



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:58 AM GMT

PDB ID : 2F1Z  
Title : Crystal structure of HAUSP  
Authors : Hu, M.; Gu, L.; Jeffrey, P.D.; Shi, Y.  
Deposited on : 2005-11-15  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

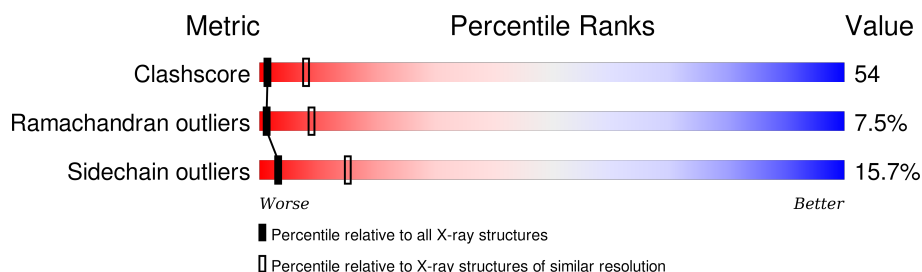
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

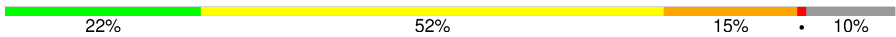
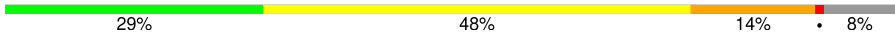
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	522	
1	B	522	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8015 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3842	2442	652	726	22			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2500	668	743	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	CLONING ARTIFACT	UNP Q93009
A	40	SER	-	CLONING ARTIFACT	UNP Q93009
A	41	HIS	-	CLONING ARTIFACT	UNP Q93009
A	42	MET	-	CLONING ARTIFACT	UNP Q93009
B	39	GLY	-	CLONING ARTIFACT	UNP Q93009
B	40	SER	-	CLONING ARTIFACT	UNP Q93009
B	41	HIS	-	CLONING ARTIFACT	UNP Q93009
B	42	MET	-	CLONING ARTIFACT	UNP Q93009

- Molecule 2 is water.

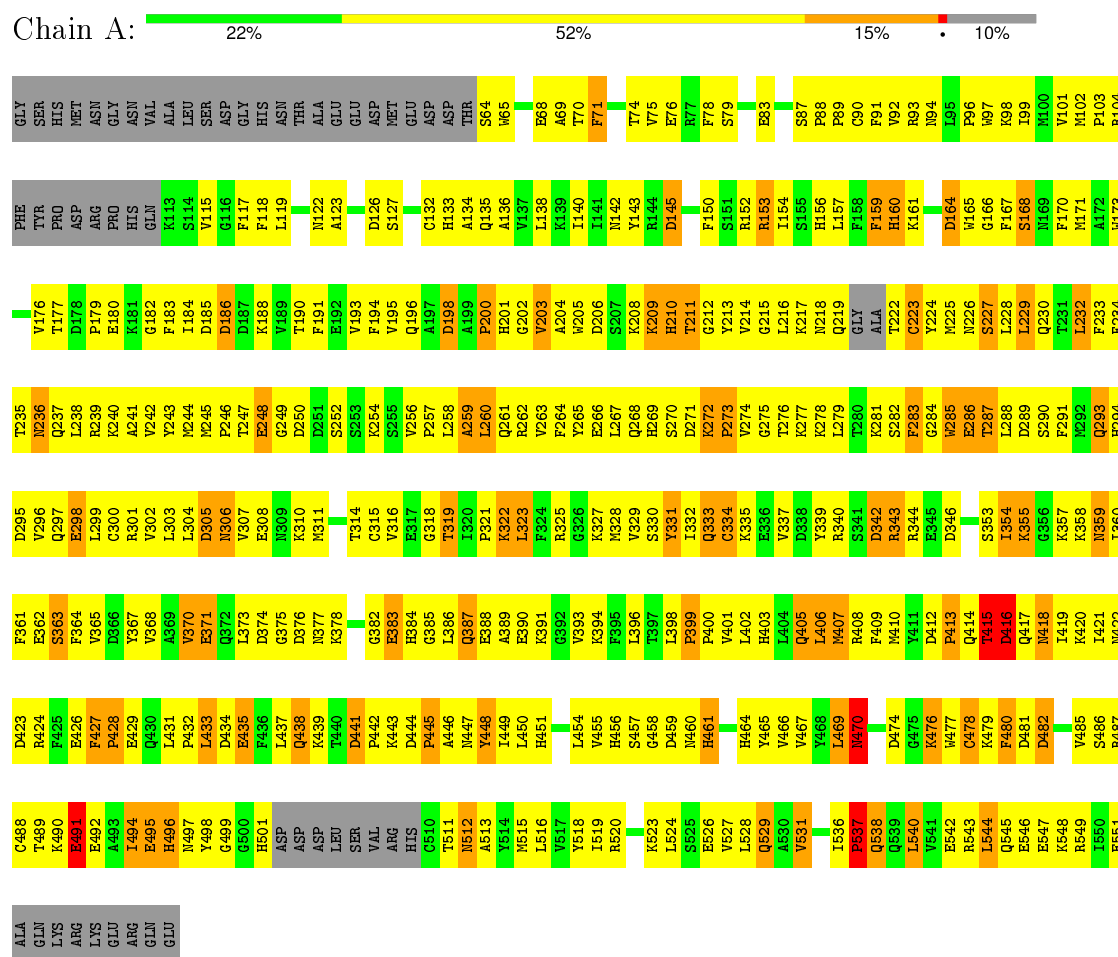
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		
2	B	122	Total	O	0	0
			122	122		

### 3 Residue-property plots

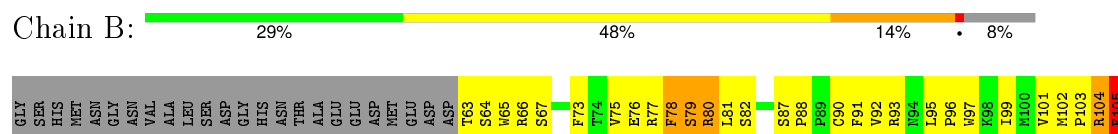
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



N512	I449	K378	V242	K312	G182	Y106
A513	L450	Y379	Y243	G313	G183	P107
Y514	H451	D380	H244	T314	D184	D108
M515	A452	A381	C315	C315	I184	R109
L516	V453	C382	P246	V316	D185	P110
V517	L454	E383	T247	E517	D186	H111
Y518	H455	H384	G318	G318	D187	Q112
H456	V456	C385	T319	T319	K188	K113
L524	D459	L386	D250	I320	V189	V115
S525	D459	Q387	S255	P321	T190	G116
E526	N460	C388	V256	K322	F191	F117
V527	H461	A389	P257	I323	E192	F118
L528	G462	C390	T258	F324	V193	L119
Q529	G463	K391	A259	K327	F194	L119
A530	H464	L392	L260	L260	V195	N122
V531	V465	T397	D261	M328	D198	W130
T532	V466	L398	P262	V329	A199	W130
D533	V467	P399	V263	S330	P200	Q135
H534	L468	P400	F264	Y331	H201	A136
D535	L469	L393		I332	G203	V137
I536	M470	H403	L267	C334	V204	L138
Q539	K471	L404	D268	C334	A204	K139
L540	K472	Q405	H269	K335	V205	D206
L544	K473	L406	S270	E336	K207	I141
E547	D474	M407		V337	K208	N142
E551	K475	R408	V274	Y339	K209	Y143
A552	K476	H410	T276		H210	R144
Q553	D481	Y411	K277	D342	T211	D145
LYS	D482	D412	K278	R343	G212	K148
ARG	D483	P413	L279	R344	Y213	S149
LYS	K484	T415	K281	Y347	G215	F150
GLU	V485	D416	F283		L216	S151
ARG		Q350		I350	K217	R152
GLN	T489	Q351	T287	K351	M218	R153
GLU	K490	L419	L288	L352	Q219	K154
	E491	K420	D289	S353	G220	S155
	E492	L421	D290	L354	A221	K156
	A493	D422	K291	K355	T222	L157
	L494	N423	H292	G356	G223	F158
	H496	E424	C293	K357	Y224	F159
	N497	F425	K358	L359	M225	H160
	Y498	F427	C360	H294	N226	K161
	G499	F428	V295	V361	S227	D164
	GLY	F429	C297	E362	L228	D164
	H15	Q430	E298	S363	L229	F167
	ASP	P432	F364	C300	Q230	S168
	ASP	L433	D366	R301	T231	N169
	ASP		Y367		P233	F170
	LEU	F436	L304	A369	F234	M171
	SER	P442	D305		T235	A172
	VAL	K443	H306	V370	M236	W173
	HIS	D444	E308	Q372	L238	V176
	ARG	P445	N309		R239	T177
	C510	T511	K310	D376	K240	D178
	T514	Y418	N311	P377	A241	P179

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.62Å 219.86Å 130.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.265 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	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	0.46	0/3935	0.74	1/5312 (0.0%)
1	B	0.50	2/4032 (0.0%)	0.81	9/5449 (0.2%)
All	All	0.48	2/7967 (0.0%)	0.78	10/10761 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	ARG	CZ-NH1	5.37	1.40	1.33
1	B	104	ARG	CB-CG	5.26	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	B	414	GLN	N-CA-C	-9.00	86.71	111.00
1	B	104	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	105	PHE	N-CA-C	7.61	131.54	111.00
1	B	387	GLN	CB-CA-C	-6.44	97.52	110.40
1	B	412	ASP	C-N-CA	-6.03	96.66	122.00
1	B	412	ASP	N-CA-C	-5.68	95.66	111.00
1	B	413	PRO	N-CA-C	5.44	126.24	112.10
1	B	90	CYS	N-CA-C	-5.26	96.80	111.00
1	A	470	ASN	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	TYR	Sidechain

## 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	3842	0	3710	428	1
1	B	3933	0	3794	406	0
2	A	118	0	0	44	0
2	B	122	0	0	41	0
All	All	8015	0	7504	821	1

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 54.

