Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 08:13 AM EDT

PDB ID	:	5CSC
Title	:	STRUCTURE OF AN OPEN FORM OF CHICKEN HEART CITRATE SYNTHASE AT 2.8 ANGSTROMS RESOLUTION
Authors	:	Liao, D.-I.; Karpusas, M.; Remington, S.J.
Deposited on	:	1990-05-07
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

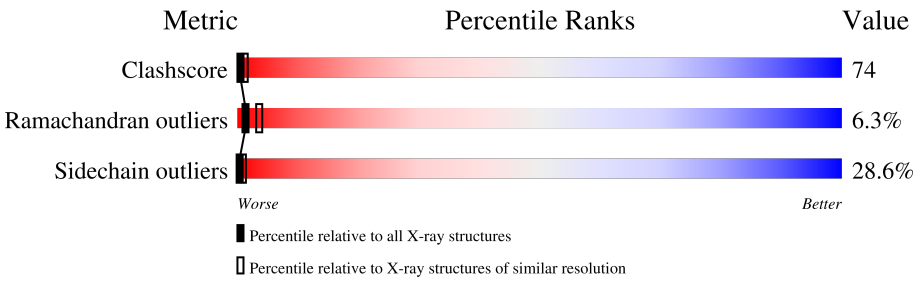
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	18% 42% 29% 10% •
2	B	429	18% 44% 28% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6606 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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3303	2112	571	603	17	0	0	0

- Molecule 2 is a protein called CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	429	3303	2112	571	603	17	0	0	0

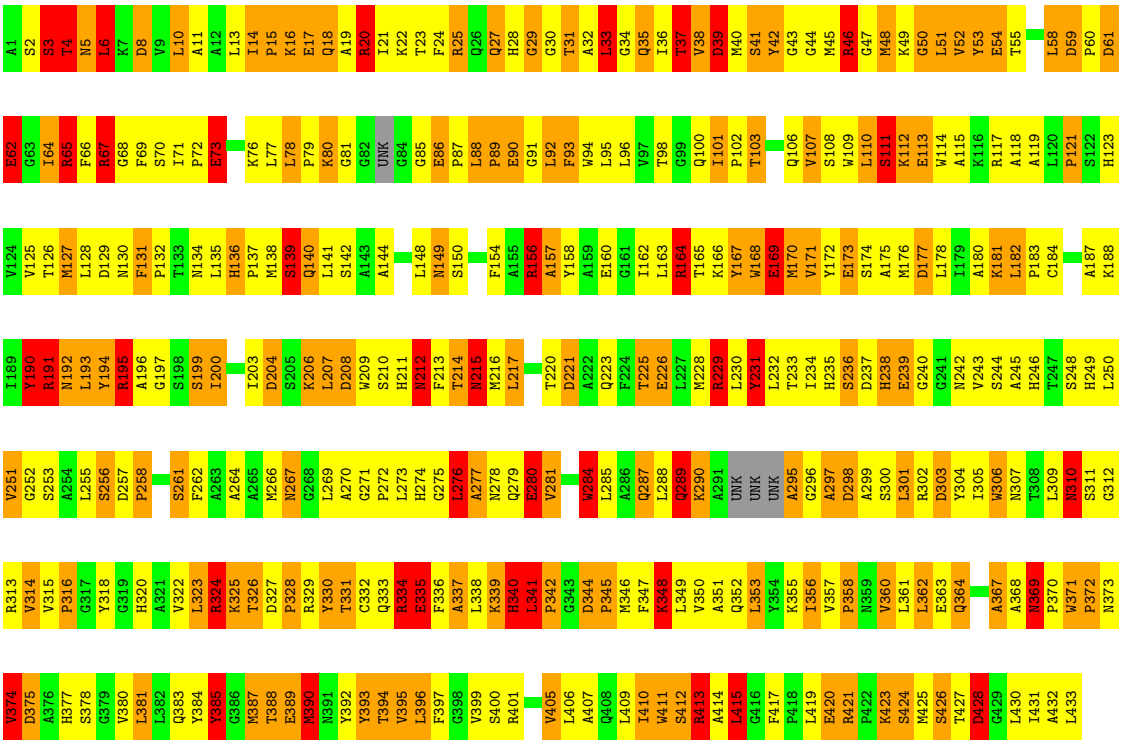
3 Residue-property plots (i)

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

Note EDS was not executed.

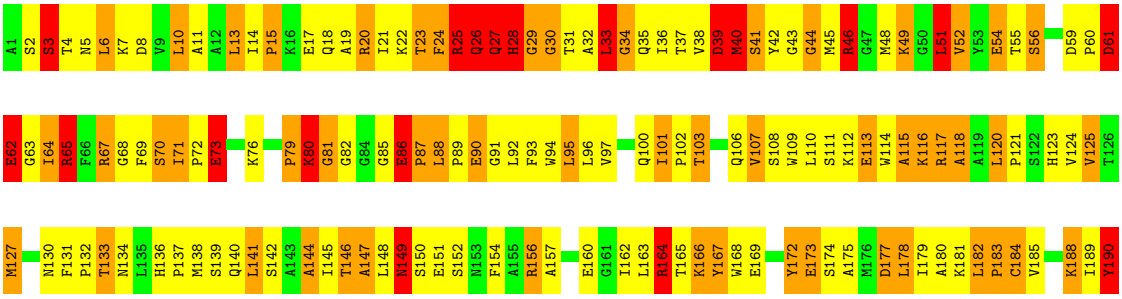
• Molecule 1: CITRATE SYNTHASE

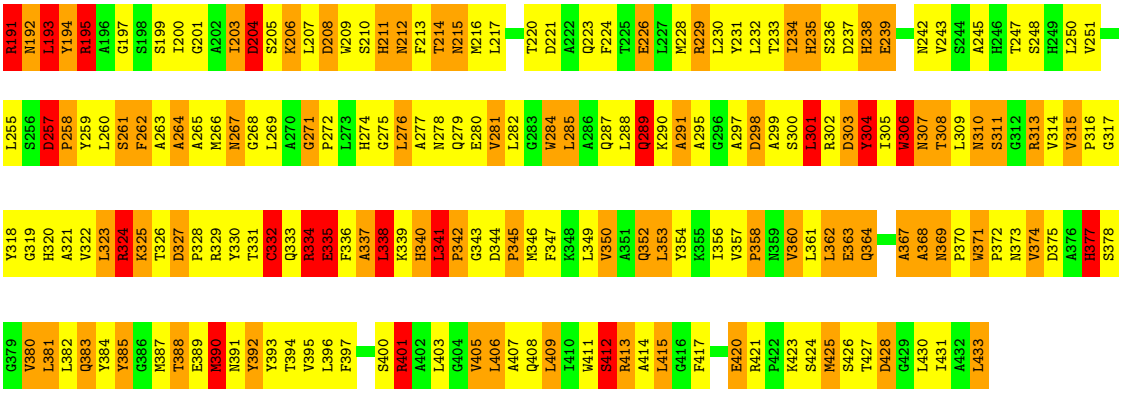
Chain A: 18% 42% 29% 10%



• Molecule 2: CITRATE SYNTHASE

Chain B: 18% 44% 28% 9%




R191 N192 L193 Y194 R195 A196 G197 S198 S199 I200 G201 A202 I203 D204 S205 K206 L207 D208 W209 S210 H211 N212 F213 T214 N215 M216 L217 T220 D221 A222 Q223 F224 T225 E226 L227 M228 R229 L230 Y231 L232 T233 I234 H235 S236 D237 H238 E239 N242 V243 S244 A245 H246 T247 S248 H249 L250 V251
L255 S256 D257 P258 Y259 L260 S261 F262 A263 A264 A265 M266 N267 G268 L269 A270 G271 P272 L273 H274 G275 L276 A277 N278 Q279 E280 V281 L282 G283 W284 L285 A286 Q287 L288 Q289 K290 A291 A295 G296 A297 D298 A299 S300 L301 R302 D303 Y304 I305 W306 N307 T308 L309 N310 S311 G312 R313 V314 V315 P316 G317
Y318 G319 H320 A321 V322 L323 R324 K325 T326 D327 P328 R329 Y330 T331 G332 Q333 R334 E335 F336 A337 L338 K339 H340 L341 P342 G343 D344 P345 M346 F347 K348 L349 V350 A351 Q352 L353 Y354 K355 I356 V357 P358 N359 V360 L361 L362 E363 Q364 A367 A368 N369 P370 W371 P372 N373 V374 D375 A376 H377 S378
G379 V380 L381 L382 Q383 Y384 Y385 G386 M387 T388 E389 H390 N391 Y392 Y393 T394 V395 L396 F397 S400 R401 A402 L403 G404 V405 L406 A407 Q408 L409 I410 W411 S412 R413 A414 L415 G416 F417 E420 R421 P422 K423 S424 M425 S426 T427 D428 G429 L430 I431 A432 L433

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	58.85Å 58.85Å 259.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6606	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.84	51/3383 (1.5%)	2.05	103/4594 (2.2%)
2	B	1.92	67/3383 (2.0%)	2.06	96/4594 (2.1%)
All	All	1.88	118/6766 (1.7%)	2.05	199/9188 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	7	5
2	B	5	3
All	All	12	8

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	363	GLU	CD-OE2	13.68	1.40	1.25
1	A	239	GLU	CD-OE2	10.55	1.37	1.25
2	B	173	GLU	CD-OE2	9.92	1.36	1.25
1	A	226	GLU	CD-OE2	9.82	1.36	1.25
1	A	73	GLU	CD-OE2	9.64	1.36	1.25
2	B	17	GLU	CD-OE2	9.58	1.36	1.25
2	B	239	GLU	CD-OE2	9.28	1.35	1.25
2	B	335	GLU	CD-OE2	8.95	1.35	1.25
2	B	151	GLU	CD-OE2	8.69	1.35	1.25
1	A	280	GLU	CD-OE2	8.60	1.35	1.25
2	B	86	GLU	CD-OE2	8.36	1.34	1.25
2	B	226	GLU	CD-OE2	8.29	1.34	1.25
2	B	412	SER	CA-CB	-8.13	1.40	1.52
2	B	20	ARG	CZ-NH1	8.07	1.43	1.33
1	A	160	GLU	CD-OE2	8.04	1.34	1.25
2	B	20	ARG	NE-CZ	7.68	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	GLU	CD-OE2	7.52	1.33	1.25
1	A	62	GLU	CD-OE2	7.46	1.33	1.25
1	A	330	TYR	CE2-CZ	7.33	1.48	1.38
1	A	375	ASP	CG-OD2	7.31	1.42	1.25
1	A	389	GLU	CD-OE2	7.26	1.33	1.25
1	A	156	ARG	CD-NE	7.18	1.58	1.46
2	B	28	HIS	C-N	7.12	1.45	1.33
1	A	17	GLU	CD-OE2	7.09	1.33	1.25
1	A	420	GLU	CD-OE2	7.07	1.33	1.25
2	B	317	GLY	CA-C	7.06	1.63	1.51
2	B	62	GLU	CD-OE2	7.00	1.33	1.25
2	B	268	GLY	CA-C	6.97	1.62	1.51
2	B	177	ASP	C-O	-6.86	1.10	1.23
1	A	330	TYR	CG-CD2	6.84	1.48	1.39
1	A	328	PRO	CA-C	-6.78	1.39	1.52
1	A	113	GLU	CD-OE2	6.72	1.33	1.25
1	A	330	TYR	CD1-CE1	6.67	1.49	1.39
1	A	17	GLU	CG-CD	-6.65	1.42	1.51
2	B	284	TRP	CD2-CE2	6.51	1.49	1.41
2	B	401	ARG	NE-CZ	-6.47	1.24	1.33
1	A	363	GLU	CD-OE2	6.46	1.32	1.25
1	A	78	LEU	C-N	6.46	1.46	1.34
2	B	208	ASP	CG-OD2	6.29	1.39	1.25
2	B	332	CYS	CB-SG	6.28	1.93	1.82
1	A	358	PRO	N-CD	6.26	1.56	1.47
1	A	411	TRP	CE2-CZ2	6.25	1.50	1.39
1	A	335	GLU	CD-OE2	6.24	1.32	1.25
2	B	211	HIS	N-CA	-6.17	1.34	1.46
1	A	89	PRO	N-CD	6.12	1.56	1.47
1	A	195	ARG	CZ-NH2	6.10	1.41	1.33
2	B	54	GLU	CD-OE1	-6.04	1.19	1.25
1	A	173	GLU	CD-OE2	6.02	1.32	1.25
1	A	47	GLY	CA-C	5.96	1.61	1.51
1	A	420	GLU	CD-OE1	-5.94	1.19	1.25
1	A	334	ARG	NE-CZ	5.92	1.40	1.33
2	B	24	PHE	C-N	5.92	1.47	1.34
2	B	67	ARG	CZ-NH1	5.91	1.40	1.33
1	A	364	GLN	C-N	5.91	1.43	1.33
2	B	34	GLY	N-CA	5.90	1.54	1.46
2	B	178	LEU	C-O	-5.90	1.12	1.23
2	B	33	LEU	N-CA	-5.86	1.34	1.46
1	A	199	SER	CA-CB	-5.80	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	CYS	CB-SG	5.78	1.92	1.82
2	B	377	HIS	CB-CG	-5.78	1.39	1.50
2	B	15	PRO	N-CD	5.77	1.55	1.47
2	B	195	ARG	CZ-NH1	5.76	1.40	1.33
2	B	342	PRO	C-N	5.74	1.43	1.33
2	B	271	GLY	N-CA	-5.72	1.37	1.46
2	B	28	HIS	CG-CD2	5.68	1.45	1.35
1	A	157	ALA	C-O	-5.67	1.12	1.23
1	A	277	ALA	N-CA	5.64	1.57	1.46
2	B	25	ARG	CZ-NH2	5.61	1.40	1.33
1	A	90	GLU	CD-OE1	-5.60	1.19	1.25
2	B	428	ASP	CG-OD2	5.59	1.38	1.25
2	B	115	ALA	C-O	5.58	1.33	1.23
1	A	81	GLY	C-N	5.57	1.43	1.33
1	A	156	ARG	N-CA	-5.53	1.35	1.46
1	A	54	GLU	CD-OE2	5.52	1.31	1.25
1	A	169	GLU	CD-OE1	-5.52	1.19	1.25
1	A	393	TYR	CB-CG	-5.52	1.43	1.51
2	B	44	GLY	C-N	5.46	1.46	1.34
2	B	95	LEU	C-N	5.45	1.46	1.34
1	A	367	ALA	CA-C	-5.45	1.38	1.52
2	B	278	ASN	C-N	5.45	1.46	1.34
1	A	27	GLN	N-CA	-5.45	1.35	1.46
2	B	103	THR	CB-OG1	5.44	1.54	1.43
2	B	182	LEU	C-N	-5.43	1.24	1.34
2	B	368	ALA	CA-C	5.42	1.67	1.52
2	B	160	GLU	CD-OE1	-5.40	1.19	1.25
2	B	311	SER	CB-OG	5.40	1.49	1.42
2	B	238	HIS	CB-CG	-5.39	1.40	1.50
1	A	324	ARG	NE-CZ	5.36	1.40	1.33
2	B	304	TYR	C-N	5.36	1.46	1.34
2	B	304	TYR	C-O	5.35	1.33	1.23
2	B	421	ARG	CZ-NH1	5.34	1.40	1.33
1	A	3	SER	CA-CB	-5.30	1.45	1.52
2	B	258	PRO	N-CD	5.30	1.55	1.47
2	B	358	PRO	CA-C	-5.30	1.42	1.52
1	A	395	VAL	C-O	-5.27	1.13	1.23
2	B	369	ASN	N-CA	-5.26	1.35	1.46
2	B	229	ARG	CZ-NH2	5.22	1.39	1.33
2	B	183	PRO	N-CA	-5.21	1.38	1.47
2	B	420	GLU	CD-OE1	-5.18	1.20	1.25
2	B	62	GLU	N-CA	-5.18	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	25	ARG	CZ-NH1	5.17	1.39	1.33
2	B	65	ARG	NE-CZ	5.16	1.39	1.33
2	B	62	GLU	C-O	5.15	1.33	1.23
1	A	296	GLY	N-CA	-5.12	1.38	1.46
1	A	150	SER	CA-CB	5.12	1.60	1.52
2	B	303	ASP	CG-OD2	5.11	1.37	1.25
1	A	127	MET	C-O	-5.11	1.13	1.23
2	B	364	GLN	C-O	5.10	1.33	1.23
2	B	306	TRP	NE1-CE2	5.08	1.44	1.37
1	A	164	ARG	CZ-NH2	5.07	1.39	1.33
2	B	30	GLY	CA-C	5.07	1.59	1.51
1	A	225	THR	C-O	-5.07	1.13	1.23
2	B	380	VAL	CA-CB	5.06	1.65	1.54
1	A	284	TRP	CA-CB	5.05	1.65	1.53
2	B	190	TYR	CE2-CZ	5.04	1.45	1.38
2	B	29	GLY	CA-C	5.01	1.59	1.51
2	B	190	TYR	CG-CD2	5.01	1.45	1.39
1	A	41	SER	CA-CB	5.01	1.60	1.52

