



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID : 1NYQ
Title : Structure of Staphylococcus aureus threonyl-tRNA synthetase complexed with an analogue of threonyl adenylate
Authors : Torres-Larios, A.; Sankaranarayanan, R.; Rees, B.; Dock-Bregeon, A.C.; Moras, D.
Deposited on : 2003-02-13
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
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

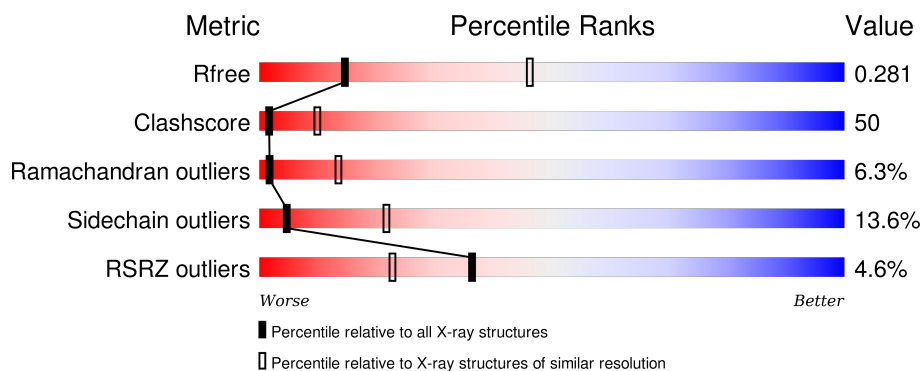
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

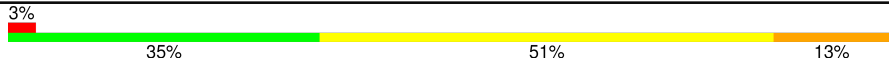
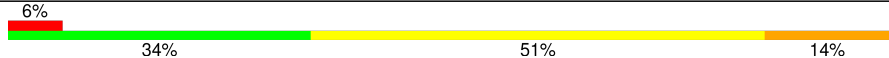
The reported resolution of this entry is 3.20 Å.

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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	 3% 35% 51% 13%
1	B	645	 6% 34% 51% 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10663 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.

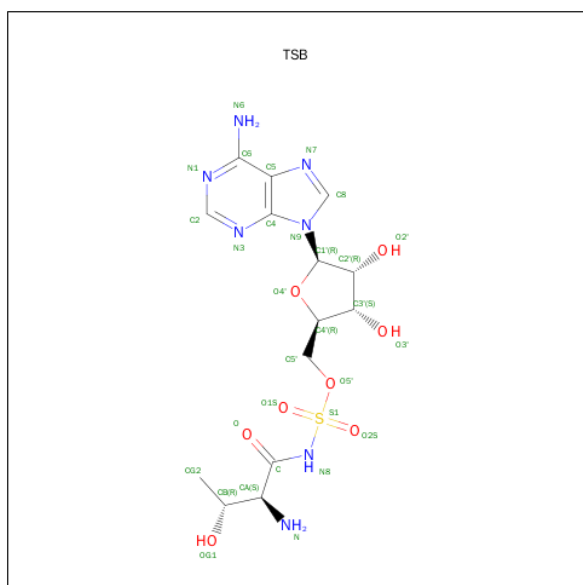
- Molecule 1 is a protein called threonyl-tRNA synthetase 1.

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	645	Total	C	N	O	S	0	0	0
			5242	3311	898	1009	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	1	Total	Zn	0	0
			1	1		

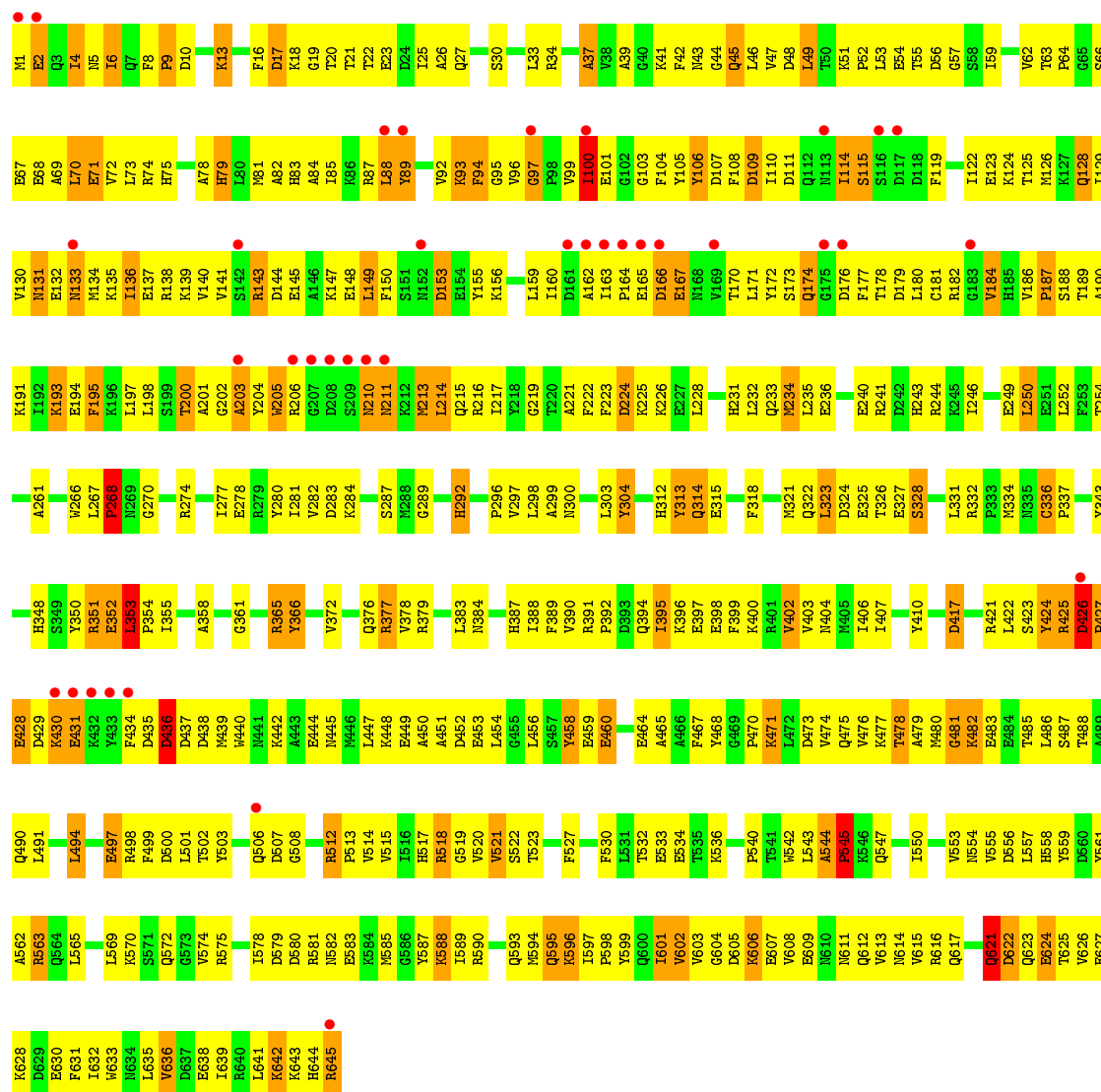
- Molecule 3 is 5'-O-(N-(L-THREONYL)-SULFAMOYL)ADENOSINE (three-letter code: TSB) (formula: C₁₄H₂₁N₇O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
3	B	1	Total	C	N	O	S	0	0
			30	14	7	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	68	Total	O	0	0
			68	68		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.28Å 122.73Å 149.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 19.89 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-3.20) 95.1 (19.89-3.19)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 3.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.285 0.204 , 0.281	Depositor DCC
R_{free} test set	3076 reflections (10.04%)	DCC
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 32007 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10663	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, TSB

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	0.61	0/5325	0.83	4/7182 (0.1%)
1	B	0.56	0/5351	0.78	5/7216 (0.1%)
All	All	0.59	0/10676	0.81	9/14398 (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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	GLY	N-CA-C	6.84	130.20	113.10
1	A	353	LEU	C-N-CA	-6.16	96.14	122.00
1	B	353	LEU	N-CA-C	5.77	126.59	111.00
1	B	519	GLY	N-CA-C	-5.61	99.07	113.10
1	A	353	LEU	N-CA-C	5.44	125.68	111.00
1	B	377	ARG	N-CA-C	-5.41	96.39	111.00
1	A	322	GLN	N-CA-C	5.37	125.51	111.00
1	B	424	TYR	N-CA-C	5.22	125.09	111.00
1	A	360	LEU	N-CA-C	-5.16	97.06	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	TYR	Sidechain
1	A	304	TYR	Sidechain
1	A	350	TYR	Sidechain
1	B	304	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	5105	486	0
1	B	5242	0	5131	563	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	20	3	0
3	B	30	0	20	3	0
4	A	75	0	0	19	0
4	B	68	0	0	21	0
All	All	10663	0	10276	1035	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 50.