All (821) 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:B:109:ARG:HE	1:B:110:PRO:HD2	1.21	1.04
1:B:491:GLU:HA	1:B:495:GLU:HG3	1.39	1.03
1:A:501:HIS:HB3	1:B:413:PRO:HG3	1.38	1.01
1:B:214:VAL:HG22	1:B:215:GLY:H	1.27	1.00
1:A:294:HIS:HB3	1:A:298:GLU:HG3	1.47	0.97
1:A:257:PRO:HG2	1:A:310:LYS:HG3	1.47	0.96
1:B:380:ASP:O	1:B:386:LEU:HA	1.65	0.96
1:B:237:GLN:HE21	1:B:527:VAL:HA	1.29	0.95
1:A:239:ARG:O	1:A:242:VAL:HG12	1.66	0.95
1:B:526:GLU:O	1:B:529:GLN:HG3	1.68	0.94
1:A:489:THR:HG22	1:A:492:GLU:OE2	1.68	0.92
1:A:256:VAL:HG22	1:A:282:SER:HB3	1.53	0.89
1:A:370:VAL:HG23	1:B:344:ARG:O	1.72	0.88
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.58	0.86
1:A:225:MET:HG3	1:A:299:LEU:HD21	1.58	0.86
1:A:302:VAL:O	1:A:306:ASN:HB2	1.76	0.86
1:B:92:VAL:HB	1:B:97:TRP:NE1	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HB2	2:A:626:HOH:O	1.76	0.85
1:B:327:LYS:HB2	1:B:397:THR:HG23	1.57	0.84
1:B:382:GLY:HA3	2:B:659:HOH:O	1.76	0.84
1:A:412:ASP:HA	1:B:386:LEU:HD21	1.59	0.84
1:A:494:ILE:HG22	1:A:495:GLU:N	1.91	0.84
1:B:142:ASN:HD21	1:B:182:GLY:HA3	1.41	0.84
1:B:262:ARG:NH1	1:B:278:LYS:HD3	1.92	0.83
1:B:109:ARG:NE	1:B:110:PRO:HD2	1.93	0.83
1:B:142:ASN:ND2	1:B:182:GLY:HA3	1.93	0.83
1:A:354:ILE:HD13	1:A:355:LYS:N	1.93	0.82
1:A:135:GLN:HB2	1:A:196:GLN:HB2	1.61	0.82
1:B:184:ILE:HD11	1:B:187:ASP:HA	1.61	0.81
1:B:242:VAL:HG13	1:B:245:MET:HE2	1.60	0.81
1:A:266:GLU:HG2	1:A:270:SER:HB2	1.62	0.81
1:B:489:THR:OG1	1:B:492:GLU:HG3	1.80	0.81
1:A:323:LEU:O	1:A:400:PRO:HD2	1.80	0.81
1:A:210:HIS:H	1:A:210:HIS:CD2	1.99	0.80
1:A:239:ARG:NH2	1:A:531:VAL:HG11	1.97	0.80
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.64	0.79
1:A:115:VAL:HG21	1:A:176:VAL:HG11	1.64	0.79
1:A:429:GLU:H	1:B:293:GLN:NE2	1.79	0.79
1:A:415:THR:O	1:A:416:ASP:HB3	1.82	0.78
1:A:434:ASP:HB3	1:A:446:ALA:HB3	1.63	0.78
1:B:332:ILE:HG12	1:B:391:LYS:CB	2.13	0.78
1:A:333:GLN:HE22	1:A:340:ARG:HD2	1.49	0.78
1:A:412:ASP:HB3	1:A:415:THR:CG2	2.13	0.78
1:A:153:ARG:H	1:A:153:ARG:HD3	1.49	0.77
1:B:331:TYR:CD2	1:B:342:ASP:HB3	2.19	0.77
1:A:371:GLU:HB2	2:B:672:HOH:O	1.84	0.77
1:B:203:VAL:HG23	1:B:204:ALA:H	1.49	0.77
1:A:431:LEU:HG	1:A:433:LEU:HD13	1.65	0.77
1:A:413:PRO:HG3	1:B:386:LEU:O	1.85	0.77
1:B:221:ALA:HB1	1:B:288:LEU:HA	1.67	0.77
1:A:96:PRO:HG2	1:A:122:ASN:HA	1.68	0.76
1:A:529:GLN:HB2	2:A:673:HOH:O	1.85	0.76
1:B:324:PHE:HZ	2:B:585:HOH:O	1.66	0.76
1:B:119:LEU:CD1	1:B:193:VAL:HG11	2.15	0.76
1:B:217:LYS:HE2	1:B:275:GLY:HA2	1.67	0.76
1:B:332:ILE:HG12	1:B:391:LYS:HB3	1.68	0.76
1:B:350:ILE:HB	1:B:404:LEU:HD23	1.65	0.76
1:B:117:PHE:CE2	1:B:138:LEU:HB3	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ILE:O	1:A:496:HIS:N	2.19	0.76
1:A:224:TYR:HB3	1:A:465:TYR:CE1	2.22	0.75
1:A:401:VAL:HG11	2:A:638:HOH:O	1.87	0.74
1:B:381:ALA:HB1	2:B:576:HOH:O	1.88	0.74
1:A:286:GLU:O	1:A:287:THR:HG22	1.87	0.74
1:B:308:GLU:OE1	1:B:320:ILE:HB	1.88	0.74
1:B:214:VAL:HG22	1:B:215:GLY:N	2.03	0.74
1:B:327:LYS:HB2	1:B:397:THR:CG2	2.16	0.73
1:B:481:ASP:HB3	1:B:484:VAL:HG23	1.70	0.73
1:B:493:ALA:O	1:B:497:ASN:ND2	2.21	0.73
1:A:531:VAL:HG21	2:A:567:HOH:O	1.88	0.73
1:B:79:SER:HA	2:B:662:HOH:O	1.87	0.73
1:A:182:GLY:O	1:A:184:ILE:N	2.22	0.73
1:B:200:PRO:HG2	1:B:203:VAL:HG21	1.70	0.73
1:A:354:ILE:HG22	2:A:603:HOH:O	1.87	0.73
1:B:237:GLN:NE2	1:B:527:VAL:HA	2.03	0.73
1:A:429:GLU:H	1:B:293:GLN:HE22	1.34	0.73
1:A:153:ARG:HH11	1:A:153:ARG:HG2	1.54	0.73
1:B:481:ASP:O	1:B:482:ASP:HB2	1.89	0.73
1:A:262:ARG:HG3	1:A:544:LEU:HD11	1.71	0.72
1:A:359:ASN:HD21	1:A:362:GLU:HG3	1.53	0.72
1:B:378:LYS:HE2	2:B:638:HOH:O	1.89	0.72
1:A:103:PRO:HD2	2:A:624:HOH:O	1.89	0.72
1:B:239:ARG:HA	2:B:639:HOH:O	1.90	0.71
1:B:308:GLU:HB2	1:B:320:ILE:HD12	1.71	0.71
1:A:449:ILE:HD11	1:A:524:LEU:HD13	1.71	0.71
1:A:247:THR:HG21	1:A:261:GLN:HE22	1.52	0.71
1:B:287:THR:HG22	1:B:288:LEU:N	2.05	0.71
1:A:546:GLU:O	1:A:549:ARG:HG2	1.91	0.71
1:A:367:TYR:HB3	2:A:610:HOH:O	1.89	0.71
1:B:460:ASN:O	1:B:462:GLY:N	2.22	0.71
1:A:353:SER:O	1:A:363:SER:OG	2.09	0.71
1:A:407:MET:HA	2:A:653:HOH:O	1.89	0.71
1:A:361:PHE:O	1:A:365:VAL:HG23	1.90	0.71
1:A:89:PRO:HD3	1:A:98:LYS:HE3	1.73	0.71
1:A:495:GLU:HB3	2:A:591:HOH:O	1.90	0.71
1:B:221:ALA:HB1	1:B:288:LEU:CA	2.20	0.71
1:A:286:GLU:OE1	1:A:286:GLU:HA	1.90	0.71
1:A:316:VAL:HG13	1:A:316:VAL:O	1.90	0.71
1:B:450:LEU:HD23	1:B:451:HIS:N	2.06	0.70
1:B:494:ILE:HG22	1:B:495:GLU:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HB2	2:A:626:HOH:O	1.90	0.70
1:A:236:ASN:HB3	2:A:673:HOH:O	1.90	0.70
1:B:103:PRO:HB3	1:B:173:TRP:HZ3	1.55	0.70
1:A:307:VAL:O	1:A:311:MET:HG3	1.90	0.70
1:A:333:GLN:NE2	1:A:340:ARG:HD2	2.06	0.70
1:A:409:PHE:CE1	1:A:420:LYS:HD2	2.27	0.70
1:B:357:LYS:HD2	1:B:362:GLU:HB3	1.72	0.70
1:A:441:ASP:OD2	1:A:444:ASP:HB3	1.92	0.70
1:A:83:GLU:HA	2:A:624:HOH:O	1.91	0.69
1:B:87:SER:HB2	1:B:88:PRO:HD2	1.73	0.69
1:A:234:PHE:HE1	1:A:480:PHE:CE2	2.10	0.69
1:A:247:THR:CG2	1:A:261:GLN:HE22	2.05	0.69
1:A:117:PHE:CE2	1:A:138:LEU:HB3	2.28	0.69
1:B:351:GLN:HG3	2:B:591:HOH:O	1.92	0.69
1:A:247:THR:HG21	1:A:261:GLN:NE2	2.07	0.69
1:A:93:ARG:NH1	1:A:205:TRP:HH2	1.90	0.69
1:B:365:VAL:HG22	2:B:643:HOH:O	1.93	0.69
1:A:333:GLN:NE2	1:A:340:ARG:HB2	2.07	0.69
1:A:223:CYS:HB3	1:A:465:TYR:CE2	2.28	0.69
1:A:201:HIS:HB3	2:A:599:HOH:O	1.93	0.68
1:B:333:GLN:O	1:B:389:ALA:HB1	1.94	0.68
1:B:420:LYS:HE2	1:B:512:ASN:HD21	1.56	0.68
1:A:398:LEU:HG	1:A:437:LEU:HD21	1.76	0.68
1:A:200:PRO:HG2	1:A:203:VAL:HG11	1.75	0.68
1:A:216:LEU:HD11	1:A:230:GLN:HG2	1.75	0.68
1:A:177:THR:HG22	2:A:674:HOH:O	1.94	0.68
1:B:267:LEU:HG	2:B:657:HOH:O	1.93	0.68
1:B:76:GLU:HA	1:B:188:LYS:HG2	1.76	0.68
1:A:160:HIS:NE2	1:A:161:LYS:HG3	2.09	0.67
1:B:287:THR:CG2	1:B:288:LEU:N	2.57	0.67
1:A:91:PHE:HB3	2:A:576:HOH:O	1.93	0.67
1:B:405:GLN:HE21	1:B:515:MET:CE	2.07	0.67
1:B:217:LYS:NZ	1:B:277:LYS:HE3	2.09	0.67
1:B:539:GLN:H	1:B:539:GLN:CD	1.97	0.67
1:B:114:SER:HB3	2:B:593:HOH:O	1.94	0.66
1:B:96:PRO:HG2	1:B:122:ASN:HA	1.77	0.66
1:B:73:PHE:CG	1:B:87:SER:HB3	2.31	0.66
1:B:235:THR:HG21	2:B:585:HOH:O	1.94	0.66
1:B:206:ASP:O	1:B:209:LYS:HG2	1.95	0.66
1:B:328:MET:HE2	2:B:619:HOH:O	1.95	0.66
1:B:364:PHE:HB3	1:B:436:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HD22	1:B:477:TRP:HH2	1.60	0.66
1:B:413:PRO:C	1:B:415:THR:H	1.82	0.66
1:A:260:LEU:C	1:A:260:LEU:HD23	2.16	0.66
1:A:331:TYR:O	1:A:332:ILE:HG13	1.95	0.66
1:A:123:ALA:HB3	2:A:575:HOH:O	1.96	0.66
1:A:412:ASP:OD2	1:A:413:PRO:HD3	1.96	0.66
1:A:334:CYS:HA	1:A:389:ALA:HB2	1.78	0.66
1:B:297:GLN:HG2	1:B:405:GLN:OE1	1.96	0.66
1:A:219:GLN:HE22	1:A:464:HIS:HA	1.59	0.66
1:B:228:LEU:HD12	1:B:299:LEU:CD1	2.25	0.66
1:A:489:THR:HG22	1:A:492:GLU:CD	2.16	0.65
1:B:114:SER:HB2	2:B:617:HOH:O	1.95	0.65
1:B:167:PHE:HB2	1:B:170:PHE:HB2	1.79	0.65
1:B:219:GLN:HE22	1:B:465:TYR:N	1.93	0.65
1:A:233:PHE:CG	1:A:267:LEU:HD23	2.31	0.65
1:A:136:ALA:HB3	1:A:154:ILE:CG1	2.27	0.65
1:A:466:VAL:HG12	1:A:467:VAL:H	1.62	0.65
1:B:152:ARG:HA	2:B:572:HOH:O	1.97	0.65
1:A:328:MET:O	1:A:344:ARG:HA	1.97	0.65
1:A:282:SER:HB2	2:A:630:HOH:O	1.96	0.65
1:A:494:ILE:HG22	1:A:495:GLU:H	1.59	0.65
