



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:25 AM UTC

PDB ID : 1A5U / pdb_00001a5u
Title : PYRUVATE KINASE COMPLEX WITH BIS MG-ATP-NA-OXALATE
Authors : Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.
Deposited on : 1998-02-18
Resolution : 2.35 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

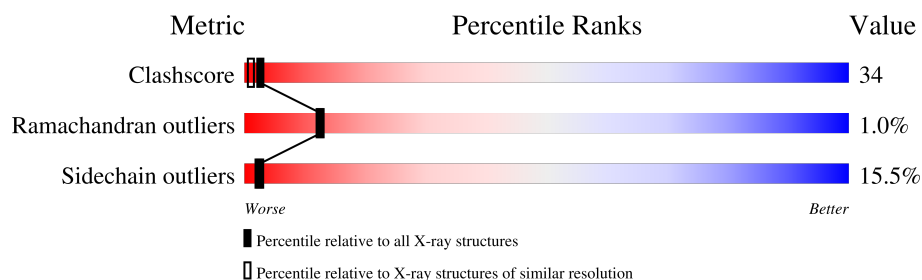
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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	530	35% 44% 17% ..
1	B	530	49% 40% 9% .
1	C	530	34% 48% 15% ..
1	D	530	49% 38% 10% .
1	E	530	45% 41% 10% ..
1	F	530	43% 44% 10% ..
1	G	530	41% 45% 12% ..
1	H	530	54% 37% 7% .

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
3	OXL	A	533	-	X	X	-
3	OXL	B	1133	-	X	-	-
3	OXL	C	1733	-	X	-	-
3	OXL	D	2333	-	X	-	-
3	OXL	E	3533	-	X	-	-
3	OXL	F	4133	-	X	X	-
3	OXL	G	4733	-	X	X	-
3	OXL	H	5333	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 33890 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	B	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	C	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	D	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	E	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	F	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	G	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

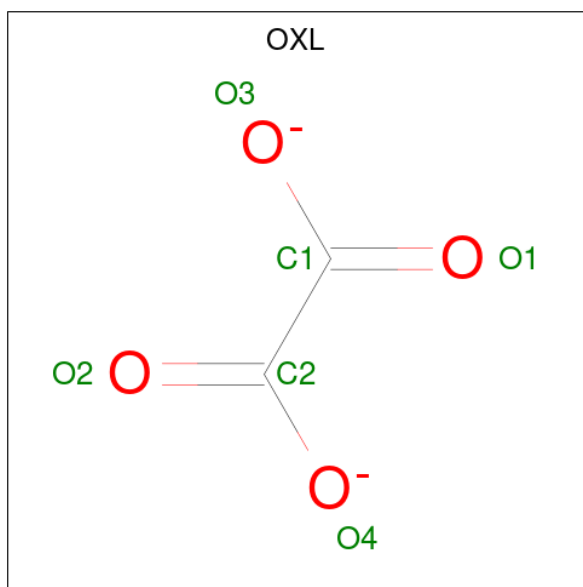
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).

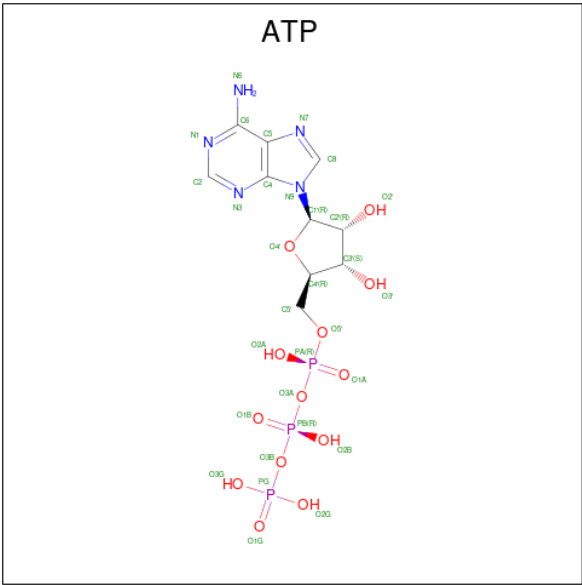


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		
4	G	2	Total	Mg	0	0
			2	2		
4	H	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is water.

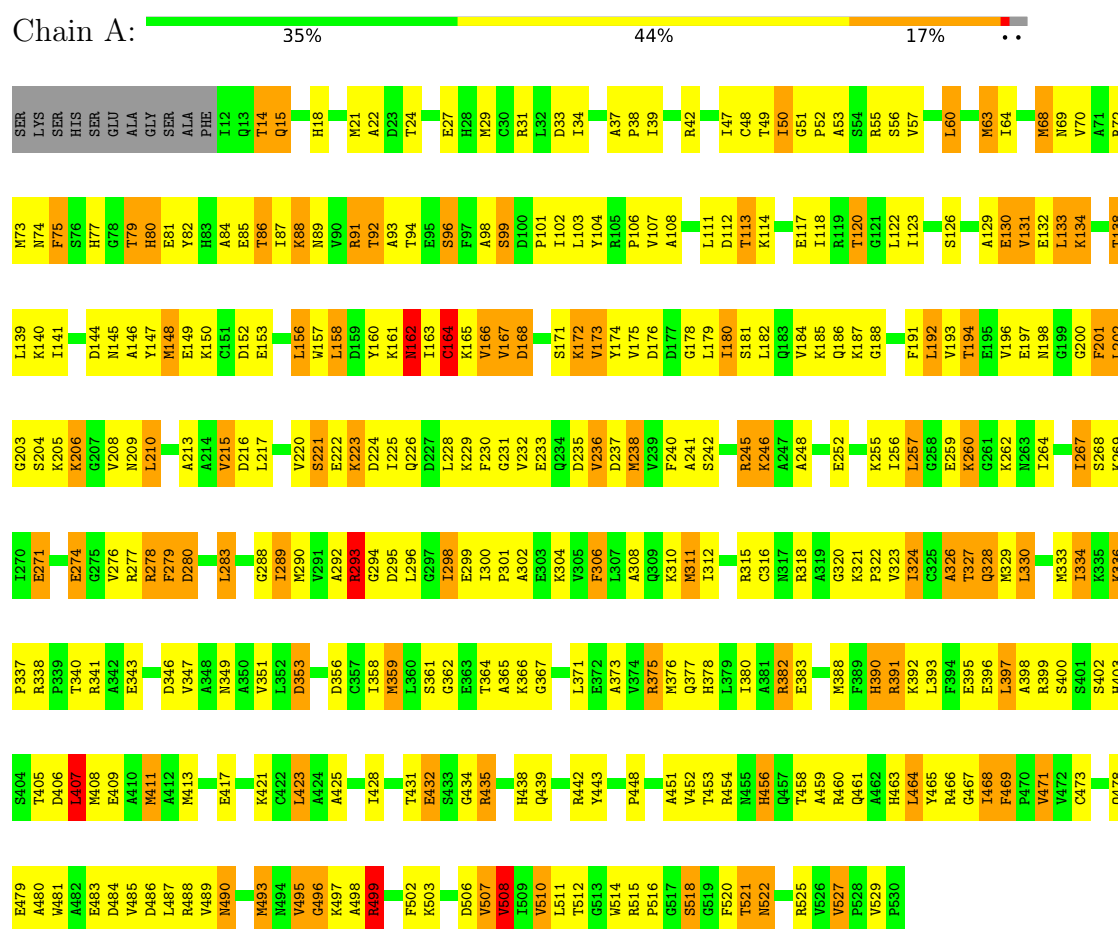
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	260	Total	O	0	0
			260	260		
6	C	166	Total	O	0	0
			166	166		
6	D	250	Total	O	0	0
			250	250		
6	E	267	Total	O	0	0
			267	267		
6	F	185	Total	O	0	0
			185	185		
6	G	210	Total	O	0	0
			210	210		
6	H	296	Total	O	0	0
			296	296		

3 Residue-property plots

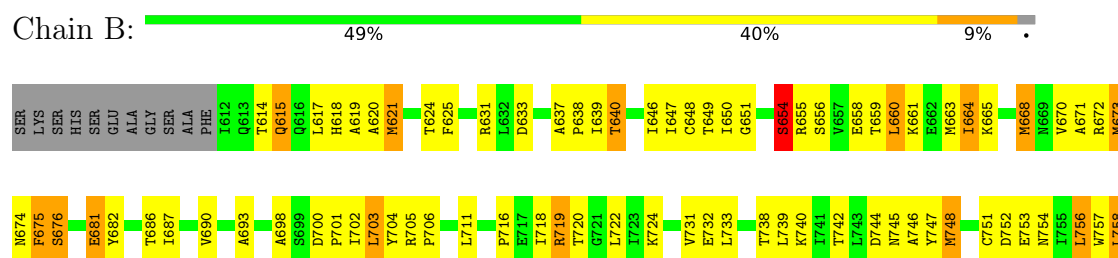
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

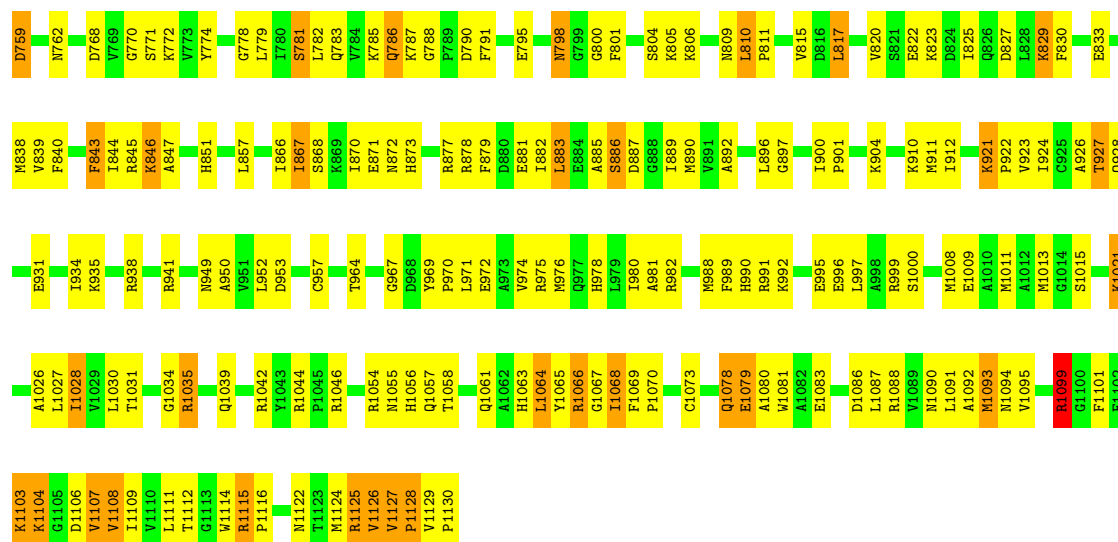
Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