All (1035) 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:593:GLN:NE2	1:B:616:ARG:HH21	1.41	1.18
1:B:395:ILE:HD11	1:B:514:VAL:HG21	1.28	1.15
1:B:478:THR:HG22	1:B:479:ALA:H	1.08	1.13
1:A:426:ASP:HB3	1:A:427:PRO:HD2	1.31	1.10
1:B:74:ARG:HG2	1:B:221:ALA:HB3	1.28	1.08
1:B:135:LYS:HG2	1:B:136:ILE:H	1.19	1.08
1:B:322:GLN:HA	1:B:328:SER:HA	1.34	1.05
1:A:113:ASN:HA	1:A:215:GLN:HE22	1.25	1.01
1:B:593:GLN:HE21	1:B:616:ARG:NH2	1.58	1.00
1:B:27:GLN:NE2	1:B:34:ARG:HH11	1.59	1.00
1:A:20:THR:HG23	1:A:24:ASP:HB2	1.46	0.96
1:A:482:LYS:HZ2	1:A:483:GLU:H	1.08	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:HD22	1:A:521:VAL:H	0.97	0.95
1:B:580:ASP:HB3	4:B:2024:HOH:O	1.66	0.95
1:B:554:ASN:HB3	1:B:557:LEU:HB3	1.48	0.94
1:B:43:ASN:HD21	1:B:57:GLY:HA3	1.34	0.93
1:B:170:THR:HG23	1:B:182:ARG:NH1	1.85	0.92
1:B:303:LEU:HD21	1:B:337:PRO:HB2	1.50	0.92
1:B:27:GLN:HE22	1:B:34:ARG:HH11	1.16	0.91
1:A:554:ASN:ND2	1:A:556:ASP:H	1.69	0.91
1:A:18:LYS:HE2	1:A:54:GLU:HG3	1.50	0.90
1:B:601:ILE:HD11	1:B:615:VAL:HG12	1.54	0.90
1:B:593:GLN:HE21	1:B:616:ARG:HH21	0.94	0.89
1:B:170:THR:HG23	1:B:182:ARG:HH11	1.37	0.89
1:A:531:LEU:O	1:A:535:THR:HG22	1.69	0.89
1:B:4:ILE:HG23	1:B:5:ASN:N	1.88	0.89
1:A:74:ARG:NH2	1:A:102:GLY:HA2	1.87	0.88
1:A:384:ASN:ND2	1:A:521:VAL:H	1.71	0.88
1:B:4:ILE:HG12	1:B:5:ASN:H	1.35	0.88
1:A:478:THR:HG22	1:A:480:MET:H	1.37	0.88
1:A:482:LYS:HZ2	1:A:483:GLU:N	1.71	0.88
1:A:550:ILE:HD13	1:A:565:LEU:HD23	1.56	0.88
1:B:550:ILE:HG23	1:B:601:ILE:HG22	1.55	0.87
1:B:471:LYS:HG3	1:B:473:ASP:OD1	1.75	0.87
1:A:478:THR:HG21	1:A:480:MET:HG2	1.56	0.87
1:B:478:THR:HG22	1:B:479:ALA:N	1.90	0.86
1:B:4:ILE:HD11	1:B:55:THR:O	1.74	0.86
1:A:256:SER:HB3	1:A:259:VAL:HG23	1.55	0.86
1:A:554:ASN:C	1:A:554:ASN:HD22	1.78	0.85
1:B:497:GLU:HA	1:B:512:ARG:HE	1.39	0.85
1:B:163:ILE:N	1:B:164:PRO:HD3	1.92	0.85
1:A:312:HIS:NE2	1:A:429:ASP:HB2	1.93	0.83
1:B:6:ILE:O	1:B:13:LYS:HB2	1.79	0.83
1:A:406:ILE:HD13	1:A:487:SER:HB3	1.60	0.83
1:B:123:GLU:HB2	1:B:197:LEU:HD12	1.60	0.83
1:B:85:ILE:HG13	1:B:108:PHE:CZ	2.14	0.83
1:B:593:GLN:NE2	1:B:616:ARG:NH2	2.18	0.82
1:A:614:ASN:HD21	1:A:623:GLN:HG3	1.44	0.82
1:B:471:LYS:CB	1:B:490:GLN:HG2	2.09	0.82
1:B:43:ASN:ND2	1:B:57:GLY:HA3	1.94	0.82
1:B:494:LEU:HD11	4:B:2005:HOH:O	1.78	0.82
1:A:204:TYR:HE1	1:A:207:GLY:HA2	1.46	0.81
1:A:440:TRP:O	1:A:444:GLU:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LYS:HD2	1:B:436:ASP:OD2	1.80	0.81
1:B:156:LYS:HG2	1:B:180:LEU:HD12	1.62	0.81
1:A:566:GLN:HE21	1:A:577:SER:HA	1.46	0.81
1:B:521:VAL:HG22	1:B:527:PHE:CE1	2.15	0.81
1:A:616:ARG:HH21	1:A:623:GLN:HE22	1.28	0.81
1:A:553:VAL:HB	1:A:558:HIS:CE1	2.16	0.81
1:A:304:TYR:HE1	1:A:337:PRO:HG3	1.44	0.80
1:A:85:ILE:HG13	1:A:108:PHE:CE2	2.17	0.80
1:A:518:ARG:O	1:A:518:ARG:HD3	1.81	0.80
1:A:553:VAL:HB	1:A:558:HIS:ND1	1.97	0.80
1:A:482:LYS:NZ	1:A:483:GLU:H	1.79	0.80
1:A:544:ALA:O	1:A:575:ARG:NH1	2.15	0.80
1:B:563:ARG:HD3	1:B:563:ARG:O	1.81	0.79
1:B:353:LEU:HD13	1:B:390:VAL:HA	1.63	0.79
1:B:27:GLN:HE22	1:B:34:ARG:NH1	1.79	0.79
1:B:27:GLN:NE2	1:B:34:ARG:HD3	1.96	0.79
1:B:48:ASP:HB2	1:B:138:ARG:NH1	1.97	0.79
1:B:471:LYS:HB2	1:B:490:GLN:HG2	1.64	0.79
1:A:321:MET:O	1:A:322:GLN:HB2	1.79	0.79
1:B:421:ARG:HH21	1:B:464:GLU:HB3	1.45	0.79
1:A:445:ASN:O	1:A:449:GLU:HG3	1.83	0.79
1:B:160:ILE:HD11	1:B:180:LEU:CD1	2.13	0.79
1:A:426:ASP:HB3	1:A:427:PRO:CD	2.13	0.78
1:B:140:VAL:HA	1:B:170:THR:HG22	1.64	0.78
1:B:46:LEU:O	1:B:184:VAL:HG11	1.84	0.78
1:B:615:VAL:HG23	1:B:623:GLN:HB3	1.63	0.78
1:A:140:VAL:HG13	1:A:170:THR:HG22	1.63	0.78
1:B:92:VAL:HB	1:B:109:ASP:HB2	1.66	0.78
1:B:399:PHE:O	1:B:403:VAL:HG23	1.84	0.77
1:A:612:GLN:NE2	1:A:625:THR:HG21	1.98	0.77
1:A:400:LYS:HG2	1:A:454:LEU:HD13	1.66	0.77
1:A:204:TYR:CD2	1:A:209:SER:HA	2.20	0.77
1:B:395:ILE:CD1	1:B:514:VAL:HG21	2.13	0.77
1:B:421:ARG:NH2	1:B:464:GLU:HB3	1.99	0.77
1:B:395:ILE:CG2	1:B:491:LEU:HD11	2.14	0.76
1:B:627:GLU:HG3	1:B:630:GLU:H	1.50	0.76
1:A:163:ILE:N	1:A:164:PRO:HD3	1.99	0.76
1:B:135:LYS:HG2	1:B:136:ILE:N	1.97	0.76
1:A:113:ASN:HA	1:A:215:GLN:NE2	2.00	0.76
1:B:353:LEU:CD1	1:B:390:VAL:HA	2.15	0.76
1:B:454:LEU:HB3	1:B:456:LEU:HD13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:CE1	4:A:1003:HOH:O	2.38	0.76
1:A:604:GLY:O	1:A:608:VAL:HG23	1.86	0.76
1:B:490:GLN:HB2	1:B:517:HIS:HB2	1.68	0.76
1:A:618:TYR:O	1:A:620:SER:N	2.18	0.75
1:B:43:ASN:HD21	1:B:57:GLY:CA	1.98	0.75
1:A:616:ARG:HH21	1:A:623:GLN:NE2	1.84	0.75
1:B:521:VAL:HG22	1:B:527:PHE:CZ	2.21	0.75
1:B:323:LEU:HD12	1:B:324:ASP:H	1.52	0.75
1:A:554:ASN:HD22	1:A:556:ASP:H	1.33	0.75
1:B:478:THR:CG2	1:B:479:ALA:H	1.92	0.75
1:A:113:ASN:CA	1:A:215:GLN:HE22	1.99	0.74
1:B:223:PHE:O	1:B:224:ASP:HB3	1.88	0.74
1:B:143:ARG:HG2	1:B:167:GLU:OE2	1.85	0.73
1:B:18:LYS:HE3	1:B:54:GLU:OE1	1.87	0.73
1:B:353:LEU:O	1:B:353:LEU:HD13	1.88	0.73
1:B:477:LYS:HG3	1:B:483:GLU:HG2	1.70	0.73
1:A:20:THR:HG23	1:A:24:ASP:CB	2.19	0.73
1:B:4:ILE:HG22	1:B:16:PHE:H	1.54	0.73
1:B:384:ASN:HD22	1:B:521:VAL:H	1.36	0.73
1:A:589:ILE:HG23	1:A:600:GLN:HE22	1.54	0.72
1:B:312:HIS:CE1	1:B:429:ASP:HB2	2.23	0.72
1:A:262:GLY:O	1:A:263:LEU:HD23	1.90	0.72
1:A:128:GLN:HA	1:A:131:ASN:ND2	2.04	0.71
1:B:110:ILE:HB	1:B:215:GLN:HG2	1.70	0.71
1:A:256:SER:HB3	1:A:259:VAL:CG2	2.20	0.71
1:B:540:PRO:HG2	1:B:543:LEU:HD12	1.72	0.71
1:B:477:LYS:HE3	1:B:483:GLU:OE2	1.89	0.71
1:B:84:ALA:HB2	1:B:126:MET:HG2	1.72	0.71
1:A:478:THR:CG2	1:A:480:MET:HG2	2.19	0.71
1:A:591:GLU:O	1:A:595:GLN:HG3	1.91	0.71
1:A:5:ASN:O	1:A:56:ASP:HB2	1.90	0.70
1:B:85:ILE:HD11	1:B:122:ILE:HD13	1.73	0.70
1:B:428:GLU:HG2	1:B:440:TRP:HE1	1.56	0.70
1:B:174:GLN:HG3	1:B:189:THR:HG21	1.74	0.70
1:B:22:THR:HB	1:B:49:LEU:HD23	1.73	0.70
1:B:261:ALA:HB3	1:B:379:ARG:NH2	2.07	0.70
1:B:563:ARG:HA	1:B:578:ILE:HD11	1.74	0.70
1:A:601:ILE:HD12	1:A:615:VAL:HG22	1.74	0.70
1:A:89:TYR:HB2	1:A:92:VAL:CG2	2.22	0.70
1:A:114:ILE:HD11	1:A:215:GLN:CB	2.21	0.69
1:B:141:VAL:CG1	1:B:145:GLU:HB3	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:HIS:CD2	1:B:177:PHE:HB2	2.27	0.69
1:B:231:HIS:O	1:B:232:LEU:HD23	1.92	0.69
1:B:431:GLU:O	1:B:431:GLU:HG2	1.92	0.69
1:A:301:VAL:HG23	1:A:328:SER:O	1.91	0.69
1:A:589:ILE:HG23	1:A:600:GLN:NE2	2.07	0.69
1:A:424:TYR:OH	1:A:448:LYS:HE3	1.92	0.69
1:A:478:THR:HG22	1:A:479:ALA:N	2.05	0.69
1:A:114:ILE:HD11	1:A:215:GLN:HB2	1.74	0.69
1:A:384:ASN:HD22	1:A:521:VAL:N	1.82	0.69
1:A:18:LYS:CE	1:A:54:GLU:HG3	2.23	0.68
1:B:156:LYS:CG	1:B:180:LEU:HD12	2.22	0.68
1:A:449:GLU:O	1:A:453:GLU:HG3	1.93	0.68
1:B:4:ILE:CG2	1:B:16:PHE:H	2.05	0.68
1:A:298:LEU:HD23	1:B:331:LEU:HD11	1.75	0.68
1:B:490:GLN:N	1:B:517:HIS:O	2.22	0.68
1:A:488:THR:O	1:A:518:ARG:HA	1.94	0.68
1:B:110:ILE:HB	1:B:215:GLN:HE21	1.59	0.68
1:B:274:ARG:O	1:B:278:GLU:HG3	1.93	0.68
1:A:616:ARG:NH2	1:A:623:GLN:HE22	1.90	0.68
1:B:351:ARG:HH11	1:B:351:ARG:HG3	1.59	0.68
1:B:160:ILE:HD11	1:B:180:LEU:HD11	1.73	0.68
1:B:518:ARG:O	1:B:518:ARG:HD3	1.93	0.68
1:A:410:TYR:OH	1:A:486:LEU:HD23	1.94	0.68
1:A:322:GLN:OE1	1:A:323:LEU:HD12	1.94	0.68
1:B:512:ARG:HH11	1:B:512:ARG:HG3	1.58	0.67
1:B:353:LEU:HD12	1:B:391:ARG:N	2.09	0.67
1:A:185:HIS:NE2	4:A:1003:HOH:O	2.27	0.67
1:B:74:ARG:HD2	1:B:103:GLY:HA2	1.77	0.67
1:A:8:PHE:CD2	1:A:9:PRO:HD2	2.29	0.67
1:B:494:LEU:CD2	1:B:498:ARG:HD2	2.25	0.67
1:A:406:ILE:HD13	1:A:487:SER:CB	2.24	0.67
1:A:526:ARG:HH11	1:A:526:ARG:HB2	1.60	0.67
1:B:612:GLN:HG2	1:B:627:GLU:HA	1.78	0.66
1:A:473:ASP:HB3	1:A:475:GLN:NE2	2.10	0.66
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.59	0.66
1:A:174:GLN:HE22	1:A:189:THR:HG21	1.60	0.66
1:B:214:LEU:HD13	1:B:214:LEU:N	2.10	0.66
1:A:319:PRO:HG2	1:B:321:MET:HB2	1.77	0.66
1:A:113:ASN:O	1:A:114:ILE:HG23	1.96	0.66
1:A:8:PHE:CE2	1:A:29:ILE:HD11	2.30	0.66
1:B:488:THR:O	1:B:518:ARG:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLU:HG2	1:B:440:TRP:NE1	2.10	0.66
1:B:476:VAL:HG21	1:B:530:PHE:CZ	2.30	0.66
1:A:204:TYR:CE2	1:A:209:SER:HA	2.30	0.65
1:B:48:ASP:HB2	1:B:138:ARG:HH11	1.57	0.65
1:B:4:ILE:HG21	1:B:16:PHE:O	1.97	0.65
1:A:304:TYR:CE1	1:A:337:PRO:HG3	2.29	0.65
1:B:303:LEU:CD2	1:B:337:PRO:HB2	2.24	0.65
1:A:80:LEU:HG	1:A:126:MET:HB2	1.77	0.65
1:B:497:GLU:HA	1:B:512:ARG:NE	2.10	0.65
1:A:323:LEU:HD13	1:A:323:LEU:O	1.95	0.65
1:A:75:HIS:NE2	4:A:1003:HOH:O	2.30	0.65
1:B:428:GLU:OE1	1:B:435:ASP:HA	1.97	0.65
1:B:75:HIS:CE1	1:B:181:CYS:SG	2.90	0.65
1:A:323:LEU:HG	1:B:366:TYR:OH	1.96	0.65
1:A:454:LEU:HB3	1:A:456:LEU:CD1	2.27	0.65
1:A:36:LYS:NZ	1:A:36:LYS:HB2	2.12	0.65
1:B:579:ASP:OD2	1:B:581:ARG:NH2	2.29	0.65
1:B:160:ILE:HD11	1:B:180:LEU:HD13	1.78	0.65
1:A:281:ILE:CG2	1:A:282:VAL:N	2.60	0.65
1:A:146:ALA:O	1:A:149:LEU:HB3	1.96	0.65
1:A:8:PHE:CB	1:A:9:PRO:HD2	2.27	0.64
1:A:312:HIS:CE1	1:A:429:ASP:HB2	2.33	0.64
1:A:353:LEU:O	1:A:355:ILE:N	2.30	0.64
1:B:75:HIS:CE1	1:B:181:CYS:HG	2.15	0.64
1:A:554:ASN:ND2	1:A:554:ASN:C	2.51	0.64
1:A:403:VAL:HG12	1:A:407:ILE:CD1	2.28	0.64
1:A:403:VAL:HG12	1:A:407:ILE:HD12	1.80	0.64
1:B:89:TYR:OH	1:B:114:ILE:HG22	1.97	0.64
1:A:170:THR:OG1	1:A:182:ARG:HG2	1.97	0.64
1:B:406:ILE:HD13	1:B:487:SER:HB2	1.78	0.64
1:A:305:LYS:HD3	1:A:310:TRP:CG	2.33	0.64
1:A:621:GLN:HG2	1:A:622:ASP:N	2.13	0.64
1:A:323:LEU:HD11	1:A:326:THR:HG21	1.79	0.64
1:B:376:GLN:NE2	4:B:2055:HOH:O	2.31	0.64
1:B:156:LYS:CB	1:B:180:LEU:HD12	2.28	0.64
1:B:392:PRO:HA	1:B:395:ILE:HG13	1.79	0.63
1:B:287:SER:C	1:B:289:GLY:H	1.99	0.63
1:A:478:THR:CG2	1:A:479:ALA:N	2.62	0.63
1:B:429:ASP:N	4:B:2005:HOH:O	2.32	0.63
1:B:604:GLY:O	1:B:608:VAL:HG23	1.98	0.63
1:B:126:MET:O	1:B:130:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD13	1:A:353:LEU:O	1.99	0.63
1:A:517:HIS:HB3	3:A:1002:TSB:OG1	1.99	0.63
1:A:194:GLU:HG3	1:A:225:LYS:HA	1.81	0.63
1:A:258:LEU:HD23	1:A:258:LEU:O	1.99	0.63
1:B:645:ARG:HD3	1:B:645:ARG:C	2.19	0.63
1:B:171:LEU:HD22	1:B:178:THR:CG2	2.28	0.63
1:B:601:ILE:HG22	1:B:601:ILE:O	1.97	0.62
1:B:25:ILE:HG21	1:B:59:ILE:CD1	2.29	0.62
1:B:323:LEU:HD12	1:B:324:ASP:N	2.14	0.62
1:A:467:PHE:CD1	1:A:467:PHE:C	2.72	0.62
1:A:522:SER:OG	1:A:523:THR:N	2.31	0.62
1:A:391:ARG:NH1	1:A:393:ASP:OD1	2.32	0.62
1:A:621:GLN:HG2	1:A:622:ASP:H	1.64	0.62
1:A:482:LYS:NZ	1:A:482:LYS:HA	2.14	0.62
1:B:606:LYS:HD2	1:B:606:LYS:H	1.64	0.62
1:A:110:ILE:HG22	1:A:112:GLN:H	1.65	0.62
1:B:4:ILE:HG12	1:B:5:ASN:N	2.12	0.62
1:A:323:LEU:HD13	1:A:326:THR:OG1	2.00	0.62
1:B:604:GLY:N	1:B:607:GLU:OE1	2.31	0.62
1:B:417:ASP:N	1:B:417:ASP:OD1	2.26	0.62
1:B:215:GLN:OE1	1:B:215:GLN:N	2.33	0.62
1:B:480:MET:C	1:B:482:LYS:H	2.03	0.62
1:A:566:GLN:HB2	1:A:578:ILE:HD11	1.81	0.62
1:A:143:ARG:HH11	1:A:163:ILE:HA	1.63	0.62
1:A:160:ILE:HD13	1:A:180:LEU:HD11	1.81	0.62
1:B:9:PRO:HD3	1:B:59:ILE:O	2.00	0.61
1:A:8:PHE:CG	1:A:9:PRO:HD2	2.34	0.61
1:A:129:ILE:O	1:A:129:ILE:HD12	2.01	0.61
1:B:471:LYS:HB3	1:B:490:GLN:HG2	1.82	0.61
1:B:130:VAL:O	1:B:132:GLU:N	2.34	0.61
1:B:518:ARG:C	1:B:518:ARG:HD3	2.21	0.61
1:B:587:TYR:C	1:B:589:ILE:H	2.04	0.61
1:A:584:LYS:O	1:A:587:TYR:N	2.34	0.61
1:B:488:THR:HG23	1:B:488:THR:O	2.01	0.61
1:A:143:ARG:NH1	1:A:163:ILE:HA	2.16	0.61
1:A:645:ARG:HG2	1:A:645:ARG:O	2.00	0.61
1:A:326:THR:HG22	1:A:327:GLU:HG3	1.82	0.61
1:A:222:PHE:HD2	1:A:228:LEU:HD12	1.64	0.61
1:A:42:PHE:O	1:A:43:ASN:HB2	2.01	0.60
