



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:35 AM 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 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/ValidationPDFNotes.html>

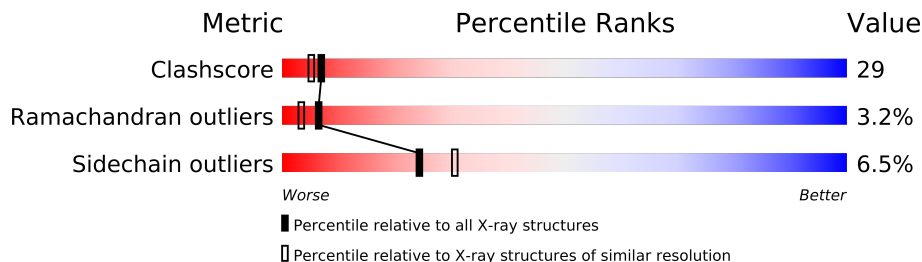
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.



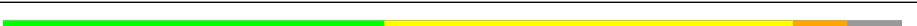

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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		

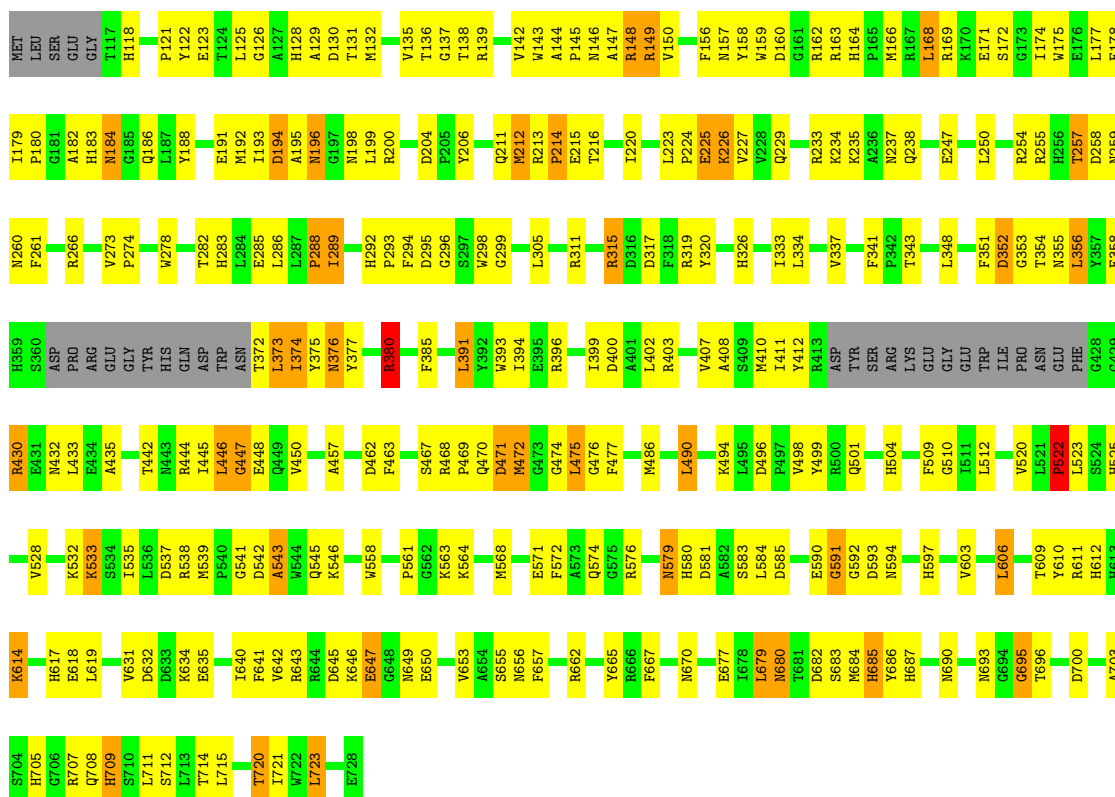
3 Residue-property plots

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

Note EDS was not executed.

