



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID : 1NYR  
Title : Structure of Staphylococcus aureus threonyl-tRNA synthetase complexed with ATP  
Authors : Torres-Larios, A.; Sankaranarayanan, R.; Rees, B.; Dock-Bregeon, A.C.; Moras, D.  
Deposited on : 2003-02-13  
Resolution : 2.80 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

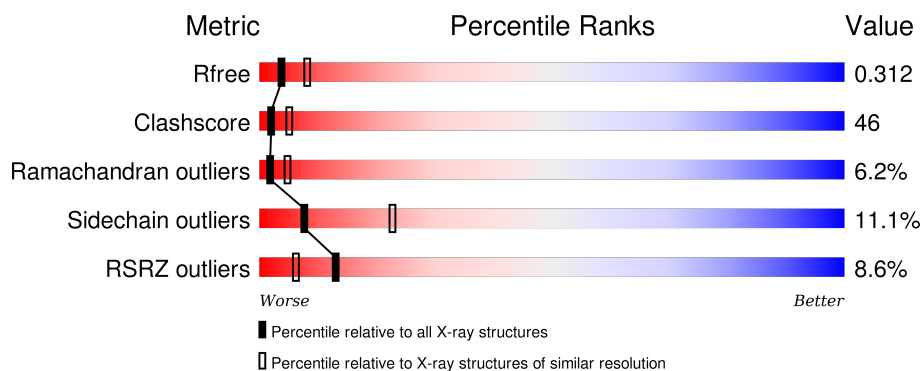
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	645	
1	B	645	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	THR	A	1004	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10684 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.

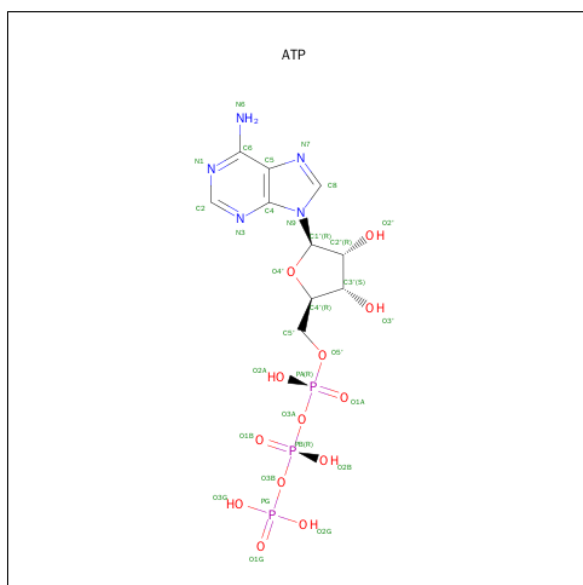
- Molecule 1 is a protein called threonyl-tRNA synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5216	3296	894	1003	23			
1	B	637	Total	C	N	O	S	0	0	0
			5171	3265	888	994	24			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

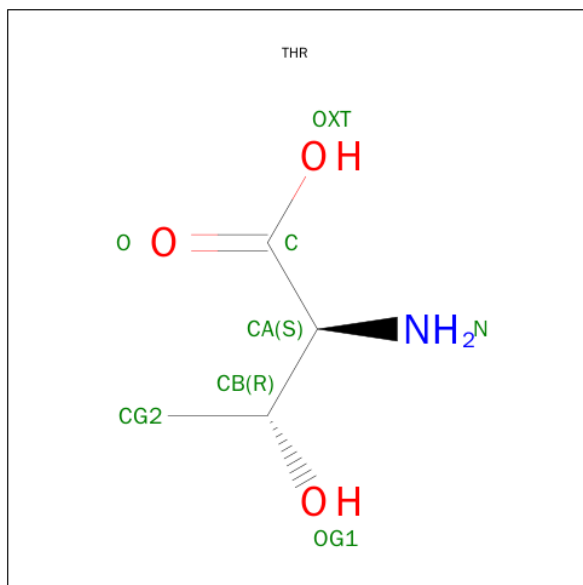
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is THREONINE (three-letter code: THR) (formula:  $C_4H_9NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

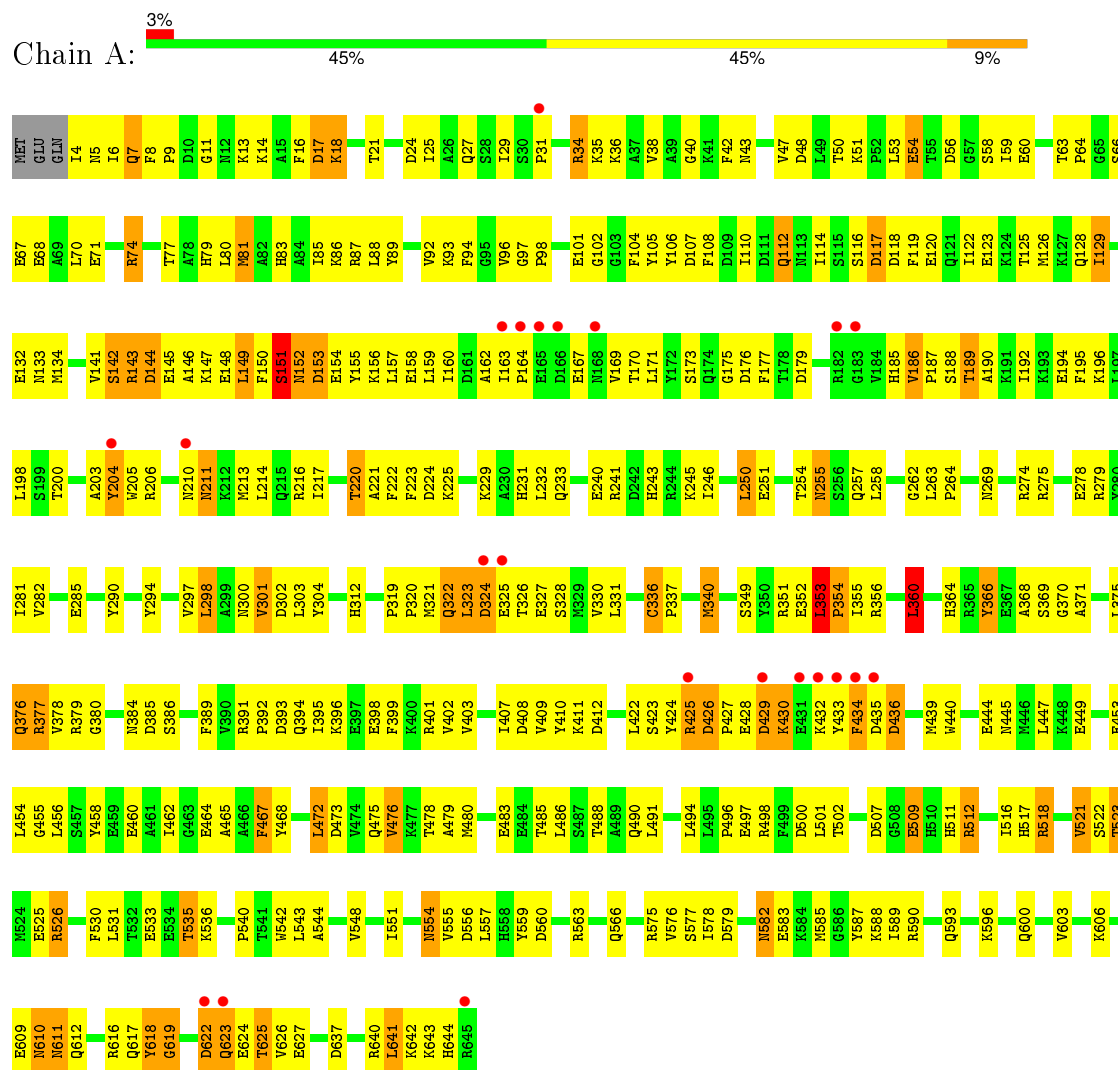
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	97	Total	O	0	0
			97	97		

### 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.

#### • Molecule 1: threonyl-tRNA synthetase 1



Y618	G619	S620	Q621	D622	Q623	E624	T625	V626	E627	K628	L632	K633	N634	L635	V636	D637	E638	L641	K642	K643	H644	R645																																								
V555	D556	L557	H558	Y559	D560	Y561	A562	R563	Q564	L565	Q566	D567	E568	L569	S570	Q571	Q572	G573	V574	H575	V576	S577	I578	D579	D580																																					
Q490	L491	D492	F493	L494	L495	P496	E497	R498	F499	D500	L501	T502	Y503	Q504	D505	G506	E507	H508	H509	R510	H511	R512	P513	V514	V515	I516	H517	R518	G519	V520	V521	S522	T523	E524	R525	E526	F527	F528	L529	T530	L531	T532	E533	E534	T535	K536	G537	A538	G539	D540	K541	D542	E543	A544	P545	V546	V547	V548	Q549	I550	V551	D552
D429	K430	E431	K432	F433	A434	D435	D436	D437	D438	M439	M440	M441	K442	A443	E444	M445	M446	L447	K448	E449	A450	A451	D452	E453	L454	G455	L456	G457	Y458	Y459	E460	A461	I462	E463	E464	A465	A466	F467	Y468	G469	P470	K471	L472	D473	V474	Q475	V476	K477	T478	A479	M480	E481	E482	E483	E484	T485	L486	S487	T488	A489		
Y366	E367	A368	S369	G370	A371	V372	S373	G374	L375	Q376	K377	V378	I383	I384	D385	S386	H387	I388	F389	V390	R391	P392	D393	Q394	I395	K396	E397	E398	E399	K400	R401	V402	V403	M404	M405	T406	I407	D408	V409	Y410	K411	D412	F413	G414	F415	E416	D417	S418	S419	F420	R421	L422	S423	Y424	R425	D426	P427	E428				
G207	D208	S209	N210	N211	K212	M213	L214	Q215	R216	Y217	T220	A221	D224	K225	K229	M234	L235	E236	E237	R238	R241	D242	H243	R244	K245	L246	E249	L250	E251	L252	F253	T254	N255	S256	P257	L258	V259	G260	A261	G262	W266	L267	P268	N269	G270	R274	R275	E276	I277	E278	R279											
Y280	M288	P296	V297	L298	A299	N300	V301	D302	L303	Y304	S307	G308	H309	H312	Y313	Q314	E315	D316	M317	F318	P319	M320	M321	Q322	L323	Q324	E325	T326	E327	S328	M329	P333	M334	N335	C336	P337	H338	H339	M340	S349	Y350	R351	E352	L353	P354	R355	R356	L360	M363	H364	R365											
A146	K147	E148	L149	PHE	SER	ASN	ASP	GLU	TYR	LYS	LEU	E158	L159	I160	D161	A162	I163	P164	E165	D166	E167	N168	V169	T170	L171	Y172	S173	Q174	G175	D176	F177	T178	D179	L180	C181	R182	G183	V184	H185	V186	P187	S188	T189	A190	K191	I192	K193	E194	F195	K196	S199	T200	K201	G202	A203	Y204	R205	D206				
M81	A82	H83	A84	I85	K86	H87	L88	Y89	G90	N91	V92	K93	F94	P98	V99	I100	E101	F104	Y105	Y106	D107	F108	D109	I110	D111	Q112	Q113	I114	S115	S116	D117	D118	F119	I122	E123	K124	T125	M126	S127	Q128	I129	V130	N131	E132	N133	I136	E137	R138	K139	V140	V141	S142	R143	D144	E145							

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.13Å 122.52Å 148.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.80) 98.8 (14.99-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.313 0.239 , 0.312	Depositor DCC
$R_{free}$ test set	2311 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 80.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46622 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP

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	0.59	0/5325	0.84	11/7182 (0.2%)
1	B	0.51	0/5277	0.75	4/7115 (0.1%)
All	All	0.56	0/10602	0.80	15/14297 (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	B	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	353	LEU	C-N-CA	-6.53	94.58	122.00
1	A	557	LEU	CA-CB-CG	6.33	129.85	115.30
1	A	353	LEU	N-CA-C	6.28	127.95	111.00
1	A	619	GLY	N-CA-C	6.12	128.40	113.10
1	A	353	LEU	C-N-CD	5.72	140.41	128.40
1	A	425	ARG	N-CA-C	5.64	126.22	111.00
1	B	447	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	360	LEU	N-CA-C	-5.52	96.11	111.00
1	A	472	LEU	N-CA-C	-5.49	96.17	111.00
1	A	625	THR	N-CA-C	-5.48	96.20	111.00
1	B	355	ILE	N-CA-C	5.31	125.33	111.00
1	A	275	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	360	LEU	N-CA-C	-5.13	97.14	111.00
1	B	415	PHE	N-CA-C	5.08	124.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	PRO	N-CA-C	-5.07	98.93	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	TYR	Sidechain
1	B	418	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	5216	0	5104	386	0
1	B	5171	0	5067	567	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	3	0
3	B	31	0	12	3	0
4	A	8	0	5	4	0
4	B	8	0	5	2	0
5	A	119	0	0	9	0
5	B	97	0	0	15	0
All	All	10684	0	10205	952	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (952) 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:A:426:ASP:HB3	1:A:427:PRO:HD2	1.31	1.11
1:B:518:ARG:HG3	1:B:518:ARG:HH11	1.12	1.09
1:B:471:LYS:HB3	1:B:490:GLN:HB3	1.32	1.09
1:B:606:LYS:HA	1:B:609:GLU:HB2	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:HG2	1:A:435:ASP:HB3	1.34	1.05
1:A:322:GLN:HG3	1:A:323:LEU:H	1.18	1.04
1:B:82:ALA:HB2	1:B:106:TYR:HE1	1.21	1.03
1:A:449:GLU:O	1:A:453:GLU:HG3	1.62	1.00
1:B:353:LEU:O	1:B:353:LEU:HD13	1.63	0.97
1:B:82:ALA:HB2	1:B:106:TYR:CE1	1.97	0.97
1:B:589:ILE:H	1:B:589:ILE:HD12	1.28	0.97
1:B:6:ILE:HD13	1:B:25:ILE:HD11	1.47	0.96
1:B:418:TYR:H	1:B:418:TYR:HD2	1.12	0.94
1:B:444:GLU:HB2	1:B:448:LYS:HE2	1.49	0.93
1:B:410:TYR:OH	1:B:486:LEU:HD23	1.69	0.92
1:B:430:LYS:NZ	1:B:497:GLU:HG3	1.87	0.90
1:B:616:ARG:NH1	1:B:622:ASP:HB3	1.86	0.90
1:B:354:PRO:HG3	1:B:394:GLN:HE22	1.36	0.88
1:A:371:ALA:HB1	1:A:377:ARG:HD3	1.53	0.88
1:A:94:PHE:HB2	1:A:156:LYS:HE3	1.54	0.88
1:B:349:SER:OG	1:B:351:ARG:HG3	1.73	0.88
1:B:446:MET:HA	1:B:449:GLU:HG3	1.56	0.88
1:A:110:ILE:HD12	1:A:114:ILE:HD11	1.53	0.87
1:A:319:PRO:HG2	1:B:321:MET:HB2	1.55	0.87
1:B:465:ALA:HA	1:B:471:LYS:HE2	1.56	0.87
1:A:158:GLU:HB3	1:A:206:ARG:NH2	1.90	0.87
1:A:322:GLN:CG	1:A:323:LEU:H	1.85	0.86
1:A:322:GLN:HG3	1:A:323:LEU:N	1.90	0.86
1:B:617:GLN:HE22	1:B:645:ARG:HD3	1.39	0.86
1:B:592:ALA:HB3	1:B:600:GLN:HE21	1.40	0.86
1:A:322:GLN:HG2	1:A:327:GLU:HB2	1.55	0.86
1:A:554:ASN:HD21	1:A:556:ASP:HB2	1.38	0.86
1:A:428:GLU:CG	1:A:435:ASP:HB3	2.05	0.86
1:B:428:GLU:HB3	1:B:440:TRP:HE1	1.40	0.86
1:B:337:PRO:HG2	5:B:2007:HOH:O	1.75	0.86
1:B:406:ILE:HD11	1:B:487:SER:OG	1.74	0.85
1:B:442:LYS:NZ	1:B:446:MET:HB2	1.90	0.85
1:B:4:ILE:HG22	1:B:16:PHE:O	1.76	0.85
1:B:422:LEU:HD22	1:B:448:LYS:HG2	1.59	0.85
1:A:554:ASN:HD22	1:A:556:ASP:H	1.25	0.84
1:B:490:GLN:HG3	1:B:517:HIS:HB2	1.60	0.83
1:B:426:ASP:CG	1:B:427:PRO:HD2	1.98	0.83
1:A:426:ASP:HB3	1:A:427:PRO:CD	2.09	0.83
1:A:616:ARG:NH1	1:A:619:GLY:H	1.77	0.82
1:B:80:LEU:HG	1:B:126:MET:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:GLN:HE21	1:B:623:GLN:HG2	1.44	0.82
1:B:544:ALA:O	1:B:575:ARG:NH1	2.13	0.82
1:A:523:THR:HG22	1:A:526:ARG:HB3	1.59	0.82
1:A:554:ASN:ND2	1:A:556:ASP:HB2	1.94	0.82
1:B:429:ASP:HB3	1:B:494:LEU:HD21	1.61	0.82
1:B:585:MET:SD	1:B:589:ILE:HD11	2.20	0.82
1:B:169:VAL:HG12	1:B:170:THR:H	1.42	0.82
1:B:212:LYS:H	1:B:212:LYS:HD2	1.43	0.81
1:B:643:LYS:HG2	1:B:644:HIS:H	1.44	0.81
1:B:450:ALA:HA	1:B:453:GLU:HG2	1.62	0.81
1:B:500:ASP:HA	1:B:512:ARG:NH2	1.96	0.81
1:A:70:LEU:O	1:A:74:ARG:HG3	1.81	0.81
1:B:163:ILE:H	1:B:164:PRO:HD3	1.46	0.80
1:B:443:ALA:O	1:B:447:LEU:HB2	1.81	0.80
1:A:246:ILE:HG23	1:A:250:LEU:HD22	1.64	0.80
1:B:354:PRO:HG3	1:B:394:GLN:NE2	1.97	0.80
1:B:340:MET:HE3	1:B:495:LEU:HD13	1.64	0.79
1:B:85:ILE:HG22	1:B:92:VAL:HG21	1.64	0.79
1:B:261:ALA:HB1	1:B:372:VAL:HG11	1.65	0.79
1:B:403:VAL:O	1:B:403:VAL:HG12	1.81	0.79
1:B:323:LEU:HD12	1:B:329:MET:HG3	1.63	0.79
1:B:390:VAL:HG12	1:B:391:ARG:H	1.46	0.79
1:A:436:ASP:HB3	1:A:439:MET:HB3	1.64	0.79
1:A:5:ASN:H	1:A:56:ASP:HB3	1.48	0.78
1:B:84:ALA:HB2	1:B:126:MET:HB3	1.66	0.78
1:B:523:THR:CG2	1:B:526:ARG:H	1.96	0.78
1:B:507:ASP:O	1:B:509:GLU:HG2	1.83	0.78
1:B:445:ASN:O	1:B:449:GLU:HG2	1.83	0.78
1:B:89:TYR:CD2	1:B:92:VAL:HG11	2.19	0.78
1:A:153:ASP:HB3	1:A:156:LYS:HB2	1.66	0.77
1:B:336:CYS:HA	1:B:387:HIS:CE1	2.19	0.77
1:A:132:GLU:OE1	1:A:134:MET:HE2	1.84	0.77
1:A:440:TRP:O	1:A:444:GLU:HG3	1.84	0.77
1:B:606:LYS:HA	1:B:609:GLU:CB	2.11	0.77
1:A:340:MET:HG3	1:A:501:LEU:HD11	1.66	0.77
1:A:141:VAL:HB	1:A:145:GLU:HB2	1.67	0.77
1:A:610:ASN:HB2	1:A:612:GLN:NE2	2.00	0.77
1:B:474:VAL:HG21	1:B:487:SER:HB2	1.65	0.77
1:A:337:PRO:HG2	5:A:1009:HOH:O	1.85	0.76
1:B:443:ALA:O	1:B:470:PRO:HG3	1.85	0.76
1:B:446:MET:HA	1:B:449:GLU:CG	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:CD1	1:A:114:ILE:HD11	2.15	0.76
1:B:340:MET:CE	1:B:495:LEU:HD13	2.16	0.76
1:B:85:ILE:HB	5:B:2021:HOH:O	1.84	0.76
1:B:106:TYR:HB3	1:B:108:PHE:CE1	2.21	0.75
1:A:93:LYS:HD3	1:A:155:TYR:HE1	1.50	0.75
1:B:114:ILE:HD12	1:B:217:ILE:HD11	1.66	0.75
1:B:430:LYS:HZ2	1:B:497:GLU:HG3	1.52	0.75
1:B:126:MET:O	1:B:130:VAL:HG23	1.87	0.75
1:B:161:ASP:O	1:B:164:PRO:HD3	1.86	0.75
1:B:55:THR:OG1	1:B:56:ASP:N	2.21	0.74
1:B:604:GLY:H	1:B:607:GLU:HB2	1.52	0.74
1:B:395:ILE:HD11	1:B:514:VAL:HG11	1.68	0.74
1:B:83:HIS:HE1	1:B:176:ASP:HB2	1.53	0.74
1:B:205:TRP:H	1:B:214:LEU:HG	1.52	0.74
1:B:169:VAL:HG12	1:B:170:THR:N	2.02	0.74
1:B:559:TYR:HE2	1:B:563:ARG:HG2	1.53	0.74
1:B:118:ASP:O	1:B:122:ILE:HG13	1.89	0.73
1:A:110:ILE:HG22	1:A:112:GLN:H	1.53	0.73
1:A:141:VAL:HG21	1:A:146:ALA:HB2	1.70	0.73
1:A:579:ASP:OD1	1:A:588:LYS:HG2	1.89	0.73
1:B:518:ARG:CG	1:B:518:ARG:HH11	1.94	0.73
1:A:27:GLN:HE22	1:A:31:PRO:HG3	1.53	0.73
1:B:471:LYS:CB	1:B:490:GLN:HB3	2.14	0.72
1:A:428:GLU:CG	1:A:440:TRP:HE1	2.02	0.72
1:A:152:ASN:N	1:A:152:ASN:HD22	1.86	0.72
1:B:422:LEU:HD23	1:B:447:LEU:HD12	1.71	0.72
1:B:523:THR:HG22	1:B:526:ARG:HB3	1.71	0.72
1:B:512:ARG:HH11	1:B:512:ARG:HG3	1.55	0.72
1:A:18:LYS:HG3	1:A:54:GLU:O	1.88	0.72
1:B:616:ARG:HH12	1:B:622:ASP:HB3	1.52	0.71
1:A:107:ASP:OD2	1:A:216:ARG:HB2	1.89	0.71
1:A:436:ASP:HB3	1:A:439:MET:CB	2.20	0.71
1:A:622:ASP:O	1:A:624:GLU:N	2.18	0.71
1:A:38:VAL:O	1:A:187:PRO:HD3	1.90	0.71
1:B:632:ILE:HD12	5:B:2070:HOH:O	1.91	0.71
1:B:420:PHE:CE2	1:B:474:VAL:HG22	2.26	0.70
1:B:68:GLU:HA	1:B:71:GLU:HG3	1.71	0.70
1:B:89:TYR:HD2	1:B:92:VAL:HG11	1.55	0.70
1:B:601:ILE:HD11	1:B:615:VAL:HG12	1.72	0.70
4:A:1004:THR:OXT	4:A:1004:THR:HG22	1.91	0.70
1:A:428:GLU:OE1	1:A:435:ASP:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:HG23	1:B:328:SER:O	1.92	0.69
1:A:428:GLU:HA	1:A:467:PHE:O	1.92	0.69
1:A:622:ASP:C	1:A:624:GLU:H	1.95	0.69
1:A:102:GLY:O	1:A:220:THR:HG23	1.92	0.69
1:B:47:VAL:HG23	1:B:48:ASP:O	1.93	0.69
1:B:31:PRO:O	1:B:35:LYS:HG3	1.93	0.69
1:B:100:ILE:HG13	1:B:104:PHE:HA	1.75	0.69
1:B:205:TRP:HB3	1:B:211:ASN:CG	2.13	0.69
1:A:427:PRO:O	1:A:467:PHE:HA	1.93	0.68
1:B:395:ILE:HD13	1:B:491:LEU:HD21	1.75	0.68
1:A:200:THR:HG22	1:A:217:ILE:HG12	1.74	0.68
1:B:390:VAL:HG12	1:B:394:GLN:HB2	1.76	0.68
1:B:396:LYS:O	1:B:400:LYS:HG3	1.94	0.68
1:B:174:GLN:HG2	1:B:177:PHE:HB3	1.76	0.68
1:A:298:LEU:H	1:A:298:LEU:HD12	1.59	0.68
1:B:66:SER:HB3	1:B:69:ALA:HB2	1.76	0.68
1:A:301:VAL:HG23	1:A:328:SER:O	1.94	0.68
1:A:66:SER:OG	1:A:68:GLU:HG3	1.94	0.68
1:A:186:VAL:HG22	1:A:187:PRO:HD2	1.76	0.67
1:A:97:GLY:HA3	1:A:106:TYR:CD2	2.29	0.67
1:B:644:HIS:O	1:B:645:ARG:HG3	1.93	0.67
1:B:98:PRO:HD2	1:B:105:TYR:CE1	2.29	0.67
1:A:554:ASN:ND2	1:A:556:ASP:H	1.90	0.67
1:B:163:ILE:H	1:B:164:PRO:CD	2.06	0.67
1:A:298:LEU:HD12	1:A:298:LEU:N	2.10	0.67
1:A:83:HIS:CE1	1:A:129:ILE:HD13	2.29	0.67
1:A:157:LEU:HA	1:A:160:ILE:HG22	1.77	0.67
1:B:390:VAL:HG12	1:B:391:ARG:N	2.09	0.67
1:B:376:GLN:OE1	1:B:478:THR:HB	1.95	0.67
1:B:596:LYS:HD3	1:B:618:TYR:CZ	2.30	0.67
1:A:384:ASN:HD22	1:A:521:VAL:H	1.43	0.67
1:B:589:ILE:N	1:B:589:ILE:HD12	2.06	0.67
1:B:430:LYS:HZ1	1:B:497:GLU:HG3	1.59	0.66
4:A:1004:THR:CG2	4:A:1004:THR:OXT	2.43	0.66
1:A:326:THR:HG22	1:A:327:GLU:HG3	1.77	0.66
1:B:119:PHE:CD1	1:B:122:ILE:HD12	2.30	0.66
1:B:485:THR:HB	5:B:2068:HOH:O	1.96	0.66
1:B:471:LYS:HA	1:B:490:GLN:HA	1.77	0.66
1:A:377:ARG:NH2	3:A:1003:ATP:O3G	2.29	0.66
1:B:262:GLY:N	1:B:372:VAL:HG13	2.10	0.66
1:A:410:TYR:OH	1:A:486:LEU:HD23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:N	1:B:164:PRO:CD	2.58	0.65
1:B:433:TYR:C	1:B:435:ASP:H	2.00	0.65
1:B:563:ARG:HG3	1:B:563:ARG:HH11	1.61	0.65
1:A:110:ILE:HD12	1:A:114:ILE:CD1	2.24	0.65
1:A:395:ILE:CG2	1:A:491:LEU:HD21	2.26	0.65
1:B:584:LYS:N	1:B:584:LYS:HD3	2.10	0.65
1:A:154:GLU:O	1:A:158:GLU:HG3	1.96	0.65
1:A:5:ASN:O	1:A:6:ILE:HD13	1.96	0.65
1:B:350:TYR:CE2	1:B:506:GLN:HA	2.32	0.65
1:B:119:PHE:HD1	1:B:122:ILE:HD12	1.60	0.65
1:B:643:LYS:HG2	1:B:644:HIS:N	2.12	0.65
1:B:167:GLU:C	1:B:168:ASN:HD22	1.99	0.65
1:A:87:ARG:NE	1:A:176:ASP:OD2	2.29	0.65
1:A:34:ARG:HG3	1:A:35:LYS:N	2.13	0.64
1:A:476:VAL:HG13	1:A:530:PHE:CE1	2.31	0.64
1:A:118:ASP:O	1:A:122:ILE:HG13	1.97	0.64
1:B:428:GLU:HB3	1:B:440:TRP:NE1	2.12	0.64
1:B:133:ASN:HA	1:B:190:ALA:HB2	1.79	0.64
1:B:6:ILE:HD12	1:B:16:PHE:CD1	2.33	0.64
1:B:3:GLN:O	1:B:4:ILE:HB	1.98	0.64
1:A:518:ARG:HD3	1:A:518:ARG:C	2.17	0.64
1:A:322:GLN:CG	1:A:323:LEU:N	2.51	0.64
1:B:492:ASP:OD1	1:B:495:LEU:HD12	1.98	0.63
1:B:554:ASN:HB3	1:B:557:LEU:HB2	1.80	0.63
1:B:621:GLN:NE2	1:B:623:GLN:HG2	2.12	0.63
1:A:157:LEU:O	1:A:160:ILE:HG22	1.99	0.63
1:B:420:PHE:O	1:B:421:ARG:HB3	1.98	0.63
1:A:616:ARG:HH12	1:A:619:GLY:H	1.45	0.63
1:B:236:GLU:C	1:B:238:ARG:H	2.02	0.63
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.64	0.63
1:B:75:HIS:HB2	1:B:99:VAL:HG22	1.81	0.63
1:B:129:ILE:O	1:B:132:GLU:HB2	1.98	0.63
1:B:146:ALA:C	1:B:148:GLU:H	2.02	0.63
1:A:153:ASP:O	1:A:157:LEU:HB2	1.99	0.63
1:B:242:ASP:OD1	1:B:244:ARG:HB2	1.97	0.63
1:A:17:ASP:N	1:A:17:ASP:OD2	2.31	0.63
1:B:616:ARG:HG2	1:B:616:ARG:O	1.99	0.62
1:A:96:VAL:O	1:A:98:PRO:HD3	1.99	0.62
1:A:143:ARG:O	1:A:144:ASP:HB2	1.98	0.62
1:B:507:ASP:O	1:B:509:GLU:N	2.32	0.62
1:B:565:LEU:CD2	1:B:601:ILE:HG21	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:SER:O	1:B:488:THR:HB	1.99	0.62
1:B:83:HIS:CE1	1:B:176:ASP:HB2	2.33	0.62
1:B:407:ILE:HG23	1:B:408:ASP:OD2	2.00	0.62