1:B:621:GLN:O	1:B:623:GLN:N	2.35	0.60
1:A:31:PRO:HA	1:A:34:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:HB2	4:A:1043:HOH:O	2.00	0.60
1:A:478:THR:HG22	1:A:480:MET:N	2.13	0.60
1:A:336:CYS:HB2	1:A:337:PRO:CD	2.31	0.60
1:B:110:ILE:HB	1:B:215:GLN:CG	2.31	0.60
1:B:95:GLY:HA2	1:B:155:TYR:HB2	1.83	0.60
1:B:404:ASN:HA	1:B:407:ILE:HD12	1.83	0.60
1:B:241:ARG:HG3	1:B:536:LYS:HG2	1.83	0.60
1:B:554:ASN:HB3	1:B:557:LEU:CB	2.25	0.60
1:A:390:VAL:HB	1:A:394:GLN:HG3	1.83	0.60
1:B:304:TYR:HE1	1:B:337:PRO:HG3	1.66	0.60
1:B:545:PRO:O	1:B:575:ARG:HD2	2.01	0.60
3:A:1002:TSB:H4'	4:A:1040:HOH:O	2.01	0.60
1:B:66:SER:HB3	1:B:69:ALA:HB3	1.82	0.60
1:A:105:TYR:HA	1:A:217:ILE:O	2.02	0.60
1:B:391:ARG:HB3	1:B:503:TYR:CZ	2.37	0.60
1:B:388:ILE:O	1:B:515:VAL:HA	2.01	0.60
1:B:186:VAL:CG1	1:B:191:LYS:HB3	2.31	0.59
1:B:326:THR:HB	4:B:2069:HOH:O	2.02	0.59
1:A:21:THR:HG22	1:A:50:THR:O	2.03	0.59
1:A:473:ASP:HB3	1:A:475:GLN:HE21	1.67	0.59
1:A:403:VAL:O	1:A:407:ILE:HD12	2.01	0.59
1:B:353:LEU:HD12	1:B:391:ARG:H	1.67	0.59
1:B:141:VAL:HG11	1:B:145:GLU:HB3	1.84	0.59
1:B:234:MET:SD	1:B:235:LEU:HD23	2.42	0.59
1:A:323:LEU:HD13	1:A:326:THR:CB	2.32	0.59
1:B:137:GLU:HG3	1:B:137:GLU:O	2.03	0.59
1:B:171:LEU:HD22	1:B:178:THR:HG22	1.83	0.59
1:B:41:LYS:HA	1:B:45:GLN:O	2.03	0.59
1:A:73:LEU:HD22	1:A:223:PHE:CE1	2.37	0.59
1:B:322:GLN:HB3	1:B:328:SER:HB3	1.83	0.59
1:A:20:THR:HG21	1:A:25:ILE:HG13	1.83	0.59
1:A:321:MET:HE3	1:B:321:MET:SD	2.43	0.59
1:B:612:GLN:HA	1:B:628:LYS:H	1.68	0.59
1:A:181:CYS:HB3	4:A:1003:HOH:O	2.02	0.59
1:B:27:GLN:HE21	1:B:27:GLN:HA	1.68	0.58
1:A:285:GLU:OE2	1:A:518:ARG:NH2	2.36	0.58
1:B:83:HIS:NE2	1:B:177:PHE:HB2	2.19	0.58
1:B:81:MET:HA	1:B:126:MET:SD	2.43	0.58
1:A:235:LEU:O	1:A:239:LYS:HG3	2.03	0.58
1:A:316:ASP:OD1	1:A:316:ASP:N	2.36	0.58
1:A:398:GLU:O	1:A:402:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ILE:HG23	1:A:588:LYS:HD3	1.85	0.58
1:B:582:ASN:O	1:B:583:GLU:HG2	2.04	0.58
1:B:4:ILE:CG2	1:B:16:PHE:O	2.52	0.58
1:B:579:ASP:OD1	1:B:581:ARG:NE	2.36	0.58
1:A:388:ILE:HD12	1:A:388:ILE:N	2.17	0.58
1:A:308:GLY:O	1:A:312:HIS:HD2	1.87	0.58
1:B:550:ILE:HG23	1:B:601:ILE:CG2	2.30	0.58
1:B:422:LEU:HG	1:B:447:LEU:HD11	1.86	0.58
1:A:306:THR:O	1:A:498:ARG:HB3	2.04	0.58
1:B:565:LEU:CD2	1:B:601:ILE:HG21	2.34	0.57
1:A:322:GLN:HG2	1:A:329:MET:HG2	1.84	0.57
1:B:336:CYS:N	1:B:337:PRO:HD2	2.19	0.57
1:B:383:LEU:HD22	3:B:2002:TSB:H5'1	1.85	0.57
1:A:601:ILE:CD1	1:A:615:VAL:HG22	2.33	0.57
1:B:471:LYS:NZ	1:B:473:ASP:OD2	2.37	0.57
1:A:612:GLN:HE22	1:A:625:THR:HG21	1.67	0.57
1:B:428:GLU:CG	1:B:440:TRP:HE1	2.16	0.57
1:B:422:LEU:HG	1:B:447:LEU:CD1	2.35	0.57
1:B:110:ILE:HB	1:B:215:GLN:NE2	2.19	0.57
1:B:198:LEU:HG	1:B:219:GLY:HA2	1.86	0.57
1:A:242:ASP:OD1	1:A:244:ARG:HB2	2.04	0.57
1:A:186:VAL:HG13	1:A:188:SER:H	1.69	0.57
1:B:194:GLU:HG3	1:B:225:LYS:N	2.19	0.57
1:B:125:THR:O	1:B:129:ILE:HG13	2.04	0.57
1:A:410:TYR:CZ	1:A:486:LEU:HD23	2.39	0.57
1:A:366:TYR:CE2	1:B:323:LEU:HB2	2.40	0.57
1:A:8:PHE:HE2	1:A:29:ILE:HD11	1.69	0.57
1:B:553:VAL:HG23	1:B:603:VAL:O	2.04	0.57
1:A:559:TYR:O	1:A:562:ALA:N	2.37	0.57
1:A:563:ARG:HG3	1:A:563:ARG:HH11	1.69	0.57
1:A:342:ILE:HD13	1:B:267:LEU:HD23	1.87	0.57
1:B:134:MET:HB2	1:B:174:GLN:OE1	2.04	0.57
1:B:521:VAL:O	1:B:521:VAL:HG13	2.05	0.57
1:B:585:MET:HA	1:B:588:LYS:HB2	1.85	0.57
1:B:82:ALA:HB2	1:B:106:TYR:CD2	2.39	0.57
1:A:4:ILE:HD13	1:A:18:LYS:HA	1.86	0.57
1:A:163:ILE:HG22	1:A:163:ILE:O	2.04	0.57
1:B:139:LYS:HE3	1:B:141:VAL:HG21	1.86	0.57
1:A:423:SER:HB2	1:A:464:GLU:C	2.25	0.57
1:A:554:ASN:HD22	1:A:555:VAL:N	2.02	0.57
1:A:157:LEU:O	1:A:160:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASN:HB3	1:B:56:ASP:OD1	2.03	0.57
1:B:569:LEU:CD2	1:B:632:ILE:HG13	2.35	0.57
1:A:89:TYR:HB2	1:A:92:VAL:HG21	1.86	0.57
1:A:424:TYR:O	1:A:462:ILE:HD12	2.05	0.57
1:A:554:ASN:ND2	1:A:557:LEU:H	2.03	0.56
1:A:324:ASP:O	1:A:326:THR:N	2.37	0.56
1:B:66:SER:HB3	1:B:69:ALA:CB	2.34	0.56
1:A:288:MET:SD	1:A:405:MET:CE	2.93	0.56
1:A:454:LEU:HB3	1:A:456:LEU:HD13	1.85	0.56
1:B:139:LYS:HE3	1:B:141:VAL:CG2	2.36	0.56
1:A:313:TYR:CE1	1:A:316:ASP:HB2	2.41	0.56
1:A:115:SER:C	1:A:117:ASP:H	2.09	0.56
1:A:259:VAL:O	1:B:299:ALA:HA	2.05	0.56
1:A:456:LEU:CD1	1:A:456:LEU:N	2.69	0.56
1:A:621:GLN:HG2	1:A:622:ASP:CG	2.25	0.56
1:A:323:LEU:CD1	1:A:326:THR:CB	2.83	0.56
1:B:162:ALA:HB1	1:B:164:PRO:HD3	1.87	0.56
1:B:148:GLU:O	1:B:150:PHE:N	2.38	0.56
1:A:353:LEU:O	1:A:389:PHE:O	2.23	0.56
1:B:49:LEU:HD12	1:B:187:PRO:HG3	1.86	0.56
1:B:234:MET:SD	1:B:234:MET:C	2.85	0.56
1:B:322:GLN:CA	1:B:328:SER:HA	2.23	0.56
1:B:473:ASP:HB3	1:B:485:THR:HG23	1.87	0.55
1:A:336:CYS:N	1:A:337:PRO:HD2	2.21	0.55
1:B:390:VAL:HB	1:B:394:GLN:OE1	2.05	0.55
1:B:114:ILE:HD11	1:B:200:THR:HG21	1.88	0.55
1:A:637:ASP:OD2	1:A:640:ARG:NH2	2.37	0.55
1:B:327:GLU:OE1	1:B:327:GLU:HA	2.05	0.55
1:B:351:ARG:NH1	1:B:351:ARG:HG3	2.21	0.55
1:A:130:VAL:HG13	1:A:189:THR:O	2.07	0.55
1:A:34:ARG:HG3	1:A:35:LYS:N	2.21	0.55
1:B:136:ILE:HG13	1:B:136:ILE:O	2.05	0.55
1:A:204:TYR:CE1	1:A:207:GLY:HA2	2.35	0.55
1:B:522:SER:OG	1:B:523:THR:N	2.39	0.55
1:B:73:LEU:HD21	1:B:222:PHE:O	2.06	0.55
1:A:409:VAL:O	1:A:412:ASP:HB2	2.06	0.55
1:A:119:PHE:O	1:A:123:GLU:HB2	2.07	0.55
1:B:193:LYS:HD2	1:B:193:LYS:N	2.22	0.55
1:A:579:ASP:OD1	1:A:588:LYS:HE2	2.07	0.55
1:A:428:GLU:CB	1:A:440:TRP:HE1	2.19	0.55
1:A:384:ASN:ND2	1:A:521:VAL:HG12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG13	1:B:292:HIS:CE1	2.41	0.55
1:A:4:ILE:O	1:A:6:ILE:HG13	2.07	0.55
1:B:6:ILE:HD13	1:B:25:ILE:HD13	1.88	0.55
1:A:376:GLN:NE2	1:A:484:GLU:OE1	2.40	0.55
1:A:162:ALA:HB3	1:A:167:GLU:OE2	2.06	0.55
1:A:340:MET:HG3	1:A:501:LEU:HD11	1.88	0.55
1:A:584:LYS:O	1:A:585:MET:C	2.46	0.54
1:A:480:MET:HE3	1:A:482:LYS:HG3	1.89	0.54
1:A:115:SER:C	1:A:117:ASP:N	2.61	0.54
1:A:288:MET:SD	1:A:405:MET:HE3	2.48	0.54
1:B:430:LYS:CG	1:B:431:GLU:H	2.20	0.54
1:A:163:ILE:N	1:A:164:PRO:CD	2.69	0.54
1:A:561:TYR:O	1:A:564:GLN:HB3	2.07	0.54
1:A:45:GLN:NE2	4:A:1062:HOH:O	2.40	0.54
1:B:556:ASP:HB2	4:B:2033:HOH:O	2.07	0.54
1:A:425:ARG:NH2	1:A:437:ASP:HA	2.23	0.54
1:B:83:HIS:CE1	1:B:177:PHE:HB2	2.42	0.54
1:B:143:ARG:O	1:B:147:LYS:HB2	2.07	0.54
1:A:324:ASP:C	1:A:326:THR:H	2.10	0.54
1:A:323:LEU:CD1	1:A:326:THR:HB	2.37	0.54
1:B:423:SER:HB3	1:B:465:ALA:N	2.22	0.54
1:A:29:ILE:O	1:A:30:SER:HB3	2.08	0.54
1:B:214:LEU:HD13	1:B:214:LEU:H	1.71	0.54
1:B:149:LEU:HG	1:B:150:PHE:CD1	2.42	0.54
1:B:448:LYS:O	1:B:451:ALA:HB3	2.08	0.54
1:B:8:PHE:CE1	1:B:59:ILE:HD11	2.43	0.54
1:A:181:CYS:SG	4:A:1003:HOH:O	2.59	0.54
1:B:449:GLU:O	1:B:453:GLU:HG3	2.08	0.54
1:A:429:ASP:O	1:A:494:LEU:HD11	2.08	0.54
1:A:155:TYR:CD1	1:A:205:TRP:CZ3	2.96	0.54
1:B:428:GLU:CB	1:B:440:TRP:HE1	2.21	0.54
1:B:644:HIS:CD2	1:B:644:HIS:N	2.74	0.54
1:B:147:LYS:HA	1:B:160:ILE:HG21	1.90	0.53
1:B:445:ASN:O	1:B:449:GLU:HG3	2.08	0.53
1:A:344:ALA:O	1:A:346:LYS:N	2.41	0.53
1:B:250:LEU:HD11	1:B:595:GLN:HA	1.89	0.53
1:B:163:ILE:N	1:B:164:PRO:CD	2.68	0.53
1:B:231:HIS:ND1	1:B:231:HIS:O	2.41	0.53
1:A:490:GLN:CG	1:A:517:HIS:HB2	2.38	0.53
1:A:174:GLN:O	1:A:176:ASP:N	2.38	0.53
1:B:244:ARG:HB3	4:B:2015:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:GLN:HG3	1:B:575:ARG:HB2	1.90	0.53
1:A:467:PHE:O	1:A:467:PHE:HD1	1.92	0.53
1:A:342:ILE:CD1	1:B:267:LEU:HD23	2.38	0.53
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.74	0.53
1:B:132:GLU:OE1	1:B:134:MET:HE1	2.08	0.53
1:B:87:ARG:HD2	1:B:125:THR:HG23	1.90	0.53
1:A:85:ILE:HG13	1:A:108:PHE:CZ	2.43	0.53
1:A:20:THR:CG2	1:A:21:THR:N	2.70	0.53
1:A:566:GLN:NE2	1:A:578:ILE:HD12	2.24	0.53
1:A:21:THR:CG2	1:A:50:THR:O	2.57	0.53
1:A:554:ASN:CG	1:A:557:LEU:HB2	2.28	0.53
1:B:494:LEU:HD22	1:B:498:ARG:HD2	1.91	0.53
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.23	0.53
1:A:212:LYS:HG3	1:A:213:MET:N	2.24	0.53
1:A:367:GLU:OE1	1:A:377:ARG:HD2	2.09	0.53
1:B:590:ARG:O	1:B:594:MET:HG3	2.08	0.53
1:B:475:GLN:NE2	1:B:485:THR:HG23	2.23	0.53
1:A:391:ARG:HD3	1:A:503:TYR:CE1	2.43	0.53
1:B:136:ILE:HD12	1:B:136:ILE:C	2.29	0.53
1:B:354:PRO:HA	1:B:390:VAL:HG12	1.91	0.53
1:A:37:ALA:HB3	1:A:49:LEU:HD11	1.89	0.53
1:B:402:VAL:O	1:B:406:ILE:HG13	2.09	0.52
1:B:105:TYR:HA	1:B:217:ILE:O	2.09	0.52
1:B:21:THR:HG22	1:B:52:PRO:HA	1.91	0.52
1:A:526:ARG:HH11	1:A:526:ARG:CB	2.20	0.52
1:A:253:PHE:CE2	1:A:375:LEU:HG	2.45	0.52
1:B:570:LYS:C	1:B:572:GLN:N	2.61	0.52
1:B:479:ALA:O	1:B:480:MET:HG3	2.09	0.52
1:A:618:TYR:C	1:A:620:SER:H	2.12	0.52
1:A:115:SER:O	1:A:117:ASP:N	2.42	0.52
1:A:70:LEU:HD23	1:A:74:ARG:CZ	2.40	0.52
1:B:631:PHE:HD2	1:B:632:ILE:HD12	1.74	0.52
1:B:298:LEU:CD2	1:B:331:LEU:HD23	2.39	0.52
1:A:245:LYS:O	1:A:249:GLU:HB2	2.10	0.52
1:B:22:THR:HB	1:B:49:LEU:CD2	2.38	0.52
1:B:21:THR:O	1:B:25:ILE:HG13	2.09	0.52
1:A:132:GLU:OE1	1:A:134:MET:HE2	2.09	0.52
1:A:135:LYS:HE2	1:A:137:GLU:HG2	1.92	0.52
1:A:20:THR:CG2	1:A:25:ILE:HG13	2.40	0.52
1:A:337:PRO:O	1:A:340:MET:HB2	2.10	0.52
1:B:223:PHE:O	1:B:224:ASP:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.23	0.52
1:B:561:TYR:CD2	1:B:608:VAL:HG22	2.45	0.52
1:B:570:LYS:C	1:B:572:GLN:H	2.13	0.52
1:A:518:ARG:HD3	1:A:518:ARG:C	2.27	0.52
1:A:612:GLN:NE2	1:A:625:THR:CG2	2.69	0.52
1:B:542:TRP:CZ2	1:B:543:LEU:HD21	2.45	0.52
1:A:281:ILE:HG23	1:A:282:VAL:N	2.24	0.52
1:A:388:ILE:CD1	1:A:388:ILE:N	2.72	0.52
1:A:186:VAL:HG13	1:A:188:SER:O	2.09	0.52
1:B:598:PRO:HB2	1:B:599:TYR:HD1	1.75	0.52
1:B:174:GLN:CG	1:B:189:THR:HG21	2.40	0.52
1:B:429:ASP:O	1:B:430:LYS:HB2	2.09	0.52
1:A:322:GLN:CB	1:A:327:GLU:O	2.58	0.52
1:A:79:HIS:CD2	1:A:185:HIS:NE2	2.78	0.52
1:B:434:PHE:HE2	1:B:438:ASP:OD1	1.92	0.52
1:B:246:ILE:HG21	1:B:532:THR:CG2	2.40	0.52
1:A:243:HIS:HB3	1:A:533:GLU:HG3	1.92	0.52
1:B:224:ASP:OD2	1:B:226:LYS:HB3	2.10	0.51
1:A:426:ASP:OD1	1:A:463:GLY:HA2	2.09	0.51
1:A:4:ILE:HG23	1:A:18:LYS:HB2	1.91	0.51
1:B:563:ARG:HG3	1:B:563:ARG:HH11	1.75	0.51
1:A:515:VAL:HG12	1:A:517:HIS:CD2	2.45	0.51
1:A:392:PRO:HG3	4:A:1075:HOH:O	2.09	0.51
1:B:481:GLY:O	1:B:483:GLU:N	2.43	0.51
1:B:95:GLY:O	1:B:155:TYR:HB2	2.11	0.51
1:A:384:ASN:HD21	1:A:520:VAL:HB	1.75	0.51
1:B:565:LEU:HD21	1:B:601:ILE:HG21	1.93	0.51
1:A:157:LEU:HA	1:A:160:ILE:HG22	1.92	0.51
1:B:392:PRO:HA	1:B:395:ILE:CD1	2.40	0.51
1:A:258:LEU:HD21	1:B:303:LEU:HA	1.93	0.51
1:A:114:ILE:HD11	1:A:215:GLN:HB3	1.91	0.51
1:B:615:VAL:HG23	1:B:623:GLN:CB	2.37	0.51
1:A:321:MET:O	1:A:328:SER:HA	2.11	0.51
1:B:477:LYS:CE	1:B:483:GLU:OE2	2.59	0.51
1:B:261:ALA:HB3	1:B:379:ARG:HH21	1.73	0.51
1:B:458:TYR:N	1:B:458:TYR:CD1	2.79	0.51
1:B:186:VAL:O	1:B:188:SER:N	2.44	0.51
1:B:188:SER:C	1:B:190:ALA:H	2.14	0.51
1:B:83:HIS:CE1	1:B:174:GLN:HE21	2.29	0.51
1:A:554:ASN:OD1	1:A:557:LEU:HB2	2.11	0.51
1:A:591:GLU:HG2	1:A:595:GLN:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:O	1:A:475:GLN:N	2.40	0.51
1:A:73:LEU:HD22	1:A:223:PHE:CD1	2.46	0.51
1:B:84:ALA:HA	1:B:129:ILE:CD1	2.41	0.51
1:B:42:PHE:H	1:B:47:VAL:CG1	2.24	0.51
1:A:336:CYS:HA	1:A:387:HIS:CE1	2.46	0.51
1:B:543:LEU:O	1:B:544:ALA:C	2.48	0.51
1:A:426:ASP:O	1:A:428:GLU:N	2.44	0.50
1:A:482:LYS:HZ3	1:A:482:LYS:HA	1.75	0.50
1:A:422:LEU:HD22	1:A:447:LEU:HD21	1.93	0.50
1:B:459:GLU:O	1:B:460:GLU:C	2.49	0.50
1:B:131:ASN:ND2	1:B:131:ASN:H	2.10	0.50
1:B:97:GLY:HA3	1:B:106:TYR:CD1	2.45	0.50
