



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:16 am GMT

PDB ID : 3GQB  
Title : Crystal Structure of the A3B3 complex from V-ATPase  
Authors : Meher, M.; Akimoto, S.; Iwata, M.; Nagata, K.; Hori, Y.; Yoshida, M.;  
Yokoyama, S.; Iwata, S.; Yokoyama, K.  
Deposited on : 2009-03-24  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

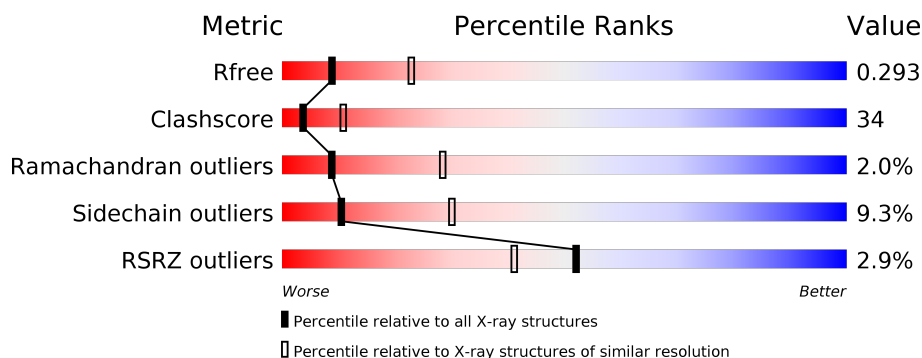
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	578	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>41%</div> <div>7%</div> </div> </div>
1	C	578	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>44%</div> <div>7%</div> </div> </div>
2	B	464	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>6%</div> </div> </div>
2	D	464	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16863 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4477	2856	763	839	19			
1	C	578	Total	C	N	O	S	0	0	0
			4477	2856	763	839	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	CYS	ENGINEERED	UNP Q56403
A	235	SER	THR	ENGINEERED	UNP Q56403
A	255	SER	CYS	ENGINEERED	UNP Q56403
A	507	SER	CYS	ENGINEERED	UNP Q56403
C	28	SER	CYS	ENGINEERED	UNP Q56403
C	235	SER	THR	ENGINEERED	UNP Q56403
C	255	SER	CYS	ENGINEERED	UNP Q56403
C	507	SER	CYS	ENGINEERED	UNP Q56403

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	460	Total	C	N	O	S	0	0	0
			3601	2280	623	689	9			
2	D	460	Total	C	N	O	S	0	0	0
			3601	2280	623	689	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	SER	CYS	ENGINEERED	UNP Q56404
D	264	SER	CYS	ENGINEERED	UNP Q56404

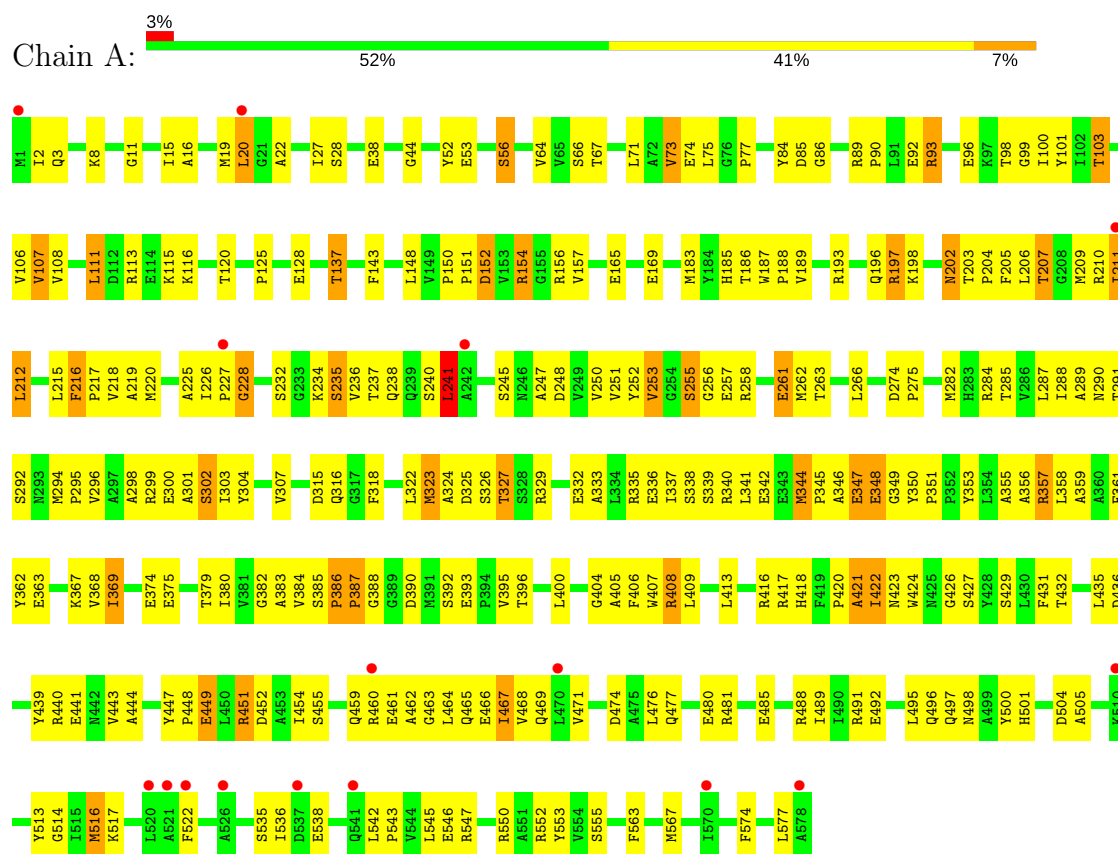
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total 199	O 199	0	0
3	B	135	Total 135	O 135	0	0
3	C	239	Total 239	O 239	0	0
3	D	134	Total 134	O 134	0	0

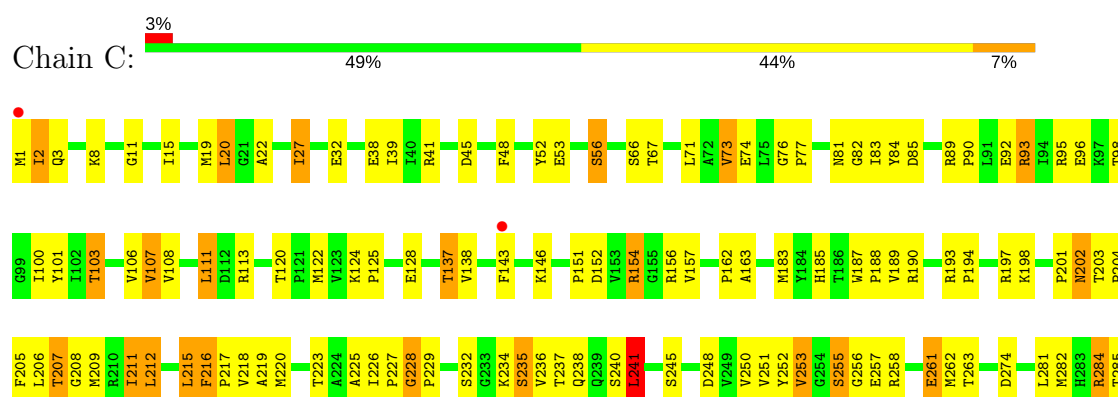
### 3 Residue-property plots

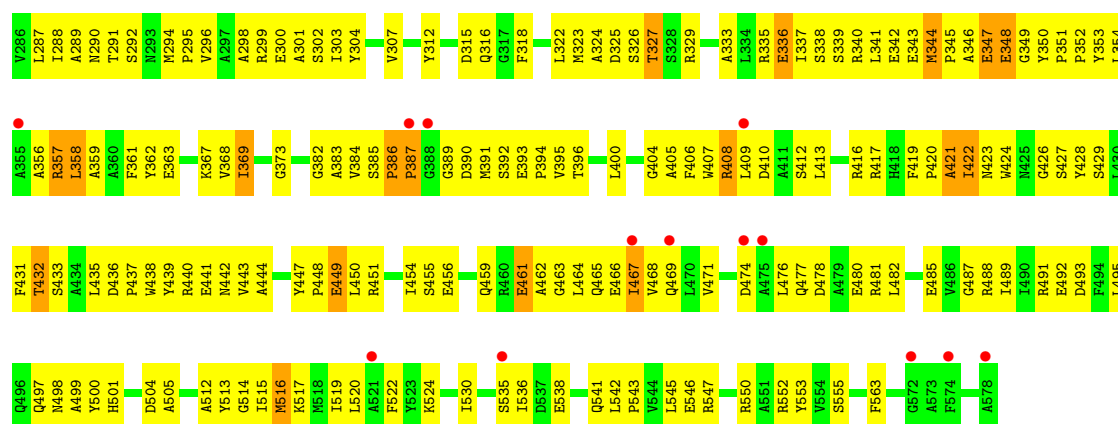
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: V-type ATP synthase alpha chain

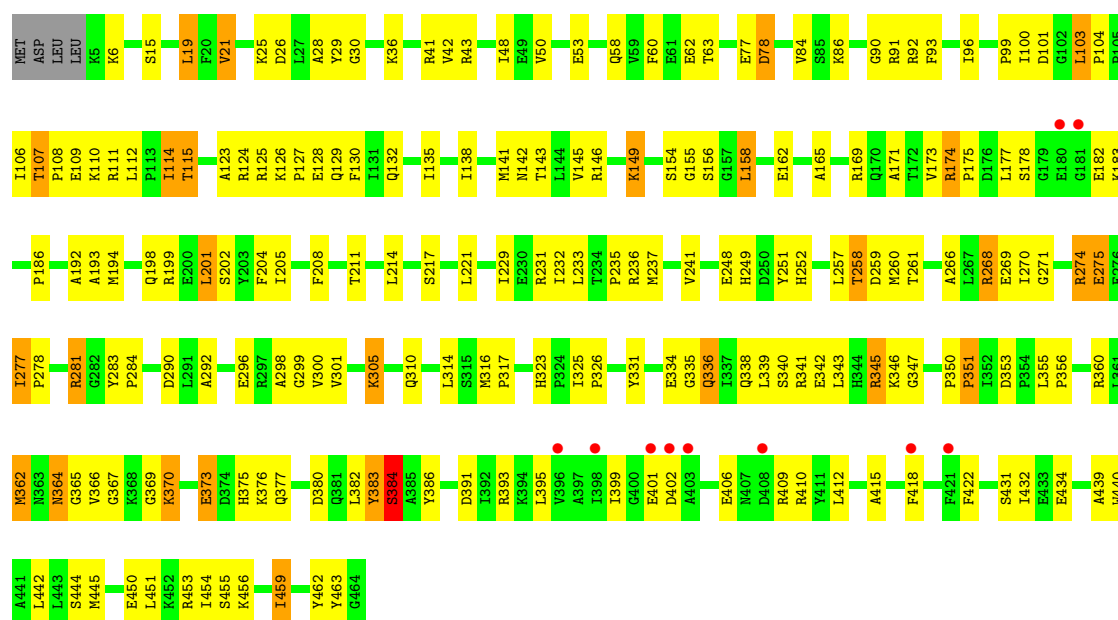


#### • Molecule 1: V-type ATP synthase alpha chain

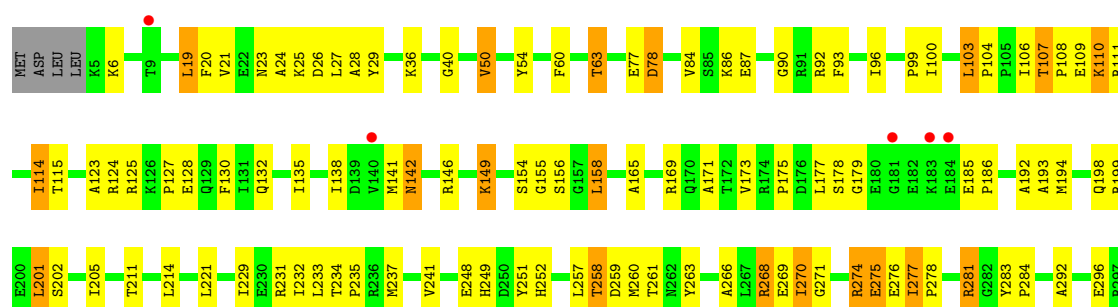


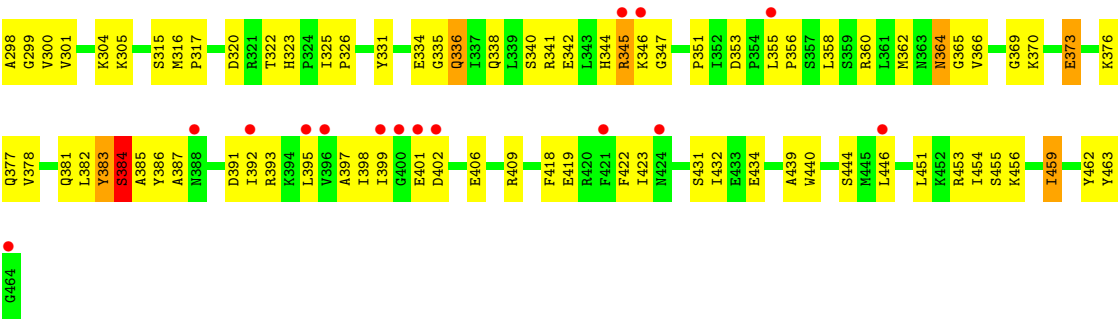


• Molecule 2: V-type ATP synthase beta chain



• Molecule 2: V-type ATP synthase beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.37Å 199.37Å 179.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.95-2.80) 97.7 (19.94-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.250 , 0.281 0.263 , 0.293	Depositor DCC
$R_{free}$ test set	4941 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 8.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
Reported twinning fraction	0.845 for 1.000H, 1.000K, L 0.155 for -1.000H, -1.000K, L	Depositor
Outliers	0 of 98400 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	16863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	0/4573	0.71	1/6203 (0.0%)
1	C	0.58	0/4573	0.72	2/6203 (0.0%)
2	B	0.54	0/3668	0.67	0/4965
2	D	0.50	0/3668	0.65	0/4965
All	All	0.55	0/16482	0.69	3/22336 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	241	LEU	CA-CB-CG	5.42	127.76	115.30
1	C	215	LEU	CA-CB-CG	-5.13	103.49	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4477	0	4494	367	0
1	C	4477	0	4494	374	1
2	B	3601	0	3627	193	1
2	D	3601	0	3627	197	0
3	A	199	0	0	120	1
3	B	135	0	0	60	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	239	0	0	135	0
3	D	134	0	0	70	0
All	All	16863	0	16242	1107	2

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 34.