1:A:442:PRO:O	1:A:443:LYS:HB2	1.96	0.64
1:B:260:LEU:HG	1:B:264:PHE:CE2	2.31	0.64
1:A:384:HIS:HB3	1:A:387:GLN:OE1	1.98	0.64
1:A:233:PHE:CD1	1:A:267:LEU:HD23	2.33	0.64
1:A:236:ASN:HD22	1:A:236:ASN:H	1.43	0.64
1:B:355:LYS:CD	1:B:356:GLY:H	2.10	0.64
1:B:470:ASN:ND2	1:B:470:ASN:O	2.30	0.64
1:A:263:VAL:HG13	1:A:264:PHE:N	2.13	0.64
1:A:211:THR:HG22	1:A:213:TYR:HB2	1.79	0.64
1:A:455:VAL:CG1	1:A:466:VAL:HB	2.27	0.64
1:A:198:ASP:HB3	2:A:642:HOH:O	1.97	0.64
1:A:308:GLU:C	1:A:310:LYS:H	1.98	0.64
1:A:308:GLU:OE1	1:A:318:GLY:HA2	1.97	0.64
1:B:350:ILE:HA	2:B:646:HOH:O	1.97	0.64
1:B:411:TYR:CD1	1:B:411:TYR:O	2.51	0.64
1:B:217:LYS:HE2	1:B:275:GLY:CA	2.28	0.64
1:A:355:LYS:NZ	1:B:377:ASN:O	2.27	0.64
1:B:247:THR:HA	1:B:250:ASP:OD2	1.98	0.64
1:B:350:ILE:HG22	1:B:352:LEU:HD13	1.80	0.64
1:B:219:GLN:O	1:B:220:GLY:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:ND2	1:A:236:ASN:H	1.94	0.63
1:B:318:GLY:O	1:B:321:PRO:HD2	1.97	0.63
1:B:193:VAL:HG23	2:B:635:HOH:O	1.98	0.63
1:B:103:PRO:HB3	1:B:173:TRP:CZ3	2.33	0.63
1:A:364:PHE:O	1:A:368:VAL:HG22	1.98	0.63
1:B:354:ILE:HG22	1:B:425:PHE:CE2	2.33	0.63
1:A:294:HIS:CB	1:A:298:GLU:HG3	2.27	0.63
1:B:308:GLU:CB	1:B:320:ILE:HD12	2.28	0.63
1:B:119:LEU:HD13	1:B:193:VAL:HG11	1.79	0.63
1:A:421:ILE:CG2	1:A:423:ASP:OD2	2.47	0.63
1:A:329:VAL:CG2	1:A:396:LEU:HD11	2.28	0.63
1:A:359:ASN:C	1:A:359:ASN:HD22	2.02	0.63
1:A:415:THR:OG1	1:A:417:GLN:HG2	1.98	0.63
1:B:153:ARG:HG2	1:B:153:ARG:HH11	1.62	0.63
1:A:153:ARG:CD	1:A:153:ARG:H	2.11	0.62
1:A:225:MET:HG2	1:A:229:LEU:HD22	1.80	0.62
1:A:295:ASP:O	1:A:298:GLU:HG2	1.99	0.62
1:A:237:GLN:HE22	1:A:526:GLU:HG2	1.65	0.62
1:A:156:HIS:ND1	1:A:165:TRP:HB2	2.14	0.62
1:B:365:VAL:HA	1:B:368:VAL:CG2	2.30	0.62
1:A:476:LYS:HE3	1:A:476:LYS:HA	1.82	0.62
1:A:285:TRP:HA	1:A:290:SER:OG	1.98	0.62
1:B:421:ILE:HG22	1:B:421:ILE:O	2.00	0.62
1:B:78:PHE:CE2	1:B:173:TRP:CH2	2.87	0.62
1:A:360:ILE:HD11	1:A:427:PHE:HB3	1.81	0.62
1:B:105:PHE:HE1	1:B:107:PRO:HB3	1.63	0.62
1:B:228:LEU:HD12	1:B:299:LEU:HD13	1.82	0.62
1:B:329:VAL:HG22	1:B:344:ARG:HG3	1.81	0.62
1:B:318:GLY:C	1:B:321:PRO:HD2	2.19	0.62
1:A:245:MET:CE	1:A:257:PRO:HB3	2.29	0.62
1:A:267:LEU:HD12	1:A:274:VAL:HG21	1.82	0.61
1:B:455:VAL:HG22	1:B:512:ASN:O	2.00	0.61
1:B:308:GLU:OE1	1:B:321:PRO:HD3	2.00	0.61
1:A:71:PHE:CE2	1:A:193:VAL:HB	2.35	0.61
1:B:217:LYS:HZ3	1:B:277:LYS:HE3	1.66	0.61
1:A:136:ALA:HB3	1:A:154:ILE:HG13	1.82	0.61
1:A:227:SER:HB3	1:A:467:VAL:HB	1.82	0.61
1:A:449:ILE:HD11	1:A:524:LEU:CD1	2.30	0.61
1:A:470:ASN:HD22	1:A:470:ASN:N	1.97	0.61
1:B:200:PRO:HG2	1:B:203:VAL:CG2	2.29	0.61
1:B:354:ILE:HD12	1:B:355:LYS:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:NE2	1:A:526:GLU:HG2	2.15	0.61
1:B:332:ILE:HG12	1:B:391:LYS:HB2	1.80	0.61
1:B:453:VAL:HG13	1:B:468:TYR:HB2	1.81	0.61
1:B:323:LEU:O	1:B:400:PRO:HD2	2.01	0.61
1:A:236:ASN:HD22	1:A:236:ASN:N	1.98	0.61
1:A:94:ASN:HA	2:A:576:HOH:O	2.01	0.61
1:B:92:VAL:HB	1:B:97:TRP:HE1	1.64	0.60
1:A:283:PHE:HB2	1:A:285:TRP:CD1	2.36	0.60
1:A:526:GLU:O	1:A:529:GLN:HG3	2.00	0.60
1:A:185:ASP:O	1:A:186:ASP:HB2	1.99	0.60
1:A:288:LEU:HD13	2:A:593:HOH:O	2.02	0.60
1:B:371:GLU:OE2	1:B:391:LYS:HE3	2.01	0.60
1:A:334:CYS:HA	1:A:389:ALA:CB	2.32	0.60
1:B:203:VAL:HG23	1:B:204:ALA:N	2.14	0.60
1:B:532:THR:C	1:B:534:HIS:H	2.04	0.60
1:B:547:GLU:O	1:B:551:GLU:HG3	2.01	0.60
1:A:494:ILE:C	1:A:496:HIS:H	2.05	0.60
1:B:256:VAL:HG22	1:B:282:SER:HB3	1.82	0.60
1:A:298:GLU:O	1:A:302:VAL:HG23	2.01	0.60
1:A:333:GLN:NE2	1:A:340:ARG:CD	2.65	0.60
1:B:184:ILE:HG12	1:B:185:ASP:N	2.17	0.60
1:A:71:PHE:CD1	1:A:90:CYS:HB2	2.37	0.60
1:B:93:ARG:HG3	1:B:198:ASP:O	2.02	0.60
1:A:537:PRO:O	1:A:538:GLN:HB2	2.02	0.60
1:B:382:GLY:O	1:B:384:HIS:N	2.35	0.60
1:B:78:PHE:HD1	1:B:189:VAL:HG21	1.67	0.60
1:A:431:LEU:CG	1:A:433:LEU:HD13	2.32	0.59
1:A:263:VAL:O	1:A:267:LEU:HB2	2.01	0.59
1:A:210:HIS:H	1:A:210:HIS:HD2	1.49	0.59
1:A:211:THR:HG23	1:A:478:CYS:SG	2.42	0.59
1:B:156:HIS:HD2	2:B:680:HOH:O	1.84	0.59
1:A:160:HIS:CG	1:A:161:LYS:H	2.20	0.59
1:A:217:LYS:HB3	2:A:628:HOH:O	2.02	0.59
1:B:406:LEU:N	1:B:514:TYR:O	2.36	0.59
1:B:450:LEU:HD22	1:B:477:TRP:CH2	2.37	0.59
1:B:295:ASP:O	1:B:296:VAL:C	2.41	0.59
1:B:245:MET:SD	1:B:307:VAL:HG13	2.43	0.59
1:A:232:LEU:HD23	1:A:238:LEU:HD23	1.85	0.58
1:B:242:VAL:HG13	1:B:245:MET:CE	2.31	0.58
1:A:470:ASN:H	1:A:470:ASN:HD22	1.50	0.58
1:B:383:GLU:C	1:B:385:GLY:H	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:O	1:B:320:ILE:HD13	2.03	0.58
1:B:93:ARG:NE	1:B:198:ASP:O	2.34	0.58
1:B:383:GLU:C	1:B:385:GLY:N	2.57	0.58
1:B:405:GLN:HE21	1:B:515:MET:HE3	1.69	0.58
1:B:354:ILE:HD12	1:B:355:LYS:H	1.67	0.58
1:B:78:PHE:O	1:B:79:SER:C	2.41	0.58
1:A:210:HIS:N	1:A:210:HIS:CD2	2.71	0.58
1:A:446:ALA:HA	1:A:520:ARG:HE	1.68	0.58
1:B:413:PRO:HB2	1:B:415:THR:HB	1.86	0.58
1:A:225:MET:HG3	1:A:299:LEU:CD2	2.32	0.58
1:B:355:LYS:HD3	1:B:356:GLY:H	1.69	0.58
1:B:307:VAL:O	1:B:310:LYS:HB3	2.04	0.58
1:B:171:MET:HG2	1:B:172:ALA:H	1.68	0.58
1:A:259:ALA:HA	1:A:262:ARG:HH21	1.69	0.58
1:B:337:VAL:HG12	1:B:338:ASP:N	2.18	0.58
1:A:260:LEU:O	1:A:263:VAL:HG12	2.03	0.58
1:A:523:LYS:O	1:A:527:VAL:HG23	2.02	0.58
1:A:434:ASP:HB3	1:A:446:ALA:CB	2.31	0.57
1:A:421:ILE:HG23	1:A:423:ASP:OD2	2.04	0.57
1:A:154:ILE:HG13	1:A:154:ILE:O	2.03	0.57
1:B:103:PRO:CB	1:B:173:TRP:HZ3	2.16	0.57
1:A:332:ILE:HA	1:A:390:GLU:O	2.03	0.57
1:A:368:VAL:HG13	2:A:610:HOH:O	2.04	0.57
1:B:73:PHE:CD2	1:B:87:SER:HB3	2.39	0.57
1:B:295:ASP:O	1:B:297:GLN:N	2.37	0.57
1:A:501:HIS:CB	1:B:413:PRO:HG3	2.24	0.57
1:A:353:SER:HA	2:A:603:HOH:O	2.02	0.57
1:A:455:VAL:HG12	1:A:466:VAL:HB	1.85	0.57
1:A:333:GLN:O	1:A:334:CYS:C	2.42	0.57
1:B:263:VAL:O	1:B:267:LEU:HD13	2.05	0.57
1:B:153:ARG:HG2	1:B:153:ARG:NH1	2.19	0.57
1:B:109:ARG:HD3	2:B:571:HOH:O	2.04	0.57
1:B:243:TYR:OH	1:B:268:GLN:NE2	2.38	0.57
1:A:153:ARG:NH1	1:A:153:ARG:HG2	2.17	0.57
1:B:169:ASN:HA	2:B:593:HOH:O	2.05	0.57
1:A:168:SER:HB3	2:A:645:HOH:O	2.03	0.57
1:A:214:VAL:HG12	1:A:215:GLY:H	1.69	0.57
1:A:308:GLU:C	1:A:310:LYS:N	2.58	0.57
1:B:354:ILE:HG22	1:B:425:PHE:CD2	2.39	0.57
1:A:374:ASP:HA	1:A:378:LYS:HG3	1.86	0.57
1:B:102:MET:SD	1:B:104:ARG:NH1	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HG3	1:B:313:GLY:N	2.18	0.57
1:A:420:LYS:HE2	1:A:422:ASN:OD1	2.05	0.57
1:B:78:PHE:HD1	1:B:189:VAL:CG2	2.18	0.57
1:B:99:ILE:HG12	1:B:193:VAL:HG21	1.87	0.57
1:A:467:VAL:HG13	1:A:467:VAL:O	2.03	0.57
1:B:287:THR:CG2	1:B:288:LEU:H	2.18	0.57
1:B:452:ALA:CB	1:B:469:LEU:HG	2.35	0.57
1:B:308:GLU:CD	1:B:321:PRO:HD3	2.25	0.56
1:A:76:GLU:HA	1:A:188:LYS:HG2	1.86	0.56
1:B:495:GLU:HA	1:B:498:TYR:CD1	2.41	0.56
1:A:519:ILE:HD13	1:A:527:VAL:HG11	1.87	0.56
1:A:333:GLN:O	1:A:334:CYS:O	2.24	0.56
1:B:365:VAL:O	1:B:369:ALA:N	2.38	0.56
1:B:156:HIS:CD2	1:B:157:LEU:H	2.23	0.56
1:A:406:LEU:HD12	1:A:406:LEU:N	2.20	0.56
1:A:248:GLU:O	1:A:250:ASP:N	2.37	0.56
1:A:288:LEU:HA	1:A:291:PHE:HD2	1.70	0.56
1:A:224:TYR:HB3	1:A:465:TYR:CD1	2.40	0.56
1:B:267:LEU:HD12	1:B:274:VAL:HG21	1.88	0.56
1:A:78:PHE:HD2	2:A:674:HOH:O	1.88	0.56
1:B:150:PHE:HD2	1:B:171:MET:CE	2.18	0.56
1:B:299:LEU:O	1:B:299:LEU:HD22	2.06	0.56