1:B:449:GLU:O	1:B:453:GLU:CG	2.60	0.50
1:A:132:GLU:OE1	1:A:134:MET:CE	2.59	0.50
1:A:21:THR:H	1:A:24:ASP:HB2	1.76	0.50
1:B:13:LYS:O	1:B:13:LYS:HD3	2.12	0.50
1:B:114:ILE:O	1:B:115:SER:HB3	2.11	0.50
1:A:154:GLU:O	1:A:158:GLU:HG2	2.11	0.50
1:A:428:GLU:HB3	1:A:440:TRP:HE1	1.75	0.50
1:B:1:MET:HG2	1:B:1:MET:O	2.11	0.50
1:B:392:PRO:HA	1:B:395:ILE:CG1	2.42	0.50
1:B:383:LEU:HD12	1:B:384:ASN:H	1.77	0.50
1:A:322:GLN:OE1	1:A:323:LEU:CD1	2.59	0.50
1:B:139:LYS:HG2	1:B:141:VAL:HG23	1.93	0.50
1:B:376:GLN:HG2	4:B:2059:HOH:O	2.10	0.50
1:B:249:GLU:O	1:B:595:GLN:NE2	2.45	0.50
1:B:439:MET:O	1:B:442:LYS:HB3	2.12	0.50
1:A:261:ALA:O	1:A:379:ARG:HD2	2.11	0.50
1:A:181:CYS:CB	4:A:1003:HOH:O	2.60	0.50
1:A:630:GLU:O	1:A:633:TRP:HB3	2.10	0.50
1:B:303:LEU:HD23	1:B:304:TYR:CZ	2.46	0.50
1:A:555:VAL:CG2	1:A:555:VAL:O	2.59	0.50
1:A:313:TYR:CD1	1:A:316:ASP:HB2	2.47	0.50
1:A:8:PHE:HB3	1:A:9:PRO:HD2	1.92	0.50
1:B:129:ILE:HG22	1:B:129:ILE:O	2.12	0.49
1:B:5:ASN:HB3	1:B:56:ASP:CG	2.32	0.49
1:A:84:ALA:HB2	1:A:126:MET:HB3	1.94	0.49
1:B:428:GLU:OE1	1:B:435:ASP:CA	2.60	0.49
1:A:242:ASP:OD1	1:A:244:ARG:N	2.35	0.49
1:B:444:GLU:HG2	1:B:470:PRO:HB3	1.94	0.49
1:B:132:GLU:HB2	1:B:134:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:CG	1:B:136:ILE:H	2.04	0.49
1:B:83:HIS:HE1	1:B:174:GLN:HE21	1.58	0.49
1:B:287:SER:C	1:B:289:GLY:N	2.66	0.49
1:B:422:LEU:CD1	1:B:422:LEU:N	2.75	0.49
1:B:470:PRO:HD2	1:B:491:LEU:O	2.11	0.49
1:A:288:MET:SD	1:A:405:MET:HE1	2.53	0.49
1:B:500:ASP:HA	1:B:512:ARG:NH2	2.26	0.49
1:B:139:LYS:HG2	1:B:141:VAL:CG2	2.42	0.49
1:A:4:ILE:C	1:A:56:ASP:HB3	2.32	0.49
1:B:163:ILE:H	1:B:164:PRO:HD3	1.71	0.49
1:A:383:LEU:HD23	1:A:385:ASP:HB2	1.94	0.49
1:B:569:LEU:HD21	1:B:632:ILE:HG13	1.93	0.49
1:A:110:ILE:HB	1:A:112:GLN:O	2.13	0.49
1:A:490:GLN:HG2	1:A:517:HIS:HB2	1.94	0.49
1:B:132:GLU:HB2	1:B:134:MET:CE	2.42	0.49
1:A:155:TYR:HB3	1:A:205:TRP:CZ3	2.48	0.49
1:A:424:TYR:HH	1:A:448:LYS:HE3	1.77	0.49
1:A:174:GLN:NE2	1:A:189:THR:HG21	2.28	0.49
1:A:621:GLN:CG	1:A:622:ASP:H	2.21	0.49
1:A:7:GLN:HG2	1:A:13:LYS:HG2	1.95	0.49
1:B:187:PRO:HA	4:B:2045:HOH:O	2.12	0.49
1:B:27:GLN:HE21	1:B:34:ARG:HD3	1.76	0.49
1:A:5:ASN:HB3	1:A:56:ASP:OD2	2.13	0.49
1:A:500:ASP:HA	1:A:512:ARG:NH1	2.27	0.49
1:A:322:GLN:HB3	1:A:327:GLU:O	2.13	0.49
1:B:137:GLU:HG2	4:B:2021:HOH:O	2.12	0.49
1:B:422:LEU:HD12	1:B:422:LEU:N	2.27	0.49
1:A:568:GLU:O	1:A:571:SER:OG	2.25	0.49
1:B:480:MET:O	1:B:482:LYS:N	2.40	0.49
1:B:323:LEU:HD13	1:B:324:ASP:OD2	2.12	0.49
1:B:583:GLU:O	1:B:588:LYS:HE2	2.11	0.49
1:B:195:PHE:N	1:B:195:PHE:CD1	2.81	0.49
1:B:210:ASN:O	1:B:211:ASN:CG	2.51	0.49
1:B:318:PHE:HE1	1:B:365:ARG:O	1.96	0.49
1:A:428:GLU:CG	1:A:440:TRP:HE1	2.26	0.49
1:B:325:GLU:O	1:B:327:GLU:HG2	2.12	0.49
1:A:569:LEU:HB3	1:A:574:VAL:HB	1.94	0.49
1:B:2:GLU:HA	1:B:17:ASP:HB3	1.95	0.48
1:A:313:TYR:O	1:A:315:GLU:N	2.45	0.48
1:B:148:GLU:O	1:B:149:LEU:C	2.51	0.48
1:A:432:LYS:O	1:A:434:PHE:CD2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:HD11	1:B:514:VAL:CG2	2.20	0.48
1:A:554:ASN:HD21	1:A:556:ASP:HB2	1.79	0.48
1:A:602:VAL:O	1:A:614:ASN:HB3	2.12	0.48
1:B:397:GLU:OE1	1:B:398:GLU:N	2.46	0.48
1:A:187:PRO:O	1:A:188:SER:HB2	2.13	0.48
1:B:593:GLN:O	1:B:596:LYS:N	2.46	0.48
1:B:601:ILE:CD1	1:B:615:VAL:HG12	2.36	0.48
1:B:355:ILE:N	4:B:2048:HOH:O	2.45	0.48
1:A:399:PHE:HE2	1:A:472:LEU:HD12	1.79	0.48
1:B:312:HIS:HE1	1:B:429:ASP:HB2	1.75	0.48
1:A:122:ILE:O	1:A:126:MET:HG2	2.13	0.48
1:B:140:VAL:HG22	1:B:170:THR:CG2	2.44	0.48
1:A:531:LEU:O	1:A:535:THR:CG2	2.54	0.48
1:B:473:ASP:HB3	1:B:475:GLN:HE21	1.77	0.48
1:A:486:LEU:O	1:A:522:SER:HB2	2.13	0.48
1:B:203:ALA:O	1:B:214:LEU:HD22	2.13	0.48
1:B:558:HIS:NE2	1:B:604:GLY:C	2.67	0.48
1:B:210:ASN:O	1:B:211:ASN:ND2	2.46	0.48
1:B:410:TYR:H	1:B:410:TYR:HD1	1.61	0.48
1:A:555:VAL:HG23	1:A:555:VAL:O	2.13	0.48
1:A:194:GLU:HG3	1:A:225:LYS:CA	2.44	0.48
1:B:277:ILE:O	1:B:280:TYR:HB3	2.14	0.48
1:A:169:VAL:HG23	1:A:169:VAL:O	2.13	0.48
1:A:458:TYR:CD1	1:A:458:TYR:N	2.81	0.48
1:B:593:GLN:O	1:B:594:MET:C	2.51	0.48
1:A:281:ILE:HG22	1:A:282:VAL:H	1.77	0.48
1:A:356:ARG:NH1	1:A:398:GLU:OE2	2.46	0.48
1:B:281:ILE:HG23	1:B:282:VAL:N	2.29	0.48
1:A:395:ILE:HG21	1:A:491:LEU:HD21	1.95	0.48
1:B:96:VAL:HG23	1:B:107:ASP:OD2	2.14	0.48
1:B:313:TYR:O	1:B:314:GLN:C	2.52	0.48
1:A:210:ASN:O	1:A:211:ASN:O	2.32	0.48
1:B:392:PRO:O	1:B:395:ILE:HG13	2.14	0.48
1:A:49:LEU:HA	1:A:49:LEU:HD23	1.73	0.48
1:B:587:TYR:C	1:B:589:ILE:N	2.67	0.48
1:B:587:TYR:HA	1:B:590:ARG:HG2	1.96	0.48
1:A:176:ASP:OD1	1:A:176:ASP:C	2.52	0.48
1:A:428:GLU:OE2	1:A:435:ASP:C	2.53	0.47
1:B:46:LEU:O	1:B:184:VAL:CG1	2.58	0.47
1:B:389:PHE:HE2	1:B:501:LEU:HD13	1.78	0.47
1:B:130:VAL:C	1:B:132:GLU:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:HH22	1:A:102:GLY:HA2	1.77	0.47
1:B:394:GLN:O	1:B:396:LYS:N	2.48	0.47
1:B:579:ASP:CG	1:B:581:ARG:HH21	2.17	0.47
1:B:595:GLN:O	1:B:597:ILE:HG13	2.15	0.47
1:B:502:THR:HA	1:B:513:PRO:HD3	1.96	0.47
1:B:87:ARG:O	1:B:88:LEU:HB2	2.15	0.47
1:B:55:THR:HB	1:B:56:ASP:H	1.58	0.47
1:B:110:ILE:CB	1:B:215:GLN:HE21	2.26	0.47
1:B:85:ILE:CD1	1:B:122:ILE:HD13	2.44	0.47
1:B:473:ASP:HB3	1:B:475:GLN:NE2	2.29	0.47
1:B:574:VAL:HG12	1:B:575:ARG:N	2.30	0.47
1:B:606:LYS:HD3	1:B:607:GLU:CD	2.35	0.47
1:B:172:TYR:CD1	1:B:173:SER:N	2.82	0.47
1:B:561:TYR:HE2	1:B:603:VAL:HG11	1.78	0.47
1:A:253:PHE:HA	1:A:267:LEU:HG	1.95	0.47
1:A:349:SER:O	1:A:352:GLU:HG2	2.13	0.47
1:A:425:ARG:HA	1:A:440:TRP:CZ3	2.50	0.47
1:B:297:VAL:HG22	4:B:2004:HOH:O	2.14	0.47
1:A:602:VAL:HG23	4:A:1019:HOH:O	2.13	0.47
1:A:500:ASP:HA	1:A:512:ARG:HH12	1.79	0.47
1:B:93:LYS:NZ	1:B:93:LYS:HB2	2.29	0.47
1:A:262:GLY:C	1:A:263:LEU:HD23	2.35	0.47
1:A:471:LYS:HA	1:A:490:GLN:HA	1.97	0.47
1:A:399:PHE:CE2	1:A:472:LEU:HD12	2.49	0.47
1:B:410:TYR:CD1	1:B:410:TYR:N	2.81	0.47
1:A:549:GLN:OE1	1:A:549:GLN:HA	2.14	0.47
1:B:130:VAL:HG13	1:B:190:ALA:HA	1.97	0.47
1:B:174:GLN:NE2	1:B:174:GLN:O	2.47	0.47
1:B:46:LEU:HG	1:B:184:VAL:HG11	1.97	0.47
1:A:610:ASN:HB3	4:A:1004:HOH:O	2.15	0.47
1:B:155:TYR:CZ	1:B:159:LEU:HD22	2.50	0.47
1:A:423:SER:HB3	1:A:464:GLU:CB	2.44	0.47
1:A:391:ARG:H	1:A:394:GLN:CG	2.28	0.47
1:A:125:THR:C	1:A:127:LYS:N	2.66	0.47
1:A:625:THR:CG2	1:A:626:VAL:N	2.78	0.47
1:A:298:LEU:HD12	1:A:298:LEU:C	2.35	0.47
1:A:581:ARG:O	1:A:588:LYS:NZ	2.45	0.47
1:A:71:GLU:HB3	4:A:1068:HOH:O	2.15	0.47
1:B:123:GLU:HB2	1:B:197:LEU:CD1	2.37	0.47
1:A:611:ASN:HD22	1:A:611:ASN:HA	1.56	0.47
1:A:386:SER:HB3	1:A:518:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PHE:O	1:A:403:VAL:HG23	2.15	0.46
1:A:46:LEU:HG	4:A:1021:HOH:O	2.14	0.46
1:A:297:VAL:HG23	1:A:362:THR:O	2.14	0.46
1:B:395:ILE:HG23	1:B:491:LEU:HD11	1.96	0.46
1:A:205:TRP:O	1:A:207:GLY:N	2.47	0.46
1:A:323:LEU:O	1:A:324:ASP:O	2.33	0.46
1:B:643:LYS:C	1:B:644:HIS:HD2	2.18	0.46
1:A:502:THR:HA	1:A:513:PRO:HD3	1.96	0.46
1:B:202:GLY:O	1:B:203:ALA:HB2	2.15	0.46
1:B:8:PHE:C	1:B:10:ASP:H	2.19	0.46
1:A:454:LEU:HB3	1:A:456:LEU:HD11	1.97	0.46
1:B:222:PHE:CD2	1:B:228:LEU:HD13	2.51	0.46
1:A:8:PHE:CZ	1:A:29:ILE:HD11	2.51	0.46
1:B:459:GLU:O	1:B:460:GLU:O	2.33	0.46
1:A:191:LYS:HE3	4:A:1007:HOH:O	2.14	0.46
1:B:140:VAL:HG22	1:B:170:THR:HG22	1.98	0.46
1:B:388:ILE:HG21	1:B:398:GLU:HG2	1.97	0.46
1:B:93:LYS:HZ2	1:B:93:LYS:HB2	1.81	0.46
1:A:34:ARG:O	1:A:36:LYS:N	2.47	0.46
1:B:467:PHE:CD1	1:B:468:TYR:N	2.84	0.46
1:A:406:ILE:HG21	1:A:474:VAL:HG21	1.97	0.46
1:A:471:LYS:NZ	1:A:473:ASP:OD2	2.48	0.46
1:A:476:VAL:HG13	1:A:530:PHE:CE1	2.50	0.46
1:A:157:LEU:O	1:A:160:ILE:CG2	2.64	0.46
1:A:469:GLY:HA3	1:A:491:LEU:O	2.16	0.46
1:A:113:ASN:C	1:A:215:GLN:HE22	2.18	0.46
1:B:396:LYS:HG3	1:B:397:GLU:N	2.31	0.46
1:A:150:PHE:O	1:A:157:LEU:HD21	2.15	0.46
1:A:177:PHE:CZ	1:A:179:ASP:HB2	2.51	0.46
1:B:478:THR:CG2	1:B:479:ALA:N	2.62	0.46
1:B:550:ILE:HG21	1:B:562:ALA:HB1	1.97	0.46
1:B:39:ALA:O	1:B:62:VAL:HB	2.16	0.46
1:A:38:VAL:O	1:A:187:PRO:HD3	2.16	0.46
1:B:467:PHE:C	1:B:467:PHE:CD1	2.88	0.46
1:B:236:GLU:O	1:B:240:GLU:HG2	2.16	0.46
1:B:27:GLN:HA	1:B:27:GLN:NE2	2.29	0.46
1:B:156:LYS:HB3	1:B:180:LEU:HD12	1.96	0.46
1:A:478:THR:CG2	1:A:479:ALA:H	2.29	0.45
1:A:323:LEU:CG	1:B:366:TYR:OH	2.63	0.45
1:A:125:THR:O	1:A:129:ILE:HG23	2.17	0.45
1:A:471:LYS:HG2	1:A:490:GLN:HB3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASP:O	1:B:609:GLU:HB2	2.16	0.45
1:B:70:LEU:HD22	1:B:74:ARG:CZ	2.46	0.45
1:B:383:LEU:HA	1:B:523:THR:HA	1.98	0.45
1:A:335:ASN:HB2	1:A:385:ASP:OD2	2.16	0.45
1:A:73:LEU:HB2	1:A:223:PHE:CZ	2.50	0.45
1:B:547:GLN:OE1	1:B:574:VAL:HG13	2.16	0.45
1:A:298:LEU:CD2	1:B:331:LEU:HD11	2.44	0.45
1:A:186:VAL:HG22	1:A:187:PRO:HD2	1.98	0.45
1:B:124:LYS:O	1:B:128:GLN:HB2	2.17	0.45
1:B:17:ASP:OD1	1:B:17:ASP:N	2.50	0.45
1:B:73:LEU:HD22	1:B:223:PHE:CD1	2.51	0.45
1:B:636:VAL:HA	1:B:639:ILE:HD12	1.98	0.45
1:A:503:TYR:CE2	1:A:511:HIS:HB3	2.51	0.45
1:A:203:ALA:O	1:A:214:LEU:HB2	2.16	0.45
1:B:234:MET:SD	1:B:235:LEU:N	2.90	0.45
1:A:195:PHE:HA	1:A:221:ALA:HA	1.98	0.45
1:B:303:LEU:HD23	1:B:304:TYR:CE1	2.51	0.45
1:A:204:TYR:HE2	1:A:209:SER:HG	1.63	0.45
1:A:97:GLY:HA3	1:A:106:TYR:CE2	2.52	0.45
1:B:501:LEU:O	1:B:513:PRO:HD2	2.16	0.45
1:A:40:GLY:HA2	1:A:62:VAL:HG23	1.98	0.45
1:A:93:LYS:HB3	1:A:153:ASP:OD1	2.16	0.45
1:B:130:VAL:C	1:B:132:GLU:H	2.20	0.45
1:B:83:HIS:CE1	1:B:174:GLN:NE2	2.84	0.45
1:A:521:VAL:HG22	1:A:527:PHE:CE1	2.52	0.45
1:B:614:ASN:HB2	1:B:625:THR:HG22	1.98	0.45
1:B:99:VAL:HG12	1:B:104:PHE:HB3	1.97	0.45
1:A:428:GLU:HG2	1:A:429:ASP:N	2.32	0.45
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.27	0.45
1:B:430:LYS:CG	1:B:431:GLU:N	2.79	0.45
1:B:487:SER:HB3	1:B:520:VAL:O	2.16	0.45
1:B:602:VAL:O	1:B:614:ASN:HB3	2.17	0.45
1:B:614:ASN:HA	1:B:625:THR:HA	1.99	0.45
1:B:425:ARG:NH1	4:B:2003:HOH:O	2.49	0.45
1:A:589:ILE:HG22	1:A:589:ILE:O	2.16	0.45
1:B:143:ARG:CG	1:B:143:ARG:HH11	2.27	0.45
1:B:62:VAL:HG13	1:B:69:ALA:HB2	1.98	0.45
1:B:66:SER:O	1:B:67:GLU:C	2.54	0.45
1:A:388:ILE:HG21	1:A:398:GLU:HG2	1.98	0.45
1:B:298:LEU:HD23	1:B:331:LEU:HD23	1.97	0.45
1:B:75:HIS:O	1:B:78:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LEU:HD13	1:B:458:TYR:HB3	1.99	0.45
1:B:27:GLN:HE21	1:B:27:GLN:CA	2.26	0.44
1:A:521:VAL:HG22	1:A:527:PHE:CD1	2.52	0.44
1:B:473:ASP:HB3	1:B:485:THR:CG2	2.47	0.44
1:A:353:LEU:CD1	1:A:390:VAL:HA	2.47	0.44
1:B:452:ASP:C	1:B:454:LEU:N	2.70	0.44
1:B:222:PHE:HD2	1:B:228:LEU:HD13	1.82	0.44
1:B:641:LEU:O	1:B:642:LYS:C	2.52	0.44
1:A:404:ASN:O	1:A:408:ASP:N	2.42	0.44
1:A:114:ILE:HG12	1:A:215:GLN:NE2	2.32	0.44
1:B:43:ASN:ND2	1:B:57:GLY:CA	2.69	0.44
1:B:167:GLU:CG	1:B:167:GLU:O	2.65	0.44
1:A:566:GLN:CD	1:A:578:ILE:HD12	2.37	0.44
1:A:123:GLU:HA	1:A:126:MET:HG2	1.98	0.44
1:A:398:GLU:HA	1:A:401:ARG:HH21	1.81	0.44
1:A:249:GLU:HB3	1:A:250:LEU:HD13	2.00	0.44
1:A:255:ASN:N	1:A:255:ASN:ND2	2.64	0.44
1:B:388:ILE:HG22	1:B:390:VAL:HG13	1.98	0.44
1:B:612:GLN:HB3	1:B:626:VAL:O	2.17	0.44
1:A:180:LEU:HD23	1:A:180:LEU:O	2.18	0.44
1:B:315:GLU:HG2	1:B:315:GLU:H	1.48	0.44
1:B:313:TYR:O	1:B:315:GLU:N	2.50	0.44
1:A:589:ILE:CG2	1:A:589:ILE:O	2.66	0.44
1:A:205:TRP:NE1	1:A:206:ARG:HG3	2.33	0.44
1:B:147:LYS:CA	1:B:160:ILE:HG21	2.47	0.44
1:A:340:MET:HE1	1:A:389:PHE:CZ	2.51	0.44
1:A:326:THR:O	1:A:327:GLU:CG	2.65	0.44
1:A:181:CYS:SG	1:A:182:ARG:N	2.90	0.44
