



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:58 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

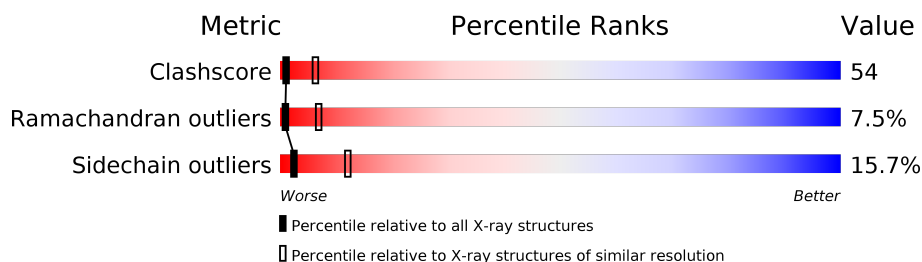
1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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

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		

N512	A513	Y514	M515	L516	V517	Y518		L524	S525	E526	V527	Q529	A530	V531	T532	D533	H534	D535	L536	Q539	L540	L544	E547	E551	A552	Q553	LYS	ARG	LYS	GLU	ARG	GLN	GLU																									
I449	L450	H451	A452	V453	L454	V455	H456	D459	P460	H461	G462	G463	H464	Y465	V466	V467	Y468	L469	N470	K471	K472	G473	D474	G475	K476	K477	C478	K479	F480	L481	D482	D483	V484	V485	T489	K490	E491	E492	A493	I494	E495	H496	N497	Y498	G499	GLY	HIS	ASP	ASP	ASP	LEU	SER	VAL	ARG	HIS	C510	T511	
K378	Y379	D380	A381	V382	E383	H384	G385	L386	Q387	E388	A389	E390	K391	T397	L398	P399	P400		H403	L404	Q405	L406	M407	H408	F409	M410	Y411	D412	P413	Q414	T415	D416	Q417	M418	I419	K420	I421	N422	D423	R424	A425	E426	F427	P428	E429	Q430	L431	P432	L433	F436	P442	K443	D444	P445		Y448		
K312	G313	T314	C315	V316	E317	G318	T319	I320	K321	K322	A323	F324		K327	M328	V329	S330	Y331	I332	Q333	C334	K335	E336	V337	D338	Y339		D342	R343	R344		Y347		I350	Q351	L352	S353	I354	K355	G356	K357	K358	K359	I360	F361	E362	F364	V365	D366	Y367	V368	A369	E371	Q372		D376	N377	
V242	Y243	M244	M245	P246	T247		D250		S255	V256	P257	L258	E259	L260	Q261	R262	V263	F264		L267	Q268	H269	S270		V274	G275	K276	K277	K278	L279	T280	K281	S282	F283		T287	L288	D289	S290	F291	M292	Q293	E294	D295	V296	Q297	E298	L299	C300	R301		L304	D305	V307	E308	N309	K310	M311
Y106	F107	D108	R109	P110	H111	Q112	K113	S114	V115	G116	F117	L118	L119	N122	M130	Q135	A136	V137	L138	K139	I140	L141	M142	Y143	R144	D145	K148	S149	F150	S151	R152	R153	L154	S155	H156	L157	F158	F159	H160	K161		D164		F167	S168	M169	F170	M171	A172	M173	V176	T177	D178	P179				

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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:225:MET:HG3	1:A:299:LEU:HD21	1.58	0.86
1:A:448:TYR:HB3	1:A:518:TYR:HB3	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:A:333:GLN:HE22	1:A:340:ARG:HD2	1.49	0.78
1:B:332:ILE:HG12	1:B:391:LYS:CB	2.13	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:B:221:ALA:HB1	1:B:288:LEU:HA	1.67	0.77
1:A:413:PRO:HG3	1:B:386:LEU:O	1.85	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:119:LEU:CD1	1:B:193:VAL:HG11	2.15	0.76
1:B:324:PHE:HZ	2:B:585:HOH:O	1.66	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:A:286:GLU:O	1:A:287:THR:HG22	1.87	0.74
1:B:381:ALA:HB1	2:B:576:HOH:O	1.88	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:182:GLY:O	1:A:184:ILE:N	2.22	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: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:A:153:ARG:HH11	1:A:153:ARG:HG2	1.54	0.73
1:A:429:GLU:H	1:B:293:GLN:HE22	1.34	0.73
1:B:237:GLN:NE2	1:B:527:VAL:HA	2.03	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:A:449:ILE:HD11	1:A:524:LEU:HD13	1.71	0.71
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:247:THR:HG21	1:A:261:GLN:HE22	1.52	0.71
1:A:546:GLU:O	1:A:549:ARG:HG2	1.91	0.71
1:B:287:THR:HG22	1:B:288:LEU:N	2.05	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:A:447:ASN:HB2	2:A:626:HOH:O	1.90	0.70