1:B:386:LEU:O	1:B:386:LEU:HG	2.04	0.56
1:A:177:THR:HA	1:A:184:ILE:HD13	1.87	0.56
1:B:427:PHE:H	1:B:498:TYR:HE2	1.53	0.56
1:A:454:LEU:N	1:A:454:LEU:HD12	2.21	0.56
1:A:103:PRO:HB3	1:A:173:TRP:CZ3	2.41	0.56
1:A:406:LEU:CD1	1:A:406:LEU:N	2.69	0.56
1:A:494:ILE:CG2	1:A:495:GLU:N	2.63	0.55
1:B:411:TYR:HD1	1:B:411:TYR:O	1.88	0.55
1:A:284:GLY:O	1:A:286:GLU:N	2.40	0.55
1:B:118:PHE:HB3	1:B:164:ASP:OD1	2.07	0.55
1:B:405:GLN:HE21	1:B:515:MET:HE2	1.72	0.55
1:B:334:CYS:HB2	1:B:339:TYR:O	2.07	0.55
1:A:414:GLN:C	1:A:415:THR:HG22	2.27	0.55
1:B:412:ASP:HB3	2:B:647:HOH:O	2.06	0.55
1:A:398:LEU:HD13	1:A:433:LEU:HD23	1.87	0.55
1:A:407:MET:HB2	2:A:603:HOH:O	2.05	0.55
1:A:160:HIS:CG	1:A:161:LYS:N	2.73	0.55
1:A:438:GLN:N	1:A:438:GLN:OE1	2.40	0.55
1:A:467:VAL:HG22	1:A:469:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLN:HE22	1:B:465:TYR:H	1.54	0.55
1:B:214:VAL:O	1:B:485:VAL:HG21	2.06	0.55
1:A:283:PHE:CE2	1:A:303:LEU:HD21	2.42	0.55
1:A:479:LYS:O	1:A:485:VAL:HA	2.07	0.55
1:A:339:TYR:HE2	2:A:623:HOH:O	1.89	0.54
1:A:279:LEU:HG	1:A:283:PHE:CZ	2.42	0.54
1:A:408:ARG:NH2	1:A:513:ALA:O	2.41	0.54
1:A:241:ALA:CB	1:A:316:VAL:HG21	2.36	0.54
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.89	0.54
1:A:214:VAL:HG21	1:A:270:SER:O	2.07	0.54
1:A:248:GLU:OE2	1:A:543:ARG:HD2	2.07	0.54
1:A:242:VAL:CG1	1:A:243:TYR:N	2.71	0.54
1:B:143:TYR:HD1	1:B:185:ASP:HB2	1.73	0.54
1:A:314:THR:HA	2:A:596:HOH:O	2.07	0.54
1:B:453:VAL:HG22	1:B:453:VAL:O	2.07	0.54
1:A:458:GLY:C	1:A:460:ASN:H	2.09	0.54
1:B:376:ASP:HA	1:B:379:TYR:CD1	2.42	0.54
1:B:75:VAL:O	1:B:188:LYS:HA	2.07	0.54
1:B:308:GLU:HG3	2:B:653:HOH:O	2.07	0.54
1:B:289:ASP:HA	1:B:292:MET:HB2	1.89	0.54
1:A:258:LEU:O	1:A:261:GLN:N	2.40	0.54
1:B:383:GLU:O	1:B:385:GLY:N	2.41	0.54
1:B:524:LEU:HD22	1:B:528:LEU:HD12	1.90	0.53
1:B:219:GLN:O	1:B:220:GLY:C	2.47	0.53
1:A:308:GLU:OE2	1:A:321:PRO:HD3	2.08	0.53
1:B:99:ILE:HD13	2:B:635:HOH:O	2.08	0.53
1:A:228:LEU:HD13	1:A:299:LEU:HD23	1.89	0.53
1:B:78:PHE:N	1:B:187:ASP:O	2.38	0.53
1:A:374:ASP:HA	1:A:378:LYS:CG	2.38	0.53
1:B:73:PHE:CG	1:B:87:SER:CB	2.91	0.53
1:A:515:MET:CG	1:A:516:LEU:N	2.72	0.53
1:B:228:LEU:CD1	1:B:299:LEU:HD13	2.38	0.53
1:A:329:VAL:HG22	1:A:344:ARG:HG2	1.90	0.53
1:B:452:ALA:HB2	1:B:469:LEU:HG	1.90	0.53
1:A:289:ASP:O	1:A:293:GLN:HB2	2.09	0.53
1:B:173:TRP:HE1	1:B:177:THR:HG21	1.73	0.53
1:B:222:THR:HB	1:B:225:MET:HE2	1.91	0.53
1:A:234:PHE:HE1	1:A:480:PHE:CZ	2.27	0.52
1:B:365:VAL:HA	1:B:368:VAL:HG23	1.91	0.52
1:A:487:ARG:HD3	2:A:612:HOH:O	2.09	0.52
1:B:204:ALA:C	1:B:206:ASP:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HG	1:B:264:PHE:CD2	2.43	0.52
1:A:262:ARG:NH2	1:A:278:LYS:HB3	2.24	0.52
1:A:269:HIS:HD2	2:A:678:HOH:O	1.92	0.52
1:A:180:GLU:O	1:A:180:GLU:HG2	2.09	0.52
1:A:117:PHE:HD2	1:A:170:PHE:CZ	2.27	0.52
1:A:333:GLN:HG3	1:A:333:GLN:O	2.10	0.52
1:B:364:PHE:HB3	1:B:436:PHE:CE2	2.45	0.52
1:A:211:THR:HG21	1:A:485:VAL:HG12	1.92	0.52
1:A:150:PHE:HB3	1:A:171:MET:HE2	1.92	0.52
1:A:152:ARG:NH1	1:A:170:PHE:O	2.42	0.52
1:A:218:ASN:HB3	2:A:590:HOH:O	2.09	0.52
1:A:295:ASP:H	1:A:298:GLU:CG	2.23	0.52
1:A:295:ASP:HB3	1:A:297:GLN:OE1	2.10	0.52
1:A:263:VAL:CG1	1:A:264:PHE:N	2.72	0.52
1:A:455:VAL:HG22	1:A:456:HIS:N	2.25	0.52
1:B:160:HIS:NE2	1:B:161:LYS:HG3	2.25	0.52
1:B:235:THR:O	1:B:238:LEU:N	2.38	0.52
1:B:78:PHE:O	1:B:80:ARG:N	2.43	0.52
1:A:455:VAL:HB	1:A:497:ASN:HD21	1.75	0.52
1:B:67:SER:HA	1:B:93:ARG:CZ	2.40	0.52
1:A:335:LYS:NZ	1:B:344:ARG:HH22	2.08	0.52
1:B:232:LEU:HD13	1:B:304:LEU:HD21	1.91	0.52
1:A:211:THR:CG2	1:A:213:TYR:HB2	2.40	0.52
1:B:255:SER:OG	1:B:257:PRO:HD2	2.09	0.52
1:A:239:ARG:HH22	1:A:531:VAL:HG11	1.75	0.51
1:B:206:ASP:HB3	1:B:209:LYS:HE3	1.92	0.51
1:B:191:PHE:N	1:B:191:PHE:CD1	2.76	0.51
1:B:230:GLN:O	1:B:234:PHE:HD1	1.93	0.51
1:A:157:LEU:HB3	2:A:657:HOH:O	2.10	0.51
1:A:536:ILE:CG2	1:A:540:LEU:HD12	2.40	0.51
1:B:409:PHE:HB3	2:B:628:HOH:O	2.09	0.51
1:B:105:PHE:CE1	1:B:107:PRO:HB3	2.46	0.51
1:A:412:ASP:OD2	1:A:413:PRO:CD	2.58	0.51
1:A:279:LEU:HD12	2:A:630:HOH:O	2.09	0.51
1:B:431:LEU:HG	1:B:433:LEU:HD13	1.91	0.51
1:A:410:MET:HE1	1:B:381:ALA:O	2.11	0.51
1:A:407:MET:HA	1:A:407:MET:HE2	1.92	0.51
1:B:78:PHE:O	1:B:81:LEU:N	2.43	0.51
1:B:466:VAL:HG11	1:B:479:LYS:HE3	1.92	0.51
1:A:140:ILE:HG13	1:A:170:PHE:HE2	1.75	0.51
1:A:333:GLN:HE21	1:A:340:ARG:NE	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PHE:CD1	1:A:90:CYS:CB	2.94	0.51
1:A:359:ASN:ND2	1:A:362:GLU:HG3	2.23	0.51
1:B:335:LYS:HG2	1:B:390:GLU:OE2	2.11	0.51
1:A:279:LEU:HA	2:A:630:HOH:O	2.10	0.51
1:B:414:GLN:O	1:B:416:ASP:N	2.44	0.51
1:A:495:GLU:HG3	2:A:573:HOH:O	2.09	0.51
1:A:102:MET:CE	1:A:104:ARG:HD3	2.40	0.51
1:B:191:PHE:HB3	2:B:635:HOH:O	2.10	0.51
1:A:480:PHE:N	1:A:480:PHE:CD1	2.79	0.51
1:B:420:LYS:HE2	1:B:512:ASN:ND2	2.24	0.51
1:A:203:VAL:HG13	1:A:203:VAL:O	2.11	0.51
1:A:152:ARG:HD3	1:A:167:PHE:CE1	2.45	0.50
1:A:118:PHE:HB3	1:A:164:ASP:OD1	2.11	0.50
1:B:357:LYS:NZ	1:B:366:ASP:HB2	2.25	0.50
1:A:226:ASN:HD21	1:A:276:THR:HG21	1.76	0.50
1:A:426:GLU:HG2	1:A:498:TYR:CD1	2.47	0.50
1:A:488:CYS:HB2	1:A:492:GLU:OE1	2.12	0.50
1:B:357:LYS:HE3	1:B:366:ASP:CB	2.40	0.50
1:A:427:PHE:N	1:A:427:PHE:CD2	2.78	0.50
1:B:416:ASP:O	1:B:417:GLN:HB2	2.10	0.50
1:B:213:TYR:CZ	1:B:471:PRO:HG2	2.47	0.50
1:B:361:PHE:C	1:B:361:PHE:CD2	2.85	0.50
1:B:429:GLU:CG	1:B:430:GLN:N	2.74	0.50
1:B:335:LYS:NZ	1:B:372:GLN:HE22	2.09	0.50
1:A:256:VAL:O	1:A:257:PRO:C	2.50	0.50
1:B:330:SER:O	1:B:342:ASP:HA	2.11	0.50
1:A:329:VAL:O	1:A:393:VAL:HA	2.12	0.50
1:B:155:SER:O	1:B:156:HIS:HB2	2.12	0.50
1:A:285:TRP:HE3	1:A:291:PHE:CD1	2.30	0.50
1:B:239:ARG:HD2	1:B:531:VAL:HG11	1.94	0.50
1:B:277:LYS:H	1:B:277:LYS:HD3	1.76	0.50
1:B:405:GLN:HA	1:B:515:MET:HA	1.93	0.50
1:A:458:GLY:C	1:A:460:ASN:N	2.65	0.50
1:A:214:VAL:HG12	1:A:215:GLY:N	2.26	0.50
1:A:241:ALA:HB1	1:A:316:VAL:HG21	1.93	0.50
1:A:327:LYS:HE2	1:A:346:ASP:OD1	2.12	0.50
1:B:139:LYS:HB2	1:B:151:SER:HB3	1.93	0.50
1:B:413:PRO:HD2	2:B:647:HOH:O	2.11	0.49
1:A:415:THR:O	1:A:416:ASP:CB	2.55	0.49
1:A:318:GLY:O	1:A:321:PRO:HD2	2.12	0.49
1:B:173:TRP:NE1	1:B:177:THR:HG21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TYR:C	1:A:332:ILE:HG13	2.32	0.49
1:A:412:ASP:HB3	1:A:415:THR:HG23	1.93	0.49
1:B:347:TYR:OH	1:B:398:LEU:HD23	2.13	0.49
1:A:409:PHE:HE1	1:A:420:LYS:HD2	1.73	0.49
1:A:314:THR:O	1:A:316:VAL:N	2.46	0.49
1:A:160:HIS:CE1	1:A:161:LYS:HG3	2.47	0.49
1:A:133:HIS:ND1	1:A:134:ALA:N	2.60	0.49
1:B:135:GLN:O	1:B:136:ALA:HB2	2.12	0.49
1:B:532:THR:C	1:B:534:HIS:N	2.66	0.49
1:B:160:HIS:CG	1:B:161:LYS:N	2.81	0.49
1:B:454:LEU:HD12	1:B:454:LEU:H	1.78	0.49
1:A:240:LYS:HD3	1:A:529:GLN:NE2	2.28	0.49
1:A:419:ILE:CG2	1:A:420:LYS:N	2.74	0.49
1:B:358:LYS:NZ	1:B:358:LYS:HB2	2.27	0.49
1:B:367:TYR:O	1:B:367:TYR:HD1	1.95	0.49
1:A:490:LYS:C	1:A:492:GLU:H	2.16	0.48
1:A:359:ASN:C	1:A:359:ASN:ND2	2.67	0.48
1:B:311:MET:HB2	2:B:653:HOH:O	2.12	0.48
1:A:450:LEU:HG	1:A:477:TRP:HH2	1.78	0.48
1:A:99:ILE:HG23	1:A:117:PHE:HE1	1.77	0.48
1:B:65:TRP:HH2	1:B:204:ALA:HB3	1.78	0.48
1:B:459:ASP:OD2	1:B:459:ASP:N	2.46	0.48
