Full wwPDB X-ray Structure Validation Report (i)

Dec 11, 2022 – 12:29 AM EST

PDB ID	:	1M7X
Title	:	The X-ray Crystallographic Structure of Branching Enzyme
Authors	:	Abad, M.C.; Binderup, K.; Rios-Steiner, J.; Arni, R.K.; Preiss, J.; Geiger, J.H.
Deposited on	:	2002-07-23
Resolution	:	2.30 Å(reported)

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

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

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

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

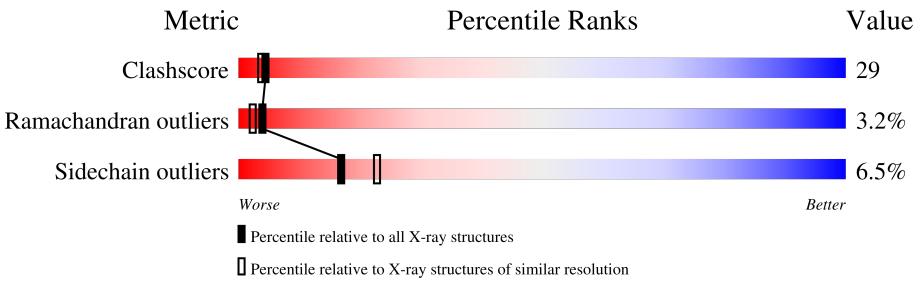
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	617	51% 37% 7% 5%
1	B	617	54% 35% 7% .
1	C	617	42% 45% 6% 6%
1	D	617	53% 37% 5% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20372 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 1,4-alpha-glucan Branching Enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	587	4823	3083	857	867	16	0	0	0
1	B	591	4852	3102	859	876	15	0	0	0
1	C	578	4750	3041	840	854	15	0	0	0
1	D	585	4805	3072	853	864	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	MET	-	initiating methionine	UNP P07762
B	112	MET	-	initiating methionine	UNP P07762
C	112	MET	-	initiating methionine	UNP P07762
D	112	MET	-	initiating methionine	UNP P07762

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	301	301	301	0	0
2	B	425	425	425	0	0
2	C	108	108	108	0	0
2	D	308	308	308	0	0

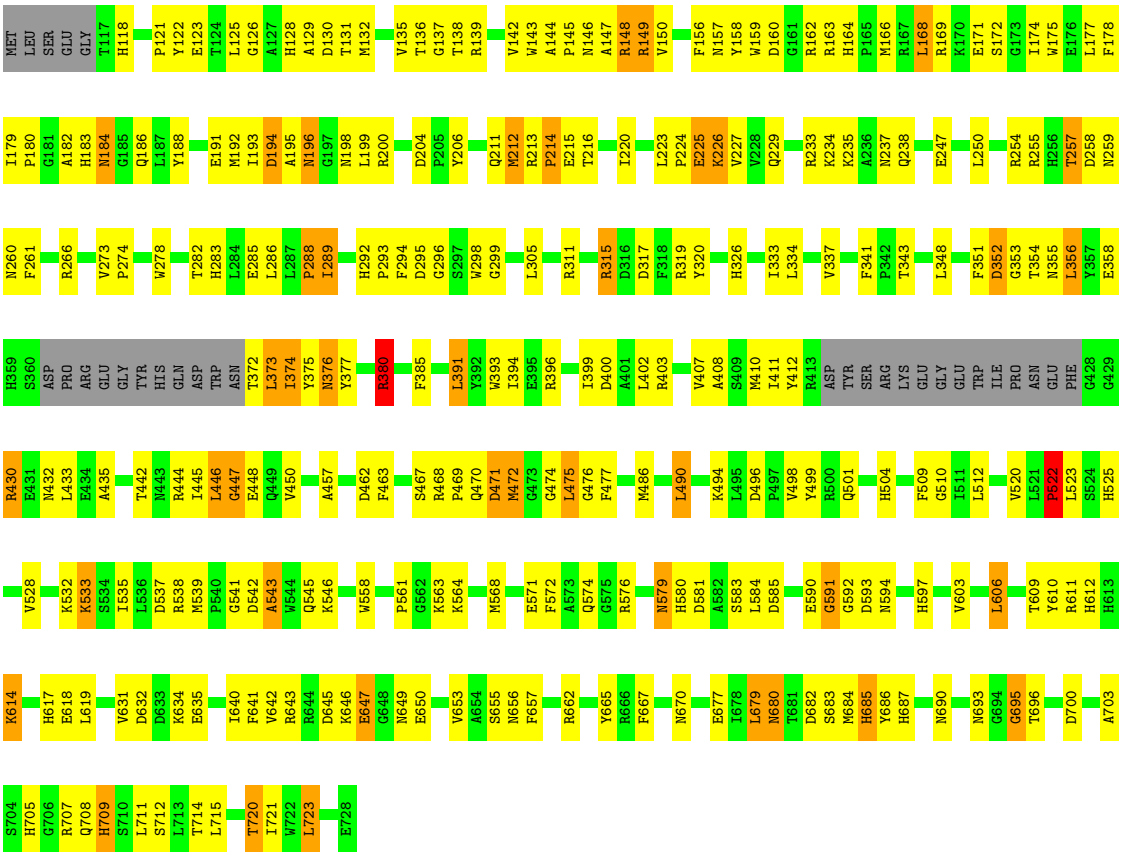
3 Residue-property plots (i)

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

Note EDS was not executed.

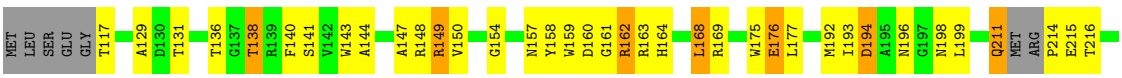
• Molecule 1: 1,4-alpha-glucan Branching Enzyme

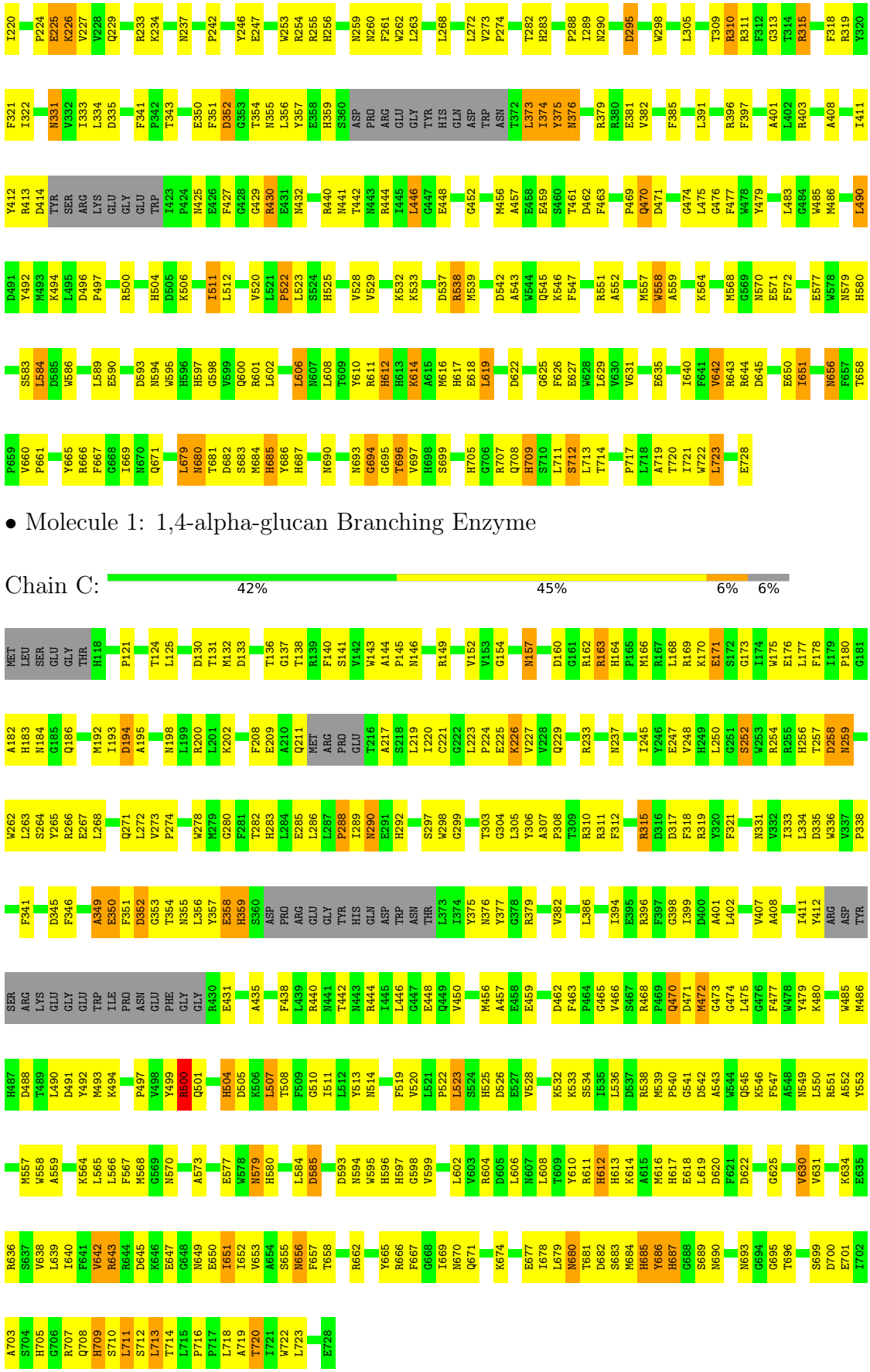
Chain A: 51% 37% 7% 5%



• Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain B: 54% 35% 7% •



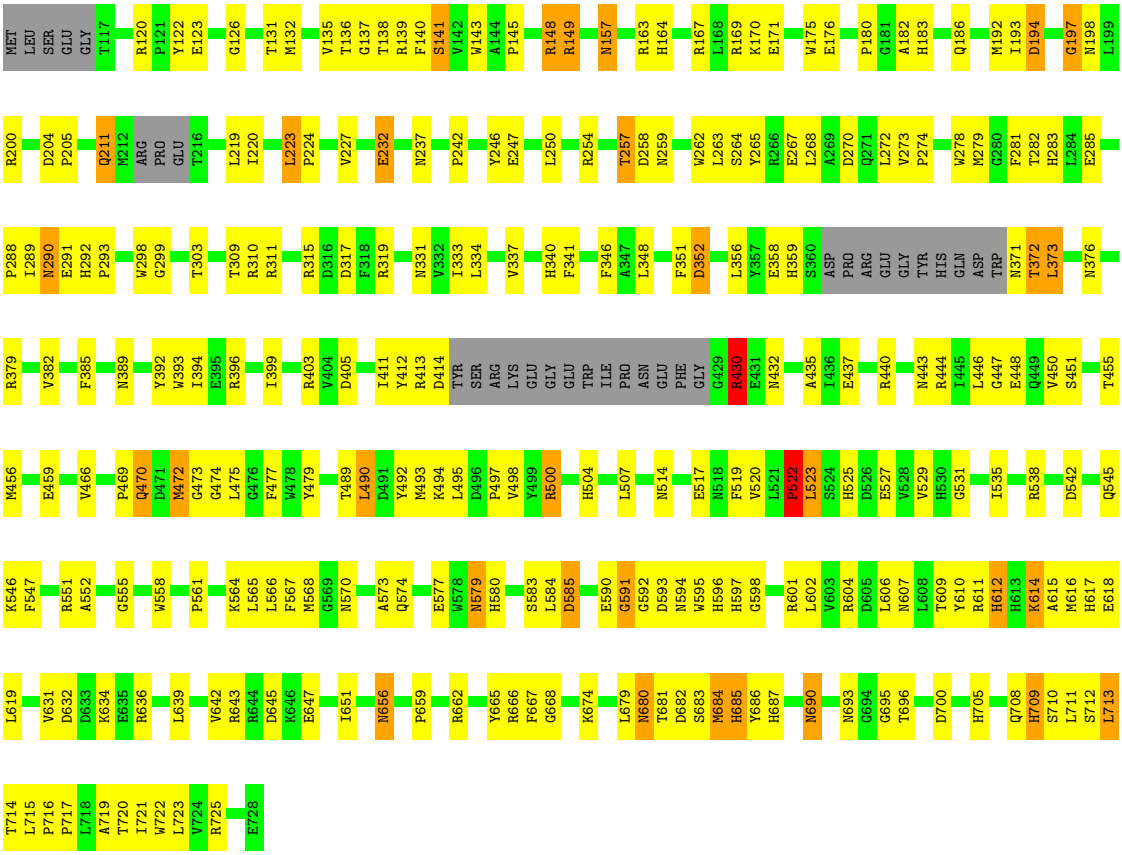


• Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain C: 42% 45% 6% 6%

• Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain D: 53% 37% 5% 5%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.47Å 102.62Å 185.06Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20372	wwPDB-VP
Average B, all atoms ($Å^2$)	23.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.40	0/4976	0.68	1/6756 (0.0%)
1	B	0.42	0/5006	0.70	2/6797 (0.0%)
1	C	0.39	0/4900	0.61	0/6653
1	D	0.42	0/4956	0.69	1/6728 (0.0%)
All	All	0.41	0/19838	0.67	4/26934 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	375	TYR	N-CA-C	6.06	127.35	111.00
1	A	685	HIS	N-CA-C	-5.83	95.25	111.00
1	B	685	HIS	N-CA-C	-5.75	95.46	111.00
1	D	685	HIS	N-CA-C	-5.36	96.53	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4823	0	4559	263	0
1	B	4852	0	4571	255	0
1	C	4750	0	4485	325	0
1	D	4805	0	4537	240	0
2	A	301	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	425	0	0	33	0
2	C	108	0	0	21	0
2	D	308	0	0	20	0
All	All	20372	0	18152	1077	0

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 29.