All (1107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:O	1:A:329:ARG:HD2	1.24	1.32
1:A:574:PHE:HB3	3:A:697:HOH:O	1.33	1.29
1:A:447:TYR:HA	3:A:651:HOH:O	1.17	1.27
1:C:124:LYS:HD3	3:C:714:HOH:O	1.25	1.26
1:C:256:GLY:O	1:C:329:ARG:HD2	1.22	1.25
1:C:405:ALA:HA	3:C:773:HOH:O	1.38	1.23
2:B:106:ILE:HD11	3:B:559:HOH:O	1.41	1.21
1:C:443:VAL:HB	3:C:707:HOH:O	1.31	1.21
2:D:132:GLN:NE2	3:D:522:HOH:O	1.74	1.21
1:C:22:ALA:HA	3:C:681:HOH:O	1.41	1.21
1:C:89:ARG:HD2	3:C:667:HOH:O	1.37	1.19
2:D:386:TYR:HB3	3:D:687:HOH:O	1.41	1.18
1:C:255:SER:HB2	1:C:290:ASN:HB2	1.16	1.16
1:A:255:SER:HB2	1:A:290:ASN:HB2	1.17	1.15
1:C:93:ARG:HB3	3:C:651:HOH:O	1.44	1.15
1:C:546:GLU:HG3	3:C:654:HOH:O	1.46	1.14
2:D:125:ARG:HD2	3:D:515:HOH:O	1.45	1.14
1:C:255:SER:HB2	1:C:290:ASN:CB	1.80	1.11
2:B:456:LYS:HG2	3:B:465:HOH:O	1.49	1.11
1:A:250:VAL:HG12	3:A:603:HOH:O	1.47	1.11
2:B:351:PRO:HB2	3:B:501:HOH:O	1.49	1.10
2:D:356:PRO:HB3	3:D:518:HOH:O	1.52	1.10
2:D:232:ILE:HD11	2:D:270:ILE:HG13	1.30	1.09
1:A:380:ILE:HA	3:A:688:HOH:O	1.49	1.08
1:A:448:PRO:HB3	3:A:635:HOH:O	1.50	1.08
1:A:207:THR:HG21	1:A:212:LEU:HD12	1.25	1.08
1:A:255:SER:HB2	1:A:290:ASN:CB	1.84	1.07
1:A:335:ARG:HD2	3:A:623:HOH:O	1.52	1.07
1:A:357:ARG:CG	1:A:357:ARG:HH11	1.67	1.07
2:B:232:ILE:HD11	2:B:270:ILE:HG13	1.29	1.06
1:A:298:ALA:HB3	3:A:717:HOH:O	1.54	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:THR:HG21	1:C:212:LEU:HD12	1.29	1.06
1:C:447:TYR:HA	3:C:806:HOH:O	1.55	1.05
1:A:386:PRO:HD3	3:A:639:HOH:O	1.56	1.04
1:A:384:VAL:HG11	1:A:396:THR:OG1	1.58	1.04
1:C:256:GLY:O	1:C:329:ARG:CD	2.05	1.04
1:C:346:ALA:O	3:C:799:HOH:O	1.76	1.03
2:B:274:ARG:O	2:B:275:GLU:HG3	1.56	1.03
1:C:296:VAL:HG23	3:C:605:HOH:O	1.58	1.03
2:D:344:HIS:HE1	3:D:538:HOH:O	1.41	1.02
2:D:355:LEU:HD23	2:D:383:TYR:CE1	1.94	1.02
1:C:384:VAL:HG11	1:C:396:THR:OG1	1.60	1.02
1:A:322:LEU:HG	3:A:679:HOH:O	1.60	1.01
2:D:179:GLY:HA2	3:D:517:HOH:O	1.59	1.01
1:C:82:GLY:HA2	3:C:611:HOH:O	1.59	1.01
1:A:296:VAL:HG23	3:A:652:HOH:O	1.59	1.01
1:A:211:ILE:HG22	1:A:495:LEU:HD22	1.39	1.01
2:B:355:LEU:HD23	2:B:383:TYR:CE1	1.95	1.01
1:A:151:PRO:O	1:A:152:ASP:HB2	1.60	1.00
2:D:364:ASN:HB3	3:D:496:HOH:O	1.60	1.00
1:A:386:PRO:CD	3:A:639:HOH:O	2.08	1.00
1:C:151:PRO:O	1:C:152:ASP:HB2	1.61	1.00
2:B:41:ARG:HG2	3:B:510:HOH:O	1.59	1.00
1:C:419:PHE:CB	3:C:683:HOH:O	2.08	1.00
1:C:282:MET:HA	1:C:282:MET:HE2	1.43	1.00
1:C:362:TYR:HD1	3:C:666:HOH:O	1.44	1.00
1:C:211:ILE:HG22	1:C:495:LEU:HD22	1.45	0.99
2:D:274:ARG:O	2:D:275:GLU:HG3	1.62	0.99
1:A:211:ILE:CG2	1:A:495:LEU:HD22	1.92	0.99
2:B:342:GLU:HB2	3:B:532:HOH:O	1.59	0.99
2:D:271:GLY:HA2	3:D:465:HOH:O	1.63	0.98
2:B:442:LEU:HA	3:B:551:HOH:O	1.62	0.98
1:C:362:TYR:CD1	3:C:666:HOH:O	2.16	0.97
2:D:86:LYS:HG2	3:D:656:HOH:O	1.63	0.97
1:C:209:MET:CE	1:C:241:LEU:CD2	2.42	0.97
2:D:232:ILE:HG22	3:D:524:HOH:O	1.62	0.97
1:A:256:GLY:O	1:A:329:ARG:CD	2.12	0.97
2:B:278:PRO:HB3	3:B:473:HOH:O	1.64	0.97
2:B:146:ARG:HH11	2:B:252:HIS:CE1	1.83	0.96
1:C:255:SER:CB	1:C:290:ASN:HB2	1.96	0.95
1:A:255:SER:CB	1:A:290:ASN:HB2	1.97	0.94
1:C:298:ALA:HB3	3:C:596:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:PRO:HB3	3:D:468:HOH:O	1.65	0.94
1:C:357:ARG:HH11	1:C:357:ARG:HG2	1.29	0.94
2:B:393:ARG:HA	3:B:552:HOH:O	1.68	0.94
1:C:209:MET:HE1	1:C:241:LEU:CD2	1.98	0.93
1:A:294:MET:HB2	3:A:594:HOH:O	1.68	0.93
1:A:468:VAL:HG11	3:A:765:HOH:O	1.66	0.93
1:A:282:MET:HE1	1:A:285:THR:HB	1.50	0.93
1:C:357:ARG:HH11	1:C:357:ARG:CG	1.80	0.93
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.31	0.93
1:C:517:LYS:HD3	1:C:563:PHE:HZ	1.34	0.92
1:C:347:GLU:HA	3:C:622:HOH:O	1.70	0.92
2:B:106:ILE:CD1	3:B:559:HOH:O	2.01	0.92
1:A:517:LYS:HD3	1:A:563:PHE:HZ	1.34	0.91
1:C:209:MET:HE1	1:C:241:LEU:HD23	1.51	0.91
2:D:277:ILE:HG12	3:D:655:HOH:O	1.70	0.91
1:A:380:ILE:CA	3:A:688:HOH:O	2.11	0.91
1:C:353:TYR:HD1	3:C:616:HOH:O	1.53	0.91
1:C:209:MET:CE	1:C:241:LEU:HD22	2.00	0.91
3:A:650:HOH:O	2:B:126:LYS:HD2	1.71	0.90
1:A:423:ASN:HA	3:A:706:HOH:O	1.70	0.90
1:C:294:MET:HB2	3:C:588:HOH:O	1.72	0.90
1:C:466:GLU:HB3	3:C:744:HOH:O	1.72	0.90
1:C:299:ARG:CZ	3:C:649:HOH:O	2.20	0.90
1:C:209:MET:HE3	1:C:241:LEU:HD22	1.52	0.89
2:B:232:ILE:CD1	2:B:270:ILE:HG13	2.03	0.89
1:C:333:ALA:O	1:C:337:ILE:HD12	1.73	0.88
1:C:185:HIS:NE2	1:C:193:ARG:NH2	2.22	0.88
1:A:234:LYS:HB3	3:A:585:HOH:O	1.75	0.87
1:A:353:TYR:HD1	3:A:671:HOH:O	1.54	0.87
2:D:146:ARG:HH11	2:D:252:HIS:CE1	1.92	0.87
1:A:209:MET:CE	1:A:241:LEU:CD2	2.52	0.87
1:A:99:GLY:HA2	1:C:124:LYS:HZ1	1.39	0.87
1:C:354:LEU:HD23	3:C:694:HOH:O	1.73	0.87
1:A:215:LEU:HD21	3:A:647:HOH:O	1.75	0.86
1:A:550:ARG:HG2	3:A:597:HOH:O	1.75	0.86
1:C:190:ARG:HD2	3:C:599:HOH:O	1.73	0.86
1:A:209:MET:HE1	1:A:241:LEU:CD2	2.06	0.86
1:C:288:ILE:HG22	3:C:633:HOH:O	1.76	0.86
2:D:232:ILE:CD1	2:D:270:ILE:HG13	2.06	0.85
1:A:333:ALA:O	1:A:337:ILE:HD12	1.75	0.85
1:C:393:GLU:HG2	1:C:395:VAL:HB	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ARG:HH12	1:C:96:GLU:CD	1.80	0.85
2:B:274:ARG:O	2:B:275:GLU:CG	2.25	0.85
1:C:282:MET:HA	1:C:282:MET:CE	2.06	0.85
1:C:76:GLY:C	3:C:686:HOH:O	2.15	0.85
1:A:185:HIS:NE2	1:A:193:ARG:NH2	2.25	0.85
2:D:355:LEU:HD23	2:D:383:TYR:HE1	1.42	0.85
1:A:93:ARG:HH12	1:A:96:GLU:CD	1.79	0.84
2:B:299:GLY:HA3	3:B:469:HOH:O	1.78	0.84
1:C:137:THR:HG23	3:C:785:HOH:O	1.75	0.84
1:A:248:ASP:HB2	1:A:318:PHE:HB3	1.56	0.84
2:B:360:ARG:HD2	3:B:486:HOH:O	1.76	0.84
1:C:373:GLY:CA	3:C:734:HOH:O	2.25	0.84
1:C:481:ARG:NH1	1:C:536:ILE:HD12	1.91	0.84
1:C:211:ILE:CG2	1:C:495:LEU:HD22	2.08	0.84
1:C:209:MET:HE3	1:C:241:LEU:CD2	2.08	0.84
1:A:346:ALA:HB2	3:A:690:HOH:O	1.78	0.84
2:B:125:ARG:HD2	3:B:503:HOH:O	1.75	0.83
1:C:545:LEU:HA	3:C:738:HOH:O	1.76	0.83
1:C:291:THR:OG1	1:C:294:MET:HG3	1.79	0.83
2:B:338:GLN:HG2	3:B:565:HOH:O	1.77	0.83
1:A:404:GLY:HA3	1:A:431:PHE:CZ	2.13	0.83
1:C:408:ARG:CZ	3:C:679:HOH:O	2.25	0.83
1:C:419:PHE:CD2	3:C:635:HOH:O	2.31	0.83
1:A:447:TYR:HB3	1:A:448:PRO:HD3	1.59	0.83
1:A:220:MET:HB3	3:A:728:HOH:O	1.77	0.83
1:C:248:ASP:HB2	1:C:318:PHE:HB3	1.60	0.83
1:C:335:ARG:HD2	3:C:699:HOH:O	1.77	0.83
2:D:392:ILE:HG13	3:D:470:HOH:O	1.78	0.83
1:C:205:PHE:CD1	3:C:621:HOH:O	2.30	0.82
1:A:380:ILE:HG12	3:A:688:HOH:O	1.77	0.82
1:C:107:VAL:O	1:C:107:VAL:HG22	1.79	0.82
1:A:481:ARG:NH1	1:A:536:ILE:HD12	1.95	0.82
2:D:128:GLU:O	2:D:365:GLY:HA2	1.79	0.81
1:C:295:PRO:HB3	3:C:659:HOH:O	1.78	0.81
2:D:274:ARG:O	2:D:275:GLU:CG	2.27	0.81
1:C:419:PHE:HB2	3:C:683:HOH:O	1.73	0.81
1:A:266:LEU:O	3:A:600:HOH:O	1.99	0.81
1:A:282:MET:CE	1:A:282:MET:HA	2.10	0.81
1:C:447:TYR:HB3	1:C:448:PRO:HD3	1.63	0.81
1:C:538:GLU:HA	3:C:632:HOH:O	1.80	0.81
1:C:550:ARG:HG2	3:C:654:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:ASN:HB3	3:D:500:HOH:O	1.79	0.81
1:C:447:TYR:HB2	3:C:707:HOH:O	1.81	0.81
1:C:456:GLU:HG2	3:C:580:HOH:O	1.81	0.81
1:A:356:ALA:CB	3:A:763:HOH:O	2.29	0.80
2:B:445:MET:SD	3:B:551:HOH:O	2.38	0.80
1:C:299:ARG:NE	3:C:649:HOH:O	2.14	0.80
1:C:419:PHE:HB3	3:C:683:HOH:O	1.75	0.80
2:B:277:ILE:HG12	3:B:544:HOH:O	1.81	0.80
1:A:209:MET:CE	1:A:241:LEU:HD22	2.12	0.80
2:B:355:LEU:HD23	2:B:383:TYR:HE1	1.43	0.80
1:A:99:GLY:HA2	1:C:124:LYS:NZ	1.95	0.80
1:C:205:PHE:HD1	3:C:621:HOH:O	1.63	0.80
1:A:209:MET:HE1	1:A:241:LEU:HD23	1.62	0.79
1:A:406:PHE:CD2	3:A:668:HOH:O	2.35	0.79
2:D:344:HIS:CD2	3:D:554:HOH:O	2.36	0.79
1:A:393:GLU:HG2	1:A:395:VAL:HB	1.64	0.79
2:D:40:GLY:HA2	3:D:499:HOH:O	1.80	0.79
2:D:274:ARG:HB3	3:D:465:HOH:O	1.81	0.79
2:B:128:GLU:O	2:B:365:GLY:HA2	1.83	0.78
1:A:546:GLU:HG3	3:A:597:HOH:O	1.83	0.78
2:D:201:LEU:CD1	2:D:221:LEU:HD13	2.14	0.78
1:A:356:ALA:HB1	3:A:763:HOH:O	1.83	0.78
1:A:93:ARG:NH1	1:A:96:GLU:CD	2.36	0.78
1:A:292:SER:HB2	2:B:296:GLU:HG3	1.64	0.78
1:C:404:GLY:HA3	1:C:431:PHE:CE1	2.18	0.78
1:C:373:GLY:HA3	3:C:734:HOH:O	1.83	0.78
2:B:373:GLU:HG3	3:B:513:HOH:O	1.84	0.78
1:C:262:MET:HE3	1:C:290:ASN:H	1.48	0.78
1:A:8:LYS:HE3	3:A:746:HOH:O	1.84	0.77
1:C:406:PHE:HZ	3:C:739:HOH:O	1.67	0.77
1:C:111:LEU:HG	3:C:686:HOH:O	1.83	0.77
1:C:501:HIS:O	1:C:505:ALA:HB2	1.83	0.77
1:C:428:TYR:CD2	3:C:773:HOH:O	2.37	0.77
1:A:574:PHE:CB	3:A:697:HOH:O	2.07	0.77
2:B:323:HIS:HD2	2:B:325:ILE:H	1.33	0.77
1:A:405:ALA:CB	3:A:752:HOH:O	2.32	0.76
1:A:404:GLY:HA3	1:A:431:PHE:CE1	2.20	0.76
1:C:89:ARG:NH1	3:C:667:HOH:O	2.05	0.76
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.50	0.76
1:C:481:ARG:HH11	1:C:536:ILE:HD12	1.49	0.76
1:A:405:ALA:HB1	3:A:750:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:LEU:HB3	2:D:104:PRO:CD	2.15	0.76
2:B:125:ARG:CD	3:B:503:HOH:O	2.32	0.76
1:C:281:LEU:HG	3:C:689:HOH:O	1.85	0.76
1:C:93:ARG:NH1	1:C:96:GLU:CD	2.38	0.76
1:C:416:ARG:NH2	3:C:690:HOH:O	2.18	0.75
1:C:404:GLY:HA3	1:C:431:PHE:CZ	2.21	0.75
2:B:103:LEU:HB3	2:B:104:PRO:CD	2.15	0.75
1:A:93:ARG:NH1	1:A:96:GLU:OE1	2.20	0.75
2:D:158:LEU:HD13	2:D:341:ARG:HH11	1.51	0.74
1:C:282:MET:HE2	1:C:285:THR:HB	1.69	0.74
1:A:8:LYS:CE	3:A:746:HOH:O	2.35	0.74
1:A:405:ALA:HB3	3:A:752:HOH:O	1.87	0.74
1:A:215:LEU:HD11	3:A:647:HOH:O	1.87	0.74
2:D:19:LEU:C	2:D:19:LEU:HD12	2.08	0.74
1:C:32:GLU:HG3	3:C:775:HOH:O	1.88	0.73
1:C:390:ASP:HB2	3:C:761:HOH:O	1.86	0.73
1:A:386:PRO:CG	3:A:639:HOH:O	2.31	0.73
1:A:418:HIS:HB2	3:A:701:HOH:O	1.89	0.73
2:B:158:LEU:HD13	2:B:341:ARG:HH11	1.53	0.73
2:D:373:GLU:HG3	3:D:565:HOH:O	1.87	0.73
2:B:19:LEU:HD12	2:B:19:LEU:C	2.09	0.73
1:A:209:MET:HE3	1:A:241:LEU:HD22	1.69	0.73
1:A:387:PRO:HB2	3:B:566:HOH:O	1.89	0.73
2:B:149:LYS:HE2	3:B:557:HOH:O	1.87	0.73
2:D:193:ALA:HA	2:D:258:THR:O	1.88	0.73
1:A:501:HIS:O	1:A:505:ALA:HB2	1.89	0.72
1:A:332:GLU:HG2	3:A:677:HOH:O	1.89	0.72
2:B:146:ARG:NH1	2:B:252:HIS:CE1	2.56	0.72
1:A:207:THR:OG1	1:A:241:LEU:HD13	1.89	0.72
1:C:207:THR:OG1	1:C:241:LEU:HD13	1.90	0.72
2:D:398:ILE:HG13	3:D:479:HOH:O	1.88	0.72
1:C:390:ASP:CB	3:C:761:HOH:O	2.36	0.72
1:C:32:GLU:CG	3:C:775:HOH:O	2.37	0.71
1:A:209:MET:HE3	1:A:241:LEU:CD2	2.20	0.71
1:A:481:ARG:HH11	1:A:536:ILE:HD12	1.53	0.71
1:A:107:VAL:O	1:A:107:VAL:HG22	1.89	0.71
2:B:201:LEU:CD1	2:B:221:LEU:HD13	2.20	0.71
1:C:111:LEU:CG	3:C:686:HOH:O	2.38	0.71
1:A:407:TRP:CD1	3:A:750:HOH:O	2.43	0.70
2:B:283:TYR:HB3	2:B:284:PRO:CD	2.21	0.70
1:C:83:ILE:N	3:C:611:HOH:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:HD3	3:A:720:HOH:O	1.91	0.70
1:C:128:GLU:OE2	1:C:156:ARG:NE	2.20	0.70
1:C:440:ARG:NH2	1:C:449:GLU:OE2	2.23	0.70
1:A:440:ARG:NH2	1:A:449:GLU:OE2	2.24	0.70
2:B:266:ALA:O	2:B:270:ILE:HG12	1.91	0.70
1:C:362:TYR:HB3	3:C:666:HOH:O	1.91	0.70
1:A:324:ALA:N	3:A:679:HOH:O	2.24	0.70
1:A:218:VAL:HG13	3:A:752:HOH:O	1.91	0.70
1:A:332:GLU:CG	3:A:677:HOH:O	2.38	0.70
1:A:489:ILE:HD11	3:A:723:HOH:O	1.91	0.70
2:D:201:LEU:HD12	2:D:221:LEU:HD13	1.74	0.70
2:B:386:TYR:CE1	3:B:529:HOH:O	2.46	0.69
1:C:296:VAL:HG12	1:C:337:ILE:HD11	1.74	0.69
1:A:291:THR:OG1	1:A:294:MET:HG3	1.92	0.69
2:B:269:GLU:C	3:B:511:HOH:O	2.30	0.69
1:A:345:PRO:HA	3:A:715:HOH:O	1.93	0.69
2:B:96:ILE:O	2:B:96:ILE:HG22	1.90	0.69
1:C:190:ARG:NH1	3:C:779:HOH:O	2.25	0.69
1:A:262:MET:HE3	1:A:290:ASN:H	1.56	0.68
1:A:384:VAL:CG1	1:A:396:THR:OG1	2.40	0.68
1:C:333:ALA:O	1:C:337:ILE:CD1	2.40	0.68
1:A:275:PRO:HA	3:A:667:HOH:O	1.93	0.68
2:B:77:GLU:OE2	2:B:111:ARG:NH1	2.26	0.68
2:D:338:GLN:CB	3:D:559:HOH:O	2.40	0.68
1:A:463:GLY:HA2	1:A:466:GLU:HG3	1.76	0.68
2:B:193:ALA:HA	2:B:258:THR:O	1.92	0.68
1:A:99:GLY:CA	1:C:124:LYS:NZ	2.55	0.68
2:D:338:GLN:HB3	3:D:559:HOH:O	1.92	0.68
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.39	0.68
1:A:485:GLU:OE1	1:A:488:ARG:NE	2.25	0.68
1:C:292:SER:HB2	2:D:296:GLU:HG3	1.76	0.68
1:C:111:LEU:CD2	3:C:686:HOH:O	2.42	0.68
2:D:142:ASN:ND2	3:D:550:HOH:O	2.26	0.68
1:C:151:PRO:O	1:C:152:ASP:CB	2.36	0.68
2:D:146:ARG:NH1	2:D:252:HIS:CE1	2.62	0.68
2:D:456:LYS:HA	2:D:459:ILE:HD12	1.76	0.68
1:A:467:ILE:O	1:A:471:VAL:HG12	1.94	0.68
1:C:96:GLU:HG2	3:C:670:HOH:O	1.92	0.68
1:A:151:PRO:O	1:A:152:ASP:CB	2.36	0.67
