



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:04 PM UTC

PDB ID : 1JKM / pdb_00001jkm
Title : BREFELDIN A ESTERASE, A BACTERIAL HOMOLOGUE OF HUMAN HORMONE SENSITIVE LIPASE
Authors : Wei, Y.; Contreras, A.J.; Sheffield, P.; Osterlund, T.; Derewenda, U.; Matern, U.O.; Derewenda, Z.S.
Deposited on : 1998-02-04
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

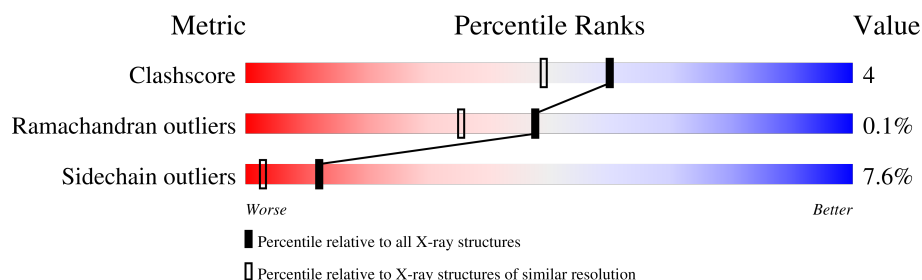
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	 69% 23% 6% ..
1	B	361	 60% 35% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5947 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 BREFELDIN A ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2695	1693	478	518	6			
1	B	361	Total	C	N	O	S	0	0	0
			2721	1711	481	523	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	GLU	conflict	GB 3025874
B	44	ALA	GLU	conflict	GB 3025874

- Molecule 2 is water.

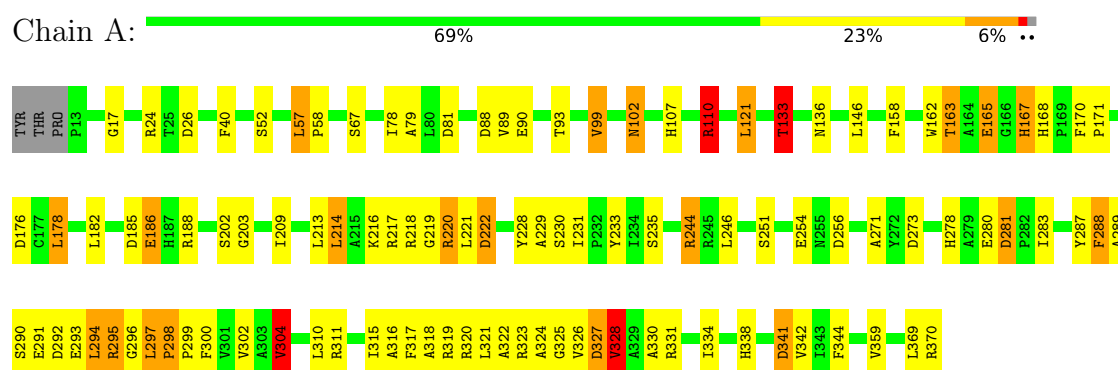
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	292	Total	O	0	0
			292	292		
2	B	239	Total	O	0	0
			239	239		

3 Residue-property plots

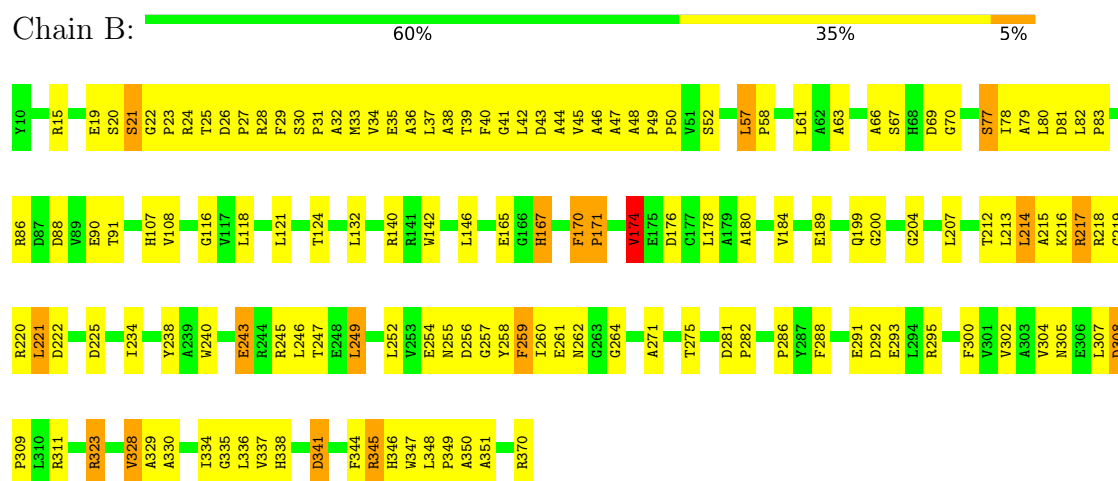
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: BREFELDIN A ESTERASE



• Molecule 1: BREFELDIN A ESTERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.70Å 82.60Å 81.50Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	8.00 – 1.85	Depositor
% Data completeness (in resolution range)	85.8 (8.00-1.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	SHELX-90	Depositor
R, R_{free}	0.169 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5947	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/2758	1.75	45/3767 (1.2%)
1	B	0.82	2/2786 (0.1%)	1.61	33/3808 (0.9%)
All	All	0.93	2/5544 (0.0%)	1.68	78/7575 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	ALA	N-CA	5.61	1.52	1.46
1	B	328	VAL	CA-C	5.45	1.59	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	HIS	CA-CB-CG	12.26	126.06	113.80
1	A	328	VAL	CB-CA-C	-11.29	93.80	110.62
1	A	304	VAL	N-CA-CB	-10.96	94.02	112.44
1	A	220	ARG	CD-NE-CZ	10.96	139.74	124.40
1	B	328	VAL	CB-CA-C	-10.63	94.78	110.62
1	B	341	ASP	CA-CB-CG	9.77	122.37	112.60
1	A	133	THR	N-CA-CB	-8.48	97.41	110.29
1	A	167	HIS	CA-CB-CG	7.62	121.42	113.80
1	B	116	GLY	CA-C-O	-7.37	116.69	122.52
1	B	174	VAL	N-CA-CB	7.17	120.28	110.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	24	ARG	CD-NE-CZ	6.94	134.12	124.40
1	A	79	ALA	CA-C-O	-6.93	113.57	121.19
1	A	222	ASP	CA-CB-CG	-6.85	105.75	112.60
1	B	234	ILE	CA-C-O	-6.81	114.14	119.46
1	B	170	PHE	O-C-N	6.81	126.96	121.38
1	B	311	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	B	176	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	69	ASP	CA-C-N	6.53	127.19	119.94
1	B	69	ASP	C-N-CA	6.53	127.19	119.94
1	B	311	ARG	NE-CZ-NH1	-6.46	115.04	121.50
1	A	230	SER	O-C-N	-6.39	115.71	123.19
1	A	256	ASP	CA-C-O	-6.38	113.64	120.92
1	B	328	VAL	CA-C-N	-6.37	113.69	122.93
1	B	328	VAL	C-N-CA	-6.37	113.69	122.93
1	A	121	LEU	CA-CB-CG	6.29	138.31	116.30
1	B	305	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	273	ASP	O-C-N	-6.23	115.80	121.34
1	A	233	TYR	CA-CB-CG	6.18	125.03	113.90
1	B	170	PHE	CA-C-O	-6.17	114.53	119.71
1	A	298	PRO	O-C-N	5.97	128.51	121.46
1	A	170	PHE	CA-C-O	-5.92	114.01	120.17
1	A	158	PHE	O-C-N	-5.87	116.33	122.96
1	B	308	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	88	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	88	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	185	ASP	CA-CB-CG	-5.76	106.84	112.60
1	A	359	VAL	O-C-N	-5.66	116.00	121.83
1	B	304	VAL	CA-C-N	-5.66	113.77	122.87
1	B	304	VAL	C-N-CA	-5.66	113.77	122.87
1	A	328	VAL	CA-C-O	-5.63	114.08	120.67
1	A	24	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	288	PHE	CA-CB-CG	-5.56	108.24	113.80
1	B	328	VAL	O-C-N	5.54	129.16	123.18
1	A	81	ASP	CA-CB-CG	-5.51	107.08	112.60
1	A	90	GLU	CA-C-O	-5.49	114.70	120.80
1	A	162	TRP	CA-C-O	5.45	126.32	120.38
1	A	26	ASP	CA-C-O	5.43	123.64	119.46
1	A	341	ASP	CA-C-O	-5.39	112.63	119.31
1	A	186	GLU	CB-CG-CD	5.36	121.72	112.60
1	B	323	ARG	CD-NE-CZ	5.35	131.89	124.40
1	A	331	ARG	CD-NE-CZ	-5.34	116.92	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	VAL	CA-C-N	-5.31	115.50	122.99
1	B	302	VAL	C-N-CA	-5.31	115.50	122.99
1	A	99	VAL	N-CA-CB	-5.30	99.73	111.50
1	A	202	SER	CA-C-O	-5.29	112.94	120.51
1	A	146	LEU	N-CA-C	5.29	117.46	111.11
1	A	176	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	110	ARG	O-C-N	5.28	125.54	121.85
1	A	273	ASP	CA-C-O	5.21	127.70	121.02
1	A	229	ALA	CA-C-N	-5.19	114.92	122.65
1	A	229	ALA	C-N-CA	-5.19	114.92	122.65
1	A	342	VAL	CA-C-O	-5.18	114.30	120.78
1	A	228	TYR	O-C-N	-5.17	116.29	123.12
1	B	259	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	249	LEU	CA-C-N	5.14	124.81	119.56
1	B	249	LEU	C-N-CA	5.14	124.81	119.56
1	B	288	PHE	CA-CB-CG	-5.14	108.66	113.80
1	B	217	ARG	NH1-CZ-NH2	5.13	125.97	119.30
1	B	174	VAL	CB-CA-C	-5.12	105.23	112.14
1	A	344	PHE	CA-C-N	5.11	131.30	121.54
1	A	344	PHE	C-N-CA	5.11	131.30	121.54
1	B	238	TYR	CA-CB-CG	-5.07	104.77	113.90
1	A	203	GLY	O-C-N	-5.07	116.87	122.24
1	B	140	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	345	ARG	CD-NE-CZ	5.02	131.43	124.40
1	A	244	ARG	CG-CD-NE	5.00	123.00	112.00
1	A	327	ASP	CA-C-O	-5.00	115.58	120.98

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLY	Mainchain
1	A	235	SER	Mainchain
1	A	294	LEU	Mainchain
1	B	200	GLY	Mainchain
1	B	225	ASP	Mainchain
1	B	286	PRO	Mainchain
1	B	300	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2695	0	2606	27	546
1	B	2721	0	2628	21	773
2	A	292	0	0	8	81
2	B	239	0	0	2	83
All	All	5947	0	5234	46	800

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 4.

