



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:04 PM GMT

PDB ID : 1DXI
Title : STRUCTURE DETERMINATION OF GLUCOSE ISOMERASE FROM STREPTOMYCES MURINUS AT 2.6 ANGSTROMS RESOLUTION
Authors : Rasmussen, H.; La Cour, T.; Nyborg, J.; Schulein, M.
Deposited on : 1993-09-30
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

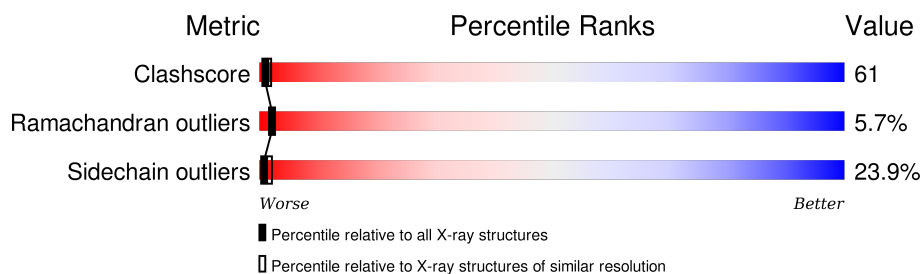
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6054 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 D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3023	1908	536	570	9			
1	B	388	Total	C	N	O	S	0	0	0
			3023	1908	536	570	9			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

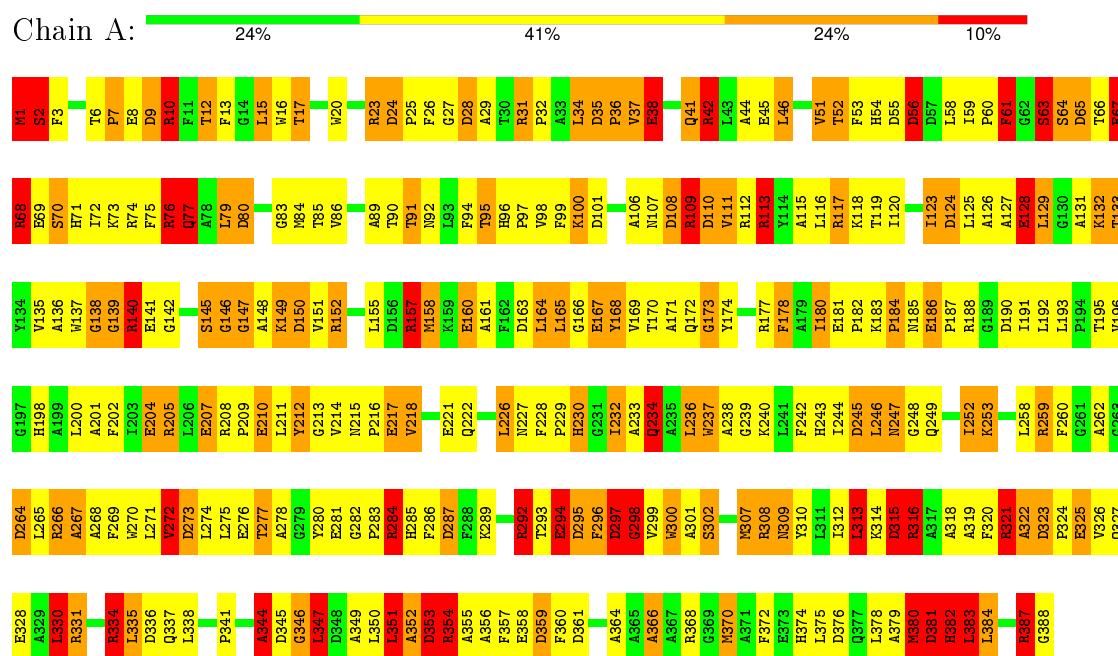
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		

3 Residue-property plots

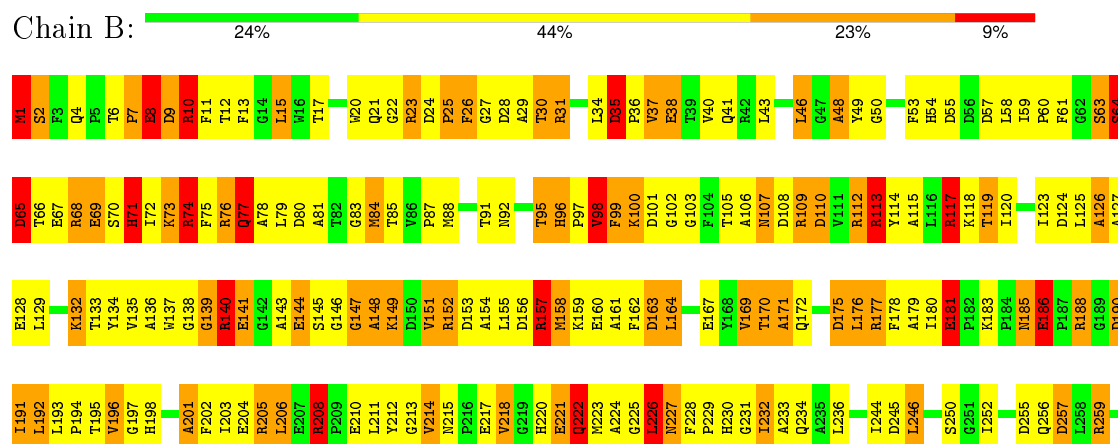
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: D-XYLOSE ISOMERASE



• Molecule 1: D-XYLOSE ISOMERASE



G388	V326 Q327 D264 A329 L330 R331 A332 R334 L335 D336 Q337 L338 A339 Q340 P341 T342 A343 A344 D345 G346 L347 D348 A349 L350 P351 A352 D353 R354 A355 A356 F357 R358 D359	V262 Q327 D264 A329 L330 R331 A332 R334 L335 D336 Q337 L338 A339 Q340 P341 T342 A343 A344 D345 G346 L347 D348 A349 L350 P351 A352 D353 R354 A355 A356 F357 R358 D359	G263 D264 L265 R266 A267 D268 F269 W270 L271 V272 D273 L274 L275 E276 T277 A278	P283 R284 H285 F286 D287 F288 K289 P290 P291 R292 T293 E294 D295 F296 D297 G298 V299 H300 A301 S302 A303	G306 R307 R308 N309 Y310 L311 T312 L313 R314 D315 R316 A317 A318 A319 F320 R321 A322 D323 P324 R325
------	--	--	--	--	--

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.65Å 137.65Å 132.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6054	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.60	11/3097 (0.4%)	2.47	175/4198 (4.2%)
1	B	2.07	8/3097 (0.3%)	2.54	178/4198 (4.2%)
All	All	1.85	19/6194 (0.3%)	2.50	353/8396 (4.2%)

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	2	16
1	B	0	13
All	All	2	29

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CA-CB	67.37	3.02	1.53
1	B	1	MET	N-CA	64.25	2.74	1.46
1	A	1	MET	N-CA	42.74	2.31	1.46
1	A	1	MET	C-O	39.00	1.97	1.23
1	A	1	MET	CA-CB	-10.09	1.31	1.53
1	B	1	MET	C-O	7.95	1.38	1.23
1	B	382	HIS	N-CA	7.00	1.60	1.46
1	A	213	GLY	N-CA	6.21	1.55	1.46
1	B	381	ASP	C-O	6.04	1.34	1.23
1	A	346	GLY	CA-C	5.98	1.61	1.51
1	A	381	ASP	N-CA	5.53	1.57	1.46
1	A	370	MET	C-O	5.42	1.33	1.23
1	B	46	LEU	C-O	5.42	1.33	1.23
1	A	139	GLY	N-CA	5.39	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLY	N-CA	-5.39	1.38	1.46
1	B	38	GLU	CD-OE2	5.32	1.31	1.25
1	A	347	LEU	N-CA	-5.16	1.36	1.46
1	B	328	GLU	CB-CG	-5.14	1.42	1.52
1	A	64	SER	CB-OG	5.04	1.48	1.42