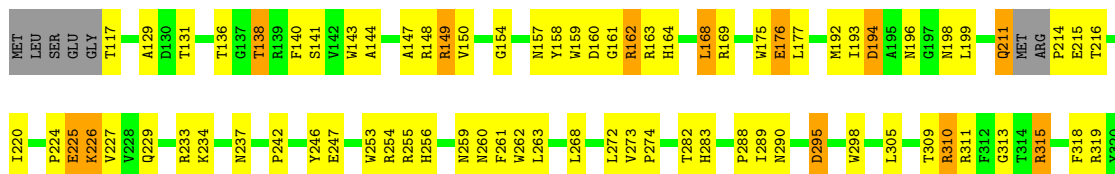
• Molecule 1: 1,4-alpha-glucan Branching Enzyme

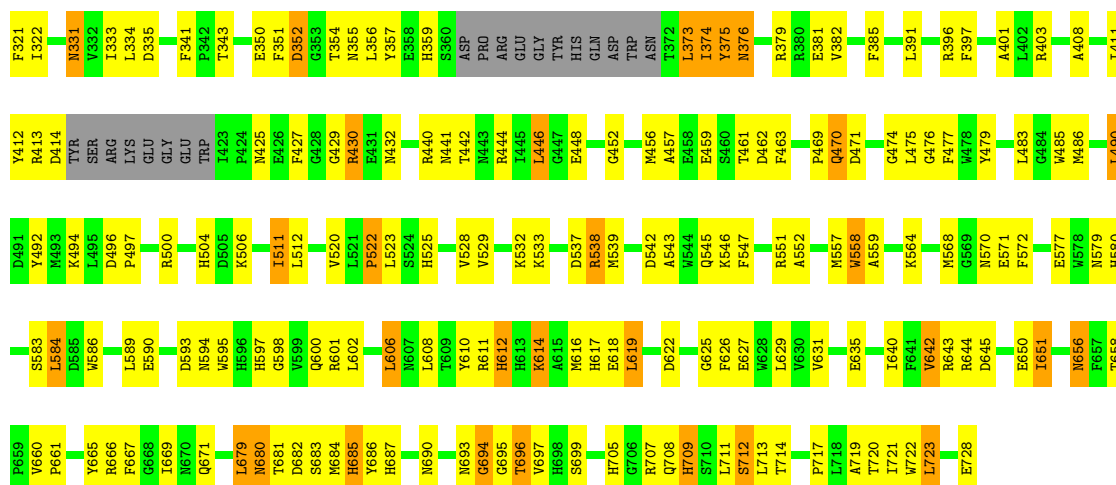
Chain A:



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

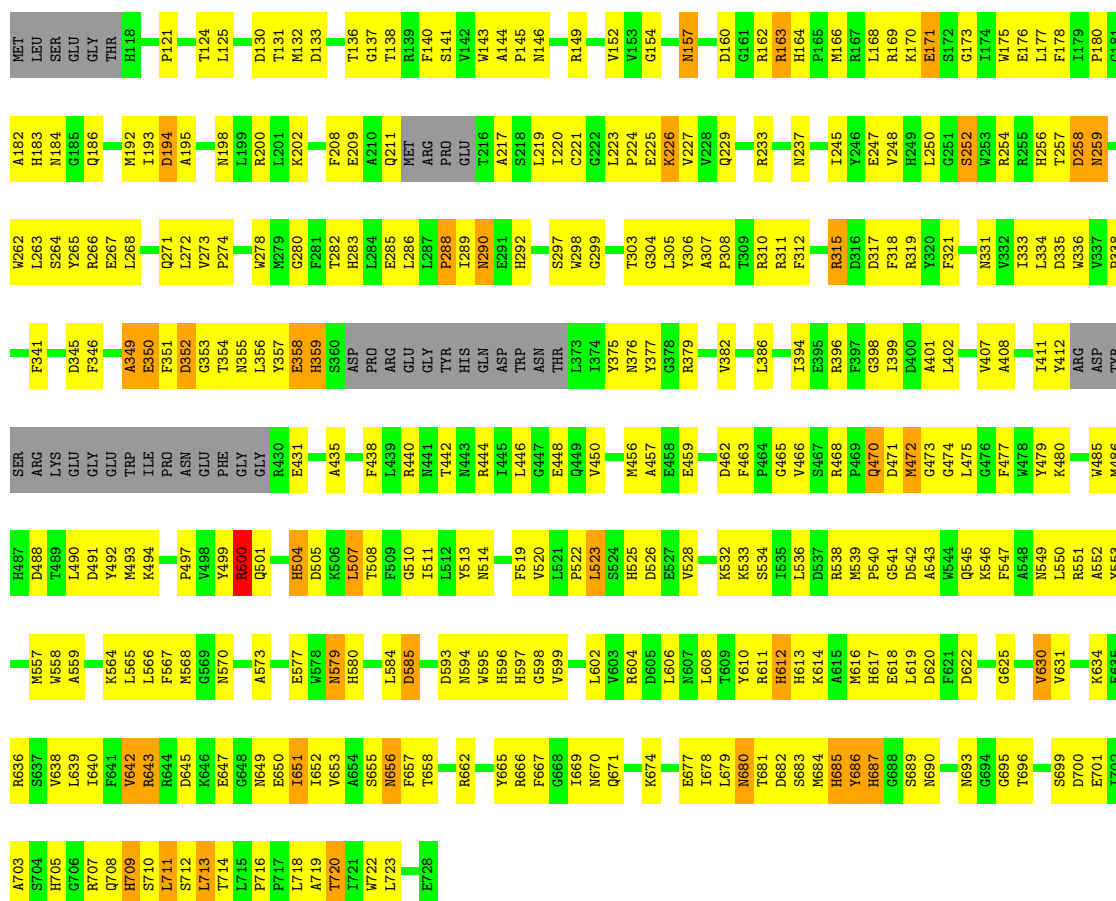
Chain B:





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

Chain C:



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

Chain D:



T714	L619	K546	M456	R379	P288	R200
L715	V631	F547	E459	V382	I289	
P717	D632	R551	V466	F385	N290	D204
L718	K633	A552	P469	R389	E291	P205
A719	R635	G555	Q470	Y392	H292	Q211
T720	R636	W558	M472	K393	PRD	W212
T721	L639	P561	G473	I394	GLU	ARG
W722	V642	K564	G474	R396	T216	GLU
L723	R643	L565	L475	T399	L219	
W724	R644	L566	G476	R403	T220	
R725	D645	F567	P477	R404	L223	
E726	K646	M568	Y479	V404	P224	
	E647	G569	T489	D405	V227	
	I651	N570	L490	I411	E232	
	N656	A573	D491	Y412	R319	
	P659	Q574	M492	R413	N331	
	R662	E577	K494	D414	V332	
	Y665	N578	L495	TYR	I333	
	R666	N579	D496	SER	L334	
	F667	H580	P497	ARG	Y246	
	G668	S583	V498	LYS	E247	
	K674	L584	Y499	GLY	L250	
	L679	D585	R500	GLY	F341	
	N680	E590	H504	TRP	R254	
	T681	G591	L507	ILE	T257	
	D682	D592	N514	PRD	D258	
	S683	N594	E517	ASN	N259	
	M684	N595	N518	PHE	F351	
	H685	H596	F519	GLY	D352	
	Y686	G598	V520	G429	L356	
	H687	L601	L521	R430	Y357	
	N690	L602	P522	E431	E358	
	N693	V603	L523	N432	H359	
	G694	R604	S524	A435	S359	
	G695	D605	H525	I436	ASP	
	T696	L606	D526	E437	PRD	
	D700	N607	W527	R440	ARG	
	H705	L608	V528	N443	GLY	
	Q708	T609	H529	N444	TYR	
	H709	Y610	G531	R445	HIS	
	S710	R611	I535	I446	GLN	
	L711	H612	R538	G447	ASP	
	S712	H613	D542	L448	TRP	
	L713	K614	Q545	E449	N371	
		A615		V450	F281	
		H616		S451	T282	
		H617		T455	L373	
					H283	
					L284	
					E285	

4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4805	0	4537	240	0
2	A	301	0	0	19	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (1077) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:C:551:ARG:HB3	1:C:681:THR:CG2	2.16	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

5.3.1 Protein backbone ⓘ

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%)	4	1
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	10	7
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	6	3
1	D	577/617 (94%)	522 (90%)	40 (7%)	15 (3%)	8	5
All	All	2311/2468 (94%)	2040 (88%)	197 (8%)	74 (3%)	6	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	25	31
1	B	501/525 (95%)	464 (93%)	37 (7%)	20	24
1	C	490/525 (93%)	460 (94%)	30 (6%)	26	34
1	D	496/525 (94%)	466 (94%)	30 (6%)	27	35
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	24	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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.