1:B:450:LEU:HD23	1:B:451:HIS:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ILE:HG22	1:B:495:GLU:N	2.06	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:A:441:ASP:OD2	1:A:444:ASP:HB3	1.92	0.70
1:B:357:LYS:HD2	1:B:362:GLU:HB3	1.72	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:200:PRO:HG2	1:A:203:VAL:HG11	1.75	0.68
1:A:398:LEU:HG	1:A:437:LEU:HD21	1.76	0.68
1:A:177:THR:HG22	2:A:674:HOH:O	1.94	0.68
1:A:216:LEU:HD11	1:A:230:GLN:HG2	1.75	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:A:91:PHE:HB3	2:A:576:HOH:O	1.93	0.67
1:B:287:THR:CG2	1:B:288:LEU:N	2.57	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:206:ASP:O	1:B:209:LYS:HG2	1.95	0.66
1:B:235:THR:HG21	2:B:585:HOH:O	1.94	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:A:123:ALA:HB3	2:A:575:HOH:O	1.96	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:B:413:PRO:C	1:B:415:THR:H	1.82	0.66
1:B:450:LEU:HD22	1:B:477:TRP:HH2	1.60	0.66
1:A:412:ASP:OD2	1:A:413:PRO:HD3	1.96	0.66
1:A:219:GLN:HE22	1:A:464:HIS:HA	1.59	0.66
1:A:334:CYS:HA	1:A:389:ALA:HB2	1.78	0.66
1:B:228:LEU:HD12	1:B:299:LEU:CD1	2.25	0.66
1:B:297:GLN:HG2	1:B:405:GLN:OE1	1.96	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:236:ASN:HD22	1:A:236:ASN:H	1.43	0.64
1:A:233:PHE:CD1	1:A:267:LEU:HD23	2.33	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:211:THR:HG22	1:A:213:TYR:HB2	1.79	0.64
1:A:263:VAL:HG13	1:A:264:PHE:N	2.13	0.64
1:A:198:ASP:HB3	2:A:642:HOH:O	1.97	0.64
1:A:455:VAL:CG1	1:A:466:VAL:HB	2.27	0.64
1:A:308:GLU:OE1	1:A:318:GLY:HA2	1.97	0.64
1:A:308:GLU:C	1:A:310:LYS:H	1.98	0.64
1:B:350:ILE:HA	2:B:646:HOH:O	1.97	0.64
1:B:217:LYS:HE2	1:B:275:GLY:CA	2.28	0.64
1:B:411:TYR:CD1	1:B:411:TYR:O	2.51	0.64
1:B:219:GLN:O	1:B:220:GLY:O	2.16	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:A:355:LYS:NZ	1:B:377:ASN:O	2.27	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:193:VAL:HG23	2:B:635:HOH:O	1.98	0.63
1:B:318:GLY:O	1:B:321:PRO:HD2	1.97	0.63
1:A:364:PHE:O	1:A:368:VAL:HG22	1.98	0.63
1:B:103:PRO:HB3	1:B:173:TRP:CZ3	2.33	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:119:LEU:HD13	1:B:193:VAL:HG11	1.79	0.63
1:B:308:GLU:CB	1:B:320:ILE:HD12	2.28	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:156:HIS:ND1	1:A:165:TRP:HB2	2.14	0.62
1:A:237:GLN:HE22	1:A:526:GLU:HG2	1.65	0.62
1:A:295:ASP:O	1:A:298:GLU:HG2	1.99	0.62
1:A:476:LYS:HE3	1:A:476:LYS:HA	1.82	0.62
1:B:365:VAL:HA	1:B:368:VAL:CG2	2.30	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:318:GLY:C	1:B:321:PRO:HD2	2.19	0.62
1:B:329:VAL:HG22	1:B:344:ARG:HG3	1.81	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: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:B:308:GLU:OE1	1:B:321:PRO:HD3	2.00	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:470:ASN:HD22	1:A:470:ASN:N	1.97	0.61
1:A:449:ILE:HD11	1:A:524:LEU:CD1	2.30	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:323:LEU:O	1:B:400:PRO:HD2	2.01	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: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:185:ASP:O	1:A:186:ASP:HB2	1.99	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:288:LEU:HD13	2:A:593:HOH:O	2.02	0.60
1:A:334:CYS:HA	1:A:389:ALA:CB	2.32	0.60