All (353) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	CD-NE-CZ	37.36	175.90	123.60
1	B	68	ARG	NE-CZ-NH1	28.72	134.66	120.30
1	A	146	GLY	C-N-CA	27.20	179.43	122.30
1	A	157	ARG	NE-CZ-NH1	22.99	131.80	120.30
1	A	349	ALA	C-N-CA	20.62	173.24	121.70
1	B	266	ARG	NE-CZ-NH2	-17.59	111.51	120.30
1	B	316	ARG	NE-CZ-NH2	17.42	129.01	120.30
1	A	140	ARG	NE-CZ-NH1	17.32	128.96	120.30
1	A	346	GLY	C-N-CA	16.96	164.11	121.70
1	B	266	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	A	152	ARG	NE-CZ-NH1	15.99	128.29	120.30
1	B	68	ARG	NE-CZ-NH2	-15.94	112.33	120.30
1	B	316	ARG	CD-NE-CZ	15.46	145.24	123.60
1	B	84	MET	CA-CB-CG	15.32	139.35	113.30
1	A	63	SER	N-CA-CB	-14.76	88.36	110.50
1	A	177	ARG	NE-CZ-NH1	14.63	127.62	120.30
1	B	328	GLU	CA-CB-CG	14.54	145.40	113.40
1	B	68	ARG	CD-NE-CZ	14.42	143.79	123.60
1	B	157	ARG	NE-CZ-NH1	14.09	127.35	120.30
1	A	292	ARG	NE-CZ-NH1	13.99	127.29	120.30
1	A	76	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	B	117	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	B	294	GLU	C-N-CA	13.57	155.63	121.70
1	B	308	ARG	NE-CZ-NH2	13.49	127.04	120.30
1	A	31	ARG	NE-CZ-NH2	-13.41	113.59	120.30
1	A	259	ARG	CA-CB-CG	13.26	142.57	113.40
1	A	316	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	B	384	LEU	CB-CA-C	13.10	135.08	110.20
1	A	68	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	B	284	ARG	NE-CZ-NH1	12.51	126.56	120.30
1	A	149	LYS	CB-CG-CD	12.18	143.26	111.60
1	B	1	MET	N-CA-CB	-12.14	88.75	110.60
1	A	177	ARG	NE-CZ-NH2	-12.11	114.25	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH1	11.83	126.21	120.30
1	B	334	ARG	NE-CZ-NH1	-11.43	114.59	120.30
1	B	347	LEU	N-CA-C	10.92	140.48	111.00
1	A	1	MET	CB-CA-C	10.92	132.23	110.40
1	B	74	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	A	152	ARG	CD-NE-CZ	10.74	138.63	123.60
1	B	287	ASP	CB-CG-OD1	10.61	127.84	118.30
1	B	152	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	316	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	A	330	LEU	CA-CB-CG	10.46	139.37	115.30
1	A	334	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	A	387	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	B	1	MET	N-CA-C	10.31	138.84	111.00
1	B	76	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	A	352	ALA	C-N-CA	10.18	147.15	121.70
1	A	42	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	B	109	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	B	38	GLU	OE1-CD-OE2	-10.05	111.24	123.30
1	B	186	GLU	CA-CB-CG	9.93	135.24	113.40
1	A	150	ASP	CB-CG-OD2	-9.92	109.37	118.30
1	B	354	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	387	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	297	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	A	141	GLU	CA-CB-CG	9.52	134.34	113.40
1	A	1	MET	O-C-N	9.44	137.80	122.70
1	A	284	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	308	ARG	CD-NE-CZ	9.34	136.67	123.60
1	A	259	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	B	349	ALA	C-N-CA	9.24	144.81	121.70
1	A	56	ASP	CB-CG-OD1	9.15	126.53	118.30
1	A	226	LEU	CB-CA-C	9.13	127.55	110.20
1	A	167	GLU	CA-CB-CG	9.13	133.48	113.40
1	A	266	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	140	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	205	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	B	37	VAL	CB-CA-C	9.05	128.59	111.40
1	B	110	ASP	N-CA-CB	9.05	126.89	110.60
1	A	10	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	157	ARG	CA-CB-CG	8.99	133.19	113.40
1	A	108	ASP	CB-CG-OD2	8.98	126.38	118.30
1	A	146	GLY	O-C-N	-8.90	108.07	123.20
1	A	335	LEU	C-N-CA	8.88	143.91	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	A	168	TYR	CB-CG-CD2	8.84	126.31	121.00
1	A	259	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	B	257	ASP	CB-CG-OD1	8.80	126.22	118.30
1	A	347	LEU	N-CA-C	8.76	134.65	111.00
1	B	298	GLY	N-CA-C	-8.75	91.22	113.10
1	B	192	LEU	CA-CB-CG	8.73	135.38	115.30
1	A	353	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	387	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	1	MET	CG-SD-CE	8.61	113.97	100.20
1	B	144	GLU	CA-CB-CG	8.52	132.15	113.40
1	A	336	ASP	N-CA-CB	-8.52	95.27	110.60
1	B	110	ASP	CB-CG-OD2	8.51	125.95	118.30
1	B	387	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	28	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	A	1	MET	CA-C-O	-8.40	102.45	120.10
1	A	344	ALA	N-CA-C	8.40	133.69	111.00
1	B	145	SER	O-C-N	8.32	137.35	123.20
1	A	284	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	B	163	ASP	CB-CG-OD1	8.30	125.78	118.30
1	B	287	ASP	CB-CG-OD2	-8.29	110.83	118.30
1	B	363	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	B	382	HIS	CB-CA-C	8.21	126.83	110.40
1	A	157	ARG	NH1-CZ-NH2	-8.20	110.38	119.40
1	A	128	GLU	CA-CB-CG	8.18	131.40	113.40
1	B	46	LEU	CA-C-N	8.18	132.55	116.20
1	B	388	GLY	CA-C-O	-8.12	105.98	120.60
1	B	65	ASP	CB-CG-OD1	8.07	125.56	118.30
1	A	297	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	144	GLU	OE1-CD-OE2	-8.03	113.66	123.30
1	A	42	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	15	LEU	CA-CB-CG	7.97	133.64	115.30
1	A	298	GLY	N-CA-C	-7.97	93.17	113.10
1	B	64	SER	N-CA-CB	7.97	122.45	110.50
1	B	273	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	101	ASP	CB-CG-OD1	-7.86	111.22	118.30
1	A	281	GLU	CA-CB-CG	7.83	130.63	113.40
1	A	322	ALA	CB-CA-C	7.80	121.80	110.10
1	B	316	ARG	NH1-CZ-NH2	-7.79	110.83	119.40
1	A	382	HIS	N-CA-CB	7.71	124.48	110.60
1	A	46	LEU	CB-CA-C	7.65	124.73	110.20
1	A	384	LEU	CB-CA-C	7.62	124.67	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	LEU	CB-CA-C	7.61	124.67	110.20
1	A	167	GLU	N-CA-CB	7.59	124.26	110.60
1	A	334	ARG	CD-NE-CZ	7.59	134.22	123.60
1	A	61	PHE	N-CA-CB	7.57	124.23	110.60
1	A	210	GLU	OE1-CD-OE2	7.57	132.38	123.30
1	B	145	SER	N-CA-CB	7.57	121.85	110.50
1	A	297	ASP	C-N-CA	7.56	138.17	122.30
1	B	370	MET	CA-C-N	7.56	133.83	117.20
1	A	381	ASP	CA-C-O	-7.54	104.26	120.10
1	B	74	ARG	CD-NE-CZ	7.49	134.08	123.60
1	B	224	ALA	CB-CA-C	7.46	121.30	110.10
1	B	201	ALA	CB-CA-C	7.46	121.29	110.10
1	B	297	ASP	N-CA-CB	7.45	124.01	110.60
1	A	24	ASP	CB-CA-C	7.42	125.24	110.40
1	A	359	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	A	302	SER	N-CA-CB	7.39	121.58	110.50
1	B	358	GLU	OE1-CD-OE2	-7.37	114.46	123.30
1	B	144	GLU	CB-CG-CD	7.32	133.97	114.20
1	B	289	LYS	CB-CG-CD	7.32	130.63	111.60
1	A	349	ALA	CB-CA-C	7.28	121.02	110.10
1	A	34	LEU	CA-CB-CG	7.26	132.01	115.30
1	B	383	LEU	CB-CA-C	7.26	124.00	110.20
1	A	292	ARG	CG-CD-NE	7.26	127.04	111.80
1	A	150	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	266	ARG	CD-NE-CZ	7.23	133.72	123.60
1	B	157	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	B	143	ALA	CB-CA-C	7.22	120.93	110.10
1	A	65	ASP	CB-CA-C	7.19	124.79	110.40
1	A	380	MET	CB-CA-C	7.12	124.65	110.40
1	A	157	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	23	ARG	CD-NE-CZ	7.08	133.51	123.60
1	A	186	GLU	CA-CB-CG	7.05	128.91	113.40
1	A	351	LEU	CA-C-N	7.04	132.69	117.20
1	A	354	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	76	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	313	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	149	LYS	CA-CB-CG	6.99	128.77	113.40
1	A	100	LYS	CA-CB-CG	6.97	128.73	113.40
1	B	328	GLU	CB-CG-CD	6.94	132.94	114.20
1	A	9	ASP	CB-CA-C	6.93	124.26	110.40
1	A	42	ARG	CD-NE-CZ	6.92	133.29	123.60
1	B	245	ASP	CB-CG-OD1	6.88	124.49	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	B	190	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	38	GLU	N-CA-CB	6.80	122.84	110.60
1	A	387	ARG	N-CA-C	6.79	129.34	111.00
1	A	160	GLU	OE1-CD-OE2	6.75	131.40	123.30
1	A	236	LEU	CA-CB-CG	6.74	130.81	115.30
1	B	382	HIS	CA-C-O	6.73	134.24	120.10
1	A	63	SER	N-CA-C	-6.73	92.82	111.00
1	B	2	SER	N-CA-C	6.73	129.17	111.00
1	B	354	ARG	CD-NE-CZ	6.70	132.97	123.60
1	A	110	ASP	N-CA-CB	6.68	122.62	110.60
1	A	259	ARG	CD-NE-CZ	6.66	132.92	123.60
1	B	140	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	148	ALA	CB-CA-C	-6.60	100.20	110.10
1	B	35	ASP	CB-CG-OD2	6.58	124.23	118.30
1	B	31	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	354	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	175	ASP	CB-CA-C	6.54	123.47	110.40
1	A	287	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	A	79	LEU	CB-CA-C	6.49	122.52	110.20
1	B	292	ARG	CD-NE-CZ	6.48	132.67	123.60
1	A	334	ARG	CB-CG-CD	6.47	128.41	111.60
1	B	15	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	267	ALA	CB-CA-C	6.45	119.78	110.10
1	A	315	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	208	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	381	ASP	C-N-CA	-6.44	105.59	121.70
1	A	2	SER	C-N-CA	6.43	137.79	121.70
1	A	212	TYR	CA-C-N	6.43	129.05	116.20
1	B	30	THR	CA-CB-CG2	6.42	121.38	112.40
1	B	344	ALA	C-N-CA	6.38	137.65	121.70
1	A	110	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	10	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	128	GLU	CA-CB-CG	6.34	127.35	113.40
1	B	350	LEU	O-C-N	6.34	132.84	122.70
1	A	334	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	372	PHE	CA-CB-CG	6.29	129.01	113.90
1	B	381	ASP	CA-C-N	6.29	131.04	117.20
1	B	208	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	381	ASP	N-CA-C	-6.29	94.02	111.00
1	B	98	VAL	CB-CA-C	-6.28	99.48	111.40
1	A	264	ASP	CB-CG-OD1	-6.26	112.66	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	LEU	O-C-N	-6.25	112.57	123.20
1	A	294	GLU	CA-CB-CG	6.22	127.08	113.40
1	A	308	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	124	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	351	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	339	ALA	CB-CA-C	6.14	119.31	110.10
1	A	292	ARG	CA-CB-CG	6.14	126.90	113.40
1	B	353	ASP	CB-CA-C	6.12	122.63	110.40
1	B	245	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	152	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	B	84	MET	CB-CA-C	-6.09	98.23	110.40
1	B	222	GLN	CB-CG-CD	6.07	127.39	111.60
1	A	344	ALA	N-CA-CB	-6.05	101.63	110.10
1	A	217	GLU	CG-CD-OE2	-6.05	106.21	118.30
1	B	386	ALA	O-C-N	6.05	132.37	122.70
1	A	152	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	157	ARG	N-CA-CB	6.04	121.47	110.60
1	A	76	ARG	CD-NE-CZ	6.03	132.05	123.60
1	A	140	ARG	CB-CA-C	6.02	122.45	110.40
1	B	181	GLU	CG-CD-OE1	6.02	130.34	118.30
1	B	363	ASP	N-CA-CB	6.02	121.44	110.60
1	A	366	ALA	O-C-N	6.01	132.31	122.70
1	A	376	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	9	ASP	C-N-CA	6.00	136.70	121.70
1	A	246	LEU	CB-CA-C	5.95	121.50	110.20
1	A	266	ARG	CD-NE-CZ	5.90	131.87	123.60
1	A	139	GLY	N-CA-C	-5.90	98.36	113.10
1	B	311	LEU	CB-CA-C	5.90	121.41	110.20
1	A	68	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	210	GLU	CG-CD-OE1	-5.88	106.54	118.30
1	A	101	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	178	PHE	CB-CA-C	5.87	122.15	110.40
1	B	188	ARG	CD-NE-CZ	-5.87	115.39	123.60
1	A	109	ARG	CA-C-O	-5.86	107.79	120.10
1	A	323	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	46	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	297	ASP	N-CA-CB	5.84	121.11	110.60
1	B	8	GLU	O-C-N	5.83	132.03	122.70
1	A	146	GLY	CA-C-O	5.82	131.08	120.60
1	A	272	VAL	CA-CB-CG2	5.82	119.63	110.90
1	B	68	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	A	140	ARG	NH1-CZ-NH2	-5.79	113.03	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ALA	CB-CA-C	5.79	118.78	110.10
1	B	46	LEU	CB-CA-C	5.79	121.19	110.20
1	A	245	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	217	GLU	CG-CD-OE1	5.76	129.82	118.30
1	B	26	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	B	334	ARG	NH1-CZ-NH2	5.76	125.73	119.40
1	B	2	SER	C-N-CA	5.75	136.07	121.70
1	A	65	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	149	LYS	CA-C-O	-5.72	108.09	120.10
1	A	129	LEU	CB-CA-C	5.71	121.06	110.20
1	A	204	GLU	CA-CB-CG	5.71	125.96	113.40
1	B	353	ASP	N-CA-CB	5.70	120.87	110.60
1	A	64	SER	CB-CA-C	5.70	120.92	110.10
1	B	38	GLU	CB-CA-C	5.69	121.78	110.40
1	B	35	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	B	38	GLU	O-C-N	-5.69	113.60	122.70
1	B	191	ILE	O-C-N	5.68	131.78	122.70
1	B	353	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	212	TYR	O-C-N	-5.67	113.56	123.20
1	B	146	GLY	CA-C-O	-5.66	110.41	120.60
1	B	226	LEU	CB-CA-C	5.66	120.96	110.20
1	B	349	ALA	CB-CA-C	5.66	118.60	110.10
1	B	353	ASP	CA-CB-CG	5.66	125.86	113.40
1	B	100	LYS	CA-C-N	-5.66	104.75	117.20
1	A	3	PHE	N-CA-CB	-5.66	100.41	110.60
1	A	168	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	B	143	ALA	CA-C-O	5.65	131.97	120.10
1	B	1	MET	CA-CB-CG	-5.65	103.70	113.30
1	B	77	GLN	CB-CG-CD	5.63	126.24	111.60
1	A	113	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	211	LEU	CA-CB-CG	5.63	128.24	115.30
1	A	296	PHE	CA-C-N	5.62	129.57	117.20
1	B	321	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	165	LEU	CB-CA-C	5.62	120.87	110.20
1	B	385	GLY	C-N-CA	5.60	135.70	121.70
1	B	117	ARG	O-C-N	5.59	131.65	122.70
1	B	113	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	A	292	ARG	NH1-CZ-NH2	-5.58	113.26	119.40
1	A	31	ARG	CD-NE-CZ	5.58	131.41	123.60
1	B	69	GLU	CG-CD-OE2	5.58	129.46	118.30
1	A	205	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	157	ARG	CA-CB-CG	5.56	125.62	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ALA	CB-CA-C	-5.55	101.78	110.10
1	A	77	GLN	N-CA-CB	-5.55	100.61	110.60
1	B	163	ASP	OD1-CG-OD2	-5.53	112.79	123.30
1	A	325	GLU	CG-CD-OE1	-5.53	107.24	118.30
1	B	259	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	329	ALA	O-C-N	5.52	131.53	122.70
1	B	147	GLY	O-C-N	-5.52	113.87	122.70
1	B	145	SER	CA-C-O	-5.50	108.55	120.10
1	B	255	ASP	CB-CA-C	5.50	121.39	110.40
1	B	9	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	331	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	10	ARG	NH1-CZ-NH2	5.47	125.42	119.40
1	A	334	ARG	CA-CB-CG	5.47	125.44	113.40
1	B	368	ARG	CB-CA-C	5.46	121.31	110.40
1	A	277	THR	CA-CB-OG1	-5.44	97.58	109.00
1	B	177	ARG	CA-C-O	5.43	131.51	120.10
1	B	128	GLU	CG-CD-OE1	-5.42	107.46	118.30
1	B	84	MET	N-CA-CB	5.41	120.33	110.60
1	B	374	HIS	N-CA-CB	5.41	120.33	110.60
1	B	48	ALA	N-CA-CB	5.41	117.67	110.10
1	B	370	MET	N-CA-CB	-5.41	100.87	110.60
1	A	68	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	352	ALA	N-CA-CB	5.39	117.65	110.10
1	B	190	ASP	O-C-N	5.39	131.33	122.70
1	B	128	GLU	CB-CA-C	-5.38	99.63	110.40
1	B	381	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	B	99	PHE	C-N-CA	5.34	135.06	121.70
1	B	69	GLU	N-CA-CB	5.34	120.22	110.60
1	A	247	ASN	N-CA-CB	-5.32	101.02	110.60
1	A	109	ARG	CA-C-N	5.31	128.88	117.20
1	A	368	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	B	308	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	A	346	GLY	CA-C-N	-5.30	105.53	117.20
1	B	296	PHE	N-CA-CB	5.30	120.13	110.60
1	A	370	MET	C-N-CA	-5.25	108.58	121.70
1	B	329	ALA	CA-C-N	-5.24	105.68	117.20
1	A	173	GLY	CA-C-N	5.23	128.70	117.20
1	A	109	ARG	CD-NE-CZ	-5.22	116.29	123.60
1	A	344	ALA	O-C-N	-5.21	114.36	122.70
1	B	151	VAL	CA-CB-CG2	5.21	118.72	110.90
1	B	375	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	315	ASP	O-C-N	5.20	131.01	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	VAL	CB-CA-C	5.20	121.27	111.40
1	A	297	ASP	N-CA-C	-5.18	97.00	111.00
1	B	353	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	B	383	LEU	N-CA-CB	-5.18	100.05	110.40
1	B	35	ASP	CB-CA-C	5.16	120.72	110.40
1	B	330	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	176	LEU	C-N-CA	5.15	134.56	121.70
1	A	76	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	A	300	TRP	CB-CA-C	5.12	120.64	110.40
1	B	110	ASP	OD1-CG-OD2	-5.12	113.58	123.30
1	A	67	GLU	CA-CB-CG	5.10	124.62	113.40
1	B	366	ALA	N-CA-CB	-5.10	102.96	110.10
1	A	150	ASP	N-CA-CB	5.09	119.76	110.60
1	B	84	MET	O-C-N	5.08	130.83	122.70
1	A	309	ASN	CB-CA-C	5.08	120.55	110.40
1	A	321	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	347	LEU	CB-CA-C	5.06	119.81	110.20
1	B	10	ARG	CD-NE-CZ	5.06	130.69	123.60
1	B	321	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	10	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	99	PHE	CB-CA-C	5.04	120.48	110.40
1	B	224	ALA	CA-C-O	5.04	130.68	120.10
1	A	234	GLN	CA-CB-CG	5.03	124.46	113.40
1	B	338	LEU	CA-C-N	-5.02	106.15	117.20
1	A	177	ARG	N-CA-CB	5.02	119.63	110.60
1	B	109	ARG	CD-NE-CZ	5.01	130.62	123.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	347	LEU	CA
1	A	382	HIS	CA