1:A:157:LEU:HA	1:A:160:ILE:CG2	2.47	0.44
1:A:296:PRO:HG3	4:B:2009:HOH:O	2.16	0.44
1:B:126:MET:HE1	1:B:197:LEU:HD21	2.00	0.44
1:B:84:ALA:HB2	1:B:126:MET:CG	2.44	0.44
1:B:16:PHE:O	1:B:17:ASP:C	2.55	0.44
1:B:378:VAL:HG23	1:B:379:ARG:N	2.33	0.44
1:B:379:ARG:NH2	4:B:2038:HOH:O	2.31	0.44
1:B:202:GLY:HA2	1:B:214:LEU:O	2.17	0.44
1:B:79:HIS:CD2	1:B:172:TYR:OH	2.71	0.44
1:A:548:VAL:O	1:A:576:VAL:HA	2.17	0.44
1:B:283:ASP:HB2	4:B:2026:HOH:O	2.18	0.44
1:B:534:GLU:HA	1:B:534:GLU:OE1	2.18	0.44
1:B:350:TYR:CE2	1:B:506:GLN:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ASN:O	1:B:557:LEU:N	2.47	0.44
1:A:84:ALA:HB1	1:A:125:THR:HG22	1.97	0.44
1:A:561:TYR:CD2	1:A:608:VAL:HG22	2.53	0.44
1:B:434:PHE:O	1:B:435:ASP:HB2	2.17	0.44
1:B:561:TYR:CE2	1:B:603:VAL:HG11	2.53	0.44
1:B:602:VAL:HG23	1:B:614:ASN:OD1	2.18	0.44
1:B:597:ILE:HA	1:B:598:PRO:HD2	1.74	0.44
1:B:410:TYR:HD1	1:B:410:TYR:N	2.16	0.44
1:B:479:ALA:C	1:B:480:MET:HG3	2.38	0.44
1:B:42:PHE:HD1	1:B:59:ILE:HG23	1.83	0.44
1:B:8:PHE:O	1:B:10:ASP:N	2.51	0.44
1:A:589:ILE:HG21	1:A:616:ARG:HH12	1.83	0.44
1:A:323:LEU:O	1:A:323:LEU:CD1	2.66	0.44
1:A:612:GLN:HB2	1:A:626:VAL:O	2.18	0.44
1:B:540:PRO:CG	1:B:543:LEU:HD12	2.45	0.44
1:B:434:PHE:CD1	1:B:434:PHE:O	2.71	0.44
1:B:261:ALA:N	4:B:2038:HOH:O	2.48	0.44
1:B:297:VAL:O	1:B:332:ARG:HG2	2.18	0.44
1:B:377:ARG:HA	3:B:2002:TSB:N1	2.32	0.44
1:A:558:HIS:NE2	1:A:605:ASP:OD1	2.43	0.44
1:A:323:LEU:HD13	1:A:326:THR:HB	1.99	0.44
1:B:331:LEU:HB3	4:B:2032:HOH:O	2.18	0.44
1:B:422:LEU:HD13	1:B:458:TYR:CB	2.48	0.44
1:B:131:ASN:ND2	1:B:131:ASN:N	2.64	0.44
1:B:638:GLU:O	1:B:638:GLU:HG2	2.18	0.44
1:B:186:VAL:HG11	1:B:191:LYS:HB3	2.00	0.44
1:B:172:TYR:O	1:B:178:THR:HG23	2.17	0.44
1:B:322:GLN:N	1:B:322:GLN:OE1	2.51	0.43
1:B:163:ILE:HG22	1:B:163:ILE:O	2.18	0.43
1:A:34:ARG:HG3	1:A:35:LYS:H	1.83	0.43
1:A:186:VAL:CG1	1:A:188:SER:O	2.66	0.43
1:B:598:PRO:O	1:B:617:GLN:HA	2.18	0.43
1:A:259:VAL:O	1:B:300:ASN:N	2.46	0.43
1:A:338:HIS:O	1:A:341:MET:HB2	2.19	0.43
1:A:353:LEU:CD1	1:A:390:VAL:C	2.87	0.43
1:B:353:LEU:C	1:B:355:ILE:H	2.21	0.43
1:A:80:LEU:CG	1:A:126:MET:HB2	2.48	0.43
1:B:458:TYR:HD2	1:B:460:GLU:HG3	1.83	0.43
1:B:42:PHE:H	1:B:47:VAL:HG13	1.83	0.43
1:A:499:PHE:HB2	1:A:501:LEU:HG	2.00	0.43
1:B:569:LEU:HD23	1:B:632:ILE:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:LYS:HD3	1:B:607:GLU:OE2	2.17	0.43
1:B:250:LEU:HD13	1:B:250:LEU:HA	1.66	0.43
1:B:598:PRO:C	1:B:599:TYR:CD1	2.91	0.43
1:A:524:MET:HA	1:A:524:MET:CE	2.49	0.43
1:A:494:LEU:O	1:A:497:GLU:HB2	2.19	0.43
1:A:410:TYR:OH	1:A:486:LEU:HB3	2.18	0.43
1:B:559:TYR:CE2	1:B:563:ARG:HG3	2.53	0.43
1:A:224:ASP:OD1	1:A:226:LYS:HB2	2.19	0.43
1:B:422:LEU:HD21	1:B:451:ALA:CB	2.48	0.43
1:B:450:ALA:HA	1:B:453:GLU:HG3	2.00	0.43
1:A:250:LEU:N	1:A:250:LEU:CD1	2.81	0.43
1:A:442:LYS:HE3	1:A:493:PHE:CE1	2.53	0.43
1:B:42:PHE:CD1	1:B:53:LEU:HD13	2.53	0.43
1:A:337:PRO:O	1:A:338:HIS:C	2.57	0.43
1:B:613:VAL:HG13	1:B:628:LYS:HA	2.00	0.43
1:A:374:GLY:O	1:A:376:GLN:N	2.47	0.43
1:A:423:SER:HB3	1:A:464:GLU:HB2	2.01	0.43
1:B:343:TYR:O	1:B:348:HIS:NE2	2.48	0.43
1:B:132:GLU:O	1:B:133:ASN:C	2.56	0.43
1:A:47:VAL:HB	1:A:51:LYS:HG2	2.01	0.43
1:B:243:HIS:HB3	1:B:533:GLU:HG3	1.99	0.43
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.82	0.43
1:A:138:ARG:C	1:A:138:ARG:HD2	2.39	0.43
1:B:204:TYR:HA	1:B:213:MET:HA	1.99	0.43
1:A:229:LYS:O	1:A:233:GLN:HG3	2.18	0.43
1:A:80:LEU:CD1	1:A:129:ILE:HG12	2.49	0.43
1:A:526:ARG:NH1	1:A:526:ARG:CG	2.81	0.43
1:A:110:ILE:HG22	1:A:112:GLN:N	2.32	0.43
1:A:311:ASP:HB2	1:A:312:HIS:CD2	2.54	0.43
1:A:106:TYR:CD1	1:A:108:PHE:CE1	3.06	0.43
1:B:292:HIS:HA	1:B:358:ALA:O	2.19	0.43
1:B:119:PHE:O	1:B:123:GLU:N	2.48	0.43
1:B:45:GLN:HB3	1:B:47:VAL:HG12	1.99	0.43
1:A:155:TYR:O	1:A:159:LEU:HD13	2.18	0.43
1:B:72:VAL:HG22	1:B:184:VAL:HG22	2.00	0.43
1:A:79:HIS:O	1:A:80:LEU:C	2.56	0.43
1:B:298:LEU:HD21	1:B:331:LEU:HD23	2.01	0.43
1:A:36:LYS:HZ2	1:A:36:LYS:HB2	1.82	0.43
1:A:236:GLU:OE2	1:A:239:LYS:HD2	2.19	0.43
1:B:48:ASP:OD1	1:B:49:LEU:N	2.52	0.43
1:B:167:GLU:O	1:B:167:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLN:O	1:A:526:ARG:NH1	2.52	0.43
1:B:281:ILE:CG2	1:B:282:VAL:N	2.82	0.43
1:B:478:THR:HG21	1:B:480:MET:HE2	2.01	0.42
1:A:554:ASN:ND2	1:A:556:ASP:N	2.51	0.42
1:A:353:LEU:HD22	1:A:353:LEU:HA	1.78	0.42
1:A:385:ASP:OD1	1:A:386:SER:N	2.52	0.42
1:B:631:PHE:CD2	1:B:632:ILE:HD12	2.54	0.42
1:A:128:GLN:HA	1:A:131:ASN:HD22	1.81	0.42
1:A:374:GLY:C	1:A:376:GLN:H	2.23	0.42
1:B:458:TYR:CD2	1:B:460:GLU:HG3	2.54	0.42
1:A:151:SER:O	1:A:153:ASP:N	2.52	0.42
1:B:165:GLU:O	1:B:166:ASP:HB3	2.19	0.42
1:B:87:ARG:HH12	1:B:128:GLN:HG3	1.83	0.42
1:B:42:PHE:CB	1:B:47:VAL:HG11	2.49	0.42
1:B:384:ASN:ND2	1:B:521:VAL:H	2.12	0.42
1:A:326:THR:O	1:A:327:GLU:HG2	2.20	0.42
1:B:428:GLU:OE2	1:B:435:ASP:HB3	2.18	0.42
1:B:231:HIS:O	1:B:231:HIS:CG	2.71	0.42
1:A:157:LEU:CA	1:A:160:ILE:HG22	2.49	0.42
1:B:186:VAL:HA	1:B:187:PRO:HD2	1.76	0.42
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.86	0.42
1:A:6:ILE:HD13	1:A:25:ILE:HD11	2.02	0.42
1:B:494:LEU:HD21	1:B:498:ARG:HD2	1.99	0.42
1:A:300:ASN:HD22	1:A:327:GLU:HB3	1.84	0.42
1:A:162:ALA:O	1:A:167:GLU:OE1	2.38	0.42
1:A:265:LEU:HD23	1:B:296:PRO:CD	2.49	0.42
1:A:20:THR:HG22	1:A:21:THR:N	2.33	0.42
1:B:336:CYS:HA	1:B:387:HIS:CE1	2.55	0.42
1:A:605:ASP:O	1:A:606:LYS:C	2.55	0.42
1:B:391:ARG:HB3	1:B:503:TYR:OH	2.19	0.42
1:A:155:TYR:HB3	1:A:205:TRP:HZ3	1.84	0.42
1:A:108:PHE:O	1:A:214:LEU:HG	2.19	0.42
1:A:281:ILE:HA	1:A:281:ILE:HD12	1.74	0.42
1:B:74:ARG:CG	1:B:221:ALA:HB3	2.20	0.42
1:B:81:MET:O	1:B:85:ILE:HG12	2.20	0.42
1:B:471:LYS:HB2	1:B:490:GLN:CG	2.41	0.42
1:B:51:LYS:HA	1:B:52:PRO:HD3	1.87	0.42
1:A:625:THR:HG22	1:A:626:VAL:N	2.35	0.42
1:A:79:HIS:NE2	4:A:1003:HOH:O	2.11	0.42
1:B:71:GLU:O	1:B:75:HIS:N	2.43	0.42
1:A:563:ARG:CG	1:A:563:ARG:HH11	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TRP:HB2	1:B:211:ASN:ND2	2.35	0.42
1:B:19:GLY:O	1:B:20:THR:C	2.58	0.42
1:A:258:LEU:O	1:A:258:LEU:CD2	2.67	0.42
1:B:153:ASP:HB2	1:B:156:LYS:HD2	2.01	0.42
1:A:566:GLN:NE2	1:A:577:SER:HA	2.23	0.42
1:A:353:LEU:HD12	1:A:391:ARG:N	2.34	0.42
1:B:352:GLU:O	1:B:355:ILE:HG13	2.19	0.42
1:B:553:VAL:HG21	1:B:604:GLY:HA3	2.02	0.42
1:A:265:LEU:HD23	1:B:296:PRO:HD3	2.02	0.42
1:A:363:MET:O	1:A:381:MET:HG2	2.20	0.42
1:A:627:GLU:O	1:A:628:LYS:C	2.54	0.42
1:B:135:LYS:O	1:B:174:GLN:HG2	2.19	0.42
1:B:85:ILE:HG13	1:B:108:PHE:CE2	2.54	0.42
1:A:546:LYS:HE2	1:A:577:SER:OG	2.20	0.42
1:B:92:VAL:HB	1:B:109:ASP:CB	2.44	0.42
1:A:460:GLU:HA	1:A:460:GLU:OE1	2.20	0.42
1:B:633:TRP:CD1	1:B:633:TRP:C	2.93	0.42
1:B:8:PHE:HB3	1:B:10:ASP:OD1	2.20	0.41
1:A:589:ILE:CG2	1:A:616:ARG:NH1	2.83	0.41
1:B:423:SER:HB3	1:B:464:GLU:C	2.40	0.41
1:A:34:ARG:NH2	4:A:1045:HOH:O	2.48	0.41
1:A:447:LEU:HD11	1:A:471:LYS:C	2.40	0.41
1:A:72:VAL:O	1:A:73:LEU:C	2.58	0.41
1:B:194:GLU:CD	1:B:225:LYS:HG2	2.40	0.41
1:B:334:MET:SD	3:B:2002:TSB:N	2.83	0.41
1:A:400:LYS:CG	1:A:454:LEU:HD13	2.43	0.41
1:B:545:PRO:HB2	4:B:2012:HOH:O	2.19	0.41
1:A:644:HIS:ND1	1:A:645:ARG:N	2.68	0.41
1:B:448:LYS:HD3	1:B:460:GLU:OE2	2.19	0.41
1:A:364:HIS:HA	1:A:379:ARG:O	2.20	0.41
1:B:107:ASP:OD1	1:B:216:ARG:HB2	2.20	0.41
1:B:33:LEU:O	1:B:37:ALA:N	2.42	0.41
1:B:94:PHE:CE2	1:B:108:PHE:HE1	2.39	0.41
1:A:70:LEU:CD2	1:A:74:ARG:CZ	2.99	0.41
1:B:430:LYS:HG2	1:B:431:GLU:H	1.85	0.41
1:A:645:ARG:O	1:A:645:ARG:CG	2.62	0.41
1:B:82:ALA:HB1	1:B:94:PHE:CD2	2.55	0.41
1:B:402:VAL:HG22	1:B:403:VAL:N	2.34	0.41
1:A:490:GLN:H	1:A:490:GLN:HG2	1.55	0.41
1:B:114:ILE:HG13	1:B:115:SER:N	2.35	0.41
1:A:410:TYR:HH	1:A:487:SER:HG	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CB	1:A:9:PRO:CD	2.98	0.41
1:B:203:ALA:O	1:B:214:LEU:CD2	2.69	0.41
1:A:83:HIS:ND1	1:A:177:PHE:HB3	2.36	0.41
1:B:636:VAL:O	1:B:639:ILE:HB	2.20	0.41
1:B:23:GLU:O	1:B:26:ALA:HB3	2.21	0.41
1:A:27:GLN:HA	1:A:27:GLN:OE1	2.21	0.41
1:A:204:TYR:HE1	1:A:207:GLY:CA	2.25	0.41
1:A:340:MET:CE	1:A:389:PHE:CE2	3.04	0.41
1:A:340:MET:CE	1:A:389:PHE:CZ	3.04	0.41
1:B:72:VAL:HG22	1:B:184:VAL:CG2	2.50	0.41
1:A:36:LYS:HE3	1:A:63:THR:OG1	2.21	0.41
1:A:414:GLY:HA3	1:A:644:HIS:CE1	2.55	0.41
1:B:422:LEU:HD21	1:B:451:ALA:HB2	2.03	0.41
1:B:252:LEU:HD22	1:B:270:GLY:HA2	2.03	0.41
1:B:174:GLN:HE21	1:B:174:GLN:HB3	1.64	0.41
1:B:304:TYR:OH	1:B:332:ARG:HB3	2.21	0.41
1:B:47:VAL:CG2	1:B:47:VAL:O	2.69	0.41
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.31	0.41
1:B:143:ARG:NH2	1:B:160:ILE:O	2.54	0.41
1:B:521:VAL:CG2	1:B:527:PHE:CE1	2.97	0.41
1:A:584:LYS:O	1:A:587:TYR:HB3	2.21	0.41
1:B:267:LEU:HB3	4:B:2014:HOH:O	2.20	0.41
1:A:45:GLN:O	1:A:47:VAL:HG13	2.21	0.41
1:B:105:TYR:CD1	1:B:105:TYR:C	2.93	0.41
1:A:7:GLN:O	1:A:58:SER:HA	2.20	0.41
1:B:480:MET:C	1:B:482:LYS:N	2.72	0.41
1:B:94:PHE:HE2	1:B:108:PHE:HE1	1.69	0.41
1:A:521:VAL:CG2	1:A:527:PHE:CE1	3.03	0.41
1:B:623:GLN:O	1:B:624:GLU:C	2.59	0.41
1:A:353:LEU:HD13	1:A:390:VAL:HA	2.03	0.41
1:A:499:PHE:O	1:A:500:ASP:C	2.59	0.41
1:B:628:LYS:O	1:B:632:ILE:HD13	2.21	0.41
1:B:581:ARG:HB2	1:B:581:ARG:HE	1.75	0.41
1:B:585:MET:CE	1:B:602:VAL:HG11	2.51	0.41
1:A:348:HIS:HA	1:A:352:GLU:OE2	2.21	0.41
1:B:100:ILE:HB	1:B:101:GLU:H	1.49	0.41
1:B:426:ASP:O	1:B:427:PRO:C	2.59	0.41
1:A:120:GLU:HG2	1:A:120:GLU:O	2.20	0.41
1:A:482:LYS:HZ2	1:A:482:LYS:CA	2.34	0.41
1:B:424:TYR:O	1:B:465:ALA:HB3	2.20	0.41
1:A:467:PHE:CD1	1:A:467:PHE:O	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:TRP:CE2	1:A:543:LEU:HG	2.55	0.41
1:A:435:ASP:O	1:A:436:ASP:C	2.60	0.40
1:B:83:HIS:CG	1:B:177:PHE:HB2	2.55	0.40
1:B:336:CYS:HB2	1:B:337:PRO:CD	2.50	0.40
1:B:454:LEU:HB3	1:B:456:LEU:CD1	2.44	0.40
1:B:544:ALA:O	1:B:545:PRO:C	2.59	0.40
1:B:155:TYR:OH	1:B:159:LEU:HD22	2.21	0.40
1:B:268:PRO:N	4:B:2014:HOH:O	2.53	0.40
1:B:131:ASN:HD22	1:B:131:ASN:N	2.18	0.40
1:A:293:VAL:HB	1:B:266:TRP:O	2.20	0.40
1:A:81:MET:SD	1:A:197:LEU:HD21	2.61	0.40
1:A:603:VAL:O	1:A:603:VAL:HG12	2.21	0.40
1:B:122:ILE:O	1:B:126:MET:HE3	2.21	0.40
1:B:85:ILE:HG22	1:B:85:ILE:O	2.21	0.40
1:B:622:ASP:O	1:B:623:GLN:C	2.60	0.40
1:A:405:MET:SD	1:A:520:VAL:HG21	2.61	0.40
1:B:143:ARG:NH1	1:B:143:ARG:CG	2.83	0.40
1:A:324:ASP:C	1:A:326:THR:N	2.75	0.40
1:A:612:GLN:HB3	4:A:1004:HOH:O	2.22	0.40
1:A:30:SER:HA	1:A:31:PRO:HD3	1.88	0.40
1:A:498:ARG:HG2	1:A:498:ARG:H	1.69	0.40
1:B:499:PHE:HB2	1:B:501:LEU:HG	2.03	0.40
1:B:4:ILE:HG22	1:B:16:PHE:N	2.29	0.40
1:B:93:LYS:H	1:B:109:ASP:HB2	1.86	0.40
1:B:474:VAL:HB	1:B:487:SER:OG	2.21	0.40
1:A:526:ARG:NH1	3:A:1002:TSB:N3	2.69	0.40
1:B:343:TYR:CG	1:B:389:PHE:CD2	3.10	0.40
1:A:191:LYS:CE	4:A:1007:HOH:O	2.70	0.40
1:B:68:GLU:H	1:B:68:GLU:HG2	1.74	0.40
1:A:357:ILE:HD13	1:A:357:ILE:N	2.37	0.40
1:B:392:PRO:HA	1:B:395:ILE:HD11	2.03	0.40
1:B:126:MET:C	1:B:128:GLN:H	2.24	0.40
1:B:83:HIS:HE1	1:B:174:GLN:NE2	2.19	0.40
1:A:386:SER:HB3	1:A:518:ARG:NH1	2.37	0.40
1:B:396:LYS:HD3	1:B:400:LYS:NZ	2.36	0.40
1:B:477:LYS:HB3	1:B:481:GLY:HA2	2.04	0.40
1:B:326:THR:HG22	1:B:326:THR:O	2.21	0.40
1:A:430:LYS:HB3	1:A:434:PHE:O	2.21	0.40
1:A:627:GLU:HG3	1:A:629:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/645 (99%)	525 (82%)	81 (13%)	34 (5%)	2	19
1	B	643/645 (100%)	471 (73%)	125 (19%)	47 (7%)	1	9
All	All	1283/1290 (100%)	996 (78%)	206 (16%)	81 (6%)	2	13