All (1077) 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:C:643:ARG:HB3	1:C:643:ARG:HH11	1.12	1.08
1:A:430:ARG:HB3	1:A:430:ARG:HH21	1.22	1.02
1:C:497:PRO:HA	1:C:500:ARG:HD3	1.42	1.02
1:A:224:PRO:HG2	1:A:396:ARG:HB3	1.38	1.01
1:B:430:ARG:H	1:B:430:ARG:HD2	1.22	1.01
1:A:393:TRP:HB3	1:A:399:ILE:HD12	1.44	1.00
1:D:430:ARG:HB2	1:D:430:ARG:HH11	1.27	0.99
1:D:693:ASN:HD21	1:D:714:THR:H	1.10	0.99
1:B:194:ASP:HB2	1:B:198:ASN:H	1.28	0.99
1:D:470:GLN:H	1:D:470:GLN:NE2	1.59	0.99
1:B:658:THR:HG22	1:B:660:VAL:H	1.24	0.98
1:C:656:ASN:HD21	1:C:658:THR:HG22	1.22	0.98
1:C:224:PRO:HG2	1:C:396:ARG:HB3	1.45	0.97
1:D:211:GLN:HB2	2:D:1534:HOH:O	1.65	0.97
1:B:470:GLN:HA	1:B:474:GLY:HA2	1.45	0.96
1:B:511:ILE:HB	2:B:1888:HOH:O	1.64	0.95
1:C:606:LEU:HD23	1:C:679:LEU:HD11	1.48	0.94
1:B:373:LEU:H	1:B:373:LEU:HD23	1.33	0.91
1:D:470:GLN:H	1:D:470:GLN:HE21	1.00	0.91
1:B:594:ASN:H	1:B:597:HIS:HD2	1.16	0.90
1:B:470:GLN:H	1:B:470:GLN:NE2	1.68	0.90
1:D:376:ASN:ND2	1:D:379:ARG:HB2	1.86	0.90
1:B:164:HIS:HB3	1:B:177:LEU:HD21	1.52	0.89
1:D:594:ASN:H	1:D:597:HIS:HD2	1.18	0.89
1:B:470:GLN:HE21	1:B:470:GLN:N	1.70	0.89
1:C:643:ARG:HH11	1:C:643:ARG:CB	1.86	0.89
1:C:470:GLN:HE21	1:C:470:GLN:H	0.93	0.88
1:C:695:GLY:HA3	1:D:591:GLY:HA2	1.52	0.88
1:C:551:ARG:HG2	1:C:602:LEU:HD22	1.53	0.88
1:C:693:ASN:HD21	1:C:714:THR:H	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ASN:H	1:A:597:HIS:HD2	1.15	0.86
1:C:466:VAL:HA	1:C:475:LEU:HD12	1.58	0.85
1:C:290:ASN:HB3	2:C:833:HOH:O	1.76	0.84
1:C:470:GLN:H	1:C:470:GLN:NE2	1.74	0.84
1:B:430:ARG:H	1:B:430:ARG:CD	1.91	0.84
1:C:229:GLN:HA	1:C:233:ARG:NH1	1.92	0.84
1:A:168:LEU:HD12	1:A:169:ARG:H	1.40	0.83
1:C:643:ARG:HB3	1:C:643:ARG:NH1	1.92	0.83
1:A:224:PRO:CG	1:A:396:ARG:HB3	2.09	0.83
1:C:656:ASN:ND2	1:C:658:THR:HG22	1.94	0.83
1:C:470:GLN:HE21	1:C:470:GLN:N	1.76	0.82
1:C:536:LEU:HD22	1:C:573:ALA:HB1	1.62	0.81
1:C:183:HIS:H	1:C:186:GLN:HE21	1.28	0.81
1:D:470:GLN:HE21	1:D:470:GLN:N	1.78	0.81
1:A:684:MET:H	1:A:690:ASN:HD22	1.22	0.81
1:D:535:ILE:HA	1:D:538:ARG:HD2	1.63	0.81
1:A:684:MET:H	1:A:690:ASN:ND2	1.78	0.81
1:C:520:VAL:O	1:C:522:PRO:HD3	1.81	0.81
1:C:636:ARG:HG2	1:C:662:ARG:NH2	1.96	0.81
1:C:528:VAL:O	1:C:577:GLU:HB2	1.81	0.80
1:A:693:ASN:HD21	1:A:714:THR:H	1.28	0.80
1:A:680:ASN:ND2	1:A:682:ASP:H	1.80	0.80
1:D:674:LYS:HB3	1:D:696:THR:HG21	1.61	0.80
1:A:394:ILE:CD1	1:A:446:LEU:HD21	2.12	0.79
1:A:430:ARG:HB3	1:A:430:ARG:NH2	1.98	0.79
1:C:494:LYS:HG2	1:C:538:ARG:HG2	1.65	0.78
1:D:552:ALA:HA	1:D:720:THR:HG22	1.64	0.78
1:B:594:ASN:H	1:B:597:HIS:CD2	2.01	0.77
1:B:558:TRP:HA	1:B:564:LYS:HE3	1.67	0.77
1:D:469:PRO:HG2	1:D:472:MET:HG3	1.66	0.77
1:B:194:ASP:HB2	1:B:198:ASN:N	1.99	0.77
1:D:358:GLU:HG3	1:D:373:LEU:HD12	1.66	0.76
1:C:229:GLN:HA	1:C:233:ARG:HH11	1.47	0.76
1:C:505:ASP:HA	1:C:508:THR:OG1	1.85	0.76
1:D:594:ASN:H	1:D:597:HIS:CD2	2.01	0.76
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.18	0.76
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.65	0.76
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.67	0.76
1:C:552:ALA:HA	1:C:720:THR:HG22	1.66	0.76
1:A:594:ASN:H	1:A:597:HIS:CD2	2.02	0.76
1:C:611:ARG:O	1:C:612:HIS:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.20	0.76
1:C:551:ARG:HB3	1:C:681:THR:CG2	2.16	0.76
1:A:683:SER:O	1:A:685:HIS:O	2.04	0.76
1:A:305:LEU:HD11	2:A:1198:HOH:O	1.85	0.76
1:D:192:MET:SD	1:D:352:ASP:HA	2.25	0.76
1:B:528:VAL:O	1:B:577:GLU:HB2	1.85	0.76
1:C:542:ASP:O	1:C:546:LYS:HG2	1.86	0.75
1:D:667:PHE:HA	1:D:705:HIS:CD2	2.22	0.75
1:A:238:GLN:HG2	2:A:1759:HOH:O	1.87	0.75
1:C:594:ASN:H	1:C:597:HIS:HD2	1.35	0.75
1:D:292:HIS:O	1:D:311:ARG:NH1	2.19	0.75
1:C:639:LEU:HD12	1:C:639:LEU:H	1.52	0.75
1:A:709:HIS:N	2:A:1907:HOH:O	2.20	0.75
1:B:225:GLU:O	1:B:226:LYS:HB2	1.85	0.75
1:C:211:GLN:HG3	1:C:217:ALA:H	1.52	0.74
1:A:680:ASN:HD22	1:A:682:ASP:H	1.35	0.74
1:A:233:ARG:HD2	1:A:400:ASP:OD2	1.87	0.74
1:B:470:GLN:H	1:B:470:GLN:HE21	0.84	0.74
1:B:168:LEU:HD22	1:B:169:ARG:N	2.02	0.74
1:B:357:TYR:O	1:B:375:TYR:O	2.06	0.73
1:B:589:LEU:O	1:B:590:GLU:HB3	1.88	0.73
1:B:684:MET:H	1:B:690:ASN:HD22	1.36	0.73
1:A:520:VAL:O	1:A:522:PRO:HD3	1.88	0.73
1:C:248:VAL:HG23	1:C:286:LEU:HD23	1.71	0.73
1:C:145:PRO:HB3	1:C:173:GLY:HA3	1.72	0.72
1:A:212:MET:SD	1:A:293:PRO:HA	2.30	0.72
1:B:520:VAL:O	1:B:522:PRO:HD3	1.88	0.72
1:C:456:MET:HG2	1:C:479:TYR:HB2	1.71	0.72
1:A:162:ARG:O	1:A:162:ARG:HG2	1.90	0.72
1:C:198:ASN:HB3	1:C:200:ARG:NH1	2.04	0.72
1:D:145:PRO:HD2	1:D:356:LEU:HD11	1.71	0.72
1:C:334:LEU:HD22	2:C:1891:HOH:O	1.89	0.71
1:A:149:ARG:CZ	1:A:193:ILE:HD11	2.21	0.71
1:B:194:ASP:CB	1:B:198:ASN:H	2.03	0.71
1:A:148:ARG:O	1:A:149:ARG:HB3	1.89	0.71
1:C:680:ASN:ND2	1:C:682:ASP:H	1.89	0.71
1:D:674:LYS:HB3	1:D:696:THR:CG2	2.21	0.71
1:C:440:ARG:HG2	1:C:475:LEU:H	1.55	0.71
1:A:680:ASN:HD22	1:A:680:ASN:C	1.94	0.71
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.89	0.71
1:A:380:ARG:HG2	1:A:380:ARG:HH21	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASP:OD2	1:B:311:ARG:NH2	2.23	0.70
1:C:667:PHE:HA	1:C:705:HIS:HD2	1.57	0.70
1:B:149:ARG:HD3	2:B:1846:HOH:O	1.90	0.70
1:B:658:THR:HG22	1:B:660:VAL:N	2.02	0.69
1:D:139:ARG:HD3	1:D:176:GLU:OE1	1.92	0.69
1:A:708:GLN:O	1:A:709:HIS:HB2	1.92	0.69
1:B:533:LYS:HD2	1:B:537:ASP:HB3	1.74	0.69
1:A:684:MET:N	1:A:690:ASN:HD22	1.90	0.69
1:A:618:GLU:OE2	1:A:645:ASP:HB2	1.92	0.69
1:B:373:LEU:H	1:B:373:LEU:CD2	2.03	0.69
1:D:430:ARG:HB2	1:D:430:ARG:NH1	2.05	0.69
1:D:616:MET:SD	1:D:651:ILE:HG12	2.32	0.69
1:B:237:ASN:ND2	1:B:283:HIS:HE1	1.91	0.69
1:B:644:ARG:HG2	1:B:650:GLU:HB3	1.74	0.69
1:C:490:LEU:O	1:C:494:LYS:HG3	1.93	0.69
1:D:232:GLU:H	1:D:232:GLU:CD	1.94	0.69
1:B:147:ALA:O	1:B:193:ILE:O	2.11	0.68
1:B:355:ASN:HB2	2:B:1485:HOH:O	1.92	0.68
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.22	0.68
1:C:552:ALA:HB2	1:C:719:ALA:HA	1.74	0.68
1:B:568:MET:HB2	1:B:584:LEU:HD11	1.73	0.68
1:D:611:ARG:O	1:D:612:HIS:HB3	1.93	0.68
1:A:132:MET:HB2	1:A:135:VAL:HG13	1.74	0.68
1:C:593:ASP:HA	1:C:597:HIS:CD2	2.28	0.68
1:A:168:LEU:CD1	1:A:169:ARG:H	2.07	0.68
1:A:213:ARG:HB2	1:A:214:PRO:HD3	1.75	0.68
1:A:118:HIS:CE1	1:A:380:ARG:HH22	2.12	0.68
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.76	0.68
1:D:594:ASN:N	1:D:597:HIS:HD2	1.92	0.68
1:A:535:ILE:HD11	2:A:1206:HOH:O	1.93	0.68
1:A:618:GLU:HG2	1:A:646:LYS:HE3	1.76	0.67
1:D:250:LEU:HD22	1:D:268:LEU:HD13	1.76	0.67
1:C:647:GLU:HB3	1:C:649:ASN:ND2	2.10	0.67
1:A:132:MET:HB2	1:A:135:VAL:CG1	2.25	0.67
1:D:574:GLN:NE2	1:D:584:LEU:O	2.27	0.67
1:C:444:ARG:O	1:C:448:GLU:HG3	1.94	0.67
1:C:639:LEU:HD12	1:C:639:LEU:N	2.10	0.67
1:C:504:HIS:CD2	1:C:634:LYS:HA	2.30	0.66
1:D:555:GLY:HA3	1:D:720:THR:HG21	1.76	0.66
1:A:470:GLN:C	1:A:472:MET:H	1.98	0.66
1:D:285:GLU:OE1	1:D:403:ARG:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:O	1:A:226:LYS:HB2	1.96	0.66
1:C:193:ILE:HA	1:C:198:ASN:O	1.94	0.66
1:B:606:LEU:HD13	1:B:679:LEU:HD11	1.76	0.66
1:B:440:ARG:HE	1:B:474:GLY:HA3	1.60	0.66
1:C:265:TYR:HB2	1:C:317:ASP:HB3	1.76	0.66
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.78	0.66
1:D:373:LEU:HD23	1:D:373:LEU:H	1.61	0.66
1:D:520:VAL:O	1:D:522:PRO:HD3	1.96	0.66
1:B:229:GLN:HG2	1:B:234:LYS:HG3	1.78	0.66
1:B:310:ARG:HH11	1:B:313:GLY:HA2	1.61	0.66
1:A:471:ASP:O	1:A:472:MET:HG3	1.96	0.66
1:C:141:SER:HA	1:C:175:TRP:O	1.96	0.66
1:A:212:MET:HG2	1:A:213:ARG:N	2.11	0.65
1:B:642:VAL:HG22	1:B:650:GLU:HB2	1.78	0.65
1:D:602:LEU:O	1:D:606:LEU:HB2	1.96	0.65
1:D:680:ASN:ND2	1:D:682:ASP:H	1.94	0.65
1:B:693:ASN:HD21	1:B:713:LEU:HB3	1.60	0.65
1:B:224:PRO:HG2	1:B:396:ARG:HB3	1.78	0.65
1:B:247:GLU:OE1	1:B:525:HIS:HD2	1.79	0.65
1:C:650:GLU:HG2	1:C:671:GLN:OE1	1.95	0.65
1:B:225:GLU:HG2	2:B:1464:HOH:O	1.96	0.65
1:A:160:ASP:OD1	1:A:162:ARG:HB3	1.97	0.64
1:A:259:ASN:HB3	1:A:261:PHE:CG	2.32	0.64
1:A:126:GLY:HA2	1:A:204:ASP:OD2	1.97	0.64
1:A:295:ASP:HA	1:A:311:ARG:HH22	1.61	0.64
1:A:655:SER:OG	1:A:720:THR:HB	1.98	0.64
1:B:211:GLN:O	1:B:216:THR:HA	1.97	0.64
1:B:259:ASN:HB3	1:B:261:PHE:CE2	2.33	0.64
1:C:667:PHE:HA	1:C:705:HIS:CD2	2.32	0.64
1:B:289:ILE:HG13	1:B:334:LEU:HD11	1.79	0.64
1:B:350:GLU:HA	1:B:354:THR:O	1.97	0.63
1:B:551:ARG:NH2	2:B:1476:HOH:O	2.32	0.63
1:B:619:LEU:HG	1:B:622:ASP:HB3	1.80	0.63
1:D:376:ASN:HD22	1:D:379:ARG:HB2	1.62	0.63
1:A:149:ARG:HD3	1:A:193:ILE:CG1	2.28	0.63
1:B:627:GLU:HB3	1:B:642:VAL:HG12	1.80	0.63
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.81	0.63
1:B:611:ARG:O	1:B:612:HIS:HB3	1.98	0.63
1:C:140:PHE:O	1:C:176:GLU:HA	1.97	0.63
1:C:551:ARG:HD3	1:C:686:TYR:HB3	1.81	0.63
1:D:469:PRO:HG2	1:D:472:MET:CG	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HG3	1:A:171:GLU:OE1	1.98	0.63
1:B:425:ASN:HD22	1:B:427:PHE:H	1.46	0.63
1:C:168:LEU:HD22	1:C:169:ARG:N	2.13	0.63
1:B:683:SER:O	1:B:685:HIS:O	2.16	0.63
1:C:237:ASN:HD22	1:C:283:HIS:HE1	1.46	0.63
1:A:178:PHE:HE1	1:A:180:PRO:HG3	1.63	0.63
1:C:536:LEU:HB2	1:C:550:LEU:HD22	1.80	0.63
1:A:442:THR:O	1:A:446:LEU:HB2	1.99	0.63
1:D:149:ARG:HG2	2:D:1484:HOH:O	1.99	0.63
1:D:440:ARG:HG2	1:D:475:LEU:H	1.63	0.63
1:B:708:GLN:O	1:B:709:HIS:ND1	2.32	0.62
1:D:665:TYR:O	1:D:712:SER:HA	1.98	0.62
1:B:233:ARG:NH1	2:B:1117:HOH:O	2.32	0.62
1:B:619:LEU:HB3	1:B:625:GLY:HA3	1.80	0.62
1:A:214:PRO:O	1:A:216:THR:N	2.32	0.62
1:B:147:ALA:O	1:B:148:ARG:HB3	1.99	0.62
1:B:611:ARG:O	1:B:612:HIS:CB	2.47	0.62
1:C:684:MET:H	1:C:690:ASN:HD22	1.47	0.62