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	117	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	297	ASP	Mainchain
1	A	298	GLY	Mainchain
1	A	316	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	334	ARG	Sidechain
1	A	344	ALA	Mainchain
1	A	354	ARG	Sidechain
1	A	380	MET	Mainchain
1	A	381	ASP	Mainchain
1	A	382	HIS	Mainchain
1	A	51	VAL	Mainchain
1	A	61	PHE	Mainchain
1	A	67	GLU	Mainchain
1	A	76	ARG	Sidechain
1	B	113	ARG	Sidechain
1	B	117	ARG	Sidechain
1	B	140	ARG	Sidechain
1	B	157	ARG	Sidechain
1	B	175	ASP	Sidechain
1	B	177	ARG	Sidechain
1	B	196	VAL	Mainchain
1	B	298	GLY	Mainchain
1	B	316	ARG	Sidechain
1	B	380	MET	Mainchain
1	B	71	HIS	Mainchain
1	B	74	ARG	Sidechain
1	B	98	VAL	Mainchain

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	3023	0	2889	391	31
1	B	3023	0	2893	388	32
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	6054	0	5782	721	34

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 61.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HD2	1:B:382:HIS:CD2	1.36	1.55
1:A:345:ASP:HB3	1:A:347:LEU:CD2	1.44	1.48
1:A:316:ARG:NE	1:A:382:HIS:NE2	1.74	1.31
1:A:381:ASP:HB2	1:A:383:LEU:O	1.26	1.30
1:A:316:ARG:HB3	1:A:382:HIS:CD2	1.69	1.26
1:A:70:SER:O	1:A:74:ARG:HG3	1.37	1.22
1:A:382:HIS:O	1:A:383:LEU:HD23	1.39	1.21
1:A:345:ASP:CB	1:A:347:LEU:HD22	1.68	1.21
1:A:8:GLU:HA	1:A:10:ARG:NH1	1.59	1.18
1:B:316:ARG:CD	1:B:382:HIS:HD2	1.58	1.16
1:B:316:ARG:CD	1:B:382:HIS:CD2	2.29	1.16
1:A:316:ARG:CD	1:A:382:HIS:NE2	2.08	1.15
1:A:73:LYS:HE2	1:A:74:ARG:HE	1.12	1.14
1:B:323:ASP:HB2	1:B:383:LEU:HD11	1.18	1.12
1:B:347:LEU:CD1	1:B:349:ALA:HB3	1.80	1.11
1:A:382:HIS:C	1:A:383:LEU:HD23	1.72	1.10
1:A:320:PHE:HA	1:A:383:LEU:HD22	1.32	1.09
1:B:323:ASP:CB	1:B:383:LEU:HD11	1.84	1.08
1:A:73:LYS:CE	1:A:74:ARG:HE	1.65	1.08
1:B:323:ASP:OD2	1:B:383:LEU:HD13	1.54	1.06
1:B:347:LEU:HD11	1:B:349:ALA:HB3	1.37	1.05
1:A:382:HIS:CD2	1:A:388:GLY:HA2	1.93	1.04
1:B:96:HIS:HB3	1:B:98:VAL:HG23	1.36	1.04
1:A:316:ARG:CG	1:A:382:HIS:NE2	2.21	1.03
1:A:387:ARG:HG3	1:A:388:GLY:H	1.20	1.03
1:A:1:MET:C	1:A:1:MET:O	1.97	1.03
1:A:316:ARG:NE	1:A:382:HIS:CE1	2.27	1.02
1:A:132:LYS:CG	1:A:133:THR:HG23	1.91	1.00
1:B:316:ARG:HB3	1:B:382:HIS:CD2	1.96	1.00
1:A:345:ASP:HB3	1:A:347:LEU:HD22	1.01	1.00
1:B:149:LYS:HE2	1:B:154:ALA:HB2	1.38	1.00
1:B:347:LEU:HD13	1:B:349:ALA:CA	1.93	0.98
1:A:316:ARG:HB3	1:A:382:HIS:NE2	1.78	0.98
1:B:25:PRO:HB2	1:B:26:PHE:CD1	1.97	0.98
1:B:319:ALA:O	1:B:383:LEU:HG	1.63	0.98
1:B:310:TYR:O	1:B:314:LYS:HB2	1.64	0.97
1:A:132:LYS:HG2	1:A:133:THR:HG23	1.45	0.96
1:A:92:ASN:HD21	1:A:95:THR:HG23	1.29	0.96
1:A:370:MET:HE3	1:B:101:ASP:OD2	1.66	0.96
1:A:316:ARG:CB	1:A:382:HIS:NE2	2.31	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HG3	1:A:388:GLY:N	1.81	0.94
1:A:345:ASP:CB	1:A:347:LEU:CD2	2.37	0.94
1:A:1:MET:CA	1:A:1:MET:N	2.31	0.93
1:B:347:LEU:CD2	1:B:349:ALA:HB3	1.99	0.92
1:B:229:PRO:HA	1:B:232:ILE:HD11	1.47	0.92
1:A:316:ARG:CB	1:A:382:HIS:CD2	2.52	0.92
1:B:115:ALA:O	1:B:119:THR:HG23	1.68	0.92
1:A:259:ARG:O	1:A:262:ALA:HB3	1.67	0.92
1:A:25:PRO:HG2	1:A:26:PHE:CD1	2.04	0.92
1:B:61:PHE:CZ	1:B:96:HIS:HD2	1.86	0.92
1:B:61:PHE:CZ	1:B:96:HIS:CD2	2.58	0.92
1:A:2:SER:HA	1:A:308:ARG:NH2	1.85	0.92
1:A:113:ARG:NH1	1:B:342:THR:O	2.02	0.92
1:A:92:ASN:HD21	1:A:95:THR:CG2	1.83	0.91
1:A:316:ARG:HE	1:A:382:HIS:CE1	1.86	0.91
1:A:218:VAL:O	1:A:222:GLN:HG3	1.71	0.90
1:A:44:ALA:HB2	1:A:84:MET:HE2	1.53	0.90
1:B:323:ASP:HB2	1:B:383:LEU:CD1	2.01	0.89
1:A:8:GLU:HA	1:A:10:ARG:HH11	1.32	0.89
1:A:72:ILE:O	1:A:76:ARG:HG3	1.72	0.89
1:B:115:ALA:O	1:B:119:THR:CG2	2.21	0.89
1:A:42:ARG:O	1:A:46:LEU:HD13	1.72	0.88
1:A:382:HIS:CD2	1:A:388:GLY:CA	2.56	0.88
1:A:73:LYS:HE2	1:A:74:ARG:NE	1.87	0.88
1:A:345:ASP:HB3	1:A:347:LEU:HD23	1.55	0.87
1:B:347:LEU:CD1	1:B:349:ALA:CB	2.52	0.87
1:B:374:HIS:NE2	1:B:378:LEU:HD11	1.89	0.87
1:B:25:PRO:HB2	1:B:26:PHE:CE1	2.10	0.87
1:A:378:LEU:O	1:A:381:ASP:O	1.92	0.87
1:B:232:ILE:CD1	1:B:274:LEU:HD23	2.05	0.86
1:B:96:HIS:CB	1:B:98:VAL:HG23	2.06	0.86
1:A:341:PRO:HA	1:B:157:ARG:NH2	1.91	0.85
1:B:382:HIS:HB3	1:B:387:ARG:O	1.76	0.85
1:A:96:HIS:HD2	1:A:98:VAL:H	1.23	0.85
1:A:155:LEU:HD21	1:B:234:GLN:HG3	1.59	0.84
1:B:320:PHE:HA	1:B:383:LEU:CD2	2.08	0.83
1:A:68:ARG:NH2	1:A:125:LEU:HD22	1.93	0.83
1:B:387:ARG:HG3	1:B:388:GLY:H	1.43	0.83
1:B:6:THR:O	1:B:8:GLU:N	2.12	0.83
1:A:330:LEU:HD12	1:A:335:LEU:CD1	2.08	0.83
1:A:354:ARG:HA	1:A:358:GLU:OE1	1.77	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HD2	1:B:382:HIS:NE2	1.94	0.82
1:B:347:LEU:HD11	1:B:349:ALA:CB	2.08	0.82
1:A:320:PHE:HA	1:A:383:LEU:CD2	2.09	0.82
1:A:190:ASP:CG	1:B:227:ASN:HD22	1.83	0.82
1:A:338:LEU:O	1:B:157:ARG:HD3	1.80	0.81
1:B:99:PHE:HE1	1:B:115:ALA:HB2	1.45	0.81
1:B:323:ASP:OD2	1:B:383:LEU:CD1	2.27	0.81
1:B:196:VAL:HG23	1:B:221:GLU:OE1	1.78	0.81
1:B:149:LYS:CE	1:B:154:ALA:HB2	2.09	0.81
1:B:164:LEU:HD12	1:B:167:GLU:OE1	1.79	0.81
1:B:66:THR:HG23	1:B:67:GLU:N	1.96	0.81
1:A:12:THR:HG21	1:A:52:THR:HG22	1.62	0.81
1:A:195:THR:OG1	1:A:198:HIS:HD2	1.63	0.80
1:A:65:ASP:O	1:A:69:GLU:HG2	1.81	0.80
1:A:73:LYS:HG3	1:A:74:ARG:N	1.94	0.80
1:A:42:ARG:HG3	1:A:46:LEU:HD13	1.63	0.80
1:A:96:HIS:CD2	1:A:98:VAL:HG12	2.16	0.80
1:B:149:LYS:NZ	1:B:149:LYS:HB3	1.96	0.80
1:B:96:HIS:CG	1:B:98:VAL:CG2	2.64	0.80
1:B:268:ALA:O	1:B:272:VAL:HG23	1.80	0.80
1:A:345:ASP:CA	1:A:347:LEU:HD22	2.12	0.80
1:A:117:ARG:NH1	1:B:350:LEU:O	2.15	0.80
1:B:229:PRO:HA	1:B:232:ILE:CD1	2.13	0.79
1:A:96:HIS:CD2	1:A:98:VAL:H	2.01	0.79
1:A:353:ASP:OD2	1:A:356:ALA:HB2	1.82	0.79
1:A:8:GLU:HA	1:A:10:ARG:HH12	1.45	0.79
1:B:320:PHE:HA	1:B:383:LEU:HD23	1.65	0.79
1:B:149:LYS:CE	1:B:154:ALA:CB	2.62	0.78
1:B:381:ASP:OD2	1:B:384:LEU:CD2	2.31	0.78
1:B:36:PRO:O	1:B:40:VAL:HG23	1.84	0.78
1:A:132:LYS:HG3	1:A:133:THR:CG2	2.12	0.78
1:B:232:ILE:HD12	1:B:274:LEU:HD23	1.66	0.78
1:B:347:LEU:HD21	1:B:349:ALA:HB3	1.64	0.78
1:A:94:PHE:O	1:A:140:ARG:HD2	1.84	0.77
1:B:149:LYS:HZ3	1:B:149:LYS:HB3	1.48	0.77
1:A:382:HIS:HD2	1:A:388:GLY:HA2	1.46	0.77
1:B:66:THR:HG23	1:B:67:GLU:H	1.49	0.77
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.49	0.77
1:A:25:PRO:HG2	1:A:26:PHE:HD1	1.50	0.76
1:A:230:HIS:O	1:A:233:ALA:HB3	1.85	0.76
1:A:354:ARG:O	1:A:359:ASP:N	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:SER:O	1:B:67:GLU:N	2.18	0.76
1:B:77:GLN:O	1:B:81:ALA:HB2	1.85	0.76
1:A:132:LYS:HZ3	1:A:133:THR:CG2	2.00	0.75
1:B:96:HIS:CG	1:B:98:VAL:HG23	2.22	0.75
1:A:370:MET:CE	1:B:101:ASP:OD2	2.34	0.75
1:A:92:ASN:ND2	1:A:95:THR:HG23	2.00	0.75
1:B:323:ASP:HB3	1:B:326:VAL:HB	1.67	0.75
1:A:132:LYS:HG3	1:A:133:THR:HG23	1.67	0.74
1:A:338:LEU:HD22	1:B:107:ASN:HD21	1.52	0.74
1:B:303:ALA:O	1:B:306:CYS:HB2	1.87	0.74
1:B:97:PRO:O	1:B:100:LYS:HG3	1.88	0.74
1:B:316:ARG:CB	1:B:382:HIS:CD2	2.70	0.74
1:A:9:ASP:O	1:A:10:ARG:HB2	1.86	0.74
1:A:341:PRO:HB2	1:A:344:ALA:HB2	1.70	0.74
1:B:348:ASP:OD1	1:B:351:LEU:CD2	2.36	0.74
1:A:190:ASP:CG	1:B:227:ASN:ND2	2.41	0.74
1:B:149:LYS:HE2	1:B:154:ALA:CB	2.13	0.73
1:A:142:GLY:HA3	1:A:190:ASP:O	1.89	0.73
1:A:382:HIS:C	1:A:383:LEU:CD2	2.57	0.73
1:B:183:LYS:NZ	1:B:186:GLU:HG3	2.04	0.73
1:A:296:PHE:O	1:A:299:VAL:HB	1.89	0.73
1:B:30:THR:HG23	1:B:292:ARG:NH1	2.03	0.73
1:B:153:ASP:O	1:B:156:ASP:HB2	1.88	0.72
1:B:124:ASP:O	1:B:127:ALA:HB3	1.89	0.72
1:A:357:PHE:HB2	1:B:117:ARG:HG2	1.72	0.72
1:B:323:ASP:CG	1:B:383:LEU:CD1	2.58	0.72
1:A:354:ARG:NH1	1:A:359:ASP:OD2	2.22	0.72
1:B:382:HIS:HB3	1:B:387:ARG:C	2.10	0.72
1:B:323:ASP:CG	1:B:383:LEU:HD11	2.10	0.71
1:B:64:SER:OG	1:B:67:GLU:HG3	1.89	0.71
1:A:59:ILE:HG21	1:A:68:ARG:HG2	1.71	0.71
1:B:159:LYS:HG2	1:B:206:LEU:HD12	1.73	0.71
1:A:167:GLU:O	1:A:171:ALA:N	2.21	0.71
1:A:217:GLU:OE1	1:A:247:ASN:ND2	2.24	0.71
1:A:232:ILE:HD11	1:A:274:LEU:HG	1.71	0.71
1:B:64:SER:HB2	1:B:66:THR:HG22	1.71	0.71
1:B:316:ARG:CB	1:B:382:HIS:HD2	2.02	0.71
1:B:232:ILE:HD12	1:B:274:LEU:CD2	2.20	0.71
1:B:347:LEU:CD1	1:B:349:ALA:CA	2.69	0.70
1:A:151:VAL:HG13	1:B:233:ALA:CB	2.21	0.70
1:B:194:PRO:HD2	1:B:198:HIS:CG	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ILE:HA	1:B:206:LEU:HD22	1.72	0.70
1:A:150:ASP:OD1	1:A:152:ARG:NH1	2.24	0.70
1:A:272:VAL:HG13	1:A:310:TYR:CZ	2.25	0.70
1:A:124:ASP:OD1	1:A:168:TYR:OH	2.06	0.70
1:B:316:ARG:CG	1:B:382:HIS:HD2	2.03	0.70
1:B:387:ARG:CG	1:B:388:GLY:H	2.02	0.70
1:B:336:ASP:O	1:B:340:GLN:NE2	2.25	0.70
1:A:132:LYS:NZ	1:A:133:THR:HG23	2.07	0.70
1:B:347:LEU:HD13	1:B:349:ALA:C	2.12	0.69
1:B:24:ASP:HB2	1:B:25:PRO:HD2	1.73	0.69
1:B:64:SER:CB	1:B:67:GLU:HG3	2.22	0.69
1:A:319:ALA:O	1:A:383:LEU:HD13	1.92	0.69
1:B:348:ASP:OD1	1:B:351:LEU:HD21	1.91	0.69
1:A:113:ARG:HD2	1:B:342:THR:O	1.92	0.69
1:A:42:ARG:HG3	1:A:46:LEU:CD1	2.22	0.69
1:B:151:VAL:O	1:B:155:LEU:HB2	1.92	0.69
1:B:363:ASP:HA	1:B:366:ALA:CB	2.23	0.69
1:B:269:PHE:CE1	1:B:317:ALA:HB2	2.27	0.68
1:A:2:SER:HA	1:A:308:ARG:HH22	1.56	0.68
1:A:25:PRO:HG2	1:A:26:PHE:CE1	2.28	0.68
1:B:347:LEU:CD2	1:B:349:ALA:CB	2.70	0.68
1:A:139:GLY:O	1:A:188:ARG:HG2	1.94	0.68
1:A:107:ASN:O	1:B:334:ARG:HB3	1.94	0.68
1:A:195:THR:OG1	1:A:198:HIS:CD2	2.47	0.68
1:A:381:ASP:O	1:A:383:LEU:N	2.27	0.68
1:A:52:THR:HG21	1:A:285:HIS:CD2	2.28	0.68
1:A:325:GLU:OE1	1:A:384:LEU:HD12	1.93	0.68
1:A:132:LYS:HZ3	1:A:133:THR:HG23	1.59	0.67
1:A:135:VAL:HG12	1:A:136:ALA:N	2.07	0.67
1:B:220:HIS:O	1:B:223:MET:HB2	1.94	0.67
1:B:21:GLN:HB3	1:B:29:ALA:HB1	1.76	0.67
1:A:372:PHE:CE1	1:B:148:ALA:HB1	2.29	0.67
1:B:92:ASN:OD1	1:B:95:THR:HG23	1.94	0.67
1:B:362:VAL:CG1	1:B:363:ASP:N	2.57	0.67
1:A:96:HIS:HD2	1:A:98:VAL:HG12	1.57	0.67
1:B:195:THR:OG1	1:B:198:HIS:ND1	2.24	0.67
1:B:183:LYS:HE2	1:B:185:ASN:O	1.95	0.66
1:A:99:PHE:CE1	1:A:115:ALA:HB2	2.30	0.66
1:B:144:GLU:HB3	1:B:188:ARG:HH21	1.60	0.66
1:A:151:VAL:HG13	1:B:233:ALA:HB3	1.78	0.66
1:A:100:LYS:NZ	1:B:368:ARG:O	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:O	1:A:90:THR:HG22	1.96	0.66
1:A:73:LYS:HG3	1:A:74:ARG:HG2	1.77	0.66
1:A:249:GLN:NE2	1:A:253:LYS:HG2	2.11	0.66
1:B:159:LYS:NZ	1:B:163:ASP:OD2	2.28	0.66
1:A:119:THR:HG22	1:A:123:ILE:HD12	1.78	0.66
1:B:191:ILE:HG22	1:B:192:LEU:O	1.94	0.66
1:B:109:ARG:O	1:B:113:ARG:HG3	1.96	0.66
1:B:1:MET:O	1:B:2:SER:OG	2.14	0.65
1:A:356:ALA:O	1:B:114:TYR:HA	1.95	0.65
1:B:181:GLU:OE2	1:B:220:HIS:CE1	2.49	0.65
1:A:79:LEU:O	1:A:83:GLY:N	2.29	0.65
1:A:273:ASP:O	1:A:277:THR:N	2.17	0.65
1:B:208:ARG:HB2	1:B:210:GLU:OE2	1.96	0.65
1:A:1:MET:O	1:A:2:SER:OG	2.14	0.65
1:B:363:ASP:HA	1:B:366:ALA:HB3	1.79	0.65
1:A:135:VAL:CG1	1:A:136:ALA:N	2.58	0.65
1:A:132:LYS:CG	1:A:133:THR:CG2	2.68	0.65
1:A:168:TYR:CE1	1:A:172:GLN:HG3	2.31	0.64
1:B:244:ILE:O	1:B:285:HIS:HB3	1.98	0.64
1:B:387:ARG:HG3	1:B:388:GLY:N	2.13	0.64
