



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:53 pm BST

PDB ID : 1JKM
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

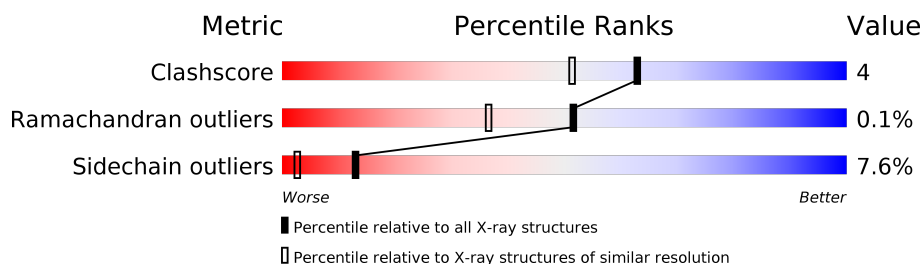
1 Overall quality at a glance

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	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (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 on 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	
1	B	361	

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.

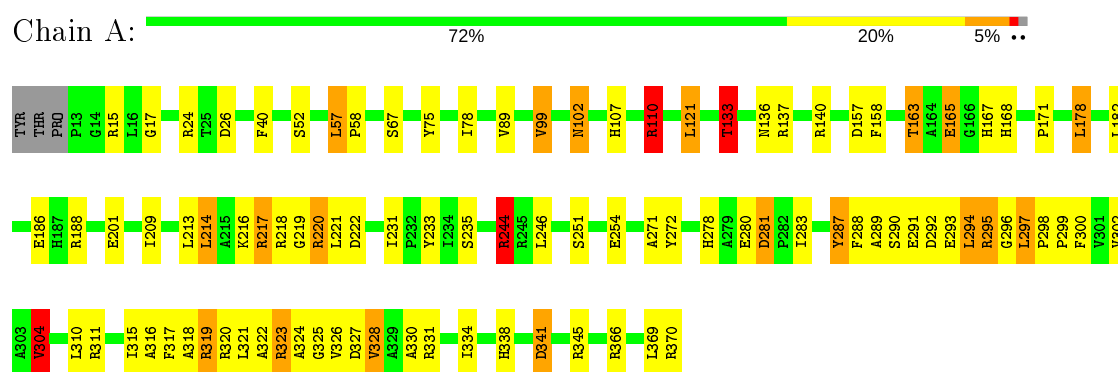
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	292	Total	O	0	0
			292	292		
2	B	239	Total	O	0	0
			239	239		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



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	140.70 Å 82.60 Å 81.50 Å 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	0.75	0/2758	1.53	39/3767 (1.0%)
1	B	0.61	0/2786	1.33	32/3808 (0.8%)
All	All	0.68	0/5544	1.43	71/7575 (0.9%)

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

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	B	141	ARG	NE-CZ-NH1	11.57	126.08	120.30
1	A	220	ARG	CD-NE-CZ	11.53	139.74	123.60
1	B	311	ARG	NE-CZ-NH1	-10.52	115.04	120.30
1	B	137	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	B	311	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	121	LEU	CA-CB-CG	10.01	138.31	115.30
1	A	244	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	A	15	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	24	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	328	VAL	CB-CA-C	-9.27	93.80	111.40
1	B	319	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	140	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	A	110	ARG	NE-CZ-NH2	-8.83	115.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	VAL	CB-CA-C	-8.75	94.78	111.40
1	A	319	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	A	281	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	331	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	304	VAL	N-CA-CB	-7.95	94.02	111.50
1	B	110	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	A	75	TYR	CB-CG-CD1	7.67	125.60	121.00
1	A	75	TYR	CB-CG-CD2	-7.57	116.46	121.00
1	A	24	ARG	CD-NE-CZ	7.51	134.12	123.60
1	B	357	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	167	HIS	CA-CB-CG	7.33	126.06	113.60
1	A	272	TYR	CB-CG-CD1	7.27	125.36	121.00
1	A	137	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	110	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	217	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	137	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	133	THR	N-CA-CB	-6.79	97.41	110.30
1	A	366	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	15	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	323	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	341	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	328	VAL	CG1-CB-CG2	6.48	121.26	110.90
1	B	245	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	272	TYR	CD1-CE1-CZ	-6.22	114.20	119.80
1	B	272	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	B	217	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	233	TYR	CA-CB-CG	6.12	125.03	113.40
1	A	220	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	345	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	A	331	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	217	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	A	201	GLU	OE1-CD-OE2	-5.95	116.17	123.30
1	B	323	ARG	CD-NE-CZ	5.92	131.89	123.60
1	B	28	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	158	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	B	75	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	A	341	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	140	ARG	CD-NE-CZ	5.60	131.44	123.60
1	B	345	ARG	CD-NE-CZ	5.59	131.43	123.60
1	B	370	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	159	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	15	ARG	NE-CZ-NH2	-5.49	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	26	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	141	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	99	VAL	N-CA-CB	-5.35	99.73	111.50
1	A	304	VAL	CG1-CB-CG2	5.35	119.46	110.90
1	A	244	ARG	CG-CD-NE	5.33	123.00	111.80
1	B	24	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	157	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	244	ARG	NH1-CZ-NH2	5.24	125.16	119.40