All (46) 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:57:LEU:HB3	1:B:58:PRO:HD3	1.66	0.76
1:A:102:ASN:HD22	1:A:102:ASN:H	1.43	0.67
1:A:304:VAL:HG13	1:A:311:ARG:HG3	1.86	0.57
1:A:133:THR:HG22	1:A:136:ASN:HB3	1.87	0.56
1:A:278:HIS:HD2	1:A:281:ASP:OD2	1.88	0.56
1:B:57:LEU:HD22	1:B:61:LEU:HG	1.86	0.55
1:A:186:GLU:HG2	2:A:608:HOH:O	2.06	0.55
1:B:91:THR:HA	1:B:108:VAL:O	2.09	0.53
1:A:163:THR:CG2	1:A:165:GLU:HG3	2.38	0.53
1:A:216:LYS:HG3	1:A:221:LEU:HD22	1.91	0.52
1:A:57:LEU:HB3	1:A:58:PRO:HD3	1.90	0.52
1:B:142:TRP:HE1	1:B:199:GLN:HE22	1.58	0.51
1:A:178:LEU:HD12	1:A:214:LEU:HD13	1.93	0.50
1:A:107:HIS:HD2	2:A:588:HOH:O	1.93	0.50
1:A:40:PHE:HE2	1:A:78:ILE:HD12	1.77	0.49
1:B:252:LEU:HD22	1:B:262:ASN:HD21	1.78	0.49
1:A:216:LYS:HD3	2:A:621:HOH:O	2.13	0.49
1:A:334:ILE:HB	1:B:330:ALA:HB3	1.96	0.48
1:B:174:VAL:HG13	1:B:207:LEU:HD23	1.96	0.48
1:A:167:HIS:HE1	1:A:271:ALA:O	1.96	0.47
1:B:243:GLU:O	1:B:247:THR:HG23	2.15	0.47
1:B:170:PHE:HA	1:B:171:PRO:HA	1.71	0.47
1:B:121:LEU:HD13	1:B:146:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:O	1:A:186:GLU:HG3	2.16	0.46
1:A:107:HIS:HE1	2:A:438:HOH:O	1.97	0.46
1:A:330:ALA:HB3	1:B:334:ILE:HB	1.97	0.45
1:B:124:THR:O	1:B:204:GLY:HA3	2.16	0.45
1:B:57:LEU:HB3	1:B:58:PRO:CD	2.43	0.45
1:B:167:HIS:HE1	1:B:271:ALA:O	2.00	0.45
1:A:110:ARG:NH2	2:A:643:HOH:O	2.50	0.44
1:B:240:TRP:O	1:B:245:ARG:HD3	2.17	0.43
1:A:231:ILE:HD12	1:A:338:HIS:CE1	2.54	0.43
2:A:634:HOH:O	1:B:86:ARG:HD2	2.19	0.43
1:B:291:GLU:OE2	1:B:323:ARG:HD2	2.19	0.43
1:A:168:HIS:HD2	2:A:567:HOH:O	2.02	0.42
1:A:188:ARG:HD3	2:A:424:HOH:O	2.18	0.42
1:A:244:ARG:HH11	1:A:244:ARG:HD3	1.54	0.42
1:A:341:ASP:N	1:A:341:ASP:OD1	2.52	0.42
1:A:102:ASN:H	1:A:102:ASN:ND2	2.12	0.42
1:B:281:ASP:HA	1:B:282:PRO:HD2	1.85	0.42
1:A:163:THR:HG23	1:A:165:GLU:HG3	2.02	0.41
1:A:310:LEU:HD12	1:A:338:HIS:CE1	2.55	0.41
1:B:107:HIS:HE1	2:B:447:HOH:O	2.02	0.41
1:B:275:THR:HG23	2:B:545:HOH:O	2.22	0.40
1:A:251:SER:HA	1:A:254:GLU:HB3	2.03	0.40
1:B:180:ALA:O	1:B:184:VAL:HG23	2.21	0.40

All (800) 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:217:ARG:CD	1:B:48:ALA:CA[2_656]	0.12	2.08
1:A:295:ARG:NH1	1:B:337:VAL:C[2_656]	0.17	2.03
1:A:296:GLY:CA	1:B:259:PHE:CE1[2_656]	0.34	1.86
1:B:346:HIS:CB	2:B:542:HOH:O[2_656]	0.36	1.84
1:A:288:PHE:O	1:B:15:ARG:NH1[2_656]	0.37	1.83
1:A:321:LEU:CD1	1:B:43:ASP:CB[2_656]	0.37	1.83
1:B:261:GLU:N	2:A:649:HOH:O[2_656]	0.40	1.80
1:B:215:ALA:CA	1:B:218:ARG:CA[2_655]	0.41	1.79
1:B:81:ASP:CB	1:B:83:PRO:CA[2_656]	0.42	1.78
1:A:300:PHE:N	1:B:38:ALA:C[2_656]	0.43	1.77
1:B:81:ASP:N	1:B:83:PRO:CG[2_656]	0.46	1.74
1:A:297:LEU:C	1:B:42:LEU:CD1[2_656]	0.48	1.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:CG2	1:B:34:VAL:C[2_656]	0.51	1.69
1:B:26:ASP:OD2	2:A:642:HOH:O[2_656]	0.52	1.68
1:A:322:ALA:O	1:B:33:MET:CG[2_656]	0.53	1.67
1:A:326:VAL:CG2	1:B:37:LEU:CD2[2_656]	0.53	1.67
1:B:27:PRO:CG	2:A:635:HOH:O[2_656]	0.57	1.63
1:A:292:ASP:OD1	1:B:309:PRO:CD[2_656]	0.58	1.62
1:A:324:ALA:CA	1:B:337:VAL:CG1[2_656]	0.58	1.62
1:A:327:ASP:CA	1:B:36:ALA:CA[2_656]	0.59	1.61
1:B:35:GLU:OE2	1:B:351:ALA:N[2_656]	0.59	1.61
1:A:287:TYR:O	1:B:20:SER:O[2_656]	0.60	1.60
1:A:291:GLU:CA	1:B:258:TYR:CG[2_656]	0.60	1.60
1:A:295:ARG:CA	1:B:259:PHE:CB[2_656]	0.60	1.60
1:A:300:PHE:CE1	1:B:41:GLY:C[2_656]	0.60	1.60
1:A:324:ALA:O	1:B:337:VAL:CG2[2_656]	0.62	1.58
1:A:293:GLU:CB	1:B:257:GLY:CA[2_656]	0.63	1.57
1:B:344:PHE:CD1	2:A:564:HOH:O[2_656]	0.65	1.55
1:A:328:VAL:N	1:B:35:GLU:C[2_656]	0.68	1.52
1:A:213:LEU:CD1	1:B:45:VAL:O[2_656]	0.70	1.50
1:A:320:ARG:NH1	1:B:22:GLY:N[2_656]	0.71	1.49
1:B:218:ARG:NE	1:B:221:LEU:N[2_655]	0.72	1.48
1:A:320:ARG:N	1:B:23:PRO:O[2_656]	0.74	1.46
1:A:327:ASP:N	1:B:36:ALA:C[2_656]	0.75	1.45
1:A:295:ARG:C	1:B:259:PHE:CG[2_656]	0.76	1.44
1:A:317:PHE:CD1	2:B:421:HOH:O[2_656]	0.77	1.43
1:B:347:TRP:O	1:B:347:TRP:O[2_656]	0.77	1.43
1:B:255:ASN:CA	2:A:469:HOH:O[2_656]	0.78	1.42
1:A:296:GLY:N	1:B:259:PHE:CD1[2_656]	0.80	1.40
1:A:296:GLY:N	1:B:259:PHE:CG[2_656]	0.82	1.38
1:A:316:ALA:O	1:B:25:THR:N[2_656]	0.82	1.38
1:B:27:PRO:CA	2:A:602:HOH:O[2_656]	0.83	1.37
1:A:316:ALA:C	1:B:24:ARG:C[2_656]	0.86	1.34
1:A:319:ARG:CB	2:B:426:HOH:O[2_656]	0.86	1.34
1:B:31:PRO:CA	2:A:421:HOH:O[2_656]	0.86	1.34
1:A:298:PRO:CA	1:B:40:PHE:CB[2_656]	0.87	1.33
1:A:326:VAL:CG1	1:B:37:LEU:CA[2_656]	0.87	1.33
1:B:29:PHE:C	2:A:393:HOH:O[2_656]	0.87	1.33
1:A:300:PHE:CA	1:B:38:ALA:O[2_656]	0.88	1.32
1:A:320:ARG:CZ	1:B:22:GLY:N[2_656]	0.88	1.32
1:B:21:SER:N	2:A:519:HOH:O[2_656]	0.88	1.32
1:A:316:ALA:C	1:B:25:THR:N[2_656]	0.89	1.31
1:A:320:ARG:NH1	1:B:22:GLY:CA[2_656]	0.89	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ASN:CB	2:A:469:HOH:O[2_656]	0.89	1.31
1:B:31:PRO:CD	2:B:449:HOH:O[2_656]	0.89	1.31
1:A:291:GLU:C	1:B:258:TYR:CB[2_656]	0.90	1.30
1:A:300:PHE:CZ	1:B:41:GLY:O[2_656]	0.90	1.30
1:A:300:PHE:CD2	1:B:43:ASP:OD1[2_656]	0.90	1.30
1:A:299:PRO:CB	1:B:39:THR:CB[2_656]	0.91	1.29
1:B:29:PHE:O	2:A:393:HOH:O[2_656]	0.91	1.29
1:A:297:LEU:CB	1:B:42:LEU:CG[2_656]	0.92	1.28
1:B:77:SER:CB	2:A:609:HOH:O[2_656]	0.93	1.27
1:B:214:LEU:CD2	2:B:519:HOH:O[2_655]	0.94	1.26
1:A:320:ARG:O	1:B:29:PHE:CE2[2_656]	0.95	1.25
1:A:289:ALA:CB	1:B:45:VAL:CG2[2_656]	0.96	1.24
1:A:294:LEU:C	1:B:259:PHE:N[2_656]	0.96	1.24
1:B:218:ARG:CD	1:B:220:ARG:C[2_655]	0.97	1.23
1:B:221:LEU:CG	2:B:496:HOH:O[2_655]	0.97	1.23
1:A:291:GLU:CB	1:B:258:TYR:CD2[2_656]	0.99	1.21
1:B:350:ALA:CA	2:B:527:HOH:O[2_656]	0.99	1.21
1:A:323:ARG:NH1	1:B:26:ASP:O[2_656]	1.00	1.20
1:A:325:GLY:CA	1:B:33:MET:CE[2_656]	1.00	1.20
1:B:215:ALA:C	1:B:218:ARG:N[2_655]	1.01	1.19
1:B:344:PHE:CZ	2:A:436:HOH:O[2_656]	1.02	1.18
1:B:30:SER:CB	1:B:30:SER:CB[2_656]	1.02	1.18
1:A:288:PHE:CD1	1:B:20:SER:N[2_656]	1.03	1.17
1:A:317:PHE:C	1:B:24:ARG:CA[2_656]	1.03	1.17
1:B:218:ARG:CD	1:B:221:LEU:N[2_655]	1.03	1.17
1:A:292:ASP:OD1	1:B:309:PRO:N[2_656]	1.04	1.16
1:A:300:PHE:N	1:B:39:THR:N[2_656]	1.04	1.16
