



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

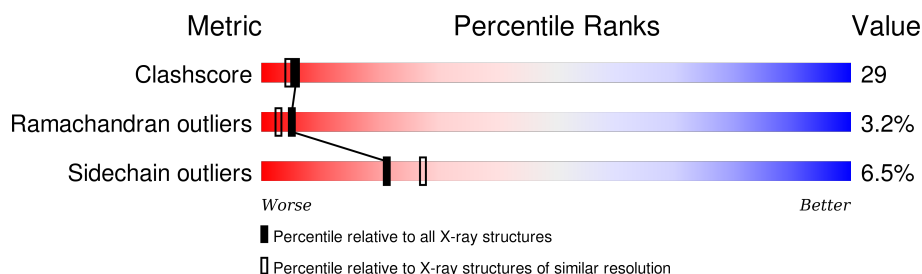
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	617	
1	B	617	
1	C	617	
1	D	617	

2 Entry composition

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

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



T714	L619	K546	M456	R379	P288	R200	RET
L715	V631	F547	E459	V352	I289	D204	LEU
P716	D632	R551	E466	F385	N290	P205	SER
L718	D633	A552	P469	N389	H298	Q211	GLY
A719	K634	G555	Q470	Y392	G299	R212	GLY
T720	E635	W558	D471	W393	W298	ARG	R120
T721	R636	P561	G473	I394	G299	PRO	P121
L723	L639	K564	G474	W393	T303	GLU	Y122
V724	V642	L565	L475	I394	T303	T216	E123
R725	R643	L566	G476	E395	T309	L219	G126
E728	D644	L567	F477	R396	R310	I220	
	D645	F567	Y478	I399	R311	L223	T131
	E647	M568	Y479	R403	R315	P224	M132
	I651	N570	T489	D405	R316	V227	V135
	N656	A573	L490	D405	D317	E232	T136
	P659	Q574	Y492	I411	R319	N237	G137
	R662	E577	K494	Y412	N331	P242	T138
Y665	Y665	M578	L495	R413	N332	Y246	R139
R666	F667	N579	D496	D414	T333	E247	F140
F667	G668	H580	P497	T333	I334	Y250	S141
G668	K674	S583	Y498	SER	T334	L250	V142
		L584	B500	ARG	T334	L250	W143
		D685	H504	LYS	Y337	L250	A144
		E590	L507	GLY	H340	L250	P145
		G591	N514	TRP	F341	R254	R148
		S592	E517	ILE	F346	T257	R149
		D593	H519	PRO	L347	D258	N157
		N594	F519	ASN	L348	N259	R163
		W595	V520	GLU	F351		H164
		H596	L521	PHE	D352	W262	R167
		G597	P522	GLY	L356	L263	L168
		G598	L522	G429	R430	S264	R169
		R601	L523	R431	E431	Y265	K170
		L602	S524	N432	E358	R266	E171
		V603	H525	A435	H359	E267	H175
		D605	D526	I436	ASP	L268	E176
		L606	E527	E437	PRQ	A269	
		N607	V528	R440	ARG	D270	P180
		L608	V529	R443	GLY	Q271	G181
		T609	H530	N443	GLY	V273	A182
		Y610	G531	R444	TYR	P274	H183
		R611	I535	I445	HIS	W278	Q186
		H612	I535	L446	GLN	M279	M192
		H613	I535	G447	TRP	G280	M192
		K614	R538	E448	ASP	F281	I193
		A615	B538	Q449	N371	T282	D194
		M616	D542	V450	L373	H283	
		H617	G545	S451	N376	E284	G197
		E618		T455		N198	I198
						L199	

4 Data and refinement statistics

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

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	0.40	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(°)	Ideal(°)
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

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:C:497:PRO:HA	1:C:500:ARG:HD3	1.42	1.02
1:A:430:ARG:HH21	1:A:430:ARG:HB3	1.22	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:693:ASN:HD21	1:D:714:THR:H	1.10	0.99
1:D:430:ARG:HH11	1:D:430:ARG:HB2	1.27	0.99
1:B:194:ASP:HB2	1:B:198:ASN:H	1.28	0.99
1:D:470:GLN:NE2	1:D:470:GLN:H	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:HD23	1:B:373:LEU:H	1.33	0.91
1:D:470:GLN:HE21	1:D:470:GLN:H	1.00	0.91
1:B:594:ASN:H	1:B:597:HIS:HD2	1.16	0.90
1:B:470:GLN:NE2	1:B:470:GLN:H	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:C:643:ARG:HH11	1:C:643:ARG:CB	1.86	0.89
1:B:470:GLN:HE21	1:B:470:GLN:N	1.70	0.89
1:C:470:GLN:H	1:C:470:GLN:HE21	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:NH1	1:C:643:ARG:HB3	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:N	1:C:470:GLN:HE21	1.76	0.82
1:C:536:LEU:HD22	1:C:573:ALA:HB1	1.62	0.81
1:D:470:GLN:HE21	1:D:470:GLN:N	1.78	0.81
1:C:183:HIS:H	1:C:186:GLN:HE21	1.28	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:D:674:LYS:HB3	1:D:696:THR:HG21	1.61	0.80
1:A:680:ASN:ND2	1:A:682:ASP:H	1.80	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:D:594:ASN:H	1:D:597:HIS:CD2	2.01	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:A:295:ASP:OD2	1:A:311:ARG:NH2	2.18	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:C:273:VAL:HB	1:C:274:PRO:HD3	1.65	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:C:551:ARG:HB3	1:C:681:THR:CG2	2.16	0.76
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.20	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:C:594:ASN:H	1:C:597:HIS:HD2	1.35	0.75
1:A:238:GLN:HG2	2:A:1759:HOH:O	1.87	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:B:225:GLU:O	1:B:226:LYS:HB2	1.85	0.75
1:A:709:HIS:N	2:A:1907:HOH:O	2.20	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:HE21	1:B:470:GLN:H	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:C:456:MET:HG2	1:C:479:TYR:HB2	1.71	0.72
1:B:520:VAL:O	1:B:522:PRO:HD3	1.88	0.72
1:A:212:MET:SD	1:A:293:PRO:HA	2.30	0.72
1:A:162:ARG:O	1:A:162:ARG:HG2	1.90	0.72
1:D:145:PRO:HD2	1:D:356:LEU:HD11	1.71	0.72
1:C:198:ASN:HB3	1:C:200:ARG:NH1	2.04	0.72
1:C:334:LEU:HD22	2:C:1891:HOH:O	1.89	0.71
1:B:194:ASP:CB	1:B:198:ASN:H	2.03	0.71
1:A:149:ARG:CZ	1:A:193:ILE:HD11	2.21	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:A:148:ARG:O	1:A:149:ARG:HB3	1.89	0.71
1:C:440:ARG:HG2	1:C:475:LEU:H	1.55	0.71
1:A:680:ASN:C	1:A:680:ASN:HD22	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:B:373:LEU:H	1:B:373:LEU:CD2	2.03	0.69
1:A:618:GLU:OE2	1:A:645:ASP:HB2	1.92	0.69
1:D:430:ARG:NH1	1:D:430:ARG:HB2	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:C:490:LEU:O	1:C:494:LYS:HG3	1.93	0.69
1:B:644:ARG:HG2	1:B:650:GLU:HB3	1.74	0.69
1:D:232:GLU:CD	1:D:232:GLU:H	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:D:611:ARG:O	1:D:612:HIS:HB3	1.93	0.68
1:B:568:MET:HB2	1:B:584:LEU:HD11	1.73	0.68
1:C:593:ASP:HA	1:C:597:HIS:CD2	2.28	0.68
1:A:132:MET:HB2	1:A:135:VAL:HG13	1.74	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:D:594:ASN:N	1:D:597:HIS:HD2	1.92	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: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:N	1:C:639:LEU:HD12	2.10	0.67
1:D:555:GLY:HA3	1:D:720:THR:HG21	1.76	0.66
1:C:504:HIS:CD2	1:C:634:LYS:HA	2.30	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:D:373:LEU:H	1:D:373:LEU:HD23	1.61	0.66
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.78	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:C:141:SER:HA	1:C:175:TRP:O	1.96	0.66
1:A:471:ASP:O	1:A:472:MET:HG3	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:680:ASN:ND2	1:D:682:ASP:H	1.94	0.65
1:D:602:LEU:O	1:D:606:LEU:HB2	1.96	0.65
1:B:693:ASN:HD21	1:B:713:LEU:HB3	1.60	0.65
1:C:650:GLU:HG2	1:C:671:GLN:OE1	1.95	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: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:C:667:PHE:HA	1:C:705:HIS:CD2	2.32	0.64
1:B:259:ASN:HB3	1:B:261:PHE:CE2	2.33	0.64
1:B:211:GLN:O	1:B:216:THR:HA	1.97	0.64
1:B:289:ILE:HG13	1:B:334:LEU:HD11	1.79	0.64
1:D:376:ASN:HD22	1:D:379:ARG:HB2	1.62	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:B:350:GLU:HA	1:B:354:THR:O	1.97	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: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
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

