



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:33 PM UTC

PDB ID : 4FT2 / pdb_00004ft2
Title : crystal structure of Zea mays ZMET2 in complex H3(1-15)K9me2 peptide and SAH
Authors : Du, J.; Patel, D.J.
Deposited on : 2012-06-27
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

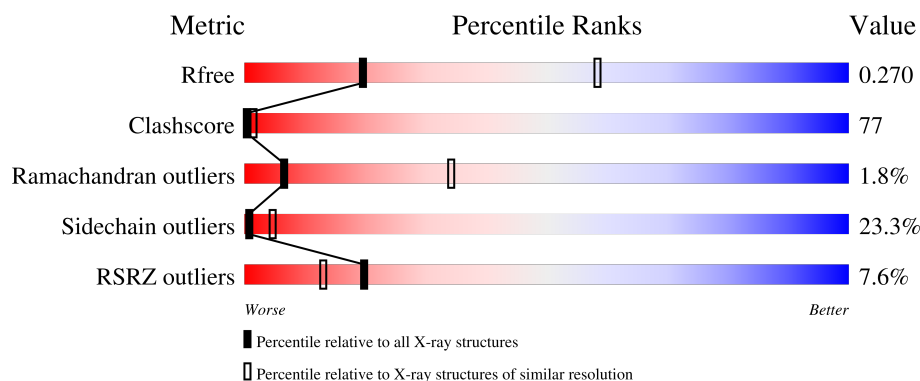
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	784	
1	B	784	
2	P	15	

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
2	MLY	P	9	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10657 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5303	3385	901	984	33			
1	B	670	Total	C	N	O	S	0	0	0
			5246	3349	892	972	33			

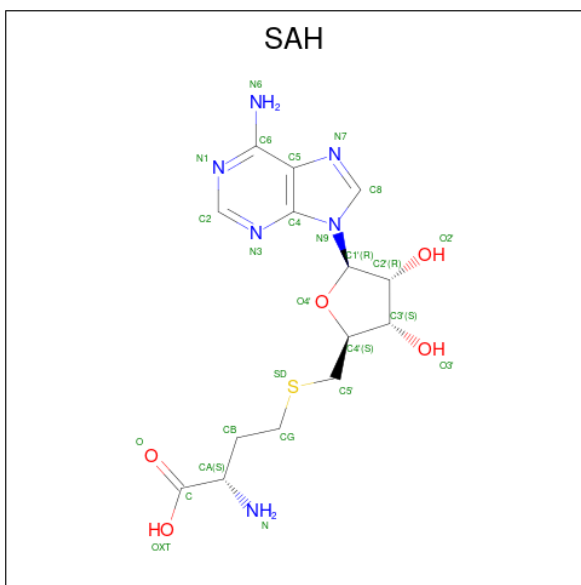
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	-	expression tag	UNP Q9AXT8
B	129	SER	-	expression tag	UNP Q9AXT8

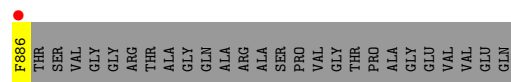
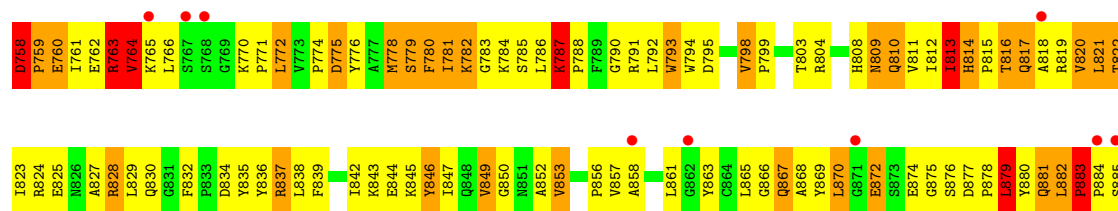
- Molecule 2 is a protein called H3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			56	33	12	11			

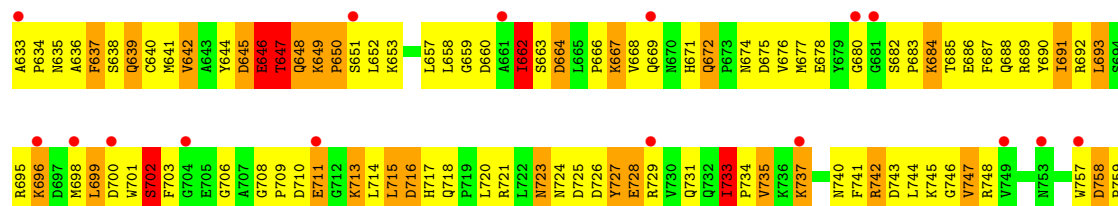
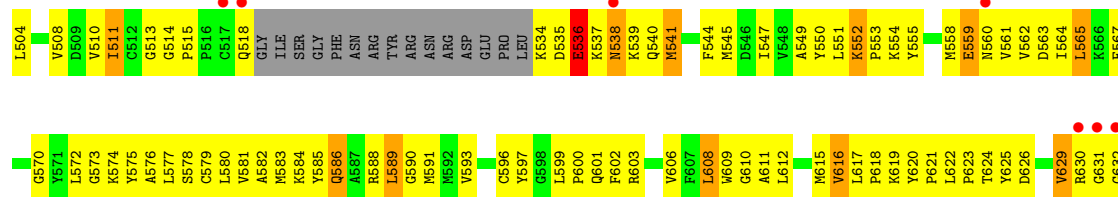
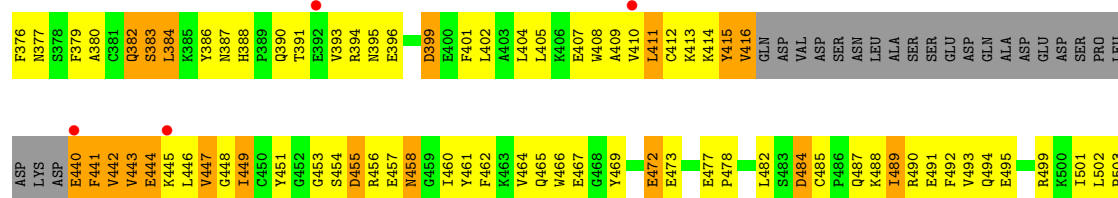
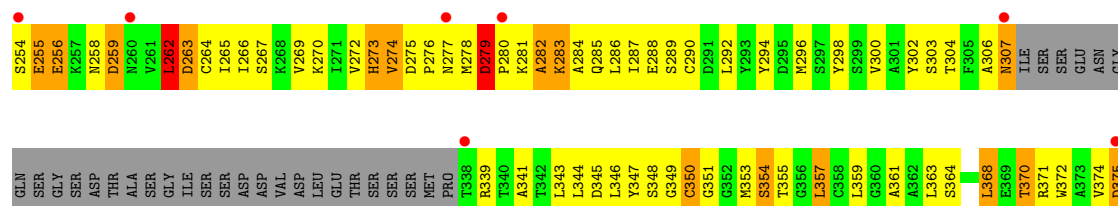
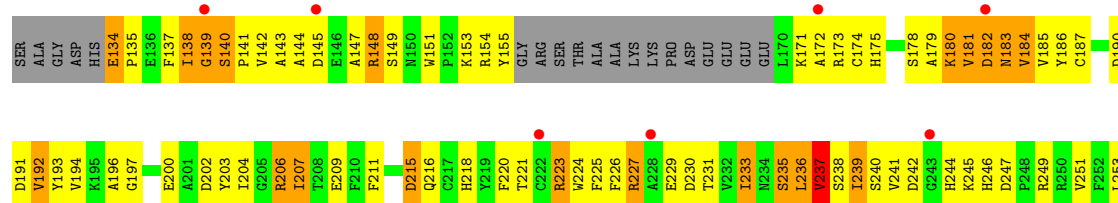
- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	B	1	Total 26	C 14	N 6	O 5	S 1	0	0



• Molecule 1: DNA (cytosine-5)-methyltransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.86Å 88.86Å 113.50Å 93.15° 95.72° 110.70°	Depositor
Resolution (Å)	40.10 – 3.20 40.10 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.10-3.20) 98.9 (40.10-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.235 , 0.277 0.232 , 0.270	Depositor DCC
R_{free} test set	1949 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10657	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SAH, MLY

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	0.68	1/5432 (0.0%)	1.15	45/7362 (0.6%)
1	B	0.58	0/5375	1.09	41/7290 (0.6%)
2	P	0.45	0/44	0.77	0/58
All	All	0.63	1/10851 (0.0%)	1.12	86/14710 (0.6%)

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	4
1	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	ALA	CA-CB	-5.53	1.44	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	SER	N-CA-C	-15.45	87.08	110.10
1	A	596	CYS	N-CA-C	-11.03	94.95	110.50
1	A	632	GLY	N-CA-C	-10.47	94.64	110.97
1	B	733	ILE	CA-C-N	10.23	132.63	119.84
1	B	733	ILE	C-N-CA	10.23	132.63	119.84
1	B	649	LYS	N-CA-C	-10.16	87.98	109.01
1	A	810	GLN	N-CA-C	10.09	126.83	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	773	VAL	CB-CA-C	-9.20	94.61	111.36
1	B	727	TYR	N-CA-C	-8.96	101.51	111.28
1	A	883	PRO	N-CA-C	8.91	121.57	110.70
1	A	651	SER	N-CA-C	-8.50	92.00	107.98
1	B	770	LYS	CA-C-N	8.46	130.42	119.84
1	B	770	LYS	C-N-CA	8.46	130.42	119.84
1	A	456	ARG	N-CA-C	-8.42	92.86	110.80
1	B	282	ALA	N-CA-C	-8.19	102.43	111.36
1	B	810	GLN	N-CA-C	8.15	123.40	113.38
1	B	733	ILE	N-CA-C	7.83	117.58	108.96
1	B	793	TRP	N-CA-C	7.74	119.89	108.60
1	B	651	SER	N-CA-C	-7.67	98.81	110.70
1	B	662	ILE	N-CA-C	7.45	120.20	112.83
1	A	552	LYS	CA-C-N	-7.44	111.78	120.11
1	A	552	LYS	C-N-CA	-7.44	111.78	120.11
1	A	684	LYS	N-CA-C	7.38	119.41	111.36
1	B	650	PRO	N-CA-C	-7.36	105.26	114.68
1	A	763	ARG	CB-CA-C	-7.34	108.10	116.54
1	B	237	VAL	N-CA-C	-7.25	104.30	113.22
1	B	183	ASN	N-CA-C	7.23	122.28	113.17
1	B	747	VAL	N-CA-C	7.20	119.37	109.80
1	A	146	GLU	N-CA-C	-7.17	104.14	113.17
1	A	787	LYS	N-CA-C	7.11	125.52	109.81
1	A	817	GLN	N-CA-C	7.09	122.11	113.17
1	A	136	GLU	N-CA-C	7.06	119.48	108.96
1	B	796	GLU	N-CA-C	6.80	117.22	108.24
1	A	798	VAL	CA-C-N	-6.76	111.93	118.97
1	A	798	VAL	C-N-CA	-6.76	111.93	118.97
1	B	702	SER	N-CA-C	-6.73	104.03	111.36
1	A	454	SER	CA-C-N	-6.69	111.12	121.02
1	A	454	SER	C-N-CA	-6.69	111.12	121.02
1	A	625	TYR	N-CA-C	6.66	119.30	109.24
1	A	763	ARG	N-CA-C	6.60	118.35	108.31
1	A	237	VAL	N-CA-C	-6.51	102.51	111.89
1	A	598	GLY	N-CA-C	6.49	128.57	113.18
1	A	646	GLU	N-CA-C	-6.43	96.41	107.61
1	A	779	SER	N-CA-C	6.43	118.37	111.36
1	A	814	HIS	CA-C-N	-6.42	112.29	118.97
1	A	814	HIS	C-N-CA	-6.42	112.29	118.97
1	B	728	GLU	N-CA-C	6.36	118.01	111.14
1	A	782	LYS	N-CA-C	-6.34	104.75	113.56
1	B	806	GLU	CA-C-N	6.24	125.65	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	806	GLU	C-N-CA	6.24	125.65	118.85
1	A	453	GLY	N-CA-C	6.21	120.00	112.49
1	B	823	ILE	CB-CA-C	-6.17	104.07	111.97
1	A	816	THR	N-CA-C	6.17	120.97	113.38
1	B	647	THR	N-CA-C	-6.07	100.92	109.96
1	A	133	HIS	N-CA-C	6.06	120.29	112.41
1	B	262	LEU	N-CA-C	6.01	118.63	111.71
1	A	762	GLU	N-CA-C	6.01	118.71	108.02
1	A	455	ASP	N-CA-C	-5.99	101.03	109.96
1	A	813	ILE	N-CA-C	5.90	116.98	108.48
1	A	282	ALA	N-CA-C	-5.73	105.12	111.36
1	B	876	SER	N-CA-C	5.71	118.12	110.35
1	A	649	LYS	N-CA-C	-5.68	105.09	113.16
1	A	303	SER	N-CA-C	-5.64	104.36	111.92
1	A	758	ASP	N-CA-C	5.63	122.26	109.81
1	B	737	LYS	N-CA-C	5.60	117.46	111.36
1	B	649	LYS	CB-CA-C	5.55	115.99	110.33
1	B	758	ASP	N-CA-C	-5.50	101.42	109.50
1	A	809	ASN	N-CA-C	5.47	120.83	113.72
1	A	137	PHE	CB-CA-C	-5.46	102.11	109.71
1	B	139	GLY	N-CA-C	-5.45	106.14	115.08
1	B	787	LYS	CA-C-N	5.37	126.55	119.84
1	B	787	LYS	C-N-CA	5.37	126.55	119.84
1	B	808	HIS	N-CA-C	5.28	117.72	111.33
1	A	289	SER	CB-CA-C	-5.27	103.52	112.00
1	B	772	LEU	N-CA-C	-5.25	106.90	113.15
1	A	137	PHE	N-CA-C	5.25	118.08	110.42
1	A	144	ALA	N-CA-C	-5.19	99.75	110.80
1	B	809	ASN	N-CA-C	5.18	119.75	113.38
1	B	773	VAL	N-CA-C	5.17	120.05	108.88
1	A	173	ARG	N-CA-C	-5.17	105.56	111.14
1	B	784	LYS	CB-CA-C	-5.16	110.61	116.54
1	B	255	GLU	N-CA-C	-5.15	106.84	113.02
1	B	767	SER	N-CA-C	-5.06	107.07	113.20
1	A	879	LEU	N-CA-C	5.04	117.34	109.52
1	B	477	GLU	CA-C-N	5.04	124.97	119.78
1	B	477	GLU	C-N-CA	5.04	124.97	119.78

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	SER	Peptide
1	A	145	ASP	Peptide
1	A	758	ASP	Peptide
1	A	883	PRO	Peptide
1	B	279	ASP	Peptide

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	5303	0	5167	856	0
1	B	5246	0	5059	750	0
2	P	56	0	60	24	0
3	A	26	0	19	5	0
3	B	26	0	19	3	0
All	All	10657	0	10324	1607	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 77.