1:D:143:TRP:CH2	1:D:356:LEU:HD22	2.34	0.62
1:A:494:LYS:HD3	1:A:538:ARG:HG2	1.80	0.62
1:B:282:THR:OG1	1:B:283:HIS:HD2	1.83	0.62
1:B:708:GLN:O	1:B:709:HIS:CB	2.47	0.62
1:C:680:ASN:HD22	1:C:682:ASP:H	1.46	0.62
1:C:693:ASN:ND2	1:C:714:THR:H	1.96	0.62
1:D:138:THR:HG23	1:D:182:ALA:O	2.00	0.62
1:C:500:ARG:HG2	1:C:500:ARG:HH21	1.65	0.62
1:D:711:LEU:O	1:D:712:SER:HB3	1.99	0.62
1:A:266:ARG:HD2	2:D:1816:HOH:O	1.99	0.62
1:B:552:ALA:HB2	1:B:719:ALA:HA	1.82	0.62
1:B:684:MET:H	1:B:690:ASN:ND2	1.96	0.62
1:C:152:VAL:CG2	1:C:177:LEU:HD23	2.30	0.62
1:A:147:ALA:O	1:A:195:ALA:HA	2.01	0.61
1:C:248:VAL:CG2	1:C:286:LEU:HD23	2.30	0.61
1:B:616:MET:SD	1:B:651:ILE:HG12	2.39	0.61
1:D:183:HIS:H	1:D:186:GLN:HE21	1.46	0.61
1:B:494:LYS:HG2	1:B:538:ARG:HG2	1.81	0.61
1:C:618:GLU:OE1	1:C:645:ASP:HB2	2.00	0.61
1:B:194:ASP:HB3	1:B:196:ASN:H	1.66	0.61
1:B:684:MET:N	1:B:690:ASN:HD22	1.98	0.61
1:C:442:THR:O	1:C:446:LEU:HD13	2.01	0.61
1:D:615:ALA:O	1:D:643:ARG:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:GLN:HA	1:B:474:GLY:CA	2.25	0.60
1:C:209:GLU:HB3	1:C:219:LEU:HB3	1.83	0.60
1:A:121:PRO:HB2	1:A:125:LEU:HD12	1.82	0.60
1:B:644:ARG:CG	1:B:650:GLU:HB3	2.31	0.60
1:C:610:TYR:O	1:C:617:HIS:HD2	1.85	0.60
1:A:122:TYR:CE1	1:A:123:GLU:HG3	2.36	0.60
1:B:457:ALA:HB2	1:B:477:PHE:CE2	2.36	0.60
1:C:686:TYR:O	1:C:687:HIS:HB2	2.00	0.60
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.36	0.60
1:B:255:ARG:HB2	1:B:583:SER:HB2	1.82	0.60
1:C:211:GLN:CG	1:C:217:ALA:H	2.14	0.60
1:A:237:ASN:ND2	1:A:283:HIS:HE1	2.00	0.60
1:C:614:LYS:HB3	1:C:618:GLU:OE1	2.02	0.60
1:C:630:VAL:HG21	1:C:640:ILE:HD12	1.83	0.60
1:B:635:GLU:HG2	2:B:937:HOH:O	2.01	0.60
1:D:611:ARG:O	1:D:612:HIS:CB	2.48	0.60
1:A:157:ASN:ND2	1:A:163:ARG:HB3	2.16	0.60
1:A:650:GLU:OE2	1:A:670:ASN:HB2	2.01	0.60
1:C:642:VAL:HG13	1:C:650:GLU:HB2	1.83	0.60
1:B:529:VAL:O	1:B:532:LYS:HG3	2.02	0.59
1:C:227:VAL:HG22	1:C:319:ARG:NH1	2.17	0.59
1:A:150:VAL:HG22	1:A:192:MET:CB	2.32	0.59
1:B:598:GLY:CA	1:B:686:TYR:HA	2.33	0.59
1:C:656:ASN:HD21	1:C:658:THR:CG2	2.07	0.59
1:D:393:TRP:HB3	1:D:399:ILE:HG12	1.84	0.59
1:A:351:PHE:O	1:A:353:GLY:N	2.35	0.59
1:C:379:ARG:HB3	1:C:382:VAL:HG23	1.85	0.59
1:C:534:SER:HB2	2:C:1251:HOH:O	2.03	0.59
1:D:614:LYS:H	1:D:614:LYS:HD2	1.67	0.59
1:A:402:LEU:HD12	1:A:446:LEU:HD11	1.84	0.59
1:C:336:TRP:HZ2	1:C:386:LEU:O	1.86	0.59
1:C:510:GLY:HA2	1:C:513:TYR:CE2	2.37	0.59
1:C:278:TRP:O	1:C:604:ARG:HD2	2.02	0.59
1:D:456:MET:HG2	1:D:479:TYR:HB2	1.85	0.59
1:A:292:HIS:O	1:A:311:ARG:NH1	2.32	0.59
1:C:262:TRP:CZ3	1:C:311:ARG:HB3	2.38	0.59
1:D:140:PHE:HZ	1:D:220:ILE:HD11	1.67	0.59
1:D:298:TRP:HE1	1:D:580:HIS:CD2	2.20	0.59
1:D:667:PHE:HA	1:D:705:HIS:NE2	2.18	0.58
1:A:193:ILE:HA	1:A:198:ASN:O	2.03	0.58
1:C:492:TYR:CE2	1:C:507:LEU:HD21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ASP:H	1:C:545:GLN:HE21	1.51	0.58
1:C:542:ASP:H	1:C:545:GLN:NE2	2.00	0.58
1:A:592:GLY:N	2:A:1880:HOH:O	2.35	0.58
1:B:430:ARG:CD	1:B:430:ARG:N	2.63	0.58
1:B:708:GLN:O	1:B:709:HIS:CG	2.57	0.58
1:D:568:MET:HB2	1:D:584:LEU:HD11	1.85	0.58
1:C:594:ASN:N	1:C:597:HIS:HD2	2.00	0.58
1:D:708:GLN:O	1:D:709:HIS:HB2	2.04	0.58
1:B:242:PRO:HB3	1:B:617:HIS:CD2	2.39	0.58
1:C:611:ARG:O	1:C:612:HIS:CB	2.52	0.58
1:A:128:HIS:HE1	1:A:223:LEU:HD13	1.68	0.58
1:A:144:ALA:HB1	1:A:352:ASP:HB3	1.86	0.58
1:A:194:ASP:C	1:A:196:ASN:H	2.07	0.58
1:A:579:ASN:ND2	1:A:581:ASP:H	2.01	0.58
1:C:334:LEU:HD13	2:C:1891:HOH:O	2.04	0.58
1:A:614:LYS:H	1:A:614:LYS:HD2	1.69	0.57
1:B:708:GLN:O	1:B:709:HIS:HB2	2.04	0.57
1:D:680:ASN:HD22	1:D:680:ASN:C	2.06	0.57
1:D:693:ASN:ND2	1:D:714:THR:H	1.92	0.57
1:B:504:HIS:HD2	2:B:801:HOH:O	1.86	0.57
1:C:290:ASN:OD1	1:C:305:LEU:HD13	2.04	0.57
1:C:545:GLN:HB3	2:C:1308:HOH:O	2.04	0.57
1:B:494:LYS:CG	1:B:538:ARG:HG2	2.34	0.57
1:C:598:GLY:CA	1:C:686:TYR:HA	2.34	0.57
1:A:146:ASN:HB3	1:A:195:ALA:HB2	1.86	0.57
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.87	0.57
1:A:470:GLN:O	1:A:472:MET:N	2.33	0.57
1:B:373:LEU:HD23	1:B:373:LEU:N	2.13	0.57
1:B:425:ASN:ND2	1:B:427:PHE:H	2.01	0.57
1:A:149:ARG:NH2	1:A:193:ILE:HD11	2.20	0.57
1:A:199:LEU:C	1:A:199:LEU:HD13	2.25	0.57
1:A:298:TRP:HE1	1:A:580:HIS:CD2	2.22	0.56
1:D:182:ALA:HA	1:D:186:GLN:HE22	1.70	0.56
1:D:668:GLY:H	1:D:705:HIS:CD2	2.23	0.56
1:A:199:LEU:HD13	1:A:200:ARG:N	2.19	0.56
1:C:282:THR:OG1	1:C:283:HIS:HD2	1.88	0.56
1:D:614:LYS:O	1:D:618:GLU:HB2	2.05	0.56
1:B:154:GLY:H	1:B:157:ASN:HB2	1.70	0.56
1:B:693:ASN:ND2	1:B:713:LEU:HB3	2.20	0.56
1:C:680:ASN:HD22	1:C:680:ASN:C	2.08	0.56
1:A:118:HIS:CG	1:A:380:ARG:HH12	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ARG:NH1	2:D:942:HOH:O	2.38	0.56
1:B:533:LYS:O	1:B:538:ARG:NH2	2.39	0.56
1:D:167:ARG:HB3	1:D:169:ARG:NH1	2.21	0.56
1:D:193:ILE:CG2	1:D:197:GLY:HA2	2.34	0.56
1:A:561:PRO:HA	1:A:643:ARG:NH2	2.21	0.56
1:B:483:LEU:HB2	2:B:1744:HOH:O	2.04	0.56
1:D:242:PRO:HB3	1:D:617:HIS:CD2	2.40	0.56
1:B:163:ARG:HB3	1:B:164:HIS:CD2	2.41	0.56
1:C:195:ALA:H	1:C:353:GLY:HA3	1.70	0.56
1:D:610:TYR:O	1:D:617:HIS:HD2	1.89	0.56
1:D:389:ASN:O	1:D:392:TYR:HB3	2.06	0.55
1:A:229:GLN:HG2	1:A:234:LYS:HE2	1.88	0.55
1:B:642:VAL:CG2	1:B:650:GLU:HB2	2.36	0.55
1:D:183:HIS:H	1:D:186:GLN:NE2	2.04	0.55
1:B:712:SER:N	2:B:1924:HOH:O	2.23	0.55
1:C:508:THR:O	1:C:511:ILE:HG22	2.06	0.55
1:B:262:TRP:HB3	2:B:1055:HOH:O	2.06	0.55
1:B:570:ASN:ND2	2:B:826:HOH:O	2.38	0.55
1:B:651:ILE:HD13	1:B:722:TRP:HB3	1.89	0.55
1:D:224:PRO:HG2	1:D:396:ARG:HB3	1.88	0.55
1:D:565:LEU:HD23	1:D:565:LEU:C	2.25	0.55
1:A:509:PHE:HA	1:A:512:LEU:HD23	1.88	0.55
1:B:375:TYR:O	1:B:376:ASN:HB3	2.06	0.55
1:B:474:GLY:O	1:B:476:GLY:N	2.39	0.55
1:C:665:TYR:O	1:C:712:SER:HA	2.05	0.55
1:C:674:LYS:HB3	1:C:696:THR:HG21	1.88	0.55
1:A:693:ASN:ND2	1:A:714:THR:H	2.02	0.55
1:C:289:ILE:HG13	1:C:334:LEU:CD1	2.36	0.55
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.89	0.55
1:B:382:VAL:O	1:B:385:PHE:HB3	2.06	0.55
1:C:345:ASP:O	1:C:346:PHE:C	2.45	0.55
1:A:486:MET:O	1:A:490:LEU:HB2	2.06	0.55
1:B:602:LEU:HG	1:B:606:LEU:HD22	1.87	0.55
1:A:147:ALA:O	1:A:148:ARG:CB	2.54	0.55
1:A:150:VAL:HG22	1:A:192:MET:HB3	1.88	0.55
1:A:259:ASN:HB3	1:A:261:PHE:CD2	2.42	0.55
1:A:403:ARG:NH1	2:A:1194:HOH:O	2.40	0.55
1:A:611:ARG:O	1:A:612:HIS:HB3	2.06	0.55
1:B:351:PHE:O	1:B:352:ASP:CB	2.54	0.55
1:C:289:ILE:HD12	1:C:289:ILE:C	2.26	0.55
1:C:594:ASN:H	1:C:597:HIS:CD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:GLY:HA3	1:D:720:THR:CG2	2.37	0.55
1:A:138:THR:HG23	1:A:182:ALA:O	2.07	0.54
1:A:708:GLN:O	1:A:709:HIS:CB	2.55	0.54
1:D:193:ILE:HG22	1:D:197:GLY:HA2	1.89	0.54
1:A:147:ALA:H	1:A:352:ASP:HB2	1.72	0.54
1:A:194:ASP:HB2	1:A:198:ASN:H	1.72	0.54
1:A:273:VAL:HB	1:A:274:PRO:HD3	1.88	0.54
1:A:293:PRO:HG2	1:A:294:PHE:HD1	1.71	0.54
1:B:608:LEU:O	1:B:611:ARG:O	2.25	0.54
1:B:666:ARG:HA	2:B:1924:HOH:O	2.07	0.54
1:D:247:GLU:HB3	1:D:567:PHE:HA	1.89	0.54
1:D:373:LEU:N	1:D:373:LEU:CD2	2.71	0.54
1:A:229:GLN:HE22	1:A:233:ARG:NH1	2.05	0.54
1:A:282:THR:OG1	1:A:283:HIS:HD2	1.91	0.54
1:A:579:ASN:HD21	1:A:581:ASP:HB2	1.72	0.54
1:B:686:TYR:N	2:B:805:HOH:O	2.22	0.54
1:C:194:ASP:HB2	1:C:198:ASN:HB2	1.90	0.54
1:C:335:ASP:HB3	2:C:1699:HOH:O	2.08	0.54
1:C:695:GLY:HA3	1:D:591:GLY:CA	2.31	0.54
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.41	0.54
1:B:157:ASN:O	1:B:158:TYR:HB2	2.06	0.54
1:B:161:GLY:C	1:B:163:ARG:N	2.59	0.54
1:A:149:ARG:H	1:A:175:TRP:HH2	1.54	0.54
1:A:183:HIS:N	1:A:186:GLN:OE1	2.40	0.54
1:A:635:GLU:H	1:A:635:GLU:CD	2.09	0.54
1:B:440:ARG:HE	1:B:474:GLY:CA	2.20	0.54
1:C:305:LEU:N	1:C:305:LEU:HD22	2.21	0.54
1:A:131:THR:OG1	1:A:136:THR:HG22	2.06	0.54
1:C:639:LEU:H	1:C:639:LEU:CD1	2.20	0.54
1:D:157:ASN:O	1:D:157:ASN:ND2	2.41	0.54
1:B:162:ARG:HG2	1:B:163:ARG:N	2.22	0.54
1:B:661:PRO:HB3	1:B:717:PRO:HD3	1.90	0.54
1:A:695:GLY:O	1:A:696:THR:HB	2.08	0.54
1:C:209:GLU:HB2	1:C:221:CYS:SG	2.48	0.54
1:C:493:MET:O	1:C:540:PRO:HD3	2.08	0.54
1:A:235:LYS:HA	1:A:238:GLN:HG3	1.90	0.54
1:A:711:LEU:N	2:A:1917:HOH:O	2.38	0.54
1:B:680:ASN:ND2	1:B:682:ASP:H	2.04	0.54
1:B:148:ARG:HD3	2:B:1626:HOH:O	2.08	0.54
1:B:150:VAL:HG22	1:B:192:MET:CB	2.38	0.53
1:C:679:LEU:HA	2:C:1519:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ASN:HB3	1:D:200:ARG:NH1	2.22	0.53
1:C:157:ASN:HD21	1:C:163:ARG:CB	2.22	0.53
1:C:619:LEU:HB3	1:C:622:ASP:HB3	1.90	0.53
1:D:547:PHE:CD2	1:D:595:TRP:HB3	2.42	0.53
1:D:610:TYR:CE1	1:D:617:HIS:HB3	2.43	0.53
1:C:486:MET:O	1:C:490:LEU:HD13	2.08	0.53
1:D:120:ARG:HG2	1:D:122:TYR:OH	2.08	0.53
1:D:379:ARG:HB3	1:D:382:VAL:HG23	1.90	0.53
1:D:683:SER:O	1:D:685:HIS:O	2.26	0.53
1:A:118:HIS:HA	2:A:1243:HOH:O	2.07	0.53
1:A:171:GLU:CD	1:A:171:GLU:H	2.11	0.53
1:A:194:ASP:C	1:A:196:ASN:N	2.62	0.53
1:C:272:LEU:HD23	1:C:321:PHE:CZ	2.43	0.53
1:C:349:ALA:O	1:C:351:PHE:N	2.40	0.53
1:C:399:ILE:HD11	1:C:402:LEU:CD2	2.39	0.53
1:C:412:TYR:CE2	1:C:431:GLU:HG2	2.44	0.53
1:C:457:ALA:HB2	1:C:477:PHE:CD2	2.42	0.53
1:A:157:ASN:HD21	1:A:164:HIS:CD2	2.27	0.53
1:A:341:PHE:CE1	1:A:348:LEU:HD23	2.43	0.53
1:A:721:ILE:HD12	1:A:723:LEU:HD11	1.91	0.53
1:B:551:ARG:HG2	1:B:602:LEU:HD23	1.89	0.53
1:C:305:LEU:HD22	1:C:305:LEU:H	1.73	0.53
1:D:584:LEU:O	1:D:585:ASP:CB	2.55	0.53
1:A:212:MET:CE	1:A:213:ARG:HG3	2.38	0.53
1:B:695:GLY:O	1:B:696:THR:HB	2.08	0.53
1:C:184:ASN:ND2	1:C:221:CYS:HA	2.23	0.53
1:C:264:SER:OG	1:C:267:GLU:HG3	2.08	0.53
1:C:333:ILE:HD13	1:C:456:MET:CE	2.38	0.53
1:D:193:ILE:HA	1:D:198:ASN:O	2.08	0.53