1:B:371:GLU:OE2	1:B:391:LYS:HE3	2.01	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:A:537:PRO:O	1:A:538:GLN:HB2	2.02	0.60
1:A:71:PHE:CD1	1:A:90:CYS:HB2	2.37	0.60
1:B:184:ILE:HG12	1:B:185:ASP:N	2.17	0.60
1:B:93:ARG:HG3	1:B:198:ASP:O	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:210:HIS:H	1:A:210:HIS:HD2	1.49	0.59
1:A:263:VAL:O	1:A:267:LEU:HB2	2.01	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:295:ASP:O	1:B:296:VAL:C	2.41	0.59
1:B:450:LEU:HD22	1:B:477:TRP:CH2	2.37	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:A:470:ASN:H	1:A:470:ASN:HD22	1.50	0.58
1:B:242:VAL:HG13	1:B:245:MET:CE	2.31	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:93:ARG:NE	1:B:198:ASP:O	2.34	0.58
1:B:304:LEU:O	1:B:320:ILE:HD13	2.03	0.58
1:B:383:GLU:C	1:B:385:GLY:N	2.57	0.58
1:B:354:ILE:HD12	1:B:355:LYS:H	1.67	0.58
1:B:405:GLN:HE21	1:B:515:MET:HE3	1.69	0.58
1:A:210:HIS:N	1:A:210:HIS:CD2	2.71	0.58
1:B:78:PHE:O	1:B:79:SER:C	2.41	0.58
1:A:446:ALA:HA	1:A:520:ARG:HE	1.68	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:413:PRO:HB2	1:B:415:THR:HB	1.86	0.58
1:B:171:MET:HG2	1:B:172:ALA:H	1.68	0.58
1:B:307:VAL:O	1:B:310:LYS:HB3	2.04	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:421:ILE:HG23	1:A:423:ASP:OD2	2.04	0.57
1:A:434:ASP:HB3	1:A:446:ALA:CB	2.31	0.57
1:A:154:ILE:HG13	1:A:154:ILE:O	2.03	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:103:PRO:CB	1:B:173:TRP:HZ3	2.16	0.57
1:B:295:ASP:O	1:B:297:GLN:N	2.37	0.57
1:B:73:PHE:CD2	1:B:87:SER:HB3	2.39	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:501:HIS:CB	1:B:413:PRO:HG3	2.24	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:A:153:ARG:NH1	1:A:153:ARG:HG2	2.17	0.57
1:A:168:SER:HB3	2:A:645:HOH:O	2.03	0.57
1:B:109:ARG:HD3	2:B:571:HOH:O	2.04	0.57
1:B:169:ASN:HA	2:B:593:HOH:O	2.05	0.57
1:B:243:TYR:OH	1:B:268:GLN:NE2	2.38	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: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
1:B:312:LYS:HG3	1:B:313:GLY:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ILE:HG22	1:B:425:PHE:CD2	2.39	0.57
1:A:420:LYS:HE2	1:A:422:ASN:OD1	2.05	0.57
1:A:467:VAL:HG13	1:A:467:VAL:O	2.03	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: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:A:76:GLU:HA	1:A:188:LYS:HG2	1.86	0.56
1:B:308:GLU:CD	1:B:321:PRO:HD3	2.25	0.56
1:A:248:GLU:O	1:A:250:ASP:N	2.37	0.56
1:A:333:GLN:O	1:A:334:CYS:O	2.24	0.56
1:A:406:LEU:HD12	1:A:406:LEU:N	2.20	0.56
1:A:519:ILE:HD13	1:A:527:VAL:HG11	1.87	0.56
1:B:156:HIS:CD2	1:B:157:LEU:H	2.23	0.56
1:B:365:VAL:O	1:B:369:ALA:N	2.38	0.56
1:B:495:GLU:HA	1:B:498:TYR:CD1	2.41	0.56
1:A:224:TYR:HB3	1:A:465:TYR:CD1	2.40	0.56
1:A:288:LEU:HA	1:A:291:PHE:HD2	1.70	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: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:411:TYR:HD1	1:B:411:TYR:O	1.88	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:A:160:HIS:CG	1:A:161:LYS:N	2.73	0.55
1:A:407:MET:HB2	2:A:603:HOH:O	2.05	0.55
1:A:398:LEU:HD13	1:A:433:LEU:HD23	1.87	0.55
1:A:438:GLN:N	1:A:438:GLN:OE1	2.40	0.55
1:B:412:ASP:HB3	2:B:647:HOH:O	2.06	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:241:ALA:CB	1:A:316:VAL:HG21	2.36	0.54
1:A:408:ARG:NH2	1:A:513:ALA:O	2.41	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:A:314:THR:HA	2:A:596:HOH:O	2.07	0.54