1:B:123:ILE:HG23	1:B:176:LEU:HD13	1.78	0.64
1:B:149:LYS:HE3	1:B:154:ALA:CB	2.27	0.64
1:B:137:TRP:HD1	1:B:181:GLU:O	1.81	0.64
1:A:312:ILE:O	1:A:316:ARG:HG3	1.98	0.64
1:A:1:MET:C	1:A:2:SER:OG	2.36	0.63
1:A:272:VAL:HG12	1:A:276:GLU:HG2	1.80	0.63
1:B:382:HIS:CB	1:B:387:ARG:O	2.46	0.63
1:B:347:LEU:CG	1:B:349:ALA:HB3	2.27	0.63
1:A:265:LEU:O	1:A:268:ALA:HB3	1.98	0.63
1:B:6:THR:OG1	1:B:8:GLU:HG2	1.98	0.63
1:B:324:PRO:HA	1:B:327:GLN:NE2	2.13	0.63
1:B:30:THR:CG2	1:B:292:ARG:NH1	2.61	0.63
1:A:169:VAL:O	1:A:172:GLN:O	2.16	0.63
1:A:325:GLU:OE1	1:A:384:LEU:CD1	2.47	0.62
1:A:387:ARG:CG	1:A:388:GLY:N	2.61	0.62
1:B:157:ARG:NH2	1:B:160:GLU:OE1	2.31	0.62
1:B:66:THR:CG2	1:B:67:GLU:H	2.11	0.62
1:B:308:ARG:HG3	1:B:312:ILE:HD11	1.80	0.62
1:B:105:THR:OG1	1:B:141:GLU:HG3	2.00	0.62
1:A:345:ASP:H	1:A:347:LEU:HB2	1.65	0.62
1:B:183:LYS:HZ1	1:B:186:GLU:HG3	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:HB3	1:B:31:ARG:O	1.99	0.62
1:B:266:ARG:HH12	1:B:376:ASP:CG	2.02	0.62
1:A:372:PHE:CD1	1:B:148:ALA:HB1	2.34	0.62
1:B:31:ARG:NH2	1:B:291:PRO:O	2.33	0.61
1:B:381:ASP:OD2	1:B:384:LEU:HD23	2.00	0.61
1:B:266:ARG:NH1	1:B:376:ASP:OD1	2.33	0.61
1:A:12:THR:CG2	1:A:52:THR:HG22	2.31	0.61
1:A:59:ILE:CD1	1:A:71:HIS:HB2	2.30	0.61
1:B:383:LEU:O	1:B:384:LEU:CG	2.49	0.61
1:B:350:LEU:N	1:B:350:LEU:HD23	2.16	0.61
1:A:319:ALA:O	1:A:383:LEU:CD1	2.49	0.61
1:B:96:HIS:CD2	1:B:98:VAL:CG2	2.84	0.61
1:B:66:THR:CG2	1:B:67:GLU:N	2.63	0.60
1:B:12:THR:CG2	1:B:49:TYR:HD1	2.14	0.60
1:A:380:MET:O	1:A:382:HIS:N	2.35	0.60
1:B:323:ASP:CB	1:B:383:LEU:CD1	2.67	0.60
1:B:99:PHE:CE1	1:B:115:ALA:HB2	2.31	0.60
1:A:15:LEU:HD23	1:A:51:VAL:CG1	2.30	0.60
1:B:30:THR:HG21	1:B:292:ARG:O	2.02	0.60
1:A:260:PHE:HE1	1:A:313:LEU:CD1	2.14	0.60
1:B:11:PHE:HZ	1:B:311:LEU:HD13	1.65	0.60
1:A:35:ASP:OD2	1:A:37:VAL:CG2	2.50	0.60
1:A:59:ILE:HD12	1:A:71:HIS:HB2	1.83	0.60
1:A:119:THR:HG22	1:A:123:ILE:CD1	2.31	0.60
1:B:362:VAL:HG12	1:B:363:ASP:H	1.66	0.60
1:B:208:ARG:CB	1:B:210:GLU:OE2	2.50	0.60
1:A:140:ARG:HA	1:A:188:ARG:HD3	1.84	0.59
1:B:324:PRO:HA	1:B:327:GLN:HE21	1.67	0.59
1:A:17:THR:HG21	1:A:286:PHE:O	2.02	0.59
1:B:382:HIS:O	1:B:383:LEU:HB2	2.02	0.59
1:A:35:ASP:OD2	1:A:37:VAL:HG23	2.03	0.59
1:A:58:LEU:HD11	1:A:75:PHE:CD1	2.37	0.59
1:A:190:ASP:OD1	1:B:227:ASN:ND2	2.35	0.59
1:A:172:GLN:O	1:A:174:TYR:N	2.35	0.59
1:A:381:ASP:C	1:A:383:LEU:N	2.55	0.59
1:A:354:ARG:O	1:A:359:ASP:HB2	2.02	0.59
1:A:280:TYR:CZ	1:A:282:GLY:HA3	2.37	0.59
1:A:35:ASP:O	1:A:38:GLU:N	2.36	0.59
1:B:346:GLY:O	1:B:347:LEU:HD23	2.01	0.59
1:B:12:THR:HG22	1:B:49:TYR:HD1	1.66	0.59
1:B:92:ASN:OD1	1:B:95:THR:CG2	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ALA:O	1:B:112:ARG:HD3	2.03	0.59
1:A:191:ILE:HG22	1:A:192:LEU:O	2.03	0.58
1:B:217:GLU:OE2	1:B:220:HIS:NE2	2.37	0.58
1:A:269:PHE:HE1	1:A:270:TRP:CZ3	2.20	0.58
1:A:338:LEU:HB2	1:B:107:ASN:ND2	2.19	0.58
1:B:70:SER:HA	1:B:73:LYS:HG3	1.85	0.58
1:A:8:GLU:CA	1:A:10:ARG:HH11	2.13	0.58
1:B:149:LYS:HE3	1:B:154:ALA:HB1	1.86	0.58
1:A:218:VAL:HG21	1:A:247:ASN:O	2.03	0.58
1:B:21:GLN:HG2	1:B:31:ARG:O	2.03	0.58
1:B:383:LEU:O	1:B:384:LEU:HG	2.04	0.58
1:B:348:ASP:OD1	1:B:351:LEU:HD23	2.02	0.58
1:B:363:ASP:O	1:B:366:ALA:HB3	2.03	0.57
1:A:125:LEU:HD12	1:A:129:LEU:HD13	1.86	0.57
1:A:370:MET:HE2	1:B:101:ASP:HB3	1.86	0.57
1:A:337:GLN:NE2	1:B:109:ARG:H	2.02	0.57
1:A:366:ALA:HB1	1:B:97:PRO:HB2	1.85	0.57
1:B:25:PRO:CB	1:B:26:PHE:CD1	2.81	0.57
1:A:233:ALA:CB	1:B:151:VAL:HG22	2.34	0.57
1:A:264:ASP:HB3	1:A:267:ALA:HB3	1.86	0.57
1:B:326:VAL:HG21	1:B:383:LEU:CD2	2.34	0.57
1:B:387:ARG:CB	1:B:387:ARG:HH11	2.17	0.57
1:A:326:VAL:HG22	1:A:378:LEU:HD13	1.87	0.57
1:A:99:PHE:HE1	1:A:115:ALA:HB2	1.69	0.57
1:A:2:SER:HA	1:A:308:ARG:HH21	1.67	0.57
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.70	0.57
1:A:151:VAL:HG11	1:B:230:HIS:HA	1.87	0.57
1:A:207:GLU:O	1:A:208:ARG:HG3	2.05	0.57
1:A:214:VAL:O	1:A:216:PRO:HD3	2.05	0.57
1:B:347:LEU:HD21	1:B:349:ALA:CB	2.33	0.56
1:B:217:GLU:OE2	1:B:220:HIS:CD2	2.58	0.56
1:A:116:LEU:CD2	1:A:165:LEU:HD13	2.35	0.56
1:A:316:ARG:CG	1:A:382:HIS:CE1	2.89	0.56
1:A:44:ALA:N	1:A:84:MET:HE1	2.20	0.56
1:B:370:MET:HG3	1:B:372:PHE:CE2	2.40	0.56
1:B:228:PHE:HB3	1:B:229:PRO:HD3	1.86	0.56
1:B:194:PRO:HD2	1:B:198:HIS:CB	2.34	0.56
1:A:73:LYS:HE3	1:A:74:ARG:HE	1.62	0.56
1:A:218:VAL:HG22	1:A:247:ASN:CB	2.35	0.56
1:B:138:GLY:O	1:B:140:ARG:N	2.38	0.56
1:B:63:SER:O	1:B:65:ASP:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HB2	1:A:286:PHE:CD1	2.41	0.55
1:A:320:PHE:HE2	1:A:321:ARG:HH21	1.53	0.55
1:A:330:LEU:HD12	1:A:335:LEU:HD12	1.85	0.55
1:A:183:LYS:HG2	1:A:184:PRO:HD2	1.89	0.55
1:A:20:TRP:CD2	1:A:289:LYS:HG2	2.41	0.55
1:B:158:MET:HG2	1:B:202:PHE:CZ	2.42	0.55
1:B:137:TRP:HZ2	1:B:183:LYS:HD3	1.72	0.55
1:A:312:ILE:CG2	1:A:316:ARG:HD2	2.36	0.55
1:A:233:ALA:HB1	1:B:151:VAL:HG22	1.88	0.55
1:A:346:GLY:H	1:A:347:LEU:CB	2.20	0.55
1:B:185:ASN:HD22	1:B:186:GLU:N	2.05	0.55
1:A:106:ALA:O	1:A:112:ARG:HD3	2.06	0.55
1:B:316:ARG:HB3	1:B:382:HIS:HD2	1.48	0.55
1:A:1:MET:C	1:A:2:SER:HG	2.11	0.55
1:A:338:LEU:HD11	1:B:154:ALA:HA	1.88	0.55
1:A:309:ASN:O	1:A:313:LEU:HG	2.07	0.55
1:A:381:ASP:C	1:A:383:LEU:H	2.10	0.55
1:A:319:ALA:HB1	1:A:383:LEU:HD11	1.89	0.55
1:A:204:GLU:HG3	1:B:204:GLU:HG3	1.88	0.55
1:B:256:GLN:O	1:B:257:ASP:HB2	2.05	0.55
1:A:326:VAL:O	1:A:330:LEU:HD22	2.07	0.54
1:B:158:MET:HG3	1:B:162:PHE:HE2	1.72	0.54
1:B:362:VAL:HG12	1:B:363:ASP:N	2.22	0.54
1:B:308:ARG:O	1:B:312:ILE:HG13	2.07	0.54
1:B:308:ARG:CG	1:B:312:ILE:HD11	2.36	0.54
1:B:61:PHE:CE2	1:B:96:HIS:CD2	2.95	0.54
1:A:185:ASN:HA	1:A:191:ILE:HG13	1.88	0.54
1:A:260:PHE:CE1	1:A:313:LEU:CD1	2.90	0.54
1:B:123:ILE:HG23	1:B:176:LEU:CD1	2.36	0.54
1:A:387:ARG:CG	1:A:388:GLY:H	2.07	0.54
1:A:218:VAL:HG22	1:A:247:ASN:HB3	1.90	0.54
1:A:351:LEU:HD21	1:B:120:ILE:HG21	1.89	0.54
1:A:284:ARG:HG2	1:A:310:TYR:CE2	2.43	0.54
1:B:25:PRO:CB	1:B:26:PHE:CE1	2.86	0.54
1:A:272:VAL:HG21	1:A:313:LEU:HB2	1.90	0.54
1:B:181:GLU:HB2	1:B:215:ASN:O	2.08	0.54
1:B:20:TRP:O	1:B:31:ARG:NH1	2.41	0.54
1:B:134:TYR:O	1:B:178:PHE:HA	2.08	0.54
1:A:341:PRO:CB	1:A:344:ALA:HB2	2.38	0.54
1:B:296:PHE:O	1:B:299:VAL:HB	2.08	0.54
1:A:180:ILE:O	1:A:182:PRO:HD3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASP:OD2	1:B:384:LEU:HD21	2.06	0.53
1:A:387:ARG:HG2	1:A:387:ARG:NH1	2.21	0.53
1:B:61:PHE:CE2	1:B:96:HIS:HD2	2.23	0.53
1:A:354:ARG:NH2	1:A:358:GLU:HB3	2.23	0.53
1:A:357:PHE:CD1	1:B:117:ARG:HB3	2.43	0.53
1:A:32:PRO:HD2	1:A:296:PHE:CZ	2.43	0.53
1:A:52:THR:CG2	1:A:285:HIS:CD2	2.91	0.53
1:A:6:THR:O	1:A:8:GLU:N	2.42	0.53
1:B:179:ALA:HA	1:B:213:GLY:O	2.08	0.53
1:A:146:GLY:HA2	1:A:148:ALA:H	1.72	0.53
1:B:323:ASP:HB2	1:B:383:LEU:HD21	1.89	0.53
1:A:249:GLN:HE21	1:A:253:LYS:HG2	1.72	0.53
1:B:380:MET:O	1:B:387:ARG:HD2	2.08	0.53
1:B:15:LEU:HD22	1:B:53:PHE:HB2	1.89	0.53
1:A:387:ARG:HG2	1:A:387:ARG:HH11	1.74	0.53
1:A:357:PHE:CE1	1:B:118:LYS:HA	2.44	0.53
1:B:336:ASP:OD1	1:B:337:GLN:N	2.42	0.53
1:A:178:PHE:O	1:A:212:TYR:O	2.27	0.53
1:B:320:PHE:O	1:B:326:VAL:HG11	2.07	0.53
1:A:54:HIS:HA	1:A:90:THR:O	2.09	0.53
1:B:159:LYS:HE2	1:B:205:ARG:O	2.09	0.53
1:B:354:ARG:C	1:B:356:ALA:H	2.11	0.53
1:B:347:LEU:HD13	1:B:349:ALA:N	2.23	0.53
1:A:259:ARG:O	1:A:262:ALA:CB	2.48	0.53
1:B:158:MET:HG3	1:B:162:PHE:CE2	2.44	0.53
1:B:87:PRO:O	1:B:132:LYS:N	2.37	0.53
1:A:380:MET:O	1:A:381:ASP:C	2.47	0.53
1:A:73:LYS:HG3	1:A:74:ARG:CG	2.39	0.53
1:A:341:PRO:HA	1:B:157:ARG:HH22	1.70	0.53
1:B:78:ALA:HA	1:B:81:ALA:HB3	1.89	0.53
1:A:20:TRP:CG	1:A:289:LYS:HG2	2.44	0.53
1:B:236:LEU:HD13	1:B:278:ALA:CB	2.38	0.52
1:A:319:ALA:CB	1:A:383:LEU:HD11	2.39	0.52
1:B:354:ARG:O	1:B:359:ASP:HB2	2.09	0.52
1:A:77:GLN:O	1:A:80:ASP:OD1	2.27	0.52
1:A:183:LYS:HE2	1:A:185:ASN:O	2.08	0.52
1:A:346:GLY:H	1:A:347:LEU:HB2	1.74	0.52
1:A:355:ALA:O	1:A:360:PHE:HB2	2.10	0.52
1:A:272:VAL:HG13	1:A:310:TYR:CE1	2.43	0.52
1:A:35:ASP:OD1	1:A:36:PRO:HD2	2.09	0.52
1:B:350:LEU:HA	1:B:353:ASP:OD1	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TRP:HB2	1:A:181:GLU:HB3	1.92	0.52
1:A:132:LYS:HZ3	1:A:133:THR:HG21	1.74	0.52
1:B:244:ILE:HG12	1:B:246:LEU:HD13	1.91	0.52
1:B:320:PHE:CE1	1:B:379:ALA:HB2	2.45	0.52
1:B:96:HIS:ND1	1:B:97:PRO:HD2	2.24	0.52
1:A:132:LYS:HG3	1:A:133:THR:HG22	1.90	0.52
1:A:326:VAL:HG12	1:A:330:LEU:CD2	2.40	0.52
1:A:232:ILE:HG13	1:A:274:LEU:CD2	2.40	0.52
1:B:382:HIS:CG	1:B:387:ARG:O	2.64	0.51
1:A:361:ASP:CG	1:A:364:ALA:HB2	2.30	0.51
1:B:132:LYS:HE2	1:B:133:THR:N	2.26	0.51
1:A:228:PHE:O	1:A:232:ILE:HG23	2.10	0.51
1:B:194:PRO:HG2	1:B:198:HIS:CE1	2.45	0.51
1:A:23:ARG:HG2	1:A:29:ALA:HB2	1.93	0.51
1:B:92:ASN:O	1:B:118:LYS:HE2	2.11	0.51
1:B:324:PRO:O	1:B:325:GLU:C	2.50	0.51
1:B:370:MET:HB3	1:B:372:PHE:CD2	2.46	0.51
1:B:181:GLU:OE2	1:B:220:HIS:HE1	1.94	0.51
1:A:381:ASP:O	1:A:382:HIS:C	2.50	0.51
1:B:115:ALA:O	1:B:119:THR:HG22	2.07	0.50
1:B:64:SER:HB2	1:B:67:GLU:HG3	1.93	0.50
1:A:272:VAL:O	1:A:276:GLU:N	2.37	0.50
1:A:209:PRO:O	1:A:240:LYS:NZ	2.44	0.50
1:A:234:GLN:HG2	1:B:155:LEU:HD21	1.93	0.50
1:B:276:GLU:HG3	1:B:314:LYS:HG2	1.93	0.50
1:A:67:GLU:O	1:A:68:ARG:C	2.49	0.50
1:B:1:MET:N	1:B:1:MET:CA	2.74	0.50
1:B:79:LEU:O	1:B:83:GLY:N	2.44	0.50
1:A:320:PHE:CA	1:A:383:LEU:CD2	2.88	0.50
1:A:15:LEU:HD21	1:A:51:VAL:HG11	1.94	0.50
1:B:226:LEU:HD12	1:B:227:ASN:H	1.75	0.50
1:A:91:THR:HG21	1:A:119:THR:HA	1.93	0.50
1:A:312:ILE:HG23	1:A:316:ARG:HD2	1.94	0.50
1:B:347:LEU:HD22	1:B:349:ALA:N	2.27	0.50
1:A:12:THR:CG2	1:A:52:THR:CG2	2.89	0.50
1:A:321:ARG:O	1:A:322:ALA:HB2	2.12	0.50
1:B:228:PHE:HB3	1:B:229:PRO:CD	2.42	0.50
1:A:284:ARG:HD3	1:A:310:TYR:CZ	2.47	0.50
1:A:15:LEU:CD2	1:A:51:VAL:HG11	2.41	0.50
1:A:140:ARG:HH21	1:A:187:PRO:CB	2.24	0.50
1:A:238:ALA:O	1:A:240:LYS:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ASP:CG	1:B:383:LEU:HD13	2.24	0.49
1:A:272:VAL:CG1	1:A:310:TYR:CE1	2.95	0.49
1:A:316:ARG:HG2	1:A:382:HIS:CE1	2.47	0.49
1:A:116:LEU:O	1:A:120:ILE:HD12	2.12	0.49
1:A:140:ARG:HH21	1:A:187:PRO:HB3	1.78	0.49
1:B:11:PHE:CZ	1:B:311:LEU:HD13	2.47	0.49
1:A:73:LYS:HE2	1:A:74:ARG:CG	2.42	0.49
1:A:309:ASN:O	1:A:313:LEU:CG	2.60	0.49
1:B:20:TRP:CH2	1:B:22:GLY:HA2	2.47	0.49
1:B:330:LEU:HD12	1:B:335:LEU:HD13	1.95	0.49
1:A:319:ALA:C	1:A:383:LEU:HD11	2.33	0.49
1:B:183:LYS:O	1:B:191:ILE:HB	2.13	0.49
1:A:45:GLU:OE1	1:A:46:LEU:HD12	2.12	0.49
1:A:201:ALA:HB2	1:B:201:ALA:HB2	1.95	0.49
1:A:232:ILE:HG12	1:A:271:LEU:CD1	2.42	0.49
1:B:308:ARG:O	1:B:312:ILE:CG1	2.61	0.49
1:A:184:PRO:O	1:A:191:ILE:HB	2.12	0.48
1:A:323:ASP:OD1	1:A:325:GLU:N	2.46	0.48
1:B:170:THR:HG21	1:B:208:ARG:NH2	2.27	0.48
1:A:37:VAL:O	1:A:41:GLN:HB2	2.12	0.48
1:B:309:ASN:O	1:B:313:LEU:HG	2.13	0.48