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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:C:168:LEU:HD22	1:C:169:ARG:N	2.13	0.63
1:B:425:ASN:HD22	1:B:427:PHE:H	1.46	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:C:536:LEU:HB2	1:C:550:LEU:HD22	1.80	0.63
1:A:178:PHE:HE1	1:A:180:PRO:HG3	1.63	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:619:LEU:HB3	1:B:625:GLY:HA3	1.80	0.62
1:B:233:ARG:NH1	2:B:1117:HOH:O	2.32	0.62
1:C:684:MET:H	1:C:690:ASN:HD22	1.47	0.62
1:A:214:PRO:O	1:A:216:THR:N	2.32	0.62
1:D:143:TRP:CH2	1:D:356:LEU:HD22	2.34	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: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:A:494:LYS:HD3	1:A:538:ARG:HG2	1.80	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:B:684:MET:H	1:B:690:ASN:ND2	1.96	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:C:152:VAL:CG2	1:C:177:LEU:HD23	2.30	0.62
1:C:248:VAL:CG2	1:C:286:LEU:HD23	2.30	0.61
1:A:147:ALA:O	1:A:195:ALA:HA	2.01	0.61
1:D:183:HIS:H	1:D:186:GLN:HE21	1.46	0.61
1:B:616:MET:SD	1:B:651:ILE:HG12	2.39	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:C:686:TYR:O	1:C:687:HIS:HB2	2.00	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:211:GLN:CG	1:C:217:ALA:H	2.14	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: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:A:237:ASN:ND2	1:A:283:HIS:HE1	2.00	0.60
1:D:611:ARG:O	1:D:612:HIS:CB	2.48	0.60
1:B:635:GLU:HG2	2:B:937:HOH:O	2.01	0.60
1:A:157:ASN:ND2	1:A:163:ARG:HB3	2.16	0.60
1:C:642:VAL:HG13	1:C:650:GLU:HB2	1.83	0.60
1:A:650:GLU:OE2	1:A:670:ASN:HB2	2.01	0.60
1:C:227:VAL:HG22	1:C:319:ARG:NH1	2.17	0.59
1:B:529:VAL:O	1:B:532:LYS:HG3	2.02	0.59
1:C:656:ASN:HD21	1:C:658:THR:CG2	2.07	0.59
1:B:598:GLY:CA	1:B:686:TYR:HA	2.33	0.59
1:A:150:VAL:HG22	1:A:192:MET:CB	2.32	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:534:SER:HB2	2:C:1251:HOH:O	2.03	0.59
1:C:379:ARG:HB3	1:C:382:VAL:HG23	1.85	0.59
1:D:614:LYS:HD2	1:D:614:LYS:H	1.67	0.59
1:A:402:LEU:HD12	1:A:446:LEU:HD11	1.84	0.59
1:C:510:GLY:HA2	1:C:513:TYR:CE2	2.37	0.59
1:C:336:TRP:HZ2	1:C:386:LEU:O	1.86	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:D:140:PHE:HZ	1:D:220:ILE:HD11	1.67	0.59
1:C:262:TRP:CZ3	1:C:311:ARG:HB3	2.38	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:C:492:TYR:CE2	1:C:507:LEU:HD21	2.39	0.58
1:C:542:ASP:H	1:C:545:GLN:HE21	1.51	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:NE2	2.00	0.58
1:A:193:ILE:HA	1:A:198:ASN:O	2.03	0.58
1:B:430:ARG:CD	1:B:430:ARG:N	2.63	0.58
1:A:592:GLY:N	2:A:1880:HOH:O	2.35	0.58
1:D:568:MET:HB2	1:D:584:LEU:HD11	1.85	0.58
1:B:708:GLN:O	1:B:709:HIS:CG	2.57	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:C:611:ARG:O	1:C:612:HIS:CB	2.52	0.58
1:B:242:PRO:HB3	1:B:617:HIS:CD2	2.39	0.58
1:A:194:ASP:C	1:A:196:ASN:H	2.07	0.58
1:A:144:ALA:HB1	1:A:352:ASP:HB3	1.86	0.58
1:A:579:ASN:ND2	1:A:581:ASP:H	2.01	0.58
1:A:128:HIS:HE1	1:A:223:LEU:HD13	1.68	0.58
1:C:334:LEU:HD13	2:C:1891:HOH:O	2.04	0.58
1:D:693:ASN:ND2	1:D:714:THR:H	1.92	0.57
1:D:680:ASN:C	1:D:680:ASN:HD22	2.06	0.57
1:B:708:GLN:O	1:B:709:HIS:HB2	2.04	0.57
1:A:614:LYS:HD2	1:A:614:LYS:H	1.69	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:504:HIS:HD2	2:B:801:HOH:O	1.86	0.57
1:C:598:GLY:CA	1:C:686:TYR:HA	2.34	0.57
1:B:494:LYS:CG	1:B:538:ARG:HG2	2.34	0.57
1:A:146:ASN:HB3	1:A:195:ALA:HB2	1.86	0.57
1:B:373:LEU:HD23	1:B:373:LEU:N	2.13	0.57
1:A:470:GLN:O	1:A:472:MET:N	2.33	0.57
1:B:425:ASN:ND2	1:B:427:PHE:H	2.01	0.57
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.87	0.57
1:A:149:ARG:NH2	1:A:193:ILE:HD11	2.20	0.57
1:A:199:LEU:HD13	1:A:199:LEU:C	2.25	0.57
1:D:668:GLY:H	1:D:705:HIS:CD2	2.23	0.56
1:D:182:ALA:HA	1:D:186:GLN:HE22	1.70	0.56
1:A:298:TRP:HE1	1:A:580:HIS:CD2	2.22	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:A:199:LEU:HD13	1:A:200:ARG:N	2.19	0.56
1:C:680:ASN:HD22	1:C:680:ASN:C	2.08	0.56
1:B:693:ASN:ND2	1:B:713:LEU:HB3	2.20	0.56
1:B:154:GLY:H	1:B:157:ASN:HB2	1.70	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:C:508:THR:O	1:C:511:ILE:HG22	2.06	0.55
1:B:712:SER:N	2:B:1924:HOH:O	2.23	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:B:570:ASN:ND2	2:B:826:HOH:O	2.38	0.55
1:B:262:TRP:HB3	2:B:1055:HOH:O	2.06	0.55
1:D:565:LEU:C	1:D:565:LEU:HD23	2.25	0.55
1:B:474:GLY:O	1:B:476:GLY:N	2.39	0.55
1:B:375:TYR:O	1:B:376:ASN:HB3	2.06	0.55
1:A:509:PHE:HA	1:A:512:LEU:HD23	1.88	0.55
1:C:674:LYS:HB3	1:C:696:THR:HG21	1.88	0.55
1:C:665:TYR:O	1:C:712:SER:HA	2.05	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:C:345:ASP:O	1:C:346:PHE:C	2.45	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:B:602:LEU:HG	1:B:606:LEU:HD22	1.87	0.55