1	B	118	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	308	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	201	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	217	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	287	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	B	75	TYR	CB-CG-CD1	5.07	124.04	121.00

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:H	1:A:102:ASN:HD22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASP:N	1:A:341:ASP:OD1	2.52	0.42
1:A:102:ASN:ND2	1:A:102:ASN:H	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
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:326:VAL:CG2	1:B:37:LEU:CD2[2_656]	0.53	1.67
1:A:322:ALA:O	1:B:33:MET:CG[2_656]	0.53	1.67
1:B:27:PRO:CG	2:A:635:HOH:O[2_656]	0.57	1.63
1:A:324:ALA:CA	1:B:337:VAL:CG1[2_656]	0.58	1.62
1:A:292:ASP:OD1	1:B:309:PRO:CD[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: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:291:GLU:CA	1:B:258:TYR:CG[2_656]	0.60	1.60
1:A:324:ALA:O	1:B:337:VAL:CG2[2_656]	0.62	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:31:PRO:CA	2:A:421:HOH:O[2_656]	0.86	1.34
1:A:319:ARG:CB	2:B:426:HOH:O[2_656]	0.86	1.34
1:B:29:PHE:C	2:A:393:HOH:O[2_656]	0.87	1.33
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: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:300:PHE:CA	1:B:38:ALA:O[2_656]	0.88	1.32
1:B:255:ASN:CB	2:A:469:HOH:O[2_656]	0.89	1.31
1:A:320:ARG:NH1	1:B:22:GLY:CA[2_656]	0.89	1.31
1:B:31:PRO:CD	2:B:449:HOH:O[2_656]	0.89	1.31
1:A:316:ALA:C	1:B:25:THR:N[2_656]	0.89	1.31
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:291:GLU:C	1:B:258:TYR:CB[2_656]	0.90	1.30
1:B:29:PHE:O	2:A:393:HOH:O[2_656]	0.91	1.29
1:A:299:PRO:CB	1:B:39:THR:CB[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:325:GLY:CA	1:B:33:MET:CE[2_656]	1.00	1.20
1:A:323:ARG:NH1	1:B:26:ASP:O[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:317:PHE:C	1:B:24:ARG:CA[2_656]	1.03	1.17
1:A:288:PHE:CD1	1:B:20:SER:N[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:B:344:PHE:CE1	2:A:564:HOH:O[2_656]	1.04	1.16
1:A:319:ARG:O	1:B:29:PHE:CB[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:317:PHE:CZ	1:B:44:ALA:CA[2_656]	1.07	1.13
1:B:30:SER:CA	1:B:30:SER:CB[2_656]	1.07	1.13
1:A:300:PHE:CE1	1:B:42:LEU:N[2_656]	1.07	1.13
1:A:216:LYS:CE	2:B:466:HOH:O[2_656]	1.07	1.13
1:B:81:ASP:OD2	1:B:83:PRO:O[2_656]	1.07	1.13
1:B:26:ASP:N	2:A:515:HOH:O[2_656]	1.07	1.13
1:B:348:LEU:CA	2:B:472:HOH:O[2_656]	1.08	1.12
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: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:B:81:ASP:C	1:B:83: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:216:LYS:NZ	1:B:217:ARG:CZ[2_655]	1.10	1.10
1:A:218:ARG:CD	1:B:50:PRO:CD[2_656]	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: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:316:ALA:O	1:B:24:ARG:C[2_656]	1.12	1.08
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:322:ALA:O	1:B:33:MET:CB[2_656]	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:323:ARG:NH2	1:B:26:ASP: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:B:81:ASP:CA	1:B:83:PRO:CG[2_656]	1.17	1.03
1:A:327:ASP:CA	1:B:36:ALA:C[2_656]	1.17	1.03
1:A:300:PHE:CA	1:B:38:ALA:C[2_656]	1.17	1.03
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:217:ARG:NE	1:B:48:ALA:N[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:317:PHE:C	1:B:24:ARG:N[2_656]	1.21	0.99
1:A:299:PRO:CD	1:B:40:PHE:CD1[2_656]	1.21	0.99
1:A:299:PRO:CG	1:B:39:THR:CG2[2_656]	1.22	0.98
1:A:295:ARG:N	1:B:259:PHE:N[2_656]	1.22	0.98
1:A:323:ARG:NH2	1:B:26:ASP:CG[2_656]	1.22	0.98
1:B:30:SER:CA	1:B:30:SER:CA[2_656]	1.23	0.97
1:A:296:GLY:CA	1:B:259:PHE:CZ[2_656]	1.23	0.97
1:B:216:LYS:CE	1:B:217:ARG:CZ[2_655]	1.23	0.97
1:A:292:ASP:CG	1:B:309:PRO:CD[2_656]	1.24	0.96
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:B:40:PHE:CZ	2:A:599:HOH:O[2_656]	1.24	0.96
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: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:216:LYS:CG	1:B:217:ARG:CD[2_655]	1.26	0.94
1:B:32:ALA:CA	2:B:494:HOH:O[2_656]	1.26	0.94
1:B:216:LYS:CE	1:B:217:ARG:NE[2_655]	1.26	0.94
1:B:28:ARG:O	2:B:508:HOH:O[2_656]	1.27	0.93
1:A:297:LEU:CA	1:B:42:LEU:CG[2_656]	1.27	0.93
1:B:81:ASP:CA	1:B:83:PRO:CB[2_656]	1.28	0.92
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:A:295:ARG:NE	2:B:381:HOH:O[2_656]	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:547:HOH:O	2:B:470:HOH:O[2_656]	1.29	0.91
1:A:219:GLY:O	1:B:66:ALA:C[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
