



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 1VFP / pdb_00001vfp
Title : Crystal structure of the SR CA2+-ATPase with bound AMPPCP
Authors : Toyoshima, C.; Mizutani, T.
Deposited on : 2004-04-18
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

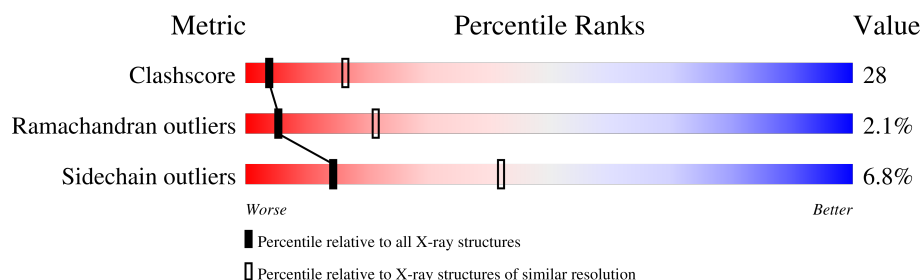
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	
1	B	994	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15418 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	B	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191
B	994	GLY	ASP	SEE REMARK 999	UNP P04191

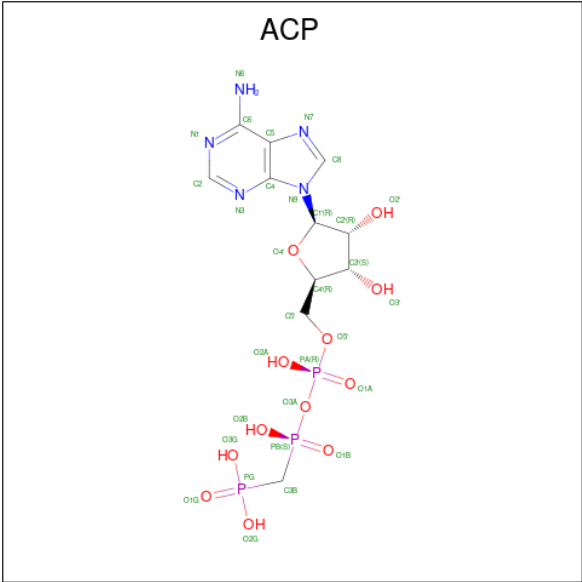
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is water.

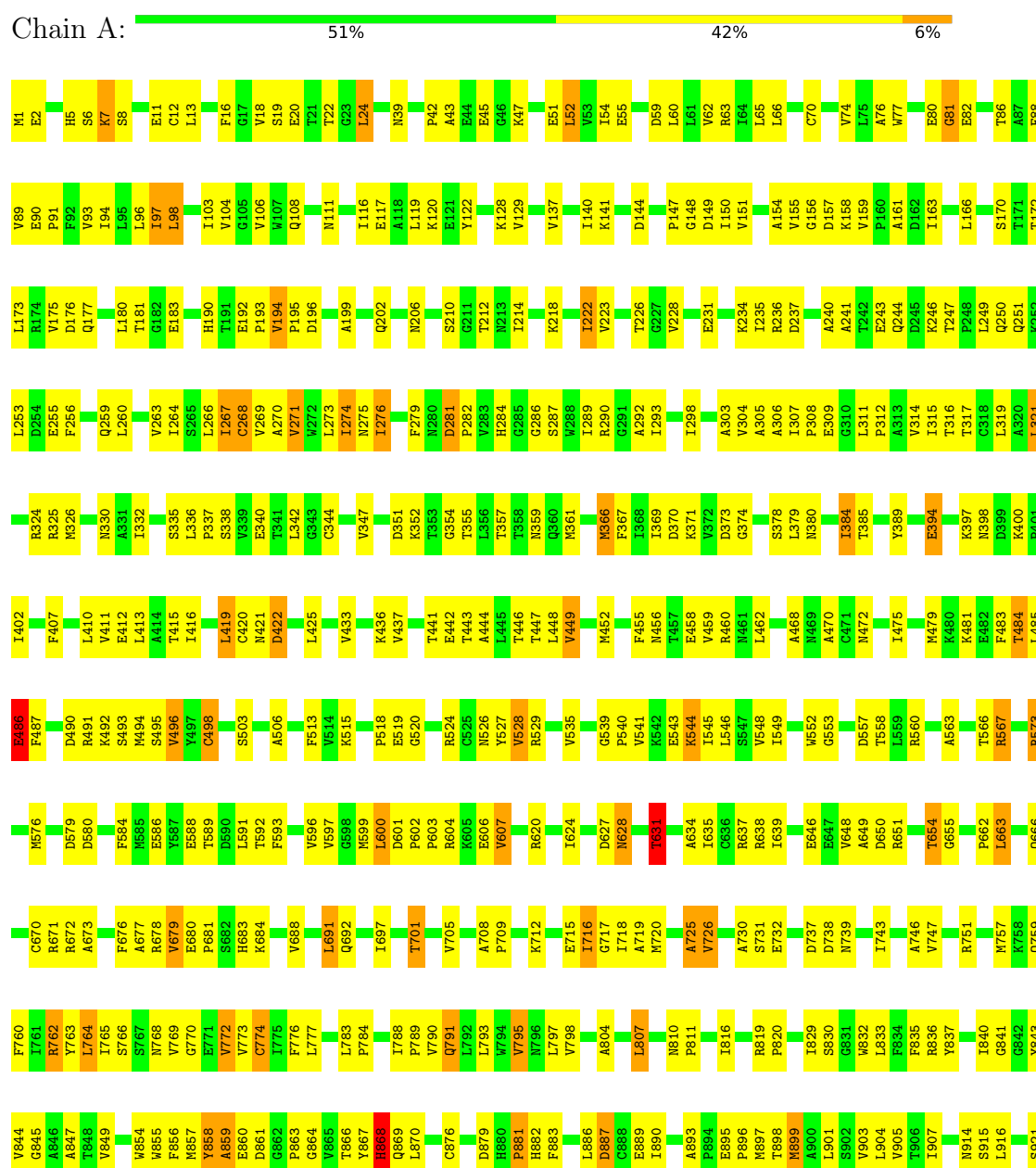
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

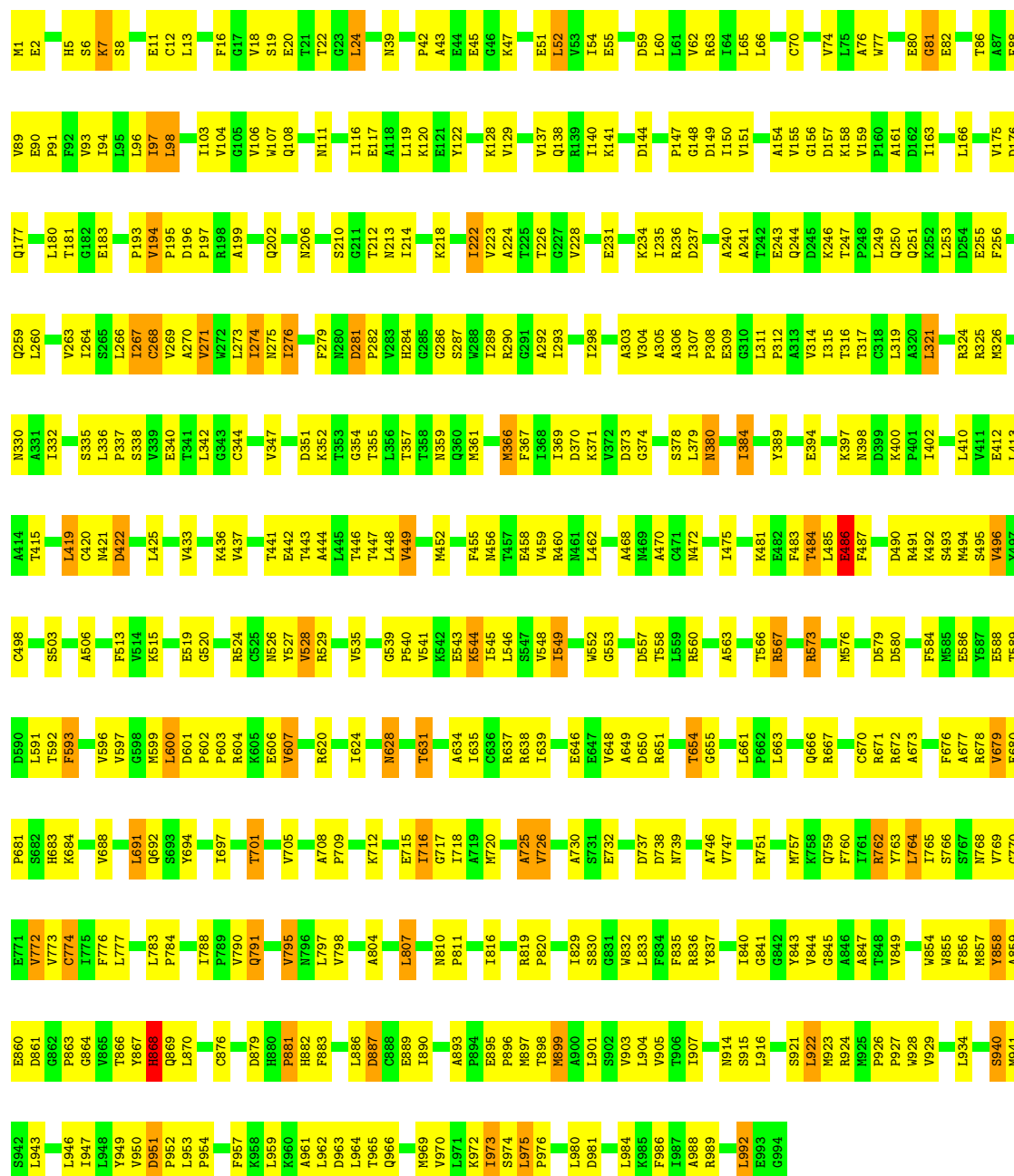
- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain B: 52% 42% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.92Å 123.62Å 151.82Å 90.00° 107.21° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.9 (15.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15418	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACP, MG