1:A:486:MET:O	1:A:490:LEU:HB2	2.06	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:D:555:GLY:HA3	1:D:720:THR:CG2	2.37	0.55
1:C:594:ASN:H	1:C:597:HIS:CD2	2.20	0.55
1:C:289:ILE:C	1:C:289:ILE:HD12	2.26	0.55
1:B:351:PHE:O	1:B:352:ASP:CB	2.54	0.55
1:A:611:ARG:O	1:A:612:HIS:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH1	2:A:1194:HOH:O	2.40	0.55
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:138:THR:HG23	1:A:182:ALA:O	2.07	0.54
1:D:373:LEU:CD2	1:D:373:LEU:N	2.71	0.54
1:A:293:PRO:HG2	1:A:294:PHE:HD1	1.71	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:D:247:GLU:HB3	1:D:567:PHE:HA	1.89	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:A:273:VAL:HB	1:A:274:PRO:HD3	1.88	0.54
1:B:686:TYR:N	2:B:805:HOH:O	2.22	0.54
1:C:695:GLY:HA3	1:D:591:GLY:CA	2.31	0.54
1:A:229:GLN:HE22	1:A:233:ARG:NH1	2.05	0.54
1:C:194:ASP:HB2	1:C:198:ASN:HB2	1.90	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:D:492:TYR:CZ	1:D:500:ARG:HG2	2.41	0.54
1:C:335:ASP:HB3	2:C:1699:HOH:O	2.08	0.54
1:B:161:GLY:C	1:B:163:ARG:N	2.59	0.54
1:B:157:ASN:O	1:B:158:TYR:HB2	2.06	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: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:CD	1:A:635:GLU:H	2.09	0.54
1:C:639:LEU:CD1	1:C:639:LEU:H	2.20	0.54
1:D:157:ASN:O	1:D:157:ASN:ND2	2.41	0.54
1:A:131:THR:OG1	1:A:136:THR:HG22	2.06	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:C:493:MET:O	1:C:540:PRO:HD3	2.08	0.54
1:C:209:GLU:HB2	1:C:221:CYS:SG	2.48	0.54
1:A:695:GLY:O	1:A:696:THR:HB	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:C:679:LEU:HA	2:C:1519:HOH:O	2.07	0.53
1:B:150:VAL:HG22	1:B:192:MET:CB	2.38	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:D:610:TYR:CE1	1:D:617:HIS:HB3	2.43	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: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: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:A:171:GLU:H	1:A:171:GLU:CD	2.11	0.53
1:C:399:ILE:HD11	1:C:402:LEU:CD2	2.39	0.53
1:C:349:ALA:O	1:C:351:PHE:N	2.40	0.53
1:A:194:ASP:C	1:A:196:ASN:N	2.62	0.53
1:A:118:HIS:HA	2:A:1243:HOH:O	2.07	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:C:272:LEU:HD23	1:C:321:PHE:CZ	2.43	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:B:551:ARG:HG2	1:B:602:LEU:HD23	1.89	0.53
1:A:157:ASN:HD21	1:A:164:HIS:CD2	2.27	0.53
1:A:721:ILE:HD12	1:A:723:LEU:HD11	1.91	0.53
1:A:341:PHE:CE1	1:A:348:LEU:HD23	2.43	0.53
1:C:333:ILE:HD13	1:C:456:MET:CE	2.38	0.53
1:A:212:MET:CE	1:A:213:ARG:HG3	2.38	0.53
1:C:184:ASN:ND2	1:C:221:CYS:HA	2.23	0.53
1:D:193:ILE:HA	1:D:198:ASN:O	2.08	0.53
1:B:695:GLY:O	1:B:696:THR:HB	2.08	0.53
1:C:264:SER:OG	1:C:267:GLU:HG3	2.08	0.53
1:D:721:ILE:HD12	1:D:723:LEU:HD21	1.90	0.53
1:B:247:GLU:OE1	1:B:525:HIS:CD2	2.60	0.53
1:A:647:GLU:HG2	2:A:1787:HOH:O	2.09	0.53
1:C:564:LYS:N	1:C:564:LYS:HD2	2.24	0.53
1:C:711:LEU:O	1:C:712:SER:HB3	2.08	0.53
1:C:247:GLU:OE1	1:C:525:HIS:HD2	1.92	0.53
1:D:475:LEU:N	1:D:475:LEU:HD12	2.24	0.53
1:A:532:LYS:O	1:A:533:LYS:HB2	2.09	0.53
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.91	0.53
1:C:137:GLY:HA3	1:C:180:PRO:HA	1.90	0.53
1:D:668:GLY:H	1:D:705:HIS:HD2	1.56	0.53
1:C:192:MET:O	1:C:193:ILE:HD13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LYS:HB2	2:C:1359:HOH:O	2.09	0.53
1:D:542:ASP:H	1:D:545:GLN:HE21	1.55	0.53
1:B:225:GLU:OE2	1:B:225:GLU:HA	2.09	0.52
1:D:459:GLU:HA	2:D:1011:HOH:O	2.09	0.52
1:C:138:THR:HG23	1:C:182:ALA:O	2.09	0.52
1:B:234:LYS:HG2	1:B:452:GLY:HA3	1.91	0.52
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.27	0.52
1:B:492:TYR:CE2	1:B:500:ARG:HG2	2.44	0.52
1:A:229:GLN:NE2	1:A:233:ARG:NH1	2.57	0.52
1:D:443:ASN:ND2	1:D:455:THR:OG1	2.42	0.52
1:D:373:LEU:N	1:D:373:LEU:HD23	2.24	0.52
1:C:149:ARG:HB3	1:C:193:ILE:CG1	2.40	0.52
1:C:647:GLU:HB3	1:C:649:ASN:HD22	1.75	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: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:233:ARG:HD3	1:A:326:HIS:CD2	2.45	0.52
1:A:172:SER:O	1:A:174:ILE:HG13	2.10	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:D:351:PHE:O	1:D:352:ASP:OD2	2.28	0.52
1:C:157:ASN:HD21	1:C:163:ARG:HB3	1.73	0.52
1:D:618:GLU:HB3	1:D:619:LEU:HD22	1.90	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:184:ASN:HA	1:A:220:ILE:HG22	1.91	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: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:A:610:TYR:CE1	1:A:617:HIS:HB3	2.45	0.51
1:D:446:LEU:C	1:D:448:GLU:H	2.14	0.51
1:C:169:ARG:HB2	2:C:1849:HOH:O	2.09	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: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:593:ASP:HA	1:B:597:HIS:CD2	2.46	0.51