1:A:458:GLY:C	1:A:460:ASN:H	2.09	0.54
1:B:143:TYR:HD1	1:B:185:ASP:HB2	1.73	0.54
1:B:376:ASP:HA	1:B:379:TYR:CD1	2.42	0.54
1:B:453:VAL:HG22	1:B:453:VAL:O	2.07	0.54
1:B:75:VAL:O	1:B:188:LYS:HA	2.07	0.54
1:B:289:ASP:HA	1:B:292:MET:HB2	1.89	0.54
1:B:308:GLU:HG3	2:B:653:HOH:O	2.07	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:219:GLN:O	1:B:220:GLY:C	2.47	0.53
1:B:524:LEU:HD22	1:B:528:LEU:HD12	1.90	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:A:374:ASP:HA	1:A:378:LYS:CG	2.38	0.53
1:B:78:PHE:N	1:B:187:ASP:O	2.38	0.53
1:B:73:PHE:CG	1:B:87:SER:CB	2.91	0.53
1:A:289:ASP:O	1:A:293:GLN:HB2	2.09	0.53
1:A:329:VAL:HG22	1:A:344:ARG:HG2	1.90	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:B:452:ALA:HB2	1:B:469:LEU:HG	1.90	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:269:HIS:HD2	2:A:678:HOH:O	1.92	0.52
1:A:262:ARG:NH2	1:A:278:LYS:HB3	2.24	0.52
1:A:180:GLU:HG2	1:A:180:GLU:O	2.09	0.52
1:A:117:PHE:HD2	1:A:170:PHE:CZ	2.27	0.52
1:A:150:PHE:HB3	1:A:171:MET:HE2	1.92	0.52
1:A:211:THR:HG21	1:A:485:VAL:HG12	1.92	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: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:263:VAL:CG1	1:A:264:PHE:N	2.72	0.52
1:A:295:ASP:HB3	1:A:297:GLN:OE1	2.10	0.52
1:A:295:ASP:H	1:A:298:GLU:CG	2.23	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:A:455:VAL:HB	1:A:497:ASN:HD21	1.75	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:B:67:SER:HA	1:B:93:ARG:CZ	2.40	0.52
1:A:211:THR:CG2	1:A:213:TYR:HB2	2.40	0.52
1:B:232:LEU:HD13	1:B:304:LEU:HD21	1.91	0.52
1:B:255:SER:OG	1:B:257:PRO:HD2	2.09	0.52
1:A:335:LYS:NZ	1:B:344:ARG:HH22	2.08	0.52
1:A:239:ARG:HH22	1:A:531:VAL:HG11	1.75	0.51
1:B:191:PHE:N	1:B:191:PHE:CD1	2.76	0.51
1:B:206:ASP:HB3	1:B:209:LYS:HE3	1.92	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:A:412:ASP:OD2	1:A:413:PRO:CD	2.58	0.51
1:B:105:PHE:CE1	1:B:107:PRO:HB3	2.46	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:407:MET:HA	1:A:407:MET:HE2	1.92	0.51
1:A:410:MET:HE1	1:B:381:ALA:O	2.11	0.51
1:B:466:VAL:HG11	1:B:479:LYS:HE3	1.92	0.51
1:B:78:PHE:O	1:B:81:LEU:N	2.43	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:359:ASN:ND2	1:A:362:GLU:HG3	2.23	0.51
1:A:71:PHE:CD1	1:A:90:CYS:CB	2.94	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:102:MET:CE	1:A:104:ARG:HD3	2.40	0.51
1:A:203:VAL:HG13	1:A:203:VAL:O	2.11	0.51
1:A:480:PHE:N	1:A:480:PHE:CD1	2.79	0.51
1:A:495:GLU:HG3	2:A:573:HOH:O	2.09	0.51
1:B:191:PHE:HB3	2:B:635:HOH:O	2.10	0.51
1:B:420:LYS:HE2	1:B:512:ASN:ND2	2.24	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: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:B:357:LYS:NZ	1:B:366:ASP:HB2	2.25	0.50
1:A:427:PHE:N	1:A:427:PHE:CD2	2.78	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:B:361:PHE:C	1:B:361:PHE:CD2	2.85	0.50
1:B:416:ASP:O	1:B:417:GLN:HB2	2.10	0.50
1:B:429:GLU:CG	1:B:430:GLN:N	2.74	0.50
1:B:213:TYR:CZ	1:B:471:PRO:HG2	2.47	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: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:B:330:SER:O	1:B:342:ASP:HA	2.11	0.50
1:A:285:TRP:HE3	1:A:291:PHE:CD1	2.30	0.50
1:A:458:GLY:C	1:A:460:ASN:N	2.65	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: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:A:415:THR:O	1:A:416:ASP:CB	2.55	0.49