1:A:235:SER:N	3:A:585:HOH:O	2.25	0.67
1:A:488:ARG:HD2	3:A:710:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:CD1	3:A:671:HOH:O	2.35	0.67
2:B:201:LEU:HD12	2:B:221:LEU:HD13	1.77	0.67
2:D:261:THR:HG23	2:D:325:ILE:HD13	1.77	0.67
1:A:282:MET:HA	1:A:282:MET:HE2	1.75	0.67
2:D:376:LYS:HB2	3:D:477:HOH:O	1.92	0.67
1:C:122:MET:CE	3:C:776:HOH:O	2.43	0.67
1:A:386:PRO:HB3	1:A:393:GLU:OE1	1.95	0.66
1:C:406:PHE:CZ	3:C:739:HOH:O	2.43	0.66
2:D:419:GLU:N	3:D:615:HOH:O	2.28	0.66
1:A:327:THR:HB	1:A:383:ALA:O	1.96	0.66
1:C:352:PRO:HG2	3:C:718:HOH:O	1.95	0.66
2:D:96:ILE:O	2:D:96:ILE:HG22	1.95	0.66
1:A:340:ARG:C	1:A:342:GLU:H	1.99	0.66
1:A:379:THR:O	3:A:688:HOH:O	2.14	0.66
1:C:11:GLY:HA2	2:D:29:TYR:OH	1.94	0.66
1:C:340:ARG:C	1:C:342:GLU:H	1.99	0.66
2:D:356:PRO:HD3	3:D:590:HOH:O	1.96	0.66
1:A:266:LEU:HB3	3:A:758:HOH:O	1.95	0.66
1:C:122:MET:HE1	3:C:776:HOH:O	1.96	0.66
1:C:492:GLU:O	1:C:552:ARG:NH1	2.29	0.66
2:D:77:GLU:OE2	2:D:111:ARG:NH1	2.29	0.65
1:C:258:ARG:HB3	3:D:551:HOH:O	1.97	0.65
1:A:460:ARG:HA	3:A:615:HOH:O	1.96	0.65
2:D:266:ALA:O	2:D:270:ILE:HG12	1.97	0.65
2:D:87:GLU:HG3	3:D:546:HOH:O	1.95	0.65
2:B:406:GLU:O	2:B:409:ARG:HB2	1.96	0.65
1:C:203:THR:O	1:C:219:ALA:HA	1.96	0.65
1:C:384:VAL:CG1	1:C:396:THR:OG1	2.42	0.65
2:B:192:ALA:HB3	2:B:257:LEU:HD23	1.78	0.65
1:C:421:ALA:HB2	3:C:635:HOH:O	1.97	0.65
2:D:28:ALA:HB3	2:D:78:ASP:OD1	1.97	0.65
2:B:323:HIS:CD2	2:B:325:ILE:H	2.15	0.65
2:D:344:HIS:CE1	3:D:538:HOH:O	2.28	0.65
1:A:143:PHE:CD2	3:A:756:HOH:O	2.50	0.65
1:A:406:PHE:HD2	3:A:668:HOH:O	1.73	0.65
1:A:492:GLU:O	1:A:552:ARG:NH1	2.30	0.65
1:C:137:THR:CG2	3:C:785:HOH:O	2.38	0.64
1:A:388:GLY:N	3:A:626:HOH:O	2.25	0.64
1:A:128:GLU:OE2	1:A:156:ARG:NE	2.25	0.64
1:A:367:LYS:HE3	3:A:713:HOH:O	1.98	0.64
2:B:283:TYR:HB3	2:B:284:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:GLU:HB3	3:C:603:HOH:O	1.97	0.64
1:C:449:GLU:H	1:C:449:GLU:CD	1.98	0.64
2:D:345:ARG:C	2:D:347:GLY:H	2.01	0.64
2:D:383:TYR:O	3:D:687:HOH:O	2.14	0.64
1:A:203:THR:O	1:A:219:ALA:HA	1.97	0.64
1:C:255:SER:HB2	1:C:290:ASN:HB3	1.78	0.64
1:A:379:THR:C	3:A:688:HOH:O	2.36	0.64
2:B:345:ARG:C	2:B:347:GLY:H	2.01	0.64
1:C:15:ILE:HB	3:C:809:HOH:O	1.97	0.64
1:C:327:THR:HB	1:C:383:ALA:O	1.98	0.64
1:C:538:GLU:CA	3:C:632:HOH:O	2.41	0.64
1:C:93:ARG:NH1	1:C:96:GLU:OE1	2.30	0.64
1:A:143:PHE:CE2	3:A:756:HOH:O	2.50	0.64
2:B:182:GLU:N	3:B:588:HOH:O	2.31	0.64
1:C:74:GLU:OE1	1:C:113:ARG:NH2	2.31	0.64
1:C:450:LEU:HB3	3:C:642:HOH:O	1.96	0.64
2:D:194:MET:SD	2:D:235:PRO:HG3	2.37	0.64
1:A:326:SER:OG	1:A:385:SER:HB2	1.98	0.64
1:C:197:ARG:HB3	1:C:369:ILE:HG23	1.79	0.64
1:C:545:LEU:HD23	3:C:738:HOH:O	1.97	0.64
1:C:485:GLU:OE1	1:C:488:ARG:NE	2.31	0.63
2:D:406:GLU:O	2:D:409:ARG:HB2	1.97	0.63
1:A:489:ILE:CD1	3:A:723:HOH:O	2.47	0.63
2:B:382:LEU:HD11	2:B:439:ALA:HB1	1.79	0.63
2:D:36:LYS:HB2	3:D:499:HOH:O	1.97	0.63
1:A:329:ARG:HH12	2:B:331:TYR:HB3	1.63	0.63
1:A:347:GLU:HA	3:A:693:HOH:O	1.97	0.63
1:A:413:LEU:HD13	1:A:416:ARG:NH1	2.13	0.63
1:A:253:VAL:O	1:A:324:ALA:HA	1.99	0.62
1:A:203:THR:HG23	1:A:204:PRO:HD2	1.79	0.62
1:A:501:HIS:CE1	1:A:553:TYR:HD2	2.16	0.62
1:C:107:VAL:O	1:C:107:VAL:CG2	2.46	0.62
1:A:296:VAL:HG12	1:A:337:ILE:HD11	1.80	0.62
1:C:111:LEU:HD21	3:C:686:HOH:O	1.97	0.62
1:C:92:GLU:OE2	3:C:663:HOH:O	2.16	0.62
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.11	0.62
1:A:19:MET:HE1	1:A:66:SER:HB2	1.81	0.62
2:D:323:HIS:HD2	2:D:325:ILE:H	1.45	0.62
1:A:115:LYS:HD2	3:A:662:HOH:O	1.98	0.62
1:A:406:PHE:CE2	3:A:668:HOH:O	2.53	0.62
1:A:447:TYR:HB3	1:A:448:PRO:CD	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:MET:CE	2:B:338:GLN:HE21	2.13	0.62
2:D:192:ALA:HB3	2:D:257:LEU:HD23	1.82	0.62
1:C:253:VAL:O	1:C:324:ALA:HA	2.00	0.62
2:D:364:ASN:HB2	3:D:539:HOH:O	1.99	0.62
1:C:439:TYR:CE2	3:C:801:HOH:O	2.51	0.62
2:D:451:LEU:HB3	2:D:454:ILE:HD12	1.81	0.62
1:C:187:TRP:CD2	1:C:188:PRO:HD2	2.35	0.62
1:C:358:LEU:O	1:C:362:TYR:HB2	2.00	0.62
2:D:419:GLU:HG3	3:D:615:HOH:O	2.00	0.62
1:C:428:TYR:CE2	3:C:773:HOH:O	2.50	0.61
1:C:467:ILE:O	1:C:471:VAL:HG12	2.00	0.61
2:B:114:ILE:HG21	2:B:237:MET:CE	2.31	0.61
1:C:8:LYS:HD2	1:C:15:ILE:HD12	1.82	0.61
1:A:11:GLY:HA2	2:B:29:TYR:OH	2.00	0.61
1:A:234:LYS:CE	3:A:718:HOH:O	2.49	0.61
2:B:305:LYS:HD2	3:B:553:HOH:O	1.99	0.61
1:C:433:SER:HB3	3:C:614:HOH:O	2.00	0.61
2:B:194:MET:SD	2:B:235:PRO:HG3	2.41	0.61
1:A:300:GLU:HB3	3:A:607:HOH:O	2.01	0.61
1:A:333:ALA:O	1:A:337:ILE:CD1	2.46	0.61
1:C:413:LEU:HD13	1:C:416:ARG:NH1	2.16	0.61
3:A:650:HOH:O	2:B:126:LYS:CD	2.37	0.61
1:A:358:LEU:O	1:A:362:TYR:HD2	1.83	0.60
2:B:261:THR:HG23	2:B:325:ILE:HD13	1.81	0.60
1:C:357:ARG:NH1	1:C:357:ARG:HG2	2.10	0.60
1:C:386:PRO:HB3	1:C:393:GLU:OE1	2.00	0.60
2:D:154:SER:OG	2:D:155:GLY:N	2.34	0.60
2:D:283:TYR:HB3	2:D:284:PRO:CD	2.30	0.60
2:B:375:HIS:HB3	3:B:509:HOH:O	1.99	0.60
1:C:362:TYR:CB	3:C:666:HOH:O	2.49	0.60
2:D:320:ASP:CB	3:D:697:HOH:O	2.48	0.60
2:D:385:ALA:HB2	3:D:552:HOH:O	2.02	0.60
1:C:463:GLY:HA2	1:C:466:GLU:HG3	1.83	0.60
1:A:234:LYS:HE3	3:A:718:HOH:O	2.01	0.60
1:A:417:ARG:HH21	2:B:453:ARG:HD3	1.67	0.60
1:C:350:TYR:HB2	3:C:673:HOH:O	2.02	0.60
1:C:74:GLU:HB3	1:C:111:LEU:HD22	1.84	0.60
2:D:345:ARG:O	2:D:347:GLY:N	2.34	0.60
2:B:345:ARG:O	2:B:347:GLY:N	2.35	0.60
1:A:424:TRP:CH2	1:A:491:ARG:HD2	2.37	0.60
2:B:268:ARG:HG3	2:B:269:GLU:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LYS:CD	3:A:746:HOH:O	2.49	0.59
2:B:6:LYS:NZ	2:B:26:ASP:OD2	2.30	0.59
1:C:2:ILE:HG21	1:C:20:LEU:O	2.01	0.59
1:C:500:TYR:HD1	3:C:758:HOH:O	1.84	0.59
2:D:114:ILE:HG21	2:D:237:MET:CE	2.32	0.59
2:B:268:ARG:O	2:B:271:GLY:N	2.33	0.59
1:A:90:PRO:HD2	1:A:108:VAL:CG2	2.32	0.59
1:A:258:ARG:NH1	2:B:360:ARG:CZ	2.66	0.59
1:A:2:ILE:HG21	1:A:20:LEU:O	2.03	0.59
1:A:303:ILE:HD12	1:A:361:PHE:CG	2.37	0.59
1:A:92:GLU:HB2	3:A:642:HOH:O	2.02	0.59
1:A:329:ARG:NH2	2:B:331:TYR:O	2.35	0.59
1:C:294:MET:O	1:C:299:ARG:HD3	2.02	0.59
1:A:449:GLU:CD	1:A:449:GLU:H	2.05	0.59
1:C:143:PHE:HE1	1:C:248:ASP:O	1.85	0.59
1:C:501:HIS:CE1	1:C:553:TYR:HD2	2.21	0.59
1:A:500:TYR:HD1	3:A:744:HOH:O	1.84	0.59
2:B:154:SER:OG	2:B:155:GLY:N	2.36	0.58
1:A:485:GLU:OE1	1:A:488:ARG:NH2	2.35	0.58
1:C:226:ILE:HG22	1:C:407:TRP:HB2	1.86	0.58
2:B:456:LYS:HA	2:B:459:ILE:HD12	1.85	0.58
1:C:357:ARG:NH1	1:C:357:ARG:CG	2.49	0.58
2:D:194:MET:SD	2:D:260:MET:CE	2.91	0.58
1:A:193:ARG:NH1	1:A:315:ASP:OD2	2.35	0.58
1:A:346:ALA:CB	3:A:690:HOH:O	2.42	0.58
1:C:251:VAL:O	1:C:322:LEU:HA	2.04	0.58
2:D:165:ALA:O	2:D:169:ARG:HG3	2.04	0.58
1:C:303:ILE:HD12	1:C:361:PHE:CG	2.38	0.58
1:C:428:TYR:HD2	3:C:773:HOH:O	1.82	0.58
1:C:536:ILE:HD13	3:C:664:HOH:O	2.04	0.58
2:D:186:PRO:HB2	2:D:251:TYR:CE2	2.38	0.58
2:D:440:TRP:CE2	2:D:462:TYR:HB2	2.38	0.58
1:C:100:ILE:HD11	1:C:101:TYR:CE1	2.39	0.58
2:D:268:ARG:HG3	2:D:269:GLU:N	2.18	0.58
2:D:399:ILE:HG13	3:D:692:HOH:O	2.03	0.58
1:A:209:MET:HG2	3:A:608:HOH:O	2.04	0.57
1:A:99:GLY:CA	1:C:124:LYS:HZ3	2.17	0.57
1:C:203:THR:HG23	1:C:204:PRO:HD2	1.85	0.57
2:D:418:PHE:O	2:D:422:PHE:HB3	2.04	0.57
1:A:251:VAL:O	1:A:322:LEU:HA	2.04	0.57
2:B:316:MET:HE1	2:B:338:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:PHE:CE2	3:C:635:HOH:O	2.54	0.57
2:D:323:HIS:CD2	2:D:325:ILE:H	2.22	0.57
1:C:358:LEU:O	1:C:362:TYR:HD2	1.87	0.57
1:C:520:LEU:HD12	3:C:642:HOH:O	2.03	0.57
1:C:354:LEU:CD2	3:C:694:HOH:O	2.41	0.57
1:A:426:GLY:HA3	3:A:604:HOH:O	2.04	0.57
2:B:440:TRP:CE2	2:B:462:TYR:HB2	2.39	0.57
2:D:234:THR:HB	2:D:235:PRO:HD3	1.87	0.57
2:D:28:ALA:CB	2:D:78:ASP:OD1	2.53	0.57
1:A:344:MET:HG2	3:A:586:HOH:O	2.04	0.57
1:A:353:TYR:HE1	3:A:590:HOH:O	1.85	0.57
1:A:497:GLN:HG2	3:A:608:HOH:O	2.05	0.57
2:B:182:GLU:HB2	3:B:588:HOH:O	2.05	0.57
2:B:340:SER:OG	2:B:342:GLU:HB3	2.05	0.57
2:D:201:LEU:HD11	2:D:221:LEU:HD13	1.86	0.57
1:A:90:PRO:HD2	1:A:108:VAL:HG21	1.84	0.57
1:A:19:MET:CE	1:A:66:SER:HB2	2.34	0.57
2:D:362:MET:CE	2:D:366:VAL:HG11	2.35	0.57
1:A:301:ALA:O	1:A:304:TYR:N	2.37	0.57
2:B:451:LEU:HB3	2:B:454:ILE:HD12	1.87	0.57
1:C:90:PRO:HD2	1:C:108:VAL:CG2	2.35	0.57
1:C:223:THR:HG21	3:C:666:HOH:O	2.04	0.57
1:C:56:SER:HA	2:D:29:TYR:HD2	1.70	0.57
2:B:43:ARG:HG3	3:B:510:HOH:O	2.05	0.57
1:A:202:ASN:HB2	3:A:702:HOH:O	2.05	0.56
1:A:205:PHE:HB3	1:A:218:VAL:HG23	1.85	0.56
2:B:186:PRO:HB2	2:B:251:TYR:CE2	2.40	0.56
1:C:250:VAL:O	1:C:285:THR:HA	2.05	0.56
1:A:344:MET:CE	3:A:653:HOH:O	2.53	0.56
1:C:103:THR:HG22	1:C:106:VAL:HG23	1.87	0.56
1:C:413:LEU:HD11	3:C:690:HOH:O	2.05	0.56
1:A:212:LEU:O	1:A:217:PRO:HA	2.06	0.56
2:B:58:GLN:HG2	3:B:517:HOH:O	2.05	0.56
1:C:301:ALA:O	1:C:304:TYR:N	2.37	0.56
2:D:283:TYR:HB3	2:D:284:PRO:HD2	1.87	0.56
1:A:408:ARG:NE	3:A:775:HOH:O	2.38	0.56
1:C:391:MET:SD	3:C:739:HOH:O	2.58	0.56
1:C:93:ARG:NH1	1:C:96:GLU:OE2	2.35	0.56
1:A:226:ILE:HG22	1:A:407:TRP:HB2	1.88	0.56
1:C:304:TYR:HA	1:C:307:VAL:HG12	1.87	0.56
1:C:326:SER:OG	1:C:385:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:NH1	2:D:360:ARG:CZ	2.69	0.56
2:D:6:LYS:HE2	3:D:509:HOH:O	2.06	0.56
1:A:426:GLY:CA	3:A:604:HOH:O	2.53	0.56
1:C:424:TRP:CH2	1:C:491:ARG:HD2	2.41	0.56
2:D:142:ASN:ND2	3:D:634:HOH:O	2.21	0.56
1:A:103:THR:HG22	1:A:106:VAL:HG23	1.88	0.55
2:B:165:ALA:O	2:B:169:ARG:HG3	2.07	0.55
1:A:74:GLU:HB3	1:A:111:LEU:HD22	1.88	0.55
1:C:257:GLU:HB2	1:C:262:MET:HE2	1.86	0.55
1:A:282:MET:HE1	1:A:285:THR:CB	2.29	0.55
1:A:346:ALA:HB3	1:A:350:TYR:O	2.05	0.55
1:A:292:SER:HB3	2:B:292:ALA:HB1	1.87	0.55
1:C:227:PRO:HB3	3:C:739:HOH:O	2.06	0.55
1:C:541:GLN:NE2	3:C:632:HOH:O	2.39	0.55
1:A:237:THR:O	1:A:241:LEU:HD23	2.07	0.55
1:A:358:LEU:O	1:A:362:TYR:HB2	2.05	0.55
1:C:229:PRO:HG3	3:C:668:HOH:O	2.04	0.55
1:C:423:ASN:HA	3:C:653:HOH:O	2.06	0.55
1:C:462:ALA:O	1:C:466:GLU:HG2	2.06	0.55
3:A:673:HOH:O	2:B:126:LYS:HD3	2.05	0.55
1:C:143:PHE:CE1	1:C:248:ASP:O	2.60	0.55
1:C:84:TYR:O	1:C:288:ILE:HA	2.07	0.55
1:C:299:ARG:NH2	3:C:649:HOH:O	2.34	0.55
2:D:198:GLN:NE2	3:D:511:HOH:O	2.39	0.55
2:B:370:LYS:O	3:B:560:HOH:O	2.18	0.55
1:C:237:THR:O	1:C:241:LEU:HD23	2.06	0.55
2:D:320:ASP:HB3	3:D:697:HOH:O	2.04	0.55
2:D:340:SER:OG	2:D:342:GLU:HB3	2.07	0.55
2:D:268:ARG:O	2:D:271:GLY:N	2.35	0.55
2:B:86:LYS:HZ2	2:B:249:HIS:CE1	2.25	0.54
1:C:206:LEU:O	1:C:245:SER:HA	2.07	0.54
1:C:346:ALA:C	3:C:799:HOH:O	2.32	0.54
1:A:143:PHE:HE1	1:A:248:ASP:O	1.90	0.54
2:B:86:LYS:NZ	2:B:249:HIS:CE1	2.76	0.54
2:D:77:GLU:CD	2:D:111:ARG:HH12	2.11	0.54
2:D:6:LYS:NZ	2:D:26:ASP:OD2	2.27	0.54
1:A:207:THR:CG2	1:A:212:LEU:HD12	2.18	0.54
1:C:436:ASP:O	1:C:440:ARG:HG3	2.08	0.54
2:D:36:LYS:HE3	3:D:499:HOH:O	2.08	0.54
1:A:100:ILE:HD11	1:A:101:TYR:CE1	2.42	0.54
1:A:462:ALA:O	1:A:466:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLN:HB3	3:A:608:HOH:O	2.07	0.54
1:C:202:ASN:HD22	1:C:202:ASN:C	2.09	0.54
2:D:398:ILE:CG1	3:D:479:HOH:O	2.50	0.54
1:A:197:ARG:HB3	1:A:369:ILE:HG23	1.90	0.54
1:A:257:GLU:HB2	1:A:262:MET:HE2	1.89	0.54
1:A:274:ASP:OD2	1:A:284:ARG:HD3	2.08	0.54
1:C:329:ARG:HH12	2:D:331:TYR:HB3	1.72	0.54
2:B:268:ARG:HA	2:B:284:PRO:HG3	1.90	0.54
2:B:386:TYR:HE1	3:B:529:HOH:O	1.89	0.54
2:D:316:MET:CE	2:D:338:GLN:HE21	2.20	0.54
1:A:386:PRO:HG3	3:A:639:HOH:O	2.03	0.54
2:B:248:GLU:C	2:B:249:HIS:HD2	2.10	0.54
1:C:234:LYS:HE3	3:C:646:HOH:O	2.07	0.54
1:C:447:TYR:HB3	1:C:448:PRO:CD	2.35	0.54
1:C:76:GLY:CA	3:C:686:HOH:O	2.54	0.54
2:D:142:ASN:CG	3:D:550:HOH:O	2.45	0.54
1:C:329:ARG:NH2	2:D:331:TYR:O	2.40	0.54
1:A:206:LEU:O	1:A:245:SER:HA	2.07	0.54
1:A:250:VAL:O	1:A:285:THR:HA	2.08	0.53
2:B:367:GLY:HA2	3:B:509:HOH:O	2.08	0.53
1:C:335:ARG:HG3	1:C:350:TYR:HA	1.89	0.53
1:C:408:ARG:HG3	1:C:408:ARG:O	2.08	0.53
2:B:410:ARG:CB	3:B:524:HOH:O	2.57	0.53
1:C:416:ARG:NH1	3:C:688:HOH:O	2.37	0.53
1:A:285:THR:HG22	1:A:287:LEU:HD23	1.91	0.53
1:A:335:ARG:HG3	1:A:350:TYR:HA	1.89	0.53
2:B:96:ILE:CG2	2:B:96:ILE:O	2.56	0.53
1:C:190:ARG:CD	3:C:599:HOH:O	2.43	0.53
1:A:436:ASP:O	1:A:440:ARG:HG3	2.07	0.53
1:C:432:THR:HA	1:C:435:LEU:HD12	1.91	0.53