1:B:539:MET:O	1:B:546:LYS:HE3	2.10	0.51
1:C:650:GLU:OE1	1:C:670:ASN:HB2	2.11	0.51
1:C:290:ASN:CB	2:C:833:HOH:O	2.48	0.51
1:C:247:GLU:OE1	1:C:525:HIS:CD2	2.63	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:B:441:ASN:OD1	1:B:444:ARG:NH2	2.40	0.51
1:D:636:ARG:HG2	1:D:662:ARG:NH2	2.26	0.51
1:C:350:GLU:HA	1:C:354:THR:O	2.11	0.51
1:A:354:THR:O	1:A:356:LEU:N	2.43	0.51
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:A:380:ARG:CG	1:A:380:ARG:HH21	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:D:182:ALA:HA	1:D:186:GLN:NE2	2.25	0.50
1:B:680:ASN:HD22	1:B:680:ASN:C	2.15	0.50
1:B:411:ILE:HG13	1:B:412:TYR:CD1	2.46	0.50
1:B:196:ASN:HB2	1:B:198:ASN:ND2	2.26	0.50
1:B:192:MET:SD	1:B:352:ASP:HA	2.51	0.50
1:C:272:LEU:HD23	1:C:321:PHE:HZ	1.76	0.50
1:C:254:ARG:O	1:C:263:LEU:HG	2.12	0.50
1:C:500:ARG:HG2	1:C:500:ARG:NH2	2.26	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:D:495:LEU:O	1:D:500:ARG:NH1	2.44	0.50
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.95	0.50
1:D:264:SER:H	1:D:267:GLU:HB2	1.74	0.50
1:C:656:ASN:C	1:C:656:ASN:HD22	2.14	0.50
1:C:399:ILE:HD12	1:C:401:ALA:O	2.11	0.50
1:B:552:ALA:HA	1:B:720:THR:HG23	1.93	0.50
1:C:568:MET:HB2	1:C:584:LEU:HD11	1.92	0.50
1:D:278:TRP:O	1:D:604:ARG:HD2	2.11	0.50
1:D:601:ARG:HD3	2:D:1124:HOH:O	2.11	0.50
1:C:183:HIS:H	1:C:186:GLN:NE2	2.03	0.50
1:A:212:MET:HE2	1:A:213:ARG:HG3	1.93	0.50
1:D:527:GLU:HB3	2:D:1112:HOH:O	2.10	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:B:658:THR:HB	2:B:865:HOH:O	2.11	0.50
1:B:440:ARG:CG	1:B:475:LEU:H	2.25	0.50
1:C:290:ASN:OD1	1:C:305:LEU:HA	2.12	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:693:ASN:HD21	1:B:714:THR:H	1.60	0.50
1:C:514:ASN:ND2	2:C:1127:HOH:O	2.45	0.50
1:C:351:PHE:O	1:C:352:ASP:OD2	2.29	0.49
1:D:666:ARG:HA	1:D:712:SER:HA	1.93	0.49
1:D:183:HIS:ND1	1:D:186:GLN:NE2	2.60	0.49
1:B:617:HIS:HE1	2:B:1920:HOH:O	1.95	0.49
1:C:497:PRO:CA	1:C:500:ARG:HD3	2.29	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:558:TRP:HA	1:C:564:LYS:HE3	1.93	0.49
1:D:679:LEU:HD22	1:D:722:TRP:CE2	2.46	0.49
1:C:708:GLN:HG2	1:C:709:HIS:ND1	2.27	0.49
1:B:341:PHE:CD2	1:B:373:LEU:HD12	2.47	0.49
1:A:211:GLN:NE2	1:A:214:PRO:O	2.44	0.49
1:D:293:PRO:HD3	1:D:303:THR:CG2	2.43	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:B:343:THR:HG22	1:B:373:LEU:HD21	1.95	0.49
1:C:315:ARG:HH11	1:C:315:ARG:HG2	1.77	0.49
1:A:225:GLU:O	1:A:396:ARG:NH2	2.46	0.49
1:C:655:SER:HB3	1:C:657:PHE:CE2	2.48	0.49
1:B:511:ILE:HD13	1:B:626:PHE:CD2	2.48	0.49
1:B:381:GLU:OE2	1:B:381:GLU:N	2.42	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:D:470:GLN:HA	1:D:474:GLY:HA2	1.94	0.49
1:D:440:ARG:CG	1:D:475:LEU:H	2.26	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:C:564:LYS:HE2	1:C:610:TYR:CE1	2.48	0.49
1:A:542:ASP:O	1:A:545:GLN:N	2.46	0.49
1:D:337:VAL:HG23	1:D:337:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ILE:O	1:C:398:GLY:HA2	2.13	0.49
1:B:594:ASN:N	1:B:597:HIS:HD2	1.96	0.49
1:B:160:ASP:OD2	1:B:162:ARG:HD2	2.13	0.49
1:A:247:GLU:OE1	1:A:525:HIS:CD2	2.66	0.49
1:A:632:ASP:HB2	2:A:1911:HOH:O	2.12	0.49
1:A:504:HIS:CG	1:A:634:LYS:HG2	2.47	0.49
1:C:685:HIS:N	1:C:685:HIS:ND1	2.60	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:A:432:ASN:ND2	1:A:435:ALA:HB2	2.28	0.49
1:C:636:ARG:CB	1:C:638:VAL:HG23	2.42	0.49
1:D:547:PHE:CE2	1:D:595:TRP:HB3	2.48	0.49
1:C:708:GLN:O	1:C:709:HIS:HB2	2.13	0.49
1:C:499:TYR:O	1:C:501:GLN:N	2.46	0.49
1:C:685:HIS:O	1:C:686:TYR:CB	2.61	0.48
1:B:708:GLN:O	1:B:708:GLN:HG2	2.13	0.48
1:B:408:ALA:HB2	1:B:459:GLU:OE2	2.13	0.48
1:D:489:THR:O	1:D:493:MET:HG2	2.13	0.48
1:B:403:ARG:NH2	2:B:809:HOH:O	2.46	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:A:341:PHE:HD1	1:A:375:TYR:CD2	2.31	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:A:374:ILE:HD13	1:A:374:ILE:H	1.78	0.48
1:A:374:ILE:N	1:A:374:ILE:HD13	2.27	0.48
1:C:259:ASN:HD22	1:C:259:ASN:N	2.11	0.48
1:C:683:SER:HA	2:C:1568:HOH:O	2.12	0.48
1:B:254:ARG:O	1:B:255:ARG:HG2	2.14	0.48
1:A:609:THR:O	1:A:611:ARG:O	2.31	0.48
1:A:504:HIS:HD2	2:A:991:HOH:O	1.94	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:D:135:VAL:HG12	1:D:180:PRO:HB3	1.95	0.48
1:C:551:ARG:HB3	1:C:681:THR:HG22	1.95	0.48
1:C:545:GLN:O	1:C:549:ASN:ND2	2.46	0.48
1:A:665:TYR:O	1:A:712:SER:HA	2.13	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:C:318:PHE:HZ	2:C:1891:HOH:O	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:568:MET:HB2	1:A:584:LEU:HD11	1.95	0.48
1:A:315:ARG:HD2	1:A:315:ARG:C	2.34	0.48
1:C:471:ASP:HB2	1:C:472:MET:HE3	1.94	0.48
1:A:224:PRO:O	1:A:225:GLU:C	2.52	0.48
1:D:341:PHE:CZ	1:D:358:GLU:HB3	2.48	0.48
