



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:48 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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

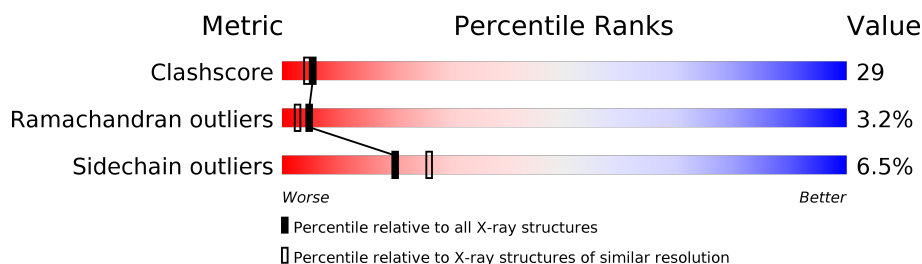
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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.

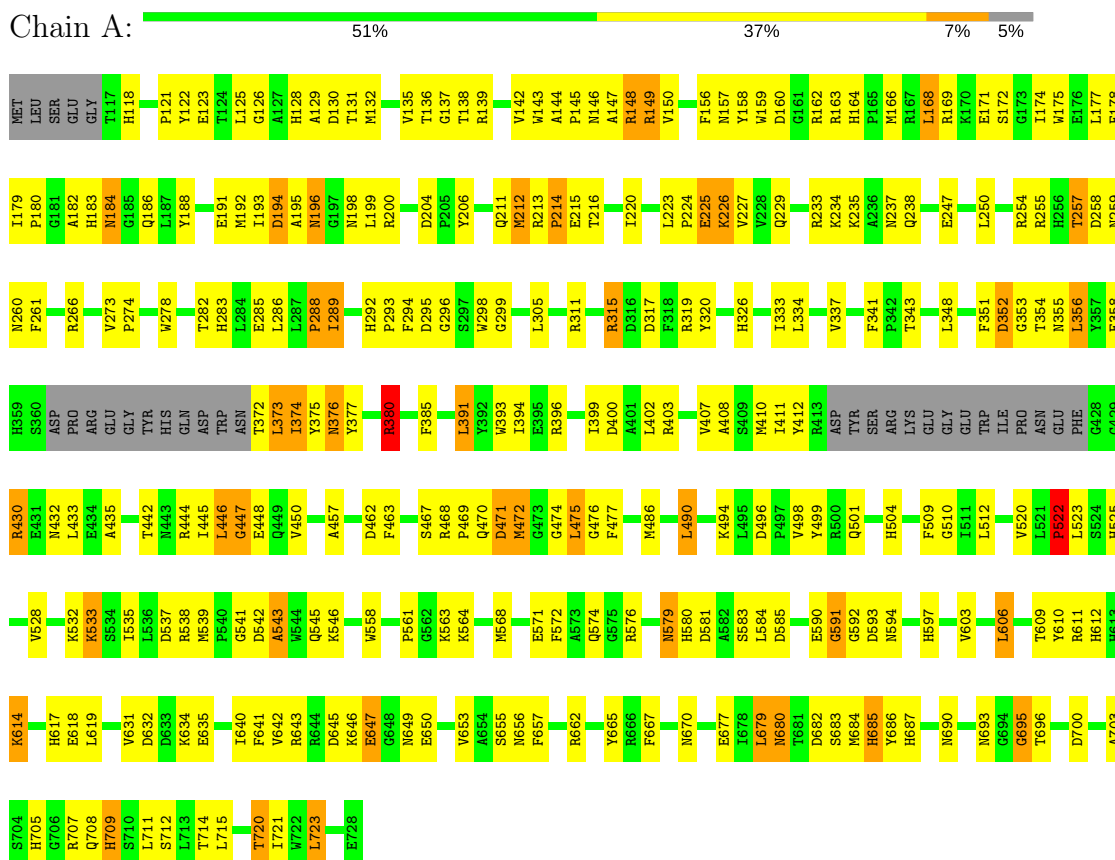
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	301	Total	O	0	0
			301	301		
2	B	425	Total	O	0	0
			425	425		
2	C	108	Total	O	0	0
			108	108		
2	D	308	Total	O	0	0
			308	308		