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	113	ASN
1	A	114	ILE
1	A	206	ARG
1	A	211	ASN
1	A	322	GLN
1	A	324	ASP
1	A	325	GLU
1	A	345	ASN
1	A	425	ARG
1	A	436	ASP
1	A	619	GLY
1	B	4	ILE
1	B	88	LEU
1	B	131	ASN
1	B	149	LEU
1	B	210	ASN
1	B	224	ASP
1	B	430	LYS
1	B	460	GLU
1	B	478	THR
1	B	482	LYS
1	B	555	VAL
1	B	596	LYS
1	B	622	ASP

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Mol	Chain	Res	Type
1	A	35	LYS
1	A	151	SER
1	A	152	ASN
1	A	162	ALA
1	A	164	PRO
1	A	175	GLY
1	A	188	SER
1	A	314	GLN
1	A	374	GLY
1	A	375	LEU
1	A	395	ILE
1	A	536	LYS
1	B	187	PRO
1	B	205	TRP
1	B	206	ARG
1	B	211	ASN
1	B	314	GLN
1	B	621	GLN
1	B	635	LEU
1	A	116	SER
1	A	427	PRO
1	A	508	GLY
1	A	559	TYR
1	B	100	ILE
1	B	352	GLU
1	B	436	ASP
1	B	544	ALA
1	B	642	LYS
1	A	62	VAL
1	A	209	SER
1	A	560	ASP
1	A	585	MET
1	B	9	PRO
1	B	115	SER
1	B	166	ASP
1	B	203	ALA
1	B	426	ASP
1	B	624	GLU
1	B	37	ALA
1	B	97	GLY
1	B	114	ILE
1	B	201	ALA