1:B:413:PRO:HD2	2:B:647:HOH:O	2.11	0.49
1:A:318:GLY:O	1:A:321:PRO:HD2	2.12	0.49
1:A:331:TYR:C	1:A:332:ILE:HG13	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:TRP:NE1	1:B:177:THR:HG21	2.27	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:133:HIS:ND1	1:A:134:ALA:N	2.60	0.49
1:A:160:HIS:CE1	1:A:161:LYS:HG3	2.47	0.49
1:A:314:THR:O	1:A:316:VAL:N	2.46	0.49
1:A:409:PHE:HE1	1:A:420:LYS:HD2	1.73	0.49
1:B:135:GLN:O	1:B:136:ALA:HB2	2.12	0.49
1:B:160:HIS:CG	1:B:161:LYS:N	2.81	0.49
1:B:532:THR:C	1:B:534:HIS:N	2.66	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:359:ASN:C	1:A:359:ASN:ND2	2.67	0.48
1:A:490:LYS:C	1:A:492:GLU:H	2.16	0.48
1:A:450:LEU:HG	1:A:477:TRP:HH2	1.78	0.48
1:B:311:MET:HB2	2:B:653:HOH:O	2.12	0.48
1:A:99:ILE:HG23	1:A:117:PHE:HE1	1.77	0.48
1:B:459:ASP:OD2	1:B:459:ASP:N	2.46	0.48
1:B:65:TRP:HH2	1:B:204:ALA:HB3	1.78	0.48
1:B:308:GLU:CG	2:B:653:HOH:O	2.61	0.48
1:A:177:THR:O	1:A:179:PRO:HD3	2.14	0.48
1:A:322:LYS:O	1:A:400:PRO:HG2	2.14	0.48
1:A:422:ASN:HD21	1:A:459:ASP:HA	1.76	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:355:LYS:CG	1:B:356:GLY:N	2.76	0.48
1:B:426:GLU:HA	1:B:498:TYR:CD2	2.48	0.48
1:B:465:TYR:CD1	1:B:465:TYR:N	2.81	0.48
1:A:143:TYR:N	1:A:143:TYR:CD2	2.80	0.48
1:A:344:ARG:HD2	1:A:396:LEU:CD1	2.44	0.48
1:B:228:LEU:HD12	1:B:299:LEU:HD12	1.94	0.48
1:B:425:PHE:HB2	2:B:648:HOH:O	2.14	0.48
1:B:191:PHE:N	1:B:191:PHE:HD1	2.12	0.48
1:B:489:THR:HG1	1:B:492:GLU:HG3	1.77	0.48
1:B:456:HIS:O	1:B:511:THR:HA	2.14	0.48
1:A:461:HIS:H	1:A:461:HIS:CD2	2.30	0.48
1:B:113:LYS:C	1:B:173:TRP:HB2	2.34	0.48
1:B:211:THR:HG21	1:B:485:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:CYS:SG	1:A:200:PRO:HB3	2.53	0.48
1:B:364:PHE:O	1:B:368:VAL:HG22	2.14	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:256:VAL:N	1:B:257:PRO:CD	2.77	0.47
1:B:528:LEU:O	1:B:529:GLN:C	2.53	0.47
1:B:391:LYS:NZ	2:B:569:HOH:O	2.47	0.47
1:B:413:PRO:CA	1:B:415:THR:H	2.27	0.47
1:B:452:ALA:HB2	1:B:469:LEU:CD2	2.45	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:A:424:ARG:HA	1:A:499:GLY:HA3	1.96	0.47
1:B:105:PHE:HD1	1:B:107:PRO:N	2.12	0.47
1:B:115:VAL:HG21	1:B:176:VAL:HG11	1.96	0.47
1:B:387:GLN:HG3	2:B:563:HOH:O	2.14	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:102:MET:O	1:B:116:GLY:N	2.45	0.47
1:B:386:LEU:O	1:B:386:LEU:CG	2.63	0.47
1:A:173:TRP:HA	1:A:176:VAL:HG12	1.96	0.47
1:A:235:THR:O	1:A:235:THR:HG22	2.14	0.47
1:A:434:ASP:CB	1:A:446:ALA:HB3	2.41	0.47
1:A:451:HIS:HA	1:A:470:ASN:HD21	1.80	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:65:TRP:CD1	1:A:94:ASN:HB2	2.49	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:A:211:THR:HG21	1:A:485:VAL:CG1	2.45	0.47
1:A:223:CYS:HB3	1:A:465:TYR:CZ	2.49	0.47
1:B:225:MET:HE1	1:B:280:THR:HG22	1.97	0.47
1:B:78:PHE:C	1:B:78:PHE:CD2	2.88	0.47
1:B:142:ASN:HB3	1:B:145:ASP:O	2.15	0.47
1:A:439:LYS:HZ3	1:A:439:LYS:HB3	1.81	0.46
1:B:454:LEU:HD12	1:B:454:LEU:N	2.29	0.46
1:A:202:GLY:O	1:A:203:VAL:HB	2.15	0.46
1:A:216:LEU:HD21	1:A:267:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:CG	1:A:544:LEU:HD11	2.42	0.46
1:B:308:GLU:O	1:B:311:MET:N	2.47	0.46
1:A:115:VAL:O	1:A:170:PHE:HB3	2.15	0.46
1:A:222:THR:HA	1:A:291:PHE:CD1	2.51	0.46
1:A:262:ARG:HH22	1:A:278:LYS:HB3	1.80	0.46