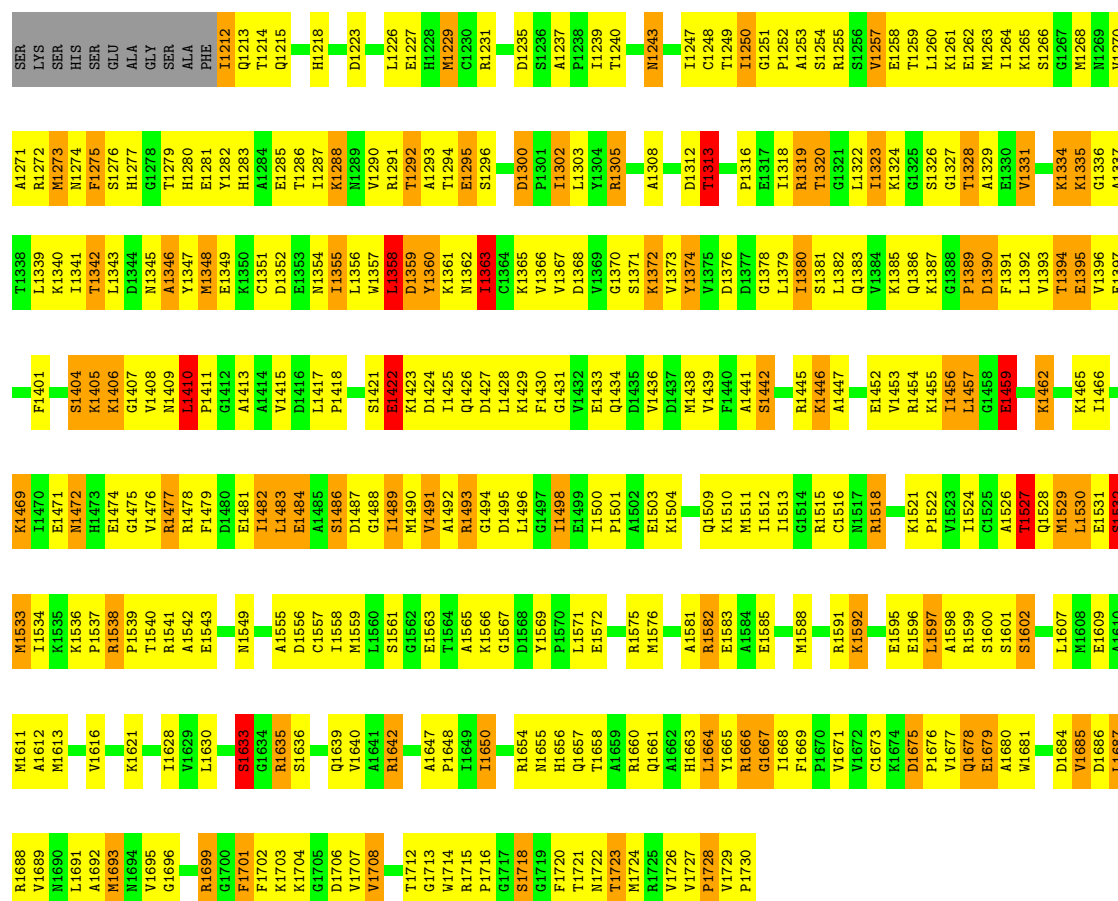
• Molecule 1: PYRUVATE KINASE





• Molecule 1: PYRUVATE KINASE

Chain C: 34% 48% 15% 0%



• Molecule 1: PYRUVATE KINASE

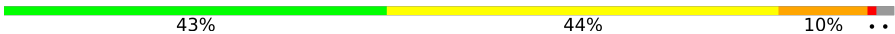
Chain D: 49% 38% 10% 0%

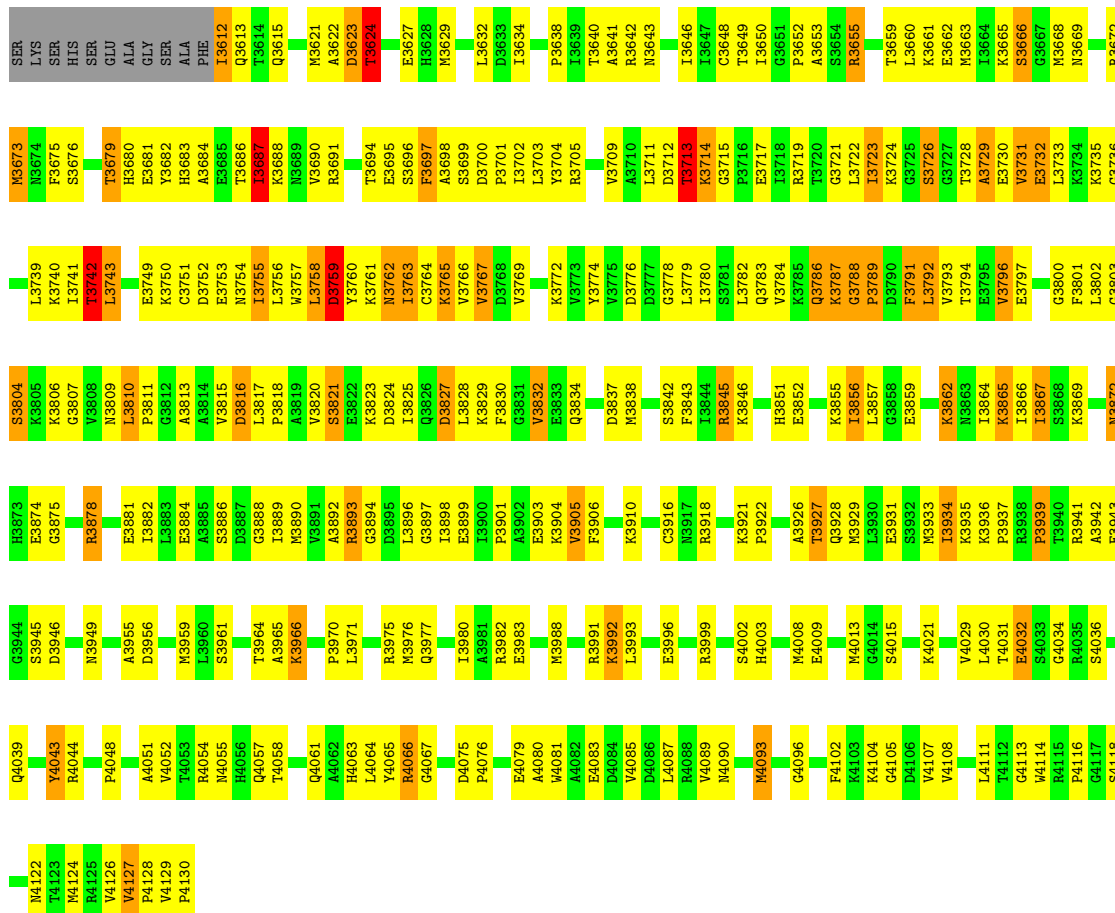


Chain E: 45% 41% 10% ..

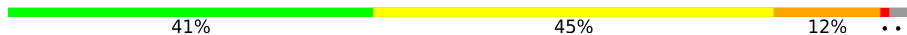


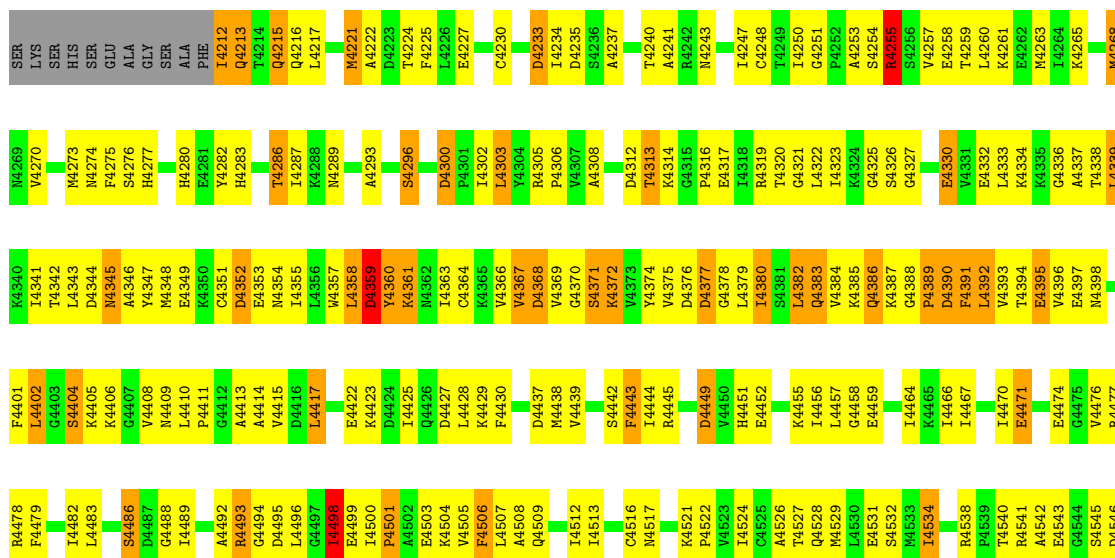
● Molecule 1: PYRUVATE KINASE

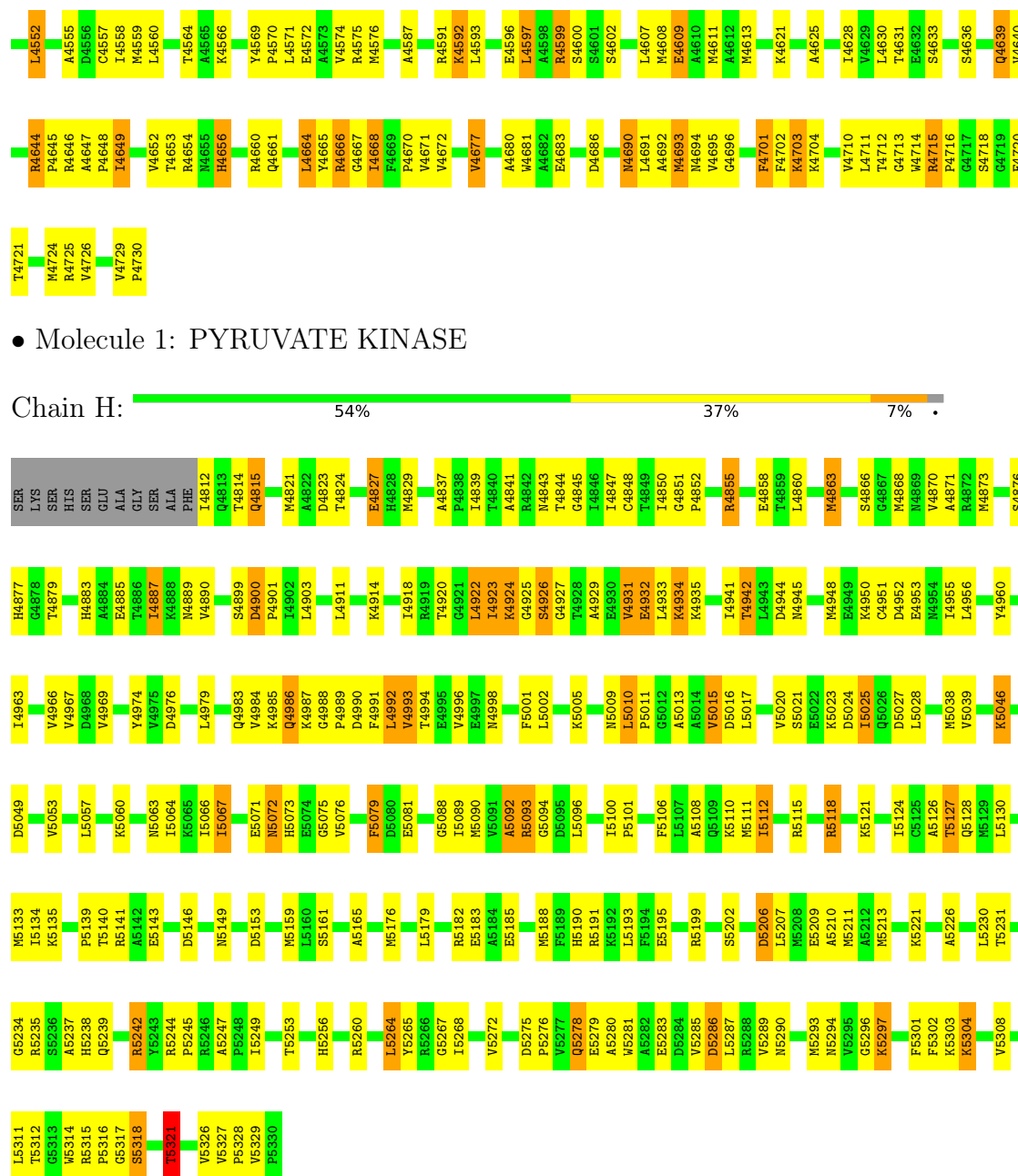
Chain F:  43% 44% 10% ..



● Molecule 1: PYRUVATE KINASE

Chain G:  41% 45% 12% ..





