



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 09:01 AM EDT

PDB ID : 5NUG
EMDB ID: : EMD-3698
Title : Motor domains from human cytoplasmic dynein-1 in the phi-particle conformation
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on : unknown
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

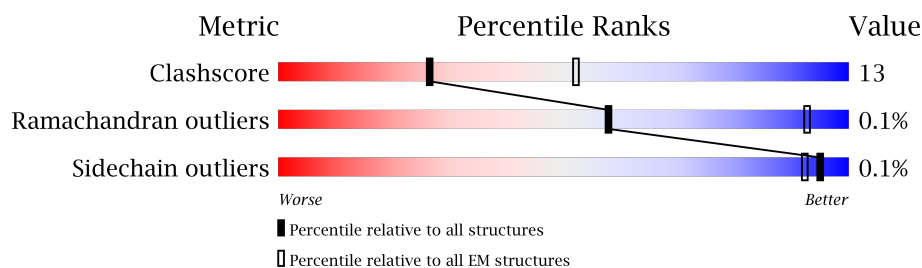
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	4646	
1	B	4646	

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	ADP	A	4801	-	-	X	-
2	ADP	B	4801	-	-	X	-

2 Entry composition [i](#)

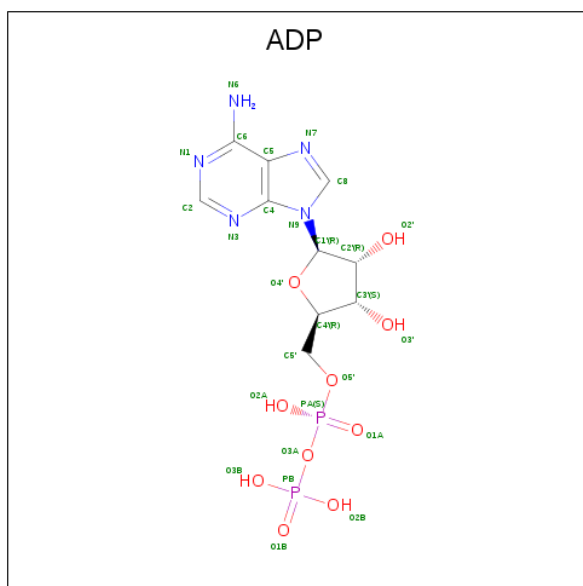
There are 4 unique types of molecules in this entry. The entry contains 46232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		
1	B	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



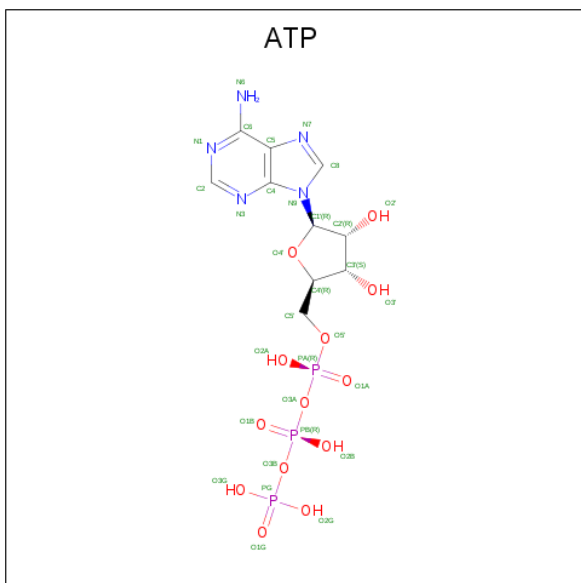
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

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



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	




[illegible]

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain B:









C4644	T4645	E4646	THR	THR	ALA	TRP	PRO	L4138	T3895	L3770	L3572	GLU	SER
			THR	GLN	MET	ARG	ALA	L4139	VAL	L3773	ASP	ASP	ASP
			GLY	GLY	ALA	T4379	TRP	R4143	G3897	E3776	ALA	ALA	ILE
			ALA	ALA	THR	THR	ARG	R4176	F3905	V3797	LYS	ASP	GLU
			LEU	THR	THR	THR	ARG	A4177	I3924	I3578	ASN	ASN	LYS
			ASP	LEU	THR	THR	ARG	R4178	I3924	I3578	GLN	GLN	MET
			ALA	THR	THR	THR	ARG	F4186	W3974	Y3801	LYS	LYS	LYS
			CYS	THR	THR	THR	ARG	S4557	SER	I3802	ALA	ALA	ASN
				THR	THR	THR	ARG	I4190	GLU	P3803	ASN	ASN	TYR
				THR	THR	THR	ARG	T3978	GLU	L3804	GLU	GLU	MET
				THR	THR	THR	ARG	V4009	T3978	I3588	VAL	VAL	SER
				THR	THR	THR	ARG	W4012	T3978	I3589	GLU	GLU	ASN
				THR	THR	THR	ARG	L4013	T3978	Q3435	GLU	GLU	PRO
				THR	THR	THR	ARG	L4027	T3978	F3599	GLU	GLU	SER
				THR	THR	THR	ARG	Y4251	T3978	I3609	TYR	TYR	ASN
				THR	THR	THR	ARG	Y4252	T3978	P3632	THR	THR	THR
				THR	THR	THR	ARG	L4265	T3978	L3455	GLU	GLU	ILE
				THR	THR	THR	ARG	W4266	T3978	S3456	VAL	VAL	VAL
				THR	THR	THR	ARG	F4273	T3978	Q3459	ASN	ASN	ARG
				THR	THR	THR	ARG	F4278	T3978	E3639	ALA	ALA	ALA
				THR	THR	THR	ARG	W4339	T3978	L3645	SER	SER	LEU
				THR	THR	THR	ARG	K4342	T3978	V3648	ALA	ALA	ALA
				THR	THR	THR	ARG	L4349	T3978	R3654	CYS	CYS	GLY
				THR	THR	THR	ARG	E4350	T3978	L3661	PRO	PRO	GLY
				THR	THR	THR	ARG	ASP	T3978	L3508	MET	MET	VAL
				THR	THR	THR	ARG	GLU	T3978	L3509	VAL	VAL	VAL
				THR	THR	THR	ARG	ASP	T3978	Y3516	LYS	LYS	LYS
				THR	THR	THR	ARG	LEU	T3978	A3517	TRP	TRP	TRP
				THR	THR	THR	ARG	ALA	T3978	S3680	ALA	ALA	ALA
				THR	THR	THR	ARG	TYR	T3978	T3681	ILE	ILE	ILE
				THR	THR	THR	ARG	THR	T3978	D3521	ALA	ALA	ALA
				THR	THR	THR	ARG	THR	T3978	Q3522	LEU	LEU	LEU
				THR	THR	THR	ARG	THR	T3978	R3525	ASN	ASN	ASN
				THR	THR	THR	ARG	THR	T3978	F3529	TYR	TYR	TYR
				THR	THR	THR	ARG	THR	T3978	W3532	ALA	ALA	ALA
				THR	THR	THR	ARG	THR	T3978	L3536	ASP	ASP	ASP
				THR	THR	THR	ARG	THR	T3978	N3540	MET	MET	MET
				THR	THR	THR	ARG	THR	T3978	T3550	LYS	LYS	LYS
				THR	THR	THR	ARG	THR	T3978	L3553	LEU	LEU	LEU
				THR	THR	THR	ARG	THR	T3978	S3554	GLN	GLN	GLN
				THR	THR	THR	ARG	THR	T3978	W3562	LYS	LYS	LYS
				THR	THR	THR	ARG	THR	T3978	T3769	LEU	LEU	LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	233227	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	106061	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

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: MG, ATP, ADP

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 >2	RMSZ	# Z >2
1	A	0.43	0/23474	0.71	4/31851 (0.0%)
1	B	0.43	0/23474	0.71	4/31851 (0.0%)
All	All	0.43	0/46948	0.71	8/63702 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3821	ILE	N-CA-C	5.74	126.51	111.00
1	B	3821	ILE	N-CA-C	5.74	126.51	111.00
1	A	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	3578	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	3578	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	2019	ASN	C-N-CD	5.02	138.94	128.40
1	B	2019	ASN	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23003	0	22805	587	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	23003	0	22805	582	0
2	A	81	0	36	13	0
2	B	81	0	36	13	0
3	A	31	0	12	4	0
3	B	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	46232	0	45706	1155	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 13.