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	0.54	6/7812 (0.1%)	0.95	28/10592 (0.3%)
1	B	0.58	5/7812 (0.1%)	0.97	32/10592 (0.3%)
All	All	0.56	11/15624 (0.1%)	0.96	60/21184 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	ASN	CG-OD1	5.70	1.34	1.23
1	B	628	ASN	CG-OD1	5.37	1.33	1.23
1	A	631	THR	CA-CB	5.36	1.62	1.53
1	A	628	ASN	CG-OD1	5.32	1.33	1.23
1	A	421	ASN	CG-OD1	5.31	1.33	1.23
1	A	526	ASN	CG-OD1	5.30	1.33	1.23
1	B	398	ASN	CG-OD1	5.22	1.33	1.23
1	A	259	GLN	CD-OE1	5.21	1.33	1.23
1	B	259	GLN	CD-OE1	5.18	1.33	1.23
1	B	421	ASN	CG-OD1	5.16	1.33	1.23
1	A	398	ASN	CG-OD1	5.14	1.33	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	GLU	N-CA-C	7.72	122.73	113.16
1	A	82	GLU	N-CA-C	7.61	122.60	113.16
1	A	80	GLU	N-CA-C	7.43	121.59	109.85
1	B	80	GLU	N-CA-C	7.42	121.58	109.85
1	A	194	VAL	CA-C-N	7.10	127.09	119.28
1	A	194	VAL	C-N-CA	7.10	127.09	119.28
1	A	539	GLY	CA-C-N	6.67	126.18	119.24
1	A	539	GLY	C-N-CA	6.67	126.18	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	774	CYS	N-CA-C	-6.66	105.69	113.88
1	A	774	CYS	N-CA-C	-6.65	105.70	113.88
1	B	194	VAL	CA-C-N	6.49	126.42	119.28
1	B	194	VAL	C-N-CA	6.49	126.42	119.28
1	A	81	GLY	N-CA-C	6.32	128.17	113.18
1	A	607	VAL	N-CA-C	6.28	116.45	110.42
1	B	81	GLY	N-CA-C	6.27	128.04	113.18
1	A	468	ALA	N-CA-C	6.16	117.66	111.07
1	A	400	LYS	CA-C-N	6.15	126.17	119.90
1	A	400	LYS	C-N-CA	6.15	126.17	119.90
1	B	539	GLY	CA-C-N	6.15	125.63	119.24
1	B	539	GLY	C-N-CA	6.15	125.63	119.24
1	B	468	ALA	N-CA-C	6.12	117.62	111.07
1	A	419	LEU	N-CA-C	6.03	118.75	111.40
1	A	666	GLN	N-CA-C	-5.89	104.78	111.14
1	A	498	CYS	N-CA-C	5.80	118.66	109.50
1	B	861	ASP	N-CA-C	-5.79	106.20	113.20
1	B	490	ASP	N-CA-C	-5.76	104.44	112.45
1	B	607	VAL	N-CA-C	5.73	115.92	110.53
1	A	654	THR	N-CA-C	-5.72	100.08	109.40
1	A	490	ASP	N-CA-C	-5.72	104.50	112.45
1	B	593	PHE	CA-C-N	-5.70	117.39	122.97
1	B	593	PHE	C-N-CA	-5.70	117.39	122.97
1	A	861	ASP	N-CA-C	-5.67	106.34	113.20
1	B	666	GLN	N-CA-C	-5.67	105.02	111.14
1	B	419	LEU	N-CA-C	5.65	118.63	111.69
1	A	725	ALA	N-CA-C	-5.64	104.76	111.69
1	B	654	THR	N-CA-C	-5.64	100.21	109.40
1	A	922	LEU	N-CA-C	-5.62	106.50	113.19
1	B	498	CYS	N-CA-C	5.59	118.34	109.50
1	A	835	PHE	N-CA-C	-5.58	105.12	111.14
1	B	159	VAL	CA-C-N	5.56	125.08	119.19
1	B	159	VAL	C-N-CA	5.56	125.08	119.19
1	B	772	VAL	N-CA-C	-5.56	106.78	111.56
1	B	835	PHE	N-CA-C	-5.54	105.16	111.14
1	B	715	GLU	N-CA-C	-5.51	105.36	111.36
1	B	922	LEU	N-CA-C	-5.49	106.66	113.19
1	A	13	LEU	N-CA-C	-5.47	105.21	111.07
1	A	715	GLU	N-CA-C	-5.40	105.48	111.36
1	B	549	ILE	N-CA-C	-5.40	105.24	110.42
1	B	725	ALA	N-CA-C	-5.34	105.13	111.69
1	B	400	LYS	CA-C-N	5.28	125.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	LYS	C-N-CA	5.28	125.29	119.90
1	A	772	VAL	N-CA-C	-5.27	107.03	111.56
1	A	159	VAL	CA-C-N	5.25	124.75	119.19
1	A	159	VAL	C-N-CA	5.25	124.75	119.19
1	A	546	LEU	N-CA-C	5.23	116.98	111.28
1	B	661	LEU	CA-C-N	-5.20	114.60	119.85
1	B	661	LEU	C-N-CA	-5.20	114.60	119.85
1	B	546	LEU	N-CA-C	5.19	116.94	111.28
1	A	627	ASP	N-CA-C	5.10	116.91	110.33
1	B	13	LEU	N-CA-C	-5.07	105.64	111.07

There are no chirality outliers.

There are no planarity outliers.

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	7671	0	7763	445	0
1	B	7671	0	7763	434	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	1	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	15418	0	15554	876	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 28.