● Molecule 1: PYRUVATE KINASE

Chain H: 54% 37% 7%

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.30Å 216.50Å 258.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35	Depositor
% Data completeness (in resolution range)	85.0 (30.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, NA, MG, OXL

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	1.27	5/4041 (0.1%)	1.66	58/5452 (1.1%)
1	B	1.19	4/4041 (0.1%)	1.61	36/5452 (0.7%)
1	C	1.13	2/4041 (0.0%)	1.64	30/5452 (0.6%)
1	D	1.19	0/4041	1.63	42/5452 (0.8%)
1	E	1.17	0/4041	1.67	38/5452 (0.7%)
1	F	1.14	0/4041	1.62	32/5452 (0.6%)
1	G	1.17	2/4041 (0.0%)	1.65	42/5452 (0.8%)
1	H	1.19	3/4041 (0.1%)	1.58	26/5452 (0.5%)
All	All	1.18	16/32328 (0.0%)	1.63	304/43616 (0.7%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ASN	N-CA	25.81	1.82	1.46
1	A	241	ALA	C-N	-14.20	1.15	1.33
1	A	162	ASN	C-N	-7.63	1.23	1.33
1	A	162	ASN	CA-CB	7.43	1.66	1.53
1	G	4713	GLY	CA-C	6.00	1.56	1.52
1	H	5161	SER	CA-C	5.99	1.55	1.52
1	G	4287	ILE	CA-CB	-5.87	1.47	1.54
1	A	164	CYS	CA-C	-5.57	1.45	1.52
1	C	1368	ASP	N-CA	5.56	1.52	1.45
1	H	4993	VAL	CA-C	-5.40	1.46	1.52
1	B	1044	ARG	C-O	-5.36	1.21	1.23
1	B	1044	ARG	N-CA	-5.19	1.42	1.46
1	B	1026	ALA	CA-C	-5.14	1.46	1.52
1	C	1374	TYR	CA-C	-5.09	1.46	1.52
1	B	633	ASP	CG-OD1	5.06	1.34	1.25
1	H	4984	VAL	CA-CB	-5.01	1.47	1.54

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	CYS	O-C-N	13.88	141.05	122.59
1	A	162	ASN	N-CA-CB	-11.01	91.04	110.42
1	C	1368	ASP	CB-CA-C	-10.24	92.74	110.45
1	E	3367	GLY	N-CA-C	10.03	123.36	112.33
1	A	222	GLU	N-CA-C	-9.72	100.76	111.36
1	C	1368	ASP	CA-CB-CG	9.45	122.05	112.60
1	H	5290	ASN	CA-CB-CG	-8.92	103.68	112.60
1	E	3490	ASN	CA-CB-CG	-8.44	104.16	112.60
1	C	1275	PHE	CA-CB-CG	-8.42	105.38	113.80
1	F	3624	THR	N-CA-CB	-8.32	97.54	110.85
1	E	3279	PHE	CA-CB-CG	-8.18	105.62	113.80
1	G	4352	ASP	N-CA-C	8.12	119.33	107.88
1	H	5318	SER	N-CA-C	-7.85	103.51	113.72
1	G	4368	ASP	CA-CB-CG	7.85	120.45	112.60
1	A	75	PHE	CA-CB-CG	-7.74	106.06	113.80
1	A	37	ALA	N-CA-C	7.73	119.52	109.93
1	D	2051	HIS	CA-CB-CG	-7.73	106.07	113.80
1	A	279	PHE	CA-CB-CG	-7.68	106.12	113.80
1	G	4361	LYS	N-CA-C	7.60	120.64	111.82
1	H	4927	GLY	N-CA-C	-7.56	103.87	115.66
1	H	4837	ALA	N-CA-C	7.55	119.17	109.65
1	D	2087	ASP	N-CA-C	-7.41	104.04	113.23
1	H	5294	ASN	CA-CB-CG	-7.40	105.20	112.60
1	D	2105	VAL	N-CA-C	7.37	118.09	110.36
1	A	508	VAL	N-CA-CB	-7.36	99.37	111.44
1	B	1127	VAL	C-N-CD	-7.30	95.06	125.00
1	B	872	ASN	CA-CB-CG	7.28	119.88	112.60
1	F	3712	ASP	CA-C-N	7.26	131.19	120.87
1	F	3712	ASP	C-N-CA	7.26	131.19	120.87
1	H	5079	PHE	N-CA-C	7.24	119.80	111.11
1	B	1068	ILE	N-CA-CB	7.20	119.02	110.95
1	B	901	PRO	N-CA-CB	7.20	109.72	103.31
1	C	1243	ASN	N-CA-C	7.12	118.83	111.14
1	A	168	ASP	CA-CB-CG	7.10	119.70	112.60
1	G	4300	ASP	CA-C-N	7.04	127.03	119.28
1	G	4300	ASP	C-N-CA	7.04	127.03	119.28
1	H	4976	ASP	CA-CB-CG	7.04	119.64	112.60
1	E	3164	CYS	O-C-N	6.96	131.84	122.59
1	G	4377	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	1701	PHE	CA-CB-CG	-6.92	106.88	113.80
1	C	1667	GLY	CA-C-N	-6.92	113.72	122.37
1	C	1667	GLY	C-N-CA	-6.92	113.72	122.37
1	F	4090	ASN	N-CA-C	6.87	118.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4609	GLU	N-CA-C	-6.87	103.72	111.14
1	A	469	PHE	CA-C-N	6.86	126.78	119.85
1	A	469	PHE	C-N-CA	6.86	126.78	119.85
1	F	3759	ASP	CA-CB-CG	6.86	119.45	112.60
1	D	2203	HIS	CA-CB-CG	-6.84	106.96	113.80
1	G	4505	VAL	N-CA-C	6.84	120.61	111.17
1	F	3763	ILE	N-CA-C	6.83	117.53	110.36
1	F	4003	HIS	CA-CB-CG	-6.80	107.00	113.80
1	F	3687	ILE	CB-CA-C	-6.80	103.14	112.04
1	E	3015	GLN	CB-CA-C	-6.79	101.88	111.80
1	A	293	ARG	N-CA-C	6.76	120.79	112.54
1	C	1360	TYR	N-CA-C	6.76	120.69	107.98
1	C	1237	ALA	N-CA-C	6.75	118.41	109.83
1	D	1958	LEU	CA-C-N	6.75	129.87	120.29
1	D	1958	LEU	C-N-CA	6.75	129.87	120.29
1	E	3382	ARG	N-CA-CB	6.65	120.59	110.28
1	D	2093	ARG	N-CA-C	6.65	120.26	111.75
1	C	1328	THR	N-CA-C	-6.64	105.21	113.38
1	D	1864	ILE	N-CA-C	-6.64	104.29	110.53
1	E	3147	TYR	CA-CB-CG	-6.62	101.98	113.90
1	A	321	LYS	O-C-N	6.60	127.87	121.66
1	A	510	VAL	N-CA-C	6.58	117.35	107.80
1	H	5093	ARG	N-CA-C	6.58	120.41	112.38
1	A	402	SER	N-CA-C	6.57	120.89	112.34
1	A	432	GLU	CB-CA-C	6.53	120.33	110.08
1	E	3293	ARG	N-CA-C	6.52	119.22	111.33
1	G	4498	ILE	CB-CA-C	-6.50	103.75	111.94
1	D	1919	ARG	CD-NE-CZ	6.50	133.50	124.40
1	E	3243	PHE	N-CA-C	6.50	120.38	111.54
1	F	3791	PHE	CA-CB-CG	-6.49	107.31	113.80
1	C	1482	ILE	N-CA-C	-6.48	104.33	110.42
1	G	4644	ARG	CB-CA-C	-6.46	105.38	111.00
1	C	1602	SER	N-CA-C	6.45	120.01	111.75
1	G	4398	ASN	CA-CB-CG	6.42	119.02	112.60
1	G	4255	ARG	N-CA-C	6.38	119.05	111.71
1	G	4677	VAL	N-CA-C	6.38	117.54	108.93
1	A	469	PHE	O-C-N	6.36	127.61	120.68
1	G	4283	HIS	CA-CB-CG	-6.35	107.45	113.80
1	F	3643	ASN	N-CA-C	6.34	120.75	112.89
1	G	4701	PHE	CA-CB-CG	-6.33	107.47	113.80
1	C	1316	PRO	N-CA-CB	6.33	106.84	102.35
1	H	5079	PHE	CA-CB-CG	-6.30	107.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1837	ALA	N-CA-C	6.29	117.58	109.65
1	A	280	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	403	HIS	CA-CB-CG	-6.28	107.52	113.80
1	B	759	ASP	CB-CA-C	-6.27	98.63	110.67
1	A	298	ILE	CB-CA-C	6.27	117.39	111.44
1	G	4501	PRO	N-CA-CB	6.25	108.90	103.27
1	F	4127	VAL	N-CA-C	6.24	114.31	109.19
1	B	1070	PRO	CB-CA-C	-6.22	103.94	111.46
1	G	4498	ILE	N-CA-CB	6.21	121.90	110.40
1	D	1968	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	495	VAL	N-CA-CB	6.19	117.79	110.55
1	E	3349	ASN	CA-CB-CG	-6.19	106.41	112.60
1	B	1127	VAL	N-CA-C	6.19	116.00	109.01
1	E	3322	PRO	N-CA-CB	6.17	108.68	103.25
1	B	758	LEU	CA-C-N	6.12	129.61	120.31
1	B	758	LEU	C-N-CA	6.12	129.61	120.31
1	C	1726	VAL	CB-CA-C	6.12	118.50	110.91
1	H	4815	GLN	CB-CA-C	-6.11	102.06	111.66
1	A	336	LYS	N-CA-C	6.10	119.36	110.14
1	H	5015	VAL	CA-C-N	6.10	130.91	120.72
1	H	5015	VAL	C-N-CA	6.10	130.91	120.72
1	G	4390	ASP	CA-CB-CG	6.10	118.70	112.60
1	D	1919	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	A	220	VAL	N-CA-C	6.07	115.59	106.42
1	C	1401	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	495	VAL	N-CA-C	6.01	116.19	110.42
1	A	336	LYS	CA-C-N	5.99	125.70	119.05
1	A	336	LYS	C-N-CA	5.99	125.70	119.05
1	F	4090	ASN	N-CA-CB	5.99	118.92	110.12
1	F	3788	GLY	C-N-CD	-5.98	100.48	125.00
1	B	633	ASP	N-CA-C	5.97	118.14	108.34
1	H	5326	VAL	CB-CA-C	5.96	119.14	110.98
1	G	4237	ALA	N-CA-C	5.96	118.06	109.48
1	G	4360	TYR	N-CA-C	5.95	118.00	108.41
1	D	2315	ARG	O-C-N	5.93	125.51	121.71
1	B	668	MET	CG-SD-CE	-5.93	87.85	100.90
1	C	1512	ILE	N-CA-C	5.92	116.70	110.72
1	B	1126	VAL	N-CA-CB	5.91	117.16	110.72
1	A	162	ASN	N-CA-C	5.90	120.21	113.19
1	A	496	GLY	N-CA-C	-5.89	105.51	112.64
1	A	298	ILE	N-CA-C	-5.89	106.49	111.56
1	F	3759	ASP	N-CA-CB	-5.89	101.22	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4607	LEU	N-CA-C	5.89	118.66	111.82
1	F	3742	THR	N-CA-C	5.88	118.34	109.23
1	A	80	HIS	N-CA-C	-5.87	104.96	111.71
1	H	5153	ASP	CA-CB-CG	5.87	118.47	112.60
1	G	4443	PHE	N-CA-C	5.85	119.62	111.90
1	E	3075	PHE	CA-CB-CG	-5.84	107.96	113.80
1	F	3898	ILE	CB-CA-C	5.84	116.91	111.30
1	A	276	VAL	N-CA-CB	5.82	116.96	110.62
1	G	4670	PRO	N-CA-C	5.81	119.58	110.80
1	C	1527	THR	N-CA-C	5.81	123.17	110.80
1	B	1081	TRP	CA-C-N	5.80	129.52	120.82