### 3 Residue-property plots

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

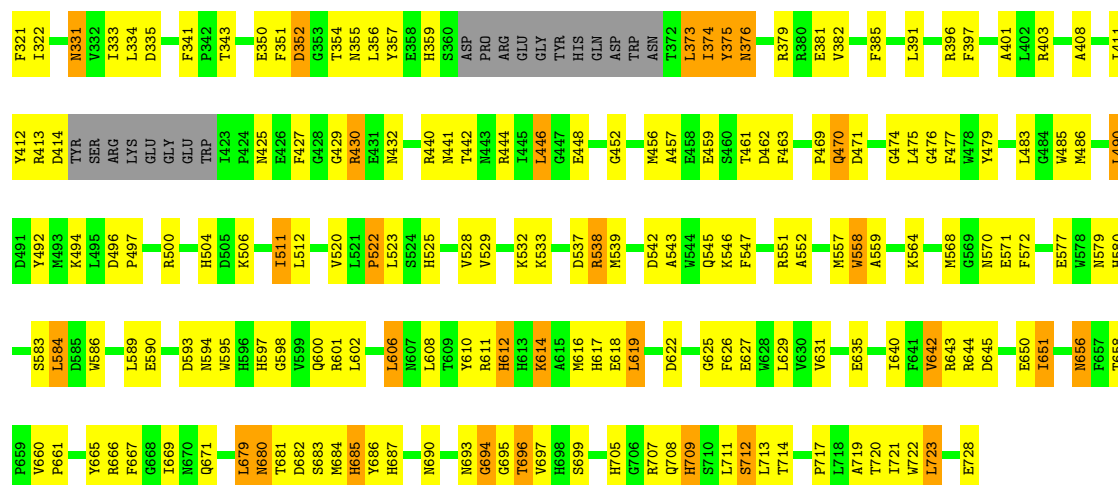
Note EDS was not executed.