1:A:111:VAL:O	1:A:112:ARG:C	2.52	0.48
1:A:15:LEU:CD2	1:A:51:VAL:CG1	2.91	0.48
1:A:309:ASN:O	1:A:313:LEU:HD12	2.13	0.48
1:A:73:LYS:HE2	1:A:74:ARG:HG2	1.95	0.48
1:A:73:LYS:HG3	1:A:74:ARG:H	1.74	0.48
1:A:338:LEU:HD22	1:B:107:ASN:ND2	2.23	0.48
1:B:137:TRP:HE1	1:B:183:LYS:HB2	1.78	0.48
1:A:357:PHE:HE1	1:B:118:LYS:HA	1.78	0.48
1:B:330:LEU:HD13	1:B:375:LEU:HD11	1.95	0.48
1:A:370:MET:HB3	1:A:372:PHE:CE2	2.49	0.48
1:A:35:ASP:OD1	1:A:36:PRO:N	2.47	0.48
1:B:181:GLU:HB2	1:B:215:ASN:HD22	1.79	0.48
1:A:68:ARG:HH21	1:A:125:LEU:HD22	1.71	0.48
1:B:21:GLN:CB	1:B:31:ARG:O	2.61	0.48
1:B:159:LYS:CE	1:B:205:ARG:O	2.61	0.48
1:A:309:ASN:O	1:A:313:LEU:CD1	2.62	0.48
1:B:15:LEU:HD22	1:B:53:PHE:CB	2.43	0.48
1:B:347:LEU:HD22	1:B:349:ALA:CB	2.44	0.47
1:A:128:GLU:O	1:A:129:LEU:HD12	2.14	0.47
1:A:59:ILE:CD1	1:A:71:HIS:CB	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:O	1:B:112:ARG:HG2	2.13	0.47
1:A:248:GLY:O	1:A:258:LEU:HB2	2.14	0.47
1:A:232:ILE:HG13	1:A:274:LEU:HD21	1.96	0.47
1:A:357:PHE:HD1	1:B:117:ARG:HB3	1.80	0.47
1:B:228:PHE:O	1:B:231:GLY:N	2.45	0.47
1:A:44:ALA:CB	1:A:84:MET:HE2	2.36	0.47
1:A:97:PRO:O	1:A:100:LYS:HB2	2.14	0.47
1:A:51:VAL:N	1:A:85:THR:O	2.45	0.47
1:B:64:SER:O	1:B:66:THR:N	2.48	0.47
1:A:135:VAL:CG1	1:A:136:ALA:H	2.27	0.47
1:B:325:GLU:O	1:B:328:GLU:HB3	2.15	0.47
1:A:35:ASP:OD1	1:A:36:PRO:CD	2.63	0.47
1:A:269:PHE:HE1	1:A:270:TRP:CH2	2.32	0.47
1:A:148:ALA:HB1	1:B:372:PHE:CE1	2.49	0.47
1:B:88:MET:HA	1:B:133:THR:O	2.14	0.47
1:A:297:ASP:OD1	1:A:301:ALA:N	2.47	0.47
1:B:13:PHE:HB2	1:B:43:LEU:HD13	1.96	0.47
1:A:24:ASP:OD1	1:A:27:GLY:N	2.47	0.47
1:A:316:ARG:HB3	1:A:382:HIS:CE1	2.46	0.47
1:A:387:ARG:CG	1:A:387:ARG:HH11	2.27	0.47
1:B:24:ASP:O	1:B:25:PRO:C	2.53	0.47
1:B:354:ARG:CG	1:B:354:ARG:HH11	2.27	0.47
1:A:351:LEU:O	1:A:352:ALA:C	2.53	0.47
1:A:89:ALA:HB3	1:A:126:ALA:HB2	1.97	0.47
1:A:379:ALA:O	1:A:380:MET:HG2	2.15	0.47
1:B:323:ASP:CB	1:B:383:LEU:HD21	2.43	0.47
1:A:166:GLY:O	1:A:170:THR:HG23	2.15	0.47
1:A:374:HIS:O	1:A:378:LEU:HG	2.15	0.46
1:A:260:PHE:HE1	1:A:313:LEU:HD12	1.79	0.46
1:B:110:ASP:OD1	1:B:110:ASP:O	2.33	0.46
1:B:326:VAL:HG21	1:B:383:LEU:HD22	1.97	0.46
1:B:271:LEU:O	1:B:274:LEU:HB3	2.16	0.46
1:B:64:SER:OG	1:B:67:GLU:CG	2.60	0.46
1:A:237:TRP:H	1:A:239:GLY:H	1.63	0.46
1:B:135:VAL:CG1	1:B:136:ALA:N	2.79	0.46
1:A:259:ARG:HG3	1:A:302:SER:O	2.16	0.46
1:A:75:PHE:CE2	1:A:79:LEU:HD21	2.49	0.46
1:B:21:GLN:CG	1:B:31:ARG:O	2.63	0.46
1:A:337:GLN:HE21	1:B:109:ARG:H	1.62	0.46
1:A:53:PHE:O	1:A:90:THR:CG2	2.64	0.46
1:A:31:ARG:NH2	1:A:294:GLU:O	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PHE:O	1:B:229:PRO:C	2.54	0.46
1:B:36:PRO:O	1:B:40:VAL:CG2	2.59	0.46
1:A:337:GLN:O	1:B:112:ARG:NH1	2.45	0.46
1:B:370:MET:HB3	1:B:372:PHE:CE2	2.50	0.46
1:B:46:LEU:O	1:B:48:ALA:N	2.49	0.46
1:A:328:GLU:O	1:A:331:ARG:HB2	2.16	0.46
1:B:316:ARG:HB3	1:B:382:HIS:CG	2.45	0.46
1:B:96:HIS:O	1:B:97:PRO:C	2.54	0.46
1:B:332:ALA:O	1:B:334:ARG:NH1	2.48	0.46
1:B:218:VAL:HG13	1:B:246:LEU:HA	1.98	0.46
1:A:315:ASP:O	1:A:318:ALA:HB3	2.16	0.46
1:A:168:TYR:CZ	1:A:172:GLN:HG3	2.51	0.45
1:B:363:ASP:HA	1:B:366:ALA:HB2	1.96	0.45
1:A:35:ASP:OD1	1:A:37:VAL:HG22	2.15	0.45
1:A:178:PHE:HB2	1:A:212:TYR:CD2	2.51	0.45
1:B:132:LYS:CE	1:B:133:THR:OG1	2.63	0.45
1:A:109:ARG:NH1	1:A:113:ARG:CZ	2.80	0.45
1:A:296:PHE:O	1:A:300:TRP:CD1	2.69	0.45
1:B:295:ASP:O	1:B:299:VAL:HG23	2.15	0.45
1:B:125:LEU:O	1:B:126:ALA:C	2.55	0.45
1:A:117:ARG:HD3	1:B:350:LEU:O	2.17	0.45
1:B:10:ARG:HB3	1:B:283:PRO:HA	1.99	0.45
1:A:382:HIS:HD2	1:A:388:GLY:CA	2.15	0.45
1:B:226:LEU:HD13	1:B:226:LEU:HA	1.88	0.45
1:A:227:ASN:O	1:A:230:HIS:HB2	2.16	0.45
1:A:227:ASN:HD22	1:B:190:ASP:CG	2.20	0.45
1:B:382:HIS:O	1:B:383:LEU:CB	2.65	0.45
1:A:345:ASP:N	1:A:347:LEU:HB2	2.31	0.45
1:A:86:VAL:O	1:A:131:ALA:HA	2.17	0.45
1:B:132:LYS:HE3	1:B:133:THR:OG1	2.16	0.45
1:A:294:GLU:HB3	1:A:298:GLY:HA3	1.99	0.45
1:B:35:ASP:O	1:B:38:GLU:N	2.50	0.45
1:B:135:VAL:HG22	1:B:179:ALA:HB3	1.97	0.45
1:A:370:MET:HB3	1:A:372:PHE:CD2	2.51	0.45
1:B:250:SER:N	1:B:256:GLN:OE1	2.41	0.45
1:B:298:GLY:O	1:B:299:VAL:C	2.55	0.45
1:A:53:PHE:HD1	1:A:54:HIS:O	2.00	0.45
1:A:361:ASP:O	1:A:364:ALA:HB3	2.17	0.45
1:A:244:ILE:HD13	1:A:275:LEU:HD11	1.99	0.45
1:B:64:SER:HB2	1:B:66:THR:CG2	2.45	0.45
1:A:132:LYS:HE2	1:A:283:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:CB	1:A:140:ARG:HG3	2.47	0.45
1:B:144:GLU:HB2	1:B:188:ARG:HE	1.81	0.45
1:B:179:ALA:HB1	1:B:215:ASN:HB2	1.99	0.44
1:A:109:ARG:NH1	1:A:113:ARG:CD	2.80	0.44
1:A:205:ARG:HD3	1:A:205:ARG:HA	1.85	0.44
1:A:157:ARG:HD2	1:B:338:LEU:O	2.18	0.44
1:B:259:ARG:O	1:B:262:ALA:HB3	2.17	0.44
1:A:334:ARG:NH1	1:B:108:ASP:OD2	2.50	0.44
1:B:236:LEU:HD13	1:B:278:ALA:HB1	1.99	0.44
1:A:158:MET:HG2	1:A:202:PHE:CZ	2.52	0.44
1:B:107:ASN:HA	1:B:107:ASN:HD22	1.27	0.44
1:A:60:PRO:HG2	1:A:63:SER:OG	2.18	0.44
1:A:354:ARG:O	1:A:359:ASP:CB	2.65	0.44
1:A:237:TRP:CG	1:B:155:LEU:HD23	2.52	0.44
1:B:383:LEU:O	1:B:384:LEU:HD23	2.18	0.44
1:A:59:ILE:HA	1:A:60:PRO:HD2	1.73	0.44
1:B:22:GLY:O	1:B:292:ARG:NE	2.51	0.44
1:A:382:HIS:HB3	1:A:388:GLY:HA3	1.99	0.44
1:A:196:VAL:O	1:A:200:LEU:HG	2.17	0.44
1:B:137:TRP:HE1	1:B:183:LYS:CB	2.31	0.44
1:A:354:ARG:HB3	1:A:358:GLU:HB2	2.00	0.44
1:B:54:HIS:HB2	1:B:57:ASP:OD2	2.18	0.44
1:B:294:GLU:HA	1:B:294:GLU:OE1	2.18	0.44
1:A:28:ASP:O	1:A:292:ARG:NH2	2.49	0.44
1:B:137:TRP:CZ2	1:B:183:LYS:HD3	2.50	0.43
1:A:113:ARG:HH12	1:B:343:ALA:HA	1.83	0.43
1:A:217:GLU:O	1:A:228:PHE:CE1	2.71	0.43
1:A:46:LEU:HD21	1:A:300:TRP:HE3	1.81	0.43
1:A:245:ASP:OD1	1:A:285:HIS:ND1	2.33	0.43
1:B:195:THR:HA	1:B:221:GLU:OE2	2.17	0.43
1:B:180:ILE:O	1:B:214:VAL:HA	2.19	0.43
1:B:72:ILE:H	1:B:72:ILE:HG13	1.71	0.43
1:B:59:ILE:HA	1:B:60:PRO:HD2	1.70	0.43
1:B:60:PRO:HD2	1:B:71:HIS:CD2	2.53	0.43
1:A:157:ARG:CD	1:B:338:LEU:O	2.65	0.43
1:A:326:VAL:HG12	1:A:330:LEU:HD22	2.00	0.43
1:B:22:GLY:O	1:B:292:ARG:HD2	2.18	0.43
1:B:222:GLN:O	1:B:225:GLY:HA2	2.18	0.43
1:A:316:ARG:CZ	1:A:382:HIS:CE1	2.97	0.43
1:A:109:ARG:HH11	1:A:113:ARG:CD	2.32	0.43
1:B:374:HIS:NE2	1:B:378:LEU:CD1	2.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ALA:HB3	1:B:117:ARG:HH21	1.82	0.43
1:B:159:LYS:NZ	1:B:206:LEU:HA	2.34	0.43
1:B:298:GLY:O	1:B:301:ALA:HB3	2.19	0.43
1:A:215:ASN:OD1	1:A:243:HIS:ND1	2.52	0.43
1:A:322:ALA:O	1:A:324:PRO:HD3	2.19	0.43
1:B:383:LEU:HD22	1:B:383:LEU:HA	1.67	0.43
1:A:382:HIS:CD2	1:A:388:GLY:HA3	2.52	0.43
1:A:125:LEU:O	1:A:128:GLU:N	2.52	0.43
1:B:283:PRO:O	1:B:285:HIS:N	2.51	0.43
1:B:354:ARG:C	1:B:356:ALA:N	2.71	0.43
1:A:148:ALA:CB	1:B:372:PHE:CD1	3.01	0.43
1:A:85:THR:OG1	1:A:86:VAL:N	2.52	0.43
1:A:59:ILE:HD11	1:A:72:ILE:HG13	2.00	0.43
1:B:327:GLN:HE21	1:B:327:GLN:HB2	1.71	0.43
1:B:307:MET:O	1:B:311:LEU:HB2	2.19	0.43
1:B:381:ASP:HB2	1:B:384:LEU:HD23	2.00	0.42
1:B:300:TRP:O	1:B:303:ALA:HB3	2.19	0.42
1:A:361:ASP:OD1	1:A:364:ALA:N	2.43	0.42
1:B:197:GLY:O	1:B:201:ALA:N	2.45	0.42
1:B:50:GLY:CA	1:B:85:THR:O	2.66	0.42
1:A:323:ASP:O	1:A:324:PRO:C	2.56	0.42
1:B:24:ASP:OD1	1:B:27:GLY:N	2.51	0.42
1:B:26:PHE:CD1	1:B:26:PHE:N	2.87	0.42
1:A:360:PHE:CE2	1:B:114:TYR:HB2	2.53	0.42
1:B:134:TYR:HB2	1:B:176:LEU:HD22	2.02	0.42
1:B:323:ASP:HB2	1:B:383:LEU:CD2	2.49	0.42
1:A:274:LEU:O	1:A:278:ALA:CB	2.68	0.42
1:A:229:PRO:O	1:A:230:HIS:C	2.58	0.42
1:A:214:VAL:N	1:A:240:LYS:O	2.45	0.42
1:B:380:MET:C	1:B:381:ASP:O	2.56	0.42
1:A:312:ILE:HG22	1:A:316:ARG:HD2	2.01	0.42
1:B:349:ALA:N	1:B:350:LEU:HD23	2.34	0.42
1:B:4:GLN:O	1:B:6:THR:HG23	2.19	0.42
1:A:139:GLY:O	1:A:187:PRO:HD2	2.20	0.42
1:A:13:PHE:HE2	1:A:307:MET:CE	2.31	0.42
1:A:160:GLU:O	1:A:164:LEU:HB2	2.20	0.42
1:A:346:GLY:N	1:A:347:LEU:HD13	2.34	0.42
1:A:217:GLU:OE2	1:A:287:ASP:OD2	2.38	0.42
1:A:84:MET:HG3	1:A:85:THR:H	1.84	0.42
1:B:1:MET:C	1:B:2:SER:OG	2.58	0.42
1:B:264:ASP:OD1	1:B:267:ALA:CB	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:O	1:B:29:ALA:C	2.55	0.42
1:B:203:ILE:HG23	1:B:212:TYR:HB2	2.00	0.42
1:B:13:PHE:HB2	1:B:43:LEU:CD1	2.49	0.42
1:A:316:ARG:HG3	1:A:316:ARG:H	1.59	0.42
1:A:387:ARG:CG	1:A:387:ARG:NH1	2.83	0.42
1:A:184:PRO:HB3	1:B:226:LEU:HD21	2.01	0.42
1:B:30:THR:HG23	1:B:292:ARG:CZ	2.50	0.42
1:A:212:TYR:O	1:A:242:PHE:CE2	2.72	0.42
1:A:319:ALA:C	1:A:383:LEU:CD1	2.89	0.42
1:B:96:HIS:CG	1:B:98:VAL:HG22	2.51	0.42
1:B:137:TRP:CH2	1:B:139:GLY:HA2	2.55	0.42
1:A:56:ASP:CG	1:A:118:LYS:HZ1	2.23	0.42
1:A:320:PHE:CA	1:A:383:LEU:HD22	2.23	0.42
1:B:350:LEU:HG	1:B:351:LEU:N	2.35	0.42
1:A:193:LEU:HD11	1:A:202:PHE:CD2	2.55	0.41
1:A:382:HIS:CG	1:A:388:GLY:CA	3.02	0.41
1:A:191:ILE:O	1:A:192:LEU:C	2.56	0.41
1:A:16:TRP:CE3	1:A:54:HIS:HD2	2.39	0.41
1:A:148:ALA:HB1	1:B:372:PHE:CD1	2.55	0.41
1:B:158:MET:O	1:B:161:ALA:HB3	2.20	0.41
1:B:158:MET:CG	1:B:202:PHE:CZ	3.03	0.41
1:B:266:ARG:NH2	1:B:380:MET:HB2	2.35	0.41
1:B:135:VAL:HG12	1:B:136:ALA:N	2.36	0.41
1:A:218:VAL:HG13	1:A:247:ASN:HB2	2.01	0.41
1:A:272:VAL:O	1:A:273:ASP:C	2.58	0.41
1:B:208:ARG:HB3	1:B:210:GLU:OE2	2.19	0.41
1:B:387:ARG:CG	1:B:387:ARG:HH11	2.33	0.41
1:A:338:LEU:HD22	1:B:149:LYS:HG2	2.01	0.41
1:A:198:HIS:CD2	1:A:198:HIS:H	2.39	0.41
1:A:124:ASP:O	1:A:127:ALA:HB3	2.19	0.41
1:A:264:ASP:CG	1:A:267:ALA:HB2	2.41	0.41
1:A:163:ASP:HA	1:A:208:ARG:HH12	1.84	0.41
1:B:350:LEU:CD2	1:B:351:LEU:HD23	2.51	0.41
1:A:357:PHE:HB2	1:B:117:ARG:CG	2.46	0.41
1:B:144:GLU:H	1:B:188:ARG:NH2	2.19	0.41
1:A:188:ARG:HE	1:A:188:ARG:HA	1.86	0.41
1:B:50:GLY:HA3	1:B:85:THR:O	2.21	0.41
1:B:350:LEU:HD21	1:B:351:LEU:CD2	2.51	0.41
1:B:96:HIS:CD2	1:B:98:VAL:HG21	2.55	0.41
1:B:149:LYS:HZ1	1:B:192:LEU:HD21	1.85	0.41
1:B:336:ASP:O	1:B:339:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:H	1:B:188:ARG:HH21	1.67	0.41
1:B:193:LEU:HD11	1:B:202:PHE:CD2	2.56	0.41
1:A:106:ALA:C	1:A:108:ASP:H	2.24	0.41
1:A:137:TRP:CD2	1:A:138:GLY:O	2.74	0.41
1:B:43:LEU:O	1:B:46:LEU:O	2.38	0.41
1:B:54:HIS:O	1:B:55:ASP:C	2.58	0.41
1:B:270:TRP:CE3	1:B:270:TRP:HA	2.56	0.41
1:A:236:LEU:O	1:B:152:ARG:HG2	2.20	0.41
1:B:159:LYS:NZ	1:B:205:ARG:O	2.50	0.41
1:B:350:LEU:HD21	1:B:351:LEU:HD23	2.02	0.40
1:A:338:LEU:CD2	1:B:149:LYS:HG2	2.51	0.40
1:A:310:TYR:O	1:A:314:LYS:N	2.50	0.40
1:A:295:ASP:O	1:A:299:VAL:HG23	2.21	0.40
1:B:6:THR:HA	1:B:7:PRO:HD2	1.90	0.40
1:B:208:ARG:O	1:B:211:LEU:HB2	2.21	0.40
1:B:185:ASN:O	1:B:186:GLU:HB3	2.21	0.40
1:A:259:ARG:HD3	1:A:302:SER:HB2	2.02	0.40
1:A:109:ARG:NH1	1:A:113:ARG:NE	2.70	0.40
1:A:227:ASN:HB2	1:B:190:ASP:OD1	2.21	0.40
1:A:116:LEU:HD11	1:A:161:ALA:HA	2.04	0.40
1:B:24:ASP:HB2	1:B:25:PRO:CD	2.47	0.40
1:A:79:LEU:HD22	1:A:86:VAL:HG23	2.03	0.40
1:A:140:ARG:HA	1:A:188:ARG:CD	2.51	0.40
1:B:110:ASP:HA	1:B:113:ARG:HB2	2.04	0.40
1:B:170:THR:HG22	1:B:171:ALA:N	2.35	0.40