1:A:323:LEU:HG	1:A:326:THR:HB	1.80	0.62
1:A:155:TYR:O	1:A:159:LEU:HB2	1.99	0.62
1:A:5:ASN:O	1:A:56:ASP:HB2	2.00	0.62
1:B:403:VAL:CG1	1:B:403:VAL:O	2.48	0.62
1:A:5:ASN:N	1:A:56:ASP:HB3	2.15	0.62
1:B:402:VAL:O	1:B:406:ILE:HG22	2.00	0.62
1:A:158:GLU:HB3	1:A:206:ARG:HH21	1.63	0.62
1:A:14:LYS:HE3	1:A:16:PHE:CZ	2.35	0.62
1:A:433:TYR:CG	1:A:434:PHE:N	2.68	0.62
1:A:303:LEU:HD21	1:A:337:PRO:HB2	1.82	0.61
1:A:473:ASP:HB3	1:A:485:THR:HG23	1.80	0.61
1:B:74:ARG:C	1:B:76:SER:H	2.04	0.61
1:B:288:MET:HE3	1:B:405:MET:HB2	1.81	0.61
1:A:500:ASP:OD1	1:A:512:ARG:NH2	2.31	0.61
1:B:205:TRP:HB3	1:B:211:ASN:ND2	2.15	0.61
1:B:288:MET:SD	1:B:405:MET:SD	2.98	0.61
1:A:105:TYR:HA	1:A:217:ILE:O	2.00	0.61
1:B:234:MET:SD	1:B:234:MET:C	2.78	0.61
1:A:353:LEU:O	1:A:355:ILE:N	2.34	0.61
1:B:159:LEU:HD11	1:B:162:ALA:HB3	1.82	0.61
1:A:303:LEU:CD2	1:A:337:PRO:HB2	2.31	0.61
1:A:297:VAL:O	1:A:297:VAL:HG22	2.00	0.61
1:B:105:TYR:HA	1:B:217:ILE:O	2.00	0.61
1:B:7:GLN:O	1:B:58:SER:HA	2.00	0.61
1:A:141:VAL:CG2	1:A:146:ALA:HB2	2.31	0.61
1:B:143:ARG:N	1:B:168:ASN:HB3	2.16	0.60
1:B:386:SER:HB3	1:B:518:ARG:HG2	1.83	0.60
1:A:246:ILE:CG2	1:A:250:LEU:HD22	2.31	0.60
1:A:488:THR:O	1:A:518:ARG:HA	2.01	0.60
1:B:317:MET:HG2	1:B:333:PRO:HB3	1.84	0.60
1:B:612:GLN:HG2	1:B:627:GLU:HA	1.82	0.60
1:B:518:ARG:HG3	1:B:518:ARG:NH1	1.94	0.60
1:A:554:ASN:HD22	1:A:556:ASP:N	1.97	0.60
1:B:80:LEU:CG	1:B:126:MET:HB2	2.31	0.60
1:A:433:TYR:CE2	1:A:434:PHE:HB2	2.37	0.60
1:B:478:THR:HG21	1:B:484:GLU:HG3	1.84	0.59
1:B:304:TYR:HA	1:B:307:SER:HG	1.67	0.59
1:B:589:ILE:CD1	1:B:589:ILE:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:N	1:A:428:GLU:OE2	2.35	0.59
1:B:447:LEU:HD11	1:B:471:LYS:O	2.02	0.59
1:B:442:LYS:HZ2	1:B:446:MET:HB2	1.63	0.59
1:B:406:ILE:HD11	1:B:487:SER:CB	2.31	0.59
1:A:392:PRO:HD2	5:A:1025:HOH:O	2.02	0.59
1:B:430:LYS:HB3	1:B:436:ASP:HB2	1.84	0.59
1:B:312:HIS:HD2	1:B:427:PRO:HB2	1.67	0.59
1:B:453:GLU:O	1:B:454:LEU:HD13	2.03	0.59
1:A:433:TYR:CD2	1:A:434:PHE:N	2.70	0.59
1:B:27:GLN:OE1	1:B:34:ARG:HD3	2.02	0.59
1:A:321:MET:O	1:A:322:GLN:HB2	2.03	0.59
1:A:523:THR:CG2	1:A:526:ARG:H	2.16	0.59
1:B:454:LEU:HD22	1:B:454:LEU:N	2.18	0.59
1:A:257:GLN:HG3	1:A:258:LEU:H	1.66	0.59
1:A:158:GLU:HB3	1:A:206:ARG:HH22	1.66	0.58
1:B:254:THR:HG23	1:B:267:LEU:HD11	1.85	0.58
1:A:399:PHE:O	1:A:403:VAL:HG23	2.02	0.58
1:B:80:LEU:HD11	1:B:129:ILE:HG21	1.84	0.58
1:A:85:ILE:HD11	1:A:122:ILE:HD13	1.85	0.58
1:B:107:ASP:OD2	1:B:216:ARG:HB2	2.03	0.58
1:A:241:ARG:HD2	1:A:536:LYS:NZ	2.18	0.58
1:A:428:GLU:CB	1:A:440:TRP:HE1	2.16	0.58
1:A:324:ASP:C	1:A:326:THR:H	2.06	0.58
1:B:110:ILE:HG22	1:B:111:ASP:N	2.19	0.58
1:B:125:THR:C	1:B:127:LYS:H	2.06	0.58
1:A:445:ASN:HB3	5:A:1031:HOH:O	2.03	0.58
1:B:82:ALA:CB	1:B:106:TYR:HE1	2.07	0.58
1:B:114:ILE:CD1	1:B:217:ILE:HD11	2.33	0.58
1:A:585:MET:HG3	1:A:589:ILE:HD13	1.85	0.58
1:A:478:THR:CG2	1:A:479:ALA:N	2.67	0.58
1:A:582:ASN:HD22	1:A:582:ASN:C	2.04	0.58
1:A:152:ASN:N	1:A:152:ASN:ND2	2.52	0.58
1:B:430:LYS:HG2	1:B:436:ASP:OD1	2.03	0.58
1:B:300:ASN:HD21	1:B:327:GLU:CD	2.06	0.58
1:A:196:LYS:HD3	1:A:232:LEU:HD11	1.85	0.58
1:A:143:ARG:H	1:A:169:VAL:HG22	1.67	0.57
1:B:262:GLY:N	1:B:372:VAL:CG1	2.67	0.57
1:A:7:GLN:HG2	1:A:13:LYS:CD	2.33	0.57
1:A:324:ASP:O	1:A:326:THR:N	2.37	0.57
1:B:82:ALA:HB1	1:B:177:PHE:CZ	2.38	0.57
1:B:425:ARG:HD2	1:B:425:ARG:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:O	1:A:323:LEU:HG	2.03	0.57
1:B:522:SER:OG	1:B:523:THR:N	2.36	0.57
1:B:488:THR:O	1:B:518:ARG:HA	2.04	0.57
1:B:441:ASN:O	1:B:445:ASN:ND2	2.38	0.57
1:B:606:LYS:CA	1:B:609:GLU:HB2	2.20	0.57
1:B:56:ASP:C	1:B:56:ASP:OD2	2.42	0.57
1:B:395:ILE:CD1	1:B:514:VAL:HG11	2.34	0.57
1:A:87:ARG:HH21	1:A:176:ASP:CB	2.16	0.57
1:B:404:ASN:O	1:B:407:ILE:CG2	2.52	0.57
1:B:182:ARG:HD2	1:B:182:ARG:N	2.20	0.57
1:B:105:TYR:HD1	1:B:106:TYR:N	2.03	0.57
1:B:169:VAL:CG1	1:B:170:THR:H	2.13	0.57
1:B:453:GLU:CB	1:B:454:LEU:HD22	2.34	0.57
1:A:454:LEU:HB3	1:A:456:LEU:HD13	1.87	0.57
1:A:531:LEU:O	1:A:535:THR:HB	2.04	0.57
1:B:429:ASP:O	1:B:430:LYS:HB2	2.04	0.57
1:A:427:PRO:O	1:A:467:PHE:O	2.22	0.57
1:A:323:LEU:O	1:A:324:ASP:O	2.23	0.57
1:B:422:LEU:HD23	1:B:447:LEU:CD1	2.35	0.56
1:A:4:ILE:N	1:A:16:PHE:O	2.39	0.56
1:B:604:GLY:O	1:B:608:VAL:HG23	2.05	0.56
1:B:404:ASN:O	1:B:407:ILE:HG22	2.04	0.56
1:B:353:LEU:CD1	1:B:353:LEU:O	2.45	0.56
1:A:110:ILE:HG22	1:A:112:GLN:N	2.20	0.56
1:A:399:PHE:O	1:A:402:VAL:CG1	2.52	0.56
1:B:570:LYS:C	1:B:572:GLN:H	2.08	0.56
1:A:617:GLN:O	1:A:618:TYR:C	2.43	0.56
1:A:423:SER:HB3	1:A:464:GLU:HB2	1.88	0.56
1:B:403:VAL:C	5:B:2026:HOH:O	2.43	0.56
1:B:83:HIS:ND1	1:B:177:PHE:HB2	2.21	0.56
1:A:304:TYR:HE2	1:A:337:PRO:HG3	1.70	0.56
1:B:565:LEU:HD21	1:B:601:ILE:HG21	1.87	0.56
1:B:601:ILE:HG22	1:B:601:ILE:O	2.03	0.56
1:A:566:GLN:NE2	1:A:578:ILE:HG13	2.21	0.56
1:B:86:LYS:O	1:B:86:LYS:HG2	2.05	0.56
1:B:386:SER:HB2	1:B:518:ARG:NH1	2.20	0.56
1:B:492:ASP:OD2	1:B:492:ASP:C	2.43	0.56
1:A:351:ARG:HH22	1:B:580:ASP:HB3	1.70	0.56
1:A:97:GLY:HA2	1:A:105:TYR:O	2.06	0.56
1:B:98:PRO:HD2	1:B:105:TYR:CZ	2.41	0.56
1:B:496:PRO:HG3	1:B:515:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:HIS:ND1	1:A:427:PRO:HB2	2.20	0.56
1:A:198:LEU:HD11	1:A:220:THR:OG1	2.05	0.56
1:A:163:ILE:N	1:A:164:PRO:HD3	2.21	0.56
1:A:436:ASP:CB	1:A:439:MET:HB3	2.34	0.55
1:A:122:ILE:O	1:A:126:MET:HG2	2.06	0.55
1:A:279:ARG:HH11	1:A:279:ARG:HG3	1.70	0.55
1:B:621:GLN:O	1:B:623:GLN:N	2.34	0.55
1:A:617:GLN:HG2	1:A:623:GLN:CD	2.27	0.55
1:B:229:LYS:HA	1:B:229:LYS:HE2	1.88	0.55
1:B:558:HIS:CD2	1:B:604:GLY:HA2	2.42	0.55
1:B:416:GLU:CD	1:B:416:GLU:O	2.44	0.55
1:A:254:THR:HG22	1:A:255:ASN:O	2.06	0.55
1:B:336:CYS:HB2	1:B:337:PRO:CD	2.35	0.55
1:A:428:GLU:HB3	1:A:440:TRP:HE1	1.71	0.55
1:B:338:HIS:HD2	5:B:2007:HOH:O	1.89	0.55
1:B:4:ILE:HG22	1:B:16:PHE:H	1.70	0.55
1:B:471:LYS:HD3	1:B:490:GLN:NE2	2.22	0.55
1:B:195:PHE:N	1:B:195:PHE:HD1	2.05	0.55
1:B:496:PRO:HG3	1:B:515:VAL:HG23	1.89	0.55
1:B:144:ASP:HA	1:B:147:LYS:HG3	1.89	0.55
1:B:520:VAL:HG12	1:B:521:VAL:N	2.21	0.55
1:B:490:GLN:CG	1:B:517:HIS:HB2	2.33	0.55
1:B:604:GLY:H	1:B:607:GLU:CB	2.18	0.55
1:A:214:LEU:N	1:A:214:LEU:HD12	2.22	0.55
1:A:399:PHE:O	1:A:402:VAL:HG13	2.07	0.55
1:A:81:MET:HE2	1:A:104:PHE:HE2	1.72	0.55
1:A:322:GLN:HB3	1:A:327:GLU:O	2.07	0.54
1:A:163:ILE:HG22	1:A:163:ILE:O	2.07	0.54
1:A:89:TYR:O	1:A:92:VAL:HG23	2.07	0.54
1:A:494:LEU:HD11	1:A:498:ARG:HD3	1.90	0.54
1:A:622:ASP:C	1:A:624:GLU:N	2.59	0.54
1:A:467:PHE:CD1	1:A:467:PHE:C	2.80	0.54
1:B:83:HIS:CG	1:B:177:PHE:HB2	2.43	0.54
1:B:195:PHE:N	1:B:195:PHE:CD1	2.75	0.54
1:B:621:GLN:O	1:B:623:GLN:HG3	2.07	0.54
1:B:110:ILE:HG22	1:B:111:ASP:H	1.71	0.54
1:B:592:ALA:HB3	1:B:600:GLN:NE2	2.19	0.54
1:B:303:LEU:HD11	1:B:337:PRO:HB2	1.88	0.54
1:A:152:ASN:H	1:A:152:ASN:ND2	2.05	0.54
1:B:548:VAL:O	1:B:576:VAL:HG23	2.07	0.54
1:B:436:ASP:OD2	1:B:438:ASP:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:C	1:A:159:LEU:H	2.11	0.54
1:B:100:ILE:HG22	1:B:101:GLU:N	2.22	0.54
1:B:440:TRP:CE3	1:B:440:TRP:HA	2.42	0.54
1:B:323:LEU:HD12	1:B:329:MET:CG	2.34	0.54
1:B:169:VAL:CG1	1:B:170:THR:N	2.71	0.54
1:B:523:THR:HG22	1:B:526:ARG:H	1.73	0.54
1:B:304:TYR:HA	1:B:307:SER:OG	2.08	0.54
1:A:150:PHE:O	1:A:157:LEU:HD13	2.07	0.54
1:B:442:LYS:HZ1	1:B:446:MET:HB2	1.71	0.54
1:B:312:HIS:O	1:B:314:GLN:N	2.41	0.54
1:B:41:LYS:HB3	1:B:60:GLU:HB2	1.88	0.54
1:B:535:THR:O	1:B:536:LYS:HB2	2.07	0.54
1:A:304:TYR:CE2	1:A:337:PRO:HG3	2.43	0.54
1:B:159:LEU:O	1:B:159:LEU:HD13	2.08	0.54
1:A:93:LYS:HD3	1:A:155:TYR:CE1	2.38	0.54
1:B:404:ASN:ND2	1:B:404:ASN:O	2.41	0.54
1:A:42:PHE:CD2	1:A:53:LEU:HD22	2.43	0.54
1:B:566:GLN:HG3	1:B:576:VAL:HG13	1.90	0.53
1:A:59:ILE:HG13	1:A:60:GLU:H	1.74	0.53
1:B:407:ILE:HG23	1:B:408:ASP:H	1.74	0.53
1:B:472:LEU:O	1:B:472:LEU:HG	2.07	0.53
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.23	0.53
1:B:339:HIS:ND1	1:B:387:HIS:ND1	2.53	0.53
1:B:426:ASP:OD2	1:B:427:PRO:HD2	2.08	0.53
1:B:146:ALA:O	1:B:148:GLU:N	2.40	0.53
1:B:274:ARG:O	1:B:278:GLU:HG3	2.08	0.53
1:B:125:THR:C	1:B:127:LYS:N	2.59	0.53
1:B:200:THR:O	1:B:201:ALA:O	2.26	0.53
1:A:521:VAL:HG13	1:A:521:VAL:O	2.08	0.53
1:A:395:ILE:HG21	1:A:491:LEU:HD21	1.90	0.53
1:A:43:ASN:ND2	1:A:58:SER:H	2.07	0.53
1:B:143:ARG:HB2	1:B:168:ASN:HA	1.90	0.53
1:B:436:ASP:OD2	1:B:439:MET:HG2	2.08	0.53
1:B:472:LEU:O	1:B:473:ASP:O	2.27	0.53
1:B:406:ILE:CD1	1:B:487:SER:HB3	2.38	0.53
1:A:323:LEU:CG	1:A:323:LEU:O	2.56	0.53
1:B:299:ALA:HB1	1:B:303:LEU:HD23	1.90	0.53
1:B:212:LYS:N	1:B:212:LYS:HD2	2.21	0.53
1:B:395:ILE:HD11	1:B:514:VAL:HG21	1.90	0.53
1:B:606:LYS:O	1:B:610:ASN:OD1	2.27	0.53
1:B:611:ASN:H	1:B:611:ASN:HD22	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASP:OD1	1:B:147:LYS:HE2	2.08	0.53
1:A:210:ASN:HD22	1:A:210:ASN:N	2.06	0.53
1:B:7:GLN:N	1:B:57:GLY:O	2.35	0.53
1:B:205:TRP:C	1:B:205:TRP:CE3	2.83	0.53
1:B:593:GLN:HG3	1:B:600:GLN:HE22	1.74	0.53
1:A:589:ILE:HG23	1:A:600:GLN:HE22	1.74	0.53
1:A:133:ASN:HD22	1:A:189:THR:HG22	1.73	0.53
1:B:139:LYS:HG2	1:B:140:VAL:N	2.23	0.53
1:A:123:GLU:HA	1:A:126:MET:HG2	1.91	0.52
1:B:391:ARG:HD3	1:B:503:TYR:CE2	2.44	0.52
1:A:59:ILE:HG13	1:A:60:GLU:N	2.25	0.52
1:A:86:LYS:HD3	1:A:177:PHE:HD1	1.74	0.52
1:B:540:PRO:HG2	1:B:543:LEU:HD12	1.91	0.52
1:A:368:ALA:HA	5:B:2010:HOH:O	2.09	0.52
1:A:264:PRO:HG3	1:A:375:LEU:HD23	1.90	0.52
1:A:455:GLY:O	1:A:456:LEU:HD12	2.09	0.52
1:B:532:THR:HG1	1:B:539:PHE:HZ	1.56	0.52
1:A:428:GLU:HG3	1:A:440:TRP:HE1	1.72	0.52
1:A:304:TYR:HE2	1:A:337:PRO:CG	2.21	0.52
1:B:407:ILE:HG23	1:B:408:ASP:N	2.25	0.52
1:B:323:LEU:CD1	1:B:329:MET:HG3	2.35	0.52
1:B:74:ARG:O	1:B:76:SER:N	2.42	0.52
1:B:641:LEU:O	1:B:642:LYS:HB2	2.10	0.52
1:A:386:SER:HB3	1:A:518:ARG:HD2	1.90	0.52
1:B:390:VAL:CG1	1:B:394:GLN:HB2	2.39	0.52
1:B:159:LEU:HD21	1:B:162:ALA:HB3	1.91	0.52
1:B:144:ASP:HA	1:B:147:LYS:HE2	1.92	0.52
1:B:542:TRP:CH2	1:B:543:LEU:HD21	2.45	0.52
1:B:521:VAL:O	1:B:522:SER:HB3	2.09	0.52
1:A:478:THR:HG22	1:A:479:ALA:N	2.24	0.52
1:B:428:GLU:HG2	1:B:429:ASP:N	2.25	0.52
1:B:617:GLN:NE2	1:B:645:ARG:HD3	2.16	0.51
1:A:433:TYR:CZ	1:A:434:PHE:HB2	2.45	0.51
1:B:404:ASN:C	1:B:407:ILE:HG22	2.30	0.51
1:B:444:GLU:HB2	1:B:448:LYS:CE	2.33	0.51
1:A:68:GLU:HA	1:A:71:GLU:HG3	1.92	0.51
1:B:251:GLU:O	1:B:269:ASN:HB2	2.10	0.51
1:B:80:LEU:HD11	1:B:129:ILE:CG2	2.41	0.51
1:A:544:ALA:O	1:A:575:ARG:NH1	2.43	0.51
1:A:490:GLN:O	1:A:516:ILE:HA	2.11	0.51
1:B:432:LYS:O	1:B:435:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:CD1	1:B:129:ILE:HD13	2.40	0.51
1:B:542:TRP:CZ2	1:B:543:LEU:HD21	2.46	0.51
1:B:335:ASN:HB2	1:B:385:ASP:OD1	2.11	0.51
1:A:157:LEU:C	1:A:159:LEU:N	2.63	0.51