All (876) 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:52:LEU:HB3	1:A:106:VAL:HG23	1.41	1.01
1:B:52:LEU:HB3	1:B:106:VAL:HG23	1.41	1.00
1:B:600:LEU:HD12	1:B:602:PRO:HD3	1.50	0.92
1:B:140:ILE:HD12	1:B:141:LYS:H	1.36	0.90
1:A:773:VAL:HG23	1:A:845:GLY:HA3	1.54	0.90
1:A:246:LYS:HE3	1:A:251:GLN:HG2	1.54	0.89
1:A:600:LEU:HD12	1:A:602:PRO:HD3	1.53	0.89
1:A:573:ARG:HG2	1:A:573:ARG:HH11	1.37	0.88
1:B:246:LYS:HE3	1:B:251:GLN:HG2	1.54	0.87
1:B:773:VAL:HG23	1:B:845:GLY:HA3	1.54	0.87
1:A:963:ASP:HB2	1:A:966:GLN:HG3	1.57	0.86
1:A:952:PRO:HG3	1:B:111:ASN:HD21	1.41	0.86
1:B:573:ARG:HG2	1:B:573:ARG:HH11	1.41	0.84
1:A:140:ILE:HD12	1:A:141:LYS:H	1.41	0.84
1:B:963:ASP:HB2	1:B:966:GLN:HG3	1.58	0.83
1:A:156:GLY:HA2	1:A:726:VAL:CG1	2.07	0.83
1:B:156:GLY:HA2	1:B:726:VAL:CG1	2.09	0.82
1:B:65:LEU:CD2	1:B:309:GLU:HG2	2.09	0.82
1:A:65:LEU:CD2	1:A:309:GLU:HG2	2.10	0.82
1:A:247:THR:HG22	1:A:337:PRO:HG3	1.61	0.82
1:B:770:GLY:HA3	1:B:844:VAL:HG23	1.63	0.81
1:A:287:SER:HB2	1:A:289:ILE:HG22	1.62	0.81
1:A:947:ILE:HA	1:A:953:LEU:HD23	1.62	0.81
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.63	0.81
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.63	0.81
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.63	0.81
1:B:947:ILE:HA	1:B:953:LEU:HD23	1.61	0.81
1:B:558:THR:HG22	1:B:634:ALA:HB1	1.63	0.80
1:A:161:ALA:HA	1:A:210:SER:HB2	1.64	0.80
1:B:287:SER:HB2	1:B:289:ILE:HG22	1.62	0.80
1:B:247:THR:HG22	1:B:337:PRO:HG3	1.62	0.80
1:B:679:VAL:HG22	1:B:683:HIS:CB	2.11	0.80
1:B:903:VAL:HA	1:B:970:VAL:HG13	1.64	0.80
1:B:355:THR:HG23	1:B:720:MET:HE3	1.62	0.79
1:A:355:THR:HG23	1:A:720:MET:HE3	1.62	0.79
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.63	0.79
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.64	0.79
1:A:840:ILE:HD13	1:A:980:LEU:HD23	1.65	0.79
1:B:181:THR:OG1	1:B:183:GLU:HG2	1.83	0.79
1:B:65:LEU:HD22	1:B:309:GLU:HG2	1.65	0.79
1:B:161:ALA:HA	1:B:210:SER:HB2	1.65	0.78
1:A:679:VAL:HG22	1:A:683:HIS:CB	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:VAL:HG12	1:B:907:ILE:HD13	1.66	0.78
1:B:964:LEU:HD12	1:B:964:LEU:H	1.49	0.78
1:B:541:VAL:O	1:B:545:ILE:HG12	1.85	0.77
1:A:65:LEU:HD22	1:A:309:GLU:HG2	1.66	0.77
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.67	0.77
1:A:181:THR:OG1	1:A:183:GLU:HG2	1.85	0.77
1:A:964:LEU:H	1:A:964:LEU:HD12	1.50	0.77
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.67	0.76
1:B:624:ILE:HG21	1:B:684:LYS:HG2	1.67	0.76
1:A:271:VAL:HG22	1:A:776:PHE:HE1	1.50	0.76
1:A:773:VAL:CG2	1:A:845:GLY:HA3	2.15	0.76
1:B:876:CYS:HB3	1:B:883:PHE:CE2	2.21	0.76
1:A:567:ARG:HG2	1:A:591:LEU:HD23	1.68	0.76
1:A:847:ALA:HB1	1:A:973:ILE:HD12	1.68	0.75
1:B:773:VAL:CG2	1:B:845:GLY:HA3	2.15	0.75
1:A:876:CYS:HB3	1:A:883:PHE:CE2	2.20	0.75
1:A:705:VAL:HG12	1:A:726:VAL:CG1	2.17	0.75
1:B:271:VAL:HG22	1:B:776:PHE:HE1	1.50	0.75
1:B:567:ARG:HG2	1:B:591:LEU:HD23	1.68	0.75
1:B:847:ALA:HB1	1:B:973:ILE:HD12	1.67	0.75
1:A:90:GLU:HG2	1:A:790:VAL:HG22	1.68	0.74
1:A:844:VAL:HG12	1:A:907:ILE:HD13	1.67	0.74
1:A:777:LEU:HD23	1:A:777:LEU:O	1.87	0.74
1:B:840:ILE:HD13	1:B:980:LEU:HD23	1.67	0.74
1:A:541:VAL:O	1:A:545:ILE:HG12	1.88	0.74
1:B:90:GLU:HG2	1:B:790:VAL:HG22	1.68	0.74
1:B:129:VAL:HG12	1:B:151:VAL:HG22	1.70	0.74
1:B:777:LEU:O	1:B:777:LEU:HD23	1.87	0.73
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.70	0.73
1:A:705:VAL:HG12	1:A:726:VAL:HG11	1.71	0.73
1:B:549:ILE:HD11	1:B:596:VAL:HG21	1.70	0.73
1:B:705:VAL:HG12	1:B:726:VAL:CG1	2.18	0.73
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.71	0.73
1:B:679:VAL:HG22	1:B:683:HIS:HB3	1.71	0.73
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.70	0.73
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.69	0.73
1:A:855:TRP:O	1:A:859:ALA:HB2	1.89	0.72
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.71	0.72
1:B:495:SER:HB2	1:B:588:GLU:OE1	1.89	0.72
1:B:895:GLU:HB2	1:B:896:PRO:HD3	1.72	0.72
1:A:271:VAL:HG22	1:A:776:PHE:CE1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:TRP:HE1	1:A:858:TYR:HD2	1.38	0.72
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.72	0.72
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.71	0.72
1:A:366:MET:HE2	1:A:448:LEU:HD11	1.71	0.72
1:B:420:CYS:O	1:B:515:LYS:HE2	1.90	0.71
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.25	0.71
1:B:855:TRP:O	1:B:859:ALA:HB2	1.90	0.71
1:B:1:MET:HG3	1:B:2:GLU:N	2.05	0.71
1:B:705:VAL:HG12	1:B:726:VAL:HG11	1.73	0.71
1:B:957:PHE:O	1:B:959:LEU:HG	1.91	0.71
1:B:855:TRP:CE3	1:B:896:PRO:HG3	2.25	0.71
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.91	0.70
1:B:366:MET:HE2	1:B:448:LEU:HD11	1.72	0.70
1:B:271:VAL:HG22	1:B:776:PHE:CE1	2.25	0.70
1:A:895:GLU:HB2	1:A:896:PRO:HD3	1.71	0.70
1:A:957:PHE:O	1:A:959:LEU:HG	1.91	0.70
1:B:96:LEU:HD23	1:B:797:LEU:HD11	1.74	0.70
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.92	0.70
1:A:620:ARG:NH2	1:A:671:ARG:HA	2.06	0.70
1:A:308:PRO:CB	1:A:764:LEU:HD23	2.22	0.70
1:A:840:ILE:HD13	1:A:980:LEU:CD2	2.21	0.69
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.75	0.69
1:A:528:VAL:HG11	1:A:541:VAL:HG11	1.72	0.69
1:A:306:ALA:HA	1:A:768:ASN:HD22	1.57	0.69
1:B:166:LEU:HD11	1:B:222:ILE:HB	1.74	0.69
1:B:628:ASN:HB3	1:B:631:THR:HG23	1.75	0.69
1:B:308:PRO:CB	1:B:764:LEU:HD23	2.22	0.69
1:B:854:TRP:HE1	1:B:858:TYR:HD2	1.39	0.69
1:A:420:CYS:O	1:A:515:LYS:HE2	1.93	0.69
1:B:306:ALA:HA	1:B:768:ASN:ND2	2.08	0.69
1:B:528:VAL:HG11	1:B:541:VAL:HG11	1.72	0.69
1:B:620:ARG:NH2	1:B:671:ARG:HA	2.08	0.68
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.75	0.68
1:A:770:GLY:HA2	1:A:773:VAL:HG22	1.74	0.68
1:A:679:VAL:HG22	1:A:683:HIS:HB3	1.74	0.68
1:B:840:ILE:HD13	1:B:980:LEU:CD2	2.23	0.68
1:A:306:ALA:HA	1:A:768:ASN:ND2	2.08	0.68
1:A:495:SER:HB2	1:A:588:GLU:OE1	1.94	0.68
1:A:628:ASN:HB3	1:A:631:THR:HG23	1.75	0.68
1:B:306:ALA:HA	1:B:768:ASN:HD22	1.57	0.68
1:B:389:TYR:HB3	1:B:425:LEU:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:893:ALA:O	1:B:896:PRO:HD2	1.95	0.67
1:A:96:LEU:HD23	1:A:797:LEU:HD11	1.75	0.67
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.76	0.67
1:B:770:GLY:HA2	1:B:773:VAL:HG22	1.75	0.67
1:B:366:MET:HG2	1:B:384:ILE:HD11	1.77	0.67
1:B:804:ALA:O	1:B:807:LEU:HB2	1.93	0.67
1:B:716:ILE:HD13	1:B:717:GLY:N	2.10	0.66
1:A:308:PRO:HB3	1:A:764:LEU:HD23	1.77	0.66
1:B:86:THR:HG22	1:B:790:VAL:HG21	1.78	0.66
1:A:893:ALA:O	1:A:896:PRO:HD2	1.96	0.66
1:A:716:ILE:HD13	1:A:717:GLY:N	2.11	0.66
1:A:737:ASP:O	1:A:738:ASP:HB2	1.96	0.66
1:B:366:MET:HE1	1:B:452:MET:SD	2.36	0.66
1:B:128:LYS:HD3	1:B:437:VAL:HG13	1.78	0.65
1:B:369:ILE:HD11	1:B:545:ILE:HD11	1.78	0.65
1:A:86:THR:HG22	1:A:790:VAL:HG21	1.78	0.65
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.76	0.65
1:A:65:LEU:HG	1:A:304:VAL:HG13	1.79	0.65
1:A:804:ALA:O	1:A:807:LEU:HB2	1.95	0.65
1:B:90:GLU:CG	1:B:790:VAL:HG22	2.27	0.65
1:A:128:LYS:HD3	1:A:437:VAL:HG13	1.77	0.65
1:A:90:GLU:CG	1:A:790:VAL:HG22	2.27	0.64
1:B:65:LEU:HG	1:B:304:VAL:HG13	1.79	0.64
1:B:308:PRO:HB3	1:B:764:LEU:HD23	1.78	0.64
1:A:1:MET:HG3	1:A:2:GLU:N	2.11	0.64
1:B:163:ILE:CD1	1:B:223:VAL:HG22	2.27	0.64
1:A:42:PRO:HG2	1:A:236:ARG:HH12	1.62	0.64
1:A:163:ILE:CD1	1:A:223:VAL:HG22	2.27	0.64
1:B:737:ASP:OD2	1:B:739:ASN:HB2	1.98	0.64
1:B:156:GLY:HA2	1:B:726:VAL:HG12	1.80	0.64
1:B:449:VAL:HG21	1:B:472:ASN:OD1	1.96	0.64
1:B:276:ILE:HD13	1:B:276:ILE:H	1.62	0.63
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.28	0.63
1:A:553:GLY:O	1:A:558:THR:HA	1.97	0.63
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.81	0.63
1:A:276:ILE:HD13	1:A:276:ILE:H	1.63	0.63
1:A:8:SER:OG	1:A:11:GLU:HG3	1.99	0.63
1:B:335:SER:OG	1:B:337:PRO:HD2	1.99	0.63
1:B:646:GLU:OE1	1:B:651:ARG:NH1	2.32	0.63
1:B:737:ASP:O	1:B:738:ASP:HB2	1.96	0.63
1:A:737:ASP:OD2	1:A:739:ASN:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:O	1:B:212:THR:HB	1.99	0.63
1:B:8:SER:OG	1:B:11:GLU:HG3	1.98	0.63
1:B:42:PRO:HG2	1:B:236:ARG:HH12	1.64	0.63
1:A:864:GLY:HA3	1:A:890:ILE:HD11	1.81	0.62
1:B:864:GLY:HA3	1:B:890:ILE:HD11	1.81	0.62
1:A:335:SER:OG	1:A:337:PRO:HD2	1.99	0.62
1:A:854:TRP:NE1	1:A:858:TYR:HD2	1.98	0.62
1:B:573:ARG:HG2	1:B:573:ARG:NH1	2.14	0.62
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.31	0.62
1:B:916:LEU:CD1	1:B:927:PRO:HA	2.28	0.62
1:A:156:GLY:HA2	1:A:726:VAL:HG12	1.78	0.62
1:B:881:PRO:HG2	1:B:882:HIS:H	1.64	0.62
1:A:352:LYS:HD2	1:A:635:ILE:HD12	1.82	0.62
1:A:573:ARG:HG2	1:A:573:ARG:NH1	2.11	0.62
1:B:352:LYS:HD2	1:B:635:ILE:HD12	1.81	0.62
1:B:553:GLY:O	1:B:558:THR:HA	1.98	0.62
1:A:881:PRO:HG2	1:A:882:HIS:H	1.64	0.62
1:A:51:GLU:O	1:A:54:ILE:HG22	2.01	0.61
1:A:361:MET:CE	1:A:560:ARG:HD3	2.30	0.61
1:B:321:LEU:HD13	1:B:325:ARG:HH22	1.65	0.61
1:B:361:MET:CE	1:B:560:ARG:HD3	2.30	0.61
1:A:810:ASN:ND2	1:A:916:LEU:HA	2.16	0.61
1:B:51:GLU:O	1:B:54:ILE:HG22	2.00	0.61
1:A:42:PRO:HG2	1:A:236:ARG:NH1	2.15	0.60
1:B:854:TRP:NE1	1:B:858:TYR:HD2	1.98	0.60
1:A:366:MET:CE	1:A:448:LEU:HD11	2.31	0.60
1:A:65:LEU:HD21	1:A:309:GLU:HG2	1.84	0.60
1:A:486:GLU:O	1:A:491:ARG:NH2	2.33	0.60
1:B:819:ARG:HG3	1:B:820:PRO:HD2	1.84	0.60
1:B:975:LEU:N	1:B:976:PRO:HD2	2.16	0.60
1:A:975:LEU:N	1:A:976:PRO:HD2	2.15	0.60
1:B:24:LEU:HD22	1:B:149:ASP:HB3	1.83	0.60
1:B:243:GLU:HG2	1:B:244:GLN:N	2.16	0.60
1:B:273:LEU:O	1:B:276:ILE:HG23	2.02	0.60
1:B:402:ILE:C	1:B:402:ILE:HD12	2.27	0.60
1:A:243:GLU:HG2	1:A:244:GLN:N	2.17	0.60
1:A:273:LEU:O	1:A:276:ILE:HG23	2.02	0.60
1:A:321:LEU:HD13	1:A:325:ARG:HH22	1.67	0.60
1:B:366:MET:CE	1:B:448:LEU:HD11	2.31	0.60
1:B:810:ASN:ND2	1:B:916:LEU:HA	2.17	0.60
1:A:249:LEU:HD22	1:A:340:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:HG2	1:B:236:ARG:NH1	2.17	0.60
1:B:357:THR:HA	1:B:603:PRO:HA	1.84	0.59
1:A:156:GLY:HA2	1:A:726:VAL:HG11	1.85	0.59
1:A:176:ASP:O	1:A:212:THR:HB	2.00	0.59
1:B:1:MET:HE1	1:B:7:LYS:HZ3	1.67	0.59