All (34) 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:345:ASP:CB	1:B:35:ASP:N[3_555]	0.82	1.38
1:A:345:ASP:CG	1:B:35:ASP:N[3_555]	0.86	1.34
1:A:345:ASP:CG	1:B:35:ASP:CA[3_555]	0.90	1.30
1:A:345:ASP:OD1	1:B:35:ASP:C[3_555]	1.12	1.08
1:A:345:ASP:OD1	1:B:35:ASP:O[3_555]	1.33	0.87
1:A:345:ASP:OD2	1:B:35:ASP:CA[3_555]	1.34	0.86
1:B:308:ARG:NH1	1:B:381:ASP:OD2[7_555]	1.49	0.71
1:A:345:ASP:C	1:B:35:ASP:CB[3_555]	1.53	0.67
1:A:345:ASP:OD1	1:B:35:ASP:CA[3_555]	1.56	0.64
1:A:345:ASP:CG	1:B:34:LEU:C[3_555]	1.60	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:CB	1:B:34:LEU:C[3_555]	1.65	0.55
1:A:345:ASP:OD1	1:B:35:ASP:N[3_555]	1.65	0.55
1:A:346:GLY:N	1:B:35:ASP:CB[3_555]	1.68	0.52
1:A:346:GLY:CA	1:B:35:ASP:OD2[3_555]	1.75	0.45
1:A:345:ASP:O	1:B:35:ASP:OD2[3_555]	1.75	0.45
1:A:345:ASP:CG	1:B:35:ASP:C[3_555]	1.82	0.38
1:B:308:ARG:NH1	1:B:381:ASP:CG[7_555]	1.89	0.31
1:A:345:ASP:CA	1:B:35:ASP:N[3_555]	1.94	0.26
1:A:345:ASP:OD2	1:B:35:ASP:N[3_555]	1.94	0.26
1:A:345:ASP:CB	1:B:35:ASP:CA[3_555]	1.96	0.24
1:A:345:ASP:O	1:B:35:ASP:CG[3_555]	1.97	0.23
1:A:292:ARG:NH1	1:B:140:ARG:NH1[7_555]	1.99	0.21
1:A:345:ASP:OD2	1:B:34:LEU:O[3_555]	1.99	0.21
1:A:346:GLY:N	1:B:35:ASP:CG[3_555]	2.03	0.17
1:A:346:GLY:CA	1:B:35:ASP:CG[3_555]	2.04	0.16
1:A:345:ASP:O	1:B:35:ASP:CB[3_555]	2.04	0.16
1:A:345:ASP:OD2	1:B:34:LEU:C[3_555]	2.13	0.07
1:B:308:ARG:NH1	1:B:381:ASP:OD1[7_555]	2.13	0.07
1:A:345:ASP:CG	1:B:34:LEU:O[3_555]	2.13	0.07
1:A:293:THR:O	1:A:370:MET:N[7_555]	2.13	0.07
1:A:140:ARG:NH2	1:B:24:ASP:OD2[7_555]	2.13	0.07
1:A:316:ARG:NH2	1:A:387:ARG:N[7_555]	2.14	0.06
1:A:345:ASP:C	1:B:35:ASP:CG[3_555]	2.15	0.05
1:A:346:GLY:CA	1:B:74:ARG:NH1[3_555]	2.16	0.04