1:A:319:ARG:O	1:B:29:PHE:CB[2_656]	1.04	1.16
1:B:344:PHE:CE1	2:A:564:HOH:O[2_656]	1.04	1.16
1:A:218:ARG:CG	1:B:50:PRO:CD[2_656]	1.05	1.15
1:A:289:ALA:CB	1:B:45:VAL:CB[2_656]	1.05	1.15
1:A:293:GLU:OE1	2:B:573:HOH:O[2_656]	1.06	1.14
1:A:216:LYS:CE	2:B:466:HOH:O[2_656]	1.07	1.13
1:A:300:PHE:CE1	1:B:42:LEU:N[2_656]	1.07	1.13
1:A:317:PHE:CZ	1:B:44:ALA:CA[2_656]	1.07	1.13
1:B:26:ASP:N	2:A:515:HOH:O[2_656]	1.07	1.13
1:B:30:SER:CA	1:B:30:SER:CB[2_656]	1.07	1.13
1:B:81:ASP:OD2	1:B:83:PRO:O[2_656]	1.07	1.13
1:A:295:ARG:N	1:B:259:PHE:CA[2_656]	1.08	1.12
1:B:217:ARG:N	1:B:217:ARG:N[2_655]	1.08	1.12
1:B:348:LEU:CA	2:B:472:HOH:O[2_656]	1.08	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:B:35:GLU:CA[2_656]	1.09	1.11
1:A:216:LYS:CD	2:B:466:HOH:O[2_656]	1.10	1.10
1:A:218:ARG:CD	1:B:50:PRO:CD[2_656]	1.10	1.10
1:A:298:PRO:CB	1:B:40:PHE:CB[2_656]	1.10	1.10
1:B:81:ASP:C	1:B:83:PRO:CD[2_656]	1.10	1.10
1:B:216:LYS:NZ	1:B:217:ARG:CZ[2_655]	1.10	1.10
1:A:327:ASP:C	1:B:35:GLU:O[2_656]	1.11	1.09
1:A:297:LEU:CA	1:B:42:LEU:CD1[2_656]	1.12	1.08
1:A:316:ALA:O	1:B:24:ARG:C[2_656]	1.12	1.08
1:B:261:GLU:CA	2:A:649:HOH:O[2_656]	1.12	1.08
1:B:35:GLU:OE2	1:B:350:ALA:C[2_656]	1.12	1.08
1:A:322:ALA:O	1:B:33:MET:CB[2_656]	1.13	1.07
1:A:326:VAL:CB	1:B:37:LEU:CG[2_656]	1.13	1.07
1:B:348:LEU:N	2:B:472:HOH:O[2_656]	1.13	1.07
1:A:317:PHE:O	1:B:24:ARG:N[2_656]	1.14	1.06
1:B:81:ASP:O	1:B:83:PRO:CD[2_656]	1.14	1.06
1:A:323:ARG:NH2	1:B:26:ASP:CB[2_656]	1.15	1.05
1:A:326:VAL:C	1:B:37:LEU:N[2_656]	1.15	1.05
1:A:326:VAL:CB	1:B:37:LEU:CB[2_656]	1.15	1.05
1:A:297:LEU:CB	1:B:42:LEU:CB[2_656]	1.16	1.04
1:B:216:LYS:NZ	1:B:217:ARG:NH1[2_655]	1.16	1.04
1:A:300:PHE:CA	1:B:38:ALA:C[2_656]	1.17	1.03
1:A:327:ASP:CA	1:B:36:ALA:C[2_656]	1.17	1.03
1:B:81:ASP:CA	1:B:83:PRO:CG[2_656]	1.17	1.03
1:A:217:ARG:NE	1:B:48:ALA:N[2_656]	1.18	1.02
1:A:328:VAL:O	1:B:35:GLU:CB[2_656]	1.18	1.02
1:A:328:VAL:CG2	1:B:34:VAL:O[2_656]	1.18	1.02
1:A:287:TYR:C	1:B:20:SER:O[2_656]	1.19	1.01
1:A:294:LEU:C	1:B:259:PHE:CA[2_656]	1.20	1.00
1:A:291:GLU:N	1:B:258:TYR:CG[2_656]	1.21	0.99
1:A:299:PRO:CD	1:B:40:PHE:CD1[2_656]	1.21	0.99
1:A:317:PHE:C	1:B:24:ARG:N[2_656]	1.21	0.99
1:A:295:ARG:N	1:B:259:PHE:N[2_656]	1.22	0.98
1:A:299:PRO:CG	1:B:39:THR:CG2[2_656]	1.22	0.98
1:A:323:ARG:NH2	1:B:26:ASP:CG[2_656]	1.22	0.98
1:A:296:GLY:CA	1:B:259:PHE:CZ[2_656]	1.23	0.97
1:B:30:SER:CA	1:B:30:SER:CA[2_656]	1.23	0.97
1:B:216:LYS:CE	1:B:217:ARG:CZ[2_655]	1.23	0.97
1:A:291:GLU:O	1:B:258:TYR:CB[2_656]	1.24	0.96
1:A:291:GLU:CA	1:B:258:TYR:CD2[2_656]	1.24	0.96
1:A:292:ASP:CG	1:B:309:PRO:CD[2_656]	1.24	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:C	1:B:259:PHE:CE1[2_656]	1.24	0.96
1:A:299:PRO:N	1:B:40:PHE:N[2_656]	1.24	0.96
1:B:40:PHE:CZ	2:A:599:HOH:O[2_656]	1.24	0.96
1:A:300:PHE:N	1:B:38:ALA:O[2_656]	1.25	0.95
1:B:15:ARG:NH2	2:A:490:HOH:O[2_656]	1.25	0.95
1:B:32:ALA:CA	2:B:494:HOH:O[2_656]	1.26	0.94
1:B:216:LYS:CG	1:B:217:ARG:CD[2_655]	1.26	0.94
1:B:216:LYS:CE	1:B:217:ARG:NE[2_655]	1.26	0.94
1:A:297:LEU:CA	1:B:42:LEU:CG[2_656]	1.27	0.93
1:B:28:ARG:O	2:B:508:HOH:O[2_656]	1.27	0.93
1:A:294:LEU:CA	1:B:259:PHE:N[2_656]	1.28	0.92
1:A:318:ALA:N	1:B:24:ARG:CB[2_656]	1.28	0.92
1:B:81:ASP:CA	1:B:83:PRO:CB[2_656]	1.28	0.92
1:A:219:GLY:O	1:B:66:ALA:C[2_656]	1.29	0.91
1:A:295:ARG:NE	2:B:381:HOH:O[2_656]	1.29	0.91
1:B:40:PHE:CE2	2:A:432:HOH:O[2_656]	1.29	0.91
1:B:32:ALA:O	2:A:456:HOH:O[2_656]	1.29	0.91
2:A:547:HOH:O	2:B:470:HOH:O[2_656]	1.29	0.91
1:A:291:GLU:CA	1:B:258:TYR:CB[2_656]	1.30	0.90
1:A:292:ASP:CG	1:B:309:PRO:N[2_656]	1.31	0.89
1:B:25:THR:C	2:A:515:HOH:O[2_656]	1.31	0.89
1:A:217:ARG:CB	1:B:49:PRO:N[2_656]	1.32	0.88
1:A:290:SER:C	1:B:258:TYR:CD1[2_656]	1.32	0.88
1:A:295:ARG:NH1	1:B:338:HIS:N[2_656]	1.32	0.88
1:A:296:GLY:CA	1:B:259:PHE:CD1[2_656]	1.32	0.88
1:A:299:PRO:CB	1:B:39:THR:CA[2_656]	1.32	0.88
1:A:317:PHE:CG	2:B:421:HOH:O[2_656]	1.32	0.88
1:A:321:LEU:N	1:B:23:PRO:CB[2_656]	1.32	0.88
1:B:80:LEU:C	1:B:83:PRO:CG[2_656]	1.32	0.88
1:B:215:ALA:C	1:B:218:ARG:CA[2_655]	1.32	0.88
1:A:290:SER:OG	1:B:256:ASP:C[2_656]	1.33	0.87
1:A:299:PRO:CA	1:B:39:THR:CA[2_656]	1.33	0.87
1:A:300:PHE:CB	1:B:38:ALA:CA[2_656]	1.33	0.87
1:B:32:ALA:C	2:B:494:HOH:O[2_656]	1.33	0.87
1:A:288:PHE:C	1:B:15:ARG:NH1[2_656]	1.35	0.85
1:A:297:LEU:CB	1:B:42:LEU:CD2[2_656]	1.36	0.84
1:A:315:ILE:O	1:B:24:ARG:O[2_656]	1.36	0.84
1:A:328:VAL:CB	1:B:34:VAL:O[2_656]	1.36	0.84
1:A:328:VAL:C	1:B:35:GLU:CA[2_656]	1.36	0.84
1:B:221:LEU:CB	2:B:496:HOH:O[2_655]	1.36	0.84
1:A:297:LEU:O	1:B:42:LEU:CD1[2_656]	1.37	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PRO:CB	1:B:39:THR:CG2[2_656]	1.37	0.83
1:B:216:LYS:CB	1:B:217:ARG:CB[2_655]	1.37	0.83
1:A:291:GLU:N	1:B:258:TYR:CD1[2_656]	1.38	0.82
1:A:295:ARG:NH1	1:B:337:VAL:O[2_656]	1.38	0.82
1:A:295:ARG:C	1:B:259:PHE:CB[2_656]	1.38	0.82
1:A:295:ARG:N	1:B:259:PHE:CB[2_656]	1.38	0.82
1:A:317:PHE:C	1:B:24:ARG:CB[2_656]	1.38	0.82
1:A:318:ALA:N	1:B:24:ARG:CA[2_656]	1.38	0.82
1:A:321:LEU:CD2	1:B:43:ASP:CA[2_656]	1.38	0.82
1:A:328:VAL:N	1:B:35:GLU:O[2_656]	1.38	0.82
1:B:15:ARG:CZ	2:A:490:HOH:O[2_656]	1.39	0.81
1:B:81:ASP:N	1:B:83:PRO:CB[2_656]	1.39	0.81
1:A:294:LEU:N	1:B:257:GLY:O[2_656]	1.40	0.80
1:A:295:ARG:NH1	1:B:337:VAL:CA[2_656]	1.40	0.80
1:A:299:PRO:CA	1:B:39:THR:C[2_656]	1.40	0.80
1:A:299:PRO:C	1:B:39:THR:C[2_656]	1.40	0.80
1:A:327:ASP:N	1:B:37:LEU:N[2_656]	1.40	0.80
1:B:347:TRP:CD1	2:B:418:HOH:O[2_656]	1.40	0.80
1:A:292:ASP:N	1:B:255:ASN:O[2_656]	1.41	0.79
1:A:295:ARG:CZ	1:B:337:VAL:CA[2_656]	1.41	0.79
1:A:321:LEU:CG	1:B:43:ASP:CA[2_656]	1.41	0.79
1:A:218:ARG:CD	1:B:50:PRO:CG[2_656]	1.42	0.78
1:A:288:PHE:CD1	1:B:19:GLU:C[2_656]	1.42	0.78
1:A:302:VAL:CG2	1:B:24:ARG:NE[2_656]	1.42	0.78
1:A:318:ALA:O	1:B:34:VAL:CG2[2_656]	1.42	0.78
1:B:216:LYS:N	1:B:217:ARG:C[2_655]	1.42	0.78
1:A:213:LEU:CD2	1:B:46:ALA:CA[2_656]	1.43	0.77
1:A:293:GLU:OE2	1:B:46:ALA:O[2_656]	1.43	0.77
1:A:295:ARG:CZ	1:B:337:VAL:C[2_656]	1.43	0.77