1:A:234:LYS:HD2	3:A:718:HOH:O	2.08	0.53
1:A:85:ASP:OD1	1:A:85:ASP:C	2.47	0.53
2:B:28:ALA:CB	2:B:78:ASP:OD1	2.57	0.53
2:D:383:TYR:O	2:D:384:SER:C	2.47	0.53
1:A:304:TYR:HA	1:A:307:VAL:HG12	1.90	0.53
1:C:193:ARG:NH1	1:C:315:ASP:OD2	2.41	0.53
1:A:295:PRO:HB3	3:A:629:HOH:O	2.08	0.53
2:B:270:ILE:HG22	2:B:270:ILE:O	2.09	0.53
2:B:353:ASP:HB2	3:B:466:HOH:O	2.09	0.53
1:C:205:PHE:HB3	1:C:218:VAL:HG23	1.91	0.53
2:D:358:LEU:HB3	3:D:473:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:MET:CE	1:C:285:THR:HB	2.39	0.52
1:C:335:ARG:HD3	1:C:349:GLY:O	2.09	0.52
1:A:203:THR:HG23	1:A:204:PRO:CD	2.39	0.52
2:B:431:SER:OG	2:B:434:GLU:HG3	2.09	0.52
1:A:408:ARG:CZ	3:A:775:HOH:O	2.56	0.52
1:A:73:VAL:CG1	1:A:75:LEU:HD21	2.39	0.52
1:A:339:SER:O	1:A:342:GLU:N	2.43	0.52
1:A:408:ARG:O	1:A:408:ARG:HG3	2.08	0.52
1:C:413:LEU:CD1	1:C:416:ARG:NH1	2.73	0.52
1:C:404:GLY:CA	1:C:431:PHE:CE1	2.91	0.52
1:A:291:THR:N	3:A:594:HOH:O	2.42	0.52
1:A:357:ARG:HG2	1:A:357:ARG:NH1	2.10	0.52
1:C:90:PRO:HD2	1:C:108:VAL:HG21	1.91	0.52
1:A:207:THR:HB	3:A:691:HOH:O	2.09	0.52
1:A:296:VAL:HG12	1:A:337:ILE:CD1	2.39	0.52
1:C:462:ALA:O	1:C:466:GLU:CG	2.58	0.52
2:D:335:GLY:O	2:D:336:GLN:HB3	2.07	0.52
1:A:77:PRO:HG2	1:A:183:MET:HE2	1.90	0.52
2:B:391:ASP:O	2:B:395:LEU:HD13	2.09	0.52
2:B:410:ARG:HB2	3:B:524:HOH:O	2.10	0.52
2:B:41:ARG:NH1	2:B:62:GLU:OE2	2.40	0.52
1:C:82:GLY:CA	3:C:611:HOH:O	2.37	0.52
2:D:123:ALA:O	2:D:301:VAL:HG13	2.09	0.52
1:A:74:GLU:OE1	1:A:113:ARG:NH2	2.44	0.51
2:B:92:ARG:HD2	2:B:205:ILE:HD11	1.91	0.51
2:B:28:ALA:HB3	2:B:78:ASP:OD1	2.10	0.51
2:D:444:SER:HA	2:D:463:TYR:CE1	2.45	0.51
2:B:103:LEU:HB3	2:B:104:PRO:HD2	1.91	0.51
2:B:141:MET:HB2	2:B:142:ASN:HD22	1.75	0.51
1:C:253:VAL:HG12	1:C:322:LEU:HD11	1.91	0.51
2:D:401:GLU:O	2:D:402:ASP:HB2	2.11	0.51
2:B:135:ILE:HG22	2:B:138:ILE:H	1.75	0.51
1:C:262:MET:SD	1:C:289:ALA:HB1	2.49	0.51
1:C:216:PHE:CZ	1:C:424:TRP:HA	2.46	0.51
1:C:274:ASP:OD2	1:C:284:ARG:HD3	2.10	0.51
1:A:462:ALA:O	1:A:466:GLU:CG	2.59	0.51
1:A:154:ARG:HD3	3:A:661:HOH:O	2.10	0.51
1:A:340:ARG:C	1:A:342:GLU:N	2.64	0.51
1:A:387:PRO:HD2	2:B:331:TYR:CE2	2.45	0.51
1:C:252:TYR:CD2	1:C:252:TYR:O	2.64	0.51
1:C:281:LEU:HB3	3:C:680:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:VAL:HG11	1:C:396:THR:HG1	1.74	0.51
1:C:513:TYR:HA	3:C:585:HOH:O	2.10	0.51
1:C:517:LYS:HD3	1:C:563:PHE:CZ	2.26	0.51
1:A:107:VAL:O	1:A:107:VAL:CG2	2.58	0.51
1:A:439:TYR:CE2	3:A:771:HOH:O	2.63	0.51
2:B:339:LEU:C	3:B:565:HOH:O	2.49	0.51
2:B:84:VAL:HG11	2:B:112:LEU:HD12	1.91	0.51
1:C:426:GLY:HA3	3:C:787:HOH:O	2.09	0.51
2:B:444:SER:HA	2:B:463:TYR:CE1	2.46	0.51
1:C:485:GLU:OE1	1:C:488:ARG:NH2	2.44	0.51
2:D:109:GLU:HA	2:D:109:GLU:OE1	2.11	0.51
2:D:382:LEU:HD11	2:D:439:ALA:HB1	1.92	0.51
1:A:8:LYS:HD2	1:A:15:ILE:HD12	1.92	0.51
2:D:399:ILE:CG1	3:D:692:HOH:O	2.59	0.51
2:B:345:ARG:C	2:B:347:GLY:N	2.64	0.51
2:B:418:PHE:O	2:B:422:PHE:HB3	2.11	0.51
1:C:359:ALA:O	1:C:363:GLU:HB2	2.10	0.51
2:D:261:THR:HG23	2:D:325:ILE:CD1	2.41	0.51
1:A:232:SER:OG	1:A:409:LEU:HD22	2.11	0.50
1:C:296:VAL:HG12	1:C:337:ILE:CD1	2.39	0.50
1:C:215:LEU:HD21	1:C:455:SER:HB3	1.92	0.50
2:D:345:ARG:C	2:D:347:GLY:N	2.64	0.50
2:D:40:GLY:CA	3:D:499:HOH:O	2.47	0.50
2:B:173:VAL:O	2:B:175:PRO:HD3	2.10	0.50
2:B:77:GLU:CD	2:B:111:ARG:HH12	2.14	0.50
2:D:179:GLY:CA	3:D:517:HOH:O	2.36	0.50
1:C:212:LEU:O	1:C:217:PRO:HA	2.12	0.50
1:C:226:ILE:O	1:C:383:ALA:HA	2.12	0.50
1:C:410:ASP:OD1	3:C:674:HOH:O	2.19	0.50
1:A:323:MET:C	3:A:679:HOH:O	2.47	0.50
2:D:268:ARG:HA	2:D:284:PRO:HG3	1.94	0.50
2:D:418:PHE:HD1	3:D:615:HOH:O	1.93	0.50
1:A:216:PHE:CZ	1:A:424:TRP:HA	2.47	0.50
2:D:364:ASN:OD1	2:D:364:ASN:N	2.44	0.50
1:C:400:LEU:HD21	1:C:406:PHE:CD1	2.47	0.50
1:C:408:ARG:NH1	3:C:679:HOH:O	2.42	0.50
2:D:305:LYS:HD3	3:D:563:HOH:O	2.11	0.50
1:A:216:PHE:HZ	1:A:424:TRP:HA	1.76	0.50
1:C:498:ASN:ND2	3:C:608:HOH:O	2.45	0.50
2:B:141:MET:HE3	3:B:527:HOH:O	2.11	0.50
2:B:248:GLU:C	2:B:249:HIS:CD2	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:HG21	1:A:287:LEU:HD21	1.93	0.50
1:A:77:PRO:HG2	1:A:183:MET:CE	2.42	0.50
1:C:252:TYR:HD2	1:C:252:TYR:O	1.93	0.50
2:D:397:ALA:HB1	3:D:528:HOH:O	2.12	0.50
1:C:198:LYS:HD3	1:C:368:VAL:HG12	1.93	0.49
1:C:489:ILE:HD11	1:C:545:LEU:HD22	1.94	0.49
2:D:96:ILE:O	2:D:96:ILE:CG2	2.60	0.49
1:A:22:ALA:HA	3:A:609:HOH:O	2.12	0.49
1:A:294:MET:O	1:A:299:ARG:HD3	2.11	0.49
2:B:334:GLU:C	2:B:360:ARG:HD3	2.32	0.49
2:B:380:ASP:HB3	3:B:507:HOH:O	2.11	0.49
1:C:77:PRO:HG2	1:C:183:MET:CE	2.42	0.49
2:D:124:ARG:NH2	2:D:298:ALA:O	2.46	0.49
2:D:353:ASP:HB2	3:D:466:HOH:O	2.12	0.49
1:A:228:GLY:HA3	1:A:234:LYS:HE2	1.95	0.49
2:B:399:ILE:HA	3:B:521:HOH:O	2.11	0.49
2:D:19:LEU:C	2:D:19:LEU:CD1	2.80	0.49
1:A:56:SER:HA	2:B:29:TYR:HD2	1.77	0.49
1:C:367:LYS:HE3	3:C:749:HOH:O	2.12	0.49
1:C:464:LEU:C	1:C:466:GLU:H	2.16	0.49
2:D:103:LEU:HB3	2:D:104:PRO:HD2	1.92	0.49
2:D:198:GLN:NE2	2:D:201:LEU:HD23	2.27	0.49
2:D:334:GLU:C	2:D:360:ARG:HD3	2.32	0.49
2:D:178:SER:HA	2:D:369:GLY:O	2.13	0.49
1:A:226:ILE:O	1:A:383:ALA:HA	2.12	0.49
1:A:362:TYR:HE1	3:A:599:HOH:O	1.96	0.49
2:B:123:ALA:O	2:B:301:VAL:HG13	2.12	0.49
1:C:216:PHE:HZ	1:C:424:TRP:HA	1.76	0.49
1:C:461:GLU:HG3	1:C:487:GLY:HA3	1.94	0.49
2:D:320:ASP:HB3	3:D:685:HOH:O	2.13	0.49
1:A:432:THR:HA	1:A:435:LEU:HD12	1.94	0.49
2:D:248:GLU:C	2:D:249:HIS:HD2	2.16	0.49
1:A:116:LYS:HE3	3:A:735:HOH:O	2.12	0.49
1:A:84:TYR:O	1:A:288:ILE:HA	2.12	0.49
1:A:357:ARG:C	1:A:359:ALA:N	2.65	0.49
2:B:109:GLU:HA	2:B:109:GLU:OE1	2.13	0.49
2:B:373:GLU:CG	3:B:513:HOH:O	2.50	0.49
1:C:340:ARG:C	1:C:342:GLU:N	2.66	0.49
1:C:394:PRO:HB2	3:C:694:HOH:O	2.13	0.49
2:B:364:ASN:OD1	2:B:364:ASN:N	2.46	0.49
2:B:401:GLU:O	2:B:402:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PRO:HA	1:C:384:VAL:O	2.12	0.49
1:C:236:VAL:CG2	3:C:656:HOH:O	2.60	0.49
1:A:16:ALA:HB2	1:A:64:VAL:HG11	1.95	0.49
1:A:143:PHE:CE1	1:A:248:ASP:O	2.66	0.49
1:C:524:LYS:HE2	3:C:790:HOH:O	2.13	0.49
1:A:298:ALA:CB	3:A:717:HOH:O	2.35	0.48
1:A:423:ASN:OD1	1:A:426:GLY:N	2.32	0.48
2:D:269:GLU:C	2:D:271:GLY:H	2.17	0.48
1:A:186:THR:HG23	3:A:740:HOH:O	2.14	0.48
1:A:210:ARG:HA	3:A:638:HOH:O	2.13	0.48
1:A:329:ARG:CZ	3:B:504:HOH:O	2.61	0.48
1:A:367:LYS:CE	3:A:720:HOH:O	2.60	0.48
1:A:367:LYS:NZ	1:A:375:GLU:OE1	2.46	0.48
1:C:338:SER:OG	1:C:351:PRO:HB3	2.13	0.48
1:A:301:ALA:N	3:A:607:HOH:O	2.46	0.48
1:C:207:THR:HG1	1:C:241:LEU:HD13	1.77	0.48
1:C:413:LEU:HD22	3:C:653:HOH:O	2.12	0.48
1:A:338:SER:OG	1:A:351:PRO:HB3	2.12	0.48
1:C:74:GLU:CD	1:C:113:ARG:HH22	2.16	0.48
1:C:232:SER:OG	1:C:409:LEU:HD22	2.13	0.48
1:C:459:GLN:HA	3:C:619:HOH:O	2.13	0.48
1:A:517:LYS:HD3	1:A:563:PHE:CZ	2.27	0.48
1:C:22:ALA:HB1	1:C:39:ILE:CD1	2.44	0.48
2:D:274:ARG:O	2:D:275:GLU:CB	2.61	0.48
2:B:355:LEU:HB2	2:B:356:PRO:HD3	1.94	0.48
1:A:211:ILE:HG23	1:A:495:LEU:HD22	1.89	0.48
2:B:19:LEU:CD1	2:B:19:LEU:C	2.81	0.48
2:B:30:GLY:O	3:B:488:HOH:O	2.20	0.48
2:D:317:PRO:HG2	2:D:323:HIS:CE1	2.49	0.48
1:A:227:PRO:HA	1:A:384:VAL:O	2.13	0.48
2:B:201:LEU:HD11	2:B:221:LEU:HD13	1.94	0.48
1:C:356:ALA:HB1	3:C:756:HOH:O	2.12	0.48
1:A:2:ILE:HB	1:A:19:MET:HE2	1.96	0.48
1:A:424:TRP:CE3	1:A:495:LEU:CD1	2.97	0.48
2:B:19:LEU:HD11	2:B:21:VAL:HG22	1.95	0.48
2:B:48:ILE:HD12	2:B:274:ARG:HD2	1.96	0.48
1:C:235:SER:O	1:C:238:GLN:HB2	2.14	0.48
1:C:497:GLN:HA	1:C:504:ASP:OD2	2.14	0.48
2:D:135:ILE:HG22	2:D:138:ILE:H	1.79	0.48
2:D:90:GLY:HA2	2:D:214:LEU:O	2.14	0.48
1:A:413:LEU:CD1	1:A:416:ARG:NH1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:TYR:CA	3:B:473:HOH:O	2.61	0.48
2:B:362:MET:CE	2:B:366:VAL:HG11	2.43	0.48
1:C:339:SER:O	1:C:342:GLU:N	2.46	0.48
1:C:464:LEU:C	1:C:466:GLU:N	2.67	0.48
1:C:19:MET:CE	1:C:66:SER:HB2	2.44	0.48
2:D:125:ARG:CZ	2:D:300:VAL:HB	2.44	0.48
1:C:357:ARG:C	1:C:359:ALA:N	2.65	0.47
1:C:535:SER:HB3	1:C:538:GLU:HB2	1.96	0.47
2:D:362:MET:HE2	2:D:366:VAL:HG11	1.95	0.47
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.14	0.47
1:A:38:GLU:CD	1:A:52:TYR:OH	2.51	0.47
1:C:357:ARG:C	1:C:359:ALA:H	2.16	0.47
2:D:431:SER:OG	2:D:434:GLU:HG3	2.14	0.47
1:A:443:VAL:HG11	1:A:447:TYR:CD1	2.50	0.47
2:B:283:TYR:C	3:B:473:HOH:O	2.53	0.47
2:B:351:PRO:O	3:B:501:HOH:O	2.20	0.47
2:D:364:ASN:CB	3:D:496:HOH:O	2.36	0.47
1:A:165:GLU:HG3	3:A:695:HOH:O	2.13	0.47
1:A:216:PHE:N	1:A:217:PRO:CD	2.77	0.47
2:B:143:THR:N	2:B:362:MET:HG3	2.30	0.47
1:A:212:LEU:O	1:A:217:PRO:CA	2.62	0.47
1:A:258:ARG:HB2	1:A:261:GLU:HB2	1.97	0.47
1:A:407:TRP:NE1	3:A:750:HOH:O	2.45	0.47
1:A:420:PRO:O	1:A:422:ILE:N	2.39	0.47
2:D:142:ASN:HD22	2:D:142:ASN:N	2.12	0.47
2:B:53:GLU:HG3	3:B:485:HOH:O	2.14	0.47
1:C:32:GLU:HG2	3:C:775:HOH:O	2.07	0.47
2:D:92:ARG:HD2	2:D:205:ILE:HD11	1.94	0.47
1:C:454:ILE:HG13	1:C:516:MET:CG	2.45	0.47
1:A:262:MET:SD	1:A:289:ALA:HB1	2.54	0.47
1:C:358:LEU:O	1:C:362:TYR:CD2	2.67	0.47
1:A:358:LEU:O	1:A:362:TYR:CD2	2.64	0.47
1:A:198:LYS:HD3	1:A:368:VAL:HG12	1.96	0.47
1:C:241:LEU:O	1:C:245:SER:HB3	2.15	0.47
1:C:550:ARG:HA	1:C:550:ARG:HD3	1.66	0.47
1:A:357:ARG:C	1:A:359:ALA:H	2.18	0.47
1:A:476:LEU:HB3	1:A:480:GLU:HB2	1.97	0.47
2:B:274:ARG:O	2:B:275:GLU:CB	2.62	0.47
1:C:228:GLY:HA3	1:C:234:LYS:HE2	1.97	0.47
1:C:461:GLU:OE1	3:C:810:HOH:O	2.21	0.47
2:D:299:GLY:HA3	3:D:471:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HG3	1:A:185:HIS:HB3	1.98	0.46
1:A:285:THR:CG2	1:A:287:LEU:CD2	2.93	0.46
1:C:530:ILE:HG21	3:C:664:HOH:O	2.13	0.46
2:B:275:GLU:HA	3:B:534:HOH:O	2.14	0.46
2:B:383:TYR:O	2:B:384:SER:C	2.53	0.46
1:C:19:MET:HE3	1:C:66:SER:N	2.30	0.46
1:C:422:ILE:HG13	1:C:423:ASN:N	2.30	0.46
2:D:173:VAL:O	2:D:175:PRO:HD3	2.14	0.46
2:D:233:LEU:O	2:D:237:MET:HG2	2.16	0.46
1:C:416:ARG:O	1:C:417:ARG:HB2	2.15	0.46
1:C:466:GLU:O	1:C:469:GLN:HB3	2.16	0.46
1:C:499:ALA:N	3:C:730:HOH:O	2.33	0.46
1:A:113:ARG:HD2	1:A:169:GLU:OE2	2.15	0.46
2:D:355:LEU:HB2	2:D:356:PRO:HD3	1.98	0.46
1:A:216:PHE:HA	1:A:429:SER:HB2	1.97	0.46
1:A:454:ILE:HG13	1:A:516:MET:CG	2.46	0.46
1:C:27:ILE:HD13	1:C:71:LEU:HA	1.97	0.46
2:D:100:ILE:O	2:D:100:ILE:HG22	2.15	0.46
1:A:464:LEU:C	1:A:466:GLU:H	2.16	0.46
1:A:464:LEU:C	1:A:466:GLU:N	2.68	0.46
2:B:412:LEU:HG	3:B:563:HOH:O	2.15	0.46
1:C:437:PRO:HD3	3:C:724:HOH:O	2.14	0.46
1:A:125:PRO:HA	1:A:157:VAL:HG12	1.98	0.46
1:A:148:LEU:HD11	1:A:316:GLN:HG2	1.97	0.46
1:A:392:SER:O	1:A:393:GLU:C	2.53	0.46
2:B:194:MET:SD	2:B:260:MET:CE	3.04	0.46
1:C:120:THR:HB	1:C:137:THR:HG22	1.97	0.46
1:C:154:ARG:HD3	3:C:687:HOH:O	2.15	0.46
1:C:232:SER:OG	1:C:421:ALA:HB3	2.16	0.46
1:C:98:THR:HG21	1:C:106:VAL:HG21	1.97	0.46
1:A:235:SER:O	1:A:238:GLN:HB2	2.16	0.46
1:A:550:ARG:HA	1:A:550:ARG:HD3	1.66	0.46
2:B:281:ARG:HD3	3:B:623:HOH:O	2.16	0.46
1:C:146:LYS:HG3	1:C:316:GLN:HB3	1.98	0.46
1:C:522:PHE:CD2	1:C:522:PHE:C	2.89	0.46
1:A:424:TRP:HH2	1:A:491:ARG:HD2	1.76	0.46
2:B:103:LEU:HB3	2:B:104:PRO:HD3	1.96	0.46
1:A:400:LEU:HD21	1:A:406:PHE:CD1	2.51	0.46
2:B:456:LYS:HA	3:B:499:HOH:O	2.15	0.46
2:B:78:ASP:CB	3:B:482:HOH:O	2.64	0.46
1:A:85:ASP:OD2	1:A:89:ARG:NE	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HB	1:A:137:THR:HG22	1.98	0.45
1:A:380:ILE:HG22	3:A:599:HOH:O	2.16	0.45
2:B:15:SER:HB3	3:B:570:HOH:O	2.15	0.45
1:C:285:THR:HG21	1:C:287:LEU:HD21	1.97	0.45
2:D:258:THR:HA	2:D:259:ASP:HA	1.74	0.45
1:A:325:ASP:HA	1:A:326:SER:HA	1.57	0.45
1:A:485:GLU:OE1	1:A:488:ARG:CZ	2.63	0.45
2:B:236:ARG:NH2	2:B:290:ASP:OD1	2.49	0.45
1:C:187:TRP:CG	1:C:188:PRO:HD2	2.52	0.45
1:C:500:TYR:CD1	3:C:758:HOH:O	2.55	0.45
2:D:362:MET:HE3	2:D:366:VAL:HG11	1.97	0.45
2:D:393:ARG:HB2	3:D:467:HOH:O	2.15	0.45
2:D:40:GLY:C	3:D:499:HOH:O	2.54	0.45
1:A:215:LEU:HD21	1:A:455:SER:HB3	1.98	0.45
1:A:420:PRO:HB3	3:A:737:HOH:O	2.17	0.45
2:B:178:SER:HA	2:B:369:GLY:O	2.16	0.45
1:C:318:PHE:HE1	3:C:657:HOH:O	2.00	0.45
1:C:348:GLU:OE1	1:C:348:GLU:HA	2.17	0.45
1:C:387:PRO:HB3	3:C:645:HOH:O	2.15	0.45
1:C:424:TRP:HH2	1:C:491:ARG:HD2	1.81	0.45