1:D:721:ILE:HD12	1:D:723:LEU:HD21	1.90	0.53
1:A:647:GLU:HG2	2:A:1787:HOH:O	2.09	0.53
1:B:247:GLU:OE1	1:B:525:HIS:CD2	2.60	0.53
1:C:247:GLU:OE1	1:C:525:HIS:HD2	1.92	0.53
1:C:564:LYS:HD2	1:C:564:LYS:N	2.24	0.53
1:C:711:LEU:O	1:C:712:SER:HB3	2.08	0.53
1:A:532:LYS:O	1:A:533:LYS:HB2	2.09	0.53
1:C:137:GLY:HA3	1:C:180:PRO:HA	1.90	0.53
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.91	0.53
1:D:475:LEU:N	1:D:475:LEU:HD12	2.24	0.53
1:C:192:MET:O	1:C:193:ILE:HD13	2.09	0.53
1:C:226:LYS:HB2	2:C:1359:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:ASP:H	1:D:545:GLN:HE21	1.55	0.53
1:D:668:GLY:H	1:D:705:HIS:HD2	1.56	0.53
1:B:225:GLU:HA	1:B:225:GLU:OE2	2.09	0.52
1:D:459:GLU:HA	2:D:1011:HOH:O	2.09	0.52
1:B:234:LYS:HG2	1:B:452:GLY:HA3	1.91	0.52
1:C:138:THR:HG23	1:C:182:ALA:O	2.09	0.52
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.27	0.52
1:A:229:GLN:NE2	1:A:233:ARG:NH1	2.57	0.52
1:B:492:TYR:CE2	1:B:500:ARG:HG2	2.44	0.52
1:D:443:ASN:ND2	1:D:455:THR:OG1	2.42	0.52
1:C:149:ARG:HB3	1:C:193:ILE:CG1	2.40	0.52
1:D:373:LEU:HD23	1:D:373:LEU:N	2.24	0.52
1:A:445:ILE:C	1:A:447:GLY:H	2.13	0.52
1:B:542:ASP:H	1:B:545:GLN:HE21	1.56	0.52
1:C:647:GLU:HB3	1:C:649:ASN:HD22	1.75	0.52
1:B:194:ASP:OD1	1:B:198:ASN:HB2	2.10	0.52
1:C:290:ASN:ND2	1:C:304:GLY:O	2.42	0.52
1:D:558:TRP:HA	1:D:564:LYS:HE3	1.90	0.52
1:A:172:SER:O	1:A:174:ILE:HG13	2.10	0.52
1:A:233:ARG:HD3	1:A:326:HIS:CD2	2.45	0.52
1:B:194:ASP:HB2	1:B:198:ASN:HB2	1.91	0.52
1:B:196:ASN:HB2	1:B:198:ASN:HD22	1.75	0.52
1:C:157:ASN:HD21	1:C:163:ARG:HB3	1.73	0.52
1:D:351:PHE:O	1:D:352:ASP:OD2	2.28	0.52
1:D:618:GLU:HB3	1:D:619:LEU:HD22	1.90	0.52
1:A:184:ASN:HA	1:A:220:ILE:HG22	1.91	0.52
1:B:686:TYR:O	1:B:687:HIS:HB2	2.09	0.52
1:D:167:ARG:NH1	2:D:1310:HOH:O	2.43	0.52
1:A:351:PHE:HB3	1:A:356:LEU:HD12	1.92	0.51
1:A:700:ASP:O	1:A:709:HIS:HA	2.10	0.51
1:C:146:ASN:HB2	1:C:352:ASP:CG	2.31	0.51
1:C:149:ARG:HB3	1:C:193:ILE:HG13	1.91	0.51
1:A:610:TYR:CE1	1:A:617:HIS:HB3	2.45	0.51
1:B:214:PRO:C	1:B:216:THR:H	2.13	0.51
1:D:186:GLN:HA	2:D:1309:HOH:O	2.09	0.51
1:D:446:LEU:C	1:D:448:GLU:H	2.14	0.51
1:A:610:TYR:O	1:A:617:HIS:HD2	1.92	0.51
1:B:656:ASN:C	1:B:656:ASN:HD22	2.14	0.51
1:C:169:ARG:HB2	2:C:1849:HOH:O	2.09	0.51
1:A:118:HIS:CD2	1:A:380:ARG:HH12	2.29	0.51
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:ARG:HB3	1:D:681:THR:HB	1.93	0.51
1:A:145:PRO:HD2	1:A:356:LEU:HD11	1.92	0.51
1:C:164:HIS:HB3	1:C:177:LEU:HD21	1.92	0.51
1:B:539:MET:O	1:B:546:LYS:HE3	2.10	0.51
1:B:593:ASP:HA	1:B:597:HIS:CD2	2.46	0.51
1:C:247:GLU:OE1	1:C:525:HIS:CD2	2.63	0.51
1:C:290:ASN:CB	2:C:833:HOH:O	2.48	0.51
1:C:650:GLU:OE1	1:C:670:ASN:HB2	2.11	0.51
1:B:441:ASN:OD1	1:B:444:ARG:NH2	2.40	0.51
1:C:144:ALA:HA	1:C:356:LEU:HD11	1.92	0.51
1:D:607:ASN:O	1:D:611:ARG:HG3	2.10	0.51
1:D:636:ARG:HG2	1:D:662:ARG:NH2	2.26	0.51
1:A:354:THR:O	1:A:356:LEU:N	2.43	0.51
1:C:350:GLU:HA	1:C:354:THR:O	2.11	0.51
1:A:380:ARG:HH21	1:A:380:ARG:CG	2.19	0.50
1:A:528:VAL:HA	1:A:533:LYS:O	2.11	0.50
1:A:539:MET:O	1:A:546:LYS:HE3	2.11	0.50
1:B:430:ARG:HD2	1:B:430:ARG:N	2.04	0.50
1:C:198:ASN:HB3	1:C:200:ARG:HH12	1.73	0.50
1:B:411:ILE:HG13	1:B:412:TYR:CD1	2.46	0.50
1:B:680:ASN:C	1:B:680:ASN:HD22	2.15	0.50
1:D:182:ALA:HA	1:D:186:GLN:NE2	2.25	0.50
1:B:192:MET:SD	1:B:352:ASP:HA	2.51	0.50
1:B:196:ASN:HB2	1:B:198:ASN:ND2	2.26	0.50
1:C:254:ARG:O	1:C:263:LEU:HG	2.12	0.50
1:C:272:LEU:HD23	1:C:321:PHE:HZ	1.76	0.50
1:C:333:ILE:HD13	1:C:456:MET:HE3	1.94	0.50
1:C:493:MET:HE3	1:C:549:ASN:HB3	1.93	0.50
1:C:500:ARG:HG2	1:C:500:ARG:NH2	2.26	0.50
1:D:495:LEU:O	1:D:500:ARG:NH1	2.44	0.50
1:D:264:SER:H	1:D:267:GLU:HB2	1.74	0.50
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.95	0.50
1:B:552:ALA:HA	1:B:720:THR:HG23	1.93	0.50
1:C:399:ILE:HD12	1:C:401:ALA:O	2.11	0.50
1:C:568:MET:HB2	1:C:584:LEU:HD11	1.92	0.50
1:C:656:ASN:HD22	1:C:656:ASN:C	2.14	0.50
1:D:278:TRP:O	1:D:604:ARG:HD2	2.11	0.50
1:A:212:MET:HE2	1:A:213:ARG:HG3	1.93	0.50
1:C:183:HIS:H	1:C:186:GLN:NE2	2.03	0.50
1:D:527:GLU:HB3	2:D:1112:HOH:O	2.10	0.50
1:D:601:ARG:HD3	2:D:1124:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:MET:O	1:B:490:LEU:HB2	2.12	0.50
1:D:450:VAL:O	1:D:451:SER:C	2.48	0.50
1:A:394:ILE:HD13	1:A:446:LEU:HD21	1.94	0.50
1:B:246:TYR:CE2	1:B:568:MET:HA	2.47	0.50
1:B:440:ARG:CG	1:B:475:LEU:H	2.25	0.50
1:B:658:THR:HB	2:B:865:HOH:O	2.11	0.50
1:B:693:ASN:HD21	1:B:714:THR:H	1.60	0.50
1:C:290:ASN:OD1	1:C:305:LEU:HA	2.12	0.50
1:C:514:ASN:ND2	2:C:1127:HOH:O	2.45	0.50
1:B:617:HIS:HE1	2:B:1920:HOH:O	1.95	0.49
1:C:351:PHE:O	1:C:352:ASP:OD2	2.29	0.49
1:D:183:HIS:ND1	1:D:186:GLN:NE2	2.60	0.49
1:D:666:ARG:HA	1:D:712:SER:HA	1.93	0.49
1:A:132:MET:O	1:A:135:VAL:HG12	2.12	0.49
1:B:693:ASN:O	1:B:694:GLY:O	2.30	0.49
1:C:497:PRO:CA	1:C:500:ARG:HD3	2.29	0.49
1:C:558:TRP:HA	1:C:564:LYS:HE3	1.93	0.49
1:C:708:GLN:HG2	1:C:709:HIS:ND1	2.27	0.49
1:D:679:LEU:HD22	1:D:722:TRP:CE2	2.46	0.49
1:A:211:GLN:NE2	1:A:214:PRO:O	2.44	0.49
1:B:341:PHE:CD2	1:B:373:LEU:HD12	2.47	0.49
1:B:631:VAL:HG22	1:B:631:VAL:O	2.11	0.49
1:C:488:ASP:O	1:C:491:ASP:HB2	2.11	0.49
1:D:293:PRO:HD3	1:D:303:THR:CG2	2.43	0.49
1:B:343:THR:HG22	1:B:373:LEU:HD21	1.95	0.49
1:C:315:ARG:HG2	1:C:315:ARG:HH11	1.77	0.49
1:A:225:GLU:O	1:A:396:ARG:NH2	2.46	0.49
1:A:677:GLU:HG2	1:A:723:LEU:CD1	2.43	0.49
1:B:140:PHE:O	1:B:176:GLU:HA	2.12	0.49
1:B:381:GLU:OE2	1:B:381:GLU:N	2.42	0.49
1:B:511:ILE:HD13	1:B:626:PHE:CD2	2.48	0.49
1:C:655:SER:HB3	1:C:657:PHE:CE2	2.48	0.49
1:C:264:SER:HB2	2:C:1100:HOH:O	2.13	0.49
1:C:584:LEU:O	1:C:585:ASP:OD2	2.30	0.49
1:C:701:GLU:HA	1:C:709:HIS:HA	1.94	0.49
1:D:290:ASN:ND2	2:D:861:HOH:O	2.44	0.49
1:D:440:ARG:CG	1:D:475:LEU:H	2.26	0.49
1:D:470:GLN:HA	1:D:474:GLY:HA2	1.94	0.49
1:A:542:ASP:O	1:A:545:GLN:N	2.46	0.49
1:C:394:ILE:O	1:C:398:GLY:HA2	2.13	0.49
1:C:564:LYS:HE2	1:C:610:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:VAL:HG23	1:D:337:VAL:O	2.12	0.49
1:A:247:GLU:OE1	1:A:525:HIS:CD2	2.66	0.49
1:A:504:HIS:CG	1:A:634:LYS:HG2	2.47	0.49
1:A:632:ASP:HB2	2:A:1911:HOH:O	2.12	0.49
1:B:160:ASP:OD2	1:B:162:ARG:HD2	2.13	0.49
1:B:594:ASN:N	1:B:597:HIS:HD2	1.96	0.49
1:A:432:ASN:ND2	1:A:435:ALA:HB2	2.28	0.49
1:A:470:GLN:C	1:A:472:MET:N	2.65	0.49
1:C:208:PHE:HA	1:C:306:TYR:O	2.13	0.49
1:C:685:HIS:ND1	1:C:685:HIS:N	2.60	0.49
1:C:499:TYR:O	1:C:501:GLN:N	2.46	0.49
1:C:636:ARG:CB	1:C:638:VAL:HG23	2.42	0.49
1:C:708:GLN:O	1:C:709:HIS:HB2	2.13	0.49
1:D:547:PHE:CE2	1:D:595:TRP:HB3	2.48	0.49
1:B:403:ARG:NH2	2:B:809:HOH:O	2.46	0.48
1:B:408:ALA:HB2	1:B:459:GLU:OE2	2.13	0.48
1:B:708:GLN:O	1:B:708:GLN:HG2	2.13	0.48
1:C:685:HIS:O	1:C:686:TYR:CB	2.61	0.48
1:D:489:THR:O	1:D:493:MET:HG2	2.13	0.48
1:A:341:PHE:HD1	1:A:375:TYR:CD2	2.31	0.48
1:A:374:ILE:HD13	1:A:374:ILE:H	1.78	0.48
1:A:374:ILE:HD13	1:A:374:ILE:N	2.27	0.48
1:A:564:LYS:HD2	1:A:564:LYS:N	2.28	0.48
1:A:571:GLU:HA	1:A:603:VAL:HG21	1.94	0.48
1:A:686:TYR:N	2:A:1474:HOH:O	2.22	0.48
1:B:147:ALA:O	1:B:148:ARG:CB	2.61	0.48
1:C:209:GLU:HG2	1:C:219:LEU:HD22	1.95	0.48
1:C:259:ASN:N	1:C:259:ASN:HD22	2.11	0.48
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.77	0.48
1:A:358:GLU:OE2	1:A:358:GLU:N	2.45	0.48
1:A:504:HIS:HD2	2:A:991:HOH:O	1.94	0.48
1:A:609:THR:O	1:A:611:ARG:O	2.31	0.48
1:B:254:ARG:O	1:B:255:ARG:HG2	2.14	0.48
1:C:683:SER:HA	2:C:1568:HOH:O	2.12	0.48
1:D:135:VAL:HG12	1:D:180:PRO:HB3	1.95	0.48
1:A:665:TYR:O	1:A:712:SER:HA	2.13	0.48
1:C:545:GLN:O	1:C:549:ASN:ND2	2.46	0.48
1:C:551:ARG:HB3	1:C:681:THR:HG22	1.95	0.48
1:D:631:VAL:O	1:D:631:VAL:HG22	2.12	0.48
1:A:211:GLN:CG	1:A:214:PRO:HB2	2.42	0.48
1:A:315:ARG:C	1:A:315:ARG:HD2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:MET:HB2	1:A:584:LEU:HD11	1.95	0.48
1:C:252:SER:HB3	1:C:580:HIS:O	2.14	0.48
1:C:259:ASN:H	1:C:259:ASN:ND2	2.12	0.48
1:C:318:PHE:HZ	2:C:1891:HOH:O	1.95	0.48
1:C:471:ASP:HB2	1:C:472:MET:HE3	1.94	0.48
1:C:613:HIS:CD2	1:C:678:ILE:HD12	2.48	0.48
1:D:579:ASN:ND2	2:D:1033:HOH:O	2.47	0.48
1:A:224:PRO:O	1:A:225:GLU:C	2.52	0.48
1:C:143:TRP:CH2	1:C:356:LEU:HD22	2.49	0.48
1:D:341:PHE:CZ	1:D:358:GLU:HB3	2.48	0.48
1:A:150:VAL:HG22	1:A:192:MET:HB2	1.94	0.48
1:C:700:ASP:O	1:C:709:HIS:HA	2.13	0.48
1:D:444:ARG:O	1:D:448:GLU:HB2	2.14	0.48
1:B:442:THR:O	1:B:446:LEU:HB2	2.12	0.48
1:C:209:GLU:HG2	1:C:219:LEU:HD13	1.96	0.48
1:C:685:HIS:O	1:C:686:TYR:CG	2.66	0.48
1:A:512:LEU:HD22	1:A:512:LEU:H	1.79	0.48
1:A:693:ASN:HD21	1:A:714:THR:N	2.04	0.48
1:B:351:PHE:O	1:B:352:ASP:HB3	2.13	0.48
1:B:618:GLU:OE1	1:B:645:ASP:HB2	2.13	0.48
1:B:728:GLU:HG2	2:B:1862:HOH:O	2.13	0.48
1:C:166:MET:HG2	1:C:177:LEU:HB2	1.96	0.48
1:C:480:LYS:O	1:C:519:PHE:HD2	1.97	0.48
1:D:684:MET:HB3	1:D:684:MET:HE3	1.66	0.48
1:B:651:ILE:O	1:B:651:ILE:HG13	2.14	0.48
1:C:192:MET:SD	1:C:352:ASP:HA	2.54	0.48
2:C:1199:HOH:O	1:D:695:GLY:HA2	2.13	0.48
1:D:371:ASN:CG	1:D:372:THR:N	2.67	0.47
1:D:552:ALA:HA	1:D:720:THR:CG2	2.41	0.47
1:A:147:ALA:HB3	1:A:175:TRP:HZ2	1.79	0.47
1:B:413:ARG:O	1:B:414:ASP:HB2	2.14	0.47
1:B:665:TYR:O	1:B:712:SER:HA	2.14	0.47
1:D:684:MET:C	1:D:685:HIS:O	2.49	0.47
1:A:474:GLY:O	1:A:476:GLY:N	2.46	0.47
1:A:576:ARG:NH1	1:A:585:ASP:OD2	2.47	0.47
1:D:148:ARG:O	1:D:193:ILE:HB	2.14	0.47
1:D:219:LEU:HD23	1:D:220:ILE:O	2.14	0.47
1:D:514:ASN:ND2	1:D:561:PRO:HB2	2.28	0.47
1:D:564:LYS:N	1:D:564:LYS:HD2	2.29	0.47
1:A:149:ARG:HD3	1:A:193:ILE:HG13	1.95	0.47