All (1607) 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:456:ARG:HD3	1:A:461:TYR:CE2	1.48	1.48
1:A:173:ARG:NH1	1:A:212:GLU:HG2	1.34	1.42
1:A:648:GLN:C	1:A:650:PRO:HD2	1.43	1.39
1:B:648:GLN:C	1:B:650:PRO:HD3	1.46	1.38
1:A:287:ILE:HD12	1:A:288:GLU:N	1.36	1.38
1:B:883:PRO:CG	1:B:884:PRO:HD2	1.52	1.36
1:A:456:ARG:HD3	1:A:461:TYR:CD2	1.61	1.34
1:A:624:THR:O	1:A:625:TYR:CD2	1.85	1.29
1:B:780:PHE:CZ	1:B:809:ASN:HB3	1.71	1.25
1:B:883:PRO:HG2	1:B:884:PRO:CD	1.67	1.25
1:A:649:LYS:N	1:A:650:PRO:HD2	1.48	1.22
1:A:456:ARG:CD	1:A:461:TYR:CE2	2.23	1.21
1:A:170:LEU:O	1:A:171:LYS:HG3	1.34	1.21
1:A:456:ARG:CD	1:A:461:TYR:HE2	1.55	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASP:O	1:A:744:LEU:HD23	1.37	1.20
1:B:859:ARG:HH11	1:B:859:ARG:CG	1.54	1.20
1:A:755:VAL:CB	1:A:778:MET:HE1	1.70	1.19
1:A:136:GLU:HG3	1:A:218:HIS:CD2	1.77	1.19
1:A:460:ILE:H	1:A:460:ILE:CD1	1.53	1.18
1:A:752:ASN:CA	1:A:784:LYS:HE2	1.74	1.17
1:A:415:TYR:CD1	1:A:490:ARG:HG2	1.79	1.16
1:B:518:GLN:OE1	1:B:537:LYS:HG2	1.40	1.16
1:A:456:ARG:CG	1:A:461:TYR:HE2	1.60	1.15
1:A:460:ILE:HD12	1:A:460:ILE:N	1.58	1.14
1:A:752:ASN:O	1:A:784:LYS:HG2	1.44	1.14
1:B:882:LEU:HD12	1:B:882:LEU:N	1.63	1.13
1:B:859:ARG:HG3	1:B:859:ARG:NH1	1.39	1.13
1:A:487:GLN:HB3	1:A:491:GLU:OE2	1.50	1.11
1:A:274:VAL:HG12	1:A:275:ASP:H	1.16	1.10
1:B:148:ARG:HG2	1:B:148:ARG:HH11	1.03	1.10
1:A:452:GLY:HA2	1:A:456:ARG:NH1	1.68	1.09
1:A:452:GLY:CA	1:A:456:ARG:HD2	1.83	1.09
1:A:588:ARG:HH21	1:A:617:LEU:HD11	1.11	1.09
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.04	1.09
1:A:415:TYR:HD1	1:A:490:ARG:HG2	1.09	1.09
1:A:752:ASN:HA	1:A:784:LYS:HE2	1.10	1.08
1:A:605:ARG:HG2	1:A:605:ARG:HH11	1.13	1.08
1:B:814:HIS:HD2	1:B:819:ARG:NH2	1.49	1.08
1:A:236:LEU:HD23	1:A:239:ILE:HG12	1.30	1.08
1:A:171:LYS:HD2	1:A:214:THR:HG21	1.34	1.07
1:B:748:ARG:HE	1:B:759:PRO:HD2	1.13	1.07
1:A:350:CYS:O	1:A:384:LEU:HD22	1.55	1.06
1:B:883:PRO:CB	1:B:884:PRO:CD	2.32	1.06
1:B:262:LEU:HD12	1:B:262:LEU:H	1.20	1.06
1:A:648:GLN:C	1:A:650:PRO:CD	2.28	1.06
1:B:444:GLU:OE1	1:B:444:GLU:HA	1.52	1.06
1:A:416:VAL:HG12	1:A:416:VAL:O	1.54	1.06
1:A:452:GLY:HA3	1:A:456:ARG:HD2	1.09	1.05
1:A:452:GLY:CA	1:A:456:ARG:HH11	1.69	1.05
1:B:883:PRO:HB2	1:B:884:PRO:HD3	1.38	1.05
1:B:819:ARG:O	1:B:820:VAL:HG12	1.56	1.05
1:A:136:GLU:HG3	1:A:218:HIS:NE2	1.71	1.04
1:A:781:ILE:HG22	1:A:781:ILE:O	1.57	1.04
1:B:880:TYR:CE2	1:B:881:GLN:O	2.10	1.04
1:A:644:TYR:CD2	1:A:649:LYS:HD3	1.91	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:H	1:A:460:ILE:HD12	0.87	1.03
1:A:755:VAL:CB	1:A:778:MET:CE	2.36	1.03
1:A:664:ASP:CG	1:A:692:ARG:HH11	1.66	1.03
1:B:883:PRO:CG	1:B:884:PRO:CD	2.30	1.03
1:B:883:PRO:HB2	1:B:884:PRO:CD	1.87	1.02
1:B:648:GLN:O	1:B:650:PRO:HD3	1.56	1.02
1:A:154:ARG:HH12	1:A:209:GLU:CD	1.67	1.02
1:B:414:LYS:HG3	1:B:416:VAL:H	1.25	1.02
1:B:560:ASN:HD22	1:B:564:ILE:HD11	1.19	1.01
1:B:236:LEU:HD13	1:B:574:LYS:HB2	1.39	1.01
1:B:487:GLN:HG3	1:B:490:ARG:NH2	1.74	1.01
1:A:764:VAL:CG1	1:A:772:LEU:HB2	1.90	1.00
1:A:136:GLU:HG2	1:A:137:PHE:H	1.25	1.00
1:A:764:VAL:HG11	1:A:772:LEU:HB2	1.02	1.00
1:A:173:ARG:CZ	1:A:212:GLU:HG2	1.91	0.99
1:B:748:ARG:HE	1:B:759:PRO:CD	1.75	0.99
1:A:560:ASN:HB3	1:A:564:ILE:HD11	1.44	0.98
1:A:664:ASP:HB3	1:A:688:GLN:OE1	1.63	0.98
1:A:452:GLY:HA2	1:A:456:ARG:HH11	0.84	0.98
1:B:780:PHE:HZ	1:B:809:ASN:HB3	1.12	0.97
1:A:485:CYS:SG	1:A:488:LYS:NZ	2.38	0.97
1:A:287:ILE:HD12	1:A:288:GLU:H	1.30	0.97
1:A:764:VAL:HG11	1:A:772:LEU:CB	1.95	0.96
1:B:408:TRP:O	1:B:412:CYS:HB2	1.64	0.96
1:A:136:GLU:CG	1:A:218:HIS:CD2	2.47	0.96
1:A:452:GLY:HA3	1:A:456:ARG:CD	1.94	0.96
1:B:440:GLU:OE1	1:B:441:PHE:HE1	1.47	0.96
1:B:441:PHE:CE2	2:P:9:MLY:CH1	2.49	0.96
1:B:444:GLU:OE1	1:B:488:LYS:HE2	1.65	0.95
1:A:412:CYS:O	1:A:416:VAL:HB	1.67	0.95
1:B:645:ASP:O	1:B:646:GLU:HB3	1.64	0.95
1:A:740:ASN:HD22	1:A:742:ARG:HG3	1.30	0.95
1:A:134:GLU:HG2	1:A:180:LYS:HE3	1.48	0.94
1:A:599:LEU:HD11	1:A:856:PRO:HG2	1.49	0.94
1:A:604:MET:HE1	1:A:641:MET:HE1	1.50	0.94
1:B:466:TRP:HB2	1:B:469:TYR:HD1	1.32	0.93
1:A:355:THR:HG22	1:A:388:HIS:CE1	2.03	0.93
1:A:171:LYS:HD2	1:A:214:THR:CG2	1.97	0.93
1:A:478:PRO:HG2	1:A:481:ASN:HB2	1.49	0.93
1:A:287:ILE:CD1	1:A:288:GLU:N	2.30	0.93
1:B:648:GLN:C	1:B:648:GLN:HE21	1.77	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASP:C	1:A:744:LEU:HD23	1.94	0.92
1:A:173:ARG:NH1	1:A:212:GLU:CG	2.30	0.92
1:A:748:ARG:CB	1:A:756:GLU:H	1.83	0.92
1:A:456:ARG:HB3	1:A:461:TYR:OH	1.68	0.92
1:A:495:GLU:O	1:A:498:LYS:HG2	1.68	0.91
1:A:170:LEU:O	1:A:171:LYS:CG	2.18	0.91
1:B:733:ILE:HG13	1:B:734:PRO:HD2	1.49	0.91
1:B:560:ASN:HD22	1:B:564:ILE:CD1	1.81	0.91
1:A:457:GLU:O	1:A:458:ASN:HB2	1.68	0.91
1:A:667:LYS:HA	1:A:817:GLN:OE1	1.71	0.91
1:A:171:LYS:CD	1:A:214:THR:HG21	2.01	0.90
1:B:182:ASP:CG	1:B:183:ASN:H	1.79	0.90
1:A:837:ARG:HG3	1:A:837:ARG:HH11	1.35	0.90
1:A:648:GLN:N	1:A:648:GLN:CD	2.30	0.90
1:A:659:GLY:O	1:A:663:SER:HB2	1.71	0.90
1:B:589:LEU:HA	1:B:620:TYR:OH	1.72	0.90
1:B:648:GLN:HE21	1:B:648:GLN:CA	1.85	0.90
1:A:355:THR:HG22	1:A:388:HIS:HE1	1.37	0.89
1:A:456:ARG:CG	1:A:461:TYR:CE2	2.52	0.89
1:A:173:ARG:HH11	1:A:212:GLU:HG2	1.25	0.89
1:A:649:LYS:N	1:A:650:PRO:CD	2.30	0.89
1:B:148:ARG:HG2	1:B:148:ARG:NH1	1.83	0.89
1:B:560:ASN:ND2	1:B:564:ILE:HD11	1.85	0.89
1:A:154:ARG:NH1	1:A:209:GLU:CD	2.31	0.89
1:B:134:GLU:OE1	1:B:134:GLU:N	2.05	0.89
1:A:447:VAL:HG23	1:A:463:LYS:HB3	1.54	0.88
1:B:440:GLU:N	1:B:440:GLU:CD	2.30	0.88
1:A:404:LEU:HD21	1:A:502:LEU:HD11	1.56	0.88
1:A:457:GLU:OE2	1:A:457:GLU:HA	1.73	0.88
1:A:879:LEU:HD22	1:A:879:LEU:H	1.39	0.88
1:B:814:HIS:HD2	1:B:819:ARG:HH21	1.19	0.88
1:A:136:GLU:HG2	1:A:137:PHE:N	1.86	0.88
1:A:652:LEU:O	1:A:653:LYS:C	2.15	0.88
1:A:664:ASP:CG	1:A:692:ARG:NH1	2.31	0.88
1:A:715:LEU:HD22	1:A:837:ARG:HG2	1.52	0.88
1:B:182:ASP:CG	1:B:183:ASN:N	2.31	0.88
1:B:880:TYR:CZ	1:B:881:GLN:O	2.27	0.88
1:B:821:LEU:HD23	1:B:825:GLU:OE1	1.72	0.88
1:B:748:ARG:NE	1:B:759:PRO:HD2	1.88	0.87
1:A:605:ARG:HH11	1:A:605:ARG:CG	1.88	0.87
1:A:648:GLN:CA	1:A:650:PRO:HD2	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:SER:O	1:B:788:PRO:HD3	1.74	0.87
1:A:560:ASN:CB	1:A:564:ILE:HD11	2.05	0.87
1:A:596:CYS:HB3	1:A:623:PRO:HB3	1.55	0.87
1:B:140:SER:OG	1:B:141:PRO:HD3	1.74	0.87
1:B:814:HIS:CD2	1:B:819:ARG:NH2	2.41	0.87
1:B:737:LYS:HG3	1:B:793:TRP:NE1	1.90	0.87
1:B:442:VAL:HA	2:P:6:THR:HG22	1.56	0.86
1:B:206:ARG:HG3	1:B:206:ARG:NH1	1.84	0.86
1:A:134:GLU:HG2	1:A:180:LYS:CE	2.05	0.86
1:A:384:LEU:CD1	1:A:384:LEU:C	2.49	0.86
1:A:592:MET:HG3	1:A:642:VAL:HG21	1.56	0.86
1:A:759:PRO:O	1:A:760:GLU:HB2	1.75	0.86
1:B:619:LYS:HG3	1:B:880:TYR:HB2	1.57	0.86
1:A:281:LYS:HA	1:A:284:ALA:HB3	1.57	0.86
1:B:236:LEU:O	1:B:239:ILE:HD11	1.75	0.86
1:A:487:GLN:CB	1:A:491:GLU:OE2	2.23	0.86
1:A:541:MET:SD	1:A:558:MET:HE1	2.16	0.85
1:A:752:ASN:CB	1:A:784:LYS:HE2	2.05	0.85
1:A:379:PHE:CD2	1:A:844:GLU:HG2	2.10	0.85
1:B:596:CYS:HB3	1:B:623:PRO:HB3	1.56	0.85
1:B:206:ARG:HH11	1:B:206:ARG:CG	1.89	0.85
1:B:725:ASP:OD1	1:B:726:ASP:N	2.10	0.85
1:A:781:ILE:O	1:A:782:LYS:HB3	1.74	0.84
1:B:440:GLU:OE1	1:B:441:PHE:CE1	2.30	0.84
1:A:755:VAL:C	1:A:778:MET:HE1	2.02	0.84
1:A:136:GLU:HG3	1:A:218:HIS:CE1	2.12	0.84
1:A:592:MET:HE2	1:A:857:VAL:HG13	1.59	0.83
1:B:218:HIS:C	1:B:262:LEU:HD11	2.03	0.83
1:A:666:PRO:HG3	1:A:679:TYR:O	1.78	0.83
1:B:534:LYS:O	1:B:538:ASN:HB3	1.76	0.83
1:A:752:ASN:CB	1:A:784:LYS:CE	2.56	0.83
1:B:699:LEU:N	1:B:699:LEU:HD12	1.92	0.83
1:A:714:LEU:HD21	1:A:717:HIS:HB2	1.58	0.83
1:B:882:LEU:N	1:B:882:LEU:CD1	2.38	0.83
1:B:444:GLU:OE1	1:B:488:LYS:CE	2.25	0.83
1:B:879:LEU:H	1:B:879:LEU:HD22	1.41	0.83
1:A:212:GLU:OE1	1:A:218:HIS:HA	1.77	0.83
1:A:877:ASP:OD1	1:A:878:PRO:HD2	1.79	0.83
1:A:274:VAL:HG12	1:A:275:ASP:N	1.94	0.82
1:A:405:LEU:HD21	1:A:503:PRO:HG2	1.58	0.82
1:A:588:ARG:NH2	1:A:617:LEU:HD11	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ARG:HG2	1:A:605:ARG:NH1	1.92	0.82
1:B:648:GLN:C	1:B:650:PRO:CD	2.43	0.82
1:A:284:ALA:O	1:A:287:ILE:HG13	1.79	0.82
1:A:218:HIS:HB2	1:A:262:LEU:HD12	1.62	0.82
1:A:537:LYS:C	1:A:539:LYS:H	1.88	0.82
1:B:375:ASP:OD1	1:B:375:ASP:C	2.22	0.82
1:B:444:GLU:OE1	1:B:444:GLU:CA	2.27	0.82
1:A:221:THR:HB	1:A:259:ASP:OD1	1.80	0.82
1:A:490:ARG:O	1:A:494:GLN:HG2	1.80	0.82
1:A:278:MET:HG2	1:A:282:ALA:HB3	1.61	0.82
1:A:465:GLN:HG3	1:A:474:ASP:OD1	1.79	0.82
1:A:484:ASP:OD1	1:A:484:ASP:N	2.09	0.82
1:A:646:GLU:CD	1:A:646:GLU:C	2.47	0.82
1:A:624:THR:O	1:A:625:TYR:HD2	1.56	0.81
1:A:648:GLN:CA	1:A:648:GLN:NE2	2.43	0.81
1:A:487:GLN:O	1:A:491:GLU:CD	2.22	0.81
1:A:502:LEU:HD23	1:A:503:PRO:HD2	1.60	0.81
1:A:664:ASP:O	1:A:665:LEU:HG	1.80	0.81
1:A:714:LEU:HD21	1:A:717:HIS:CB	2.09	0.81
1:B:142:VAL:HG12	1:B:143:ALA:H	1.45	0.81
1:B:399:ASP:OD1	1:B:399:ASP:N	2.14	0.81
1:A:782:LYS:HG3	1:A:782:LYS:O	1.79	0.81
1:A:456:ARG:HD3	1:A:461:TYR:HD2	1.42	0.81
1:A:154:ARG:HH21	1:A:170:LEU:HD11	1.45	0.80
1:B:881:GLN:C	1:B:882:LEU:HD12	2.06	0.80
1:A:534:LYS:NZ	1:A:535:ASP:HB3	1.96	0.80
1:A:692:ARG:O	1:A:693:LEU:HD12	1.80	0.80
1:A:877:ASP:OD1	1:A:878:PRO:CD	2.30	0.80
1:B:601:GLN:OE1	1:B:801:VAL:HG12	1.81	0.80
1:A:803:THR:HA	1:A:850:GLY:HA3	1.62	0.80
1:A:704:GLY:O	1:A:705:GLU:CD	2.24	0.80
1:A:457:GLU:OE2	1:A:457:GLU:CA	2.30	0.80
1:A:466:TRP:CD1	1:A:466:TRP:N	2.50	0.80
1:A:261:VAL:HG22	1:A:263:ASP:H	1.47	0.80
1:A:284:ALA:O	1:A:287:ILE:CD1	2.30	0.80
1:A:781:ILE:O	1:A:781:ILE:CG2	2.30	0.80
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.47	0.79
1:A:685:THR:OG1	1:A:688:GLN:HG3	1.82	0.79
1:A:564:ILE:HG23	1:A:572:LEU:HB2	1.64	0.79
1:A:596:CYS:O	1:A:597:TYR:HB2	1.81	0.79
1:A:648:GLN:N	1:A:648:GLN:NE2	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:CD1	1:A:384:LEU:O	2.30	0.79
1:A:236:LEU:CD2	1:A:239:ILE:HG12	2.12	0.79
1:B:648:GLN:O	1:B:650:PRO:CD	2.29	0.79
1:B:819:ARG:O	1:B:820:VAL:CG1	2.30	0.79
1:A:740:ASN:ND2	1:A:742:ARG:HG3	1.98	0.79
1:A:778:MET:HE3	1:A:778:MET:HA	1.63	0.79
1:A:410:VAL:O	1:A:413:LYS:HB3	1.82	0.79
1:A:416:VAL:O	1:A:416:VAL:CG1	2.27	0.79
1:A:645:ASP:CG	1:A:646:GLU:H	1.89	0.79
1:A:823:ILE:HD11	1:A:842:ILE:HG23	1.62	0.79
1:A:308:ILE:CG2	1:A:308:ILE:O	2.30	0.79
1:A:837:ARG:HB3	1:A:839:PHE:HE1	1.47	0.79
1:A:852:ALA:HA	3:A:1000:SAH:OXT	1.83	0.79
1:B:209:GLU:HB2	1:B:221:THR:HB	1.62	0.79
1:B:349:GLY:HA2	1:B:380:ALA:HB1	1.63	0.79
1:B:466:TRP:HB2	1:B:469:TYR:CD1	2.17	0.79
1:B:649:LYS:N	1:B:650:PRO:HD3	1.93	0.79
1:A:287:ILE:HD12	1:A:288:GLU:CA	2.13	0.78
1:A:486:PRO:HB2	1:A:490:ARG:HD2	1.63	0.78
1:B:792:LEU:HD23	1:B:811:VAL:O	1.83	0.78
1:A:227:ARG:HB3	1:A:229:GLU:OE1	1.84	0.78
1:B:485:CYS:HB3	2:P:6:THR:N	1.99	0.78
1:A:671:HIS:CD2	1:A:721:ARG:HH21	2.01	0.78
1:A:717:HIS:CE1	1:A:822:THR:HG21	2.19	0.78
1:B:218:HIS:O	1:B:262:LEU:CD1	2.32	0.78
1:B:622:LEU:HD12	1:B:880:TYR:O	1.84	0.78
1:B:648:GLN:N	1:B:648:GLN:NE2	2.32	0.78
1:A:236:LEU:HD23	1:A:239:ILE:CG1	2.11	0.77
1:B:536:GLU:OE2	1:B:536:GLU:CA	2.30	0.77
1:A:171:LYS:CD	1:A:214:THR:CG2	2.62	0.77
1:A:154:ARG:HH21	1:A:170:LEU:CD1	1.97	0.77
1:A:136:GLU:CG	1:A:218:HIS:NE2	2.48	0.77
1:B:442:VAL:HG12	1:B:442:VAL:O	1.83	0.77
1:B:134:GLU:HB3	1:B:135:PRO:HD2	1.67	0.77
1:B:564:ILE:HG23	1:B:572:LEU:HB2	1.64	0.77
1:B:814:HIS:CD2	1:B:819:ARG:HH21	2.02	0.77
1:A:136:GLU:HG3	1:A:218:HIS:CG	2.20	0.77
1:A:196:ALA:HB2	1:A:201:ALA:O	1.85	0.77
1:A:308:ILE:O	1:A:309:SER:CB	2.33	0.77
1:A:384:LEU:C	1:A:384:LEU:HD12	2.09	0.77
1:B:262:LEU:H	1:B:262:LEU:CD1	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:PHE:CD1	1:B:441:PHE:N	2.50	0.76
1:A:141:PRO:O	1:A:142:VAL:HG22	1.86	0.76
1:A:596:CYS:O	1:A:597:TYR:CB	2.30	0.76
1:B:646:GLU:OE2	1:B:647:THR:HA	1.86	0.76
1:A:646:GLU:CD	1:A:646:GLU:O	2.28	0.76
1:A:817:GLN:NE2	1:A:819:ARG:HE	1.84	0.76
1:B:772:LEU:C	1:B:774:PRO:HD3	2.10	0.76
1:A:153:LYS:HE2	1:A:170:LEU:HD22	1.67	0.76
1:A:883:PRO:HB2	1:A:884:PRO:CD	2.15	0.76
1:B:645:ASP:OD1	1:B:645:ASP:C	2.29	0.76
1:B:733:ILE:CG2	1:B:791:ARG:HE	1.98	0.76
1:A:755:VAL:O	1:A:778:MET:CE	2.34	0.76
1:A:242:ASP:OD1	1:A:243:GLY:N	2.18	0.76
1:A:456:ARG:CB	1:A:461:TYR:HE2	1.98	0.76
1:A:534:LYS:HZ2	1:A:535:ASP:N	1.84	0.76
1:A:381:CYS:HB3	1:A:393:VAL:HG11	1.67	0.75
1:B:786:LEU:C	1:B:788:PRO:HD2	2.11	0.75
1:B:536:GLU:OE2	1:B:536:GLU:C	2.30	0.75
1:A:136:GLU:CB	1:A:218:HIS:CD2	2.69	0.75
1:A:879:LEU:HD22	1:A:879:LEU:N	2.00	0.75
1:B:202:ASP:O	1:B:227:ARG:NH2	2.20	0.75
1:B:821:LEU:CD2	1:B:825:GLU:OE1	2.33	0.75
1:B:375:ASP:OD1	1:B:377:ASN:N	2.20	0.75
1:A:209:GLU:CD	1:A:221:THR:HG21	2.11	0.75
1:A:460:ILE:O	1:A:461:TYR:HD1	1.68	0.75
1:B:723:ASN:OD1	1:B:723:ASN:N	2.20	0.75
1:A:384:LEU:O	1:A:384:LEU:HD13	1.87	0.74
1:B:443:VAL:CG2	1:B:488:LYS:HG3	2.16	0.74
1:B:808:HIS:ND1	1:B:809:ASN:OD1	2.20	0.74
1:B:883:PRO:CB	1:B:884:PRO:HD3	2.09	0.74
1:A:867:GLN:NE2	1:A:872:GLU:OE1	2.20	0.74
1:B:487:GLN:CG	1:B:490:ARG:NH2	2.51	0.74
1:A:192:VAL:HG11	1:A:207:ILE:HD11	1.69	0.74
1:B:820:VAL:HG13	1:B:821:LEU:N	2.02	0.74
1:B:883:PRO:HG2	1:B:884:PRO:HD2	0.77	0.74
1:A:389:PRO:HG3	1:A:703:PHE:CE1	2.23	0.74
1:A:755:VAL:O	1:A:778:MET:HE2	1.88	0.74
1:B:281:LYS:HA	1:B:284:ALA:HB3	1.70	0.74
1:B:735:VAL:O	1:B:735:VAL:HG22	1.88	0.74
1:B:690:TYR:OH	1:B:859:ARG:NH2	2.21	0.73
1:B:650:PRO:C	1:B:652:LEU:H	1.96	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:HG2	1:A:212:GLU:HB3	1.69	0.73
1:A:443:VAL:HA	1:A:466:TRP:HB3	1.70	0.73
1:B:138:ILE:HG12	1:B:139:GLY:H	1.51	0.73
1:B:740:ASN:C	1:B:740:ASN:OD1	2.30	0.73
1:A:381:CYS:HB3	1:A:393:VAL:CG1	2.19	0.73
1:A:287:ILE:HD12	1:A:287:ILE:C	2.10	0.73
1:A:350:CYS:C	1:A:384:LEU:CD2	2.61	0.73
1:A:663:SER:HB3	1:A:688:GLN:HE22	1.53	0.73
1:B:648:GLN:HE21	1:B:648:GLN:N	1.86	0.73
1:A:136:GLU:HB2	1:A:218:HIS:CD2	2.24	0.73
1:A:376:PHE:O	1:A:395:ASN:ND2	2.22	0.73
1:B:227:ARG:HB2	1:B:230:ASP:OD2	1.87	0.73
1:B:536:GLU:OE2	1:B:536:GLU:HA	1.86	0.73
1:A:456:ARG:CB	1:A:461:TYR:CE2	2.72	0.73
1:A:764:VAL:HG13	1:A:772:LEU:H	1.53	0.73
1:B:376:PHE:O	1:B:395:ASN:ND2	2.21	0.72
1:A:277:ASN:OD1	1:A:277:ASN:N	2.22	0.72
1:A:837:ARG:HG3	1:A:837:ARG:NH1	1.99	0.72
1:B:560:ASN:HD22	1:B:564:ILE:CG1	2.02	0.72
1:B:711:GLU:N	1:B:711:GLU:OE1	2.22	0.72
1:A:672:GLN:NE2	1:A:674:ASN:HB2	2.05	0.72
1:A:534:LYS:HD3	1:A:535:ASP:H	1.54	0.72
1:A:828:ARG:NH2	1:A:834:ASP:OD1	2.23	0.72
1:B:148:ARG:HH11	1:B:148:ARG:CG	1.92	0.72
1:B:207:ILE:HD12	1:B:207:ILE:H	1.52	0.72
1:B:725:ASP:O	1:B:728:GLU:HB2	1.90	0.72
1:A:191:ASP:OD1	1:A:206:ARG:NH1	2.22	0.72
1:A:308:ILE:O	1:A:309:SER:HB2	1.88	0.72
1:A:389:PRO:HD2	1:A:702:SER:OG	1.90	0.72
1:A:577:LEU:O	1:A:581:VAL:HG12	1.89	0.72
1:A:725:ASP:HA	1:A:766:LEU:HD23	1.71	0.72
1:B:741:PHE:CE2	1:B:788:PRO:HG3	2.25	0.72
1:A:351:GLY:O	1:A:355:THR:HG23	1.90	0.72
1:A:362:ALA:HB1	1:A:699:LEU:HD22	1.72	0.72
1:B:809:ASN:OD1	1:B:809:ASN:N	2.23	0.72
1:B:837:ARG:O	1:B:838:LEU:HD12	1.90	0.72
1:A:453:GLY:O	1:A:454:SER:C	2.30	0.72
1:A:460:ILE:O	1:A:461:TYR:CD1	2.43	0.72
1:A:790:GLY:O	1:A:813:ILE:HG23	1.90	0.72
1:B:444:GLU:HA	1:B:488:LYS:HE2	1.72	0.72
1:B:466:TRP:CB	1:B:469:TYR:HD1	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:O	1:A:367:LYS:HE3	1.90	0.71
1:B:191:ASP:OD1	1:B:206:ARG:NH1	2.23	0.71
1:A:539:LYS:O	1:A:542:VAL:N	2.23	0.71
1:A:339:ARG:O	1:A:367:LYS:HB3	1.90	0.71
1:A:743:ASP:O	1:A:744:LEU:CD2	2.30	0.71
1:A:812:ILE:HG23	1:A:820:VAL:HG22	1.71	0.71
1:B:307:ASN:H	1:B:307:ASN:HD22	1.38	0.71
1:A:350:CYS:O	1:A:384:LEU:CD2	2.34	0.71
1:A:685:THR:O	1:A:689:ARG:HG3	1.90	0.71
1:A:580:LEU:O	1:A:585:TYR:HB2	1.90	0.71
1:B:223:ARG:HD2	1:B:254:SER:O	1.90	0.71
1:B:388:HIS:HB3	1:B:391:THR:HG23	1.71	0.71
1:B:484:ASP:HB2	2:P:6:THR:O	1.89	0.71
1:B:561:VAL:HG12	1:B:562:VAL:H	1.54	0.71
1:A:487:GLN:O	1:A:491:GLU:CG	2.38	0.71
1:A:517:CYS:HB2	1:A:538:ASN:HA	1.71	0.71
1:B:880:TYR:CG	1:B:881:GLN:N	2.59	0.71
1:A:880:TYR:HD1	1:A:881:GLN:N	1.88	0.70
1:A:560:ASN:HB3	1:A:564:ILE:CD1	2.21	0.70
1:B:375:ASP:OD1	1:B:376:PHE:N	2.23	0.70
1:A:766:LEU:HD13	1:A:770:LYS:O	1.91	0.70
1:A:699:LEU:O	1:A:701:TRP:HB2	1.90	0.70
1:A:746:GLY:HA2	1:A:758:ASP:CB	2.21	0.70
1:A:645:ASP:OD1	1:A:646:GLU:N	2.24	0.70
1:A:598:GLY:N	1:A:625:TYR:CD2	2.59	0.70
1:A:823:ILE:HD13	1:A:845:LYS:HG3	1.74	0.70
1:A:874:GLU:OE2	1:A:875:GLY:O	2.09	0.70
1:B:485:CYS:HB2	2:P:5:GLN:N	2.06	0.70
1:A:284:ALA:O	1:A:287:ILE:CG1	2.39	0.70
1:B:193:TYR:CE1	1:B:269:VAL:HG22	2.26	0.70
1:B:867:GLN:NE2	1:B:872:GLU:OE1	2.25	0.70
1:A:564:ILE:O	1:A:570:GLY:HA2	1.92	0.69
1:B:440:GLU:C	1:B:441:PHE:CD1	2.70	0.69
1:B:626:ASP:OD1	1:B:626:ASP:O	2.11	0.69
1:B:726:ASP:OD1	1:B:729:ARG:NH1	2.24	0.69
1:A:250:ARG:NH2	1:A:295:ASP:OD2	2.25	0.69
1:B:677:MET:HE3	1:B:717:HIS:HB3	1.75	0.69
1:B:741:PHE:CD2	1:B:788:PRO:HG2	2.28	0.69
1:A:648:GLN:HE21	1:A:648:GLN:HA	1.56	0.69
1:A:537:LYS:C	1:A:539:LYS:N	2.48	0.69
1:A:647:THR:C	1:A:648:GLN:NE2	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:SER:OG	1:B:236:LEU:N	2.22	0.69
1:B:442:VAL:CG1	1:B:467:GLU:HG3	2.22	0.69
1:A:151:TRP:HE1	1:A:175:HIS:CE1	2.11	0.69
1:B:664:ASP:CG	1:B:692:ARG:NH1	2.51	0.69
1:A:646:GLU:C	1:A:646:GLU:OE2	2.36	0.69
1:A:537:LYS:CG	1:A:538:ASN:H	2.06	0.69
1:A:648:GLN:NE2	1:A:648:GLN:HA	2.06	0.69
1:B:828:ARG:HH22	1:B:834:ASP:CG	2.01	0.69
1:A:148:ARG:HG2	1:A:155:TYR:CD2	2.29	0.68
1:A:353:MET:HB2	1:A:853:VAL:HG11	1.73	0.68
1:B:218:HIS:O	1:B:262:LEU:HD12	1.94	0.68
1:B:671:HIS:CD2	1:B:721:ARG:HD2	2.28	0.68
1:A:279:ASP:OD1	1:A:279:ASP:N	2.27	0.68
1:A:454:SER:O	1:A:455:ASP:C	2.30	0.68
1:B:485:CYS:N	2:P:6:THR:O	2.26	0.68