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:321:LEU:N	1:B:23:PRO:CB[2_656]	1.32	0.88
1:A:299:PRO:CB	1:B:39:THR:CA[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:217:ARG:CB	1:B:49:PRO: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:290:SER:C	1:B:258:TYR:CD1[2_656]	1.32	0.88
1:A:317:PHE:CG	2:B:421:HOH:O[2_656]	1.32	0.88
1:A:295:ARG:NH1	1:B:338:HIS:N[2_656]	1.32	0.88
1:A:290:SER:OG	1:B:256:ASP:C[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:299:PRO:CA	1:B:39:THR:CA[2_656]	1.33	0.87
1:A:288:PHE:C	1:B:15:ARG:NH1[2_656]	1.35	0.85
1:B:221:LEU:CB	2:B:496:HOH:O[2_655]	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:A:297:LEU:CB	1:B:42:LEU:CD2[2_656]	1.36	0.84
1:A:297:LEU:O	1:B:42:LEU:CD1[2_656]	1.37	0.83
1:B:216:LYS:CB	1:B:217:ARG:CB[2_655]	1.37	0.83
1:A:299:PRO:CB	1:B:39:THR:CG2[2_656]	1.37	0.83
1:A:295:ARG:NH1	1:B:337:VAL:O[2_656]	1.38	0.82
1:A:318:ALA:N	1:B:24:ARG:CA[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:291:GLU:N	1:B:258:TYR:CD1[2_656]	1.38	0.82
1:A:328:VAL:N	1:B:35:GLU:O[2_656]	1.38	0.82
1:A:321:LEU:CD2	1:B:43:ASP:CA[2_656]	1.38	0.82
1:A:317:PHE:C	1:B:24:ARG:CB[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:295:ARG:NH1	1:B:337:VAL:CA[2_656]	1.40	0.80
1:B:347:TRP:CD1	2:B:418:HOH:O[2_656]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:N	1:B:37:LEU:N[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:294:LEU:N	1:B:257:GLY:O[2_656]	1.40	0.80
1:A:321:LEU:CG	1:B:43:ASP:CA[2_656]	1.41	0.79
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:302:VAL:CG2	1:B:24:ARG:NE[2_656]	1.42	0.78
1:B:216:LYS:N	1:B:217:ARG:C[2_655]	1.42	0.78
1:A:318:ALA:O	1:B:34:VAL:CG2[2_656]	1.42	0.78
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:328:VAL:CG2	1:B:34:VAL:CA[2_656]	1.43	0.77
1:A:299:PRO:O	1:B:39:THR:C[2_656]	1.43	0.77
1:B:215:ALA:CA	1:B:218:ARG:C[2_655]	1.43	0.77
1:A:293:GLU:OE2	1:B:46:ALA:O[2_656]	1.43	0.77
1:A:325:GLY:C	1:B:33:MET:CE[2_656]	1.43	0.77
1:A:295:ARG:CZ	1:B:337:VAL:C[2_656]	1.43	0.77
1:A:213:LEU:CD2	1:B:46:ALA:CA[2_656]	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:B:344:PHE:CG	2:A:564:HOH: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: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:290:SER:OG	1:B:256:ASP:N[2_656]	1.46	0.74
1:A:321:LEU:O	1:B:37:LEU:CD1[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: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: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: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:350:ALA:C	2:B:527:HOH:O[2_656]	1.47	0.73
1:A:219:GLY:O	1:B:66:ALA:O[2_656]	1.48	0.72
1:A:216:LYS:CG	2:B:466:HOH:O[2_656]	1.48	0.72
1:A:292:ASP:O	1:B:260:ILE:O[2_656]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:GLU:OE1	1:B:19:GLU:OE2[2_656]	1.49	0.71
1:A:213:LEU:CG	1:B:45:VAL:O[2_656]	1.49	0.71
1:A:287:TYR:CD2	1:B:20:SER:OG[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:B:30:SER:C	1:B:30:SER:CB[2_656]	1.51	0.69
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:A:287:TYR:O	1:B:20:SER:C[2_656]	1.52	0.68
1:A:327:ASP:O	1:B:35:GLU:O[2_656]	1.52	0.68
1:A:323:ARG:CG	1:B:29:PHE:CA[2_656]	1.52	0.68
1:A:290:SER:OG	1:B:256:ASP:CA[2_656]	1.52	0.68
1:B:81:ASP:CG	1:B:83:PRO: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:OD2	1:B:347:TRP:CZ3[2_656]	1.52	0.68
1:A:318:ALA:N	1:B:24:ARG:CG[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:328:VAL:N	1:B:36:ALA:N[2_656]	1.54	0.66
1:B:220:ARG:CA	2:B:473:HOH:O[2_655]	1.54	0.66
1:A:299:PRO:C	1:B:39:THR:N[2_656]	1.54	0.66
1:B:81:ASP:CB	1:B:83:PRO:CB[2_656]	1.54	0.66
1:A:217:ARG:CD	1:B:48:ALA:C[2_656]	1.55	0.65
1:B:346:HIS:CD2	1:B:349:PRO:CB[2_656]	1.55	0.65
1:A:291:GLU:CG	1:B:258:TYR:CD2[2_656]	1.55	0.65
1:B:347:TRP:CH2	2:A:491:HOH:O[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:316:ALA:CB	1:B:25:THR:CB[2_656]	1.55	0.65
1:A:326:VAL:CG1	1:B:37:LEU:CB[2_656]	1.55	0.65
1:B:178:LEU:CB	2:B:563:HOH:O[2_655]	1.55	0.65
1:A:299:PRO:C	1:B:40:PHE:N[2_656]	1.55	0.65
1:B:347:TRP:CE3	2:A:578:HOH:O[2_656]	1.55	0.65
1:A:317:PHE:CA	1:B:24:ARG: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:ARG:CD	1:B:48:ALA:CB[2_656]	1.56	0.64
1:B:215:ALA:CA	1:B:218:ARG:N[2_655]	1.56	0.64
1:A:299:PRO:CA	1:B:40:PHE:N[2_656]	1.57	0.63
1:B:77:SER:CA	2:A:609:HOH:O[2_656]	1.57	0.63
1:A:294:LEU:CA	2:B:417:HOH:O[2_656]	1.57	0.63
1:B:347:TRP:NE1	1:B:350:ALA:N[2_656]	1.57	0.63
1:B:213:LEU:O	1:B:217:ARG:CA[2_655]	1.57	0.63