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	386/388 (100%)	309 (80%)	53 (14%)	24 (6%)	2	2
1	B	386/388 (100%)	312 (81%)	54 (14%)	20 (5%)	2	3
All	All	772/776 (100%)	621 (80%)	107 (14%)	44 (6%)	2	2

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PHE
1	A	186	GLU
1	A	347	LEU
1	A	351	LEU
1	A	387	ARG
1	B	7	PRO
1	B	8	GLU
1	B	102	GLY
1	B	295	ASP
1	B	345	ASP
1	B	383	LEU
1	B	386	ALA
1	A	138	GLY
1	A	173	GLY
1	A	237	TRP
1	A	353	ASP
1	A	382	HIS
1	B	65	ASP
1	B	139	GLY
1	B	329	ALA
1	A	17	THR
1	A	23	ARG
1	A	147	GLY
1	A	184	PRO
1	A	354	ARG
1	A	380	MET
1	A	383	LEU
1	B	76	ARG
1	B	171	ALA
1	B	252	ILE
1	A	56	ASP
1	A	68	ARG
1	A	252	ILE
1	B	17	THR
1	B	75	PHE
1	B	147	GLY
1	B	172	GLN
1	A	2	SER
1	B	25	PRO
1	A	7	PRO
1	A	145	SER
1	A	298	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	64	SER
1	B	186	GLU