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

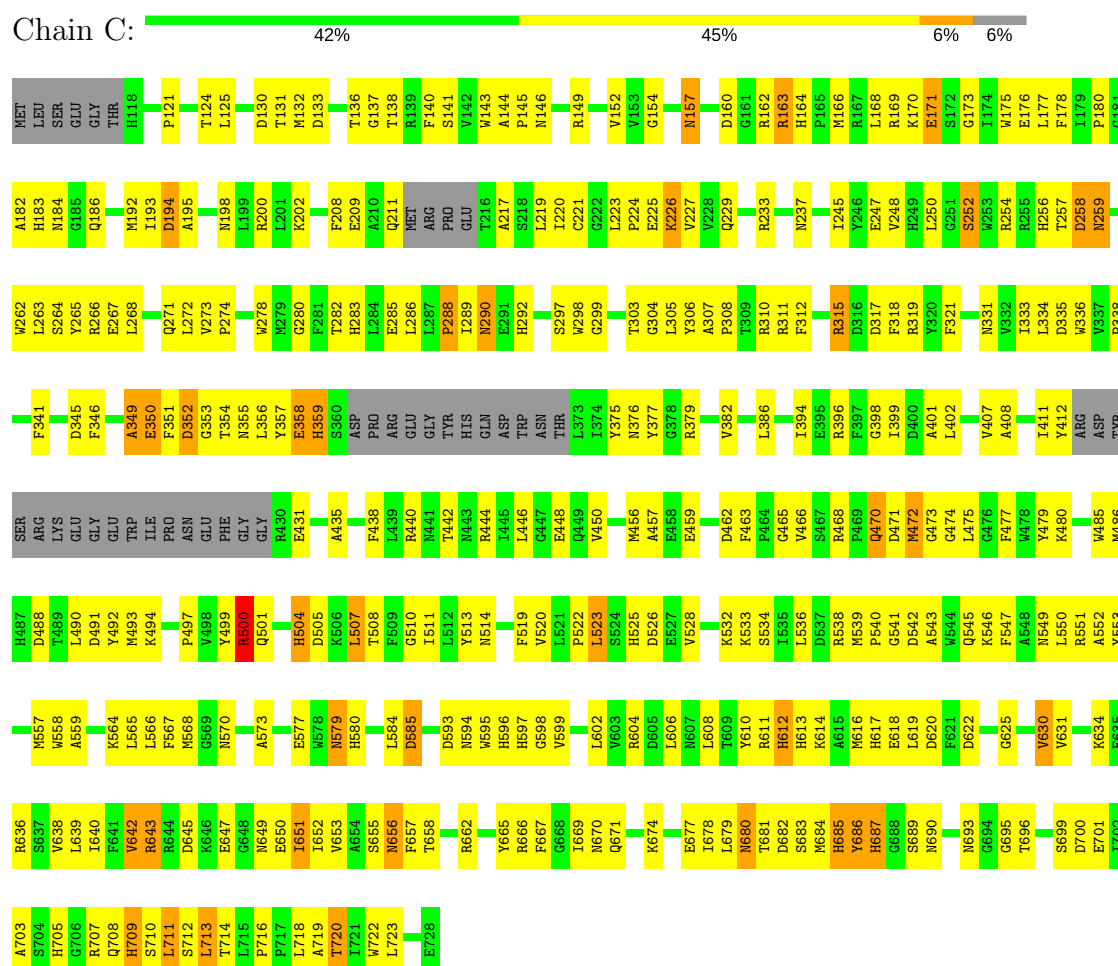


#### • Molecule 1: 1,4-alpha-glucan Branching Enzyme





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



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



T714	L619	K546	M456	R379	P288	R200	MET
L715	V631	F547	E459	V382	I289	D204	LEU
P716	D632	R551	E471	F385	N290	P205	SER
L717	D633	A552	V466	N389	H291	Q211	GLU
A718	K634	G555	P469	Y392	P293	W212	GLY
T720	E635	W558	Q470	W393	W298	ARG	
I721	R636	P561	D471	I394	G299	PRO	R120
W722	L639	K564	M472	E395	T303	T216	P121
L723	V642	L565	G474	R396	R309	L219	Y122
V724	R643	L566	L475	I399	R310	I220	E123
R725	D645	F567	F477	R403	R311	L223	
E728	K646	M568	Y479	R404	R315	P224	G126
	E647	G569	T489	D405	D316	V227	T131
	I651	N570	L490	I411	D317	E232	M132
	N656	A573	D491	Y412	R319	N237	V135
	P659	Q574	M493	R413	N331	Y246	T136
	R662	E577	K494	D414	N332	E247	G137
	Y665	W578	L495	TYR	T333	L250	T138
	R666	N579	D496	SER	L334	R264	R139
	F667	H580	P497	ARG	Y337	W262	F140
	G668	S583	Y498	LYS	H340	L263	S141
	K674	L584	R500	GLU	F341	S264	W142
		D585	H504	GLY	TRP	E267	W143
		E590	L507	ILE	I346	L268	A144
	L679	G591	N514	ASN	L348	E269	P145
	N680	G592	E517	GLU	F351	Q271	R163
	T681	D593	N518	PHE	D352	L272	H164
	D682	N594	F519	GLY	L356	V273	R167
	S683	W595	V520	GLY	E357	P274	L168
	M684	H596	L521	ASP	Y358	W278	R169
	H685	H597	P522	ASP	H359	M279	K170
	Y686	G598	L523	ARG	S360	T281	E171
	H687	R601	H524	GLY	PRO	T282	
		L602	D526	TYR	D270	H283	G175
	N690	R603	H528	R440	ARG	L284	E176
	N693	D605	V529	N443	GLY	W285	P180
	G694	L606	H530	R444	TYR	E286	G181
	G695	N607	G531	L445	HIS	L287	A182
	T696	I608	L535	E446	GLN	P274	H183
	D700	T609	R538	Q448	ASP	W278	Q186
		Y610	D542	L447	TRP	M279	
	H705	R611	E545	E449	ASP	F281	M192
	Q708	H613	R538	Q449	T372	T282	I193
	W709	K614	D542	V450	N371	H283	D194
	S710	A615	D542	S451	L373	E285	G197
	L711	M616	D542	T455	N376	L199	N198
	S712	H617	D542				
	L713	E618	D542				