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	117	ARG	NE-CZ-NH1	16.55	128.57	120.30
1	A	334	ARG	NE-CZ-NH1	15.57	128.09	120.30
2	B	421	ARG	NE-CZ-NH1	14.51	127.55	120.30
2	B	413	ARG	NE-CZ-NH1	13.73	127.17	120.30
2	B	413	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	A	334	ARG	NE-CZ-NH2	-13.04	113.78	120.30
2	B	8	ASP	CB-CG-OD2	-11.77	107.71	118.30
1	A	413	ARG	NE-CZ-NH2	-11.39	114.61	120.30
2	B	117	ARG	NE-CZ-NH2	-11.25	114.67	120.30
2	B	421	ARG	NE-CZ-NH2	-10.87	114.86	120.30
2	B	324	ARG	NE-CZ-NH1	-10.76	114.92	120.30
2	B	298	ASP	CB-CG-OD2	-10.66	108.70	118.30
1	A	20	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	A	324	ARG	CB-CA-C	10.05	130.50	110.40
2	B	65	ARG	NE-CZ-NH1	9.98	125.29	120.30
2	B	191	ARG	NE-CZ-NH2	-9.89	115.36	120.30
2	B	156	ARG	NE-CZ-NH1	9.64	125.12	120.30
2	B	315	VAL	C-N-CD	-9.63	99.41	120.60
1	A	257	ASP	CB-CG-OD2	-9.47	109.77	118.30
1	A	229	ARG	NE-CZ-NH1	9.43	125.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	A	39	ASP	CB-CG-OD1	9.11	126.50	118.30
1	A	59	ASP	CB-CG-OD1	9.11	126.50	118.30
1	A	229	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	413	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	304	TYR	CB-CG-CD1	-8.71	115.78	121.00
1	A	231	TYR	CB-CG-CD2	-8.66	115.81	121.00
1	A	107	VAL	CA-CB-CG2	-8.49	98.16	110.90
2	B	303	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	A	191	ARG	NE-CZ-NH1	8.43	124.52	120.30
2	B	327	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	231	TYR	CB-CG-CD1	8.31	125.99	121.00
1	A	318	TYR	CB-CG-CD1	-8.16	116.10	121.00
2	B	8	ASP	CB-CG-OD1	8.11	125.60	118.30
1	A	428	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	190	TYR	CB-CG-CD2	-8.01	116.19	121.00
2	B	39	ASP	CB-CG-OD1	7.98	125.48	118.30
2	B	25	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	4	THR	N-CA-CB	7.86	125.23	110.30
1	A	276	LEU	CB-CA-C	-7.83	95.31	110.20
1	A	432	ALA	CB-CA-C	-7.75	98.47	110.10
1	A	428	ASP	CB-CG-OD1	7.72	125.25	118.30
2	B	298	ASP	CB-CG-OD1	7.63	125.16	118.30
2	B	264	ALA	N-CA-CB	7.61	120.76	110.10
1	A	20	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	364	GLN	C-N-CA	7.58	138.22	122.30
2	B	237	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	167	TYR	CB-CG-CD1	7.57	125.54	121.00
2	B	51	LEU	N-CA-C	7.54	131.36	111.00
1	A	156	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	B	303	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	344	ASP	CB-CG-OD1	7.49	125.04	118.30
2	B	425	MET	CB-CA-C	7.44	125.27	110.40
1	A	46	ARG	N-CA-CB	-7.43	97.22	110.60
1	A	367	ALA	O-C-N	7.42	134.58	122.70
1	A	298	ASP	CB-CG-OD1	7.42	124.98	118.30
2	B	374	VAL	CB-CA-C	-7.36	97.41	111.40
1	A	303	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	136	HIS	CB-CA-C	-7.31	95.79	110.40
1	A	330	TYR	CB-CG-CD2	-7.27	116.64	121.00
2	B	33	LEU	CB-CA-C	7.21	123.89	110.20
1	A	221	ASP	CB-CG-OD2	-7.15	111.87	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	368	ALA	CB-CA-C	7.11	120.77	110.10
2	B	367	ALA	CB-CA-C	-7.11	99.44	110.10
2	B	281	VAL	CA-CB-CG2	-7.10	100.25	110.90
1	A	295	ALA	N-CA-CB	7.10	120.03	110.10
1	A	177	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	367	ALA	CB-CA-C	-7.04	99.53	110.10
1	A	298	ASP	CB-CG-OD2	-7.04	111.97	118.30
2	B	237	ASP	CB-CG-OD2	-6.96	112.03	118.30
2	B	340	HIS	CA-CB-CG	-6.96	101.78	113.60
2	B	177	ASP	CB-CA-C	-6.95	96.49	110.40
2	B	194	TYR	CB-CG-CD1	6.88	125.13	121.00
2	B	3	SER	CB-CA-C	-6.85	97.08	110.10
2	B	167	TYR	N-CA-CB	6.85	122.93	110.60
2	B	204	ASP	CB-CA-C	6.82	124.04	110.40
1	A	61	ASP	CB-CG-OD2	-6.78	112.20	118.30
2	B	156	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	167	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	A	421	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	B	291	ALA	N-CA-CB	6.71	119.49	110.10
2	B	413	ARG	CD-NE-CZ	6.70	132.98	123.60
2	B	156	ARG	CD-NE-CZ	6.67	132.93	123.60
2	B	39	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	208	ASP	CB-CG-OD1	6.60	124.24	118.30
2	B	262	PHE	CB-CG-CD1	6.50	125.35	120.80
1	A	3	SER	CB-CA-C	-6.50	97.75	110.10
2	B	164	ARG	NE-CZ-NH2	-6.49	117.05	120.30
2	B	133	THR	N-CA-CB	6.49	122.63	110.30
1	A	387	MET	CB-CA-C	6.48	123.36	110.40
1	A	6	LEU	N-CA-CB	6.47	123.35	110.40
2	B	194	TYR	CB-CG-CD2	-6.46	117.12	121.00
2	B	25	ARG	N-CA-CB	6.46	122.23	110.60
1	A	46	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	B	301	LEU	N-CA-CB	6.43	123.27	110.40
1	A	93	PHE	CB-CG-CD2	6.40	125.28	120.80
2	B	334	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	B	193	LEU	CB-CG-CD2	-6.37	100.17	111.00
2	B	195	ARG	NE-CZ-NH2	-6.37	117.12	120.30
2	B	204	ASP	CB-CG-OD1	6.34	124.01	118.30
2	B	407	ALA	N-CA-CB	6.34	118.97	110.10
2	B	412	SER	N-CA-CB	-6.26	101.10	110.50
2	B	327	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	212	ASN	CB-CA-C	-6.21	97.99	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	328	PRO	O-C-N	6.19	132.60	122.70
1	A	194	TYR	CG-CD1-CE1	6.14	126.21	121.30
1	A	258	PRO	N-CA-CB	6.12	110.64	103.30
2	B	243	VAL	CG1-CB-CG2	-6.11	101.12	110.90
2	B	229	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	A	204	ASP	CB-CA-C	6.09	122.58	110.40
1	A	130	ASN	N-CA-CB	6.06	121.50	110.60
2	B	46	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	A	65	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	326	THR	N-CA-CB	6.04	121.78	110.30
1	A	180	ALA	CB-CA-C	6.01	119.12	110.10
2	B	164	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	B	141	LEU	CB-CG-CD2	-5.94	100.91	111.00
1	A	61	ASP	CB-CG-OD1	5.93	123.64	118.30
2	B	40	MET	N-CA-CB	5.91	121.24	110.60
2	B	32	ALA	N-CA-CB	5.89	118.35	110.10
1	A	196	ALA	CB-CA-C	5.88	118.93	110.10
2	B	353	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	169	GLU	N-CA-CB	5.84	121.11	110.60
1	A	204	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	168	TRP	CD1-NE1-CE2	5.83	114.25	109.00
1	A	117	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	8	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	31	THR	CA-CB-CG2	-5.80	104.28	112.40
2	B	385	TYR	CA-CB-CG	-5.76	102.46	113.40
2	B	377	HIS	CA-CB-CG	-5.73	103.85	113.60
1	A	51	LEU	N-CA-C	5.73	126.48	111.00
2	B	27	GLN	N-CA-CB	5.73	120.92	110.60
1	A	204	ASP	CB-CG-OD1	5.72	123.45	118.30
2	B	107	VAL	CA-CB-CG1	5.71	119.47	110.90
2	B	338	LEU	N-CA-CB	5.70	121.79	110.40
2	B	267	ASN	CA-CB-CG	-5.68	100.90	113.40
1	A	42	TYR	CB-CG-CD2	-5.67	117.59	121.00
1	A	111	SER	N-CA-CB	5.65	118.97	110.50
1	A	310	ASN	CB-CA-C	5.64	121.68	110.40
1	A	66	PHE	C-N-CA	5.61	135.73	121.70
1	A	37	THR	CA-CB-CG2	-5.60	104.56	112.40
2	B	242	ASN	N-CA-CB	5.58	120.65	110.60
1	A	18	GLN	N-CA-CB	-5.51	100.67	110.60
1	A	73	GLU	N-CA-CB	5.50	120.50	110.60
2	B	257	ASP	CB-CG-OD2	-5.49	113.36	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	79	PRO	N-CA-CB	5.49	109.89	103.30
1	A	369	ASN	N-CA-C	-5.48	96.19	111.00
1	A	191	ARG	CD-NE-CZ	5.48	131.27	123.60
1	A	303	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	410	ILE	CB-CA-C	-5.46	100.69	111.60
2	B	332	CYS	CB-CA-C	5.45	121.30	110.40
2	B	334	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	B	26	GLN	CB-CA-C	5.44	121.28	110.40
2	B	164	ARG	CA-C-O	5.43	131.51	120.10
2	B	235	HIS	CA-CB-CG	-5.40	104.42	113.60
1	A	39	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	B	172	TYR	CG-CD1-CE1	5.38	125.60	121.30
1	A	385	TYR	CA-CB-CG	-5.37	103.19	113.40
1	A	53	TYR	N-CA-C	-5.37	96.50	111.00
1	A	208	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	390	MET	CB-CA-C	5.34	121.08	110.40
1	A	419	LEU	CB-CA-C	-5.34	100.06	110.20
1	A	118	ALA	CB-CA-C	5.34	118.10	110.10
2	B	65	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
2	B	152	SER	N-CA-CB	5.33	118.50	110.50
2	B	313	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	330	TYR	CB-CG-CD1	5.30	124.18	121.00
1	A	257	ASP	CB-CG-OD1	5.27	123.04	118.30
2	B	390	MET	N-CA-CB	5.26	120.07	110.60
2	B	337	ALA	N-CA-CB	-5.26	102.74	110.10
2	B	367	ALA	CA-C-N	-5.23	105.69	117.20
1	A	267	ASN	CA-CB-CG	-5.23	101.89	113.40
2	B	315	VAL	CB-CA-C	-5.22	101.47	111.40
1	A	139	SER	O-C-N	5.22	131.06	122.70
1	A	415	LEU	CB-CA-C	5.22	120.11	110.20
2	B	147	ALA	N-CA-CB	-5.20	102.82	110.10
1	A	297	ALA	CA-C-N	-5.18	105.80	117.20
1	A	207	LEU	CA-CB-CG	-5.17	103.40	115.30
2	B	61	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	67	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	107	VAL	CA-CB-CG2	-5.14	103.19	110.90
2	B	215	ASN	N-CA-CB	-5.13	101.36	110.60
1	A	33	LEU	CA-CB-CG	-5.10	103.58	115.30
1	A	51	LEU	N-CA-CB	5.08	120.57	110.40
2	B	392	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	B	33	LEU	CB-CG-CD2	-5.08	102.37	111.00
2	B	80	LYS	C-N-CA	5.08	132.96	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	342	PRO	CA-N-CD	-5.06	104.41	111.50
1	A	304	TYR	CB-CG-CD2	5.06	124.04	121.00
2	B	88	LEU	O-C-N	-5.05	111.51	121.10
1	A	332	CYS	CB-CA-C	5.04	120.49	110.40
1	A	164	ARG	CA-CB-CG	5.04	124.49	113.40
2	B	324	ARG	CD-NE-CZ	-5.04	116.55	123.60
1	A	121	PRO	N-CA-CB	5.04	109.34	103.30
2	B	387	MET	N-CA-CB	5.04	119.67	110.60
1	A	374	VAL	CG1-CB-CG2	5.03	118.94	110.90
2	B	113	GLU	CG-CD-OE1	5.01	128.32	118.30
1	A	372	PRO	C-N-CA	5.01	134.22	121.70

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	THR	CA
1	A	5	ASN	CA
1	A	51	LEU	CA
1	A	289	GLN	CA
1	A	340	HIS	CA
1	A	390	MET	CA
1	A	425	MET	CA
2	B	26	GLN	CA
2	B	46	ARG	CA
2	B	51	LEU	CA
2	B	390	MET	CA
2	B	425	MET	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASN	Sidechain
1	A	337	ALA	Mainchain
1	A	339	LYS	Mainchain
1	A	348	LYS	Mainchain
1	A	385	TYR	Sidechain
2	B	149	ASN	Sidechain
2	B	231	TYR	Sidechain
2	B	354	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3303	0	3288	489	26
2	B	3303	0	3288	535	26
All	All	6606	0	6576	972	26

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 74.