All (1155) 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:3638:VAL:HG12	1:A:3681:THR:CG2	1.29	1.60
1:B:3638:VAL:HG12	1:B:3681:THR:CG2	1.29	1.54
1:B:3749:LEU:HD13	1:B:3773:LEU:CD1	1.44	1.46
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG2	1.50	1.45
1:A:3749:LEU:HD13	1:A:3773:LEU:CD1	1.44	1.43
1:A:2584:TRP:CZ3	1:A:2732:PRO:HG2	1.50	1.43
1:A:1931:ASN:ND2	1:A:2317:SER:HB3	1.28	1.42
1:B:1931:ASN:ND2	1:B:2317:SER:HB3	1.28	1.41
1:A:3815:MET:CE	1:A:3871:VAL:CG2	2.07	1.33
1:B:3815:MET:CE	1:B:3871:VAL:CG2	2.07	1.32
1:A:3815:MET:HE2	1:A:3871:VAL:CG2	1.61	1.29
1:A:3456:SER:CB	1:B:3459:GLN:HG3	1.64	1.27
1:A:2584:TRP:CZ3	1:A:2732:PRO:CG	2.17	1.25
1:A:3459:GLN:HG3	1:B:3456:SER:CB	1.65	1.25
1:A:3638:VAL:CG1	1:A:3681:THR:CG2	2.14	1.25
1:B:2584:TRP:CZ3	1:B:2732:PRO:CG	2.18	1.24
1:B:3638:VAL:CG1	1:B:3681:THR:CG2	2.14	1.24
1:A:3115:LEU:HD13	1:A:3143:ILE:CD1	1.67	1.24
1:B:3115:LEU:HD13	1:B:3143:ILE:CD1	1.67	1.24
1:A:3456:SER:OG	1:B:3459:GLN:HG3	1.34	1.22
1:A:4622:VAL:HG12	1:A:4624:PHE:CE2	1.75	1.21
1:A:3459:GLN:HG3	1:B:3456:SER:OG	1.38	1.19
1:B:4622:VAL:HG12	1:B:4624:PHE:CE2	1.76	1.19
1:A:2609:LEU:HD11	1:A:2615:MET:HB2	1.23	1.17
1:B:3815:MET:CE	1:B:3871:VAL:HG21	1.72	1.16
1:B:2325:LEU:HD23	1:B:2333:LEU:HD12	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3821:ILE:HD12	1:A:4342:LYS:CG	1.77	1.14
1:B:3815:MET:HE1	1:B:3871:VAL:CG2	1.70	1.14
1:A:3749:LEU:HD13	1:A:3773:LEU:HD11	1.26	1.13
1:A:3815:MET:CE	1:A:3871:VAL:HG21	1.72	1.13
1:B:3821:ILE:HD12	1:B:4342:LYS:CG	1.78	1.12
1:A:3456:SER:OG	1:B:3459:GLN:CG	1.96	1.12
1:A:2549:GLN:NE2	1:A:2572:LEU:HD22	1.65	1.12
1:A:4607:LEU:HD21	1:A:4635:PHE:HZ	1.08	1.11
1:A:4511:LEU:HD22	1:A:4644:CYS:SG	1.90	1.11
1:B:2549:GLN:NE2	1:B:2572:LEU:HD22	1.65	1.11
1:B:2196:GLY:HA2	1:B:2201:GLY:HA3	1.32	1.11
1:A:3821:ILE:HD12	1:A:4342:LYS:HG3	1.33	1.10
1:B:2457:SER:HB3	1:B:2584:TRP:CH2	1.86	1.10
1:B:2457:SER:CB	1:B:2584:TRP:HH2	1.63	1.10
1:A:2457:SER:HB3	1:A:2584:TRP:CH2	1.86	1.10
1:B:3821:ILE:CD1	1:B:4342:LYS:HD2	1.81	1.10
1:A:2457:SER:CB	1:A:2584:TRP:HH2	1.63	1.10
1:A:3115:LEU:HD13	1:A:3143:ILE:HD11	1.31	1.10
1:A:4607:LEU:HD21	1:A:4635:PHE:CZ	1.85	1.10
1:B:2609:LEU:HD11	1:B:2615:MET:HB2	1.23	1.10
1:A:3459:GLN:CG	1:B:3456:SER:OG	1.99	1.10
1:B:4511:LEU:HD22	1:B:4644:CYS:SG	1.90	1.10
1:B:4607:LEU:HD21	1:B:4635:PHE:CZ	1.85	1.10
1:B:3115:LEU:HD13	1:B:3143:ILE:HD11	1.31	1.09
1:A:3749:LEU:HD13	1:A:3773:LEU:HD13	1.33	1.09
1:B:1931:ASN:ND2	1:B:2317:SER:CB	2.14	1.09
1:B:4424:LEU:HD13	1:B:4486:ILE:CD1	1.83	1.09
1:A:3821:ILE:CD1	1:A:4342:LYS:HD2	1.81	1.09
1:A:2196:GLY:HA2	1:A:2201:GLY:HA3	1.32	1.09
1:A:1931:ASN:ND2	1:A:2317:SER:CB	2.14	1.09
1:A:3815:MET:HE1	1:A:3871:VAL:CG2	1.80	1.09
1:A:4622:VAL:CG1	1:A:4624:PHE:CE2	2.34	1.08
1:B:4622:VAL:CG1	1:B:4624:PHE:CE2	2.34	1.08
1:B:4607:LEU:HD21	1:B:4635:PHE:HZ	1.08	1.08
1:A:3815:MET:HE2	1:A:3871:VAL:HG21	1.13	1.08
1:A:4424:LEU:HD13	1:A:4486:ILE:CD1	1.83	1.08
1:B:3749:LEU:HD13	1:B:3773:LEU:HD11	1.26	1.08
1:B:3815:MET:HE2	1:B:3871:VAL:CG2	1.71	1.08
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.28	1.08
1:B:3821:ILE:HD12	1:B:4342:LYS:HG3	1.34	1.08
1:B:3749:LEU:HD13	1:B:3773:LEU:HD13	1.33	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3815:MET:HE1	1:B:3871:VAL:HG23	1.29	1.07
1:B:1766:LEU:HD23	1:B:1833:ALA:HA	1.36	1.07
1:B:2580:LEU:O	1:B:2584:TRP:HD1	1.36	1.07
1:B:3815:MET:HE2	1:B:3871:VAL:HG21	1.17	1.06
1:A:1879:LEU:HD12	1:A:1918:ALA:HB2	1.36	1.06
1:B:3638:VAL:CG1	1:B:3681:THR:HG23	1.79	1.06
1:A:3638:VAL:CG1	1:A:3681:THR:HG23	1.79	1.05
1:A:3815:MET:HE1	1:A:3871:VAL:HG23	1.37	1.05
1:A:1766:LEU:HD23	1:A:1833:ALA:HA	1.36	1.05
1:A:2580:LEU:O	1:A:2584:TRP:HD1	1.36	1.04
1:B:1879:LEU:HD12	1:B:1918:ALA:HB2	1.36	1.03
1:A:2609:LEU:HD11	1:A:2615:MET:CB	1.87	1.03
1:A:2549:GLN:HE21	1:A:2572:LEU:HD22	1.18	1.03
1:B:4605:VAL:CG1	1:B:4635:PHE:CE2	2.42	1.03
1:B:4424:LEU:HD13	1:B:4486:ILE:HD11	1.38	1.02
1:A:4605:VAL:CG1	1:A:4635:PHE:CE2	2.42	1.02
1:A:3749:LEU:CD1	1:A:3773:LEU:CD1	2.37	1.01
1:B:2609:LEU:HD11	1:B:2615:MET:CB	1.88	1.01
1:B:3749:LEU:CD1	1:B:3773:LEU:CD1	2.37	1.01
1:A:4424:LEU:HD13	1:A:4486:ILE:HD11	1.38	1.01
1:B:2549:GLN:HE21	1:B:2572:LEU:HD22	1.18	1.01
1:A:3099:THR:HG22	1:A:3152:GLN:NE2	1.75	1.01
1:B:3099:THR:HG22	1:B:3152:GLN:NE2	1.75	1.01
1:A:1778:LEU:CD1	1:A:1830:ILE:HD12	1.91	1.00
1:B:4605:VAL:HG11	1:B:4635:PHE:CE2	1.96	1.00
1:B:1778:LEU:CD1	1:B:1830:ILE:HD12	1.91	1.00
1:A:3638:VAL:CG1	1:A:3681:THR:HG21	1.91	0.99
1:A:4605:VAL:HG11	1:A:4635:PHE:CE2	1.96	0.99
1:A:2549:GLN:HG3	1:A:2572:LEU:HD13	1.44	0.98
1:B:1879:LEU:HD12	1:B:1918:ALA:CB	1.93	0.98
1:A:3638:VAL:HG12	1:A:3681:THR:HG21	1.45	0.98
1:B:2819:GLU:OE2	1:B:2862:ASP:CB	2.12	0.98
1:B:3638:VAL:CG1	1:B:3681:THR:HG21	1.91	0.97
1:B:2457:SER:CB	1:B:2584:TRP:CH2	2.44	0.97
1:B:3638:VAL:HG12	1:B:3681:THR:HG21	1.45	0.97
1:B:2584:TRP:HZ3	1:B:2732:PRO:HG2	1.15	0.97
1:A:3749:LEU:CD1	1:A:3773:LEU:HD11	1.95	0.97
1:B:2358:ARG:NH2	2:B:4801:ADP:O1B	1.97	0.97
1:A:2819:GLU:OE2	1:A:2862:ASP:CB	2.12	0.97
1:A:3817:SER:OG	1:A:4349:LEU:HD12	1.65	0.97
1:B:2549:GLN:HG3	1:B:2572:LEU:HD13	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2358:ARG:NH2	2:A:4801:ADP:O1B	1.97	0.96
1:A:1879:LEU:HD12	1:A:1918:ALA:CB	1.93	0.96
1:A:2302:VAL:HG22	1:A:2342:MET:HB2	1.46	0.96
1:A:3459:GLN:HG3	1:B:3456:SER:HB3	1.46	0.96
1:B:3817:SER:OG	1:B:4349:LEU:CD1	2.14	0.96
1:B:3822:HIS:O	1:B:3823:PHE:CG	2.19	0.96
1:B:3749:LEU:CD1	1:B:3773:LEU:HD11	1.95	0.95
1:A:3172:THR:HG21	1:A:3694:SER:OG	1.66	0.95
1:A:3822:HIS:O	1:A:3823:PHE:CG	2.19	0.95
1:A:3817:SER:OG	1:A:4349:LEU:CD1	2.14	0.95
1:A:3821:ILE:HD12	1:A:4342:LYS:CD	1.97	0.95
1:A:2457:SER:CB	1:A:2584:TRP:CH2	2.44	0.95
1:B:1931:ASN:HD22	1:B:2317:SER:HB3	1.15	0.95
1:A:2609:LEU:CD1	1:A:2615:MET:HB2	1.97	0.95
1:A:2220:LEU:HD23	1:A:2342:MET:HG2	1.48	0.95
1:A:3456:SER:HB3	1:B:3459:GLN:HG3	1.49	0.95
1:A:3638:VAL:HG12	1:A:3681:THR:HG23	0.97	0.95
1:B:3817:SER:OG	1:B:4349:LEU:HD12	1.65	0.94
1:B:1981:ALA:HB2	1:B:1999:CYS:SG	2.07	0.94
1:B:3638:VAL:HG12	1:B:3681:THR:HG23	0.97	0.94
1:B:2302:VAL:HG22	1:B:2342:MET:HB2	1.46	0.94
1:B:3822:HIS:O	1:B:3823:PHE:CD2	2.21	0.94
1:A:4622:VAL:HG11	1:A:4624:PHE:CZ	2.03	0.94
1:B:3821:ILE:HD12	1:B:4342:LYS:CD	1.97	0.94
1:B:2609:LEU:CD1	1:B:2615:MET:HB2	1.97	0.94
1:B:1931:ASN:HD22	1:B:2317:SER:CB	1.76	0.94
1:B:3172:THR:HG21	1:B:3694:SER:OG	1.66	0.94
1:A:1981:ALA:HB2	1:A:1999:CYS:SG	2.07	0.93
1:A:3822:HIS:O	1:A:3823:PHE:CD2	2.21	0.93
1:B:4622:VAL:HG11	1:B:4624:PHE:CZ	2.03	0.93
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.48	0.93
1:A:3115:LEU:CD1	1:A:3143:ILE:HD11	1.99	0.92
1:A:1778:LEU:HD11	1:A:1830:ILE:HD12	1.52	0.92
1:A:1931:ASN:HD22	1:A:2317:SER:HB3	1.15	0.92
1:A:1931:ASN:HD22	1:A:2317:SER:CB	1.77	0.92
1:A:4622:VAL:CG1	1:A:4624:PHE:CZ	2.53	0.92
1:B:3115:LEU:CD1	1:B:3143:ILE:HD11	1.99	0.91
1:B:4622:VAL:CG1	1:B:4624:PHE:CZ	2.53	0.91
1:B:2220:LEU:HD23	1:B:2342:MET:HG2	1.49	0.91
1:B:2464:GLN:HG2	1:B:2583:THR:HG23	1.51	0.91
1:B:2605:LEU:CD2	1:B:2662:PHE:CE1	2.54	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.49	0.91
1:B:1778:LEU:HD11	1:B:1830:ILE:HD12	1.52	0.91
1:A:2584:TRP:HZ3	1:A:2732:PRO:HG2	1.15	0.90
1:A:3123:PRO:HB3	1:A:3540:ASN:ND2	1.85	0.90
1:A:2605:LEU:CD2	1:A:2662:PHE:CE1	2.54	0.90
1:B:3123:PRO:HB3	1:B:3540:ASN:ND2	1.85	0.90
1:B:2580:LEU:O	1:B:2584:TRP:CD1	2.24	0.90
1:A:2584:TRP:HZ3	1:A:2732:PRO:CG	1.70	0.89
1:A:2580:LEU:O	1:A:2584:TRP:CD1	2.24	0.89
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.51	0.89
1:B:3115:LEU:CD1	1:B:3143:ILE:CD1	2.50	0.89
1:A:4186:PHE:HZ	1:A:4265:LEU:CD1	1.85	0.89
1:B:4186:PHE:HZ	1:B:4265:LEU:CD1	1.85	0.89
1:A:2457:SER:HB3	1:A:2584:TRP:HH2	1.29	0.89
1:A:1632:VAL:CG1	1:A:1636:ASP:HB2	2.03	0.88
1:A:4186:PHE:HZ	1:A:4265:LEU:HD11	1.39	0.88
1:B:2584:TRP:HZ3	1:B:2732:PRO:CG	1.70	0.88
1:B:1632:VAL:CG1	1:B:1636:ASP:HB2	2.03	0.88
1:B:2752:ASN:ND2	1:B:2770:THR:HG22	1.90	0.87
1:A:4067:THR:HB	1:A:4094:VAL:HG22	1.56	0.87
1:B:4186:PHE:HZ	1:B:4265:LEU:HD11	1.38	0.87
1:A:3115:LEU:HD13	1:A:3143:ILE:HD13	1.55	0.87
1:B:3115:LEU:HD13	1:B:3143:ILE:HD13	1.55	0.87
1:A:3638:VAL:HG12	1:A:3681:THR:HG22	1.57	0.86
1:A:3708:LEU:CD2	1:A:3809:SER:HA	2.05	0.86
1:B:2612:LEU:HD13	1:B:2615:MET:HE3	1.56	0.86
1:A:2612:LEU:HD13	1:A:2615:MET:HE3	1.56	0.85
1:B:4067:THR:HB	1:B:4094:VAL:HG22	1.56	0.85
1:A:4424:LEU:CD1	1:A:4486:ILE:HD13	2.07	0.85
1:B:3821:ILE:HD13	1:B:4342:LYS:HD2	1.59	0.85
1:B:3708:LEU:CD2	1:B:3809:SER:HA	2.05	0.85
1:B:2863:ARG:O	1:B:2863:ARG:HD3	1.76	0.85
1:B:3808:CYS:SG	1:B:3836:TYR:OH	2.35	0.85
1:A:2863:ARG:HD3	1:A:2863:ARG:O	1.76	0.85
1:B:4424:LEU:CD1	1:B:4486:ILE:HD13	2.07	0.85
1:A:2091:ARG:NH1	2:A:4801:ADP:O1A	2.10	0.84
1:A:2752:ASN:ND2	1:A:2770:THR:HG22	1.90	0.84
1:A:3115:LEU:CD1	1:A:3143:ILE:CD1	2.50	0.84
1:A:3821:ILE:HD13	1:A:4342:LYS:HD2	1.59	0.84
1:B:2091:ARG:NH1	2:B:4801:ADP:O1A	2.10	0.84
1:A:3821:ILE:CD1	1:A:4342:LYS:CD	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4605:VAL:HG11	1:A:4635:PHE:CZ	2.13	0.83
1:B:4605:VAL:HG11	1:B:4635:PHE:CZ	2.13	0.83
1:B:2091:ARG:NH1	2:B:4801:ADP:H5'2	1.94	0.83
1:A:3808:CYS:SG	1:A:3836:TYR:OH	2.35	0.83
1:A:2446:ILE:HD11	1:A:2735:TYR:CD1	2.14	0.82
1:A:3815:MET:HE2	1:A:3871:VAL:HG22	1.59	0.82
1:B:1879:LEU:CD1	1:B:1918:ALA:HB2	2.10	0.82
1:B:2446:ILE:HD11	1:B:2735:TYR:CD1	2.14	0.82
1:A:2851:ASP:OD2	1:A:2863:ARG:NH1	2.12	0.82
1:A:2091:ARG:NH1	2:A:4801:ADP:H5'2	1.94	0.81
1:B:3821:ILE:CD1	1:B:4342:LYS:CD	2.55	0.81
1:A:1879:LEU:CD1	1:A:1918:ALA:HB2	2.10	0.81
1:B:2851:ASP:OD2	1:B:2863:ARG:NH1	2.12	0.81
1:B:3638:VAL:HG12	1:B:3681:THR:HG22	1.57	0.81
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.64	0.80
1:B:3822:HIS:ND1	1:B:3824:LEU:HB3	1.97	0.80
1:B:4424:LEU:HD13	1:B:4486:ILE:HD13	1.61	0.80
1:B:2609:LEU:CD2	1:B:2617:VAL:HG23	2.12	0.80
1:A:1931:ASN:OD1	1:A:1958:ASP:HB2	1.82	0.80
1:B:2551:LYS:HD3	1:B:2551:LYS:O	1.82	0.80
1:B:3882:THR:HG22	1:B:4339:MET:HG3	1.64	0.80
1:B:3175:HIS:CD2	1:B:3585:ARG:NH2	2.50	0.80
1:B:2609:LEU:CD2	1:B:2617:VAL:CG2	2.60	0.79
1:A:1636:ASP:OD2	1:A:1656:LYS:NZ	2.14	0.79
1:A:2609:LEU:CD2	1:A:2617:VAL:HG23	2.12	0.79
1:B:1879:LEU:HD11	1:B:1914:GLU:O	1.83	0.79
1:A:3822:HIS:ND1	1:A:3824:LEU:HB3	1.97	0.79
1:A:2551:LYS:HD3	1:A:2551:LYS:O	1.82	0.79
1:B:1636:ASP:OD2	1:B:1656:LYS:NZ	2.14	0.79
1:B:2593:LEU:HD23	1:B:2734:VAL:CG2	2.13	0.79
1:A:2609:LEU:CD2	1:A:2617:VAL:CG2	2.60	0.79
1:B:1931:ASN:OD1	1:B:1958:ASP:HB2	1.82	0.78
1:A:3675:PHE:O	1:A:3676:VAL:HG13	1.83	0.78
1:B:3675:PHE:O	1:B:3676:VAL:HG13	1.83	0.78
1:A:1825:LEU:HD12	1:A:1830:ILE:HD11	1.64	0.78
1:A:2605:LEU:CD2	1:A:2662:PHE:CD1	2.66	0.78
1:A:1879:LEU:HD11	1:A:1914:GLU:O	1.83	0.78
1:A:3175:HIS:CD2	1:A:3585:ARG:NH2	2.50	0.78
1:A:2265:TYR:CE2	1:A:2314:ASN:ND2	2.52	0.78
1:A:2609:LEU:HD21	1:A:2617:VAL:HG23	1.66	0.78
1:B:2265:TYR:CE2	1:B:2314:ASN:ND2	2.52	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2605:LEU:CD2	1:B:2662:PHE:CD1	2.66	0.78
1:A:2593:LEU:HD23	1:A:2734:VAL:CG2	2.13	0.78
1:B:2549:GLN:HE21	1:B:2572:LEU:CD2	1.97	0.78
1:A:3008:MET:HE2	1:A:3066:PHE:CZ	2.19	0.77
1:B:3815:MET:CE	1:B:3871:VAL:HG22	2.14	0.77
1:B:1825:LEU:HD12	1:B:1830:ILE:HD11	1.64	0.77
1:B:2609:LEU:HD21	1:B:2617:VAL:HG23	1.66	0.77
1:B:2058:GLY:O	1:B:2104:LYS:HE3	1.85	0.77
1:B:3151:HIS:HD1	1:B:3516:TYR:HH	1.30	0.77
1:B:4622:VAL:HG11	1:B:4624:PHE:CE2	2.17	0.77
1:A:2581:LEU:HD21	1:A:2593:LEU:HD21	1.67	0.76
1:B:2581:LEU:HD21	1:B:2593:LEU:HD21	1.67	0.76
1:A:4622:VAL:HG11	1:A:4624:PHE:CE2	2.17	0.76
1:B:4605:VAL:HG13	1:B:4635:PHE:CE2	2.19	0.76
1:A:4605:VAL:HG13	1:A:4635:PHE:CE2	2.19	0.76
1:A:2584:TRP:CE3	1:A:2732:PRO:HG2	2.17	0.76
1:A:4035:VAL:HG22	1:A:4143:ARG:HG3	1.68	0.76
1:B:2609:LEU:CD1	1:B:2615:MET:CB	2.59	0.76
1:B:2549:GLN:CG	1:B:2572:LEU:HD13	2.16	0.76
1:A:2571:THR:HG1	1:A:2574:THR:HG1	1.29	0.75
1:A:3562:TRP:HB3	1:A:3567:LEU:HD23	1.69	0.75
1:A:4424:LEU:CD1	1:A:4486:ILE:CD1	2.61	0.75
1:A:2058:GLY:O	1:A:2104:LYS:HE3	1.85	0.75
1:A:4190:ILE:HD11	1:A:4252:TYR:HE1	1.52	0.75
1:B:2149:LEU:HD11	1:B:2157:LEU:HD22	1.68	0.75
1:B:4035:VAL:HG22	1:B:4143:ARG:HG3	1.68	0.75
1:A:2609:LEU:CD1	1:A:2615:MET:CB	2.59	0.75
1:A:3008:MET:CE	1:A:3066:PHE:CZ	2.69	0.75
1:A:1778:LEU:HD13	1:A:1830:ILE:HD12	1.68	0.75
1:B:3008:MET:CE	1:B:3066:PHE:CZ	2.69	0.75
1:B:4190:ILE:HD11	1:B:4252:TYR:HE1	1.52	0.75
1:A:1933:ASP:OD1	1:A:1962:ARG:NH2	2.20	0.75
1:A:2549:GLN:CG	1:A:2572:LEU:HD13	2.16	0.75
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.68	0.74
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG3	2.20	0.74
1:B:2584:TRP:CE3	1:B:2732:PRO:HG2	2.17	0.74
1:B:1933:ASP:OD1	1:B:1962:ARG:NH2	2.20	0.74
1:B:1778:LEU:HD13	1:B:1830:ILE:HD12	1.68	0.74
1:B:2749:GLY:HA2	1:B:2770:THR:HG21	1.70	0.74
1:B:2605:LEU:HD23	1:B:2662:PHE:CE1	2.21	0.74
1:B:3562:TRP:HB3	1:B:3567:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2549:GLN:HE21	1:A:2572:LEU:CD2	1.97	0.74
1:A:2605:LEU:HD23	1:A:2662:PHE:CE1	2.21	0.74
1:A:3082:SER:OG	1:A:3085:LEU:HD12	1.87	0.74
1:B:4388:LEU:O	1:B:4392:PRO:HD3	1.88	0.74
1:A:4388:LEU:O	1:A:4392:PRO:HD3	1.88	0.73
1:A:3459:GLN:CG	1:B:3456:SER:CB	2.58	0.73
1:B:2457:SER:OG	1:B:2584:TRP:HH2	1.71	0.73
1:B:3082:SER:OG	1:B:3085:LEU:HD12	1.87	0.73
1:B:3154:LEU:HD22	1:B:3516:TYR:CD2	2.23	0.73
1:B:4424:LEU:CD1	1:B:4486:ILE:CD1	2.61	0.73
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.30	0.72
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.70	0.72
1:A:3154:LEU:HD22	1:A:3516:TYR:CD2	2.23	0.72
1:A:2312:VAL:HG11	1:A:2355:THR:HG23	1.70	0.72
1:A:2078:GLU:OE1	1:A:4522:THR:HG21	1.90	0.72