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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

*Continued on next page...*



*Continued from previous page...*

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:HH11	1:C:643:ARG:HB3	1.12	1.08
1:A:430:ARG:HH21	1:A:430:ARG:HB3	1.22	1.02
1:C:497:PRO:HA	1:C:500:ARG:HD3	1.42	1.02
1:A:224:PRO:HG2	1:A:396:ARG:HB3	1.38	1.01
1:B:430:ARG:H	1:B:430:ARG:HD2	1.22	1.01
1:A:393:TRP:HB3	1:A:399:ILE:HD12	1.44	1.00
1:D:430:ARG:HH11	1:D:430:ARG:HB2	1.27	0.99
1:D:693:ASN:HD21	1:D:714:THR:H	1.10	0.99
1:B:194:ASP:HB2	1:B:198:ASN:H	1.28	0.99
1:D:470:GLN: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:B:470:GLN:HE21	1:B:470:GLN:N	1.70	0.89
1:C:643:ARG:HH11	1:C:643:ARG:CB	1.86	0.89
1:C:470:GLN: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

*Continued on next page...*

*Continued from previous page...*

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:C:183:HIS:H	1:C:186:GLN:HE21	1.28	0.81
1:D:470:GLN:HE21	1:D:470:GLN:N	1.78	0.81
1:A:684:MET:H	1:A:690:ASN:HD22	1.22	0.81
1:D:535:ILE:HA	1:D:538:ARG:HD2	1.63	0.81
1:A:684:MET:H	1:A:690:ASN:ND2	1.78	0.81
1:C:520:VAL:O	1:C:522:PRO:HD3	1.81	0.81
1:C:636:ARG:HG2	1:C:662:ARG:NH2	1.96	0.81
1:C:528:VAL:O	1:C:577:GLU:HB2	1.81	0.80
1:A:693:ASN:HD21	1:A:714:THR:H	1.28	0.80
1:A:680:ASN:ND2	1:A:682:ASP:H	1.80	0.80
1:D:674:LYS:HB3	1:D:696:THR:HG21	1.61	0.80
1:A:394:ILE:CD1	1:A:446:LEU:HD21	2.12	0.79
1:A:430:ARG:HB3	1:A:430:ARG:NH2	1.98	0.79
1:C:494:LYS:HG2	1:C:538:ARG:HG2	1.65	0.78
1:D:552:ALA:HA	1:D:720:THR:HG22	1.64	0.78
1:B:594:ASN:H	1:B:597:HIS:CD2	2.01	0.77
1:B:558:TRP:HA	1:B:564:LYS:HE3	1.67	0.77
1:D:469:PRO:HG2	1:D:472:MET:HG3	1.66	0.77
1:B:194:ASP:HB2	1:B:198:ASN:N	1.99	0.77
1:D:358:GLU:HG3	1:D:373:LEU:HD12	1.66	0.76
1:C:229:GLN:HA	1:C:233:ARG:HH11	1.47	0.76
1:C:505:ASP:HA	1:C:508:THR:OG1	1.85	0.76
1:D:594:ASN:H	1:D:597:HIS:CD2	2.01	0.76
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.18	0.76
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.65	0.76
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.67	0.76
1:C:552:ALA:HA	1:C:720:THR:HG22	1.66	0.76
1:A:594:ASN:H	1:A:597:HIS:CD2	2.02	0.76
1:C:611:ARG:O	1:C:612:HIS:HB3	1.86	0.76

