



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:59 pm BST

PDB ID : 4FT2
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

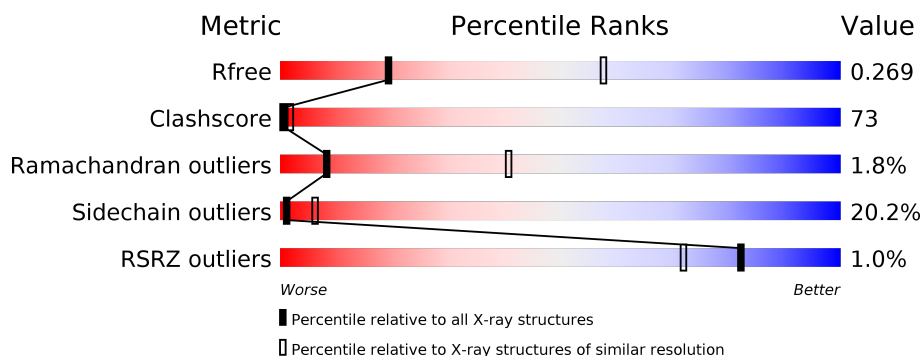
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>22%</div> <div>49%</div> <div>15%</div> <div>14%</div> </div>
1	B	784	<div> <div>26%</div> <div>47%</div> <div>12%</div> <div>15%</div> </div>
2	P	15	<div> <div>13%</div> <div>27%</div> <div>7%</div> <div>53%</div> </div>

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			

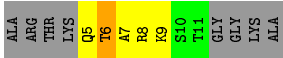
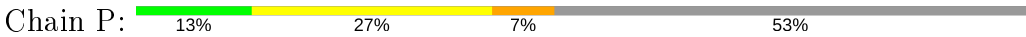
- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



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



● Molecule 2: H3 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.86 Å 88.86 Å 113.50 Å 93.15° 95.72° 110.70°	Depositor
Resolution (Å)	40.10 – 3.20 48.74 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.10-3.20) 98.3 (48.74-3.18)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.235 , 0.277 0.231 , 0.269	Depositor DCC
R_{free} test set	1949 reflections (5.02%)	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)	0.27 , 58.8	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	0.89	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	0.52	2/5432 (0.0%)	0.74	11/7362 (0.1%)
1	B	0.45	1/5375 (0.0%)	0.67	2/7290 (0.0%)
2	P	0.42	0/44	0.72	0/58
All	All	0.48	3/10851 (0.0%)	0.70	13/14710 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	CYS	CB-SG	-5.65	1.72	1.81
1	A	625	TYR	CB-CG	5.57	1.59	1.51
1	B	264	CYS	CB-SG	-5.12	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	SER	N-CA-C	-8.86	87.08	111.00
1	B	773	VAL	CB-CA-C	-8.84	94.61	111.40
1	B	649	LYS	N-CA-C	-8.53	87.98	111.00
1	A	632	GLY	N-CA-C	-7.38	94.64	113.10
1	A	651	SER	N-CA-C	-7.04	92.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ARG	N-CA-C	-6.72	92.86	111.00
1	A	598	GLY	N-CA-C	6.19	128.57	113.10
1	A	596	CYS	N-CA-C	-5.94	94.95	111.00
1	A	810	GLN	N-CA-C	5.86	126.83	111.00
1	A	646	GLU	N-CA-C	-5.40	96.41	111.00
1	A	787	LYS	N-CA-C	5.38	125.52	111.00
1	A	134	GLU	C-N-CD	-5.25	109.04	120.60
1	A	132	ASP	CB-CG-OD2	5.20	122.98	118.30

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	815	0
1	B	5246	0	5059	709	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	1525	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 73.

