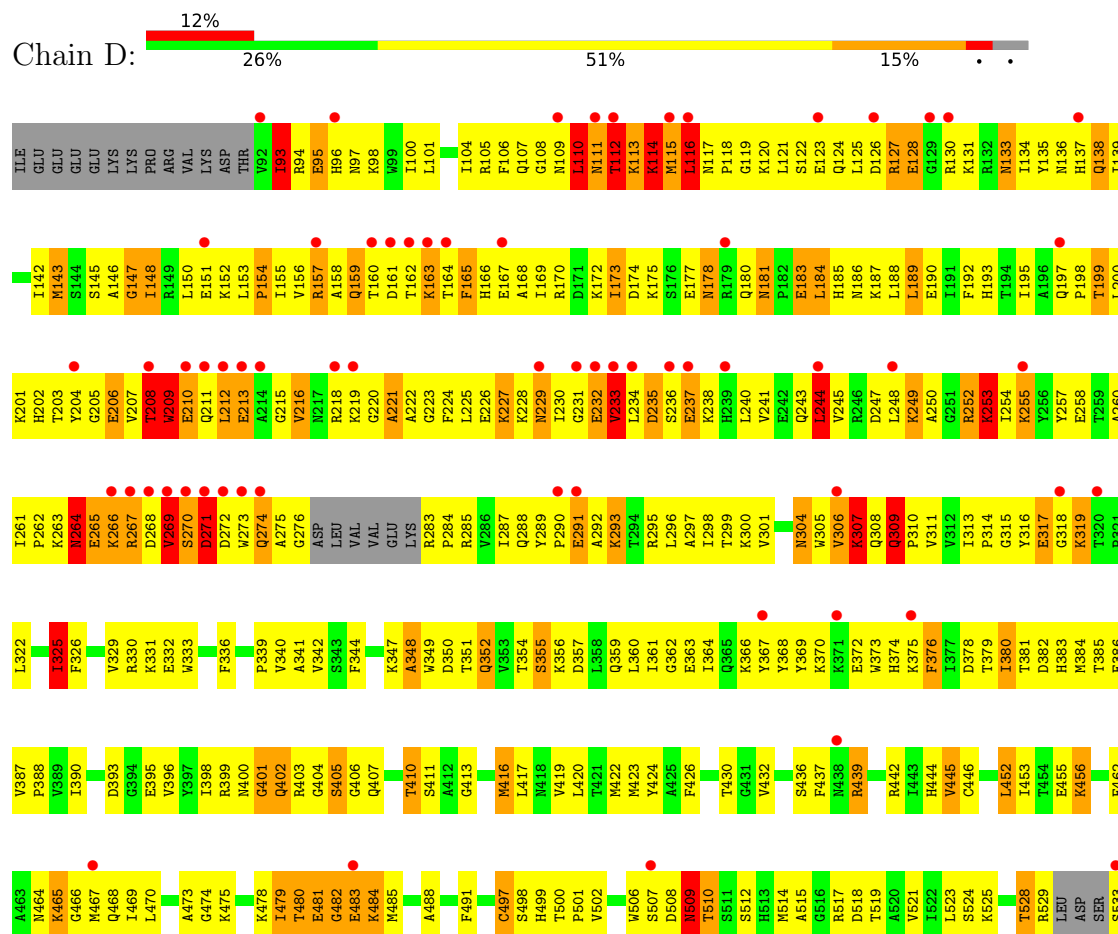


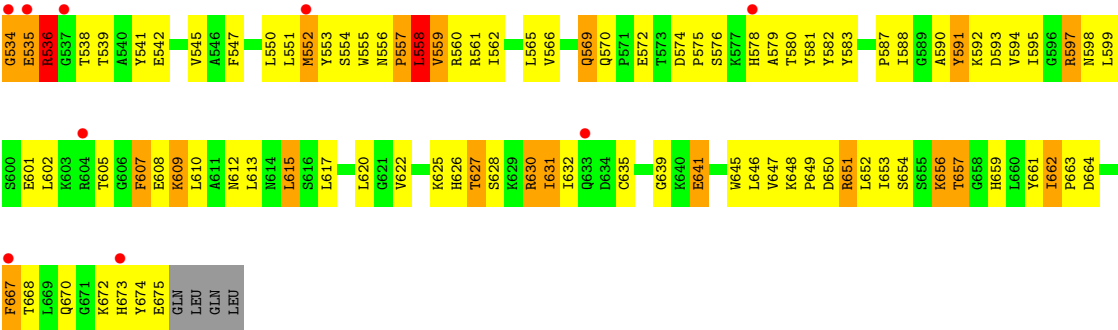
• Molecule 1: RNA-dependent RNA polymerase





• Molecule 1: RNA-dependent RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	412.27Å 412.27Å 95.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.69 – 3.00 29.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.69-3.00) 91.0 (29.69-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.303 0.251 , 0.299	Depositor DCC
R_{free} test set	10559 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18714	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/4799	1.14	36/6475 (0.6%)
1	B	0.53	0/4799	1.06	27/6475 (0.4%)
1	C	0.50	0/4785	1.18	53/6455 (0.8%)
1	D	0.54	0/4736	1.18	41/6386 (0.6%)
All	All	0.53	0/19119	1.14	157/25791 (0.6%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	GLN	N-CA-C	-16.92	85.11	109.48
1	C	233	VAL	N-CA-C	-14.21	98.76	112.83
1	D	309	GLN	CA-C-N	-12.96	106.30	119.90
1	D	309	GLN	C-N-CA	-12.96	106.30	119.90
1	C	232	GLU	N-CA-C	-12.89	96.21	114.12
1	A	309	GLN	CA-C-N	12.80	135.84	119.84
1	A	309	GLN	C-N-CA	12.80	135.84	119.84
1	C	175	LYS	N-CA-C	12.27	125.17	108.23
1	C	210	GLU	N-CA-C	-11.79	98.15	111.82
1	C	286	VAL	N-CA-C	11.36	132.97	109.34
1	C	177	GLU	N-CA-C	-11.25	86.84	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	ILE	N-CA-C	-10.92	94.63	109.37
1	C	219	LYS	N-CA-C	-10.87	97.51	112.30
1	C	163	LYS	N-CA-C	-10.50	99.37	111.03
1	A	309	GLN	C-N-CD	-9.68	85.32	125.00
1	D	232	GLU	N-CA-C	-9.47	101.89	113.15
1	C	376	PHE	N-CA-C	-9.39	100.44	112.93
1	D	97	ASN	N-CA-C	-9.29	98.51	112.54
1	B	338	GLU	CA-C-N	9.23	129.31	119.89
1	B	338	GLU	C-N-CA	9.23	129.31	119.89
1	D	112	THR	N-CA-C	-8.93	97.89	111.56
1	D	610	LEU	N-CA-C	-8.54	102.06	111.36
1	D	558	LEU	N-CA-C	-8.53	97.05	109.59
1	A	475	LYS	CA-C-N	8.47	128.23	119.76
1	A	475	LYS	C-N-CA	8.47	128.23	119.76
1	D	480	THR	N-CA-C	-8.46	103.48	113.21
1	B	533	SER	N-CA-C	-8.16	102.56	114.39
1	C	176	SER	N-CA-C	8.10	128.06	110.80
1	D	355	SER	N-CA-C	-8.04	102.46	111.14
1	A	117	ASN	CA-C-N	8.00	128.75	119.47
1	A	117	ASN	C-N-CA	8.00	128.75	119.47
1	A	402	GLN	N-CA-C	-7.94	97.09	107.73
1	D	657	THR	N-CA-C	-7.84	103.85	113.41
1	C	673	HIS	N-CA-C	7.68	123.13	107.69
1	B	181	ASN	CA-C-N	7.61	129.35	119.84
1	B	181	ASN	C-N-CA	7.61	129.35	119.84
1	A	310	PRO	CA-N-CD	-7.50	101.50	112.00
1	D	605	THR	N-CA-C	-7.43	104.34	113.41
1	D	233	VAL	N-CA-C	-7.38	105.79	111.62
1	A	171	ASP	N-CA-C	7.32	119.26	111.28
1	B	387	VAL	N-CA-C	7.25	116.60	108.05
1	D	528	THR	N-CA-C	7.20	120.27	110.55
1	D	186	ASN	N-CA-C	-7.16	103.08	111.03
1	B	431	GLY	N-CA-C	-6.95	105.47	114.85
1	C	146	ALA	N-CA-C	-6.79	101.39	110.55
1	C	610	LEU	N-CA-C	-6.73	103.94	111.28
1	A	285	ARG	N-CA-C	-6.66	99.67	110.20
1	D	662	ILE	CA-C-N	6.63	127.02	119.92
1	D	662	ILE	C-N-CA	6.63	127.02	119.92
1	A	173	ILE	N-CA-C	6.59	118.19	111.00
1	C	183	GLU	N-CA-C	6.57	120.40	112.38
1	D	163	LYS	N-CA-C	-6.55	103.97	112.68
1	C	639	GLY	N-CA-C	6.50	121.82	114.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	ASN	N-CA-C	6.50	119.67	110.50
1	D	250	ALA	N-CA-C	-6.50	105.49	113.41
1	A	235	ASP	N-CA-C	6.45	118.00	110.97
1	C	531	ASP	N-CA-C	6.41	124.44	110.80
1	C	446	CYS	N-CA-C	-6.38	99.55	108.54
1	D	376	PHE	N-CA-C	-6.36	103.48	111.11
1	C	673	HIS	CA-C-N	6.36	133.15	121.70
1	C	673	HIS	C-N-CA	6.36	133.15	121.70
1	C	178	ASN	N-CA-C	6.31	119.07	110.55
1	C	539	THR	N-CA-C	-6.30	104.64	112.90
1	D	309	GLN	N-CA-C	-6.29	95.91	109.81
1	D	208	THR	N-CA-C	6.26	118.50	108.41
1	D	157	ARG	N-CA-C	-6.24	101.06	110.24
1	C	95	GLU	N-CA-C	6.19	118.53	111.11
1	C	366	LYS	N-CA-C	-6.17	105.85	113.19
1	A	534	GLY	N-CA-C	-6.17	102.49	110.69
1	D	307	LYS	N-CA-C	-6.16	99.15	109.07
1	D	165	PHE	N-CA-C	-6.14	104.89	112.38
1	B	539	THR	N-CA-C	-6.14	105.28	112.89
1	B	112	THR	N-CA-C	-6.13	101.20	110.28
1	D	502	VAL	CA-C-N	6.13	125.89	119.76
1	D	502	VAL	C-N-CA	6.13	125.89	119.76
1	C	309	GLN	CA-C-N	-6.09	112.22	119.84
1	C	309	GLN	C-N-CA	-6.09	112.22	119.84
1	A	650	ASP	N-CA-C	-6.07	100.67	109.59
1	D	93	ILE	N-CA-C	6.05	121.92	109.34
1	A	553	TYR	N-CA-C	6.04	120.52	112.30
1	C	461	LYS	N-CA-C	-6.04	104.62	112.23
1	B	402	GLN	N-CA-C	-6.01	100.31	108.24
1	C	373	TRP	N-CA-C	-6.00	96.69	107.98
1	A	197	GLN	CA-C-N	5.99	127.32	119.84
1	A	197	GLN	C-N-CA	5.99	127.32	119.84
1	D	244	LEU	N-CA-C	-5.99	104.10	111.40
1	D	552	MET	N-CA-C	5.93	118.70	111.82
1	B	274	GLN	N-CA-C	-5.92	104.83	111.28
1	B	445	VAL	N-CA-C	5.90	116.78	108.17
1	A	338	GLU	CA-C-N	5.87	126.69	120.11
1	A	338	GLU	C-N-CA	5.87	126.69	120.11
1	A	245	VAL	N-CA-C	-5.87	104.13	110.23
1	B	310	PRO	N-CA-C	-5.87	100.39	112.47
1	C	209	TRP	N-CA-C	5.86	123.29	110.80
1	C	275	ALA	N-CA-C	-5.82	106.31	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLN	N-CA-C	-5.82	98.93	108.76
1	B	209	TRP	N-CA-C	-5.81	104.31	111.75
1	A	431	GLY	N-CA-C	-5.80	106.77	114.95
1	B	473	ALA	N-CA-C	-5.78	106.23	113.28
1	C	441	ALA	N-CA-C	5.76	117.83	109.07
1	D	160	THR	N-CA-C	-5.74	98.58	110.80
1	A	480	THR	N-CA-C	5.73	120.55	112.93
1	C	169	ILE	N-CA-C	-5.73	104.35	110.36
1	C	372	GLU	N-CA-C	-5.68	103.86	112.04
1	C	176	SER	CA-C-N	5.65	132.34	121.54
1	C	176	SER	C-N-CA	5.65	132.34	121.54
1	D	158	ALA	N-CA-C	5.63	117.83	108.99
1	B	594	VAL	CB-CA-C	-5.59	106.14	111.06
1	B	253	LYS	N-CA-C	5.57	122.67	110.80
1	D	269	VAL	N-CA-C	5.56	120.90	109.34
1	D	133	ASN	N-CA-C	-5.54	102.08	110.28
1	C	139	ILE	N-CA-C	5.53	115.73	110.42
1	C	150	LEU	N-CA-C	-5.48	105.70	112.38
1	B	263	LYS	N-CA-C	5.47	118.12	109.96
1	D	249	LYS	N-CA-C	-5.45	106.68	113.38
1	A	357	ASP	N-CA-C	-5.42	105.27	111.07
1	C	135	TYR	N-CA-C	5.42	119.01	109.80
1	D	265	GLU	N-CA-C	5.40	122.31	110.80
1	A	325	ILE	N-CA-C	5.39	115.59	110.42
1	A	137	HIS	N-CA-C	5.39	117.59	111.02
1	C	410	THR	N-CA-C	5.39	117.59	111.02
1	B	645	TRP	N-CA-C	5.39	117.49	108.23
1	C	175	LYS	CB-CA-C	-5.37	102.80	113.80
1	A	469	ILE	N-CA-C	-5.36	105.28	110.42
1	B	275	ALA	N-CA-C	-5.33	102.64	110.52
1	D	656	LYS	N-CA-C	-5.33	107.80	114.56
1	C	349	TRP	N-CA-C	5.32	116.76	111.07
1	A	322	LEU	N-CA-C	5.30	119.23	112.87
1	A	532	SER	N-CA-C	-5.29	105.57	112.23
1	B	570	GLN	CA-C-N	5.28	124.95	119.56
1	B	570	GLN	C-N-CA	5.28	124.95	119.56
1	B	322	LEU	N-CA-C	5.28	118.82	112.38
1	B	586	ASP	CA-C-N	5.28	124.73	119.24
1	B	586	ASP	C-N-CA	5.28	124.73	119.24
1	C	286	VAL	CB-CA-C	-5.28	102.64	111.29
1	C	608	GLU	N-CA-C	5.23	117.73	111.71
1	C	544	ALA	N-CA-C	-5.20	105.67	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	VAL	N-CA-C	5.18	116.09	109.30
1	D	484	LYS	N-CA-C	5.17	116.85	108.26
1	A	461	LYS	N-CA-C	-5.17	105.56	111.14
1	C	338	GLU	CA-C-N	5.16	126.28	119.84
1	C	338	GLU	C-N-CA	5.16	126.28	119.84
1	C	664	ASP	N-CA-C	-5.12	102.88	110.46
1	C	423	MET	N-CA-C	-5.10	105.72	111.28
1	D	536	ARG	N-CA-C	5.08	121.62	110.80
1	D	500	THR	N-CA-C	-5.08	102.33	110.10
1	C	244	LEU	N-CA-C	-5.07	105.41	111.03
1	C	354	THR	N-CA-C	5.06	117.37	109.52
1	A	522	ILE	N-CA-C	-5.06	105.56	110.42
1	A	473	ALA	N-CA-C	-5.05	107.12	113.28
1	B	375	LYS	N-CA-C	-5.04	105.86	111.36
1	B	323	PHE	N-CA-C	5.04	119.18	113.19
1	D	367	TYR	N-CA-C	-5.03	105.26	111.40
1	A	186	ASN	N-CA-C	-5.01	105.70	111.07
1	A	638	ILE	CB-CA-C	-5.01	105.48	112.04
1	C	672	LYS	CA-C-N	-5.00	115.58	123.13
1	C	672	LYS	C-N-CA	-5.00	115.58	123.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	369	TYR	Sidechain
1	C	369	TYR	Sidechain
1	D	591	TYR	Sidechain

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	4697	0	4737	367	0
1	B	4697	0	4735	326	0
1	C	4684	0	4725	584	1
1	D	4636	0	4667	577	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18714	0	18864	1808	1

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 48.