1:B:564:GLN:O	1:B:568:GLU:HG3	2.11	0.51
1:A:7:GLN:HE22	1:A:11:GLY:HA2	1.76	0.51
1:A:424:TYR:C	1:A:462:ILE:HD12	2.31	0.50
1:B:213:MET:HE3	1:B:213:MET:HA	1.93	0.50
1:B:105:TYR:CD1	1:B:106:TYR:N	2.79	0.50
1:A:7:GLN:HG2	1:A:13:LYS:HD2	1.92	0.50
1:B:415:PHE:CZ	1:B:530:PHE:CE2	2.99	0.50
1:B:200:THR:O	1:B:200:THR:HG22	2.10	0.50
1:A:392:PRO:O	1:A:395:ILE:HG13	2.11	0.50
1:A:312:HIS:CE1	1:A:428:GLU:O	2.65	0.50
1:B:497:GLU:HA	1:B:512:ARG:HE	1.76	0.50
1:B:478:THR:O	1:B:480:MET:N	2.45	0.50
1:B:484:GLU:HB3	1:B:526:ARG:HD3	1.93	0.50
1:B:277:ILE:HD13	1:B:527:PHE:CD2	2.47	0.50
1:A:579:ASP:OD2	1:A:588:LYS:HE2	2.11	0.50
1:A:643:LYS:HG2	1:A:644:HIS:N	2.27	0.50
1:A:8:PHE:HB3	1:A:9:PRO:HD2	1.93	0.50
1:A:555:VAL:HG23	1:A:555:VAL:O	2.12	0.50
1:A:79:HIS:CD2	1:A:185:HIS:NE2	2.79	0.50
1:B:439:MET:HE1	1:B:494:LEU:HB2	1.94	0.50
1:B:499:PHE:HB3	1:B:501:LEU:HD21	1.93	0.50
1:A:156:LYS:HE2	1:A:179:ASP:OD2	2.12	0.50
1:B:299:ALA:CB	1:B:303:LEU:HD23	2.41	0.50
1:A:494:LEU:O	1:A:497:GLU:HB2	2.12	0.50
1:A:566:GLN:NE2	1:A:577:SER:HA	2.26	0.50
1:A:143:ARG:CZ	1:A:163:ILE:HG23	2.42	0.50
1:A:143:ARG:N	1:A:169:VAL:HG22	2.25	0.50
1:B:559:TYR:HE2	1:B:563:ARG:CG	2.22	0.50
1:A:67:GLU:O	1:A:71:GLU:HG2	2.12	0.50
1:B:254:THR:CG2	1:B:267:LEU:HD11	2.42	0.50
1:B:404:ASN:HD22	1:B:407:ILE:HG21	1.77	0.50
1:A:143:ARG:HD3	1:A:163:ILE:HG12	1.93	0.50
1:B:187:PRO:HD2	1:B:191:LYS:HD2	1.94	0.50
1:B:403:VAL:HA	1:B:406:ILE:HG22	1.94	0.50
1:B:503:TYR:HE1	1:B:512:ARG:O	1.95	0.50
1:A:153:ASP:CB	1:A:156:LYS:HB2	2.39	0.50
1:A:399:PHE:HE2	1:A:472:LEU:HD12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:HB2	1:B:266:TRP:HB2	1.92	0.50
1:B:550:ILE:CD1	1:B:565:LEU:HD23	2.42	0.49
1:A:525:GLU:H	1:A:525:GLU:CD	2.14	0.49
1:A:637:ASP:O	1:A:641:LEU:HB2	2.11	0.49
1:A:428:GLU:OE1	1:A:435:ASP:CB	2.59	0.49
1:B:312:HIS:CD2	1:B:427:PRO:HB2	2.47	0.49
1:B:163:ILE:HG12	1:B:163:ILE:O	2.12	0.49
1:A:274:ARG:O	1:A:278:GLU:HG3	2.13	0.49
1:A:426:ASP:CB	1:A:427:PRO:HD2	2.22	0.49
1:B:643:LYS:NZ	1:B:645:ARG:HD2	2.28	0.49
1:B:521:VAL:O	1:B:521:VAL:HG12	2.11	0.49
1:B:42:PHE:CB	1:B:47:VAL:HG11	2.42	0.49
1:B:419:SER:C	1:B:420:PHE:CD1	2.86	0.49
1:A:257:GLN:HG3	1:A:258:LEU:N	2.28	0.49
1:B:499:PHE:HB3	1:B:501:LEU:CD2	2.42	0.49
1:A:326:THR:HG22	1:A:327:GLU:CG	2.42	0.49
1:A:155:TYR:HD2	1:A:205:TRP:CE2	2.30	0.49
1:B:442:LYS:CE	1:B:446:MET:HB2	2.42	0.49
1:B:41:LYS:HD2	1:B:60:GLU:CD	2.32	0.49
1:B:7:GLN:HA	1:B:13:LYS:CB	2.43	0.49
1:B:443:ALA:HA	1:B:493:PHE:HE2	1.77	0.49
1:B:585:MET:CE	1:B:589:ILE:HD11	2.42	0.49
1:A:376:GLN:HE22	1:A:526:ARG:HD2	1.76	0.49
1:B:336:CYS:CA	1:B:387:HIS:CE1	2.94	0.49
1:B:545:PRO:O	1:B:575:ARG:HD2	2.12	0.49
1:B:550:ILE:HD13	1:B:565:LEU:HD23	1.95	0.49
1:A:194:GLU:HB2	1:A:222:PHE:O	2.12	0.49
1:B:386:SER:HB3	1:B:518:ARG:CG	2.43	0.49
1:B:171:LEU:HD21	1:B:178:THR:CG2	2.43	0.49
1:B:616:ARG:CZ	1:B:622:ASP:HB3	2.43	0.49
1:A:205:TRP:HB3	1:A:211:ASN:HB3	1.94	0.49
1:A:391:ARG:NH1	1:A:393:ASP:OD2	2.45	0.49
1:B:424:TYR:N	1:B:424:TYR:CD1	2.80	0.49
1:B:4:ILE:HG12	1:B:56:ASP:HB2	1.94	0.49
1:A:143:ARG:H	1:A:169:VAL:CG2	2.25	0.49
1:A:4:ILE:HG13	1:A:56:ASP:CA	2.42	0.49
1:A:583:GLU:HG3	1:A:587:TYR:CE2	2.47	0.49
1:B:391:ARG:HB2	1:B:394:GLN:HG3	1.95	0.48
1:A:194:GLU:OE2	1:A:225:LYS:HE3	2.12	0.48
1:A:540:PRO:HG2	1:A:543:LEU:HD12	1.95	0.48
1:B:610:ASN:N	1:B:610:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD11	1:A:169:VAL:HG11	1.95	0.48
1:A:593:GLN:HE22	1:A:616:ARG:NH1	2.11	0.48
1:B:521:VAL:O	1:B:521:VAL:CG1	2.60	0.48
1:A:385:ASP:OD2	1:A:386:SER:N	2.46	0.48
1:A:353:LEU:HD13	1:A:353:LEU:O	2.13	0.48
1:A:281:ILE:O	1:A:285:GLU:HG3	2.13	0.48
1:B:1:MET:O	1:B:2:GLU:HG2	2.13	0.48
1:B:494:LEU:CD1	1:B:498:ARG:HG3	2.44	0.48
1:A:110:ILE:C	1:A:112:GLN:H	2.16	0.48
1:A:616:ARG:NH1	1:A:619:GLY:N	2.56	0.48
1:B:125:THR:O	1:B:128:GLN:N	2.35	0.48
1:A:157:LEU:CA	1:A:160:ILE:HG22	2.42	0.48
1:B:59:ILE:H	1:B:59:ILE:HD12	1.78	0.48
1:B:173:SER:OG	1:B:174:GLN:N	2.47	0.48
1:B:262:GLY:CA	1:B:372:VAL:HG13	2.42	0.48
1:B:563:ARG:HG3	1:B:563:ARG:NH1	2.25	0.48
1:B:395:ILE:HD11	1:B:514:VAL:CG1	2.42	0.48
1:B:635:LEU:O	1:B:638:GLU:N	2.47	0.48
1:A:290:TYR:HA	1:A:356:ARG:HB2	1.95	0.48
1:A:263:LEU:O	1:B:296:PRO:HG2	2.14	0.48
1:A:596:LYS:HD3	1:A:618:TYR:CZ	2.48	0.48
1:B:241:ARG:HH22	1:B:536:LYS:HZ2	1.61	0.48
1:B:92:VAL:HB	1:B:110:ILE:CD1	2.43	0.48
1:B:277:ILE:HD13	1:B:527:PHE:HD2	1.78	0.48
1:B:561:TYR:HD2	1:B:603:VAL:CG1	2.26	0.48
1:A:262:GLY:O	1:A:263:LEU:HD23	2.13	0.48
1:A:396:LYS:HE2	1:A:449:GLU:HB2	1.96	0.48
1:A:319:PRO:HA	1:A:320:PRO:HD3	1.67	0.48
1:A:610:ASN:CB	1:A:612:GLN:NE2	2.73	0.48
1:A:517:HIS:HB3	4:A:1004:THR:OG1	2.14	0.48
1:B:229:LYS:CA	1:B:229:LYS:HE2	2.43	0.48
1:B:126:MET:HE2	1:B:195:PHE:HE2	1.79	0.48
1:B:536:LYS:O	1:B:596:LYS:NZ	2.47	0.48
1:A:389:PHE:N	1:A:389:PHE:CD1	2.81	0.48
1:A:384:ASN:ND2	1:A:521:VAL:H	2.09	0.48
1:A:409:VAL:O	1:A:412:ASP:HB2	2.14	0.48
1:B:180:LEU:HD23	1:B:180:LEU:C	2.34	0.48
1:B:622:ASP:O	1:B:623:GLN:C	2.52	0.48
1:A:610:ASN:O	1:A:611:ASN:C	2.51	0.48
1:A:38:VAL:HG21	1:A:223:PHE:HZ	1.79	0.48
1:A:222:PHE:HZ	1:A:231:HIS:CD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:O	1:A:35:LYS:HG3	2.14	0.47
1:A:38:VAL:HG21	1:A:223:PHE:CZ	2.49	0.47
1:B:439:MET:O	1:B:443:ALA:N	2.47	0.47
1:A:322:GLN:CG	1:A:327:GLU:HB2	2.35	0.47
1:B:585:MET:O	1:B:589:ILE:CD1	2.62	0.47
1:A:189:THR:HG21	5:A:1028:HOH:O	2.14	0.47
1:B:398:GLU:O	1:B:401:ARG:N	2.39	0.47
1:B:368:ALA:C	1:B:370:GLY:H	2.16	0.47
1:B:428:GLU:CD	1:B:428:GLU:H	2.18	0.47
1:B:472:LEU:O	1:B:472:LEU:CG	2.63	0.47
1:B:487:SER:HA	1:B:519:GLY:O	2.14	0.47
1:A:142:SER:O	1:A:143:ARG:HB3	2.13	0.47
1:B:386:SER:CB	1:B:518:ARG:NH1	2.78	0.47
1:B:559:TYR:HD2	1:B:559:TYR:C	2.18	0.47
1:A:589:ILE:HG22	1:A:590:ARG:N	2.29	0.47
1:A:63:THR:HB	1:A:64:PRO:HD2	1.96	0.47
1:A:143:ARG:HD3	1:A:163:ILE:CD1	2.44	0.47
1:B:433:TYR:C	1:B:435:ASP:N	2.63	0.47
1:A:616:ARG:HH12	1:A:619:GLY:N	2.11	0.47
1:A:353:LEU:HD22	1:A:353:LEU:HA	1.55	0.47
1:B:187:PRO:CG	1:B:191:LYS:HD2	2.43	0.47
1:B:174:GLN:HG3	1:B:174:GLN:O	2.14	0.47
1:B:7:GLN:HA	1:B:13:LYS:HB3	1.97	0.47
1:A:154:GLU:HG3	1:A:155:TYR:CD1	2.50	0.47
1:B:450:ALA:CA	1:B:453:GLU:HG2	2.41	0.47
1:A:54:GLU:OE1	1:A:54:GLU:HA	2.15	0.47
1:B:70:LEU:C	1:B:72:VAL:N	2.66	0.47
1:B:8:PHE:N	1:B:8:PHE:CD1	2.83	0.47
1:A:195:PHE:HA	1:A:221:ALA:HA	1.96	0.47
1:B:620:SER:O	1:B:621:GLN:C	2.53	0.47
1:B:604:GLY:N	1:B:607:GLU:HB2	2.26	0.47
1:B:136:ILE:HD12	1:B:136:ILE:N	2.28	0.47
1:B:204:TYR:HA	1:B:214:LEU:HG	1.96	0.47
1:B:476:VAL:CG1	1:B:484:GLU:HB2	2.45	0.47
1:B:75:HIS:CD2	1:B:75:HIS:O	2.68	0.47
1:B:8:PHE:C	1:B:10:ASP:H	2.17	0.47
1:B:196:LYS:O	1:B:220:THR:N	2.40	0.47
1:B:205:TRP:N	1:B:214:LEU:HG	2.25	0.47
1:B:181:CYS:SG	1:B:185:HIS:NE2	2.85	0.47
1:A:429:ASP:O	1:A:430:LYS:HB2	2.14	0.47
1:B:518:ARG:CG	1:B:518:ARG:NH1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLN:NE2	1:A:526:ARG:HD2	2.30	0.46
1:B:559:TYR:CD2	1:B:559:TYR:C	2.88	0.46
1:A:279:ARG:NH1	1:A:279:ARG:HG3	2.30	0.46
1:A:398:GLU:OE1	1:A:401:ARG:NH2	2.42	0.46
1:B:7:GLN:CB	1:B:13:LYS:HB3	2.45	0.46
1:B:644:HIS:O	1:B:645:ARG:CG	2.63	0.46
1:B:509:GLU:O	1:B:511:HIS:ND1	2.48	0.46
1:A:108:PHE:O	1:A:214:LEU:HB3	2.14	0.46
1:B:389:PHE:N	1:B:389:PHE:CD1	2.84	0.46
1:A:360:LEU:HB2	5:A:1088:HOH:O	2.16	0.46
1:B:241:ARG:NH2	1:B:536:LYS:HZ2	2.13	0.46
1:A:464:GLU:OE1	1:A:464:GLU:HA	2.15	0.46
1:B:210:ASN:ND2	1:B:210:ASN:O	2.48	0.46
1:B:129:ILE:HD11	1:B:189:THR:HG21	1.97	0.46
1:B:617:GLN:O	1:B:618:TYR:C	2.54	0.46
1:A:119:PHE:O	1:A:123:GLU:HB2	2.16	0.46
1:A:518:ARG:O	1:A:518:ARG:HD3	2.15	0.46
1:B:355:ILE:HG13	1:B:356:ARG:N	2.30	0.46
1:B:114:ILE:HD12	1:B:217:ILE:CD1	2.40	0.46
1:B:56:ASP:OD2	1:B:56:ASP:O	2.32	0.46
1:A:157:LEU:O	1:A:159:LEU:N	2.48	0.46
1:A:92:VAL:HG12	1:A:93:LYS:O	2.16	0.46
1:B:204:TYR:O	1:B:205:TRP:C	2.53	0.46
1:A:70:LEU:HD13	1:A:74:ARG:NH2	2.31	0.46
1:A:7:GLN:HG2	1:A:13:LYS:HD3	1.97	0.46
1:B:521:VAL:HG13	1:B:527:PHE:CD2	2.51	0.46
1:A:42:PHE:O	1:A:43:ASN:HB2	2.14	0.46
1:B:415:PHE:CZ	1:B:530:PHE:HE2	2.34	0.46
1:B:470:PRO:O	1:B:490:GLN:HB2	2.16	0.46
1:B:418:TYR:CD2	1:B:418:TYR:N	2.65	0.46
1:B:167:GLU:C	1:B:168:ASN:ND2	2.68	0.46
1:B:123:GLU:C	1:B:125:THR:H	2.19	0.46
1:A:467:PHE:CD1	1:A:468:TYR:N	2.84	0.46
1:B:474:VAL:O	1:B:485:THR:HA	2.16	0.46
1:B:42:PHE:HB3	1:B:47:VAL:HG11	1.97	0.46
1:B:146:ALA:C	1:B:148:GLU:N	2.69	0.46
1:B:159:LEU:CD1	1:B:162:ALA:HB3	2.45	0.46
1:B:515:VAL:O	1:B:515:VAL:HG12	2.14	0.46
1:B:471:LYS:HB2	1:B:472:LEU:H	1.59	0.46
1:B:598:PRO:HA	1:B:618:TYR:HB2	1.98	0.46
1:B:214:LEU:N	1:B:214:LEU:HD22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:O	1:A:458:TYR:CD2	2.68	0.46
1:B:390:VAL:CG1	1:B:391:ARG:H	2.23	0.45
1:B:420:PHE:CD2	1:B:474:VAL:HG22	2.51	0.45
1:B:74:ARG:C	1:B:76:SER:N	2.68	0.45
1:B:363:MET:HA	5:B:2022:HOH:O	2.15	0.45
1:A:428:GLU:O	1:A:435:ASP:OD2	2.35	0.45
1:B:430:LYS:HD3	1:B:439:MET:SD	2.56	0.45
1:A:40:GLY:O	1:A:47:VAL:HG22	2.16	0.45
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.86	0.45
1:B:394:GLN:O	1:B:396:LYS:N	2.49	0.45
1:B:616:ARG:NH1	1:B:622:ASP:CB	2.71	0.45
1:B:523:THR:HG22	1:B:526:ARG:CB	2.43	0.45
1:B:213:MET:HA	1:B:213:MET:CE	2.46	0.45
1:A:80:LEU:CD2	1:A:192:ILE:HG21	2.46	0.45
1:B:206:ARG:HG3	1:B:208:ASP:OD1	2.17	0.45
1:A:224:ASP:N	1:A:224:ASP:OD1	2.49	0.45
1:A:424:TYR:CE2	1:A:444:GLU:HB3	2.52	0.45
1:B:105:TYR:O	1:B:106:TYR:HB2	2.15	0.45
1:B:7:GLN:O	1:B:58:SER:CA	2.64	0.45
1:B:641:LEU:O	1:B:642:LYS:CB	2.62	0.45
1:B:439:MET:CE	1:B:494:LEU:HB2	2.46	0.45
1:B:80:LEU:CD1	1:B:129:ILE:HG21	2.46	0.45
1:A:526:ARG:NH2	3:A:1003:ATP:H2'	2.30	0.45
1:A:97:GLY:HA2	1:A:106:TYR:HA	1.99	0.45
1:A:210:ASN:ND2	1:A:210:ASN:N	2.64	0.45
1:B:194:GLU:OE1	1:B:225:LYS:HG3	2.17	0.45
1:B:88:LEU:O	1:B:88:LEU:HG	2.16	0.45
1:A:229:LYS:O	1:A:233:GLN:HG3	2.17	0.45
1:B:402:VAL:CG2	1:B:403:VAL:N	2.79	0.45
1:B:443:ALA:O	1:B:447:LEU:CB	2.59	0.45
1:A:423:SER:HB3	1:A:464:GLU:CB	2.46	0.45
1:A:523:THR:HG21	3:A:1003:ATP:N3	2.32	0.45
1:B:607:GLU:C	5:B:2040:HOH:O	2.54	0.45
1:A:282:VAL:CG2	1:A:360:LEU:HD21	2.46	0.45
1:A:282:VAL:CG2	1:A:360:LEU:CD2	2.95	0.45
1:A:498:ARG:HG2	1:A:498:ARG:H	1.47	0.45
1:B:395:ILE:HD13	1:B:491:LEU:CD2	2.46	0.45
1:A:476:VAL:CG1	1:A:530:PHE:CE1	2.99	0.45
1:A:606:LYS:CE	1:A:625:THR:HG21	2.47	0.45
1:A:349:SER:O	1:A:352:GLU:HG2	2.17	0.45
1:B:406:ILE:CD1	1:B:487:SER:CB	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:MET:CA	1:B:126:MET:HE3	2.47	0.45
1:A:142:SER:O	1:A:143:ARG:CB	2.64	0.45
1:B:569:LEU:HD22	1:B:574:VAL:HG21	1.98	0.45
1:B:587:TYR:CD1	1:B:587:TYR:C	2.90	0.45
1:B:597:ILE:O	1:B:597:ILE:HG22	2.17	0.45
1:B:113:ASN:O	1:B:114:ILE:HG23	2.17	0.45
1:B:589:ILE:O	1:B:600:GLN:NE2	2.50	0.45