1:C:143:TRP:CH2	1:C:356:LEU:HD22	2.49	0.48
1:A:150:VAL:HG22	1:A:192:MET:HB2	1.94	0.48
1:D:444:ARG:O	1:D:448:GLU:HB2	2.14	0.48
1:C:700:ASP:O	1:C:709:HIS:HA	2.13	0.48
1:C:685:HIS:O	1:C:686:TYR:CG	2.66	0.48
1:C:209:GLU:HG2	1:C:219:LEU:HD13	1.96	0.48
1:B:442:THR:O	1:B:446:LEU:HB2	2.12	0.48
1:D:684:MET:HE3	1:D:684:MET:HB3	1.66	0.48
1:A:693:ASN:HD21	1:A:714:THR:N	2.04	0.48
1:C:166:MET:HG2	1:C:177:LEU:HB2	1.96	0.48
1:B:351:PHE:O	1:B:352:ASP:HB3	2.13	0.48
1:A:512:LEU:H	1:A:512:LEU:HD22	1.79	0.48
1:B:728:GLU:HG2	2:B:1862:HOH:O	2.13	0.48
1:B:618:GLU:OE1	1:B:645:ASP:HB2	2.13	0.48
1:C:480:LYS:O	1:C:519:PHE:HD2	1.97	0.48
1:C:192:MET:SD	1:C:352:ASP:HA	2.54	0.48
1:B:651:ILE:HG13	1:B:651:ILE:O	2.14	0.48
2:C:1199:HOH:O	1:D:695:GLY:HA2	2.13	0.48
1:D:552:ALA:HA	1:D:720:THR:CG2	2.41	0.47
1:D:371:ASN:CG	1:D:372:THR:N	2.67	0.47
1:D:684:MET:C	1:D:685:HIS:O	2.49	0.47
1:A:147:ALA:HB3	1:A:175:TRP:HZ2	1.79	0.47
1:B:665:TYR:O	1:B:712:SER:HA	2.14	0.47
1:B:413:ARG:O	1:B:414:ASP:HB2	2.14	0.47
1:D:219:LEU:HD23	1:D:220:ILE:O	2.14	0.47
1:D:148:ARG:O	1:D:193:ILE:HB	2.14	0.47
1:D:564:LYS:HD2	1:D:564:LYS:N	2.29	0.47
1:A:576:ARG:NH1	1:A:585:ASP:OD2	2.47	0.47
1:A:474:GLY:O	1:A:476:GLY:N	2.46	0.47
1:D:514:ASN:ND2	1:D:561:PRO:HB2	2.28	0.47
1:A:149:ARG:HD3	1:A:193:ILE:HG13	1.95	0.47
1:D:680:ASN:HD22	1:D:682:ASP:H	1.62	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:A:457:ALA:HB2	1:A:477:PHE:CE2	2.49	0.47
1:D:686:TYR:O	1:D:687:HIS:HB2	2.15	0.47
1:A:211:GLN:O	1:A:216:THR:HA	2.13	0.47
1:B:697:VAL:HG11	1:B:713:LEU:HD23	1.95	0.47
1:B:211:GLN:HG3	1:B:211:GLN:O	2.14	0.47
1:C:225:GLU:O	1:C:225:GLU:HG3	2.14	0.47
1:C:666:ARG:NH1	1:C:700:ASP:HB2	2.29	0.47
1:C:594:ASN:OD1	1:C:596:HIS:HB2	2.15	0.47
1:C:292:HIS:O	1:C:311:ARG:NH1	2.47	0.47
1:D:135:VAL:CG1	1:D:180:PRO:HB3	2.44	0.47
1:D:379:ARG:HB3	1:D:382:VAL:CG2	2.44	0.47
1:C:683:SER:O	1:C:685:HIS:O	2.33	0.47
1:D:684:MET:HB2	1:D:690:ASN:CG	2.35	0.47
1:C:305:LEU:CD2	1:C:305:LEU:H	2.27	0.47
1:A:168:LEU:CG	1:A:169:ARG:N	2.78	0.47
1:D:490:LEU:O	1:D:494:LYS:HG3	2.14	0.47
1:B:149:ARG:HB3	1:B:193:ILE:HB	1.95	0.47
1:D:346:PHE:HA	2:D:1211:HOH:O	2.14	0.47
1:B:374:ILE:HD13	1:B:374:ILE:H	1.78	0.47
1:D:141:SER:HA	1:D:175:TRP:O	2.13	0.47
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.97	0.47
1:D:237:ASN:ND2	1:D:283:HIS:HE1	2.13	0.47
1:C:551:ARG:C	1:C:681:THR:HG21	2.35	0.47
1:B:572:PHE:HB2	1:B:589:LEU:HD21	1.96	0.47
1:B:335:ASP:OD1	1:B:403:ARG:HD3	2.14	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:A:463:PHE:CE2	1:A:475:LEU:HD13	2.49	0.47
1:A:376:ASN:C	1:A:376:ASN:HD22	2.18	0.47
1:B:163:ARG:NH2	2:B:1006:HOH:O	2.47	0.47
1:C:602:LEU:HA	1:C:686:TYR:CE1	2.49	0.47
1:A:680:ASN:C	1:A:680:ASN:ND2	2.65	0.47
1:A:144:ALA:HB1	1:A:352:ASP:CB	2.45	0.47
1:C:157:ASN:OD1	1:C:164:HIS:HD2	1.98	0.47
1:B:298:TRP:HE1	1:B:580:HIS:CD2	2.33	0.47
1:D:273:VAL:HB	1:D:274:PRO:HD3	1.96	0.47
1:B:598:GLY:HA3	1:B:686:TYR:HA	1.96	0.47
1:A:229:GLN:HG2	1:A:234:LYS:HG2	1.95	0.47
1:B:551:ARG:HG2	1:B:602:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:ARG:HH12	1:C:700:ASP:HB2	1.79	0.47
1:A:504:HIS:CD2	1:A:634:LYS:HA	2.50	0.47
1:C:259:ASN:N	1:C:259:ASN:ND2	2.59	0.47
1:B:268:LEU:O	1:B:272:LEU:HB3	2.15	0.47
1:D:412:TYR:C	1:D:414:ASP:H	2.18	0.47
1:D:205:PRO:HB3	1:D:348:LEU:HD11	1.97	0.47
1:C:579:ASN:C	1:C:579:ASN:HD22	2.19	0.47
1:C:681:THR:HG22	2:C:1864:HOH:O	2.15	0.46
1:C:493:MET:HE2	1:C:553:TYR:HB2	1.96	0.46
1:A:614:LYS:HD2	1:A:614:LYS:N	2.30	0.46
1:D:265:TYR:HB2	1:D:317:ASP:HB3	1.97	0.46
1:C:166:MET:HG2	1:C:177:LEU:CB	2.45	0.46
1:B:711:LEU:O	1:B:712:SER:HB3	2.15	0.46
1:B:543:ALA:O	1:B:547:PHE:HD1	1.98	0.46
1:C:551:ARG:HD2	1:C:681:THR:O	2.15	0.46
1:C:349:ALA:HA	1:C:358:GLU:OE1	2.14	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:651:ILE:HD12	1:C:651:ILE:C	2.34	0.46
1:D:667:PHE:O	1:D:710:SER:HB2	2.14	0.46
1:D:584:LEU:O	1:D:585:ASP:HB2	2.15	0.46
1:A:490:LEU:O	1:A:494:LYS:HG3	2.14	0.46
1:A:257:THR:HG22	1:A:258:ASP:N	2.30	0.46
1:C:703:ALA:HA	1:C:707:ARG:O	2.15	0.46
1:D:639:LEU:N	1:D:639:LEU:HD12	2.29	0.46
1:C:273:VAL:CB	1:C:274:PRO:HD3	2.40	0.46
1:A:118:HIS:O	1:A:121:PRO:HD3	2.16	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:B:379:ARG:HB3	1:B:382:VAL:HG23	1.97	0.46
1:A:593:ASP:OD2	1:A:687:HIS:HE1	1.99	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:B:168:LEU:HD22	1:B:168:LEU:C	2.35	0.46
1:A:211:GLN:HG2	1:A:211:GLN:O	2.14	0.46
1:A:289:ILE:H	1:A:289:ILE:HG13	1.63	0.46
1:C:341:PHE:HE1	1:C:357:TYR:HB3	1.80	0.46
1:B:456:MET:HG2	1:B:479:TYR:HB2	1.97	0.46
1:C:631:VAL:HG22	1:C:631:VAL:O	2.14	0.46
1:B:658:THR:CG2	1:B:660:VAL:HG23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG12	1:A:233:ARG:HH22	1.80	0.46