All (1808) 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:C:170:ARG:HD3	1:D:111:ASN:HD22	1.07	1.13
1:C:218:ARG:HB3	1:C:231:GLY:HA3	1.28	1.12
1:D:580:THR:HA	1:D:673:HIS:HB3	1.28	1.12
1:A:311:VAL:HG21	1:A:319:LYS:HD2	1.28	1.10
1:A:625:LYS:H	1:A:625:LYS:HD2	0.94	1.09
1:C:309:GLN:HB3	1:C:310:PRO:HD2	1.34	1.08
1:D:227:LYS:HD2	1:D:228:LYS:H	1.09	1.08
1:C:370:LYS:HG3	1:C:371:LYS:H	1.15	1.07
1:A:143:MET:HE3	1:A:523:LEU:HD22	1.32	1.06
1:D:266:LYS:HD3	1:D:267:ARG:N	1.69	1.06
1:B:253:LYS:H	1:B:253:LYS:HD2	1.10	1.06
1:D:307:LYS:NZ	1:D:319:LYS:HG2	1.71	1.05
1:D:253:LYS:HD3	1:D:253:LYS:H	1.22	1.05
1:D:204:TYR:OH	1:D:310:PRO:HD2	1.55	1.05
1:A:625:LYS:H	1:A:625:LYS:CD	1.68	1.04
1:C:370:LYS:HG3	1:C:371:LYS:N	1.67	1.04
1:B:336:PHE:HB2	1:B:339:PRO:HG3	1.40	1.04
1:C:227:LYS:HD3	1:C:227:LYS:H	1.22	1.04
1:D:159:GLN:HG2	1:D:161:ASP:HB2	1.37	1.03
1:C:167:GLU:CA	1:C:170:ARG:HH12	1.72	1.03
1:C:167:GLU:HA	1:C:170:ARG:NH1	1.72	1.03
1:D:95:GLU:HG3	1:D:96:HIS:H	1.20	1.02
1:C:167:GLU:HA	1:C:170:ARG:HH12	1.23	1.02
1:A:147:GLY:HA3	1:A:624:THR:HG23	1.38	1.02
1:D:298:ILE:HG12	1:D:380:ILE:HD11	1.41	1.01
1:C:422:MET:HE2	1:C:422:MET:HA	1.42	1.01
1:C:183:GLU:HA	1:C:186:ASN:HD22	1.26	1.00
1:D:229:ASN:H	1:D:229:ASN:HD22	1.09	1.00
1:D:266:LYS:HE2	1:D:269:VAL:HG12	1.40	1.00
1:A:625:LYS:HD2	1:A:625:LYS:N	1.75	1.00
1:C:179:ARG:HD3	1:C:179:ARG:H	1.27	0.99
1:C:116:LEU:HB3	1:D:398:ILE:HD12	1.43	0.99
1:C:170:ARG:HD3	1:D:111:ASN:ND2	1.78	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:VAL:HG12	1:B:208:THR:H	1.28	0.98
1:C:309:GLN:HB3	1:C:310:PRO:CD	1.91	0.98
1:D:648:LYS:HB2	1:D:661:TYR:HB2	1.45	0.98
1:C:229:ASN:HB2	1:C:232:GLU:HG3	1.43	0.98
1:A:237:GLU:HB3	1:A:240:LEU:HD12	1.46	0.98
1:D:114:LYS:HA	1:D:114:LYS:CE	1.94	0.98
1:D:143:MET:HG2	1:D:148:ILE:HG21	1.47	0.97
1:C:325:ILE:HG23	1:C:326:PHE:H	1.24	0.97
1:D:143:MET:HE3	1:D:523:LEU:HD22	1.47	0.96
1:D:336:PHE:HB2	1:D:339:PRO:HG3	1.46	0.96
1:C:309:GLN:O	1:C:311:VAL:N	1.98	0.96
1:C:404:GLY:H	1:C:407:GLN:NE2	1.65	0.95
1:C:190:GLU:HA	1:C:193:HIS:HD2	1.31	0.94
1:D:309:GLN:HB3	1:D:310:PRO:HD3	1.49	0.94
1:C:352:GLN:HG2	1:C:476:PRO:HD2	1.47	0.93
1:C:283:ARG:HG2	1:C:285:ARG:HH21	1.31	0.93
1:C:230:ILE:HG13	1:C:292:ALA:HB1	1.50	0.93
1:B:175:LYS:HD3	1:B:351:THR:HG23	1.52	0.92
1:B:253:LYS:HD2	1:B:253:LYS:N	1.81	0.92
1:D:673:HIS:O	1:D:674:TYR:HD1	1.53	0.92
1:A:229:ASN:ND2	1:A:232:GLU:HB2	1.85	0.92
1:C:212:LEU:HD22	1:C:300:LYS:HB2	1.49	0.92
1:D:227:LYS:CD	1:D:228:LYS:H	1.84	0.91
1:B:200:LEU:O	1:B:203:THR:HG23	1.70	0.90
1:C:336:PHE:HB2	1:C:339:PRO:HG3	1.51	0.89
1:B:213:GLU:O	1:B:216:VAL:HG22	1.72	0.89
1:C:105:ARG:HG3	1:C:122:SER:HB3	1.53	0.89
1:C:236:SER:O	1:C:237:GLU:HB2	1.70	0.89
1:C:173:ILE:HD11	1:C:286:VAL:HG21	1.53	0.88
1:D:157:ARG:NH2	1:D:275:ALA:HB1	1.89	0.88
1:B:146:ALA:HA	1:B:630:ARG:HD2	1.53	0.88
1:C:648:LYS:HE2	1:C:659:HIS:HB2	1.55	0.88
1:D:209:TRP:HZ3	1:D:300:LYS:HZ1	1.22	0.88
1:A:229:ASN:HD22	1:A:232:GLU:HB2	1.38	0.87
1:D:227:LYS:HD2	1:D:228:LYS:N	1.89	0.87
1:C:227:LYS:HD3	1:C:227:LYS:N	1.88	0.87
1:A:118:PRO:HG2	1:B:398:ILE:HD13	1.56	0.87
1:C:231:GLY:HA2	1:C:234:LEU:HB2	1.56	0.87
1:D:536:ARG:N	1:D:536:ARG:HH11	1.71	0.87
1:C:370:LYS:CG	1:C:372:GLU:H	1.87	0.86
1:A:665:LYS:HD3	1:A:665:LYS:H	1.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ALA:HB1	1:C:627:THR:HA	1.55	0.86
1:D:307:LYS:HZ3	1:D:319:LYS:HG2	1.38	0.86
1:A:668:THR:O	1:A:669:LEU:HD23	1.76	0.86
1:C:155:ILE:HG13	1:C:266:LYS:HG2	1.57	0.86
1:C:116:LEU:O	1:C:118:PRO:HD3	1.76	0.86
1:D:307:LYS:HZ1	1:D:319:LYS:HG2	1.41	0.86
1:C:202:HIS:HA	1:C:368:TYR:O	1.76	0.85
1:D:266:LYS:HE2	1:D:269:VAL:CG1	2.05	0.85
1:C:422:MET:HE1	1:C:470:LEU:HD11	1.58	0.85
1:C:229:ASN:O	1:C:233:VAL:HG23	1.75	0.84
1:B:133:ASN:H	1:B:536:ARG:HH12	1.25	0.84
1:D:94:ARG:HD2	1:D:95:GLU:HG2	1.57	0.84
1:B:317:GLU:OE2	1:B:320:THR:HB	1.77	0.84
1:D:211:GLN:HG3	1:D:211:GLN:O	1.76	0.84
1:B:154:PRO:HG3	1:B:620:LEU:HD13	1.60	0.84
1:C:308:GLN:O	1:C:319:LYS:HD2	1.76	0.84
1:B:159:GLN:NE2	1:B:164:THR:HG21	1.92	0.84
1:C:204:TYR:HD2	1:C:368:TYR:HB3	1.43	0.83
1:B:648:LYS:HE2	1:B:657:THR:OG1	1.79	0.83
1:B:143:MET:HE3	1:B:523:LEU:HD22	1.61	0.83
1:C:375:LYS:HA	1:C:378:ASP:HB2	1.59	0.83
1:D:127:ARG:C	1:D:127:ARG:HD3	2.04	0.83
1:D:253:LYS:H	1:D:253:LYS:CD	1.92	0.83
1:C:283:ARG:HB2	1:C:283:ARG:HH11	1.44	0.83
1:A:354:THR:HG22	1:A:357:ASP:H	1.44	0.82
1:B:237:GLU:HB3	1:B:240:LEU:HD12	1.61	0.82
1:C:556:ASN:HD22	1:C:559:VAL:H	1.26	0.82
1:D:114:LYS:HE2	1:D:115:MET:H	1.42	0.82
1:C:183:GLU:HA	1:C:186:ASN:ND2	1.94	0.82
1:C:224:PHE:HD2	1:C:225:LEU:HD23	1.43	0.82
1:D:675:GLU:O	1:D:675:GLU:HG2	1.79	0.82
1:B:244:LEU:HD22	1:B:248:LEU:HD22	1.62	0.82
1:C:301:VAL:O	1:C:302:MET:HG3	1.81	0.81
1:D:269:VAL:HG23	1:D:270:SER:N	1.94	0.81
1:C:399:ARG:HD2	1:C:402:GLN:HB2	1.62	0.81
1:D:536:ARG:HH11	1:D:536:ARG:H	1.22	0.81
1:D:95:GLU:CG	1:D:96:HIS:H	1.92	0.81
1:B:254:ILE:HD13	1:B:255:LYS:N	1.95	0.81
1:C:190:GLU:HA	1:C:193:HIS:CD2	2.15	0.81
1:C:556:ASN:ND2	1:C:559:VAL:H	1.79	0.81
1:D:113:LYS:O	1:D:114:LYS:HB2	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:TRP:HB2	1:C:648:LYS:NZ	1.96	0.81
1:D:298:ILE:CG1	1:D:380:ILE:HD11	2.11	0.81
1:C:370:LYS:HG2	1:C:372:GLU:H	1.45	0.81
1:B:155:ILE:HD13	1:B:528:THR:HG21	1.61	0.81
1:D:136:ASN:HB3	1:D:542:GLU:OE2	1.81	0.81
1:D:326:PHE:CD2	1:D:501:PRO:HG3	2.16	0.80
1:A:218:ARG:HA	1:A:230:ILE:HG22	1.61	0.80
1:C:283:ARG:HD3	1:C:283:ARG:N	1.96	0.80
1:D:204:TYR:HB2	1:D:368:TYR:O	1.81	0.80
1:D:226:GLU:OE2	1:D:293:LYS:HG2	1.81	0.80
1:B:229:ASN:O	1:B:233:VAL:HG23	1.82	0.80
1:B:570:GLN:HB3	1:B:573:THR:HG23	1.64	0.80
1:D:161:ASP:C	1:D:163:LYS:H	1.89	0.80
1:B:159:GLN:HE22	1:B:164:THR:HG21	1.48	0.79
1:C:155:ILE:CG1	1:C:266:LYS:HG2	2.12	0.79
1:C:283:ARG:HG2	1:C:285:ARG:NH2	1.97	0.79
1:B:309:GLN:HB2	1:B:310:PRO:HD3	1.65	0.79
1:C:272:ASP:HB3	1:C:279:VAL:HG11	1.65	0.79
1:C:163:LYS:O	1:C:167:GLU:HG3	1.82	0.78
1:C:165:PHE:C	1:C:165:PHE:CD2	2.59	0.78
1:B:146:ALA:HB1	1:B:627:THR:HG23	1.64	0.78
1:D:114:LYS:HA	1:D:114:LYS:HE3	1.65	0.78
1:D:135:TYR:OH	1:D:274:GLN:HG3	1.84	0.78
1:C:350:ASP:HB3	1:C:403:ARG:O	1.84	0.78
1:B:354:THR:HB	1:B:357:ASP:OD2	1.84	0.78
1:D:109:ASN:HD21	1:D:110:LEU:HD23	1.49	0.77
1:C:575:PRO:HG2	1:C:583:TYR:CZ	2.20	0.77
1:B:207:VAL:HG12	1:B:208:THR:N	1.98	0.77
1:C:199:THR:O	1:C:200:LEU:HB2	1.84	0.77
1:D:112:THR:HG23	1:D:113:LYS:H	1.49	0.77
1:B:648:LYS:HB2	1:B:661:TYR:HB2	1.67	0.77
1:C:645:TRP:HB2	1:C:648:LYS:HZ2	1.48	0.77
1:D:94:ARG:HD3	1:D:95:GLU:H	1.50	0.77
1:D:159:GLN:C	1:D:161:ASP:H	1.93	0.77
1:C:650:ASP:HB3	1:C:653:ILE:HB	1.67	0.77
1:D:114:LYS:HA	1:D:114:LYS:HE2	1.64	0.77
1:C:212:LEU:CD2	1:C:300:LYS:HB2	2.15	0.76
1:D:325:ILE:CG2	1:D:326:PHE:N	2.49	0.76
1:D:248:LEU:O	1:D:376:PHE:HA	1.84	0.76
1:A:538:THR:HG23	1:A:541:TYR:H	1.51	0.76
1:C:170:ARG:HB2	1:C:170:ARG:HH11	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLU:N	1:C:170:ARG:HH12	1.82	0.76
1:C:283:ARG:HB3	1:C:285:ARG:HE	1.49	0.76
1:D:210:GLU:H	1:D:210:GLU:CD	1.94	0.76
1:D:266:LYS:HD3	1:D:267:ARG:H	1.47	0.76
1:C:227:LYS:H	1:C:227:LYS:CD	1.99	0.76
1:C:592:LYS:HA	1:C:597:ARG:O	1.86	0.76
1:C:138:GLN:HE21	1:C:539:THR:CG2	1.99	0.75
1:C:374:HIS:C	1:C:376:PHE:H	1.95	0.75
1:D:184:LEU:C	1:D:184:LEU:HD12	2.11	0.75
1:A:355:SER:OG	1:A:385:THR:HG22	1.86	0.75
1:D:116:LEU:HD23	1:D:116:LEU:H	1.51	0.75
1:B:181:ASN:O	1:B:184:LEU:HB2	1.87	0.75
1:B:301:VAL:HG11	1:B:376:PHE:CE1	2.21	0.75
1:C:149:ARG:HG2	1:C:151:GLU:OE2	1.84	0.75
1:C:398:ILE:O	1:D:115:MET:HB3	1.86	0.75
1:B:175:LYS:CD	1:B:351:THR:HG23	2.16	0.75
1:A:178:ASN:ND2	1:A:352:GLN:HG3	2.01	0.75
1:D:533:SER:C	1:D:535:GLU:H	1.95	0.75
1:C:370:LYS:CG	1:C:371:LYS:N	2.49	0.74
1:A:336:PHE:HB2	1:A:339:PRO:HG3	1.69	0.74
1:B:336:PHE:CB	1:B:339:PRO:HG3	2.16	0.74
1:C:178:ASN:ND2	1:C:352:GLN:HG3	2.02	0.74
1:C:273:TRP:CD1	1:C:279:VAL:HG13	2.23	0.74
1:D:142:ILE:O	1:D:145:SER:HB3	1.87	0.74
1:C:312:VAL:HG11	1:C:368:TYR:HE2	1.52	0.74
1:D:233:VAL:HG12	1:D:234:LEU:N	2.00	0.74
1:D:247:ASP:HA	1:D:252:ARG:HH21	1.52	0.74
1:A:532:SER:C	1:A:534:GLY:H	1.92	0.74
1:C:143:MET:HE1	1:C:523:LEU:HB3	1.68	0.74
1:B:526:MET:HG3	1:B:549:PHE:CD2	2.22	0.74
1:C:154:PRO:HG3	1:C:620:LEU:HD23	1.70	0.74
1:C:422:MET:CE	1:C:470:LEU:HD21	2.18	0.74
1:A:175:LYS:HD3	1:A:351:THR:HG23	1.68	0.74
1:C:204:TYR:HB2	1:C:369:TYR:HA	1.69	0.74
1:C:325:ILE:HG23	1:C:326:PHE:N	1.98	0.73
1:D:155:ILE:HG21	1:D:528:THR:HG21	1.70	0.73
1:D:200:LEU:O	1:D:203:THR:HG23	1.87	0.73
1:D:309:GLN:HB3	1:D:310:PRO:CD	2.18	0.73
1:B:325:ILE:HG23	1:B:326:PHE:H	1.52	0.73
1:C:212:LEU:HD13	1:C:300:LYS:HA	1.70	0.73
1:D:558:LEU:O	1:D:559:VAL:HG23	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:HIS:O	1:D:674:TYR:CD1	2.40	0.73
1:D:229:ASN:H	1:D:229:ASN:ND2	1.86	0.73
1:B:222:ALA:O	1:B:226:GLU:HB3	1.89	0.73
1:D:95:GLU:HG3	1:D:96:HIS:N	2.01	0.72
1:A:196:ALA:O	1:A:198:PRO:HD3	1.89	0.72
1:A:104:ILE:HD11	1:A:118:PRO:HB2	1.71	0.72
1:B:570:GLN:HB3	1:B:573:THR:CG2	2.20	0.72
1:C:249:LYS:HA	1:C:376:PHE:HB2	1.70	0.72
1:D:94:ARG:CD	1:D:95:GLU:HG2	2.20	0.72
1:C:233:VAL:HG12	1:C:237:GLU:HB3	1.70	0.72
1:D:354:THR:HG22	1:D:355:SER:N	2.03	0.72
1:B:229:ASN:HD22	1:B:232:GLU:HB2	1.55	0.72
1:D:580:THR:HA	1:D:673:HIS:CB	2.14	0.72
1:B:133:ASN:H	1:B:536:ARG:NH1	1.88	0.72
1:B:366:LYS:HD3	1:B:378:ASP:OD1	1.90	0.72
1:D:204:TYR:CD1	1:D:368:TYR:HB3	2.23	0.72
1:D:452:LEU:O	1:D:452:LEU:HD23	1.89	0.72
1:D:325:ILE:HG22	1:D:326:PHE:H	1.55	0.71
1:A:609:LYS:O	1:A:613:LEU:HG	1.90	0.71
1:C:165:PHE:CD1	1:C:262:PRO:HG3	2.25	0.71
1:D:109:ASN:ND2	1:D:110:LEU:HD23	2.05	0.71
1:D:231:GLY:C	1:D:233:VAL:H	1.95	0.71
1:D:597:ARG:HH11	1:D:597:ARG:HG3	1.54	0.71
1:D:98:LYS:HB3	1:D:101:LEU:HD12	1.73	0.71
1:D:234:LEU:O	1:D:238:LYS:HG3	1.90	0.71
1:A:181:ASN:ND2	1:A:184:LEU:HB2	2.05	0.71
1:B:164:THR:HA	1:B:167:GLU:HG3	1.71	0.71
1:D:138:GLN:HE22	1:D:539:THR:HG23	1.55	0.71
1:D:541:TYR:O	1:D:545:VAL:HG23	1.90	0.71
1:A:310:PRO:O	1:A:312:VAL:HG13	1.91	0.71
1:D:325:ILE:CG2	1:D:326:PHE:H	2.03	0.71
1:A:648:LYS:O	1:A:654:SER:HB2	1.90	0.71
1:B:165:PHE:CD1	1:B:262:PRO:HB3	2.25	0.71
1:C:661:TYR:O	1:C:663:PRO:HD3	1.91	0.71
1:B:592:LYS:HD3	1:B:598:ASN:ND2	2.06	0.70
1:B:163:LYS:O	1:B:167:GLU:HG3	1.92	0.70
1:D:159:GLN:C	1:D:161:ASP:N	2.49	0.70
1:D:307:LYS:HD3	1:D:308:GLN:N	2.06	0.70
1:D:479:ILE:C	1:D:481:GLU:H	1.99	0.70
1:A:530:LEU:HD22	1:A:530:LEU:N	2.07	0.70
1:C:541:TYR:HA	1:C:576:SER:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:TRP:CD2	1:C:597:ARG:HD2	2.27	0.70
1:A:229:ASN:O	1:A:233:VAL:HG23	1.92	0.70
1:A:575:PRO:HG3	1:A:583:TYR:CZ	2.26	0.70
1:C:243:GLN:HE22	1:C:246:ARG:HD3	1.56	0.69
1:A:607:PHE:CD2	1:A:607:PHE:N	2.60	0.69
1:B:106:PHE:HE1	1:B:122:SER:HA	1.56	0.69
1:D:184:LEU:CD1	1:D:188:LEU:HG	2.22	0.69
1:D:380:ILE:O	1:D:384:MET:HG2	1.92	0.69
1:A:664:ASP:HB3	1:A:665:LYS:HD3	1.74	0.69
1:B:204:TYR:CD2	1:B:368:TYR:HB3	2.27	0.69
1:D:354:THR:HG22	1:D:356:LYS:H	1.57	0.69
1:C:366:LYS:HB3	1:C:374:HIS:NE2	2.07	0.69
1:D:209:TRP:HB2	1:D:210:GLU:CD	2.18	0.69
1:C:636:VAL:HG22	1:C:657:THR:HG23	1.72	0.69
1:D:93:ILE:HG12	1:D:116:LEU:HD12	1.74	0.69
1:A:200:LEU:O	1:A:203:THR:HG23	1.93	0.69
1:A:224:PHE:CE1	1:B:125:LEU:HD13	2.28	0.69
1:A:231:GLY:HA2	1:A:234:LEU:HD12	1.74	0.69
1:B:351:THR:HG22	1:B:352:GLN:NE2	2.08	0.69
1:C:336:PHE:CB	1:C:339:PRO:HG3	2.21	0.69
1:C:439:ARG:HB3	1:C:439:ARG:NH1	2.07	0.69
1:D:226:GLU:HG3	1:D:227:LYS:HZ3	1.57	0.69
1:C:370:LYS:HG3	1:C:372:GLU:H	1.58	0.68
1:D:112:THR:O	1:D:114:LYS:N	2.26	0.68
1:A:309:GLN:O	1:A:310:PRO:HG2	1.90	0.68
1:A:539:THR:O	1:A:543:LYS:HG3	1.93	0.68
1:B:592:LYS:HB2	1:B:598:ASN:ND2	2.06	0.68
1:D:266:LYS:CE	1:D:269:VAL:HG12	2.22	0.68
1:D:304:ASN:HB3	1:D:309:GLN:OE1	1.93	0.68
1:A:317:GLU:HG2	1:A:325:ILE:HD11	1.74	0.68
1:C:181:ASN:HD22	1:C:181:ASN:C	2.02	0.68
1:D:215:GLY:O	1:D:216:VAL:HG22	1.93	0.68
1:B:204:TYR:HB2	1:B:368:TYR:O	1.94	0.68
1:D:244:LEU:HD22	1:D:248:LEU:HD22	1.76	0.68
1:A:143:MET:O	1:A:148:ILE:HB	1.94	0.68
1:B:580:THR:HA	1:B:673:HIS:HB2	1.76	0.68
1:C:583:TYR:CZ	1:C:587:PRO:HG3	2.29	0.68
1:A:226:GLU:OE1	1:A:291:GLU:HG2	1.94	0.68
1:A:650:ASP:HB3	1:A:653:ILE:HB	1.76	0.68
1:B:298:ILE:HD13	1:B:380:ILE:HD11	1.76	0.68
1:C:93:ILE:HG21	1:D:398:ILE:HD13	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:HG11	1:C:368:TYR:CE2	2.28	0.68
1:C:620:LEU:N	1:C:620:LEU:HD12	2.09	0.68
1:D:126:ASP:HB3	1:D:130:ARG:O	1.94	0.68
1:C:244:LEU:O	1:C:248:LEU:HB2	1.94	0.67
1:C:430:THR:OG1	1:C:432:VAL:HG23	1.94	0.67
1:D:608:GLU:O	1:D:609:LYS:CB	2.42	0.67
1:C:178:ASN:HD21	1:C:352:GLN:HE21	1.42	0.67
1:D:215:GLY:O	1:D:216:VAL:HG13	1.94	0.67
1:B:221:ALA:O	1:B:295:ARG:NH2	2.24	0.67
1:C:361:ILE:HD11	1:C:417:LEU:HD13	1.76	0.67
1:B:229:ASN:ND2	1:B:232:GLU:HB2	2.09	0.67
1:D:109:ASN:HB3	1:D:273:TRP:NE1	2.09	0.67
1:D:204:TYR:HD1	1:D:368:TYR:HB3	1.60	0.67