1:B:604:ARG:HB2	1:B:607:VAL:HG23	1.83	0.59
1:A:819:ARG:HG3	1:A:820:PRO:HD2	1.83	0.59
1:B:486:GLU:O	1:B:491:ARG:NH2	2.35	0.59
1:B:119:LEU:HB3	1:B:332:ILE:HD11	1.83	0.59
1:B:442:GLU:HG2	1:B:515:LYS:NZ	2.18	0.59
1:B:624:ILE:CG2	1:B:684:LYS:HG2	2.32	0.59
1:A:351:ASP:O	1:A:355:THR:HB	2.01	0.59
1:A:788:ILE:HG23	1:A:897:MET:HE1	1.85	0.59
1:B:836:ARG:HD3	1:B:984:LEU:HD13	1.85	0.59
1:B:351:ASP:O	1:B:355:THR:HB	2.03	0.59
1:A:357:THR:HA	1:A:603:PRO:HA	1.85	0.59
1:B:24:LEU:HD22	1:B:149:ASP:CB	2.33	0.59
1:B:70:CYS:O	1:B:74:VAL:HG23	2.02	0.59
1:B:947:ILE:HD12	1:B:953:LEU:HD23	1.85	0.59
1:B:65:LEU:HD21	1:B:309:GLU:HG2	1.83	0.58
1:B:788:ILE:HG23	1:B:897:MET:HE1	1.84	0.58
1:A:181:THR:HB	1:A:202:GLN:HG2	1.86	0.58
1:A:442:GLU:HG2	1:A:515:LYS:NZ	2.18	0.58
1:A:449:VAL:HG21	1:A:472:ASN:OD1	2.03	0.58
1:A:326:MET:CE	1:A:746:ALA:HB2	2.34	0.58
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.86	0.58
1:B:783:LEU:HB3	1:B:784:PRO:HD2	1.85	0.58
1:A:458:GLU:HA	1:A:460:ARG:HH12	1.69	0.58
1:B:458:GLU:HA	1:B:460:ARG:HH12	1.68	0.58
1:A:716:ILE:HD13	1:A:716:ILE:C	2.28	0.58
1:B:140:ILE:CD1	1:B:141:LYS:H	2.12	0.58
1:B:147:PRO:HA	1:B:223:VAL:HG12	1.86	0.58
1:B:1:MET:HE1	1:B:7:LYS:NZ	2.18	0.58
1:B:596:VAL:HG12	1:B:597:VAL:N	2.18	0.58
1:B:249:LEU:HD22	1:B:340:GLU:HG3	1.84	0.58
1:B:716:ILE:HD13	1:B:716:ILE:C	2.29	0.58
1:B:757:MET:HE2	1:B:757:MET:HA	1.86	0.58
1:A:20:GLU:HA	1:A:150:ILE:HG12	1.85	0.58
1:A:119:LEU:HB3	1:A:332:ILE:HD11	1.86	0.58
1:B:51:GLU:O	1:B:55:GLU:HG3	2.04	0.58
1:B:963:ASP:C	1:B:965:THR:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:C	1:A:275:ASN:H	2.12	0.57
1:A:757:MET:HE2	1:A:757:MET:HA	1.86	0.57
1:B:361:MET:HE2	1:B:599:MET:SD	2.44	0.57
1:B:515:LYS:O	1:B:515:LYS:HG3	2.03	0.57
1:B:760:PHE:HA	1:B:807:LEU:HD23	1.86	0.57
1:A:70:CYS:O	1:A:74:VAL:HG23	2.04	0.57
1:A:974:SER:C	1:A:976:PRO:HD2	2.29	0.57
1:A:51:GLU:O	1:A:55:GLU:HG3	2.04	0.57
1:A:76:ALA:HB1	1:A:88:PHE:CD1	2.40	0.57
1:B:1:MET:HG3	1:B:2:GLU:H	1.68	0.57
1:B:326:MET:CE	1:B:746:ALA:HB2	2.33	0.57
1:A:347:VAL:HG11	1:A:691:LEU:HD21	1.87	0.57
1:A:947:ILE:HD12	1:A:953:LEU:HD23	1.87	0.57
1:A:963:ASP:C	1:A:965:THR:H	2.10	0.57
1:B:844:VAL:HG12	1:B:907:ILE:CD1	2.33	0.57
1:A:788:ILE:HG12	1:A:791:GLN:HB2	1.86	0.57
1:B:181:THR:HB	1:B:202:GLN:HG2	1.87	0.57
1:B:24:LEU:HB2	1:B:149:ASP:HB3	1.87	0.57
1:B:156:GLY:HA2	1:B:726:VAL:HG11	1.87	0.57
1:B:788:ILE:HG12	1:B:791:GLN:HB2	1.86	0.57
1:B:86:THR:CG2	1:B:790:VAL:HG21	2.35	0.56
1:B:315:ILE:HG23	1:B:316:THR:N	2.20	0.56
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.36	0.56
1:A:836:ARG:HD3	1:A:984:LEU:HD13	1.86	0.56
1:B:354:GLY:HA2	1:B:359:ASN:HB2	1.87	0.56
1:B:701:THR:HG23	1:B:718:ILE:HB	1.88	0.56
1:B:974:SER:C	1:B:976:PRO:HD2	2.30	0.56
1:A:515:LYS:O	1:A:515:LYS:HG3	2.03	0.56
1:A:903:VAL:HG22	1:A:970:VAL:HG13	1.87	0.56
1:B:119:LEU:HD23	1:B:332:ILE:HD13	1.87	0.56
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.36	0.56
1:A:628:ASN:HB3	1:A:631:THR:CG2	2.35	0.56
1:B:76:ALA:HB1	1:B:88:PHE:CD1	2.40	0.56
1:B:266:LEU:C	1:B:268:CYS:H	2.14	0.56
1:B:903:VAL:HG22	1:B:970:VAL:HG13	1.87	0.56
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.87	0.56
1:A:266:LEU:C	1:A:268:CYS:H	2.14	0.56
1:A:402:ILE:C	1:A:402:ILE:HD12	2.30	0.56
1:A:86:THR:CG2	1:A:790:VAL:HG21	2.36	0.56
1:A:760:PHE:HA	1:A:807:LEU:HD23	1.87	0.56
1:B:20:GLU:HA	1:B:150:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:ILE:HD12	1:B:953:LEU:CD2	2.36	0.56
1:A:330:ASN:HB2	1:A:737:ASP:HB2	1.87	0.56
1:A:620:ARG:HH22	1:A:671:ARG:HA	1.70	0.56
1:B:247:THR:O	1:B:251:GLN:HG3	2.06	0.56
1:B:330:ASN:HB2	1:B:737:ASP:HB2	1.88	0.56
1:B:147:PRO:HA	1:B:223:VAL:CG1	2.35	0.56
1:B:273:LEU:C	1:B:275:ASN:H	2.13	0.56
1:B:281:ASP:OD1	1:B:282:PRO:HD2	2.06	0.56
1:B:584:PHE:N	1:B:584:PHE:CD2	2.72	0.56
1:B:810:ASN:HD22	1:B:916:LEU:HA	1.71	0.56
1:A:222:ILE:HD13	1:A:223:VAL:N	2.20	0.56
1:B:140:ILE:HD12	1:B:141:LYS:N	2.13	0.56
1:A:161:ALA:CA	1:A:210:SER:HB2	2.35	0.55
1:B:140:ILE:HD11	1:B:144:ASP:OD2	2.06	0.55
1:A:810:ASN:HD22	1:A:916:LEU:HA	1.70	0.55
1:A:24:LEU:HB2	1:A:149:ASP:HB3	1.88	0.55
1:A:952:PRO:HG3	1:B:111:ASN:ND2	2.17	0.55
1:A:1:MET:HE1	1:A:7:LYS:NZ	2.22	0.55
1:A:140:ILE:HD12	1:A:141:LYS:N	2.17	0.55
1:A:763:TYR:HB2	1:A:915:SER:OG	2.06	0.55
1:B:161:ALA:CA	1:B:210:SER:HB2	2.37	0.55
1:B:975:LEU:O	1:B:975:LEU:HD13	2.06	0.55
1:B:347:VAL:HG11	1:B:691:LEU:HD21	1.89	0.55
1:B:436:LYS:CB	1:B:443:THR:HG21	2.36	0.55
1:B:843:TYR:OH	1:B:976:PRO:HG2	2.07	0.55
1:A:158:LYS:HE2	1:A:725:ALA:HB1	1.89	0.54
1:B:867:TYR:HD2	1:B:868:HIS:CE1	2.25	0.54
1:A:111:ASN:HB3	1:A:324:ARG:NE	2.22	0.54
1:A:119:LEU:HD23	1:A:332:ILE:HD13	1.89	0.54
1:A:315:ILE:HG23	1:A:316:THR:N	2.22	0.54
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.90	0.54
1:A:247:THR:O	1:A:251:GLN:HG3	2.07	0.54
1:A:811:PRO:HG2	1:A:929:VAL:HG12	1.90	0.54
1:B:947:ILE:HD11	1:B:957:PHE:CE1	2.43	0.54
1:A:281:ASP:OD1	1:A:282:PRO:HD2	2.07	0.54
1:A:947:ILE:HD12	1:A:953:LEU:CD2	2.37	0.54
1:B:491:ARG:NH1	1:B:588:GLU:OE1	2.40	0.54
1:B:951:ASP:HB3	1:B:952:PRO:HD3	1.89	0.54
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.89	0.54
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.89	0.54
1:B:111:ASN:HB3	1:B:324:ARG:NE	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASP:HA	1:B:240:ALA:O	2.08	0.54
1:B:326:MET:HE2	1:B:746:ALA:HB2	1.90	0.54
1:A:705:VAL:HG12	1:A:726:VAL:HG13	1.90	0.54
1:B:620:ARG:HH22	1:B:671:ARG:HA	1.73	0.54
1:B:628:ASN:HB3	1:B:631:THR:CG2	2.37	0.54
1:A:237:ASP:HA	1:A:240:ALA:O	2.07	0.53
1:A:361:MET:HE1	1:A:560:ARG:HD3	1.90	0.53
1:A:436:LYS:CB	1:A:443:THR:HG21	2.38	0.53
1:B:222:ILE:HD13	1:B:223:VAL:N	2.23	0.53
1:A:24:LEU:HD22	1:A:149:ASP:CB	2.38	0.53
1:B:763:TYR:HB2	1:B:915:SER:OG	2.07	0.53
1:A:688:VAL:O	1:A:692:GLN:HG3	2.09	0.53
1:A:867:TYR:HD2	1:A:868:HIS:CE1	2.26	0.53
1:B:158:LYS:HE2	1:B:725:ALA:HB1	1.90	0.53
1:B:688:VAL:O	1:B:692:GLN:HG3	2.08	0.53
1:A:338:SER:OG	1:A:732:GLU:HB3	2.08	0.53
1:A:366:MET:HE3	1:A:384:ILE:HD12	1.89	0.53
1:A:584:PHE:CD2	1:A:584:PHE:N	2.72	0.53
1:B:491:ARG:O	1:B:492:LYS:HB2	2.09	0.53
1:A:326:MET:HE2	1:A:746:ALA:HB2	1.89	0.53
1:A:879:ASP:OD1	1:A:881:PRO:HD3	2.09	0.53
1:B:679:VAL:HG22	1:B:683:HIS:HB2	1.89	0.53
1:A:515:LYS:O	4:A:1001:ACP:H2	2.09	0.53
1:A:844:VAL:HG12	1:A:907:ILE:CD1	2.35	0.53
1:A:235:ILE:O	1:A:240:ALA:HB3	2.08	0.53
1:A:947:ILE:HD11	1:A:957:PHE:CE1	2.44	0.53
1:B:366:MET:HE3	1:B:384:ILE:HD12	1.90	0.53
1:B:545:ILE:O	1:B:549:ILE:HG12	2.09	0.53
1:A:975:LEU:HD13	1:A:975:LEU:O	2.09	0.53
1:B:367:PHE:HD1	1:B:552:TRP:CH2	2.26	0.53
1:B:6:SER:HA	1:B:194:VAL:O	2.09	0.53
1:B:338:SER:OG	1:B:732:GLU:HB3	2.08	0.53
1:B:235:ILE:O	1:B:240:ALA:HB3	2.10	0.52
1:B:361:MET:HE1	1:B:560:ARG:HD3	1.90	0.52
1:B:895:GLU:O	1:B:899:MET:HB2	2.09	0.52
1:A:321:LEU:O	1:A:325:ARG:HG3	2.08	0.52
1:B:879:ASP:OD1	1:B:881:PRO:HD3	2.09	0.52
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.41	0.52
1:A:807:LEU:HD21	1:A:915:SER:CB	2.39	0.52
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.39	0.52
1:B:635:ILE:O	1:B:639:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:TYR:C	1:B:869:GLN:H	2.17	0.52
1:A:76:ALA:HB1	1:A:88:PHE:CE1	2.45	0.52
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.09	0.52
1:A:712:LYS:HG3	1:A:730:ALA:HB1	1.91	0.52
1:B:119:LEU:HB3	1:B:332:ILE:CD1	2.40	0.52
1:B:903:VAL:HG23	1:B:970:VAL:HG22	1.92	0.52
1:A:6:SER:HA	1:A:194:VAL:O	2.10	0.52
1:B:712:LYS:HG3	1:B:730:ALA:HB1	1.92	0.52
1:A:491:ARG:O	1:A:492:LYS:HB2	2.10	0.51
1:A:867:TYR:C	1:A:869:GLN:H	2.17	0.51
1:B:276:ILE:H	1:B:276:ILE:CD1	2.23	0.51
1:B:389:TYR:HA	1:B:447:THR:HG21	1.92	0.51
1:B:515:LYS:O	4:B:2001:ACP:H2	2.10	0.51
1:B:705:VAL:HG12	1:B:726:VAL:HG13	1.90	0.51
1:A:701:THR:HG23	1:A:718:ILE:HB	1.92	0.51
1:A:596:VAL:HG12	1:A:597:VAL:N	2.23	0.51
1:B:389:TYR:O	1:B:447:THR:CG2	2.59	0.51
1:B:637:ARG:HG2	1:B:637:ARG:HH11	1.76	0.51
1:B:76:ALA:HB1	1:B:88:PHE:CE1	2.45	0.51
1:B:950:VAL:O	1:B:954:PRO:HD2	2.11	0.51
1:B:484:THR:HB	1:B:496:VAL:HG22	1.92	0.51
1:B:485:LEU:HB2	1:B:495:SER:HB3	1.92	0.51
1:B:963:ASP:C	1:B:965:THR:N	2.69	0.51
1:A:903:VAL:HG23	1:A:970:VAL:HG22	1.91	0.51
1:A:963:ASP:C	1:A:965:THR:N	2.69	0.51
1:B:777:LEU:HD22	1:B:849:VAL:HG21	1.93	0.51
1:B:540:PRO:O	1:B:543:GLU:HB3	2.10	0.51
1:B:276:ILE:HA	1:B:279:PHE:CE2	2.45	0.51
1:B:903:VAL:HA	1:B:970:VAL:CG1	2.39	0.51
1:A:243:GLU:HG2	1:A:244:GLN:H	1.75	0.51
1:A:540:PRO:O	1:A:543:GLU:HB3	2.11	0.51
1:A:768:ASN:O	1:A:772:VAL:HG23	2.11	0.51
1:A:276:ILE:H	1:A:276:ILE:CD1	2.24	0.50
1:B:24:LEU:HD22	1:B:149:ASP:N	2.26	0.50
1:A:367:PHE:HD1	1:A:552:TRP:CH2	2.29	0.50
1:B:811:PRO:HG2	1:B:929:VAL:HG12	1.92	0.50
1:B:807:LEU:HD21	1:B:915:SER:CB	2.41	0.50
1:A:276:ILE:HA	1:A:279:PHE:CE2	2.46	0.50
1:A:389:TYR:HA	1:A:447:THR:HG21	1.93	0.50
1:B:243:GLU:HG2	1:B:244:GLN:H	1.75	0.50
1:B:342:LEU:O	1:B:747:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:THR:HG22	1:A:962:LEU:CD1	2.42	0.50
1:A:903:VAL:HA	1:A:970:VAL:CG1	2.39	0.50
1:B:768:ASN:O	1:B:772:VAL:HG23	2.11	0.50
1:B:772:VAL:C	1:B:774:CYS:H	2.20	0.50
1:A:867:TYR:O	1:A:869:GLN:N	2.45	0.50
1:A:950:VAL:HB	1:A:953:LEU:HD22	1.94	0.50
1:B:214:ILE:HD12	1:B:214:ILE:N	2.27	0.50
1:B:361:MET:CE	1:B:599:MET:HG3	2.41	0.50
1:A:19:SER:HB2	1:A:22:THR:HB	1.93	0.50
1:A:140:ILE:HD11	1:A:144:ASP:OD2	2.12	0.50
1:A:260:LEU:O	1:A:264:ILE:HG12	2.12	0.50
1:A:679:VAL:HG22	1:A:683:HIS:HB2	1.91	0.50
1:B:276:ILE:HD13	1:B:276:ILE:N	2.27	0.50
1:B:762:ARG:HG2	1:B:837:TYR:HE1	1.77	0.50
1:A:60:LEU:O	1:A:63:ARG:HB2	2.12	0.50
1:A:950:VAL:O	1:A:954:PRO:HD2	2.12	0.50
1:B:19:SER:HB2	1:B:22:THR:HB	1.93	0.50
1:A:361:MET:HE2	1:A:560:ARG:HD3	1.94	0.49
1:A:772:VAL:C	1:A:774:CYS:H	2.19	0.49
1:B:797:LEU:HD23	1:B:797:LEU:C	2.37	0.49
1:A:119:LEU:HD21	1:A:330:ASN:HA	1.94	0.49
1:B:558:THR:HG22	1:B:634:ALA:CB	2.40	0.49
1:A:545:ILE:O	1:A:549:ILE:HG12	2.11	0.49