1:A:457:ALA:HB2	1:A:477:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:HE	1:B:432:ASN:HA	1.79	0.47
1:C:407:VAL:O	1:C:411:ILE:HG12	2.15	0.47
1:D:680:ASN:HD22	1:D:682:ASP:H	1.62	0.47
1:A:211:GLN:O	1:A:216:THR:HA	2.13	0.47
1:B:211:GLN:O	1:B:211:GLN:HG3	2.14	0.47
1:B:697:VAL:HG11	1:B:713:LEU:HD23	1.95	0.47
1:C:225:GLU:HG3	1:C:225:GLU:O	2.14	0.47
1:C:666:ARG:NH1	1:C:700:ASP:HB2	2.29	0.47
1:D:686:TYR:O	1:D:687:HIS:HB2	2.15	0.47
1:C:292:HIS:O	1:C:311:ARG:NH1	2.47	0.47
1:C:594:ASN:OD1	1:C:596:HIS:HB2	2.15	0.47
1:D:135:VAL:CG1	1:D:180:PRO:HB3	2.44	0.47
1:A:168:LEU:CG	1:A:169:ARG:N	2.78	0.47
1:B:149:ARG:HB3	1:B:193:ILE:HB	1.95	0.47
1:B:374:ILE:HD13	1:B:374:ILE:H	1.78	0.47
1:C:305:LEU:H	1:C:305:LEU:CD2	2.27	0.47
1:C:683:SER:O	1:C:685:HIS:O	2.33	0.47
1:D:141:SER:HA	1:D:175:TRP:O	2.13	0.47
1:D:237:ASN:ND2	1:D:283:HIS:HE1	2.13	0.47
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.97	0.47
1:D:346:PHE:HA	2:D:1211:HOH:O	2.14	0.47
1:D:379:ARG:HB3	1:D:382:VAL:CG2	2.44	0.47
1:D:490:LEU:O	1:D:494:LYS:HG3	2.14	0.47
1:D:684:MET:HB2	1:D:690:ASN:CG	2.35	0.47
1:A:376:ASN:C	1:A:376:ASN:HD22	2.18	0.47
1:A:463:PHE:CE2	1:A:475:LEU:HD13	2.49	0.47
1:B:335:ASP:OD1	1:B:403:ARG:HD3	2.14	0.47
1:B:572:PHE:HB2	1:B:589:LEU:HD21	1.96	0.47
1:C:408:ALA:HB2	1:C:459:GLU:OE2	2.15	0.47
1:C:465:GLY:HA2	1:C:468:ARG:CG	2.45	0.47
1:C:551:ARG:C	1:C:681:THR:HG21	2.35	0.47
1:A:144:ALA:HB1	1:A:352:ASP:CB	2.45	0.47
1:A:680:ASN:ND2	1:A:680:ASN:C	2.65	0.47
1:B:163:ARG:NH2	2:B:1006:HOH:O	2.47	0.47
1:B:298:TRP:HE1	1:B:580:HIS:CD2	2.33	0.47
1:C:157:ASN:OD1	1:C:164:HIS:HD2	1.98	0.47
1:C:602:LEU:HA	1:C:686:TYR:CE1	2.49	0.47
1:D:273:VAL:HB	1:D:274:PRO:HD3	1.96	0.47
1:A:229:GLN:HG2	1:A:234:LYS:HG2	1.95	0.47
1:A:504:HIS:CD2	1:A:634:LYS:HA	2.50	0.47
1:B:268:LEU:O	1:B:272:LEU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:HG2	1:B:602:LEU:CD2	2.45	0.47
1:B:598:GLY:HA3	1:B:686:TYR:HA	1.96	0.47
1:C:259:ASN:N	1:C:259:ASN:ND2	2.59	0.47
1:C:579:ASN:HD22	1:C:579:ASN:C	2.19	0.47
1:C:666:ARG:HH12	1:C:700:ASP:HB2	1.79	0.47
1:D:205:PRO:HB3	1:D:348:LEU:HD11	1.97	0.47
1:D:412:TYR:C	1:D:414:ASP:H	2.18	0.47
1:A:614:LYS:HD2	1:A:614:LYS:N	2.30	0.46
1:C:493:MET:HE2	1:C:553:TYR:HB2	1.96	0.46
1:C:681:THR:HG22	2:C:1864:HOH:O	2.15	0.46
1:D:265:TYR:HB2	1:D:317:ASP:HB3	1.97	0.46
1:B:543:ALA:O	1:B:547:PHE:HD1	1.98	0.46
1:B:711:LEU:O	1:B:712:SER:HB3	2.15	0.46
1:C:166:MET:HG2	1:C:177:LEU:CB	2.45	0.46
1:A:147:ALA:HB3	1:A:175:TRP:CZ2	2.50	0.46
1:C:160:ASP:OD2	1:C:162:ARG:HG2	2.16	0.46
1:C:349:ALA:HA	1:C:358:GLU:OE1	2.14	0.46
1:C:551:ARG:HD2	1:C:681:THR:O	2.15	0.46
1:C:651:ILE:HD12	1:C:651:ILE:C	2.34	0.46
1:A:257:THR:HG22	1:A:258:ASP:N	2.30	0.46
1:A:490:LEU:O	1:A:494:LYS:HG3	2.14	0.46
1:C:703:ALA:HA	1:C:707:ARG:O	2.15	0.46
1:D:584:LEU:O	1:D:585:ASP:HB2	2.15	0.46
1:D:639:LEU:N	1:D:639:LEU:HD12	2.29	0.46
1:D:667:PHE:O	1:D:710:SER:HB2	2.14	0.46
1:A:118:HIS:O	1:A:121:PRO:HD3	2.16	0.46
1:C:273:VAL:CB	1:C:274:PRO:HD3	2.40	0.46
1:C:595:TRP:O	1:C:599:VAL:HG23	2.16	0.46
1:D:246:TYR:HB2	1:D:281:PHE:CD2	2.50	0.46
1:A:593:ASP:OD2	1:A:687:HIS:HE1	1.99	0.46
1:B:379:ARG:HB3	1:B:382:VAL:HG23	1.97	0.46
1:B:446:LEU:C	2:B:1835:HOH:O	2.53	0.46
1:D:283:HIS:ND1	1:D:333:ILE:HD11	2.31	0.46
1:D:289:ILE:C	1:D:289:ILE:HD12	2.36	0.46
1:A:211:GLN:O	1:A:211:GLN:HG2	2.14	0.46
1:A:289:ILE:H	1:A:289:ILE:HG13	1.63	0.46
1:B:168:LEU:HD22	1:B:168:LEU:C	2.35	0.46
1:B:456:MET:HG2	1:B:479:TYR:HB2	1.97	0.46
1:C:341:PHE:HE1	1:C:357:TYR:HB3	1.80	0.46
1:C:631:VAL:HG22	1:C:631:VAL:O	2.14	0.46
1:A:148:ARG:O	1:A:149:ARG:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG12	1:A:166:MET:SD	2.56	0.46
1:A:227:VAL:HG12	1:A:233:ARG:HH22	1.80	0.46
1:A:237:ASN:HD22	1:A:283:HIS:HE1	1.63	0.46
1:B:131:THR:OG1	1:B:136:THR:HG22	2.16	0.46
1:B:237:ASN:ND2	1:B:283:HIS:CE1	2.79	0.46
1:B:602:LEU:HG	1:B:606:LEU:CD2	2.46	0.46
1:B:658:THR:CG2	1:B:660:VAL:HG23	2.45	0.46
1:D:662:ARG:HB2	1:D:715:LEU:HB2	1.98	0.46
1:B:150:VAL:HG22	1:B:192:MET:HB2	1.97	0.46
1:B:259:ASN:HB3	1:B:261:PHE:CD2	2.50	0.46
1:B:333:ILE:HG12	1:B:401:ALA:HB3	1.97	0.46
1:B:643:ARG:O	1:B:650:GLU:HA	2.16	0.46
1:C:245:ILE:HG21	1:C:285:GLU:HB2	1.98	0.46
1:C:680:ASN:HD22	1:C:681:THR:N	2.14	0.46
1:C:684:MET:HE3	1:D:684:MET:CE	2.46	0.46
1:D:432:ASN:HB3	1:D:435:ALA:HB3	1.98	0.46
1:A:214:PRO:C	1:A:216:THR:H	2.18	0.46
1:B:117:THR:N	2:B:1682:HOH:O	2.48	0.46
1:B:310:ARG:HE	1:B:313:GLY:C	2.18	0.46
1:B:610:TYR:O	1:B:617:HIS:HD2	1.98	0.46
1:C:620:ASP:OD2	1:C:643:ARG:NH2	2.49	0.46
1:D:310:ARG:NE	2:D:1482:HOH:O	2.49	0.46
1:D:382:VAL:O	1:D:385:PHE:HB3	2.16	0.46
1:D:659:PRO:O	1:D:717:PRO:HB3	2.16	0.46
1:A:278:TRP:HB2	1:B:612:HIS:CE1	2.51	0.45
1:A:450:VAL:HG23	1:A:450:VAL:O	2.15	0.45
1:B:194:ASP:HB2	1:B:198:ASN:CA	2.46	0.45
1:C:290:ASN:HD21	1:C:305:LEU:HA	1.80	0.45
1:D:194:ASP:OD2	1:D:198:ASN:HB2	2.15	0.45
1:D:601:ARG:HG2	1:D:685:HIS:CE1	2.51	0.45
1:D:618:GLU:OE1	1:D:645:ASP:HB2	2.16	0.45
1:A:647:GLU:HB3	1:A:649:ASN:ND2	2.31	0.45
1:B:194:ASP:C	1:B:196:ASN:N	2.66	0.45
1:D:598:GLY:CA	1:D:686:TYR:HA	2.47	0.45
1:B:685:HIS:HA	2:B:805:HOH:O	2.15	0.45
1:D:309:THR:OG1	1:D:311:ARG:HB2	2.16	0.45
1:D:609:THR:O	1:D:611:ARG:O	2.34	0.45
1:A:147:ALA:O	1:A:195:ALA:CA	2.63	0.45
1:A:496:ASP:HB3	1:A:499:TYR:CD1	2.50	0.45
1:B:159:TRP:HB3	2:B:1734:HOH:O	2.17	0.45
1:C:336:TRP:CE3	1:C:338:PRO:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ALA:O	1:C:350:GLU:C	2.54	0.45
1:C:493:MET:CE	1:C:553:TYR:HB2	2.47	0.45
1:C:619:LEU:HB2	1:C:625:GLY:HA3	1.99	0.45
1:D:358:GLU:OE2	1:D:358:GLU:N	2.44	0.45
1:C:485:TRP:CH2	1:C:557:MET:HG3	2.51	0.45
1:C:552:ALA:HB2	1:C:718:LEU:O	2.16	0.45
1:A:563:LYS:C	1:A:564:LYS:HD2	2.36	0.45
1:A:584:LEU:O	1:A:585:ASP:HB2	2.16	0.45
1:B:194:ASP:CG	1:B:198:ASN:HB2	2.37	0.45
1:C:355:ASN:HB3	1:C:358:GLU:OE2	2.16	0.45
1:A:341:PHE:HD1	1:A:375:TYR:CE2	2.35	0.45
1:A:712:SER:N	2:A:1917:HOH:O	2.15	0.45
1:C:121:PRO:HB2	1:C:125:LEU:HD12	1.97	0.45
1:C:463:PHE:O	1:C:466:VAL:HG23	2.17	0.45
1:C:492:TYR:CZ	1:C:500:ARG:HG3	2.52	0.45
1:C:669:ILE:HD11	1:C:699:SER:HB2	1.98	0.45
1:D:311:ARG:HB2	1:D:311:ARG:HE	1.61	0.45
1:D:466:VAL:O	1:D:477:PHE:HB2	2.17	0.45
1:A:156:PHE:HE1	1:A:188:TYR:HB3	1.82	0.45
1:A:164:HIS:HB3	1:A:177:LEU:HD21	1.99	0.45
1:A:194:ASP:OD1	1:A:198:ASN:HB2	2.16	0.45
1:A:468:ARG:HB3	1:A:469:PRO:HD2	1.99	0.45
1:A:667:PHE:HA	1:A:705:HIS:CD2	2.52	0.45
1:C:593:ASP:HA	1:C:597:HIS:HD2	1.80	0.45
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.66	0.45
1:D:614:LYS:HD2	1:D:614:LYS:N	2.31	0.45
1:D:651:ILE:C	1:D:651:ILE:HD12	2.36	0.45
1:A:227:VAL:HG22	1:A:319:ARG:NH2	2.31	0.45
1:A:255:ARG:HB2	1:A:583:SER:HB2	1.99	0.45
1:B:253:TRP:CE3	1:B:254:ARG:HB2	2.52	0.45
1:B:459:GLU:OE1	1:B:461:THR:O	2.35	0.45
1:B:469:PRO:HB2	1:B:471:ASP:OD2	2.16	0.45
1:C:712:SER:N	2:C:1490:HOH:O	2.38	0.45
1:D:372:THR:HG23	1:D:372:THR:O	2.16	0.45
1:A:289:ILE:HD11	1:A:334:LEU:HD21	1.98	0.45
1:B:227:VAL:HG22	1:B:319:ARG:NH1	2.32	0.45
1:C:716:PRO:HB2	1:C:719:ALA:HB3	1.98	0.45
1:D:257:THR:HG22	1:D:258:ASP:N	2.32	0.45
1:B:256:HIS:NE2	1:B:263:LEU:HD22	2.32	0.44
1:B:429:GLY:HA2	1:B:430:ARG:CZ	2.46	0.44
1:C:169:ARG:HD3	1:C:171:GLU:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:LEU:HD22	1:D:722:TRP:CD2	2.52	0.44
1:A:194:ASP:CG	1:A:198:ASN:HB2	2.38	0.44
1:A:337:VAL:HG23	1:A:337:VAL:O	2.16	0.44
1:B:168:LEU:HB2	1:B:175:TRP:CZ3	2.52	0.44
1:C:700:ASP:O	1:C:710:SER:N	2.45	0.44
1:D:268:LEU:O	1:D:272:LEU:HB3	2.16	0.44
1:A:285:GLU:HA	1:A:333:ILE:O	2.17	0.44
1:A:317:ASP:O	1:A:320:TYR:HB3	2.17	0.44
1:A:351:PHE:HD2	1:A:356:LEU:HD12	1.83	0.44
1:A:411:ILE:HG13	1:A:412:TYR:CD1	2.52	0.44
1:A:467:SER:HA	1:A:477:PHE:O	2.16	0.44
1:D:126:GLY:HA2	1:D:204:ASP:OD2	2.17	0.44
1:D:590:GLU:O	1:D:591:GLY:O	2.35	0.44
1:D:593:ASP:HA	1:D:597:HIS:CD2	2.52	0.44
1:D:618:GLU:C	1:D:619:LEU:HD22	2.38	0.44
1:A:186:GLN:HB2	1:A:220:ILE:HD12	1.99	0.44
1:B:441:ASN:OD1	1:B:444:ARG:NH1	2.48	0.44
1:C:225:GLU:O	1:C:226:LYS:HB2	2.16	0.44
1:C:351:PHE:HD2	1:C:356:LEU:HD12	1.81	0.44
1:A:590:GLU:HG3	1:A:591:GLY:H	1.83	0.44
1:B:713:LEU:HA	2:B:1397:HOH:O	2.17	0.44
1:A:137:GLY:HA3	1:A:179:ILE:O	2.18	0.44
1:A:224:PRO:HG2	1:A:396:ARG:CB	2.28	0.44
1:B:194:ASP:C	1:B:196:ASN:H	2.21	0.44
1:B:614:LYS:HD2	2:B:1920:HOH:O	2.17	0.44
1:D:291:GLU:OE1	1:D:291:GLU:HA	2.17	0.44
1:D:716:PRO:HB2	1:D:719:ALA:HB3	1.98	0.44
1:A:182:ALA:HA	1:A:186:GLN:OE1	2.18	0.44
1:A:684:MET:HG3	1:A:685:HIS:N	2.32	0.44
1:B:669:ILE:HD11	1:B:699:SER:CB	2.48	0.44
1:C:132:MET:HB3	1:C:178:PHE:CE1	2.53	0.44
1:C:528:VAL:HA	1:C:533:LYS:O	2.18	0.44
1:D:573:ALA:O	1:D:596:HIS:CE1	2.71	0.44
1:A:430:ARG:HH21	1:A:430:ARG:CB	2.10	0.44
1:B:584:LEU:HB2	1:B:586:TRP:NE1	2.33	0.44
1:C:154:GLY:H	1:C:157:ASN:CB	2.31	0.44
1:B:685:HIS:CA	2:B:805:HOH:O	2.65	0.44
1:C:168:LEU:HD21	1:C:173:GLY:HA2	1.99	0.44
1:C:532:LYS:O	1:C:533:LYS:HB2	2.16	0.44
1:C:693:ASN:HD21	1:C:714:THR:N	2.02	0.44
1:A:444:ARG:O	1:A:448:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASN:CG	1:C:164:HIS:HD2	2.21	0.43
1:C:237:ASN:ND2	1:C:283:HIS:CE1	2.79	0.43
1:C:656:ASN:ND2	1:C:656:ASN:C	2.71	0.43
1:D:523:LEU:HD12	1:D:523:LEU:HA	1.81	0.43
1:A:294:PHE:N	1:A:294:PHE:CD1	2.86	0.43
1:A:655:SER:HB3	1:A:657:PHE:CE1	2.53	0.43
1:B:129:ALA:HB2	2:B:839:HOH:O	2.18	0.43
1:B:351:PHE:O	1:B:356:LEU:HD12	2.18	0.43
1:D:262:TRP:CZ3	1:D:311:ARG:HG3	2.53	0.43
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.99	0.43