1:A:6:ILE:O	1:A:13:LYS:HA	2.17	0.45
1:A:473:ASP:HB3	1:A:475:GLN:NE2	2.32	0.45
1:A:606:LYS:HE3	1:A:625:THR:HG21	1.99	0.45
1:A:364:HIS:CD2	1:A:380:GLY:HA2	2.52	0.45
1:A:321:MET:O	1:A:321:MET:CG	2.64	0.44
1:B:82:ALA:HB2	1:B:106:TYR:CD1	2.50	0.44
1:B:561:TYR:CD2	1:B:608:VAL:HG22	2.53	0.44
1:B:70:LEU:C	1:B:72:VAL:H	2.21	0.44
1:B:595:GLN:HB3	1:B:597:ILE:HD13	1.98	0.44
1:B:439:MET:O	1:B:443:ALA:HB2	2.17	0.44
1:B:494:LEU:HD12	1:B:498:ARG:HG3	1.99	0.44
1:B:570:LYS:C	1:B:572:GLN:N	2.70	0.44
1:B:186:VAL:HG13	1:B:187:PRO:N	2.32	0.44
1:A:88:LEU:HD11	1:A:125:THR:OG1	2.17	0.44
1:B:419:SER:O	1:B:474:VAL:HG13	2.17	0.44
1:A:439:MET:HE2	1:A:494:LEU:N	2.33	0.44
1:A:422:LEU:HD12	1:A:458:TYR:CE1	2.53	0.44
1:A:81:MET:CE	1:A:104:PHE:HE2	2.31	0.44
1:A:36:LYS:HG2	1:A:64:PRO:HD2	1.98	0.44
1:B:420:PHE:CE1	1:B:474:VAL:HG13	2.52	0.44
1:B:236:GLU:C	1:B:238:ARG:N	2.71	0.44
1:B:186:VAL:HG11	1:B:191:LYS:HB3	1.99	0.44
1:B:587:TYR:HD1	1:B:587:TYR:C	2.20	0.44
1:B:470:PRO:O	1:B:490:GLN:CB	2.66	0.44
1:B:81:MET:HA	1:B:126:MET:HE3	2.00	0.44
1:A:4:ILE:HD11	1:A:56:ASP:N	2.32	0.44
1:A:336:CYS:SG	4:A:1004:THR:N	2.91	0.44
1:B:166:ASP:O	1:B:167:GLU:HG3	2.18	0.44
1:B:21:THR:HB	1:B:49:LEU:O	2.18	0.44
1:B:402:VAL:C	1:B:404:ASN:H	2.20	0.44
1:B:309:HIS:CE1	1:B:467:PHE:CD2	3.06	0.44
1:A:472:LEU:C	1:A:472:LEU:HD23	2.38	0.44
1:A:566:GLN:HE21	1:A:577:SER:HA	1.83	0.44
1:B:186:VAL:HG13	1:B:187:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD11	1:A:56:ASP:H	1.83	0.44
1:B:570:LYS:O	1:B:572:GLN:N	2.51	0.44
1:B:275:ARG:HD2	5:B:2006:HOH:O	2.18	0.44
1:B:177:PHE:CD2	1:B:178:THR:N	2.85	0.44
1:B:94:PHE:HE2	5:B:2021:HOH:O	2.00	0.44
1:A:14:LYS:HE3	1:A:16:PHE:CE1	2.52	0.44
1:B:523:THR:HG23	1:B:525:GLU:N	2.33	0.44
1:A:303:LEU:HG	1:A:337:PRO:HB2	2.00	0.44
1:B:601:ILE:HG13	1:B:613:VAL:HB	1.99	0.44
1:A:582:ASN:ND2	1:A:582:ASN:C	2.71	0.44
1:A:637:ASP:OD2	1:A:640:ARG:NH2	2.50	0.44
1:B:194:GLU:HG3	1:B:224:ASP:C	2.38	0.44
1:A:354:PRO:HD3	1:A:394:GLN:HE22	1.83	0.44
1:B:535:THR:HB	1:B:538:ALA:O	2.18	0.43
1:B:644:HIS:O	1:B:645:ARG:CB	2.66	0.43
1:A:158:GLU:CB	1:A:206:ARG:HH21	2.29	0.43
1:B:365:ARG:HG2	1:B:365:ARG:HH11	1.82	0.43
1:A:117:ASP:N	1:A:117:ASP:OD1	2.49	0.43
1:B:558:HIS:O	1:B:559:TYR:C	2.57	0.43
1:A:576:VAL:HG22	1:A:577:SER:N	2.32	0.43
1:B:637:ASP:OD2	1:B:641:LEU:HD23	2.18	0.43
1:B:186:VAL:CG1	1:B:191:LYS:HB3	2.49	0.43
3:B:2003:ATP:C5'	4:B:2004:THR:OXT	2.66	0.43
1:B:366:TYR:CD1	1:B:366:TYR:C	2.91	0.43
1:B:467:PHE:HD2	1:B:468:TYR:HD1	1.66	0.43
1:A:399:PHE:O	1:A:402:VAL:HG12	2.17	0.43
1:B:531:LEU:HD21	1:B:543:LEU:HD13	2.01	0.43
1:A:559:TYR:OH	1:A:563:ARG:NH1	2.45	0.43
1:A:243:HIS:HB3	1:A:533:GLU:HG3	2.00	0.43
1:B:404:ASN:HD22	1:B:407:ILE:CG2	2.30	0.43
1:B:408:ASP:N	1:B:408:ASP:OD2	2.50	0.43
1:B:428:GLU:OE2	1:B:435:ASP:HB3	2.17	0.43
1:B:443:ALA:HB1	1:B:470:PRO:CD	2.47	0.43
1:B:241:ARG:HH12	1:B:536:LYS:HZ2	1.67	0.43
1:B:85:ILE:O	1:B:89:TYR:CB	2.66	0.43
1:A:497:GLU:CD	1:A:512:ARG:HH11	2.22	0.43
1:A:146:ALA:O	1:A:147:LYS:C	2.56	0.43
4:B:2004:THR:N	5:B:2016:HOH:O	2.51	0.43
1:B:17:ASP:O	1:B:20:THR:OG1	2.28	0.43
1:B:353:LEU:N	1:B:354:PRO:CD	2.82	0.43
1:B:372:VAL:HG12	5:B:2013:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:HB3	1:A:108:PHE:CE1	2.53	0.43
1:A:116:SER:HA	1:A:119:PHE:CD1	2.54	0.43
1:B:30:SER:HA	1:B:31:PRO:HD3	1.82	0.43
1:B:74:ARG:NH1	1:B:221:ALA:O	2.51	0.43
1:B:333:PRO:HG2	1:B:334:MET:HG2	1.99	0.43
1:B:391:ARG:O	1:B:394:GLN:HB2	2.19	0.43
1:A:143:ARG:HD3	1:A:163:ILE:HD11	2.00	0.43
1:B:468:TYR:HB2	1:B:492:ASP:CG	2.38	0.43
1:B:371:ALA:O	1:B:372:VAL:C	2.57	0.43
1:A:107:ASP:HB3	1:A:214:LEU:HD22	2.00	0.43
1:B:66:SER:HB3	1:B:69:ALA:CB	2.45	0.43
1:B:418:TYR:HD2	1:B:418:TYR:N	1.94	0.43
1:B:75:HIS:HB2	1:B:99:VAL:CG2	2.48	0.43
1:B:634:ASN:O	1:B:638:GLU:HB2	2.19	0.43
1:A:141:VAL:CB	1:A:145:GLU:HB2	2.45	0.43
1:A:478:THR:CG2	1:A:480:MET:HG2	2.48	0.43
1:B:425:ARG:C	1:B:425:ARG:HD2	2.40	0.43
1:B:206:ARG:HD2	1:B:206:ARG:O	2.19	0.43
1:B:405:MET:C	1:B:407:ILE:H	2.21	0.43
1:B:421:ARG:O	1:B:421:ARG:HG3	2.19	0.43
1:A:321:MET:HB2	1:B:319:PRO:HG2	2.00	0.43
1:B:212:LYS:O	1:B:214:LEU:HD22	2.18	0.43
1:A:551:ILE:HG23	1:A:588:LYS:HD3	2.01	0.43
1:B:253:PHE:O	1:B:254:THR:HG22	2.19	0.43
1:A:643:LYS:HG2	1:A:644:HIS:H	1.84	0.43
1:A:641:LEU:HD13	5:A:1050:HOH:O	2.19	0.43
1:A:424:TYR:HE1	1:A:460:GLU:OE2	2.02	0.42
1:A:157:LEU:HA	1:A:160:ILE:CG2	2.47	0.42
1:B:192:ILE:C	1:B:193:LYS:HD2	2.40	0.42
1:A:149:LEU:HD23	1:A:171:LEU:HD21	2.01	0.42
1:B:6:ILE:O	1:B:13:LYS:HA	2.19	0.42
1:A:376:GLN:NE2	5:A:1101:HOH:O	2.35	0.42
1:A:27:GLN:NE2	1:A:31:PRO:HG3	2.29	0.42
1:A:392:PRO:CD	5:A:1025:HOH:O	2.66	0.42
1:B:612:GLN:HB3	1:B:626:VAL:O	2.19	0.42
1:B:36:LYS:HE3	1:B:63:THR:CG2	2.49	0.42
1:A:50:THR:O	1:A:51:LYS:C	2.55	0.42
1:B:420:PHE:CE2	1:B:474:VAL:CG2	3.01	0.42
1:A:322:GLN:HE21	1:A:323:LEU:HB3	1.84	0.42
1:B:171:LEU:C	1:B:171:LEU:HD13	2.40	0.42
1:A:70:LEU:O	1:A:74:ARG:CG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD22	1:B:74:ARG:HG3	2.00	0.42
1:A:375:LEU:HB3	1:A:525:GLU:HB2	2.00	0.42
1:A:80:LEU:HD23	1:A:192:ILE:HG21	2.01	0.42
1:A:331:LEU:HD11	1:B:298:LEU:HD21	2.01	0.42
1:B:391:ARG:NH1	1:B:393:ASP:OD2	2.52	0.42
1:B:471:LYS:NZ	5:B:2091:HOH:O	2.53	0.42
1:B:7:GLN:HG3	1:B:13:LYS:HB3	2.01	0.42
1:B:574:VAL:HG12	1:B:575:ARG:N	2.34	0.42
1:A:85:ILE:HG21	1:A:108:PHE:CD2	2.54	0.42
1:A:83:HIS:ND1	1:A:129:ILE:HD13	2.34	0.42
1:B:84:ALA:CB	1:B:126:MET:HB3	2.44	0.42
1:B:299:ALA:O	1:B:329:MET:HA	2.20	0.42
1:A:204:TYR:HE1	5:A:1064:HOH:O	2.03	0.42
1:B:439:MET:HE3	1:B:494:LEU:N	2.35	0.42
1:B:241:ARG:NH1	1:B:536:LYS:HZ2	2.18	0.42
1:B:204:TYR:HA	1:B:214:LEU:HD23	2.02	0.42
1:A:4:ILE:HG13	1:A:56:ASP:HB3	2.02	0.42
1:A:54:GLU:OE1	1:A:54:GLU:CA	2.68	0.42
1:A:203:ALA:O	1:A:213:MET:HG3	2.19	0.42
1:B:86:LYS:HE3	1:B:91:ASN:HA	2.01	0.42
1:A:606:LYS:O	1:A:609:GLU:HB2	2.20	0.42
1:B:378:VAL:H	3:B:2003:ATP:HN62	1.68	0.42
1:A:626:VAL:HG12	1:A:627:GLU:O	2.19	0.42
1:B:610:ASN:O	1:B:611:ASN:C	2.57	0.42
1:B:4:ILE:HG23	1:B:4:ILE:O	2.20	0.42
1:B:324:ASP:O	1:B:326:THR:N	2.45	0.42
1:B:438:ASP:CG	1:B:439:MET:N	2.73	0.42
1:B:171:LEU:O	1:B:171:LEU:HD13	2.19	0.42
1:A:303:LEU:CG	1:A:337:PRO:HB2	2.49	0.42
1:A:151:SER:HB2	1:A:152:ASN:H	1.72	0.42
1:B:141:VAL:HG11	1:B:146:ALA:HB2	2.02	0.42
1:A:360:LEU:HA	1:A:360:LEU:HD13	1.92	0.42
1:A:444:GLU:O	1:A:445:ASN:C	2.58	0.42
1:B:492:ASP:OD1	1:B:495:LEU:HB2	2.20	0.42
1:A:203:ALA:O	1:A:214:LEU:N	2.53	0.42
1:B:74:ARG:HH11	1:B:74:ARG:CG	2.29	0.42
1:B:8:PHE:O	1:B:10:ASP:N	2.51	0.42
3:B:2003:ATP:O2B	3:B:2003:ATP:O2A	2.38	0.42
1:A:25:ILE:O	1:A:29:ILE:HG13	2.20	0.42
1:B:137:GLU:H	1:B:137:GLU:HG2	1.51	0.42
1:B:4:ILE:HG22	1:B:16:PHE:C	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:HH12	1:B:536:LYS:NZ	2.16	0.41
1:B:616:ARG:CZ	1:B:622:ASP:CB	2.98	0.41
1:A:152:ASN:H	1:A:152:ASN:HD22	1.55	0.41
1:A:456:LEU:O	1:A:458:TYR:HD2	2.03	0.41
1:A:254:THR:HG22	1:A:255:ASN:N	2.35	0.41
1:A:188:SER:C	1:A:190:ALA:H	2.23	0.41
1:B:80:LEU:HD13	1:B:129:ILE:HD13	2.03	0.41
1:A:143:ARG:NH1	1:A:163:ILE:HG23	2.35	0.41
1:A:340:MET:CE	1:A:389:PHE:CE2	3.03	0.41
1:B:559:TYR:O	1:B:559:TYR:HD2	2.02	0.41
1:A:486:LEU:O	1:A:522:SER:HB2	2.20	0.41
1:B:186:VAL:HG13	1:B:187:PRO:HD2	2.01	0.41
1:A:262:GLY:O	1:A:378:VAL:HB	2.20	0.41
1:A:251:GLU:O	1:A:269:ASN:HB2	2.20	0.41
1:B:474:VAL:O	1:B:486:LEU:N	2.52	0.41
1:A:480:MET:HG3	1:A:480:MET:O	2.21	0.41
1:A:509:GLU:CD	1:A:509:GLU:H	2.24	0.41
1:B:474:VAL:HG21	1:B:487:SER:CB	2.45	0.41
1:B:501:LEU:O	1:B:512:ARG:HG2	2.19	0.41
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.87	0.41
1:B:204:TYR:O	1:B:207:GLY:N	2.53	0.41
1:A:340:MET:CG	1:A:501:LEU:HD11	2.45	0.41
1:B:255:ASN:HD21	1:B:374:GLY:HA2	1.86	0.41
1:A:300:ASN:O	1:A:302:ASP:N	2.54	0.41
1:A:240:GLU:HA	1:A:245:LYS:HE2	2.02	0.41
1:B:429:ASP:HA	1:B:435:ASP:OD2	2.20	0.41
1:B:444:GLU:O	1:B:448:LYS:HG3	2.20	0.41
1:B:212:LYS:H	1:B:212:LYS:CD	2.25	0.41
1:B:453:GLU:HB2	1:B:454:LEU:HD22	2.00	0.41
1:B:383:LEU:HA	1:B:523:THR:HA	2.02	0.41
1:B:115:SER:HA	1:B:200:THR:HG21	2.03	0.41
1:B:399:PHE:O	1:B:403:VAL:HB	2.21	0.41
1:B:4:ILE:CG2	1:B:16:PHE:O	2.60	0.41
1:B:4:ILE:O	1:B:4:ILE:CG2	2.68	0.41
1:B:262:GLY:H	1:B:372:VAL:HG13	1.81	0.41
1:B:47:VAL:HG23	1:B:48:ASP:N	2.35	0.41
1:B:280:TYR:OH	1:B:409:VAL:HA	2.20	0.41
1:B:584:LYS:O	1:B:585:MET:C	2.58	0.41
1:B:623:GLN:O	1:B:624:GLU:O	2.39	0.41
1:B:252:LEU:O	1:B:270:GLY:HA3	2.21	0.41
1:A:502:THR:HA	1:A:511:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:HG22	1:B:250:LEU:HD22	2.03	0.41
1:A:428:GLU:HG3	1:A:440:TRP:NE1	2.35	0.41
1:A:542:TRP:CE3	1:A:642:LYS:HE3	2.56	0.41
1:B:486:LEU:HB3	1:B:487:SER:H	1.57	0.41
1:B:400:LYS:O	1:B:404:ASN:HB2	2.21	0.41
1:B:241:ARG:O	1:B:533:GLU:HG2	2.21	0.41
1:A:143:ARG:HD3	1:A:163:ILE:CG1	2.51	0.41
1:B:211:ASN:HB2	1:B:214:LEU:HD21	2.03	0.41
1:A:340:MET:HE2	1:A:389:PHE:CE2	2.56	0.41
1:B:100:ILE:HG22	1:B:101:GLU:H	1.85	0.41
1:B:182:ARG:HD2	1:B:182:ARG:H	1.82	0.41
1:A:548:VAL:HB	1:A:576:VAL:HG23	2.03	0.41
1:B:186:VAL:CG1	1:B:188:SER:O	2.69	0.41
1:A:282:VAL:HG23	1:A:360:LEU:HD21	2.03	0.41
1:A:603:VAL:O	1:A:603:VAL:HG12	2.20	0.41
1:A:21:THR:O	1:A:24:ASP:HB2	2.20	0.41
1:A:97:GLY:CA	1:A:105:TYR:O	2.69	0.41
1:B:191:LYS:O	1:B:191:LYS:CG	2.70	0.41
1:B:256:SER:OG	1:B:259:VAL:HG23	2.21	0.41
1:A:408:ASP:HA	1:A:411:LYS:HE3	2.02	0.41
1:B:430:LYS:CB	1:B:436:ASP:HB2	2.49	0.40
1:B:585:MET:O	1:B:589:ILE:HD12	2.21	0.40
1:B:561:TYR:HD2	1:B:603:VAL:HG11	1.85	0.40
1:A:434:PHE:HD2	1:A:434:PHE:HA	1.63	0.40
1:B:540:PRO:CG	1:B:543:LEU:HD12	2.51	0.40
1:A:368:ALA:O	1:A:370:GLY:N	2.54	0.40
1:A:583:GLU:HG3	1:A:587:TYR:CD2	2.56	0.40
1:A:364:HIS:HA	1:A:379:ARG:O	2.22	0.40
1:B:598:PRO:C	1:B:599:TYR:CD1	2.95	0.40
1:B:204:TYR:CD1	1:B:204:TYR:N	2.90	0.40
1:B:563:ARG:HA	1:B:578:ILE:HD11	2.02	0.40
1:A:585:MET:O	1:A:588:LYS:HB2	2.22	0.40
1:B:554:ASN:CG	1:B:557:LEU:HD12	2.41	0.40
1:B:114:ILE:HG22	1:B:118:ASP:OD2	2.22	0.40
1:B:129:ILE:CD1	1:B:174:GLN:HE22	2.35	0.40
1:B:6:ILE:HA	1:B:57:GLY:O	2.21	0.40
1:A:13:LYS:HE3	1:A:13:LYS:HB3	1.91	0.40
1:B:245:LYS:O	1:B:249:GLU:HB2	2.22	0.40
1:B:288:MET:CE	1:B:405:MET:HB2	2.51	0.40
1:B:79:HIS:CD2	1:B:174:GLN:OE1	2.74	0.40
1:A:93:LYS:CD	1:A:155:TYR:HE1	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:O	1:A:108:PHE:CE1	2.74	0.40
1:A:77:THR:HA	1:A:80:LEU:HB3	2.04	0.40
1:B:616:ARG:O	1:B:617:GLN:C	2.58	0.40
1:A:407:ILE:O	1:A:410:TYR:HB2	2.21	0.40
1:B:573:GLY:O	5:B:2093:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/645 (99%)	552 (86%)	62 (10%)	26 (4%)	3	11
1	B	633/645 (98%)	466 (74%)	114 (18%)	53 (8%)	1	2
All	All	1273/1290 (99%)	1018 (80%)	176 (14%)	79 (6%)	2	5