1:B:637:PHE:HB3	1:B:640:CYS:SG	2.34	0.68
1:B:441:PHE:CE2	2:P:9:MLY:HH12	2.28	0.68
1:B:729:ARG:NH2	1:B:773:VAL:HG11	2.07	0.68
1:A:195:LYS:HB2	1:A:266:ILE:HD11	1.75	0.68
1:B:140:SER:CB	1:B:141:PRO:CD	2.71	0.68
1:B:414:LYS:HG3	1:B:416:VAL:N	2.06	0.68
1:B:733:ILE:CG1	1:B:734:PRO:HD2	2.23	0.68
1:A:541:MET:HE1	1:A:558:MET:HE1	1.76	0.68
1:A:296:MET:HG2	1:A:306:ALA:O	1.93	0.68
1:B:154:ARG:O	1:B:171:LYS:HG2	1.94	0.68
1:B:441:PHE:CZ	2:P:9:MLY:HH12	2.28	0.68
1:A:170:LEU:HG	1:A:171:LYS:N	2.08	0.68
1:B:812:ILE:O	1:B:821:LEU:HD12	1.93	0.68
1:A:274:VAL:CG1	1:A:275:ASP:H	1.98	0.68
1:B:180:LYS:NZ	1:B:182:ASP:O	2.21	0.68
1:B:599:LEU:HD23	1:B:829:LEU:O	1.94	0.68
1:B:788:PRO:O	1:B:789:PHE:C	2.35	0.68
1:B:813:ILE:HA	1:B:820:VAL:HA	1.77	0.68
1:B:441:PHE:CD2	2:P:9:MLY:HH13	2.29	0.67
1:A:449:ILE:HD11	1:A:460:ILE:CG2	2.25	0.67
1:A:737:LYS:NZ	1:A:795:ASP:OD1	2.25	0.67
1:B:142:VAL:HG13	1:B:175:HIS:H	1.59	0.67
1:B:819:ARG:NH1	1:B:822:THR:HG22	2.09	0.67
1:A:752:ASN:CB	1:A:784:LYS:HE3	2.25	0.67
1:B:536:GLU:O	1:B:539:LYS:HG3	1.95	0.67
1:B:648:GLN:NE2	1:B:648:GLN:H	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:HIS:CD2	1:A:721:ARG:NH2	2.63	0.67
1:B:142:VAL:CG1	1:B:175:HIS:H	2.06	0.67
1:B:570:GLY:O	1:B:574:LYS:HG3	1.95	0.67
1:A:151:TRP:NE1	1:A:175:HIS:CE1	2.63	0.67
1:B:147:ALA:O	1:B:151:TRP:N	2.27	0.67
1:B:345:ASP:CG	1:B:348:SER:HB3	2.20	0.67
1:A:154:ARG:NE	1:A:170:LEU:HD21	2.09	0.67
1:A:755:VAL:CA	1:A:778:MET:HE1	2.24	0.67
1:A:133:HIS:O	1:A:135:PRO:HG3	1.93	0.67
1:A:287:ILE:O	1:A:290:CYS:SG	2.51	0.66
1:B:688:GLN:HA	1:B:691:ILE:HD11	1.77	0.66
1:A:556:VAL:HB	1:A:610:GLY:HA3	1.77	0.66
1:A:641:MET:HG3	1:A:642:VAL:N	2.09	0.66
1:B:793:TRP:O	1:B:795:ASP:N	2.28	0.66
1:A:233:ILE:HG13	1:A:233:ILE:O	1.94	0.66
1:A:443:VAL:HG23	1:A:466:TRP:CE3	2.30	0.66
1:A:464:VAL:HG22	1:A:475:THR:O	1.95	0.66
1:A:534:LYS:CD	1:A:535:ASP:H	2.08	0.66
1:A:648:GLN:O	1:A:650:PRO:HG2	1.94	0.66
1:B:279:ASP:HB2	1:B:280:PRO:HD3	1.77	0.66
1:A:879:LEU:H	1:A:879:LEU:CD2	2.08	0.66
1:B:415:TYR:O	1:B:490:ARG:HA	1.95	0.66
1:A:664:ASP:OD1	1:A:692:ARG:NH1	2.28	0.66
1:A:781:ILE:HD13	1:A:781:ILE:N	2.10	0.66
1:B:581:VAL:O	1:B:584:LYS:N	2.26	0.66
1:B:741:PHE:CD2	1:B:788:PRO:CG	2.78	0.66
1:A:592:MET:HG3	1:A:642:VAL:CG2	2.24	0.66
1:B:805:ALA:O	1:B:806:GLU:HG3	1.95	0.66
1:A:384:LEU:O	1:A:384:LEU:HD12	1.96	0.66
1:A:880:TYR:CD1	1:A:881:GLN:N	2.64	0.66
1:A:350:CYS:C	1:A:384:LEU:HD22	2.20	0.66
1:B:279:ASP:HB2	1:B:280:PRO:CD	2.26	0.66
1:B:867:GLN:CD	1:B:872:GLU:OE1	2.38	0.66
1:A:444:GLU:HB3	1:A:466:TRP:HA	1.78	0.65
1:A:782:LYS:O	1:A:782:LYS:CG	2.43	0.65
1:A:140:SER:O	1:A:142:VAL:N	2.30	0.65
1:A:884:PRO:O	1:A:885:SER:C	2.39	0.65
1:B:622:LEU:CD1	1:B:880:TYR:O	2.44	0.65
1:B:444:GLU:O	1:B:465:GLN:HB2	1.96	0.65
1:B:657:LEU:HB3	1:B:794:TRP:O	1.96	0.65
1:A:270:LYS:HE3	1:A:291:ASP:OD1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:HIS:CE1	1:B:822:THR:HG21	2.32	0.65
1:A:591:MET:HG2	1:A:606:VAL:HG22	1.78	0.65
1:A:755:VAL:C	1:A:778:MET:CE	2.70	0.65
1:B:802:VAL:HG23	1:B:810:GLN:NE2	2.12	0.65
1:B:819:ARG:NH1	1:B:820:VAL:O	2.30	0.65
1:B:819:ARG:HG3	1:B:819:ARG:HH11	1.62	0.65
1:B:882:LEU:HD12	1:B:882:LEU:H	1.60	0.65
1:A:879:LEU:N	1:A:879:LEU:CD2	2.60	0.65
1:B:599:LEU:HD11	1:B:856:PRO:HG2	1.78	0.65
1:B:344:LEU:HD12	1:B:372:TRP:HB2	1.77	0.65
1:A:250:ARG:HG3	1:A:293:TYR:CE1	2.32	0.65
1:A:445:LYS:C	1:A:446:LEU:HD23	2.22	0.65
1:A:817:GLN:NE2	1:A:819:ARG:NE	2.44	0.65
1:B:565:LEU:HB3	1:B:637:PHE:CE2	2.31	0.65
1:B:593:VAL:HG23	1:B:641:MET:HE1	1.77	0.65
1:B:637:PHE:N	1:B:637:PHE:CD2	2.65	0.65
1:A:487:GLN:CA	1:A:491:GLU:OE2	2.45	0.64
1:A:136:GLU:HB2	1:A:218:HIS:NE2	2.12	0.64
1:A:209:GLU:OE1	1:A:221:THR:HG21	1.97	0.64
1:A:241:VAL:HG11	1:A:583:MET:HE2	1.78	0.64
1:A:486:PRO:HB2	1:A:490:ARG:CD	2.26	0.64
1:A:541:MET:CE	1:A:558:MET:HE1	2.28	0.64
1:A:776:TYR:HA	1:A:779:SER:OG	1.96	0.64
1:B:440:GLU:OE1	1:B:440:GLU:N	2.30	0.64
1:B:635:ASN:OD1	1:B:636:ALA:N	2.29	0.64
1:B:672:GLN:OE1	1:B:674:ASN:HB2	1.97	0.64
1:A:242:ASP:CG	1:A:243:GLY:H	2.04	0.64
1:A:278:MET:HG2	1:A:282:ALA:CB	2.27	0.64
1:B:262:LEU:HD12	1:B:262:LEU:N	2.04	0.64
1:B:664:ASP:CG	1:B:692:ARG:HH11	2.05	0.64
1:B:140:SER:CB	1:B:141:PRO:HD3	2.27	0.64
1:A:592:MET:CG	1:A:642:VAL:HG21	2.27	0.64
1:A:874:GLU:CD	1:A:875:GLY:N	2.56	0.64
1:B:696:LYS:HZ2	1:B:706:GLY:C	2.05	0.64
1:A:755:VAL:CB	1:A:778:MET:HE3	2.27	0.64
1:B:648:GLN:O	1:B:648:GLN:NE2	2.30	0.64
1:A:148:ARG:HG3	1:A:148:ARG:NH1	2.12	0.64
1:A:457:GLU:O	1:A:458:ASN:CB	2.39	0.64
1:A:154:ARG:HE	1:A:170:LEU:HD11	1.63	0.64
1:A:211:PHE:CE1	1:A:219:TYR:HD2	2.16	0.64
1:A:677:MET:HG3	1:A:714:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:VAL:CG1	1:A:772:LEU:H	2.11	0.64
1:B:197:GLY:HA3	1:B:200:GLU:OE2	1.98	0.64
1:B:215:ASP:O	1:B:216:GLN:HB2	1.97	0.64
1:A:534:LYS:HZ1	1:A:535:ASP:HB3	1.63	0.64
1:A:534:LYS:HZ2	1:A:535:ASP:H	1.44	0.63
1:A:209:GLU:CD	1:A:221:THR:CG2	2.71	0.63
1:A:308:ILE:O	1:A:308:ILE:HG23	1.94	0.63
1:B:246:HIS:CE1	1:B:582:ALA:HB2	2.33	0.63
1:B:692:ARG:O	1:B:693:LEU:HD12	1.98	0.63
1:B:879:LEU:HD22	1:B:879:LEU:N	2.12	0.63
1:B:650:PRO:C	1:B:652:LEU:N	2.51	0.63
1:B:441:PHE:N	1:B:441:PHE:HD1	1.96	0.63
1:B:562:VAL:HG22	1:B:591:MET:HE3	1.79	0.63
1:B:675:ASP:OD1	1:B:676:VAL:N	2.31	0.63
1:A:741:PHE:O	1:A:744:LEU:HG	1.97	0.63
1:B:259:ASP:OD1	1:B:259:ASP:N	2.32	0.63
1:B:699:LEU:HD12	1:B:699:LEU:H	1.59	0.63
1:A:186:TYR:CE2	1:A:265:ILE:HG21	2.33	0.63
1:A:347:TYR:O	3:A:1000:SAH:HG1	1.97	0.63
1:A:664:ASP:OD2	1:A:692:ARG:NH1	2.25	0.63
1:B:273:HIS:HB2	1:B:294:TYR:CZ	2.34	0.63
1:B:561:VAL:HG12	1:B:562:VAL:N	2.13	0.63
1:A:580:LEU:HD21	1:A:610:GLY:HA2	1.80	0.63
1:B:349:GLY:O	1:B:351:GLY:N	2.32	0.63
1:A:176:TYR:O	1:A:210:PHE:HB2	1.99	0.62
1:A:353:MET:HB2	1:A:853:VAL:CG1	2.28	0.62
1:B:192:VAL:HG13	1:B:193:TYR:N	2.14	0.62
1:A:456:ARG:C	1:A:457:GLU:OE2	2.42	0.62
1:B:485:CYS:CB	2:P:5:GLN:N	2.62	0.62
1:B:565:LEU:HB3	1:B:637:PHE:CD2	2.34	0.62
1:A:134:GLU:CG	1:A:180:LYS:HE3	2.27	0.62
1:A:227:ARG:HB2	1:A:230:ASP:OD2	2.00	0.62
1:A:351:GLY:HA3	1:A:384:LEU:CD2	2.29	0.62
1:A:351:GLY:HA3	1:A:384:LEU:HD21	1.81	0.62
1:A:557:LEU:HD21	1:A:861:LEU:HD13	1.80	0.62
1:A:137:PHE:HE1	1:A:210:PHE:HB3	1.63	0.62
1:A:456:ARG:HB3	1:A:461:TYR:CZ	2.34	0.62
1:A:491:GLU:HA	1:A:494:GLN:HG3	1.81	0.62
1:A:512:CYS:HA	1:A:557:LEU:O	2.00	0.62
1:B:413:LYS:O	1:B:415:TYR:CD2	2.53	0.62
1:B:648:GLN:H	1:B:648:GLN:CD	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ARG:NH2	1:B:773:VAL:CG1	2.62	0.62
1:A:644:TYR:CD2	1:A:649:LYS:CD	2.76	0.62
1:B:589:LEU:C	1:B:589:LEU:HD12	2.24	0.62
1:B:664:ASP:OD1	1:B:692:ARG:NH1	2.29	0.62
1:A:600:PRO:HG2	1:A:661:ALA:HB2	1.80	0.62
1:B:349:GLY:CA	1:B:380:ALA:HB1	2.29	0.62
1:A:375:ASP:OD2	1:A:376:PHE:N	2.32	0.62
1:B:586:GLN:NE2	1:B:612:LEU:O	2.20	0.62
1:A:234:ASN:C	1:A:236:LEU:H	2.05	0.61
1:A:284:ALA:O	1:A:287:ILE:HD11	2.00	0.61
1:A:478:PRO:O	1:A:482:LEU:HD23	1.99	0.61
1:B:572:LEU:HD12	1:B:572:LEU:H	1.64	0.61
1:A:384:LEU:C	1:A:384:LEU:HD13	2.23	0.61
1:B:415:TYR:HD2	1:B:415:TYR:N	1.98	0.61
1:B:668:VAL:CG2	1:B:672:GLN:HB2	2.30	0.61
1:B:143:ALA:HB3	1:B:147:ALA:HB2	1.82	0.61
1:B:442:VAL:HG11	1:B:467:GLU:HG3	1.82	0.61
1:A:234:ASN:O	1:A:236:LEU:N	2.31	0.61
1:B:347:TYR:OH	1:B:540:GLN:NE2	2.33	0.61
1:A:350:CYS:C	1:A:384:LEU:HD23	2.24	0.61
1:A:703:PHE:CE2	1:A:709:PRO:HD2	2.35	0.61
1:A:714:LEU:HD23	1:A:714:LEU:C	2.25	0.61
1:B:383:SER:O	1:B:387:ASN:ND2	2.30	0.61
1:B:737:LYS:HG3	1:B:793:TRP:HE1	1.65	0.61
1:B:859:ARG:CG	1:B:859:ARG:NH1	2.27	0.61
1:A:140:SER:O	1:A:142:VAL:HG13	2.00	0.61
1:A:491:GLU:O	1:A:495:GLU:HB2	2.00	0.61
1:B:671:HIS:HD2	1:B:721:ARG:HD2	1.65	0.61
1:A:133:HIS:O	1:A:135:PRO:HD3	2.00	0.61
1:A:279:ASP:CB	1:A:280:PRO:HD2	2.30	0.61
1:A:788:PRO:HB3	1:A:808:HIS:O	2.01	0.61
1:B:349:GLY:C	1:B:351:GLY:H	2.09	0.61
1:B:379:PHE:O	1:B:382:GLN:N	2.33	0.61
1:A:249:ARG:CG	1:A:249:ARG:O	2.49	0.61
1:B:676:VAL:HG23	1:B:715:LEU:HD12	1.83	0.61
1:A:211:PHE:HE1	1:A:219:TYR:HD2	1.49	0.61
1:B:780:PHE:C	1:B:782:LYS:H	2.09	0.61
1:A:206:ARG:HH11	1:A:206:ARG:CG	2.14	0.61
1:A:730:VAL:HG11	1:A:818:ALA:O	2.00	0.61
1:A:790:GLY:C	1:A:811:VAL:HG23	2.25	0.61
1:A:883:PRO:HB2	1:A:884:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:HIS:CD2	1:B:274:VAL:N	2.68	0.61
1:A:138:ILE:CG2	1:A:139:GLY:N	2.63	0.60
1:A:143:ALA:O	1:A:144:ALA:C	2.44	0.60
1:A:825:GLU:O	1:A:829:LEU:HG	2.01	0.60
1:B:444:GLU:N	1:B:465:GLN:O	2.34	0.60
1:B:446:LEU:HD12	1:B:489:ILE:HA	1.82	0.60
1:B:819:ARG:O	1:B:820:VAL:CB	2.48	0.60
1:B:181:VAL:O	1:B:182:ASP:OD1	2.19	0.60
1:B:196:ALA:HB1	1:B:203:TYR:CZ	2.36	0.60
1:A:399:ASP:OD1	1:A:399:ASP:N	2.34	0.60
1:B:402:LEU:HD13	1:B:547:ILE:HD13	1.82	0.60
1:B:811:VAL:O	1:B:811:VAL:HG13	2.01	0.60
1:B:464:VAL:HG12	1:B:465:GLN:N	2.16	0.60
1:A:483:SER:OG	1:A:484:ASP:OD1	2.18	0.60
1:A:794:TRP:HZ2	1:A:816:THR:HG23	1.66	0.60
1:A:192:VAL:CG1	1:A:207:ILE:HD11	2.31	0.60
1:A:485:CYS:SG	1:A:488:LYS:HD2	2.42	0.60
1:B:609:TRP:CD1	1:B:620:TYR:CE1	2.89	0.60
1:B:283:LYS:C	1:B:287:ILE:HD12	2.26	0.60
1:B:410:VAL:HG13	1:B:411:LEU:H	1.67	0.60
1:B:441:PHE:CE2	2:P:9:MLY:HH11	2.36	0.60
1:A:154:ARG:NH1	1:A:209:GLU:OE1	2.34	0.60
1:B:402:LEU:O	1:B:405:LEU:HB2	2.02	0.60
1:A:173:ARG:HG3	1:A:174:CYS:N	2.16	0.59
1:A:469:TYR:N	1:A:469:TYR:HD2	1.98	0.59
1:B:485:CYS:O	1:B:485:CYS:SG	2.60	0.59
1:B:780:PHE:C	1:B:782:LYS:N	2.60	0.59
1:A:466:TRP:CD1	1:A:466:TRP:H	2.17	0.59
1:A:192:VAL:HA	1:A:268:LYS:HA	1.85	0.59
1:A:487:GLN:O	1:A:491:GLU:HG3	2.01	0.59
1:B:142:VAL:HG12	1:B:143:ALA:N	2.15	0.59
1:B:819:ARG:HH11	1:B:819:ARG:CG	2.15	0.59
1:A:664:ASP:CG	1:A:664:ASP:O	2.44	0.59
1:B:456:ARG:HB3	1:B:461:TYR:CZ	2.37	0.59
1:B:489:ILE:HG12	1:B:490:ARG:N	2.16	0.59
1:B:740:ASN:OD1	1:B:742:ARG:N	2.30	0.59
1:B:134:GLU:N	1:B:180:LYS:HZ1	2.01	0.59
1:B:283:LYS:O	1:B:287:ILE:HD12	2.02	0.59
1:B:786:LEU:C	1:B:788:PRO:CD	2.75	0.59
1:A:138:ILE:HG23	1:A:139:GLY:N	2.18	0.59
1:A:624:THR:O	1:A:624:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ARG:C	1:A:764:VAL:HG12	2.26	0.59
1:B:404:LEU:HB2	1:B:451:TYR:HB3	1.84	0.59
1:B:138:ILE:CG1	1:B:139:GLY:H	2.16	0.59
1:B:413:LYS:O	1:B:415:TYR:CE2	2.56	0.59
1:A:232:VAL:HG23	1:A:233:ILE:HG22	1.85	0.59
1:A:509:ASP:OD1	1:A:554:LYS:HE3	2.01	0.59
1:B:748:ARG:NE	1:B:758:ASP:HA	2.17	0.59
1:B:441:PHE:CD2	2:P:9:MLY:CH1	2.85	0.59
1:B:555:TYR:HE2	1:B:618:PRO:HD3	1.66	0.59
1:A:209:GLU:OE1	1:A:221:THR:CG2	2.51	0.59
1:B:388:HIS:HB3	1:B:391:THR:CG2	2.32	0.59
1:B:448:GLY:O	1:B:462:PHE:HA	2.01	0.59
1:B:579:CYS:O	1:B:583:MET:HG3	2.03	0.59
1:A:148:ARG:CG	1:A:155:TYR:CD2	2.86	0.58
1:A:232:VAL:O	1:A:574:LYS:HD3	2.03	0.58
1:A:668:VAL:CG1	1:A:669:GLN:N	2.66	0.58
1:B:224:TRP:CZ2	1:B:258:ASN:HB2	2.38	0.58
1:B:415:TYR:CD2	1:B:415:TYR:N	2.71	0.58
1:B:773:VAL:HG23	1:B:773:VAL:O	2.02	0.58
1:A:450:CYS:SG	1:A:451:TYR:N	2.75	0.58
1:A:496:GLY:HA3	1:A:501:ILE:HD13	1.85	0.58
1:B:565:LEU:HB2	1:B:634:PRO:HG2	1.85	0.58
1:A:291:ASP:O	1:A:292:LEU:HD23	2.03	0.58
1:A:345:ASP:OD2	1:A:354:SER:HB2	2.02	0.58
1:A:469:TYR:N	1:A:469:TYR:CD2	2.71	0.58
1:B:233:ILE:HG13	1:B:233:ILE:O	2.03	0.58
1:B:240:SER:HB3	1:B:245:LYS:CE	2.34	0.58
1:B:603:ARG:CZ	1:B:830:GLN:HE22	2.16	0.58
1:A:137:PHE:CE2	1:A:218:HIS:HB3	2.38	0.58
1:A:250:ARG:HH21	1:A:295:ASP:CG	2.11	0.58
1:A:345:ASP:CG	1:A:348:SER:HB3	2.28	0.58
1:A:415:TYR:CD1	1:A:490:ARG:CG	2.71	0.58
1:A:454:SER:O	1:A:456:ARG:N	2.36	0.58
1:B:617:LEU:HD12	1:B:618:PRO:HD2	1.85	0.58
1:B:804:ARG:O	1:B:810:GLN:OE1	2.20	0.58
1:A:218:HIS:CB	1:A:262:LEU:HD12	2.32	0.58
1:A:341:ALA:O	1:A:368:LEU:HD23	2.03	0.58
1:A:586:GLN:NE2	1:A:615:MET:O	2.36	0.58
1:A:617:LEU:HD12	1:A:617:LEU:O	2.03	0.58
1:A:645:ASP:CG	1:A:646:GLU:N	2.60	0.58
1:A:683:PRO:HB2	1:A:689:ARG:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LEU:HD21	1:A:717:HIS:HB3	1.86	0.58
1:A:874:GLU:OE1	1:A:875:GLY:N	2.37	0.58
1:B:780:PHE:CE1	1:B:809:ASN:HB3	2.31	0.58
1:B:791:ARG:NH2	1:B:814:HIS:O	2.36	0.58
1:B:819:ARG:HH12	1:B:821:LEU:HA	1.68	0.58
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.67	0.58
1:A:495:GLU:OE1	1:A:498:LYS:NZ	2.24	0.58
1:A:557:LEU:HD12	1:A:558:MET:H	1.68	0.58
1:B:508:VAL:HG21	1:B:551:LEU:HD13	1.84	0.58
1:B:780:PHE:HZ	1:B:809:ASN:CB	2.01	0.58
1:B:812:ILE:HG23	1:B:820:VAL:HG23	1.85	0.58
1:A:154:ARG:NH2	1:A:170:LEU:HD11	2.14	0.58
1:A:456:ARG:HB3	1:A:461:TYR:HH	1.67	0.58
1:A:508:VAL:HG13	1:A:553:PRO:HA	1.86	0.58
1:A:748:ARG:CB	1:A:755:VAL:HA	2.33	0.58
1:B:236:LEU:O	1:B:239:ILE:CD1	2.51	0.58
1:B:269:VAL:HG12	1:B:270:LYS:N	2.18	0.58
1:B:485:CYS:HA	2:P:5:GLN:N	2.19	0.58
1:A:450:CYS:HB3	1:A:476:TRP:CH2	2.38	0.58
1:A:456:ARG:HB3	1:A:461:TYR:CE2	2.39	0.58
1:A:781:ILE:O	1:A:782:LYS:CB	2.48	0.58
1:B:740:ASN:HA	1:B:790:GLY:CA	2.34	0.58
1:A:225:PHE:CE1	1:A:253:LEU:HG	2.38	0.58
1:A:353:MET:HE3	1:A:512:CYS:SG	2.44	0.58
1:A:200:GLU:HG3	1:A:201:ALA:N	2.17	0.57
1:A:517:CYS:CB	1:A:538:ASN:HA	2.35	0.57
1:B:700:ASP:OD1	1:B:702:SER:HB2	2.03	0.57
1:B:190:ASP:O	1:B:207:ILE:HD12	2.03	0.57
1:A:744:LEU:HD13	1:A:772:LEU:HD13	1.86	0.57
1:B:780:PHE:H	1:B:783:GLY:H	1.52	0.57
1:A:596:CYS:CB	1:A:623:PRO:HB3	2.32	0.57
1:A:537:LYS:HA	1:A:539:LYS:HG3	1.85	0.57
1:B:275:ASP:OD2	1:B:277:ASN:HB2	2.05	0.57
1:B:485:CYS:HB3	2:P:6:THR:H	1.68	0.57
1:A:509:ASP:OD2	1:A:869:TYR:OH	2.23	0.57
1:A:810:GLN:O	1:A:811:VAL:HG12	2.05	0.57
1:A:154:ARG:CZ	1:A:209:GLU:OE1	2.52	0.57
1:B:478:PRO:O	1:B:482:LEU:CD1	2.53	0.57
1:B:726:ASP:HA	1:B:729:ARG:HD2	1.86	0.57
1:A:534:LYS:CE	1:A:535:ASP:H	2.18	0.56
1:B:155:TYR:C	1:B:171:LYS:HZ1	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLN:HB2	1:B:537:LYS:HB3	1.87	0.56
1:B:402:LEU:HB2	1:B:547:ILE:HD11	1.87	0.56
1:B:541:MET:CE	1:B:576:ALA:HB2	2.35	0.56
1:A:144:ALA:O	1:A:145:ASP:OD1	2.24	0.56
1:A:308:ILE:O	1:A:308:ILE:HG22	2.05	0.56
1:A:579:CYS:O	1:A:583:MET:HG3	2.05	0.56
1:A:588:ARG:HE	1:A:617:LEU:HD13	1.70	0.56
1:A:603:ARG:CZ	1:A:830:GLN:HE22	2.18	0.56
1:A:748:ARG:CB	1:A:756:GLU:N	2.63	0.56
1:B:446:LEU:HD11	1:B:489:ILE:HG22	1.87	0.56
1:B:650:PRO:O	1:B:652:LEU:N	2.29	0.56
1:B:668:VAL:O	1:B:817:GLN:NE2	2.38	0.56
1:A:555:TYR:HE2	1:A:618:PRO:HD3	1.70	0.56
1:B:263:ASP:OD2	1:B:263:ASP:N	2.35	0.56
1:B:757:TRP:H	1:B:757:TRP:CD1	2.22	0.56
1:A:588:ARG:HH21	1:A:617:LEU:CD1	2.01	0.56
1:A:824:ARG:NH2	1:A:836:TYR:O	2.24	0.56
1:A:279:ASP:HB3	1:A:280:PRO:HD2	1.87	0.56
1:B:410:VAL:HG13	1:B:411:LEU:N	2.20	0.56
1:B:741:PHE:HD2	1:B:788:PRO:HG2	1.68	0.56
1:A:483:SER:HG	1:A:484:ASP:H	1.54	0.56
1:A:657:LEU:HD13	1:A:795:ASP:HA	1.86	0.56
1:B:218:HIS:O	1:B:262:LEU:HD11	1.98	0.56
1:B:285:GLN:O	1:B:288:GLU:HB2	2.05	0.56
1:A:774:PRO:HB2	1:A:776:TYR:CE2	2.41	0.56
1:B:286:LEU:O	1:B:289:SER:N	2.38	0.56
1:B:538:ASN:OD1	1:B:538:ASN:C	2.49	0.56
1:A:226:PHE:CD1	1:A:230:ASP:HB2	2.41	0.56
1:B:646:GLU:O	1:B:646:GLU:HG2	2.05	0.56
1:A:137:PHE:CE1	1:A:210:PHE:HB3	2.41	0.55
1:A:487:GLN:C	1:A:491:GLU:CD	2.74	0.55
1:A:580:LEU:HD21	1:A:610:GLY:CA	2.36	0.55
1:A:598:GLY:CA	1:A:625:TYR:CD2	2.89	0.55
1:B:644:TYR:O	1:B:645:ASP:CG	2.49	0.55
1:A:173:ARG:CZ	1:A:212:GLU:CG	2.75	0.55
1:A:624:THR:C	1:A:625:TYR:CD2	2.76	0.55
1:B:687:PHE:O	1:B:690:TYR:N	2.38	0.55
1:A:247:ASP:OD1	1:A:249:ARG:HG2	2.07	0.55
1:A:602:PHE:O	1:A:799:PRO:O	2.24	0.55
1:A:742:ARG:NH2	1:A:753:ASN:O	2.40	0.55
1:B:735:VAL:O	1:B:735:VAL:CG2	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ASN:O	1:A:784:LYS:CG	2.37	0.55
1:B:140:SER:HB3	1:B:141:PRO:CD	2.37	0.55
1:B:224:TRP:HZ2	1:B:258:ASN:HB2	1.70	0.55
1:B:812:ILE:HG23	1:B:820:VAL:CG2	2.37	0.55
1:A:369:GLU:OE2	1:A:371:ARG:NH1	2.39	0.55
1:A:596:CYS:O	1:A:597:TYR:CD2	2.59	0.55
1:B:724:ASN:O	1:B:727:TYR:N	2.39	0.55
1:B:733:ILE:CG2	1:B:791:ARG:NE	2.69	0.55
1:A:810:GLN:O	1:A:811:VAL:CG1	2.54	0.55
1:B:518:GLN:OE1	1:B:537:LYS:CG	2.34	0.55
1:A:648:GLN:C	1:A:650:PRO:CG	2.80	0.55
1:A:672:GLN:HE21	1:A:674:ASN:HB2	1.71	0.55
1:B:142:VAL:HG21	1:B:174:CYS:SG	2.47	0.55
1:A:442:VAL:O	1:A:467:GLU:HG2	2.07	0.55
1:A:599:LEU:HD23	1:A:829:LEU:O	2.06	0.55
1:A:823:ILE:HG12	1:A:846:TYR:CE2	2.42	0.55
1:B:621:PRO:HG3	1:B:860:ALA:HB1	1.88	0.55
1:B:838:LEU:C	1:B:839:PHE:CD2	2.85	0.55
1:A:715:LEU:CD2	1:A:837:ARG:HG2	2.33	0.55
1:A:534:LYS:HD3	1:A:535:ASP:N	2.21	0.55
1:B:144:ALA:O	1:B:145:ASP:HB2	2.06	0.55
1:A:137:PHE:HE2	1:A:212:GLU:OE1	1.90	0.54
1:A:273:HIS:HE1	1:A:308:ILE:CG2	2.20	0.54
1:A:735:VAL:O	1:A:735:VAL:CG1	2.55	0.54
1:B:407:GLU:HA	1:B:410:VAL:HG12	1.88	0.54
1:B:793:TRP:CB	1:B:815:PRO:HB3	2.37	0.54
1:A:877:ASP:OD1	1:A:878:PRO:HD3	2.07	0.54
1:B:487:GLN:HA	1:B:490:ARG:NH1	2.22	0.54
1:A:154:ARG:NH2	1:A:209:GLU:OE1	2.39	0.54
1:A:170:LEU:C	1:A:171:LYS:HG3	2.27	0.54
1:A:212:GLU:CD	1:A:218:HIS:HD1	2.13	0.54
1:A:781:ILE:HD13	1:A:781:ILE:H	1.70	0.54
1:B:478:PRO:O	1:B:482:LEU:HD12	2.07	0.54
1:B:588:ARG:NH1	1:B:618:PRO:O	2.40	0.54
1:A:690:TYR:O	1:A:693:LEU:HD13	2.08	0.54
1:B:411:LEU:C	1:B:411:LEU:HD23	2.32	0.54
1:B:878:PRO:HB2	1:B:879:LEU:HD13	1.90	0.54
1:A:592:MET:HE2	1:A:857:VAL:CG1	2.32	0.54
1:A:803:THR:OG1	1:A:847:ILE:HA	2.07	0.54
1:B:272:VAL:HG13	1:B:290:CYS:HB3	1.90	0.54
1:B:677:MET:O	1:B:714:LEU:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:ILE:O	1:B:824:ARG:C	2.48	0.54
1:A:173:ARG:HH11	1:A:212:GLU:CG	2.09	0.54
1:A:280:PRO:O	1:A:281:LYS:CB	2.56	0.54
1:A:172:ALA:HA	1:A:212:GLU:O	2.06	0.54
1:A:537:LYS:CG	1:A:538:ASN:N	2.68	0.54
1:A:565:LEU:HA	1:A:570:GLY:CA	2.38	0.54
1:A:599:LEU:CD1	1:A:856:PRO:HG2	2.31	0.54
1:A:752:ASN:C	1:A:754:ILE:H	2.14	0.54