1:B:308:GLU:CG	2:B:653:HOH:O	2.61	0.48
1:B:426:GLU:HA	1:B:498:TYR:CD2	2.48	0.48
1:A:422:ASN:HD21	1:A:459:ASP:HA	1.76	0.48
1:A:322:LYS:O	1:A:400:PRO:HG2	2.14	0.48
1:A:177:THR:O	1:A:179:PRO:HD3	2.14	0.48
1:B:465:TYR:CD1	1:B:465:TYR:N	2.81	0.48
1:B:355:LYS:CG	1:B:356:GLY:N	2.76	0.48
1:A:476:LYS:HE3	1:A:477:TRP:H	1.77	0.48
1:B:338:ASP:OD1	1:B:338:ASP:C	2.51	0.48
1:B:228:LEU:HD12	1:B:299:LEU:HD12	1.94	0.48
1:A:344:ARG:HD2	1:A:396:LEU:CD1	2.44	0.48
1:B:425:PHE:HB2	2:B:648:HOH:O	2.14	0.48
1:A:143:TYR:N	1:A:143:TYR:CD2	2.80	0.48
1:B:489:THR:HG1	1:B:492:GLU:HG3	1.77	0.48
1:B:191:PHE:N	1:B:191:PHE:HD1	2.12	0.48
1:B:456:HIS:O	1:B:511:THR:HA	2.14	0.48
1:B:211:THR:HG21	1:B:485:VAL:HG12	1.96	0.48
1:B:113:LYS:C	1:B:173:TRP:HB2	2.34	0.48
1:A:461:HIS:H	1:A:461:HIS:CD2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PHE:O	1:B:368:VAL:HG22	2.14	0.48
1:A:132:CYS:SG	1:A:200:PRO:HB3	2.53	0.48
1:B:474:ASP:OD1	1:B:476:LYS:HD3	2.14	0.48
1:A:283:PHE:N	1:A:283:PHE:CD2	2.81	0.48
1:A:432:PRO:HA	1:A:447:ASN:OD1	2.14	0.48
1:B:534:HIS:C	1:B:536:ILE:H	2.17	0.48
1:B:528:LEU:O	1:B:529:GLN:C	2.53	0.47
1:B:256:VAL:N	1:B:257:PRO:CD	2.77	0.47
1:B:413:PRO:CA	1:B:415:THR:H	2.27	0.47
1:B:391:LYS:NZ	2:B:569:HOH:O	2.47	0.47
1:B:452:ALA:HB2	1:B:469:LEU:CD2	2.45	0.47
1:B:105:PHE:HD1	1:B:107:PRO:N	2.12	0.47
1:A:236:ASN:ND2	1:A:236:ASN:N	2.58	0.47
1:A:374:ASP:O	1:A:377:ASN:N	2.47	0.47
1:B:387:GLN:HG3	2:B:563:HOH:O	2.14	0.47
1:B:115:VAL:HG21	1:B:176:VAL:HG11	1.96	0.47
1:A:424:ARG:HA	1:A:499:GLY:HA3	1.96	0.47
1:A:87:SER:O	1:A:98:LYS:HE2	2.14	0.47
1:B:416:ASP:OD1	1:B:416:ASP:C	2.53	0.47
1:B:422:ASN:ND2	1:B:510:CYS:SG	2.88	0.47
1:A:481:ASP:O	1:A:482:ASP:HB2	2.14	0.47
1:B:386:LEU:O	1:B:386:LEU:CG	2.63	0.47
1:B:102:MET:O	1:B:116:GLY:N	2.45	0.47
1:B:214:VAL:CG2	1:B:215:GLY:H	2.11	0.47
1:A:405:GLN:HE21	1:A:405:GLN:HB2	1.55	0.47
1:A:173:TRP:HA	1:A:176:VAL:HG12	1.96	0.47
1:A:434:ASP:CB	1:A:446:ALA:HB3	2.41	0.47
1:A:65:TRP:CD1	1:A:94:ASN:HB2	2.49	0.47
1:A:451:HIS:HA	1:A:470:ASN:HD21	1.80	0.47
1:A:235:THR:O	1:A:235:THR:HG22	2.14	0.47
1:B:63:THR:OG1	1:B:64:SER:N	2.47	0.47
1:B:460:ASN:O	1:B:461:HIS:C	2.53	0.47
1:B:78:PHE:C	1:B:78:PHE:CD2	2.88	0.47
1:A:223:CYS:HB3	1:A:465:TYR:CZ	2.49	0.47
1:A:211:THR:HG21	1:A:485:VAL:CG1	2.45	0.47
1:B:225:MET:HE1	1:B:280:THR:HG22	1.97	0.47
1:B:142:ASN:HB3	1:B:145:ASP:O	2.15	0.47
1:B:454:LEU:HD12	1:B:454:LEU:N	2.29	0.46
1:A:439:LYS:HZ3	1:A:439:LYS:HB3	1.81	0.46
1:A:216:LEU:HD21	1:A:267:LEU:HD11	1.96	0.46
1:A:262:ARG:CG	1:A:544:LEU:HD11	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:O	1:B:311:MET:N	2.47	0.46
1:A:202:GLY:O	1:A:203:VAL:HB	2.15	0.46
1:A:262:ARG:HH22	1:A:278:LYS:HB3	1.80	0.46
1:A:222:THR:HA	1:A:291:PHE:CD1	2.51	0.46
1:B:308:GLU:C	1:B:310:LYS:N	2.67	0.46
1:A:115:VAL:O	1:A:170:PHE:HB3	2.15	0.46
1:B:225:MET:C	1:B:227:SER:N	2.68	0.46
1:A:382:GLY:O	1:A:385:GLY:N	2.45	0.46
1:A:491:GLU:HG3	1:A:495:GLU:HB2	1.97	0.46
1:A:337:VAL:HG12	1:A:387:GLN:HG2	1.98	0.46
1:B:337:VAL:CG1	1:B:338:ASP:N	2.78	0.46
1:B:118:PHE:CD1	1:B:118:PHE:N	2.83	0.46
1:A:92:VAL:HG21	1:A:195:VAL:HG11	1.97	0.46
1:A:242:VAL:HG21	1:A:260:LEU:CD2	2.45	0.46
1:A:531:VAL:HG12	2:A:621:HOH:O	2.15	0.46
1:A:408:ARG:O	1:A:420:LYS:HA	2.16	0.46
1:B:308:GLU:HB2	1:B:320:ILE:CD1	2.43	0.46
1:B:320:ILE:N	1:B:321:PRO:CD	2.78	0.46
1:A:332:ILE:O	1:A:340:ARG:HA	2.15	0.46
1:B:355:LYS:N	1:B:355:LYS:HD3	2.30	0.46
1:A:331:TYR:C	1:A:331:TYR:CD1	2.89	0.46
1:A:316:VAL:HG22	1:A:319:THR:OG1	2.15	0.46
1:B:156:HIS:CD2	1:B:157:LEU:N	2.83	0.46
1:A:494:ILE:CG2	1:A:495:GLU:OE1	2.64	0.46
1:A:442:PRO:C	1:A:444:ASP:H	2.18	0.46
1:B:63:THR:O	1:B:66:ARG:NH2	2.48	0.46
1:B:241:ALA:CB	1:B:319:THR:HG21	2.46	0.46
1:B:240:LYS:HD2	1:B:529:GLN:OE1	2.16	0.46
1:A:494:ILE:C	1:A:496:HIS:N	2.66	0.46
1:A:117:PHE:CD2	1:A:138:LEU:HB3	2.51	0.46
1:A:71:PHE:CD2	1:A:71:PHE:N	2.83	0.46
1:A:87:SER:HB2	1:A:88:PRO:HD2	1.98	0.46
1:B:355:LYS:HG2	1:B:356:GLY:N	2.31	0.46
1:B:443:LYS:C	1:B:445:PRO:HD3	2.36	0.46
1:B:450:LEU:HD23	1:B:451:HIS:H	1.77	0.46
1:A:208:LYS:CG	1:A:214:VAL:HG22	2.46	0.46
1:A:536:ILE:O	1:A:537:PRO:C	2.54	0.45
1:B:224:TYR:C	1:B:224:TYR:CD1	2.90	0.45
1:B:475:GLY:O	1:B:477:TRP:HD1	1.98	0.45
1:A:459:ASP:O	1:A:459:ASP:OD2	2.34	0.45
1:B:449:ILE:N	1:B:449:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:HE3	1:B:366:ASP:HB2	1.97	0.45
1:A:448:TYR:HA	1:A:519:ILE:O	2.16	0.45
1:A:71:PHE:HD2	1:A:71:PHE:N	2.14	0.45
1:A:455:VAL:HB	1:A:497:ASN:ND2	2.30	0.45
1:A:156:HIS:CD2	1:A:157:LEU:H	2.34	0.45
1:A:206:ASP:O	1:A:209:LYS:HB2	2.17	0.45
1:A:242:VAL:HG13	1:A:243:TYR:N	2.32	0.45
1:B:79:SER:OG	1:B:187:ASP:OD1	2.28	0.45
1:A:176:VAL:HG22	1:A:176:VAL:O	2.16	0.45
1:A:301:ARG:O	1:A:305:ASP:HB2	2.16	0.45
1:A:233:PHE:HA	1:A:264:PHE:CZ	2.51	0.45
1:A:416:ASP:OD2	1:A:416:ASP:C	2.55	0.45
1:B:386:LEU:HD23	1:B:386:LEU:N	2.31	0.45
1:A:115:VAL:CG2	1:A:176:VAL:HG11	2.39	0.45
1:B:257:PRO:O	1:B:261:GLN:HG3	2.17	0.45
1:A:418:ASN:HA	1:A:418:ASN:HD22	1.58	0.45
1:B:448:TYR:C	1:B:449:ILE:HD12	2.37	0.45
1:B:150:PHE:HD2	1:B:171:MET:HE2	1.81	0.45
1:B:208:LYS:O	1:B:212:GLY:N	2.45	0.45
1:B:239:ARG:HG2	1:B:243:TYR:CE1	2.51	0.45
1:B:239:ARG:HD3	1:B:268:GLN:NE2	2.32	0.45
1:B:92:VAL:HB	1:B:97:TRP:CD1	2.50	0.45
1:A:551:GLU:HG2	2:A:648:HOH:O	2.16	0.45
1:B:217:LYS:O	1:B:218:ASN:O	2.34	0.45
1:A:455:VAL:HG23	1:A:512:ASN:C	2.36	0.45
1:A:343:ARG:HG3	1:A:343:ARG:O	2.16	0.45
1:A:208:LYS:HE3	1:A:212:GLY:O	2.17	0.45
1:B:258:LEU:HD13	1:B:262:ARG:NH2	2.31	0.45
1:B:81:LEU:HG	1:B:82:SER:H	1.82	0.45
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.32	0.45
1:A:216:LEU:O	1:A:482:ASP:C	2.54	0.45
1:B:529:GLN:HB3	2:B:629:HOH:O	2.16	0.45
1:A:153:ARG:CD	1:A:153:ARG:N	2.75	0.45
1:A:281:LYS:O	1:A:284:GLY:N	2.47	0.45
1:B:411:TYR:CE1	1:B:413:PRO:HB3	2.51	0.44
1:B:238:LEU:CD2	2:B:585:HOH:O	2.64	0.44
1:B:376:ASP:HA	1:B:379:TYR:CE1	2.51	0.44
1:B:141:ILE:HA	1:B:149:SER:OG	2.17	0.44
1:A:243:TYR:OH	1:A:268:GLN:NE2	2.50	0.44
1:B:245:MET:HA	1:B:246:PRO:HD3	1.59	0.44
1:B:99:ILE:HD11	1:B:193:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:CG1	1:A:316:VAL:O	2.62	0.44
1:A:480:PHE:N	1:A:480:PHE:HD1	2.16	0.44
1:B:283:PHE:CE2	1:B:299:LEU:HD23	2.52	0.44
1:B:466:VAL:CG1	1:B:467:VAL:N	2.80	0.44
1:A:256:VAL:CG2	1:A:282:SER:HB3	2.36	0.44
1:A:528:LEU:O	1:A:529:GLN:O	2.36	0.44
1:A:414:GLN:O	1:A:415:THR:CB	2.65	0.44
1:A:153:ARG:HD3	1:A:153:ARG:N	2.20	0.44
1:A:373:LEU:HB3	1:A:377:ASN:O	2.17	0.44
1:B:361:PHE:HD2	1:B:361:PHE:C	2.20	0.44
1:B:111:HIS:O	1:B:111:HIS:ND1	2.51	0.44
1:B:91:PHE:HA	1:B:95:LEU:O	2.17	0.44
1:B:421:ILE:O	1:B:423:ASP:N	2.50	0.44
1:A:245:MET:HE1	1:A:257:PRO:HB3	2.00	0.44
1:B:250:ASP:OD1	1:B:310:LYS:NZ	2.48	0.44
1:B:235:THR:CB	2:B:585:HOH:O	2.65	0.44
1:B:235:THR:O	1:B:236:ASN:C	2.55	0.44
1:A:211:THR:HG22	1:A:213:TYR:CB	2.47	0.44
1:A:300:CYS:O	1:A:304:LEU:HB2	2.18	0.44
1:B:466:VAL:HG12	1:B:467:VAL:N	2.32	0.44
1:B:177:THR:O	1:B:179:PRO:HD3	2.17	0.44
1:B:143:TYR:CD1	1:B:185:ASP:HB2	2.52	0.44
1:B:360:ILE:HD11	1:B:516:LEU:HD12	2.00	0.44
1:A:297:GLN:HG3	1:A:405:GLN:NE2	2.33	0.44