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	A	324	ASP
1	A	425	ARG
1	A	430	LYS
1	A	432	LYS
1	A	465	ALA
1	B	4	ILE
1	B	90	GLY
1	B	91	ASN
1	B	147	LYS
1	B	167	GLU
1	B	201	ALA
1	B	205	TRP

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Mol	Chain	Res	Type
1	B	313	TYR
1	B	324	ASP
1	B	325	GLU
1	B	415	PHE
1	B	421	ARG
1	B	430	LYS
1	B	465	ALA
1	B	473	ASP
1	B	479	ALA
1	B	508	GLY
1	B	605	ASP
1	B	617	GLN
1	B	621	GLN
1	B	624	GLU
1	A	18	LYS
1	A	143	ARG
1	A	144	ASP
1	A	151	SER
1	A	175	GLY
1	A	322	GLN
1	A	325	GLU
1	A	436	ASP
1	A	618	TYR
1	A	623	GLN
1	B	75	HIS
1	B	106	TYR
1	B	114	ILE
1	B	355	ILE
1	B	464	GLU
1	B	488	THR
1	B	520	VAL
1	B	611	ASN
1	A	149	LEU
1	A	189	THR
1	B	9	PRO
1	B	143	ARG
1	B	166	ASP
1	B	203	ALA
1	B	369	SER
1	B	395	ILE
1	B	436	ASP
1	B	471	LYS