1:A:2605:LEU:HD22	1:A:2662:PHE:HE1	1.55	0.72
1:B:2078:GLU:OE1	1:B:4522:THR:HG21	1.90	0.72
1:A:2457:SER:OG	1:A:2584:TRP:HH2	1.71	0.72
1:B:2312:VAL:HG11	1:B:2355:THR:HG23	1.70	0.72
1:B:3550:THR:OG1	1:B:3574:THR:HG22	1.90	0.72
1:A:3638:VAL:HG13	1:A:3681:THR:HG21	1.71	0.72
1:B:2605:LEU:HD22	1:B:2662:PHE:HE1	1.55	0.71
1:A:3822:HIS:CE1	1:A:3824:LEU:HB3	2.25	0.71
1:B:3099:THR:HG22	1:B:3152:GLN:HE22	1.54	0.71
1:A:3550:THR:OG1	1:A:3574:THR:HG22	1.89	0.71
1:B:3099:THR:CG2	1:B:3152:GLN:NE2	2.52	0.71
1:A:3099:THR:CG2	1:A:3152:GLN:HE22	2.04	0.71
1:B:3638:VAL:HG13	1:B:3681:THR:HG21	1.71	0.70
1:B:3008:MET:HE2	1:B:3066:PHE:CZ	2.25	0.70
1:B:4607:LEU:CD2	1:B:4635:PHE:CZ	2.70	0.70
1:B:3822:HIS:CE1	1:B:3824:LEU:HB3	2.25	0.70
1:A:2584:TRP:CZ3	1:A:2732:PRO:HG3	2.20	0.70
1:B:2571:THR:HG1	1:B:2574:THR:HG1	1.22	0.70
1:A:3562:TRP:HB3	1:A:3567:LEU:CD2	2.22	0.70
1:A:2933:LEU:HD23	1:A:3065:VAL:HG13	1.73	0.70
1:A:3099:THR:CG2	1:A:3152:GLN:NE2	2.52	0.70
1:A:1762:VAL:O	1:A:1766:LEU:HD13	1.92	0.69
1:B:3099:THR:CG2	1:B:3152:GLN:HE22	2.04	0.69
1:B:1766:LEU:CD2	1:B:1833:ALA:HA	2.19	0.69
1:B:2912:PHE:HB2	1:B:3104:GLN:OE1	1.93	0.69
1:B:3815:MET:HE2	1:B:3871:VAL:HG22	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:CD2	1:A:1833:ALA:HA	2.19	0.69
1:A:3456:SER:OG	1:B:3459:GLN:CD	2.30	0.69
1:B:2457:SER:HB3	1:B:2584:TRP:CZ2	2.28	0.69
1:A:3456:SER:CB	1:B:3459:GLN:CG	2.58	0.69
1:A:4607:LEU:CD2	1:A:4635:PHE:CZ	2.70	0.69
1:B:3562:TRP:HB3	1:B:3567:LEU:CD2	2.22	0.69
1:B:2933:LEU:HD23	1:B:3065:VAL:HG13	1.73	0.69
1:A:1931:ASN:HD21	1:A:2317:SER:HB3	1.51	0.69
1:A:4190:ILE:HD11	1:A:4252:TYR:CE1	2.28	0.69
1:A:3099:THR:HG22	1:A:3152:GLN:HE22	1.54	0.69
1:B:1762:VAL:O	1:B:1766:LEU:HD13	1.92	0.69
1:A:2912:PHE:HB2	1:A:3104:GLN:OE1	1.93	0.69
1:B:3824:LEU:CD2	1:B:4130:ILE:HG12	2.23	0.69
1:B:1632:VAL:CG1	1:B:1636:ASP:CB	2.71	0.68
1:B:2995:ASP:OD1	1:B:3067:THR:HB	1.94	0.68
1:A:2626:THR:O	1:A:2627:THR:HG23	1.93	0.68
1:A:1632:VAL:CG1	1:A:1636:ASP:CB	2.71	0.68
1:A:2995:ASP:OD1	1:A:3067:THR:HB	1.94	0.68
1:B:2626:THR:O	1:B:2627:THR:HG23	1.93	0.68
1:A:2457:SER:HB3	1:A:2584:TRP:CZ2	2.28	0.68
1:A:2196:GLY:CA	1:A:2201:GLY:HA3	2.19	0.68
1:A:3550:THR:OG1	1:A:3574:THR:CG2	2.42	0.68
1:B:3478:LEU:HD13	1:B:3770:LEU:HD13	1.75	0.68
1:B:4247:MET:HE2	1:B:4252:TYR:CE2	2.28	0.68
1:A:3824:LEU:CD2	1:A:4130:ILE:HG12	2.23	0.68
1:A:3459:GLN:CD	1:B:3456:SER:OG	2.32	0.68
1:B:3522:GLN:OE1	1:B:3704:THR:HG21	1.94	0.68
1:A:4247:MET:CE	1:A:4252:TYR:HE2	2.07	0.68
1:B:2196:GLY:CA	1:B:2201:GLY:HA3	2.19	0.68
1:B:3550:THR:OG1	1:B:3574:THR:CG2	2.42	0.68
1:B:4190:ILE:HD11	1:B:4252:TYR:CE1	2.28	0.68
1:B:4247:MET:CE	1:B:4252:TYR:HE2	2.07	0.68
1:A:2580:LEU:HG	1:A:2584:TRP:HE1	1.59	0.67
1:A:3815:MET:CE	1:A:3871:VAL:HG22	2.14	0.67
1:A:2605:LEU:HD22	1:A:2662:PHE:CE1	2.27	0.67
1:A:3522:GLN:OE1	1:A:3704:THR:HG21	1.94	0.67
1:B:2549:GLN:NE2	1:B:2572:LEU:CD2	2.53	0.67
1:B:3175:HIS:HD2	1:B:3585:ARG:NH2	1.92	0.67
1:A:4186:PHE:CZ	1:A:4265:LEU:HD11	2.28	0.67
1:B:2555:ILE:HG21	1:B:2570:PRO:HD2	1.76	0.67
1:B:2580:LEU:HG	1:B:2584:TRP:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2910:VAL:HG11	1:A:3105:VAL:HG23	1.77	0.67
1:A:2555:ILE:HG21	1:A:2570:PRO:HD2	1.76	0.67
1:A:2612:LEU:HD13	1:A:2615:MET:CE	2.25	0.67
1:A:3200:HIS:O	1:A:3204:GLY:N	2.28	0.67
1:B:1931:ASN:HD21	1:B:2317:SER:HB3	1.51	0.67
1:A:3675:PHE:O	1:A:3676:VAL:CG1	2.43	0.66
1:B:2910:VAL:HG11	1:B:3105:VAL:HG23	1.77	0.66
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.77	0.66
1:B:3200:HIS:O	1:B:3204:GLY:N	2.28	0.66
1:B:4186:PHE:CZ	1:B:4265:LEU:HD11	2.28	0.66
1:A:3924:ILE:HG22	1:A:3924:ILE:O	1.95	0.66
1:A:4247:MET:HE2	1:A:4252:TYR:CE2	2.30	0.66
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.77	0.66
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.16	0.66
1:A:3478:LEU:HD13	1:A:3770:LEU:HD13	1.76	0.66
1:B:1632:VAL:HG12	1:B:1636:ASP:HB2	1.77	0.66
1:B:3675:PHE:O	1:B:3676:VAL:CG1	2.43	0.66
1:A:3021:PHE:CD1	1:A:3029:LEU:HD12	2.31	0.65
1:B:3021:PHE:CD1	1:B:3029:LEU:HD12	2.31	0.65
1:A:2584:TRP:CH2	1:A:2732:PRO:CG	2.79	0.65
1:A:2593:LEU:HD23	1:A:2734:VAL:HG23	1.78	0.65
1:B:2863:ARG:C	1:B:2863:ARG:HD3	2.16	0.65
1:A:2787:ASP:OD1	1:A:2787:ASP:O	2.15	0.65
1:A:3175:HIS:HD2	1:A:3585:ARG:NH2	1.92	0.65
1:B:3021:PHE:CE1	1:B:3029:LEU:HD12	2.32	0.65
1:A:2609:LEU:HD22	1:A:2617:VAL:CG2	2.27	0.65
1:B:2091:ARG:NH1	2:B:4801:ADP:C5'	2.60	0.65
1:B:2593:LEU:HD23	1:B:2734:VAL:HG23	1.78	0.65
1:A:3021:PHE:CE1	1:A:3029:LEU:HD12	2.32	0.64
1:B:2612:LEU:HD13	1:B:2615:MET:CE	2.25	0.64
1:B:3924:ILE:HG22	1:B:3924:ILE:O	1.95	0.64
1:A:1632:VAL:HG12	1:A:1636:ASP:HB2	1.77	0.64
1:B:2584:TRP:HZ3	1:B:2732:PRO:HG3	1.60	0.64
1:B:4388:LEU:HD21	1:B:4434:VAL:HG13	1.79	0.64
1:B:4565:LEU:HD23	1:B:4642:VAL:HG22	1.79	0.64
1:B:2584:TRP:CH2	1:B:2732:PRO:CG	2.79	0.64
1:A:1778:LEU:HD11	1:A:1830:ILE:CD1	2.27	0.64
1:B:2602:THR:OG1	2:B:4804:ADP:O1A	2.16	0.64
1:A:2091:ARG:NH1	2:A:4801:ADP:C5'	2.60	0.64
1:B:2609:LEU:HD22	1:B:2617:VAL:CG2	2.27	0.64
1:B:2787:ASP:OD1	1:B:2787:ASP:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3580:LEU:HD21	1:A:3589:ILE:HD11	1.80	0.64
1:A:1766:LEU:HD23	1:A:1833:ALA:CA	2.22	0.63
1:A:4560:VAL:O	1:A:4587:LEU:HD12	1.98	0.63
1:A:4388:LEU:HD21	1:A:4434:VAL:HG13	1.79	0.63
1:B:3817:SER:HG	1:B:4349:LEU:HD12	1.62	0.63
1:A:2602:THR:OG1	2:A:4804:ADP:O1A	2.16	0.63
1:A:2667:ASN:ND2	1:A:2713:ASN:O	2.32	0.63
1:B:4560:VAL:O	1:B:4587:LEU:HD12	1.98	0.63
1:B:2667:ASN:ND2	1:B:2713:ASN:O	2.32	0.63
1:B:3580:LEU:HD21	1:B:3589:ILE:HD11	1.81	0.63
1:A:4565:LEU:HD23	1:A:4642:VAL:HG22	1.79	0.63
1:B:3708:LEU:HD23	1:B:3809:SER:CA	2.26	0.63
1:B:4190:ILE:CD1	1:B:4252:TYR:CE1	2.82	0.62
1:A:3811:ILE:HD12	1:A:3887:LEU:HD22	1.81	0.62
1:B:2612:LEU:CD1	1:B:2615:MET:HE3	2.29	0.62
1:B:3824:LEU:HD22	1:B:4130:ILE:HG12	1.79	0.62
1:B:3482:LEU:O	1:B:3486:ARG:N	2.32	0.62
1:A:3824:LEU:HD22	1:A:4130:ILE:HG12	1.80	0.62
1:B:2605:LEU:HD22	1:B:2662:PHE:CE1	2.27	0.62
1:B:3008:MET:HE1	1:B:3066:PHE:CZ	2.35	0.62
1:A:1879:LEU:HD12	1:A:1918:ALA:HB3	1.82	0.62
1:A:4508:HIS:CE1	1:A:4587:LEU:HD21	2.35	0.62
1:B:3811:ILE:CD1	1:B:3887:LEU:HD22	2.30	0.62
1:A:2568:VAL:HG22	1:A:2603:MET:CE	2.30	0.61
1:B:2568:VAL:HG22	1:B:2603:MET:CE	2.30	0.61
1:A:2549:GLN:NE2	1:A:2572:LEU:CD2	2.53	0.61
1:B:2103:VAL:HG13	1:B:2136:ILE:HG23	1.82	0.61
1:B:2593:LEU:CD1	1:B:2605:LEU:HB2	2.30	0.61
1:A:1931:ASN:ND2	1:A:2317:SER:CA	2.63	0.61
1:A:4190:ILE:CD1	1:A:4252:TYR:CE1	2.82	0.61
1:B:3811:ILE:HD12	1:B:3887:LEU:HD22	1.81	0.61
1:A:2072:PHE:HZ	1:A:2157:LEU:HD11	1.64	0.61
1:B:2100:ALA:HA	1:B:2140:SER:OG	2.01	0.61
1:A:1927:VAL:HG12	1:A:1954:TRP:HB2	1.83	0.61
1:A:2103:VAL:HG13	1:A:2136:ILE:HG23	1.82	0.61
1:A:3482:LEU:O	1:A:3486:ARG:N	2.32	0.61
1:B:3824:LEU:HD22	1:B:4130:ILE:HG23	1.82	0.60
1:B:4508:HIS:CE1	1:B:4587:LEU:HD21	2.35	0.60
1:A:2593:LEU:CD1	1:A:2605:LEU:HB2	2.30	0.60
1:A:2612:LEU:CD1	1:A:2615:MET:HE3	2.29	0.60
1:B:1879:LEU:HD12	1:B:1918:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1931:ASN:ND2	1:B:2317:SER:CA	2.63	0.60
1:A:3459:GLN:CG	1:B:3456:SER:HB3	2.28	0.60
1:A:2549:GLN:CD	1:A:2572:LEU:HD22	2.22	0.60
1:A:2571:THR:CG2	1:A:2747:ILE:HG12	2.32	0.60
1:B:1766:LEU:HD23	1:B:1833:ALA:CA	2.22	0.60
1:B:2571:THR:CG2	1:B:2747:ILE:HG12	2.32	0.60
1:A:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.36	0.60
1:A:3708:LEU:HD23	1:A:3809:SER:CA	2.26	0.60
1:A:3824:LEU:HD22	1:A:4130:ILE:HG23	1.82	0.60
1:B:2072:PHE:HZ	1:B:2157:LEU:HD11	1.64	0.60
1:B:2936:ILE:HG21	1:B:3093:TRP:CZ3	2.36	0.60
1:A:3639:GLU:OE2	1:A:4137:ASN:ND2	2.22	0.60
1:A:4561:THR:CG2	1:A:4587:LEU:HD13	2.32	0.60
1:B:2540:SER:OG	1:B:2544:GLU:O	2.16	0.60
1:A:2551:LYS:HD3	1:A:2551:LYS:C	2.22	0.60
1:A:3811:ILE:CD1	1:A:3887:LEU:HD22	2.30	0.60
1:B:4561:THR:CG2	1:B:4587:LEU:HD13	2.32	0.60
1:A:2100:ALA:HA	1:A:2140:SER:OG	2.01	0.60
1:A:2605:LEU:HD21	1:A:2662:PHE:CD1	2.37	0.60
1:B:2549:GLN:CD	1:B:2572:LEU:HD22	2.22	0.60
1:B:2830:LEU:HD12	1:B:2871:ILE:HG21	1.84	0.60
1:B:4622:VAL:HG12	1:B:4624:PHE:CZ	2.28	0.59
1:B:1927:VAL:HG12	1:B:1954:TRP:HB2	1.83	0.59
1:B:4507:ILE:HG13	1:B:4509:VAL:HG23	1.83	0.59
1:A:4507:ILE:HG13	1:A:4509:VAL:HG23	1.83	0.59
1:B:2472:TYR:HB2	1:B:2541:ILE:HD11	1.84	0.59
1:B:3822:HIS:CE1	1:B:3824:LEU:CB	2.86	0.59
1:B:2551:LYS:HD3	1:B:2551:LYS:C	2.22	0.59
1:B:3099:THR:HG22	1:B:3152:GLN:HE21	1.65	0.59
1:A:3099:THR:HG22	1:A:3152:GLN:HE21	1.65	0.59
1:A:3822:HIS:CE1	1:A:3824:LEU:CB	2.86	0.59
1:B:4186:PHE:CZ	1:B:4265:LEU:CD1	2.77	0.59
1:B:1778:LEU:HD11	1:B:1830:ILE:CD1	2.27	0.59
1:B:1830:ILE:HG22	1:B:1831:ASP:N	2.18	0.59
1:B:2584:TRP:CZ3	1:B:2732:PRO:CB	2.86	0.59
1:B:3150:VAL:HG22	1:B:3532:TRP:CD1	2.38	0.59
1:B:4247:MET:CE	1:B:4252:TYR:CE2	2.86	0.59
1:B:3822:HIS:HB3	1:B:3825:TYR:CZ	2.38	0.59
1:A:3150:VAL:HG22	1:A:3532:TRP:CD1	2.38	0.58
1:B:2549:GLN:HG3	1:B:2572:LEU:CD1	2.29	0.58
1:A:2830:LEU:HD12	1:A:2871:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3683:ASP:HB2	1:A:4137:ASN:OD1	2.03	0.58
1:A:2294:GLU:OE1	1:A:2299:GLN:NE2	2.37	0.58
1:A:4247:MET:CE	1:A:4252:TYR:CE2	2.86	0.58
1:B:3639:GLU:OE2	1:B:4137:ASN:ND2	2.22	0.58
1:A:2472:TYR:HB2	1:A:2541:ILE:HD11	1.84	0.58
1:A:4027:LEU:HD23	1:A:4058:LEU:HD13	1.86	0.58
1:B:2588:HIS:HA	1:B:2707:GLN:NE2	2.18	0.58
1:A:2588:HIS:HA	1:A:2707:GLN:NE2	2.18	0.58
1:B:2279:LEU:O	1:B:2283:VAL:HG23	2.04	0.58
1:A:3822:HIS:HB3	1:A:3825:TYR:CZ	2.38	0.58
1:B:2294:GLU:OE1	1:B:2299:GLN:NE2	2.37	0.58
1:B:4027:LEU:HD23	1:B:4058:LEU:HD13	1.86	0.58
1:A:1896:LEU:HD21	1:A:1954:TRP:CZ2	2.39	0.58
1:A:2963:VAL:HG23	1:A:2967:TYR:CD2	2.39	0.58
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.36	0.58
1:B:2605:LEU:HD21	1:B:2662:PHE:CD1	2.37	0.58
1:B:4388:LEU:CD2	1:B:4434:VAL:HG13	2.33	0.58
1:A:1830:ILE:HG22	1:A:1831:ASP:N	2.18	0.58
1:A:2295:LEU:C	1:A:2338:ASN:HD21	2.07	0.58
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.36	0.58
1:B:1935:THR:HG22	1:B:2328:PRO:HG2	1.86	0.58
1:B:2295:LEU:C	1:B:2338:ASN:HD21	2.07	0.58
1:B:2912:PHE:CE2	1:B:3101:ALA:HB1	2.39	0.58
1:A:2912:PHE:CE2	1:A:3101:ALA:HB1	2.39	0.57
1:A:4388:LEU:CD2	1:A:4434:VAL:HG13	2.33	0.57
1:A:4424:LEU:HD11	1:A:4486:ILE:HD13	1.86	0.57
1:B:2963:VAL:HG23	1:B:2967:TYR:CD2	2.39	0.57
1:A:2295:LEU:HA	1:A:2338:ASN:HD22	1.70	0.57
1:A:4605:VAL:HG13	1:A:4635:PHE:CD2	2.39	0.57
1:A:2279:LEU:O	1:A:2283:VAL:HG23	2.04	0.57
1:B:1889:TYR:O	1:B:1893:THR:HG23	2.05	0.57
1:B:3683:ASP:HB2	1:B:4137:ASN:OD1	2.04	0.57
1:B:4605:VAL:HG13	1:B:4635:PHE:CD2	2.39	0.57
1:A:1571:ILE:HD13	1:A:1607:LEU:HD22	1.87	0.57
1:B:1896:LEU:HD21	1:B:1954:TRP:CZ2	2.39	0.57
1:B:2568:VAL:HG22	1:B:2603:MET:HE2	1.87	0.57
1:B:2571:THR:HG21	1:B:2747:ILE:HG12	1.87	0.57
1:B:3203:VAL:C	1:B:3204:GLY:N	2.58	0.57
1:B:4086:THR:O	1:B:4090:SER:N	2.37	0.57
1:B:4186:PHE:HE2	1:B:4252:TYR:CD2	2.23	0.57
1:A:4247:MET:HE3	1:A:4252:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4508:HIS:CE1	1:A:4587:LEU:CD2	2.88	0.57
1:B:1571:ILE:HD13	1:B:1607:LEU:HD22	1.87	0.57
1:A:1935:THR:HG22	1:A:2328:PRO:HG2	1.86	0.57
1:A:3082:SER:OG	1:A:3085:LEU:CD1	2.53	0.57
1:B:4508:HIS:CE1	1:B:4587:LEU:CD2	2.88	0.57
1:A:4186:PHE:HE2	1:A:4252:TYR:CD2	2.23	0.56
1:B:1778:LEU:CD1	1:B:1830:ILE:CD1	2.75	0.56
1:A:3451:TYR:CE1	1:A:3455:ILE:HD11	2.40	0.56
1:A:4067:THR:HG21	1:A:4083:ALA:HB1	1.87	0.56
1:B:2499:LEU:HD12	1:B:2514:LEU:HD23	1.87	0.56
1:A:2571:THR:OG1	1:A:2574:THR:OG1	2.06	0.56
1:A:3203:VAL:C	1:A:3204:GLY:N	2.58	0.56
1:B:2295:LEU:HA	1:B:2338:ASN:HD22	1.70	0.56
1:A:1892:MET:O	1:A:1896:LEU:HD13	2.05	0.56
1:A:2499:LEU:HD12	1:A:2514:LEU:HD23	1.87	0.56
1:A:2584:TRP:CZ3	1:A:2732:PRO:CB	2.86	0.56
1:A:2626:THR:O	1:A:2627:THR:CG2	2.53	0.56
1:B:3451:TYR:CE1	1:B:3455:ILE:HD11	2.40	0.56
1:A:3818:LEU:O	1:A:3821:ILE:HG22	2.06	0.56
1:A:4507:ILE:CD1	1:A:4509:VAL:CG2	2.84	0.56
1:A:1778:LEU:CD1	1:A:1830:ILE:CD1	2.75	0.56
1:A:1889:TYR:O	1:A:1893:THR:HG23	2.05	0.56
1:A:2591:LEU:HG	1:A:2709:VAL:HG12	1.88	0.56
1:A:3456:SER:HB3	1:B:3459:GLN:CG	2.30	0.56
1:B:4067:THR:HG21	1:B:4083:ALA:HB1	1.87	0.56
1:B:4560:VAL:HG12	1:B:4563:LEU:HD11	1.88	0.56
1:A:1644:SER:HA	1:A:1650:LEU:HD11	1.88	0.56
1:A:3822:HIS:HB3	1:A:3825:TYR:CE1	2.41	0.56
1:A:4186:PHE:CZ	1:A:4265:LEU:CD1	2.77	0.56
1:B:1644:SER:HA	1:B:1650:LEU:HD11	1.88	0.56
1:B:1879:LEU:HD11	1:B:1914:GLU:C	2.27	0.56
1:B:4507:ILE:CD1	1:B:4509:VAL:CG2	2.84	0.56
1:B:2626:THR:O	1:B:2627:THR:CG2	2.53	0.56
1:A:2571:THR:HG21	1:A:2747:ILE:HG12	1.87	0.55
1:B:2461:MET:HE3	1:B:2584:TRP:CZ2	2.41	0.55
1:B:2994:MET:CE	1:B:3008:MET:SD	2.94	0.55
1:B:4561:THR:HG22	1:B:4587:LEU:HD13	1.88	0.55
1:A:1879:LEU:HD11	1:A:1914:GLU:C	2.27	0.55
1:A:2091:ARG:CZ	2:A:4801:ADP:H5'2	2.36	0.55
1:B:2609:LEU:HD11	1:B:2615:MET:HB3	1.83	0.55
1:A:2994:MET:CE	1:A:3008:MET:SD	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2591:LEU:HG	1:B:2709:VAL:HG12	1.88	0.55
1:A:1830:ILE:CG2	1:A:1831:ASP:N	2.69	0.55
1:A:4561:THR:HG22	1:A:4587:LEU:HD13	1.88	0.55
1:B:2464:GLN:HG2	1:B:2583:THR:CG2	2.32	0.55
1:A:2897:LEU:HD23	1:A:2901:TYR:OH	2.07	0.55
1:A:2091:ARG:HH11	2:A:4801:ADP:H5'2	1.71	0.55
1:B:1892:MET:O	1:B:1896:LEU:HD13	2.05	0.55
1:A:1765:ALA:CB	1:A:1778:LEU:HD23	2.37	0.55
1:B:2897:LEU:HD23	1:B:2901:TYR:OH	2.07	0.55
1:B:1830:ILE:CG2	1:B:1831:ASP:N	2.69	0.55
1:B:3082:SER:OG	1:B:3085:LEU:CD1	2.53	0.55
1:B:4395:LEU:HD21	1:B:4483:SER:HA	1.88	0.55
1:A:2609:LEU:HD11	1:A:2615:MET:HB3	1.83	0.55
1:A:4560:VAL:HG12	1:A:4563:LEU:HD11	1.88	0.55
1:B:3822:HIS:HB3	1:B:3825:TYR:CE1	2.41	0.55
1:B:4424:LEU:HD11	1:B:4486:ILE:HD13	1.86	0.55
1:A:3008:MET:HE1	1:A:3066:PHE:CZ	2.41	0.55
1:A:3236:ALA:HB1	1:A:3451:TYR:HE1	1.72	0.55
1:A:4186:PHE:HZ	1:A:4265:LEU:HD12	1.71	0.54