1:B:308:GLU:C	1:B:310:LYS:N	2.67	0.46
1:A:382:GLY:O	1:A:385:GLY:N	2.45	0.46
1:B:225:MET:C	1:B:227:SER:N	2.68	0.46
1:A:337:VAL:HG12	1:A:387:GLN:HG2	1.98	0.46
1:A:491:GLU:HG3	1:A:495:GLU:HB2	1.97	0.46
1:A:92:VAL:HG21	1:A:195:VAL:HG11	1.97	0.46
1:B:118:PHE:CD1	1:B:118:PHE:N	2.83	0.46
1:B:337:VAL:CG1	1:B:338:ASP:N	2.78	0.46
1:A:242:VAL:HG21	1:A:260:LEU:CD2	2.45	0.46
1:A:332:ILE:O	1:A:340:ARG:HA	2.15	0.46
1:A:408:ARG:O	1:A:420:LYS:HA	2.16	0.46
1:A:531:VAL:HG12	2:A:621:HOH:O	2.15	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:B:355:LYS:N	1:B:355:LYS:HD3	2.30	0.46
1:A:316:VAL:HG22	1:A:319:THR:OG1	2.15	0.46
1:A:331:TYR:C	1:A:331:TYR:CD1	2.89	0.46
1:B:156:HIS:CD2	1:B:157:LEU:N	2.83	0.46
1:A:442:PRO:C	1:A:444:ASP:H	2.18	0.46
1:A:494:ILE:CG2	1:A:495:GLU:OE1	2.64	0.46
1:B:241:ALA:CB	1:B:319:THR:HG21	2.46	0.46
1:B:63:THR:O	1:B:66:ARG:NH2	2.48	0.46
1:A:117:PHE:CD2	1:A:138:LEU:HB3	2.51	0.46
1:A:494:ILE:C	1:A:496:HIS:N	2.66	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:240:LYS:HD2	1:B:529:GLN:OE1	2.16	0.46
1:A:208:LYS:CG	1:A:214:VAL:HG22	2.46	0.46
1:B:450:LEU:HD23	1:B:451:HIS:H	1.77	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:A:459:ASP:O	1:A:459:ASP:OD2	2.34	0.45
1:B:357:LYS:HE3	1:B:366:ASP:HB2	1.97	0.45
1:B:449:ILE:HD12	1:B:449:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLY:O	1:B:477:TRP:HD1	1.98	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:455:VAL:HB	1:A:497:ASN:ND2	2.30	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:176:VAL:O	1:A:176:VAL:HG22	2.16	0.45
1:A:242:VAL:HG13	1:A:243:TYR:N	2.32	0.45
1:A:301:ARG:O	1:A:305:ASP:HB2	2.16	0.45
1:B:79:SER:OG	1:B:187:ASP:OD1	2.28	0.45
1:A:115:VAL:CG2	1:A:176:VAL:HG11	2.39	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:A:418:ASN:HA	1:A:418:ASN:HD22	1.58	0.45
1:B:257:PRO:O	1:B:261:GLN:HG3	2.17	0.45
1:B:386:LEU:HD23	1:B:386:LEU:N	2.31	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:448:TYR:C	1:B:449:ILE:HD12	2.37	0.45
1:A:551:GLU:HG2	2:A:648:HOH:O	2.16	0.45
1:B:239:ARG:HD3	1:B:268:GLN:NE2	2.32	0.45
1:B:239:ARG:HG2	1:B:243:TYR:CE1	2.51	0.45
1:B:92:VAL:HB	1:B:97:TRP:CD1	2.50	0.45
1:A:343:ARG:HG3	1:A:343:ARG:O	2.16	0.45
1:A:455:VAL:HG23	1:A:512:ASN:C	2.36	0.45
1:B:217:LYS:O	1:B:218:ASN:O	2.34	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:301:ARG:HG2	1:B:301:ARG:NH1	2.32	0.45
1:B:81:LEU:HG	1:B:82:SER:H	1.82	0.45
1:A:153:ARG:CD	1:A:153:ARG:N	2.75	0.45
1:A:216:LEU:O	1:A:482:ASP:C	2.54	0.45
1:A:281:LYS:O	1:A:284:GLY:N	2.47	0.45
1:B:529:GLN:HB3	2:B:629:HOH:O	2.16	0.45
1:B:141:ILE:HA	1:B:149:SER:OG	2.17	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:411:TYR:CE1	1:B:413:PRO:HB3	2.51	0.44
1:A:243:TYR:OH	1:A:268:GLN:NE2	2.50	0.44
1:A:316:VAL:CG1	1:A:316:VAL:O	2.62	0.44
1:B:245:MET:HA	1:B:246:PRO:HD3	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HD11	1:B:193:VAL:HG23	1.99	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:153:ARG:HD3	1:A:153:ARG:N	2.20	0.44
1:A:256:VAL:CG2	1:A:282:SER:HB3	2.36	0.44
1:A:373:LEU:HB3	1:A:377:ASN:O	2.17	0.44
1:A:414:GLN:O	1:A:415:THR:CB	2.65	0.44
1:A:528:LEU:O	1:A:529:GLN:O	2.36	0.44
1:B:111:HIS:O	1:B:111:HIS:ND1	2.51	0.44
1:B:361:PHE:HD2	1:B:361:PHE:C	2.20	0.44
1:B:421:ILE:O	1:B:423:ASP:N	2.50	0.44