1:A:319:ARG:CA	2:B:426: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: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:296:GLY:N	1:B:259:PHE:CD2[2_656]	1.58	0.62
1:A:280:GLU:OE1	1:B:19:GLU:CD[2_656]	1.58	0.62
1:A:320:ARG:NH1	1:B:21:SER:C[2_656]	1.58	0.62
1:A:299:PRO:C	1:B:39:THR:CA[2_656]	1.58	0.62
1:A:218:ARG:NE	1:B:50:PRO: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:320:ARG:O	1:B:29:PHE:CZ[2_656]	1.58	0.62
1:A:315:ILE:C	1:B:24:ARG:O[2_656]	1.59	0.61
1:A:298:PRO:CB	1:B:40:PHE:CG[2_656]	1.59	0.61
1:B:30:SER:OG	1:B:30:SER:OG[2_656]	1.59	0.61
1:B:27:PRO:CD	2:A:635:HOH:O[2_656]	1.59	0.61
1:A:295:ARG:C	1:B:259:PHE:CD1[2_656]	1.59	0.61
1:A:326:VAL:CG1	1:B:37:LEU:C[2_656]	1.59	0.61
1:A:217:ARG:CG	1:B:48:ALA:CA[2_656]	1.59	0.61
1:A:328:VAL:CB	1:B:34:VAL:C[2_656]	1.59	0.61
1:A:294:LEU:CB	2:B:417:HOH:O[2_656]	1.60	0.60
1:B:35:GLU:CD	1:B:351:ALA:N[2_656]	1.60	0.60
1:A:326:VAL:CB	1:B:37:LEU:CD2[2_656]	1.60	0.60
1:B:348:LEU:C	2:B:590:HOH:O[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:A:291:GLU:OE1	1:B:307:LEU:CD2[2_656]	1.61	0.59
1:B:347:TRP:CZ3	2:A:578:HOH:O[2_656]	1.61	0.59
1:A:320:ARG:NH2	1:B:22:GLY:N[2_656]	1.61	0.59
1:A:326:VAL:O	1:B:33:MET:O[2_656]	1.61	0.59
1:A:323:ARG:NH1	1:B:26:ASP:C[2_656]	1.61	0.59
1:B:216:LYS:CE	1:B:217:ARG:NH1[2_655]	1.61	0.59
1:B:79:ALA:CB	2:A:552:HOH:O[2_656]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:CB	1:B:30:SER:OG[2_656]	1.62	0.58
1:B:26:ASP:CG	2:A:642:HOH:O[2_656]	1.62	0.58
1:B:292:ASP:CB	2:B:557:HOH:O[2_655]	1.62	0.58
1:A:327:ASP:N	1:B:36:ALA:CA[2_656]	1.62	0.58
1:B:216:LYS:C	1:B:217:ARG:CB[2_655]	1.62	0.58
1:A:322:ALA:C	1:B:33:MET:CG[2_656]	1.62	0.58
1:A:300:PHE:CD1	1:B:42:LEU:N[2_656]	1.62	0.58
1:A:296:GLY:N	1:B:259:PHE:CE1[2_656]	1.62	0.58
1:A:293:GLU:N	1:B:258:TYR:N[2_656]	1.63	0.57
1:A:217:ARG:O	1:B:49:PRO:CG[2_656]	1.63	0.57
1:B:214:LEU:C	1:B:219:GLY:N[2_655]	1.63	0.57
1:B:220:ARG:CG	2:B:473:HOH:O[2_655]	1.63	0.57
1:A:316:ALA:CA	1:B:24:ARG:O[2_656]	1.63	0.57
1:A:216:LYS:NZ	1:B:260:ILE:CA[2_656]	1.63	0.57
1:B:348:LEU:CA	2:B:590:HOH:O[2_656]	1.63	0.57
1:A:295:ARG:CA	1:B:259:PHE:CG[2_656]	1.63	0.57
1:B:81:ASP:C	1:B:83:PRO:N[2_656]	1.63	0.57
1:B:216:LYS:N	1:B:218:ARG:N[2_655]	1.63	0.57
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: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:A:287:TYR:CE2	1:B:20:SER:OG[2_656]	1.64	0.56
1:B:78:ILE:CD1	2:A:636:HOH:O[2_656]	1.64	0.56
1:A:295:ARG:NH2	1:B:337:VAL:CA[2_656]	1.64	0.56
1:B:345:ARG:O	2:B:574:HOH:O[2_656]	1.64	0.56
1:B:260:ILE:C	2:A:649:HOH:O[2_656]	1.64	0.56
1:A:293:GLU:CA	1:B:257:GLY:CA[2_656]	1.64	0.56
1:A:209:ILE:CG2	1:B:44:ALA:CB[2_656]	1.64	0.56
1:A:289:ALA:CB	1:B:45:VAL:CG1[2_656]	1.64	0.56
1:A:324:ALA:C	1:B:337:VAL:CG2[2_656]	1.65	0.55
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: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:323:ARG:CG	1:B:29:PHE:N[2_656]	1.65	0.55
1:B:21:SER:CA	2:A:519:HOH:O[2_656]	1.65	0.55
1:B:27:PRO:N	2:A:602:HOH:O[2_656]	1.66	0.54
1:A:316:ALA:CA	1:B:25:THR:CA[2_656]	1.66	0.54
1:B:347:TRP:C	2:B:472:HOH:O[2_656]	1.66	0.54
1:A:293:GLU:CD	2:B:573:HOH:O[2_656]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:O	1:B:259:PHE:C[2_656]	1.66	0.54
1:B:218:ARG:NE	1:B:221:LEU:CA[2_655]	1.66	0.54
1:A:300:PHE:CG	1:B:43:ASP:OD1[2_656]	1.67	0.53
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:328:VAL:CA	1:B:35:GLU:CA[2_656]	1.67	0.53
1:A:316:ALA:CB	1:B:25:THR:CG2[2_656]	1.68	0.52
1:B:348:LEU:O	2:B:541:HOH:O[2_656]	1.68	0.52
1:A:320:ARG:N	1:B:23:PRO:C[2_656]	1.68	0.52
1:A:295:ARG:CD	1:B:338:HIS:N[2_656]	1.68	0.52
1:B:81:ASP:CA	1:B:83:PRO:CA[2_656]	1.68	0.52
1:A:317:PHE:O	1:B:23:PRO:C[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:291:GLU:N	1:B:258:TYR:CD2[2_656]	1.69	0.51
1:B:31:PRO:CG	2:B:449:HOH:O[2_656]	1.69	0.51
1:A:321:LEU:CD2	1:B:42:LEU:O[2_656]	1.69	0.51
1:A:290:SER:O	1:B:258:TYR:N[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:CB	1:B:47:ALA:N[2_656]	1.70	0.50
1:A:320:ARG:CZ	1:B:21:SER:C[2_656]	1.70	0.50
1:A:288:PHE:CG	1:B:20:SER:CA[2_656]	1.70	0.50
1:A:319:ARG:C	1:B:23:PRO:O[2_656]	1.70	0.50
1:B:220:ARG:CB	2:B:473:HOH:O[2_655]	1.71	0.49
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:A:213:LEU:CD2	1:B:46:ALA:N[2_656]	1.71	0.49
1:A:299:PRO:CA	1:B:39:THR:CB[2_656]	1.71	0.49
1:A:290:SER:O	1:B:258:TYR:CD1[2_656]	1.71	0.49
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:294:LEU:N	1:B:259:PHE:N[2_656]	1.72	0.48
1:A:217:ARG:C	1:B:49:PRO:CB[2_656]	1.72	0.48
1:B:216:LYS:CD	1:B:217:ARG:CD[2_655]	1.72	0.48
1:B:255:ASN:N	2:A:469:HOH:O[2_656]	1.72	0.48