1:D:94:ARG:HD3	1:D:95:GLU:N	2.10	0.67
1:D:304:ASN:HA	1:D:309:GLN:HG3	1.76	0.67
1:D:583:TYR:CE1	1:D:587:PRO:HG3	2.30	0.67
1:A:648:LYS:HA	1:A:648:LYS:NZ	2.09	0.67
1:B:325:ILE:HG23	1:B:326:PHE:N	2.10	0.67
1:C:213:GLU:O	1:C:215:GLY:N	2.28	0.67
1:C:283:ARG:HD3	1:C:283:ARG:H	1.58	0.67
1:C:159:GLN:HG3	1:C:281:GLU:HB2	1.77	0.67
1:A:347:LYS:HD3	1:A:478:LYS:HA	1.76	0.67
1:B:340:VAL:HG13	1:B:487:VAL:HG13	1.75	0.67
1:C:170:ARG:CD	1:D:111:ASN:ND2	2.57	0.67
1:D:298:ILE:CD1	1:D:380:ILE:HD11	2.25	0.67
1:A:146:ALA:HB1	1:A:627:THR:HG23	1.76	0.66
1:C:173:ILE:HD11	1:C:286:VAL:CG2	2.25	0.66
1:C:268:ASP:OD2	1:C:270:SER:HB2	1.95	0.66
1:D:307:LYS:HD3	1:D:307:LYS:C	2.20	0.66
1:B:153:LEU:O	1:B:155:ILE:HG22	1.95	0.66
1:C:159:GLN:N	1:C:282:LYS:O	2.29	0.66
1:C:167:GLU:CA	1:C:170:ARG:NH1	2.42	0.66
1:C:277:ASP:O	1:C:279:VAL:HG12	1.95	0.66
1:C:370:LYS:HE3	1:C:372:GLU:CD	2.20	0.66
1:D:157:ARG:HA	1:D:265:GLU:CG	2.25	0.66
1:D:229:ASN:HD22	1:D:229:ASN:N	1.87	0.66
1:A:309:GLN:CB	1:A:310:PRO:HD2	2.26	0.66
1:A:648:LYS:N	1:A:649:PRO:CD	2.58	0.66
1:C:212:LEU:HD22	1:C:300:LYS:CB	2.25	0.66
1:D:254:ILE:C	1:D:255:LYS:HE2	2.20	0.66
1:C:419:VAL:HG12	1:C:445:VAL:CG1	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HB3	1:B:524:SER:OG	1.96	0.66
1:C:239:HIS:CD2	1:C:239:HIS:H	2.13	0.66
1:C:354:THR:HB	1:C:357:ASP:OD1	1.94	0.66
1:C:354:THR:HG22	1:C:355:SER:N	2.09	0.66
1:D:112:THR:HG23	1:D:113:LYS:N	2.11	0.66
1:D:547:PHE:HZ	1:D:668:THR:HG22	1.60	0.66
1:B:298:ILE:CD1	1:B:380:ILE:HD11	2.25	0.66
1:C:159:GLN:CG	1:C:281:GLU:HB2	2.24	0.66
1:A:337:ASN:O	1:A:339:PRO:HD3	1.95	0.66
1:D:547:PHE:CZ	1:D:551:LEU:HD21	2.30	0.66
1:A:311:VAL:CG2	1:A:319:LYS:HD2	2.18	0.66
1:B:506:TRP:CD2	1:B:597:ARG:HD2	2.30	0.66
1:C:479:ILE:N	1:C:479:ILE:HD12	2.10	0.66
1:A:147:GLY:HA3	1:A:624:THR:CG2	2.21	0.65
1:C:355:SER:HB3	1:C:385:THR:HG23	1.78	0.65
1:C:165:PHE:C	1:C:165:PHE:HD2	2.02	0.65
1:C:282:LYS:HG2	1:C:283:ARG:H	1.60	0.65
1:C:578:HIS:O	1:C:672:LYS:HB3	1.96	0.65
1:C:642:GLU:HA	1:C:659:HIS:HE2	1.60	0.65
1:B:560:ARG:HD2	1:B:599:LEU:HD21	1.76	0.65
1:B:330:ARG:HD3	1:B:513:HIS:CE1	2.31	0.65
1:D:258:GLU:HG2	1:D:290:PRO:HG3	1.78	0.65
1:B:153:LEU:HD13	1:B:524:SER:HA	1.78	0.65
1:D:254:ILE:HG22	1:D:383:HIS:HE2	1.61	0.65
1:B:274:GLN:HE21	1:B:619:THR:HG21	1.62	0.65
1:C:301:VAL:O	1:C:301:VAL:HG22	1.96	0.65
1:D:380:ILE:HG22	1:D:381:THR:N	2.11	0.65
1:C:422:MET:HE1	1:C:470:LEU:HD21	1.79	0.65
1:C:557:PRO:HD2	1:C:610:LEU:HD21	1.79	0.65
1:C:560:ARG:HD2	1:C:599:LEU:HD21	1.77	0.65
1:A:118:PRO:HG2	1:B:398:ILE:CD1	2.25	0.65
1:A:592:LYS:HA	1:A:597:ARG:O	1.96	0.65
1:C:322:LEU:O	1:C:325:ILE:HG22	1.97	0.65
1:D:233:VAL:CG1	1:D:234:LEU:N	2.60	0.65
1:D:325:ILE:HG23	1:D:326:PHE:N	2.11	0.65
1:D:575:PRO:HG3	1:D:583:TYR:CZ	2.31	0.65
1:C:376:PHE:O	1:C:380:ILE:HG22	1.97	0.65
1:D:536:ARG:H	1:D:536:ARG:NH1	1.94	0.65
1:C:362:GLY:O	1:C:365:GLN:HB2	1.97	0.64
1:C:470:LEU:HD13	1:C:477:GLN:NE2	2.12	0.64
1:D:116:LEU:C	1:D:118:PRO:HD3	2.21	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ILE:HD11	1:D:416:MET:HE1	1.79	0.64
1:D:482:GLY:O	1:D:484:LYS:N	2.29	0.64
1:C:637:ALA:O	1:C:640:LYS:HG2	1.98	0.64
1:D:127:ARG:HD3	1:D:127:ARG:O	1.96	0.64
1:A:116:LEU:O	1:A:118:PRO:HD3	1.97	0.64
1:C:230:ILE:HG23	1:C:296:LEU:HD22	1.77	0.64
1:C:439:ARG:HB3	1:C:439:ARG:HH11	1.63	0.64
1:C:517:ARG:C	1:C:613:LEU:HD22	2.22	0.64
1:D:465:LYS:O	1:D:469:ILE:HG13	1.97	0.64
1:A:159:GLN:OE1	1:A:164:THR:HG21	1.97	0.64
1:A:270:SER:O	1:A:274:GLN:HB2	1.97	0.64
1:D:556:ASN:C	1:D:556:ASN:HD22	2.06	0.64
1:C:283:ARG:HB3	1:C:285:ARG:NE	2.12	0.64
1:C:309:GLN:O	1:C:310:PRO:C	2.41	0.64
1:C:325:ILE:CG2	1:C:326:PHE:H	2.08	0.64
1:C:342:VAL:HB	1:C:452:LEU:CD2	2.28	0.64
1:C:648:LYS:C	1:C:650:ASP:H	2.06	0.64
1:D:165:PHE:CD1	1:D:262:PRO:HG3	2.32	0.64
1:C:106:PHE:HE1	1:C:122:SER:HA	1.63	0.64
1:D:419:VAL:HG23	1:D:420:LEU:N	2.13	0.64
1:A:163:LYS:O	1:A:167:GLU:HG3	1.98	0.64
1:A:224:PHE:O	1:B:131:LYS:HD3	1.97	0.64
1:B:584:LYS:HB2	1:B:669:LEU:HD11	1.80	0.64
1:C:570:GLN:C	1:C:572:GLU:H	2.06	0.64
1:A:118:PRO:CG	1:B:398:ILE:HD13	2.26	0.64
1:A:519:THR:HA	1:A:522:ILE:HD12	1.79	0.64
1:C:115:MET:HG3	1:D:174:ASP:HA	1.79	0.64
1:D:297:ALA:O	1:D:301:VAL:HG23	1.98	0.64
1:A:648:LYS:HA	1:A:648:LYS:HZ3	1.62	0.63
1:A:670:GLN:CD	1:A:673:HIS:HE2	2.05	0.63
1:C:570:GLN:OE1	1:C:573:THR:HG21	1.98	0.63
1:D:553:TYR:HA	1:D:555:TRP:CD1	2.32	0.63
1:B:237:GLU:CB	1:B:240:LEU:HD12	2.28	0.63
1:C:234:LEU:O	1:C:238:LYS:HE3	1.99	0.63
1:C:580:THR:HA	1:C:673:HIS:HB2	1.80	0.63
1:D:218:ARG:HG2	1:D:231:GLY:HA3	1.81	0.63
1:A:532:SER:C	1:A:534:GLY:N	2.56	0.63
1:A:635:CYS:CB	1:A:653:ILE:HG12	2.29	0.63
1:B:349:TRP:CZ3	1:B:475:LYS:HD2	2.34	0.63
1:C:519:THR:HG21	1:C:617:LEU:HD11	1.81	0.63
1:D:109:ASN:O	1:D:117:ASN:ND2	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HD13	1:A:118:PRO:C	2.24	0.63
1:B:380:ILE:O	1:B:384:MET:HG3	1.98	0.63
1:C:167:GLU:N	1:C:170:ARG:NH1	2.45	0.63
1:A:351:THR:HG22	1:A:352:GLN:NE2	2.13	0.63
1:C:392:ALA:HB1	1:D:125:LEU:HB3	1.80	0.63
1:A:237:GLU:CB	1:A:240:LEU:HD12	2.27	0.63
1:A:648:LYS:N	1:A:649:PRO:HD3	2.13	0.63
1:B:648:LYS:C	1:B:650:ASP:N	2.57	0.63
1:C:583:TYR:CE1	1:C:587:PRO:HG3	2.33	0.63
1:C:599:LEU:HB3	1:C:649:PRO:HB3	1.81	0.63
1:D:227:LYS:HD3	1:D:228:LYS:HD2	1.80	0.63
1:D:519:THR:HG21	1:D:617:LEU:HD11	1.80	0.63
1:A:127:ARG:CB	1:A:127:ARG:HH11	2.12	0.63
1:A:155:ILE:HD13	1:A:528:THR:HG21	1.80	0.63
1:C:123:GLU:OE1	1:C:131:LYS:HE3	1.98	0.63
1:D:93:ILE:HG22	1:D:94:ARG:H	1.64	0.63
1:D:153:LEU:HD13	1:D:524:SER:HA	1.80	0.63
1:D:159:GLN:O	1:D:161:ASP:N	2.29	0.63
1:C:183:GLU:O	1:C:184:LEU:C	2.41	0.62
1:D:326:PHE:CG	1:D:501:PRO:HG3	2.34	0.62
1:A:598:ASN:HB2	1:A:601:GLU:OE2	1.97	0.62
1:B:648:LYS:O	1:B:650:ASP:N	2.33	0.62
1:B:191:ILE:HA	1:B:194:THR:HG23	1.81	0.62
1:B:348:ALA:O	1:B:351:THR:HB	2.00	0.62
1:D:536:ARG:N	1:D:536:ARG:NH1	2.46	0.62
1:C:169:ILE:C	1:C:171:ASP:H	2.07	0.62
1:D:200:LEU:C	1:D:203:THR:HG23	2.25	0.62
1:A:648:LYS:HZ3	1:A:653:ILE:HG22	1.63	0.62
1:A:352:GLN:HG2	1:A:476:PRO:CD	2.30	0.62
1:B:208:THR:HB	1:B:210:GLU:CD	2.24	0.62
1:D:258:GLU:OE2	1:D:399:ARG:NH2	2.31	0.62
1:C:153:LEU:O	1:C:154:PRO:C	2.43	0.62
1:B:132:ARG:HA	1:B:536:ARG:NH2	2.15	0.62
1:C:138:GLN:HB2	1:C:542:GLU:OE2	1.99	0.62
1:C:354:THR:CG2	1:C:355:SER:N	2.62	0.62
1:C:366:LYS:HB3	1:C:374:HIS:CD2	2.35	0.62
1:C:419:VAL:HG12	1:C:445:VAL:HG11	1.82	0.62
1:A:149:ARG:HB2	1:A:152:LYS:HG2	1.82	0.62
1:B:164:THR:HA	1:B:167:GLU:CG	2.29	0.62
1:B:535:GLU:HG2	1:B:537:GLY:H	1.64	0.62
1:D:244:LEU:O	1:D:248:LEU:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:ASN:HB2	1:D:601:GLU:OE2	1.99	0.62
1:B:210:GLU:OE1	1:B:210:GLU:N	2.33	0.62
1:C:181:ASN:C	1:C:181:ASN:ND2	2.57	0.62
1:D:148:ILE:HA	1:D:622:VAL:O	2.00	0.62
1:D:506:TRP:CD2	1:D:597:ARG:HD2	2.35	0.62
1:B:648:LYS:CE	1:B:657:THR:OG1	2.47	0.61
1:D:112:THR:C	1:D:114:LYS:H	2.08	0.61
1:D:114:LYS:CE	1:D:115:MET:HE2	2.30	0.61
1:A:648:LYS:HD3	1:A:659:HIS:HB2	1.82	0.61
1:D:349:TRP:CZ2	1:D:417:LEU:HD23	2.34	0.61
1:B:207:VAL:CG1	1:B:208:THR:H	2.07	0.61
1:C:636:VAL:HG12	1:C:637:ALA:N	2.14	0.61
1:A:610:LEU:HD13	1:A:614:ASN:ND2	2.15	0.61
1:B:530:LEU:HD22	1:B:530:LEU:N	2.15	0.61
1:C:165:PHE:O	1:C:166:HIS:C	2.43	0.61
1:C:446:CYS:HB2	1:C:496:PHE:CE1	2.36	0.61
1:A:258:GLU:O	1:A:389:VAL:HA	1.99	0.61
1:C:163:LYS:HG2	1:C:167:GLU:OE2	2.00	0.61
1:C:173:ILE:O	1:C:175:LYS:N	2.29	0.61
1:C:218:ARG:HA	1:C:230:ILE:O	2.00	0.61
1:D:184:LEU:HD12	1:D:185:HIS:N	2.16	0.61
1:A:452:LEU:O	1:A:452:LEU:HD23	2.01	0.61
1:C:368:TYR:O	1:C:369:TYR:C	2.43	0.61
1:D:212:LEU:CD1	1:D:299:THR:HG22	2.30	0.61
1:A:244:LEU:HD22	1:A:248:LEU:CD2	2.30	0.61
1:A:302:MET:HA	1:A:369:TYR:OH	2.01	0.61
1:D:612:ASN:HA	1:D:615:LEU:HD12	1.82	0.61
1:B:149:ARG:HB2	1:B:152:LYS:HG2	1.81	0.61
1:C:370:LYS:CD	1:C:372:GLU:HB3	2.30	0.61
1:D:184:LEU:HD13	1:D:188:LEU:HG	1.83	0.61
1:D:341:ALA:HB3	1:D:488:ALA:HB3	1.82	0.61
1:D:470:LEU:O	1:D:473:ALA:HB3	2.01	0.61
1:A:309:GLN:O	1:A:310:PRO:CG	2.49	0.61
1:A:490:ARG:HB3	1:A:492:GLU:OE1	2.01	0.61
1:B:298:ILE:HG12	1:B:380:ILE:HD12	1.81	0.61
1:A:208:THR:HB	1:A:210:GLU:OE2	2.00	0.61
1:C:106:PHE:HB3	1:C:151:GLU:OE1	2.01	0.61
1:C:233:VAL:CG1	1:C:237:GLU:HB3	2.29	0.61
1:C:556:ASN:ND2	1:C:559:VAL:HG23	2.16	0.61
1:D:157:ARG:HA	1:D:265:GLU:HG3	1.83	0.61
1:C:354:THR:HG22	1:C:356:LYS:H	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TRP:O	1:A:648:LYS:HG2	2.01	0.60
1:D:380:ILE:CG2	1:D:381:THR:N	2.64	0.60
1:C:330:ARG:HH11	1:C:513:HIS:HE1	1.50	0.60
1:C:344:PHE:CE1	1:C:422:MET:HG3	2.36	0.60
1:D:93:ILE:CG1	1:D:116:LEU:HD12	2.30	0.60
1:D:173:ILE:HD13	1:D:288:GLN:NE2	2.16	0.60
1:D:212:LEU:HD11	1:D:299:THR:HG22	1.84	0.60
1:A:181:ASN:HD21	1:A:184:LEU:HG	1.66	0.60
1:A:249:LYS:HE3	1:A:373:TRP:CZ3	2.37	0.60
1:A:341:ALA:HB3	1:A:488:ALA:HB3	1.82	0.60
1:A:492:GLU:CD	1:A:492:GLU:H	2.10	0.60
1:B:207:VAL:HG21	1:B:303:TYR:HB3	1.83	0.60
1:C:143:MET:O	1:C:148:ILE:HB	2.00	0.60
1:C:172:LYS:HE3	1:C:285:ARG:HG2	1.83	0.60
1:C:369:TYR:O	1:C:370:LYS:HB3	2.01	0.60
1:B:322:LEU:HB3	1:B:552:MET:HE1	1.84	0.60
1:B:556:ASN:HD22	1:B:556:ASN:C	2.10	0.60
1:C:421:THR:O	1:C:424:TYR:HB3	2.01	0.60
1:A:317:GLU:HG2	1:A:325:ILE:CD1	2.31	0.60
1:B:648:LYS:C	1:B:650:ASP:H	2.07	0.60
1:C:541:TYR:HA	1:C:576:SER:CB	2.31	0.60
1:D:506:TRP:HE1	1:D:512:SER:HB3	1.66	0.60
1:A:209:TRP:CD2	1:A:238:LYS:HE2	2.36	0.60
1:A:482:GLY:O	1:A:484:LYS:HG2	2.02	0.60
1:C:178:ASN:ND2	1:C:352:GLN:HA	2.16	0.60
1:C:231:GLY:HA2	1:C:234:LEU:CB	2.30	0.60
1:A:302:MET:HE3	1:A:377:ILE:HG12	1.84	0.60
1:B:132:ARG:HA	1:B:536:ARG:HH22	1.65	0.60
1:C:161:ASP:O	1:C:164:THR:N	2.35	0.60
1:C:300:LYS:C	1:C:302:MET:H	2.10	0.60
1:C:518:ASP:O	1:C:522:ILE:HG13	2.01	0.60
1:C:636:VAL:O	1:C:637:ALA:C	2.44	0.60
1:D:213:GLU:C	1:D:215:GLY:H	2.10	0.60
1:B:298:ILE:HG12	1:B:380:ILE:CD1	2.31	0.60
1:B:641:GLU:HG3	1:B:645:TRP:HE1	1.65	0.60
1:C:390:ILE:HD11	1:D:100:ILE:HD11	1.84	0.60
1:A:146:ALA:CB	1:A:627:THR:HG23	2.32	0.59
1:A:592:LYS:HD3	1:A:598:ASN:ND2	2.17	0.59
1:B:646:LEU:O	1:B:649:PRO:HD2	2.01	0.59
1:C:422:MET:HA	1:C:422:MET:CE	2.27	0.59
1:B:526:MET:HG3	1:B:549:PHE:CE2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:GLN:O	1:C:572:GLU:N	2.33	0.59
1:D:249:LYS:HD2	1:D:373:TRP:CH2	2.37	0.59
1:B:220:GLY:O	1:B:229:ASN:HB2	2.01	0.59
1:C:146:ALA:HA	1:C:630:ARG:HD2	1.84	0.59
1:A:497:CYS:O	1:A:498:SER:HB2	2.02	0.59
1:B:415:SER:O	1:B:419:VAL:HG13	2.02	0.59
1:B:673:HIS:O	1:B:674:TYR:O	2.20	0.59
1:C:162:THR:HB	1:D:276:GLY:C	2.28	0.59
1:D:147:GLY:HA3	1:D:627:THR:OG1	2.01	0.59
1:D:154:PRO:HG3	1:D:620:LEU:HD13	1.84	0.59
1:D:264:ASN:H	1:D:264:ASN:ND2	1.95	0.59
1:A:302:MET:CE	1:A:377:ILE:HG12	2.32	0.59
1:C:650:ASP:OD2	1:C:653:ILE:HD13	2.03	0.59
1:D:590:ALA:O	1:D:593:ASP:HB3	2.02	0.59
1:B:185:HIS:HE1	1:B:357:ASP:OD1	1.86	0.59
1:B:187:LYS:HD2	1:B:424:TYR:HE1	1.67	0.59
1:C:357:ASP:O	1:C:361:ILE:HD13	2.01	0.59
1:D:93:ILE:HG22	1:D:94:ARG:N	2.18	0.59
1:D:116:LEU:O	1:D:118:PRO:HD3	2.02	0.59
1:D:267:ARG:NH1	1:D:285:ARG:HH12	2.00	0.59
1:C:189:LEU:O	1:C:192:PHE:HB3	2.03	0.59
1:D:646:LEU:O	1:D:649:PRO:HD2	2.03	0.59
1:B:556:ASN:CG	1:B:559:VAL:HG23	2.28	0.59
1:A:108:GLY:N	1:A:119:GLY:HA2	2.18	0.59
1:C:230:ILE:HD11	1:C:295:ARG:CZ	2.33	0.59
1:C:365:GLN:C	1:C:367:TYR:H	2.10	0.59
1:D:226:GLU:HG3	1:D:227:LYS:NZ	2.17	0.59
1:D:263:LYS:HB2	1:D:287:ILE:HD12	1.84	0.59
1:D:594:VAL:HG11	1:D:668:THR:OG1	2.02	0.59
1:A:149:ARG:NH1	1:A:621:GLY:O	2.36	0.59
1:C:181:ASN:HD21	1:C:184:LEU:H	1.50	0.59
1:D:241:VAL:O	1:D:245:VAL:HG23	2.03	0.59
1:A:116:LEU:C	1:A:118:PRO:HD3	2.28	0.58
1:B:154:PRO:CG	1:B:620:LEU:HD13	2.31	0.58
1:B:139:ILE:O	1:B:143:MET:HG3	2.03	0.58
1:C:253:LYS:CE	1:D:96:HIS:HB2	2.33	0.58
1:C:648:LYS:C	1:C:650:ASP:N	2.59	0.58
1:D:561:ARG:HE	1:D:650:ASP:CG	2.11	0.58
1:D:309:GLN:CB	1:D:310:PRO:CD	2.82	0.58
1:D:517:ARG:C	1:D:613:LEU:HD22	2.28	0.58
1:A:154:PRO:HG3	1:A:620:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASN:C	1:A:556:ASN:HD22	2.11	0.58
1:C:99:TRP:CD2	1:D:255:LYS:HG3	2.39	0.58
1:D:142:ILE:HD13	1:D:565:LEU:HB3	1.86	0.58
1:D:230:ILE:HA	1:D:233:VAL:HB	1.85	0.58
1:A:200:LEU:C	1:A:203:THR:HG23	2.29	0.58
1:A:230:ILE:HG12	1:A:296:LEU:HD11	1.85	0.58
1:A:400:ASN:O	1:A:401:GLY:O	2.22	0.58
1:C:181:ASN:ND2	1:C:184:LEU:H	2.01	0.58
1:D:254:ILE:HG22	1:D:383:HIS:NE2	2.18	0.58
1:D:354:THR:CG2	1:D:355:SER:N	2.66	0.58
1:B:661:TYR:O	1:B:663:PRO:HD3	2.04	0.58
1:C:204:TYR:CD2	1:C:368:TYR:HB3	2.32	0.58
1:D:469:ILE:O	1:D:473:ALA:HB2	2.04	0.58
1:C:222:ALA:HB1	1:C:226:GLU:HG2	1.86	0.58
1:C:501:PRO:O	1:C:609:LYS:HE2	2.04	0.58
1:A:218:ARG:O	1:A:230:ILE:O	2.21	0.58
1:B:127:ARG:O	1:B:127:ARG:HG2	2.04	0.58
1:B:183:GLU:HB2	1:B:187:LYS:HE3	1.84	0.58
1:B:206:GLU:HB2	1:B:373:TRP:CZ2	2.38	0.58
1:B:301:VAL:HG22	1:B:302:MET:HG3	1.84	0.58
1:C:430:THR:HA	1:C:461:LYS:HD3	1.85	0.58
1:C:652:LEU:HD11	1:C:656:LYS:HE2	1.86	0.58