2:B:146:ARG:NH1	2:B:252:HIS:NE2	2.64	0.45
1:C:74:GLU:CD	1:C:113:ARG:NH2	2.69	0.45
2:D:93:PHE:N	2:D:93:PHE:CD1	2.83	0.45
2:B:183:LYS:HG2	3:B:577:HOH:O	2.16	0.45
1:C:216:PHE:HA	1:C:429:SER:HB2	1.97	0.45
1:C:408:ARG:HG2	1:C:408:ARG:NH1	2.31	0.45
2:D:141:MET:HB2	2:D:142:ASN:HD22	1.81	0.45
1:A:404:GLY:CA	1:A:431:PHE:CE1	2.94	0.45
1:A:248:ASP:CB	1:A:318:PHE:HB3	2.40	0.45
2:B:132:GLN:O	2:B:171:ALA:HA	2.17	0.45
2:B:248:GLU:O	2:B:249:HIS:CD2	2.69	0.45
1:C:501:HIS:O	1:C:505:ALA:CB	2.59	0.45
2:D:334:GLU:HG2	3:D:678:HOH:O	2.17	0.45
1:A:406:PHE:O	1:A:427:SER:HB3	2.17	0.45
1:A:489:ILE:HD11	1:A:545:LEU:HD22	1.99	0.45
2:B:127:PRO:HB3	2:B:146:ARG:O	2.16	0.45
1:C:20:LEU:HD23	3:C:600:HOH:O	2.17	0.45
1:C:45:ASP:N	1:C:45:ASP:OD1	2.48	0.45
1:C:85:ASP:OD2	1:C:89:ARG:NE	2.40	0.45
1:C:95:ARG:HD2	3:C:663:HOH:O	2.16	0.45
2:D:316:MET:HE2	2:D:338:GLN:HE21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:ILE:HB	2:D:326:PRO:CD	2.47	0.45
2:B:124:ARG:NH2	2:B:298:ALA:O	2.50	0.45
1:C:535:SER:HB3	1:C:538:GLU:CB	2.46	0.45
1:A:255:SER:HB2	1:A:290:ASN:HB3	1.86	0.44
1:A:451:ARG:HG2	1:A:452:ASP:N	2.31	0.44
1:A:424:TRP:CE3	1:A:495:LEU:HD13	2.52	0.44
1:A:74:GLU:CD	1:A:113:ARG:HH22	2.21	0.44
2:B:258:THR:HA	2:B:259:ASP:HA	1.80	0.44
2:B:93:PHE:CD1	2:B:93:PHE:N	2.85	0.44
1:C:203:THR:HG23	1:C:204:PRO:CD	2.46	0.44
1:C:392:SER:O	1:C:393:GLU:C	2.55	0.44
1:C:516:MET:HG2	3:C:642:HOH:O	2.17	0.44
1:C:550:ARG:HD3	1:C:553:TYR:HD1	1.82	0.44
2:D:391:ASP:O	2:D:395:LEU:HD13	2.17	0.44
1:A:103:THR:HG22	1:A:106:VAL:CG2	2.47	0.44
1:A:234:LYS:O	1:A:235:SER:C	2.56	0.44
1:A:253:VAL:HG12	1:A:322:LEU:HD11	2.00	0.44
1:A:257:GLU:HG2	1:A:262:MET:CE	2.47	0.44
1:A:408:ARG:HD2	1:A:409:LEU:O	2.17	0.44
1:A:535:SER:HB3	1:A:538:GLU:CB	2.46	0.44
1:A:98:THR:HG21	1:A:106:VAL:HG21	1.99	0.44
2:B:342:GLU:HA	2:B:345:ARG:CZ	2.47	0.44
1:A:99:GLY:N	1:C:124:LYS:HE2	2.33	0.44
2:D:398:ILE:HG22	3:D:692:HOH:O	2.17	0.44
1:A:252:TYR:HB2	3:A:603:HOH:O	2.15	0.44
1:A:390:ASP:C	1:A:392:SER:H	2.21	0.44
2:D:124:ARG:NE	3:D:471:HOH:O	2.43	0.44
1:A:203:THR:HG22	1:A:220:MET:HB2	1.99	0.44
1:A:496:GLN:NE2	3:A:610:HOH:O	2.50	0.44
2:B:298:ALA:HB2	2:B:310:GLN:HE21	1.83	0.44
2:B:376:LYS:O	2:B:380:ASP:OD1	2.35	0.44
2:D:342:GLU:HA	2:D:345:ARG:CZ	2.48	0.44
2:D:86:LYS:NZ	2:D:249:HIS:CE1	2.86	0.44
1:A:247:ALA:O	1:A:284:ARG:NH2	2.51	0.44
2:B:377:GLN:HE22	2:B:455:SER:HB3	1.82	0.44
1:C:1:MET:HA	1:C:66:SER:O	2.18	0.44
1:C:476:LEU:HB3	1:C:480:GLU:HB2	2.00	0.44
1:C:208:GLY:O	1:C:497:GLN:NE2	2.48	0.44
2:D:103:LEU:HB3	2:D:104:PRO:HD3	1.95	0.44
2:D:248:GLU:C	2:D:249:HIS:CD2	2.90	0.44
2:D:260:MET:HE1	2:D:263:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:ILE:HA	2:D:278:PRO:HD3	1.81	0.44
1:A:154:ARG:HG2	3:A:661:HOH:O	2.17	0.44
1:A:497:GLN:HA	1:A:504:ASP:OD2	2.17	0.44
1:A:93:ARG:NH1	1:A:96:GLU:OE2	2.38	0.44
2:B:231:ARG:HD2	2:B:266:ALA:HB2	2.00	0.44
2:B:128:GLU:HG3	2:B:129:GLN:HE21	1.82	0.44
2:B:99:PRO:O	2:B:100:ILE:HD13	2.16	0.44
1:C:8:LYS:HB3	3:C:809:HOH:O	2.17	0.44
1:A:465:GLN:HG3	3:A:582:HOH:O	2.17	0.44
1:A:468:VAL:HG22	1:A:476:LEU:HD11	2.00	0.44
2:B:269:GLU:C	2:B:271:GLY:H	2.20	0.44
2:B:335:GLY:O	2:B:336:GLN:HB3	2.18	0.44
1:C:103:THR:HG22	1:C:106:VAL:CG2	2.47	0.44
1:C:387:PRO:HD2	2:D:331:TYR:CE2	2.53	0.44
2:D:20:PHE:CD2	2:D:54:TYR:CE2	3.06	0.44
1:A:359:ALA:O	1:A:363:GLU:HB2	2.18	0.44
1:C:225:ALA:HA	1:C:382:GLY:O	2.18	0.44
1:C:471:VAL:O	1:C:471:VAL:HG22	2.17	0.44
2:D:276:GLU:HA	3:D:655:HOH:O	2.17	0.44
1:C:296:VAL:HA	3:C:649:HOH:O	2.17	0.43
2:D:378:VAL:HG12	2:D:382:LEU:HD12	2.00	0.43
2:D:84:VAL:HG23	2:D:241:VAL:HG22	2.00	0.43
1:A:285:THR:CG2	1:A:287:LEU:HD23	2.48	0.43
1:A:471:VAL:O	1:A:471:VAL:HG22	2.18	0.43
1:C:346:ALA:HB3	1:C:350:TYR:O	2.17	0.43
1:C:465:GLN:HG3	3:C:590:HOH:O	2.18	0.43
1:C:482:LEU:HA	3:C:647:HOH:O	2.18	0.43
2:D:231:ARG:HD2	2:D:266:ALA:HB2	1.99	0.43
2:D:336:GLN:OE1	3:D:473:HOH:O	2.21	0.43
1:C:291:THR:HG1	1:C:294:MET:HG3	1.79	0.43
2:B:115:THR:HB	3:B:568:HOH:O	2.19	0.43
2:B:198:GLN:NE2	2:B:201:LEU:HD23	2.34	0.43
2:B:204:PHE:O	2:B:208:PHE:HD1	2.01	0.43
1:C:406:PHE:O	1:C:427:SER:HB3	2.18	0.43
1:A:187:TRP:CD2	1:A:188:PRO:HD2	2.54	0.43
1:A:227:PRO:O	1:A:228:GLY:C	2.57	0.43
1:A:257:GLU:CG	1:A:262:MET:CE	2.96	0.43
1:A:390:ASP:OD1	1:A:390:ASP:N	2.51	0.43
2:B:450:GLU:HB3	3:B:490:HOH:O	2.18	0.43
1:A:202:ASN:C	1:A:202:ASN:HD22	2.21	0.43
1:A:498:ASN:CG	1:A:501:HIS:HB2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LYS:O	1:C:235:SER:C	2.57	0.43
1:C:252:TYR:CD2	1:C:252:TYR:C	2.92	0.43
1:C:404:GLY:C	1:C:431:PHE:CE1	2.92	0.43
1:A:73:VAL:HB	1:A:189:VAL:HG12	1.99	0.43
1:A:285:THR:HG22	1:A:287:LEU:CD2	2.49	0.43
2:B:343:LEU:HD11	2:B:353:ASP:HB3	2.01	0.43
1:C:203:THR:HG22	1:C:220:MET:HB2	2.01	0.43
1:C:258:ARG:HB2	1:C:261:GLU:HB2	2.00	0.43
1:C:481:ARG:NH1	1:C:536:ILE:CD1	2.72	0.43
1:C:85:ASP:OD1	1:C:85:ASP:C	2.56	0.43
2:D:377:GLN:HE22	2:D:455:SER:HB3	1.83	0.43
1:A:351:PRO:HB3	3:A:601:HOH:O	2.19	0.43
1:A:466:GLU:O	1:A:469:GLN:HB3	2.19	0.43
1:A:535:SER:HB3	1:A:538:GLU:HB2	2.01	0.43
2:B:229:ILE:HG22	3:B:505:HOH:O	2.19	0.43
1:C:285:THR:HG22	1:C:287:LEU:HD23	2.01	0.43
1:C:338:SER:O	1:C:343:GLU:HG3	2.19	0.43
1:C:352:PRO:HD2	3:C:762:HOH:O	2.18	0.43
1:C:514:GLY:HA2	1:C:563:PHE:CE2	2.54	0.43
2:D:63:THR:N	3:D:571:HOH:O	2.47	0.43
1:A:344:MET:HA	1:A:345:PRO:HD3	1.88	0.42
1:C:424:TRP:HH2	3:C:690:HOH:O	2.02	0.42
1:A:86:GLY:HA2	1:A:288:ILE:HG21	2.01	0.42
2:B:174:ARG:NH1	2:B:177:LEU:HG	2.34	0.42
2:B:84:VAL:HG23	2:B:241:VAL:HG22	2.02	0.42
1:C:125:PRO:HA	1:C:157:VAL:HG12	2.00	0.42
1:C:285:THR:CG2	1:C:287:LEU:HD23	2.49	0.42
1:C:447:TYR:CB	3:C:707:HOH:O	2.55	0.42
1:C:27:ILE:HD11	1:C:71:LEU:HB2	2.01	0.42
2:D:335:GLY:N	2:D:360:ARG:HD3	2.35	0.42
1:A:234:LYS:CD	3:A:718:HOH:O	2.67	0.42
1:A:241:LEU:O	1:A:245:SER:HB3	2.20	0.42
1:A:349:GLY:HA3	3:A:588:HOH:O	2.19	0.42
2:B:336:GLN:HB3	2:B:336:GLN:HE21	1.61	0.42
1:C:285:THR:CG2	1:C:287:LEU:CD2	2.98	0.42
1:C:81:ASN:O	1:C:81:ASN:ND2	2.52	0.42
2:D:149:LYS:HG2	2:D:149:LYS:H	1.67	0.42
2:D:387:ALA:N	3:D:687:HOH:O	2.45	0.42
1:A:196:GLN:HE21	1:A:196:GLN:HB2	1.68	0.42
1:A:252:TYR:CD2	1:A:252:TYR:O	2.72	0.42
1:A:357:ARG:O	1:A:359:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:PHE:C	1:A:522:PHE:CD2	2.92	0.42
2:D:107:THR:HA	2:D:108:PRO:HD3	1.89	0.42
2:D:185:GLU:N	2:D:186:PRO:CD	2.82	0.42
2:D:60:PHE:CD1	2:D:229:ILE:HG21	2.55	0.42
1:C:417:ARG:HH21	2:D:453:ARG:HD3	1.84	0.42
1:A:513:TYR:HD1	3:A:726:HOH:O	2.02	0.42
2:B:125:ARG:O	2:B:300:VAL:HG23	2.19	0.42
2:B:143:THR:H	2:B:362:MET:HG3	1.84	0.42
2:B:269:GLU:CB	3:B:511:HOH:O	2.67	0.42
2:B:36:LYS:HB3	2:B:42:VAL:HG22	2.02	0.42
1:C:20:LEU:CD2	3:C:600:HOH:O	2.66	0.42
1:C:438:TRP:O	1:C:442:ASN:HB2	2.20	0.42
1:C:498:ASN:CG	1:C:501:HIS:HB2	2.40	0.42
2:D:269:GLU:C	2:D:271:GLY:N	2.72	0.42
2:D:304:LYS:HE2	3:D:543:HOH:O	2.19	0.42
1:C:344:MET:HA	1:C:345:PRO:HD3	1.89	0.42
1:C:468:VAL:HG22	1:C:476:LEU:HD11	2.01	0.42
1:C:90:PRO:HD2	1:C:108:VAL:HG23	2.01	0.42
2:D:233:LEU:HD23	3:D:524:HOH:O	2.19	0.42
2:B:340:SER:N	3:B:501:HOH:O	2.52	0.42
2:D:106:ILE:HB	3:D:504:HOH:O	2.19	0.42
2:D:281:ARG:NH2	2:D:322:THR:OG1	2.53	0.42
1:A:418:HIS:CB	3:A:701:HOH:O	2.59	0.42
2:B:339:LEU:HA	2:B:351:PRO:O	2.19	0.42
2:B:91:ARG:NH1	2:B:106:ILE:CG2	2.83	0.42
1:C:77:PRO:HG2	1:C:183:MET:HE3	2.01	0.42
1:A:355:ALA:O	1:A:356:ALA:C	2.58	0.42
2:B:107:THR:HA	2:B:108:PRO:HD3	1.87	0.42
2:B:162:GLU:OE2	3:B:468:HOH:O	2.22	0.42
1:C:447:TYR:CB	1:C:448:PRO:HD3	2.42	0.42
2:D:125:ARG:O	2:D:300:VAL:HG23	2.20	0.42
2:B:60:PHE:CD1	2:B:229:ILE:HG21	2.54	0.42
2:D:127:PRO:HB3	2:D:146:ARG:O	2.20	0.42
2:D:24:ALA:O	2:D:26:ASP:N	2.53	0.42
2:D:304:LYS:HE3	3:D:530:HOH:O	2.20	0.42
2:D:99:PRO:O	2:D:100:ILE:HD13	2.19	0.42
1:A:150:PRO:HG3	1:A:185:HIS:CB	2.50	0.41
1:A:301:ALA:O	1:A:302:SER:C	2.58	0.41
1:A:367:LYS:CD	3:A:720:HOH:O	2.57	0.41
1:A:422:ILE:HG13	1:A:423:ASN:N	2.35	0.41
1:C:450:LEU:HD13	3:C:642:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:LEU:O	2:D:369:GLY:O	2.38	0.41
1:A:216:PHE:CA	1:A:429:SER:HB2	2.50	0.41
1:C:390:ASP:C	1:C:392:SER:H	2.24	0.41
1:C:485:GLU:OE1	1:C:488:ARG:CZ	2.68	0.41
1:C:76:GLY:HA2	1:C:312:TYR:OH	2.20	0.41
2:D:20:PHE:CD1	2:D:20:PHE:N	2.88	0.41
2:D:27:LEU:O	2:D:50:VAL:HG11	2.20	0.41
1:A:27:ILE:HD13	1:A:71:LEU:HA	2.02	0.41
1:C:325:ASP:HA	1:C:326:SER:HA	1.58	0.41
1:C:336:GLU:HG3	3:D:472:HOH:O	2.20	0.41
1:C:408:ARG:HB2	3:C:682:HOH:O	2.20	0.41
1:C:512:ALA:HB3	3:C:623:HOH:O	2.20	0.41
1:C:515:ILE:O	1:C:519:ILE:HG13	2.21	0.41
2:D:248:GLU:O	2:D:249:HIS:CD2	2.73	0.41
2:D:277:ILE:H	2:D:277:ILE:HG12	1.55	0.41
1:A:338:SER:N	3:A:627:HOH:O	2.47	0.41
1:A:367:LYS:CE	3:A:713:HOH:O	2.65	0.41
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.39	0.41
1:A:443:VAL:HG21	3:A:771:HOH:O	2.20	0.41
1:A:481:ARG:NH1	1:A:536:ILE:CD1	2.75	0.41
2:B:233:LEU:O	2:B:237:MET:HG2	2.20	0.41
1:C:162:PRO:O	1:C:163:ALA:C	2.58	0.41
1:C:8:LYS:CB	3:C:809:HOH:O	2.68	0.41
1:A:257:GLU:CG	1:A:262:MET:HE2	2.50	0.41
1:C:212:LEU:O	1:C:217:PRO:CA	2.68	0.41
1:C:410:ASP:O	1:C:421:ALA:HB1	2.21	0.41
1:C:439:TYR:CD2	3:C:801:HOH:O	2.74	0.41
2:D:132:GLN:O	2:D:171:ALA:HA	2.20	0.41
1:A:252:TYR:O	1:A:252:TYR:HD2	2.03	0.41
1:A:454:ILE:HG13	1:A:516:MET:HG3	2.02	0.41
1:A:514:GLY:HA2	1:A:563:PHE:CE2	2.56	0.41
2:B:90:GLY:HA2	2:B:214:LEU:O	2.20	0.41
1:A:542:LEU:HD21	1:A:577:LEU:HD11	2.03	0.41
1:A:93:ARG:HA	1:A:93:ARG:HH11	1.85	0.41
2:B:314:LEU:O	2:B:314:LEU:HD12	2.21	0.41
2:B:325:ILE:HB	2:B:326:PRO:CD	2.50	0.41
1:C:193:ARG:HA	1:C:194:PRO:HD3	1.91	0.41
2:D:338:GLN:HB2	3:D:559:HOH:O	2.13	0.41
2:D:381:GLN:NE2	3:D:552:HOH:O	2.49	0.41
1:A:322:LEU:HB3	3:A:688:HOH:O	2.20	0.41
1:A:447:TYR:CB	1:A:448:PRO:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ARG:NE	2:B:101:ASP:OD2	2.47	0.41
2:B:362:MET:HE3	2:B:366:VAL:HG11	2.02	0.41
2:B:78:ASP:HB2	3:B:482:HOH:O	2.20	0.41
1:C:542:LEU:HA	1:C:543:PRO:HD3	1.80	0.41
1:A:232:SER:OG	1:A:421:ALA:HB3	2.20	0.41
1:A:74:GLU:CD	1:A:113:ARG:NH2	2.74	0.41
1:A:90:PRO:HD2	1:A:108:VAL:HG23	2.02	0.41
1:A:99:GLY:HA3	1:C:124:LYS:HZ3	1.85	0.41
1:C:346:ALA:HB2	1:C:352:PRO:HD3	2.03	0.41
1:C:420:PRO:O	1:C:422:ILE:N	2.47	0.41
2:D:110:LYS:HE2	2:D:110:LYS:HB3	1.97	0.41
1:A:501:HIS:O	1:A:505:ALA:CB	2.63	0.41
1:A:542:LEU:HA	1:A:543:PRO:HD3	1.82	0.41
1:A:567:MET:HE3	1:A:567:MET:HB2	1.86	0.41
2:B:277:ILE:HG12	2:B:277:ILE:H	1.51	0.41
1:C:216:PHE:N	1:C:217:PRO:CD	2.83	0.41
1:C:282:MET:HE1	1:C:287:LEU:HD21	2.03	0.41
1:C:41:ARG:HB3	1:C:48:PHE:HB2	2.02	0.41
1:C:73:VAL:HB	1:C:189:VAL:HG12	2.02	0.41
1:A:183:MET:HB3	1:A:183:MET:HE2	1.71	0.40
1:A:332:GLU:HG3	3:A:677:HOH:O	2.13	0.40
1:A:374:GLU:HB2	3:A:730:HOH:O	2.20	0.40
1:A:416:ARG:HB3	3:A:701:HOH:O	2.20	0.40
2:D:325:ILE:HB	2:D:326:PRO:HD3	2.02	0.40
1:A:335:ARG:HD3	1:A:349:GLY:O	2.21	0.40
1:C:292:SER:HB3	2:D:292:ALA:HB1	2.02	0.40
1:A:348:GLU:OE1	1:A:348:GLU:CA	2.68	0.40
1:A:464:LEU:O	1:A:468:VAL:HG23	2.21	0.40
2:B:317:PRO:HG2	2:B:323:HIS:CE1	2.57	0.40
2:B:340:SER:HB3	2:B:343:LEU:HG	2.03	0.40
2:B:353:ASP:O	2:B:356:PRO:HD2	2.22	0.40
2:B:415:ALA:HB2	3:B:472:HOH:O	2.21	0.40
2:B:442:LEU:HD23	3:B:551:HOH:O	2.20	0.40
1:C:337:ILE:HD12	1:C:337:ILE:H	1.85	0.40
1:C:74:GLU:OE2	1:C:113:ARG:NH2	2.53	0.40
1:A:225:ALA:HA	1:A:382:GLY:O	2.21	0.40
1:A:86:GLY:N	1:A:290:ASN:OD1	2.53	0.40
1:A:447:TYR:CB	1:A:448:PRO:CD	2.93	0.40
1:A:459:GLN:O	1:A:462:ALA:HB3	2.21	0.40
1:A:466:GLU:HB3	3:A:698:HOH:O	2.21	0.40
2:B:350:PRO:HA	2:B:351:PRO:HD2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLY:HA3	3:C:743:HOH:O	2.21	0.40
1:C:394:PRO:CD	3:C:780:HOH:O	2.69	0.40
1:C:454:ILE:HG13	1:C:516:MET:HG3	2.04	0.40
2:D:419:GLU:HA	2:D:423:ILE:HB	2.03	0.40
2:D:86:LYS:HZ2	2:D:249:HIS:CE1	2.39	0.40
2:B:277:ILE:HA	2:B:278:PRO:HD3	1.83	0.40
1:C:357:ARG:NH1	1:C:357:ARG:HG3	2.32	0.40
1:C:357:ARG:O	1:C:359:ALA:N	2.54	0.40
1:C:38:GLU:CD	1:C:52:TYR:OH	2.59	0.40
2:D:154:SER:CB	3:D:566:HOH:O	2.68	0.40