1:A:295:ARG:N	1:B:258:TYR:C[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:A:298:PRO:C	1:B:40:PHE:CA[2_656]	1.73	0.47
1:A:294:LEU:CD1	1:B:23:PRO:CG[2_656]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:OD1	1:B:347:TRP:CE3[2_656]	1.73	0.47
1:A:294:LEU:CD2	1:B:44:ALA:O[2_656]	1.73	0.47
1:A:293:GLU:CA	1:B:257:GLY:C[2_656]	1.73	0.47
1:A:316:ALA:CB	1:B:25:THR:CA[2_656]	1.73	0.47
1:A:291:GLU:OE1	1:B:307:LEU:CB[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: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:298:PRO:N	1:B:42:LEU:CD1[2_656]	1.73	0.47
1:A:293:GLU:CB	1:B:257:GLY:N[2_656]	1.74	0.46
1:A:299:PRO:C	1:B:38:ALA:O[2_656]	1.74	0.46
1:B:347:TRP:CA	1:B:349:PRO:CD[2_656]	1.74	0.46
1:A:299:PRO:C	1:B:38:ALA:C[2_656]	1.74	0.46
1:A:297:LEU:CD1	1:B:42:LEU:CD2[2_656]	1.74	0.46
1:A:288:PHE:CE1	1:B:20:SER:N[2_656]	1.74	0.46
1:B:347:TRP:CG	2:B:418:HOH:O[2_656]	1.75	0.45
1:A:316:ALA:N	1:B:24:ARG:O[2_656]	1.75	0.45
1:A:291:GLU:O	1:B:258:TYR:C[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
2:A:387:HOH:O	2:B:568:HOH:O[2_656]	1.75	0.45
1:A:320:ARG:CB	1:B:23:PRO:CA[2_656]	1.76	0.44
1:A:291:GLU:O	1:B:258:TYR:O[2_656]	1.76	0.44
1:A:326:VAL:C	1:B:36:ALA:C[2_656]	1.76	0.44
1:A:328:VAL:CG2	1:B:35:GLU:N[2_656]	1.76	0.44
1:A:327:ASP:OD2	1:B:347:TRP:CH2[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:A:216:LYS:NZ	1:B:259:PHE:O[2_656]	1.76	0.44
1:B:215:ALA:N	1:B:219:GLY:N[2_655]	1.76	0.44
1:B:33:MET:CA	2:A:596:HOH:O[2_656]	1.76	0.44
1:B:346:HIS:CA	2:B:542:HOH:O[2_656]	1.76	0.44
1:A:289:ALA:CA	1:B:45:VAL:CG2[2_656]	1.76	0.44
1:B:346:HIS:CG	2:B:560:HOH:O[2_656]	1.76	0.44
1:B:344:PHE:CE2	2:A:436:HOH:O[2_656]	1.76	0.44
1:B:81:ASP:CG	1:B:83:PRO:CB[2_656]	1.77	0.43
1:A:295:ARG:CD	2:B:381:HOH:O[2_656]	1.77	0.43
1:A:288:PHE:CD1	1:B:20:SER:CA[2_656]	1.77	0.43
1:A:322:ALA:C	1:B:33:MET:CB[2_656]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:CB	1:B:22:GLY:O[2_656]	1.77	0.43
1:A:291:GLU:OE1	1:B:307:LEU:CG[2_656]	1.77	0.43
1:A:327:ASP:C	1:B:36:ALA:N[2_656]	1.77	0.43
1:A:302:VAL:CB	1:B:24:ARG:CZ[2_656]	1.78	0.42
1:B:214:LEU:CA	1:B:216:LYS:O[2_655]	1.78	0.42
1:B:255:ASN:C	2:A:469:HOH:O[2_656]	1.78	0.42
1:B:216:LYS:CE	1:B:217:ARG:CD[2_655]	1.78	0.42
1:A:299:PRO:CG	1:B:39:THR:CB[2_656]	1.78	0.42
1:A:216:LYS:CE	1:B:259:PHE:O[2_656]	1.78	0.42
1:B:15:ARG:NE	2:A:490:HOH:O[2_656]	1.78	0.42
1:A:321:LEU:CD2	1:B:43:ASP:N[2_656]	1.78	0.42
1:A:300:PHE:CE1	1:B:41:GLY:CA[2_656]	1.79	0.41
1:B:216:LYS:CD	2:B:603:HOH:O[2_655]	1.79	0.41
1:B:77:SER:N	2:A:609:HOH:O[2_656]	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:B:31:PRO:CG	1:B:335:GLY:CA[2_656]	1.81	0.39
1:A:299:PRO:CB	1:B:39:THR:C[2_656]	1.81	0.39
1:A:291:GLU:CG	1:B:258:TYR:CE2[2_656]	1.81	0.39
2:B:407:HOH:O	2:B:442:HOH:O[2_656]	1.81	0.39
1:B:221:LEU:CD1	2:B:496:HOH:O[2_655]	1.81	0.39
1:A:293:GLU:C	1:B:257:GLY:C[2_656]	1.81	0.39
1:B:349:PRO:C	2:B:541:HOH:O[2_656]	1.81	0.39
1:A:318:ALA:CB	1:B:24:ARG:NH1[2_656]	1.81	0.39
1:A:294:LEU:N	1:B:257:GLY:C[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:A:218:ARG:NE	1:B:50:PRO:CB[2_656]	1.81	0.39
1:A:320:ARG:C	1:B:23:PRO:CA[2_656]	1.82	0.38
1:A:297:LEU:C	1:B:42:LEU:CG[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:324:ALA:C	1:B:337:VAL:CB[2_656]	1.82	0.38
1:A:217:ARG:NE	1:B:48:ALA:CB[2_656]	1.82	0.38
1:A:280:GLU:OE1	1:B:19:GLU:OE1[2_656]	1.83	0.37
1:B:215:ALA:C	1:B:218:ARG:CB[2_655]	1.83	0.37
1:B:30:SER:N	2:A:393:HOH:O[2_656]	1.83	0.37
1:A:318:ALA:O	1:B:34:VAL:CG1[2_656]	1.83	0.37
1:A:298:PRO:CG	1:B:40:PHE:O[2_656]	1.83	0.37
1:B:344:PHE:CZ	2:A:564:HOH:O[2_656]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:505:HOH:O	2:B:462: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:A:219:GLY:O	1:B:67:SER:N[2_656]	1.83	0.37
1:A:300:PHE:CD1	1:B:41:GLY:C[2_656]	1.83	0.37
1:A:322:ALA:CB	1:B:30:SER:O[2_656]	1.83	0.37
1:A:327:ASP:OD1	1:B:347:TRP:CD2[2_656]	1.84	0.36
1:B:32:ALA:CB	2:B:494:HOH:O[2_656]	1.84	0.36
1:A:320:ARG:CZ	1:B:22:GLY:CA[2_656]	1.84	0.36
1:A:299:PRO:N	1:B:39:THR:C[2_656]	1.84	0.36
1:A:213:LEU:CD1	1:B:45:VAL:C[2_656]	1.84	0.36
1:B:347:TRP:C	1:B:347:TRP:O[2_656]	1.84	0.36
1:B:217:ARG:N	1:B:217:ARG:CB[2_655]	1.84	0.36
1:A:295:ARG:C	1:B:259:PHE:CD2[2_656]	1.84	0.36
1:A:294:LEU:N	1:B:258:TYR:C[2_656]	1.84	0.36
1:A:327:ASP:CB	1:B:36:ALA:CA[2_656]	1.84	0.36
1:B:348:LEU:CB	2:B:472:HOH:O[2_656]	1.84	0.36
1:A:292:ASP:CG	1:B:309:PRO:CA[2_656]	1.85	0.35
1:B:214:LEU:O	1:B:218:ARG:N[2_655]	1.85	0.35
1:A:296:GLY:C	1:B:259:PHE:CD1[2_656]	1.85	0.35