All (972) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HB2	1:A:46:ARG:NH1	1.52	1.22
1:A:33:LEU:HD11	2:B:433:LEU:HD21	1.16	1.13
2:B:86:GLU:HG3	2:B:230:LEU:HB2	1.31	1.12
2:B:79:PRO:HG2	2:B:107:VAL:HG21	1.33	1.11
2:B:341:LEU:HD22	2:B:384:TYR:CD2	1.85	1.10
1:A:178:LEU:HD23	1:A:406:LEU:HD11	1.28	1.09
1:A:323:LEU:HD22	1:A:324:ARG:H	1.18	1.08
1:A:25:ARG:HD2	2:B:42:TYR:CD2	1.89	1.07
1:A:424:SER:HB2	2:B:51:LEU:HB2	1.32	1.07
2:B:350:VAL:HG21	2:B:380:VAL:HG21	1.34	1.04
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.35	1.03
1:A:92:LEU:HG	1:A:233:THR:HG23	1.34	1.03
2:B:327:ASP:OD2	2:B:329:ARG:HG3	1.54	1.03
2:B:320:HIS:N	2:B:369:ASN:OD1	1.90	1.03
1:A:94:TRP:CE3	1:A:110:LEU:HD21	1.94	1.02
1:A:298:ASP:HA	1:A:356:ILE:HD11	1.40	1.02
2:B:329:ARG:HH21	2:B:374:VAL:HG21	1.24	1.02
2:B:329:ARG:HH21	2:B:374:VAL:CG2	1.73	1.00
2:B:323:LEU:O	2:B:369:ASN:ND2	1.93	0.99
2:B:124:VAL:HG21	2:B:148:LEU:CD2	1.91	0.99
2:B:281:VAL:CG2	2:B:316:PRO:HB2	1.92	0.99
2:B:125:VAL:CG1	2:B:188:LYS:HE2	1.94	0.96
1:A:33:LEU:HD11	2:B:433:LEU:CD2	1.95	0.96
2:B:339:LYS:HB3	2:B:340:HIS:CD2	2.00	0.96
2:B:124:VAL:HG21	2:B:148:LEU:HD21	1.46	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:LEU:HD11	2:B:370:PRO:HG3	1.48	0.95
1:A:109:TRP:CE3	1:A:110:LEU:HD23	2.01	0.95
2:B:412:SER:HA	2:B:417:PHE:CD2	2.01	0.95
1:A:340:HIS:O	1:A:342:PRO:HD3	1.67	0.94
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.50	0.94
2:B:33:LEU:C	2:B:33:LEU:HD12	1.87	0.94
2:B:269:LEU:HD11	2:B:397:PHE:CE2	2.02	0.94
2:B:136:HIS:CD2	2:B:137:PRO:HD2	2.03	0.94
2:B:92:LEU:HD13	2:B:233:THR:HG23	1.50	0.93
1:A:326:THR:HG22	1:A:327:ASP:O	1.68	0.93
1:A:98:THR:HG22	1:A:100:GLN:HG3	1.48	0.93
2:B:281:VAL:HG22	2:B:316:PRO:HB2	1.50	0.93
1:A:34:GLY:O	2:B:36:ILE:N	2.03	0.92
2:B:329:ARG:NH2	2:B:374:VAL:HG21	1.85	0.91
1:A:425:MET:HA	2:B:52:VAL:H	1.36	0.91
1:A:33:LEU:CD1	2:B:433:LEU:HD21	2.01	0.90
2:B:141:LEU:HD22	2:B:395:VAL:HG13	1.50	0.90
1:A:273:LEU:HD13	2:B:255:LEU:HD12	1.54	0.90
2:B:125:VAL:HG13	2:B:188:LYS:HE2	1.51	0.90
2:B:271:GLY:O	2:B:275:GLY:N	2.03	0.90
2:B:22:LYS:O	2:B:26:GLN:HB2	1.71	0.90
2:B:362:LEU:HD12	2:B:367:ALA:HB2	1.54	0.90
2:B:174:SER:HB2	2:B:258:PRO:HG2	1.53	0.89
1:A:126:THR:O	1:A:129:ASP:HB2	1.70	0.89
2:B:424:SER:O	2:B:425:MET:HG3	1.71	0.89
2:B:251:VAL:HG11	2:B:261:SER:HA	1.53	0.89
2:B:64:ILE:HG13	2:B:65:ARG:H	1.37	0.88
1:A:46:ARG:HB2	1:A:46:ARG:CZ	2.04	0.88
2:B:342:PRO:HD2	2:B:343:GLY:H	1.38	0.88
1:A:273:LEU:CD1	2:B:255:LEU:HD12	2.04	0.88
2:B:64:ILE:HG13	2:B:65:ARG:N	1.86	0.88
1:A:30:GLY:HA2	2:B:37:THR:CG2	2.04	0.87
2:B:131:PHE:CD2	2:B:140:GLN:HB3	2.10	0.87
1:A:80:LYS:HG2	1:A:85:GLY:O	1.75	0.87
1:A:109:TRP:CH2	1:A:113:GLU:HG2	2.09	0.87
1:A:135:LEU:HD11	1:A:139:SER:HB3	1.57	0.86
1:A:125:VAL:HG13	1:A:188:LYS:HE2	1.57	0.85
1:A:192:ASN:HA	1:A:197:GLY:HA2	1.55	0.85
1:A:329:ARG:NH2	1:A:374:VAL:HG21	1.92	0.85
1:A:243:VAL:HB	1:A:274:HIS:CD2	2.12	0.85
1:A:182:LEU:HD22	1:A:399:VAL:HG22	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:NH1	1:A:216:MET:O	2.09	0.84
2:B:412:SER:HB3	2:B:417:PHE:HD2	1.42	0.84
1:A:94:TRP:HE3	1:A:110:LEU:HD21	1.38	0.84
1:A:136:HIS:HD2	1:A:138:MET:H	1.23	0.84
2:B:305:ILE:HD13	2:B:357:VAL:HG22	1.60	0.84
2:B:311:SER:HB3	2:B:313:ARG:CZ	2.08	0.84
1:A:46:ARG:HB2	1:A:46:ARG:HH11	1.42	0.83
2:B:94:TRP:CD1	2:B:102:PRO:HB3	2.14	0.83
2:B:301:LEU:CD1	2:B:356:ILE:HD13	2.08	0.83
1:A:279:GLN:HG2	1:A:390:MET:HG3	1.59	0.83
1:A:411:TRP:CE3	1:A:415:LEU:HD21	2.14	0.83
2:B:174:SER:CB	2:B:258:PRO:HG2	2.07	0.82
1:A:362:LEU:CD1	1:A:370:PRO:HG3	2.08	0.82
1:A:369:ASN:N	1:A:370:PRO:HD3	1.93	0.82
2:B:301:LEU:HG	2:B:356:ILE:HD13	1.62	0.82
2:B:319:GLY:HA2	2:B:369:ASN:O	1.79	0.82
1:A:6:LEU:HB2	1:A:94:TRP:CZ3	2.14	0.82
2:B:340:HIS:O	2:B:342:PRO:HD3	1.78	0.82
2:B:357:VAL:HB	2:B:358:PRO:HD3	1.62	0.82
1:A:334:ARG:O	1:A:334:ARG:HG3	1.76	0.81
1:A:424:SER:HB2	2:B:51:LEU:CB	2.08	0.81
1:A:330:TYR:HB2	1:A:373:ASN:O	1.80	0.80
1:A:251:VAL:HG12	1:A:261:SER:HB3	1.61	0.80
1:A:109:TRP:CZ3	1:A:110:LEU:HD23	2.16	0.80
1:A:25:ARG:HD2	2:B:42:TYR:CG	2.16	0.80
2:B:301:LEU:CG	2:B:356:ILE:HD13	2.11	0.80
2:B:377:HIS:O	2:B:381:LEU:HD22	1.81	0.80
2:B:6:LEU:HD23	2:B:172:TYR:OH	1.81	0.80
1:A:281:VAL:HG22	1:A:316:PRO:O	1.82	0.80
2:B:131:PHE:CE2	2:B:140:GLN:HB3	2.16	0.80
2:B:192:ASN:HA	2:B:197:GLY:HA2	1.64	0.80
1:A:281:VAL:HG22	1:A:316:PRO:HB2	1.63	0.80
2:B:302:ARG:O	2:B:306:TRP:HB2	1.82	0.80
1:A:277:ALA:HB3	1:A:375:ASP:OD1	1.82	0.79
1:A:191:ARG:HA	1:A:195:ARG:HB2	1.65	0.79
2:B:311:SER:HB3	2:B:313:ARG:NH1	1.97	0.79
2:B:65:ARG:HG3	2:B:68:GLY:O	1.81	0.79
1:A:341:LEU:HD22	1:A:384:TYR:CD2	2.16	0.79
1:A:109:TRP:HE3	1:A:110:LEU:HD23	1.47	0.79
1:A:236:SER:O	1:A:401:ARG:HA	1.82	0.79
1:A:431:ILE:HD12	2:B:20:ARG:NH2	1.98	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD12	1:A:367:ALA:HB2	1.63	0.79
2:B:350:VAL:CG2	2:B:380:VAL:HG21	2.12	0.79
1:A:370:PRO:HD2	1:A:371:TRP:NE1	1.97	0.79
2:B:285:LEU:HG	2:B:346:MET:HE2	1.65	0.79
2:B:412:SER:HB3	2:B:417:PHE:CD2	2.17	0.79
2:B:145:ILE:HG22	2:B:263:ALA:HB2	1.63	0.78
1:A:204:ASP:OD2	1:A:206:LYS:HD3	1.83	0.78
1:A:323:LEU:HD22	1:A:324:ARG:N	1.96	0.78
2:B:157:ALA:HB1	2:B:162:ILE:HG21	1.65	0.78
2:B:300:SER:O	2:B:303:ASP:HB2	1.84	0.78
2:B:2:SER:O	2:B:3:SER:HB3	1.82	0.78
1:A:94:TRP:CD1	1:A:102:PRO:HB3	2.18	0.78
2:B:86:GLU:CG	2:B:230:LEU:HB2	2.10	0.78
1:A:329:ARG:HH21	1:A:374:VAL:CG2	1.96	0.78
2:B:330:TYR:HB2	2:B:373:ASN:O	1.83	0.78
1:A:136:HIS:CD2	1:A:138:MET:H	2.02	0.78
2:B:149:ASN:CG	2:B:149:ASN:O	2.21	0.78
1:A:54:GLU:OE2	2:B:427:THR:OG1	2.02	0.77
2:B:276:LEU:HB3	2:B:280:GLU:OE2	1.85	0.77
1:A:223:GLN:NE2	1:A:340:HIS:CG	2.53	0.77
1:A:362:LEU:HD13	1:A:370:PRO:HG3	1.66	0.77
2:B:65:ARG:NH1	2:B:70:SER:HB3	2.00	0.77
1:A:178:LEU:CD2	1:A:406:LEU:HD11	2.11	0.77
2:B:307:ASN:O	2:B:311:SER:HB2	1.85	0.77
1:A:347:PHE:O	1:A:348:LYS:O	2.02	0.77
2:B:236:SER:O	2:B:401:ARG:HA	1.84	0.77
1:A:269:LEU:HD11	1:A:397:PHE:CD2	2.21	0.76
2:B:154:PHE:HE1	2:B:167:TYR:HB3	1.46	0.76
1:A:347:PHE:O	1:A:348:LYS:C	2.23	0.76
1:A:323:LEU:CD2	1:A:324:ARG:H	1.98	0.76
2:B:81:GLY:HA2	2:B:88:LEU:HD11	1.67	0.76
2:B:415:LEU:HD12	2:B:417:PHE:CZ	2.21	0.76
2:B:157:ALA:HB1	2:B:162:ILE:CG2	2.15	0.75
1:A:94:TRP:CZ3	1:A:110:LEU:HD21	2.21	0.75
2:B:146:THR:O	2:B:149:ASN:HB3	1.86	0.75
2:B:182:LEU:N	2:B:183:PRO:CD	2.50	0.75
2:B:223:GLN:NE2	2:B:340:HIS:ND1	2.33	0.75
1:A:411:TRP:HE3	1:A:415:LEU:HD21	1.48	0.75
2:B:411:TRP:O	2:B:415:LEU:N	2.18	0.75
1:A:119:ALA:O	1:A:181:LYS:HE3	1.87	0.74
1:A:223:GLN:NE2	1:A:340:HIS:ND1	2.34	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:N	1:A:207:LEU:HD23	2.00	0.74
2:B:362:LEU:HD12	2:B:367:ALA:CB	2.17	0.74
1:A:311:SER:O	1:A:313:ARG:NH1	2.20	0.74
2:B:33:LEU:C	2:B:33:LEU:CD1	2.56	0.74
2:B:79:PRO:CG	2:B:107:VAL:HG21	2.13	0.74
1:A:424:SER:CB	2:B:51:LEU:HB2	2.15	0.74
1:A:5:ASN:HA	1:A:8:ASP:HB2	1.68	0.74
1:A:79:PRO:HG2	1:A:107:VAL:HG21	1.69	0.74
1:A:168:TRP:CE2	1:A:169:GLU:HG3	2.23	0.74
1:A:329:ARG:HH21	1:A:374:VAL:HG21	1.53	0.74
1:A:172:TYR:O	1:A:175:ALA:HB3	1.87	0.73
1:A:157:ALA:HB1	1:A:162:ILE:CG2	2.19	0.73
2:B:107:VAL:O	2:B:110:LEU:N	2.21	0.73
2:B:124:VAL:HG21	2:B:148:LEU:HD23	1.70	0.73
2:B:301:LEU:HD21	2:B:352:GLN:HB3	1.69	0.73
1:A:131:PHE:CE2	1:A:140:GLN:HB3	2.24	0.73
2:B:288:LEU:HD23	2:B:349:LEU:HD21	1.70	0.73
1:A:121:PRO:O	1:A:125:VAL:HG23	1.90	0.72
1:A:51:LEU:HB2	2:B:424:SER:HA	1.71	0.72
1:A:174:SER:HB2	1:A:258:PRO:HG2	1.72	0.72
2:B:65:ARG:NH1	2:B:68:GLY:O	2.22	0.72
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.18	0.72
1:A:42:TYR:CG	2:B:25:ARG:HD2	2.25	0.72
2:B:333:GLN:NE2	2:B:377:HIS:HB3	2.05	0.72
2:B:56:SER:HB2	2:B:64:ILE:HD11	1.72	0.72
1:A:390:MET:HB2	1:A:393:TYR:CE2	2.24	0.72
2:B:207:LEU:N	2:B:207:LEU:HD23	2.04	0.72
1:A:102:PRO:HB2	1:A:107:VAL:HG23	1.72	0.71
2:B:324:ARG:CZ	2:B:324:ARG:CB	2.67	0.71
1:A:340:HIS:C	1:A:342:PRO:HD3	2.09	0.71
2:B:94:TRP:CE3	2:B:110:LEU:HD11	2.25	0.71
2:B:115:ALA:O	2:B:118:ALA:HB3	1.88	0.71
1:A:348:LYS:O	1:A:351:ALA:HB3	1.90	0.71
2:B:109:TRP:CE3	2:B:110:LEU:HD23	2.24	0.71
2:B:339:LYS:HB3	2:B:340:HIS:NE2	2.05	0.71
1:A:95:LEU:HA	1:A:100:GLN:O	1.90	0.71
2:B:27:GLN:HE21	2:B:28:HIS:CE1	2.09	0.71
2:B:384:TYR:HD2	2:B:385:TYR:CE2	2.09	0.71
2:B:269:LEU:HD11	2:B:397:PHE:CD2	2.25	0.71
2:B:357:VAL:O	2:B:361:LEU:HB2	1.89	0.71
2:B:349:LEU:O	2:B:353:LEU:HD22	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:O	1:A:170:MET:N	2.24	0.70
1:A:30:GLY:HA2	2:B:37:THR:HG22	1.72	0.70
2:B:412:SER:CA	2:B:417:PHE:CD2	2.74	0.70
1:A:285:LEU:HG	1:A:346:MET:CE	2.21	0.70
2:B:46:ARG:HH11	2:B:46:ARG:HA	1.56	0.70
2:B:93:PHE:O	2:B:97:VAL:HG23	1.90	0.70
2:B:184:CYS:O	2:B:188:LYS:HB2	1.91	0.70
2:B:94:TRP:HE3	2:B:110:LEU:HD11	1.55	0.70
2:B:181:LYS:C	2:B:183:PRO:HD2	2.11	0.70
2:B:18:GLN:O	2:B:22:LYS:HG2	1.92	0.70
1:A:311:SER:HB2	1:A:313:ARG:CZ	2.21	0.70
2:B:322:VAL:HG12	2:B:322:VAL:O	1.91	0.70
2:B:315:VAL:CG1	2:B:316:PRO:HD2	2.20	0.69
2:B:349:LEU:HG	2:B:353:LEU:HD22	1.74	0.69
1:A:178:LEU:HD23	1:A:406:LEU:CD1	2.17	0.69
2:B:281:VAL:HG23	2:B:316:PRO:HB2	1.74	0.69
1:A:162:ILE:HD12	1:A:167:TYR:HD1	1.57	0.69
2:B:46:ARG:HH11	2:B:46:ARG:CA	2.06	0.69
2:B:214:THR:HG22	2:B:215:ASN:N	2.08	0.69
2:B:350:VAL:O	2:B:353:LEU:HB2	1.92	0.69
1:A:94:TRP:CG	1:A:102:PRO:HB3	2.27	0.69
1:A:320:HIS:HB3	1:A:369:ASN:OD1	1.92	0.69
2:B:125:VAL:HG12	2:B:188:LYS:HE2	1.72	0.69
1:A:131:PHE:CD2	1:A:140:GLN:HB3	2.28	0.69
1:A:86:GLU:HG2	1:A:230:LEU:CB	2.19	0.69
2:B:36:ILE:HG23	2:B:48:MET:HE2	1.73	0.69
1:A:297:ALA:HB1	1:A:299:ALA:H	1.57	0.68
1:A:384:TYR:HD2	1:A:385:TYR:CE2	2.12	0.68
2:B:320:HIS:O	2:B:369:ASN:HB3	1.93	0.68
1:A:86:GLU:CG	1:A:230:LEU:HB2	2.20	0.68
1:A:98:THR:HG21	1:A:100:GLN:HB2	1.74	0.68
1:A:245:ALA:HA	1:A:405:VAL:CG2	2.23	0.68
2:B:102:PRO:HB2	2:B:107:VAL:HG23	1.76	0.68
2:B:301:LEU:HD11	2:B:356:ILE:HD13	1.75	0.68
1:A:190:TYR:O	1:A:193:LEU:N	2.27	0.68
1:A:412:SER:HB3	1:A:417:PHE:CD2	2.29	0.68
1:A:377:HIS:O	1:A:377:HIS:ND1	2.24	0.68
2:B:279:GLN:HG2	2:B:390:MET:HG3	1.75	0.68
1:A:162:ILE:HD12	1:A:167:TYR:CD1	2.29	0.68
2:B:109:TRP:CZ3	2:B:110:LEU:HD23	2.28	0.68
2:B:92:LEU:HD22	2:B:233:THR:HA	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:PHE:CZ	2:B:97:VAL:HG21	2.28	0.68
1:A:98:THR:CG2	1:A:100:GLN:HG3	2.21	0.68
2:B:301:LEU:HD23	2:B:352:GLN:NE2	2.09	0.68
2:B:326:THR:HG22	2:B:327:ASP:O	1.94	0.68
1:A:69:PHE:HA	1:A:73:GLU:OE1	1.93	0.67
2:B:212:ASN:O	2:B:216:MET:HG3	1.94	0.67
2:B:204:ASP:OD2	2:B:206:LYS:N	2.28	0.67
2:B:362:LEU:CD1	2:B:370:PRO:HG3	2.22	0.67
2:B:245:ALA:HA	2:B:405:VAL:CG2	2.24	0.67
2:B:251:VAL:CG1	2:B:261:SER:HA	2.24	0.67
1:A:80:LYS:HE2	1:A:85:GLY:O	1.94	0.67
1:A:184:CYS:O	1:A:188:LYS:HB2	1.94	0.67
2:B:46:ARG:HA	2:B:46:ARG:NH1	2.09	0.67
2:B:298:ASP:O	2:B:302:ARG:HB2	1.95	0.67
1:A:339:LYS:HB3	1:A:340:HIS:CD2	2.29	0.67
1:A:14:ILE:O	1:A:17:GLU:N	2.27	0.67
1:A:157:ALA:HB1	1:A:162:ILE:HG23	1.77	0.67
1:A:274:HIS:O	1:A:274:HIS:ND1	2.27	0.67
2:B:178:LEU:HD23	2:B:406:LEU:HD11	1.76	0.67
2:B:327:ASP:OD1	2:B:374:VAL:HG22	1.95	0.67
1:A:266:MET:HA	1:A:266:MET:HE2	1.77	0.66
1:A:271:GLY:O	1:A:275:GLY:N	2.23	0.66
1:A:136:HIS:HB3	1:A:139:SER:HB2	1.77	0.66
2:B:211:HIS:O	2:B:215:ASN:HB3	1.95	0.66
2:B:221:ASP:OD2	2:B:223:GLN:N	2.27	0.66
2:B:257:ASP:HB2	2:B:258:PRO:HD2	1.75	0.66
1:A:65:ARG:HH11	1:A:70:SER:HB3	1.59	0.66
1:A:213:PHE:O	1:A:217:LEU:HB2	1.95	0.66
2:B:311:SER:O	2:B:313:ARG:NH1	2.28	0.66
2:B:163:LEU:HD12	2:B:164:ARG:N	2.10	0.66
2:B:306:TRP:CZ3	2:B:364:GLN:NE2	2.64	0.66
1:A:10:LEU:O	1:A:14:ILE:HG13	1.95	0.66
2:B:107:VAL:O	2:B:109:TRP:N	2.28	0.66
1:A:13:LEU:O	1:A:16:LYS:HB2	1.96	0.66
1:A:27:GLN:HG2	1:A:28:HIS:N	2.11	0.66
1:A:384:TYR:CE2	1:A:385:TYR:CZ	2.83	0.66
2:B:109:TRP:CH2	2:B:113:GLU:HG2	2.31	0.66
2:B:193:LEU:HB3	2:B:194:TYR:CD2	2.31	0.66
1:A:243:VAL:HB	1:A:274:HIS:HD2	1.59	0.65
1:A:311:SER:HB3	1:A:313:ARG:HH12	1.62	0.65
2:B:412:SER:HA	2:B:417:PHE:CE2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLY:O	1:A:51:LEU:HG	1.96	0.65
2:B:6:LEU:HD13	2:B:94:TRP:CE3	2.32	0.65
1:A:433:LEU:CD2	2:B:33:LEU:HD22	2.27	0.65
1:A:352:GLN:O	1:A:355:LYS:N	2.29	0.65
1:A:421:ARG:N	2:B:44:GLY:O	2.29	0.65
2:B:369:ASN:N	2:B:370:PRO:HD3	2.10	0.65
2:B:285:LEU:HB3	2:B:346:MET:HE1	1.78	0.64
1:A:128:LEU:HD23	1:A:131:PHE:CE2	2.32	0.64
1:A:362:LEU:HD12	1:A:367:ALA:CB	2.27	0.64
2:B:97:VAL:HG12	2:B:97:VAL:O	1.97	0.64
2:B:235:HIS:O	2:B:401:ARG:NH2	2.27	0.64
1:A:301:LEU:HD12	1:A:356:ILE:HG21	1.80	0.64
2:B:320:HIS:H	2:B:369:ASN:CG	2.01	0.64
1:A:177:ASP:O	1:A:181:LYS:HG3	1.97	0.64
1:A:266:MET:HA	1:A:266:MET:CE	2.28	0.64
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.77	0.64
2:B:121:PRO:HB2	2:B:123:HIS:CD2	2.32	0.64
1:A:162:ILE:CD1	1:A:167:TYR:CD1	2.81	0.64
1:A:362:LEU:HD11	1:A:370:PRO:HG3	1.79	0.64
1:A:301:LEU:HD21	1:A:352:GLN:HB3	1.78	0.64
2:B:288:LEU:O	2:B:291:ALA:N	2.29	0.63
1:A:53:TYR:CD2	1:A:240:GLY:HA3	2.33	0.63
1:A:149:ASN:ND2	2:B:139:SER:OG	2.31	0.63
2:B:323:LEU:O	2:B:369:ASN:HB2	1.98	0.63
1:A:411:TRP:HA	1:A:414:ALA:HB3	1.81	0.63
2:B:223:GLN:NE2	2:B:340:HIS:CG	2.66	0.63
2:B:311:SER:O	2:B:313:ARG:HD3	1.99	0.63
2:B:2:SER:O	2:B:3:SER:CB	2.47	0.63
1:A:44:GLY:O	1:A:45:MET:HB2	1.99	0.63
2:B:349:LEU:HG	2:B:353:LEU:CD2	2.29	0.63
1:A:306:TRP:CD1	1:A:360:VAL:HG13	2.33	0.63
2:B:92:LEU:HG	2:B:92:LEU:O	1.97	0.63
2:B:106:GLN:O	2:B:109:TRP:HB3	1.99	0.63
1:A:52:VAL:H	2:B:425:MET:HA	1.63	0.62
1:A:53:TYR:CG	1:A:240:GLY:HA3	2.34	0.62
1:A:306:TRP:CE2	1:A:364:GLN:NE2	2.67	0.62
2:B:232:LEU:HD23	2:B:400:SER:HB2	1.82	0.62
2:B:305:ILE:HD11	2:B:353:LEU:HD12	1.81	0.62
1:A:284:TRP:CG	1:A:316:PRO:HG3	2.34	0.62
2:B:326:THR:O	2:B:327:ASP:C	2.38	0.62
2:B:193:LEU:HD23	2:B:194:TYR:CE2	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:SER:CB	2:B:417:PHE:CD2	2.82	0.62
1:A:167:TYR:CE2	1:A:255:LEU:HD11	2.35	0.62
1:A:323:LEU:HD13	1:A:325:LYS:O	2.00	0.62
2:B:131:PHE:HD2	2:B:140:GLN:NE2	1.97	0.62
1:A:64:ILE:HG13	1:A:65:ARG:H	1.65	0.62
2:B:7:LYS:NZ	2:B:173:GLU:OE1	2.33	0.62
2:B:65:ARG:HH11	2:B:70:SER:HB3	1.64	0.62
2:B:149:ASN:O	2:B:149:ASN:OD1	2.17	0.62