All (1525) 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: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:648:GLN:C	1:A:650:PRO:HD2	1.43	1.34
1:B:648:GLN:C	1:B:650:PRO:HD3	1.46	1.33
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:743:ASP:O	1:A:744:LEU:HD23	1.37	1.20
1:A:456:ARG:CD	1:A:461:TYR:HE2	1.55	1.20
1:B:859:ARG:CG	1:B:859:ARG:HH11	1.54	1.20
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:N	1:B:882:LEU:HD12	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:588:ARG:HH21	1:A:617:LEU:HD11	1.11	1.09
1:A:452:GLY:CA	1:A:456:ARG:HD2	1.83	1.09
1:B:206:ARG:HH11	1:B:206:ARG:HG3	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:B:883:PRO:CB	1:B:884:PRO:CD	2.32	1.06
1:A:350:CYS:O	1:A:384:LEU:HD22	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:H	1:B:262:LEU:HD12	1.20	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:B:880:TYR:CE2	1:B:881:GLN:O	2.10	1.04
1:A:781:ILE:O	1:A:781:ILE:HG22	1.57	1.04
1:A:644:TYR:CD2	1:A:649:LYS:HD3	1.91	1.04
1:A:755:VAL:CB	1:A:778:MET:CE	2.36	1.04
1:A:460:ILE:H	1:A:460:ILE:HD12	0.87	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:B:414:LYS:HG3	1:B:416:VAL:H	1.25	1.02
1:A:648:GLN:C	1:A:650:PRO:CD	2.28	1.01
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:664:ASP:CG	1:A:692:ARG:HH11	1.66	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:154:ARG:HH12	1:A:209:GLU:CD	1.67	0.97
1:A:287:ILE:HD12	1:A:288:GLU:H	1.30	0.97
1:A:755:VAL:CB	1:A:778:MET:HE1	1.94	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:837:ARG:HG3	1:A:837:ARG:HH11	1.35	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:A:755:VAL:C	1:A:778:MET:HE1	1.92	0.89
1:B:148:ARG:NH1	1:B:148:ARG:HG2	1.83	0.89
1:B:560:ASN:ND2	1:B:564:ILE:HD11	1.85	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:A:457:GLU:OE2	1:A:457:GLU:HA	1.73	0.88
1:A:404:LEU:HD21	1:A:502:LEU:HD11	1.56	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:755:VAL:CB	1:A:778:MET:HE3	2.01	0.88
1:A:136:GLU:HG2	1:A:137:PHE:N	1.86	0.88
1:A:715:LEU:HD22	1:A:837:ARG:HG2	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:743:ASP:C	1:A:744:LEU:HD23	1.94	0.87
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:648:GLN:C	1:B:648:GLN:HE21	1.77	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:NH1	1:B:206:ARG:HG3	1.84	0.86
1:A:134:GLU:HG2	1:A:180:LYS:CE	2.05	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:B:182:ASP:CG	1:B:183:ASN:H	1.79	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:A:648:GLN:CD	1:A:648:GLN:N	2.30	0.85
1:B:206:ARG:CG	1:B:206:ARG:HH11	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:136:GLU:HG3	1:A:218:HIS:CE1	2.12	0.84
1:A:154:ARG:NH1	1:A:209:GLU:CD	2.31	0.84
1:B:440:GLU:CD	1:B:440:GLU:N	2.30	0.84
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:B:182:ASP:CG	1:B:183:ASN:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:LEU:O	1:A:653:LYS:C	2.15	0.83
1:B:444:GLU:OE1	1:B:488:LYS:CE	2.25	0.83
1:B:879:LEU:HD22	1:B:879:LEU:H	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:664:ASP:CG	1:A:692:ARG:NH1	2.31	0.82
1:A:605:ARG:NH1	1:A:605:ARG:HG2	1.92	0.82
1:A:588:ARG:NH2	1:A:617:LEU:HD11	1.93	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: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:N	1:A:484:ASP:OD1	2.09	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: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:O	1:A:782:LYS:HG3	1.79	0.81
1:A:456:ARG:HD3	1:A:461:TYR:HD2	1.42	0.81
1:B:649:LYS:N	1:B:650:PRO:HD3	1.93	0.80
1:A:384:LEU:C	1:A:384:LEU:CD1	2.49	0.80
1:A:154:ARG:HH21	1:A:170:LEU:HD11	1.45	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: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:HH11	1:A:148:ARG:HG3	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:410:VAL:O	1:A:413:LYS:HB3	1.82	0.79
1:A:416:VAL:CG1	1:A:416:VAL:O	2.27	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:218:HIS:C	1:B:262:LEU:HD11	2.03	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: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:A:487:GLN:O	1:A:491:GLU:CD	2.22	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:CA	1:B:536:GLU:OE2	2.30	0.77
1:A:171:LYS:CD	1:A:214:THR:CG2	2.62	0.77
1:A:537:LYS:C	1:A:539:LYS:H	1.88	0.77
1:B:375:ASP:C	1:B:375:ASP:OD1	2.22	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:O	1:B:442:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:262:LEU:H	1:B:262:LEU:CD1	1.97	0.77
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:817:GLN:NE2	1:A:819:ARG:HE	1.84	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: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:B:881:GLN:C	1:B:882:LEU:HD12	2.06	0.75
1:A:381:CYS:HB3	1:A:393:VAL:HG11	1.67	0.75
1:A:704:GLY:O	1:A:705:GLU:CD	2.24	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: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:HD13	1:A:384:LEU:O	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:A:645:ASP:CG	1:A:646:GLU:H	1.89	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:B:281:LYS:HA	1:B:284:ALA:HB3	1.70	0.74
1:B:735:VAL:HG22	1:B:735:VAL:O	1.88	0.74
1:B:690:TYR:OH	1:B:859:ARG:NH2	2.21	0.73
1:A:173:ARG:HG2	1:A:212:GLU:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HA	1:A:466:TRP:HB3	1.70	0.73
1:A:646:GLU:CD	1:A:646:GLU:C	2.47	0.73
1:B:138:ILE:HG12	1:B:139:GLY:H	1.51	0.73
1:A:381:CYS:HB3	1:A:393:VAL:CG1	2.19	0.73
1:A:308:ILE:O	1:A:309:SER:HB2	1.88	0.73
1:A:384:LEU:C	1:A:384:LEU:HD12	2.09	0.73
1:A:663:SER:HB3	1:A:688:GLN:HE22	1.53	0.73
1:B:648:GLN:N	1:B:648:GLN:HE21	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:HA	1:B:536:GLU:OE2	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:226:PHE:HE2	1:B:254:SER:HG	1.36	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:577:LEU:O	1:A:581:VAL:HG12	1.89	0.72
1:A:389:PRO:HD2	1:A:702:SER:OG	1.90	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LYS:O	1:A:542:VAL:N	2.23	0.71
1:A:646:GLU:CD	1:A:646:GLU:O	2.28	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:HD22	1:B:307:ASN:H	1.38	0.71
1:B:645:ASP:C	1:B:645:ASP:OD1	2.29	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:B:772:LEU:C	1:B:774:PRO:HD3	2.10	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:235:SER:OG	1:B:236:LEU:N	2.22	0.70
1:B:375:ASP:OD1	1:B:376:PHE:N	2.23	0.70
1:B:786:LEU:C	1:B:788:PRO:HD2	2.11	0.70
1:A:766:LEU:HD13	1:A:770:LYS:O	1.91	0.70
1:B:536:GLU:C	1:B:536:GLU:OE2	2.30	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:209:GLU:CD	1:A:221:THR:HG21	2.11	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: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:741:PHE:CD2	1:B:788:PRO:HG2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:GLN:HE21	1:A:648:GLN:HA	1.56	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:650:PRO:C	1:B:652:LEU:H	1.96	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:740:ASN:C	1:B:740:ASN:OD1	2.30	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:350:CYS:C	1:A:384:LEU:CD2	2.61	0.68
1:A:279:ASP:OD1	1:A:279:ASP:N	2.27	0.68
1:A:287:ILE:C	1:A:287:ILE:HD12	2.10	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:729:ARG:NH2	1:B:773:VAL:HG11	2.07	0.68
1:B:441:PHE:CE2	2:P:9:MLY:HH12	2.28	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: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:813:ILE:HA	1:B:820:VAL:HA	1.77	0.68
1:B:599:LEU:HD23	1:B:829:LEU:O	1.94	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:648:GLN:C	1:B:650:PRO:CD	2.43	0.67
1:B:819:ARG:NH1	1:B:822:THR:HG22	2.09	0.67
1:A:308:ILE:HG23	1:A:308:ILE:O	1.94	0.67
1:A:453:GLY:O	1:A:454:SER:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:GLN:NE2	1:B:648:GLN:H	1.92	0.67
1:A:671:HIS:CD2	1:A:721:ARG:NH2	2.63	0.67
1:A:664:ASP:OD1	1:A:692:ARG:NH1	2.28	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:A:154:ARG:NE	1:A:170:LEU:HD21	2.09	0.67
1:B:648:GLN:NE2	1:B:648:GLN:CA	2.58	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:O	1:A:233:ILE:HG13	1.94	0.66
1:A:464:VAL:HG22	1:A:475:THR:O	1.95	0.66
1:A:443:VAL:HG23	1:A:466:TRP:CE3	2.30	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:781:ILE:N	1:A:781:ILE:HD13	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:HD12	1:A:384:LEU:O	1.96	0.66
1:A:880:TYR:CD1	1:A:881:GLN:N	2.64	0.66
1:B:279:ASP:HB2	1:B:280:PRO:CD	2.26	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:B:622:LEU:CD1	1:B:880:TYR:O	2.44	0.65
1:A:537:LYS:C	1:A:539:LYS:N	2.48	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:778:MET:HE3	1:A:778:MET:HA	1.77	0.65
1:A:270:LYS:HE3	1:A:291:ASP:OD1	1.95	0.65
1:B:717:HIS:CE1	1:B:822:THR:HG21	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:MET:HG2	1:A:606:VAL:HG22	1.78	0.65
1:A:647:THR:C	1:A:648:GLN:NE2	2.50	0.65
1:B:802:VAL:HG23	1:B:810:GLN:NE2	2.12	0.65
1:B:819:ARG:HG3	1:B:819:ARG:HH11	1.62	0.65
1:B:819:ARG:NH1	1:B:820:VAL:O	2.30	0.65
1:B:882:LEU:H	1:B:882:LEU:HD12	1.60	0.65
1:A:879:LEU:N	1:A:879:LEU:CD2	2.60	0.65
1:B:440:GLU:C	1:B:441:PHE:CD1	2.70	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: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: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:486:PRO:HB2	1:A:490:ARG:CD	2.26	0.64
1:A:776:TYR:HA	1:A:779:SER:OG	1.96	0.64
1:B:440:GLU:N	1:B:440:GLU:OE1	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: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:140:SER:CB	1:B:141:PRO:HD3	2.27	0.64
1:B:664:ASP:CG	1:B:692:ARG:NH1	2.51	0.64
1:A:592:MET:CG	1:A:642:VAL:HG21	2.27	0.64
1:A:646:GLU:OE2	1:A:646:GLU:C	2.36	0.64
1:A:755:VAL:O	1:A:778:MET:HE1	1.96	0.64
1:B:648:GLN:O	1:B:648:GLN:NE2	2.30	0.64
1:A:148:ARG:NH1	1:A:148:ARG:HG3	2.12	0.64
1:A:457:GLU:O	1:A:458:ASN:CB	2.39	0.64
1:B:215:ASP:O	1:B:216:GLN:HB2	1.97	0.64
1:B:828:ARG:HH22	1:B:834:ASP:CG	2.01	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