1:A:148:ARG:O	1:A:149:ARG:CB	2.62	0.46
1:A:150:VAL:HG12	1:A:166:MET:SD	2.56	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:A:237:ASN:HD22	1:A:283:HIS:HE1	1.63	0.46
1:D:662:ARG:HB2	1:D:715:LEU:HB2	1.98	0.46
1:B:131:THR:OG1	1:B:136:THR:HG22	2.16	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:B:643:ARG:O	1:B:650:GLU:HA	2.16	0.46
1:B:259:ASN:HB3	1:B:261:PHE:CD2	2.50	0.46
1:B:150:VAL:HG22	1:B:192:MET:HB2	1.97	0.46
1:C:245:ILE:HG21	1:C:285:GLU:HB2	1.98	0.46
1:D:432:ASN:HB3	1:D:435:ALA:HB3	1.98	0.46
1:B:333:ILE:HG12	1:B:401:ALA:HB3	1.97	0.46
1:C:620:ASP:OD2	1:C:643:ARG:NH2	2.49	0.46
1:D:382:VAL:O	1:D:385:PHE:HB3	2.16	0.46
1:A:214:PRO:C	1:A:216:THR:H	2.18	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:D:310:ARG:NE	2:D:1482:HOH:O	2.49	0.46
1:D:659:PRO:O	1:D:717:PRO:HB3	2.16	0.46
1:B:117:THR:N	2:B:1682:HOH:O	2.48	0.46
1:B:194:ASP:HB2	1:B:198:ASN:CA	2.46	0.45
1:D:601:ARG:HG2	1:D:685:HIS:CE1	2.51	0.45
1:C:290:ASN:HD21	1:C:305:LEU:HA	1.80	0.45
1:A:278:TRP:HB2	1:B:612:HIS:CE1	2.51	0.45
1:D:618:GLU:OE1	1:D:645:ASP:HB2	2.16	0.45
1:D:194:ASP:OD2	1:D:198:ASN:HB2	2.15	0.45
1:A:450:VAL:O	1:A:450:VAL:HG23	2.15	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:A:647:GLU:HB3	1:A:649:ASN:ND2	2.31	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:D:358:GLU:N	1:D:358:GLU:OE2	2.44	0.45
1:C:493:MET:CE	1:C:553:TYR:HB2	2.47	0.45
1:C:349:ALA:O	1:C:350:GLU:C	2.54	0.45
1:A:147:ALA:O	1:A:195:ALA:CA	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:TRP:CE3	1:C:338:PRO:HG2	2.52	0.45
1:C:619:LEU:HB2	1:C:625:GLY:HA3	1.99	0.45
1:B:159:TRP:HB3	2:B:1734:HOH:O	2.17	0.45
1:A:496:ASP:HB3	1:A:499:TYR:CD1	2.50	0.45
1:C:552:ALA:HB2	1:C:718:LEU:O	2.16	0.45
1:C:485:TRP:CH2	1:C:557:MET:HG3	2.51	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: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:C:492:TYR:CZ	1:C:500:ARG:HG3	2.52	0.45
1:C:463:PHE:O	1:C:466:VAL:HG23	2.17	0.45
1:D:311:ARG:HE	1:D:311:ARG:HB2	1.61	0.45
1:D:466:VAL:O	1:D:477:PHE:HB2	2.17	0.45
1:A:712:SER:N	2:A:1917:HOH:O	2.15	0.45
1:A:341:PHE:HD1	1:A:375:TYR:CE2	2.35	0.45
1:C:121:PRO:HB2	1:C:125:LEU:HD12	1.97	0.45
1:C:669:ILE:HD11	1:C:699:SER:HB2	1.98	0.45
1:C:593:ASP:HA	1:C:597:HIS:HD2	1.80	0.45
1:A:194:ASP:OD1	1:A:198:ASN:HB2	2.16	0.45
1:D:651:ILE:HD12	1:D:651:ILE:C	2.36	0.45
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.66	0.45
1:A:164:HIS:HB3	1:A:177:LEU:HD21	1.99	0.45
1:D:614:LYS:N	1:D:614:LYS:HD2	2.31	0.45
1:A:667:PHE:HA	1:A:705:HIS:CD2	2.52	0.45
1:A:156:PHE:HE1	1:A:188:TYR:HB3	1.82	0.45
1:A:468:ARG:HB3	1:A:469:PRO:HD2	1.99	0.45
1:A:227:VAL:HG22	1:A:319:ARG:NH2	2.31	0.45
1:B:253:TRP:CE3	1:B:254:ARG:HB2	2.52	0.45
1:C:712:SER:N	2:C:1490:HOH:O	2.38	0.45
1:B:459:GLU:OE1	1:B:461:THR:O	2.35	0.45
1:D:372:THR:HG23	1:D:372:THR:O	2.16	0.45
1:B:469:PRO:HB2	1:B:471:ASP:OD2	2.16	0.45
1:A:255:ARG:HB2	1:A:583:SER:HB2	1.99	0.45
1:C:716:PRO:HB2	1:C:719:ALA:HB3	1.98	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:D:257:THR:HG22	1:D:258:ASP:N	2.32	0.45
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
1:D:679:LEU:HD22	1:D:722:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:HIS:NE2	1:B:263:LEU:HD22	2.32	0.44
1:B:168:LEU:HB2	1:B:175:TRP:CZ3	2.52	0.44
1:A:194:ASP:CG	1:A:198:ASN:HB2	2.38	0.44
1:D:268:LEU:O	1:D:272:LEU:HB3	2.16	0.44
1:C:700:ASP:O	1:C:710:SER:N	2.45	0.44
1:A:337:VAL:HG23	1:A:337:VAL:O	2.16	0.44
1:D:593:ASP:HA	1:D:597:HIS:CD2	2.52	0.44
1:D:590:GLU:O	1:D:591:GLY:O	2.35	0.44
1:A:351:PHE:HD2	1:A:356:LEU:HD12	1.83	0.44
1:D:618:GLU:C	1:D:619:LEU:HD22	2.38	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:A:285:GLU:HA	1:A:333:ILE:O	2.17	0.44
1:A:411:ILE:HG13	1:A:412:TYR:CD1	2.52	0.44
1:A:317:ASP:O	1:A:320:TYR:HB3	2.17	0.44
1:C:351:PHE:HD2	1:C:356:LEU:HD12	1.81	0.44
1:A:186:GLN:HB2	1:A:220:ILE:HD12	1.99	0.44
1:C:225:GLU:O	1:C:226:LYS:HB2	2.16	0.44
1:B:441:ASN:OD1	1:B:444:ARG:NH1	2.48	0.44
1:B:713:LEU:HA	2:B:1397:HOH:O	2.17	0.44
1:A:590:GLU:HG3	1:A:591:GLY:H	1.83	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:A:137:GLY:HA3	1:A:179:ILE:O	2.18	0.44
1:D:716:PRO:HB2	1:D:719:ALA:HB3	1.98	0.44
1:D:291:GLU:OE1	1:D:291:GLU:HA	2.17	0.44
1:A:684:MET:HG3	1:A:685:HIS:N	2.32	0.44
1:C:528:VAL:HA	1:C:533:LYS:O	2.18	0.44
1:A:182:ALA:HA	1:A:186:GLN:OE1	2.18	0.44
1:D:573:ALA:O	1:D:596:HIS:CE1	2.71	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:A:430:ARG:CB	1:A:430:ARG:HH21	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:693:ASN:HD21	1:C:714:THR:N	2.02	0.44
1:C:532:LYS:O	1:C:533:LYS:HB2	2.16	0.44
1:C:168:LEU:HD21	1:C:173:GLY:HA2	1.99	0.44