1:B:155:TYR:C	1:B:171:LYS:NZ	2.66	0.54
1:B:786:LEU:O	1:B:788:PRO:HD2	2.08	0.54
1:A:444:GLU:HG2	1:A:445:LYS:N	2.23	0.54
1:A:537:LYS:HA	1:A:539:LYS:CG	2.37	0.54
1:A:703:PHE:C	1:A:705:GLU:H	2.15	0.54
1:A:668:VAL:H	1:A:817:GLN:HE22	1.54	0.54
1:A:817:GLN:HE22	1:A:819:ARG:HE	1.56	0.54
1:B:819:ARG:NH1	1:B:822:THR:CG2	2.71	0.54
1:A:193:TYR:CE1	1:A:269:VAL:HB	2.43	0.54
1:A:700:ASP:O	1:A:702:SER:N	2.39	0.54
1:B:174:CYS:O	1:B:211:PHE:HB2	2.08	0.54
1:B:386:TYR:CE2	1:B:837:ARG:HD3	2.43	0.54
1:B:787:LYS:N	1:B:788:PRO:CD	2.70	0.54
1:A:196:ALA:HA	1:A:203:TYR:HE2	1.72	0.53
1:B:514:GLY:N	1:B:515:PRO:CD	2.71	0.53
1:B:726:ASP:O	1:B:727:TYR:C	2.50	0.53
1:A:609:TRP:CD1	1:A:620:TYR:CE1	2.96	0.53
1:B:629:VAL:HG21	1:B:641:MET:CE	2.38	0.53
1:B:715:LEU:O	1:B:824:ARG:HD3	2.08	0.53
1:B:802:VAL:CG2	1:B:810:GLN:NE2	2.71	0.53
1:A:136:GLU:CB	1:A:218:HIS:NE2	2.71	0.53
1:A:348:SER:O	1:A:351:GLY:N	2.42	0.53
1:B:353:MET:CE	1:B:559:GLU:HG2	2.38	0.53
1:A:211:PHE:CD1	1:A:211:PHE:C	2.86	0.53
1:A:280:PRO:O	1:A:281:LYS:HB2	2.08	0.53
1:A:450:CYS:HB3	1:A:476:TRP:CZ3	2.43	0.53
1:B:137:PHE:CE2	1:B:218:HIS:HB3	2.43	0.53
1:B:370:THR:O	1:B:391:THR:HG22	2.08	0.53
1:A:874:GLU:CD	1:A:875:GLY:O	2.51	0.53
1:B:472:GLU:C	1:B:473:GLU:HG2	2.33	0.53
1:A:133:HIS:O	1:A:135:PRO:CD	2.57	0.53
1:B:251:VAL:HG23	1:B:294:TYR:HB3	1.90	0.53
1:A:221:THR:HG23	1:A:221:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:MET:HE2	1:A:282:ALA:O	2.08	0.53
1:A:557:LEU:HD12	1:A:558:MET:N	2.23	0.53
1:A:664:ASP:O	1:A:665:LEU:CG	2.53	0.53
1:B:134:GLU:HB3	1:B:135:PRO:CD	2.37	0.53
1:B:602:PHE:O	1:B:799:PRO:O	2.27	0.53
1:B:630:ARG:NH1	1:B:632:GLY:HA3	2.24	0.53
1:A:134:GLU:HG2	1:A:180:LYS:HE2	1.86	0.53
1:A:296:MET:HG2	1:A:306:ALA:C	2.34	0.53
1:A:514:GLY:O	1:A:515:PRO:C	2.52	0.53
1:A:542:VAL:HG22	1:A:575:TYR:OH	2.08	0.53
1:A:734:PRO:O	1:A:791:ARG:HD2	2.08	0.53
1:A:852:ALA:CA	3:A:1000:SAH:OXT	2.55	0.53
1:B:240:SER:HB3	1:B:245:LYS:HE2	1.90	0.53
1:B:304:THR:HG23	1:B:588:ARG:HB2	1.90	0.53
1:B:660:ASP:O	1:B:685:THR:HG21	2.08	0.53
1:A:208:THR:OG1	1:A:221:THR:HG23	2.09	0.53
1:A:596:CYS:O	1:A:597:TYR:CG	2.61	0.53
1:A:698:MET:O	1:A:699:LEU:HB2	2.09	0.53
1:B:789:PHE:CE2	1:B:807:PRO:HB2	2.44	0.53
1:A:817:GLN:HE21	1:A:819:ARG:NE	2.06	0.53
1:B:645:ASP:OD1	1:B:647:THR:N	2.42	0.53
1:B:741:PHE:CD2	1:B:788:PRO:HG3	2.42	0.53
1:A:133:HIS:O	1:A:135:PRO:CG	2.57	0.52
1:A:568:ALA:O	1:A:569:ASP:C	2.52	0.52
1:A:775:ASP:OD1	1:A:775:ASP:N	2.37	0.52
1:A:852:ALA:HA	3:A:1000:SAH:C	2.38	0.52
1:B:218:HIS:HB2	1:B:262:LEU:CD1	2.39	0.52
1:A:145:ASP:OD2	1:A:148:ARG:NH1	2.41	0.52
1:A:624:THR:C	1:A:625:TYR:HD2	2.16	0.52
1:B:143:ALA:CB	1:B:147:ALA:HB2	2.38	0.52
1:B:280:PRO:C	1:B:282:ALA:H	2.17	0.52
1:B:699:LEU:N	1:B:699:LEU:CD1	2.58	0.52
1:A:249:ARG:O	1:A:249:ARG:HG2	2.09	0.52
1:A:564:ILE:CG2	1:A:573:GLY:N	2.72	0.52
1:A:569:ASP:O	1:A:570:GLY:C	2.52	0.52
1:B:695:ARG:HD2	1:B:708:GLY:HA3	1.92	0.52
1:A:155:TYR:CE1	1:A:172:ALA:HB3	2.44	0.52
1:B:148:ARG:HB3	1:B:155:TYR:CD2	2.44	0.52
1:B:559:GLU:OE1	1:B:853:VAL:HG22	2.09	0.52
1:B:744:LEU:O	1:B:745:LYS:CB	2.58	0.52
1:A:490:ARG:O	1:A:494:GLN:CG	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:HD21	1:B:503:PRO:HG2	1.91	0.52
1:B:828:ARG:NH2	1:B:834:ASP:OD1	2.43	0.52
1:B:830:GLN:HB3	1:B:832:PHE:HD2	1.74	0.52
1:A:541:MET:HE1	1:A:558:MET:CE	2.39	0.52
1:B:193:TYR:CD1	1:B:269:VAL:HG22	2.44	0.52
1:B:716:ASP:OD1	1:B:716:ASP:N	2.41	0.52
1:A:604:MET:HE1	1:A:641:MET:CE	2.32	0.52
1:B:220:PHE:CE2	1:B:262:LEU:HA	2.44	0.52
1:B:304:THR:HG21	1:B:588:ARG:HH21	1.75	0.52
1:B:440:GLU:HG3	2:P:8:ARG:NH1	2.25	0.52
1:B:589:LEU:C	1:B:589:LEU:CD1	2.83	0.52
1:B:884:PRO:O	1:B:885:SER:C	2.53	0.52
1:A:215:ASP:C	1:A:216:GLN:OE1	2.52	0.52
1:A:642:VAL:HG23	1:A:642:VAL:O	2.09	0.52
1:B:225:PHE:HE1	1:B:294:TYR:CD2	2.27	0.52
1:B:349:GLY:O	3:B:1000:SAH:O	2.28	0.52
1:B:444:GLU:OE1	1:B:488:LYS:HE3	2.06	0.52
1:B:455:ASP:OD2	1:B:455:ASP:C	2.52	0.52
1:A:469:TYR:CE2	1:B:808:HIS:CE1	2.98	0.52
1:A:483:SER:HB3	1:A:485:CYS:SG	2.50	0.52
1:A:534:LYS:NZ	1:A:534:LYS:HB2	2.24	0.52
1:A:535:ASP:OD1	1:A:535:ASP:C	2.52	0.52
1:B:351:GLY:HA3	1:B:384:LEU:HD22	1.92	0.52
1:B:619:LYS:HG3	1:B:880:TYR:CB	2.35	0.52
1:A:466:TRP:H	1:A:466:TRP:HD1	1.58	0.52
1:B:364:SER:CB	1:B:866:GLY:HA3	2.40	0.52
1:B:443:VAL:HG23	1:B:488:LYS:HG3	1.90	0.52
1:B:554:LYS:HD3	1:B:615:MET:CE	2.39	0.52
1:B:589:LEU:HD12	1:B:589:LEU:O	2.10	0.52
1:A:196:ALA:HB1	1:A:200:GLU:CG	2.40	0.51
1:A:534:LYS:NZ	1:A:535:ASP:H	2.06	0.51
1:A:874:GLU:CD	1:A:875:GLY:H	2.18	0.51
1:B:733:ILE:HG13	1:B:734:PRO:CD	2.32	0.51
1:B:877:ASP:OD1	1:B:877:ASP:N	2.43	0.51
1:B:580:LEU:O	1:B:585:TYR:HB2	2.10	0.51
1:B:672:GLN:HG3	1:B:672:GLN:O	2.11	0.51
1:B:808:HIS:CE1	1:B:809:ASN:OD1	2.63	0.51
1:B:828:ARG:HH21	1:B:828:ARG:HG3	1.73	0.51
1:A:173:ARG:HG3	1:A:174:CYS:SG	2.50	0.51
1:A:486:PRO:O	1:A:487:GLN:C	2.53	0.51
1:A:535:ASP:OD1	1:A:537:LYS:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ILE:HG22	1:A:791:ARG:HH11	1.75	0.51
1:B:727:TYR:HD2	1:B:727:TYR:O	1.93	0.51
1:A:668:VAL:O	1:A:817:GLN:NE2	2.44	0.51
1:A:817:GLN:O	1:A:818:ALA:HB3	2.10	0.51
1:B:138:ILE:HG12	1:B:139:GLY:N	2.23	0.51
1:B:793:TRP:HB2	1:B:815:PRO:HB3	1.92	0.51
1:A:198:GLU:O	1:A:199:ASN:HB2	2.10	0.51
1:A:214:THR:O	1:A:215:ASP:OD2	2.28	0.51
1:A:453:GLY:O	1:A:455:ASP:N	2.44	0.51
1:A:486:PRO:O	1:A:489:ILE:N	2.44	0.51
1:A:587:ALA:HA	1:A:609:TRP:O	2.10	0.51
1:B:458:ASN:N	1:B:458:ASN:OD1	2.40	0.51
1:B:676:VAL:HG23	1:B:715:LEU:CD1	2.41	0.51
1:A:140:SER:CB	1:A:141:PRO:CD	2.89	0.51
1:A:534:LYS:HZ2	1:A:535:ASP:HB3	1.70	0.51
1:A:764:VAL:HG22	1:A:765:LYS:N	2.24	0.51
1:B:138:ILE:CG1	1:B:139:GLY:N	2.73	0.51
1:B:490:ARG:O	1:B:494:GLN:HG3	2.10	0.51
1:A:151:TRP:NE1	1:A:175:HIS:ND1	2.59	0.51
1:A:460:ILE:CD1	1:A:460:ILE:N	2.30	0.51
1:A:804:ARG:O	1:A:804:ARG:HG2	2.10	0.51
1:A:823:ILE:HG12	1:A:846:TYR:CD2	2.45	0.51
1:B:717:HIS:C	1:B:718:GLN:HG3	2.36	0.51
1:B:364:SER:OG	1:B:863:TYR:O	2.29	0.51
1:B:635:ASN:O	1:B:636:ALA:C	2.54	0.51
1:A:202:ASP:O	1:A:227:ARG:NH2	2.44	0.51
1:A:596:CYS:C	1:A:597:TYR:CG	2.88	0.51
1:A:735:VAL:O	1:A:735:VAL:HG13	2.11	0.51
1:A:764:VAL:CG2	1:A:765:LYS:N	2.74	0.51
1:B:453:GLY:HA3	1:B:456:ARG:HE	1.76	0.51
1:B:725:ASP:O	1:B:728:GLU:N	2.43	0.51
1:A:284:ALA:C	1:A:287:ILE:HG13	2.35	0.51
1:A:601:GLN:HB3	1:A:798:VAL:HG23	1.93	0.51
1:A:611:ALA:HB3	1:A:617:LEU:HB3	1.93	0.51
1:A:668:VAL:H	1:A:817:GLN:NE2	2.09	0.51
1:A:695:ARG:HB3	1:A:700:ASP:HB3	1.93	0.51
1:B:563:ASP:O	1:B:567:PHE:N	2.40	0.51
1:B:668:VAL:H	1:B:817:GLN:HE22	1.59	0.51
1:A:302:TYR:O	1:A:303:SER:HB2	2.12	0.50
1:A:752:ASN:C	1:A:754:ILE:N	2.68	0.50
1:B:374:VAL:HG22	1:B:394:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LEU:HD11	1:B:606:VAL:CG2	2.41	0.50
1:B:725:ASP:OD1	1:B:725:ASP:C	2.53	0.50
1:B:733:ILE:HG21	1:B:791:ARG:NE	2.26	0.50
1:B:771:PRO:C	1:B:773:VAL:H	2.18	0.50
1:B:819:ARG:HH22	1:B:825:GLU:CD	2.19	0.50
1:B:842:ILE:HG23	1:B:846:TYR:CE2	2.47	0.50
1:A:283:LYS:O	1:A:287:ILE:HG13	2.11	0.50
1:B:664:ASP:OD2	1:B:692:ARG:NH1	2.44	0.50
1:B:838:LEU:O	1:B:839:PHE:CD2	2.64	0.50
1:B:402:LEU:HB2	1:B:547:ILE:CD1	2.42	0.50
1:B:510:VAL:HG11	1:B:865:LEU:HD21	1.94	0.50
1:B:644:TYR:CE1	1:B:649:LYS:HD2	2.46	0.50
1:B:776:TYR:O	1:B:779:SER:O	2.30	0.50
1:A:136:GLU:CG	1:A:137:PHE:N	2.65	0.50
1:A:511:ILE:HD11	1:A:548:VAL:HG22	1.92	0.50
1:A:145:ASP:CG	1:A:148:ARG:NH1	2.69	0.50
1:A:357:LEU:HD23	1:A:858:ALA:O	2.11	0.50
1:A:555:TYR:CE2	1:A:618:PRO:HD3	2.46	0.50
1:B:672:GLN:HG3	1:B:718:GLN:HG2	1.93	0.50
1:A:460:ILE:C	1:A:461:TYR:CD1	2.90	0.50
1:B:237:VAL:HG22	1:B:246:HIS:CD2	2.47	0.50
1:A:456:ARG:O	1:A:457:GLU:OE2	2.30	0.50
1:A:885:SER:O	1:A:885:SER:OG	2.21	0.50
1:B:302:TYR:CD2	1:B:878:PRO:HB3	2.47	0.50
1:B:363:LEU:CD1	1:B:699:LEU:HD13	2.42	0.50
1:B:872:GLU:O	1:B:873:SER:OG	2.23	0.50
1:A:279:ASP:H	1:A:282:ALA:HB3	1.76	0.50
1:A:648:GLN:CA	1:A:650:PRO:CD	2.83	0.50
1:B:675:ASP:O	1:B:715:LEU:HA	2.12	0.50
1:B:734:PRO:O	1:B:735:VAL:HG13	2.12	0.50
1:A:191:ASP:O	1:A:269:VAL:N	2.41	0.49
1:A:646:GLU:O	1:A:647:THR:OG1	2.30	0.49
1:A:226:PHE:HD1	1:A:230:ASP:HB2	1.77	0.49
1:A:287:ILE:CD1	1:A:287:ILE:C	2.77	0.49
1:B:287:ILE:HA	1:B:290:CYS:SG	2.52	0.49
1:B:343:LEU:HB2	1:B:368:LEU:CD2	2.42	0.49
1:B:554:LYS:HD3	1:B:615:MET:HE3	1.94	0.49
1:B:685:THR:HG22	1:B:688:GLN:CD	2.36	0.49
1:B:710:ASP:HB3	1:B:715:LEU:HD21	1.94	0.49
1:B:821:LEU:HD23	1:B:825:GLU:CB	2.43	0.49
1:A:278:MET:HB3	1:A:283:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:CB	1:A:280:PRO:CD	2.89	0.49
1:A:457:GLU:OE2	1:A:457:GLU:N	2.45	0.49
1:A:464:VAL:O	1:A:474:ASP:OD1	2.30	0.49
1:A:581:VAL:O	1:A:584:LYS:N	2.39	0.49
1:B:659:GLY:CA	1:B:794:TRP:HB3	2.42	0.49
1:B:675:ASP:O	1:B:716:ASP:N	2.41	0.49
1:B:787:LYS:O	1:B:788:PRO:O	2.29	0.49
1:A:496:GLY:O	1:A:501:ILE:HG23	2.13	0.49
1:A:594:ALA:O	1:A:596:CYS:O	2.30	0.49
1:A:626:ASP:C	1:A:626:ASP:OD1	2.56	0.49
1:A:646:GLU:O	1:A:646:GLU:OE1	2.30	0.49
1:B:207:ILE:HD12	1:B:207:ILE:N	2.25	0.49
1:B:218:HIS:CB	1:B:262:LEU:HD11	2.42	0.49
1:B:272:VAL:CG1	1:B:290:CYS:HB3	2.43	0.49
1:B:508:VAL:HG12	1:B:553:PRO:HB3	1.95	0.49
1:B:740:ASN:HA	1:B:789:PHE:O	2.13	0.49
1:B:830:GLN:OE1	1:B:830:GLN:HA	2.11	0.49
1:A:281:LYS:HA	1:A:284:ALA:CB	2.35	0.49
1:A:585:TYR:CD1	1:A:610:GLY:O	2.66	0.49
1:B:269:VAL:HG12	1:B:270:LYS:H	1.77	0.49
1:A:569:ASP:O	1:A:571:TYR:N	2.46	0.49
1:A:598:GLY:HA3	1:A:625:TYR:CE2	2.48	0.49
1:A:730:VAL:CG1	1:A:818:ALA:O	2.60	0.49
1:B:269:VAL:HG11	1:B:292:LEU:HD12	1.95	0.49
1:B:442:VAL:CA	2:P:6:THR:HG22	2.36	0.49
1:B:464:VAL:CG1	1:B:465:GLN:N	2.75	0.49
1:A:150:ASN:HB3	1:A:151:TRP:CE3	2.48	0.49
1:A:288:GLU:OE1	1:A:288:GLU:O	2.30	0.49
1:A:609:TRP:HD1	1:A:620:TYR:CE1	2.31	0.49
1:B:190:ASP:HB2	1:B:207:ILE:HD13	1.94	0.49
1:B:343:LEU:HD12	1:B:510:VAL:O	2.13	0.49
1:B:511:ILE:HG21	1:B:553:PRO:HG3	1.93	0.49
1:B:737:LYS:HB2	1:B:793:TRP:CZ2	2.46	0.49
1:A:236:LEU:C	1:A:238:SER:N	2.64	0.49
1:A:442:VAL:O	1:A:467:GLU:CG	2.61	0.49
1:A:739:ALA:HB3	1:A:791:ARG:HB2	1.94	0.49
1:B:239:ILE:HG21	1:B:575:TYR:CE1	2.48	0.49
1:A:206:ARG:NH1	1:A:206:ARG:CG	2.76	0.48
1:A:211:PHE:CE1	1:A:219:TYR:HB2	2.47	0.48
1:A:447:VAL:HG11	1:A:465:GLN:OE1	2.13	0.48
1:A:560:ASN:CG	1:A:564:ILE:HD11	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ARG:NE	1:B:396:GLU:OE2	2.46	0.48
1:B:659:GLY:O	1:B:663:SER:OG	2.30	0.48
1:A:704:GLY:O	1:A:705:GLU:OE1	2.31	0.48
1:B:545:MET:HE3	1:B:576:ALA:HA	1.95	0.48
1:B:597:TYR:OH	1:B:621:PRO:O	2.25	0.48
1:B:718:GLN:O	1:B:822:THR:HA	2.13	0.48
1:A:270:LYS:HE3	1:A:291:ASP:CG	2.38	0.48
1:A:652:LEU:O	1:A:654:LYS:N	2.45	0.48
1:A:653:LYS:O	1:A:654:LYS:C	2.56	0.48
1:A:827:ALA:HB1	1:A:832:PHE:HB2	1.95	0.48
1:A:853:VAL:N	3:A:1000:SAH:OXT	2.42	0.48
1:B:307:ASN:H	1:B:307:ASN:ND2	2.08	0.48
1:B:353:MET:O	1:B:357:LEU:HB2	2.13	0.48
1:B:774:PRO:O	1:B:777:ALA:N	2.46	0.48
1:B:143:ALA:O	1:B:144:ALA:HB3	2.12	0.48
1:B:513:GLY:HA3	1:B:558:MET:HA	1.94	0.48
1:B:553:PRO:O	1:B:585:TYR:OH	2.25	0.48
1:A:593:VAL:HG12	1:A:595:GLY:H	1.77	0.48
1:A:671:HIS:HE1	1:A:673:PRO:HB3	1.79	0.48
1:B:345:ASP:OD2	1:B:348:SER:HB3	2.13	0.48
1:B:793:TRP:C	1:B:795:ASP:N	2.68	0.48
1:A:404:LEU:CD2	1:A:502:LEU:HD11	2.35	0.48
1:A:550:TYR:HD1	1:A:551:LEU:HG	1.79	0.48
1:A:867:GLN:HA	1:A:870:LEU:HD12	1.95	0.48
1:B:624:THR:HG22	1:B:624:THR:O	2.12	0.48
1:A:347:TYR:CD1	1:A:515:PRO:HA	2.48	0.48
1:A:671:HIS:CG	1:A:721:ARG:HH21	2.30	0.48
1:B:501:ILE:O	1:B:502:LEU:HD23	2.13	0.48
1:A:456:ARG:HG2	1:A:461:TYR:CE2	2.41	0.48
1:A:879:LEU:O	1:A:879:LEU:HD23	2.14	0.48
1:B:278:MET:C	1:B:279:ASP:CG	2.82	0.48
1:B:284:ALA:O	1:B:288:GLU:HG3	2.13	0.48
1:B:353:MET:HB2	1:B:853:VAL:HG21	1.96	0.48
1:B:748:ARG:CZ	1:B:759:PRO:HD2	2.44	0.48
1:A:170:LEU:HG	1:A:171:LYS:H	1.79	0.48
1:A:344:LEU:HD12	1:A:372:TRP:HB2	1.94	0.48
1:A:384:LEU:HD11	1:A:388:HIS:ND1	2.29	0.48
1:B:241:VAL:O	1:B:242:ASP:C	2.57	0.48
1:B:666:PRO:HB3	1:B:680:GLY:HA3	1.96	0.48
1:A:140:SER:OG	1:A:141:PRO:HD3	2.13	0.48
1:A:364:SER:OG	1:A:867:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:C	1:A:839:PHE:CD1	2.92	0.48
1:B:231:THR:OG1	1:B:233:ILE:HG23	2.14	0.48
1:B:691:ILE:HD12	1:B:692:ARG:N	2.29	0.48
1:A:763:ARG:HB3	1:A:764:VAL:H	1.24	0.47
1:B:223:ARG:HA	1:B:256:GLU:O	2.14	0.47
1:B:262:LEU:C	1:B:264:CYS:N	2.69	0.47
1:B:445:LYS:HB2	1:B:465:GLN:OE1	2.14	0.47
1:B:723:ASN:O	1:B:724:ASN:C	2.56	0.47
1:B:725:ASP:OD1	1:B:729:ARG:CZ	2.61	0.47
1:A:154:ARG:NE	1:A:170:LEU:HD11	2.28	0.47
1:A:375:ASP:O	1:A:395:ASN:HA	2.14	0.47
1:A:798:VAL:O	1:A:799:PRO:C	2.54	0.47
1:B:658:LEU:HB3	1:B:794:TRP:HA	1.96	0.47
1:B:741:PHE:N	1:B:789:PHE:O	2.47	0.47
1:A:141:PRO:C	1:A:143:ALA:N	2.70	0.47
1:A:363:LEU:N	1:A:363:LEU:CD2	2.76	0.47
1:A:793:TRP:HA	1:A:793:TRP:CE3	2.49	0.47
1:A:812:ILE:CG2	1:A:820:VAL:HG22	2.43	0.47
1:B:139:GLY:HA3	1:B:178:SER:HB3	1.96	0.47
1:B:664:ASP:OD2	1:B:664:ASP:C	2.57	0.47
1:B:814:HIS:ND1	1:B:815:PRO:HD2	2.29	0.47
1:A:232:VAL:HG13	1:A:298:TYR:OH	2.14	0.47
1:A:404:LEU:O	1:A:405:LEU:C	2.56	0.47
1:A:456:ARG:CD	1:A:461:TYR:CD2	2.58	0.47
1:A:879:LEU:HD23	1:A:879:LEU:C	2.39	0.47
1:B:266:ILE:HG22	1:B:267:SER:N	2.28	0.47
1:B:443:VAL:HG23	1:B:444:GLU:N	2.28	0.47
1:B:534:LYS:O	1:B:538:ASN:CB	2.57	0.47
1:B:599:LEU:HD11	1:B:856:PRO:CG	2.44	0.47
1:B:668:VAL:HG21	1:B:672:GLN:HB2	1.97	0.47
1:A:622:LEU:HD13	1:A:644:TYR:CE1	2.49	0.47
1:A:645:ASP:OD1	1:A:645:ASP:N	2.45	0.47
1:B:304:THR:HG21	1:B:588:ARG:NH2	2.28	0.47
1:B:442:VAL:HA	2:P:6:THR:CG2	2.38	0.47
1:A:604:MET:O	1:A:605:ARG:HG2	2.15	0.47
1:B:414:LYS:HD2	1:B:416:VAL:C	2.39	0.47
1:B:590:GLY:HA2	1:B:640:CYS:O	2.15	0.47
1:B:658:LEU:CD1	1:B:829:LEU:HD11	2.44	0.47
1:B:740:ASN:HA	1:B:790:GLY:HA3	1.96	0.47
1:A:196:ALA:CB	1:A:201:ALA:O	2.60	0.47
1:A:206:ARG:NH2	1:A:294:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HD23	1:A:446:LEU:N	2.29	0.47
1:A:509:ASP:OD1	1:A:554:LYS:CE	2.63	0.47
1:B:192:VAL:CG1	1:B:193:TYR:N	2.76	0.47
1:B:226:PHE:CD2	1:B:254:SER:HB2	2.50	0.47
1:B:235:SER:O	1:B:236:LEU:C	2.56	0.47
1:B:286:LEU:HA	1:B:289:SER:OG	2.15	0.47
1:B:361:ALA:CB	1:B:368:LEU:HB2	2.45	0.47
1:B:407:GLU:O	1:B:410:VAL:HG12	2.15	0.47
1:B:411:LEU:HD21	1:B:493:VAL:CG2	2.44	0.47
1:B:440:GLU:N	1:B:441:PHE:CD1	2.83	0.47
1:B:447:VAL:O	1:B:447:VAL:HG23	2.14	0.47
1:B:541:MET:HE3	1:B:576:ALA:HB2	1.97	0.47
1:B:646:GLU:OE2	1:B:647:THR:CA	2.60	0.47
1:A:204:ILE:O	1:A:224:TRP:HE3	1.98	0.47
1:A:280:PRO:C	1:A:281:LYS:HG2	2.40	0.47
1:A:495:GLU:HA	1:A:498:LYS:HE3	1.97	0.47
1:B:601:GLN:HB2	1:B:798:VAL:O	2.15	0.47
1:A:212:GLU:OE2	1:A:218:HIS:N	2.48	0.47
1:A:236:LEU:O	1:A:239:ILE:HB	2.15	0.47
1:A:239:ILE:N	1:A:239:ILE:HD13	2.29	0.47
1:A:488:LYS:HG3	1:A:489:ILE:H	1.80	0.47
1:B:343:LEU:HB2	1:B:368:LEU:HD22	1.97	0.47
1:B:603:ARG:NH2	1:B:830:GLN:HE22	2.13	0.47
1:B:658:LEU:HD11	1:B:662:ILE:HD13	1.97	0.47
1:B:696:LYS:C	1:B:698:MET:O	2.58	0.47
1:B:747:VAL:O	1:B:748:ARG:CG	2.62	0.47
1:A:394:ARG:NE	1:A:396:GLU:OE1	2.40	0.47
1:A:465:GLN:HG3	1:A:474:ASP:CG	2.40	0.47
1:B:279:ASP:CB	1:B:280:PRO:HD3	2.43	0.47
1:B:487:GLN:CG	1:B:490:ARG:HH22	2.24	0.47
1:B:684:LYS:HG2	1:B:688:GLN:OE1	2.13	0.47
1:A:154:ARG:HD2	1:A:175:HIS:HE1	1.80	0.46
1:A:247:ASP:HB3	1:A:250:ARG:HB2	1.98	0.46
1:A:445:LYS:HB2	1:A:445:LYS:HE3	1.57	0.46
1:A:759:PRO:C	1:A:761:ILE:H	2.23	0.46
1:B:144:ALA:O	1:B:145:ASP:CB	2.62	0.46
1:B:154:ARG:NE	1:B:209:GLU:OE1	2.48	0.46
1:B:346:LEU:HD12	1:B:544:PHE:CE1	2.49	0.46
1:B:359:LEU:HD23	1:B:859:ARG:NH1	2.30	0.46
1:B:757:TRP:CD1	1:B:757:TRP:N	2.82	0.46
1:A:224:TRP:NE1	1:A:258:ASN:OD1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:C	1:A:416:VAL:H	2.24	0.46
1:A:449:ILE:HD12	1:A:461:TYR:O	2.15	0.46
1:A:599:LEU:HD11	1:A:856:PRO:CG	2.33	0.46
1:B:280:PRO:O	1:B:282:ALA:N	2.49	0.46
1:B:349:GLY:C	1:B:351:GLY:N	2.73	0.46
1:A:286:LEU:O	1:A:289:SER:OG	2.30	0.46
1:A:624:THR:O	1:A:625:TYR:CE2	2.57	0.46
1:B:596:CYS:HB3	1:B:623:PRO:CB	2.37	0.46
1:B:821:LEU:HD23	1:B:825:GLU:HB2	1.96	0.46
1:A:191:ASP:HB2	1:A:269:VAL:O	2.16	0.46
1:A:407:GLU:O	1:A:410:VAL:HB	2.16	0.46
1:A:648:GLN:C	1:A:650:PRO:HG2	2.41	0.46
1:B:307:ASN:ND2	1:B:586:GLN:CD	2.73	0.46
1:B:413:LYS:O	1:B:415:TYR:HD2	1.98	0.46
1:B:686:GLU:HA	1:B:689:ARG:NH2	2.31	0.46
1:B:792:LEU:O	1:B:793:TRP:HB3	2.15	0.46
1:A:780:PHE:O	1:A:783:GLY:N	2.46	0.46
1:A:781:ILE:HG12	1:A:785:SER:HB2	1.96	0.46
1:B:660:ASP:O	1:B:688:GLN:NE2	2.48	0.46
1:A:154:ARG:HD2	1:A:175:HIS:CE1	2.51	0.46
1:A:363:LEU:C	1:A:365:GLY:N	2.72	0.46
1:B:511:ILE:CG2	1:B:553:PRO:HG3	2.46	0.46
1:B:740:ASN:OD1	1:B:742:ARG:HG3	2.16	0.46
1:B:805:ALA:HB2	1:B:846:TYR:CE1	2.50	0.46
1:A:140:SER:HB3	1:A:141:PRO:HD2	1.97	0.46
1:A:250:ARG:NH2	1:A:295:ASP:CG	2.71	0.46
1:A:537:LYS:HG3	1:A:538:ASN:N	2.31	0.46
1:A:774:PRO:CB	1:A:776:TYR:CE2	2.98	0.46
1:B:485:CYS:HB3	2:P:6:THR:C	2.40	0.46
1:B:616:VAL:O	1:B:868:ALA:HB1	2.16	0.46
1:B:672:GLN:HG2	1:B:717:HIS:O	2.16	0.46
1:B:817:GLN:O	1:B:818:ALA:HB3	2.15	0.46
1:A:495:GLU:CD	1:A:499:ARG:HH21	2.23	0.46
1:A:671:HIS:CE1	1:A:673:PRO:HD3	2.50	0.46
1:A:830:GLN:NE2	1:A:852:ALA:O	2.49	0.46
1:B:239:ILE:HD13	1:B:578:SER:CB	2.46	0.46
1:B:485:CYS:CA	2:P:5:GLN:N	2.79	0.46
1:B:596:CYS:O	1:B:625:TYR:N	2.49	0.46
1:A:537:LYS:HG2	1:A:538:ASN:H	1.80	0.46
1:A:589:LEU:C	1:A:589:LEU:HD23	2.41	0.46
1:B:247:ASP:O	1:B:249:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ASN:O	1:B:727:TYR:HB3	2.15	0.46
1:A:234:ASN:C	1:A:236:LEU:N	2.72	0.46
1:A:347:TYR:CD2	1:A:347:TYR:N	2.84	0.46
1:A:415:TYR:CE1	1:A:490:ARG:HG2	2.45	0.46