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:A:454:SER:O	1:A:455:ASP:C	2.30	0.64
1:A:534:LYS:HZ1	1:A:535:ASP:HB3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LYS:HZ2	1:A:535:ASP:H	1.44	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:N	1:B:879:LEU:HD22	2.12	0.63
1:B:441:PHE:N	1:B:441:PHE:HD1	1.96	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:H	1:B:699:LEU:HD12	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:B:788:PRO:O	1:B:789:PHE:C	2.35	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:B:565:LEU:HB3	1:B:637:PHE:CD2	2.34	0.62
1:B:485:CYS:CB	2:P:5:GLN:N	2.62	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:345:ASP:CG	1:B:348:SER:HB3	2.20	0.62
1:B:413:LYS:O	1:B:415:TYR:CD2	2.53	0.62
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: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:284:ALA:O	1:A:287:ILE:HD11	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PRO:O	1:A:482:LEU:HD23	1.99	0.61
1:B:572:LEU:H	1:B:572:LEU:HD12	1.64	0.61
1:B:593:VAL:HG23	1:B:641:MET:HE1	1.81	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:703:PHE:CE2	1:A:709:PRO:HD2	2.35	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:379:PHE:O	1:B:382:GLN:N	2.33	0.61
1:B:867:GLN:CD	1:B:872:GLU:OE1	2.38	0.61
1:A:249:ARG:CG	1:A:249:ARG:O	2.49	0.61
1:A:350:CYS:C	1:A:384:LEU:HD22	2.20	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: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:883:PRO:HB2	1:A:884:PRO:HD3	1.81	0.61
1:A:884:PRO:O	1:A:885:SER:C	2.39	0.61
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: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:811:VAL:HG13	1:B:811:VAL:O	2.01	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:N	1:A:399:ASP:OD1	2.34	0.60
1:B:402:LEU:HD13	1:B:547:ILE:HD13	1.82	0.60
1:B:464:VAL:HG12	1:B:465:GLN:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:445:LYS:C	1:A:446:LEU:HD23	2.22	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:650:PRO:C	1:B:652:LEU:N	2.51	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:A:209:GLU:CD	1:A:221:THR:CG2	2.71	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:242:ASP:CG	1:A:243:GLY:H	2.04	0.59
1:A:469:TYR:HD2	1:A:469:TYR:N	1.98	0.59
1:B:485:CYS:SG	1:B:485:CYS:O	2.60	0.59
1:B:664:ASP:CG	1:B:692:ARG:HH11	2.05	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:A:755:VAL:O	1:A:778:MET:HE2	2.03	0.59
1:A:874:GLU:CD	1:A:875:GLY:N	2.56	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: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:648:GLN:CD	1:B:648:GLN:H	2.06	0.59
1:B:696:LYS:HZ1	1:B:706:GLY:C	2.05	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
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:555:TYR:HE2	1:B:618:PRO:HD3	1.66	0.59
1:B:441:PHE:CD2	2:P:9:MLY:CH1	2.85	0.59
1:A:209:GLU:OE1	1:A:221:THR:CG2	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:415:TYR:CD2	2.71	0.58
1:B:773:VAL:O	1:B:773:VAL:HG23	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:CD2	1:A:469:TYR:N	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:B:558:MET:HE1	1:B:608:LEU:HD22	1.85	0.58
1:A:137:PHE:CE2	1:A:218:HIS:HB3	2.38	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:O	1:A:617:LEU:HD12	2.03	0.58
1:A:683:PRO:HB2	1:A:689:ARG:HG2	1.86	0.58
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:791:ARG:NH2	1:B:814:HIS:O	2.36	0.58
1:B:780:PHE:CE1	1:B:809:ASN:HB3	2.31	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: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:234:ASN:C	1:A:236:LEU:H	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:CYS:C	1:A:384:LEU:HD23	2.24	0.58
1:A:384:LEU:HD13	1:A:384:LEU:C	2.23	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:B:650:PRO:O	1:B:652:LEU:N	2.29	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:456:ARG:C	1:A:457:GLU:OE2	2.42	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:755:VAL:CA	1:A:778:MET:HE1	2.33	0.57
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:B:589:LEU:C	1:B:589:LEU:HD12	2.24	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:241:VAL:HG11	1:A:583:MET:HE2	1.86	0.57
1:A:534:LYS:CE	1:A:535:ASP:H	2.18	0.56
1:B:518:GLN:HB2	1:B:537:LYS:HB3	1.87	0.56
1:A:714:LEU:C	1:A:714:LEU:HD23	2.25	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:579:CYS:O	1:A:583:MET:HG3	2.05	0.56
1:A:603:ARG:CZ	1:A:830:GLN:HE22	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:308:ILE:HG22	1:A:308:ILE:O	2.05	0.56
1:A:588:ARG:HE	1:A:617:LEU:HD13	1.70	0.56
1:B:349:GLY:C	1:B:351:GLY:H	2.09	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:A:588:ARG:HH21	1:A:617:LEU:CD1	2.01	0.56
1:A:790:GLY:C	1:A:811:VAL:HG23	2.25	0.56
1:A:824:ARG:NH2	1:A:836:TYR:O	2.24	0.56
1:B:780:PHE:C	1:B:782:LYS:H	2.09	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:143:ALA:O	1:A:144:ALA:C	2.44	0.56
1:A:483:SER:HG	1:A:484:ASP:H	1.54	0.56
1:A:537:LYS:CG	1:A:538:ASN:N	2.68	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:A:226:PHE:CD1	1:A:230:ASP:HB2	2.41	0.56
1:B:646:GLU:HG2	1:B:646:GLU:O	2.05	0.56
1:A:137:PHE:CE1	1:A:210:PHE:HB3	2.41	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:A:173:ARG:CZ	1:A:212:GLU:CG	2.75	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:742:ARG:NH2	1:A:753:ASN:O	2.40	0.55
1:A:602:PHE:O	1:A:799:PRO:O	2.24	0.55
1:B:735:VAL:CG2	1:B:735:VAL:O	2.52	0.55
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:283:LYS:C	1:B:287:ILE:HD12	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:144:ALA:O	1:B:145:ASP:HB2	2.06	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: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:A:664:ASP:CG	1:A:664:ASP:O	2.44	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:786:LEU:C	1:B:788:PRO:CD	2.75	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:781:ILE:H	1:A:781:ILE:HD13	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:878:PRO:HB2	1:B:879:LEU:HD13	1.90	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
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: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: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:763:ARG:C	1:A:764:VAL:HG12	2.26	0.54
1:B:780:PHE:C	1:B:782:LYS:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:THR:HG23	1:A:221:THR:O	2.08	0.54
1:A:250:ARG:HH21	1:A:295:ASP:CG	2.11	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:787:LYS:N	1:B:788:PRO:CD	2.70	0.54
1:B:386:TYR:CE2	1:B:837:ARG:HD3	2.43	0.54
1:A:196:ALA:HA	1:A:203:TYR:HE2	1.72	0.53
1:A:345:ASP:CG	1:A:348:SER:HB3	2.28	0.53
1:B:514:GLY:N	1:B:515:PRO:CD	2.71	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: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: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: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:630:ARG:NH1	1:B:632:GLY:HA3	2.24	0.53
1:B:602:PHE:O	1:B:799:PRO:O	2.27	0.53
1:A:134:GLU:HG2	1:A:180:LYS:HE2	1.86	0.53
1:A:542:VAL:HG22	1:A:575:TYR:OH	2.08	0.53
1:A:645:ASP:CG	1:A:646:GLU:N	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:775:ASP:N	1:A:775:ASP:OD1	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:B:143:ALA:CB	1:B:147:ALA:HB2	2.38	0.52
1:B:699:LEU:N	1:B:699:LEU:CD1	2.58	0.52
1:A:249:ARG:HG2	1:A:249:ARG:O	2.09	0.52
1:A:564:ILE:CG2	1:A:573:GLY:N	2.72	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
1:B:405:LEU:HD21	1:B:503:PRO:HG2	1.91	0.52
1:B:830:GLN:HB3	1:B:832:PHE:HD2	1.74	0.52
1:B:828:ARG:NH2	1:B:834:ASP:OD1	2.43	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: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:A:642:VAL:O	1:A:642:VAL:HG23	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: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: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:469:TYR:CE2	1:B:808:HIS:CE1	2.98	0.52
1:A:466:TRP:HD1	1:A:466:TRP:H	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:589:LEU:O	1:B:589:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:HD3	1:B:615:MET:CE	2.39	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:B:733:ILE:HG13	1:B:734:PRO:CD	2.32	0.51
1:B:877:ASP:N	1:B:877:ASP:OD1	2.43	0.51
1:B:580:LEU:O	1:B:585:TYR:HB2	2.10	0.51
1:B:672:GLN:O	1:B:672:GLN:HG3	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:236:LEU:C	1:A:238:SER:N	2.64	0.51
1:A:535:ASP:OD1	1:A:537:LYS:O	2.28	0.51
1:A:733:ILE:HG22	1:A:791:ARG:HH11	1.75	0.51
1:B:727:TYR:O	1:B:727:TYR:HD2	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:B:538:ASN:OD1	1:B:538:ASN:C	2.49	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:HG2	1:A:804:ARG:O	2.10	0.51
1:A:823:ILE:HG12	1:A:846:TYR:CD2	2.45	0.51
1:B:364:SER:OG	1:B:863:TYR:O	2.29	0.51
1:A:202:ASP:O	1:A:227:ARG:NH2	2.44	0.51
1:A:592:MET:CE	1:A:857:VAL:HG13	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:TYR:O	1:B:645:ASP:CG	2.49	0.51
1:B:725:ASP:O	1:B:728:GLU:N	2.43	0.51
1:A:611:ALA:HB3	1:A:617:LEU:HB3	1.93	0.51
1:A:624:THR:C	1:A:625:TYR:CD2	2.76	0.51
1:A:695:ARG:HB3	1:A:700:ASP:HB3	1.93	0.51
1:A:601:GLN:HB3	1:A:798:VAL:HG23	1.93	0.51
1:A:668:VAL:H	1:A:817:GLN:NE2	2.09	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:B:830:GLN:HA	1:B:830:GLN:OE1	2.11	0.51
1:A:302:TYR:O	1:A:303:SER:HB2	2.12	0.50
1:B:374:VAL:HG22	1:B:394:ARG:HB2	1.93	0.50
1:B:565:LEU:HD11	1:B:606:VAL:CG2	2.41	0.50
1:B:733:ILE:HG21	1:B:791:ARG:NE	2.26	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:A:648:GLN:C	1:A:650:PRO:CG	2.80	0.50
1:B:510:VAL:HG11	1:B:865:LEU:HD21	1.94	0.50
1:B:402:LEU:HB2	1:B:547:ILE:CD1	2.42	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:B:838:LEU:C	1:B:839:PHE:CD2	2.85	0.50
1:A:357:LEU:HD23	1:A:858:ALA:O	2.11	0.50
1:A:541:MET:SD	1:A:558:MET:HE1	2.51	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:752:ASN:C	1:A:754:ILE:H	2.14	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