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:HA2	1:A:580:HIS:CE1	2.54	0.43
1:B:309:THR:OG1	1:B:311:ARG:HG3	2.19	0.43
1:B:490:LEU:O	1:B:494:LYS:HG3	2.18	0.43
1:B:571:GLU:O	1:B:600:GLN:HA	2.18	0.43
1:C:194:ASP:HB2	1:C:198:ASN:H	1.83	0.43
1:C:245:ILE:CG2	1:C:285:GLU:HB2	2.48	0.43
1:C:652:ILE:HB	1:C:723:LEU:HB2	2.00	0.43
1:D:668:GLY:N	1:D:705:HIS:HD2	2.16	0.43
1:B:315:ARG:C	1:B:315:ARG:HD2	2.40	0.43
1:C:657:PHE:O	1:C:658:THR:HB	2.19	0.43
1:B:707:ARG:NH1	2:B:950:HOH:O	2.52	0.42
1:C:266:ARG:HB3	2:C:1337:HOH:O	2.19	0.42
1:C:307:ALA:HA	1:C:308:PRO:HD3	1.86	0.42
1:C:463:PHE:CD2	1:C:475:LEU:HD11	2.54	0.42
1:C:493:MET:HB3	1:C:539:MET:HE1	2.00	0.42
1:C:693:ASN:HD21	1:C:713:LEU:HB2	1.84	0.42
1:D:289:ILE:HG13	1:D:334:LEU:HD11	2.01	0.42
1:D:466:VAL:HA	1:D:475:LEU:HD22	2.01	0.42
1:D:529:VAL:HA	1:D:577:GLU:OE1	2.19	0.42
1:A:157:ASN:C	1:A:159:TRP:N	2.71	0.42
1:A:143:TRP:CZ3	1:A:356:LEU:HD22	2.55	0.42
1:A:662:ARG:HB2	1:A:715:LEU:HB2	2.00	0.42
1:B:233:ARG:HA	1:B:331:ASN:HD21	1.84	0.42
1:B:322:ILE:HG21	1:B:397:PHE:O	2.19	0.42
1:C:288:PRO:C	1:C:290:ASN:H	2.22	0.42
1:C:541:GLY:CA	1:C:545:GLN:HE21	2.33	0.42
1:A:380:ARG:CG	1:A:380:ARG:NH2	2.78	0.42
1:C: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:C:566:LEU:HG	1:C:570:ASN:HB2	2.02	0.42
1:A:641:PHE:CD1	1:A:641:PHE:C	2.92	0.42
1:B:160:ASP:CG	1:B:162:ARG:HD2	2.40	0.42
1:D:164:HIS:HE1	2:D:1447:HOH:O	2.02	0.42
1:D:531:GLY:CA	1:D:577:GLU:OE2	2.66	0.42
1:A:178:PHE:CE1	1:A:180:PRO:HG3	2.48	0.42
1:B:511:ILE:HG23	2:B:1218:HOH:O	2.19	0.42
1:C:149:ARG:O	1:C:192:MET:HA	2.20	0.42
1:C:297:SER:C	1:C:299:GLY:H	2.23	0.42
1:C:435:ALA:O	1:C:438:PHE:HB3	2.19	0.42
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.42
1:A:168:LEU:HG	1:A:169:ARG:N	2.35	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:O	1:A:192:MET:HA	2.19	0.42
1:A:703:ALA:HA	1:A:707:ARG:O	2.19	0.42
1:C:130:ASP:CG	1:C:131:THR:H	2.22	0.42
1:C:359:HIS:CD2	1:C:376:ASN:HB2	2.55	0.42
1:C:375:TYR:HB2	1:C:377:TYR:CZ	2.55	0.42
1:C: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:C:598:GLY:HA3	1:C:686:TYR:HA	2.01	0.42
1:A:194:ASP:N	1:A:198:ASN:O	2.47	0.42