1:C:723:LEU:N	1:C:723:LEU:HD22	2.32	0.43
1:D:447:GLY:HA2	1:D:451:SER:HA	2.01	0.43
1:D:525:HIS:HB3	1:D:567:PHE:CE1	2.53	0.43
1:A:168:LEU:HD12	1:A:169:ARG:N	2.21	0.43
1:A:564:LYS:HE2	1:A:610:TYR:CE1	2.53	0.43
1:C:152:VAL:HG21	1:C:177:LEU:HD23	1.99	0.43
1:B:144:ALA:HB1	1:B:147:ALA:HB2	2.01	0.43
1:B:551:ARG:HB3	1:B:681:THR:HB	2.00	0.43
1:C:192:MET:HE2	1:C:202:LYS:HG3	2.00	0.43
1:C:219:LEU:HD23	1:C:220:ILE:O	2.18	0.43
1:C:474:GLY:O	1:C:475:LEU:HB2	2.19	0.43
1:D:263:LEU:HB3	1:D:267:GLU:HB3	2.00	0.43
1:D:615:ALA:HB1	1:D:643:ARG:O	2.18	0.43
1:A:150:VAL:HA	1:A:191:GLU:O	2.18	0.43
1:A:168:LEU:CG	1:A:169:ARG:H	2.31	0.43
1:A:408:ALA:HA	1:A:411:ILE:HG12	1.99	0.43
1:C:352:ASP:OD2	1:C:352:ASP:C	2.56	0.43
1:C:608:LEU:O	1:C:611:ARG:O	2.37	0.43
1:D:123:GLU:HA	1:D:223:LEU:HD21	2.01	0.43
1:D:288:PRO:HB2	1:D:299:GLY:HA3	2.01	0.43
1:D:685:HIS:C	1:D:687:HIS:H	2.21	0.43
1:B:667:PHE:HA	1:B:705:HIS:CD2	2.54	0.43
1:C:256:HIS:HE1	1:C:267:GLU:OE1	2.02	0.43
1:C:486:MET:O	1:C:490:LEU:HB2	2.18	0.43
1:D:371:ASN:O	1:D:372:THR:C	2.55	0.43
1:D:430:ARG:HH11	1:D:430:ARG:CB	2.15	0.43
1:A:250:LEU:HD21	1:A:286:LEU:HD22	1.99	0.43
1:A:667:PHE:HA	1:A:705:HIS:HD2	1.84	0.43
1:A:708:GLN:HA	2:A:1907:HOH:O	2.18	0.43
1:B:194:ASP:CB	1:B:198:ASN:HB2	2.48	0.43
1:D:517:GLU:HB2	1:D:519:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:HA2	1:A:580:HIS:CE1	2.54	0.43
1:B:309:THR:OG1	1:B:311:ARG:HG3	2.19	0.43
1:B:490:LEU:O	1:B:494:LYS:HG3	2.18	0.43
1:B:571:GLU:O	1:B:600:GLN:HA	2.18	0.43
1:C:194:ASP:HB2	1:C:198:ASN:H	1.83	0.43
1:C:245:ILE:CG2	1:C:285:GLU:HB2	2.48	0.43
1:C:652:ILE:HB	1:C:723:LEU:HB2	2.00	0.43
1:D:668:GLY:N	1:D:705:HIS:HD2	2.16	0.43
1:B:315:ARG:HD2	1:B:315:ARG:C	2.40	0.43
1:C:657:PHE:O	1:C:658:THR:HB	2.19	0.43
1:B:707:ARG:NH1	2:B:950:HOH:O	2.52	0.42
1:C:266:ARG:HB3	2:C:1337:HOH:O	2.19	0.42
1:C:307:ALA:HA	1:C:308:PRO:HD3	1.86	0.42
1:C:463:PHE:CD2	1:C:475:LEU:HD11	2.54	0.42
1:C:493:MET:HB3	1:C:539:MET:HE1	2.00	0.42
1:C:693:ASN:HD21	1:C:713:LEU:HB2	1.84	0.42
1:D:289:ILE:HG13	1:D:334:LEU:HD11	2.01	0.42
1:D:466:VAL:HA	1:D:475:LEU:HD22	2.01	0.42
1:D:529:VAL:HA	1:D:577:GLU:OE1	2.19	0.42
1:A:143:TRP:CZ3	1:A:356:LEU:HD22	2.55	0.42
1:A:157:ASN:C	1:A:159:TRP:N	2.71	0.42
1:A:662:ARG:HB2	1:A:715:LEU:HB2	2.00	0.42
1:B:233:ARG:HA	1:B:331:ASN:HD21	1.84	0.42
1:B:322:ILE:HG21	1:B:397:PHE:O	2.19	0.42
1:C:288:PRO:C	1:C:290:ASN:H	2.22	0.42
1:C:541:GLY:CA	1:C:545:GLN:HE21	2.33	0.42
1:A:380:ARG:CG	1:A:380:ARG:NH2	2.78	0.42
1:C:146:ASN:HB2	1:C:352:ASP:OD1	2.19	0.42
1:C:280:GLY:O	1:C:611:ARG:NH1	2.41	0.42
1:C:566:LEU:HG	1:C:570:ASN:HB2	2.02	0.42
1:A:641:PHE:CD1	1:A:641:PHE:C	2.92	0.42
1:B:160:ASP:CG	1:B:162:ARG:HD2	2.40	0.42
1:D:164:HIS:HE1	2:D:1447:HOH:O	2.02	0.42
1:D:531:GLY:CA	1:D:577:GLU:OE2	2.66	0.42
1:A:178:PHE:CE1	1:A:180:PRO:HG3	2.48	0.42
1:B:511:ILE:HG23	2:B:1218:HOH:O	2.19	0.42
1:C:149:ARG:O	1:C:192:MET:HA	2.20	0.42
1:C:297:SER:C	1:C:299:GLY:H	2.23	0.42
1:C:435:ALA:O	1:C:438:PHE:HB3	2.19	0.42
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.42
1:A:149:ARG:O	1:A:192:MET:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HG	1:A:169:ARG:N	2.35	0.42
1:A:703:ALA:HA	1:A:707:ARG:O	2.19	0.42
1:C:130:ASP:CG	1:C:131:THR:H	2.22	0.42
1:C:359:HIS:CD2	1:C:376:ASN:HB2	2.55	0.42
1:C:375:TYR:HB2	1:C:377:TYR:CZ	2.55	0.42
1:C:598:GLY:HA3	1:C:686:TYR:HA	2.01	0.42
1:C:604:ARG:NH2	2:C:1576:HOH:O	2.52	0.42
1:C:666:ARG:HH12	1:C:700:ASP:CB	2.33	0.42
1:A:194:ASP:N	1:A:198:ASN:O	2.47	0.42
1:A:206:TYR:CZ	1:A:385:PHE:HD1	2.36	0.42
1:A:341:PHE:O	1:A:343:THR:HG23	2.20	0.42
1:B:259:ASN:O	1:B:260:ASN:HB3	2.19	0.42
1:B:552:ALA:O	1:B:720:THR:HG21	2.20	0.42
1:D:437:GLU:OE2	1:D:437:GLU:HA	2.19	0.42
1:D:504:HIS:CD2	1:D:634:LYS:HA	2.54	0.42
1:A:541:GLY:HA2	2:A:1350:HOH:O	2.19	0.42
1:C:182:ALA:HA	1:C:186:GLN:NE2	2.35	0.42
1:D:183:HIS:CE1	1:D:186:GLN:NE2	2.88	0.42
1:D:413:ARG:O	1:D:414:ASP:CB	2.68	0.42
1:C:457:ALA:HB2	1:C:477:PHE:CE2	2.55	0.42
1:D:140:PHE:O	1:D:176:GLU:HA	2.20	0.42
1:C:265:TYR:CE2	1:C:312:PHE:HB2	2.55	0.42
1:C:315:ARG:HG2	1:C:315:ARG:NH1	2.35	0.42
1:C:679:LEU:HB3	1:C:722:TRP:HB2	2.02	0.42
1:D:198:ASN:HB3	1:D:200:ARG:HH12	1.85	0.42
1:D:722:TRP:C	1:D:723:LEU:HD22	2.40	0.42
1:B:295:ASP:OD2	1:B:295:ASP:N	2.52	0.41
1:B:352:ASP:OD2	1:B:352:ASP:C	2.57	0.41
1:B:594:ASN:HB2	2:B:1233:HOH:O	2.20	0.41
1:B:629:LEU:HB2	1:B:640:ILE:HG22	2.02	0.41
1:C:722:TRP:C	1:C:723:LEU:HD22	2.40	0.41
1:D:136:THR:HG22	1:D:137:GLY:N	2.35	0.41
1:D:713:LEU:HA	2:D:1624:HOH:O	2.20	0.41
1:D:721:ILE:CD1	1:D:723:LEU:HD21	2.50	0.41
1:A:147:ALA:O	1:A:148:ARG:HB2	2.19	0.41
1:A:509:PHE:HA	1:A:512:LEU:CD2	2.50	0.41
1:B:138:THR:HG21	1:B:220:ILE:HD13	2.02	0.41
1:B:462:ASP:O	1:B:463:PHE:C	2.59	0.41
1:B:606:LEU:HD13	1:B:679:LEU:CD1	2.49	0.41
1:C:463:PHE:HD2	1:C:475:LEU:HD11	1.84	0.41
1:C:541:GLY:HA3	1:C:545:GLN:HE21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ASP:N	1:C:545:GLN:HE21	2.18	0.41
1:A:259:ASN:O	1:A:260:ASN:HB3	2.19	0.41
1:B:143:TRP:CZ2	1:B:356:LEU:HD22	2.55	0.41
1:B:150:VAL:HG22	1:B:192:MET:HB3	2.03	0.41
1:C:523:LEU:HD22	1:C:557:MET:SD	2.61	0.41
1:D:246:TYR:HB2	1:D:281:PHE:CG	2.55	0.41
1:D:293:PRO:HD3	1:D:303:THR:HG23	2.01	0.41
1:A:686:TYR:O	1:A:687:HIS:HB2	2.21	0.41
1:B:457:ALA:HB2	1:B:477:PHE:CD2	2.55	0.41
1:B:485:TRP:CH2	1:B:557:MET:HG3	2.55	0.41
1:B:593:ASP:OD2	1:B:687:HIS:CE1	2.74	0.41
1:C:168:LEU:HB2	1:C:175:TRP:CE3	2.55	0.41
1:C:223:LEU:HD23	1:C:396:ARG:CZ	2.50	0.41
1:C:336:TRP:CZ3	1:C:338:PRO:HG2	2.55	0.41
1:C:351:PHE:O	1:C:353:GLY:N	2.54	0.41
1:A:351:PHE:CD2	1:A:356:LEU:HD12	2.56	0.41
1:B:448:GLU:HB2	2:B:1637:HOH:O	2.20	0.41
1:B:680:ASN:HA	1:B:721:ILE:HG22	2.03	0.41
1:C:131:THR:OG1	1:C:136:THR:HG22	2.19	0.41
1:C:168:LEU:CD1	1:C:170:LYS:HA	2.50	0.41
1:C:247:GLU:HB3	1:C:567:PHE:HA	2.03	0.41
1:C:543:ALA:HB1	1:C:595:TRP:CH2	2.56	0.41
1:C:684:MET:N	1:C:690:ASN:HD22	2.17	0.41
1:D:140:PHE:CZ	1:D:220:ILE:HD11	2.52	0.41
1:D:679:LEU:HB3	1:D:722:TRP:HB2	2.02	0.41
1:B:547:PHE:CD2	1:B:595:TRP:HB3	2.55	0.41
1:C:262:TRP:CG	1:C:312:PHE:HE2	2.38	0.41
1:C:375:TYR:O	1:C:376:ASN:HB3	2.20	0.41
1:C:480:LYS:O	1:C:519:PHE:HA	2.20	0.41
1:C:565:LEU:HD23	1:C:565:LEU:C	2.40	0.41
1:D:394:ILE:HG21	1:D:450:VAL:HG11	2.01	0.41
1:A:572:PHE:HZ	1:A:584:LEU:O	2.03	0.41
1:A:631:VAL:HG22	1:A:631:VAL:O	2.21	0.41
1:B:141:SER:HA	1:B:175:TRP:O	2.21	0.41
1:B:490:LEU:HD12	1:B:490:LEU:HA	1.95	0.41
1:B:496:ASP:O	1:B:497:PRO:C	2.58	0.41
1:B:506:LYS:NZ	2:B:1487:HOH:O	2.53	0.41
1:D:267:GLU:O	1:D:270:ASP:OD2	2.39	0.41
1:A:407:VAL:HA	1:A:410:MET:CE	2.50	0.41
1:B:143:TRP:CE2	1:B:381:GLU:HG2	2.56	0.41
1:B:559:ALA:HA	1:B:616:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:VAL:HG23	1:C:177:LEU:HD23	2.02	0.41
1:A:129:ALA:HA	1:A:138:THR:HG22	2.03	0.41
1:A:157:ASN:ND2	1:A:164:HIS:CD2	2.88	0.41
1:A:606:LEU:CD1	1:A:679:LEU:HD11	2.51	0.41
1:C:252:SER:OG	1:C:568:MET:HE1	2.21	0.41
1:C:450:VAL:HG23	1:C:450:VAL:O	2.21	0.41
1:C:547:PHE:O	1:C:551:ARG:HB2	2.21	0.41
1:C:579:ASN:C	1:C:579:ASN:ND2	2.75	0.41
1:C:643:ARG:HD2	1:C:643:ARG:HA	1.86	0.41
1:D:163:ARG:HD2	2:D:1502:HOH:O	2.20	0.41
1:D:566:LEU:HG	1:D:570:ASN:HB2	2.01	0.41
1:D:725:ARG:CZ	2:D:1544:HOH:O	2.69	0.41
1:A:144:ALA:HA	1:A:145:PRO:HD2	1.91	0.41
1:A:288:PRO:HB2	1:A:299:GLY:HA3	2.03	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.92	0.41
1:A:447:GLY:N	2:A:1483:HOH:O	2.54	0.41
1:A:542:ASP:O	1:A:543:ALA:C	2.59	0.41
1:B:597:HIS:O	1:B:601:ARG:HB2	2.20	0.41
1:D:227:VAL:HG22	1:D:319:ARG:NH1	2.36	0.41
1:D:254:ARG:HA	1:D:583:SER:HB2	2.03	0.41
1:D:279:MET:O	1:D:604:ARG:HA	2.21	0.41
1:D:289:ILE:HG13	1:D:334:LEU:CD1	2.51	0.41
1:D:494:LYS:HG2	1:D:538:ARG:HB3	2.03	0.41
1:D:497:PRO:HA	1:D:500:ARG:HD3	2.01	0.41
1:D:542:ASP:H	1:D:545:GLN:NE2	2.18	0.41
1:A:254:ARG:NH2	2:A:1871:HOH:O	2.43	0.40
1:B:318:PHE:O	1:B:321:PHE:HB3	2.20	0.40
1:B:494:LYS:CD	1:B:538:ARG:HG2	2.51	0.40
1:C:192:MET:CE	1:C:202:LYS:HG3	2.51	0.40
1:C:669:ILE:HD11	1:C:699:SER:CB	2.50	0.40
1:C:685:HIS:NE2	1:D:685:HIS:HD2	2.19	0.40
1:D:593:ASP:OD2	1:D:687:HIS:CE1	2.73	0.40
1:D:656:ASN:ND2	2:D:844:HOH:O	2.36	0.40
1:B:168:LEU:HB2	1:B:175:TRP:CE3	2.57	0.40
1:B:425:ASN:HD21	1:B:427:PHE:HB2	1.86	0.40
1:C:351:PHE:HB3	1:C:356:LEU:HD12	2.02	0.40
1:C:526:ASP:O	1:C:532:LYS:NZ	2.48	0.40
1:C:619:LEU:HA	2:C:1152:HOH:O	2.21	0.40
1:D:170:LYS:HG2	2:D:1613:HOH:O	2.19	0.40
1:D:709:HIS:HD2	2:D:1905:HOH:O	2.04	0.40
1:A:130:ASP:OD1	1:A:132:MET:HE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:THR:HG22	1:A:373:LEU:HD23	2.03	0.40
1:B:289:ILE:C	1:B:289:ILE:HD12	2.42	0.40
2:C:1747:HOH:O	1:D:254:ARG:HD3	2.21	0.40
1:D:131:THR:HG22	1:D:132:MET:N	2.36	0.40
1:D:546:LYS:HB3	1:D:546:LYS:HE3	1.94	0.40
1:D:690:ASN:HD22	1:D:690:ASN:HA	1.63	0.40
1:A:640:ILE:HA	1:A:653:VAL:O	2.21	0.40
1:B:552:ALA:O	1:B:720:THR:CG2	2.69	0.40
1:B:721:ILE:HD12	1:B:723:LEU:HD21	2.03	0.40
1:C:263:LEU:HD13	1:C:271:GLN:NE2	2.37	0.40
1:C:642:VAL:HG23	1:C:652:ILE:HG12	2.02	0.40
1:C:677:GLU:HA	1:C:722:TRP:O	2.22	0.40
1:C:682:ASP:OD2	1:C:689:SER:N	2.55	0.40
1:D:293:PRO:CD	1:D:303:THR:HG23	2.52	0.40
1:A:377:TYR:HD1	2:A:1382:HOH:O	2.04	0.40
1:A:542:ASP:HB3	2:A:1800:HOH:O	2.20	0.40
1:A:574:GLN:HE21	1:A:574:GLN:HB2	1.70	0.40
1:B:671:GLN:HB3	1:D:498:VAL:HG11	2.04	0.40
1:C:333:ILE:HD13	1:C:456:MET:HE1	2.03	0.40
1:D:411:ILE:HG13	1:D:412:TYR:CD1	2.56	0.40
1:D:440:ARG:HG2	1:D:475:LEU:N	2.34	0.40
1:D:700:ASP:O	1:D:709:HIS:HA	2.22	0.40