1:B:76:GLU:O	1:B:77:ARG:C	2.56	0.44
1:A:340:ARG:HD3	1:A:342:ASP:OD1	2.17	0.44
1:A:361:PHE:CG	1:B:298:GLU:HG2	2.52	0.44
1:B:157:LEU:HD13	1:B:157:LEU:C	2.39	0.44
1:A:237:GLN:HE21	1:A:527:VAL:HA	1.82	0.43
1:A:490:LYS:O	1:A:492:GLU:N	2.50	0.43
1:A:466:VAL:HG12	1:A:467:VAL:N	2.32	0.43
1:A:258:LEU:O	1:A:260:LEU:N	2.51	0.43
1:B:193:VAL:O	1:B:193:VAL:HG12	2.17	0.43
1:B:413:PRO:C	1:B:415:THR:N	2.54	0.43
1:B:238:LEU:HD22	2:B:585:HOH:O	2.16	0.43
1:A:70:THR:HG1	1:A:194:PHE:HD1	1.64	0.43
1:A:435:GLU:HB3	1:B:305:ASP:OD2	2.18	0.43
1:A:354:ILE:HD13	1:A:355:LYS:CA	2.46	0.43
1:B:184:ILE:CG1	1:B:185:ASP:N	2.80	0.43
1:A:470:ASN:N	1:A:470:ASN:ND2	2.66	0.43
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TRP:CG	1:B:130:TRP:O	2.71	0.43
1:B:242:VAL:O	1:B:245:MET:HG3	2.18	0.43
1:A:265:TYR:CE2	1:A:536:ILE:HD13	2.54	0.43
1:B:130:TRP:HA	1:B:201:HIS:O	2.18	0.43
1:A:329:VAL:HG23	1:A:396:LEU:HD11	1.99	0.43
1:A:393:VAL:CG1	1:A:394:LYS:N	2.81	0.43
1:B:464:HIS:CD2	2:B:650:HOH:O	2.72	0.43
1:A:242:VAL:O	1:A:245:MET:HG3	2.19	0.43
1:A:285:TRP:HE3	1:A:291:PHE:CE1	2.37	0.43
1:A:69:ALA:O	1:A:194:PHE:HD1	2.02	0.43
1:B:459:ASP:O	1:B:460:ASN:HB2	2.17	0.43
1:A:64:SER:N	2:A:632:HOH:O	2.51	0.43
1:A:416:ASP:O	1:A:416:ASP:CG	2.57	0.43
1:A:136:ALA:HA	1:A:194:PHE:O	2.18	0.43
1:B:63:THR:HG23	1:B:64:SER:H	1.84	0.43
1:A:133:HIS:O	1:A:134:ALA:HB2	2.19	0.43
1:B:77:ARG:O	1:B:77:ARG:HG2	2.19	0.42
1:B:287:THR:HG23	1:B:288:LEU:H	1.84	0.42
1:A:262:ARG:O	1:A:263:VAL:C	2.57	0.42
1:A:263:VAL:CG1	1:A:264:PHE:H	2.32	0.42
1:B:339:TYR:CE1	1:B:384:HIS:NE2	2.84	0.42
1:B:105:PHE:CD1	1:B:107:PRO:N	2.87	0.42
1:B:484:VAL:O	1:B:484:VAL:HG23	2.19	0.42
1:A:185:ASP:O	1:A:186:ASP:CB	2.65	0.42
1:A:232:LEU:HD21	1:A:304:LEU:HD21	2.01	0.42
1:A:75:VAL:HA	2:A:574:HOH:O	2.19	0.42
1:B:236:ASN:O	1:B:239:ARG:N	2.52	0.42
1:A:118:PHE:HB3	1:A:165:TRP:O	2.19	0.42
1:A:542:GLU:O	1:A:545:GLN:HB2	2.20	0.42
1:B:472:LYS:HB3	2:B:642:HOH:O	2.19	0.42
1:A:142:ASN:HB3	1:A:145:ASP:O	2.20	0.42
1:B:524:LEU:HD23	1:B:524:LEU:HA	1.83	0.42
1:A:69:ALA:O	1:A:194:PHE:CD1	2.73	0.42
1:B:103:PRO:CB	1:B:173:TRP:CZ3	2.98	0.42
1:B:101:VAL:HG22	1:B:191:PHE:CE2	2.55	0.42
1:A:88:PRO:HA	1:A:89:PRO:HD2	1.87	0.42
1:A:198:ASP:OD2	1:A:198:ASP:N	2.53	0.42
1:B:426:GLU:HB3	1:B:498:TYR:CD2	2.55	0.42
1:A:405:GLN:OE1	1:A:515:MET:CE	2.68	0.42
1:B:92:VAL:O	1:B:95:LEU:HB2	2.20	0.42
1:B:73:PHE:CD1	1:B:87:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:HG3	2:A:612:HOH:O	2.19	0.42
1:A:242:VAL:HG21	1:A:260:LEU:HD21	2.00	0.42
1:A:239:ARG:CZ	1:A:531:VAL:HG11	2.47	0.42
1:A:135:GLN:O	1:A:136:ALA:HB2	2.20	0.42
1:A:156:HIS:CD2	2:A:657:HOH:O	2.72	0.42
1:B:105:PHE:HD1	1:B:106:TYR:C	2.23	0.42
1:B:106:TYR:CD1	1:B:112:GLN:O	2.72	0.42
1:A:410:MET:O	1:A:419:ILE:N	2.53	0.42
1:B:78:PHE:HE2	1:B:173:TRP:CH2	2.35	0.42
1:B:150:PHE:HD2	1:B:171:MET:HE3	1.85	0.42
1:B:429:GLU:HG3	1:B:430:GLN:N	2.35	0.42
1:B:148:LYS:O	1:B:148:LYS:HG2	2.20	0.42
1:A:403:HIS:HE1	2:A:618:HOH:O	2.02	0.42
1:B:350:ILE:HG22	1:B:352:LEU:CD1	2.50	0.42
1:B:159:PHE:O	1:B:160:HIS:C	2.57	0.42
1:B:418:ASN:N	1:B:418:ASN:OD1	2.51	0.42
1:B:411:TYR:CZ	1:B:413:PRO:HB3	2.54	0.42
1:B:239:ARG:O	1:B:240:LYS:C	2.57	0.42
1:B:308:GLU:C	1:B:310:LYS:H	2.23	0.42
1:B:206:ASP:HB3	1:B:209:LYS:CE	2.50	0.42
1:B:225:MET:C	1:B:227:SER:H	2.23	0.42
1:A:101:VAL:HG11	1:A:191:PHE:CZ	2.55	0.42
1:B:216:LEU:CD1	1:B:226:ASN:HB3	2.50	0.42
1:A:331:TYR:O	1:A:391:LYS:HA	2.20	0.41
1:B:357:LYS:CE	1:B:366:ASP:HB2	2.50	0.41
1:B:296:VAL:HG23	1:B:297:GLN:H	1.85	0.41
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.90	0.41
1:B:63:THR:HG23	1:B:64:SER:N	2.35	0.41
1:B:443:LYS:O	1:B:445:PRO:HD3	2.19	0.41
1:A:222:THR:N	1:A:288:LEU:HD22	2.35	0.41
1:A:448:TYR:CB	1:A:518:TYR:HB3	2.39	0.41
1:B:459:ASP:O	1:B:460:ASN:CB	2.68	0.41
1:A:474:ASP:OD2	1:A:474:ASP:N	2.43	0.41
1:B:411:TYR:C	1:B:411:TYR:CD1	2.93	0.41
1:B:77:ARG:HA	1:B:187:ASP:HB3	2.02	0.41
1:B:242:VAL:CG1	1:B:245:MET:HE2	2.40	0.41
1:A:102:MET:HE1	1:A:104:ARG:HD3	2.01	0.41
1:A:234:PHE:CE1	1:A:480:PHE:CZ	3.07	0.41
1:B:258:LEU:HD13	1:B:262:ARG:HH21	1.85	0.41
1:B:81:LEU:HG	1:B:82:SER:N	2.36	0.41
1:B:532:THR:HG22	1:B:533:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:O	1:A:273:PRO:C	2.59	0.41
1:B:233:PHE:CD1	1:B:233:PHE:C	2.93	0.41
1:A:224:TYR:CD1	1:A:224:TYR:C	2.94	0.41
1:A:159:PHE:O	1:A:160:HIS:C	2.58	0.41
1:B:201:HIS:N	1:B:201:HIS:ND1	2.68	0.41
1:A:457:SER:HB2	1:A:511:THR:HG23	2.02	0.41
1:A:266:GLU:HB3	1:A:274:VAL:HG13	2.03	0.41
1:A:490:LYS:C	1:A:492:GLU:N	2.73	0.41
1:A:393:VAL:HG12	1:A:394:LYS:N	2.34	0.41
1:B:388:GLU:HG2	2:B:563:HOH:O	2.20	0.41
1:A:92:VAL:HB	1:A:97:TRP:NE1	2.35	0.41
1:A:383:GLU:H	1:A:383:GLU:HG2	1.57	0.41
1:B:495:GLU:HA	1:B:498:TYR:CE1	2.55	0.41
1:B:78:PHE:C	1:B:78:PHE:HD2	2.24	0.41
1:B:288:LEU:C	1:B:290:SER:H	2.24	0.41
1:A:159:PHE:CD2	1:A:159:PHE:N	2.88	0.41
1:B:139:LYS:CB	1:B:151:SER:HB3	2.51	0.41
1:A:254:LYS:HB2	2:A:569:HOH:O	2.21	0.41
1:B:106:TYR:HB3	1:B:109:ARG:O	2.20	0.41
1:B:477:TRP:CZ2	1:B:494:ILE:HD11	2.56	0.41
1:A:245:MET:HA	1:A:246:PRO:HD3	1.88	0.41
1:B:78:PHE:CD1	1:B:189:VAL:HG21	2.51	0.41
1:B:245:MET:HG2	1:B:311:MET:HG2	2.02	0.41
1:A:102:MET:HE2	1:A:104:ARG:HD3	2.03	0.41
1:B:297:GLN:H	1:B:297:GLN:HG3	1.63	0.41
1:A:394:LYS:HD3	1:A:394:LYS:HA	1.90	0.41
1:A:118:PHE:N	1:A:118:PHE:CD1	2.88	0.41
1:B:414:GLN:C	1:B:416:ASP:N	2.74	0.41
1:B:301:ARG:O	1:B:305:ASP:CB	2.69	0.41
1:A:75:VAL:CG1	2:A:671:HOH:O	2.69	0.41
1:A:398:LEU:HB2	1:A:448:TYR:OH	2.21	0.41
1:A:417:GLN:HB3	1:A:419:ILE:HG12	2.02	0.41
1:B:92:VAL:HG21	1:B:195:VAL:CG1	2.50	0.41
1:A:103:PRO:O	1:A:104:ARG:HG2	2.20	0.41
1:A:118:PHE:HA	1:A:166:GLY:HA3	2.02	0.41
1:A:405:GLN:OE1	1:A:515:MET:HE1	2.21	0.40
1:A:68:GLU:O	1:A:69:ALA:HB2	2.21	0.40
1:B:223:CYS:HB3	1:B:465:TYR:CE1	2.57	0.40
1:B:150:PHE:HZ	1:B:152:ARG:NH2	2.19	0.40
1:A:360:ILE:CD1	1:A:427:PHE:HB3	2.51	0.40
1:A:217:LYS:HD3	1:A:275:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:PHE:HZ	1:B:456:HIS:ND1	2.19	0.40
1:A:294:HIS:HB3	1:A:298:GLU:CG	2.34	0.40
1:A:233:PHE:HB2	1:A:267:LEU:HD23	2.03	0.40
1:A:266:GLU:OE2	1:A:274:VAL:HG13	2.21	0.40
1:A:398:LEU:HA	1:A:399:PRO:HD3	1.91	0.40
1:A:218:ASN:HB3	1:A:219:GLN:H	1.35	0.40
1:A:236:ASN:O	1:A:239:ARG:HB3	2.21	0.40
1:A:414:GLN:O	1:A:415:THR:HB	2.21	0.40
1:A:99:ILE:HG12	1:A:193:VAL:HG21	2.03	0.40
1:A:98:LYS:O	1:A:119:LEU:HD12	2.22	0.40
1:B:470:ASN:ND2	1:B:473:GLY:HA2	2.37	0.40
1:B:159:PHE:CE1	1:B:161:LYS:HB2	2.56	0.40
1:B:315:CYS:SG	1:B:316:VAL:HG13	2.62	0.40
1:A:407:MET:HG2	2:B:637:HOH:O	2.20	0.40
1:A:358:LYS:NZ	1:B:295:ASP:OD2	2.42	0.40
1:B:153:ARG:HG3	2:B:572:HOH:O	2.21	0.40
1:B:67:SER:HB3	1:B:93:ARG:NH2	2.37	0.40
1:A:74:THR:OG1	1:A:190:THR:HG23	2.20	0.40
1:B:109:ARG:HE	1:B:110:PRO:CD	2.10	0.40
1:B:204:ALA:O	1:B:205:TRP:HB3	2.22	0.40
1:B:350:ILE:HG23	2:B:646:HOH:O	2.20	0.40
1:B:138:LEU:N	1:B:138:LEU:HD12	2.36	0.40
1:A:78:PHE:O	1:A:79:SER:C	2.59	0.40
1:B:354:ILE:CD1	1:B:355:LYS:N	2.85	0.40
1:A:301:ARG:HA	1:A:301:ARG:HD3	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:O	1:A:287:THR:O[4_555]	1.83	0.37