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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	0.50
1:A:191:ASP:O	1:A:269:VAL:N	2.41	0.49
1:A:212:GLU:CD	1:A:218:HIS:HD1	2.13	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: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:411:LEU:C	1:B:411:LEU:HD23	2.32	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:279:ASP:CB	1:A:280:PRO:CD	2.89	0.49
1:A:278:MET:HB3	1:A:283:LYS:HE3	1.94	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:646:GLU:OE1	1:A:646:GLU:O	2.30	0.49
1:B:155:TYR:C	1:B:171:LYS:NZ	2.66	0.49
1:A:703:PHE:C	1:A:705:GLU:H	2.15	0.49
1:B:207:ILE:N	1:B:207:ILE:HD12	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: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:B:472:GLU:C	1:B:473:GLU:HG2	2.33	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:143:ALA:O	1:B:144:ALA:HB3	2.12	0.49
1:B:269:VAL:HG11	1:B:292:LEU:HD12	1.95	0.49
1:B:464:VAL:CG1	1:B:465:GLN:N	2.75	0.49
1:B:442:VAL:CA	2:P:6:THR:HG22	2.36	0.49
1:A:150:ASN:HB3	1:A:151:TRP:CE3	2.48	0.49
1:A:288:GLU:O	1:A:288:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:726:ASP:O	1:B:727:TYR:C	2.50	0.49
1:B:737:LYS:HB2	1:B:793:TRP:CZ2	2.46	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:B:394:ARG:NE	1:B:396:GLU:OE2	2.46	0.48
1:A:211:PHE:CD1	1:A:211:PHE:C	2.86	0.48
1:A:704:GLY:O	1:A:705:GLU:OE1	2.31	0.48
1:B:155:TYR:C	1:B:171:LYS:HZ1	2.16	0.48
1:B:280:PRO:C	1:B:282:ALA:H	2.17	0.48
1:B:718:GLN:O	1:B:822:THR:HA	2.13	0.48
1:A:853:VAL:N	3:A:1000:SAH:OXT	2.42	0.48
1:A:652:LEU:O	1:A:654:LYS:N	2.45	0.48
1:A:827:ALA:HB1	1:A:832:PHE:HB2	1.95	0.48
1:B:307:ASN:ND2	1:B:307:ASN:H	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:A:288:GLU:HG3	1:A:289:SER:N	2.28	0.48
1:A:874:GLU:CD	1:A:875:GLY:O	2.51	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:A:296:MET:HG2	1:A:306:ALA:C	2.34	0.48
1:A:404:LEU:CD2	1:A:502:LEU:HD11	2.35	0.48
1:A:514:GLY:O	1:A:515:PRO:C	2.52	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:O	1:B:624:THR:HG22	2.12	0.48
1:A:286:LEU:O	1:A:289:SER:OG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:284:ALA:O	1:B:288:GLU:HG3	2.13	0.48
1:B:748:ARG:CZ	1:B:759:PRO:HD2	2.44	0.48
1:B:353:MET:HB2	1:B:853:VAL:HG21	1.96	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:A:568:ALA:O	1:A:569:ASP:C	2.52	0.48
1:B:666:PRO:HB3	1:B:680:GLY:HA3	1.96	0.48
1:B:793:TRP:C	1:B:795:ASP:N	2.68	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
1:A:624:THR:C	1:A:625:TYR:HD2	2.16	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:569:ASP:O	1:A:570:GLY:C	2.52	0.47
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:445:LYS:HB2	1:B:465:GLN:OE1	2.14	0.47
1:B:589:LEU:C	1:B:589:LEU:CD1	2.83	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: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:363:LEU:N	1:A:363:LEU:CD2	2.76	0.47
1:A:793:TRP:CE3	1:A:793:TRP:HA	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: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:456:ARG:CD	1:A:461:TYR:CD2	2.58	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:N	1:A:645:ASP:OD1	2.45	0.47
1:B:304:THR:HG21	1:B:588:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HA	2:P:6:THR:CG2	2.38	0.47
1:B:884:PRO:O	1:B:885:SER:C	2.53	0.47
1:A:215:ASP:C	1:A:216:GLN:OE1	2.52	0.47
1:A:604:MET:O	1:A:605:ARG:HG2	2.15	0.47
1:B:455:ASP:OD2	1:B:455:ASP:C	2.52	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:509:ASP:OD1	1:A:554:LYS:CE	2.63	0.47
1:A:535:ASP:C	1:A:535:ASP:OD1	2.52	0.47
1:B:226:PHE:CD2	1:B:254:SER:HB2	2.50	0.47
1:B:447:VAL:O	1:B:447:VAL:HG23	2.14	0.47
1:A:206:ARG:NH2	1:A:294:TYR:OH	2.48	0.47
1:A:446:LEU:HD23	1:A:446:LEU:N	2.29	0.47
1:B:192:VAL:CG1	1:B:193:TYR:N	2.76	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:440:GLU:N	1:B:441:PHE:CD1	2.83	0.47
1:B:411:LEU:HD21	1:B:493:VAL:CG2	2.44	0.47
1:B:646:GLU:OE2	1:B:647:THR:CA	2.60	0.47
1:B:771:PRO:C	1:B:773:VAL:H	2.18	0.47
1:A:204:ILE:O	1:A:224:TRP:HE3	1.98	0.47
1:A:495:GLU:HA	1:A:498:LYS:HE3	1.97	0.47
1:A:874:GLU:CD	1:A:875:GLY:H	2.18	0.47
1:B:717:HIS:C	1:B:718:GLN:HG3	2.36	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:HD13	1:A:239:ILE:N	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:658:LEU:HD11	1:B:662:ILE:HD13	1.97	0.47
1:B:747:VAL:O	1:B:748:ARG:CG	2.62	0.47
1:B:603:ARG:NH2	1:B:830:GLN:HE22	2.13	0.47
1:A:394:ARG:NE	1:A:396:GLU:OE1	2.40	0.47
1:A:486:PRO:O	1:A:487:GLN:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:A:445:LYS:HB2	1.57	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:N	1:B:757:TRP:CD1	2.82	0.46
1:B:817:GLN:O	1:B:818:ALA:HB3	2.15	0.46
1:A:224:TRP:NE1	1:A:258:ASN:OD1	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:A:752:ASN:C	1:A:754:ILE:N	2.68	0.46
1:B:280:PRO:O	1:B:282:ALA:N	2.49	0.46
1:A:233:ILE:CG1	1:A:233:ILE:O	2.61	0.46
1:A:624:THR:O	1:A:625:TYR:CE2	2.57	0.46
1:B:353:MET:HE1	1:B:559:GLU:HG2	1.96	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: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:781:ILE:HG12	1:A:785:SER:HB2	1.96	0.46
1:A:780:PHE:O	1:A:783:GLY:N	2.46	0.46
1:B:635:ASN:O	1:B:636:ALA:C	2.54	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:596:CYS:C	1:A:597:TYR:CG	2.88	0.46
1:B:511:ILE:CG2	1:B:553:PRO:HG3	2.46	0.46
1:B:629:VAL:HG21	1:B:641:MET:HE2	1.98	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:284:ALA:C	1:A:287:ILE:HG13	2.35	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:672:GLN:HG2	1:B:717:HIS:O	2.16	0.46
1:B:616:VAL:O	1:B:868:ALA:HB1	2.16	0.46
1:A:495:GLU:OE1	1:A:498:LYS:NZ	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:CYS:CA	2:P:5:GLN:N	2.79	0.46
1:B:239:ILE:HD13	1:B:578:SER:CB	2.46	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:B:247:ASP:O	1:B:249:ARG:N	2.48	0.46
1:B:685:THR:HG22	1:B:688:GLN:CD	2.36	0.46
1:B:724:ASN:O	1:B:727:TYR:HB3	2.15	0.46
1:B:725:ASP:OD1	1:B:725:ASP:C	2.53	0.46
1:B:819:ARG:HH22	1:B:825:GLU:CD	2.19	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:A:798:VAL:HG23	1:A:798:VAL:O	2.16	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: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:580:LEU:HD21	1:B:610:GLY:HA3	1.98	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: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:A:487:GLN:C	1:A:491:GLU:CD	2.74	0.45
1:B:235:SER:O	1:B:237:VAL:N	2.50	0.45
1:B:281:LYS:HE3	1:B:281:LYS:HB3	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:A:460:ILE:C	1:A:461:TYR:CD1	2.90	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:145:ASP:CG	1:A:148:ARG:NH1	2.69	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:645:ASP:OD1	1:A:647:THR:OG1	2.31	0.45
1:A:386:TYR:OH	1:A:710:ASP:OD2	2.35	0.45
1:A:875:GLY:O	1:A:876:SER:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:142:VAL:CG2	1:B:174:CYS:SG	3.04	0.45
1:B:218:HIS:HB2	1:B:262:LEU:HD13	1.99	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: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:472:GLU:O	1:B:473:GLU:CB	2.64	0.45
1:B:589:LEU:HA	1:B:620:TYR:HH	1.78	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: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:626:ASP:C	1:A:626:ASP:OD1	2.56	0.45
1:B:204:ILE:HD13	1:B:292:LEU:HD11	1.99	0.45
1:B:842:ILE:HG22	1:B:843:LYS:N	2.31	0.45
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:287:ILE:C	1:A:287:ILE:CD1	2.77	0.44
1:A:665:LEU:HA	1:A:665:LEU:HD23	1.84	0.44
1:B:278:MET:HB3	1:B:282:ALA:HB3	2.00	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:NH1	1:A:605:ARG:CG	2.57	0.44
1:A:719:PRO:HG3	1:A:819:ARG:HD2	1.98	0.44
1:A:717:HIS:ND1	1:A:822:THR:HG21	2.32	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:ND1	1:A:218:HIS:N	2.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:609:TRP:CE3	1:A:618:PRO:HG2	2.53	0.44
1:B:355:THR:O	1:B:359:LEU:HD13	2.18	0.44