1	B	1081	TRP	C-N-CA	5.80	129.52	120.82
1	D	1919	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	E	3049	THR	CA-C-N	-5.79	115.64	122.93
1	E	3049	THR	C-N-CA	-5.79	115.64	122.93
1	E	3168	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	527	VAL	O-C-N	5.77	125.33	121.69
1	A	469	PHE	CA-CB-CG	-5.76	108.04	113.80
1	B	843	PHE	N-CA-C	5.76	119.61	112.24
1	B	1094	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	274	GLU	CA-C-N	5.73	126.34	119.98
1	A	274	GLU	C-N-CA	5.73	126.34	119.98
1	D	2310	VAL	N-CA-C	5.73	116.11	107.80
1	G	4286	THR	N-CA-C	-5.73	104.94	111.07
1	G	4668	ILE	CA-CB-CG2	-5.73	100.77	110.50
1	E	3168	ASP	CB-CA-C	-5.72	100.56	111.48
1	G	4339	LEU	N-CA-CB	5.71	121.34	111.00
1	E	3103	LEU	CA-C-O	5.71	124.80	118.52
1	F	3901	PRO	N-CA-CB	5.71	108.39	103.31
1	G	4439	VAL	N-CA-C	5.70	116.33	108.12
1	A	467	GLY	CA-C-N	-5.70	115.61	122.90
1	A	467	GLY	C-N-CA	-5.70	115.61	122.90
1	D	2328	PRO	CB-CA-C	-5.70	102.48	110.63
1	G	4670	PRO	CB-CA-C	-5.69	104.57	111.46
1	D	2249	ILE	CA-C-N	-5.68	115.63	122.90
1	D	2249	ILE	C-N-CA	-5.68	115.63	122.90
1	D	2090	MET	CA-C-N	-5.67	115.39	122.48
1	D	2090	MET	C-N-CA	-5.67	115.39	122.48
1	E	3528	PRO	CB-CA-C	-5.67	102.85	110.85
1	H	5127	THR	N-CA-C	5.67	122.89	110.80
1	G	4391	PHE	N-CA-C	5.66	115.87	107.88
1	H	5272	VAL	N-CA-CB	5.65	117.28	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4672	VAL	N-CA-C	5.65	116.90	108.54
1	C	1313	THR	N-CA-CB	-5.64	101.87	110.45
1	F	3796	VAL	N-CA-CB	5.63	117.24	110.31
1	G	4359	ASP	CB-CA-C	-5.63	100.19	109.65
1	E	3172	LYS	CA-C-N	-5.62	116.22	123.19
1	E	3172	LYS	C-N-CA	-5.62	116.22	123.19
1	D	2043	PHE	N-CA-C	5.61	118.92	111.30
1	B	1069	PHE	CA-C-N	5.60	125.78	119.90
1	B	1069	PHE	C-N-CA	5.60	125.78	119.90
1	F	3713	THR	N-CA-CB	-5.59	101.76	109.97
1	E	3312	ILE	N-CA-C	5.56	115.75	110.42
1	B	633	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	786	GLN	CB-CG-CD	-5.55	103.17	112.60
1	D	1954	ASN	CA-C-N	-5.55	114.72	122.71
1	D	1954	ASN	C-N-CA	-5.55	114.72	122.71
1	G	4233	ASP	CA-CB-CG	5.54	118.14	112.60
1	G	4415	VAL	N-CA-C	5.54	115.52	106.72
1	A	138	THR	CB-CA-C	5.53	118.85	109.50
1	A	306	PHE	CA-CB-CG	-5.53	108.27	113.80
1	F	3758	LEU	CA-C-N	5.52	130.07	120.68
1	F	3758	LEU	C-N-CA	5.52	130.07	120.68
1	A	152	ASP	CA-CB-CG	5.52	118.12	112.60
1	E	3454	ARG	N-CA-C	-5.51	106.56	113.28
1	G	4215	GLN	N-CA-CB	-5.50	103.64	111.84
1	E	3066	SER	CB-CA-C	5.50	120.89	109.95
1	E	3113	THR	N-CA-CB	-5.50	102.40	110.26
1	H	5101	PRO	N-CA-CB	5.49	108.08	103.25
1	E	3305	VAL	N-CA-C	5.49	116.12	110.36
1	G	4486	SER	N-CA-C	5.49	118.58	110.46
1	D	1855	ARG	CB-CA-C	-5.48	101.36	110.68
1	B	625	PHE	CA-CB-CG	-5.48	108.32	113.80
1	B	654	SER	N-CA-C	5.48	120.98	113.97
1	A	359	MET	N-CA-C	5.47	118.50	109.85
1	F	3939	PRO	CB-CA-C	-5.46	103.06	110.60
1	B	681	GLU	CB-CA-C	5.45	119.83	110.79
1	E	3210	LEU	CA-C-N	5.43	126.63	119.84
1	E	3210	LEU	C-N-CA	5.43	126.63	119.84
1	A	490	ASN	CA-CB-CG	-5.42	107.18	112.60
1	H	5206	ASP	CB-CA-C	5.42	118.71	109.72
1	C	1663	HIS	CA-CB-CG	-5.41	108.39	113.80
1	D	2112	ILE	N-CA-C	5.41	115.61	110.42
1	H	4900	ASP	CA-C-N	5.40	126.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	4900	ASP	C-N-CA	5.40	126.59	119.84
1	B	675	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	507	VAL	N-CA-CB	5.36	118.81	111.41
1	B	1115	ARG	CB-CA-C	5.36	120.73	110.17
1	C	1422	GLU	N-CA-C	-5.36	105.61	111.82
1	D	2221	LYS	N-CA-C	5.34	117.54	111.02
1	B	705	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	499	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	H	5124	ILE	CB-CA-C	-5.33	102.89	110.83
1	D	1993	VAL	CB-CA-C	-5.32	105.02	111.88
1	C	1459	GLU	N-CA-C	5.32	116.76	111.07
1	H	5121	LYS	CB-CA-C	5.32	116.04	108.76
1	D	2121	LYS	CA-C-N	5.31	125.61	119.93
1	D	2121	LYS	C-N-CA	5.31	125.61	119.93
1	F	3697	PHE	CB-CA-C	-5.31	102.47	111.02
1	F	4043	TYR	N-CA-CB	5.31	118.17	110.47
1	E	3443	TYR	CB-CA-C	5.30	119.89	109.72
1	B	1099	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	2234	GLY	N-CA-C	-5.28	108.33	115.36
1	E	3510	VAL	N-CA-C	5.28	115.46	107.75
1	E	3055	ARG	N-CA-C	5.28	117.72	111.33
1	H	4996	VAL	N-CA-CB	5.28	116.56	110.49
1	D	2299	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	E	3043	ASN	N-CA-C	5.27	117.93	111.82
1	A	361	SER	O-C-N	5.26	124.73	120.83
1	C	1699	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	B	758	LEU	O-C-N	5.26	129.99	123.15
1	D	2101	PRO	N-CA-CB	5.25	108.00	103.27
1	E	3262	LYS	N-CA-C	5.25	117.08	111.36
1	C	1633	SER	N-CA-C	-5.25	105.24	111.69
1	F	3827	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	33	ASP	CA-CB-CG	5.25	117.84	112.60
1	C	1489	ILE	N-CA-C	5.24	117.40	108.86
1	D	1894	THR	N-CA-C	5.24	116.68	111.07
1	A	353	ASP	N-CA-CB	5.24	117.82	110.12
1	D	2033	GLU	N-CA-C	-5.23	105.58	111.28
1	D	1843	ASN	N-CA-C	5.23	118.81	112.23
1	E	3220	VAL	CB-CA-C	-5.23	104.20	110.99
1	F	3851	HIS	CA-CB-CG	-5.22	108.58	113.80
1	F	3816	ASP	N-CA-CB	5.22	119.31	110.49
1	C	1300	ASP	CA-C-N	5.21	126.35	119.84
1	C	1300	ASP	C-N-CA	5.21	126.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3435	ARG	N-CA-C	5.21	117.70	111.71
1	G	4633	SER	N-CA-C	-5.20	106.94	113.28
1	A	382	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	2025	ILE	CB-CA-C	-5.20	105.23	111.88
1	E	3359	MET	N-CA-C	5.19	117.08	109.24
1	C	1439	VAL	N-CA-C	5.18	115.74	108.17
1	D	2041	ALA	N-CA-C	5.18	117.11	107.99
1	D	1848	CYS	N-CA-C	5.18	117.41	109.07
1	A	328	GLN	N-CA-C	5.17	119.43	113.38
1	D	2025	ILE	N-CA-CB	5.17	116.25	110.51
1	B	1021	LYS	N-CA-CB	5.16	117.62	109.94
1	B	981	ALA	CB-CA-C	5.15	119.35	110.79
1	F	3905	VAL	N-CA-C	5.15	116.49	110.62
1	G	4506	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	326	ALA	N-CA-C	5.14	117.49	109.52
1	A	201	PHE	CA-CB-CG	-5.14	108.66	113.80
1	D	2308	VAL	N-CA-CB	-5.14	102.31	111.92
1	B	1055	ASN	CA-C-N	5.13	127.41	120.38
1	B	1055	ASN	C-N-CA	5.13	127.41	120.38
1	H	4998	ASN	N-CA-CB	5.12	118.62	110.84
1	A	356	ASP	N-CA-CB	5.12	118.18	110.30
1	A	468	ILE	N-CA-CB	5.12	117.19	111.21
1	A	324	ILE	CA-C-N	-5.10	115.68	122.72
1	A	324	ILE	C-N-CA	-5.10	115.68	122.72
1	B	646	ILE	N-CA-C	5.09	114.90	107.37
1	D	1991	PHE	N-CA-C	5.09	115.25	108.38
1	F	3791	PHE	N-CA-C	5.09	115.87	108.14
1	F	4090	ASN	CB-CA-C	5.09	119.24	110.79
1	H	5242	ARG	N-CA-CB	5.08	117.68	110.06
1	A	407	LEU	N-CA-C	5.07	116.50	111.07
1	B	1079	GLU	CA-C-N	-5.07	116.00	123.00
1	B	1079	GLU	C-N-CA	-5.07	116.00	123.00
1	E	3241	ALA	N-CA-C	5.07	116.92	107.99
1	D	1991	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	318	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	G	4710	VAL	N-CA-C	5.06	115.26	108.17
1	E	3210	LEU	C-N-CD	-5.05	104.30	125.00
1	C	1358	LEU	N-CA-C	5.05	116.86	109.24
1	A	391	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	E	3334	ILE	N-CA-C	-5.04	105.62	110.72
1	B	790	ASP	N-CA-CB	-5.04	103.05	111.06
1	A	22	ALA	N-CA-C	5.03	116.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4587	ALA	CA-C-N	-5.03	111.95	122.07
1	G	4587	ALA	C-N-CA	-5.03	111.95	122.07
1	H	5321	THR	CB-CA-C	5.03	119.74	111.50
1	F	4116	PRO	N-CA-CB	5.02	108.00	103.33
1	C	1635	ARG	N-CA-C	5.01	116.74	111.28
1	F	3686	THR	N-CA-C	-5.01	105.10	111.11
1	C	1264	ILE	CB-CA-C	-5.01	105.56	111.97
1	G	4414	ALA	N-CA-C	5.00	116.36	109.15
1	G	4225	PHE	CA-CB-CG	-5.00	108.80	113.80