1:B:91:PHE:HA	1:B:95:LEU:O	2.17	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: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: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:B:466:VAL:HG12	1:B:467:VAL:N	2.32	0.44
1:B:143:TYR:CD1	1:B:185:ASP:HB2	2.52	0.44
1:B:177:THR:O	1:B:179:PRO:HD3	2.17	0.44
1:B:360:ILE:HD11	1:B:516:LEU:HD12	2.00	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:A:297:GLN:HG3	1:A:405:GLN:NE2	2.33	0.44
1:B:157:LEU:HD13	1:B:157:LEU:C	2.39	0.44
1:B:76:GLU:O	1:B:77:ARG:C	2.56	0.44
1:A:466:VAL:HG12	1:A:467:VAL:N	2.32	0.43
1:A:490:LYS:O	1:A:492:GLU:N	2.50	0.43
1:A:237:GLN:HE21	1:A:527:VAL:HA	1.82	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:A:435:GLU:HB3	1:B:305:ASP:OD2	2.18	0.43
1:A:70:THR:HG1	1:A:194:PHE:HD1	1.64	0.43
1:B:238:LEU:HD22	2:B:585:HOH:O	2.16	0.43
1:B:413:PRO:C	1:B:415:THR:N	2.54	0.43
1:A:354:ILE:HD13	1:A:355:LYS:CA	2.46	0.43
1:A:470:ASN:N	1:A:470:ASN:ND2	2.66	0.43
1:B:130:TRP:CG	1:B:130:TRP:O	2.71	0.43
1:B:184:ILE:CG1	1:B:185:ASP:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.84	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:B:242:VAL:O	1:B:245:MET:HG3	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:64:SER:N	2:A:632:HOH:O	2.51	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:136:ALA:HA	1:A:194:PHE:O	2.18	0.43
1:A:416:ASP:O	1:A:416:ASP:CG	2.57	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:287:THR:HG23	1:B:288:LEU:H	1.84	0.42
1:B:77:ARG:O	1:B:77:ARG:HG2	2.19	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: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: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:118:PHE:HB3	1:A:165:TRP:O	2.19	0.42
1:A:142:ASN:HB3	1:A:145:ASP:O	2.20	0.42
1:A:542:GLU:O	1:A:545:GLN:HB2	2.20	0.42
1:B:236:ASN:O	1:B:239:ARG:N	2.52	0.42
1:B:472:LYS:HB3	2:B:642:HOH:O	2.19	0.42
1:A:198:ASP:OD2	1:A:198:ASP:N	2.53	0.42
1:A:69:ALA:O	1:A:194:PHE:CD1	2.73	0.42
1:A:88:PRO:HA	1:A:89:PRO:HD2	1.87	0.42
1:B:101:VAL:HG22	1:B:191:PHE:CE2	2.55	0.42
1:B:103:PRO:CB	1:B:173:TRP:CZ3	2.98	0.42
1:B:524:LEU:HD23	1:B:524:LEU:HA	1.83	0.42
1:A:476:LYS:HG3	2:A:612:HOH:O	2.19	0.42
1:A:405:GLN:OE1	1:A:515:MET:CE	2.68	0.42
1:B:426:GLU:HB3	1:B:498:TYR:CD2	2.55	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:B:92:VAL:O	1:B:95:LEU:HB2	2.20	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: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:403:HIS:HE1	2:A:618:HOH:O	2.02	0.42
1:A:410:MET:O	1:A:419:ILE:N	2.53	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:B:148:LYS:O	1:B:148:LYS:HG2	2.20	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:78:PHE:HE2	1:B:173:TRP:CH2	2.35	0.42
1:B:159:PHE:O	1:B:160:HIS:C	2.57	0.42
1:B:350:ILE:HG22	1:B:352:LEU:CD1	2.50	0.42
1:B:418:ASN:N	1:B:418:ASN:OD1	2.51	0.42
1:A:101:VAL:HG11	1:A:191:PHE:CZ	2.55	0.42
1:B:206:ASP:HB3	1:B:209:LYS:CE	2.50	0.42
1:B:216:LEU:CD1	1:B:226:ASN:HB3	2.50	0.42
1:B:225:MET:C	1:B:227:SER:H	2.23	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:411:TYR:CZ	1:B:413:PRO:HB3	2.54	0.42
1:A:331:TYR:O	1:A:391:LYS:HA	2.20	0.41
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.90	0.41
1:B:296:VAL:HG23	1:B:297:GLN:H	1.85	0.41
1:B:357:LYS:CE	1:B:366:ASP:HB2	2.50	0.41
1:B:443:LYS:O	1:B:445:PRO:HD3	2.19	0.41