1:A:299:PRO:O	1:B:39:THR:C[2_656]	1.43	0.77
1:A:325:GLY:C	1:B:33:MET:CE[2_656]	1.43	0.77
1:A:328:VAL:CG2	1:B:34:VAL:CA[2_656]	1.43	0.77
1:B:215:ALA:CA	1:B:218:ARG:C[2_655]	1.43	0.77
1:A:288:PHE:O	1:B:15:ARG:CZ[2_656]	1.44	0.76
1:A:298:PRO:C	1:B:40:PHE:CB[2_656]	1.44	0.76
1:B:78:ILE:CG1	2:A:623:HOH:O[2_656]	1.44	0.76
1:A:217:ARG:NE	1:B:48:ALA:CA[2_656]	1.45	0.75
1:A:300:PHE:CE1	1:B:41:GLY:O[2_656]	1.45	0.75
1:A:321:LEU:CD1	1:B:43:ASP:CA[2_656]	1.45	0.75
1:A:327:ASP:C	1:B:35:GLU:C[2_656]	1.45	0.75
1:B:344:PHE:CG	2:A:564:HOH:O[2_656]	1.45	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:SER:OG	1:B:256:ASP:N[2_656]	1.46	0.74
1:A:290:SER:OG	1:B:256:ASP:O[2_656]	1.46	0.74
1:A:300:PHE:CZ	1:B:41:GLY:C[2_656]	1.46	0.74
1:A:321:LEU:O	1:B:37:LEU:CD1[2_656]	1.46	0.74
1:B:81:ASP:CA	1:B:83:PRO:CD[2_656]	1.46	0.74
1:B:216:LYS:CA	1:B:217:ARG:CB[2_655]	1.46	0.74
1:A:294:LEU:CD1	1:B:23:PRO:CD[2_656]	1.47	0.73
1:A:297:LEU:CG	1:B:42:LEU:CD2[2_656]	1.47	0.73
1:B:33:MET:N	2:B:494:HOH:O[2_656]	1.47	0.73
1:B:81:ASP:CB	1:B:83:PRO:N[2_656]	1.47	0.73
1:B:350:ALA:C	2:B:527:HOH:O[2_656]	1.47	0.73
1:A:216:LYS:CG	2:B:466:HOH:O[2_656]	1.48	0.72
1:A:219:GLY:O	1:B:66:ALA:O[2_656]	1.48	0.72
1:A:292:ASP:O	1:B:260:ILE:O[2_656]	1.48	0.72
1:A:213:LEU:CG	1:B:45:VAL:O[2_656]	1.49	0.71
1:A:280:GLU:OE1	1:B:19:GLU:OE2[2_656]	1.49	0.71
1:A:287:TYR:CD2	1:B:20:SER:OG[2_656]	1.49	0.71
1:A:323:ARG:CD	1:B:28:ARG:C[2_656]	1.49	0.71
1:A:324:ALA:O	1:B:337:VAL:CB[2_656]	1.49	0.71
1:A:297:LEU:CA	1:B:42:LEU:CD2[2_656]	1.50	0.70
1:B:215:ALA:O	1:B:218:ARG:CG[2_655]	1.50	0.70
1:A:298:PRO:CA	1:B:40:PHE:CG[2_656]	1.51	0.69
1:A:316:ALA:C	1:B:24:ARG:O[2_656]	1.51	0.69
1:A:323:ARG:CD	1:B:29:PHE:N[2_656]	1.51	0.69
1:B:30:SER:C	1:B:30:SER:CB[2_656]	1.51	0.69
1:A:287:TYR:O	1:B:20:SER:C[2_656]	1.52	0.68
1:A:290:SER:OG	1:B:256:ASP:CA[2_656]	1.52	0.68
1:A:318:ALA:N	1:B:24:ARG:CG[2_656]	1.52	0.68
1:A:323:ARG:CG	1:B:29:PHE:CA[2_656]	1.52	0.68
1:A:324:ALA:C	1:B:337:VAL:CG1[2_656]	1.52	0.68
1:A:327:ASP:O	1:B:35:GLU:O[2_656]	1.52	0.68
1:A:327:ASP:OD2	1:B:347:TRP:CZ3[2_656]	1.52	0.68
1:B:81:ASP:CG	1:B:83:PRO:CA[2_656]	1.52	0.68
1:B:215:ALA:O	1:B:218:ARG:CB[2_655]	1.52	0.68
1:A:317:PHE:N	1:B:24:ARG:C[2_656]	1.53	0.67
1:A:217:ARG:CD	1:B:48:ALA:N[2_656]	1.54	0.66
1:A:299:PRO:C	1:B:39:THR:N[2_656]	1.54	0.66
1:A:328:VAL:N	1:B:36:ALA:N[2_656]	1.54	0.66
1:B:81:ASP:CB	1:B:83:PRO:CB[2_656]	1.54	0.66
1:B:220:ARG:CA	2:B:473:HOH:O[2_655]	1.54	0.66
1:A:217:ARG:CD	1:B:48:ALA:C[2_656]	1.55	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:CG	1:B:258:TYR:CD2[2_656]	1.55	0.65
1:A:299:PRO:C	1:B:40:PHE:N[2_656]	1.55	0.65
1:A:316:ALA:CB	1:B:25:THR:CB[2_656]	1.55	0.65
1:A:317:PHE:CA	1:B:24:ARG:CB[2_656]	1.55	0.65
1:A:320:ARG:O	1:B:29:PHE:CD2[2_656]	1.55	0.65
1:A:324:ALA:CB	1:B:337:VAL:CG1[2_656]	1.55	0.65
1:A:326:VAL:CG1	1:B:37:LEU:CB[2_656]	1.55	0.65
1:B:347:TRP:CH2	2:A:491:HOH:O[2_656]	1.55	0.65
1:B:347:TRP:CE3	2:A:578:HOH:O[2_656]	1.55	0.65
1:B:178:LEU:CB	2:B:563:HOH:O[2_655]	1.55	0.65
1:B:346:HIS:CD2	1:B:349:PRO:CB[2_656]	1.55	0.65
1:A:217:ARG:NH1	1:B:48:ALA:CB[2_656]	1.56	0.64
1:A:217:ARG:CD	1:B:48:ALA:CB[2_656]	1.56	0.64
1:A:293:GLU:C	1:B:257:GLY:O[2_656]	1.56	0.64
1:A:295:ARG:CZ	1:B:338:HIS:N[2_656]	1.56	0.64
1:A:299:PRO:O	1:B:40:PHE:N[2_656]	1.56	0.64
1:B:27:PRO:CB	2:A:602:HOH:O[2_656]	1.56	0.64
1:B:215:ALA:CA	1:B:218:ARG:N[2_655]	1.56	0.64
1:A:294:LEU:CA	2:B:417:HOH:O[2_656]	1.57	0.63
1:A:295:ARG:O	1:B:259:PHE:O[2_656]	1.57	0.63
1:A:299:PRO:CA	1:B:40:PHE:N[2_656]	1.57	0.63
1:A:319:ARG:CA	2:B:426:HOH:O[2_656]	1.57	0.63
1:B:77:SER:CA	2:A:609:HOH:O[2_656]	1.57	0.63
1:B:213:LEU:O	1:B:217:ARG:CA[2_655]	1.57	0.63
1:B:347:TRP:NE1	1:B:350:ALA:N[2_656]	1.57	0.63
1:A:218:ARG:NE	1:B:50:PRO:CD[2_656]	1.58	0.62
1:A:280:GLU:OE1	1:B:19:GLU:CD[2_656]	1.58	0.62
1:A:292:ASP:OD2	1:B:309:PRO:CA[2_656]	1.58	0.62
1:A:296:GLY:N	1:B:259:PHE:CD2[2_656]	1.58	0.62
1:A:299:PRO:C	1:B:39:THR:CA[2_656]	1.58	0.62
1:A:320:ARG:NH1	1:B:21:SER:C[2_656]	1.58	0.62
1:A:320:ARG:O	1:B:29:PHE:CZ[2_656]	1.58	0.62
1:A:322:ALA:CB	1:B:34:VAL:N[2_656]	1.58	0.62
1:A:327:ASP:N	1:B:36:ALA:O[2_656]	1.58	0.62
1:A:217:ARG:CG	1:B:48:ALA:CA[2_656]	1.59	0.61
1:A:295:ARG:C	1:B:259:PHE:CD1[2_656]	1.59	0.61
1:A:298:PRO:CB	1:B:40:PHE:CG[2_656]	1.59	0.61
1:A:315:ILE:C	1:B:24:ARG:O[2_656]	1.59	0.61
1:A:326:VAL:CG1	1:B:37:LEU:C[2_656]	1.59	0.61
1:A:328:VAL:CB	1:B:34:VAL:C[2_656]	1.59	0.61
1:B:27:PRO:CD	2:A:635:HOH:O[2_656]	1.59	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:OG	1:B:30:SER:OG[2_656]	1.59	0.61
1:A:294:LEU:CB	2:B:417:HOH:O[2_656]	1.60	0.60
1:A:326:VAL:CB	1:B:37:LEU:CD2[2_656]	1.60	0.60
1:A:326:VAL:CG2	1:B:37:LEU:CG[2_656]	1.60	0.60
1:A:326:VAL:CB	1:B:37:LEU:CA[2_656]	1.60	0.60
1:B:35:GLU:CD	1:B:351:ALA:N[2_656]	1.60	0.60
1:B:348:LEU:C	2:B:590:HOH:O[2_656]	1.60	0.60
1:A:291:GLU:OE1	1:B:307:LEU:CD2[2_656]	1.61	0.59
1:A:320:ARG:NH2	1:B:22:GLY:N[2_656]	1.61	0.59
1:A:323:ARG:NH1	1:B:26:ASP:C[2_656]	1.61	0.59
1:A:326:VAL:O	1:B:33:MET:O[2_656]	1.61	0.59
1:B:347:TRP:CZ3	2:A:578:HOH:O[2_656]	1.61	0.59
1:B:216:LYS:CE	1:B:217:ARG:NH1[2_655]	1.61	0.59
1:A:296:GLY:N	1:B:259:PHE:CE1[2_656]	1.62	0.58
1:A:300:PHE:CD1	1:B:42:LEU:N[2_656]	1.62	0.58
1:A:322:ALA:C	1:B:33:MET:CG[2_656]	1.62	0.58
1:A:327:ASP:N	1:B:36:ALA:CA[2_656]	1.62	0.58
1:B:79:ALA:CB	2:A:552:HOH:O[2_656]	1.62	0.58
1:B:26:ASP:CG	2:A:642:HOH:O[2_656]	1.62	0.58
1:B:30:SER:CB	1:B:30:SER:OG[2_656]	1.62	0.58
1:B:216:LYS:C	1:B:217:ARG:CB[2_655]	1.62	0.58
1:B:292:ASP:CB	2:B:557:HOH:O[2_655]	1.62	0.58
1:A:216:LYS:NZ	1:B:260:ILE:CA[2_656]	1.63	0.57
1:A:217:ARG:O	1:B:49:PRO:CG[2_656]	1.63	0.57
1:A:293:GLU:N	1:B:258:TYR:N[2_656]	1.63	0.57
1:A:295:ARG:CA	1:B:259:PHE:CG[2_656]	1.63	0.57
1:A:316:ALA:CA	1:B:24:ARG:O[2_656]	1.63	0.57
1:B:81:ASP:C	1:B:83:PRO:N[2_656]	1.63	0.57
1:B:214:LEU:C	1:B:219:GLY:N[2_655]	1.63	0.57
1:B:216:LYS:N	1:B:218:ARG:N[2_655]	1.63	0.57