1:B:2091:ARG:CZ	2:B:4801:ADP:H5'2	2.36	0.54
1:A:4395:LEU:HD21	1:A:4483:SER:HA	1.88	0.54
1:B:4560:VAL:HG12	1:B:4563:LEU:CD1	2.38	0.54
1:B:1765:ALA:CB	1:B:1778:LEU:HD23	2.37	0.54
1:B:3818:LEU:O	1:B:3821:ILE:HG22	2.06	0.54
1:A:2457:SER:CA	1:A:2584:TRP:CH2	2.91	0.54
1:A:2893:VAL:O	1:A:2897:LEU:HD13	2.07	0.54
1:A:4560:VAL:HG12	1:A:4563:LEU:CD1	2.38	0.54
1:A:4067:THR:HG21	1:A:4083:ALA:CB	2.37	0.54
1:B:2893:VAL:O	1:B:2897:LEU:HD13	2.07	0.54
1:A:2192:THR:OG1	1:A:2373:MET:HG3	2.07	0.54
1:A:2312:VAL:HG11	1:A:2355:THR:CG2	2.38	0.54
1:A:2552:VAL:HG23	1:A:2552:VAL:O	2.08	0.54
1:A:2464:GLN:OE1	1:A:2586:ALA:HB3	2.08	0.54
1:B:2464:GLN:OE1	1:B:2586:ALA:HB3	2.08	0.54
1:B:3150:VAL:O	1:B:3153:THR:OG1	2.25	0.54
1:B:4511:LEU:HD22	1:B:4644:CYS:HG	1.66	0.54
1:A:2190:TYR:O	1:A:2377:ASN:CG	2.46	0.54
1:B:3745:LEU:HD11	1:B:3773:LEU:HA	1.89	0.54
1:A:2295:LEU:HA	1:A:2338:ASN:ND2	2.23	0.54
1:A:4086:THR:O	1:A:4090:SER:N	2.37	0.54
1:B:2190:TYR:O	1:B:2377:ASN:CG	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2767:GLU:N	1:B:2768:PRO:HD2	2.23	0.54
1:B:2819:GLU:CD	1:B:2862:ASP:CB	2.77	0.54
1:A:3745:LEU:HD11	1:A:3773:LEU:HA	1.89	0.54
1:B:1765:ALA:HB3	1:B:1778:LEU:HD23	1.89	0.53
1:B:2295:LEU:HA	1:B:2338:ASN:ND2	2.23	0.53
1:B:3222:LEU:HD12	1:B:3465:LEU:HD23	1.90	0.53
1:B:3803:PRO:C	1:B:3804:LEU:N	2.62	0.53
1:B:3822:HIS:C	1:B:3823:PHE:CD2	2.81	0.53
1:B:4067:THR:HG21	1:B:4083:ALA:CB	2.37	0.53
1:A:2767:GLU:N	1:A:2768:PRO:HD2	2.23	0.53
1:A:3803:PRO:C	1:A:3804:LEU:N	2.62	0.53
1:B:4247:MET:HE3	1:B:4252:TYR:HE2	1.72	0.53
1:A:2300:TRP:CD2	1:A:2342:MET:HE3	2.43	0.53
1:A:3150:VAL:O	1:A:3153:THR:OG1	2.25	0.53
1:A:1765:ALA:HB3	1:A:1778:LEU:HD23	1.89	0.53
1:A:2265:TYR:CD2	1:A:2314:ASN:ND2	2.76	0.53
1:A:2549:GLN:HG3	1:A:2572:LEU:CD1	2.29	0.53
1:A:3822:HIS:C	1:A:3823:PHE:CD2	2.81	0.53
1:B:1879:LEU:CD1	1:B:1914:GLU:O	2.55	0.53
1:B:2552:VAL:HG23	1:B:2552:VAL:O	2.08	0.53
1:B:4622:VAL:HG11	1:B:4624:PHE:HZ	1.69	0.53
1:A:2461:MET:HE3	1:A:2584:TRP:CZ2	2.44	0.53
1:B:2091:ARG:HH11	2:B:4801:ADP:H5'2	1.71	0.53
1:A:2182:LEU:HD11	1:A:2207:VAL:HG11	1.91	0.53
1:A:3175:HIS:CD2	1:A:3585:ARG:CZ	2.92	0.53
1:B:2192:THR:OG1	1:B:2373:MET:HG3	2.07	0.53
1:B:3205:LEU:O	1:B:3208:ILE:HG22	2.09	0.53
1:A:2464:GLN:HG2	1:A:2583:THR:CG2	2.32	0.53
1:B:2457:SER:CA	1:B:2584:TRP:CH2	2.91	0.53
1:A:2238:LEU:HD13	1:A:2300:TRP:CE3	2.44	0.53
1:A:2584:TRP:HZ3	1:A:2732:PRO:HG3	1.60	0.53
1:A:3811:ILE:CD1	1:A:3887:LEU:CD2	2.87	0.53
1:B:2046:ARG:HA	1:B:2049:ILE:HG22	1.90	0.53
1:B:2238:LEU:HD13	1:B:2300:TRP:CE3	2.44	0.53
1:B:3236:ALA:HB1	1:B:3451:TYR:HE1	1.72	0.53
1:B:4607:LEU:CD2	1:B:4635:PHE:CE2	2.92	0.53
1:A:1762:VAL:O	1:A:1766:LEU:CD1	2.58	0.52
1:A:3205:LEU:O	1:A:3208:ILE:HG22	2.09	0.52
1:B:3236:ALA:HB1	1:B:3451:TYR:CE1	2.44	0.52
1:B:3749:LEU:HD13	1:B:3773:LEU:HD12	1.74	0.52
1:B:2302:VAL:HG22	1:B:2342:MET:CB	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2265:TYR:CD2	1:B:2314:ASN:ND2	2.76	0.52
1:B:3175:HIS:CD2	1:B:3585:ARG:CZ	2.92	0.52
1:B:3882:THR:OG1	1:B:4342:LYS:NZ	2.35	0.52
1:A:1825:LEU:HD12	1:A:1830:ILE:CD1	2.38	0.52
1:B:2345:VAL:HG11	1:B:2348:LEU:HD21	1.91	0.52
1:B:3010:THR:HG22	1:B:3016:GLU:O	2.10	0.52
1:A:1970:ALA:CB	1:A:4073:SER:HB2	2.40	0.52
1:A:2046:ARG:HA	1:A:2049:ILE:HG22	1.90	0.52
1:A:2584:TRP:CH2	1:A:2732:PRO:HB3	2.45	0.52
1:A:2819:GLU:CD	1:A:2862:ASP:CB	2.76	0.52
1:A:3236:ALA:HB1	1:A:3451:TYR:CE1	2.44	0.52
1:B:2312:VAL:HG11	1:B:2355:THR:CG2	2.38	0.52
1:A:4607:LEU:CD2	1:A:4635:PHE:CE2	2.92	0.52
1:B:3824:LEU:HD21	1:B:4130:ILE:HG12	1.92	0.52
1:A:2091:ARG:CZ	2:A:4801:ADP:H4'	2.40	0.52
1:A:2345:VAL:HG11	1:A:2348:LEU:HD21	1.91	0.52
1:A:2994:MET:HE1	1:A:3008:MET:SD	2.49	0.52
1:A:3222:LEU:HD12	1:A:3465:LEU:HD23	1.90	0.52
1:B:2182:LEU:HD11	1:B:2207:VAL:HG11	1.91	0.52
1:B:2307:VAL:HG13	1:B:2312:VAL:HG21	1.92	0.52
1:A:2302:VAL:HG22	1:A:2342:MET:CB	2.31	0.52
1:A:3102:LEU:O	1:A:3105:VAL:HG12	2.10	0.52
1:A:3817:SER:HG	1:A:4349:LEU:HD12	1.72	0.52
1:B:2091:ARG:CZ	2:B:4801:ADP:H4'	2.40	0.52
1:B:2300:TRP:CD2	1:B:2342:MET:HE3	2.46	0.51
1:A:2549:GLN:CG	1:A:2572:LEU:HD22	2.40	0.51
1:A:2648:VAL:HG11	1:A:2694:ARG:NH2	2.26	0.51
1:A:3882:THR:OG1	1:A:4342:LYS:NZ	2.35	0.51
1:A:2230:LYS:NZ	3:A:4802:ATP:O3G	2.43	0.51
1:B:3811:ILE:CD1	1:B:3887:LEU:CD2	2.87	0.51
1:A:4589:GLN:C	1:A:4590:LEU:HD12	2.31	0.51
1:B:2078:GLU:OE1	1:B:4522:THR:CG2	2.58	0.51
1:A:1490:TRP:CG	1:A:1538:ILE:HD12	2.45	0.51
1:A:2588:HIS:HA	1:A:2707:GLN:HE22	1.76	0.51
1:A:2849:ASN:O	1:A:2852:THR:HG22	2.11	0.51
1:A:3021:PHE:CG	1:A:3029:LEU:CD1	2.93	0.51
1:B:1970:ALA:CB	1:B:4073:SER:HB2	2.40	0.51
1:B:4589:GLN:C	1:B:4590:LEU:HD12	2.31	0.51
1:A:4186:PHE:HE2	1:A:4252:TYR:CG	2.28	0.51
1:A:4622:VAL:HG11	1:A:4624:PHE:HZ	1.70	0.51
1:B:2584:TRP:CH2	1:B:2732:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2584:TRP:CH2	1:B:2732:PRO:CB	2.93	0.51
1:B:4042:LEU:CD2	1:B:4139:LEU:HD23	2.41	0.51
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.75	0.51
1:A:4609:VAL:HG23	1:A:4622:VAL:HG23	1.93	0.51
1:A:1750:VAL:HG12	1:A:1811:LEU:HD13	1.93	0.51
1:B:1750:VAL:HG12	1:B:1811:LEU:HD13	1.93	0.51
1:B:2605:LEU:HD21	1:B:2662:PHE:HD1	1.75	0.51
1:B:3021:PHE:CG	1:B:3029:LEU:CD1	2.93	0.51
1:B:4186:PHE:HE2	1:B:4252:TYR:CG	2.28	0.51
1:B:2149:LEU:HD11	1:B:2157:LEU:CD2	2.40	0.51
1:B:2230:LYS:NZ	3:B:4802:ATP:O3G	2.43	0.51
1:A:2307:VAL:HG13	1:A:2312:VAL:HG21	1.92	0.51
1:A:2584:TRP:CH2	1:A:2732:PRO:CB	2.93	0.51
1:B:4609:VAL:HG23	1:B:4622:VAL:HG23	1.93	0.51
1:A:2568:VAL:HG22	1:A:2603:MET:HE3	1.91	0.51
1:B:1490:TRP:CG	1:B:1538:ILE:HD12	2.45	0.51
1:B:1762:VAL:O	1:B:1766:LEU:CD1	2.57	0.51
1:B:2648:VAL:HG11	1:B:2694:ARG:NH2	2.26	0.51
1:B:2588:HIS:HA	1:B:2707:GLN:HE22	1.76	0.51
1:B:3021:PHE:CG	1:B:3029:LEU:HD13	2.46	0.51
1:B:3102:LEU:O	1:B:3105:VAL:HG12	2.10	0.51
1:B:4507:ILE:HD12	1:B:4509:VAL:HG22	1.93	0.51
1:B:4560:VAL:CG1	1:B:4563:LEU:HD11	2.41	0.51
1:B:4622:VAL:CG1	1:B:4624:PHE:HE2	2.15	0.51
1:A:2593:LEU:HD11	1:A:2605:LEU:HB2	1.93	0.50
1:A:4607:LEU:HD21	1:A:4635:PHE:CE2	2.41	0.50
1:B:1752:LEU:CD2	1:B:1756:ILE:HD11	2.41	0.50
1:B:2549:GLN:CG	1:B:2572:LEU:HD22	2.41	0.50
1:A:1752:LEU:CD2	1:A:1756:ILE:HD11	2.41	0.50
1:A:2593:LEU:CD2	1:A:2734:VAL:CG2	2.89	0.50
1:A:4622:VAL:HG12	1:A:4624:PHE:CZ	2.28	0.50
1:B:3888:ALA:HB1	1:B:4012:ASN:HD22	1.75	0.50
1:B:4186:PHE:HZ	1:B:4265:LEU:HD12	1.71	0.50
1:A:3010:THR:HG22	1:A:3016:GLU:O	2.10	0.50
1:A:3021:PHE:CG	1:A:3029:LEU:HD13	2.46	0.50
1:A:3097:TRP:CE3	1:A:3173:PRO:HB3	2.47	0.50
1:A:1879:LEU:CD1	1:A:1914:GLU:O	2.55	0.50
1:B:2849:ASN:O	1:B:2852:THR:HG22	2.11	0.50
1:A:3521:ASP:OD1	1:A:3702:THR:HG21	2.11	0.50
1:A:4560:VAL:CG1	1:A:4563:LEU:HD11	2.41	0.50
1:A:2072:PHE:CZ	1:A:2157:LEU:HD11	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2635:PHE:CZ	1:A:2686:MET:HE1	2.46	0.50
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.93	0.50
1:A:3824:LEU:HD21	1:A:4130:ILE:HG12	1.92	0.50
1:A:1537:TRP:CH2	1:A:1578:LEU:HD21	2.47	0.50
1:A:4042:LEU:CD2	1:A:4139:LEU:HD23	2.41	0.50
1:B:1537:TRP:CH2	1:B:1578:LEU:HD21	2.47	0.50
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.93	0.49
1:A:3821:ILE:HG23	1:A:3822:HIS:N	2.28	0.49
1:B:3097:TRP:CE3	1:B:3173:PRO:HB3	2.47	0.49
1:B:2635:PHE:CZ	1:B:2686:MET:HE1	2.48	0.49
1:B:4447:TYR:CE2	1:B:4451:LEU:HD11	2.47	0.49
1:A:2078:GLU:OE1	1:A:4522:THR:CG2	2.58	0.49
1:B:3521:ASP:OD1	1:B:3702:THR:HG21	2.11	0.49
1:B:3478:LEU:CD1	1:B:3770:LEU:HD13	2.43	0.49
1:A:1792:LEU:HD13	1:A:1812:ILE:HG13	1.95	0.49
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.94	0.49
1:A:4507:ILE:HD12	1:A:4509:VAL:HG22	1.93	0.49
1:B:3822:HIS:C	1:B:3823:PHE:CG	2.86	0.49
1:A:3208:ILE:HD12	1:A:3482:LEU:HB3	1.95	0.49
1:A:3680:SER:O	1:A:3681:THR:HG23	2.12	0.49
1:A:3708:LEU:HD21	1:A:3809:SER:HA	1.93	0.49
1:B:1792:LEU:HD13	1:B:1812:ILE:HG13	1.95	0.49
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.94	0.49
1:B:2493:TYR:HA	1:B:2539:VAL:HG11	1.95	0.49
1:B:3821:ILE:HG23	1:B:3822:HIS:N	2.28	0.49
1:A:2457:SER:HA	1:A:2584:TRP:CH2	2.47	0.49
1:A:4434:VAL:HA	1:A:4437:VAL:HG22	1.95	0.49
1:B:2072:PHE:CZ	1:B:2157:LEU:HD11	2.45	0.49
1:B:2457:SER:HA	1:B:2584:TRP:CH2	2.47	0.49
1:B:2593:LEU:HD11	1:B:2605:LEU:HB2	1.93	0.49
1:B:2994:MET:HE2	1:B:3008:MET:SD	2.53	0.49
1:A:3509:LEU:HB3	1:A:3529:PHE:CE1	2.48	0.49
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	1.95	0.49
1:A:3639:GLU:CD	1:A:4137:ASN:HD21	2.11	0.49
1:B:3208:ILE:HD12	1:B:3482:LEU:HB3	1.95	0.49
1:A:2662:PHE:CZ	1:A:2711:ALA:HB2	2.48	0.48
1:B:1825:LEU:HD12	1:B:1830:ILE:CD1	2.38	0.48
1:B:3639:GLU:CD	1:B:4137:ASN:HD21	2.11	0.48
1:A:2585:LEU:HB2	1:A:2612:LEU:HD11	1.95	0.48
1:B:3509:LEU:HB3	1:B:3529:PHE:CE1	2.48	0.48
1:B:3680:SER:O	1:B:3681:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4635:PHE:CZ	1:B:4640:VAL:HB	2.48	0.48
1:A:2605:LEU:HD21	1:A:2662:PHE:HD1	1.75	0.48
1:A:4635:PHE:CZ	1:A:4640:VAL:HB	2.48	0.48
1:B:2662:PHE:CZ	1:B:2711:ALA:HB2	2.48	0.48
1:B:4434:VAL:HA	1:B:4437:VAL:HG22	1.95	0.48
1:A:3745:LEU:HD22	1:A:3776:GLU:CB	2.44	0.48
1:B:4248:ALA:HB1	1:B:4266:ASN:OD1	2.14	0.48
1:A:3638:VAL:H	1:A:3681:THR:HG22	1.79	0.48
1:A:2230:LYS:N	3:A:4802:ATP:O1B	2.46	0.48
1:B:4609:VAL:CG2	1:B:4622:VAL:CG2	2.92	0.48
1:A:4447:TYR:CE2	1:A:4451:LEU:HD11	2.47	0.48
1:B:2626:THR:HG22	1:B:2679:VAL:HG21	1.96	0.48
1:A:2602:THR:HG22	1:A:2662:PHE:CZ	2.49	0.48
1:B:2591:LEU:HD12	1:B:2591:LEU:C	2.34	0.48
1:A:4622:VAL:CG1	1:A:4624:PHE:HE2	2.15	0.48
1:B:3745:LEU:HD22	1:B:3776:GLU:CB	2.44	0.48
1:A:2493:TYR:HA	1:A:2539:VAL:HG11	1.95	0.48
1:A:3021:PHE:CD1	1:A:3029:LEU:CD1	2.97	0.48
1:B:2668:LEU:N	1:B:2669:PRO:CD	2.77	0.48
1:B:3811:ILE:HD12	1:B:3887:LEU:CD2	2.44	0.48
1:B:4041:VAL:HG11	1:B:4125:PHE:CE2	2.49	0.48
1:B:4186:PHE:CZ	1:B:4265:LEU:HD12	2.48	0.48
1:A:2069:ILE:HD12	1:A:2137:LEU:HD21	1.96	0.47
1:A:3822:HIS:C	1:A:3823:PHE:CG	2.86	0.47
1:A:4041:VAL:HG11	1:A:4125:PHE:CE2	2.49	0.47
1:B:2585:LEU:HB2	1:B:2612:LEU:HD11	1.95	0.47
1:B:3021:PHE:CD1	1:B:3029:LEU:CD1	2.97	0.47
1:B:3638:VAL:H	1:B:3681:THR:HG22	1.79	0.47
1:B:2599:SER:N	2:B:4804:ADP:O2A	2.43	0.47
1:A:2591:LEU:C	1:A:2591:LEU:HD12	2.34	0.47
1:A:4609:VAL:CG2	1:A:4622:VAL:CG2	2.92	0.47
1:B:2602:THR:HG22	1:B:2662:PHE:CZ	2.49	0.47
1:B:3509:LEU:HD21	1:B:3536:LEU:HD12	1.96	0.47
1:A:2149:LEU:HD11	1:A:2157:LEU:CD2	2.40	0.47
1:B:1778:LEU:HD13	1:B:1830:ILE:CD1	2.40	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.32	0.47
1:A:4387:TRP:CZ3	1:A:4391:ILE:HD13	2.49	0.47
1:A:2729:ARG:NH1	3:A:4802:ATP:O1G	2.40	0.47
1:B:4042:LEU:HD12	1:B:4126:LEU:HB2	1.95	0.47
1:B:3824:LEU:HD22	1:B:4130:ILE:CG2	2.45	0.47
1:B:2230:LYS:N	3:B:4802:ATP:O1B	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2729:ARG:NH1	3:B:4802:ATP:O1G	2.40	0.47
1:A:2191:LEU:HD22	3:A:4802:ATP:C5	2.50	0.47
1:A:2568:VAL:CG2	1:A:2603:MET:HE3	2.44	0.47
1:A:4508:HIS:ND1	1:A:4587:LEU:CD2	2.77	0.47
1:B:1766:LEU:HD12	1:B:1778:LEU:HD21	1.96	0.47
1:B:2231:SER:OG	1:B:2344:GLU:OE2	2.32	0.47
1:B:4508:HIS:ND1	1:B:4587:LEU:CD2	2.77	0.47
1:A:4248:ALA:HB1	1:A:4266:ASN:OD1	2.14	0.47
1:B:2069:ILE:HD12	1:B:2137:LEU:HD21	1.96	0.47
1:A:3554:SER:HB2	1:A:3578:ILE:HD12	1.96	0.47
1:A:4042:LEU:HD12	1:A:4126:LEU:HB2	1.95	0.47
1:B:4387:TRP:CZ3	1:B:4391:ILE:HD13	2.49	0.47
1:B:2191:LEU:HD22	3:B:4802:ATP:C5	2.50	0.47
1:A:2154:ILE:N	1:A:2155:PRO:CD	2.78	0.47
1:A:4566:GLN:HE21	1:A:4643:LEU:HD11	1.80	0.47
1:B:2154:ILE:N	1:B:2155:PRO:CD	2.78	0.47
1:B:3716:VAL:HG21	1:B:3804:LEU:HD23	1.95	0.47
1:B:3478:LEU:HD22	1:B:3770:LEU:HD13	1.96	0.47
1:A:1541:GLN:O	1:A:1545:VAL:HG23	2.15	0.47
1:A:2626:THR:HG22	1:A:2679:VAL:HG21	1.96	0.47
1:A:3478:LEU:HD22	1:A:3770:LEU:HD13	1.96	0.47
1:B:3554:SER:HB2	1:B:3578:ILE:HD12	1.96	0.47
1:A:1766:LEU:HD12	1:A:1778:LEU:HD21	1.96	0.47
1:A:2568:VAL:HG22	1:A:2603:MET:HE2	1.95	0.47
1:A:4427:VAL:O	1:A:4431:LEU:HG	2.15	0.47
1:B:3522:GLN:HB2	1:B:3704:THR:HG22	1.97	0.47
1:B:3888:ALA:HA	1:B:4013:LEU:HD21	1.97	0.47
1:A:2668:LEU:N	1:A:2669:PRO:CD	2.77	0.47
1:A:3645:LEU:HD23	1:A:3648:VAL:HB	1.97	0.47
1:A:3478:LEU:CD1	1:A:3770:LEU:HD22	2.45	0.47
1:B:2461:MET:CE	1:B:2584:TRP:CZ2	2.98	0.47
1:B:2922:ILE:HD12	1:B:2933:LEU:HD21	1.96	0.47
1:A:3888:ALA:HA	1:A:4013:LEU:HD21	1.97	0.46
1:B:1504:VAL:HG11	1:B:1524:GLU:HB2	1.97	0.46
1:B:2103:VAL:HG13	1:B:2136:ILE:CG2	2.46	0.46
1:A:2308:ASP:OD2	1:A:2310:GLU:HB3	2.15	0.46
1:A:2461:MET:CE	1:A:2584:TRP:CZ2	2.98	0.46
1:B:2752:ASN:HD22	1:B:2770:THR:HG22	1.76	0.46
1:A:3008:MET:HE2	1:A:3066:PHE:HZ	1.75	0.46
1:A:3811:ILE:HD12	1:A:3887:LEU:CD2	2.44	0.46
1:A:4507:ILE:HD12	1:A:4509:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2958:VAL:HG13	1:B:2993:ILE:HG12	1.98	0.46
1:B:4427:VAL:O	1:B:4431:LEU:HG	2.15	0.46
1:A:2058:GLY:O	1:A:2104:LYS:CE	2.61	0.46
1:A:3509:LEU:HD21	1:A:3536:LEU:HD12	1.96	0.46
1:A:2922:ILE:HD12	1:A:2933:LEU:HD21	1.96	0.46
1:A:3478:LEU:CD1	1:A:3770:LEU:HD13	2.43	0.46
1:A:3824:LEU:HD22	1:A:4130:ILE:CG2	2.45	0.46
1:B:3645:LEU:HD23	1:B:3648:VAL:HB	1.97	0.46
1:A:4387:TRP:CH2	1:A:4391:ILE:HG21	2.51	0.46
1:B:2191:LEU:HD23	1:B:2377:ASN:ND2	2.30	0.46
1:B:4566:GLN:HE21	1:B:4643:LEU:HD11	1.80	0.46
1:A:2103:VAL:HG13	1:A:2136:ILE:CG2	2.46	0.46
1:B:3478:LEU:CD1	1:B:3770:LEU:HD22	2.45	0.46
1:B:3817:SER:OG	1:B:4349:LEU:HD13	2.10	0.46
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.97	0.46
1:B:1541:GLN:O	1:B:1545:VAL:HG23	2.15	0.46
1:B:3203:VAL:O	1:B:3207:LYS:N	2.47	0.46
1:B:1792:LEU:HD22	1:B:1808:LEU:HD22	1.97	0.46
1:B:4607:LEU:HD12	1:B:4624:PHE:CE2	2.51	0.46
1:A:3522:GLN:HB2	1:A:3704:THR:HG22	1.97	0.46
1:A:3683:ASP:CB	1:A:4137:ASN:OD1	2.64	0.46
1:B:3683:ASP:CB	1:B:4137:ASN:OD1	2.64	0.46
1:A:2304:ASP:OD1	1:A:2684:ARG:NH2	2.47	0.45