1:D:209:TRP:HB2	1:D:210:GLU:OE2	2.04	0.58
1:D:541:TYR:HA	1:D:576:SER:HB3	1.86	0.58
1:D:558:LEU:HD22	1:D:631:ILE:HD12	1.85	0.58
1:A:535:GLU:O	1:A:536:ARG:HB2	2.03	0.58
1:C:170:ARG:HH11	1:C:170:ARG:CB	2.16	0.58
1:C:151:GLU:HG2	1:C:151:GLU:O	2.04	0.58
1:D:344:PHE:CE1	1:D:422:MET:HG3	2.39	0.58
1:D:583:TYR:CZ	1:D:587:PRO:HG3	2.39	0.58
1:B:132:ARG:HB3	1:B:536:ARG:HH22	1.69	0.57
1:C:202:HIS:ND1	1:C:370:LYS:HA	2.18	0.57
1:C:282:LYS:HG2	1:C:283:ARG:N	2.18	0.57
1:C:395:GLU:OE2	1:D:120:LYS:HB2	2.03	0.57
1:C:480:THR:HG22	1:C:481:GLU:H	1.69	0.57
1:D:218:ARG:HG2	1:D:218:ARG:HH11	1.69	0.57
1:A:536:ARG:HH11	1:A:536:ARG:HA	1.69	0.57
1:B:398:ILE:O	1:B:398:ILE:HG22	2.02	0.57
1:B:583:TYR:CZ	1:B:587:PRO:HG3	2.39	0.57
1:C:292:ALA:HA	1:C:295:ARG:HE	1.67	0.57
1:C:480:THR:HG22	1:C:481:GLU:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LYS:HE2	1:D:115:MET:N	2.16	0.57
1:A:146:ALA:HA	1:A:630:ARG:HD3	1.85	0.57
1:A:583:TYR:CZ	1:A:587:PRO:HG3	2.39	0.57
1:C:529:ARG:C	1:C:530:LEU:HG	2.30	0.57
1:D:230:ILE:CG1	1:D:292:ALA:HB1	2.34	0.57
1:D:316:TYR:HA	1:D:445:VAL:HG12	1.85	0.57
1:D:363:GLU:O	1:D:366:LYS:N	2.38	0.57
1:A:648:LYS:NZ	1:A:654:SER:HA	2.20	0.57
1:C:236:SER:O	1:C:237:GLU:CB	2.49	0.57
1:C:204:TYR:CB	1:C:369:TYR:HA	2.35	0.57
1:D:152:LYS:HD3	1:D:620:LEU:O	2.02	0.57
1:D:212:LEU:O	1:D:215:GLY:O	2.23	0.57
1:D:231:GLY:C	1:D:233:VAL:N	2.61	0.57
1:C:184:LEU:O	1:C:188:LEU:HG	2.04	0.57
1:C:211:GLN:HA	1:C:214:ALA:HB2	1.87	0.57
1:C:610:LEU:O	1:C:614:ASN:HB2	2.05	0.57
1:D:635:CYS:HB3	1:D:653:ILE:HD12	1.87	0.57
1:A:106:PHE:HB3	1:A:151:GLU:OE2	2.05	0.57
1:A:192:PHE:CZ	1:A:364:ILE:HG23	2.40	0.57
1:B:148:ILE:HA	1:B:622:VAL:O	2.05	0.57
1:B:209:TRP:N	1:B:210:GLU:OE1	2.36	0.57
1:B:228:LYS:HD2	1:B:237:GLU:OE1	2.04	0.57
1:B:313:ILE:HG12	1:B:416:MET:HE2	1.85	0.57
1:C:105:ARG:HB2	1:C:106:PHE:CE1	2.39	0.57
1:B:639:GLY:HA2	1:B:645:TRP:CD1	2.40	0.57
1:C:143:MET:HE3	1:C:523:LEU:HD22	1.87	0.57
1:D:401:GLY:O	1:D:402:GLN:HG3	2.04	0.57
1:A:583:TYR:CE1	1:A:587:PRO:HG3	2.40	0.57
1:B:555:TRP:CH2	1:B:613:LEU:HD13	2.40	0.57
1:C:249:LYS:NZ	1:C:372:GLU:HG3	2.19	0.57
1:C:348:ALA:O	1:C:351:THR:HB	2.04	0.57
1:C:384:MET:HA	1:C:387:VAL:CG2	2.35	0.57
1:D:404:GLY:O	1:D:406:GLY:N	2.36	0.57
1:C:241:VAL:HG13	1:C:297:ALA:HB2	1.87	0.57
1:D:347:LYS:O	1:D:352:GLN:NE2	2.37	0.57
1:A:635:CYS:HB3	1:A:653:ILE:HG12	1.85	0.56
1:B:541:TYR:HA	1:B:576:SER:HB3	1.86	0.56
1:D:360:LEU:HD12	1:D:360:LEU:O	2.05	0.56
1:B:653:ILE:O	1:B:657:THR:HG23	2.06	0.56
1:C:100:ILE:O	1:C:102:LYS:N	2.38	0.56
1:C:165:PHE:C	1:C:167:GLU:N	2.60	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ARG:CD	1:C:402:GLN:HB2	2.35	0.56
1:C:561:ARG:HH12	1:C:632:ILE:HD11	1.70	0.56
1:C:575:PRO:HG2	1:C:583:TYR:CE2	2.39	0.56
1:D:307:LYS:HZ1	1:D:319:LYS:CG	2.16	0.56
1:A:185:HIS:HE1	1:A:357:ASP:OD1	1.88	0.56
1:A:244:LEU:HD22	1:A:248:LEU:HD21	1.87	0.56
1:A:272:ASP:O	1:A:275:ALA:O	2.23	0.56
1:C:187:LYS:O	1:C:190:GLU:N	2.38	0.56
1:C:198:PRO:O	1:C:201:LYS:HB3	2.05	0.56
1:C:556:ASN:HD22	1:C:559:VAL:N	2.01	0.56
1:C:642:GLU:HA	1:C:659:HIS:NE2	2.20	0.56
1:D:112:THR:C	1:D:114:LYS:N	2.62	0.56
1:D:506:TRP:CE3	1:D:597:ARG:HD2	2.40	0.56
1:D:650:ASP:O	1:D:651:ARG:C	2.48	0.56
1:A:551:LEU:HD22	1:A:594:VAL:HG21	1.88	0.56
1:B:206:GLU:HA	1:B:301:VAL:HA	1.87	0.56
1:D:94:ARG:HD2	1:D:95:GLU:CG	2.31	0.56
1:D:124:GLN:NE2	1:D:275:ALA:HB2	2.21	0.56
1:D:211:GLN:O	1:D:211:GLN:CG	2.49	0.56
1:B:253:LYS:H	1:B:253:LYS:CD	1.97	0.56
1:C:350:ASP:OD2	1:C:403:ARG:HG3	2.05	0.56
1:A:347:LYS:HD3	1:A:478:LYS:CA	2.35	0.56
1:B:212:LEU:HD22	1:B:300:LYS:HB2	1.88	0.56
1:C:352:GLN:CG	1:C:476:PRO:HD2	2.28	0.56
1:C:581:TYR:HD2	1:C:670:GLN:HA	1.70	0.56
1:A:204:TYR:CD2	1:A:368:TYR:HB3	2.40	0.56
1:A:254:ILE:CG2	1:A:383:HIS:NE2	2.69	0.56
1:B:236:SER:O	1:B:238:LYS:N	2.35	0.56
1:C:322:LEU:HD22	1:C:515:ALA:CB	2.35	0.56
1:C:430:THR:HB	1:C:458:LEU:HD22	1.87	0.56
1:D:555:TRP:CH2	1:D:613:LEU:HD13	2.40	0.56
1:B:352:GLN:HG2	1:B:476:PRO:HD2	1.87	0.56
1:A:178:ASN:HD21	1:A:352:GLN:HG3	1.68	0.56
1:A:254:ILE:HG22	1:A:383:HIS:NE2	2.21	0.56
1:A:430:THR:OG1	1:A:432:VAL:HG23	2.04	0.56
1:C:99:TRP:CH2	1:C:100:ILE:HD13	2.40	0.56
1:C:159:GLN:HG3	1:C:281:GLU:CB	2.35	0.56
1:C:502:VAL:HG23	1:C:516:GLY:HA3	1.87	0.56
1:D:533:SER:C	1:D:535:GLU:N	2.64	0.56
1:A:508:ASP:O	1:A:510:THR:HG23	2.06	0.56
1:C:334:ASP:C	1:C:336:PHE:H	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASN:CG	1:D:110:LEU:N	2.63	0.56
1:D:553:TYR:HD2	1:D:555:TRP:HE1	1.52	0.56
1:A:311:VAL:HG21	1:A:319:LYS:CD	2.19	0.55
1:A:313:ILE:HB	1:A:316:TYR:HB2	1.88	0.55
1:B:143:MET:O	1:B:148:ILE:HB	2.06	0.55
1:C:302:MET:HA	1:C:369:TYR:CZ	2.41	0.55
1:D:208:THR:O	1:D:209:TRP:C	2.48	0.55
1:A:237:GLU:O	1:A:240:LEU:HB2	2.07	0.55
1:A:268:ASP:OD2	1:A:270:SER:HB2	2.06	0.55
1:B:436:SER:O	1:B:439:ARG:HB2	2.05	0.55
1:C:302:MET:HE3	1:C:377:ILE:HG12	1.88	0.55
1:C:322:LEU:HD12	1:C:552:MET:HE3	1.87	0.55
1:C:416:MET:O	1:C:420:LEU:HG	2.06	0.55
1:C:639:GLY:HA3	1:C:648:LYS:HE3	1.88	0.55
1:D:231:GLY:HA2	1:D:234:LEU:HD12	1.87	0.55
1:A:138:GLN:HG3	1:A:539:THR:HG22	1.88	0.55
1:B:586:ASP:HB3	1:B:664:ASP:O	2.06	0.55
1:C:239:HIS:CD2	1:C:239:HIS:N	2.74	0.55
1:C:356:LYS:HA	1:C:359:GLN:OE1	2.06	0.55
1:C:591:TYR:CE1	1:C:595:ILE:HG13	2.42	0.55
1:D:157:ARG:HA	1:D:265:GLU:HG2	1.88	0.55
1:D:309:GLN:CB	1:D:310:PRO:HD3	2.29	0.55
1:C:99:TRP:CG	1:D:255:LYS:HG3	2.41	0.55
1:D:138:GLN:HE22	1:D:539:THR:CG2	2.19	0.55
1:D:283:ARG:HG3	1:D:283:ARG:O	2.05	0.55
1:B:317:GLU:HG3	1:B:317:GLU:O	2.07	0.55
1:C:127:ARG:HH22	1:D:261:ILE:HD12	1.70	0.55
1:C:426:PHE:HA	1:C:462:PHE:CD1	2.42	0.55
1:D:106:PHE:CE2	1:D:150:LEU:HB2	2.41	0.55
1:A:589:GLY:O	1:A:592:LYS:HB3	2.05	0.55
1:D:355:SER:O	1:D:359:GLN:HG3	2.06	0.55
1:B:615:LEU:O	1:B:616:SER:C	2.50	0.55
1:D:114:LYS:HE2	1:D:115:MET:HE2	1.89	0.55
1:D:253:LYS:HD3	1:D:253:LYS:N	2.04	0.55
1:A:639:GLY:O	1:A:657:THR:HB	2.07	0.55
1:B:166:HIS:HE2	1:B:393:ASP:CG	2.15	0.55
1:B:191:ILE:HG12	1:B:434:TYR:CG	2.42	0.55
1:C:179:ARG:H	1:C:179:ARG:CD	2.06	0.55
1:C:337:ASN:C	1:C:339:PRO:HD3	2.32	0.55
1:C:507:SER:HB3	1:C:651:ARG:HH21	1.72	0.55
1:D:168:ALA:HB2	1:D:284:PRO:HD2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:HD22	1:A:229:ASN:C	2.14	0.55
1:C:216:VAL:HG23	1:C:217:ASN:N	2.22	0.55
1:D:535:GLU:HG3	1:D:541:TYR:CE1	2.42	0.55
1:B:212:LEU:HD22	1:B:300:LYS:CB	2.37	0.55
1:C:211:GLN:O	1:C:214:ALA:N	2.37	0.55
1:C:332:GLU:HB3	1:C:442:ARG:HG3	1.89	0.55
1:D:329:VAL:HG12	1:D:491:PHE:HE2	1.72	0.55
1:B:218:ARG:HA	1:B:230:ILE:HG22	1.89	0.54
1:C:155:ILE:HG12	1:C:266:LYS:HG2	1.89	0.54
1:C:305:TRP:HB2	1:C:369:TYR:HE1	1.72	0.54
1:C:369:TYR:O	1:C:370:LYS:CB	2.56	0.54
1:C:531:ASP:N	1:C:536:ARG:O	2.35	0.54
1:D:231:GLY:HA2	1:D:234:LEU:CD1	2.38	0.54
1:D:648:LYS:C	1:D:650:ASP:H	2.13	0.54
1:C:165:PHE:O	1:C:168:ALA:N	2.28	0.54
1:C:273:TRP:HD1	1:C:279:VAL:HG13	1.66	0.54
1:C:446:CYS:HB2	1:C:496:PHE:CZ	2.43	0.54
1:C:575:PRO:CG	1:C:583:TYR:CZ	2.89	0.54
1:D:249:LYS:HD2	1:D:373:TRP:CZ3	2.42	0.54
1:D:419:VAL:HG23	1:D:420:LEU:H	1.71	0.54
1:D:533:SER:O	1:D:535:GLU:N	2.40	0.54
1:A:275:ALA:O	1:A:277:ASP:N	2.40	0.54
1:A:366:LYS:HD3	1:A:378:ASP:OD1	2.07	0.54
1:A:582:TYR:CE1	1:A:669:LEU:HD12	2.42	0.54
1:B:351:THR:HG22	1:B:352:GLN:HE22	1.71	0.54
1:B:524:SER:O	1:B:528:THR:HG23	2.08	0.54
1:C:460:LEU:HD21	1:C:489:TYR:OH	2.08	0.54
1:D:230:ILE:HG12	1:D:292:ALA:HB1	1.90	0.54
1:D:535:GLU:CG	1:D:541:TYR:CZ	2.90	0.54
1:B:263:LYS:HD3	1:B:265:GLU:OE1	2.06	0.54
1:D:661:TYR:O	1:D:663:PRO:HD3	2.06	0.54
1:B:201:LYS:O	1:B:203:THR:HG22	2.07	0.54
1:B:371:LYS:HA	1:B:374:HIS:CD2	2.42	0.54
1:C:304:ASN:HB2	1:C:369:TYR:OH	2.08	0.54
1:D:588:ILE:HG12	1:D:646:LEU:HD11	1.89	0.54
1:A:306:VAL:HG12	1:A:307:LYS:HD2	1.90	0.54
1:A:316:TYR:CD2	1:A:319:LYS:HG2	2.43	0.54
1:B:578:HIS:HA	1:B:672:LYS:HG3	1.89	0.54
1:D:307:LYS:NZ	1:D:319:LYS:CG	2.59	0.54
1:B:106:PHE:CE1	1:B:122:SER:HA	2.39	0.54
1:D:135:TYR:CE2	1:D:150:LEU:HB3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LEU:HD22	1:D:515:ALA:CB	2.37	0.54
1:A:110:LEU:O	1:B:170:ARG:HD3	2.08	0.54
1:A:325:ILE:HG23	1:A:326:PHE:N	2.22	0.54
1:C:154:PRO:CG	1:C:620:LEU:CD2	2.85	0.54
1:C:393:ASP:OD2	1:C:395:GLU:HG2	2.07	0.54
1:C:500:THR:HG23	1:C:609:LYS:HE3	1.90	0.54
1:D:363:GLU:HA	1:D:366:LYS:HE3	1.90	0.54
1:A:244:LEU:O	1:A:248:LEU:HD22	2.07	0.54
1:A:349:TRP:CZ3	1:A:475:LYS:HD2	2.43	0.54
1:B:254:ILE:HD13	1:B:255:LYS:C	2.34	0.54
1:C:165:PHE:CG	1:C:262:PRO:HG3	2.43	0.54
1:D:112:THR:CG2	1:D:113:LYS:H	2.21	0.54
1:D:124:GLN:HE22	1:D:275:ALA:HB2	1.73	0.54
1:A:480:THR:O	1:A:481:GLU:HB2	2.08	0.53
1:B:164:THR:HG22	1:B:167:GLU:OE2	2.08	0.53
1:B:332:GLU:OE1	1:B:444:HIS:NE2	2.33	0.53
1:B:377:ILE:O	1:B:380:ILE:HG22	2.08	0.53
1:C:502:VAL:HG11	1:C:555:TRP:CE3	2.44	0.53
1:D:113:LYS:O	1:D:114:LYS:CB	2.55	0.53
1:A:146:ALA:HB1	1:A:627:THR:HA	1.90	0.53
1:A:586:ASP:OD2	1:A:586:ASP:C	2.51	0.53
1:C:100:ILE:C	1:C:102:LYS:H	2.16	0.53
1:C:648:LYS:HB2	1:C:661:TYR:HB2	1.90	0.53
1:D:109:ASN:O	1:D:110:LEU:O	2.26	0.53
1:D:211:GLN:O	1:D:212:LEU:HB2	2.08	0.53
1:D:231:GLY:HA2	1:D:234:LEU:HG	1.89	0.53
1:A:347:LYS:HD3	1:A:478:LYS:N	2.24	0.53
1:B:260:ALA:HA	1:B:287:ILE:O	2.07	0.53
1:C:94:ARG:HB2	1:D:386:GLU:OE1	2.08	0.53
1:D:508:ASP:O	1:D:510:THR:N	2.41	0.53
1:A:110:LEU:H	1:A:117:ASN:ND2	2.06	0.53
1:C:361:ILE:HD11	1:C:417:LEU:HB2	1.89	0.53
1:C:404:GLY:H	1:C:407:GLN:HE22	1.51	0.53
1:C:209:TRP:HB3	1:C:212:LEU:HB3	1.91	0.53
1:C:222:ALA:HB1	1:C:226:GLU:CG	2.38	0.53
1:D:148:ILE:HG13	1:D:627:THR:HG21	1.91	0.53
1:D:253:LYS:CD	1:D:253:LYS:N	2.66	0.53
1:B:138:GLN:HA	1:B:138:GLN:NE2	2.23	0.53
1:C:639:GLY:HA2	1:C:645:TRP:CD1	2.44	0.53
1:D:155:ILE:HG23	1:D:155:ILE:O	2.07	0.53
1:D:354:THR:HG22	1:D:355:SER:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PRO:CG	1:C:620:LEU:HD23	2.37	0.53
1:B:317:GLU:O	1:B:317:GLU:CG	2.57	0.53
1:B:460:LEU:HD21	1:B:489:TYR:OH	2.09	0.53
1:C:139:ILE:O	1:C:143:MET:HG3	2.08	0.53
1:C:560:ARG:HH21	1:C:561:ARG:HH21	1.57	0.53
1:D:316:TYR:O	1:D:318:GLY:N	2.37	0.53
1:D:349:TRP:HZ2	1:D:417:LEU:HD23	1.71	0.53
1:D:608:GLU:O	1:D:609:LYS:HB2	2.08	0.53
1:C:218:ARG:CB	1:C:231:GLY:HA3	2.20	0.53
1:D:139:ILE:HG13	1:D:542:GLU:OE2	2.09	0.53
1:D:139:ILE:HG12	1:D:566:VAL:HG21	1.91	0.53
1:D:308:GLN:O	1:D:309:GLN:O	2.27	0.53
1:D:317:GLU:HG2	1:D:325:ILE:HD11	1.91	0.53
1:A:352:GLN:HG2	1:A:476:PRO:HD2	1.90	0.53
1:B:229:ASN:HD22	1:B:229:ASN:C	2.15	0.53
1:B:562:ILE:O	1:B:566:VAL:HG23	2.09	0.53
1:B:582:TYR:CE1	1:B:669:LEU:HD13	2.43	0.53
1:D:152:LYS:HG2	1:D:273:TRP:CZ3	2.44	0.53
1:D:227:LYS:CD	1:D:228:LYS:HD2	2.38	0.53
1:D:319:LYS:CD	1:D:319:LYS:N	2.72	0.53
1:B:161:ASP:OD1	1:B:161:ASP:O	2.27	0.52
1:B:570:GLN:N	1:B:571:PRO:HD3	2.23	0.52
1:C:179:ARG:HD3	1:C:179:ARG:N	2.11	0.52
1:C:424:TYR:O	1:C:425:ALA:C	2.52	0.52
1:C:538:THR:O	1:C:542:GLU:HG3	2.09	0.52
1:D:558:LEU:O	1:D:559:VAL:CG2	2.56	0.52
1:A:118:PRO:HD2	1:B:396:VAL:O	2.08	0.52
1:A:664:ASP:CB	1:A:665:LYS:HD3	2.39	0.52
1:C:272:ASP:HB3	1:C:279:VAL:CG1	2.38	0.52
1:D:159:GLN:NE2	1:D:162:THR:OG1	2.43	0.52
1:D:213:GLU:C	1:D:215:GLY:N	2.67	0.52
1:D:597:ARG:HG3	1:D:597:ARG:NH1	2.21	0.52
1:A:260:ALA:HA	1:A:287:ILE:O	2.09	0.52
1:A:316:TYR:CE2	1:A:319:LYS:HG2	2.45	0.52
1:A:482:GLY:O	1:A:484:LYS:N	2.43	0.52
1:C:155:ILE:HA	1:C:267:ARG:O	2.10	0.52
1:C:184:LEU:HD11	1:C:473:ALA:CA	2.39	0.52
1:C:363:GLU:HA	1:C:366:LYS:HE2	1.91	0.52
1:D:122:SER:O	1:D:123:GLU:C	2.52	0.52
1:D:467:MET:O	1:D:470:LEU:HB2	2.09	0.52
1:D:535:GLU:HG2	1:D:541:TYR:CZ	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ALA:HA	1:A:630:ARG:CD	2.39	0.52
1:A:350:ASP:OD1	1:A:403:ARG:HB3	2.08	0.52
1:B:138:GLN:HA	1:B:138:GLN:HE21	1.74	0.52
1:B:452:LEU:HD23	1:B:452:LEU:C	2.35	0.52
1:C:173:ILE:CD1	1:C:286:VAL:HG21	2.34	0.52
1:C:672:LYS:O	1:C:672:LYS:HG2	2.08	0.52
1:D:161:ASP:C	1:D:163:LYS:N	2.59	0.52
1:D:227:LYS:HD3	1:D:228:LYS:CD	2.40	0.52
1:A:562:ILE:O	1:A:566:VAL:HG23	2.10	0.52
1:C:591:TYR:O	1:C:595:ILE:HG12	2.10	0.52
1:D:257:TYR:CD1	1:D:257:TYR:C	2.87	0.52
1:A:116:LEU:HB3	1:B:398:ILE:HB	1.91	0.52
1:A:491:PHE:HE1	1:A:513:HIS:CD2	2.28	0.52
1:D:399:ARG:HG2	1:D:399:ARG:HH11	1.74	0.52
1:D:507:SER:C	1:D:509:ASN:H	2.16	0.52
1:A:104:ILE:HD13	1:A:118:PRO:O	2.09	0.52
1:A:456:LYS:O	1:A:460:LEU:HD23	2.10	0.52
1:B:160:THR:HG23	1:B:160:THR:O	2.09	0.52
1:C:403:ARG:NH1	1:C:410:THR:HA	2.24	0.52
1:C:439:ARG:HH11	1:C:439:ARG:CB	2.21	0.52
1:C:440:VAL:HG11	1:C:458:LEU:HD13	1.92	0.52
1:D:342:VAL:HB	1:D:452:LEU:CD2	2.40	0.52
1:C:209:TRP:HH2	1:C:238:LYS:O	1.93	0.52
1:C:241:VAL:O	1:C:244:LEU:N	2.42	0.52
1:C:500:THR:CG2	1:C:609:LYS:HE3	2.40	0.52
1:C:502:VAL:CG2	1:C:516:GLY:HA3	2.39	0.52
1:C:616:SER:O	1:C:620:LEU:HD13	2.10	0.52
1:D:104:ILE:HG22	1:D:105:ARG:N	2.25	0.52
1:D:166:HIS:NE2	1:D:393:ASP:OD2	2.41	0.52
1:D:271:ASP:CG	1:D:271:ASP:O	2.52	0.52
1:D:308:GLN:HB3	1:D:311:VAL:HA	1.92	0.52
1:C:230:ILE:CG1	1:C:292:ALA:HB1	2.32	0.52