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Mol	Chain	Res	Type
1	B	588	LYS
1	B	64	PRO
1	B	133	ASN
1	B	268	PRO
1	B	481	GLY
1	B	545	PRO
1	A	372	VAL
1	B	395	ILE
1	B	427	PRO
1	B	44	GLY
1	B	508	GLY
1	A	163	ILE
1	B	30	SER
1	B	636	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	567/570 (100%)	485 (86%)	82 (14%)	4	19
1	B	570/570 (100%)	497 (87%)	73 (13%)	5	25
All	All	1137/1140 (100%)	982 (86%)	155 (14%)	5	22

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	17	ASP
1	A	34	ARG
1	A	36	LYS
1	A	46	LEU
1	A	55	THR
1	A	63	THR
1	A	66	SER
1	A	70	LEU

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Mol	Chain	Res	Type
1	A	74	ARG
1	A	86	LYS
1	A	96	VAL
1	A	106	TYR
1	A	117	ASP
1	A	125	THR
1	A	129	ILE
1	A	131	ASN
1	A	135	LYS
1	A	138	ARG
1	A	140	VAL
1	A	141	VAL
1	A	165	GLU
1	A	166	ASP
1	A	172	TYR
1	A	186	VAL
1	A	200	THR
1	A	204	TYR
1	A	208	ASP
1	A	210	ASN
1	A	211	ASN
1	A	214	LEU
1	A	226	LYS
1	A	232	LEU
1	A	236	GLU
1	A	241	ARG
1	A	249	GLU
1	A	255	ASN
1	A	258	LEU
1	A	281	ILE
1	A	287	SER
1	A	313	TYR
1	A	316	ASP
1	A	321	MET
1	A	323	LEU
1	A	328	SER
1	A	330	VAL
1	A	333	PRO
1	A	340	MET
1	A	353	LEU
1	A	356	ARG
1	A	366	TYR