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	3978	0	4054	365	2
1	B	3978	0	4056	239	0
1	C	3978	0	4056	373	5
1	D	3978	0	4055	278	5
1	E	3978	0	4056	262	12
1	F	3978	0	4056	275	2
1	G	3978	0	4056	298	2
1	H	3978	0	4056	212	18
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	0	2	0
3	B	6	0	0	1	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	6	0	0	1	0
3	F	6	0	0	3	0
3	G	6	0	0	2	0
3	H	6	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	12	4	0
5	C	31	0	12	4	0
5	D	31	0	12	1	0
5	E	31	0	12	2	0
5	F	31	0	12	0	0
5	G	31	0	12	0	0
6	A	176	0	0	10	0
6	B	260	0	0	13	0
6	C	166	0	0	12	0
6	D	250	0	0	18	0
6	E	267	0	0	17	0
6	F	185	0	0	11	0
6	G	210	0	0	6	0
6	H	296	0	0	15	2
All	All	33890	0	32517	2187	24

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 34.

All (2187) 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:162:ASN:N	1:A:162:ASN:CA	1.82	1.40
1:E:3493:MET:HE2	1:E:3530:PRO:HD2	1.23	1.14
1:C:1678:GLN:HB2	1:C:1684:ASP:HB2	1.31	1.13
1:D:1850:ILE:HD11	1:D:1868:MET:HE1	1.13	1.12
1:H:4850:ILE:HD11	1:H:4868:MET:HE1	1.16	1.12
1:A:122:LEU:HD23	1:A:204:SER:HB3	1.28	1.12
1:B:650:ILE:HD11	1:B:668:MET:HE1	1.23	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4848:CYS:HB2	1:H:4868:MET:HE3	1.21	1.11
1:G:4250:ILE:HB	1:G:4273:MET:HE3	1.36	1.08
1:C:1248:CYS:HB2	1:C:1268:MET:HE3	1.09	1.08
1:E:3142:THR:HG22	1:E:3144:ASP:H	1.06	1.07
1:G:4665:TYR:HB2	1:G:4668:ILE:HD12	1.39	1.04
1:G:4250:ILE:HD11	1:G:4268:MET:HE1	1.08	1.04
1:D:1850:ILE:HB	1:D:1873:MET:HE3	1.41	1.02
1:C:1526:ALA:HB1	1:C:1559:MET:HE2	1.39	1.01
1:F:3624:THR:HG22	1:F:3627:GLU:H	1.18	1.01
1:E:3048:CYS:HB2	1:E:3068:MET:HE3	1.40	1.00
1:A:514:TRP:H	1:A:522:ASN:HD21	1.10	1.00
1:G:4367:VAL:HG22	1:G:4371:SER:HB3	1.43	1.00
1:H:4942:THR:HG23	1:H:4944:ASP:H	1.25	0.99
1:B:928:GLN:NE2	1:D:2141:ARG:H	1.60	0.99
1:B:648:CYS:HB2	1:B:668:MET:HE3	1.43	0.98
1:A:141:ILE:HG21	1:A:158:LEU:HD22	1.44	0.98
1:A:73:MET:HE2	1:A:86:THR:HG21	1.40	0.98
1:A:113:THR:HG22	1:A:242:SER:HB2	1.40	0.98
1:A:326:ALA:HB1	1:A:359:MET:HE2	1.46	0.98
1:A:126:SER:HB3	1:A:129:ALA:HB2	1.44	0.97
1:A:160:TYR:HD2	1:A:163:ILE:HB	1.28	0.97
1:A:51:GLY:O	1:A:55:ARG:HG3	1.65	0.97
1:D:2044:ILE:HG22	1:D:2082:ILE:HD12	1.47	0.96
1:H:5133:MET:HE2	1:H:5139:PRO:HB3	1.46	0.96
1:F:3776:ASP:HB3	1:F:3779:LEU:HB3	1.47	0.95
1:D:2176:MET:HE3	1:D:2176:MET:HA	1.47	0.94
1:F:3648:CYS:HB2	1:F:3668:MET:HE2	1.46	0.94
1:F:3941:ARG:H	1:H:5128:GLN:HE21	1.15	0.93
1:D:1848:CYS:HB2	1:D:1868:MET:HE3	1.50	0.93
1:E:3186:GLN:HB3	1:E:3193:VAL:HB	1.49	0.93
1:G:4322:LEU:HD23	1:G:4404:SER:HB2	1.51	0.92
1:C:1669:PHE:HB3	1:C:1699:ARG:HH12	1.32	0.92
1:E:3376:MET:HA	1:E:3376:MET:HE3	1.50	0.91
1:G:4593:LEU:HD21	1:G:4644:ARG:HG3	1.52	0.91
1:A:431:THR:HG21	1:A:434:GLY:HA2	1.51	0.91
1:G:4250:ILE:HD11	1:G:4268:MET:CE	2.00	0.91
1:E:3050:ILE:HD11	1:E:3068:MET:HE1	1.51	0.90
1:D:1824:THR:HG22	1:D:1827:GLU:HB2	1.50	0.90
1:G:4680:ALA:HB3	1:G:4683:GLU:HG3	1.53	0.89
1:E:3493:MET:HE1	1:E:3529:VAL:HG13	1.54	0.89
1:E:3341:ARG:H	1:G:4528:GLN:HE21	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5020:VAL:HG13	1:H:5024:ASP:HB2	1.54	0.89
1:D:1986:GLN:HB3	1:D:1993:VAL:HB	1.53	0.89
1:F:3928:GLN:NE2	1:H:5141:ARG:H	1.71	0.89
1:B:1065:TYR:HB2	1:B:1068:ILE:HD12	1.53	0.89
1:C:1322:LEU:HD12	1:C:1349:GLU:HG2	1.53	0.88
1:C:1347:TYR:CD2	1:C:1355:ILE:HG21	2.07	0.88
1:C:1250:ILE:HB	1:C:1273:MET:HE3	1.55	0.88
1:F:3890:MET:HE2	1:F:3892:ALA:HB2	1.55	0.88
1:G:4389:PRO:HD2	1:G:4391:PHE:CE2	2.08	0.88
1:G:4248:CYS:HB2	1:G:4268:MET:HE3	1.56	0.88
1:G:4371:SER:H	1:G:4384:VAL:HB	1.38	0.88
1:H:4873:MET:HE3	1:H:4887:ILE:HD12	1.52	0.88
1:C:1382:LEU:HD21	1:C:1396:VAL:HG22	1.55	0.88
1:B:815:VAL:HB	1:B:817:LEU:HD12	1.55	0.87
1:E:3402:SER:HB2	1:F:3621:MET:HE1	1.54	0.87
1:A:328:GLN:NE2	1:C:1541:ARG:H	1.72	0.87
1:H:5020:VAL:HG11	1:H:5025:ILE:HG12	1.56	0.87
1:C:1693:MET:CE	1:C:1729:VAL:HG22	2.05	0.87
1:F:3733:LEU:HD11	1:F:3802:LEU:HD22	1.57	0.87
1:F:3726:SER:HB3	1:F:3729:ALA:HB2	1.57	0.86
1:G:4367:VAL:HG22	1:G:4371:SER:CB	2.06	0.86
1:H:5133:MET:HE2	1:H:5139:PRO:CB	2.04	0.86
1:G:4479:PHE:CZ	1:G:4483:LEU:HD22	2.09	0.86
1:B:720:THR:HG22	1:B:758:LEU:CD2	2.04	0.86
1:A:73:MET:HE2	1:A:86:THR:CG2	2.06	0.86
1:E:3142:THR:HG22	1:E:3144:ASP:N	1.89	0.86
1:F:3928:GLN:HE21	1:H:5141:ARG:H	1.24	0.86
1:A:141:ILE:CG2	1:A:158:LEU:HD22	2.07	0.85
1:C:1591:ARG:HH12	1:C:1592:LYS:HE3	1.42	0.85
1:A:431:THR:CG2	1:A:434:GLY:HA2	2.06	0.85
1:E:3160:TYR:HD2	1:E:3163:ILE:HB	1.41	0.85
1:C:1442:SER:HA	1:C:1469:LYS:HD3	1.59	0.84
1:E:3106:PRO:HG2	1:E:3470:PRO:HB2	1.60	0.84
1:E:3431:THR:HG21	1:E:3434:GLY:HA2	1.60	0.84
1:C:1678:GLN:HB2	1:C:1684:ASP:CB	2.08	0.84
1:H:4926:SER:HB3	1:H:4929:ALA:H	1.42	0.83
1:H:5311:LEU:HB3	1:H:5321:THR:CG2	2.08	0.83
1:C:1343:LEU:HD21	1:C:1361:LYS:HA	1.61	0.83
1:E:3050:ILE:HD11	1:E:3068:MET:CE	2.09	0.83
1:D:2304:LYS:HG3	1:D:2330:PRO:C	2.03	0.83
1:E:3245:ARG:HB3	1:E:3274:GLU:HG2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:CG2	1:A:208:VAL:HB	2.09	0.83
1:D:1824:THR:HG23	1:D:1827:GLU:H	1.44	0.83
1:E:3160:TYR:O	1:E:3163:ILE:HG22	1.78	0.83
1:B:928:GLN:HE21	1:D:2141:ARG:H	1.26	0.82
1:B:1109:ILE:CD1	1:B:1126:VAL:HG22	2.09	0.82
1:C:1534:ILE:HG23	1:C:1567:GLY:HA2	1.59	0.82
1:G:4248:CYS:HB2	1:G:4268:MET:CE	2.10	0.82
1:C:1343:LEU:CD2	1:C:1361:LYS:HA	2.10	0.82
1:G:4250:ILE:CD1	1:G:4268:MET:HE1	2.03	0.82
1:A:301:PRO:HG2	1:A:304:LYS:HD2	1.61	0.81
1:D:2201:SER:HA	1:D:2203:HIS:CE1	2.14	0.81
1:B:1104:LYS:HB3	1:B:1130:PRO:C	2.04	0.81
1:C:1270:VAL:HG22	1:C:1308:ALA:HB3	1.60	0.81
1:C:1477:ARG:NH2	1:C:1478:ARG:HH11	1.78	0.81
1:D:2265:TYR:HB2	1:D:2268:ILE:HD12	1.61	0.81
1:F:3726:SER:CB	1:F:3729:ALA:HB2	2.10	0.81
1:H:5090:MET:HE3	1:H:5126:ALA:CB	2.09	0.81
1:B:941:ARG:H	1:D:2128:GLN:HE21	1.26	0.81
1:F:3672:ARG:C	1:F:3673:MET:HE3	2.05	0.81
1:E:3341:ARG:H	1:G:4528:GLN:NE2	1.77	0.81
1:F:3713:THR:HG22	1:F:3842:SER:H	1.45	0.81
1:F:3941:ARG:H	1:H:5128:GLN:NE2	1.77	0.81
1:C:1248:CYS:CB	1:C:1268:MET:HE3	2.04	0.81
1:D:2090:MET:HE2	1:D:2092:ALA:HB2	1.62	0.81
1:G:4477:ARG:NH2	1:G:4478:ARG:NH1	2.29	0.81
1:A:113:THR:CG2	1:A:242:SER:HB2	2.10	0.80
1:C:1273:MET:HE2	1:C:1286:THR:CG2	2.10	0.80
1:C:1313:THR:HG22	1:C:1442:SER:H	1.45	0.80
1:B:648:CYS:HB2	1:B:668:MET:CE	2.10	0.80
1:D:1824:THR:HG22	1:D:1827:GLU:CB	2.10	0.80
1:F:3731:VAL:HG12	1:F:3802:LEU:HB3	1.64	0.80
1:G:4276:SER:HB3	1:G:4319:ARG:HE	1.46	0.80
1:D:1850:ILE:HD11	1:D:1868:MET:CE	2.05	0.80
1:E:3493:MET:CE	1:E:3529:VAL:HG13	2.10	0.80
1:F:3648:CYS:HB2	1:F:3668:MET:CE	2.12	0.80
1:A:163:ILE:HG23	1:A:163:ILE:O	1.82	0.80
1:C:1248:CYS:HB2	1:C:1268:MET:CE	2.03	0.80
1:H:4847:ILE:HG21	1:H:5159:MET:HE2	1.62	0.80
1:F:3624:THR:CG2	1:F:3627:GLU:H	1.93	0.80
1:F:3702:ILE:HG22	1:F:3703:LEU:HD12	1.63	0.80
1:B:890:MET:HE2	1:B:892:ALA:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:HB3	1:A:463:HIS:ND1	1.97	0.80
1:B:759:ASP:HB3	6:B:6586:HOH:O	1.82	0.79
1:C:1602:SER:HB2	1:D:1821:MET:HE1	1.62	0.79
1:B:976:MET:HE3	1:B:980:ILE:HG13	1.64	0.79
1:D:2176:MET:CE	1:D:2179:LEU:HB2	2.12	0.79
1:A:225:ILE:HG23	1:A:256:ILE:CG2	2.13	0.79