1:C:656:ASN:C	1:C:656:ASN:ND2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ASN:ND2	1:C:283:HIS:CE1	2.79	0.43
1:C:157:ASN:CG	1:C:164:HIS:HD2	2.21	0.43
1:A:444:ARG:O	1:A:448:GLU:HG3	2.18	0.43
1:D:523:LEU:HA	1:D:523:LEU:HD12	1.81	0.43
1:D:262:TRP:CZ3	1:D:311:ARG:HG3	2.53	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:351:PHE:O	1:B:356:LEU:HD12	2.18	0.43
1:B:129:ALA:HB2	2:B:839:HOH:O	2.18	0.43
1:C:723:LEU:N	1:C:723:LEU:HD22	2.32	0.43
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.99	0.43
1:D:525:HIS:HB3	1:D:567:PHE:CE1	2.53	0.43
1:D:447:GLY:HA2	1:D:451:SER:HA	2.01	0.43
1:A:168:LEU:HD12	1:A:169:ARG:N	2.21	0.43
1:C:152:VAL:HG21	1:C:177:LEU:HD23	1.99	0.43
1:A:564:LYS:HE2	1:A:610:TYR:CE1	2.53	0.43
1:C:474:GLY:O	1:C:475:LEU:HB2	2.19	0.43
1:C:192:MET:HE2	1:C:202:LYS:HG3	2.00	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:D:615:ALA:HB1	1:D:643:ARG:O	2.18	0.43
1:C:219:LEU:HD23	1:C:220:ILE:O	2.18	0.43
1:D:263:LEU:HB3	1:D:267:GLU:HB3	2.00	0.43
1:D:685:HIS:C	1:D:687:HIS:H	2.21	0.43
1:A:168:LEU:CG	1:A:169:ARG:H	2.31	0.43
1:C:608:LEU:O	1:C:611:ARG:O	2.37	0.43
1:C:352:ASP:C	1:C:352:ASP:OD2	2.56	0.43
1:A:150:VAL:HA	1:A:191:GLU:O	2.18	0.43
1:A:408:ALA:HA	1:A:411:ILE:HG12	1.99	0.43
1:D:288:PRO:HB2	1:D:299:GLY:HA3	2.01	0.43
1:D:123:GLU:HA	1:D:223:LEU:HD21	2.01	0.43
1:D:430:ARG:HH11	1:D:430:ARG:CB	2.15	0.43
1:C:486:MET:O	1:C:490:LEU:HB2	2.18	0.43
1:C:256:HIS:HE1	1:C:267:GLU:OE1	2.02	0.43
1:D:371:ASN:O	1:D:372:THR:C	2.55	0.43
1:B:667:PHE:HA	1:B:705:HIS:CD2	2.54	0.43
1:B:194:ASP:CB	1:B:198:ASN:HB2	2.48	0.43
1:A:708:GLN:HA	2:A:1907:HOH:O	2.18	0.43
1:A:667:PHE:HA	1:A:705:HIS:HD2	1.84	0.43
1:A:250:LEU:HD21	1:A:286:LEU:HD22	1.99	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: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:C:194:ASP:HB2	1:C:198:ASN:H	1.83	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:A:296:GLY:HA2	1:A:580:HIS:CE1	2.54	0.43
1:C:245:ILE:CG2	1:C:285:GLU:HB2	2.48	0.43
1:B:571:GLU:O	1:B:600:GLN:HA	2.18	0.43
1:C:657:PHE:O	1:C:658:THR:HB	2.19	0.43
1:B:315:ARG:C	1:B:315:ARG:HD2	2.40	0.43
1:C:693:ASN:HD21	1:C:713:LEU:HB2	1.84	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:D:466:VAL:HA	1:D:475:LEU:HD22	2.01	0.42
1:D:289:ILE:HG13	1:D:334:LEU:HD11	2.01	0.42
1:C:307:ALA:HA	1:C:308:PRO:HD3	1.86	0.42
1:D:529:VAL:HA	1:D:577:GLU:OE1	2.19	0.42
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: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:143:TRP:CZ3	1:A:356:LEU:HD22	2.55	0.42
1:B:233:ARG:HA	1:B:331:ASN:HD21	1.84	0.42
1:A:157:ASN:C	1:A:159:TRP:N	2.71	0.42
1:B:322:ILE:HG21	1:B:397:PHE:O	2.19	0.42
1:A:662:ARG:HB2	1:A:715:LEU:HB2	2.00	0.42
1:C:280:GLY:O	1:C:611:ARG:NH1	2.41	0.42
1:C:146:ASN:HB2	1:C:352:ASP:OD1	2.19	0.42
1:A:380:ARG:CG	1:A:380:ARG:NH2	2.78	0.42
1:C:566:LEU:HG	1:C:570:ASN:HB2	2.02	0.42
1:B:160:ASP:CG	1:B:162:ARG:HD2	2.40	0.42
1:D:531:GLY:CA	1:D:577:GLU:OE2	2.66	0.42
1:D:164:HIS:HE1	2:D:1447:HOH:O	2.02	0.42
1:A:641:PHE:CD1	1:A:641:PHE:C	2.92	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:A:178:PHE:CE1	1:A:180:PRO:HG3	2.48	0.42
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.42
1:C:435:ALA:O	1:C:438:PHE:HB3	2.19	0.42
1:C:297:SER:C	1:C:299:GLY:H	2.23	0.42
1:C:598:GLY:HA3	1:C:686:TYR:HA	2.01	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:149:ARG:O	1:A:192:MET:HA	2.19	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: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:A:194:ASP:N	1:A:198:ASN:O	2.47	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:A:341:PHE:O	1:A:343:THR:HG23	2.20	0.42
1:D:504:HIS:CD2	1:D:634:LYS:HA	2.54	0.42
1:A:206:TYR:CZ	1:A:385:PHE:HD1	2.36	0.42
1:D:437:GLU:OE2	1:D:437:GLU:HA	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:A:541:GLY:HA2	2:A:1350:HOH:O	2.19	0.42
1:D:140:PHE:O	1:D:176:GLU:HA	2.20	0.42
1:C:457:ALA:HB2	1:C:477:PHE:CE2	2.55	0.42
1:C:679:LEU:HB3	1:C:722:TRP:HB2	2.02	0.42
1:C:265:TYR:CE2	1:C:312:PHE:HB2	2.55	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:C:315:ARG:HG2	1:C:315:ARG:NH1	2.35	0.42
1:C:722:TRP:C	1:C:723:LEU:HD22	2.40	0.41
1:B:594:ASN:HB2	2:B:1233:HOH:O	2.20	0.41
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:D:721:ILE:CD1	1:D:723:LEU:HD21	2.50	0.41
1:D:136:THR:HG22	1:D:137:GLY:N	2.35	0.41
1:B:629:LEU:HB2	1:B:640:ILE:HG22	2.02	0.41
1:D:713:LEU:HA	2:D:1624:HOH:O	2.20	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
1:C:542:ASP:N	1:C:545:GLN:HE21	2.18	0.41
1:A:147:ALA:O	1:A:148:ARG:HB2	2.19	0.41
1:B:606:LEU:HD13	1:B:679:LEU:CD1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ASP:O	1:B:463:PHE:C	2.59	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:D:293:PRO:HD3	1:D:303:THR:HG23	2.01	0.41