1:B:351:GLY:CA	1:B:384:LEU:HD22	2.47	0.44
1:B:645:ASP:O	1:B:646:GLU:CB	2.47	0.44
1:A:812:ILE:HG13	1:A:812:ILE:O	2.18	0.44
1:B:831:GLY:HA3	1:B:856:PRO:HD3	1.99	0.44
1:B:442:VAL:HG23	2:P:6:THR:CG2	2.47	0.44
1:A:560:ASN:CG	1:A:564:ILE:HD11	2.38	0.44
1:A:609:TRP:CH2	1:A:865:LEU:HB2	2.53	0.44
1:A:592:MET:HE1	1:A:857:VAL:HG13	1.99	0.44
1:B:349:GLY:O	1:B:350:CYS:SG	2.74	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:B:591:MET:HE2	1:B:604:MET:SD	2.58	0.44
1:A:142:VAL:HG23	1:A:142:VAL:O	2.17	0.44
1:A:270:LYS:HE3	1:A:291:ASP:CG	2.38	0.44
1:A:565:LEU:HB3	1:A:637:PHE:CD2	2.53	0.44
1:A:653:LYS:O	1:A:654:LYS:C	2.56	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:182:ASP:OD1	1:B:184:VAL:N	2.34	0.44
1:B:138:ILE:HD12	1:B:185:VAL:HG21	2.00	0.44
1:B:239:ILE:HD13	1:B:578:SER:HB2	2.00	0.44
1:B:294:TYR:O	1:B:294:TYR:CD1	2.70	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:HG3	1:A:672:GLN:O	2.18	0.43
1:B:586:GLN:O	1:B:610:GLY:HA2	2.18	0.43
1:B:554:LYS:O	1:B:611:ALA:HA	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:HH21	1:B:748:ARG:HG2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:MET:CE	1:A:282:ALA:O	2.66	0.43
1:B:239:ILE:HD13	1:B:578:SER:OG	2.17	0.43
1:B:642:VAL:CG2	1:B:642:VAL:O	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: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:778:MET:HB3	1:A:778:MET:HE2	1.49	0.43
1:A:204:ILE:CG2	1:A:271:ILE:HD11	2.48	0.43
1:A:704:GLY:O	1:A:705:GLU:CG	2.65	0.43
1:B:218:HIS:N	1:B:218:HIS:CD2	2.86	0.43
1:B:262:LEU:C	1:B:264:CYS:N	2.69	0.43
1:B:554:LYS:HD3	1:B:615:MET:HE2	2.00	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
1:B:241:VAL:O	1:B:242:ASP:C	2.57	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:838:LEU:C	1:A:839:PHE:CD1	2.92	0.43
1:B:273:HIS:HD2	1:B:274:VAL:N	2.14	0.43
1:B:791:ARG:NH2	1:B:815:PRO:O	2.51	0.43
1:A:141:PRO:C	1:A:143:ALA:N	2.70	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:723:ASN:O	1:B:724:ASN:C	2.56	0.43
1:B:819:ARG:NH1	1:B:819:ARG:CG	2.74	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:798:VAL:O	1:A:799:PRO:C	2.54	0.43
1:A:658:LEU:HD13	1:A:829:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:716:ASP:OD1	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:664:ASP:OD2	1:B:664:ASP:C	2.57	0.43
1:A:175:HIS:CD2	1:A:211:PHE:CB	3.01	0.42
1:A:137:PHE:CZ	1:A:211:PHE:O	2.72	0.42
1:A:391:THR:HG22	1:A:392:GLU:N	2.34	0.42
1:A:780:PHE:HB3	1:A:785:SER:HB3	2.01	0.42
1:B:589:LEU:HD23	1:B:608:LEU:HD12	2.01	0.42
1:A:404:LEU:O	1:A:405:LEU:C	2.56	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
1:B:235:SER:O	1:B:236:LEU:C	2.56	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: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
1:B:720:LEU:HD22	1:B:805:ALA:O	2.19	0.42
1:B:485:CYS:HB3	2:P:6:THR:O	2.19	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:B:394:ARG:HB3	1:B:394:ARG:HE	1.58	0.42
1:B:578:SER:O	1:B:581:VAL:N	2.53	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:363:LEU:C	1:A:365:GLY:N	2.72	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:347:TYR:N	1:B:347:TYR:CD1	2.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:1000:SAH:H4'	3:B:1000:SAH:HG2	1.75	0.42
1:B:218:HIS:HB2	1:B:262:LEU:HD11	2.01	0.42
1:A:280:PRO:C	1:A:281:LYS:HG2	2.40	0.42
1:A:342:THR:OG1	1:A:508:VAL:HA	2.19	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:695:ARG:HG2	1:A:835:TYR:CE1	2.55	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:414:LYS:HD2	1:B:416:VAL:C	2.39	0.42
1:B:572:LEU:N	1:B:572:LEU:HD12	2.32	0.42
1:B:599:LEU:HD12	1:B:599:LEU:N	2.34	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:724:ASN:O	1:A:728:GLU:HG3	2.19	0.42
1:A:781:ILE:HA	1:A:781:ILE:HD12	1.79	0.42
1:A:879:LEU:C	1:A:879:LEU:HD23	2.39	0.42
1:B:696:LYS:C	1:B:698:MET:O	2.58	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:234:ASN:C	1:A:236:LEU:N	2.72	0.42
1:A:465:GLN:HG3	1:A:474:ASP:CG	2.40	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:241:VAL:HG11	1:A:583:MET:CE	2.49	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:B:513:GLY:HA2	1:B:544:PHE:CZ	2.55	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:B:302:TYR:CE2	1:B:878:PRO:HB3	2.55	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:A:414:LYS:C	1:A:416:VAL:H	2.24	0.42
1:B:279:ASP:CB	1:B:280:PRO:CD	2.97	0.42
1:B:349:GLY:C	1:B:351:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:B:239:ILE:H	1.85	0.41
1:A:143:ALA:CB	1:A:177:ARG:HH21	2.33	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:CD2	1:A:302:TYR:N	2.88	0.41
1:A:479:ILE:O	1:A:482:LEU:HB2	2.21	0.41
1:A:495:GLU:CD	1:A:499:ARG:HH21	2.23	0.41
1:A:648:GLN:C	1:A:650:PRO:HG2	2.41	0.41
1:A:759:PRO:C	1:A:761:ILE:H	2.23	0.41
1:A:791:ARG:HH21	1:A:818:ALA:H	1.69	0.41
1:B:307:ASN:ND2	1:B:586:GLN:CD	2.73	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:CG1	1:B:233:ILE:O	2.68	0.41
1:B:341:ALA:O	1:B:368:LEU:HD23	2.20	0.41
1:B:394:ARG:NH2	1:B:396:GLU:OE2	2.52	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:HG3	1:A:630:ARG:H	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: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:353:MET:HE3	1:B:559:GLU:HG2	2.02	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:386:TYR:CD2	1:B:837:ARG:HD3	2.55	0.41
1:A:255:GLU:HG3	1:A:255:GLU:O	2.20	0.41
1:A:341:ALA:HB1	1:A:509:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2.21	0.41
1:B:603:ARG:NH1	1:B:852:ALA:O	2.53	0.41
1:B:659:GLY:O	1:B:663:SER:OG	2.30	0.41
1:B:485:CYS:HB3	2:P:6:THR:C	2.40	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:619:LYS:HD2	1:A:877:ASP:O	2.21	0.41
1:A:591:MET:O	1:A:642:VAL:HG22	2.21	0.41
1:B:140:SER:HB3	1:B:141:PRO:HD2	2.00	0.41
1:B:413:LYS:HE3	1:B:413:LYS:HB2	1.79	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:A:589:LEU:HD23	1:A:589:LEU:C	2.41	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: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:714:LEU:C	1:B:715:LEU:HD12	2.41	0.41
1:A:250:ARG:NH2	1:A:295:ASP:CG	2.71	0.41
1:A:553:PRO:HB2	1:A:555:TYR:O	2.21	0.41
1:B:143:ALA:N	1:B:175:HIS:O	2.53	0.41
1:B:273:HIS:CD2	1:B:273:HIS:C	2.94	0.41
1:B:414:LYS:C	1:B:415:TYR:CD2	2.94	0.41
1:B:485:CYS:HB3	2:P:6:THR:CA	2.51	0.41
1:B:724:ASN:O	1:B:725:ASP:C	2.58	0.41
1:B:724:ASN:O	1:B:727:TYR:CB	2.69	0.41
1:B:740:ASN:OD1	1:B:741:PHE:N	2.54	0.41
1:A:408:TRP:NE1	1:A:412:CYS:SG	2.94	0.41
1:A:511:ILE:HG23	1:A:553:PRO:CB	2.51	0.41
1:A:646:GLU:OE2	1:A:646:GLU:O	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LEU:HA	1:B:600:PRO:HD3	1.85	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:674:ASN:C	1:B:718:GLN:HE21	2.24	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:440:GLU:N	1:B:441:PHE:HD1	2.18	0.40
1:B:748:ARG:NH1	1:B:759:PRO:HD2	2.36	0.40
1:B:387:ASN:CB	1:B:836:TYR:CE2	3.04	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:HA	1:B:504:LEU:HD23	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:824:ARG:O	1:B:825:GLU:C	2.60	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: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:812:ILE:CG1	1:B:812:ILE:O	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:285:GLN:O	1:A:286:LEU:C	2.58	0.40
1:A:346:LEU:C	1:A:347:TYR:HD2	2.25	0.40
1:A:843:LYS:O	1:A:846:TYR:HB2	2.22	0.40
1:B:414:LYS:C	1:B:415:TYR:HD2	2.24	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:141:PRO:C	1:A:143:ALA:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:536:GLU:O	1:A:537:LYS:C	2.60	0.40
1:A:558:MET:O	1:A:607:PHE:HA	2.21	0.40
1:A:865:LEU:O	1:A:866:GLY:C	2.59	0.40
1:B:154:ARG:HA	1:B:154:ARG:HD3	1.86	0.40
1:B:154:ARG:C	1:B:171:LYS:HG2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/784 (85%)	580 (87%)	70 (10%)	14 (2%)	7	37
1	B	660/784 (84%)	577 (87%)	73 (11%)	10 (2%)	10	44
2	P	4/15 (27%)	4 (100%)	0	0	100	100
All	All	1328/1583 (84%)	1161 (87%)	143 (11%)	24 (2%)	8	41