1:B:220:ARG:CG	2:B:473:HOH:O[2_655]	1.63	0.57
1:B:348:LEU:CA	2:B:590:HOH:O[2_656]	1.63	0.57
1:A:209:ILE:CG2	1:B:44:ALA:CB[2_656]	1.64	0.56
1:A:287:TYR:CE2	1:B:20:SER:OG[2_656]	1.64	0.56
1:A:289:ALA:CB	1:B:45:VAL:CG1[2_656]	1.64	0.56
1:A:293:GLU:CA	1:B:257:GLY:CA[2_656]	1.64	0.56
1:A:295:ARG:NH2	1:B:337:VAL:CA[2_656]	1.64	0.56
1:A:298:PRO:C	1:B:40:PHE:N[2_656]	1.64	0.56
1:A:328:VAL:N	1:B:35:GLU:CA[2_656]	1.64	0.56
1:B:78:ILE:CD1	2:A:636:HOH:O[2_656]	1.64	0.56
1:B:260:ILE:C	2:A:649:HOH:O[2_656]	1.64	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:NZ	1:B:217:ARG:NH2[2_655]	1.64	0.56
1:B:217:ARG:N	1:B:217:ARG:CA[2_655]	1.64	0.56
1:B:345:ARG:O	2:B:574:HOH:O[2_656]	1.64	0.56
1:A:292:ASP:OD2	1:B:309:PRO:N[2_656]	1.65	0.55
1:A:295:ARG:NE	1:B:338:HIS:N[2_656]	1.65	0.55
1:A:323:ARG:CG	1:B:29:PHE:N[2_656]	1.65	0.55
1:A:324:ALA:C	1:B:337:VAL:CG2[2_656]	1.65	0.55
1:B:21:SER:CA	2:A:519:HOH:O[2_656]	1.65	0.55
1:B:81:ASP:CA	1:B:83:PRO:N[2_656]	1.65	0.55
1:B:218:ARG:CD	1:B:220:ARG:CA[2_655]	1.65	0.55
1:A:293:GLU:CD	2:B:573:HOH:O[2_656]	1.66	0.54
1:A:295:ARG:O	1:B:259:PHE:C[2_656]	1.66	0.54
1:A:316:ALA:CA	1:B:25:THR:CA[2_656]	1.66	0.54
1:B:27:PRO:N	2:A:602:HOH:O[2_656]	1.66	0.54
1:B:218:ARG:NE	1:B:221:LEU:CA[2_655]	1.66	0.54
1:B:347:TRP:C	2:B:472:HOH:O[2_656]	1.66	0.54
1:A:291:GLU:O	1:B:258:TYR:CA[2_656]	1.67	0.53
1:A:294:LEU:O	1:B:259:PHE:CA[2_656]	1.67	0.53
1:A:300:PHE:CG	1:B:43:ASP:OD1[2_656]	1.67	0.53
1:A:328:VAL:CA	1:B:35:GLU:CA[2_656]	1.67	0.53
1:A:295:ARG:CD	1:B:338:HIS:N[2_656]	1.68	0.52
1:A:316:ALA:CB	1:B:25:THR:CG2[2_656]	1.68	0.52
1:A:320:ARG:N	1:B:23:PRO:C[2_656]	1.68	0.52
1:B:81:ASP:CA	1:B:83:PRO:CA[2_656]	1.68	0.52
1:B:348:LEU:O	2:B:541:HOH:O[2_656]	1.68	0.52
1:A:291:GLU:N	1:B:258:TYR:CD2[2_656]	1.69	0.51
1:A:317:PHE:O	1:B:23:PRO:C[2_656]	1.69	0.51
1:A:321:LEU:CD2	1:B:42:LEU:O[2_656]	1.69	0.51
1:B:31:PRO:CG	2:B:449:HOH:O[2_656]	1.69	0.51
1:B:82:LEU:CD2	2:B:509:HOH:O[2_656]	1.69	0.51
1:B:346:HIS:CG	2:B:542:HOH:O[2_656]	1.69	0.51
1:A:213:LEU:CB	1:B:47:ALA:N[2_656]	1.70	0.50
1:A:288:PHE:CG	1:B:20:SER:CA[2_656]	1.70	0.50
1:A:290:SER:O	1:B:258:TYR:N[2_656]	1.70	0.50
1:A:319:ARG:C	1:B:23:PRO:O[2_656]	1.70	0.50
1:A:320:ARG:CZ	1:B:21:SER:C[2_656]	1.70	0.50
1:A:322:ALA:CA	1:B:34:VAL:N[2_656]	1.70	0.50
1:A:323:ARG:NH2	1:B:26:ASP:OD1[2_656]	1.70	0.50
1:A:213:LEU:CD2	1:B:46:ALA:N[2_656]	1.71	0.49
1:A:290:SER:O	1:B:258:TYR:CD1[2_656]	1.71	0.49
1:A:299:PRO:CA	1:B:39:THR:CB[2_656]	1.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ALA:C	1:B:25:THR:CA[2_656]	1.71	0.49
1:B:215:ALA:CB	1:B:218:ARG:CA[2_655]	1.71	0.49
1:B:220:ARG:CB	2:B:473:HOH:O[2_655]	1.71	0.49
1:A:217:ARG:C	1:B:49:PRO:CB[2_656]	1.72	0.48
1:A:294:LEU:N	1:B:259:PHE:N[2_656]	1.72	0.48
1:A:295:ARG:N	1:B:258:TYR:C[2_656]	1.72	0.48
1:A:300:PHE:CA	1:B:38:ALA:CA[2_656]	1.72	0.48
1:A:317:PHE:CA	1:B:24:ARG:CA[2_656]	1.72	0.48
1:A:317:PHE:CZ	1:B:44:ALA:N[2_656]	1.72	0.48
1:A:327:ASP:CA	1:B:36:ALA:N[2_656]	1.72	0.48
1:B:255:ASN:N	2:A:469:HOH:O[2_656]	1.72	0.48
1:B:216:LYS:CD	1:B:217:ARG:CD[2_655]	1.72	0.48
1:A:291:GLU:OE1	1:B:307:LEU:CB[2_656]	1.73	0.47
1:A:293:GLU:CA	1:B:257:GLY:C[2_656]	1.73	0.47
1:A:294:LEU:CD1	1:B:23:PRO:CG[2_656]	1.73	0.47
1:A:294:LEU:CD2	1:B:44:ALA:O[2_656]	1.73	0.47
1:A:298:PRO:C	1:B:40:PHE:CA[2_656]	1.73	0.47
1:A:298:PRO:N	1:B:42:LEU:CD1[2_656]	1.73	0.47
1:A:316:ALA:CB	1:B:25:THR:CA[2_656]	1.73	0.47
1:A:323:ARG:N	1:B:29:PHE:CD2[2_656]	1.73	0.47
1:A:327:ASP:OD1	1:B:347:TRP:CE3[2_656]	1.73	0.47
1:A:327:ASP:C	1:B:36:ALA:C[2_656]	1.73	0.47
1:B:215:ALA:N	1:B:218:ARG:C[2_655]	1.73	0.47
1:A:288:PHE:CE1	1:B:20:SER:N[2_656]	1.74	0.46
1:A:293:GLU:CB	1:B:257:GLY:N[2_656]	1.74	0.46
1:A:297:LEU:CD1	1:B:42:LEU:CD2[2_656]	1.74	0.46
1:A:299:PRO:C	1:B:38:ALA:O[2_656]	1.74	0.46
1:A:299:PRO:C	1:B:38:ALA:C[2_656]	1.74	0.46
1:B:347:TRP:CA	1:B:349:PRO:CD[2_656]	1.74	0.46
1:A:291:GLU:O	1:B:258:TYR:C[2_656]	1.75	0.45
1:A:316:ALA:N	1:B:24:ARG:O[2_656]	1.75	0.45
2:A:387:HOH:O	2:B:568:HOH:O[2_656]	1.75	0.45
2:A:502:HOH:O	2:B:511:HOH:O[2_656]	1.75	0.45
1:B:32:ALA:N	2:B:494:HOH:O[2_656]	1.75	0.45
1:B:81:ASP:N	1:B:83:PRO:CD[2_656]	1.75	0.45
1:B:215:ALA:N	1:B:217:ARG:O[2_655]	1.75	0.45
1:B:347:TRP:CG	2:B:418:HOH:O[2_656]	1.75	0.45
1:A:216:LYS:NZ	1:B:259:PHE:O[2_656]	1.76	0.44
1:A:289:ALA:CA	1:B:45:VAL:CG2[2_656]	1.76	0.44
1:A:291:GLU:O	1:B:258:TYR:O[2_656]	1.76	0.44
1:A:320:ARG:CB	1:B:23:PRO:CA[2_656]	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:C	1:B:36:ALA:C[2_656]	1.76	0.44
1:A:327:ASP:OD2	1:B:347:TRP:CH2[2_656]	1.76	0.44
1:A:328:VAL:CG2	1:B:35:GLU:N[2_656]	1.76	0.44
1:B:344:PHE:CE2	2:A:436:HOH:O[2_656]	1.76	0.44
1:B:33:MET:CA	2:A:596:HOH:O[2_656]	1.76	0.44
1:B:81:ASP:OD2	1:B:83:PRO:C[2_656]	1.76	0.44
1:B:215:ALA:N	1:B:218:ARG:CA[2_655]	1.76	0.44
1:B:215:ALA:N	1:B:219:GLY:N[2_655]	1.76	0.44
1:B:346:HIS:CA	2:B:542:HOH:O[2_656]	1.76	0.44
1:B:346:HIS:CG	2:B:560:HOH:O[2_656]	1.76	0.44
1:A:288:PHE:CD1	1:B:20:SER:CA[2_656]	1.77	0.43
1:A:291:GLU:OE1	1:B:307:LEU:CG[2_656]	1.77	0.43
1:A:295:ARG:CD	2:B:381:HOH:O[2_656]	1.77	0.43
1:A:320:ARG:CB	1:B:22:GLY:O[2_656]	1.77	0.43
1:A:322:ALA:C	1:B:33:MET:CB[2_656]	1.77	0.43
1:A:327:ASP:C	1:B:36:ALA:N[2_656]	1.77	0.43
1:B:81:ASP:CG	1:B:83:PRO:CB[2_656]	1.77	0.43
1:A:216:LYS:CE	1:B:259:PHE:O[2_656]	1.78	0.42
1:A:299:PRO:CG	1:B:39:THR:CB[2_656]	1.78	0.42
1:A:302:VAL:CB	1:B:24:ARG:CZ[2_656]	1.78	0.42
1:A:321:LEU:CD2	1:B:43:ASP:N[2_656]	1.78	0.42
1:B:255:ASN:C	2:A:469:HOH:O[2_656]	1.78	0.42
1:B:15:ARG:NE	2:A:490:HOH:O[2_656]	1.78	0.42
1:B:214:LEU:CA	1:B:216:LYS:O[2_655]	1.78	0.42
1:B:216:LYS:CE	1:B:217:ARG:CD[2_655]	1.78	0.42
1:A:300:PHE:CE1	1:B:41:GLY:CA[2_656]	1.79	0.41
1:B:77:SER:N	2:A:609:HOH:O[2_656]	1.79	0.41
1:B:216:LYS:CD	2:B:603:HOH:O[2_655]	1.79	0.41
1:A:217:ARG:CG	1:B:47:ALA:O[2_656]	1.80	0.40
1:A:300:PHE:O	1:B:38:ALA:CB[2_656]	1.80	0.40
1:A:323:ARG:CB	1:B:307:LEU:CD1[2_656]	1.80	0.40
1:A:218:ARG:NE	1:B:50:PRO:CB[2_656]	1.81	0.39