1:C:231:GLY:C	1:C:234:LEU:HB3	2.34	0.52
1:C:344:PHE:CD2	1:C:344:PHE:N	2.76	0.52
1:D:366:LYS:HD3	1:D:378:ASP:OD1	2.10	0.52
1:A:209:TRP:CG	1:A:238:LYS:HE2	2.45	0.52
1:B:530:LEU:HD22	1:B:530:LEU:H	1.73	0.52
1:C:305:TRP:CB	1:C:369:TYR:HE1	2.23	0.52
1:D:114:LYS:CE	1:D:114:LYS:CA	2.77	0.52
1:D:147:GLY:HA3	1:D:627:THR:HG1	1.74	0.52
1:A:589:GLY:O	1:A:592:LYS:N	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ALA:HA	1:A:640:LYS:HE3	1.92	0.51
1:C:249:LYS:HE2	1:C:373:TRP:CZ3	2.45	0.51
1:D:218:ARG:O	1:D:230:ILE:O	2.27	0.51
1:B:127:ARG:HG3	1:B:127:ARG:NH1	2.24	0.51
1:C:635:CYS:HB3	1:C:653:ILE:HG12	1.92	0.51
1:D:198:PRO:C	1:D:200:LEU:N	2.67	0.51
1:A:159:GLN:HG2	1:A:281:GLU:OE2	2.08	0.51
1:A:223:GLY:O	1:A:224:PHE:HB2	2.10	0.51
1:A:639:GLY:O	1:A:648:LYS:HE3	2.09	0.51
1:C:93:ILE:HG13	1:C:94:ARG:N	2.25	0.51
1:C:330:ARG:HD3	1:C:491:PHE:CE1	2.45	0.51
1:A:419:VAL:HG23	1:A:420:LEU:N	2.25	0.51
1:B:228:LYS:HB3	1:B:232:GLU:HB3	1.92	0.51
1:D:245:VAL:HG13	1:D:301:VAL:HG22	1.92	0.51
1:B:100:ILE:HG23	1:B:101:LEU:N	2.26	0.51
1:B:249:LYS:HA	1:B:376:PHE:HB2	1.92	0.51
1:B:635:CYS:HB3	1:B:653:ILE:CG1	2.40	0.51
1:C:165:PHE:HD2	1:C:165:PHE:O	1.94	0.51
1:C:342:VAL:HB	1:C:452:LEU:HD21	1.90	0.51
1:C:507:SER:C	1:C:509:ASN:H	2.18	0.51
1:D:481:GLU:O	1:D:482:GLY:C	2.53	0.51
1:A:210:GLU:H	1:A:210:GLU:CD	2.15	0.51
1:A:560:ARG:O	1:A:564:LEU:HG	2.11	0.51
1:C:497:CYS:O	1:C:498:SER:HB2	2.11	0.51
1:D:639:GLY:HA2	1:D:645:TRP:CD1	2.45	0.51
1:B:146:ALA:CB	1:B:627:THR:HG23	2.36	0.51
1:C:546:ALA:HB1	1:C:563:CYS:HA	1.93	0.51
1:D:123:GLU:HB3	1:D:131:LYS:HG2	1.93	0.51
1:A:430:THR:HB	1:A:458:LEU:HD22	1.93	0.51
1:C:223:GLY:O	1:C:224:PHE:C	2.53	0.51
1:C:517:ARG:NH1	1:C:525:LYS:HE3	2.26	0.51
1:D:109:ASN:HB3	1:D:273:TRP:HE1	1.73	0.51
1:C:95:GLU:OE2	1:C:98:LYS:HE2	2.09	0.51
1:C:301:VAL:HG11	1:C:376:PHE:CZ	2.45	0.51
1:D:212:LEU:HD13	1:D:300:LYS:HA	1.93	0.51
1:D:215:GLY:C	1:D:216:VAL:HG22	2.36	0.51
1:D:468:GLN:C	1:D:470:LEU:N	2.66	0.51
1:A:339:PRO:O	1:A:340:VAL:HG23	2.11	0.51
1:C:155:ILE:HG12	1:C:266:LYS:CD	2.41	0.51
1:C:191:ILE:O	1:C:194:THR:HG23	2.10	0.51
1:D:138:GLN:CD	1:D:569:GLN:HG2	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASP:O	1:D:273:TRP:HB2	2.10	0.51
1:A:133:ASN:OD1	1:A:536:ARG:NH2	2.44	0.50
1:A:593:ASP:OD1	1:A:667:PHE:HA	2.10	0.50
1:C:324:ASN:OD1	1:C:324:ASN:O	2.28	0.50
1:D:164:THR:O	1:D:167:GLU:N	2.45	0.50
1:D:231:GLY:HA2	1:D:234:LEU:CG	2.41	0.50
1:D:181:ASN:HB2	1:D:183:GLU:OE1	2.10	0.50
1:D:558:LEU:CD2	1:D:631:ILE:HD12	2.41	0.50
1:D:560:ARG:NE	1:D:650:ASP:OD1	2.44	0.50
1:A:126:ASP:HB2	1:A:132:ARG:HD3	1.92	0.50
1:A:418:ASN:HD22	1:A:445:VAL:CG2	2.23	0.50
1:C:155:ILE:HG12	1:C:266:LYS:HD3	1.92	0.50
1:C:370:LYS:HD2	1:C:372:GLU:HB3	1.93	0.50
1:C:430:THR:HG21	1:C:458:LEU:HB3	1.93	0.50
1:C:542:GLU:O	1:C:545:VAL:HB	2.11	0.50
1:D:187:LYS:O	1:D:190:GLU:HB3	2.11	0.50
1:B:504:VAL:HG13	1:B:602:LEU:HD13	1.94	0.50
1:C:289:TYR:HD1	1:C:290:PRO:O	1.94	0.50
1:C:302:MET:HA	1:C:369:TYR:CE2	2.46	0.50
1:C:419:VAL:HG12	1:C:445:VAL:HG13	1.93	0.50
1:D:315:GLY:O	1:D:317:GLU:N	2.45	0.50
1:A:127:ARG:HH11	1:A:127:ARG:HB3	1.75	0.50
1:A:398:ILE:HG22	1:A:398:ILE:O	2.12	0.50
1:A:424:TYR:O	1:A:428:GLU:HG2	2.11	0.50
1:B:296:LEU:O	1:B:297:ALA:C	2.53	0.50
1:B:494:ILE:O	1:B:500:THR:HG22	2.11	0.50
1:C:146:ALA:CB	1:C:627:THR:HG23	2.41	0.50
1:C:223:GLY:O	1:C:226:GLU:N	2.43	0.50
1:C:459:GLY:O	1:C:462:PHE:HB3	2.12	0.50
1:D:558:LEU:O	1:D:559:VAL:CB	2.59	0.50
1:A:126:ASP:OD1	1:A:128:GLU:N	2.37	0.50
1:B:209:TRP:CD1	1:B:300:LYS:HE3	2.45	0.50
1:B:516:GLY:HA2	1:B:555:TRP:CZ2	2.47	0.50
1:C:93:ILE:CG2	1:D:398:ILE:HD13	2.42	0.50
1:C:183:GLU:O	1:C:186:ASN:HB2	2.11	0.50
1:D:157:ARG:CZ	1:D:275:ALA:HB1	2.40	0.50
1:D:184:LEU:C	1:D:184:LEU:CD1	2.85	0.50
1:D:266:LYS:CD	1:D:267:ARG:N	2.59	0.50
1:D:319:LYS:NZ	1:D:675:GLU:HA	2.27	0.50
1:A:276:GLY:O	1:A:278:LEU:HG	2.11	0.50
1:A:352:GLN:HG2	1:A:476:PRO:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:GLU:HG2	1:B:207:VAL:N	2.27	0.50
1:B:432:VAL:HG21	1:B:440:VAL:HG21	1.94	0.50
1:C:95:GLU:C	1:C:97:ASN:H	2.20	0.50
1:C:648:LYS:N	1:C:649:PRO:CD	2.75	0.50
1:D:381:THR:HA	1:D:384:MET:HG3	1.94	0.50
1:A:424:TYR:CZ	1:A:428:GLU:HG3	2.46	0.50
1:B:357:ASP:O	1:B:361:ILE:HD13	2.11	0.50
1:B:463:ALA:O	1:B:484:LYS:HB2	2.11	0.50
1:C:292:ALA:HB2	1:C:295:ARG:HH21	1.75	0.50
1:D:227:LYS:CE	1:D:228:LYS:HD2	2.42	0.50
1:A:93:ILE:HG21	1:B:398:ILE:HG12	1.92	0.50
1:A:275:ALA:O	1:A:276:GLY:C	2.54	0.50
1:A:446:CYS:SG	1:A:497:CYS:SG	3.10	0.50
1:C:239:HIS:H	1:C:239:HIS:HD2	1.59	0.50
1:C:345:ASP:OD2	1:C:478:LYS:HD2	2.11	0.50
1:D:204:TYR:HB3	1:D:369:TYR:CE2	2.47	0.50
1:A:330:ARG:HD3	1:A:513:HIS:CE1	2.46	0.49
1:B:376:PHE:C	1:B:376:PHE:CD2	2.90	0.49
1:C:104:ILE:HG21	1:C:119:GLY:HA3	1.94	0.49
1:C:153:LEU:O	1:C:155:ILE:HG22	2.12	0.49
1:C:209:TRP:CB	1:C:212:LEU:HB3	2.42	0.49
1:D:207:VAL:HG22	1:D:300:LYS:O	2.12	0.49
1:D:403:ARG:HD3	1:D:407:GLN:OE1	2.12	0.49
1:A:99:TRP:CE2	1:B:255:LYS:HB3	2.47	0.49
1:A:354:THR:HG22	1:A:357:ASP:N	2.21	0.49
1:A:536:ARG:HG3	1:A:537:GLY:H	1.77	0.49
1:B:615:LEU:O	1:B:617:LEU:N	2.45	0.49
1:C:292:ALA:HA	1:C:295:ARG:NE	2.27	0.49
1:A:218:ARG:NH1	1:A:231:GLY:HA3	2.27	0.49
1:B:159:GLN:HG2	1:B:281:GLU:CD	2.37	0.49
1:C:342:VAL:HG11	1:C:462:PHE:CD2	2.47	0.49
1:C:662:ILE:HD12	1:C:662:ILE:N	2.28	0.49
1:D:224:PHE:CE2	1:D:390:ILE:HG21	2.46	0.49
1:C:504:VAL:HG11	1:C:602:LEU:HD22	1.92	0.49
1:C:547:PHE:CE2	1:C:551:LEU:HD11	2.46	0.49
1:D:227:LYS:HD3	1:D:228:LYS:HG3	1.93	0.49
1:D:322:LEU:HD11	1:D:499:HIS:CE1	2.47	0.49
1:D:400:ASN:O	1:D:401:GLY:O	2.30	0.49
1:D:422:MET:HE1	1:D:470:LEU:HD11	1.93	0.49
1:A:206:GLU:HB2	1:A:373:TRP:CZ2	2.47	0.49
1:A:230:ILE:HG12	1:A:296:LEU:CD1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:CG2	1:A:355:SER:N	2.74	0.49
1:A:530:LEU:HD22	1:A:530:LEU:H	1.76	0.49
1:B:423:MET:HE3	1:B:437:PHE:CD2	2.48	0.49
1:C:230:ILE:CG2	1:C:296:LEU:HD13	2.42	0.49
1:C:249:LYS:HZ3	1:C:372:GLU:HG3	1.77	0.49
1:C:349:TRP:HZ2	1:C:417:LEU:HD23	1.78	0.49
1:C:620:LEU:N	1:C:620:LEU:CD1	2.75	0.49
1:C:646:LEU:O	1:C:646:LEU:HD23	2.13	0.49
1:D:218:ARG:HH11	1:D:231:GLY:CA	2.26	0.49
1:D:227:LYS:HE2	1:D:228:LYS:HD2	1.95	0.49
1:D:263:LYS:HB2	1:D:287:ILE:CD1	2.42	0.49
1:B:104:ILE:HD11	1:B:118:PRO:HB2	1.94	0.49
1:C:154:PRO:HG2	1:C:620:LEU:CD2	2.43	0.49
1:D:591:TYR:C	1:D:591:TYR:CD2	2.91	0.49
1:A:139:ILE:HG12	1:A:566:VAL:HG21	1.95	0.49
1:B:517:ARG:C	1:B:613:LEU:HD22	2.38	0.49
1:B:634:ASP:O	1:B:637:ALA:HB3	2.12	0.49
1:C:334:ASP:O	1:C:336:PHE:N	2.41	0.49
1:A:184:LEU:HD22	1:A:188:LEU:CD1	2.43	0.49
1:A:206:GLU:OE1	1:A:300:LYS:NZ	2.41	0.49
1:B:234:LEU:O	1:B:238:LYS:HB2	2.12	0.49
1:B:619:THR:HG22	1:B:620:LEU:HG	1.95	0.49
1:C:166:HIS:C	1:C:170:ARG:NH1	2.71	0.49
1:C:500:THR:HG23	1:C:609:LYS:CE	2.43	0.49
1:D:154:PRO:O	1:D:266:LYS:HG3	2.13	0.49
1:D:354:THR:CG2	1:D:355:SER:H	2.25	0.49
1:D:354:THR:H	1:D:357:ASP:HB2	1.78	0.49
1:B:144:SER:O	1:B:146:ALA:O	2.31	0.49
1:B:206:GLU:CG	1:B:207:VAL:N	2.76	0.49
1:D:590:ALA:O	1:D:668:THR:HG23	2.12	0.49
1:B:180:GLN:OE1	1:B:354:THR:HG21	2.13	0.49
1:B:354:THR:HG22	1:B:356:LYS:N	2.28	0.49
1:B:605:THR:O	1:B:607:PHE:N	2.46	0.49
1:C:648:LYS:O	1:C:650:ASP:N	2.46	0.49
1:D:351:THR:HA	1:D:402:GLN:HG2	1.95	0.49
1:D:639:GLY:O	1:D:645:TRP:HD1	1.95	0.49
1:A:95:GLU:C	1:A:97:ASN:N	2.70	0.48
1:A:95:GLU:O	1:A:97:ASN:N	2.45	0.48
1:B:153:LEU:O	1:B:155:ILE:N	2.45	0.48
1:C:330:ARG:HD3	1:C:491:PHE:CD1	2.48	0.48
1:C:379:THR:O	1:C:382:ASP:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:LEU:CD1	1:C:656:LYS:HE2	2.43	0.48
1:A:231:GLY:HA2	1:A:234:LEU:CD1	2.41	0.48
1:A:672:LYS:O	1:A:672:LYS:HD2	2.13	0.48
1:B:190:GLU:O	1:B:193:HIS:HB2	2.12	0.48
1:B:208:THR:C	1:B:210:GLU:N	2.68	0.48
1:B:303:TYR:O	1:B:307:LYS:HB2	2.12	0.48
1:C:422:MET:HE1	1:C:470:LEU:CD1	2.35	0.48
1:C:582:TYR:CE1	1:C:669:LEU:HD12	2.48	0.48
1:C:590:ALA:O	1:C:593:ASP:HB3	2.14	0.48
1:D:554:SER:HB2	1:D:599:LEU:HD11	1.94	0.48
1:A:501:PRO:O	1:A:609:LYS:HE2	2.13	0.48
1:A:555:TRP:CH2	1:A:613:LEU:HD12	2.47	0.48
1:A:631:ILE:O	1:A:634:ASP:HB2	2.13	0.48
1:C:161:ASP:O	1:C:164:THR:C	2.55	0.48
1:C:169:ILE:C	1:C:171:ASP:N	2.71	0.48
1:C:237:GLU:C	1:C:239:HIS:N	2.71	0.48
1:C:463:ALA:HA	1:C:485:MET:HB2	1.95	0.48
1:D:380:ILE:HG22	1:D:381:THR:H	1.76	0.48
1:A:138:GLN:HG3	1:A:539:THR:CG2	2.43	0.48
1:A:234:LEU:O	1:A:238:LYS:HB2	2.12	0.48
1:A:347:LYS:CD	1:A:478:LYS:HA	2.43	0.48
1:A:351:THR:HG22	1:A:352:GLN:HE22	1.76	0.48
1:A:354:THR:HG23	1:A:355:SER:N	2.27	0.48
1:A:355:SER:CB	1:A:385:THR:HG22	2.42	0.48
1:A:535:GLU:O	1:A:536:ARG:CB	2.61	0.48
1:A:590:ALA:HB1	1:A:668:THR:OG1	2.13	0.48
1:C:372:GLU:HG2	1:C:373:TRP:N	2.28	0.48
1:B:648:LYS:HE3	1:B:657:THR:HG21	1.96	0.48
1:C:301:VAL:CG1	1:C:376:PHE:CZ	2.97	0.48
1:C:561:ARG:NH1	1:C:632:ILE:HD11	2.28	0.48
1:D:106:PHE:HB3	1:D:151:GLU:OE1	2.14	0.48
1:A:228:LYS:HD2	1:A:237:GLU:CD	2.38	0.48
1:A:331:LYS:O	1:A:334:ASP:N	2.46	0.48
1:C:272:ASP:CB	1:C:279:VAL:HG11	2.42	0.48
1:C:383:HIS:O	1:C:385:THR:N	2.46	0.48
1:C:419:VAL:CG1	1:C:445:VAL:HG11	2.44	0.48
1:C:517:ARG:O	1:C:613:LEU:HD22	2.13	0.48
1:D:204:TYR:O	1:D:370:LYS:HG3	2.14	0.48
1:A:126:ASP:HB3	1:A:130:ARG:HB2	1.95	0.48
1:A:357:ASP:O	1:A:361:ILE:HD13	2.14	0.48
1:A:479:ILE:HD12	1:A:479:ILE:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:THR:O	1:A:530:LEU:HD22	2.13	0.48
1:C:212:LEU:HD13	1:C:300:LYS:CA	2.42	0.48
1:C:452:LEU:HD23	1:C:452:LEU:O	2.13	0.48
1:D:370:LYS:O	1:D:374:HIS:CD2	2.67	0.48
1:B:209:TRP:CD2	1:B:238:LYS:HE3	2.49	0.48
1:B:337:ASN:C	1:B:339:PRO:HD3	2.39	0.48
1:B:594:VAL:CG1	1:B:668:THR:HB	2.44	0.48
1:C:125:LEU:HD22	1:D:224:PHE:HD1	1.79	0.48
1:C:204:TYR:CE2	1:C:368:TYR:HD2	2.32	0.48
1:D:670:GLN:OE1	1:D:673:HIS:NE2	2.47	0.48
1:B:636:VAL:O	1:B:637:ALA:C	2.56	0.48
1:D:535:GLU:HB2	1:D:578:HIS:HB3	1.96	0.48
1:D:556:ASN:ND2	1:D:558:LEU:O	2.46	0.48
1:A:95:GLU:C	1:A:97:ASN:H	2.21	0.48
1:A:306:VAL:HG22	1:A:409:ASP:HA	1.95	0.48
1:B:229:ASN:ND2	1:B:229:ASN:C	2.69	0.48
1:C:355:SER:CB	1:C:385:THR:HG23	2.42	0.48
1:D:106:PHE:HB3	1:D:151:GLU:CD	2.39	0.48
1:D:157:ARG:HH21	1:D:275:ALA:HB1	1.73	0.48
1:D:648:LYS:HD3	1:D:648:LYS:HA	1.40	0.48
1:D:648:LYS:HZ3	1:D:659:HIS:HB2	1.79	0.48
1:A:104:ILE:HD11	1:A:118:PRO:CB	2.42	0.47
1:A:189:LEU:HD22	1:A:193:HIS:NE2	2.29	0.47
1:A:259:THR:O	1:A:288:GLN:HA	2.13	0.47
1:A:577:LYS:HG2	1:A:582:TYR:CZ	2.49	0.47
1:B:599:LEU:HB3	1:B:649:PRO:HB3	1.96	0.47
1:B:648:LYS:N	1:B:649:PRO:CD	2.77	0.47
1:C:100:ILE:C	1:C:102:LYS:N	2.72	0.47
1:D:134:ILE:HG23	1:D:135:TYR:CD1	2.49	0.47
1:D:208:THR:O	1:D:211:GLN:HG2	2.14	0.47
1:D:517:ARG:HH22	1:D:525:LYS:HZ2	1.62	0.47
1:A:605:THR:O	1:A:606:GLY:C	2.55	0.47
1:D:104:ILE:HD11	1:D:118:PRO:HB2	1.96	0.47
1:D:123:GLU:HB3	1:D:131:LYS:CG	2.44	0.47
1:D:138:GLN:NE2	1:D:539:THR:HG23	2.25	0.47
1:D:361:ILE:HD13	1:D:413:GLY:HA2	1.95	0.47
1:A:354:THR:HG22	1:A:356:LYS:N	2.29	0.47
1:B:313:ILE:HB	1:B:316:TYR:HB2	1.97	0.47
1:B:500:THR:CB	1:B:609:LYS:HZ1	2.27	0.47
1:B:629:LYS:O	1:B:632:ILE:HB	2.14	0.47
1:C:547:PHE:CZ	1:C:551:LEU:HD11	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:ALA:HB1	1:C:668:THR:OG1	2.14	0.47
1:D:147:GLY:O	1:D:148:ILE:O	2.32	0.47
1:D:497:CYS:O	1:D:498:SER:HB2	2.12	0.47
1:D:626:HIS:HB3	1:D:630:ARG:HD3	1.95	0.47
1:D:648:LYS:C	1:D:650:ASP:N	2.72	0.47
1:D:661:TYR:C	1:D:662:ILE:HD12	2.39	0.47
1:A:226:GLU:CD	1:A:291:GLU:HG2	2.39	0.47
1:B:187:LYS:O	1:B:191:ILE:HG13	2.13	0.47
1:C:149:ARG:HD3	1:C:152:LYS:HG3	1.97	0.47
1:C:160:THR:HG23	1:C:262:PRO:HB2	1.97	0.47
1:C:201:LYS:HG2	1:C:202:HIS:CD2	2.49	0.47
1:C:645:TRP:CE3	1:C:645:TRP:HA	2.49	0.47
1:D:192:PHE:HZ	1:D:368:TYR:CE1	2.31	0.47
1:D:301:VAL:HG21	1:D:376:PHE:CE1	2.50	0.47
1:A:147:GLY:O	1:A:623:TRP:HA	2.14	0.47
1:C:166:HIS:HB3	1:D:110:LEU:HD11	1.95	0.47
1:C:177:GLU:OE1	1:C:400:ASN:HB3	2.15	0.47
1:C:226:GLU:HG3	1:C:227:LYS:N	2.28	0.47
1:C:400:ASN:OD1	1:D:115:MET:SD	2.73	0.47
1:D:198:PRO:O	1:D:199:THR:C	2.57	0.47
1:D:521:VAL:O	1:D:525:LYS:HB2	2.13	0.47
1:A:569:GLN:O	1:A:570:GLN:C	2.56	0.47
1:B:598:ASN:HB2	1:B:601:GLU:OE2	2.15	0.47
1:C:482:GLY:O	1:C:483:GLU:HB2	2.14	0.47
1:D:143:MET:HG3	1:D:148:ILE:HD13	1.97	0.47
1:A:325:ILE:O	1:A:328:LYS:HG2	2.15	0.47
1:A:572:GLU:H	1:A:572:GLU:HG3	1.28	0.47
1:B:116:LEU:C	1:B:118:PRO:HD3	2.40	0.47
1:B:361:ILE:HD11	1:B:417:LEU:HB2	1.95	0.47
1:B:536:ARG:O	1:B:536:ARG:HD3	2.15	0.47
1:B:583:TYR:CE1	1:B:587:PRO:HG3	2.50	0.47
1:C:127:ARG:HA	1:C:127:ARG:HD2	1.40	0.47
1:C:352:GLN:O	1:C:353:VAL:C	2.58	0.47
1:C:365:GLN:C	1:C:367:TYR:N	2.67	0.47
1:D:245:VAL:HG13	1:D:301:VAL:CG2	2.45	0.47
1:D:363:GLU:HA	1:D:366:LYS:CE	2.44	0.47
1:D:379:THR:O	1:D:380:ILE:C	2.58	0.47
1:D:517:ARG:NH2	1:D:525:LYS:HZ2	2.12	0.47
1:D:561:ARG:O	1:D:565:LEU:HG	2.13	0.47
1:D:590:ALA:HB1	1:D:668:THR:HG22	1.97	0.47
1:D:652:LEU:O	1:D:656:LYS:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PHE:O	1:A:168:ALA:HB3	2.15	0.47