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Mol	Chain	Res	Type
1	B	472	LEU
1	B	571	SER
1	B	620	SER
1	B	628	LYS
1	A	211	ASN
1	A	301	VAL
1	A	366	TYR
1	A	369	SER
1	B	163	ILE
1	B	623	GLN
1	B	643	LYS
1	A	162	ALA
1	A	429	ASP
1	A	611	ASN
1	B	353	LEU
1	B	622	ASP
1	B	642	LYS
1	B	116	SER
1	B	427	PRO
1	B	406	ILE
1	B	470	PRO
1	B	513	PRO
1	B	519	GLY
1	A	426	ASP

### 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	567/570 (100%)	512 (90%)	55 (10%)	10	29
1	B	562/570 (99%)	491 (87%)	71 (13%)	5	17
All	All	1129/1140 (99%)	1003 (89%)	126 (11%)	8	22

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	17	ASP
1	A	34	ARG
1	A	48	ASP
1	A	54	GLU
1	A	74	ARG
1	A	81	MET
1	A	101	GLU
1	A	112	GLN
1	A	117	ASP
1	A	120	GLU
1	A	128	GLN
1	A	129	ILE
1	A	148	GLU
1	A	151	SER
1	A	152	ASN
1	A	153	ASP
1	A	167	GLU
1	A	170	THR
1	A	173	SER
1	A	186	VAL
1	A	204	TYR
1	A	220	THR
1	A	250	LEU
1	A	255	ASN
1	A	298	LEU
1	A	323	LEU
1	A	330	VAL
1	A	336	CYS
1	A	340	MET
1	A	353	LEU
1	A	360	LEU
1	A	366	TYR
1	A	376	GLN
1	A	377	ARG
1	A	434	PHE
1	A	447	LEU
1	A	467	PHE
1	A	476	VAL
1	A	483	GLU
1	A	496	PRO
1	A	507	ASP
1	A	509	GLU