There are no symmetry-related clashes.

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	581/617 (94%)	502 (86%)	52 (9%)	27 (5%)	2 1
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	6 5
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	4 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	577/617 (94%)	522 (90%)	40 (7%)	15 (3%)	5 4
All	All	2311/2468 (94%)	2040 (88%)	197 (8%)	74 (3%)	4 2

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	212	MET
1	A	215	GLU
1	A	225	GLU
1	A	257	THR
1	A	352	ASP
1	A	543	ALA
1	B	194	ASP
1	B	225	GLU
1	B	226	LYS
1	B	352	ASP
1	B	612	HIS
1	B	709	HIS
1	C	350	GLU
1	C	352	ASP
1	C	585	ASP
1	D	194	ASP
1	D	257	THR
1	D	430	ARG
1	D	585	ASP
1	D	591	GLY
1	A	226	LYS
1	A	355	ASN
1	A	471	ASP
1	A	591	GLY
1	A	695	GLY
1	A	709	HIS
1	B	694	GLY
1	C	258	ASP
1	C	288	PRO
1	C	349	ALA
1	C	500	ARG
1	C	616	MET
1	C	687	HIS
1	D	149	ARG
1	D	259	ASN

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Mol	Chain	Res	Type
1	D	592	GLY
1	D	612	HIS
1	A	194	ASP
1	A	472	MET
1	A	475	LEU
1	A	522	PRO
1	B	584	LEU
1	C	226	LYS
1	C	257	THR
1	C	612	HIS
1	D	197	GLY
1	D	290	ASN
1	D	372	THR
1	A	149	ARG
1	A	184	ASN
1	A	214	PRO
1	A	433	LEU
1	A	533	LYS
1	B	288	PRO
1	C	194	ASP
1	C	504	HIS
1	C	686	TYR
1	A	380	ARG
1	B	215	GLU
1	B	522	PRO
1	C	709	HIS
1	D	522	PRO
1	A	168	LEU
1	A	288	PRO
1	B	696	THR
1	B	712	SER
1	C	252	SER
1	D	709	HIS
1	A	447	GLY
1	C	630	VAL
1	A	510	GLY
1	C	473	GLY
1	D	473	GLY