## 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	462/522 (88%)	356 (77%)	71 (15%)	35 (8%)	1	9
1	B	477/522 (91%)	364 (76%)	78 (16%)	35 (7%)	1	9
All	All	939/1044 (90%)	720 (77%)	149 (16%)	70 (8%)	1	9

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	183	PHE
1	A	203	VAL
1	A	277	LYS
1	A	334	CYS
1	A	495	GLU
1	A	529	GLN
1	A	537	PRO
1	A	538	GLN
1	B	105	PHE
1	B	111	HIS
1	B	160	HIS
1	B	207	SER
1	B	218	ASN
1	B	220	GLY
1	B	296	VAL
1	B	383	GLU
1	B	415	THR
1	B	461	HIS
1	A	160	HIS
1	A	204	ALA
1	A	236	ASN
1	A	249	GLY
1	A	252	SER
1	A	285	TRP
1	A	315	CYS
1	A	375	GLY
1	A	415	THR
1	A	416	ASP
1	B	79	SER
1	B	183	PHE
1	B	208	LYS
1	B	270	SER

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Mol	Chain	Res	Type
1	B	382	GLY
1	B	384	HIS
1	B	422	ASN
1	B	482	ASP
1	B	535	ASP
1	A	259	ALA
1	A	273	PRO
1	A	445	PRO
1	A	491	GLU
1	B	113	LYS
1	B	413	PRO
1	B	423	ASP
1	B	471	PRO
1	B	529	GLN
1	A	211	THR
1	A	223	CYS
1	A	244	MET
1	A	355	LYS
1	B	112	GLN
1	B	178	ASP
1	B	236	ASN
1	A	209	LYS
1	A	413	PRO
1	A	428	PRO
1	A	482	ASP
1	B	108	ASP
1	B	203	VAL
1	B	442	PRO
1	B	460	ASN
1	B	524	LEU
1	A	145	ASP
1	A	200	PRO
1	A	399	PRO
1	A	494	ILE
1	B	246	PRO
1	B	399	PRO
1	B	214	VAL