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	297/297 (100%)	229 (77%)	68 (23%)	1	2
1	B	297/297 (100%)	223 (75%)	74 (25%)	1	1
All	All	594/594 (100%)	452 (76%)	142 (24%)	1	1

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	PRO
1	A	10	ARG
1	A	12	THR
1	A	34	LEU
1	A	35	ASP
1	A	36	PRO
1	A	37	VAL
1	A	38	GLU
1	A	41	GLN
1	A	42	ARG
1	A	52	THR
1	A	55	ASP
1	A	63	SER
1	A	64	SER
1	A	66	THR
1	A	70	SER
1	A	77	GLN
1	A	80	ASP
1	A	91	THR
1	A	95	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	ARG
1	A	110	ASP
1	A	111	VAL
1	A	123	ILE
1	A	128	GLU
1	A	132	LYS
1	A	133	THR
1	A	140	ARG
1	A	145	SER
1	A	149	LYS
1	A	157	ARG
1	A	158	MET
1	A	164	LEU
1	A	180	ILE
1	A	207	GLU
1	A	210	GLU
1	A	218	VAL
1	A	221	GLU
1	A	226	LEU
1	A	230	HIS
1	A	232	ILE
1	A	234	GLN
1	A	252	ILE
1	A	253	LYS
1	A	266	ARG
1	A	272	VAL
1	A	273	ASP
1	A	284	ARG
1	A	292	ARG
1	A	294	GLU
1	A	295	ASP
1	A	307	MET
1	A	313	LEU
1	A	315	ASP
1	A	321	ARG
1	A	327	GLN
1	A	330	LEU
1	A	334	ARG
1	A	347	LEU
1	A	350	LEU
1	A	353	ASP
1	A	375	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	380	MET
1	A	381	ASP
1	A	382	HIS
1	A	383	LEU
1	A	387	ARG
1	B	1	MET
1	B	9	ASP
1	B	10	ARG
1	B	23	ARG
1	B	35	ASP
1	B	37	VAL
1	B	41	GLN
1	B	58	LEU
1	B	63	SER
1	B	64	SER
1	B	68	ARG
1	B	69	GLU
1	B	71	HIS
1	B	73	LYS
1	B	74	ARG
1	B	77	GLN
1	B	80	ASP
1	B	84	MET
1	B	91	THR
1	B	95	THR
1	B	96	HIS
1	B	98	VAL
1	B	107	ASN
1	B	117	ARG
1	B	119	THR
1	B	129	LEU
1	B	132	LYS
1	B	140	ARG
1	B	141	GLU
1	B	149	LYS
1	B	157	ARG
1	B	158	MET
1	B	164	LEU
1	B	169	VAL
1	B	170	THR
1	B	181	GLU
1	B	185	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	186	GLU
1	B	205	ARG
1	B	206	LEU
1	B	208	ARG
1	B	214	VAL
1	B	218	VAL
1	B	221	GLU
1	B	222	GLN
1	B	226	LEU
1	B	227	ASN
1	B	232	ILE
1	B	246	LEU
1	B	265	LEU
1	B	288	PHE
1	B	292	ARG
1	B	293	THR
1	B	311	LEU
1	B	312	ILE
1	B	314	LYS
1	B	325	GLU
1	B	328	GLU
1	B	330	LEU
1	B	334	ARG
1	B	335	LEU
1	B	340	GLN
1	B	347	LEU
1	B	354	ARG
1	B	359	ASP
1	B	362	VAL
1	B	363	ASP
1	B	368	ARG
1	B	370	MET
1	B	375	LEU
1	B	381	ASP
1	B	382	HIS
1	B	383	LEU
1	B	387	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	54	HIS
1	A	77	GLN
1	A	92	ASN
1	A	96	HIS
1	A	172	GLN
1	A	198	HIS
1	A	337	GLN
1	A	377	GLN
1	B	21	GLN
1	B	71	HIS
1	B	96	HIS
1	B	107	ASN
1	B	185	ASN
1	B	227	ASN
1	B	230	HIS
1	B	249	GLN
1	B	309	ASN
1	B	327	GLN
1	B	382	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.