1:A:2958:VAL:HG13	1:A:2993:ILE:HG12	1.98	0.45
1:A:3745:LEU:HD22	1:A:3776:GLU:HB2	1.98	0.45
1:A:4042:LEU:HD11	1:A:4128:MET:HE3	1.98	0.45
1:B:2058:GLY:O	1:B:2104:LYS:CE	2.61	0.45
1:B:2308:ASP:OD2	1:B:2310:GLU:HB3	2.16	0.45
1:B:3745:LEU:HD11	1:B:3773:LEU:HD22	1.98	0.45
1:A:1778:LEU:HD13	1:A:1830:ILE:CD1	2.40	0.45
1:A:2191:LEU:HD23	1:A:2377:ASN:ND2	2.30	0.45
1:A:4186:PHE:CZ	1:A:4265:LEU:HD12	2.48	0.45
1:A:3814:THR:OG1	1:A:3890:ILE:HD11	2.16	0.45
1:A:3817:SER:OG	1:A:4349:LEU:HD13	2.10	0.45
1:B:4387:TRP:CH2	1:B:4391:ILE:HG21	2.51	0.45
1:B:4507:ILE:HD12	1:B:4509:VAL:CG2	2.46	0.45
1:B:3717:LEU:HD11	1:B:3797:VAL:HG11	1.99	0.45
1:A:2254:ILE:HG12	1:A:2279:LEU:HD21	1.98	0.45
1:B:1931:ASN:HD22	1:B:2317:SER:CA	2.26	0.45
1:A:2213:ILE:CG2	1:A:2220:LEU:HD13	2.47	0.45
1:A:1931:ASN:HD22	1:A:2317:SER:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4607:LEU:HD12	1:A:4624:PHE:CE2	2.51	0.45
1:B:2079:GLN:OE1	1:B:4526:GLN:NE2	2.47	0.45
1:A:2461:MET:HE3	1:A:2584:TRP:HZ2	1.80	0.45
1:A:2709:VAL:HG23	1:A:2709:VAL:O	2.17	0.45
1:A:3745:LEU:HD11	1:A:3773:LEU:HD22	1.98	0.45
1:B:1985:HIS:CD2	1:B:1997:ILE:HD12	2.52	0.45
1:B:2213:ILE:CG2	1:B:2220:LEU:HD13	2.47	0.45
1:B:2254:ILE:HG12	1:B:2279:LEU:HD21	1.98	0.45
1:B:2994:MET:HE1	1:B:3008:MET:SD	2.57	0.45
1:B:3871:VAL:HG11	1:B:3883:PHE:CE2	2.52	0.45
1:B:4042:LEU:HD11	1:B:4128:MET:CE	2.47	0.45
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	1.97	0.45
1:A:3871:VAL:HG11	1:A:3883:PHE:CE2	2.52	0.45
1:B:3814:THR:OG1	1:B:3890:ILE:HD11	2.16	0.45
1:B:4178:ARG:HG2	1:B:4278:PHE:CE1	2.52	0.45
1:A:3680:SER:O	1:A:3681:THR:CG2	2.65	0.45
1:A:3801:TYR:CD1	1:A:3856:LEU:HD22	2.52	0.45
1:B:4240:TRP:CZ3	1:B:4273:PHE:O	2.70	0.45
1:A:3203:VAL:O	1:A:3207:LYS:N	2.47	0.45
1:A:3822:HIS:NE2	1:A:3876:LEU:CD1	2.79	0.45
1:A:4097:LYS:HA	1:A:4127:THR:HG22	1.98	0.45
1:B:2593:LEU:CD2	1:B:2734:VAL:CG2	2.89	0.45
1:B:3822:HIS:NE2	1:B:3876:LEU:CD1	2.79	0.45
1:B:4088:VAL:HG22	1:B:4122:PHE:CE2	2.52	0.45
1:B:4097:LYS:HA	1:B:4127:THR:HG22	1.98	0.45
1:A:4178:ARG:HG2	1:A:4278:PHE:CE1	2.52	0.44
1:B:2569:VAL:O	1:B:2569:VAL:HG13	2.17	0.44
1:B:2568:VAL:HG22	1:B:2603:MET:HE3	1.99	0.44
1:B:3102:LEU:HB3	1:B:3148:VAL:HG22	1.99	0.44
1:B:3683:ASP:CG	1:B:4137:ASN:OD1	2.56	0.44
1:A:2458:LEU:HD13	1:A:2498:ILE:HG22	1.99	0.44
1:B:2515:GLY:HA2	1:B:2534:ILE:HD12	1.99	0.44
1:A:2358:ARG:HH22	2:A:4801:ADP:PB	2.40	0.44
1:A:2515:GLY:HA2	1:A:2534:ILE:HD12	1.99	0.44
1:A:2453:ARG:HD2	1:A:2733:VAL:HG12	2.00	0.44
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.52	0.44
1:A:4042:LEU:HD11	1:A:4128:MET:CE	2.47	0.44
1:B:2622:PHE:CE2	1:B:2679:VAL:HG11	2.52	0.44
1:A:2766:ALA:O	1:A:2770:THR:HG23	2.18	0.44
1:A:4088:VAL:HG22	1:A:4122:PHE:CE2	2.52	0.44
1:A:4508:HIS:ND1	1:A:4587:LEU:HD21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1931:ASN:ND2	1:B:2317:SER:N	2.65	0.44
1:B:3745:LEU:HD22	1:B:3776:GLU:HB2	1.98	0.44
1:A:1931:ASN:HD22	1:A:2317:SER:CA	2.27	0.44
1:A:1985:HIS:CD2	1:A:1997:ILE:HD12	2.52	0.44
1:A:3822:HIS:CG	1:A:3822:HIS:O	2.71	0.44
1:B:2304:ASP:OD1	1:B:2684:ARG:NH2	2.47	0.44
1:B:2358:ARG:NH2	2:B:4801:ADP:PB	2.89	0.44
1:B:3567:LEU:HB2	1:B:3599:PHE:CD1	2.52	0.44
1:A:2358:ARG:NH2	2:A:4801:ADP:PB	2.89	0.44
1:A:2874:SER:OG	1:A:2875:ASN:N	2.51	0.44
1:A:3717:LEU:HD11	1:A:3797:VAL:HG11	1.99	0.44
1:B:3572:LEU:C	1:B:3572:LEU:HD23	2.38	0.44
1:A:2605:LEU:HD23	1:A:2662:PHE:CD1	2.44	0.44
1:A:2622:PHE:CE2	1:A:2679:VAL:HG11	2.52	0.44
1:A:3102:LEU:HB3	1:A:3148:VAL:HG22	1.99	0.44
1:B:1931:ASN:HD22	1:B:2317:SER:N	2.15	0.44
1:B:2358:ARG:HH22	2:B:4801:ADP:PB	2.40	0.44
1:B:2461:MET:HE3	1:B:2584:TRP:HZ2	1.79	0.44
1:B:2453:ARG:HD2	1:B:2733:VAL:HG12	2.00	0.44
1:B:2874:SER:OG	1:B:2875:ASN:N	2.51	0.44
1:B:3680:SER:O	1:B:3681:THR:CG2	2.65	0.44
1:B:4609:VAL:CG2	1:B:4622:VAL:HG23	2.48	0.44
1:B:1879:LEU:HD21	1:B:1914:GLU:CG	2.47	0.44
1:B:2551:LYS:C	1:B:2551:LYS:CD	2.86	0.44
1:B:2569:VAL:HG11	1:B:2747:ILE:HG23	1.99	0.44
1:B:4508:HIS:ND1	1:B:4587:LEU:HD21	2.33	0.44
1:A:2568:VAL:CG2	1:A:2603:MET:CE	2.95	0.44
1:A:3572:LEU:C	1:A:3572:LEU:HD23	2.38	0.44
1:A:3609:ILE:HG12	1:A:3632:PRO:HG2	1.99	0.44
1:A:4240:TRP:CZ3	1:A:4273:PHE:O	2.70	0.44
1:A:2079:GLN:OE1	1:A:4526:GLN:NE2	2.47	0.44
1:B:3708:LEU:HD21	1:B:3809:SER:HA	1.93	0.44
1:B:3801:TYR:CD1	1:B:3856:LEU:HD22	2.52	0.44
1:A:2284:LEU:HB3	1:A:2333:LEU:HD13	2.00	0.43
1:A:3822:HIS:CB	1:A:3825:TYR:CZ	3.01	0.43
1:B:1550:ILE:HD13	1:B:1638:LEU:HD22	2.00	0.43
1:B:3609:ILE:HG12	1:B:3632:PRO:HG2	1.99	0.43
1:B:3822:HIS:O	1:B:3822:HIS:CG	2.71	0.43
1:A:1879:LEU:HD21	1:A:1914:GLU:CG	2.47	0.43
1:A:2335:LEU:HD11	1:A:2341:ILE:HD11	2.00	0.43
1:A:2871:ILE:HG23	1:A:2871:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2335:LEU:HD11	1:B:2341:ILE:HD11	2.00	0.43
1:B:2709:VAL:O	1:B:2709:VAL:HG23	2.17	0.43
1:B:2910:VAL:CG1	1:B:3105:VAL:HG23	2.47	0.43
1:B:3832:PHE:O	1:B:3835:ILE:HB	2.18	0.43
1:A:2519:ARG:HA	1:A:2526:LEU:CD1	2.49	0.43
1:B:2568:VAL:CG2	1:B:2603:MET:CE	2.95	0.43
1:B:3822:HIS:CB	1:B:3825:TYR:CZ	3.01	0.43
1:A:1931:ASN:ND2	1:A:2317:SER:N	2.65	0.43
1:A:3832:PHE:O	1:A:3835:ILE:HB	2.18	0.43
1:B:2220:LEU:CD2	1:B:2342:MET:HE2	2.49	0.43
1:B:2571:THR:OG1	1:B:2574:THR:OG1	2.06	0.43
1:B:3574:THR:O	1:B:3578:ILE:HG12	2.19	0.43
1:A:2635:PHE:CE1	1:A:2706:ILE:HD13	2.54	0.43
1:A:2569:VAL:HG11	1:A:2747:ILE:HG23	1.99	0.43
1:A:3825:TYR:CE2	1:A:3875:MET:SD	3.12	0.43
1:B:1818:GLN:O	1:B:1822:THR:HG23	2.19	0.43
1:A:1818:GLN:O	1:A:1822:THR:HG23	2.19	0.43
1:A:1923:LEU:HD12	1:A:1954:TRP:CZ2	2.53	0.43
1:A:2302:VAL:HG12	1:A:2303:PHE:N	2.33	0.43
1:A:2910:VAL:CG1	1:A:3105:VAL:HG23	2.47	0.43
1:B:2295:LEU:C	1:B:2338:ASN:ND2	2.72	0.43
1:B:2302:VAL:HG12	1:B:2303:PHE:N	2.33	0.43
1:B:2766:ALA:O	1:B:2770:THR:HG23	2.18	0.43
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	2.00	0.43
1:B:1526:LYS:O	1:B:1529:ARG:HG2	2.19	0.43
1:B:1632:VAL:HG13	1:B:1636:ASP:HB2	1.95	0.43
1:B:2284:LEU:HB3	1:B:2333:LEU:HD13	2.00	0.43
1:B:3654:ARG:HB2	1:B:3661:LEU:HB2	2.01	0.43
1:A:1970:ALA:HB2	1:A:4073:SER:HB2	2.00	0.43
1:A:4609:VAL:CG2	1:A:4622:VAL:HG23	2.48	0.43
1:B:1970:ALA:HB2	1:B:4073:SER:HB2	2.00	0.43
1:B:4430:ASP:O	1:B:4434:VAL:HG12	2.19	0.43
1:A:2308:ASP:HB2	1:A:2309:PRO:HD2	2.00	0.43
1:A:2569:VAL:HG13	1:A:2569:VAL:O	2.17	0.43
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.19	0.43
1:A:3683:ASP:CG	1:A:4137:ASN:OD1	2.56	0.43
1:A:4430:ASP:O	1:A:4434:VAL:HG12	2.19	0.43
1:B:1923:LEU:HD12	1:B:1954:TRP:CZ2	2.53	0.43
1:B:2458:LEU:HD13	1:B:2498:ILE:HG22	1.99	0.43
1:B:2519:ARG:HA	1:B:2526:LEU:CD1	2.49	0.43
1:B:2635:PHE:CE1	1:B:2706:ILE:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3769:THR:O	1:B:3773:LEU:HG	2.19	0.43
1:B:3825:TYR:CE2	1:B:3875:MET:SD	3.12	0.43
1:A:1632:VAL:HG11	1:A:1636:ASP:CB	2.48	0.43
1:A:2551:LYS:C	1:A:2551:LYS:CD	2.86	0.43
1:A:2213:ILE:HG21	1:A:2220:LEU:HD13	2.01	0.42
1:A:2256:PRO:HB3	1:A:2264:LEU:HD22	2.00	0.42
1:A:4088:VAL:HG13	1:A:4118:PRO:CB	2.49	0.42
1:B:1713:LEU:HD22	1:B:1749:LEU:HD21	2.00	0.42
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	2.01	0.42
1:B:2213:ILE:HG21	1:B:2220:LEU:HD13	2.01	0.42
1:A:2234:TRP:HH2	1:A:2253:ILE:HD11	1.84	0.42
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.59	0.42
1:B:2571:THR:HG22	1:B:2747:ILE:HG12	2.00	0.42
1:B:2871:ILE:HG23	1:B:2871:ILE:O	2.18	0.42
1:B:4088:VAL:HG13	1:B:4118:PRO:CB	2.49	0.42
1:A:1526:LYS:O	1:A:1529:ARG:HG2	2.19	0.42
1:A:2496:TYR:CZ	1:A:2500:TRP:CD1	3.08	0.42
1:A:3109:PHE:CD2	1:A:3180:ILE:HG21	2.54	0.42
1:B:2275:TRP:NE1	1:B:2277:ASP:OD1	2.53	0.42
1:B:3550:THR:OG1	1:B:3574:THR:HG21	2.19	0.42
1:A:2588:HIS:HB3	1:A:2658:TRP:CZ3	2.54	0.42
1:B:1961:ASN:ND2	1:B:2025:ARG:CB	2.82	0.42
1:B:2234:TRP:HH2	1:B:2253:ILE:HD11	1.84	0.42
1:B:2526:LEU:HA	1:B:2545:TRP:CZ3	2.54	0.42
1:B:2907:VAL:O	1:B:2907:VAL:HG23	2.20	0.42
1:B:4577:LEU:HD21	1:B:4635:PHE:HD1	1.84	0.42
1:A:1452:VAL:HG13	1:A:1512:TYR:CE1	2.55	0.42
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.53	0.42
1:A:3609:ILE:HG12	1:A:3632:PRO:HB2	2.01	0.42
1:B:2308:ASP:HB2	1:B:2309:PRO:HD2	2.00	0.42
1:B:3879:ASP:O	1:B:3882:THR:OG1	2.30	0.42
1:B:4529:ALA:O	1:B:4533:SER:N	2.52	0.42
1:A:1550:ILE:HD13	1:A:1638:LEU:HD22	2.00	0.42
1:A:2381:ARG:HG2	1:A:2385:ILE:HD11	2.02	0.42
1:B:1452:VAL:HG13	1:B:1512:TYR:CE1	2.55	0.42
1:B:2824:ILE:HG13	1:B:2825:TRP:N	2.34	0.42
1:B:4609:VAL:CG2	1:B:4622:VAL:HG21	2.50	0.42
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	2.01	0.42
1:A:2549:GLN:HG2	1:A:2572:LEU:HB2	2.02	0.42
1:A:2824:ILE:HG13	1:A:2825:TRP:N	2.34	0.42
1:A:3769:THR:O	1:A:3773:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1632:VAL:HG11	1:B:1636:ASP:CB	2.48	0.42
1:B:2605:LEU:HD23	1:B:2662:PHE:CD1	2.44	0.42
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	2.02	0.42
1:A:3178:ASP:OD1	1:A:3584:ASN:HB3	2.20	0.42
1:B:1861:MET:HE2	1:B:1890:LEU:HA	2.02	0.42
1:B:2256:PRO:HB3	1:B:2264:LEU:HD22	2.01	0.42
1:B:3178:ASP:OD1	1:B:3584:ASN:HB3	2.20	0.42
1:B:3588:LEU:HD23	1:B:3589:ILE:N	2.35	0.42
1:B:3609:ILE:HG12	1:B:3632:PRO:HB2	2.01	0.42
1:A:4609:VAL:CG2	1:A:4622:VAL:HG21	2.50	0.42
1:B:2285:ARG:NH1	1:B:2333:LEU:HD21	2.35	0.42
1:B:3508:LEU:HD23	1:B:3536:LEU:HD21	2.02	0.42
1:A:1961:ASN:ND2	1:A:2025:ARG:CB	2.82	0.42
1:A:2091:ARG:NH1	2:A:4801:ADP:PA	2.93	0.42
1:A:2571:THR:HG22	1:A:2747:ILE:HG12	2.00	0.42
1:A:2938:VAL:O	1:A:2941:ALA:HB2	2.20	0.42
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	2.02	0.42
1:A:3654:ARG:HB2	1:A:3661:LEU:HB2	2.01	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:B:2091:ARG:NH1	2:B:4801:ADP:PA	2.93	0.42
1:B:2220:LEU:HD23	1:B:2342:MET:HE2	2.02	0.42
1:B:2938:VAL:O	1:B:2941:ALA:HB2	2.20	0.42
1:B:3109:PHE:CD2	1:B:3180:ILE:HG21	2.54	0.42
1:B:3175:HIS:CD2	1:B:3585:ARG:HH22	2.36	0.42
1:B:1628:ARG:NH2	1:B:1871:GLU:OE2	2.53	0.41
1:B:2549:GLN:HG2	1:B:2572:LEU:HB2	2.02	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.01	0.41
1:A:1931:ASN:HD21	1:A:2317:SER:CB	2.21	0.41
1:A:2623:SER:OG	1:A:2624:SER:N	2.53	0.41
1:A:2907:VAL:O	1:A:2907:VAL:HG23	2.20	0.41
1:B:1761:ASN:HB3	1:B:1781:VAL:HG22	2.02	0.41
1:B:3713:LEU:O	1:B:3717:LEU:HG	2.20	0.41
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.59	0.41
1:B:2381:ARG:HG2	1:B:2385:ILE:HD11	2.02	0.41
1:B:2496:TYR:CZ	1:B:2500:TRP:CD1	3.08	0.41
1:A:1641:ILE:HA	1:A:1698:ILE:CD1	2.50	0.41
1:B:1960:PHE:CE1	1:B:1963:LEU:CD2	3.03	0.41
1:B:2588:HIS:HB3	1:B:2658:TRP:CZ3	2.54	0.41
1:B:4387:TRP:CZ3	1:B:4391:ILE:HG21	2.56	0.41
1:A:1632:VAL:HG11	1:A:1636:ASP:HB3	2.02	0.41
1:A:1960:PHE:CE1	1:A:1963:LEU:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	2.03	0.41
1:A:3550:THR:OG1	1:A:3574:THR:HG21	2.19	0.41
1:A:4387:TRP:CZ3	1:A:4391:ILE:HG21	2.56	0.41
1:A:4577:LEU:HD21	1:A:4635:PHE:HD1	1.84	0.41
1:B:2623:SER:OG	1:B:2624:SER:N	2.53	0.41
1:A:1628:ARG:NH2	1:A:1871:GLU:OE2	2.53	0.41
1:A:2526:LEU:HA	1:A:2545:TRP:CZ3	2.54	0.41
1:A:2538:GLU:N	1:A:2546:SER:O	2.53	0.41
1:A:4529:ALA:O	1:A:4533:SER:N	2.52	0.41
1:B:2091:ARG:HH11	2:B:4801:ADP:PA	2.43	0.41
1:B:2147:PRO:HG3	1:B:2209:GLN:HB3	2.02	0.41
1:B:4176:ARG:HD3	1:B:4223:LEU:HD22	2.03	0.41
1:A:3924:ILE:CG2	1:A:3924:ILE:O	2.67	0.41
1:A:4528:VAL:HG21	1:A:4592:TRP:CD1	2.56	0.41
1:A:2091:ARG:HH11	2:A:4801:ADP:PA	2.43	0.41
1:A:2295:LEU:C	1:A:2338:ASN:ND2	2.72	0.41
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.43	0.41
1:A:3745:LEU:CD1	1:A:3773:LEU:HD22	2.51	0.41
1:B:3633:LEU:O	1:B:3677:ILE:HA	2.21	0.41
1:B:4528:VAL:HG21	1:B:4592:TRP:CD1	2.56	0.41
1:B:4561:THR:HG23	1:B:4587:LEU:HD13	2.03	0.41
1:A:2635:PHE:O	1:A:2639:CYS:N	2.50	0.41
1:A:3151:HIS:CE1	1:A:3516:TYR:HH	2.36	0.41
1:A:3588:LEU:HD23	1:A:3589:ILE:N	2.35	0.41
1:A:3633:LEU:O	1:A:3677:ILE:HA	2.21	0.41
1:A:1761:ASN:HB3	1:A:1781:VAL:HG22	2.02	0.41
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.01	0.41
1:B:3638:VAL:N	1:B:3681:THR:HG22	2.36	0.41
1:A:1931:ASN:OD1	1:A:1958:ASP:CB	2.62	0.41
1:A:2540:SER:OG	1:A:2544:GLU:O	2.16	0.41
1:A:3871:VAL:HG11	1:A:3883:PHE:CD2	2.56	0.41
1:B:1641:ILE:HA	1:B:1698:ILE:CD1	2.50	0.41
1:B:2568:VAL:CG2	1:B:2603:MET:HE3	2.51	0.41
1:A:1632:VAL:HG13	1:A:1636:ASP:HB2	1.95	0.40
1:A:2285:ARG:NH1	1:A:2333:LEU:HD21	2.35	0.40
1:A:2752:ASN:HD22	1:A:2770:THR:HG22	1.76	0.40
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	2.03	0.40
1:A:2599:SER:N	2:A:4804:ADP:O2A	2.43	0.40
1:B:3871:VAL:HG11	1:B:3883:PHE:CD2	2.56	0.40
1:A:2370:SER:O	1:A:2373:MET:HB3	2.21	0.40
1:A:3154:LEU:HD11	1:A:3520:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4042:LEU:HD21	1:A:4139:LEU:HD23	2.03	0.40
1:B:1879:LEU:HD13	1:B:1915:SER:HA	2.03	0.40
1:B:2454:CYS:HB3	1:B:2502:LEU:HD23	2.03	0.40
1:B:2538:GLU:N	1:B:2546:SER:O	2.53	0.40
1:A:1978:ILE:HG23	1:A:2012:MET:HE1	2.02	0.40
1:A:2091:ARG:NH2	1:A:2320:ASP:OD1	2.53	0.40
1:A:2639:CYS:SG	1:A:2652:PRO:HA	2.62	0.40
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	2.03	0.40
1:A:4176:ARG:HD3	1:A:4223:LEU:HD22	2.03	0.40
1:B:3154:LEU:HD11	1:B:3520:PHE:CE2	2.56	0.40
1:B:3553:LEU:HD13	1:B:3578:ILE:HG21	2.04	0.40
1:B:3868:PHE:CE1	1:B:3884:ALA:HB2	2.56	0.40
1:B:4009:VAL:HG13	1:B:4013:LEU:HD12	2.03	0.40
1:A:2994:MET:HE2	1:A:3008:MET:SD	2.61	0.40
1:A:3868:PHE:CE1	1:A:3884:ALA:HB2	2.56	0.40
1:A:4565:LEU:CD2	1:A:4642:VAL:HG22	2.50	0.40
1:B:1632:VAL:HG11	1:B:1636:ASP:HB3	2.02	0.40
1:B:2370:SER:O	1:B:2373:MET:HB3	2.21	0.40
1:B:2635:PHE:O	1:B:2639:CYS:N	2.50	0.40
1:A:2182:LEU:O	1:A:2185:VAL:HG22	2.22	0.40
1:A:4468:THR:HG21	1:A:4611:LEU:HD23	2.04	0.40
1:B:2016:ILE:HD12	1:B:2036:PHE:CD2	2.56	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 PDB entries followed by that with respect to all EM entries.