1:A:425:MET:HA	2:B:52:VAL:N	2.11	0.62
2:B:163:LEU:O	2:B:165:THR:N	2.32	0.62
1:A:266:MET:HE2	1:A:269:LEU:HB3	1.80	0.61
1:A:311:SER:CB	1:A:313:ARG:NH1	2.63	0.61
2:B:223:GLN:HE22	2:B:340:HIS:CE1	2.18	0.61
2:B:60:PRO:O	2:B:324:ARG:HB2	2.00	0.61
1:A:39:ASP:HB2	2:B:29:GLY:O	2.01	0.61
1:A:92:LEU:HD11	1:A:236:SER:OG	1.99	0.61
2:B:36:ILE:HG21	2:B:48:MET:HE1	1.81	0.61
2:B:307:ASN:O	2:B:308:THR:O	2.18	0.61
1:A:223:GLN:HE22	1:A:340:HIS:CE1	2.18	0.61
1:A:285:LEU:HD21	1:A:350:VAL:CG2	2.30	0.61
2:B:334:ARG:O	2:B:334:ARG:HG3	1.91	0.61
2:B:384:TYR:HD2	2:B:385:TYR:CD2	2.18	0.61
2:B:88:LEU:O	2:B:89:PRO:C	2.38	0.61
2:B:94:TRP:CD1	2:B:102:PRO:CB	2.84	0.61
1:A:121:PRO:HD2	1:A:148:LEU:CD2	2.31	0.61
1:A:123:HIS:CG	2:B:132:PRO:HG3	2.35	0.61
1:A:29:GLY:O	2:B:39:ASP:N	2.33	0.61
1:A:269:LEU:HD11	1:A:397:PHE:CE2	2.35	0.61
2:B:46:ARG:HH11	2:B:46:ARG:C	2.04	0.61
2:B:182:LEU:N	2:B:183:PRO:HD2	2.15	0.61
2:B:310:ASN:ND2	2:B:364:GLN:OE1	2.34	0.61
1:A:264:ALA:HB1	2:B:264:ALA:HB1	1.82	0.61
1:A:325:LYS:HD2	1:A:326:THR:O	2.00	0.61
2:B:350:VAL:HA	2:B:353:LEU:HD23	1.82	0.61
1:A:18:GLN:O	1:A:22:LYS:HG2	2.01	0.61
2:B:45:MET:O	2:B:48:MET:HB2	2.01	0.61
2:B:109:TRP:CE3	2:B:110:LEU:CD2	2.83	0.61
2:B:320:HIS:ND1	2:B:321:ALA:N	2.49	0.61
1:A:6:LEU:HD13	1:A:94:TRP:CE3	2.35	0.60
2:B:353:LEU:O	2:B:357:VAL:HB	2.01	0.60
1:A:298:ASP:HA	1:A:356:ILE:CD1	2.26	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:SER:HB3	1:A:313:ARG:NH1	2.17	0.60
1:A:384:TYR:HE2	1:A:385:TYR:CZ	2.18	0.60
2:B:190:TYR:O	2:B:193:LEU:N	2.34	0.60
1:A:78:LEU:HD11	1:A:92:LEU:HD23	1.84	0.60
1:A:125:VAL:CG1	1:A:188:LYS:HE2	2.31	0.60
2:B:131:PHE:CD2	2:B:140:GLN:NE2	2.69	0.60
1:A:46:ARG:NH1	1:A:46:ARG:CB	2.48	0.60
2:B:163:LEU:O	2:B:166:LYS:N	2.29	0.60
1:A:13:LEU:O	1:A:16:LYS:CB	2.49	0.60
2:B:136:HIS:HD2	2:B:138:MET:H	1.50	0.60
2:B:148:LEU:C	2:B:150:SER:H	2.04	0.60
2:B:191:ARG:HA	2:B:195:ARG:HB2	1.83	0.60
1:A:311:SER:HB2	1:A:313:ARG:NH2	2.18	0.59
1:A:384:TYR:CE2	1:A:385:TYR:CE1	2.90	0.59
2:B:315:VAL:HG12	2:B:316:PRO:HD2	1.84	0.59
1:A:114:TRP:O	1:A:115:ALA:C	2.40	0.59
1:A:135:LEU:CD1	1:A:139:SER:HB3	2.30	0.59
2:B:127:MET:CE	2:B:131:PHE:CZ	2.85	0.59
2:B:269:LEU:HA	2:B:274:HIS:CD2	2.37	0.59
2:B:181:LYS:O	2:B:185:VAL:HG23	2.03	0.59
2:B:333:GLN:O	2:B:336:PHE:HB3	2.02	0.59
1:A:390:MET:HB2	1:A:393:TYR:CZ	2.37	0.59
1:A:67:ARG:HB3	1:A:69:PHE:HD2	1.68	0.59
1:A:191:ARG:HD3	1:A:200:ILE:HA	1.85	0.59
1:A:299:ALA:O	1:A:303:ASP:HB2	2.03	0.59
1:A:27:GLN:NE2	1:A:28:HIS:CE1	2.71	0.59
1:A:90:GLU:HG3	1:A:114:TRP:CZ3	2.38	0.59
1:A:431:ILE:HD12	2:B:20:ARG:HH21	1.68	0.59
2:B:70:SER:OG	2:B:72:PRO:HD2	2.02	0.59
2:B:136:HIS:CG	2:B:137:PRO:HD2	2.37	0.59
2:B:162:ILE:HD11	2:B:167:TYR:HD1	1.68	0.59
2:B:281:VAL:HG22	2:B:316:PRO:CB	2.30	0.59
2:B:397:PHE:HE1	2:B:401:ARG:NH2	2.01	0.59
1:A:420:GLU:O	1:A:421:ARG:HB2	2.03	0.58
1:A:336:PHE:O	1:A:337:ALA:C	2.40	0.58
1:A:48:MET:O	1:A:49:LYS:C	2.40	0.58
1:A:164:ARG:O	1:A:167:TYR:HB2	2.03	0.58
2:B:91:GLY:CA	2:B:102:PRO:HG3	2.33	0.58
2:B:144:ALA:O	2:B:147:ALA:N	2.36	0.58
1:A:144:ALA:O	1:A:148:LEU:N	2.34	0.58
1:A:384:TYR:HE2	1:A:385:TYR:CE1	2.22	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:HB3	2:B:258:PRO:HG2	1.85	0.58
1:A:326:THR:O	1:A:328:PRO:HD3	2.04	0.58
2:B:301:LEU:HD11	2:B:356:ILE:CD1	2.33	0.58
1:A:327:ASP:OD1	1:A:374:VAL:HG22	2.04	0.58
2:B:6:LEU:HB2	2:B:94:TRP:CZ3	2.39	0.58
2:B:145:ILE:HD11	2:B:182:LEU:HD21	1.85	0.58
1:A:413:ARG:HA	1:A:413:ARG:NE	2.19	0.58
2:B:341:LEU:HD22	2:B:384:TYR:CE2	2.36	0.58
1:A:59:ASP:OD2	1:A:61:ASP:N	2.32	0.58
1:A:149:ASN:HD21	2:B:139:SER:CB	2.16	0.58
2:B:334:ARG:O	2:B:338:LEU:HG	2.04	0.58
2:B:356:ILE:O	2:B:360:VAL:HG23	2.04	0.58
1:A:168:TRP:CZ2	1:A:169:GLU:HG3	2.38	0.58
2:B:284:TRP:CZ2	2:B:315:VAL:HG13	2.39	0.58
2:B:288:LEU:HD13	2:B:304:TYR:CE2	2.39	0.58
1:A:71:ILE:HG12	1:A:329:ARG:HG2	1.84	0.57
1:A:284:TRP:CZ3	1:A:285:LEU:CD1	2.87	0.57
1:A:302:ARG:HB2	1:A:356:ILE:HG12	1.84	0.57
1:A:13:LEU:O	1:A:16:LYS:HG3	2.05	0.57
1:A:91:GLY:CA	1:A:102:PRO:HG3	2.33	0.57
1:A:231:TYR:CD1	1:A:231:TYR:C	2.78	0.57
1:A:285:LEU:HD21	1:A:350:VAL:HG22	1.86	0.57
2:B:342:PRO:HD2	2:B:343:GLY:N	2.16	0.57
2:B:328:PRO:O	2:B:332:CYS:HB2	2.05	0.57
2:B:92:LEU:CD1	2:B:233:THR:HG23	2.32	0.57
2:B:301:LEU:HG	2:B:356:ILE:CD1	2.32	0.57
2:B:357:VAL:CB	2:B:358:PRO:HD3	2.32	0.57
2:B:381:LEU:HD13	2:B:381:LEU:N	2.20	0.57
1:A:323:LEU:O	1:A:369:ASN:HB2	2.05	0.56
2:B:142:SER:O	2:B:146:THR:OG1	2.22	0.56
1:A:206:LYS:C	1:A:207:LEU:HD23	2.24	0.56
1:A:337:ALA:HB3	1:A:347:PHE:CZ	2.41	0.56
2:B:136:HIS:O	2:B:140:GLN:HG3	2.05	0.56
2:B:288:LEU:HD13	2:B:304:TYR:CD2	2.39	0.56
1:A:48:MET:O	1:A:49:LYS:O	2.23	0.56
1:A:233:THR:O	1:A:236:SER:OG	2.14	0.56
1:A:267:ASN:O	1:A:270:ALA:HB3	2.05	0.56
1:A:333:GLN:OE1	1:A:378:SER:HA	2.05	0.56
2:B:42:TYR:OH	2:B:427:THR:HG23	2.04	0.56
2:B:103:THR:OG1	2:B:106:GLN:HG3	2.05	0.56
2:B:149:ASN:O	2:B:149:ASN:ND2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD23	2:B:390:MET:CE	2.35	0.56
2:B:285:LEU:HG	2:B:346:MET:CE	2.35	0.56
2:B:337:ALA:CB	2:B:347:PHE:CE2	2.88	0.56
1:A:305:ILE:HD11	1:A:357:VAL:HG22	1.87	0.56
2:B:59:ASP:HB3	2:B:63:GLY:O	2.04	0.56
1:A:214:THR:HA	1:A:217:LEU:HB2	1.86	0.56
2:B:127:MET:HE2	2:B:131:PHE:CZ	2.41	0.56
2:B:342:PRO:CD	2:B:343:GLY:H	2.14	0.56
1:A:284:TRP:HZ3	1:A:285:LEU:CD1	2.17	0.56
1:A:320:HIS:N	1:A:369:ASN:OD1	2.39	0.56
1:A:157:ALA:HB1	1:A:162:ILE:HG21	1.85	0.56
1:A:430:LEU:CD2	2:B:33:LEU:CD2	2.83	0.56
2:B:174:SER:HB2	2:B:258:PRO:CG	2.33	0.56
2:B:269:LEU:HD11	2:B:397:PHE:HE2	1.66	0.56
2:B:340:HIS:O	2:B:342:PRO:CD	2.51	0.56
2:B:401:ARG:HG2	2:B:401:ARG:NH1	2.21	0.56
1:A:42:TYR:CD2	2:B:25:ARG:HD2	2.40	0.56
2:B:204:ASP:OD2	2:B:204:ASP:C	2.44	0.56
1:A:425:MET:CA	2:B:52:VAL:H	2.14	0.56
2:B:65:ARG:CG	2:B:68:GLY:O	2.54	0.56
1:A:6:LEU:HB2	1:A:94:TRP:HZ3	1.66	0.55
1:A:109:TRP:HE3	1:A:110:LEU:CD2	2.18	0.55
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.42	0.55
1:A:230:LEU:HD12	1:A:230:LEU:O	2.05	0.55
2:B:190:TYR:CD2	2:B:217:LEU:HD22	2.40	0.55
2:B:223:GLN:NE2	2:B:340:HIS:CE1	2.74	0.55
2:B:318:TYR:CE1	2:B:372:PRO:HG3	2.42	0.55
2:B:349:LEU:O	2:B:350:VAL:C	2.44	0.55
1:A:221:ASP:OD2	1:A:223:GLN:HB2	2.07	0.55
1:A:234:ILE:HG13	1:A:235:HIS:CE1	2.41	0.55
2:B:305:ILE:HD13	2:B:357:VAL:CG2	2.35	0.55
2:B:369:ASN:N	2:B:370:PRO:CD	2.69	0.55
2:B:408:GLN:O	2:B:412:SER:OG	2.24	0.55
1:A:6:LEU:HD13	1:A:94:TRP:CZ3	2.41	0.55
1:A:306:TRP:HD1	1:A:360:VAL:HG13	1.72	0.55
2:B:163:LEU:HD12	2:B:164:ARG:H	1.72	0.55
2:B:305:ILE:HA	2:B:308:THR:HB	1.88	0.55
1:A:27:GLN:CG	1:A:28:HIS:N	2.66	0.55
1:A:163:LEU:O	1:A:165:THR:N	2.40	0.55
1:A:384:TYR:CD2	1:A:385:TYR:CE2	2.93	0.55
2:B:107:VAL:C	2:B:109:TRP:N	2.59	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:MET:HB2	2:B:393:TYR:CE2	2.42	0.55
2:B:415:LEU:CD1	2:B:417:PHE:CZ	2.90	0.55
2:B:19:ALA:HA	2:B:22:LYS:HG2	1.88	0.55
2:B:54:GLU:N	2:B:408:GLN:OE1	2.29	0.55
2:B:138:MET:HE1	2:B:269:LEU:HD23	1.89	0.54
2:B:13:LEU:HD11	2:B:100:GLN:NE2	2.22	0.54
2:B:138:MET:CE	2:B:269:LEU:HD23	2.37	0.54
2:B:179:ILE:O	2:B:209:TRP:NE1	2.36	0.54
1:A:327:ASP:HB3	1:A:373:ASN:HA	1.90	0.54
2:B:320:HIS:HB3	2:B:369:ASN:ND2	2.23	0.54
2:B:94:TRP:CG	2:B:102:PRO:HB3	2.41	0.54
2:B:415:LEU:HB2	2:B:417:PHE:CE1	2.43	0.54
1:A:88:LEU:CD1	1:A:229:ARG:HD3	2.37	0.54
2:B:28:HIS:O	2:B:31:THR:HB	2.06	0.54
1:A:14:ILE:HB	1:A:15:PRO:HD3	1.90	0.54
1:A:288:LEU:HD23	1:A:349:LEU:HD21	1.90	0.54
2:B:90:GLU:OE2	2:B:111:SER:OG	2.19	0.54
1:A:182:LEU:N	1:A:183:PRO:CD	2.70	0.54
2:B:33:LEU:HD12	2:B:34:GLY:N	2.23	0.54
2:B:109:TRP:CZ3	2:B:110:LEU:CD2	2.91	0.54
1:A:88:LEU:HD11	1:A:229:ARG:HD3	1.90	0.53
1:A:91:GLY:HA2	1:A:102:PRO:HG3	1.90	0.53
1:A:370:PRO:HD2	1:A:371:TRP:CD1	2.44	0.53
2:B:214:THR:CG2	2:B:215:ASN:N	2.70	0.53
1:A:37:THR:HG21	2:B:30:GLY:HA2	1.90	0.53
1:A:251:VAL:HG11	1:A:261:SER:HA	1.88	0.53
2:B:337:ALA:HB3	2:B:347:PHE:CE2	2.43	0.53
1:A:251:VAL:CG1	1:A:261:SER:HB3	2.37	0.53
1:A:430:LEU:HD23	1:A:433:LEU:HD23	1.89	0.53
2:B:27:GLN:NE2	2:B:28:HIS:CE1	2.76	0.53
2:B:54:GLU:HB2	2:B:408:GLN:OE1	2.08	0.53
2:B:87:PRO:O	2:B:229:ARG:HB3	2.08	0.53
2:B:248:SER:OG	2:B:405:VAL:HG22	2.08	0.53
1:A:187:ALA:O	1:A:191:ARG:HB2	2.08	0.53
2:B:36:ILE:HG23	2:B:48:MET:CE	2.38	0.53
1:A:301:LEU:HD12	1:A:301:LEU:C	2.28	0.53
2:B:378:SER:O	2:B:381:LEU:N	2.39	0.53
2:B:384:TYR:CD2	2:B:385:TYR:CE2	2.92	0.53
1:A:158:TYR:HE2	1:A:167:TYR:HH	1.56	0.53
1:A:411:TRP:O	1:A:415:LEU:HG	2.08	0.53
2:B:111:SER:OG	2:B:208:ASP:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD23	2:B:390:MET:HE2	1.92	0.52
2:B:329:ARG:O	2:B:333:GLN:HG3	2.08	0.52
1:A:412:SER:HB3	1:A:417:PHE:HD2	1.74	0.52
2:B:107:VAL:O	2:B:108:SER:C	2.47	0.52
2:B:168:TRP:CE2	2:B:169:GLU:HG2	2.45	0.52
2:B:324:ARG:CZ	2:B:324:ARG:HB3	2.33	0.52
1:A:306:TRP:CZ2	1:A:364:GLN:NE2	2.77	0.52
2:B:46:ARG:HH11	2:B:46:ARG:CG	2.22	0.52
1:A:86:GLU:HG3	1:A:87:PRO:HD2	1.91	0.52
1:A:305:ILE:O	1:A:309:LEU:HG	2.09	0.52
2:B:144:ALA:O	2:B:147:ALA:HB3	2.09	0.52
1:A:65:ARG:NH1	1:A:70:SER:HB3	2.25	0.52
1:A:399:VAL:HG12	1:A:399:VAL:O	2.09	0.52
1:A:162:ILE:CD1	1:A:167:TYR:CE1	2.93	0.52
1:A:162:ILE:CD1	1:A:167:TYR:HD1	2.18	0.52
1:A:405:VAL:O	1:A:405:VAL:HG13	2.09	0.52
1:A:427:THR:O	1:A:431:ILE:HG13	2.10	0.52
2:B:318:TYR:CE1	2:B:372:PRO:HB3	2.44	0.52
2:B:397:PHE:CE1	2:B:401:ARG:NH2	2.78	0.52
1:A:157:ALA:O	1:A:162:ILE:HG12	2.09	0.52
1:A:204:ASP:OD2	1:A:206:LYS:CD	2.55	0.52
1:A:347:PHE:O	1:A:350:VAL:N	2.42	0.52
2:B:95:LEU:HD12	2:B:95:LEU:O	2.10	0.52
1:A:38:VAL:O	1:A:38:VAL:CG1	2.58	0.52
2:B:40:MET:HB2	2:B:48:MET:CE	2.39	0.52
1:A:337:ALA:HB3	1:A:347:PHE:CE2	2.45	0.51
1:A:352:GLN:O	1:A:353:LEU:C	2.48	0.51
2:B:36:ILE:CG2	2:B:48:MET:CE	2.87	0.51
2:B:61:ASP:O	2:B:62:GLU:OE2	2.28	0.51
1:A:33:LEU:N	2:B:36:ILE:O	2.43	0.51
1:A:168:TRP:C	1:A:170:MET:H	2.14	0.51
1:A:322:VAL:O	1:A:323:LEU:C	2.49	0.51
1:A:428:ASP:OD2	1:A:428:ASP:N	2.43	0.51
2:B:230:LEU:O	2:B:234:ILE:HG23	2.10	0.51
2:B:371:TRP:HB3	2:B:372:PRO:CD	2.40	0.51
2:B:430:LEU:HD23	2:B:433:LEU:HD23	1.93	0.51
2:B:392:TYR:CE2	2:B:396:LEU:HD13	2.45	0.51
1:A:17:GLU:OE2	1:A:17:GLU:HA	2.11	0.51
2:B:46:ARG:NH1	2:B:46:ARG:C	2.64	0.51
2:B:223:GLN:CD	2:B:340:HIS:ND1	2.63	0.51
2:B:337:ALA:HB1	2:B:347:PHE:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLN:O	1:A:288:LEU:C	2.49	0.51
1:A:61:ASP:O	1:A:62:GLU:OE2	2.28	0.51
1:A:174:SER:CB	1:A:258:PRO:HG2	2.40	0.51
1:A:223:GLN:NE2	1:A:340:HIS:CE1	2.79	0.51
1:A:238:HIS:O	1:A:242:ASN:ND2	2.42	0.51
1:A:136:HIS:CD2	1:A:137:PRO:CD	2.93	0.51
1:A:171:VAL:HG21	1:A:413:ARG:HG2	1.93	0.51
1:A:273:LEU:HD11	2:B:255:LEU:HD12	1.91	0.51
2:B:162:ILE:CD1	2:B:167:TYR:HD1	2.24	0.51
2:B:336:PHE:O	2:B:337:ALA:C	2.48	0.51
1:A:154:PHE:CD1	1:A:171:VAL:HG23	2.46	0.51
1:A:393:TYR:CD1	1:A:393:TYR:N	2.76	0.51
1:A:46:ARG:CZ	1:A:46:ARG:CB	2.81	0.50
1:A:253:SER:C	1:A:255:LEU:H	2.14	0.50
1:A:423:LYS:NZ	2:B:239:GLU:OE1	2.38	0.50
1:A:433:LEU:HD23	2:B:33:LEU:HD22	1.92	0.50
2:B:92:LEU:HD13	2:B:233:THR:CG2	2.33	0.50
1:A:64:ILE:HG13	1:A:65:ARG:N	2.25	0.50
1:A:157:ALA:CB	1:A:170:MET:SD	3.00	0.50
1:A:223:GLN:HE22	1:A:340:HIS:CG	2.27	0.50
1:A:112:LYS:O	1:A:115:ALA:HB3	2.11	0.50
1:A:384:TYR:CD2	1:A:385:TYR:CZ	2.99	0.50
1:A:301:LEU:CD1	1:A:356:ILE:HG21	2.40	0.50
2:B:69:PHE:HA	2:B:73:GLU:OE1	2.10	0.50
2:B:145:ILE:CG2	2:B:263:ALA:HB2	2.36	0.50
2:B:236:SER:HA	2:B:400:SER:O	2.12	0.50
2:B:357:VAL:N	2:B:358:PRO:CD	2.74	0.50
1:A:250:LEU:HD13	1:A:420:GLU:CD	2.32	0.50
2:B:257:ASP:HB2	2:B:258:PRO:CD	2.40	0.50
2:B:305:ILE:CD1	2:B:357:VAL:HG22	2.39	0.50
2:B:377:HIS:O	2:B:377:HIS:ND1	2.45	0.50
1:A:92:LEU:HG	1:A:233:THR:CG2	2.24	0.50
2:B:127:MET:HE3	2:B:131:PHE:CZ	2.47	0.50
1:A:77:LEU:O	1:A:78:LEU:C	2.50	0.49
1:A:285:LEU:HG	1:A:346:MET:HE2	1.93	0.49
1:A:336:PHE:O	1:A:337:ALA:O	2.29	0.49
2:B:145:ILE:HG22	2:B:259:TYR:O	2.12	0.49
2:B:200:ILE:CG1	2:B:201:GLY:N	2.75	0.49
1:A:272:PRO:HG2	2:B:255:LEU:O	2.12	0.49
1:A:306:TRP:CD1	1:A:360:VAL:CG1	2.94	0.49
2:B:88:LEU:O	2:B:90:GLU:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:MET:HG2	2:B:395:VAL:HG22	1.94	0.49
2:B:272:PRO:C	2:B:274:HIS:H	2.14	0.49
1:A:369:ASN:N	1:A:370:PRO:CD	2.67	0.49
2:B:97:VAL:O	2:B:97:VAL:CG1	2.61	0.49
2:B:181:LYS:O	2:B:184:CYS:HB2	2.13	0.49
2:B:289:GLN:O	2:B:289:GLN:HG2	2.12	0.49
1:A:320:HIS:CB	1:A:369:ASN:OD1	2.60	0.49
2:B:269:LEU:CD1	2:B:397:PHE:CE2	2.85	0.49
2:B:306:TRP:CE3	2:B:364:GLN:NE2	2.80	0.49
2:B:388:THR:O	2:B:390:MET:N	2.44	0.49
1:A:281:VAL:CG2	1:A:316:PRO:HB2	2.37	0.49
2:B:37:THR:HB	2:B:40:MET:HG3	1.95	0.49
2:B:86:GLU:CD	2:B:230:LEU:HD22	2.32	0.49
1:A:46:ARG:O	1:A:46:ARG:HG3	2.13	0.49
2:B:46:ARG:NH1	2:B:46:ARG:HG3	2.26	0.49
2:B:392:TYR:O	2:B:395:VAL:N	2.42	0.49
1:A:64:ILE:HG22	1:A:71:ILE:HD13	1.95	0.49
2:B:130:ASN:O	2:B:131:PHE:C	2.50	0.49
2:B:301:LEU:CD2	2:B:352:GLN:NE2	2.76	0.49
2:B:346:MET:CG	2:B:380:VAL:HG13	2.42	0.49
2:B:408:GLN:HE22	2:B:417:PHE:HE2	1.59	0.49
1:A:37:THR:CG2	2:B:30:GLY:HA2	2.42	0.49
1:A:210:SER:CB	1:A:229:ARG:HG2	2.43	0.49
1:A:235:HIS:HB3	1:A:397:PHE:HD1	1.77	0.49
1:A:350:VAL:O	1:A:353:LEU:HB2	2.13	0.49
2:B:247:THR:O	2:B:251:VAL:HB	2.13	0.49
1:A:163:LEU:HD12	1:A:164:ARG:N	2.27	0.48
1:A:337:ALA:O	1:A:340:HIS:N	2.46	0.48
2:B:40:MET:HB2	2:B:48:MET:HE3	1.94	0.48
1:A:128:LEU:HD23	1:A:131:PHE:CD2	2.48	0.48
1:A:250:LEU:HD12	1:A:420:GLU:HB3	1.94	0.48
1:A:305:ILE:HD12	1:A:356:ILE:HG22	1.94	0.48
1:A:390:MET:HA	1:A:393:TYR:CE1	2.48	0.48
2:B:36:ILE:CG2	2:B:48:MET:HE1	2.43	0.48
1:A:337:ALA:O	1:A:338:LEU:C	2.52	0.48
2:B:285:LEU:O	2:B:288:LEU:HB3	2.13	0.48
1:A:98:THR:HG22	1:A:100:GLN:CG	2.34	0.48
1:A:101:ILE:HG23	1:A:101:ILE:HD13	1.48	0.48
1:A:162:ILE:HD11	1:A:167:TYR:CD1	2.48	0.48
1:A:211:HIS:O	1:A:215:ASN:HB3	2.13	0.48
1:A:323:LEU:CD2	1:A:324:ARG:N	2.65	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:O	1:A:288:LEU:N	2.47	0.48
1:A:362:LEU:HD13	1:A:370:PRO:CG	2.40	0.48
2:B:127:MET:CE	2:B:131:PHE:HZ	2.26	0.48
2:B:162:ILE:HD11	2:B:167:TYR:CD1	2.49	0.48
2:B:324:ARG:CG	2:B:324:ARG:NH1	2.73	0.48
1:A:162:ILE:HD11	1:A:167:TYR:CE1	2.48	0.48