1:A:206:TYR:CZ	1:A:385:PHE:HD1	2.36	0.42
1:A:341:PHE:O	1:A:343:THR:HG23	2.20	0.42
1:B:259:ASN:O	1:B:260:ASN:HB3	2.19	0.42
1:B:552:ALA:O	1:B:720:THR:HG21	2.20	0.42
1:D:437:GLU:OE2	1:D:437:GLU:HA	2.19	0.42
1:D:504:HIS:CD2	1:D:634:LYS:HA	2.54	0.42
1:A:541:GLY:HA2	2:A:1350:HOH:O	2.19	0.42
1:C:182:ALA:HA	1:C:186:GLN:NE2	2.35	0.42
1:D:183:HIS:CE1	1:D:186:GLN:NE2	2.88	0.42
1:D:413:ARG:O	1:D:414:ASP:CB	2.68	0.42
1:C:457:ALA:HB2	1:C:477:PHE:CE2	2.55	0.42
1:D:140:PHE:O	1:D:176:GLU:HA	2.20	0.42
1:C:265:TYR:CE2	1:C:312:PHE:HB2	2.55	0.42
1:C:315:ARG:HG2	1:C:315:ARG:NH1	2.35	0.42
1:C:679:LEU:HB3	1:C:722:TRP:HB2	2.02	0.42
1:D:198:ASN:HB3	1:D:200:ARG:HH12	1.85	0.42
1:D:722:TRP:C	1:D:723:LEU:HD22	2.40	0.42
1:B:295:ASP:OD2	1:B:295:ASP:N	2.52	0.41
1:B:352:ASP:OD2	1:B:352:ASP:C	2.57	0.41
1:B:594:ASN:HB2	2:B:1233:HOH:O	2.20	0.41
1:B:629:LEU:HB2	1:B:640:ILE:HG22	2.02	0.41
1:C:722:TRP:C	1:C:723:LEU:HD22	2.40	0.41
1:D:136:THR:HG22	1:D:137:GLY:N	2.35	0.41
1:D:713:LEU:HA	2:D:1624:HOH:O	2.20	0.41
1:D:721:ILE:CD1	1:D:723:LEU:HD21	2.50	0.41
1:A:147:ALA:O	1:A:148:ARG:HB2	2.19	0.41
1:A:509:PHE:HA	1:A:512:LEU:CD2	2.50	0.41
1:B:138:THR:HG21	1:B:220:ILE:HD13	2.02	0.41
1:B:462:ASP:O	1:B:463:PHE:C	2.59	0.41
1:B:606:LEU:HD13	1:B:679:LEU:CD1	2.49	0.41
1:C:463:PHE:HD2	1:C:475:LEU:HD11	1.84	0.41
1:C:541:GLY:HA3	1:C:545:GLN:HE21	1.84	0.41

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	581/617 (94%)	502 (86%)	52 (9%)	27 (5%)	<b>3</b> <b>1</b>
1	B	583/617 (94%)	522 (90%)	48 (8%)	13 (2%)	<b>8</b> <b>6</b>
1	C	570/617 (92%)	494 (87%)	57 (10%)	19 (3%)	<b>4</b> <b>2</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	577/617 (94%)	522 (90%)	40 (7%)	15 (3%)	6	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

*Continued on next page...*

*Continued from previous page...*

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%)	20	27
1	B	501/525 (95%)	464 (93%)	37 (7%)	16	20
1	C	490/525 (93%)	460 (94%)	30 (6%)	22	29
1	D	496/525 (94%)	466 (94%)	30 (6%)	22	30
All	All	1985/2100 (94%)	1856 (94%)	129 (6%)	20	26

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.