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

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Mol	Chain	Res	Type
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%)	448 (79%)	116 (21%)	1	6
1	B	549/668 (82%)	440 (80%)	109 (20%)	1	6
2	P	5/9 (56%)	4 (80%)	1 (20%)	1	6
All	All	1118/1345 (83%)	892 (80%)	226 (20%)	1	6

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	138	ILE
1	A	154	ARG
1	A	173	ARG
1	A	183	ASN
1	A	190	ASP
1	A	202	ASP
1	A	209	GLU

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Mol	Chain	Res	Type
1	A	214	THR
1	A	215	ASP
1	A	218	HIS
1	A	233	ILE
1	A	235	SER
1	A	236	LEU
1	A	238	SER
1	A	239	ILE
1	A	249	ARG
1	A	253	LEU
1	A	269	VAL
1	A	270	LYS
1	A	272	VAL
1	A	275	ASP
1	A	277	ASN
1	A	279	ASP
1	A	286	LEU
1	A	288	GLU
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	442	VAL
1	A	443	VAL
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

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Mol	Chain	Res	Type
1	A	485	CYS
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
1	A	563	ASP
1	A	581	VAL
1	A	585	TYR
1	A	592	MET
1	A	605	ARG
1	A	612	LEU
1	A	615	MET
1	A	617	LEU
1	A	627	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	664	ASP
1	A	668	VAL
1	A	671	HIS
1	A	675	ASP
1	A	677	MET
1	A	678	GLU
1	A	698	MET
1	A	701	TRP
1	A	710	ASP
1	A	716	ASP
1	A	720	LEU
1	A	724	ASN
1	A	731	GLN
1	A	735	VAL
1	A	760	GLU
1	A	762	GLU