1:A:243:GLN:O	1:A:243:GLN:HG3	2.15	0.47
1:B:355:SER:O	1:B:359:GLN:HG3	2.15	0.47
1:B:561:ARG:O	1:B:565:LEU:HG	2.15	0.47
1:C:155:ILE:HG23	1:C:266:LYS:HE2	1.96	0.47
1:C:330:ARG:HH11	1:C:513:HIS:CE1	2.30	0.47
1:C:529:ARG:HG3	1:C:530:LEU:N	2.30	0.47
1:D:237:GLU:O	1:D:241:VAL:HG23	2.15	0.47
1:D:344:PHE:N	1:D:344:PHE:CD2	2.80	0.47
1:A:153:LEU:HA	1:A:154:PRO:HD3	1.78	0.47
1:A:286:VAL:O	1:A:286:VAL:CG2	2.61	0.47
1:B:635:CYS:O	1:B:636:VAL:C	2.58	0.47
1:B:651:ARG:O	1:B:654:SER:HB3	2.15	0.47
1:C:149:ARG:C	1:C:151:GLU:N	2.70	0.47
1:C:189:LEU:HD22	1:C:193:HIS:CE1	2.50	0.47
1:C:591:TYR:CD1	1:C:595:ILE:HG13	2.49	0.47
1:C:592:LYS:HD3	1:C:592:LYS:C	2.40	0.47
1:D:313:ILE:HG12	1:D:416:MET:HG2	1.96	0.47
1:A:154:PRO:HB3	1:A:270:SER:HA	1.96	0.47
1:A:237:GLU:OE2	1:A:293:LYS:NZ	2.44	0.47
1:A:560:ARG:NE	1:A:650:ASP:OD1	2.47	0.47
1:A:586:ASP:H	1:A:666:GLY:N	2.13	0.47
1:C:672:LYS:O	1:C:673:HIS:ND1	2.48	0.47
1:D:218:ARG:O	1:D:220:GLY:N	2.41	0.47
1:A:347:LYS:HD3	1:A:477:GLN:C	2.40	0.46
1:C:292:ALA:HB2	1:C:295:ARG:NH2	2.30	0.46
1:D:108:GLY:CA	1:D:119:GLY:HA2	2.45	0.46
1:D:110:LEU:O	1:D:111:ASN:C	2.56	0.46
1:D:210:GLU:HA	1:D:213:GLU:HG3	1.97	0.46
1:D:404:GLY:O	1:D:405:SER:C	2.58	0.46
1:A:286:VAL:O	1:A:286:VAL:HG22	2.15	0.46
1:A:598:ASN:O	1:A:601:GLU:HB2	2.15	0.46
1:C:212:LEU:HD21	1:C:296:LEU:O	2.15	0.46
1:C:263:LYS:HD2	1:C:287:ILE:HD11	1.96	0.46
1:C:558:LEU:HD22	1:C:562:ILE:HD11	1.96	0.46
1:D:172:LYS:C	1:D:174:ASP:H	2.22	0.46
1:D:452:LEU:HD23	1:D:452:LEU:C	2.41	0.46
1:C:125:LEU:HD12	1:C:130:ARG:O	2.15	0.46
1:C:173:ILE:HD11	1:C:286:VAL:CB	2.45	0.46
1:C:263:LYS:CD	1:C:287:ILE:HD11	2.45	0.46
1:C:384:MET:HE2	1:C:407:GLN:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:ARG:O	1:C:654:SER:N	2.49	0.46
1:C:283:ARG:HB2	1:C:283:ARG:NH1	2.22	0.46
1:C:322:LEU:HD12	1:C:552:MET:CE	2.44	0.46
1:D:252:ARG:O	1:D:253:LYS:C	2.57	0.46
1:D:350:ASP:CB	1:D:403:ARG:HB3	2.46	0.46
1:B:432:VAL:HG12	1:B:433:PRO:O	2.16	0.46
1:C:377:ILE:O	1:C:380:ILE:HG23	2.14	0.46
1:C:570:GLN:N	1:C:571:PRO:HD3	2.30	0.46
1:D:287:ILE:O	1:D:287:ILE:HG22	2.16	0.46
1:D:553:TYR:C	1:D:555:TRP:N	2.71	0.46
1:D:626:HIS:C	1:D:630:ARG:HG3	2.40	0.46
1:A:234:LEU:O	1:A:238:LYS:HD2	2.16	0.46
1:C:282:LYS:CG	1:C:283:ARG:H	2.26	0.46
1:C:581:TYR:CD2	1:C:670:GLN:HA	2.49	0.46
1:D:114:LYS:HE2	1:D:114:LYS:CA	2.39	0.46
1:D:304:ASN:HD22	1:D:309:GLN:CD	2.23	0.46
1:D:379:THR:O	1:D:382:ASP:N	2.49	0.46
1:B:373:TRP:O	1:B:376:PHE:HB3	2.16	0.46
1:B:650:ASP:HB3	1:B:653:ILE:HB	1.98	0.46
1:B:664:ASP:O	1:B:665:LYS:C	2.59	0.46
1:C:170:ARG:HH11	1:C:170:ARG:CG	2.29	0.46
1:D:305:TRP:O	1:D:306:VAL:C	2.58	0.46
1:D:519:THR:CG2	1:D:617:LEU:HD11	2.45	0.46
1:A:189:LEU:O	1:A:192:PHE:HB3	2.16	0.46
1:A:303:TYR:CE2	1:A:309:GLN:HG3	2.51	0.46
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.78	0.46
1:A:416:MET:O	1:A:419:VAL:HG22	2.15	0.46
1:A:646:LEU:O	1:A:649:PRO:CD	2.64	0.46
1:A:662:ILE:HG12	1:D:436:SER:HB3	1.97	0.46
1:B:132:ARG:CA	1:B:536:ARG:HH22	2.27	0.46
1:B:210:GLU:CD	1:B:210:GLU:H	2.23	0.46
1:B:442:ARG:HG2	1:B:442:ARG:HH11	1.80	0.46
1:C:169:ILE:O	1:C:174:ASP:HB3	2.16	0.46
1:C:330:ARG:O	1:C:331:LYS:C	2.59	0.46
1:C:367:TYR:HD2	1:C:368:TYR:CD1	2.34	0.46
1:D:650:ASP:O	1:D:652:LEU:N	2.49	0.46
1:A:347:LYS:HG2	1:A:476:PRO:O	2.16	0.46
1:B:422:MET:HE1	1:B:470:LEU:CD1	2.46	0.46
1:C:111:ASN:CG	1:C:111:ASN:O	2.58	0.46
1:C:568:SER:OG	1:C:647:VAL:HG13	2.16	0.46
1:D:104:ILE:CG2	1:D:105:ARG:N	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:HG2	1:D:218:ARG:NH1	2.30	0.46
1:D:626:HIS:HB3	1:D:630:ARG:CD	2.45	0.46
1:A:127:ARG:HB3	1:A:127:ARG:NH1	2.30	0.46
1:A:648:LYS:HZ2	1:A:654:SER:HA	1.81	0.46
1:B:404:GLY:O	1:B:406:GLY:N	2.49	0.46
1:C:96:HIS:ND1	1:D:383:HIS:CE1	2.84	0.46
1:C:112:THR:HB	1:C:115:MET:HB2	1.97	0.46
1:C:209:TRP:CH2	1:C:238:LYS:HB3	2.50	0.46
1:C:440:VAL:CG1	1:C:458:LEU:HD13	2.46	0.46
1:C:645:TRP:CB	1:C:648:LYS:HZ2	2.23	0.46
1:A:333:TRP:CE2	1:A:339:PRO:HB2	2.50	0.45
1:A:586:ASP:O	1:A:589:GLY:N	2.46	0.45
1:A:645:TRP:O	1:A:648:LYS:CG	2.64	0.45
1:C:363:GLU:C	1:C:365:GLN:N	2.72	0.45
1:C:651:ARG:O	1:C:652:LEU:C	2.58	0.45
1:D:156:VAL:H	1:D:266:LYS:HB2	1.81	0.45
1:D:201:LYS:HE2	1:D:202:HIS:CD2	2.51	0.45
1:D:322:LEU:HD22	1:D:515:ALA:HB1	1.98	0.45
1:D:557:PRO:O	1:D:561:ARG:HG3	2.16	0.45
1:C:192:PHE:HD1	1:C:195:ILE:HD11	1.80	0.45
1:D:227:LYS:CD	1:D:228:LYS:N	2.65	0.45
1:D:478:LYS:HB3	1:D:480:THR:HG22	1.98	0.45
1:A:153:LEU:O	1:A:155:ILE:N	2.49	0.45
1:A:309:GLN:HB3	1:A:310:PRO:HD2	1.98	0.45
1:A:530:LEU:N	1:A:530:LEU:CD2	2.79	0.45
1:B:132:ARG:CB	1:B:536:ARG:HH22	2.28	0.45
1:B:237:GLU:CG	1:B:240:LEU:HD12	2.46	0.45
1:B:371:LYS:C	1:B:373:TRP:H	2.25	0.45
1:C:147:GLY:O	1:C:623:TRP:HA	2.16	0.45
1:C:207:VAL:HG23	1:C:208:THR:N	2.30	0.45
1:D:175:LYS:NZ	1:D:352:GLN:OE1	2.49	0.45
1:D:227:LYS:HD3	1:D:228:LYS:CG	2.46	0.45
1:B:200:LEU:C	1:B:203:THR:HG23	2.36	0.45
1:C:302:MET:CE	1:C:377:ILE:HG12	2.47	0.45
1:C:360:LEU:O	1:C:364:ILE:HG13	2.16	0.45
1:C:519:THR:HA	1:C:522:ILE:HD12	1.97	0.45
1:D:134:ILE:O	1:D:529:ARG:HA	2.17	0.45
1:D:138:GLN:HB2	1:D:542:GLU:OE1	2.16	0.45
1:D:209:TRP:CZ3	1:D:300:LYS:NZ	2.75	0.45
1:D:322:LEU:HD12	1:D:552:MET:SD	2.56	0.45
1:A:230:ILE:HD12	1:A:295:ARG:NH1	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:OH	1:A:290:PRO:HG3	2.17	0.45
1:A:502:VAL:CG2	1:A:516:GLY:HA3	2.47	0.45
1:B:215:GLY:O	1:B:216:VAL:C	2.60	0.45
1:B:463:ALA:HA	1:B:485:MET:HB2	1.98	0.45
1:C:146:ALA:HB3	1:C:627:THR:HG23	1.98	0.45
1:B:206:GLU:CG	1:B:207:VAL:H	2.29	0.45
1:C:187:LYS:O	1:C:188:LEU:C	2.58	0.45
1:C:308:GLN:NE2	1:C:313:ILE:HD12	2.31	0.45
1:C:354:THR:CG2	1:C:355:SER:H	2.28	0.45
1:D:165:PHE:O	1:D:169:ILE:HG13	2.17	0.45
1:D:172:LYS:O	1:D:174:ASP:N	2.45	0.45
1:D:455:GLU:O	1:D:456:LYS:C	2.59	0.45
1:B:325:ILE:CG2	1:B:326:PHE:N	2.79	0.45
1:B:430:THR:HB	1:B:458:LEU:HD22	1.99	0.45
1:D:95:GLU:CG	1:D:96:HIS:N	2.62	0.45
1:A:195:ILE:CD1	1:A:314:PRO:HG2	2.47	0.45
1:A:454:THR:HG23	1:A:455:GLU:O	2.17	0.45
1:A:507:SER:C	1:A:509:ASN:H	2.24	0.45
1:A:590:ALA:O	1:A:591:TYR:C	2.59	0.45
1:B:270:SER:O	1:B:274:GLN:HB2	2.16	0.45
1:B:635:CYS:HB3	1:B:653:ILE:HG12	1.97	0.45
1:C:338:GLU:OE1	1:C:456:LYS:HD3	2.16	0.45
1:D:142:ILE:HD13	1:D:565:LEU:CB	2.46	0.45
1:D:163:LYS:HG3	1:D:164:THR:HG23	1.98	0.45
1:D:192:PHE:CZ	1:D:364:ILE:HG23	2.52	0.45
1:D:645:TRP:HA	1:D:645:TRP:CE3	2.52	0.45
1:B:322:LEU:O	1:B:325:ILE:HG22	2.17	0.45
1:C:204:TYR:O	1:C:369:TYR:O	2.35	0.45
1:C:260:ALA:HB2	1:C:389:VAL:CG1	2.47	0.45
1:C:308:GLN:NE2	1:C:313:ILE:CD1	2.80	0.45
1:C:619:THR:HG22	1:C:620:LEU:HD12	1.98	0.45
1:D:94:ARG:O	1:D:95:GLU:C	2.60	0.45
1:D:189:LEU:O	1:D:192:PHE:HB3	2.17	0.45
1:D:266:LYS:HD3	1:D:267:ARG:CA	2.43	0.45
1:D:375:LYS:HA	1:D:375:LYS:HD2	1.80	0.45
1:D:535:GLU:CG	1:D:541:TYR:CE1	3.00	0.45
1:D:579:ALA:O	1:D:580:THR:C	2.60	0.45
1:A:221:ALA:O	1:A:295:ARG:NH2	2.50	0.45
1:A:580:THR:HG22	1:A:673:HIS:HB3	1.99	0.45
1:B:435:LYS:HD3	1:B:435:LYS:H	1.82	0.45
1:C:338:GLU:N	1:C:339:PRO:HD3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ILE:CD1	1:C:417:LEU:HD13	2.43	0.45
1:C:629:LYS:O	1:C:632:ILE:HB	2.18	0.45
1:A:229:ASN:ND2	1:A:229:ASN:C	2.72	0.44
1:A:590:ALA:C	1:A:592:LYS:N	2.74	0.44
1:B:212:LEU:CD2	1:B:300:LYS:HB2	2.47	0.44
1:B:554:SER:O	1:B:560:ARG:NH1	2.50	0.44
1:C:519:THR:CG2	1:C:617:LEU:HD11	2.45	0.44
1:A:345:ASP:OD2	1:A:478:LYS:HB2	2.17	0.44
1:B:100:ILE:CG2	1:B:101:LEU:N	2.79	0.44
1:C:184:LEU:HD11	1:C:473:ALA:HA	1.98	0.44
1:C:253:LYS:HE3	1:D:96:HIS:HB2	1.99	0.44
1:C:468:GLN:O	1:C:472:GLU:HG2	2.17	0.44
1:D:107:GLN:HG2	1:D:108:GLY:N	2.33	0.44
1:D:184:LEU:HD12	1:D:188:LEU:HG	1.97	0.44
1:D:187:LYS:HD2	1:D:424:TYR:HE1	1.83	0.44
1:D:190:GLU:O	1:D:193:HIS:N	2.51	0.44
1:D:292:ALA:HB2	1:D:295:ARG:HH21	1.82	0.44
1:D:607:PHE:HB3	1:D:608:GLU:H	1.59	0.44
1:B:592:LYS:HB2	1:B:598:ASN:HD22	1.78	0.44
1:C:300:LYS:C	1:C:302:MET:N	2.75	0.44
1:C:313:ILE:HD13	1:C:416:MET:N	2.32	0.44
1:C:330:ARG:NH1	1:C:513:HIS:HE1	2.13	0.44
1:D:201:LYS:HG2	1:D:202:HIS:CD2	2.52	0.44
1:D:608:GLU:O	1:D:609:LYS:HB3	2.16	0.44
1:A:204:TYR:HB2	1:A:368:TYR:O	2.18	0.44
1:A:218:ARG:NH1	1:A:231:GLY:CA	2.81	0.44
1:A:648:LYS:NZ	1:A:657:THR:OG1	2.48	0.44
1:B:136:ASN:HB3	1:B:542:GLU:CD	2.42	0.44
1:B:301:VAL:HG11	1:B:376:PHE:HE1	1.81	0.44
1:C:586:ASP:C	1:C:586:ASP:OD2	2.59	0.44
1:D:387:VAL:HA	1:D:388:PRO:HD3	1.72	0.44
1:A:594:VAL:HG23	1:A:595:ILE:H	1.82	0.44
1:B:159:GLN:O	1:B:284:PRO:HB3	2.18	0.44
1:B:185:HIS:CE1	1:B:357:ASP:OD1	2.66	0.44
1:C:118:PRO:HD2	1:D:396:VAL:O	2.17	0.44
1:C:125:LEU:HD11	1:C:129:GLY:O	2.17	0.44
1:C:230:ILE:HG21	1:C:296:LEU:HD13	1.99	0.44
1:C:376:PHE:CD2	1:C:377:ILE:N	2.86	0.44
1:D:362:GLY:C	1:D:366:LYS:HE2	2.43	0.44
1:D:506:TRP:HE1	1:D:512:SER:CB	2.28	0.44
1:A:206:GLU:HA	1:A:301:VAL:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CD1	1:B:125:LEU:HD13	2.53	0.44
1:A:229:ASN:ND2	1:A:232:GLU:CB	2.71	0.44
1:A:637:ALA:O	1:A:640:LYS:HG2	2.17	0.44
1:B:266:LYS:NZ	1:B:530:LEU:CD2	2.80	0.44
1:B:506:TRP:CE2	1:B:597:ARG:HD2	2.52	0.44
1:B:508:ASP:OD2	1:B:508:ASP:C	2.60	0.44
1:B:635:CYS:HB3	1:B:653:ILE:HG13	1.99	0.44
1:C:170:ARG:NE	1:D:110:LEU:HD11	2.33	0.44
1:C:370:LYS:HG3	1:C:372:GLU:N	2.30	0.44
1:C:404:GLY:O	1:C:405:SER:C	2.60	0.44
1:C:646:LEU:O	1:C:649:PRO:HD2	2.17	0.44
1:D:298:ILE:HG12	1:D:380:ILE:CD1	2.30	0.44
1:A:325:ILE:CG2	1:A:326:PHE:N	2.81	0.44
1:A:462:PHE:CZ	1:A:485:MET:HE1	2.53	0.44
1:B:204:TYR:HD2	1:B:368:TYR:HB3	1.81	0.44
1:B:361:ILE:N	1:B:361:ILE:HD12	2.32	0.44
1:C:109:ASN:H	1:D:395:GLU:CD	2.25	0.44
1:C:209:TRP:HA	1:C:212:LEU:HB3	1.99	0.44
1:D:104:ILE:HA	1:D:121:LEU:CD2	2.48	0.44
1:D:224:PHE:CD2	1:D:390:ILE:HG21	2.52	0.44
1:A:298:ILE:HG12	1:A:380:ILE:HD12	1.99	0.44
1:A:480:THR:O	1:A:481:GLU:CB	2.66	0.44
1:A:594:VAL:HG23	1:A:595:ILE:N	2.33	0.44
1:A:672:LYS:O	1:A:672:LYS:CG	2.65	0.44
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.83	0.44
1:C:110:LEU:HA	1:D:170:ARG:HH21	1.83	0.44
1:C:330:ARG:HA	1:C:330:ARG:HD2	1.64	0.44
1:C:561:ARG:HH11	1:C:632:ILE:HG12	1.82	0.44
1:D:143:MET:CG	1:D:148:ILE:HG21	2.33	0.44
1:D:535:GLU:HG3	1:D:541:TYR:CZ	2.51	0.44
1:A:149:ARG:HB3	1:A:151:GLU:HG3	2.00	0.44
1:A:668:THR:C	1:A:669:LEU:HD23	2.41	0.44
1:B:354:THR:HG22	1:B:356:LYS:H	1.83	0.44
1:B:619:THR:HG22	1:B:620:LEU:N	2.32	0.44
1:C:175:LYS:HB3	1:C:176:SER:H	1.20	0.44
1:C:221:ALA:O	1:C:295:ARG:NH2	2.51	0.44
1:C:224:PHE:CD2	1:C:225:LEU:HD23	2.35	0.44
1:D:212:LEU:HD22	1:D:300:LYS:HG3	2.00	0.44
1:D:230:ILE:HG22	1:D:231:GLY:N	2.33	0.44
1:D:647:VAL:HG23	1:D:653:ILE:HG21	1.99	0.44
1:A:130:ARG:HA	1:A:130:ARG:HD3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLY:O	1:A:405:SER:C	2.59	0.43
1:A:607:PHE:HD2	1:A:608:GLU:H	1.65	0.43
1:B:191:ILE:CA	1:B:194:THR:HG23	2.47	0.43
1:B:354:THR:CG2	1:B:355:SER:N	2.80	0.43
1:B:632:ILE:O	1:B:635:CYS:HB2	2.18	0.43
1:C:174:ASP:OD2	1:C:175:LYS:HG3	2.18	0.43
1:C:211:GLN:O	1:C:214:ALA:HB3	2.17	0.43
1:C:336:PHE:CE2	1:C:453:ILE:HG22	2.53	0.43
1:C:367:TYR:HD2	1:C:368:TYR:CE1	2.35	0.43
1:D:135:TYR:OH	1:D:274:GLN:CG	2.60	0.43
1:D:670:GLN:OE1	1:D:673:HIS:CE1	2.71	0.43
1:B:178:ASN:HD21	1:B:352:GLN:HA	1.82	0.43
1:B:568:SER:O	1:B:571:PRO:HG3	2.18	0.43
1:B:586:ASP:C	1:B:586:ASP:OD2	2.59	0.43
1:C:104:ILE:HD13	1:C:119:GLY:N	2.32	0.43
1:C:350:ASP:OD2	1:C:403:ARG:CG	2.67	0.43
1:D:100:ILE:CG2	1:D:101:LEU:N	2.80	0.43
1:D:180:GLN:HE21	1:D:474:GLY:HA3	1.82	0.43
1:D:209:TRP:CE3	1:D:209:TRP:N	2.81	0.43
1:D:332:GLU:OE1	1:D:444:HIS:NE2	2.43	0.43
1:D:517:ARG:O	1:D:518:ASP:C	2.62	0.43
1:A:100:ILE:HG23	1:A:101:LEU:N	2.33	0.43
1:A:127:ARG:HD2	1:B:128:GLU:OE1	2.18	0.43
1:B:595:ILE:O	1:B:595:ILE:HG22	2.18	0.43
1:C:146:ALA:HB1	1:C:627:THR:CA	2.38	0.43
1:C:147:GLY:O	1:C:624:THR:HG23	2.18	0.43
1:C:179:ARG:HH21	1:C:471:HIS:CE1	2.36	0.43
1:A:184:LEU:CD2	1:A:188:LEU:HG	2.48	0.43
1:A:273:TRP:C	1:A:275:ALA:N	2.72	0.43
1:A:371:LYS:HA	1:A:374:HIS:CD2	2.53	0.43
1:A:577:LYS:HG2	1:A:582:TYR:CE2	2.53	0.43
1:A:662:ILE:O	1:A:662:ILE:HG22	2.18	0.43
1:A:670:GLN:OE1	1:A:673:HIS:NE2	2.45	0.43
1:C:106:PHE:HE2	1:C:150:LEU:HB2	1.83	0.43
1:C:226:GLU:OE1	1:C:291:GLU:HG2	2.18	0.43
1:C:389:VAL:HG21	1:C:397:TYR:CE1	2.53	0.43
1:D:268:ASP:C	1:D:269:VAL:HG12	2.43	0.43
1:D:422:MET:HE1	1:D:470:LEU:CD1	2.48	0.43
1:A:547:PHE:CG	1:A:583:TYR:HD2	2.36	0.43
1:C:188:LEU:HB2	1:C:360:LEU:HD21	2.00	0.43
1:C:277:ASP:O	1:C:279:VAL:N	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ILE:HD11	1:C:496:PHE:HE2	1.83	0.43
1:C:372:GLU:CG	1:C:373:TRP:N	2.81	0.43
1:C:379:THR:O	1:C:380:ILE:C	2.61	0.43
1:D:111:ASN:HB3	1:D:113:LYS:HG2	2.01	0.43
1:D:143:MET:HE3	1:D:523:LEU:CD2	2.34	0.43
1:D:270:SER:O	1:D:271:ASP:C	2.61	0.43
1:D:289:TYR:HA	1:D:290:PRO:HD3	1.91	0.43
1:D:333:TRP:O	1:D:339:PRO:HG2	2.18	0.43
1:D:430:THR:OG1	1:D:432:VAL:HG23	2.18	0.43
1:D:599:LEU:HD23	1:D:649:PRO:HB2	2.01	0.43