All (2) 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)
2:B:410:ARG:NH2	1:C:478:ASP:OD2[6_555]	2.13	0.07
3:A:653:HOH:O	3:B:704:HOH:O[2_665]	2.14	0.06

## 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	576/578 (100%)	512 (89%)	51 (9%)	13 (2%)	7	25
1	C	576/578 (100%)	504 (88%)	61 (11%)	11 (2%)	9	30
2	B	458/464 (99%)	407 (89%)	43 (9%)	8 (2%)	11	34
2	D	458/464 (99%)	408 (89%)	41 (9%)	9 (2%)	9	28
All	All	2068/2084 (99%)	1831 (88%)	196 (10%)	41 (2%)	9	28

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLY
1	A	235	SER
1	A	555	SER
2	B	281	ARG
2	B	346	LYS
1	C	228	GLY
1	C	555	SER
2	D	25	LYS
2	D	281	ARG
2	D	346	LYS
1	A	302	SER
1	A	341	LEU
1	A	421	ALA
2	B	25	LYS
2	B	383	TYR
2	B	384	SER
1	C	235	SER
1	C	302	SER
1	C	341	LEU
2	D	275	GLU
2	D	383	TYR
2	D	384	SER
1	A	386	PRO
1	A	444	ALA
2	B	275	GLU
1	C	386	PRO
1	C	444	ALA
1	A	236	VAL
1	C	358	LEU
1	A	152	ASP
1	A	387	PRO
2	B	459	ILE
1	C	387	PRO
1	C	421	ALA
1	A	44	GLY
1	A	197	ARG
1	C	201	PRO
2	B	351	PRO
2	D	459	ILE
2	D	270	ILE
2	D	351	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/468 (100%)	425 (91%)	43 (9%)	11	30
1	C	468/468 (100%)	419 (90%)	49 (10%)	8	23
2	B	386/390 (99%)	352 (91%)	34 (9%)	12	33
2	D	386/390 (99%)	354 (92%)	32 (8%)	13	36
All	All	1708/1716 (100%)	1550 (91%)	158 (9%)	10	30