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	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	55	88
1	B	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	55	88
All	All	5776/9292 (62%)	5428 (94%)	342 (6%)	6 (0%)	58	88

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1647	VAL
1	B	1647	VAL
1	A	1964	GLU
1	B	1964	GLU
1	A	1511	PRO
1	B	1511	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 PDB entries followed by that with respect to all EM entries.

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	2472/4125 (60%)	2469 (100%)	3 (0%)	94	98
1	B	2472/4125 (60%)	2469 (100%)	3 (0%)	94	98
All	All	4944/8250 (60%)	4938 (100%)	6 (0%)	95	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2796	PRO
1	A	3825	TYR
1	A	3905	PHE
1	B	2796	PRO
1	B	3825	TYR
1	B	3905	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1612	GLN
1	A	1748	GLN
1	A	1784	ASN
1	A	1790	ASN
1	A	1856	GLN

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Mol	Chain	Res	Type
1	A	1863	ASN
1	A	1881	GLN
1	A	1894	GLN
1	A	1921	HIS
1	A	1931	ASN
1	A	1976	GLN
1	A	1979	GLN
1	A	1985	HIS
1	A	2079	GLN
1	A	2134	GLN
1	A	2139	GLN
1	A	2338	ASN
1	A	2549	GLN
1	A	2752	ASN
1	A	2913	ASN
1	A	2998	ASN
1	A	3014	ASN
1	A	3047	HIS
1	A	3152	GLN
1	A	3175	HIS
1	A	3182	HIS
1	A	3538	GLN
1	A	3540	ASN
1	A	3584	ASN
1	A	3646	ASN
1	A	3880	HIS
1	A	4012	ASN
1	A	4131	ASN
1	A	4393	GLN
1	A	4488	GLN
1	A	4490	GLN
1	A	4526	GLN
1	A	4566	GLN
1	B	1612	GLN
1	B	1748	GLN
1	B	1784	ASN
1	B	1790	ASN
1	B	1856	GLN
1	B	1863	ASN
1	B	1881	GLN
1	B	1894	GLN
1	B	1921	HIS