1:A:218:ARG:NE	1:B:50:PRO:CG[2_656]	1.85	0.35
1:A:217:ARG:CZ	1:B:48:ALA:CB[2_656]	1.85	0.35
1:A:300:PHE:CE2	1:B:43:ASP:OD1[2_656]	1.85	0.35
1:A:295:ARG:N	1:B:258:TYR:O[2_656]	1.86	0.34
1:A:328:VAL:CA	1:B:35:GLU:C[2_656]	1.86	0.34
1:A:317:PHE:CA	1:B:24:ARG:N[2_656]	1.86	0.34
1:A:295:ARG:CD	1:B:338:HIS:CB[2_656]	1.86	0.34
1:B:350:ALA:O	2:B:527:HOH: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:213:LEU:O	1:B:47:ALA:O[2_656]	1.86	0.34
1:A:320:ARG:CA	1:B:23:PRO:CA[2_656]	1.86	0.34
1:A:317:PHE:N	1:B:25:THR:N[2_656]	1.86	0.34
1:A:289:ALA:O	1:B:21:SER:O[2_656]	1.87	0.33
1:A:295:ARG:CA	1:B:259:PHE:CA[2_656]	1.87	0.33
1:A:292:ASP:C	1:B:260:ILE:O[2_656]	1.87	0.33
1:A:321:LEU:CG	1:B:43:ASP:CB[2_656]	1.87	0.33
1:A:319:ARG:O	1:B:29: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:B:77:SER:OG	2:A:511:HOH: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ALA:CA	1:B:33:MET:C[2_656]	1.87	0.33
1:A:325:GLY:N	1:B:33:MET:SD[2_656]	1.88	0.32
1:A:321:LEU:CD1	1:B:43:ASP:CG[2_656]	1.88	0.32
1:B:218:ARG:CZ	1:B:221:LEU:N[2_655]	1.88	0.32
1:A:318:ALA:O	1:B:34:VAL: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:217:ARG:O	1:B:49:PRO:CB[2_656]	1.88	0.32
1:B:335:GLY:O	2:A:575:HOH:O[2_656]	1.88	0.32
1:A:328:VAL:CA	1:B:34:VAL:O[2_656]	1.89	0.31
1:B:215:ALA:CA	1:B:218:ARG:CB[2_655]	1.89	0.31
1:B:214:LEU:CG	2:B:519:HOH:O[2_655]	1.89	0.31
1:A:290:SER:CB	1:B:256:ASP:N[2_656]	1.89	0.31
1:B:27:PRO:O	1:B:27:PRO:O[2_656]	1.89	0.31
1:A:292:ASP:CB	1:B:309:PRO:CG[2_656]	1.89	0.31
1:A:326:VAL:O	1:B:37:LEU:N[2_656]	1.89	0.31
1:B:215:ALA:N	1:B:218:ARG:N[2_655]	1.89	0.31
1:A:291:GLU:C	1:B:258:TYR:CG[2_656]	1.89	0.31
1:B:215:ALA:C	1:B:217:ARG:C[2_655]	1.89	0.31
1:B:81:ASP:CB	1:B:83:PRO:C[2_656]	1.89	0.31
1:A:300:PHE:N	1:B:38:ALA:CA[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:B:29:PHE:N	2:B:478:HOH:O[2_656]	1.89	0.31
1:B:28:ARG:C	2:B:508:HOH:O[2_656]	1.89	0.31
1:A:327:ASP:CA	1:B:36:ALA: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:302:VAL:CB	1:B:24:ARG:NE[2_656]	1.90	0.30
1:A:290:SER:N	1:B:256:ASP:O[2_656]	1.90	0.30
1:A:298:PRO:CB	1:B:40:PHE:CD2[2_656]	1.90	0.30
1:A:328:VAL:O	1:B:35:GLU:N[2_656]	1.90	0.30
1:A:293:GLU:CA	1:B:260:ILE:O[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:B:218:ARG:CD	1:B:220:ARG:N[2_655]	1.91	0.29
1:A:321:LEU:N	1:B:23:PRO:CA[2_656]	1.91	0.29
1:B:35:GLU:CG	1:B:350:ALA:CB[2_656]	1.91	0.29
1:B:31:PRO:C	2:A:421:HOH:O[2_656]	1.91	0.29
1:A:325:GLY:N	1:B:33:MET:CE[2_656]	1.92	0.28
1:A:293:GLU:CB	1:B:257:GLY:C[2_656]	1.92	0.28
1:A:288:PHE:CB	1:B:19:GLU:O[2_656]	1.92	0.28
1:A:327:ASP:C	1:B:36:ALA:CA[2_656]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:C	1:B:218:ARG:CG[2_655]	1.93	0.27
1:A:292:ASP:CG	1:B:309:PRO:CB[2_656]	1.93	0.27
2:B:407:HOH:O	2:B:508:HOH:O[2_656]	1.93	0.27
1:A:291:GLU:N	1:B:258:TYR:CE1[2_656]	1.93	0.27
1:B:218:ARG:NE	1:B:220:ARG:C[2_655]	1.93	0.27
1:B:20:SER:C	2:A:519:HOH:O[2_656]	1.93	0.27
1:A:317:PHE:CE1	2:B:421:HOH:O[2_656]	1.93	0.27
1:A:292:ASP:OD1	1:B:308:ASP:C[2_656]	1.93	0.27
1:A:325:GLY:CA	1:B:33:MET:SD[2_656]	1.94	0.26
1:B:63:ALA:O	2:A:540:HOH:O[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: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:222:ASP:OD1	1:B:70:GLY:N[2_656]	1.94	0.26
1:A:317:PHE:C	1:B:24:ARG:CG[2_656]	1.94	0.26
1:B:347:TRP:CZ2	2:A:491:HOH:O[2_656]	1.94	0.26
1:A:298:PRO:CG	1:B:40:PHE:CB[2_656]	1.95	0.25
1:B:29:PHE:O	2:B:478:HOH:O[2_656]	1.95	0.25
1:A:292:ASP:OD1	1:B:309:PRO:CG[2_656]	1.95	0.25
1:A:299:PRO:N	1:B:40:PHE:CA[2_656]	1.95	0.25
1:A:292:ASP:CB	1:B:309:PRO:CD[2_656]	1.95	0.25
1:B:254:GLU:O	2:A:527:HOH:O[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:A:288:PHE:CD2	1:B:20:SER:CB[2_656]	1.95	0.25
1:A:321:LEU:CD2	1:B:42:LEU:C[2_656]	1.95	0.25
1:A:298:PRO:O	1:B:37:LEU: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:B:349:PRO:O	2:B:541: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: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:77:SER:OG	2:A:609:HOH:O[2_656]	1.97	0.23
1:A:288:PHE:CE2	1:B:20:SER:CB[2_656]	1.97	0.23
1:B:292:ASP:CG	2:B:557:HOH:O[2_655]	1.97	0.23
1:A:290:SER:OG	1:B:255:ASN:C[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:A:298:PRO:N	1:B:40:PHE:CB[2_656]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:CZ	1:B:26:ASP:O[2_656]	1.97	0.23
1:A:290:SER:CB	1:B:256:ASP:O[2_656]	1.97	0.23
1:B:215:ALA:N	1:B:217:ARG:C[2_655]	1.97	0.23
1:A:319:ARG:CG	2:B:442:HOH:O[2_656]	1.97	0.23
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:A:291:GLU:CB	1:B:258:TYR:CG[2_656]	1.98	0.22