1:B:414:LYS:C	1:B:415:TYR:CD2	2.94	0.46
1:B:442:VAL:HG12	1:B:467:GLU:HG3	1.96	0.46
1:B:622:LEU:HB3	1:B:623:PRO:HD2	1.97	0.46
1:B:714:LEU:C	1:B:715:LEU:HD12	2.41	0.46
1:B:724:ASN:O	1:B:725:ASP:C	2.58	0.46
1:B:725:ASP:HA	1:B:728:GLU:HG3	1.97	0.46
1:B:879:LEU:N	1:B:879:LEU:CD2	2.79	0.46
1:B:273:HIS:CD2	1:B:273:HIS:C	2.94	0.45
1:B:580:LEU:HD21	1:B:610:GLY:HA3	1.98	0.45
1:B:674:ASN:C	1:B:718:GLN:HE21	2.24	0.45
1:A:794:TRP:CZ2	1:A:816:THR:HG23	2.48	0.45
1:A:837:ARG:HB3	1:A:839:PHE:CE1	2.39	0.45
1:B:154:ARG:HB3	1:B:172:ALA:HB3	1.98	0.45
1:B:622:LEU:HD22	1:B:644:TYR:CE1	2.51	0.45
1:B:821:LEU:O	1:B:846:TYR:OH	2.35	0.45
1:A:175:HIS:HA	1:A:211:PHE:HA	1.97	0.45
1:A:287:ILE:CD1	1:A:288:GLU:H	2.11	0.45
1:B:235:SER:O	1:B:237:VAL:N	2.50	0.45
1:B:281:LYS:HB3	1:B:281:LYS:HE3	1.65	0.45
1:A:210:PHE:CE2	1:A:262:LEU:HD21	2.50	0.45
1:A:270:LYS:HG3	1:A:291:ASP:H	1.80	0.45
1:A:354:SER:OG	1:A:370:THR:HG21	2.17	0.45
1:B:220:PHE:HE2	1:B:262:LEU:HA	1.81	0.45
1:B:667:LYS:HA	1:B:817:GLN:OE1	2.16	0.45
1:B:884:PRO:HG2	1:B:885:SER:H	1.80	0.45
1:A:153:LYS:HE3	1:A:153:LYS:HB2	1.73	0.45
1:A:379:PHE:HA	1:A:382:GLN:HG3	1.98	0.45
1:A:386:TYR:OH	1:A:710:ASP:OD2	2.35	0.45
1:A:645:ASP:OD1	1:A:647:THR:OG1	2.31	0.45
1:A:798:VAL:HG23	1:A:798:VAL:O	2.16	0.45
1:A:875:GLY:O	1:A:876:SER:CB	2.65	0.45
1:B:672:GLN:OE1	1:B:677:MET:HE2	2.16	0.45
1:B:824:ARG:O	1:B:825:GLU:C	2.60	0.45
1:A:552:LYS:HA	1:A:552:LYS:HD2	1.55	0.45
1:A:557:LEU:HA	1:A:608:LEU:O	2.17	0.45
1:B:621:PRO:CG	1:B:860:ALA:HB1	2.46	0.45
1:B:631:GLY:C	1:B:633:ALA:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:C	1:A:347:TYR:HD2	2.25	0.45
1:A:865:LEU:O	1:A:866:GLY:C	2.59	0.45
1:B:142:VAL:CG2	1:B:174:CYS:SG	3.04	0.45
1:B:154:ARG:C	1:B:171:LYS:HG2	2.42	0.45
1:B:218:HIS:HB2	1:B:262:LEU:HD13	1.99	0.45
1:B:345:ASP:OD1	1:B:354:SER:OG	2.25	0.45
1:B:538:ASN:OD1	1:B:538:ASN:O	2.35	0.45
1:B:644:TYR:O	1:B:647:THR:HG23	2.17	0.45
1:A:141:PRO:C	1:A:143:ALA:H	2.25	0.45
1:A:289:SER:OG	1:A:289:SER:O	2.30	0.45
1:A:536:GLU:O	1:A:537:LYS:C	2.60	0.45
1:A:794:TRP:CZ2	1:A:815:PRO:HB2	2.51	0.45
1:B:290:CYS:HB2	1:B:292:LEU:O	2.17	0.45
1:B:414:LYS:C	1:B:415:TYR:HD2	2.24	0.45
1:B:472:GLU:O	1:B:473:GLU:CB	2.64	0.45
1:B:729:ARG:CZ	1:B:773:VAL:HG11	2.46	0.45
1:B:819:ARG:HH12	1:B:822:THR:H	1.64	0.45
1:A:154:ARG:HE	1:A:170:LEU:HD21	1.80	0.45
1:A:242:ASP:HB3	1:A:244:HIS:HD2	1.82	0.45
1:A:511:ILE:HG23	1:A:553:PRO:HB3	1.99	0.45
1:A:668:VAL:HG13	1:A:669:GLN:N	2.31	0.45
1:A:778:MET:HE3	1:A:778:MET:CA	2.30	0.45
1:B:648:GLN:CA	1:B:648:GLN:NE2	2.58	0.45
1:B:733:ILE:HG23	1:B:735:VAL:H	1.82	0.45
1:B:747:VAL:O	1:B:748:ARG:HG3	2.17	0.45
1:A:867:GLN:O	1:A:868:ALA:C	2.60	0.45
1:B:204:ILE:HD13	1:B:292:LEU:HD11	1.99	0.45
1:B:379:PHE:O	1:B:380:ALA:C	2.60	0.45
1:B:646:GLU:C	1:B:646:GLU:CD	2.82	0.45
1:B:842:ILE:HG22	1:B:843:LYS:N	2.31	0.45
1:A:487:GLN:C	1:A:491:GLU:OE2	2.60	0.44
1:A:716:ASP:OD2	1:A:838:LEU:N	2.48	0.44
1:A:763:ARG:HD2	1:A:763:ARG:HA	1.27	0.44
1:B:383:SER:HB3	1:B:838:LEU:HA	1.99	0.44
1:A:665:LEU:HD23	1:A:665:LEU:HA	1.84	0.44
1:B:278:MET:HB3	1:B:282:ALA:HB3	2.00	0.44
1:B:444:GLU:O	1:B:445:LYS:C	2.59	0.44
1:A:241:VAL:O	1:A:242:ASP:HB3	2.18	0.44
1:A:344:LEU:CD1	1:A:372:TRP:HB2	2.48	0.44
1:A:605:ARG:CG	1:A:605:ARG:NH1	2.57	0.44
1:A:717:HIS:ND1	1:A:822:THR:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:PRO:HG3	1:A:819:ARG:HD2	1.98	0.44
1:A:752:ASN:C	1:A:784:LYS:HG2	2.33	0.44
1:A:882:LEU:HB3	1:A:886:PHE:CB	2.47	0.44
1:B:748:ARG:HE	1:B:759:PRO:HD3	1.72	0.44
1:A:218:HIS:N	1:A:218:HIS:ND1	2.65	0.44
1:A:236:LEU:C	1:A:238:SER:H	2.26	0.44
1:A:254:SER:OG	1:A:256:GLU:HB2	2.17	0.44
1:A:865:LEU:HD23	1:A:866:GLY:N	2.32	0.44
1:B:223:ARG:HG3	1:B:254:SER:O	2.18	0.44
1:B:794:TRP:CD1	1:B:794:TRP:H	2.34	0.44
1:A:364:SER:OG	1:A:863:TYR:O	2.35	0.44
1:B:276:PRO:O	1:B:279:ASP:OD2	2.35	0.44
1:B:514:GLY:H	1:B:515:PRO:HD2	1.82	0.44
1:B:561:VAL:CG1	1:B:562:VAL:H	2.24	0.44
1:B:695:ARG:O	1:B:698:MET:O	2.35	0.44
1:A:597:TYR:H	1:A:624:THR:C	2.26	0.44
1:A:609:TRP:CE3	1:A:618:PRO:HG2	2.53	0.44
1:B:351:GLY:CA	1:B:384:LEU:HD22	2.47	0.44
1:B:355:THR:O	1:B:359:LEU:HD13	2.18	0.44
1:B:645:ASP:O	1:B:646:GLU:CB	2.47	0.44
1:A:257:LYS:O	1:A:258:ASN:CG	2.60	0.44
1:A:300:VAL:O	1:A:301:ALA:C	2.61	0.44
1:A:812:ILE:HG13	1:A:812:ILE:O	2.18	0.44
1:B:442:VAL:HG23	2:P:6:THR:CG2	2.47	0.44
1:B:578:SER:O	1:B:579:CYS:C	2.60	0.44
1:B:831:GLY:HA3	1:B:856:PRO:HD3	1.99	0.44
1:B:874:GLU:O	1:B:875:GLY:C	2.59	0.44
1:A:363:LEU:O	1:A:364:SER:C	2.59	0.44
1:A:609:TRP:CH2	1:A:865:LEU:HB2	2.53	0.44
1:B:349:GLY:O	1:B:350:CYS:SG	2.74	0.44
1:B:353:MET:HE1	1:B:559:GLU:HG2	1.99	0.44
1:B:415:TYR:O	1:B:490:ARG:HG3	2.18	0.44
1:B:501:ILE:HG13	1:B:502:LEU:HG	1.99	0.44
1:B:513:GLY:HA2	1:B:544:PHE:CE1	2.53	0.44
1:A:142:VAL:HG23	1:A:142:VAL:O	2.17	0.44
1:A:565:LEU:HB3	1:A:637:PHE:CD2	2.53	0.44
1:A:812:ILE:O	1:A:821:LEU:HB2	2.18	0.44
1:B:138:ILE:HG22	1:B:179:ALA:HA	1.98	0.44
1:B:138:ILE:HD12	1:B:185:VAL:HG21	2.00	0.44
1:B:182:ASP:OD1	1:B:184:VAL:N	2.34	0.44
1:B:239:ILE:HD13	1:B:578:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:TYR:O	1:B:294:TYR:CD1	2.70	0.44
1:B:386:TYR:OH	1:B:710:ASP:OD2	2.28	0.44
1:B:404:LEU:HB2	1:B:451:TYR:CB	2.48	0.44
1:B:411:LEU:HD23	1:B:412:CYS:N	2.33	0.44
1:A:511:ILE:HG23	1:A:553:PRO:HG3	2.00	0.43
1:A:648:GLN:HA	1:A:650:PRO:HD2	1.93	0.43
1:A:672:GLN:O	1:A:672:GLN:HG3	2.18	0.43
1:A:744:LEU:O	1:A:745:LYS:C	2.57	0.43
1:B:353:MET:HE3	1:B:559:GLU:HG2	2.00	0.43
1:B:554:LYS:O	1:B:611:ALA:HA	2.18	0.43
1:B:586:GLN:O	1:B:610:GLY:HA2	2.18	0.43
1:B:675:ASP:HA	1:B:718:GLN:NE2	2.33	0.43
1:B:740:ASN:HA	1:B:790:GLY:HA2	1.99	0.43
1:B:748:ARG:HG2	1:B:748:ARG:HH21	1.82	0.43
1:A:234:ASN:C	1:A:234:ASN:OD1	2.61	0.43
1:A:536:GLU:O	1:A:538:ASN:ND2	2.51	0.43
1:B:196:ALA:HB2	1:B:203:TYR:CD2	2.52	0.43
1:B:240:SER:HB3	1:B:245:LYS:HE3	1.99	0.43
1:B:449:ILE:HD12	1:B:460:ILE:HG23	1.99	0.43
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.67	0.43
1:A:211:PHE:CE1	1:A:219:TYR:CD2	3.03	0.43
1:A:700:ASP:C	1:A:702:SER:H	2.27	0.43
1:A:838:LEU:C	1:A:839:PHE:HD1	2.25	0.43
1:B:239:ILE:HD13	1:B:578:SER:OG	2.17	0.43
1:B:642:VAL:O	1:B:642:VAL:CG2	2.66	0.43
1:B:685:THR:HG23	1:B:688:GLN:H	1.84	0.43
1:B:734:PRO:O	1:B:735:VAL:CG1	2.66	0.43
1:B:748:ARG:HH11	1:B:759:PRO:HD2	1.84	0.43
1:A:174:CYS:C	1:A:175:HIS:HD2	2.26	0.43
1:A:278:MET:CE	1:A:282:ALA:O	2.66	0.43
1:A:343:LEU:HB2	1:A:368:LEU:HD22	2.01	0.43
1:A:408:TRP:CE2	1:A:412:CYS:SG	3.11	0.43
1:A:585:TYR:CE1	1:A:612:LEU:HG	2.54	0.43
1:A:204:ILE:CG2	1:A:271:ILE:HD11	2.48	0.43
1:A:394:ARG:HH21	1:A:396:GLU:CD	2.26	0.43
1:A:704:GLY:O	1:A:705:GLU:CG	2.65	0.43
1:A:704:GLY:C	1:A:706:GLY:H	2.27	0.43
1:B:218:HIS:N	1:B:218:HIS:CD2	2.86	0.43
1:A:171:LYS:HD3	1:A:214:THR:CG2	2.46	0.43
1:A:252:PHE:HA	1:A:296:MET:O	2.18	0.43
1:A:553:PRO:O	1:A:585:TYR:OH	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:C	1:B:511:ILE:HG22	2.43	0.43
1:B:565:LEU:HD11	1:B:606:VAL:HG21	1.99	0.43
1:B:619:LYS:HB2	1:B:878:PRO:O	2.18	0.43
1:A:498:LYS:HG3	1:A:499:ARG:N	2.34	0.43
1:A:724:ASN:OD1	1:A:724:ASN:N	2.50	0.43
1:A:757:TRP:O	1:A:759:PRO:HD3	2.18	0.43
1:A:865:LEU:HD23	1:A:865:LEU:C	2.43	0.43
1:B:273:HIS:HD2	1:B:274:VAL:N	2.14	0.43
1:B:774:PRO:O	1:B:775:ASP:C	2.61	0.43
1:B:791:ARG:NH2	1:B:815:PRO:O	2.51	0.43
1:A:171:LYS:HB2	1:A:214:THR:HG23	1.99	0.43
1:A:350:CYS:O	1:A:836:TYR:OH	2.29	0.43
1:A:676:VAL:HA	1:A:714:LEU:O	2.19	0.43
1:B:223:ARG:CD	1:B:254:SER:O	2.63	0.43
1:B:793:TRP:C	1:B:795:ASP:H	2.27	0.43
1:B:819:ARG:NH1	1:B:819:ARG:CG	2.74	0.43
1:A:137:PHE:C	1:A:138:ILE:O	2.61	0.43
1:A:171:LYS:HD3	1:A:214:THR:HG21	1.96	0.43
1:A:236:LEU:HD23	1:A:239:ILE:CD1	2.49	0.43
1:A:658:LEU:HD13	1:A:829:LEU:HD21	2.01	0.43
1:A:671:HIS:ND1	1:A:671:HIS:C	2.76	0.43
1:B:227:ARG:C	1:B:229:GLU:N	2.77	0.43
1:B:629:VAL:HG21	1:B:641:MET:HE3	2.00	0.43
1:B:657:LEU:HD23	1:B:795:ASP:C	2.44	0.43
1:B:663:SER:HB2	1:B:688:GLN:HE22	1.84	0.43
1:B:735:VAL:HA	1:B:791:ARG:CD	2.49	0.43
1:A:180:LYS:HB2	1:A:185:VAL:HG12	2.00	0.43
1:A:716:ASP:OD1	1:A:716:ASP:N	2.51	0.43
1:B:409:ALA:HB2	1:B:550:TYR:OH	2.18	0.43
1:B:564:ILE:CG2	1:B:573:GLY:N	2.81	0.43
1:B:564:ILE:O	1:B:570:GLY:HA2	2.18	0.43
1:B:625:TYR:CD1	1:B:653:LYS:HB2	2.54	0.43
1:B:787:LYS:C	1:B:788:PRO:O	2.61	0.43
1:A:137:PHE:CZ	1:A:211:PHE:O	2.72	0.42
1:A:175:HIS:CD2	1:A:211:PHE:CB	3.01	0.42
1:A:780:PHE:HB3	1:A:785:SER:HB3	2.01	0.42
1:A:874:GLU:OE1	1:A:874:GLU:C	2.62	0.42
1:B:589:LEU:HD23	1:B:608:LEU:HD12	2.01	0.42
1:A:449:ILE:HD12	1:A:450:CYS:H	1.84	0.42
1:A:565:LEU:HA	1:A:570:GLY:HA2	2.02	0.42
1:A:725:ASP:O	1:A:729:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:TYR:HD1	1:A:881:GLN:C	2.27	0.42
1:B:231:THR:HB	1:B:298:TYR:CE1	2.54	0.42
1:B:379:PHE:CE2	1:B:844:GLU:OE1	2.72	0.42
1:B:485:CYS:HB3	2:P:6:THR:O	2.19	0.42
1:B:720:LEU:HD22	1:B:805:ALA:O	2.19	0.42
1:B:780:PHE:O	1:B:782:LYS:N	2.47	0.42
1:B:793:TRP:HB3	1:B:815:PRO:HB3	2.00	0.42
2:P:9:MLY:HH12	2:P:9:MLY:HD3	1.69	0.42
1:A:648:GLN:O	1:A:650:PRO:CG	2.65	0.42
1:A:835:TYR:CD1	1:A:835:TYR:C	2.97	0.42
1:B:394:ARG:HE	1:B:394:ARG:HB3	1.58	0.42
1:B:578:SER:O	1:B:581:VAL:N	2.53	0.42
1:B:881:GLN:C	1:B:882:LEU:CD1	2.84	0.42
1:A:154:ARG:HH21	1:A:170:LEU:HD13	1.78	0.42
1:A:196:ALA:HB2	1:A:203:TYR:CE2	2.54	0.42
1:A:285:GLN:O	1:A:286:LEU:C	2.58	0.42
1:A:624:THR:O	1:A:625:TYR:CG	2.57	0.42
1:A:695:ARG:O	1:A:699:LEU:N	2.53	0.42
1:A:787:LYS:HB3	1:A:809:ASN:O	2.19	0.42
1:B:196:ALA:O	1:B:200:GLU:CD	2.63	0.42
1:B:347:TYR:CD1	1:B:347:TYR:N	2.86	0.42
1:B:599:LEU:CD1	1:B:856:PRO:HG2	2.49	0.42
1:B:621:PRO:HD3	1:B:864:CYS:SG	2.59	0.42
1:B:644:TYR:O	1:B:645:ASP:CB	2.66	0.42
1:B:733:ILE:O	1:B:733:ILE:HG22	2.18	0.42
1:B:842:ILE:HG23	1:B:846:TYR:CD2	2.54	0.42
1:A:171:LYS:HD2	1:A:214:THR:HG23	1.96	0.42
1:A:173:ARG:N	1:A:212:GLU:O	2.50	0.42
1:A:875:GLY:O	1:A:876:SER:OG	2.30	0.42
1:B:218:HIS:HB2	1:B:262:LEU:HD11	2.01	0.42
1:B:726:ASP:CG	1:B:729:ARG:NH1	2.77	0.42
3:B:1000:SAH:HG2	3:B:1000:SAH:H4'	1.75	0.42
1:A:342:THR:OG1	1:A:508:VAL:HA	2.19	0.42
1:A:391:THR:HG22	1:A:392:GLU:N	2.34	0.42
1:A:695:ARG:HG2	1:A:835:TYR:CE1	2.55	0.42
1:A:714:LEU:HD11	1:A:717:HIS:HD2	1.85	0.42
1:A:758:ASP:O	1:A:759:PRO:O	2.37	0.42
1:A:866:GLY:O	1:A:870:LEU:HD12	2.19	0.42
1:B:134:GLU:OE1	1:B:134:GLU:CA	2.68	0.42
1:B:240:SER:HA	1:B:244:HIS:O	2.20	0.42
1:B:572:LEU:HD12	1:B:572:LEU:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LEU:N	1:B:599:LEU:HD12	2.34	0.42
1:B:635:ASN:CG	1:B:636:ALA:N	2.77	0.42
1:A:225:PHE:CZ	1:A:253:LEU:HG	2.55	0.42
1:A:443:VAL:CA	1:A:466:TRP:HB3	2.46	0.42
1:A:604:MET:CE	1:A:641:MET:HE1	2.37	0.42
1:A:635:ASN:O	1:A:636:ALA:C	2.63	0.42
1:A:724:ASN:O	1:A:728:GLU:HG3	2.19	0.42
1:A:778:MET:HE2	1:A:778:MET:HB3	1.71	0.42
1:A:781:ILE:HD12	1:A:781:ILE:HA	1.79	0.42
1:B:678:GLU:OE2	1:B:713:LYS:HE3	2.19	0.42
1:B:725:ASP:O	1:B:728:GLU:CB	2.64	0.42
1:A:204:ILE:HB	1:A:225:PHE:HB2	2.01	0.42
1:A:592:MET:HG2	1:A:597:TYR:OH	2.19	0.42
1:A:776:TYR:O	1:A:779:SER:OG	2.30	0.42
1:A:814:HIS:O	1:A:815:PRO:C	2.61	0.42
1:A:273:HIS:CE1	1:A:308:ILE:CG2	3.02	0.42
1:A:662:ILE:CG2	1:A:825:GLU:HG2	2.49	0.42
1:A:701:TRP:C	1:A:703:PHE:N	2.76	0.42
1:B:302:TYR:CE2	1:B:878:PRO:HB3	2.55	0.42
1:B:513:GLY:HA2	1:B:544:PHE:CZ	2.55	0.42
1:B:682:SER:O	1:B:683:PRO:C	2.60	0.42
1:B:746:GLY:O	1:B:757:TRP:HA	2.20	0.42
1:B:813:ILE:HG22	1:B:814:HIS:O	2.19	0.42
1:A:173:ARG:CG	1:A:174:CYS:N	2.81	0.42
1:A:308:ILE:O	1:A:309:SER:OG	2.38	0.42
1:B:279:ASP:CB	1:B:280:PRO:CD	2.97	0.42
1:B:518:GLN:HB2	1:B:537:LYS:CB	2.49	0.42
1:B:733:ILE:HG22	1:B:791:ARG:HH11	1.85	0.42
1:A:212:GLU:OE1	1:A:218:HIS:CA	2.59	0.41
1:A:558:MET:HB3	1:A:608:LEU:HB3	2.02	0.41
1:A:628:VAL:O	1:A:628:VAL:HG23	2.19	0.41
1:A:675:ASP:OD1	1:A:675:ASP:N	2.52	0.41
1:B:239:ILE:H	1:B:239:ILE:HD12	1.85	0.41
1:B:371:ARG:C	1:B:372:TRP:CG	2.98	0.41
1:A:143:ALA:CB	1:A:177:ARG:HH21	2.33	0.41
1:A:148:ARG:O	1:A:149:SER:C	2.63	0.41
1:A:269:VAL:CG2	1:A:270:LYS:N	2.83	0.41
1:A:294:TYR:HE1	1:A:308:ILE:CD1	2.33	0.41
1:A:302:TYR:N	1:A:302:TYR:CD2	2.88	0.41
1:A:390:GLN:O	1:A:391:THR:OG1	2.34	0.41
1:A:479:ILE:O	1:A:482:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:TRP:C	1:A:703:PHE:H	2.28	0.41
1:A:791:ARG:HH21	1:A:818:ALA:H	1.69	0.41
1:B:565:LEU:H	1:B:565:LEU:HG	1.55	0.41
1:B:837:ARG:HG2	1:B:838:LEU:N	2.35	0.41
1:A:710:ASP:HB3	1:A:715:LEU:HD21	2.01	0.41
1:A:803:THR:CA	1:A:850:GLY:HA3	2.43	0.41
1:A:849:VAL:HG12	1:A:850:GLY:N	2.35	0.41
1:B:233:ILE:O	1:B:233:ILE:CG1	2.68	0.41
1:B:341:ALA:O	1:B:368:LEU:HD23	2.20	0.41
1:B:375:ASP:OD1	1:B:376:PHE:C	2.64	0.41
1:B:394:ARG:NH2	1:B:396:GLU:OE2	2.52	0.41
1:B:725:ASP:CG	1:B:729:ARG:NH2	2.78	0.41
1:B:879:LEU:H	1:B:879:LEU:CD2	2.22	0.41
1:A:140:SER:OG	1:A:141:PRO:CD	2.69	0.41
1:A:214:THR:O	1:A:215:ASP:CB	2.68	0.41
1:A:537:LYS:O	1:A:539:LYS:N	2.54	0.41
1:A:565:LEU:O	1:A:570:GLY:N	2.53	0.41
1:A:630:ARG:H	1:A:630:ARG:HG3	1.65	0.41
1:A:708:GLY:O	1:A:711:GLU:HG2	2.20	0.41
1:A:772:LEU:HD23	1:A:772:LEU:HA	1.73	0.41
1:B:386:TYR:CD2	1:B:837:ARG:HD3	2.55	0.41
1:B:451:TYR:HD1	1:B:460:ILE:HD12	1.85	0.41
1:B:549:ALA:O	1:B:552:LYS:HE2	2.20	0.41
1:B:659:GLY:HA3	1:B:794:TRP:HB3	2.02	0.41
1:B:741:PHE:CE2	1:B:788:PRO:CG	2.97	0.41
1:B:784:LYS:O	1:B:785:SER:C	2.61	0.41
1:A:255:GLU:O	1:A:255:GLU:HG3	2.20	0.41
1:A:341:ALA:HB1	1:A:509:ASP:HB3	2.02	0.41
1:A:384:LEU:CD1	1:A:388:HIS:ND1	2.84	0.41
1:A:763:ARG:HH12	1:A:771:PRO:HB2	1.86	0.41
1:B:384:LEU:HD12	1:B:384:LEU:C	2.45	0.41
1:B:384:LEU:HD12	1:B:384:LEU:O	2.21	0.41
1:B:603:ARG:NH1	1:B:852:ALA:O	2.53	0.41
1:A:137:PHE:CE2	1:A:212:GLU:OE1	2.71	0.41
1:A:229:GLU:HG3	1:A:237:VAL:HG11	2.03	0.41
1:A:278:MET:CG	1:A:282:ALA:CB	2.96	0.41
1:A:564:ILE:HG22	1:A:573:GLY:H	1.85	0.41
1:A:591:MET:O	1:A:642:VAL:HG22	2.21	0.41
1:A:619:LYS:HD2	1:A:877:ASP:O	2.21	0.41
1:B:140:SER:HB3	1:B:141:PRO:HD2	2.00	0.41
1:B:306:ALA:O	1:B:307:ASN:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LYS:HE3	1:B:413:LYS:HB2	1.79	0.41
1:B:669:GLN:N	1:B:669:GLN:CD	2.79	0.41
1:B:695:ARG:HB3	1:B:700:ASP:HB3	2.02	0.41
1:B:822:THR:OG1	1:B:825:GLU:HG3	2.20	0.41
1:A:146:GLU:HA	1:A:149:SER:OG	2.20	0.41
1:B:262:LEU:O	1:B:263:ASP:C	2.61	0.41
1:B:286:LEU:O	1:B:289:SER:OG	2.33	0.41
1:A:273:HIS:HE1	1:A:308:ILE:HG22	1.85	0.41
1:A:658:LEU:CD1	1:A:829:LEU:HD21	2.50	0.41
1:A:737:LYS:NZ	1:A:795:ASP:CG	2.79	0.41
1:A:822:THR:HG22	1:A:825:GLU:OE2	2.21	0.41
1:B:142:VAL:HG11	1:B:174:CYS:SG	2.60	0.41
1:B:407:GLU:O	1:B:408:TRP:C	2.64	0.41
1:A:408:TRP:NE1	1:A:412:CYS:SG	2.94	0.41
1:A:492:PHE:C	1:A:492:PHE:CD1	2.97	0.41
1:A:511:ILE:HG23	1:A:553:PRO:CB	2.51	0.41
1:A:553:PRO:HB2	1:A:555:TYR:O	2.21	0.41
1:A:646:GLU:O	1:A:646:GLU:OE2	2.38	0.41
1:A:699:LEU:O	1:A:700:ASP:C	2.62	0.41
1:A:714:LEU:HD23	1:A:715:LEU:N	2.35	0.41
1:A:730:VAL:HG22	1:A:813:ILE:HD12	2.02	0.41
1:B:142:VAL:CG1	1:B:175:HIS:O	2.69	0.41
1:B:143:ALA:N	1:B:175:HIS:O	2.53	0.41
1:B:262:LEU:C	1:B:264:CYS:H	2.29	0.41
1:B:410:VAL:CG1	1:B:411:LEU:H	2.34	0.41
1:B:482:LEU:HA	2:P:7:ALA:HB2	2.03	0.41
1:B:485:CYS:HB3	2:P:6:THR:CA	2.51	0.41
1:B:599:LEU:HA	1:B:600:PRO:HD3	1.85	0.41
1:B:714:LEU:C	1:B:715:LEU:CD1	2.94	0.41
1:B:724:ASN:O	1:B:727:TYR:CB	2.69	0.41
1:B:830:GLN:HB3	1:B:832:PHE:CD2	2.56	0.41
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.85	0.41
1:A:588:ARG:HE	1:A:617:LEU:CD1	2.32	0.41
1:B:491:GLU:O	1:B:495:GLU:OE1	2.38	0.41
1:B:703:PHE:CZ	1:B:709:PRO:HD2	2.56	0.41
1:B:783:GLY:O	1:B:784:LYS:C	2.64	0.41
1:A:207:ILE:HD13	1:A:222:CYS:HB3	2.03	0.40
1:A:535:ASP:O	1:A:536:GLU:OE2	2.39	0.40
1:A:596:CYS:N	1:A:627:VAL:HG11	2.37	0.40
1:B:226:PHE:HE2	1:B:254:SER:OG	2.03	0.40
1:B:387:ASN:CB	1:B:836:TYR:CE2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:GLU:N	1:B:441:PHE:HD1	2.18	0.40
1:B:700:ASP:O	1:B:701:TRP:C	2.64	0.40
1:B:748:ARG:NH1	1:B:759:PRO:HD2	2.36	0.40
1:A:140:SER:O	1:A:141:PRO:C	2.63	0.40
1:A:192:VAL:HG23	1:A:193:TYR:N	2.36	0.40
1:A:233:ILE:O	1:A:234:ASN:O	2.38	0.40
1:B:347:TYR:O	3:B:1000:SAH:HG1	2.22	0.40
1:B:353:MET:HB2	1:B:853:VAL:CG2	2.51	0.40
1:B:374:VAL:HG21	1:B:401:PHE:CG	2.56	0.40
1:B:504:LEU:HD23	1:B:504:LEU:HA	1.83	0.40
1:B:638:SER:OG	1:B:639:GLN:HG2	2.21	0.40
1:B:740:ASN:HD21	1:B:742:ARG:HG3	1.86	0.40
1:B:827:ALA:HB1	1:B:832:PHE:HB2	2.03	0.40
1:B:855:VAL:N	1:B:856:PRO:CD	2.84	0.40
1:A:151:TRP:O	1:A:151:TRP:CD1	2.74	0.40
1:A:288:GLU:HG3	1:A:289:SER:N	2.28	0.40
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.84	0.40
1:A:598:GLY:CA	1:A:625:TYR:CE2	3.05	0.40
1:B:462:PHE:HE1	1:B:492:PHE:CD2	2.38	0.40
1:B:589:LEU:C	1:B:620:TYR:CE2	2.99	0.40
1:B:646:GLU:O	1:B:647:THR:C	2.59	0.40
1:B:810:GLN:O	1:B:811:VAL:C	2.64	0.40
1:B:812:ILE:O	1:B:812:ILE:CG1	2.69	0.40
1:B:880:TYR:CD2	1:B:881:GLN:O	2.67	0.40
1:A:175:HIS:CD2	1:A:211:PHE:HB3	2.56	0.40
1:A:175:HIS:CD2	1:A:211:PHE:HB2	2.57	0.40
1:A:843:LYS:O	1:A:846:TYR:HB2	2.22	0.40
1:B:443:VAL:HG21	1:B:485:CYS:SG	2.62	0.40
1:B:577:LEU:HD12	1:B:577:LEU:HA	1.83	0.40
1:B:621:PRO:HG3	1:B:860:ALA:CB	2.51	0.40
1:B:723:ASN:ND2	1:B:726:ASP:OD2	2.54	0.40
1:A:394:ARG:NH2	1:A:396:GLU:OE1	2.53	0.40
1:A:449:ILE:HD13	1:A:462:PHE:CE1	2.57	0.40
1:A:558:MET:O	1:A:607:PHE:HA	2.21	0.40
1:B:154:ARG:HA	1:B:154:ARG:HD3	1.86	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	664/784 (85%)	580 (87%)	70 (10%)	14 (2%)	5	31
1	B	660/784 (84%)	577 (87%)	73 (11%)	10 (2%)	8	37
2	P	4/15 (27%)	4 (100%)	0	0	100	100
All	All	1328/1583 (84%)	1161 (87%)	143 (11%)	24 (2%)	6	34