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Mol	Chain	Res	Type
1	A	512	ARG
1	A	518	ARG
1	A	521	VAL
1	A	523	THR
1	A	526	ARG
1	A	535	THR
1	A	554	ASN
1	A	560	ASP
1	A	582	ASN
1	A	610	ASN
1	A	622	ASP
1	A	641	LEU
1	B	34	ARG
1	B	47	VAL
1	B	55	THR
1	B	56	ASP
1	B	59	ILE
1	B	68	GLU
1	B	70	LEU
1	B	92	VAL
1	B	94	PHE
1	B	106	TYR
1	B	114	ILE
1	B	117	ASP
1	B	129	ILE
1	B	137	GLU
1	B	149	LEU
1	B	158	GLU
1	B	182	ARG
1	B	195	PHE
1	B	204	TYR
1	B	205	TRP
1	B	210	ASN
1	B	211	ASN
1	B	212	LYS
1	B	214	LEU
1	B	225	LYS
1	B	250	LEU
1	B	256	SER
1	B	257	GLN
1	B	279	ARG
1	B	297	VAL

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Mol	Chain	Res	Type
1	B	313	TYR
1	B	326	THR
1	B	352	GLU
1	B	353	LEU
1	B	355	ILE
1	B	360	LEU
1	B	365	ARG
1	B	366	TYR
1	B	399	PHE
1	B	401	ARG
1	B	402	VAL
1	B	404	ASN
1	B	408	ASP
1	B	412	ASP
1	B	413	PHE
1	B	416	GLU
1	B	418	TYR
1	B	428	GLU
1	B	434	PHE
1	B	435	ASP
1	B	438	ASP
1	B	440	TRP
1	B	464	GLU
1	B	467	PHE
1	B	468	TYR
1	B	473	ASP
1	B	490	GLN
1	B	492	ASP
1	B	507	ASP
1	B	518	ARG
1	B	523	THR
1	B	555	VAL
1	B	559	TYR
1	B	563	ARG
1	B	580	ASP
1	B	587	TYR
1	B	594	MET
1	B	601	ILE
1	B	609	GLU
1	B	610	ASN
1	B	611	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	43	ASN
1	A	133	ASN
1	A	152	ASN
1	A	210	ASN
1	A	231	HIS
1	A	233	GLN
1	A	322	GLN
1	A	345	ASN
1	A	364	HIS
1	A	376	GLN
1	A	384	ASN
1	A	475	GLN
1	A	490	GLN
1	A	554	ASN
1	A	566	GLN
1	A	582	ASN
1	A	593	GLN
1	A	600	GLN
1	A	612	GLN
1	A	617	GLN
1	B	12	ASN
1	B	79	HIS
1	B	83	HIS
1	B	121	GLN
1	B	128	GLN
1	B	174	GLN
1	B	210	ASN
1	B	211	ASN
1	B	255	ASN
1	B	309	HIS
1	B	404	ASN
1	B	490	GLN
1	B	506	GLN
1	B	572	GLN
1	B	595	GLN
1	B	600	GLN
1	B	611	ASN
1	B	612	GLN
1	B	617	GLN
1	B	621	GLN
1	B	634	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	A	1003	-	24,33,33	0.80	0	31,52,52	1.18	3 (9%)
4	THR	A	1004	2	4,7,7	1.05	0	3,9,9	0.74	0
3	ATP	B	2003	-	24,33,33	0.75	0	31,52,52	1.21	3 (9%)
4	THR	B	2004	2	4,7,7	0.27	0	3,9,9	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1003	-	-	0/18/38/38	0/3/3/3
4	THR	A	1004	2	-	0/4/8/8	0/0/0/0
3	ATP	B	2003	-	-	0/18/38/38	0/3/3/3
4	THR	B	2004	2	-	0/4/8/8	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	ATP	PA-O3A-PB	-3.55	122.77	132.73
3	A	1003	ATP	PA-O3A-PB	-3.49	122.94	132.73
3	B	2003	ATP	PB-O3B-PG	-3.31	121.56	132.67
3	A	1003	ATP	PB-O3B-PG	-2.94	122.80	132.67
3	B	2003	ATP	O2G-PG-O1G	2.84	119.72	110.58
3	A	1003	ATP	O2G-PG-O1G	2.93	120.00	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	ATP	3	0
4	A	1004	THR	4	0
3	B	2003	ATP	3	0
4	B	2004	THR	2	0

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	642/645 (99%)	-0.08	22 (3%) 49 36	24, 58, 103, 134	0
1	B	637/645 (98%)	0.52	88 (13%) 4 2	29, 79, 143, 157	0
All	All	1279/1290 (99%)	0.22	110 (8%) 13 6	24, 67, 135, 157	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	TYR	6.9
1	B	111	ASP	6.1
1	B	212	LYS	5.8
1	B	88	LEU	5.6
1	B	90	GLY	5.3
1	B	166	ASP	5.2
1	A	434	PHE	5.1
1	A	432	LYS	5.1
1	B	455	GLY	5.0
1	B	113	ASN	4.9
1	B	170	THR	4.8
1	A	204	TYR	4.7
1	B	447	LEU	4.7
1	A	431	GLU	4.7
1	B	209	SER	4.7
1	A	166	ASP	4.7
1	A	433	TYR	4.6
1	B	441	ASN	4.5
1	B	210	ASN	4.5
1	A	325	GLU	4.3
1	B	208	ASP	4.2
1	B	94	PHE	4.2
1	B	161	ASP	4.1
1	B	619	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	445	ASN	4.1
1	A	164	PRO	4.0
1	B	459	GLU	4.0
1	A	163	ILE	4.0
1	B	211	ASN	4.0
1	B	168	ASN	4.0
1	A	429	ASP	3.9
1	B	457	SER	3.9
1	A	623	GLN	3.8
1	B	117	ASP	3.8
1	B	183	GLY	3.8
1	B	91	ASN	3.7
1	B	440	TRP	3.6
1	B	87	ARG	3.5
1	B	92	VAL	3.4
1	B	446	MET	3.4
1	B	1	MET	3.4
1	B	2	GLU	3.4
1	B	160	ILE	3.4
1	B	165	GLU	3.3
1	B	454	LEU	3.3
1	B	431	GLU	3.3
1	B	175	GLY	3.2
1	B	169	VAL	3.2
1	B	112	GLN	3.2
1	B	204	TYR	3.1
1	B	458	TYR	3.1
1	B	434	PHE	3.1
1	B	645	ARG	3.0
1	B	141	VAL	3.0
1	B	557	LEU	3.0
1	B	167	GLU	3.0
1	B	199	SER	3.0
1	B	181	CYS	3.0
1	A	324	ASP	3.0
1	B	133	ASN	2.9
1	A	210	ASN	2.9
1	B	213	MET	2.9
1	A	182	ARG	2.9
1	B	182	ARG	2.9
1	B	312	HIS	2.9
1	B	140	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	168	ASN	2.6
1	B	89	TYR	2.6
1	B	214	LEU	2.6
1	B	10	ASP	2.6
1	A	165	GLU	2.6
1	B	416	GLU	2.4
1	A	31	PRO	2.4
1	B	174	GLN	2.4
1	B	466	ALA	2.4
1	A	183	GLY	2.4
1	B	422	LEU	2.4
1	B	606	LYS	2.4
1	B	475	GLN	2.4
1	B	480	MET	2.4
1	B	624	GLU	2.3
1	A	435	ASP	2.3
1	B	452	ASP	2.3
1	B	451	ALA	2.3
1	B	215	GLN	2.3
1	B	448	LYS	2.3
1	A	622	ASP	2.3
1	B	437	ASP	2.3
1	B	432	LYS	2.3
1	B	419	SER	2.2
1	B	149	LEU	2.2
1	B	463	GLY	2.2
1	A	645	ARG	2.2
1	B	461	ALA	2.2
1	B	108	PHE	2.1
1	B	444	GLU	2.1
1	B	201	ALA	2.1
1	B	325	GLU	2.1
1	B	418	TYR	2.1
1	B	621	GLN	2.1
1	B	477	LYS	2.1
1	A	425	ARG	2.1
1	B	128	GLN	2.1
1	B	142	SER	2.1
1	B	483	GLU	2.1
1	B	66	SER	2.0
1	B	315	GLU	2.0
1	B	469	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	423	SER	2.0
1	B	620	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	A	1003	31/31	0.89	0.22	1.85	56,63,88,91	0
4	THR	A	1004	8/8	0.98	0.18	1.34	75,75,77,77	0
4	THR	B	2004	8/8	0.97	0.21	0.60	113,114,114,115	0
3	ATP	B	2003	31/31	0.81	0.25	0.39	119,121,141,141	0
2	ZN	A	1002	1/1	0.98	0.03	-1.69	93,93,93,93	0
2	ZN	A	1001	1/1	0.99	0.08	-2.82	45,45,45,45	0
2	ZN	B	2001	1/1	0.99	0.10	-	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.