1:B:60:LEU:O	1:B:63:ARG:HB2	2.12	0.49
1:B:670:CYS:HB3	1:B:691:LEU:HD13	1.94	0.49
1:A:286:GLY:HA3	1:A:290:ARG:HD3	1.95	0.49
1:A:436:LYS:HB3	1:A:443:THR:HG21	1.95	0.49
1:A:795:VAL:HG22	1:A:901:LEU:HD11	1.94	0.49
1:A:798:VAL:HG13	1:A:940:SER:OG	2.12	0.49
1:A:103:ILE:HA	1:A:106:VAL:HG12	1.94	0.49
1:A:762:ARG:HG2	1:A:837:TYR:HE1	1.77	0.49
1:B:158:LYS:NZ	1:B:213:ASN:OD1	2.41	0.49
1:B:769:VAL:HB	1:B:841:GLY:HA3	1.95	0.49
1:B:89:VAL:O	1:B:93:VAL:HG23	2.12	0.49
1:B:306:ALA:CA	1:B:768:ASN:HD22	2.25	0.49
1:B:795:VAL:HG22	1:B:901:LEU:HD11	1.93	0.49
1:A:1:MET:HE1	1:A:7:LYS:HZ3	1.78	0.49
1:B:419:LEU:HD12	1:B:513:PHE:CE2	2.48	0.49
1:B:898:THR:HG22	1:B:962:LEU:CD1	2.42	0.49
1:A:119:LEU:HB3	1:A:332:ILE:CD1	2.42	0.49
1:A:163:ILE:HD12	1:A:223:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:O	1:A:747:VAL:HG22	2.13	0.49
1:A:366:MET:HE1	1:A:452:MET:SD	2.53	0.49
1:B:361:MET:HE2	1:B:560:ARG:HD3	1.94	0.49
1:B:389:TYR:O	1:B:447:THR:HG22	2.12	0.49
1:B:867:TYR:O	1:B:869:GLN:N	2.45	0.49
1:A:270:ALA:O	1:A:274:ILE:HG12	2.13	0.48
1:A:777:LEU:HD22	1:A:849:VAL:HG21	1.95	0.48
1:B:193:PRO:HA	1:B:206:ASN:ND2	2.28	0.48
1:A:1:MET:HG3	1:A:2:GLU:H	1.74	0.48
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.96	0.48
1:A:276:ILE:HD13	1:A:276:ILE:N	2.28	0.48
1:A:361:MET:HE2	1:A:599:MET:SD	2.53	0.48
1:A:459:VAL:HA	1:A:462:LEU:HD12	1.94	0.48
1:B:286:GLY:HA3	1:B:290:ARG:HD3	1.94	0.48
1:A:24:LEU:HD22	1:A:149:ASP:N	2.28	0.48
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.28	0.48
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.27	0.48
1:B:764:LEU:O	1:B:768:ASN:HB2	2.12	0.48
1:B:811:PRO:HG2	1:B:929:VAL:CG1	2.44	0.48
1:A:218:LYS:HD2	1:A:422:ASP:OD2	2.13	0.48
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.95	0.48
1:A:952:PRO:HG2	1:B:107:TRP:NE1	2.29	0.48
1:B:163:ILE:HD11	1:B:223:VAL:HG22	1.95	0.48
1:A:140:ILE:CD1	1:A:141:LYS:H	2.18	0.48
1:A:764:LEU:O	1:A:768:ASN:HB2	2.14	0.48
1:B:52:LEU:HB3	1:B:106:VAL:CG2	2.30	0.48
1:B:97:ILE:HD13	1:B:97:ILE:O	2.13	0.48
1:A:1:MET:HB2	1:A:16:PHE:CZ	2.49	0.48
1:A:52:LEU:HB3	1:A:106:VAL:CG2	2.29	0.48
1:B:231:GLU:OE1	1:B:231:GLU:HA	2.13	0.48
1:A:317:THR:O	1:A:321:LEU:HB2	2.14	0.48
1:A:797:LEU:C	1:A:797:LEU:HD23	2.39	0.48
1:B:119:LEU:HD21	1:B:330:ASN:HA	1.96	0.48
1:B:765:ILE:O	1:B:769:VAL:HG23	2.13	0.48
1:B:966:GLN:O	1:B:969:MET:HB3	2.14	0.48
1:A:231:GLU:OE1	1:A:231:GLU:HA	2.13	0.48
1:A:788:ILE:HG12	1:A:791:GLN:CD	2.39	0.48
1:B:1:MET:HB2	1:B:16:PHE:CZ	2.49	0.48
1:B:436:LYS:HB3	1:B:443:THR:HG21	1.95	0.48
1:B:446:THR:HG23	1:B:472:ASN:ND2	2.28	0.48
1:A:306:ALA:CA	1:A:768:ASN:HD22	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:THR:O	1:B:321:LEU:HB2	2.13	0.48
1:B:459:VAL:HA	1:B:462:LEU:HD12	1.95	0.48
1:A:97:ILE:HD13	1:A:97:ILE:O	2.14	0.47
1:A:370:ASP:HB3	1:A:378:SER:OG	2.14	0.47
1:A:557:ASP:O	1:A:558:THR:C	2.56	0.47
1:A:765:ILE:O	1:A:769:VAL:HG23	2.14	0.47
1:A:769:VAL:HB	1:A:841:GLY:HA3	1.96	0.47
1:A:895:GLU:O	1:A:899:MET:HB2	2.13	0.47
1:B:218:LYS:HD2	1:B:422:ASP:OD2	2.13	0.47
1:B:321:LEU:O	1:B:325:ARG:HG3	2.13	0.47
1:B:412:GLU:CD	1:B:529:ARG:HH11	2.22	0.47
1:B:557:ASP:O	1:B:558:THR:C	2.57	0.47
1:A:864:GLY:CA	1:A:890:ILE:HD11	2.44	0.47
1:B:260:LEU:O	1:B:264:ILE:HG12	2.14	0.47
1:A:549:ILE:CD1	1:A:596:VAL:HG11	2.44	0.47
1:A:303:ALA:O	1:A:307:ILE:HG12	2.13	0.47
1:B:39:ASN:OD1	1:B:226:THR:HB	2.14	0.47
1:B:654:THR:HA	1:B:677:ALA:O	2.15	0.47
1:B:832:TRP:CE2	1:B:988:ALA:HB2	2.49	0.47
1:B:487:PHE:HB2	1:B:494:MET:HE3	1.97	0.47
1:B:679:VAL:CG2	1:B:683:HIS:HB3	2.44	0.47
1:B:886:LEU:O	1:B:887:ASP:C	2.57	0.47
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.50	0.47
1:B:303:ALA:O	1:B:307:ILE:HG12	2.14	0.47
1:B:519:GLU:OE2	1:B:678:ARG:NH1	2.47	0.47
1:B:788:ILE:HG12	1:B:791:GLN:CD	2.40	0.47
1:A:266:LEU:C	1:A:268:CYS:N	2.72	0.47
1:A:279:PHE:CE1	1:A:292:ALA:HA	2.50	0.47
1:A:870:LEU:HD12	1:A:870:LEU:N	2.30	0.47
1:A:886:LEU:O	1:A:887:ASP:C	2.57	0.47
1:A:898:THR:HG22	1:A:962:LEU:HD11	1.96	0.47
1:B:270:ALA:O	1:B:274:ILE:HG12	2.14	0.47
1:B:321:LEU:HD22	1:B:325:ARG:CZ	2.44	0.47
1:B:361:MET:HB2	1:B:444:ALA:HB2	1.97	0.47
1:B:527:TYR:O	1:B:592:THR:HA	2.15	0.47
1:B:856:PHE:O	1:B:866:THR:HG22	2.15	0.47
1:A:832:TRP:CE2	1:A:988:ALA:HB2	2.49	0.47
1:B:336:LEU:HB2	1:B:337:PRO:HD3	1.97	0.47
1:B:701:THR:HA	1:B:718:ILE:O	2.15	0.47
1:B:798:VAL:HG13	1:B:940:SER:OG	2.15	0.47
1:B:870:LEU:N	1:B:870:LEU:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:O	1:B:155:VAL:C	2.58	0.47
1:B:970:VAL:C	1:B:972:LYS:H	2.23	0.47
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.97	0.46
1:A:361:MET:HG3	1:A:441:THR:HA	1.97	0.46
1:A:485:LEU:HB2	1:A:495:SER:HB3	1.96	0.46
1:A:986:PHE:HA	1:A:989:ARG:HH21	1.81	0.46
1:B:155:VAL:HA	1:B:214:ILE:HG22	1.97	0.46
1:B:379:LEU:CD1	1:B:544:LYS:HD2	2.44	0.46
1:B:858:TYR:CG	1:B:858:TYR:O	2.68	0.46
1:A:321:LEU:HD22	1:A:325:ARG:CZ	2.45	0.46
1:B:266:LEU:C	1:B:268:CYS:N	2.73	0.46
1:B:371:LYS:HE2	1:B:373:ASP:HB2	1.96	0.46
1:A:371:LYS:HE2	1:A:373:ASP:HB2	1.96	0.46
1:A:379:LEU:CD1	1:A:544:LYS:HD2	2.45	0.46
1:A:389:TYR:O	1:A:447:THR:CG2	2.63	0.46
1:B:579:ASP:CG	1:B:580:ASP:N	2.74	0.46
1:B:898:THR:HG22	1:B:962:LEU:HD11	1.96	0.46
1:B:904:LEU:O	1:B:907:ILE:HG22	2.15	0.46
1:A:579:ASP:CG	1:A:580:ASP:N	2.74	0.46
1:A:973:ILE:HD13	1:A:973:ILE:O	2.16	0.46
1:B:103:ILE:HA	1:B:106:VAL:HG12	1.96	0.46
1:B:950:VAL:HB	1:B:953:LEU:HD22	1.96	0.46
1:A:214:ILE:N	1:A:214:ILE:HD12	2.30	0.46
1:B:103:ILE:HG23	1:B:104:VAL:N	2.31	0.46
1:B:864:GLY:CA	1:B:890:ILE:HD11	2.46	0.46
1:B:928:TRP:HA	1:B:934:LEU:HD11	1.96	0.46
1:B:947:ILE:HD12	1:B:953:LEU:HG	1.97	0.46
1:A:264:ILE:HD12	1:A:306:ALA:HB1	1.98	0.46
1:A:484:THR:HB	1:A:496:VAL:HG22	1.98	0.46
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.98	0.46
1:A:858:TYR:CG	1:A:858:TYR:O	2.67	0.46
1:B:857:MET:HE1	1:B:868:HIS:H	1.81	0.46
1:A:249:LEU:O	1:A:253:LEU:HG	2.16	0.46
1:A:412:GLU:CD	1:A:529:ARG:HH11	2.24	0.46
1:A:654:THR:HA	1:A:677:ALA:O	2.14	0.46
1:A:856:PHE:O	1:A:866:THR:HG22	2.15	0.46
1:A:924:ARG:O	1:A:926:PRO:HD3	2.16	0.46
1:B:680:GLU:HB3	1:B:681:PRO:HD2	1.98	0.46
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.45	0.46
1:A:970:VAL:C	1:A:972:LYS:H	2.23	0.46
1:B:279:PHE:CE1	1:B:292:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:O	1:A:63:ARG:HG3	2.15	0.46
1:A:194:VAL:O	1:A:194:VAL:HG13	2.16	0.46
1:A:458:GLU:HG2	1:A:460:ARG:HH12	1.81	0.46
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.98	0.46
1:B:116:ILE:HG22	1:B:120:LYS:HE3	1.98	0.46
1:B:344:CYS:HB2	1:B:697:ILE:HG13	1.98	0.46
1:A:103:ILE:HG23	1:A:104:VAL:N	2.31	0.46
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.97	0.46
1:A:788:ILE:CG2	1:A:897:MET:HE1	2.45	0.46
1:A:904:LEU:O	1:A:907:ILE:HG22	2.16	0.46
1:A:966:GLN:O	1:A:969:MET:HB3	2.15	0.46
1:B:59:ASP:O	1:B:63:ARG:HG3	2.16	0.46
1:B:832:TRP:NE1	1:B:988:ALA:HB2	2.30	0.46
1:B:973:ILE:HD13	1:B:973:ILE:O	2.15	0.46
1:A:784:PRO:HG3	1:A:856:PHE:HE1	1.81	0.45
1:B:359:ASN:N	1:B:601:ASP:OD1	2.49	0.45
1:B:986:PHE:HA	1:B:989:ARG:HH21	1.80	0.45
1:A:366:MET:HE3	1:A:384:ILE:CD1	2.46	0.45
1:B:890:ILE:HG12	1:B:890:ILE:O	2.15	0.45
1:A:361:MET:CE	1:A:599:MET:HG3	2.45	0.45
1:B:584:PHE:N	1:B:584:PHE:HD2	2.15	0.45
1:B:788:ILE:CG2	1:B:897:MET:HE1	2.45	0.45
1:A:890:ILE:O	1:A:890:ILE:HG12	2.17	0.45
1:A:947:ILE:HD12	1:A:953:LEU:HG	1.97	0.45
1:B:905:VAL:HG12	1:B:941:MET:HE1	1.98	0.45
1:A:635:ILE:O	1:A:639:ILE:HG12	2.15	0.45
1:A:947:ILE:HD12	1:A:953:LEU:CG	2.47	0.45
1:B:596:VAL:CG1	1:B:597:VAL:N	2.79	0.45
1:A:103:ILE:HG23	1:A:104:VAL:H	1.82	0.45
1:A:558:THR:HG22	1:A:634:ALA:CB	2.40	0.45
1:A:807:LEU:HD21	1:A:915:SER:HB3	1.98	0.45
1:A:914:ASN:HB3	1:A:981:ASP:OD1	2.17	0.45
1:B:163:ILE:HD12	1:B:223:VAL:HG22	1.96	0.45
1:B:515:LYS:HA	1:B:563:ALA:O	2.17	0.45
1:A:116:ILE:HG22	1:A:120:LYS:HE3	1.97	0.45
1:A:751:ARG:C	1:A:816:ILE:HD11	2.42	0.45
1:A:857:MET:HE1	1:A:868:HIS:H	1.82	0.45
1:B:344:CYS:O	1:B:697:ILE:HB	2.17	0.45
1:B:947:ILE:HD12	1:B:953:LEU:CG	2.46	0.45
1:A:89:VAL:O	1:A:93:VAL:HG23	2.17	0.45
1:A:527:TYR:O	1:A:592:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:TRP:NE1	1:A:988:ALA:HB2	2.31	0.45
1:B:379:LEU:HD11	1:B:544:LYS:HD2	1.98	0.45
1:A:491:ARG:HD2	1:A:493:SER:OG	2.17	0.45
1:A:528:VAL:HG12	1:A:593:PHE:HB3	1.99	0.45
1:B:314:VAL:HG13	1:B:757:MET:HE1	1.98	0.45
1:B:355:THR:CG2	1:B:720:MET:HE3	2.42	0.45
1:A:39:ASN:OD1	1:A:226:THR:HB	2.17	0.45
1:A:311:LEU:HA	1:A:314:VAL:HG12	1.99	0.45
1:B:119:LEU:HD21	1:B:330:ASN:C	2.41	0.45
1:B:264:ILE:HD12	1:B:306:ALA:HB1	1.99	0.45
1:A:119:LEU:HD21	1:A:330:ASN:C	2.42	0.44
1:A:264:ILE:HD13	1:A:267:ILE:HD11	2.00	0.44
1:A:487:PHE:HB2	1:A:494:MET:HE3	1.99	0.44
1:A:503:SER:HA	1:A:506:ALA:HB2	1.99	0.44
1:B:830:SER:OG	1:B:833:LEU:HD13	2.17	0.44
1:A:52:LEU:O	1:A:55:GLU:HB2	2.17	0.44
1:A:163:ILE:HD11	1:A:223:VAL:HG22	1.99	0.44
1:A:175:VAL:HG12	1:A:176:ASP:N	2.31	0.44
1:A:389:TYR:O	1:A:447:THR:HG22	2.17	0.44
1:A:701:THR:HA	1:A:718:ILE:O	2.18	0.44
1:A:777:LEU:HD23	1:A:777:LEU:C	2.42	0.44
1:B:249:LEU:O	1:B:253:LEU:HG	2.17	0.44
1:B:528:VAL:HG12	1:B:593:PHE:HB3	2.00	0.44
1:B:549:ILE:CD1	1:B:596:VAL:HG11	2.48	0.44
1:B:751:ARG:HB3	1:B:816:ILE:HD11	1.99	0.44
1:A:545:ILE:HD12	1:A:593:PHE:CE1	2.53	0.44
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.99	0.44
1:B:103:ILE:HG23	1:B:104:VAL:H	1.82	0.44
1:B:412:GLU:OE2	1:B:566:THR:HG21	2.17	0.44
1:B:604:ARG:HB2	1:B:607:VAL:CG2	2.47	0.44
1:B:777:LEU:HD23	1:B:777:LEU:C	2.41	0.44
1:A:311:LEU:O	1:A:314:VAL:HG12	2.18	0.44
1:B:361:MET:HG3	1:B:441:THR:HA	1.97	0.44
1:B:520:GLY:O	1:B:524:ARG:HG3	2.18	0.44
1:B:807:LEU:HD21	1:B:915:SER:HB3	1.98	0.44
1:A:314:VAL:HG13	1:A:757:MET:HE1	1.99	0.44
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.17	0.44
1:A:602:PRO:HA	1:A:603:PRO:HD2	1.91	0.44
1:A:795:VAL:HG22	1:A:901:LEU:CD1	2.48	0.44
1:A:975:LEU:N	1:A:976:PRO:CD	2.80	0.44