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	PRO
1	A	650	PRO
1	A	759	PRO
1	A	764	VAL
1	B	536	GLU
1	B	820	VAL
1	A	414	LYS
1	A	653	LYS
1	B	883	PRO
1	A	415	TYR
1	A	567	PHE
1	A	635	ASN
1	A	645	ASP
1	A	883	PRO
1	B	140	SER
1	B	884	PRO
1	B	350	CYS
1	B	454	SER
1	B	646	GLU
1	B	788	PRO
1	A	138	ILE
1	A	140	SER
1	B	279	ASP
1	A	142	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	564/668 (84%)	432 (77%)	132 (23%)	1	4
1	B	549/668 (82%)	422 (77%)	127 (23%)	1	5
2	P	5/9 (56%)	3 (60%)	2 (40%)	0	0
All	All	1118/1345 (83%)	857 (77%)	261 (23%)	1	5

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	138	ILE
1	A	142	VAL
1	A	153	LYS
1	A	154	ARG
1	A	170	LEU
1	A	173	ARG
1	A	183	ASN
1	A	185	VAL
1	A	192	VAL
1	A	202	ASP
1	A	206	ARG
1	A	209	GLU
1	A	214	THR
1	A	215	ASP
1	A	218	HIS
1	A	233	ILE
1	A	236	LEU
1	A	238	SER
1	A	239	ILE
1	A	245	LYS
1	A	253	LEU
1	A	261	VAL
1	A	269	VAL
1	A	272	VAL
1	A	275	ASP