1:F:3740:LYS:HE2	1:F:3791:PHE:CD2	2.18	0.79
1:G:4680:ALA:HB3	1:G:4683:GLU:CG	2.13	0.79
1:C:1472:ASN:ND2	1:C:1475:GLY:H	1.81	0.79
1:E:3191:PHE:HE2	1:E:3193:VAL:HG23	1.46	0.79
1:D:1899:SER:O	1:D:1901:PRO:HD3	1.83	0.79
1:D:2044:ILE:CG2	1:D:2082:ILE:HD12	2.13	0.79
1:D:1824:THR:CG2	1:D:1827:GLU:H	1.95	0.79
1:E:3431:THR:CG2	1:E:3434:GLY:HA2	2.12	0.79
1:C:1609:GLU:O	1:C:1613:MET:HG3	1.84	0.78
1:H:5327:VAL:HG13	1:H:5328:PRO:HD2	1.63	0.78
1:H:5133:MET:HE2	1:H:5139:PRO:CG	2.13	0.78
1:B:650:ILE:CD1	1:B:668:MET:HE1	2.10	0.78
6:B:6064:HOH:O	1:D:1824:THR:HG21	1.84	0.78
1:C:1259:THR:O	1:C:1263:MET:HG3	1.83	0.78
1:A:126:SER:HB3	1:A:129:ALA:CB	2.12	0.78
1:H:4923:ILE:HD12	1:H:4931:VAL:HG23	1.66	0.78
1:A:511:LEU:HD22	1:A:521:THR:HG23	1.66	0.77
1:F:3949:ASN:HD21	1:H:5110:LYS:NZ	1.83	0.77
1:E:3465:TYR:HB2	1:E:3468:ILE:HD12	1.65	0.77
1:H:5209:GLU:O	1:H:5213:MET:HG3	1.84	0.77
1:F:3724:LYS:HG3	6:F:7409:HOH:O	1.85	0.77
1:H:4850:ILE:HD11	1:H:4868:MET:CE	2.08	0.77
1:G:4339:LEU:HD11	1:G:4354:ASN:CA	2.15	0.77
1:E:3225:ILE:HD12	1:E:3256:ILE:HD12	1.66	0.77
1:E:3253:VAL:HG12	1:E:3257:LEU:CD2	2.14	0.77
1:F:3787:LYS:HA	1:F:3792:LEU:HD12	1.67	0.77
1:A:277:ARG:NH2	1:A:278:ARG:NH1	2.33	0.77
1:A:515:ARG:HD2	6:A:6021:HOH:O	1.85	0.77
1:H:4848:CYS:HB2	1:H:4868:MET:CE	2.10	0.77
1:A:122:LEU:HD23	1:A:204:SER:CB	2.14	0.76
1:D:1902:ILE:HG13	1:D:2295:VAL:HG22	1.66	0.76
1:E:3479:GLU:HG3	6:E:6677:HOH:O	1.84	0.76
1:E:3246:LYS:HD2	1:E:3249:ASP:OD1	1.86	0.76
1:A:162:ASN:N	1:A:162:ASN:CB	2.49	0.76
1:E:3027:GLU:O	1:E:3031:ARG:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1665:TYR:HB2	1:C:1668:ILE:HD12	1.67	0.76
1:E:3316:CYS:HB3	1:E:3321:LYS:O	1.84	0.76
1:A:328:GLN:HE21	1:C:1541:ARG:H	1.32	0.76
1:B:873:HIS:O	1:B:877:ARG:HG3	1.86	0.76
1:C:1409:ASN:O	1:C:1411:PRO:HD3	1.85	0.76
1:A:55:ARG:HD2	1:A:82:TYR:OH	1.84	0.76
1:F:3663:MET:CE	1:F:3668:MET:HE3	2.15	0.76
1:H:5191:ARG:O	1:H:5195:GLU:HG3	1.84	0.76
1:A:48:CYS:HB2	1:A:68:MET:HE2	1.68	0.76
1:C:1250:ILE:HD11	1:C:1268:MET:HE1	1.68	0.76
1:E:3172:LYS:HE3	1:E:3183:GLN:HB2	1.67	0.76
1:G:4438:MET:HA	1:G:4464:ILE:HG23	1.66	0.76
1:H:4848:CYS:CB	1:H:4868:MET:HE3	2.09	0.76
1:G:4322:LEU:HD23	1:G:4404:SER:CB	2.15	0.76
1:G:4360:TYR:HE2	1:G:4366:VAL:HG21	1.51	0.76
1:B:1054:ARG:HD2	6:B:7369:HOH:O	1.85	0.76
1:G:4494:GLY:CA	1:G:4527:THR:HG21	2.17	0.75
1:A:221:SER:HB2	1:A:224:ASP:H	1.51	0.75
1:A:391:ARG:O	1:A:395:GLU:HG3	1.87	0.75
1:B:873:HIS:CE1	1:B:900:ILE:HG22	2.22	0.75
1:D:1850:ILE:CD1	1:D:1868:MET:HE1	2.06	0.75
1:D:2201:SER:HA	1:D:2203:HIS:HE1	1.51	0.75
1:H:4847:ILE:CG2	1:H:5159:MET:HE2	2.16	0.75
1:C:1526:ALA:CB	1:C:1559:MET:HE2	2.15	0.75
1:C:1669:PHE:HB3	1:C:1699:ARG:NH1	2.01	0.75
1:F:3650:ILE:HD11	1:F:3668:MET:HE1	1.66	0.75
1:F:3723:ILE:HA	1:F:3751:CYS:O	1.86	0.75
1:B:823:LYS:HE3	1:B:827:ASP:OD2	1.85	0.75
1:E:3493:MET:HE2	1:E:3530:PRO:CD	2.09	0.75
1:H:5130:LEU:HD13	1:H:5133:MET:CE	2.16	0.75
1:C:1693:MET:HE2	1:C:1729:VAL:HA	1.68	0.75
1:G:4408:VAL:HG12	1:G:4410:LEU:CD1	2.17	0.74
1:B:740:LYS:HE2	1:B:742:THR:HG22	1.69	0.74
1:A:145:ASN:O	1:A:148:MET:HB2	1.87	0.74
1:F:3732:GLU:HB2	1:F:3801:PHE:CD1	2.21	0.74
1:A:399:ARG:NH2	1:C:1223:ASP:HB2	2.03	0.74
1:G:4332:GLU:HA	1:G:4401:PHE:HA	1.69	0.74
1:A:122:LEU:HD12	1:A:149:GLU:HG2	1.67	0.74
1:H:5311:LEU:HB3	1:H:5321:THR:HG21	1.69	0.74
1:F:3652:PRO:HD2	1:F:3965:ALA:O	1.88	0.74
1:B:722:LEU:HA	1:B:804:SER:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1678:GLN:CB	1:C:1684:ASP:HB2	2.15	0.74
1:B:866:ILE:O	1:B:887:ASP:HB2	1.88	0.74
1:C:1421:SER:O	1:C:1425:ILE:HG13	1.88	0.74
1:G:4368:ASP:O	1:G:4371:SER:HB2	1.87	0.74
1:A:192:LEU:HD22	1:A:192:LEU:N	2.02	0.74
1:C:1376:ASP:OD2	1:C:1406:LYS:HE2	1.87	0.74
1:G:4704:LYS:HG2	1:G:4730:PRO:C	2.12	0.74
1:H:4851:GLY:O	1:H:4855:ARG:HG2	1.86	0.74
1:B:1125:ARG:HD2	6:B:7678:HOH:O	1.88	0.74
1:C:1273:MET:HE2	1:C:1286:THR:HG22	1.69	0.74
1:C:1345:ASN:O	1:C:1348:MET:HB3	1.86	0.74
1:A:55:ARG:HD2	1:A:82:TYR:CZ	2.23	0.73
1:F:3752:ASP:CG	1:F:3754:ASN:H	1.96	0.73
1:H:5090:MET:HE3	1:H:5126:ALA:HB3	1.70	0.73
1:B:897:GLY:HA3	1:D:2141:ARG:HE	1.51	0.73
1:C:1313:THR:CG2	1:C:1442:SER:H	1.99	0.73
1:H:5108:ALA:O	1:H:5112:ILE:HG13	1.88	0.73
1:B:815:VAL:HB	1:B:817:LEU:CD1	2.18	0.73
1:B:941:ARG:H	1:D:2128:GLN:NE2	1.86	0.73
1:D:1817:LEU:O	1:D:1820:ALA:HB3	1.87	0.73
1:E:3252:GLU:O	1:E:3256:ILE:HG12	1.89	0.73
1:A:147:TYR:HA	1:A:150:LYS:HB2	1.70	0.73
1:A:167:VAL:CG2	1:A:184:VAL:HG21	2.19	0.73
1:A:327:THR:HG22	1:A:328:GLN:HG3	1.69	0.73
1:C:1313:THR:HG22	1:C:1442:SER:OG	1.87	0.73
1:E:3392:LYS:O	1:E:3396:GLU:HG3	1.88	0.73
1:C:1363:ILE:O	1:C:1367:VAL:HG12	1.88	0.73
1:C:1428:LEU:HD13	1:C:1456:ILE:HB	1.71	0.73
1:C:1500:ILE:HB	1:C:1501:PRO:HD2	1.70	0.73
1:A:160:TYR:CD2	1:A:163:ILE:HB	2.19	0.73
1:B:1087:LEU:HD23	1:B:1088:ARG:N	2.04	0.73
1:G:4478:ARG:O	1:G:4482:ILE:HG13	1.89	0.73
1:B:928:GLN:NE2	1:D:2141:ARG:N	2.36	0.72
1:C:1286:THR:O	1:C:1290:VAL:HG23	1.89	0.72
1:C:1404:SER:O	1:C:1406:LYS:HD3	1.90	0.72
1:D:2284:ASP:O	1:D:2288:ARG:HG3	1.89	0.72
1:E:3426:ALA:HA	1:E:3447:ALA:HB1	1.70	0.72
1:B:950:ALA:O	1:B:953:ASP:HB2	1.89	0.72
1:C:1250:ILE:HB	1:C:1273:MET:CE	2.20	0.72
1:E:3172:LYS:HE2	1:E:3197:GLU:OE1	1.89	0.72
1:F:3999:ARG:HH12	1:H:4823:ASP:HB2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1291:ARG:O	1:C:1295:GLU:HG2	1.90	0.72
1:A:131:VAL:HG12	1:A:202:LEU:HD23	1.71	0.71
1:B:674:ASN:OD1	1:B:676:SER:HB2	1.90	0.71
1:D:2046:LYS:HB2	6:D:7775:HOH:O	1.90	0.71
1:F:3763:ILE:O	1:F:3767:VAL:HG13	1.91	0.71
1:A:118:ILE:HG22	1:A:208:VAL:HB	1.72	0.71
1:A:388:MET:HB2	1:A:390:HIS:CE1	2.24	0.71
1:C:1671:VAL:HG12	1:C:1691:LEU:HD21	1.72	0.71
1:D:1848:CYS:HB2	1:D:1868:MET:CE	2.19	0.71
1:A:310:LYS:HZ1	1:C:1549:ASN:HD21	1.39	0.71
1:A:485:VAL:O	1:A:489:VAL:HG23	1.89	0.71
1:C:1382:LEU:CD2	1:C:1396:VAL:HG22	2.21	0.71
1:C:1477:ARG:HH22	1:C:1478:ARG:NH1	1.88	0.71
1:D:1945:ASN:HD21	1:D:1961:LYS:NZ	1.88	0.71
1:E:3188:GLY:HA3	1:E:3191:PHE:CE1	2.25	0.71
1:G:4591:ARG:NH1	1:G:4592:LYS:HD2	2.06	0.71
1:H:4963:ILE:O	1:H:4967:VAL:HG22	1.90	0.71
1:B:1111:LEU:HD21	1:B:1124:MET:HB2	1.71	0.71
1:D:1851:GLY:O	1:D:1855:ARG:HG3	1.91	0.71
1:G:4409:ASN:C	1:G:4410:LEU:HD12	2.15	0.71
1:G:4715:ARG:HB3	1:G:4716:PRO:HD2	1.71	0.71
1:A:288:GLY:O	1:A:289:ILE:HD13	1.89	0.71
1:A:326:ALA:CB	1:A:359:MET:HE2	2.21	0.71
1:C:1511:MET:O	1:C:1515:ARG:HG3	1.91	0.71
1:F:3776:ASP:OD2	1:F:3806:LYS:HE3	1.91	0.71
1:A:191:PHE:HE2	1:A:193:VAL:HG23	1.56	0.70
1:G:4509:GLN:O	1:G:4513:ILE:HG13	1.90	0.70
1:D:1855:ARG:HD2	1:D:1882:TYR:OH	1.90	0.70
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.26	0.70
1:F:3752:ASP:OD1	1:F:3755:ILE:HD13	1.91	0.70
1:H:5130:LEU:HD13	1:H:5133:MET:HE3	1.73	0.70
1:D:2044:ILE:HG13	1:D:2068:SER:HB3	1.72	0.70
1:D:2116:CYS:HB3	1:D:2121:LYS:O	1.91	0.70
1:A:506:ASP:O	1:A:529:VAL:HG23	1.92	0.70
1:B:866:ILE:C	1:B:867:ILE:HD13	2.17	0.70
1:C:1257:VAL:HG21	1:C:1292:THR:HG22	1.71	0.70
1:F:3669:ASN:HB3	1:F:4063:HIS:CD2	2.27	0.70
1:F:3949:ASN:HD21	1:H:5110:LYS:HZ1	1.38	0.70
1:B:970:PRO:O	1:B:974:VAL:HG23	1.90	0.70
1:B:1091:LEU:O	1:B:1095:VAL:HG23	1.92	0.70