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Mol	Chain	Res	Type
1	A	763	ARG
1	A	772	LEU
1	A	775	ASP
1	A	780	PHE
1	A	781	ILE
1	A	787	LYS
1	A	788	PRO
1	A	792	LEU
1	A	793	TRP
1	A	804	ARG
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	853	VAL
1	A	870	LEU
1	A	872	GLU
1	A	879	LEU
1	A	881	GLN
1	A	882	LEU
1	A	885	SER
1	B	134	GLU
1	B	138	ILE
1	B	148	ARG
1	B	149	SER
1	B	173	ARG
1	B	174	CYS
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	206	ARG
1	B	207	ILE
1	B	215	ASP
1	B	223	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	273	HIS
1	B	274	VAL
1	B	279	ASP
1	B	283	LYS
1	B	296	MET
1	B	303	SER
1	B	339	ARG
1	B	354	SER
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	395	ASN
1	B	399	ASP
1	B	411	LEU
1	B	415	TYR
1	B	440	GLU
1	B	441	PHE
1	B	443	VAL
1	B	444	GLU
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

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Mol	Chain	Res	Type
1	B	535	ASP
1	B	536	GLU
1	B	538	ASN
1	B	541	MET
1	B	552	LYS
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	645	ASP
1	B	646	GLU
1	B	647	THR
1	B	648	GLN
1	B	664	ASP
1	B	667	LYS
1	B	672	GLN
1	B	693	LEU
1	B	696	LYS
1	B	699	LEU
1	B	702	SER
1	B	715	LEU
1	B	716	ASP
1	B	723	ASN
1	B	727	TYR
1	B	731	GLN
1	B	733	ILE
1	B	735	VAL
1	B	742	ARG
1	B	760	GLU
1	B	780	PHE
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	809	ASN
1	B	819	ARG

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Mol	Chain	Res	Type
1	B	820	VAL
1	B	821	LEU
1	B	822	THR
1	B	842	ILE
1	B	859	ARG
1	B	879	LEU
1	B	882	LEU
2	P	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
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	B	246	HIS
1	B	273	HIS
1	B	307	ASN
1	B	540	GLN
1	B	560	ASN
1	B	648	GLN
1	B	671	HIS
1	B	674	ASN
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	0.63	0	6,11,13	1.80	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	-3.28	104.92	113.79
2	P	9	MLY	CH1-NZ-CE	-2.05	102.60	110.74

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	1000	-	21,28,28	1.71	5 (23%)	20,40,40	1.93	5 (25%)
3	SAH	B	1000	-	21,28,28	1.70	5 (23%)	20,40,40	1.92	5 (25%)

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	A	1000	-	-	4/7/31/31	0/3/3/3
3	SAH	B	1000	-	-	1/7/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	SAH	C2-N3	5.05	1.40	1.32
3	B	1000	SAH	C2-N3	5.01	1.40	1.32
3	B	1000	SAH	C2-N1	3.26	1.40	1.33
3	A	1000	SAH	C2-N1	3.25	1.40	1.33
3	A	1000	SAH	C5-C4	-2.71	1.33	1.40
3	B	1000	SAH	C5-C4	-2.69	1.33	1.40
3	B	1000	SAH	C6-C5	-2.60	1.33	1.43
3	A	1000	SAH	C6-C5	-2.58	1.33	1.43
3	A	1000	SAH	O4'-C1'	2.05	1.43	1.41
3	B	1000	SAH	O4'-C1'	2.01	1.43	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	SAH	N3-C2-N1	-6.76	118.11	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	SAH	N3-C2-N1	-6.70	118.20	128.68
3	A	1000	SAH	C5-C6-N6	-2.69	116.26	120.35
3	B	1000	SAH	C5-C6-N6	-2.69	116.26	120.35
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
3	A	1000	SAH	C3'-C2'-C1'	2.05	104.06	100.98
3	B	1000	SAH	O4'-C1'-C2'	-2.04	103.94	106.93
3	B	1000	SAH	C3'-C2'-C1'	2.03	104.03	100.98
3	A	1000	SAH	O4'-C1'-C2'	-2.01	103.98	106.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

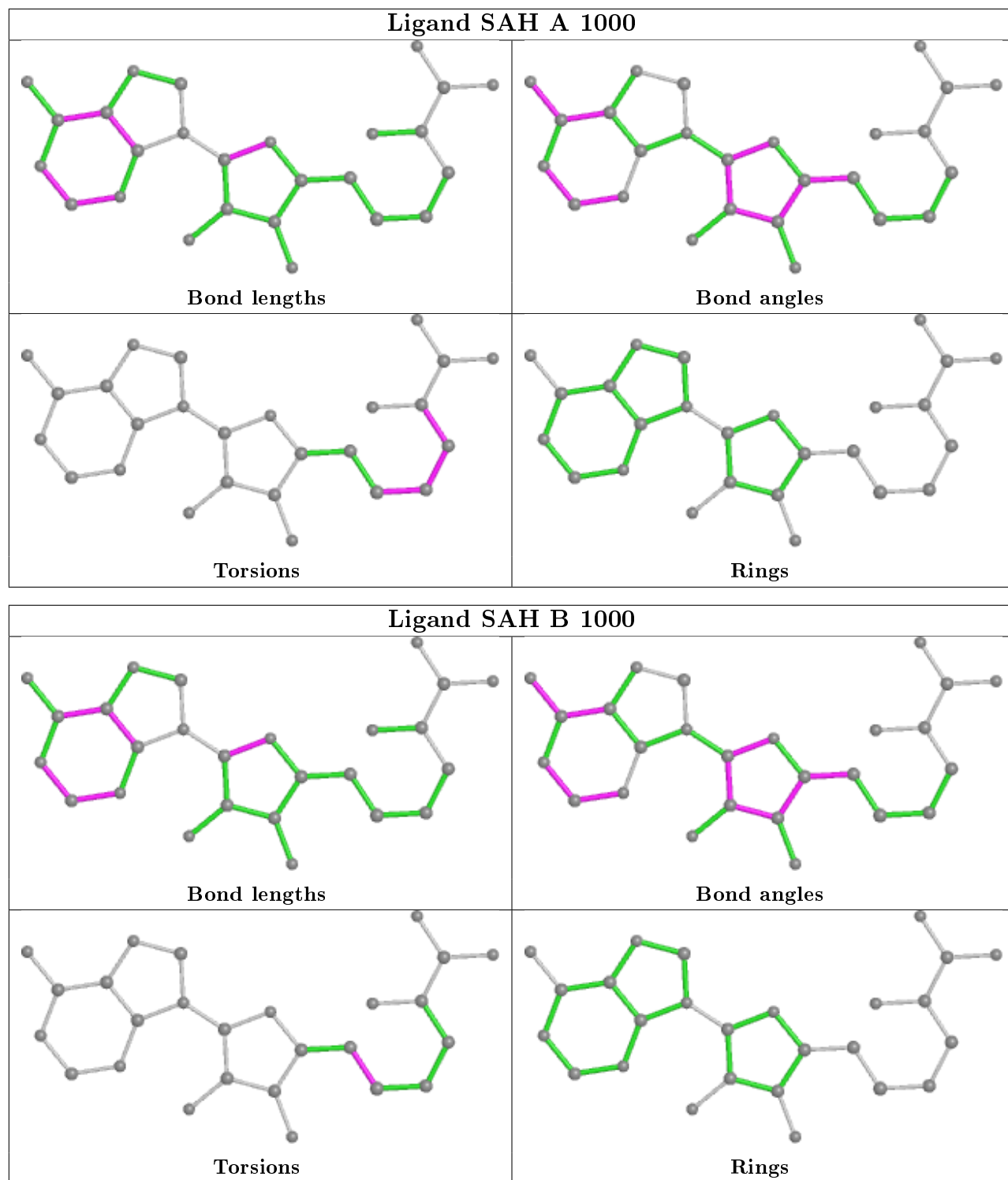
Mol	Chain	Res	Type	Atoms
3	A	1000	SAH	N-CA-CB-CG
3	A	1000	SAH	C-CA-CB-CG
3	A	1000	SAH	CA-CB-CG-SD
3	A	1000	SAH	CB-CG-SD-C5'
3	B	1000	SAH	C4'-C5'-SD-CG