1:A:310:ASN:C	1:A:312:GLY:H	2.16	0.48
1:A:322:VAL:O	1:A:323:LEU:O	2.32	0.48
1:A:53:TYR:CD2	1:A:240:GLY:CA	2.96	0.48
1:A:340:HIS:CD2	1:A:340:HIS:N	2.82	0.48
2:B:43:GLY:O	2:B:46:ARG:HG2	2.14	0.48
1:A:53:TYR:CG	1:A:240:GLY:CA	2.97	0.48
1:A:114:TRP:CD1	1:A:176:MET:HE3	2.49	0.48
1:A:284:TRP:CZ3	1:A:285:LEU:HD12	2.49	0.48
1:A:27:GLN:HG2	1:A:28:HIS:H	1.76	0.48
2:B:203:ILE:HD11	2:B:216:MET:HE1	1.95	0.47
2:B:257:ASP:O	2:B:261:SER:OG	2.31	0.47
2:B:301:LEU:CG	2:B:356:ILE:CD1	2.88	0.47
2:B:353:LEU:O	2:B:357:VAL:CG2	2.62	0.47
1:A:213:PHE:O	1:A:213:PHE:CD1	2.68	0.47
1:A:245:ALA:HA	1:A:405:VAL:HG21	1.95	0.47
1:A:246:HIS:O	1:A:249:HIS:HB3	2.14	0.47
2:B:81:GLY:HA2	2:B:88:LEU:CD1	2.41	0.47
2:B:101:ILE:O	2:B:102:PRO:C	2.51	0.47
1:A:88:LEU:CD1	1:A:229:ARG:CD	2.93	0.47
1:A:136:HIS:HD2	1:A:138:MET:N	2.03	0.47
1:A:427:THR:O	1:A:427:THR:HG22	2.13	0.47
2:B:405:VAL:O	2:B:409:LEU:HB2	2.13	0.47
1:A:20:ARG:HG3	1:A:20:ARG:HH11	1.79	0.47
1:A:103:THR:OG1	1:A:106:GLN:HG3	2.14	0.47
1:A:111:SER:HB3	1:A:208:ASP:HA	1.96	0.47
1:A:132:PRO:HG3	2:B:123:HIS:CB	2.45	0.47
2:B:59:ASP:OD2	2:B:62:GLU:N	2.48	0.47
1:A:21:ILE:O	1:A:25:ARG:HG3	2.15	0.47
1:A:157:ALA:HB3	1:A:170:MET:SD	2.55	0.47
1:A:433:LEU:HD21	2:B:33:LEU:HD22	1.96	0.47
1:A:33:LEU:HD13	1:A:33:LEU:O	2.14	0.47
1:A:55:THR:HB	1:A:96:LEU:HD22	1.95	0.47
2:B:333:GLN:O	2:B:336:PHE:N	2.41	0.47
1:A:231:TYR:CD1	1:A:231:TYR:O	2.67	0.47
1:A:331:THR:O	1:A:335:GLU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:O	1:A:339:LYS:O	2.32	0.47
2:B:80:LYS:C	2:B:82:GLY:H	2.18	0.47
2:B:248:SER:HB3	2:B:265:ALA:HB2	1.97	0.47
2:B:272:PRO:C	2:B:274:HIS:N	2.67	0.47
2:B:346:MET:HG2	2:B:380:VAL:HG13	1.97	0.47
1:A:262:PHE:O	1:A:266:MET:HG2	2.15	0.47
2:B:200:ILE:HG13	2:B:201:GLY:N	2.30	0.47
2:B:217:LEU:HD23	2:B:217:LEU:HA	1.64	0.47
1:A:89:PRO:HG3	1:A:232:LEU:HB2	1.96	0.47
1:A:121:PRO:HD2	1:A:148:LEU:HD21	1.96	0.47
1:A:248:SER:HA	1:A:261:SER:O	2.14	0.47
1:A:430:LEU:HD21	2:B:33:LEU:HD21	1.97	0.47
2:B:91:GLY:O	2:B:102:PRO:HG3	2.15	0.47
1:A:311:SER:CB	1:A:313:ARG:CZ	2.91	0.47
1:A:323:LEU:O	1:A:324:ARG:HB2	2.15	0.47
1:A:389:GLU:OE2	1:A:389:GLU:N	2.39	0.47
2:B:148:LEU:HD23	2:B:148:LEU:HA	1.60	0.47
2:B:149:ASN:HB2	2:B:260:LEU:HD13	1.98	0.47
2:B:157:ALA:HB1	2:B:162:ILE:HG23	1.91	0.47
2:B:323:LEU:HD23	2:B:324:ARG:H	1.80	0.47
1:A:91:GLY:O	1:A:102:PRO:HG3	2.16	0.46
1:A:367:ALA:HB1	1:A:368:ALA:H	1.11	0.46
2:B:238:HIS:O	2:B:239:GLU:HB2	2.14	0.46
2:B:323:LEU:HB3	2:B:369:ASN:ND2	2.30	0.46
2:B:360:VAL:O	2:B:363:GLU:HB3	2.15	0.46
1:A:24:PHE:HD2	1:A:28:HIS:HD2	1.64	0.46
1:A:168:TRP:C	1:A:170:MET:N	2.68	0.46
2:B:94:TRP:CD1	2:B:102:PRO:CA	2.98	0.46
2:B:368:ALA:C	2:B:370:PRO:HD3	2.34	0.46
1:A:58:LEU:HD23	1:A:322:VAL:HG11	1.97	0.46
1:A:59:ASP:OD2	1:A:61:ASP:HB2	2.15	0.46
1:A:168:TRP:CZ2	1:A:169:GLU:CG	2.99	0.46
1:A:226:GLU:O	1:A:229:ARG:HB2	2.14	0.46
1:A:209:TRP:CZ3	1:A:232:LEU:HD22	2.50	0.46
1:A:306:TRP:CD2	1:A:364:GLN:NE2	2.83	0.46
2:B:6:LEU:HB2	2:B:94:TRP:HZ3	1.81	0.46
2:B:38:VAL:HG22	2:B:430:LEU:HD22	1.96	0.46
2:B:269:LEU:C	2:B:271:GLY:N	2.69	0.46
2:B:86:GLU:HG3	2:B:230:LEU:CB	2.23	0.46
2:B:408:GLN:NE2	2:B:417:PHE:HE2	2.14	0.46
1:A:98:THR:CG2	1:A:100:GLN:HB2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD12	1:A:362:LEU:HA	1.59	0.46
2:B:297:ALA:C	2:B:299:ALA:N	2.67	0.46
1:A:38:VAL:HG12	2:B:29:GLY:HA2	1.98	0.46
2:B:71:ILE:HG22	2:B:72:PRO:HD3	1.97	0.46
2:B:110:LEU:O	2:B:114:TRP:N	2.42	0.46
2:B:331:THR:O	2:B:335:GLU:HB2	2.15	0.46
1:A:137:PRO:C	1:A:139:SER:H	2.19	0.46
2:B:148:LEU:O	2:B:150:SER:N	2.44	0.46
2:B:306:TRP:CH2	2:B:364:GLN:NE2	2.83	0.46
1:A:112:LYS:HE3	1:A:112:LYS:HB2	1.55	0.46
1:A:149:ASN:ND2	2:B:139:SER:CB	2.79	0.46
2:B:141:LEU:HD22	2:B:395:VAL:CG1	2.35	0.46
2:B:324:ARG:CG	2:B:324:ARG:HH11	2.27	0.46
1:A:70:SER:OG	1:A:72:PRO:HD2	2.16	0.45
1:A:89:PRO:HD3	1:A:229:ARG:O	2.16	0.45
2:B:164:ARG:HA	2:B:167:TYR:CE2	2.51	0.45
1:A:171:VAL:O	1:A:175:ALA:HB2	2.17	0.45
1:A:173:GLU:HA	1:A:173:GLU:OE2	2.14	0.45
1:A:392:TYR:HE2	1:A:396:LEU:HD13	1.82	0.45
1:A:393:TYR:N	1:A:393:TYR:HD1	2.14	0.45
2:B:89:PRO:HD3	2:B:229:ARG:O	2.16	0.45
2:B:121:PRO:O	2:B:125:VAL:HG23	2.16	0.45
2:B:267:ASN:HD22	2:B:267:ASN:HA	1.20	0.45
2:B:329:ARG:HE	2:B:374:VAL:HG22	1.81	0.45
1:A:221:ASP:OD2	1:A:223:GLN:N	2.49	0.45
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.66	0.45
1:A:314:VAL:O	1:A:314:VAL:CG1	2.58	0.45
2:B:269:LEU:C	2:B:271:GLY:H	2.18	0.45
2:B:271:GLY:HA2	2:B:272:PRO:HD2	1.58	0.45
2:B:353:LEU:O	2:B:357:VAL:CB	2.65	0.45
1:A:378:SER:O	1:A:381:LEU:N	2.41	0.45
1:A:392:TYR:CE2	1:A:396:LEU:HD13	2.52	0.45
2:B:350:VAL:O	2:B:353:LEU:N	2.49	0.45
1:A:19:ALA:HA	1:A:22:LYS:HG2	1.99	0.45
1:A:369:ASN:H	1:A:370:PRO:HD3	1.78	0.45
2:B:41:SER:C	2:B:43:GLY:H	2.20	0.45
2:B:298:ASP:HA	2:B:356:ILE:HD11	1.99	0.45
2:B:323:LEU:HD23	2:B:324:ARG:N	2.31	0.45
2:B:326:THR:HA	2:B:371:TRP:HB2	1.99	0.45
2:B:326:THR:OG1	2:B:371:TRP:HB3	2.17	0.45
2:B:371:TRP:CB	2:B:372:PRO:CD	2.95	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:O	1:A:22:LYS:HG3	2.16	0.45
1:A:53:TYR:O	2:B:425:MET:O	2.35	0.45
1:A:64:ILE:CD1	1:A:238:HIS:HA	2.47	0.45
1:A:285:LEU:CG	1:A:346:MET:HE2	2.47	0.45
1:A:344:ASP:HA	1:A:345:PRO:HD2	1.66	0.45
2:B:93:PHE:CE2	2:B:97:VAL:HG21	2.51	0.45
2:B:168:TRP:CE2	2:B:169:GLU:CG	2.98	0.45
2:B:255:LEU:HD23	2:B:255:LEU:HA	1.61	0.45
2:B:323:LEU:O	2:B:369:ASN:CB	2.64	0.45
2:B:327:ASP:O	2:B:330:TYR:HB3	2.17	0.45
1:A:334:ARG:O	1:A:338:LEU:HG	2.17	0.45
1:A:371:TRP:HA	1:A:372:PRO:HD3	1.69	0.45
1:A:223:GLN:CD	1:A:340:HIS:ND1	2.70	0.45
1:A:251:VAL:O	1:A:256:SER:HB2	2.16	0.45
2:B:149:ASN:ND2	2:B:149:ASN:C	2.67	0.45
2:B:262:PHE:O	2:B:266:MET:HG2	2.17	0.45
2:B:320:HIS:HB3	2:B:369:ASN:CG	2.37	0.45
2:B:43:GLY:O	2:B:46:ARG:CG	2.65	0.44
1:A:42:TYR:OH	1:A:427:THR:HG23	2.17	0.44
2:B:28:HIS:H	2:B:28:HIS:CD2	2.34	0.44
2:B:46:ARG:NH1	2:B:46:ARG:CG	2.73	0.44
2:B:212:ASN:O	2:B:216:MET:HB2	2.18	0.44
2:B:342:PRO:CD	2:B:343:GLY:N	2.78	0.44
1:A:2:SER:O	1:A:3:SER:HB3	2.18	0.44
1:A:98:THR:CG2	1:A:100:GLN:CG	2.92	0.44
2:B:6:LEU:O	2:B:6:LEU:HG	2.17	0.44
2:B:172:TYR:O	2:B:175:ALA:HB3	2.18	0.44
2:B:192:ASN:HA	2:B:192:ASN:HD22	1.71	0.44
2:B:392:TYR:O	2:B:393:TYR:C	2.54	0.44
1:A:181:LYS:HG3	1:A:181:LYS:H	1.72	0.44
1:A:330:TYR:CD2	1:A:377:HIS:HB2	2.52	0.44
2:B:121:PRO:HB2	2:B:123:HIS:HD2	1.81	0.44
2:B:269:LEU:O	2:B:271:GLY:N	2.50	0.44
1:A:17:GLU:O	1:A:21:ILE:HG13	2.18	0.44
1:A:33:LEU:HD12	1:A:49:LYS:HD2	1.99	0.44
1:A:38:VAL:O	1:A:42:TYR:HD2	2.00	0.44
1:A:269:LEU:O	1:A:269:LEU:HG	2.16	0.44
1:A:430:LEU:HD21	2:B:33:LEU:CD2	2.47	0.44
2:B:277:ALA:HB3	2:B:375:ASP:OD1	2.18	0.44
1:A:320:HIS:O	1:A:369:ASN:HB3	2.17	0.44
1:A:325:LYS:HD2	1:A:326:THR:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ILE:N	2:B:72:PRO:CD	2.80	0.44
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.62	0.44
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.71	0.44
2:B:188:LYS:HG3	2:B:200:ILE:HG21	1.99	0.44
2:B:224:PHE:HB2	2:B:385:TYR:CD1	2.53	0.44
2:B:405:VAL:HG12	2:B:406:LEU:HD23	1.99	0.44
1:A:64:ILE:CG2	1:A:71:ILE:CD1	2.96	0.44
2:B:91:GLY:HA3	2:B:102:PRO:HG3	1.99	0.44
2:B:116:LYS:O	2:B:117:ARG:C	2.54	0.44
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.82	0.43
1:A:285:LEU:O	1:A:288:LEU:CB	2.66	0.43
2:B:109:TRP:HE3	2:B:110:LEU:CD2	2.28	0.43
2:B:285:LEU:HB3	2:B:346:MET:CE	2.47	0.43
2:B:411:TRP:HA	2:B:414:ALA:HB3	2.00	0.43
1:A:114:TRP:NE1	1:A:176:MET:HE3	2.33	0.43
1:A:168:TRP:CG	1:A:169:GLU:N	2.86	0.43
1:A:182:LEU:HD11	1:A:262:PHE:CE2	2.53	0.43
2:B:206:LYS:C	2:B:207:LEU:HD23	2.38	0.43
1:A:13:LEU:O	1:A:16:LYS:CG	2.65	0.43
1:A:310:ASN:O	1:A:312:GLY:N	2.51	0.43
2:B:46:ARG:HH11	2:B:46:ARG:CB	2.31	0.43
2:B:371:TRP:HB3	2:B:372:PRO:HD2	2.00	0.43
1:A:40:MET:HB3	1:A:46:ARG:HG3	2.01	0.43
1:A:106:GLN:O	1:A:110:LEU:HG	2.18	0.43
1:A:141:LEU:HD22	1:A:395:VAL:HG13	2.01	0.43
1:A:232:LEU:O	1:A:400:SER:OG	2.33	0.43
1:A:251:VAL:HG12	1:A:252:GLY:N	2.32	0.43
2:B:326:THR:HG22	2:B:326:THR:O	2.18	0.43
2:B:329:ARG:NH2	2:B:374:VAL:CG2	2.52	0.43
2:B:393:TYR:CD1	2:B:393:TYR:N	2.83	0.43
2:B:86:GLU:CG	2:B:230:LEU:HD22	2.48	0.43
1:A:411:TRP:CZ3	1:A:415:LEU:HD21	2.52	0.43
2:B:213:PHE:HD1	2:B:213:PHE:HA	1.52	0.43
2:B:282:LEU:HD12	2:B:282:LEU:HA	1.83	0.43
2:B:350:VAL:HG21	2:B:380:VAL:CG2	2.26	0.43
2:B:357:VAL:CB	2:B:358:PRO:CD	2.96	0.43
1:A:64:ILE:HD13	1:A:238:HIS:CD2	2.53	0.43
1:A:246:HIS:O	1:A:246:HIS:CD2	2.72	0.43
1:A:276:LEU:HB3	1:A:280:GLU:OE2	2.17	0.43
1:A:362:LEU:CD1	1:A:367:ALA:CB	2.96	0.43
2:B:70:SER:O	2:B:71:ILE:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:VAL:HG23	2:B:125:VAL:H	1.47	0.43
2:B:313:ARG:HD3	2:B:313:ARG:N	2.34	0.43
2:B:318:TYR:HE1	2:B:372:PRO:HG3	1.83	0.43
2:B:361:LEU:HD23	2:B:361:LEU:HA	1.71	0.43
1:A:35:GLN:HA	2:B:35:GLN:HA	2.00	0.43
2:B:14:ILE:O	2:B:15:PRO:C	2.57	0.43
2:B:24:PHE:C	2:B:26:GLN:N	2.72	0.43
2:B:102:PRO:HB2	2:B:107:VAL:CG2	2.46	0.43
1:A:24:PHE:CD2	1:A:28:HIS:HD2	2.37	0.43
1:A:28:HIS:O	1:A:31:THR:HB	2.19	0.43
1:A:284:TRP:CZ3	1:A:285:LEU:HD13	2.54	0.43
2:B:94:TRP:NE1	2:B:102:PRO:HA	2.34	0.43
2:B:340:HIS:CD2	2:B:340:HIS:N	2.82	0.42
1:A:4:THR:HG22	1:A:5:ASN:H	1.84	0.42
1:A:65:ARG:HG2	1:A:68:GLY:HA2	2.00	0.42
2:B:10:LEU:HD23	2:B:10:LEU:HA	1.68	0.42
2:B:163:LEU:HD12	2:B:163:LEU:HA	1.69	0.42
1:A:427:THR:HG21	2:B:21:ILE:HG12	2.00	0.42
2:B:51:LEU:O	2:B:52:VAL:HB	2.19	0.42
2:B:367:ALA:HB1	2:B:368:ALA:H	1.00	0.42
1:A:285:LEU:O	1:A:288:LEU:HB3	2.20	0.42
1:A:315:VAL:HA	1:A:316:PRO:HD3	1.96	0.42
1:A:349:LEU:O	1:A:350:VAL:C	2.57	0.42
1:A:353:LEU:HD12	1:A:357:VAL:CG2	2.49	0.42
2:B:145:ILE:CG2	2:B:259:TYR:O	2.66	0.42
2:B:200:ILE:H	2:B:200:ILE:HG23	1.61	0.42
1:A:269:LEU:O	1:A:275:GLY:CA	2.68	0.42
1:A:288:LEU:HA	1:A:288:LEU:HD12	1.61	0.42
2:B:168:TRP:CZ2	2:B:169:GLU:HG2	2.55	0.42
2:B:341:LEU:HB3	2:B:384:TYR:CE2	2.54	0.42
1:A:36:ILE:CD1	2:B:49:LYS:O	2.68	0.42
1:A:101:ILE:CG2	1:A:102:PRO:HD2	2.49	0.42
2:B:88:LEU:HD12	2:B:229:ARG:HD2	2.01	0.42
2:B:207:LEU:HB2	2:B:212:ASN:OD1	2.20	0.42
1:A:142:SER:CB	1:A:267:ASN:HD21	2.32	0.42
1:A:269:LEU:O	1:A:275:GLY:HA3	2.20	0.42
2:B:71:ILE:HG22	2:B:328:PRO:HB2	2.02	0.42
2:B:322:VAL:O	2:B:322:VAL:CG1	2.64	0.42
1:A:329:ARG:HH21	1:A:374:VAL:HG22	1.79	0.42
1:A:390:MET:HA	1:A:393:TYR:CD1	2.55	0.42
2:B:177:ASP:O	2:B:181:LYS:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD23	2:B:390:MET:HE1	2.01	0.42
2:B:308:THR:HG22	2:B:309:LEU:N	2.34	0.42
2:B:383:GLN:HE21	2:B:383:GLN:HB3	1.55	0.42
1:A:58:LEU:CD2	1:A:322:VAL:HG11	2.49	0.42
1:A:310:ASN:HD22	1:A:310:ASN:HA	1.78	0.42
1:A:425:MET:O	1:A:426:SER:HB3	2.20	0.42
2:B:86:GLU:HB2	2:B:226:GLU:OE1	2.20	0.42
2:B:136:HIS:CG	2:B:137:PRO:CD	3.01	0.42
2:B:324:ARG:CZ	2:B:324:ARG:HB2	2.49	0.42
1:A:269:LEU:CD1	1:A:397:PHE:CE2	3.03	0.41
2:B:154:PHE:CE1	2:B:167:TYR:HB3	2.38	0.41
2:B:180:ALA:O	2:B:183:PRO:HG2	2.20	0.41
2:B:236:SER:O	2:B:401:ARG:HD3	2.20	0.41
1:A:43:GLY:O	1:A:46:ARG:HB3	2.20	0.41
1:A:168:TRP:CH2	1:A:169:GLU:HG2	2.55	0.41
1:A:410:ILE:O	1:A:410:ILE:CG2	2.66	0.41
2:B:349:LEU:O	2:B:350:VAL:O	2.37	0.41
1:A:297:ALA:CB	1:A:299:ALA:H	2.29	0.41
1:A:306:TRP:CH2	1:A:364:GLN:NE2	2.88	0.41
2:B:281:VAL:O	2:B:284:TRP:HB3	2.19	0.41
1:A:49:LYS:HG2	2:B:425:MET:SD	2.60	0.41
1:A:305:ILE:HD11	1:A:357:VAL:CG2	2.50	0.41
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.88	0.41
2:B:297:ALA:O	2:B:299:ALA:N	2.54	0.41
2:B:381:LEU:HD12	2:B:381:LEU:HA	1.75	0.41
2:B:390:MET:HB2	2:B:393:TYR:CD2	2.54	0.41
1:A:22:LYS:HE3	1:A:22:LYS:HB2	1.80	0.41
1:A:38:VAL:HG22	1:A:430:LEU:HD22	2.03	0.41
1:A:101:ILE:HD12	1:A:101:ILE:HG21	1.73	0.41
1:A:272:PRO:HA	1:A:276:LEU:HD22	2.02	0.41
2:B:133:THR:CG2	2:B:133:THR:O	2.68	0.41
2:B:182:LEU:N	2:B:183:PRO:HD3	2.33	0.41
2:B:315:VAL:HG13	2:B:316:PRO:HD2	1.98	0.41
2:B:431:ILE:HG21	2:B:431:ILE:HD13	1.73	0.41
1:A:176:MET:HE3	1:A:176:MET:HB3	1.94	0.41
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.70	0.41
2:B:267:ASN:N	2:B:267:ASN:ND2	2.63	0.41
2:B:281:VAL:O	2:B:284:TRP:N	2.38	0.41
1:A:30:GLY:HA2	2:B:37:THR:HG23	1.99	0.41
1:A:70:SER:O	1:A:71:ILE:C	2.58	0.41
1:A:356:ILE:HG22	1:A:357:VAL:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:TYR:O	1:A:392:TYR:CG	2.74	0.41
2:B:109:TRP:CZ2	2:B:113:GLU:HG2	2.55	0.41
1:A:11:ALA:HB2	1:A:168:TRP:HH2	1.86	0.41
1:A:138:MET:HG3	1:A:394:THR:HB	2.01	0.41
1:A:172:TYR:CD2	1:A:172:TYR:C	2.94	0.41
1:A:360:VAL:O	1:A:364:GLN:N	2.54	0.41
2:B:19:ALA:HA	2:B:22:LYS:CG	2.48	0.41
2:B:71:ILE:N	2:B:72:PRO:HD2	2.35	0.41
2:B:120:LEU:HD22	2:B:184:CYS:HB3	2.02	0.41
2:B:124:VAL:CG2	2:B:148:LEU:HD23	2.47	0.41
2:B:212:ASN:O	2:B:216:MET:CG	2.64	0.41
2:B:371:TRP:CD1	2:B:371:TRP:N	2.88	0.41
1:A:305:ILE:HD13	1:A:305:ILE:HG21	1.76	0.41
2:B:250:LEU:HD12	2:B:420:GLU:HB3	2.03	0.41
2:B:323:LEU:HD22	2:B:325:LYS:H	1.86	0.41
2:B:357:VAL:N	2:B:358:PRO:HD2	2.36	0.41
1:A:14:ILE:O	1:A:16:LYS:N	2.54	0.40
1:A:357:VAL:HB	1:A:358:PRO:HD3	2.02	0.40
1:A:392:TYR:O	1:A:392:TYR:CD2	2.74	0.40
1:A:431:ILE:HD13	1:A:431:ILE:HG21	1.59	0.40
2:B:390:MET:HE3	2:B:390:MET:HB3	1.93	0.40
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.70	0.40
1:A:214:THR:CA	1:A:217:LEU:HB2	2.50	0.40
1:A:328:PRO:O	1:A:331:THR:HB	2.21	0.40
2:B:25:ARG:HH11	2:B:25:ARG:HD3	1.51	0.40
2:B:356:ILE:HG22	2:B:357:VAL:N	2.36	0.40
1:A:33:LEU:HA	1:A:33:LEU:HD22	1.55	0.40
1:A:210:SER:HB2	1:A:229:ARG:HG2	2.03	0.40
1:A:212:ASN:O	1:A:216:MET:N	2.54	0.40
1:A:234:ILE:H	1:A:234:ILE:HG23	1.68	0.40
2:B:172:TYR:CD2	2:B:172:TYR:C	2.94	0.40
2:B:195:ARG:HH11	2:B:195:ARG:HD3	1.61	0.40
2:B:337:ALA:CB	2:B:347:PHE:CD2	3.04	0.40
2:B:344:ASP:HA	2:B:345:PRO:HD2	1.84	0.40
1:A:278:ASN:ND2	1:A:393:TYR:HB3	2.36	0.40
1:A:371:TRP:CB	1:A:372:PRO:CD	2.97	0.40
1:A:93:PHE:CD2	1:A:114:TRP:HZ2	2.39	0.40
1:A:193:LEU:HB3	1:A:194:TYR:CD2	2.56	0.40
1:A:255:LEU:O	2:B:272:PRO:HG2	2.22	0.40
1:A:348:LYS:O	1:A:351:ALA:N	2.54	0.40
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:MET:C	1:A:392:TYR:N	2.74	0.40
2:B:55:THR:HB	2:B:96:LEU:HD22	2.02	0.40
2:B:71:ILE:HG21	2:B:328:PRO:O	2.21	0.40
2:B:320:HIS:ND1	2:B:322:VAL:N	2.59	0.40