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	498/525 (95%)	466 (94%)	32 (6%)	17	23
1	B	501/525 (95%)	464 (93%)	37 (7%)	13	17
1	C	490/525 (93%)	460 (94%)	30 (6%)	18	25
1	D	496/525 (94%)	466 (94%)	30 (6%)	19	26
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	17	23

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	158	TYR
1	A	196	ASN
1	A	289	ILE
1	A	315	ARG
1	A	356	LEU
1	A	373	LEU
1	A	374	ILE
1	A	376	ASN
1	A	380	ARG
1	A	391	LEU
1	A	430	ARG
1	A	446	LEU
1	A	462	ASP
1	A	490	LEU
1	A	498	VAL
1	A	501	GLN
1	A	522	PRO
1	A	523	LEU
1	A	537	ASP
1	A	558	TRP
1	A	579	ASN
1	A	606	LEU
1	A	614	LYS

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Mol	Chain	Res	Type
1	A	619	LEU
1	A	642	VAL
1	A	647	GLU
1	A	656	ASN
1	A	679	LEU
1	A	680	ASN
1	A	720	THR
1	A	723	LEU
1	B	138	THR
1	B	149	ARG
1	B	162	ARG
1	B	168	LEU
1	B	176	GLU
1	B	199	LEU
1	B	211	GLN
1	B	290	ASN
1	B	295	ASP
1	B	305	LEU
1	B	310	ARG
1	B	315	ARG
1	B	331	ASN
1	B	359	HIS
1	B	373	LEU
1	B	374	ILE
1	B	376	ASN
1	B	391	LEU
1	B	430	ARG
1	B	446	LEU
1	B	470	GLN
1	B	490	LEU
1	B	511	ILE
1	B	512	LEU
1	B	523	LEU
1	B	538	ARG
1	B	558	TRP
1	B	579	ASN
1	B	606	LEU
1	B	614	LYS
1	B	619	LEU
1	B	642	VAL
1	B	651	ILE
1	B	656	ASN

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Mol	Chain	Res	Type
1	B	679	LEU
1	B	680	ASN
1	B	723	LEU
1	C	124	THR
1	C	133	ASP
1	C	157	ASN
1	C	163	ARG
1	C	171	GLU
1	C	258	ASP
1	C	259	ASN
1	C	290	ASN
1	C	303	THR
1	C	310	ARG
1	C	315	ARG
1	C	331	ASN
1	C	358	GLU
1	C	359	HIS
1	C	462	ASP
1	C	470	GLN
1	C	472	MET
1	C	500	ARG
1	C	507	LEU
1	C	523	LEU
1	C	579	ASN
1	C	642	VAL
1	C	643	ARG
1	C	651	ILE
1	C	656	ASN
1	C	680	ASN
1	C	685	HIS
1	C	711	LEU
1	C	713	LEU
1	C	720	THR
1	D	141	SER
1	D	148	ARG
1	D	157	ASN
1	D	171	GLU
1	D	211	GLN
1	D	223	LEU
1	D	232	GLU
1	D	315	ARG
1	D	331	ASN

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Mol	Chain	Res	Type
1	D	352	ASP
1	D	359	HIS
1	D	373	LEU
1	D	430	ARG
1	D	470	GLN
1	D	472	MET
1	D	490	LEU
1	D	500	ARG
1	D	507	LEU
1	D	522	PRO
1	D	523	LEU
1	D	579	ASN
1	D	614	LYS
1	D	632	ASP
1	D	642	VAL
1	D	647	GLU
1	D	656	ASN
1	D	680	ASN
1	D	684	MET
1	D	690	ASN
1	D	713	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	229	GLN
1	A	237	ASN
1	A	260	ASN
1	A	283	HIS
1	A	331	ASN
1	A	340	HIS
1	A	355	ASN
1	A	376	ASN
1	A	384	ASN
1	A	441	ASN
1	A	501	GLN
1	A	504	HIS
1	A	514	ASN
1	A	525	HIS
1	A	570	ASN
1	A	574	GLN

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Mol	Chain	Res	Type
1	A	579	ASN
1	A	580	HIS
1	A	587	HIS
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	687	HIS
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS
1	A	708	GLN
1	A	709	HIS
1	B	157	ASN
1	B	164	HIS
1	B	198	ASN
1	B	211	GLN
1	B	237	ASN
1	B	256	HIS
1	B	271	GLN
1	B	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	376	ASN
1	B	425	ASN
1	B	470	GLN
1	B	504	HIS
1	B	514	ASN
1	B	525	HIS
1	B	545	GLN
1	B	570	ASN
1	B	574	GLN
1	B	579	ASN
1	B	580	HIS
1	B	587	HIS
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	680	ASN
1	B	687	HIS
1	B	690	ASN
1	B	693	ASN

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Mol	Chain	Res	Type
1	B	705	HIS
1	B	709	HIS
1	C	146	ASN
1	C	157	ASN
1	C	164	HIS
1	C	184	ASN
1	C	186	GLN
1	C	237	ASN
1	C	256	HIS
1	C	259	ASN
1	C	283	HIS
1	C	301	GLN
1	C	331	ASN
1	C	470	GLN
1	C	514	ASN
1	C	530	HIS
1	C	545	GLN
1	C	570	ASN
1	C	574	GLN
1	C	579	ASN
1	C	580	HIS
1	C	597	HIS
1	C	613	HIS
1	C	617	HIS
1	C	649	ASN
1	C	656	ASN
1	C	680	ASN
1	C	690	ASN
1	C	693	ASN
1	C	705	HIS
1	D	164	HIS
1	D	186	GLN
1	D	211	GLN
1	D	237	ASN
1	D	238	GLN
1	D	256	HIS
1	D	283	HIS
1	D	290	ASN
1	D	331	ASN
1	D	340	HIS
1	D	359	HIS
1	D	376	ASN

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Mol	Chain	Res	Type
1	D	443	ASN
1	D	470	GLN
1	D	504	HIS
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	579	ASN
1	D	580	HIS
1	D	597	HIS
1	D	617	HIS
1	D	656	ASN
1	D	680	ASN
1	D	685	HIS
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS
1	D	708	GLN
1	D	709	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.