1:A:132:ARG:HG3	1:A:132:ARG:HH11	1.83	0.43
1:A:188:LEU:HB3	1:A:360:LEU:HD11	1.99	0.43
1:A:463:ALA:O	1:A:484:LYS:HB2	2.19	0.43
1:B:412:ALA:O	1:B:413:GLY:C	2.60	0.43
1:C:248:LEU:O	1:C:376:PHE:HA	2.19	0.43
1:D:165:PHE:CG	1:D:262:PRO:HG3	2.53	0.43
1:D:220:GLY:O	1:D:221:ALA:C	2.62	0.43
1:D:673:HIS:CG	1:D:674:TYR:N	2.85	0.43
1:A:460:LEU:N	1:A:460:LEU:CD2	2.82	0.43
1:B:325:ILE:CG2	1:B:326:PHE:H	2.23	0.43
1:B:437:PHE:C	1:B:439:ARG:H	2.27	0.43
1:C:185:HIS:O	1:C:186:ASN:C	2.62	0.43
1:C:594:VAL:HG23	1:C:595:ILE:N	2.34	0.43
1:D:136:ASN:HB3	1:D:542:GLU:CD	2.41	0.43
1:D:164:THR:C	1:D:167:GLU:H	2.26	0.43
1:D:215:GLY:O	1:D:216:VAL:CG2	2.66	0.43
1:D:301:VAL:HG21	1:D:376:PHE:CZ	2.54	0.43
1:D:553:TYR:C	1:D:555:TRP:H	2.27	0.43
1:B:127:ARG:CG	1:B:127:ARG:HH11	2.32	0.43
1:B:181:ASN:HA	1:B:182:PRO:HD3	1.71	0.43
1:B:326:PHE:CG	1:B:501:PRO:HB3	2.54	0.43
1:C:209:TRP:HA	1:C:212:LEU:CB	2.49	0.43
1:C:390:ILE:HG12	1:C:396:VAL:HG22	2.01	0.43
1:D:151:GLU:O	1:D:273:TRP:HA	2.18	0.43
1:D:556:ASN:HD22	1:D:557:PRO:N	2.17	0.43
1:B:336:PHE:CE1	1:B:454:THR:HA	2.53	0.43
1:B:414:ASN:O	1:B:415:SER:C	2.60	0.43
1:B:493:ASP:O	1:B:494:ILE:C	2.60	0.43
1:C:138:GLN:HE21	1:C:539:THR:HG21	1.79	0.43
1:C:154:PRO:O	1:C:155:ILE:HB	2.18	0.43
1:C:202:HIS:CA	1:C:368:TYR:O	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:HA	1:D:203:THR:HG21	2.01	0.43
1:D:332:GLU:HB3	1:D:442:ARG:HG3	2.01	0.43
1:D:347:LYS:O	1:D:348:ALA:C	2.62	0.43
1:A:181:ASN:HD22	1:A:184:LEU:HB2	1.81	0.43
1:A:390:ILE:HG12	1:A:396:VAL:HG22	2.01	0.43
1:A:648:LYS:HB2	1:A:661:TYR:HB2	1.99	0.43
1:B:154:PRO:HB3	1:B:270:SER:HA	2.00	0.43
1:B:226:GLU:HG3	1:B:293:LYS:NZ	2.34	0.43
1:B:528:THR:O	1:B:530:LEU:HD22	2.19	0.43
1:C:148:ILE:HA	1:C:622:VAL:O	2.19	0.43
1:C:155:ILE:HG21	1:C:528:THR:HG21	2.01	0.43
1:C:298:ILE:HD13	1:C:380:ILE:HD11	2.01	0.43
1:D:329:VAL:HG13	1:D:453:ILE:HD11	2.01	0.43
1:D:331:LYS:HD3	1:D:331:LYS:HA	1.90	0.43
1:A:217:ASN:ND2	1:A:674:TYR:OH	2.52	0.42
1:A:261:ILE:HG22	1:A:392:ALA:HB2	1.99	0.42
1:C:344:PHE:CD1	1:C:422:MET:HG3	2.53	0.42
1:C:548:SER:OG	1:C:581:TYR:HB2	2.18	0.42
1:D:221:ALA:HB1	1:D:289:TYR:CZ	2.53	0.42
1:D:266:LYS:HZ2	1:D:267:ARG:C	2.26	0.42
1:D:404:GLY:C	1:D:406:GLY:N	2.77	0.42
1:D:648:LYS:HE2	1:D:657:THR:HG21	1.99	0.42
1:A:337:ASN:C	1:A:339:PRO:HD3	2.45	0.42
1:A:664:ASP:OD1	1:D:439:ARG:NH2	2.52	0.42
1:B:159:GLN:OE1	1:B:281:GLU:HG3	2.19	0.42
1:B:191:ILE:HA	1:B:194:THR:CG2	2.49	0.42
1:B:325:ILE:HD11	1:B:496:PHE:CE2	2.54	0.42
1:C:189:LEU:HD22	1:C:193:HIS:NE2	2.34	0.42
1:D:235:ASP:OD1	1:D:235:ASP:N	2.53	0.42
1:D:641:GLU:HB2	1:D:645:TRP:HE1	1.84	0.42
1:A:180:GLN:OE1	1:A:354:THR:HG21	2.19	0.42
1:A:664:ASP:O	1:A:665:LYS:O	2.37	0.42
1:C:163:LYS:C	1:C:165:PHE:H	2.27	0.42
1:C:349:TRP:CZ2	1:C:417:LEU:HD23	2.53	0.42
1:C:366:LYS:HD3	1:C:378:ASP:OD1	2.19	0.42
1:C:422:MET:HE2	1:C:422:MET:CA	2.30	0.42
1:D:650:ASP:OD2	1:D:653:ILE:HG12	2.19	0.42
1:A:138:GLN:HB2	1:A:542:GLU:CD	2.44	0.42
1:A:330:ARG:O	1:A:331:LYS:C	2.62	0.42
1:A:361:ILE:HD11	1:A:417:LEU:HB2	2.01	0.42
1:A:364:ILE:HG21	1:A:416:MET:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ALA:HB2	1:A:566:VAL:HG11	2.00	0.42
1:B:141:THR:O	1:B:144:SER:HB2	2.19	0.42
1:C:187:LYS:H	1:C:187:LYS:HG3	1.70	0.42
1:C:325:ILE:O	1:C:326:PHE:C	2.62	0.42
1:C:349:TRP:CZ3	1:C:475:LYS:HD2	2.55	0.42
1:C:538:THR:HB	1:C:539:THR:H	1.72	0.42
1:D:166:HIS:HE2	1:D:393:ASP:CG	2.27	0.42
1:D:462:PHE:O	1:D:466:GLY:HA3	2.19	0.42
1:D:648:LYS:HB2	1:D:661:TYR:CB	2.33	0.42
1:A:280:VAL:O	1:A:280:VAL:CG1	2.67	0.42
1:A:361:ILE:HD12	1:A:361:ILE:N	2.34	0.42
1:A:590:ALA:HA	1:A:593:ASP:HB3	2.01	0.42
1:B:332:GLU:O	1:B:336:PHE:HD2	2.03	0.42
1:C:142:ILE:O	1:C:145:SER:HB2	2.19	0.42
1:C:188:LEU:HD22	1:C:420:LEU:HB3	2.02	0.42
1:C:192:PHE:O	1:C:195:ILE:HG13	2.19	0.42
1:C:323:PHE:CE1	1:C:324:ASN:ND2	2.87	0.42
1:C:334:ASP:C	1:C:336:PHE:N	2.78	0.42
1:D:155:ILE:O	1:D:155:ILE:CG2	2.68	0.42
1:D:264:ASN:O	1:D:265:GLU:HB2	2.20	0.42
1:D:349:TRP:CZ3	1:D:475:LYS:HD2	2.54	0.42
1:D:354:THR:HG22	1:D:356:LYS:N	2.30	0.42
1:D:593:ASP:OD1	1:D:667:PHE:HA	2.18	0.42
1:A:274:GLN:HA	1:A:620:LEU:HD21	2.01	0.42
1:B:570:GLN:OE1	1:B:573:THR:HG21	2.19	0.42
1:C:96:HIS:CE1	1:D:383:HIS:ND1	2.88	0.42
1:C:156:VAL:O	1:C:266:LYS:HA	2.20	0.42
1:C:370:LYS:HE3	1:C:372:GLU:CG	2.49	0.42
1:C:516:GLY:HA2	1:C:555:TRP:CZ2	2.54	0.42
1:C:541:TYR:O	1:C:545:VAL:HG23	2.19	0.42
1:D:200:LEU:HA	1:D:203:THR:CG2	2.50	0.42
1:D:401:GLY:O	1:D:402:GLN:CB	2.68	0.42
1:A:590:ALA:HA	1:A:593:ASP:CB	2.50	0.42
1:B:143:MET:CE	1:B:523:LEU:HD22	2.40	0.42
1:B:244:LEU:HD22	1:B:248:LEU:CD2	2.43	0.42
1:C:206:GLU:HA	1:C:301:VAL:HA	2.02	0.42
1:D:184:LEU:O	1:D:188:LEU:N	2.41	0.42
1:D:230:ILE:HG13	1:D:292:ALA:HB1	2.00	0.42
1:D:252:ARG:HE	1:D:252:ARG:HB2	1.49	0.42
1:D:344:PHE:CD1	1:D:422:MET:HG3	2.54	0.42
1:D:626:HIS:CB	1:D:630:ARG:HD3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLN:NE2	1:B:138:GLN:CA	2.80	0.42
1:B:261:ILE:HG22	1:B:392:ALA:HB2	2.01	0.42
1:B:574:ASP:HB3	1:B:575:PRO:HD2	2.02	0.42
1:C:169:ILE:O	1:C:171:ASP:N	2.45	0.42
1:C:192:PHE:O	1:C:193:HIS:C	2.63	0.42
1:C:479:ILE:N	1:C:479:ILE:CD1	2.79	0.42
1:D:108:GLY:HA2	1:D:119:GLY:HA2	2.02	0.42
1:D:514:MET:HE1	1:D:554:SER:OG	2.20	0.42
1:A:189:LEU:HD22	1:A:193:HIS:CD2	2.55	0.42
1:B:126:ASP:HB2	1:B:132:ARG:HG2	2.02	0.42
1:B:369:TYR:O	1:B:374:HIS:NE2	2.50	0.42
1:B:605:THR:O	1:B:606:GLY:C	2.62	0.42
1:B:652:LEU:O	1:B:653:ILE:C	2.63	0.42
1:C:113:LYS:N	1:D:174:ASP:OD1	2.51	0.42
1:C:120:LYS:HB2	1:D:395:GLU:OE2	2.20	0.42
1:C:222:ALA:C	1:C:226:GLU:HB3	2.45	0.42
1:C:235:ASP:OD1	1:C:235:ASP:N	2.49	0.42
1:C:672:LYS:C	1:C:673:HIS:HD1	2.28	0.42
1:D:195:ILE:C	1:D:195:ILE:HD12	2.45	0.42
1:D:657:THR:O	1:D:659:HIS:ND1	2.50	0.42
1:A:143:MET:HE1	1:A:523:LEU:HB3	2.01	0.42
1:A:244:LEU:HD22	1:A:248:LEU:HD22	2.00	0.42
1:B:144:SER:O	1:B:145:SER:C	2.62	0.42
1:B:212:LEU:HD11	1:B:299:THR:HG22	2.02	0.42
1:B:309:GLN:N	1:B:310:PRO:CD	2.83	0.42
1:B:443:ILE:HG12	1:B:444:HIS:N	2.35	0.42
1:C:237:GLU:O	1:C:239:HIS:N	2.52	0.42
1:D:266:LYS:CE	1:D:269:VAL:CG1	2.87	0.42
1:D:316:TYR:C	1:D:318:GLY:N	2.78	0.42
1:D:342:VAL:HG11	1:D:462:PHE:CD2	2.55	0.42
1:A:273:TRP:O	1:A:274:GLN:C	2.62	0.41
1:A:455:GLU:O	1:A:456:LYS:C	2.62	0.41
1:A:575:PRO:CG	1:A:583:TYR:CZ	2.99	0.41
1:A:610:LEU:CD1	1:A:614:ASN:ND2	2.83	0.41
1:A:646:LEU:O	1:A:649:PRO:HD2	2.19	0.41
1:B:266:LYS:NZ	1:B:530:LEU:HD23	2.34	0.41
1:B:355:SER:HB3	1:B:385:THR:HG23	2.02	0.41
1:B:486:LYS:HB2	1:B:486:LYS:HE3	1.91	0.41
1:B:504:VAL:HG13	1:B:602:LEU:CD1	2.50	0.41
1:C:127:ARG:NH2	1:D:261:ILE:HD12	2.35	0.41
1:C:165:PHE:O	1:C:167:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:THR:HA	1:C:300:LYS:HE2	2.02	0.41
1:C:313:ILE:HB	1:C:316:TYR:HB2	2.00	0.41
1:C:376:PHE:HD2	1:C:377:ILE:HG13	1.85	0.41
1:D:243:GLN:HG3	1:D:247:ASP:OD2	2.20	0.41
1:D:482:GLY:O	1:D:483:GLU:C	2.63	0.41
1:D:483:GLU:HG3	1:D:484:LYS:H	1.85	0.41
1:D:626:HIS:O	1:D:627:THR:C	2.63	0.41
1:A:301:VAL:CG2	1:A:302:MET:HG3	2.50	0.41
1:A:389:VAL:HG11	1:A:397:TYR:CZ	2.54	0.41
1:C:224:PHE:C	1:C:226:GLU:H	2.28	0.41
1:D:139:ILE:O	1:D:143:MET:HB2	2.20	0.41
1:D:177:GLU:OE1	1:D:354:THR:HG23	2.20	0.41
1:D:221:ALA:O	1:D:222:ALA:C	2.61	0.41
1:A:231:GLY:O	1:A:234:LEU:HB2	2.21	0.41
1:A:298:ILE:HD13	1:A:380:ILE:HD11	2.01	0.41
1:A:333:TRP:CZ2	1:A:339:PRO:HB2	2.55	0.41
1:A:648:LYS:CD	1:A:659:HIS:HB2	2.50	0.41
1:B:551:LEU:HD22	1:B:594:VAL:CG2	2.49	0.41
1:B:583:TYR:O	1:B:583:TYR:CD1	2.73	0.41
1:C:246:ARG:HH11	1:C:246:ARG:HB2	1.85	0.41
1:C:370:LYS:HE3	1:C:372:GLU:OE2	2.19	0.41
1:C:506:TRP:CE2	1:C:597:ARG:HD2	2.55	0.41
1:D:426:PHE:CD2	1:D:437:PHE:HE1	2.39	0.41
1:A:556:ASN:CG	1:A:559:VAL:HG23	2.45	0.41
1:B:213:GLU:OE2	1:B:234:LEU:HD13	2.20	0.41
1:B:237:GLU:O	1:B:240:LEU:HB2	2.20	0.41
1:B:442:ARG:HG2	1:B:442:ARG:NH1	2.35	0.41
1:B:535:GLU:C	1:B:537:GLY:N	2.76	0.41
1:B:623:TRP:CD1	1:B:623:TRP:C	2.97	0.41
1:C:249:LYS:HG3	1:C:373:TRP:CE3	2.56	0.41
1:C:309:GLN:NE2	1:C:319:LYS:HE2	2.34	0.41
1:C:393:ASP:O	1:D:124:GLN:HG3	2.20	0.41
1:D:169:ILE:O	1:D:172:LYS:O	2.38	0.41
1:D:200:LEU:O	1:D:201:LYS:C	2.63	0.41
1:D:244:LEU:HD21	1:D:254:ILE:CD1	2.51	0.41
1:D:283:ARG:HA	1:D:284:PRO:HD3	1.92	0.41
1:D:363:GLU:H	1:D:363:GLU:HG2	1.73	0.41
1:A:153:LEU:HB3	1:A:524:SER:OG	2.20	0.41
1:B:592:LYS:HB2	1:B:598:ASN:HD21	1.84	0.41
1:C:167:GLU:O	1:C:171:ASP:OD2	2.38	0.41
1:C:168:ALA:O	1:C:169:ILE:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ALA:O	1:C:171:ASP:HB2	2.20	0.41
1:D:416:MET:O	1:D:419:VAL:HG22	2.20	0.41
1:A:191:ILE:HD11	1:A:434:TYR:CE1	2.55	0.41
1:A:586:ASP:HA	1:A:587:PRO:HD3	1.89	0.41
1:A:589:GLY:O	1:A:592:LYS:CB	2.68	0.41
1:A:591:TYR:O	1:A:595:ILE:HB	2.21	0.41
1:B:502:VAL:HA	1:B:503:PRO:HD3	1.91	0.41
1:C:419:VAL:CG2	1:C:420:LEU:N	2.82	0.41
1:D:205:GLY:O	1:D:206:GLU:C	2.63	0.41
1:D:252:ARG:HG3	1:D:253:LYS:HE2	2.03	0.41
1:A:107:GLN:N	1:A:151:GLU:OE2	2.46	0.41
1:A:347:LYS:HE2	1:A:477:GLN:O	2.21	0.41
1:A:538:THR:CG2	1:A:540:ALA:HB3	2.51	0.41
1:B:200:LEU:HA	1:B:203:THR:HG21	2.03	0.41
1:B:452:LEU:HD23	1:B:452:LEU:O	2.20	0.41
1:C:211:GLN:O	1:C:214:ALA:CB	2.69	0.41
1:C:212:LEU:O	1:C:216:VAL:CG1	2.69	0.41
1:C:269:VAL:HG21	1:C:273:TRP:CE2	2.55	0.41
1:D:109:ASN:CB	1:D:273:TRP:NE1	2.81	0.41
1:D:260:ALA:C	1:D:261:ILE:CG2	2.93	0.41
1:D:625:LYS:HG3	1:D:626:HIS:CD2	2.56	0.41
1:D:648:LYS:HE2	1:D:653:ILE:HG22	2.03	0.41
1:D:648:LYS:N	1:D:649:PRO:CD	2.84	0.41
1:A:570:GLN:OE1	1:A:573:THR:HG21	2.20	0.41
1:B:502:VAL:CG2	1:B:516:GLY:HA3	2.51	0.41
1:B:647:VAL:HG23	1:B:653:ILE:HG21	2.01	0.41
1:B:650:ASP:O	1:B:651:ARG:C	2.63	0.41
1:C:289:TYR:HA	1:C:290:PRO:HD3	2.00	0.41
1:C:383:HIS:C	1:C:385:THR:N	2.79	0.41
1:C:470:LEU:O	1:C:473:ALA:N	2.51	0.41
1:D:257:TYR:O	1:D:291:GLU:OE2	2.38	0.41
1:D:591:TYR:O	1:D:595:ILE:HG12	2.20	0.41
1:D:592:LYS:HA	1:D:597:ARG:O	2.21	0.41
1:D:645:TRP:HA	1:D:645:TRP:HE3	1.85	0.41
1:A:165:PHE:CD1	1:A:262:PRO:HD3	2.56	0.41
1:A:313:ILE:HA	1:A:314:PRO:HD3	1.93	0.41
1:A:432:VAL:HG21	1:A:440:VAL:HG21	2.03	0.41
1:A:460:LEU:HD23	1:A:460:LEU:N	2.36	0.41
1:B:180:GLN:HG2	1:B:473:ALA:O	2.21	0.41
1:B:341:ALA:HB3	1:B:488:ALA:HB3	2.02	0.41
1:B:387:VAL:HA	1:B:388:PRO:HD3	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:PHE:CD1	1:B:667:PHE:N	2.88	0.41
1:C:165:PHE:CE2	1:C:169:ILE:HG13	2.56	0.41
1:C:178:ASN:HD22	1:C:352:GLN:HA	1.86	0.41
1:C:181:ASN:HD21	1:C:184:LEU:N	2.17	0.41
1:C:195:ILE:HG13	1:C:195:ILE:H	1.79	0.41
1:C:211:GLN:C	1:C:213:GLU:N	2.76	0.41
1:C:289:TYR:CB	1:C:406:GLY:HA3	2.51	0.41
1:C:374:HIS:C	1:C:376:PHE:N	2.65	0.41
1:C:605:THR:O	1:C:606:GLY:C	2.64	0.41
1:C:612:ASN:C	1:C:614:ASN:H	2.27	0.41
1:D:130:ARG:H	1:D:130:ARG:HG2	1.60	0.41
1:D:175:LYS:NZ	1:D:178:ASN:ND2	2.69	0.41
1:D:195:ILE:CG2	1:D:423:MET:HE1	2.51	0.41
1:D:195:ILE:HG21	1:D:423:MET:HE1	2.03	0.41
1:D:204:TYR:CZ	1:D:310:PRO:HD2	2.47	0.41
1:D:224:PHE:CD2	1:D:225:LEU:N	2.89	0.41
1:D:330:ARG:NH1	1:D:491:PHE:CB	2.84	0.41
1:D:470:LEU:HA	1:D:473:ALA:HB3	2.03	0.41
1:D:479:ILE:C	1:D:481:GLU:N	2.68	0.41
1:D:480:THR:HG23	1:D:481:GLU:OE2	2.21	0.41
1:D:594:VAL:HG23	1:D:595:ILE:HD13	2.02	0.41
1:D:608:GLU:O	1:D:608:GLU:HG3	2.20	0.41
1:A:201:LYS:HD2	1:A:367:TYR:CZ	2.56	0.41
1:A:289:TYR:HA	1:A:290:PRO:HD3	1.79	0.41
1:A:468:GLN:O	1:A:472:GLU:HG2	2.20	0.41
1:A:555:TRP:CH2	1:A:613:LEU:CD1	3.04	0.41
1:B:422:MET:HE1	1:B:470:LEU:HD11	2.03	0.41
1:B:508:ASP:OD2	1:B:510:THR:HG23	2.21	0.41
1:B:570:GLN:HB3	1:B:573:THR:HG21	2.01	0.41
1:C:296:LEU:HD12	1:C:296:LEU:HA	1.86	0.41
1:D:115:MET:O	1:D:116:LEU:C	2.64	0.41
1:D:223:GLY:HA2	1:D:289:TYR:CE1	2.56	0.41
1:D:569:GLN:O	1:D:570:GLN:C	2.63	0.41
1:A:223:GLY:O	1:A:259:THR:HG21	2.21	0.40
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.85	0.40
1:C:356:LYS:HE2	1:C:356:LYS:HB3	1.86	0.40
1:C:370:LYS:CG	1:C:372:GLU:HB3	2.51	0.40
1:C:419:VAL:HG23	1:C:420:LEU:N	2.36	0.40
1:C:592:LYS:HD3	1:C:592:LYS:O	2.20	0.40
1:D:244:LEU:CD2	1:D:248:LEU:HD22	2.47	0.40
1:D:410:THR:HG22	1:D:411:SER:N	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:THR:HG22	1:D:617:LEU:HD21	2.03	0.40
1:D:534:GLY:O	1:D:535:GLU:C	2.64	0.40
1:D:547:PHE:HZ	1:D:668:THR:CG2	2.31	0.40
1:D:551:LEU:HD12	1:D:581:TYR:CD1	2.56	0.40
1:D:582:TYR:O	1:D:582:TYR:CG	2.73	0.40
1:A:181:ASN:HD21	1:A:184:LEU:CG	2.33	0.40
1:A:210:GLU:CD	1:A:210:GLU:N	2.78	0.40
1:A:320:THR:HA	1:A:321:PRO:HD3	1.97	0.40
1:A:361:ILE:HD11	1:A:417:LEU:HD13	2.03	0.40
1:A:648:LYS:H	1:A:649:PRO:HD3	1.84	0.40
1:B:209:TRP:HH2	1:B:241:VAL:HG11	1.86	0.40
1:B:223:GLY:O	1:B:224:PHE:C	2.65	0.40
1:C:400:ASN:HD22	1:C:400:ASN:HA	1.60	0.40
1:C:470:LEU:HA	1:C:470:LEU:HD23	1.88	0.40
1:D:94:ARG:CD	1:D:95:GLU:N	2.81	0.40
1:D:218:ARG:C	1:D:220:GLY:H	2.27	0.40
1:D:228:LYS:CB	1:D:233:VAL:HG23	2.51	0.40
1:A:181:ASN:ND2	1:A:184:LEU:CB	2.80	0.40
1:A:305:TRP:NE1	1:A:409:ASP:OD1	2.47	0.40