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	SAH	5	0
3	B	1000	SAH	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.13	8 (1%) 79 67	31, 69, 145, 218	0
1	B	670/784 (85%)	-0.18	5 (0%) 87 81	29, 70, 131, 200	0
2	P	6/15 (40%)	-0.15	0 100 100	82, 97, 104, 104	0
All	All	1350/1583 (85%)	-0.16	13 (0%) 82 72	29, 70, 139, 218	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASN	3.1
1	B	729	ARG	2.8
1	A	180	LYS	2.8
1	A	487	GLN	2.8
1	A	468	GLY	2.7
1	A	740	ASN	2.6
1	A	484	ASP	2.5
1	A	218	HIS	2.4
1	A	445	LYS	2.4
1	B	228	ALA	2.3
1	B	416	VAL	2.1
1	B	744	LEU	2.1
1	B	277	ASN	2.1

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(\AA^2)	Q<0.9
2	MLY	P	9	11/12	0.91	0.29	65,75,80,80	0

6.3 Carbohydrates [i](#)

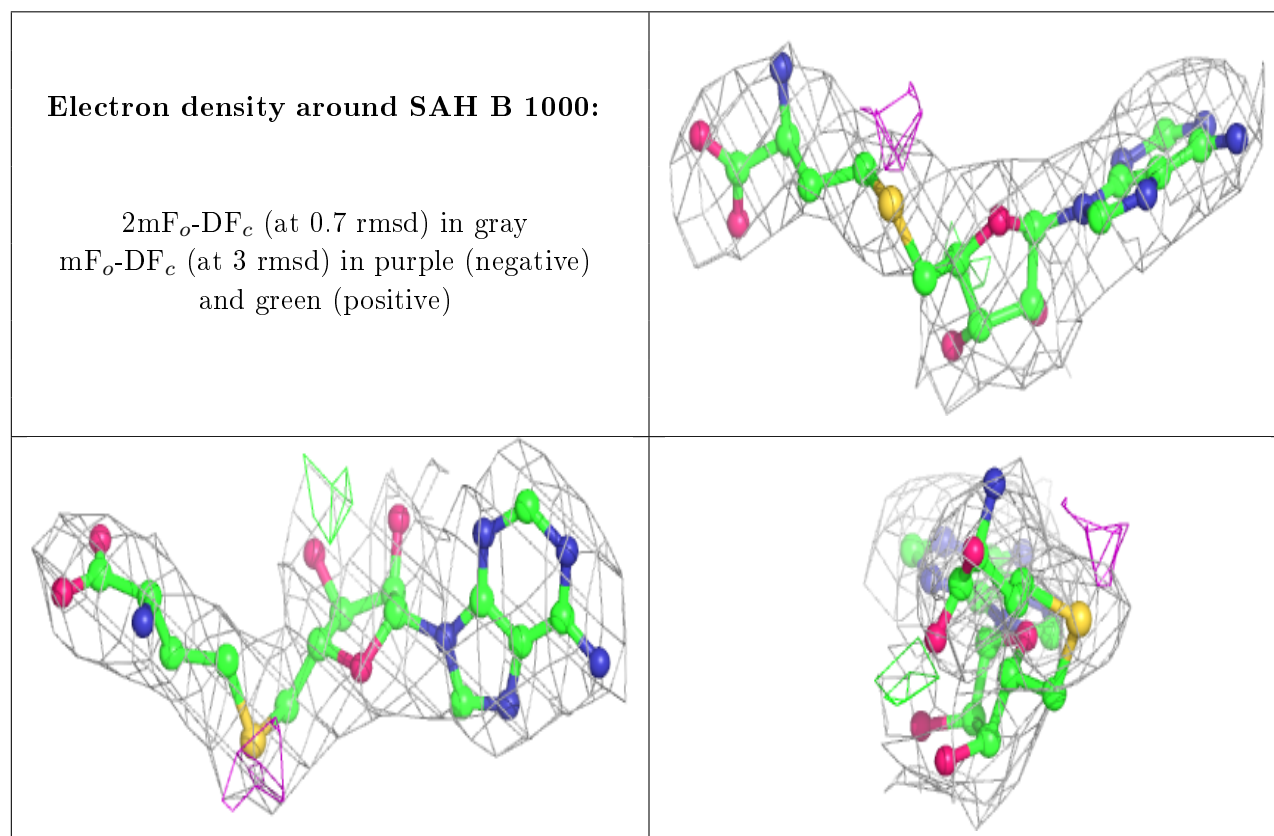
There are no carbohydrates in this entry.

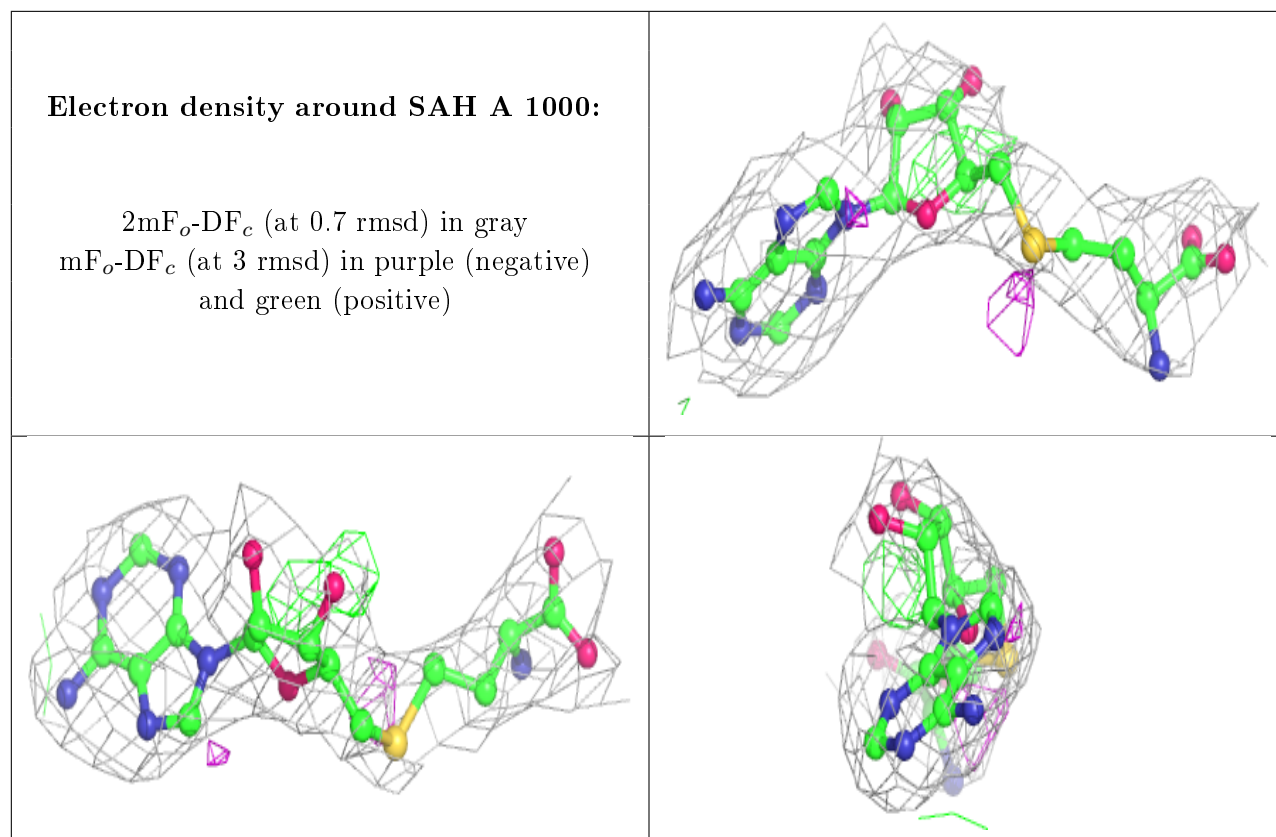
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
3	SAH	B	1000	26/26	0.92	0.23	29,66,105,146	0
3	SAH	A	1000	26/26	0.93	0.22	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.