1:B:380:ASN:HD22	1:B:380:ASN:HA	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ILE:HD12	1:B:593:PHE:CE1	2.52	0.44
1:A:326:MET:HE1	1:A:746:ALA:HB2	2.00	0.44
1:A:361:MET:HB2	1:A:444:ALA:HB2	1.99	0.44
1:A:515:LYS:HA	1:A:563:ALA:O	2.17	0.44
1:A:528:VAL:HG23	1:A:535:VAL:CG2	2.48	0.44
1:A:866:THR:OG1	1:A:867:TYR:N	2.51	0.44
1:A:648:VAL:C	1:A:650:ASP:H	2.26	0.44
1:B:1:MET:CG	1:B:2:GLU:N	2.79	0.44
1:B:314:VAL:HG22	1:B:757:MET:HE1	1.99	0.44
1:B:483:PHE:HZ	1:B:576:MET:HE1	1.83	0.44
1:B:914:ASN:HB3	1:B:981:ASP:OD1	2.18	0.44
1:A:352:LYS:HD2	1:A:635:ILE:CD1	2.48	0.44
1:A:624:ILE:CG2	1:A:679:VAL:HG11	2.48	0.44
1:B:784:PRO:HG3	1:B:856:PHE:HE1	1.82	0.44
1:B:975:LEU:N	1:B:976:PRO:CD	2.81	0.44
1:A:263:VAL:O	1:A:267:ILE:HG12	2.17	0.44
1:A:503:SER:HA	1:A:506:ALA:CB	2.48	0.44
1:A:648:VAL:C	1:A:650:ASP:N	2.76	0.44
1:B:5:HIS:CD2	1:B:194:VAL:HG13	2.53	0.44
1:B:273:LEU:O	1:B:276:ILE:HD12	2.18	0.44
1:B:458:GLU:HG2	1:B:460:ARG:HH12	1.82	0.44
1:A:90:GLU:N	1:A:91:PRO:HD2	2.33	0.43
1:A:379:LEU:HD11	1:A:544:LYS:HD2	2.00	0.43
1:A:916:LEU:HD11	1:A:927:PRO:HA	2.00	0.43
1:B:175:VAL:HG12	1:B:176:ASP:N	2.33	0.43
1:B:370:ASP:HB3	1:B:378:SER:OG	2.18	0.43
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.18	0.43
1:A:637:ARG:HG2	1:A:637:ARG:HH11	1.83	0.43
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.73	0.43
1:B:45:GLU:O	1:B:47:LYS:HG3	2.18	0.43
1:B:148:GLY:HA2	1:B:222:ILE:HD11	2.00	0.43
1:B:263:VAL:O	1:B:267:ILE:HG12	2.18	0.43
1:B:751:ARG:C	1:B:816:ILE:HD11	2.42	0.43
1:A:45:GLU:O	1:A:47:LYS:HG3	2.18	0.43
1:A:719:ALA:HB2	1:A:731:SER:OG	2.19	0.43
1:B:766:SER:HB2	1:B:840:ILE:HB	2.00	0.43
1:B:503:SER:HA	1:B:506:ALA:HB2	1.99	0.43
1:B:795:VAL:HG22	1:B:901:LEU:CD1	2.47	0.43
1:B:866:THR:OG1	1:B:867:TYR:N	2.51	0.43
1:B:970:VAL:C	1:B:972:LYS:N	2.76	0.43
1:A:483:PHE:HZ	1:A:576:MET:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLU:O	1:A:589:THR:HG22	2.18	0.43
1:B:52:LEU:O	1:B:55:GLU:HB2	2.19	0.43
1:B:924:ARG:O	1:B:926:PRO:HD3	2.18	0.43
1:A:170:SER:HB2	1:A:486:GLU:HG2	2.00	0.43
1:A:330:ASN:CB	1:A:737:ASP:HB2	2.48	0.43
1:B:311:LEU:HA	1:B:314:VAL:HG12	2.00	0.43
1:B:366:MET:HE3	1:B:384:ILE:CD1	2.49	0.43
1:A:62:VAL:O	1:A:66:LEU:HB2	2.18	0.43
1:A:177:GLN:HB3	1:A:212:THR:HG21	2.01	0.43
1:A:986:PHE:CA	1:A:989:ARG:HH21	2.32	0.43
1:B:264:ILE:HD13	1:B:267:ILE:HD11	1.99	0.43
1:B:315:ILE:CG2	1:B:316:THR:N	2.82	0.43
1:B:624:ILE:CG2	1:B:679:VAL:HG11	2.49	0.43
1:B:887:ASP:C	1:B:889:GLU:H	2.26	0.43
1:A:5:HIS:CD2	1:A:194:VAL:HG13	2.53	0.43
1:A:654:THR:O	1:A:655:GLY:C	2.62	0.43
1:B:503:SER:HA	1:B:506:ALA:CB	2.49	0.43
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.86	0.43
1:A:519:GLU:OE2	1:A:678:ARG:NH1	2.52	0.43
1:A:970:VAL:C	1:A:972:LYS:N	2.75	0.43
1:B:90:GLU:N	1:B:91:PRO:HD2	2.34	0.43
1:B:389:TYR:CA	1:B:447:THR:HG21	2.48	0.43
1:B:449:VAL:HG21	1:B:472:ASN:CG	2.43	0.43
1:B:491:ARG:HD2	1:B:493:SER:OG	2.18	0.43
1:A:273:LEU:O	1:A:276:ILE:HD12	2.18	0.43
1:A:766:SER:HB2	1:A:840:ILE:HB	2.00	0.43
1:A:830:SER:OG	1:A:833:LEU:HD13	2.18	0.43
1:B:62:VAL:O	1:B:66:LEU:HB2	2.19	0.43
1:B:855:TRP:CZ3	1:B:896:PRO:HG3	2.54	0.43
1:A:89:VAL:O	1:A:90:GLU:C	2.62	0.42
1:A:336:LEU:N	1:A:337:PRO:CD	2.82	0.42
1:A:344:CYS:O	1:A:697:ILE:HB	2.19	0.42
1:A:705:VAL:CG1	1:A:726:VAL:HG11	2.45	0.42
1:B:986:PHE:CA	1:B:989:ARG:HH21	2.32	0.42
1:B:586:GLU:O	1:B:589:THR:HG22	2.18	0.42
1:B:870:LEU:HD12	1:B:870:LEU:H	1.84	0.42
1:B:988:ALA:CA	1:B:992:LEU:HD12	2.42	0.42
1:A:234:LYS:C	1:A:236:ARG:H	2.27	0.42
1:A:269:VAL:O	1:A:273:LEU:HG	2.19	0.42
1:A:355:THR:CG2	1:A:720:MET:HE3	2.41	0.42
1:A:520:GLY:O	1:A:524:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASP:OD2	1:A:672:ARG:HD2	2.19	0.42
1:B:269:VAL:O	1:B:273:LEU:HG	2.19	0.42
1:B:943:LEU:HD12	1:B:943:LEU:HA	1.85	0.42
1:A:256:PHE:CE1	1:A:829:ILE:HD11	2.54	0.42
1:A:359:ASN:N	1:A:601:ASP:OD1	2.50	0.42
1:B:455:PHE:O	1:B:456:ASN:C	2.62	0.42
1:B:606:GLU:HG3	1:B:739:ASN:OD1	2.20	0.42
1:B:648:VAL:C	1:B:650:ASP:H	2.27	0.42
1:B:673:ALA:HB3	1:B:676:PHE:CZ	2.54	0.42
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.50	0.42
1:A:701:THR:HG21	1:A:743:ILE:HD11	2.02	0.42
1:A:887:ASP:C	1:A:889:GLU:H	2.26	0.42
1:A:904:LEU:HD12	1:A:904:LEU:HA	1.89	0.42
1:B:326:MET:HE1	1:B:746:ALA:HB2	1.99	0.42
1:B:650:ASP:OD2	1:B:672:ARG:HD2	2.19	0.42
1:A:870:LEU:HD12	1:A:870:LEU:H	1.84	0.42
1:B:289:ILE:O	1:B:293:ILE:HG13	2.19	0.42
1:B:691:LEU:HD12	1:B:691:LEU:HA	1.72	0.42
1:A:284:HIS:C	1:A:286:GLY:H	2.28	0.42
1:A:810:ASN:HA	1:A:811:PRO:HD3	1.89	0.42
1:A:905:VAL:HG12	1:A:941:MET:HE1	2.00	0.42
1:A:949:TYR:N	1:A:949:TYR:CD1	2.88	0.42
1:B:234:LYS:C	1:B:236:ARG:H	2.27	0.42
1:B:271:VAL:HA	1:B:274:ILE:HG12	2.01	0.42
1:B:330:ASN:CB	1:B:737:ASP:HB2	2.49	0.42
1:A:18:VAL:HG21	1:A:24:LEU:CD1	2.50	0.42
1:A:397:LYS:HB3	1:A:402:ILE:HG21	2.01	0.42
1:A:544:LYS:O	1:A:545:ILE:C	2.63	0.42
1:B:1:MET:HB3	1:B:224:ALA:O	2.20	0.42
1:B:18:VAL:HG21	1:B:24:LEU:CD1	2.49	0.42
1:B:140:ILE:CG1	1:B:141:LYS:N	2.82	0.42
1:B:986:PHE:HA	1:B:989:ARG:HE	1.85	0.42
1:A:158:LYS:HE2	1:A:158:LYS:HB2	1.83	0.42
1:A:247:THR:OG1	1:A:250:GLN:HB2	2.20	0.42
1:B:410:LEU:HD23	1:B:410:LEU:HA	1.89	0.42
1:A:344:CYS:HB2	1:A:697:ILE:HG13	2.00	0.42
1:A:455:PHE:O	1:A:456:ASN:C	2.62	0.42
1:A:481:LYS:HG3	1:A:496:VAL:HG13	2.01	0.42
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.54	0.42
1:B:379:LEU:CD1	1:B:548:VAL:HG21	2.50	0.42
1:B:654:THR:O	1:B:655:GLY:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ALA:O	1:A:155:VAL:C	2.62	0.41
1:A:289:ILE:O	1:A:293:ILE:HG13	2.20	0.41
1:A:458:GLU:HA	1:A:460:ARG:NH1	2.33	0.41
1:B:94:ILE:O	1:B:97:ILE:HG22	2.19	0.41
1:B:177:GLN:HB3	1:B:212:THR:HG21	2.01	0.41
1:B:311:LEU:O	1:B:314:VAL:HG12	2.19	0.41
1:B:361:MET:SD	1:B:601:ASP:HB2	2.59	0.41
1:A:94:ILE:O	1:A:97:ILE:HG22	2.20	0.41
1:A:194:VAL:HA	1:A:195:PRO:HD2	1.79	0.41
1:A:266:LEU:O	1:A:268:CYS:N	2.53	0.41
1:A:273:LEU:C	1:A:275:ASN:N	2.77	0.41
1:A:314:VAL:HG22	1:A:757:MET:HE1	2.02	0.41
1:A:347:VAL:HG11	1:A:691:LEU:CD2	2.49	0.41
1:B:305:ALA:O	1:B:768:ASN:ND2	2.53	0.41
1:B:949:TYR:N	1:B:949:TYR:CD1	2.87	0.41
1:A:783:LEU:HD22	1:A:870:LEU:HB3	2.02	0.41
1:A:986:PHE:HA	1:A:989:ARG:HE	1.84	0.41
1:B:66:LEU:HD13	1:B:98:LEU:HD23	2.02	0.41
1:B:194:VAL:O	1:B:194:VAL:HG13	2.19	0.41
1:B:336:LEU:N	1:B:337:PRO:CD	2.83	0.41
1:B:458:GLU:HA	1:B:460:ARG:NH1	2.33	0.41
1:A:315:ILE:CG2	1:A:316:THR:N	2.83	0.41
1:A:412:GLU:OE2	1:A:529:ARG:NH1	2.53	0.41
1:A:624:ILE:HG22	1:A:679:VAL:HG11	2.02	0.41
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.90	0.41
1:A:1:MET:HE1	1:A:12:CYS:HA	2.01	0.41
1:A:148:GLY:HA2	1:A:222:ILE:HD11	2.02	0.41
1:A:573:ARG:NH1	1:A:573:ARG:CG	2.78	0.41
1:A:648:VAL:O	1:A:650:ASP:N	2.53	0.41
1:A:762:ARG:NH2	1:A:836:ARG:NH1	2.69	0.41
1:B:89:VAL:O	1:B:90:GLU:C	2.63	0.41
1:B:247:THR:OG1	1:B:250:GLN:HB2	2.20	0.41
1:B:347:VAL:HG11	1:B:691:LEU:CD2	2.50	0.41
1:B:481:LYS:HG3	1:B:496:VAL:HG13	2.02	0.41
1:B:624:ILE:HG22	1:B:679:VAL:HG11	2.02	0.41
1:A:94:ILE:HG12	1:A:793:LEU:HD22	2.03	0.41
1:A:271:VAL:HA	1:A:274:ILE:HG12	2.01	0.41
1:A:857:MET:HB2	1:A:858:TYR:H	1.66	0.41
1:B:284:HIS:C	1:B:286:GLY:H	2.28	0.41
1:B:964:LEU:H	1:B:964:LEU:CD1	2.26	0.41
1:A:154:ALA:N	1:A:157:ASP:OD2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:VAL:HG23	1:B:535:VAL:CG2	2.51	0.41
1:B:783:LEU:HD22	1:B:870:LEU:HB3	2.03	0.41
1:A:305:ALA:O	1:A:768:ASN:ND2	2.54	0.41
1:A:361:MET:SD	1:A:601:ASP:HB2	2.59	0.41
1:A:385:THR:HG1	1:A:394:GLU:H	1.68	0.41
1:A:389:TYR:CA	1:A:447:THR:HG21	2.50	0.41
1:A:483:PHE:HZ	1:A:576:MET:CE	2.33	0.41
1:B:648:VAL:C	1:B:650:ASP:N	2.77	0.41
1:B:903:VAL:CG2	1:B:970:VAL:HG13	2.51	0.41
1:A:66:LEU:HD13	1:A:98:LEU:HD23	2.03	0.41
1:A:379:LEU:HD12	1:A:548:VAL:HG21	2.03	0.41
1:A:407:PHE:O	1:A:411:VAL:HG23	2.21	0.41
1:A:415:THR:HA	1:A:475:ILE:HG21	2.02	0.41
1:A:584:PHE:N	1:A:584:PHE:HD2	2.15	0.41
1:A:596:VAL:CG1	1:A:597:VAL:N	2.83	0.41
1:A:716:ILE:C	1:A:716:ILE:CD1	2.94	0.41
1:A:903:VAL:CG2	1:A:970:VAL:HG13	2.50	0.41
1:B:195:PRO:O	1:B:197:PRO:HD3	2.20	0.41
1:B:196:ASP:HB3	1:B:199:ALA:HB2	2.03	0.41
1:B:266:LEU:O	1:B:268:CYS:N	2.54	0.41
1:B:579:ASP:CG	1:B:580:ASP:H	2.29	0.41
1:B:667:ARG:HG2	1:B:694:TYR:CE2	2.56	0.41
1:B:916:LEU:HD11	1:B:927:PRO:HA	2.01	0.41
1:B:921:SER:C	1:B:923:MET:H	2.29	0.41
1:A:172:THR:HG22	1:A:173:LEU:N	2.36	0.41
1:A:192:GLU:H	1:A:192:GLU:HG3	1.69	0.41
1:A:479:MET:HE3	1:A:498:CYS:HB3	2.03	0.41
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.86	0.41
1:A:921:SER:HB2	1:A:989:ARG:HH12	1.85	0.41
1:B:256:PHE:CE1	1:B:829:ILE:HD11	2.55	0.41
1:B:602:PRO:HA	1:B:603:PRO:HD2	1.92	0.41
1:B:836:ARG:HD3	1:B:984:LEU:CD1	2.50	0.41
1:A:807:LEU:HA	1:A:810:ASN:OD1	2.21	0.40
1:B:369:ILE:HD11	1:B:545:ILE:CD1	2.50	0.40
1:A:579:ASP:CG	1:A:580:ASP:H	2.29	0.40
1:A:964:LEU:H	1:A:964:LEU:CD1	2.27	0.40
1:B:154:ALA:N	1:B:157:ASP:OD2	2.45	0.40
1:B:415:THR:HA	1:B:475:ILE:HG21	2.03	0.40
1:B:648:VAL:O	1:B:650:ASP:N	2.53	0.40
1:B:921:SER:HB2	1:B:989:ARG:HH12	1.86	0.40
1:A:379:LEU:CD1	1:A:548:VAL:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE1	1:B:12:CYS:HA	2.02	0.40
1:B:287:SER:HB2	1:B:289:ILE:CG2	2.42	0.40
1:B:397:LYS:HB3	1:B:402:ILE:HG21	2.02	0.40
1:A:190:HIS:O	1:A:206:ASN:HA	2.20	0.40
1:A:662:PRO:O	1:A:663:LEU:C	2.65	0.40
1:A:772:VAL:C	1:A:774:CYS:N	2.79	0.40
1:B:86:THR:HG22	1:B:86:THR:O	2.22	0.40
1:B:807:LEU:HA	1:B:810:ASN:OD1	2.21	0.40
1:A:1:MET:CG	1:A:2:GLU:N	2.83	0.40
1:A:673:ALA:HB3	1:A:676:PHE:CZ	2.55	0.40
1:A:988:ALA:O	1:A:993:GLU:HG2	2.21	0.40
1:B:412:GLU:OE2	1:B:529:ARG:NH1	2.54	0.40
1:B:513:PHE:HD1	1:B:566:THR:HG22	1.87	0.40
1:B:762:ARG:NH2	1:B:836:ARG:NH1	2.69	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	992/994 (100%)	875 (88%)	95 (10%)	22 (2%)	5	20
1	B	992/994 (100%)	878 (88%)	94 (10%)	20 (2%)	6	22
All	All	1984/1988 (100%)	1753 (88%)	189 (10%)	42 (2%)	5	21