1:A:355:SER:O	1:A:358:LEU:HB2	2.21	0.40
1:B:161:ASP:OD1	1:B:161:ASP:C	2.64	0.40
1:B:258:GLU:O	1:B:389:VAL:HA	2.22	0.40
1:C:355:SER:HB3	1:C:385:THR:CG2	2.50	0.40
1:C:570:GLN:C	1:C:572:GLU:N	2.75	0.40
1:D:128:GLU:H	1:D:128:GLU:HG3	1.65	0.40
1:D:354:THR:N	1:D:357:ASP:HB2	2.36	0.40
1:D:355:SER:HB3	1:D:385:THR:HG23	2.04	0.40
1:A:180:GLN:O	1:A:181:ASN:C	2.64	0.40
1:A:281:GLU:OE1	1:B:163:LYS:HG2	2.21	0.40
1:A:336:PHE:CE1	1:A:454:THR:HA	2.57	0.40
1:A:422:MET:HE1	1:A:470:LEU:CD1	2.51	0.40
1:A:446:CYS:CB	1:A:497:CYS:SG	3.10	0.40
1:B:208:THR:OG1	1:B:211:GLN:N	2.54	0.40
1:B:409:ASP:O	1:B:410:THR:C	2.64	0.40
1:B:603:LYS:HE2	1:B:604:ARG:NH2	2.36	0.40
1:B:648:LYS:O	1:B:649:PRO:C	2.64	0.40
1:C:209:TRP:CA	1:C:212:LEU:HB3	2.52	0.40
1:C:586:ASP:HA	1:C:587:PRO:HD3	1.92	0.40
1:D:313:ILE:O	1:D:314:PRO:C	2.65	0.40
1:A:222:ALA:O	1:A:226:GLU:HB3	2.21	0.40
1:A:263:LYS:HD2	1:A:287:ILE:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:LYS:O	1:A:672:LYS:CD	2.69	0.40
1:B:592:LYS:HD3	1:B:598:ASN:HD22	1.82	0.40
1:C:104:ILE:CG2	1:C:119:GLY:HA3	2.52	0.40
1:C:155:ILE:HD13	1:C:528:THR:HG21	2.04	0.40
1:C:204:TYR:HE2	1:C:368:TYR:HD2	1.68	0.40
1:C:299:THR:O	1:C:299:THR:HG22	2.22	0.40
1:D:164:THR:C	1:D:166:HIS:N	2.72	0.40
1:D:212:LEU:O	1:D:216:VAL:HG13	2.22	0.40
1:D:229:ASN:ND2	1:D:232:GLU:HB2	2.36	0.40
1:D:381:THR:HA	1:D:384:MET:CG	2.50	0.40
1:D:572:GLU:HG3	1:D:572:GLU:O	2.22	0.40
1:D:648:LYS:HD2	1:D:654:SER:HA	2.04	0.40

All (1) 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:C:199:THR:OG1	1:C:199:THR:OG1[10_666]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/601 (97%)	490 (84%)	72 (12%)	19 (3%)	3	17
1	B	581/601 (97%)	488 (84%)	67 (12%)	26 (4%)	2	12
1	C	577/601 (96%)	446 (77%)	84 (15%)	47 (8%)	1	3
1	D	569/601 (95%)	414 (73%)	95 (17%)	60 (10%)	0	2
All	All	2308/2404 (96%)	1838 (80%)	318 (14%)	152 (7%)	1	5

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PRO
1	A	221	ALA
1	A	224	PHE
1	A	276	GLY
1	A	277	ASP
1	A	310	PRO
1	A	401	GLY
1	A	483	GLU
1	A	536	ARG
1	A	665	LYS
1	B	126	ASP
1	B	130	ARG
1	B	202	HIS
1	B	224	PHE
1	B	237	GLU
1	C	118	PRO
1	C	174	ASP
1	C	176	SER
1	C	177	GLU
1	C	209	TRP
1	C	214	ALA
1	C	221	ALA
1	C	224	PHE
1	C	285	ARG
1	C	286	VAL
1	C	309	GLN
1	C	370	LYS
1	D	93	ILE
1	D	95	GLU
1	D	110	LEU
1	D	113	LYS
1	D	114	LYS
1	D	116	LEU
1	D	148	ILE
1	D	178	ASN
1	D	209	TRP
1	D	212	LEU
1	D	216	VAL
1	D	221	ALA
1	D	266	LYS
1	D	267	ARG
1	D	271	ASP
1	D	274	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	309	GLN
1	D	325	ILE
1	D	464	ASN
1	D	483	GLU
1	D	509	ASN
1	D	535	GLU
1	D	559	VAL
1	D	607	PHE
1	D	609	LYS
1	D	651	ARG
1	A	183	GLU
1	A	331	LYS
1	A	481	GLU
1	A	509	ASN
1	B	137	HIS
1	B	206	GLU
1	B	221	ALA
1	B	225	LEU
1	B	236	SER
1	B	253	LYS
1	B	401	GLY
1	B	405	SER
1	B	606	GLY
1	B	646	LEU
1	C	101	LEU
1	C	159	GLN
1	C	170	ARG
1	C	216	VAL
1	C	237	GLU
1	C	301	VAL
1	C	310	PRO
1	C	335	SER
1	C	384	MET
1	C	401	GLY
1	D	137	HIS
1	D	159	GLN
1	D	173	ILE
1	D	210	GLU
1	D	236	SER
1	D	253	LYS
1	D	270	SER
1	D	401	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	402	GLN
1	D	405	SER
1	D	465	LYS
1	D	482	GLY
1	D	536	ARG
1	D	627	THR
1	A	272	ASP
1	A	671	GLY
1	B	616	SER
1	B	637	ALA
1	C	155	ILE
1	C	164	THR
1	C	186	ASN
1	C	280	VAL
1	C	302	MET
1	C	402	GLN
1	C	456	LYS
1	C	508	ASP
1	D	146	ALA
1	D	206	GLU
1	D	237	GLU
1	A	96	HIS
1	B	154	PRO
1	B	184	LEU
1	B	227	LYS
1	B	235	ASP
1	B	277	ASP
1	C	153	LEU
1	C	278	LEU
1	D	111	ASN
1	D	115	MET
1	D	235	ASP
1	D	348	ALA
1	D	456	LYS
1	D	481	GLU
1	D	485	MET
1	D	510	THR
1	D	641	GLU
1	A	337	ASN
1	B	272	ASP
1	C	184	LEU
1	C	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	202	HIS
1	C	225	LEU
1	C	575	PRO
1	D	154	PRO
1	D	219	LYS
1	D	306	VAL
1	A	602	LEU
1	B	310	PRO
1	B	509	ASN
1	B	649	PRO
1	C	238	LYS
1	C	295	ARG
1	C	571	PRO
1	D	128	GLU
1	D	534	GLY
1	D	557	PRO
1	D	574	ASP
1	C	93	ILE
1	C	154	PRO
1	C	339	PRO
1	C	182	PRO
1	C	353	VAL
1	C	606	GLY
1	D	147	GLY
1	C	269	VAL

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	511/529 (97%)	447 (88%)	64 (12%)	4	20
1	B	511/529 (97%)	458 (90%)	53 (10%)	7	28
1	C	510/529 (96%)	444 (87%)	66 (13%)	4	19
1	D	503/529 (95%)	438 (87%)	65 (13%)	4	19
All	All	2035/2116 (96%)	1787 (88%)	248 (12%)	5	21

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	125	LEU
1	A	126	ASP
1	A	127	ARG
1	A	132	ARG
1	A	151	GLU
1	A	181	ASN
1	A	184	LEU
1	A	189	LEU
1	A	199	THR
1	A	216	VAL
1	A	229	ASN
1	A	230	ILE
1	A	244	LEU
1	A	248	LEU
1	A	265	GLU
1	A	274	GLN
1	A	277	ASP
1	A	280	VAL
1	A	286	VAL
1	A	296	LEU
1	A	301	VAL
1	A	319	LYS
1	A	322	LEU
1	A	325	ILE
1	A	340	VAL
1	A	347	LYS
1	A	351	THR
1	A	352	GLN
1	A	354	THR
1	A	360	LEU
1	A	378	ASP
1	A	385	THR
1	A	445	VAL
1	A	452	LEU
1	A	454	THR
1	A	460	LEU
1	A	468	GLN
1	A	480	THR
1	A	483	GLU
1	A	495	GLU
1	A	526	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	530	LEU
1	A	535	GLU
1	A	539	THR
1	A	550	LEU
1	A	556	ASN
1	A	558	LEU
1	A	572	GLU
1	A	574	ASP
1	A	580	THR
1	A	599	LEU
1	A	600	SER
1	A	602	LEU
1	A	607	PHE
1	A	610	LEU
1	A	615	LEU
1	A	619	THR
1	A	625	LYS
1	A	646	LEU
1	A	647	VAL
1	A	648	LYS
1	A	653	ILE
1	A	655	SER
1	B	125	LEU
1	B	127	ARG
1	B	130	ARG
1	B	132	ARG
1	B	151	GLU
1	B	160	THR
1	B	183	GLU
1	B	184	LEU
1	B	189	LEU
1	B	194	THR
1	B	199	THR
1	B	203	THR
1	B	227	LYS
1	B	229	ASN
1	B	244	LEU
1	B	248	LEU
1	B	253	LYS
1	B	254	ILE
1	B	261	ILE
1	B	283	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	284	PRO
1	B	286	VAL
1	B	296	LEU
1	B	301	VAL
1	B	322	LEU
1	B	340	VAL
1	B	351	THR
1	B	352	GLN
1	B	354	THR
1	B	360	LEU
1	B	378	ASP
1	B	385	THR
1	B	419	VAL
1	B	435	LYS
1	B	445	VAL
1	B	446	CYS
1	B	452	LEU
1	B	468	GLN
1	B	479	ILE
1	B	480	THR
1	B	526	MET
1	B	530	LEU
1	B	539	THR
1	B	550	LEU
1	B	552	MET
1	B	556	ASN
1	B	558	LEU
1	B	573	THR
1	B	580	THR
1	B	602	LEU
1	B	619	THR
1	B	655	SER
1	B	664	ASP
1	C	107	GLN
1	C	115	MET
1	C	116	LEU
1	C	121	LEU
1	C	127	ARG
1	C	151	GLU
1	C	155	ILE
1	C	157	ARG
1	C	161	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	165	PHE
1	C	170	ARG
1	C	171	ASP
1	C	179	ARG
1	C	181	ASN
1	C	184	LEU
1	C	187	LYS
1	C	189	LEU
1	C	190	GLU
1	C	194	THR
1	C	197	GLN
1	C	199	THR
1	C	207	VAL
1	C	210	GLU
1	C	218	ARG
1	C	225	LEU
1	C	227	LYS
1	C	233	VAL
1	C	234	LEU
1	C	235	ASP
1	C	237	GLU
1	C	239	HIS
1	C	244	LEU
1	C	246	ARG
1	C	279	VAL
1	C	283	ARG
1	C	285	ARG
1	C	296	LEU
1	C	308	GLN
1	C	309	GLN
1	C	317	GLU
1	C	340	VAL
1	C	345	ASP
1	C	360	LEU
1	C	363	GLU
1	C	370	LYS
1	C	372	GLU
1	C	374	HIS
1	C	378	ASP
1	C	379	THR
1	C	380	ILE
1	C	400	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	439	ARG
1	C	468	GLN
1	C	479	ILE
1	C	497	CYS
1	C	508	ASP
1	C	539	THR
1	C	550	LEU
1	C	558	LEU
1	C	572	GLU
1	C	580	THR
1	C	600	SER
1	C	602	LEU
1	C	616	SER
1	C	636	VAL
1	C	652	LEU
1	D	110	LEU
1	D	112	THR
1	D	114	LYS
1	D	116	LEU
1	D	127	ARG
1	D	133	ASN
1	D	138	GLN
1	D	143	MET
1	D	181	ASN
1	D	183	GLU
1	D	184	LEU
1	D	189	LEU
1	D	197	GLN
1	D	199	THR
1	D	208	THR
1	D	209	TRP
1	D	213	GLU
1	D	227	LYS
1	D	229	ASN
1	D	233	VAL
1	D	240	LEU
1	D	244	LEU
1	D	252	ARG
1	D	253	LYS
1	D	255	LYS
1	D	264	ASN
1	D	269	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	271	ASP
1	D	291	GLU
1	D	293	LYS
1	D	296	LEU
1	D	304	ASN
1	D	307	LYS
1	D	317	GLU
1	D	319	LYS
1	D	325	ILE
1	D	340	VAL
1	D	352	GLN
1	D	372	GLU
1	D	380	ILE
1	D	410	THR
1	D	416	MET
1	D	439	ARG
1	D	445	VAL
1	D	446	CYS
1	D	452	LEU
1	D	479	ILE
1	D	497	CYS
1	D	509	ASN
1	D	536	ARG
1	D	538	THR
1	D	550	LEU
1	D	558	LEU
1	D	562	ILE
1	D	569	GLN
1	D	597	ARG
1	D	602	LEU
1	D	615	LEU
1	D	628	SER
1	D	630	ARG
1	D	631	ILE
1	D	632	ILE
1	D	664	ASP
1	D	667	PHE
1	D	672	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	136	ASN
1	A	137	HIS
1	A	181	ASN
1	A	185	HIS
1	A	202	HIS
1	A	211	GLN
1	A	217	ASN
1	A	229	ASN
1	A	239	HIS
1	A	243	GLN
1	A	324	ASN
1	A	337	ASN
1	A	352	GLN
1	A	365	GLN
1	A	438	ASN
1	A	509	ASN
1	A	513	HIS
1	A	598	ASN
1	A	612	ASN
1	B	109	ASN
1	B	117	ASN
1	B	137	HIS
1	B	138	GLN
1	B	178	ASN
1	B	197	GLN
1	B	229	ASN
1	B	274	GLN
1	B	337	ASN
1	B	352	GLN
1	B	365	GLN
1	B	468	GLN
1	B	499	HIS
1	B	513	HIS
1	B	556	ASN
1	B	569	GLN
1	B	598	ASN
1	C	117	ASN
1	C	138	GLN
1	C	178	ASN
1	C	181	ASN
1	C	186	ASN
1	C	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	239	HIS
1	C	243	GLN
1	C	304	ASN
1	C	308	GLN
1	C	400	ASN
1	C	407	GLN
1	C	468	GLN
1	C	499	HIS
1	C	513	HIS
1	C	556	ASN
1	C	569	GLN
1	C	670	GLN
1	D	96	HIS
1	D	111	ASN
1	D	124	GLN
1	D	138	GLN
1	D	159	GLN
1	D	178	ASN
1	D	202	HIS
1	D	229	ASN
1	D	243	GLN
1	D	264	ASN
1	D	324	ASN
1	D	359	GLN
1	D	365	GLN
1	D	418	ASN
1	D	464	ASN
1	D	468	GLN
1	D	513	HIS
1	D	556	ASN
1	D	569	GLN
1	D	612	ASN
1	D	633	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	583/601 (97%)	0.11	27 (4%) 37 20	8, 36, 78, 102	0
1	B	583/601 (97%)	0.15	26 (4%) 38 20	5, 37, 77, 102	0
1	C	581/601 (96%)	0.91	90 (15%) 5 3	19, 60, 96, 102	0
1	D	575/601 (95%)	0.64	73 (12%) 8 5	15, 53, 97, 102	0
All	All	2322/2404 (96%)	0.45	216 (9%) 14 7	5, 47, 92, 102	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	THR	6.7
1	C	198	PRO	5.1
1	A	607	PHE	5.1
1	C	210	GLU	4.9
1	D	160	THR	4.6
1	A	532	SER	4.5
1	C	203	THR	4.4
1	C	533	SER	4.4
1	C	375	LYS	4.3
1	C	211	GLN	4.3
1	C	147	GLY	4.3
1	A	509	ASN	4.3
1	B	674	TYR	4.2
1	D	291	GLU	4.1
1	D	268	ASP	4.0
1	A	223	GLY	4.0
1	C	284	PRO	4.0
1	D	673	HIS	3.9
1	A	277	ASP	3.9
1	C	161	ASP	3.9
1	D	232	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	GLY	3.8
1	D	129	GLY	3.8
1	C	236	SER	3.8
1	C	218	ARG	3.8
1	C	209	TRP	3.7
1	B	320	THR	3.7
1	C	160	THR	3.7
1	D	274	GLN	3.7
1	A	674	TYR	3.7
1	B	317	GLU	3.7
1	C	205	GLY	3.7
1	C	170	ARG	3.6
1	A	482	GLY	3.6
1	B	537	GLY	3.5
1	D	208	THR	3.5
1	C	474	GLY	3.5
1	B	239	HIS	3.5
1	D	161	ASP	3.5
1	B	535	GLU	3.4
1	C	324	ASN	3.4
1	A	536	ARG	3.4
1	C	674	TYR	3.4
1	C	109	ASN	3.4
1	B	572	GLU	3.4
1	A	320	THR	3.3
1	D	438	ASN	3.3
1	C	204	TYR	3.3
1	D	164	THR	3.3
1	D	231	GLY	3.2
1	A	531	ASP	3.2
1	D	255	LYS	3.2
1	C	253	LYS	3.2
1	A	481	GLU	3.2
1	C	367	TYR	3.2
1	D	371	LYS	3.1
1	A	211	GLN	3.1
1	D	151	GLU	3.1
1	C	309	GLN	3.1
1	D	467	MET	3.1
1	C	231	GLY	3.1
1	D	112	THR	3.1
1	D	270	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	290	PRO	3.1
1	C	529	ARG	3.1
1	D	92	VAL	3.1
1	C	463	ALA	3.0
1	D	96	HIS	3.0
1	A	309	GLN	3.0
1	C	185	HIS	3.0
1	C	530	LEU	3.0
1	C	229	ASN	3.0
1	C	285	ARG	3.0
1	B	147	GLY	3.0
1	C	208	THR	3.0
1	D	162	THR	3.0
1	A	492	GLU	2.9
1	D	163	LYS	2.9
1	D	115	MET	2.9
1	D	507	SER	2.9
1	C	132	ARG	2.9
1	C	174	ASP	2.9
1	D	126	ASP	2.9
1	C	226	GLU	2.9
1	C	237	GLU	2.9
1	C	265	GLU	2.9
1	D	157	ARG	2.9
1	D	210	GLU	2.9
1	D	213	GLU	2.8
1	C	371	LYS	2.8
1	D	271	ASP	2.8
1	C	230	ILE	2.8
1	D	244	LEU	2.8
1	D	197	GLN	2.8
1	D	236	SER	2.8
1	A	667	PHE	2.8
1	C	283	ARG	2.8
1	C	111	ASN	2.7
1	A	318	GLY	2.7
1	C	275	ALA	2.7
1	C	310	PRO	2.7
1	A	222	ALA	2.7
1	C	247	ASP	2.7
1	D	552	MET	2.7
1	D	237	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	320	THR	2.7
1	D	273	TRP	2.7
1	B	218	ARG	2.6
1	A	281	GLU	2.6
1	C	187	LYS	2.6
1	C	374	HIS	2.6
1	D	167	GLU	2.6
1	C	239	HIS	2.6
1	C	217	ASN	2.5
1	D	604	ARG	2.5
1	A	642	GLU	2.5
1	D	367	TYR	2.5
1	D	318	GLY	2.5
1	D	130	ARG	2.5
1	C	373	TRP	2.5
1	C	368	TYR	2.5
1	B	215	GLY	2.5
1	C	536	ARG	2.5
1	D	212	LEU	2.5
1	B	533	SER	2.5
1	C	228	LYS	2.5
1	D	219	LYS	2.5
1	C	166	HIS	2.5
1	D	137	HIS	2.5
1	A	214	ALA	2.4
1	C	268	ASP	2.4
1	D	375	LYS	2.4
1	D	239	HIS	2.4
1	C	280	VAL	2.4
1	D	533	SER	2.4
1	C	505	ARG	2.4
1	C	277	ASP	2.4
1	C	379	THR	2.4
1	D	109	ASN	2.4
1	C	124	GLN	2.4
1	B	252	ARG	2.4
1	B	658	GLY	2.4
1	D	123	GLU	2.4
1	D	667	PHE	2.4
1	D	248	LEU	2.4
1	C	481	GLU	2.4
1	C	401	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	673	HIS	2.3
1	D	218	ARG	2.3
1	D	233	VAL	2.3
1	C	575	PRO	2.3
1	C	171	ASP	2.3
1	B	197	GLN	2.3
1	B	532	SER	2.3
1	B	321	PRO	2.3
1	B	534	GLY	2.3
1	D	537	GLY	2.3
1	B	672	LYS	2.3
1	C	272	ASP	2.3
1	C	162	THR	2.2
1	D	111	ASN	2.2
1	C	446	CYS	2.2
1	D	214	ALA	2.2
1	A	323	PHE	2.2
1	C	673	HIS	2.2
1	D	633	GLN	2.2
1	C	206	GLU	2.2
1	C	363	GLU	2.2
1	C	235	ASP	2.2
1	A	639	GLY	2.2
1	C	175	LYS	2.2
1	D	179	ARG	2.2
1	B	210	GLU	2.2
1	B	132	ARG	2.2
1	B	209	TRP	2.2
1	C	222	ALA	2.2
1	B	318	GLY	2.2
1	C	430	THR	2.1
1	C	163	LYS	2.1
1	C	472	GLU	2.1
1	D	483	GLU	2.1
1	D	229	ASN	2.1
1	D	578	HIS	2.1
1	C	165	PHE	2.1
1	C	113	LYS	2.1
1	D	266	LYS	2.1
1	B	205	GLY	2.1
1	C	182	PRO	2.1
1	D	534	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	269	VAL	2.1
1	D	234	LEU	2.1
1	D	267	ARG	2.1
1	D	204	TYR	2.1
1	A	231	GLY	2.1
1	C	262	PRO	2.1
1	C	365	GLN	2.1
1	D	211	GLN	2.1
1	A	317	GLU	2.1
1	D	306	VAL	2.0
1	C	576	SER	2.0
1	C	264	ASN	2.0
1	A	480	THR	2.0
1	B	214	ALA	2.0
1	D	272	ASP	2.0
1	A	537	GLY	2.0
1	C	180	GLN	2.0
1	C	643	GLY	2.0
1	C	347	LYS	2.0
1	C	642	GLU	2.0
1	D	535	GLU	2.0
1	C	234	LEU	2.0
1	D	116	LEU	2.0
1	B	236	SER	2.0
1	C	667	PHE	2.0
1	C	308	GLN	2.0
1	C	213	GLU	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.