1:B:63:THR:HG23	1:B:64:SER:N	2.35	0.41
1:A:222:THR:N	1:A:288:LEU:HD22	2.35	0.41
1:A:474:ASP:OD2	1:A:474:ASP:N	2.43	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: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: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:B:411:TYR:CD1	1:B:411:TYR:C	2.93	0.41
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:B:258:LEU:HD13	1:B:262:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:THR:HG22	1:B:533:ASP:N	2.35	0.41
1:B:81:LEU:HG	1:B:82:SER:N	2.36	0.41
1:A:159:PHE:O	1:A:160:HIS:C	2.58	0.41
1:A:224:TYR:CD1	1:A:224:TYR:C	2.94	0.41
1:A:457:SER:HB2	1:A:511:THR:HG23	2.02	0.41
1:B:201:HIS:ND1	1:B:201:HIS:N	2.68	0.41
1:A:266:GLU:HB3	1:A:274:VAL:HG13	2.03	0.41
1:A:383:GLU:H	1:A:383:GLU:HG2	1.57	0.41
1:A:393:VAL:HG12	1:A:394:LYS:N	2.34	0.41
1:A:490:LYS:C	1:A:492:GLU:N	2.73	0.41
1:A:92:VAL:HB	1:A:97:TRP:NE1	2.35	0.41
1:B:388:GLU:HG2	2:B:563:HOH:O	2.20	0.41
1:A:159:PHE:CD2	1:A:159:PHE:N	2.88	0.41
1:A:254:LYS:HB2	2:A:569:HOH:O	2.21	0.41
1:B:139:LYS:CB	1:B:151:SER:HB3	2.51	0.41
1:B:288:LEU:C	1:B:290:SER:H	2.24	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:A:102:MET:HE2	1:A:104:ARG:HD3	2.03	0.41
1:A:394:LYS:HD3	1:A:394:LYS:HA	1.90	0.41
1:B:78:PHE:CD1	1:B:189:VAL:HG21	2.51	0.41
1:B:301:ARG:O	1:B:305:ASP:CB	2.69	0.41
1:B:414:GLN:C	1:B:416:ASP:N	2.74	0.41
1:A:118:PHE:N	1:A:118:PHE:CD1	2.88	0.41
1:A:245:MET:HA	1:A:246:PRO:HD3	1.88	0.41
1:A:75:VAL:CG1	2:A:671:HOH:O	2.69	0.41
1:B:106:TYR:HB3	1:B:109:ARG:O	2.20	0.41
1:B:245:MET:HG2	1:B:311:MET:HG2	2.02	0.41
1:B:297:GLN:H	1:B:297:GLN:HG3	1.63	0.41
1:B:477:TRP:CZ2	1:B:494:ILE:HD11	2.56	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: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:217:LYS:HD3	1:A:275:GLY:HA2	2.02	0.40
1:A:360:ILE:CD1	1:A:427:PHE:HB3	2.51	0.40
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:150:PHE:HZ	1:B:152:ARG:NH2	2.19	0.40
1:B:223:CYS:HB3	1:B:465:TYR:CE1	2.57	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:218:ASN:HB3	1:A:219:GLN:H	1.35	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:294:HIS:HB3	1:A:298:GLU:CG	2.34	0.40
1:A:398:LEU:HA	1:A:399:PRO:HD3	1.91	0.40
1:A:99:ILE:HG12	1:A:193:VAL:HG21	2.03	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:98:LYS:O	1:A:119:LEU:HD12	2.22	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:B:470:ASN:ND2	1:B:473:GLY:HA2	2.37	0.40
1:A:74:THR:OG1	1:A:190:THR:HG23	2.20	0.40
1:A:407:MET:HG2	2:B:637:HOH:O	2.20	0.40
1:B:153:ARG:HG3	2:B:572:HOH:O	2.21	0.40
1:A:358:LYS:NZ	1:B:295:ASP:OD2	2.42	0.40
1:B:67:SER:HB3	1:B:93:ARG:NH2	2.37	0.40
1:A:301:ARG:HA	1:A:301:ARG:HD3	1.96	0.40
1:A:78:PHE:O	1:A:79:SER:C	2.59	0.40
1:B:109:ARG:HE	1:B:110:PRO:CD	2.10	0.40
1:B:138:LEU:N	1:B:138:LEU:HD12	2.36	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:354:ILE:CD1	1:B:355:LYS:N	2.85	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	7
1	B	477/522 (91%)	364 (76%)	78 (16%)	35 (7%)	1	7
All	All	939/1044 (90%)	720 (77%)	149 (16%)	70 (8%)	1	7

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	10
1	B	437/472 (93%)	374 (86%)	63 (14%)	3	15
All	All	865/944 (92%)	729 (84%)	136 (16%)	2	12

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 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.