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	TYR
1	A	486	GLU
1	A	860	GLU
1	A	881	PRO

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Mol	Chain	Res	Type
1	A	951	ASP
1	A	992	LEU
1	B	122	TYR
1	B	486	GLU
1	B	860	GLU
1	B	881	PRO
1	B	951	ASP
1	B	992	LEU
1	A	274	ILE
1	A	858	TYR
1	A	868	HIS
1	B	274	ILE
1	B	858	TYR
1	B	868	HIS
1	A	470	ALA
1	A	649	ALA
1	A	887	ASP
1	A	961	ALA
1	B	470	ALA
1	B	649	ALA
1	B	887	ASP
1	B	961	ALA
1	A	241	ALA
1	A	859	ALA
1	B	241	ALA
1	A	43	ALA
1	A	267	ILE
1	A	573	ARG
1	B	43	ALA
1	B	267	ILE
1	B	573	ARG
1	A	81	GLY
1	B	81	GLY
1	A	374	GLY
1	B	374	GLY
1	B	863	PRO
1	A	789	PRO
1	A	863	PRO

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	840/840 (100%)	782 (93%)	58 (7%)	14	41
1	B	840/840 (100%)	783 (93%)	57 (7%)	14	42
All	All	1680/1680 (100%)	1565 (93%)	115 (7%)	14	42