1:A:291:GLU:CG	1:B:258:TYR:CE2[2_656]	1.81	0.39
1:A:293:GLU:C	1:B:257:GLY:C[2_656]	1.81	0.39
1:A:294:LEU:N	1:B:257:GLY:C[2_656]	1.81	0.39
1:A:299:PRO:CB	1:B:39:THR:C[2_656]	1.81	0.39
1:A:318:ALA:CB	1:B:24:ARG:NH1[2_656]	1.81	0.39
1:B:26:ASP:CA	2:A:515:HOH:O[2_656]	1.81	0.39
1:B:27:PRO:CB	2:A:635:HOH:O[2_656]	1.81	0.39
1:B:31:PRO:CG	1:B:335:GLY:CA[2_656]	1.81	0.39
1:B:221:LEU:CD1	2:B:496:HOH:O[2_655]	1.81	0.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:PRO:C	2:B:541:HOH:O[2_656]	1.81	0.39
2:B:407:HOH:O	2:B:442:HOH:O[2_656]	1.81	0.39
1:A:217:ARG:NE	1:B:48:ALA:CB[2_656]	1.82	0.38
1:A:297:LEU:C	1:B:42:LEU:CG[2_656]	1.82	0.38
1:A:320:ARG:C	1:B:23:PRO:CA[2_656]	1.82	0.38
1:A:324:ALA:C	1:B:337:VAL:CB[2_656]	1.82	0.38
1:B:40:PHE:CE1	2:A:599:HOH:O[2_656]	1.82	0.38
1:B:215:ALA:O	1:B:218:ARG:N[2_655]	1.82	0.38
1:A:219:GLY:O	1:B:67:SER:N[2_656]	1.83	0.37
1:A:280:GLU:OE1	1:B:19:GLU:OE1[2_656]	1.83	0.37
1:A:298:PRO:CG	1:B:40:PHE:O[2_656]	1.83	0.37
1:A:300:PHE:CD1	1:B:41:GLY:C[2_656]	1.83	0.37
1:A:318:ALA:O	1:B:34:VAL:CG1[2_656]	1.83	0.37
1:A:322:ALA:CB	1:B:30:SER:O[2_656]	1.83	0.37
1:B:30:SER:N	2:A:393:HOH:O[2_656]	1.83	0.37
2:A:505:HOH:O	2:B:462:HOH:O[2_656]	1.83	0.37
1:B:344:PHE:CZ	2:A:564:HOH:O[2_656]	1.83	0.37
1:B:31:PRO:N	2:B:449:HOH:O[2_656]	1.83	0.37
1:B:215:ALA:C	1:B:218:ARG:CB[2_655]	1.83	0.37
1:A:213:LEU:CD1	1:B:45:VAL:C[2_656]	1.84	0.36
1:A:294:LEU:N	1:B:258:TYR:C[2_656]	1.84	0.36
1:A:295:ARG:C	1:B:259:PHE:CD2[2_656]	1.84	0.36
1:A:299:PRO:N	1:B:39:THR:C[2_656]	1.84	0.36
1:A:320:ARG:CZ	1:B:22:GLY:CA[2_656]	1.84	0.36
1:A:327:ASP:OD1	1:B:347:TRP:CD2[2_656]	1.84	0.36
1:A:327:ASP:CB	1:B:36:ALA:CA[2_656]	1.84	0.36
1:B:32:ALA:CB	2:B:494:HOH:O[2_656]	1.84	0.36
1:B:217:ARG:N	1:B:217:ARG:CB[2_655]	1.84	0.36
1:B:347:TRP:C	1:B:347:TRP:O[2_656]	1.84	0.36
1:B:348:LEU:CB	2:B:472:HOH:O[2_656]	1.84	0.36
1:A:217:ARG:CZ	1:B:48:ALA:CB[2_656]	1.85	0.35
1:A:218:ARG:NE	1:B:50:PRO:CG[2_656]	1.85	0.35
1:A:292:ASP:CG	1:B:309:PRO:CA[2_656]	1.85	0.35
1:A:296:GLY:C	1:B:259:PHE:CD1[2_656]	1.85	0.35
1:A:300:PHE:CE2	1:B:43:ASP:OD1[2_656]	1.85	0.35
1:B:214:LEU:O	1:B:218:ARG:N[2_655]	1.85	0.35
1:A:213:LEU:O	1:B:47:ALA:O[2_656]	1.86	0.34
1:A:217:ARG:CB	1:B:49:PRO:CD[2_656]	1.86	0.34
1:A:295:ARG:N	1:B:258:TYR:O[2_656]	1.86	0.34
1:A:295:ARG:CD	1:B:338:HIS:CB[2_656]	1.86	0.34
1:A:317:PHE:CA	1:B:24:ARG:N[2_656]	1.86	0.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:N	1:B:25:THR:N[2_656]	1.86	0.34
1:A:320:ARG:CA	1:B:23:PRO:CA[2_656]	1.86	0.34
1:A:328:VAL:CA	1:B:35:GLU:C[2_656]	1.86	0.34
1:B:350:ALA:O	2:B:527:HOH:O[2_656]	1.86	0.34
1:A:289:ALA:O	1:B:21:SER:O[2_656]	1.87	0.33
1:A:292:ASP:C	1:B:260:ILE:O[2_656]	1.87	0.33
1:A:293:GLU:N	1:B:257:GLY:N[2_656]	1.87	0.33
1:A:295:ARG:CA	1:B:259:PHE:CA[2_656]	1.87	0.33
1:A:299:PRO:CD	1:B:40:PHE:CE1[2_656]	1.87	0.33
1:A:299:PRO:CD	1:B:40:PHE:CG[2_656]	1.87	0.33
1:A:302:VAL:CG2	1:B:43:ASP:OD2[2_656]	1.87	0.33
1:A:319:ARG:O	1:B:29:PHE:CG[2_656]	1.87	0.33
1:A:321:LEU:CG	1:B:43:ASP:CB[2_656]	1.87	0.33
1:A:322:ALA:CA	1:B:33:MET:C[2_656]	1.87	0.33
1:B:77:SER:OG	2:A:511:HOH:O[2_656]	1.87	0.33
1:A:217:ARG:O	1:B:49:PRO:CB[2_656]	1.88	0.32
1:A:299:PRO:CA	1:B:39:THR:N[2_656]	1.88	0.32
1:A:318:ALA:O	1:B:34:VAL:CB[2_656]	1.88	0.32
1:A:321:LEU:CD1	1:B:43:ASP:CG[2_656]	1.88	0.32
1:A:325:GLY:N	1:B:33:MET:SD[2_656]	1.88	0.32
1:B:335:GLY:O	2:A:575:HOH:O[2_656]	1.88	0.32
1:B:218:ARG:CZ	1:B:221:LEU:N[2_655]	1.88	0.32
1:A:290:SER:CB	1:B:256:ASP:N[2_656]	1.89	0.31
1:A:291:GLU:C	1:B:258:TYR:CG[2_656]	1.89	0.31
1:A:292:ASP:CB	1:B:309:PRO:CG[2_656]	1.89	0.31
1:A:292:ASP:CG	1:B:309:PRO:CG[2_656]	1.89	0.31
1:A:294:LEU:N	1:B:258:TYR:CA[2_656]	1.89	0.31
1:A:300:PHE:N	1:B:38:ALA:CA[2_656]	1.89	0.31
1:A:326:VAL:O	1:B:37:LEU:N[2_656]	1.89	0.31
1:A:328:VAL:CA	1:B:34:VAL:O[2_656]	1.89	0.31
1:B:27:PRO:O	1:B:27:PRO:O[2_656]	1.89	0.31
1:B:28:ARG:C	2:B:508:HOH:O[2_656]	1.89	0.31
1:B:29:PHE:N	2:B:478:HOH:O[2_656]	1.89	0.31
1:B:81:ASP:CB	1:B:83:PRO:C[2_656]	1.89	0.31
1:B:214:LEU:CG	2:B:519:HOH:O[2_655]	1.89	0.31
1:B:215:ALA:CA	1:B:218:ARG:CB[2_655]	1.89	0.31
1:B:215:ALA:N	1:B:218:ARG:N[2_655]	1.89	0.31
1:B:215:ALA:C	1:B:217:ARG:C[2_655]	1.89	0.31
1:A:290:SER:N	1:B:256:ASP:O[2_656]	1.90	0.30
1:A:293:GLU:CD	1:B:46:ALA:O[2_656]	1.90	0.30
1:A:293:GLU:CA	1:B:260:ILE:O[2_656]	1.90	0.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PRO:CB	1:B:40:PHE:CD2[2_656]	1.90	0.30
1:A:302:VAL:CB	1:B:24:ARG:NE[2_656]	1.90	0.30
1:A:327:ASP:CA	1:B:36:ALA:O[2_656]	1.90	0.30
1:A:328:VAL:O	1:B:35:GLU:N[2_656]	1.90	0.30
1:A:217:ARG:CB	1:B:48:ALA:C[2_656]	1.91	0.29
1:A:317:PHE:CE2	1:B:43:ASP:O[2_656]	1.91	0.29
1:A:321:LEU:N	1:B:23:PRO:CA[2_656]	1.91	0.29
1:B:31:PRO:C	2:A:421:HOH:O[2_656]	1.91	0.29
1:B:35:GLU:CG	1:B:350:ALA:CB[2_656]	1.91	0.29
1:B:218:ARG:CD	1:B:220:ARG:N[2_655]	1.91	0.29
1:A:288:PHE:CB	1:B:19:GLU:O[2_656]	1.92	0.28
1:A:293:GLU:CB	1:B:257:GLY:C[2_656]	1.92	0.28
1:A:325:GLY:N	1:B:33:MET:CE[2_656]	1.92	0.28
1:A:327:ASP:C	1:B:36:ALA:CA[2_656]	1.92	0.28
1:A:291:GLU:N	1:B:258:TYR:CE1[2_656]	1.93	0.27
1:A:292:ASP:CG	1:B:309:PRO:CB[2_656]	1.93	0.27
1:A:292:ASP:OD1	1:B:308:ASP:C[2_656]	1.93	0.27
1:A:317:PHE:CE1	2:B:421:HOH:O[2_656]	1.93	0.27
1:B:20:SER:C	2:A:519:HOH:O[2_656]	1.93	0.27
1:B:215:ALA:C	1:B:218:ARG:CG[2_655]	1.93	0.27
1:B:218:ARG:NE	1:B:220:ARG:C[2_655]	1.93	0.27
2:B:407:HOH:O	2:B:508:HOH:O[2_656]	1.93	0.27
1:A:222:ASP:OD1	1:B:70:GLY:N[2_656]	1.94	0.26
1:A:295:ARG:O	1:B:259:PHE:CG[2_656]	1.94	0.26
1:A:299:PRO:O	1:B:38:ALA:O[2_656]	1.94	0.26
1:A:317:PHE:C	1:B:24:ARG:CG[2_656]	1.94	0.26
1:A:325:GLY:CA	1:B:33:MET:SD[2_656]	1.94	0.26
1:B:347:TRP:CZ2	2:A:491:HOH:O[2_656]	1.94	0.26
1:B:63:ALA:O	2:A:540:HOH:O[2_656]	1.94	0.26
1:B:81:ASP:OD1	1:B:83:PRO:CB[2_656]	1.94	0.26
1:B:347:TRP:O	2:B:472:HOH:O[2_656]	1.94	0.26
1:A:288:PHE:CD2	1:B:20:SER:CB[2_656]	1.95	0.25
1:A:292:ASP:OD1	1:B:309:PRO:CG[2_656]	1.95	0.25