1:D:246:TYR:HB2	1:D:281:PHE:CG	2.55	0.41
1:C:523:LEU:HD22	1:C:557:MET:SD	2.61	0.41
1:C:223:LEU:HD23	1:C:396:ARG:CZ	2.50	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:351:PHE:O	1:C:353:GLY:N	2.54	0.41
1:B:457:ALA:HB2	1:B:477:PHE:CD2	2.55	0.41
1:C:336:TRP:CZ3	1:C:338:PRO:HG2	2.55	0.41
1:A:686:TYR:O	1:A:687:HIS:HB2	2.21	0.41
1:B:485:TRP:CH2	1:B:557:MET:HG3	2.55	0.41
1:C:684:MET:N	1:C:690:ASN:HD22	2.17	0.41
1:C:168:LEU:CD1	1:C:170:LYS:HA	2.50	0.41
1:A:351:PHE:CD2	1:A:356:LEU:HD12	2.56	0.41
1:D:140:PHE:CZ	1:D:220:ILE:HD11	2.52	0.41
1:B:680:ASN:HA	1:B:721:ILE:HG22	2.03	0.41
1:D:679:LEU:HB3	1:D:722:TRP:HB2	2.02	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:131:THR:OG1	1:C:136:THR:HG22	2.19	0.41
1:B:448:GLU:HB2	2:B:1637:HOH:O	2.20	0.41
1:C:262:TRP:CG	1:C:312:PHE:HE2	2.38	0.41
1:D:394:ILE:HG21	1:D:450:VAL:HG11	2.01	0.41
1:C:480:LYS:O	1:C:519:PHE:HA	2.20	0.41
1:B:547:PHE:CD2	1:B:595:TRP:HB3	2.55	0.41
1:C:375:TYR:O	1:C:376:ASN:HB3	2.20	0.41
1:C:565:LEU:HD23	1:C:565:LEU:C	2.40	0.41
1:B:141:SER:HA	1:B:175:TRP:O	2.21	0.41
1:B:490:LEU:HA	1:B:490:LEU:HD12	1.95	0.41
1:D:267:GLU:O	1:D:270:ASP:OD2	2.39	0.41
1:A:572:PHE:HZ	1:A:584:LEU:O	2.03	0.41
1:B:506:LYS:NZ	2:B:1487:HOH:O	2.53	0.41
1:A:631:VAL:HG22	1:A:631:VAL:O	2.21	0.41
1:B:496:ASP:O	1:B:497:PRO:C	2.58	0.41
1:C:152:VAL:HG23	1:C:177:LEU:HD23	2.02	0.41
1:B:559:ALA:HA	1:B:616:MET:HE3	2.03	0.41
1:B:143:TRP:CE2	1:B:381:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HA	1:A:410:MET:CE	2.50	0.41
1:C:643:ARG:HA	1:C:643:ARG:HD2	1.86	0.41
1:C:547:PHE:O	1:C:551:ARG:HB2	2.21	0.41
1:A:157:ASN:ND2	1:A:164:HIS:CD2	2.88	0.41
1:A:129:ALA:HA	1:A:138:THR:HG22	2.03	0.41
1:C:252:SER:OG	1:C:568:MET:HE1	2.21	0.41
1:C:579:ASN:C	1:C:579:ASN:ND2	2.75	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:D:163:ARG:HD2	2:D:1502:HOH:O	2.20	0.41
1:A:606:LEU:CD1	1:A:679:LEU:HD11	2.51	0.41
1:C:450:VAL:HG23	1:C:450:VAL:O	2.21	0.41
1:B:597:HIS:O	1:B:601:ARG:HB2	2.20	0.41
1:D:494:LYS:HG2	1:D:538:ARG:HB3	2.03	0.41
1:A:144:ALA:HA	1:A:145:PRO:HD2	1.91	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:447:GLY:N	2:A:1483:HOH:O	2.54	0.41
1:D:279:MET:O	1:D:604:ARG:HA	2.21	0.41
1:A:542:ASP:O	1:A:543:ALA:C	2.59	0.41
1:D:289:ILE:HG13	1:D:334:LEU:CD1	2.51	0.41
1:D:227:VAL:HG22	1:D:319:ARG:NH1	2.36	0.41
1:A:288:PRO:HB2	1:A:299:GLY:HA3	2.03	0.41
1:D:254:ARG:HA	1:D:583:SER:HB2	2.03	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.92	0.41
1:D:593:ASP:OD2	1:D:687:HIS:CE1	2.73	0.40
1:C:685:HIS:NE2	1:D:685:HIS:HD2	2.19	0.40
1:C:192:MET:CE	1:C:202:LYS:HG3	2.51	0.40
1:B:494:LYS:CD	1:B:538:ARG:HG2	2.51	0.40
1:C:669:ILE:HD11	1:C:699:SER:CB	2.50	0.40
1:B:318:PHE:O	1:B:321:PHE:HB3	2.20	0.40
1:A:254:ARG:NH2	2:A:1871:HOH:O	2.43	0.40
1:D:656:ASN:ND2	2:D:844:HOH:O	2.36	0.40
1:C:526:ASP:O	1:C:532:LYS:NZ	2.48	0.40
1:B:168:LEU:HB2	1:B:175:TRP:CE3	2.57	0.40
1:C:351:PHE:HB3	1:C:356:LEU:HD12	2.02	0.40
1:B:425:ASN:HD21	1:B:427:PHE:HB2	1.86	0.40
1:D:709:HIS:HD2	2:D:1905:HOH:O	2.04	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:690:ASN:HA	1:D:690:ASN:HD22	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:OD1	1:A:132:MET:HE1	2.22	0.40
1:B:289:ILE:HD12	1:B:289:ILE:C	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:A:372:THR:HG22	1:A:373:LEU:HD23	2.03	0.40
1:D:546:LYS:HE3	1:D:546:LYS:HB3	1.94	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: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:D:293:PRO:CD	1:D:303:THR:HG23	2.52	0.40
1:A:640:ILE:HA	1:A:653:VAL:O	2.21	0.40
1:C:333:ILE:HD13	1:C:456:MET:HE1	2.03	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
1:A:542:ASP:HB3	2:A:1800:HOH:O	2.20	0.40
1:D:411:ILE:HG13	1:D:412:TYR:CD1	2.56	0.40
1:A:377:TYR:HD1	2:A:1382:HOH:O	2.04	0.40
1:A:574:GLN:HB2	1:A:574:GLN:HE21	1.70	0.40
1:B:671:GLN:HB3	1:D:498:VAL:HG11	2.04	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%)	3 1
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	8 6
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	5 3

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

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 ⓘ

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%)	22	28
1	B	501/525 (95%)	464 (93%)	37 (7%)	17	21
1	C	490/525 (93%)	460 (94%)	30 (6%)	23	30
1	D	496/525 (94%)	466 (94%)	30 (6%)	24	31
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	21	27

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

Some 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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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