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	24	LEU
1	A	52	LEU
1	A	77	TRP
1	A	97	ILE
1	A	98	LEU
1	A	108	GLN
1	A	117	GLU
1	A	137	VAL
1	A	180	LEU
1	A	222	ILE
1	A	228	VAL
1	A	255	GLU
1	A	268	CYS
1	A	271	VAL
1	A	276	ILE
1	A	281	ASP
1	A	298	ILE
1	A	319	LEU
1	A	321	LEU
1	A	366	MET
1	A	380	ASN
1	A	384	ILE
1	A	394	GLU
1	A	413	LEU
1	A	422	ASP
1	A	433	VAL

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Mol	Chain	Res	Type
1	A	449	VAL
1	A	484	THR
1	A	486	GLU
1	A	496	VAL
1	A	518	PRO
1	A	528	VAL
1	A	544	LYS
1	A	567	ARG
1	A	600	LEU
1	A	631	THR
1	A	638	ARG
1	A	663	LEU
1	A	679	VAL
1	A	691	LEU
1	A	701	THR
1	A	716	ILE
1	A	726	VAL
1	A	759	GLN
1	A	762	ARG
1	A	764	LEU
1	A	791	GLN
1	A	795	VAL
1	A	807	LEU
1	A	868	HIS
1	A	899	MET
1	A	922	LEU
1	A	940	SER
1	A	946	LEU
1	A	947	ILE
1	A	973	ILE
1	A	975	LEU
1	B	7	LYS
1	B	24	LEU
1	B	52	LEU
1	B	77	TRP
1	B	97	ILE
1	B	98	LEU
1	B	108	GLN
1	B	117	GLU
1	B	137	VAL
1	B	138	GLN
1	B	180	LEU

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Mol	Chain	Res	Type
1	B	222	ILE
1	B	228	VAL
1	B	255	GLU
1	B	268	CYS
1	B	271	VAL
1	B	276	ILE
1	B	281	ASP
1	B	298	ILE
1	B	319	LEU
1	B	321	LEU
1	B	366	MET
1	B	380	ASN
1	B	384	ILE
1	B	394	GLU
1	B	413	LEU
1	B	422	ASP
1	B	433	VAL
1	B	449	VAL
1	B	484	THR
1	B	486	GLU
1	B	496	VAL
1	B	528	VAL
1	B	544	LYS
1	B	567	ARG
1	B	600	LEU
1	B	631	THR
1	B	638	ARG
1	B	663	LEU
1	B	679	VAL
1	B	691	LEU
1	B	701	THR
1	B	716	ILE
1	B	726	VAL
1	B	759	GLN
1	B	762	ARG
1	B	764	LEU
1	B	791	GLN
1	B	795	VAL
1	B	807	LEU
1	B	868	HIS
1	B	899	MET
1	B	922	LEU

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Mol	Chain	Res	Type
1	B	940	SER
1	B	946	LEU
1	B	973	ILE
1	B	975	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	32	HIS
1	A	108	GLN
1	A	111	ASN
1	A	114	ASN
1	A	138	GLN
1	A	190	HIS
1	A	244	GLN
1	A	280	ASN
1	A	359	ASN
1	A	380	ASN
1	A	398	ASN
1	A	612	GLN
1	A	755	ASN
1	A	869	GLN
1	A	875	GLN
1	A	919	ASN
1	A	920	GLN
1	B	5	HIS
1	B	32	HIS
1	B	108	GLN
1	B	111	ASN
1	B	114	ASN
1	B	138	GLN
1	B	190	HIS
1	B	244	GLN
1	B	280	ASN
1	B	359	ASN
1	B	380	ASN
1	B	398	ASN
1	B	612	GLN
1	B	706	ASN
1	B	755	ASN
1	B	869	GLN

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Mol	Chain	Res	Type
1	B	875	GLN
1	B	919	ASN
1	B	920	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACP	B	2001	3	31,33,33	2.01	7 (22%)	47,52,52	1.80	8 (17%)
4	ACP	A	1001	3	31,33,33	1.93	8 (25%)	47,52,52	1.76	8 (17%)

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
4	ACP	B	2001	3	-	0/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	A	1001	3	-	0/19/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	ACP	PB-O3A	7.12	1.66	1.58
4	A	1001	ACP	PB-O3A	6.17	1.65	1.58
4	B	2001	ACP	PB-O2B	-4.11	1.46	1.56
4	B	2001	ACP	C5-N7	-3.81	1.32	1.39
4	A	1001	ACP	PB-O2B	-3.68	1.47	1.56
4	A	1001	ACP	C5-N7	-3.52	1.32	1.39
4	B	2001	ACP	C1'-N9	2.71	1.53	1.46
4	A	1001	ACP	C1'-N9	2.70	1.53	1.46
4	A	1001	ACP	PG-O2G	-2.41	1.49	1.55
4	B	2001	ACP	PA-O3A	2.39	1.62	1.59
4	A	1001	ACP	C2'-C1'	-2.25	1.46	1.53
4	A	1001	ACP	C2-N3	2.19	1.37	1.33
4	B	2001	ACP	PG-O1G	2.11	1.54	1.50
4	B	2001	ACP	C2'-C1'	-2.01	1.47	1.53
4	A	1001	ACP	C4-N3	2.00	1.38	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	ACP	C5'-C4'-C3'	-5.18	96.57	115.21
4	B	2001	ACP	C5'-C4'-C3'	-5.11	96.82	115.21
4	A	1001	ACP	O5'-C5'-C4'	4.82	125.41	108.99
4	B	2001	ACP	O5'-C5'-C4'	4.76	125.21	108.99
4	A	1001	ACP	O1B-PB-C3B	-3.89	98.80	109.05
4	B	2001	ACP	N3-C2-N1	-3.54	123.23	128.58
4	B	2001	ACP	O2B-PB-C3B	3.51	121.25	106.73
4	B	2001	ACP	O1B-PB-C3B	-3.43	100.02	109.05
4	A	1001	ACP	N3-C2-N1	-3.37	123.48	128.58
4	A	1001	ACP	O2B-PB-C3B	3.13	119.69	106.73
4	A	1001	ACP	C6-C5-C4	-2.75	113.42	117.18
4	B	2001	ACP	C6-C5-C4	-2.72	113.47	117.18
4	B	2001	ACP	C1'-N9-C8	2.37	132.35	127.09
4	A	1001	ACP	C1'-N9-C8	2.30	132.19	127.09
4	B	2001	ACP	O3G-PG-O2G	2.18	114.17	107.96
4	A	1001	ACP	O2A-PA-O5'	2.07	116.93	107.57

There are no chirality outliers.

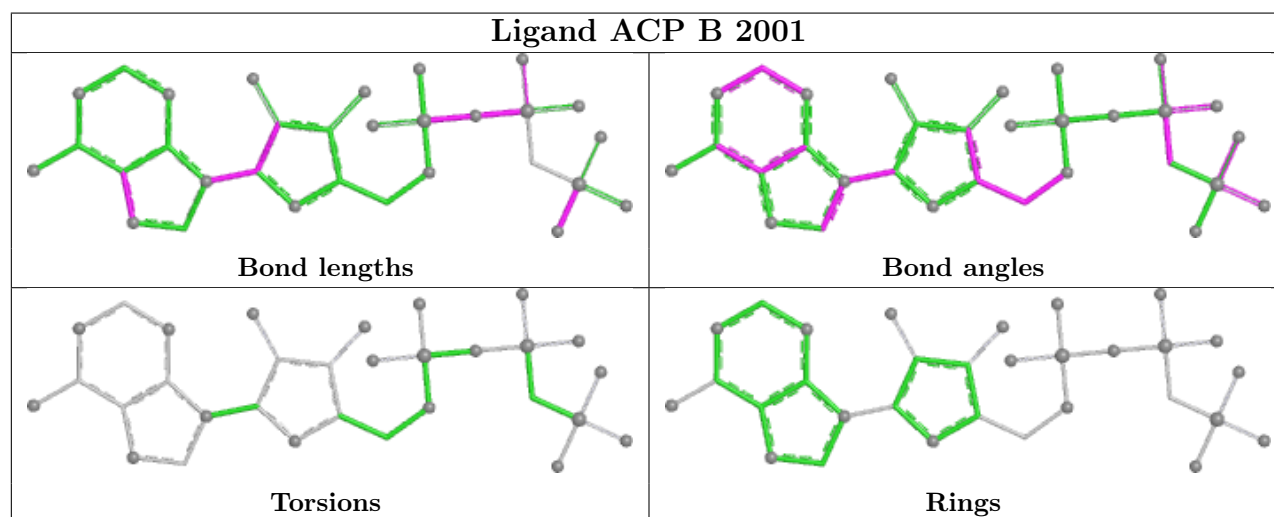
There are no torsion outliers.

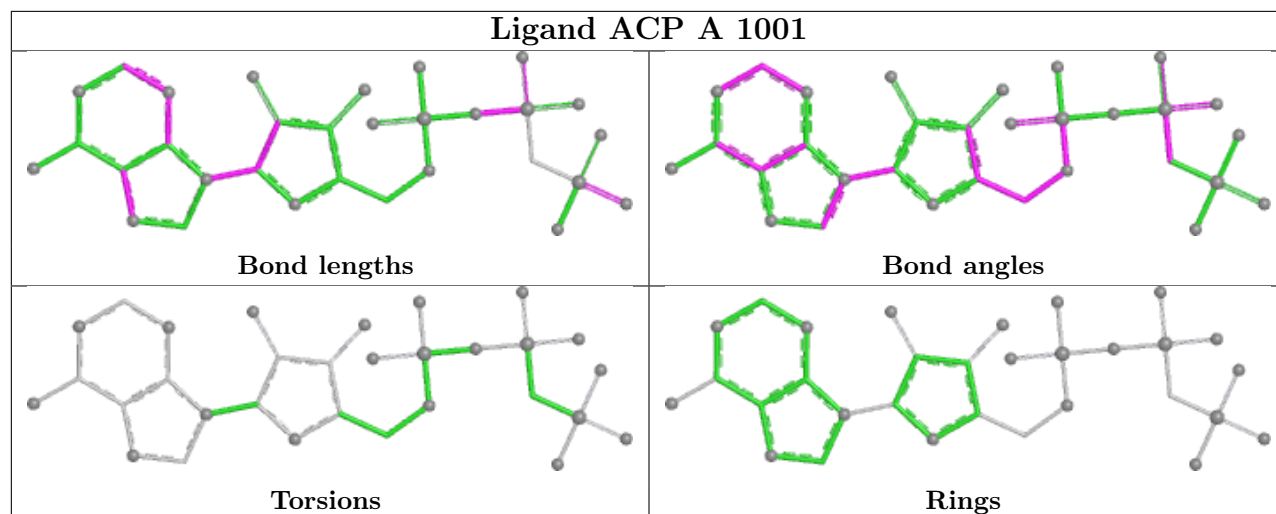
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	ACP	1	0
4	A	1001	ACP	1	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.