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	LEU
1	A	28	SER
1	A	53	GLU
1	A	56	SER
1	A	67	THR
1	A	73	VAL
1	A	93	ARG
1	A	103	THR
1	A	107	VAL
1	A	111	LEU
1	A	137	THR
1	A	154	ARG
1	A	202	ASN
1	A	207	THR
1	A	211	ILE
1	A	212	LEU
1	A	216	PHE
1	A	240	SER
1	A	241	LEU
1	A	253	VAL
1	A	255	SER
1	A	261	GLU
1	A	263	THR

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Mol	Chain	Res	Type
1	A	323	MET
1	A	327	THR
1	A	336	GLU
1	A	344	MET
1	A	347	GLU
1	A	348	GLU
1	A	357	ARG
1	A	369	ILE
1	A	408	ARG
1	A	422	ILE
1	A	441	GLU
1	A	449	GLU
1	A	451	ARG
1	A	461	GLU
1	A	467	ILE
1	A	474	ASP
1	A	477	GLN
1	A	516	MET
1	A	547	ARG
2	B	19	LEU
2	B	21	VAL
2	B	50	VAL
2	B	63	THR
2	B	78	ASP
2	B	103	LEU
2	B	107	THR
2	B	110	LYS
2	B	114	ILE
2	B	115	THR
2	B	130	PHE
2	B	145	VAL
2	B	149	LYS
2	B	156	SER
2	B	158	LEU
2	B	174	ARG
2	B	199	ARG
2	B	201	LEU
2	B	202	SER
2	B	211	THR
2	B	217	SER
2	B	258	THR
2	B	268	ARG