1:B:282:PRO:CD	2:B:575:HOH:O[2_655]	1.98	0.22
1:B:80:LEU:O	1:B:83:PRO:CG[2_656]	1.98	0.22
1:A:294:LEU:N	1:B:258:TYR:N[2_656]	1.98	0.22
1:B:35:GLU:OE2	1:B:351:ALA:CA[2_656]	1.98	0.22
1:A:291:GLU:CA	1:B:258:TYR:CD1[2_656]	1.98	0.22
1:A:302:VAL:CG2	1:B:24:ARG:CZ[2_656]	1.98	0.22
1:A:299:PRO:O	1:B:39:THR:O[2_656]	1.98	0.22
1:B:261:GLU:CB	2:A:621:HOH:O[2_656]	1.98	0.22
1:A:290:SER:C	1:B:258:TYR:CE1[2_656]	1.98	0.22
1:A:297:LEU:N	1:B:259:PHE:CD1[2_656]	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:346:HIS:CD2	2:B:560:HOH:O[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:31:PRO:CB	2:A:421:HOH:O[2_656]	2.00	0.20
1:A:324:ALA:N	1:B:337:VAL:CG1[2_656]	2.00	0.20
1:A:316:ALA:O	1:B:25:THR:CA[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
1:A:317:PHE:CE2	1:B:44:ALA:N[2_656]	2.00	0.20
2:B:467:HOH:O	2:B:590:HOH:O[2_656]	2.00	0.20
1:A:283:ILE:CD1	1:B:47:ALA:CB[2_656]	2.00	0.20
1:A:217:ARG:CZ	1:B:48:ALA: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:327:ASP:CA	1:B:36:ALA:CB[2_656]	2.01	0.19
1:A:218:ARG:NE	1:B:50:PRO:N[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:B:214:LEU:O	1:B:216:LYS:O[2_655]	2.01	0.19
1:B:261:GLU:CB	2:A:649:HOH:O[2_656]	2.01	0.19
1:A:317:PHE:N	1:B:24:ARG:CA[2_656]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:CG	1:B:48:ALA:C[2_656]	2.01	0.19
1:A:291:GLU:C	1:B:258:TYR:CA[2_656]	2.02	0.18
1:A:323:ARG:NH2	1:B:26:ASP:CA[2_656]	2.02	0.18
1:B:348:LEU:O	2:B:590:HOH:O[2_656]	2.02	0.18
1:B:35:GLU:OE2	1:B:350:ALA:CA[2_656]	2.02	0.18
1:A:320:ARG:CA	1:B:23:PRO:O[2_656]	2.02	0.18
1:A:293:GLU:N	1:B:257:GLY:C[2_656]	2.02	0.18
1:A:300:PHE:C	1:B:38:ALA:CB[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:CD1	1:B:41:GLY:CA[2_656]	2.03	0.17
1:B:256:ASP:O	2:A:433:HOH:O[2_656]	2.03	0.17
1:A:328:VAL:CA	1:B:35:GLU: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:369:LEU:O	1:B:77:SER: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:40:PHE:CZ	2:A:432:HOH:O[2_656]	2.03	0.17
1:A:290:SER:C	1:B:258:TYR:CG[2_656]	2.04	0.16
1:A:222:ASP:N	1:B:70:GLY:CA[2_656]	2.04	0.16
1:A:292:ASP:CA	1:B:255:ASN:O[2_656]	2.04	0.16
1:B:178:LEU:CD2	1:B:218:ARG:O[2_655]	2.04	0.16
1:B:81:ASP:CG	1:B:83:PRO: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:347:TRP:CD1	1:B:350:ALA:N[2_656]	2.05	0.15
1:A:324:ALA:CA	1:B:337:VAL:CB[2_656]	2.05	0.15
1:B:216:LYS:CG	2:B:603:HOH:O[2_655]	2.05	0.15
1:B:26:ASP:C	2:A:515:HOH:O[2_656]	2.05	0.15
1:A:298:PRO:O	1:B:40:PHE:N[2_656]	2.05	0.15
1:A:324:ALA:N	1:B:29:PHE:CE2[2_656]	2.05	0.15
1:A:320:ARG:C	1:B:23:PRO:CB[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:344:PHE:CD2	2:A:564: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: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:326:VAL:N	1:B:37:LEU:CG[2_656]	2.07	0.13
1:B:66:ALA:CB	2:A:540:HOH:O[2_656]	2.07	0.13
1:A:300:PHE:C	1:B:38:ALA: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:288:PHE:CG	1:B:20:SER:N[2_656]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:CG1	1:B:37:LEU:O[2_656]	2.07	0.13
1:B:70:GLY:CA	2:A:633:HOH:O[2_656]	2.07	0.13
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:295:ARG:O	1:B:259:PHE:CD1[2_656]	2.08	0.12
1:A:214:LEU:N	1:B:47:ALA:CB[2_656]	2.08	0.12
1:B:346:HIS:NE2	1:B:349:PRO:CB[2_656]	2.08	0.12
1:A:302:VAL:CB	1:B:24:ARG:NH2[2_656]	2.08	0.12
1:A:217:ARG:CG	1:B:48:ALA:N[2_656]	2.08	0.12
1:A:320:ARG:NH1	1:B:21:SER:O[2_656]	2.08	0.12
1:A:316:ALA:CA	1:B:25:THR:N[2_656]	2.08	0.12
1:A:325:GLY:O	1:B:344:PHE:CD2[2_656]	2.08	0.12
1:A:324:ALA:O	1:B:337:VAL:CG1[2_656]	2.08	0.12
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:320:ARG:NH2	1:B:21:SER:CA[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:213:LEU:CD2	1:B:45:VAL:C[2_656]	2.09	0.11
1:B:350:ALA:N	2:B:527:HOH:O[2_656]	2.09	0.11
1:B:346:HIS:ND1	2:B:560:HOH:O[2_656]	2.09	0.11
1:A:218:ARG:CZ	1:B:50:PRO:CB[2_656]	2.09	0.11
1:A:320:ARG:NH2	1:B:25:THR:OG1[2_656]	2.10	0.10
1:B:348:LEU:CB	2:B:590:HOH: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: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
1:A:296:GLY:O	1:B:259:PHE:CE1[2_656]	2.10	0.10
1:A:292:ASP:CB	1:B:255:ASN:O[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:A:316:ALA:O	1:B:24:ARG:O[2_656]	2.10	0.10
1:A:295:ARG:C	1:B:259:PHE:CA[2_656]	2.11	0.09
1:B:349:PRO:N	2:B:574:HOH:O[2_656]	2.11	0.09
1:B:81:ASP:C	1:B:83:PRO:CG[2_656]	2.11	0.09
1:A:297:LEU:N	1:B:42:LEU:CD1[2_656]	2.11	0.09
1:A:289:ALA:N	1:B:15:ARG:NH1[2_656]	2.11	0.09
1:A:302:VAL:CG2	1:B:24:ARG:NH2[2_656]	2.11	0.09