1:F:3757:TRP:C	1:F:3758:LEU:HD23	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1322:LEU:HB2	1:C:1349:GLU:HA	1.72	0.70
1:G:4323:ILE:HD13	1:G:4351:CYS:HB3	1.73	0.70
1:H:5066:ILE:C	1:H:5067:ILE:HD13	2.17	0.70
1:F:3624:THR:HG22	1:F:3627:GLU:N	2.01	0.70
1:C:1319:ARG:H	1:C:1359:ASP:HB2	1.57	0.69
1:C:1327:GLY:HA2	1:C:1404:SER:CB	2.22	0.69
1:H:4966:VAL:HB	6:H:7456:HOH:O	1.91	0.69
1:H:5130:LEU:HD22	1:H:5133:MET:CE	2.22	0.69
1:A:246:LYS:HG3	6:A:7561:HOH:O	1.90	0.69
1:E:3160:TYR:CD2	1:E:3163:ILE:HB	2.26	0.69
1:D:1814:THR:HG22	1:D:1815:GLN:HG3	1.73	0.69
1:G:4341:ILE:HB	1:G:4392:LEU:HB2	1.74	0.69
1:G:4445:ARG:O	1:G:4478:ARG:HD3	1.92	0.69
1:C:1257:VAL:HG21	1:C:1292:THR:CG2	2.22	0.69
1:C:1693:MET:HE2	1:C:1729:VAL:HG22	1.73	0.69
1:D:1873:MET:HE2	1:D:1886:THR:HG22	1.73	0.69
1:H:4873:MET:HE3	1:H:4887:ILE:CD1	2.23	0.69
1:B:1011:MET:HE2	1:B:1122:ASN:C	2.18	0.69
1:C:1459:GLU:O	1:C:1462:LYS:HG2	1.91	0.69
1:C:1493:ARG:HD3	1:C:1526:ALA:O	1.92	0.69
1:E:3411:MET:SD	1:F:4126:VAL:HG23	2.32	0.69
1:G:4477:ARG:NH2	1:G:4478:ARG:HH11	1.89	0.69
1:C:1251:GLY:O	1:C:1255:ARG:HG3	1.91	0.69
1:E:3288:GLY:C	1:E:3289:ILE:HG12	2.17	0.69
1:E:3478:GLN:HB2	1:E:3484:ASP:HB2	1.73	0.69
1:G:4216:GLN:HE22	1:G:4233:ASP:H	1.41	0.69
1:H:5314:TRP:CD1	1:H:5315:ARG:HG3	2.28	0.69
1:C:1501:PRO:HG2	1:C:1504:LYS:HD2	1.73	0.69
1:H:4952:ASP:HB2	1:H:4953:GLU:OE1	1.93	0.69
1:B:991:ARG:O	1:B:995:GLU:HG3	1.92	0.69
1:B:1093:MET:HE2	1:B:1129:VAL:HG22	1.75	0.69
1:F:3650:ILE:CD1	1:F:3668:MET:HE1	2.22	0.69
1:H:4942:THR:HG23	1:H:4944:ASP:N	2.04	0.69
1:A:328:GLN:HE22	1:C:1540:THR:HA	1.57	0.68
1:C:1723:THR:HG23	1:D:2325:ARG:HG3	1.73	0.68
1:F:3740:LYS:HE2	1:F:3791:PHE:CG	2.28	0.68
1:F:3890:MET:HE2	1:F:3892:ALA:CB	2.22	0.68
1:G:4257:VAL:O	1:G:4261:LYS:HG3	1.94	0.68
1:G:4408:VAL:HG12	1:G:4410:LEU:HD11	1.73	0.68
1:E:3432:GLU:HA	1:E:3432:GLU:OE1	1.92	0.68
1:F:3890:MET:HE3	1:F:3926:ALA:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4680:ALA:CB	1:G:4683:GLU:HG3	2.23	0.68
1:A:167:VAL:HG21	1:A:184:VAL:HG21	1.75	0.68
1:A:454:ARG:HG2	1:A:473:CYS:HB3	1.74	0.68
1:E:3222:GLU:HG2	1:E:3223:LYS:N	2.07	0.68
1:E:3475:ASP:HB3	1:E:3476:PRO:HD2	1.75	0.68
1:F:3743:LEU:HD11	1:F:3761:LYS:HA	1.76	0.68
1:B:650:ILE:HD11	1:B:668:MET:CE	2.11	0.68
1:C:1362:ASN:HD22	1:C:1365:LYS:HD2	1.59	0.68
1:D:1848:CYS:CB	1:D:1868:MET:HE3	2.24	0.68
1:D:2240:VAL:HG12	1:D:2249:ILE:CD1	2.23	0.68
1:A:225:ILE:HG23	1:A:256:ILE:HG23	1.75	0.68
1:D:2033:GLU:HG3	6:D:6665:HOH:O	1.93	0.68
1:F:3760:TYR:HE2	1:F:3766:VAL:HG21	1.58	0.68
1:F:3890:MET:HE3	1:F:3926:ALA:HB3	1.76	0.68
1:B:745:ASN:HD22	1:B:757:TRP:HE1	1.40	0.67
1:B:1078:GLN:NE2	1:B:1078:GLN:HA	2.08	0.67
1:C:1526:ALA:HB1	1:C:1559:MET:CE	2.20	0.67
1:A:122:LEU:HB2	1:A:149:GLU:HA	1.75	0.67
1:E:3145:ASN:O	1:E:3148:MET:HB2	1.93	0.67
1:G:4293:ALA:O	1:G:4296:SER:HB3	1.95	0.67
1:A:481:TRP:O	1:A:485:VAL:HG23	1.95	0.67
1:C:1423:LYS:O	1:C:1426:GLN:HB3	1.95	0.67
1:F:3845:ARG:HG2	1:F:3874:GLU:HB3	1.75	0.67
1:A:15:GLN:HG3	1:A:39:ILE:HG23	1.75	0.67
1:A:340:THR:OG1	1:A:343:GLU:HG3	1.94	0.67
1:B:716:PRO:HG2	1:B:843:PHE:CD2	2.29	0.67
1:B:999:ARG:HH12	1:D:1823:ASP:CB	2.06	0.67
1:D:2090:MET:CE	1:D:2092:ALA:HB2	2.24	0.67
1:E:3254:ARG:NH2	1:E:3287:ASP:OD2	2.28	0.67
1:G:4275:PHE:O	1:G:4314:LYS:HE3	1.94	0.67
1:A:29:MET:HE2	1:C:1510:LYS:HB3	1.75	0.67
1:C:1406:LYS:HE3	5:C:1735:ATP:O3'	1.95	0.67
1:A:290:MET:HE2	1:A:292:ALA:HB2	1.75	0.67
1:A:310:LYS:NZ	1:C:1549:ASN:HD21	1.93	0.67
1:B:844:ILE:HG13	1:B:868:SER:HB3	1.77	0.67
1:A:99:SER:O	1:A:101:PRO:HD3	1.95	0.67
1:B:999:ARG:HH12	1:D:1823:ASP:HB2	1.60	0.67
1:C:1250:ILE:HD11	1:C:1268:MET:CE	2.24	0.67
1:D:1902:ILE:HG22	1:D:1903:LEU:CD2	2.25	0.67
1:D:2141:ARG:HG2	1:D:2141:ARG:HH11	1.59	0.67
1:D:2291:LEU:O	1:D:2295:VAL:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3050:ILE:CD1	1:E:3068:MET:HE1	2.25	0.67
1:E:3440:VAL:HG12	1:E:3449:ILE:HD11	1.75	0.67
1:F:3687:ILE:HD13	1:F:3709:VAL:HG11	1.75	0.67
1:F:3999:ARG:NH1	1:H:4823:ASP:HB2	2.10	0.67
1:H:5020:VAL:HG12	1:H:5021:SER:O	1.93	0.67
1:A:333:MET:CE	1:A:373:ALA:HA	2.25	0.67
1:C:1339:LEU:HD12	1:C:1340:LYS:H	1.60	0.67
1:C:1366:VAL:CG2	1:C:1413:ALA:HB1	2.25	0.67
1:C:1693:MET:HE3	1:C:1729:VAL:HG22	1.77	0.67
1:F:3653:ALA:HB2	1:F:3966:LYS:HA	1.75	0.67
1:F:3691:ARG:O	1:F:3695:GLU:HG2	1.94	0.67
1:H:5020:VAL:CG1	1:H:5025:ILE:HG12	2.24	0.67
1:G:4360:TYR:CE2	1:G:4366:VAL:HG21	2.30	0.66
1:E:3481:TRP:HB2	1:E:3516:PRO:HG3	1.77	0.66
1:G:4665:TYR:CB	1:G:4668:ILE:HD12	2.23	0.66
1:A:484:ASP:O	1:A:487:LEU:HB3	1.95	0.66
1:C:1362:ASN:ND2	1:C:1365:LYS:HD2	2.10	0.66
1:F:3684:ALA:HB2	1:F:3830:PHE:HZ	1.60	0.66
1:G:4477:ARG:HH22	1:G:4478:ARG:NH1	1.94	0.66
1:A:84:ALA:HB2	1:A:230:PHE:HZ	1.61	0.66
1:A:120:THR:HG22	1:A:205:LYS:H	1.60	0.66
1:B:673:MET:HE3	1:B:686:THR:HG22	1.76	0.66
1:B:1111:LEU:CD2	1:B:1124:MET:HB2	2.26	0.66
1:C:1370:GLY:O	1:C:1383:GLN:NE2	2.29	0.66
1:A:203:GLY:HA3	1:A:206:LYS:HE2	1.76	0.66
1:A:292:ALA:HB1	3:A:533:OXL:C1	2.26	0.66
1:B:827:ASP:O	1:B:830:PHE:HB3	1.94	0.66
1:C:1387:LYS:HB3	1:C:1392:LEU:HD12	1.78	0.66
1:E:3448:PRO:HB3	1:E:3469:PHE:CE1	2.31	0.66
1:H:5311:LEU:HB3	1:H:5321:THR:HG23	1.75	0.66
1:B:938:ARG:HH22	1:D:1998:ASN:HD21	1.43	0.66
1:C:1323:ILE:HG22	1:C:1324:LYS:HG3	1.76	0.66
1:C:1343:LEU:HD13	1:C:1390:ASP:O	1.96	0.66
1:E:3509:ILE:CD1	1:E:3526:VAL:HG23	2.25	0.66
1:G:4342:THR:HG21	1:G:4347:TYR:CD2	2.31	0.66
1:G:4493:ARG:HD3	1:G:4526:ALA:O	1.95	0.66
1:B:768:ASP:O	1:B:771:SER:HB2	1.95	0.66
1:C:1441:ALA:O	1:C:1469:LYS:HG3	1.95	0.66
1:D:1863:MET:HE3	1:D:2174:VAL:HG21	1.76	0.66
1:D:1941:ILE:HA	1:D:1956:LEU:O	1.96	0.66
1:D:2030:PHE:CE1	1:D:2034:GLN:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3904:LYS:HD3	1:H:5183:GLU:OE2	1.96	0.66
1:B:651:GLY:O	1:B:655:ARG:HG3	1.97	0.65
1:C:1456:ILE:HD13	1:C:1456:ILE:N	2.11	0.65
1:D:1850:ILE:CB	1:D:1873:MET:HE3	2.24	0.65
1:A:173:VAL:HG13	1:A:210:LEU:HD11	1.77	0.65
1:C:1326:SER:HB3	1:C:1329:ALA:CB	2.26	0.65
1:C:1343:LEU:HD23	1:C:1361:LYS:CD	2.25	0.65
1:H:5130:LEU:HB3	1:H:5133:MET:HE3	1.78	0.65
1:H:5133:MET:HE2	1:H:5139:PRO:HG3	1.77	0.65
1:C:1313:THR:HG21	6:C:6155:HOH:O	1.95	0.65
1:D:2171:LEU:O	1:D:2175:ARG:HG3	1.96	0.65
1:E:3457:GLN:O	1:E:3461:GLN:HG3	1.96	0.65
1:A:333:MET:HG2	1:A:336:LYS:O	1.96	0.65
1:C:1581:ALA:O	1:C:1585:GLU:HG3	1.96	0.65
1:D:2072:ASN:HB2	6:D:6547:HOH:O	1.96	0.65
1:D:2126:ALA:HB1	1:D:2159:MET:HE2	1.78	0.65
1:C:1366:VAL:HG22	1:C:1413:ALA:HB1	1.77	0.65
1:E:3160:TYR:HD2	1:E:3163:ILE:CB	2.09	0.65
1:E:3402:SER:CB	1:F:3621:MET:HE1	2.27	0.65
1:G:4498:ILE:HD13	1:G:4498:ILE:N	2.11	0.65
1:G:4555:ALA:O	1:G:4666:ARG:NH1	2.29	0.65
1:C:1531:GLU:N	1:C:1543:GLU:OE2	2.30	0.65
1:A:14:THR:HG23	1:A:15:GLN:HB2	1.77	0.65
1:E:3376:MET:HE2	1:E:3380:ILE:HG13	1.78	0.65
1:G:4321:GLY:HA3	1:G:4357:TRP:HE3	1.62	0.65
1:A:103:LEU:HD11	1:A:498:ALA:HB1	1.78	0.65
1:E:3371:LEU:HB2	6:E:6190:HOH:O	1.97	0.65
1:A:160:TYR:O	1:A:163:ILE:HG22	1.96	0.65
1:A:413:MET:SD	1:B:1021:LYS:HD3	2.37	0.65
1:D:2241:ALA:O	1:D:2244:ARG:NH1	2.29	0.65
1:G:4527:THR:OG1	3:G:4733:OXL:O2	2.15	0.65
5:A:535:ATP:N7	6:A:7651:HOH:O	2.30	0.65
1:C:1427:ASP:O	1:C:1430:PHE:HB3	1.97	0.65