### 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	428/472 (91%)	355 (83%)	73 (17%)	2	12
1	B	437/472 (93%)	374 (86%)	63 (14%)	4	19
All	All	865/944 (92%)	729 (84%)	136 (16%)	3	15

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	PHE
1	A	126	ASP
1	A	153	ARG
1	A	159	PHE
1	A	164	ASP
1	A	168	SER
1	A	186	ASP
1	A	198	ASP
1	A	210	HIS
1	A	227	SER
1	A	229	LEU
1	A	232	LEU
1	A	248	GLU
1	A	260	LEU
1	A	271	ASP
1	A	272	LYS
1	A	283	PHE
1	A	286	GLU
1	A	287	THR
1	A	293	GLN
1	A	296	VAL
1	A	298	GLU
1	A	305	ASP
1	A	306	ASN
1	A	319	THR
1	A	322	LYS
1	A	323	LEU
1	A	325	ARG
1	A	330	SER
1	A	331	TYR
1	A	333	GLN

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Mol	Chain	Res	Type
1	A	342	ASP
1	A	343	ARG
1	A	354	ILE
1	A	357	LYS
1	A	359	ASN
1	A	363	SER
1	A	370	VAL
1	A	371	GLU
1	A	376	ASP
1	A	383	GLU
1	A	386	LEU
1	A	387	GLN
1	A	388	GLU
1	A	402	LEU
1	A	405	GLN
1	A	406	LEU
1	A	407	MET
1	A	415	THR
1	A	416	ASP
1	A	418	ASN
1	A	427	PHE
1	A	428	PRO
1	A	433	LEU
1	A	435	GLU
1	A	438	GLN
1	A	441	ASP
1	A	461	HIS
1	A	469	LEU
1	A	470	ASN
1	A	476	LYS
1	A	478	CYS
1	A	480	PHE
1	A	486	SER
1	A	491	GLU
1	A	496	HIS
1	A	512	ASN
1	A	531	VAL
1	A	537	PRO
1	A	540	LEU
1	A	544	LEU
1	A	547	GLU
1	A	548	LYS

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Mol	Chain	Res	Type
1	B	78	PHE
1	B	80	ARG
1	B	105	PHE
1	B	106	TYR
1	B	118	PHE
1	B	186	ASP
1	B	191	PHE
1	B	201	HIS
1	B	206	ASP
1	B	228	LEU
1	B	247	THR
1	B	258	LEU
1	B	277	LYS
1	B	282	SER
1	B	288	LEU
1	B	290	SER
1	B	296	VAL
1	B	299	LEU
1	B	301	ARG
1	B	309	ASN
1	B	312	LYS
1	B	314	THR
1	B	327	LYS
1	B	342	ASP
1	B	350	ILE
1	B	351	GLN
1	B	352	LEU
1	B	355	LYS
1	B	360	ILE
1	B	361	PHE
1	B	364	PHE
1	B	365	VAL
1	B	367	TYR
1	B	376	ASP
1	B	379	TYR
1	B	391	LYS
1	B	397	THR
1	B	403	HIS
1	B	407	MET
1	B	411	TYR
1	B	414	GLN
1	B	416	ASP

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Mol	Chain	Res	Type
1	B	418	ASN
1	B	419	ILE
1	B	422	ASN
1	B	426	GLU
1	B	450	LEU
1	B	453	VAL
1	B	459	ASP
1	B	460	ASN
1	B	469	LEU
1	B	471	PRO
1	B	474	ASP
1	B	476	LYS
1	B	495	GLU
1	B	511	THR
1	B	526	GLU
1	B	533	ASP
1	B	534	HIS
1	B	535	ASP
1	B	539	GLN
1	B	540	LEU
1	B	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	210	HIS
1	A	218	ASN
1	A	219	GLN
1	A	226	ASN
1	A	230	GLN
1	A	236	ASN
1	A	237	GLN
1	A	261	GLN
1	A	268	GLN
1	A	333	GLN
1	A	359	ASN
1	A	403	HIS
1	A	418	ASN
1	A	461	HIS
1	A	470	ASN
1	A	497	ASN

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Mol	Chain	Res	Type
1	A	512	ASN
1	A	529	GLN
1	A	538	GLN
1	A	545	GLN
1	B	156	HIS
1	B	219	GLN
1	B	237	GLN
1	B	268	GLN
1	B	293	GLN
1	B	297	GLN
1	B	351	GLN
1	B	372	GLN
1	B	387	GLN
1	B	405	GLN
1	B	414	GLN
1	B	417	GLN
1	B	422	ASN
1	B	430	GLN
1	B	464	HIS
1	B	470	ASN
1	B	539	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.