1:A:292:ASP:CB	1:B:309:PRO:CD[2_656]	1.95	0.25
1:A:298:PRO:CG	1:B:40:PHE:CB[2_656]	1.95	0.25
1:A:298:PRO:O	1:B:37:LEU:O[2_656]	1.95	0.25
1:A:299:PRO:N	1:B:40:PHE:CA[2_656]	1.95	0.25
1:A:321:LEU:CD2	1:B:42:LEU:C[2_656]	1.95	0.25
1:A:326:VAL:CA	1:B:37:LEU:CG[2_656]	1.95	0.25
1:A:327:ASP:CB	1:B:36:ALA:O[2_656]	1.95	0.25
1:B:254:GLU:O	2:A:527:HOH:O[2_656]	1.95	0.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PHE:O	2:B:478:HOH:O[2_656]	1.95	0.25
1:B:81:ASP:CG	1:B:83:PRO:C[2_656]	1.95	0.25
1:A:320:ARG:CB	1:B:22:GLY:C[2_656]	1.96	0.24
1:A:320:ARG:CB	1:B:23:PRO:N[2_656]	1.96	0.24
1:B:31:PRO:N	2:A:421:HOH:O[2_656]	1.96	0.24
1:B:214:LEU:O	1:B:219:GLY:N[2_655]	1.96	0.24
1:B:349:PRO:O	2:B:541:HOH:O[2_656]	1.96	0.24
1:A:288:PHE:CE2	1:B:20:SER:CB[2_656]	1.97	0.23
1:A:290:SER:OG	1:B:255:ASN:C[2_656]	1.97	0.23
1:A:290:SER:CB	1:B:256:ASP:O[2_656]	1.97	0.23
1:A:298:PRO:N	1:B:40:PHE:CB[2_656]	1.97	0.23
1:A:319:ARG:CG	2:B:442:HOH:O[2_656]	1.97	0.23
1:A:323:ARG:CZ	1:B:26:ASP:O[2_656]	1.97	0.23
1:B:77:SER:OG	2:A:609:HOH:O[2_656]	1.97	0.23
1:B:81:ASP:O	1:B:83:PRO:N[2_656]	1.97	0.23
1:B:214:LEU:C	1:B:217:ARG:C[2_655]	1.97	0.23
1:B:215:ALA:N	1:B:217:ARG:C[2_655]	1.97	0.23
1:B:292:ASP:CG	2:B:557:HOH:O[2_655]	1.97	0.23
1:A:290:SER:C	1:B:258:TYR:CE1[2_656]	1.98	0.22
1:A:291:GLU:CB	1:B:258:TYR:CG[2_656]	1.98	0.22
1:A:291:GLU:CA	1:B:258:TYR:CD1[2_656]	1.98	0.22
1:A:294:LEU:N	1:B:258:TYR:N[2_656]	1.98	0.22
1:A:297:LEU:N	1:B:259:PHE:CD1[2_656]	1.98	0.22
1:A:299:PRO:O	1:B:39:THR:O[2_656]	1.98	0.22
1:A:302:VAL:CG2	1:B:24:ARG:CZ[2_656]	1.98	0.22
1:A:317:PHE:O	1:B:24:ARG:CA[2_656]	1.98	0.22
1:A:321:LEU:CA	1:B:23:PRO:CB[2_656]	1.98	0.22
1:B:29:PHE:CA	2:A:393:HOH:O[2_656]	1.98	0.22
1:B:261:GLU:CB	2:A:621:HOH:O[2_656]	1.98	0.22
1:B:35:GLU:OE2	1:B:351:ALA:CA[2_656]	1.98	0.22
1:B:80:LEU:O	1:B:83:PRO:CG[2_656]	1.98	0.22
1:B:282:PRO:CD	2:B:575:HOH:O[2_655]	1.98	0.22
1:A:218:ARG:N	1:B:49:PRO:CB[2_656]	1.99	0.21
1:A:328:VAL:CB	1:B:35:GLU:N[2_656]	1.99	0.21
1:B:336:LEU:CA	2:A:575:HOH:O[2_656]	1.99	0.21
1:B:214:LEU:O	1:B:216:LYS:C[2_655]	1.99	0.21
1:B:346:HIS:CD2	2:B:560:HOH:O[2_656]	1.99	0.21
1:A:283:ILE:CD1	1:B:47:ALA:CB[2_656]	2.00	0.20
1:A:316:ALA:O	1:B:25:THR:CA[2_656]	2.00	0.20
1:A:317:PHE:CE2	1:B:44:ALA:N[2_656]	2.00	0.20
1:A:324:ALA:N	1:B:337:VAL:CG1[2_656]	2.00	0.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PRO:CB	2:A:421:HOH:O[2_656]	2.00	0.20
1:B:212:THR:O	1:B:217:ARG:O[2_655]	2.00	0.20
1:B:215:ALA:O	1:B:218:ARG:CA[2_655]	2.00	0.20
2:B:467:HOH:O	2:B:590:HOH:O[2_656]	2.00	0.20
1:A:217:ARG:CZ	1:B:48:ALA:N[2_656]	2.01	0.19
1:A:217:ARG:CG	1:B:48:ALA:C[2_656]	2.01	0.19
1:A:218:ARG:NE	1:B:50:PRO:N[2_656]	2.01	0.19
1:A:300:PHE:CB	1:B:38:ALA:CB[2_656]	2.01	0.19
1:A:317:PHE:N	1:B:24:ARG:CB[2_656]	2.01	0.19
1:A:317:PHE:CZ	1:B:43:ASP:O[2_656]	2.01	0.19
1:A:317:PHE:CE2	1:B:43:ASP:C[2_656]	2.01	0.19
1:A:317:PHE:N	1:B:24:ARG:CA[2_656]	2.01	0.19
1:A:327:ASP:CA	1:B:36:ALA:CB[2_656]	2.01	0.19
1:B:261:GLU:CB	2:A:649:HOH:O[2_656]	2.01	0.19
1:B:214:LEU:O	1:B:216:LYS:O[2_655]	2.01	0.19
1:A:291:GLU:C	1:B:258:TYR:CA[2_656]	2.02	0.18
1:A:293:GLU:N	1:B:257:GLY:C[2_656]	2.02	0.18
1:A:299:PRO:N	1:B:40:PHE:CD1[2_656]	2.02	0.18
1:A:300:PHE:C	1:B:38:ALA:CB[2_656]	2.02	0.18
1:A:320:ARG:CA	1:B:23:PRO:O[2_656]	2.02	0.18
1:A:323:ARG:NH2	1:B:26:ASP:CA[2_656]	2.02	0.18
1:B:35:GLU:OE2	1:B:350:ALA:CA[2_656]	2.02	0.18
1:B:348:LEU:O	2:B:590:HOH:O[2_656]	2.02	0.18
1:A:300:PHE:CD1	1:B:41:GLY:CA[2_656]	2.03	0.17
1:A:328:VAL:CA	1:B:35:GLU:O[2_656]	2.03	0.17
1:A:369:LEU:O	1:B:77:SER:O[2_656]	2.03	0.17
1:B:40:PHE:CZ	2:A:432:HOH:O[2_656]	2.03	0.17
1:B:256:ASP:O	2:A:433:HOH:O[2_656]	2.03	0.17
1:B:25:THR:O	2:A:515:HOH:O[2_656]	2.03	0.17
1:B:214:LEU:C	1:B:218:ARG:N[2_655]	2.03	0.17
1:A:222:ASP:N	1:B:70:GLY:CA[2_656]	2.04	0.16
1:A:290:SER:C	1:B:258:TYR:CG[2_656]	2.04	0.16
1:A:292:ASP:CA	1:B:255:ASN:O[2_656]	2.04	0.16
1:A:294:LEU:C	1:B:259:PHE:CB[2_656]	2.04	0.16
1:A:317:PHE:CB	1:B:24:ARG:CB[2_656]	2.04	0.16
1:B:81:ASP:CG	1:B:83:PRO:O[2_656]	2.04	0.16
1:B:178:LEU:CD2	1:B:218:ARG:O[2_655]	2.04	0.16
1:A:298:PRO:O	1:B:40:PHE:N[2_656]	2.05	0.15
1:A:320:ARG:C	1:B:23:PRO:CB[2_656]	2.05	0.15
1:A:324:ALA:CA	1:B:337:VAL:CB[2_656]	2.05	0.15
1:A:324:ALA:N	1:B:29:PHE:CE2[2_656]	2.05	0.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ASP:C	2:A:515:HOH:O[2_656]	2.05	0.15
1:B:216:LYS:CG	2:B:603:HOH:O[2_655]	2.05	0.15
1:B:347:TRP:CD1	1:B:350:ALA:N[2_656]	2.05	0.15
1:A:316:ALA:CA	1:B:24:ARG:C[2_656]	2.06	0.14
1:A:319:ARG:C	2:B:426:HOH:O[2_656]	2.06	0.14
1:B:33:MET:CB	2:A:508:HOH:O[2_656]	2.06	0.14
1:B:344:PHE:CD2	2:A:564:HOH:O[2_656]	2.06	0.14
1:A:288:PHE:CG	1:B:20:SER:N[2_656]	2.07	0.13
1:A:293:GLU:N	1:B:260:ILE:O[2_656]	2.07	0.13
1:A:300:PHE:N	1:B:39:THR:CA[2_656]	2.07	0.13
1:A:300:PHE:C	1:B:38:ALA:O[2_656]	2.07	0.13
1:A:326:VAL:N	1:B:37:LEU:CG[2_656]	2.07	0.13
1:A:326:VAL:CG1	1:B:37:LEU:O[2_656]	2.07	0.13
1:B:66:ALA:CB	2:A:540:HOH:O[2_656]	2.07	0.13
1:B:70:GLY:CA	2:A:633:HOH:O[2_656]	2.07	0.13
1:B:28:ARG:C	2:B:478:HOH:O[2_656]	2.07	0.13
1:A:214:LEU:N	1:B:47:ALA:CB[2_656]	2.08	0.12
1:A:217:ARG:CG	1:B:48:ALA:N[2_656]	2.08	0.12
1:A:295:ARG:O	1:B:259:PHE:CD1[2_656]	2.08	0.12
1:A:302:VAL:CB	1:B:24:ARG:NH2[2_656]	2.08	0.12
1:A:316:ALA:CA	1:B:25:THR:N[2_656]	2.08	0.12
1:A:317:PHE:CE1	1:B:44:ALA:CA[2_656]	2.08	0.12
1:A:320:ARG:NE	1:B:22:GLY:O[2_656]	2.08	0.12
1:A:320:ARG:NH1	1:B:21:SER:O[2_656]	2.08	0.12
1:A:324:ALA:O	1:B:337:VAL:CG1[2_656]	2.08	0.12
1:A:325:GLY:O	1:B:344:PHE:CD2[2_656]	2.08	0.12
1:B:346:HIS:NE2	1:B:349:PRO:CB[2_656]	2.08	0.12
1:A:213:LEU:CD2	1:B:45:VAL:C[2_656]	2.09	0.11
1:A:218:ARG:CZ	1:B:50:PRO:CB[2_656]	2.09	0.11
1:A:289:ALA:CB	1:B:45:VAL:CA[2_656]	2.09	0.11
1:A:293:GLU:CA	1:B:257:GLY:N[2_656]	2.09	0.11
1:A:293:GLU:O	1:B:46:ALA:CB[2_656]	2.09	0.11
1:A:295:ARG:NH2	1:B:336:LEU:O[2_656]	2.09	0.11
1:A:320:ARG:NH2	1:B:21:SER:CA[2_656]	2.09	0.11