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Mol	Chain	Res	Type
1	A	277	ASN
1	A	279	ASP
1	A	286	LEU
1	A	288	GLU
1	A	300	VAL
1	A	308	ILE
1	A	343	LEU
1	A	350	CYS
1	A	363	LEU
1	A	368	LEU
1	A	370	THR
1	A	377	ASN
1	A	378	SER
1	A	382	GLN
1	A	383	SER
1	A	384	LEU
1	A	385	LYS
1	A	399	ASP
1	A	416	VAL
1	A	442	VAL
1	A	443	VAL
1	A	446	LEU
1	A	447	VAL
1	A	450	CYS
1	A	457	GLU
1	A	460	ILE
1	A	466	TRP
1	A	469	TYR
1	A	472	GLU
1	A	482	LEU
1	A	484	ASP
1	A	485	CYS
1	A	491	GLU
1	A	494	GLN
1	A	495	GLU
1	A	501	ILE
1	A	502	LEU
1	A	511	ILE
1	A	534	LYS
1	A	535	ASP
1	A	536	GLU
1	A	552	LYS

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Mol	Chain	Res	Type
1	A	562	VAL
1	A	563	ASP
1	A	581	VAL
1	A	584	LYS
1	A	585	TYR
1	A	592	MET
1	A	599	LEU
1	A	605	ARG
1	A	612	LEU
1	A	615	MET
1	A	617	LEU
1	A	627	VAL
1	A	628	VAL
1	A	630	ARG
1	A	641	MET
1	A	646	GLU
1	A	648	GLN
1	A	651	SER
1	A	654	LYS
1	A	656	LEU
1	A	660	ASP
1	A	664	ASP
1	A	668	VAL
1	A	671	HIS
1	A	677	MET
1	A	678	GLU
1	A	691	ILE
1	A	698	MET
1	A	701	TRP
1	A	705	GLU
1	A	713	LYS
1	A	716	ASP
1	A	720	LEU
1	A	722	LEU
1	A	730	VAL
1	A	731	GLN
1	A	735	VAL
1	A	760	GLU
1	A	763	ARG
1	A	764	VAL
1	A	772	LEU
1	A	775	ASP