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Mol	Chain	Res	Type
1	A	401	ARG
1	A	407	ILE
1	A	421	ARG
1	A	423	SER
1	A	428	GLU
1	A	429	ASP
1	A	456	LEU
1	A	467	PHE
1	A	471	LYS
1	A	476	VAL
1	A	482	LYS
1	A	483	GLU
1	A	490	GLN
1	A	491	LEU
1	A	502	THR
1	A	509	GLU
1	A	512	ARG
1	A	518	ARG
1	A	526	ARG
1	A	545	PRO
1	A	550	ILE
1	A	554	ASN
1	A	555	VAL
1	A	563	ARG
1	A	568	GLU
1	A	594	MET
1	A	605	ASP
1	A	611	ASN
1	A	622	ASP
1	A	623	GLN
1	A	629	ASP
1	B	2	GLU
1	B	6	ILE
1	B	13	LYS
1	B	17	ASP
1	B	45	GLN
1	B	49	LEU
1	B	63	THR
1	B	70	LEU
1	B	71	GLU
1	B	79	HIS
1	B	89	TYR

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Mol	Chain	Res	Type
1	B	93	LYS
1	B	94	PHE
1	B	100	ILE
1	B	106	TYR
1	B	109	ASP
1	B	111	ASP
1	B	128	GLN
1	B	136	ILE
1	B	143	ARG
1	B	144	ASP
1	B	153	ASP
1	B	167	GLU
1	B	174	GLN
1	B	176	ASP
1	B	179	ASP
1	B	184	VAL
1	B	193	LYS
1	B	195	PHE
1	B	200	THR
1	B	213	MET
1	B	214	LEU
1	B	233	GLN
1	B	234	MET
1	B	250	LEU
1	B	254	THR
1	B	268	PRO
1	B	284	LYS
1	B	292	HIS
1	B	313	TYR
1	B	323	LEU
1	B	328	SER
1	B	336	CYS
1	B	351	ARG
1	B	353	LEU
1	B	365	ARG
1	B	366	TYR
1	B	372	VAL
1	B	402	VAL
1	B	417	ASP
1	B	425	ARG
1	B	426	ASP
1	B	428	GLU

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Mol	Chain	Res	Type
1	B	431	GLU
1	B	436	ASP
1	B	437	ASP
1	B	458	TYR
1	B	471	LYS
1	B	494	LEU
1	B	497	GLU
1	B	507	ASP
1	B	512	ARG
1	B	518	ARG
1	B	521	VAL
1	B	545	PRO
1	B	563	ARG
1	B	595	GLN
1	B	601	ILE
1	B	602	VAL
1	B	606	LYS
1	B	611	ASN
1	B	621	GLN
1	B	645	ARG

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	128	GLN
1	A	131	ASN
1	A	168	ASN
1	A	174	GLN
1	A	210	ASN
1	A	215	GLN
1	A	255	ASN
1	A	312	HIS
1	A	384	ASN
1	A	441	ASN
1	A	475	GLN
1	A	554	ASN
1	A	564	GLN
1	A	566	GLN
1	A	582	ASN
1	A	595	GLN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	611	ASN
1	A	612	GLN
1	A	623	GLN
1	B	7	GLN
1	B	27	GLN
1	B	43	ASN
1	B	83	HIS
1	B	131	ASN
1	B	211	ASN
1	B	233	GLN
1	B	269	ASN
1	B	376	GLN
1	B	384	ASN
1	B	445	ASN
1	B	475	GLN
1	B	582	ASN
1	B	593	GLN
1	B	595	GLN
1	B	600	GLN
1	B	611	ASN
1	B	612	GLN
1	B	617	GLN
1	B	634	ASN
1	B	644	HIS

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TSB	A	1002	2	24,32,32	2.46	3 (12%)	31,48,48	1.02	2 (6%)
3	TSB	B	2002	2	24,32,32	2.32	3 (12%)	31,48,48	1.03	2 (6%)

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	TSB	A	1002	2	-	0/17/39/39	0/3/3/3
3	TSB	B	2002	2	-	0/17/39/39	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	TSB	C-N8	-3.68	1.32	1.37
3	B	2002	TSB	C-N8	-3.48	1.32	1.37
3	B	2002	TSB	O1S-S1	6.50	1.48	1.42
3	A	1002	TSB	O1S-S1	6.78	1.48	1.42
3	B	2002	TSB	O2S-S1	8.20	1.49	1.42
3	A	1002	TSB	O2S-S1	8.78	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	TSB	C-N8-S1	-2.81	120.12	124.05
3	B	2002	TSB	O1S-S1-N8	-2.38	105.31	108.50
3	A	1002	TSB	C-N8-S1	-2.10	121.11	124.05
3	A	1002	TSB	C5'-O5'-S1	2.26	122.35	118.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	TSB	3	0
3	B	2002	TSB	3	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, 95th 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 ²)	Q<0.9
1	A	642/645 (99%)	-0.33	22 (3%)	49 34	19, 54, 113, 144	0
1	B	645/645 (100%)	-0.04	37 (5%)	27 15	24, 71, 156, 182	0
All	All	1287/1290 (99%)	-0.18	59 (4%)	36 23	19, 61, 144, 182	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	10.0
1	B	162	ALA	5.9
1	B	152	ASN	5.7
1	B	211	ASN	5.4
1	A	433	TYR	5.1
1	A	164	PRO	5.0
1	A	430	LYS	4.6
1	B	431	GLU	4.6
1	B	208	ASP	4.3
1	B	164	PRO	4.3
1	B	163	ILE	4.3
1	B	2	GLU	4.2
1	B	433	TYR	4.1
1	A	426	ASP	3.9
1	B	175	GLY	3.8
1	B	117	ASP	3.8
1	A	371	ALA	3.7
1	B	113	ASN	3.6
1	A	432	LYS	3.6
1	B	183	GLY	3.6
1	A	429	ASP	3.6
1	B	645	ARG	3.6
1	B	210	ASN	3.6
1	B	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	163	ILE	3.5
1	B	207	GLY	3.4
1	A	166	ASP	3.4
1	A	325	GLU	3.3
1	A	434	PHE	3.3
1	A	370	GLY	3.3
1	B	434	PHE	3.2
1	A	324	ASP	3.2
1	B	169	VAL	3.2
1	B	133	ASN	3.2
1	A	168	ASN	3.1
1	B	209	SER	3.1
1	A	431	GLU	3.0
1	B	166	ASP	3.0
1	B	116	SER	2.9
1	B	165	GLU	2.9
1	A	152	ASN	2.8
1	B	88	LEU	2.7
1	A	165	GLU	2.7
1	B	100	ILE	2.6
1	B	89	TYR	2.6
1	B	206	ARG	2.6
1	B	203	ALA	2.6
1	B	506	GLN	2.6
1	A	91	ASN	2.4
1	A	90	GLY	2.4
1	A	645	ARG	2.4
1	B	97	GLY	2.3
1	A	57	GLY	2.3
1	B	426	ASP	2.3
1	B	430	LYS	2.3
1	A	11	GLY	2.3
1	B	176	ASP	2.2
1	B	142	SER	2.2
1	B	432	LYS	2.1

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

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, 95th 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(\AA^2)	Q<0.9
3	TSB	B	2002	30/30	0.95	0.18	-0.27	41,48,50,51	0
3	TSB	A	1002	30/30	0.98	0.15	-0.94	33,37,41,41	0
2	ZN	A	1001	1/1	1.00	0.14	-1.01	40,40,40,40	0
2	ZN	B	2001	1/1	0.99	0.15	-1.18	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.