All (26) 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:A:220:THR:CB	2:B:290:LYS:O[3_664]	1.26	0.94
1:A:195:ARG:NH2	2:B:300:SER:OG[3_664]	1.27	0.93
1:A:195:ARG:CZ	2:B:300:SER:OG[3_664]	1.47	0.73
1:A:195:ARG:CD	2:B:297:ALA:CB[3_664]	1.48	0.72
1:A:290:LYS:CA	2:B:220:THR:OG1[3_764]	1.49	0.71
1:A:191:ARG:NH2	2:B:295:ALA:CB[3_664]	1.52	0.68
1:A:220:THR:OG1	2:B:290:LYS:C[3_664]	1.52	0.68
1:A:290:LYS:O	2:B:221:ASP:N[3_764]	1.52	0.68
1:A:195:ARG:NH2	2:B:300:SER:CB[3_664]	1.53	0.67
1:A:295:ALA:O	2:B:195:ARG:NE[3_764]	1.55	0.65
1:A:220:THR:OG1	2:B:291:ALA:N[3_664]	1.67	0.53
1:A:289:GLN:O	2:B:220:THR:OG1[3_764]	1.67	0.53
1:A:220:THR:CB	2:B:290:LYS:C[3_664]	1.75	0.45
1:A:220:THR:OG1	2:B:290:LYS:O[3_664]	1.76	0.44
1:A:220:THR:CA	2:B:290:LYS:O[3_664]	1.84	0.36
1:A:388:THR:CG2	2:B:303:ASP:OD1[3_664]	1.90	0.30
1:A:290:LYS:O	2:B:221:ASP:CA[3_764]	1.92	0.28
1:A:220:THR:C	2:B:290:LYS:O[3_664]	1.96	0.24
1:A:290:LYS:N	2:B:220:THR:OG1[3_764]	1.97	0.23
1:A:194:TYR:O	2:B:297:ALA:CB[3_664]	1.99	0.21
1:A:156:ARG:NH2	2:B:23:THR:O[1_455]	2.00	0.20
1:A:195:ARG:CD	2:B:297:ALA:N[3_664]	2.04	0.16
1:A:195:ARG:CD	2:B:297:ALA:CA[3_664]	2.06	0.14
1:A:289:GLN:C	2:B:220:THR:OG1[3_764]	2.06	0.14
1:A:27:GLN:NE2	2:B:156:ARG:NH1[1_545]	2.07	0.13
1:A:295:ALA:O	2:B:195:ARG:CD[3_764]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	423/433 (98%)	319 (75%)	77 (18%)	27 (6%)	1 3
2	B	423/429 (99%)	325 (77%)	72 (17%)	26 (6%)	1 4
All	All	846/862 (98%)	644 (76%)	149 (18%)	53 (6%)	1 3