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Mol	Chain	Res	Type
1	A	778	MET
1	A	780	PHE
1	A	781	ILE
1	A	786	LEU
1	A	787	LYS
1	A	792	LEU
1	A	793	TRP
1	A	813	ILE
1	A	820	VAL
1	A	821	LEU
1	A	822	THR
1	A	828	ARG
1	A	837	ARG
1	A	846	TYR
1	A	849	VAL
1	A	853	VAL
1	A	867	GLN
1	A	870	LEU
1	A	872	GLU
1	A	879	LEU
1	A	881	GLN
1	A	882	LEU
1	B	134	GLU
1	B	138	ILE
1	B	148	ARG
1	B	149	SER
1	B	153	LYS
1	B	173	ARG
1	B	180	LYS
1	B	181	VAL
1	B	182	ASP
1	B	184	VAL
1	B	186	TYR
1	B	187	CYS
1	B	192	VAL
1	B	194	VAL
1	B	206	ARG
1	B	207	ILE
1	B	215	ASP
1	B	223	ARG
1	B	227	ARG
1	B	233	ILE

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Mol	Chain	Res	Type
1	B	235	SER
1	B	236	LEU
1	B	237	VAL
1	B	238	SER
1	B	239	ILE
1	B	253	LEU
1	B	255	GLU
1	B	256	GLU
1	B	259	ASP
1	B	262	LEU
1	B	263	ASP
1	B	265	ILE
1	B	273	HIS
1	B	274	VAL
1	B	279	ASP
1	B	283	LYS
1	B	296	MET
1	B	300	VAL
1	B	303	SER
1	B	307	ASN
1	B	339	ARG
1	B	354	SER
1	B	357	LEU
1	B	368	LEU
1	B	370	THR
1	B	375	ASP
1	B	382	GLN
1	B	383	SER
1	B	384	LEU
1	B	390	GLN
1	B	393	VAL
1	B	399	ASP
1	B	411	LEU
1	B	415	TYR
1	B	416	VAL
1	B	440	GLU
1	B	441	PHE
1	B	442	VAL
1	B	443	VAL
1	B	444	GLU
1	B	447	VAL
1	B	449	ILE

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Mol	Chain	Res	Type
1	B	455	ASP
1	B	457	GLU
1	B	458	ASN
1	B	472	GLU
1	B	484	ASP
1	B	489	ILE
1	B	499	ARG
1	B	511	ILE
1	B	535	ASP
1	B	536	GLU
1	B	538	ASN
1	B	541	MET
1	B	552	LYS
1	B	559	GLU
1	B	565	LEU
1	B	586	GLN
1	B	589	LEU
1	B	608	LEU
1	B	616	VAL
1	B	629	VAL
1	B	637	PHE
1	B	639	GLN
1	B	642	VAL
1	B	645	ASP
1	B	646	GLU
1	B	647	THR
1	B	648	GLN
1	B	662	ILE
1	B	664	ASP
1	B	667	LYS
1	B	672	GLN
1	B	684	LYS
1	B	691	ILE
1	B	693	LEU
1	B	696	LYS
1	B	699	LEU
1	B	702	SER
1	B	711	GLU
1	B	713	LYS
1	B	715	LEU
1	B	716	ASP
1	B	723	ASN

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Mol	Chain	Res	Type
1	B	731	GLN
1	B	733	ILE
1	B	735	VAL
1	B	742	ARG
1	B	743	ASP
1	B	760	GLU
1	B	792	LEU
1	B	793	TRP
1	B	794	TRP
1	B	798	VAL
1	B	801	VAL
1	B	802	VAL
1	B	803	THR
1	B	809	ASN
1	B	819	ARG
1	B	820	VAL
1	B	821	LEU
1	B	822	THR
1	B	842	ILE
1	B	849	VAL
1	B	859	ARG
1	B	879	LEU
1	B	882	LEU
2	P	5	GLN
2	P	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	273	HIS
1	A	538	ASN
1	A	540	GLN
1	A	648	GLN
1	A	671	HIS
1	A	672	GLN
1	A	674	ASN
1	A	717	HIS
1	A	740	ASN
1	A	817	GLN
1	A	867	GLN
1	B	246	HIS

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Mol	Chain	Res	Type
1	B	273	HIS
1	B	307	ASN
1	B	382	GLN
1	B	540	GLN
1	B	560	ASN
1	B	648	GLN
1	B	671	HIS
1	B	731	GLN
1	B	810	GLN
1	B	817	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	MLY	P	9	2	9,10,11	0.62	0	6,11,13	1.83	2 (33%)

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
2	MLY	P	9	2	-	0/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	9	MLY	CD-CE-NZ	-3.40	104.92	113.71
2	P	9	MLY	CH1-NZ-CE	-2.05	102.60	110.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	9	MLY	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	SAH	B	1000	-	27,28,28	1.59	7 (25%)	36,40,40	2.15	12 (33%)
3	SAH	A	1000	-	27,28,28	1.56	7 (25%)	36,40,40	2.15	12 (33%)

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	SAH	B	1000	-	-	1/15/31/31	0/3/3/3
3	SAH	A	1000	-	-	5/15/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	SAH	C2-N3	3.55	1.40	1.33
3	B	1000	SAH	C2-N3	3.52	1.40	1.33
3	B	1000	SAH	C2-N1	3.40	1.40	1.33
3	A	1000	SAH	C2-N1	3.39	1.40	1.33
3	B	1000	SAH	C5-N7	-3.06	1.33	1.39
3	A	1000	SAH	C5-N7	-3.04	1.33	1.39
3	A	1000	SAH	C5-C4	-2.99	1.33	1.39
3	B	1000	SAH	C5-C4	-2.96	1.33	1.39
3	B	1000	SAH	C5-C6	-2.64	1.33	1.41
3	A	1000	SAH	C5-C6	-2.61	1.33	1.41
3	A	1000	SAH	C8-N9	-2.48	1.33	1.37
3	B	1000	SAH	C8-N9	-2.46	1.33	1.37
3	B	1000	SAH	C4-N9	-2.08	1.33	1.37
3	A	1000	SAH	C4-N9	-2.02	1.33	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	SAH	N3-C2-N1	-6.92	118.11	128.58
3	B	1000	SAH	N3-C2-N1	-6.86	118.20	128.58
3	B	1000	SAH	C5-C4-N3	-4.39	120.67	126.72
3	A	1000	SAH	C5-C4-N3	-4.36	120.71	126.72
3	A	1000	SAH	N9-C8-N7	-4.30	107.84	113.94
3	B	1000	SAH	N9-C8-N7	-4.29	107.84	113.94
3	A	1000	SAH	C2-N3-C4	3.24	119.75	111.83
3	B	1000	SAH	C2-N3-C4	3.23	119.72	111.83
3	A	1000	SAH	C5-N7-C8	3.00	108.17	103.45
3	B	1000	SAH	C5-N7-C8	3.00	108.16	103.45
3	A	1000	SAH	C5-C6-N6	-2.84	116.26	123.29
3	B	1000	SAH	C5-C6-N6	-2.84	116.26	123.29
3	A	1000	SAH	C6-C5-C4	2.62	120.76	117.18
3	B	1000	SAH	C6-C5-C4	2.61	120.75	117.18
3	B	1000	SAH	N3-C4-N9	2.55	131.50	127.17
3	A	1000	SAH	N3-C4-N9	2.54	131.49	127.17
3	A	1000	SAH	C4'-O4'-C1'	-2.51	103.92	109.47
3	B	1000	SAH	C4'-O4'-C1'	-2.49	103.97	109.47
3	B	1000	SAH	C4-N9-C8	2.43	108.29	105.74
3	A	1000	SAH	C4-N9-C8	2.43	108.28	105.74
3	B	1000	SAH	C4-C5-N7	-2.36	107.88	110.58
3	A	1000	SAH	C4-C5-N7	-2.35	107.90	110.58
3	A	1000	SAH	C5'-C4'-C3'	-2.22	109.49	115.06
3	B	1000	SAH	C5'-C4'-C3'	-2.22	109.50	115.06

There are no chirality outliers.

All (6) torsion outliers are listed below:

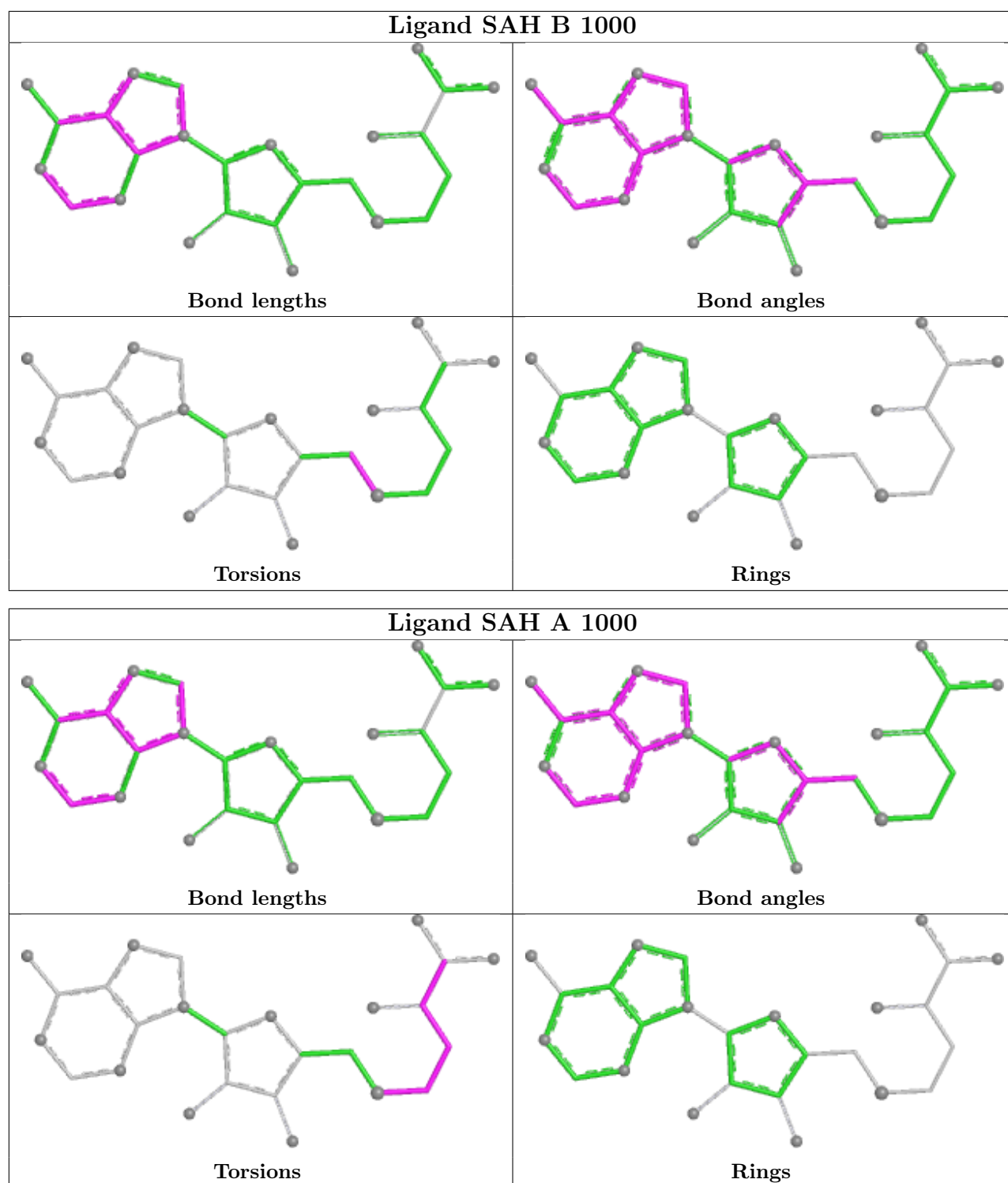
Mol	Chain	Res	Type	Atoms
3	A	1000	SAH	N-CA-CB-CG
3	A	1000	SAH	C-CA-CB-CG
3	A	1000	SAH	CA-CB-CG-SD
3	A	1000	SAH	OXT-C-CA-N
3	A	1000	SAH	CB-CG-SD-C5'
3	B	1000	SAH	C4'-C5'-SD-CG

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	SAH	3	0
3	A	1000	SAH	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	674/784 (85%)	0.68	51 (7%)	20	13	31, 69, 145, 218	0
1	B	670/784 (85%)	0.67	52 (7%)	19	12	29, 70, 131, 200	0
2	P	6/15 (40%)	0.62	0	100	100	82, 97, 104, 104	0
All	All	1350/1583 (85%)	0.67	103 (7%)	20	13	29, 70, 139, 218	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ALA	9.5
1	B	680	GLY	6.2
1	B	228	ALA	5.6
1	A	624	THR	5.6
1	A	753	ASN	5.3
1	A	740	ASN	4.6
1	A	517	CYS	4.5
1	B	517	CYS	4.4
1	A	885	SER	4.3
1	B	753	ASN	4.2
1	B	518	GLN	4.0
1	B	704	GLY	3.9
1	A	470	GLY	3.9
1	A	858	ALA	3.8
1	A	469	TYR	3.8
1	B	632	GLY	3.8
1	A	632	GLY	3.7
1	A	139	GLY	3.7
1	B	884	PRO	3.6
1	B	254	SER	3.6
1	B	700	ASP	3.6
1	B	681	GLY	3.5
1	A	652	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	862	GLY	3.5
1	A	445	LYS	3.4
1	B	538	ASN	3.4
1	A	886	PHE	3.3
1	B	661	ALA	3.3
1	A	649	LYS	3.2
1	A	473	GLU	3.2
1	A	767	SER	3.2
1	A	183	ASN	3.1
1	B	883	PRO	3.1
1	B	878	PRO	2.9
1	A	141	PRO	2.9
1	A	144	ALA	2.9
1	B	810	GLN	2.9
1	B	139	GLY	2.9
1	B	631	GLY	2.9
1	A	707	ALA	2.8
1	B	885	SER	2.8
1	A	884	PRO	2.8
1	A	453	GLY	2.8
1	B	882	LEU	2.7
1	A	636	ALA	2.7
1	B	445	LYS	2.7
1	B	729	ARG	2.7
1	A	235	SER	2.7
1	A	633	ALA	2.7
1	A	664	ASP	2.7
1	B	737	LYS	2.6
1	B	749	VAL	2.6
1	A	700	ASP	2.6
1	A	465	GLN	2.6
1	B	280	PRO	2.6
1	B	440	GLU	2.6
1	B	630	ARG	2.5
1	B	338	THR	2.5
1	A	180	LYS	2.5
1	B	277	ASN	2.5
1	A	871	GLY	2.5
1	A	507	ASP	2.5
1	A	571	TYR	2.5
1	A	309	SER	2.5
1	A	416	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	770	LYS	2.4
1	B	172	ALA	2.4
1	B	560	ASN	2.4
1	B	633	ALA	2.4
1	B	787	LYS	2.4
1	A	444	GLU	2.4
1	A	752	ASN	2.3
1	A	768	SER	2.3
1	B	375	ASP	2.3
1	B	222	CYS	2.3
1	B	243	GLY	2.3
1	A	765	LYS	2.3
1	A	295	ASP	2.3
1	A	666	PRO	2.2
1	B	757	TRP	2.2
1	A	818	ALA	2.2
1	B	790	GLY	2.2
1	A	696	LYS	2.2
1	A	690	TYR	2.2
1	B	145	ASP	2.2
1	B	698	MET	2.2
1	B	307	ASN	2.2
1	B	651	SER	2.1
1	B	765	LYS	2.1
1	B	410	VAL	2.1
1	B	392	GLU	2.1
1	B	260	ASN	2.1
1	B	182	ASP	2.1
1	A	291	ASP	2.1
1	B	669	GLN	2.1
1	B	696	LYS	2.1
1	B	793	TRP	2.1
1	A	243	GLY	2.1
1	B	711	GLU	2.1
1	A	537	LYS	2.0
1	A	276	PRO	2.0
1	A	153	LYS	2.0
1	A	185	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MLY	P	9	11/12	0.88	0.16	65,75,80,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

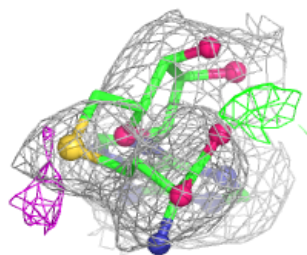
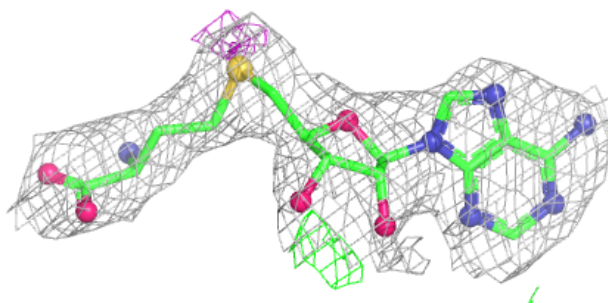
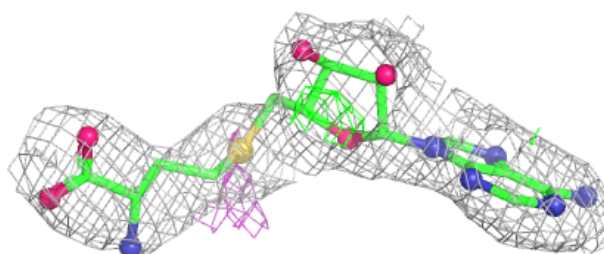
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SAH	B	1000	26/26	0.90	0.17	29,66,105,146	0
3	SAH	A	1000	26/26	0.91	0.14	15,55,89,99	0

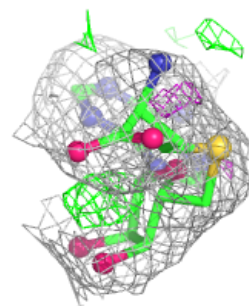
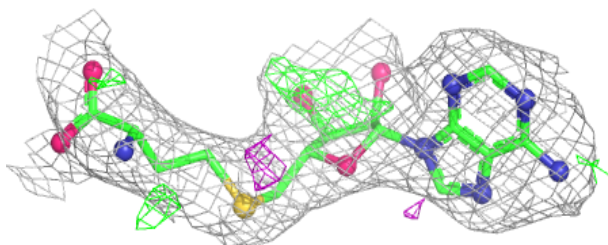
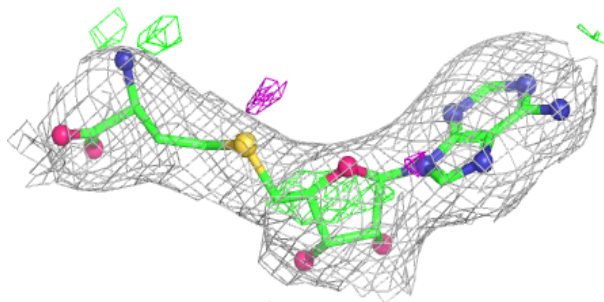
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH B 1000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SAH A 1000:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.