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Mol	Chain	Res	Type
2	B	274	ARG
2	B	277	ILE
2	B	305	LYS
2	B	336	GLN
2	B	345	ARG
2	B	362	MET
2	B	364	ASN
2	B	370	LYS
2	B	373	GLU
2	B	384	SER
2	B	432	ILE
1	C	2	ILE
1	C	3	GLN
1	C	20	LEU
1	C	27	ILE
1	C	53	GLU
1	C	56	SER
1	C	67	THR
1	C	73	VAL
1	C	93	ARG
1	C	103	THR
1	C	107	VAL
1	C	111	LEU
1	C	137	THR
1	C	138	VAL
1	C	154	ARG
1	C	202	ASN
1	C	207	THR
1	C	211	ILE
1	C	212	LEU
1	C	216	PHE
1	C	240	SER
1	C	241	LEU
1	C	253	VAL
1	C	255	SER
1	C	261	GLU
1	C	263	THR
1	C	284	ARG
1	C	323	MET
1	C	327	THR
1	C	336	GLU
1	C	344	MET

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Mol	Chain	Res	Type
1	C	347	GLU
1	C	348	GLU
1	C	357	ARG
1	C	369	ILE
1	C	408	ARG
1	C	412	SER
1	C	422	ILE
1	C	432	THR
1	C	441	GLU
1	C	449	GLU
1	C	451	ARG
1	C	461	GLU
1	C	467	ILE
1	C	474	ASP
1	C	477	GLN
1	C	493	ASP
1	C	516	MET
1	C	547	ARG
2	D	19	LEU
2	D	21	VAL
2	D	50	VAL
2	D	63	THR
2	D	78	ASP
2	D	103	LEU
2	D	107	THR
2	D	110	LYS
2	D	114	ILE
2	D	115	THR
2	D	130	PHE
2	D	142	ASN
2	D	149	LYS
2	D	156	SER
2	D	158	LEU
2	D	199	ARG
2	D	201	LEU
2	D	202	SER
2	D	211	THR
2	D	258	THR
2	D	268	ARG
2	D	274	ARG
2	D	277	ILE
2	D	315	SER

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Mol	Chain	Res	Type
2	D	336	GLN
2	D	345	ARG
2	D	364	ASN
2	D	370	LYS
2	D	373	GLU
2	D	384	SER
2	D	432	ILE
2	D	446	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	202	ASN
1	A	496	GLN
1	A	541	GLN
2	B	129	GLN
2	B	142	ASN
2	B	198	GLN
2	B	323	HIS
2	B	336	GLN
2	B	338	GLN
2	B	407	ASN
1	C	3	GLN
1	C	196	GLN
1	C	202	ASN
1	C	496	GLN
1	C	541	GLN
2	D	129	GLN
2	D	142	ASN
2	D	198	GLN
2	D	206	GLN
2	D	323	HIS
2	D	336	GLN
2	D	344	HIS
2	D	407	ASN

### 5.3.3 RNA ⓘ

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	578/578 (100%)	0.27	16 (2%) 53 43	9, 29, 57, 63	0
1	C	578/578 (100%)	0.31	15 (2%) 56 45	9, 29, 57, 63	0
2	B	460/464 (99%)	0.19	10 (2%) 62 52	5, 28, 54, 67	0
2	D	460/464 (99%)	0.26	20 (4%) 36 26	5, 28, 54, 67	0
All	All	2076/2084 (99%)	0.26	61 (2%) 52 41	5, 29, 56, 67	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	464	GLY	5.5
2	B	401	GLU	5.1
2	D	395	LEU	5.1
2	D	400	GLY	4.9
1	C	388	GLY	4.7
2	B	402	ASP	4.6
2	B	396	VAL	4.2
1	C	387	PRO	4.0
2	D	396	VAL	3.9
2	D	401	GLU	3.8
2	B	421	PHE	3.8
1	C	469	GLN	3.6
1	A	242	ALA	3.6
1	A	470	LEU	3.6
1	C	521	ALA	3.4
1	C	578	ALA	3.3
2	D	181	GLY	3.2
1	A	570	ILE	3.2
2	D	446	LEU	3.1
2	B	403	ALA	3.1
2	D	388	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	345	ARG	3.0
2	D	183	LYS	2.9
1	C	474	ASP	2.9
1	C	1	MET	2.9
1	A	20	LEU	2.9
1	C	572	GLY	2.8
2	B	180	GLU	2.8
2	D	402	ASP	2.8
1	A	537	ASP	2.8
1	A	1	MET	2.7
1	C	143	PHE	2.7
1	C	574	PHE	2.7
1	A	460	ARG	2.7
2	D	184	GLU	2.6
1	C	535	SER	2.5
2	D	421	PHE	2.5
1	A	227	PRO	2.5
2	D	392	ILE	2.5
2	B	418	PHE	2.5
1	A	578	ALA	2.5
1	A	211	ILE	2.5
1	C	467	ILE	2.5
1	A	526	ALA	2.4
1	A	522	PHE	2.3
2	B	398	ILE	2.3
1	C	355	ALA	2.3
1	A	520	LEU	2.3
1	A	541	GLN	2.3
2	D	140	VAL	2.3
2	B	181	GLY	2.3
1	A	521	ALA	2.3
2	D	399	ILE	2.2
2	D	424	ASN	2.2
2	D	346	LYS	2.2
2	B	408	ASP	2.2
1	A	510	LYS	2.1
1	C	475	ALA	2.1
2	D	9	THR	2.1
2	D	355	LEU	2.0
1	C	409	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.