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14	ILE
1	A	67	ARG
1	A	164	ARG
2	B	3	SER
2	B	6	LEU
2	B	67	ARG
2	B	118	ALA
2	B	149	ASN
2	B	164	ARG
2	B	190	TYR
2	B	341	LEU
1	A	3	SER
1	A	169	GLU
1	A	190	TYR
1	A	236	SER
1	A	340	HIS
1	A	348	LYS
2	B	11	ALA
2	B	81	GLY
2	B	191	ARG
2	B	289	GLN
2	B	308	THR
1	A	29	GLY
1	A	238	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	407	ALA
1	A	426	SER
2	B	52	VAL
2	B	85	GLY
2	B	389	GLU
1	A	32	ALA
1	A	191	ARG
1	A	239	GLU
1	A	289	GLN
2	B	304	TYR
2	B	403	LEU
1	A	280	GLU
1	A	341	LEU
1	A	345	PRO
2	B	51	LEU
2	B	90	GLU
2	B	345	PRO
2	B	426	SER
2	B	87	PRO
2	B	144	ALA
2	B	257	ASP
2	B	350	VAL
1	A	50	GLY
1	A	369	ASN
1	A	281	VAL
1	A	316	PRO
1	A	15	PRO
1	A	52	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	344/345 (100%)	240 (70%)	104 (30%)	0 1
2	B	344/345 (100%)	251 (73%)	93 (27%)	0 1
All	All	688/690 (100%)	491 (71%)	197 (29%)	0 1