1:A:297:LEU:CB	1:B:42:LEU:CD1[2_656]	2.11	0.09
1:B:30:SER:N	1:B:30:SER:CA[2_656]	2.11	0.09
1:A:320:ARG:NH2	1:B:21:SER:C[2_656]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:OE2	2:B:573: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:326:VAL:CA	1:B:37:LEU:N[2_656]	2.12	0.08
1:A:289:ALA:CA	1:B:45:VAL:CG1[2_656]	2.12	0.08
1:A:288:PHE:N	1:B:20:SER:O[2_656]	2.12	0.08
1:B:35:GLU:OE1	1:B:351:ALA: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:294:LEU:O	1:B:259:PHE:CB[2_656]	2.12	0.08
1:B:70:GLY:N	2:A:633:HOH:O[2_656]	2.12	0.08
1:B:218:ARG:CG	1:B:221:LEU:N[2_655]	2.12	0.08
1:A:327:ASP:O	1:B:36:ALA:O[2_656]	2.12	0.08
1:B:261:GLU:C	2:A:649:HOH: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:295:ARG:O	1:B:259:PHE:CA[2_656]	2.13	0.07
1:A:294:LEU:CD2	2:B:417:HOH:O[2_656]	2.13	0.07
1:A:288:PHE:CD1	1:B:19:GLU:O[2_656]	2.13	0.07
1:A:287:TYR:C	1:B:20:SER:C[2_656]	2.13	0.07
1:A:317:PHE:CZ	1:B:43:ASP:C[2_656]	2.13	0.07
1:B:218:ARG:CD	1:B:220:ARG:O[2_655]	2.13	0.07
1:A:328:VAL:C	1:B:35:GLU:CB[2_656]	2.13	0.07
1:A:320:ARG:NE	1:B:22:GLY:N[2_656]	2.13	0.07
1:A:300:PHE:CB	1:B:38:ALA:C[2_656]	2.13	0.07
1:A:294:LEU:CD2	1:B:44:ALA: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:323:ARG:CZ	1:B:26:ASP:OD1[2_656]	2.14	0.06
1:A:319:ARG:C	1:B:29:PHE:CB[2_656]	2.14	0.06
1:A:300:PHE:C	1:B:38:ALA:C[2_656]	2.14	0.06
1:A:327:ASP:O	1:B:39:THR:N[2_656]	2.14	0.06
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:296:GLY:N	1:B:259:PHE:CE2[2_656]	2.14	0.06
1:A:293:GLU:CD	1:B:261:GLU:CG[2_656]	2.14	0.06
1:A:327:ASP:OD1	1:B:36:ALA:CB[2_656]	2.14	0.06
1:B:347:TRP:CG	1:B:349:PRO:CG[2_656]	2.15	0.05
1:B:344:PHE:CE2	2:A:428: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:319:ARG:CB	2:B:442:HOH:O[2_656]	2.15	0.05
1:A:327:ASP:CB	1:B:36:ALA:C[2_656]	2.15	0.05
1:A:317:PHE:CB	2:B:421:HOH:O[2_656]	2.15	0.05
1:A:217:ARG:C	1:B:49:PRO:CG[2_656]	2.15	0.05
1:A:325:GLY:O	1:B:344:PHE:CG[2_656]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:C	1:B:216:LYS:O[2_655]	2.16	0.04
1:B:35:GLU:CD	1:B:350:ALA:C[2_656]	2.16	0.04
1:A:293:GLU:CG	1:B:257:GLY:CA[2_656]	2.16	0.04
1:B:214:LEU:C	1:B:217:ARG:O[2_655]	2.16	0.04
1:A:327:ASP:CG	1:B:347:TRP:CE3[2_656]	2.16	0.04
1:A:320:ARG:CZ	1:B:22:GLY:O[2_656]	2.16	0.04
1:B:25:THR:O	2:A:541:HOH: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:213:LEU:C	1:B:47:ALA:CB[2_656]	2.16	0.04
1:A:298:PRO:CB	1:B:40:PHE:CA[2_656]	2.17	0.03
1:B:213:LEU:C	1:B:217:ARG:O[2_655]	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:317:PHE:N	1:B:24:ARG:O[2_656]	2.17	0.03
1:A:323:ARG:CD	1:B:28:ARG:O[2_656]	2.17	0.03
1:A:297:LEU:CG	1:B:42:LEU:CG[2_656]	2.17	0.03
1:B:35:GLU:OE2	1:B:350:ALA:O[2_656]	2.17	0.03
1:A:299:PRO:N	1:B:40:PHE:CB[2_656]	2.17	0.03
1:A:327:ASP:O	1:B:36:ALA:C[2_656]	2.17	0.03
1:A:294:LEU:C	1:B:258:TYR: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:295:ARG:N	1:B:259:PHE:C[2_656]	2.18	0.02
1:A:292:ASP:O	1:B:260:ILE:C[2_656]	2.18	0.02
1:A:328:VAL:O	1:B:35:GLU:CG[2_656]	2.18	0.02
1:B:264:GLY:CA	2:A:502:HOH:O[2_656]	2.18	0.02
1:A:294:LEU:O	1:B:259:PHE:N[2_656]	2.18	0.02
1:A:320:ARG:CA	1:B:23:PRO:C[2_656]	2.18	0.02
1:A:288:PHE:CA	1:B:20:SER:CA[2_656]	2.18	0.02
1:B:344:PHE:CE1	2:A:404:HOH:O[2_656]	2.19	0.01
1:A:320:ARG:CA	1:B:29:PHE:CD1[2_656]	2.19	0.01
1:B:31:PRO:CB	2:B:449:HOH:O[2_656]	2.19	0.01
1:A:320:ARG:NH1	1:B:22:GLY:C[2_656]	2.19	0.01
1:B:27:PRO:O	2:B:478:HOH:O[2_656]	2.19	0.01
1:A:299:PRO:N	1:B:40:PHE:CG[2_656]	2.19	0.01
1:A:292:ASP:N	1:B:258:TYR:CB[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%)	41	26
All	All	715/722 (99%)	685 (96%)	29 (4%)	1 (0%)	51	36

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%)	254 (92%)	21 (8%)	13	3
1	B	278/278 (100%)	257 (92%)	21 (8%)	13	3
All	All	553/556 (100%)	511 (92%)	42 (8%)	13	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	99	VAL

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Mol	Chain	Res	Type
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	244	ARG
1	A	246	LEU
1	A	295	ARG
1	A	297	LEU
1	A	304	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	97	LEU
1	B	118	LEU
1	B	165	GLU
1	B	171	PRO
1	B	174	VAL
1	B	199	GLN
1	B	214	LEU
1	B	221	LEU
1	B	243	GLU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN

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Mol	Chain	Res	Type
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

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 carbohydrates 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.