1:B:346:HIS:ND1	2:B:560:HOH:O[2_656]	2.09	0.11
1:B:350:ALA:N	2:B:527:HOH:O[2_656]	2.09	0.11
1:A:292:ASP:CB	1:B:255:ASN:O[2_656]	2.10	0.10
1:A:296:GLY:CA	1:B:259:PHE:CE2[2_656]	2.10	0.10
1:A:296:GLY:O	1:B:259:PHE:CE1[2_656]	2.10	0.10
1:A:300:PHE:CD2	1:B:43:ASP:CG[2_656]	2.10	0.10
1:A:316:ALA:O	1:B:24:ARG:CA[2_656]	2.10	0.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ALA:O	1:B:24:ARG:O[2_656]	2.10	0.10
1:A:320:ARG:NH2	1:B:25:THR:OG1[2_656]	2.10	0.10
1:B:35:GLU:OE1	2:A:387:HOH:O[2_656]	2.10	0.10
1:B:255:ASN:CG	2:A:469:HOH:O[2_656]	2.10	0.10
1:B:348:LEU:CB	2:B:590:HOH:O[2_656]	2.10	0.10
1:A:289:ALA:N	1:B:15:ARG:NH1[2_656]	2.11	0.09
1:A:293:GLU:OE2	2:B:573:HOH:O[2_656]	2.11	0.09
1:A:295:ARG:C	1:B:259:PHE:CA[2_656]	2.11	0.09
1:A:297:LEU:N	1:B:42:LEU:CD1[2_656]	2.11	0.09
1:A:297:LEU:CB	1:B:42:LEU:CD1[2_656]	2.11	0.09
1:A:302:VAL:CG2	1:B:24:ARG:NH2[2_656]	2.11	0.09
1:A:320:ARG:NH2	1:B:21:SER:C[2_656]	2.11	0.09
1:B:30:SER:N	1:B:30:SER:CA[2_656]	2.11	0.09
1:B:81:ASP:C	1:B:83:PRO:CG[2_656]	2.11	0.09
1:B:349:PRO:N	2:B:574:HOH:O[2_656]	2.11	0.09
1:A:213:LEU:CD2	1:B:45:VAL:O[2_656]	2.12	0.08
1:A:288:PHE:N	1:B:20:SER:O[2_656]	2.12	0.08
1:A:289:ALA:CA	1:B:45:VAL:CG1[2_656]	2.12	0.08
1:A:294:LEU:O	1:B:259:PHE:CB[2_656]	2.12	0.08
1:A:295:ARG:CB	1:B:259:PHE:CB[2_656]	2.12	0.08
1:A:326:VAL:CA	1:B:37:LEU:N[2_656]	2.12	0.08
1:A:327:ASP:O	1:B:36:ALA:O[2_656]	2.12	0.08
1:B:70:GLY:N	2:A:633:HOH:O[2_656]	2.12	0.08
1:B:35:GLU:OE1	1:B:351:ALA:CB[2_656]	2.12	0.08
1:B:218:ARG:CG	1:B:221:LEU:N[2_655]	2.12	0.08
1:A:287:TYR:C	1:B:20:SER:C[2_656]	2.13	0.07
1:A:288:PHE:CD1	1:B:19:GLU:O[2_656]	2.13	0.07
1:A:291:GLU:CB	1:B:258:TYR:CE2[2_656]	2.13	0.07
1:A:294:LEU:CD2	2:B:417:HOH:O[2_656]	2.13	0.07
1:A:294:LEU:CD2	1:B:44:ALA:C[2_656]	2.13	0.07
1:A:295:ARG:O	1:B:259:PHE:CA[2_656]	2.13	0.07
1:A:300:PHE:CB	1:B:38:ALA:C[2_656]	2.13	0.07
1:A:317:PHE:CZ	1:B:43:ASP:C[2_656]	2.13	0.07
1:A:317:PHE:CE2	1:B:44:ALA:CA[2_656]	2.13	0.07
1:A:320:ARG:NE	1:B:22:GLY:N[2_656]	2.13	0.07
1:A:328:VAL:C	1:B:35:GLU:CB[2_656]	2.13	0.07
1:B:261:GLU:C	2:A:649:HOH:O[2_656]	2.13	0.07
1:B:218:ARG:CD	1:B:220:ARG:O[2_655]	2.13	0.07
1:A:216:LYS:NZ	1:B:260:ILE:N[2_656]	2.14	0.06
1:A:292:ASP:O	1:B:260:ILE:N[2_656]	2.14	0.06
1:A:293:GLU:CD	1:B:261:GLU:CG[2_656]	2.14	0.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:N	1:B:259:PHE:CE2[2_656]	2.14	0.06
1:A:300:PHE:C	1:B:38:ALA:C[2_656]	2.14	0.06
1:A:319:ARG:C	1:B:29:PHE:CB[2_656]	2.14	0.06
1:A:323:ARG:CZ	1:B:26:ASP:OD1[2_656]	2.14	0.06
1:A:327:ASP:O	1:B:39:THR:N[2_656]	2.14	0.06
1:A:327:ASP:OD1	1:B:36:ALA:CB[2_656]	2.14	0.06
1:A:217:ARG:C	1:B:49:PRO:CG[2_656]	2.15	0.05
1:A:317:PHE:CB	2:B:421:HOH:O[2_656]	2.15	0.05
1:A:319:ARG:CB	2:B:442:HOH:O[2_656]	2.15	0.05
1:A:327:ASP:N	1:B:36:ALA:CB[2_656]	2.15	0.05
1:A:327:ASP:CB	1:B:36:ALA:C[2_656]	2.15	0.05
1:B:344:PHE:CE2	2:A:428:HOH:O[2_656]	2.15	0.05
1:B:347:TRP:CG	1:B:349:PRO:CG[2_656]	2.15	0.05
1:A:213:LEU:C	1:B:47:ALA:CB[2_656]	2.16	0.04
1:A:293:GLU:CG	1:B:257:GLY:CA[2_656]	2.16	0.04
1:A:320:ARG:CZ	1:B:22:GLY:O[2_656]	2.16	0.04
1:A:323:ARG:CD	1:B:28:ARG:CA[2_656]	2.16	0.04
1:A:325:GLY:O	1:B:344:PHE:CG[2_656]	2.16	0.04
1:A:327:ASP:CG	1:B:347:TRP:CE3[2_656]	2.16	0.04
1:B:25:THR:O	2:A:541:HOH:O[2_656]	2.16	0.04
1:B:35:GLU:CD	1:B:350:ALA:C[2_656]	2.16	0.04
1:B:214:LEU:C	1:B:216:LYS:O[2_655]	2.16	0.04
1:B:214:LEU:C	1:B:217:ARG:O[2_655]	2.16	0.04
1:A:297:LEU:CG	1:B:42:LEU:CG[2_656]	2.17	0.03
1:A:298:PRO:CB	1:B:40:PHE:CA[2_656]	2.17	0.03
1:A:299:PRO:N	1:B:40:PHE:CB[2_656]	2.17	0.03
1:A:317:PHE:N	1:B:24:ARG:O[2_656]	2.17	0.03
1:A:320:ARG:C	1:B:29:PHE:CE2[2_656]	2.17	0.03
1:A:320:ARG:C	1:B:29:PHE:CD2[2_656]	2.17	0.03
1:A:323:ARG:CD	1:B:28:ARG:O[2_656]	2.17	0.03
1:A:327:ASP:O	1:B:36:ALA:C[2_656]	2.17	0.03
1:B:35:GLU:OE2	1:B:350:ALA:O[2_656]	2.17	0.03
1:B:213:LEU:C	1:B:217:ARG:O[2_655]	2.17	0.03
1:A:288:PHE:CA	1:B:20:SER:CA[2_656]	2.18	0.02
1:A:292:ASP:O	1:B:260:ILE:C[2_656]	2.18	0.02
1:A:294:LEU:C	1:B:258:TYR:C[2_656]	2.18	0.02
1:A:294:LEU:O	1:B:259:PHE:N[2_656]	2.18	0.02
1:A:295:ARG:N	1:B:259:PHE:C[2_656]	2.18	0.02
1:A:296:GLY:N	1:B:259:PHE:CZ[2_656]	2.18	0.02
1:A:320:ARG:CA	1:B:23:PRO:C[2_656]	2.18	0.02
1:A:328:VAL:O	1:B:35:GLU:CG[2_656]	2.18	0.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLY:CA	2:A:502:HOH:O[2_656]	2.18	0.02
1:A:292:ASP:N	1:B:258:TYR:CB[2_656]	2.19	0.01
1:A:299:PRO:N	1:B:40:PHE:CG[2_656]	2.19	0.01
1:A:320:ARG:CA	1:B:29:PHE:CD1[2_656]	2.19	0.01
1:A:320:ARG:NH1	1:B:22:GLY:C[2_656]	2.19	0.01
1:B:344:PHE:CE1	2:A:404:HOH:O[2_656]	2.19	0.01
1:B:27:PRO:O	2:B:478:HOH:O[2_656]	2.19	0.01
1:B:31:PRO:CB	2:B:449:HOH:O[2_656]	2.19	0.01
1:B:218:ARG:NH1	1:B:222:ASP:OD1[2_655]	2.19	0.01

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	356/361 (99%)	341 (96%)	15 (4%)	0	100	100
1	B	359/361 (99%)	344 (96%)	14 (4%)	1 (0%)	36	25
All	All	715/722 (99%)	685 (96%)	29 (4%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	LEU

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	275/278 (99%)	253 (92%)	22 (8%)	11	2
1	B	278/278 (100%)	258 (93%)	20 (7%)	13	3
All	All	553/556 (100%)	511 (92%)	42 (8%)	12	3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	57	LEU
1	A	67	SER
1	A	89	VAL
1	A	93	THR
1	A	99	VAL
1	A	102	ASN
1	A	110	ARG
1	A	121	LEU
1	A	133	THR
1	A	163	THR
1	A	165	GLU
1	A	171	PRO
1	A	178	LEU
1	A	214	LEU
1	A	220	ARG
1	A	246	LEU
1	A	295	ARG
1	A	297	LEU
1	A	304	VAL
1	A	328	VAL
1	A	370	ARG
1	B	21	SER
1	B	52	SER
1	B	57	LEU
1	B	77	SER
1	B	90	GLU
1	B	118	LEU
1	B	165	GLU
1	B	171	PRO
1	B	174	VAL
1	B	189	GLU
1	B	214	LEU
1	B	221	LEU
1	B	243	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	246	LEU
1	B	249	LEU
1	B	293	GLU
1	B	295	ARG
1	B	328	VAL
1	B	341	ASP
1	B	370	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	107	HIS
1	A	167	HIS
1	A	262	ASN
1	A	278	HIS
1	B	160	ASN
1	B	167	HIS
1	B	199	GLN
1	B	262	ASN
1	B	278	HIS
1	B	305	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.