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ASN
1	A	10	LEU
1	A	16	LYS
1	A	20	ARG
1	A	23	THR
1	A	25	ARG
1	A	33	LEU
1	A	35	GLN
1	A	37	THR
1	A	38	VAL
1	A	39	ASP
1	A	41	SER
1	A	46	ARG
1	A	48	MET
1	A	58	LEU
1	A	62	GLU
1	A	64	ILE
1	A	65	ARG
1	A	73	GLU
1	A	76	LYS
1	A	80	LYS
1	A	86	GLU
1	A	88	LEU
1	A	92	LEU
1	A	101	ILE
1	A	103	THR
1	A	108	SER
1	A	110	LEU
1	A	111	SER
1	A	112	LYS
1	A	127	MET
1	A	131	PHE
1	A	134	ASN
1	A	139	SER
1	A	140	GLN
1	A	149	ASN
1	A	156	ARG
1	A	166	LYS
1	A	170	MET
1	A	171	VAL
1	A	181	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	LEU
1	A	191	ARG
1	A	192	ASN
1	A	193	LEU
1	A	195	ARG
1	A	199	SER
1	A	200	ILE
1	A	203	ILE
1	A	206	LYS
1	A	212	ASN
1	A	214	THR
1	A	215	ASN
1	A	217	LEU
1	A	225	THR
1	A	228	MET
1	A	229	ARG
1	A	231	TYR
1	A	244	SER
1	A	251	VAL
1	A	256	SER
1	A	261	SER
1	A	276	LEU
1	A	284	TRP
1	A	287	GLN
1	A	289	GLN
1	A	290	LYS
1	A	300	SER
1	A	301	LEU
1	A	306	TRP
1	A	307	ASN
1	A	310	ASN
1	A	314	VAL
1	A	323	LEU
1	A	324	ARG
1	A	325	LYS
1	A	331	THR
1	A	334	ARG
1	A	335	GLU
1	A	340	HIS
1	A	341	LEU
1	A	342	PRO
1	A	353	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	356	ILE
1	A	360	VAL
1	A	362	LEU
1	A	371	TRP
1	A	374	VAL
1	A	381	LEU
1	A	383	GLN
1	A	387	MET
1	A	388	THR
1	A	390	MET
1	A	394	THR
1	A	396	LEU
1	A	405	VAL
1	A	409	LEU
1	A	412	SER
1	A	413	ARG
1	A	415	LEU
1	A	423	LYS
1	A	424	SER
1	A	428	ASP
2	B	4	THR
2	B	5	ASN
2	B	10	LEU
2	B	13	LEU
2	B	23	THR
2	B	25	ARG
2	B	26	GLN
2	B	27	GLN
2	B	28	HIS
2	B	33	LEU
2	B	39	ASP
2	B	40	MET
2	B	41	SER
2	B	46	ARG
2	B	49	LYS
2	B	56	SER
2	B	61	ASP
2	B	62	GLU
2	B	64	ILE
2	B	65	ARG
2	B	70	SER
2	B	71	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	73	GLU
2	B	76	LYS
2	B	80	LYS
2	B	86	GLU
2	B	101	ILE
2	B	112	LYS
2	B	116	LYS
2	B	120	LEU
2	B	125	VAL
2	B	127	MET
2	B	134	ASN
2	B	146	THR
2	B	149	ASN
2	B	166	LYS
2	B	184	CYS
2	B	188	LYS
2	B	189	ILE
2	B	191	ARG
2	B	192	ASN
2	B	193	LEU
2	B	195	ARG
2	B	199	SER
2	B	203	ILE
2	B	204	ASP
2	B	205	SER
2	B	206	LYS
2	B	210	SER
2	B	212	ASN
2	B	214	THR
2	B	228	MET
2	B	234	ILE
2	B	261	SER
2	B	276	LEU
2	B	285	LEU
2	B	287	GLN
2	B	289	GLN
2	B	301	LEU
2	B	306	TRP
2	B	307	ASN
2	B	310	ASN
2	B	314	VAL
2	B	323	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	324	ARG
2	B	325	LYS
2	B	332	CYS
2	B	334	ARG
2	B	335	GLU
2	B	338	LEU
2	B	341	LEU
2	B	352	GLN
2	B	360	VAL
2	B	362	LEU
2	B	371	TRP
2	B	377	HIS
2	B	381	LEU
2	B	382	LEU
2	B	383	GLN
2	B	388	THR
2	B	390	MET
2	B	391	ASN
2	B	394	THR
2	B	401	ARG
2	B	405	VAL
2	B	406	LEU
2	B	409	LEU
2	B	412	SER
2	B	413	ARG
2	B	415	LEU
2	B	423	LYS
2	B	428	ASP
2	B	433	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	28	HIS
1	A	134	ASN
1	A	136	HIS
1	A	140	GLN
1	A	149	ASN
1	A	192	ASN
1	A	212	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	GLN
1	A	238	HIS
1	A	267	ASN
1	A	310	ASN
1	A	352	GLN
1	A	383	GLN
1	A	391	ASN
2	B	26	GLN
2	B	28	HIS
2	B	100	GLN
2	B	136	HIS
2	B	140	GLN
2	B	149	ASN
2	B	153	ASN
2	B	192	ASN
2	B	223	GLN
2	B	238	HIS
2	B	267	ASN
2	B	278	ASN
2	B	310	ASN
2	B	352	GLN
2	B	383	GLN
2	B	391	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	291:ALA	C	295:ALA	N	9.25
1	B	82:GLY	C	84:GLY	N	3.42

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.