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Mol	Chain	Res	Type
1	B	1931	ASN
1	B	1976	GLN
1	B	1979	GLN
1	B	1985	HIS
1	B	2079	GLN
1	B	2134	GLN
1	B	2139	GLN
1	B	2338	ASN
1	B	2549	GLN
1	B	2752	ASN
1	B	2913	ASN
1	B	2998	ASN
1	B	3014	ASN
1	B	3047	HIS
1	B	3152	GLN
1	B	3175	HIS
1	B	3182	HIS
1	B	3538	GLN
1	B	3540	ASN
1	B	3584	ASN
1	B	3646	ASN
1	B	3880	HIS
1	B	4012	ASN
1	B	4131	ASN
1	B	4393	GLN
1	B	4488	GLN
1	B	4490	GLN
1	B	4526	GLN
1	B	4566	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
2	ADP	A	4801	-	25,29,29	1.14	2 (8%)	24,45,45	1.79	3 (12%)
3	ATP	A	4802	4	27,33,33	1.04	1 (3%)	25,52,52	1.91	4 (16%)
2	ADP	A	4804	-	25,29,29	0.94	1 (4%)	24,45,45	1.85	3 (12%)
2	ADP	A	4805	-	25,29,29	0.87	1 (4%)	24,45,45	1.82	4 (16%)
2	ADP	B	4801	-	25,29,29	1.14	2 (8%)	24,45,45	1.79	3 (12%)
3	ATP	B	4802	4	27,33,33	1.03	1 (3%)	25,52,52	1.91	4 (16%)
2	ADP	B	4804	-	25,29,29	0.93	1 (4%)	24,45,45	1.84	3 (12%)
2	ADP	B	4805	-	25,29,29	0.87	2 (8%)	24,45,45	1.82	4 (16%)

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	ADP	A	4801	-	-	0/12/32/32	0/3/3/3
3	ATP	A	4802	4	-	0/18/38/38	0/3/3/3
2	ADP	A	4804	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4805	-	-	0/12/32/32	0/3/3/3
2	ADP	B	4801	-	-	0/12/32/32	0/3/3/3
3	ATP	B	4802	4	-	0/18/38/38	0/3/3/3
2	ADP	B	4804	-	-	0/12/32/32	0/3/3/3
2	ADP	B	4805	-	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4805	ADP	C5-N7	-2.01	1.32	1.39
2	B	4801	ADP	C2-N3	2.31	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4801	ADP	C2-N3	2.37	1.36	1.32
2	A	4805	ADP	C5-C4	2.53	1.46	1.40
2	B	4805	ADP	C5-C4	2.53	1.46	1.40
2	B	4804	ADP	C5-C4	2.68	1.46	1.40
2	A	4804	ADP	C5-C4	2.68	1.46	1.40
3	B	4802	ATP	C5-C4	3.05	1.47	1.40
3	A	4802	ATP	C5-C4	3.09	1.47	1.40
2	A	4801	ADP	C5-C4	3.21	1.47	1.40
2	B	4801	ADP	C5-C4	3.22	1.47	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4802	ATP	N3-C2-N1	-7.51	122.31	128.86
3	A	4802	ATP	N3-C2-N1	-7.51	122.31	128.86
2	A	4805	ADP	N3-C2-N1	-6.86	122.88	128.86
2	B	4805	ADP	N3-C2-N1	-6.86	122.88	128.86
2	B	4801	ADP	N3-C2-N1	-6.47	123.22	128.86
2	A	4801	ADP	N3-C2-N1	-6.45	123.24	128.86
2	A	4804	ADP	N3-C2-N1	-6.38	123.30	128.86
2	B	4804	ADP	N3-C2-N1	-6.34	123.33	128.86
3	A	4802	ATP	C1'-N9-C4	-2.93	121.57	126.64
3	B	4802	ATP	C1'-N9-C4	-2.93	121.57	126.64
2	B	4804	ADP	C1'-N9-C4	-2.89	121.64	126.64
2	A	4801	ADP	C4-C5-N7	-2.88	106.62	109.41
2	A	4804	ADP	C1'-N9-C4	-2.88	121.67	126.64
3	A	4802	ATP	C4-C5-N7	-2.85	106.66	109.41
2	B	4801	ADP	C4-C5-N7	-2.84	106.66	109.41
3	B	4802	ATP	C4-C5-N7	-2.83	106.67	109.41
2	A	4805	ADP	C4-C5-N7	-2.82	106.69	109.41
2	B	4805	ADP	C4-C5-N7	-2.78	106.72	109.41
2	B	4804	ADP	C4-C5-N7	-2.43	107.06	109.41
2	A	4804	ADP	C4-C5-N7	-2.43	107.06	109.41
2	A	4805	ADP	N6-C6-N1	2.01	122.76	118.77
2	B	4805	ADP	N6-C6-N1	2.01	122.76	118.77
2	A	4805	ADP	O3B-PB-O2B	2.03	115.80	107.61
2	B	4805	ADP	O3B-PB-O2B	2.03	115.80	107.61
3	B	4802	ATP	C2-N1-C6	2.25	122.70	118.77
3	A	4802	ATP	C2-N1-C6	2.25	122.70	118.77
2	A	4801	ADP	C4'-O4'-C1'	2.38	112.30	109.77
2	B	4801	ADP	C4'-O4'-C1'	2.38	112.31	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4801	ADP	11	0
3	A	4802	ATP	4	0
2	A	4804	ADP	2	0
2	B	4801	ADP	11	0
3	B	4802	ATP	4	0
2	B	4804	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3803:PRO	C	3804:LEU	N	2.62
1	B	3803:PRO	C	3804:LEU	N	2.62
1	A	3203:VAL	C	3204:GLY	N	2.58
1	B	3203:VAL	C	3204:GLY	N	2.58