1:C:1477:ARG:HH22	1:C:1478:ARG:HH11	1.44	0.65
1:D:2265:TYR:HB2	1:D:2268:ILE:CD1	2.26	0.65
1:C:1442:SER:CA	1:C:1469:LYS:HD3	2.26	0.64
1:G:4247:ILE:HB	1:G:4559:MET:HG3	1.78	0.64
1:B:934:ILE:HG23	1:B:967:GLY:HA2	1.80	0.64
1:B:969:TYR:HB3	1:B:972:GLU:HB2	1.79	0.64
1:D:2176:MET:HE3	1:D:2179:LEU:HB2	1.77	0.64
1:H:5015:VAL:CG1	1:H:5017:LEU:HG	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:THR:HG21	1:B:1034:GLY:HA2	1.78	0.64
1:C:1479:PHE:HE1	1:C:1489:ILE:HD12	1.60	0.64
1:E:3315:ARG:NH1	1:G:4230:CYS:O	2.29	0.64
1:F:3838:MET:HA	1:F:3864:ILE:HG23	1.79	0.64
1:H:4850:ILE:CD1	1:H:4868:MET:HE1	2.09	0.64
1:A:246:LYS:HG3	1:A:248:ALA:HB3	1.80	0.64
1:A:57:VAL:HG22	1:A:89:ASN:HA	1.78	0.64
1:F:3731:VAL:O	1:F:3802:LEU:N	2.30	0.64
1:G:4348:MET:HA	1:G:4357:TRP:CD2	2.33	0.64
1:G:4410:LEU:O	1:G:4413:ALA:HB3	1.98	0.64
1:H:4945:ASN:HB3	1:H:4948:MET:HE2	1.77	0.64
1:A:50:ILE:HB	1:A:73:MET:CE	2.26	0.64
1:C:1319:ARG:NE	1:C:1405:LYS:O	2.30	0.64
1:E:3481:TRP:CG	1:E:3516:PRO:HD3	2.33	0.64
1:F:3787:LYS:HB3	1:F:3792:LEU:CD1	2.27	0.64
1:F:3788:GLY:N	1:F:3791:PHE:O	2.29	0.64
1:G:4374:TYR:HB3	1:G:4378:GLY:HA2	1.79	0.64
1:G:4693:MET:HE2	1:G:4729:VAL:HG22	1.79	0.64
1:C:1360:TYR:HE2	1:C:1366:VAL:HG11	1.61	0.64
1:G:4409:ASN:C	1:G:4411:PRO:HD3	2.22	0.64
1:D:1855:ARG:NH2	1:D:1885:GLU:HG2	2.11	0.64
1:A:399:ARG:HD2	6:C:6738:HOH:O	1.98	0.64
1:D:2045:ARG:C	1:D:2046:LYS:HG3	2.22	0.64
1:F:3713:THR:CG2	1:F:3842:SER:H	2.09	0.64
1:G:4389:PRO:HD2	1:G:4391:PHE:HE2	1.63	0.64
1:A:413:MET:HE3	1:A:443:TYR:CE1	2.33	0.64
1:B:867:ILE:HD13	1:B:867:ILE:N	2.13	0.64
1:E:3051:GLY:O	1:E:3055:ARG:HG3	1.97	0.64
1:F:3612:ILE:N	6:F:7416:HOH:O	2.29	0.64
1:H:5020:VAL:HG13	1:H:5024:ASP:CB	2.26	0.63
1:D:1910:ALA:HB2	1:D:2038:MET:HG3	1.80	0.63
1:E:3148:MET:HE3	1:E:3157:TRP:CH2	2.32	0.63
1:F:3698:ALA:HB2	1:F:3704:TYR:CD1	2.34	0.63
1:H:5067:ILE:HD13	1:H:5067:ILE:N	2.12	0.63
1:A:486:ASP:O	1:A:490:ASN:ND2	2.29	0.63
1:C:1273:MET:HE2	1:C:1286:THR:HG21	1.79	0.63
1:C:1530:LEU:O	1:C:1563:GLU:HG2	1.98	0.63
1:F:3688:LYS:HE3	6:F:7588:HOH:O	1.97	0.63
1:F:3722:LEU:O	1:F:3751:CYS:N	2.28	0.63
1:A:131:VAL:CG1	1:A:202:LEU:HD23	2.28	0.63
1:A:164:CYS:O	1:A:187:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2054:ARG:NH2	1:D:2062:LYS:O	2.31	0.63
1:G:4339:LEU:HD11	1:G:4354:ASN:HA	1.79	0.63
1:C:1343:LEU:HD23	1:C:1361:LYS:HD2	1.80	0.63
1:E:3172:LYS:HE2	1:E:3197:GLU:CD	2.23	0.63
1:F:3976:MET:O	1:F:3980:ILE:HG13	1.98	0.63
1:G:4339:LEU:HD11	1:G:4354:ASN:C	2.22	0.63
1:G:4493:ARG:HH12	1:G:4529:MET:HG2	1.61	0.63
1:A:238:MET:HE1	1:A:464:LEU:HD22	1.80	0.63
1:B:871:GLU:HG2	1:B:892:ALA:HB3	1.79	0.63
1:G:4322:LEU:O	1:G:4351:CYS:HB2	1.98	0.63
1:A:130:GLU:HA	1:A:202:LEU:O	1.99	0.63
1:C:1255:ARG:HD2	1:C:1282:TYR:CZ	2.33	0.63
1:D:2245:PRO:HD2	6:D:6576:HOH:O	1.99	0.63
1:E:3012:ILE:HG22	1:E:3013:GLN:N	2.14	0.63
1:E:3326:ALA:HB1	1:E:3359:MET:HE2	1.81	0.63
1:C:1509:GLN:HG2	1:C:1513:ILE:HD12	1.80	0.63
1:F:3679:THR:OG1	1:F:3680:HIS:N	2.29	0.63
1:A:280:ASP:OD1	1:A:315:ARG:NH1	2.32	0.63
1:A:421:LYS:HE2	1:B:1013:MET:SD	2.38	0.63
1:D:1860:LEU:O	1:D:1864:ILE:HG13	1.99	0.63
1:D:2190:HIS:CD2	1:D:2246:ARG:HG3	2.34	0.63
1:E:3099:SER:O	1:E:3101:PRO:HD3	1.98	0.63
1:E:3220:VAL:HG11	1:E:3225:ILE:CD1	2.29	0.63
1:F:3650:ILE:HD11	1:F:3668:MET:CE	2.29	0.63
1:H:4815:GLN:HG3	1:H:4839:ILE:HG23	1.81	0.63
1:G:4704:LYS:HE2	1:G:4730:PRO:O	1.98	0.62
1:A:57:VAL:HG22	1:A:89:ASN:CA	2.28	0.62
1:B:1099:ARG:HB3	1:B:1101:PHE:CE1	2.34	0.62
1:F:4075:ASP:CB	1:F:4087:LEU:HD21	2.30	0.62
1:F:4093:MET:HE2	1:F:4129:VAL:HG22	1.80	0.62
1:G:4322:LEU:CD2	1:G:4327:GLY:HA2	2.29	0.62
1:A:231:GLY:O	1:A:236:VAL:HG13	1.98	0.62
1:B:649:THR:OG1	1:B:672:ARG:NH1	2.30	0.62
1:F:3828:LEU:O	1:F:3832:VAL:HG23	1.99	0.62
1:A:522:ASN:HD22	1:A:522:ASN:H	1.45	0.62
1:E:3191:PHE:C	1:E:3192:LEU:HD22	2.23	0.62
1:A:411:MET:HE2	1:A:522:ASN:C	2.24	0.62
1:E:3328:GLN:HE21	1:G:4540:THR:HB	1.63	0.62
1:E:3333:MET:HA	1:E:3336:LYS:O	1.99	0.62
1:E:3355:ALA:O	1:E:3466:ARG:NH1	2.31	0.62
1:F:4113:GLY:HA2	1:F:4122:ASN:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4493:ARG:HH22	1:G:4546:ASP:CG	2.08	0.62
1:G:4508:ALA:O	1:G:4512:ILE:HG13	1.98	0.62
1:A:123:ILE:HD11	1:A:202:LEU:HG	1.81	0.62
1:C:1319:ARG:NH2	5:C:1735:ATP:O1B	2.33	0.62
1:C:1360:TYR:HD2	1:C:1363:ILE:HB	1.64	0.62
1:C:1675:ASP:HB3	1:C:1676:PRO:HD2	1.81	0.62
1:E:3372:GLU:OE1	1:E:3372:GLU:N	2.30	0.62
1:C:1339:LEU:HD12	1:C:1340:LYS:N	2.15	0.62
1:D:1814:THR:HG23	1:D:1837:ALA:O	1.98	0.62
1:D:1873:MET:HE2	1:D:1886:THR:CG2	2.30	0.62
1:F:3655:ARG:HD2	1:F:3682:TYR:OH	2.00	0.62
1:H:4876:SER:HA	1:H:4914:LYS:HG3	1.82	0.62
1:A:506:ASP:C	1:A:529:VAL:HG23	2.25	0.62
1:C:1633:SER:OG	1:C:1635:ARG:HG3	1.99	0.62
1:E:3330:LEU:HD12	1:E:3343:GLU:HB3	1.81	0.62
1:F:3750:LYS:O	1:F:3755:ILE:HD11	1.99	0.62
1:F:3825:ILE:O	1:F:3829:LYS:HG2	2.00	0.62
1:A:120:THR:HG22	1:A:205:LYS:N	2.15	0.61
1:B:658:GLU:HG3	6:B:7721:HOH:O	1.99	0.61
1:B:748:MET:HB2	1:B:757:TRP:CE2	2.35	0.61
1:B:976:MET:HE3	1:B:980:ILE:CG1	2.29	0.61
1:F:3856:ILE:HD13	1:F:3856:ILE:N	2.13	0.61
1:F:3966:LYS:O	1:F:3966:LYS:HG2	1.98	0.61
1:D:1863:MET:HG2	1:D:2171:LEU:HD23	1.81	0.61
1:H:4932:GLU:HG3	1:H:5001:PHE:CE1	2.36	0.61
1:A:223:LYS:O	1:A:226:GLN:HB2	1.99	0.61
1:C:1429:LYS:O	1:C:1433:GLU:HG2	2.00	0.61
6:A:7271:HOH:O	1:C:1542:ALA:HB3	1.99	0.61
1:B:650:ILE:HD13	1:B:650:ILE:N	2.16	0.61
1:G:4384:VAL:HA	1:G:4394:THR:HG22	1.82	0.61
1:A:108:ALA:HB2	1:A:460:ARG:HB3	1.82	0.61
1:C:1591:ARG:NH1	1:C:1592:LYS:HE3	2.15	0.61
1:D:1919:ARG:H	1:D:1959:ASP:HB2	1.66	0.61
1:D:2226:ALA:HA	1:D:2247:ALA:HB1	1.83	0.61
1:G:4367:VAL:CG2	1:G:4371:SER:HB3	2.26	0.61
1:B:654:SER:O	1:B:660:LEU:HD13	1.99	0.61
1:B:720:THR:HA	1:B:758:LEU:HD23	1.83	0.61
1:C:1532:SER:HB2	1:C:1543:GLU:OE1	2.00	0.61
1:C:1657:GLN:O	1:C:1661:GLN:HG3	2.01	0.61
1:C:1678:GLN:HA	1:C:1678:GLN:NE2	2.15	0.61
1:F:3760:TYR:CE2	1:F:3766:VAL:HG21	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4253:ALA:HB2	1:G:4566:LYS:HA	1.81	0.61
1:A:188:GLY:HA3	1:A:191:PHE:CE1	2.35	0.61
1:F:3758:LEU:HD23	1:F:3758:LEU:N	2.16	0.61
1:G:4243:ASN:HB3	1:G:4667:GLY:CA	2.31	0.61
1:G:4300:ASP:OD2	1:G:4303:LEU:HB2	1.99	0.61
1:A:113:THR:HG22	1:A:242:SER:CB	2.23	0.61
1:C:1341:ILE:HD12	1:C:1394:THR:HG21	1.81	0.61
1:D:2044:ILE:HG22	1:D:2082:ILE:CD1	2.26	0.61
1:E:3452:VAL:HG11	1:E:3488:ARG:HB3	1.83	0.61
1:F:4008:MET:HG3	1:F:4039:GLN:HG2	1.83	0.61
1:G:4703:LYS:O	1:G:4729:VAL:HB	2.01	0.61
1:E:3220:VAL:HG11	1:E:3225:ILE:HD13	1.83	0.61
1:H:4850:ILE:HD13	1:H:4850:ILE:N	2.16	0.61
1:A:173:VAL:HG13	1:A:210:LEU:CD1	2.31	0.61
1:C:1378:GLY:HA3	1:C:1498:ILE:HG13	1.83	0.61
1:F:3892:ALA:HB1	3:F:4133:OXL:C2	2.31	0.60
1:G:4388:GLY:HA3	1:G:4391:PHE:CE2	2.36	0.60
1:H:5130:LEU:HD22	1:H:5133:MET:HE3	1.83	0.60
1:A:141:ILE:HG21	1:A:158:LEU:CD2	2.24	0.60
1:B:739:LEU:HD12	1:B:754:ASN:C	2.26	0.60
1:C:1255:ARG:HD2	1:C:1282:TYR:OH	2.01	0.60
1:C:1385:LYS:HB2	1:C:1393:VAL:O	2.01	0.60
1:D:2240:VAL:HG12	1:D:2249:ILE:HD13	1.83	0.60
1:A:133:LEU:HD13	1:A:133:LEU:N	2.16	0.60
1:A:161:LYS:C	1:A:162:ASN:CA	2.68	0.60
1:B:989:PHE:CE2	1:B:992:LYS:HD2	2.36	0.60
1:B:1091:LEU:O	1:B:1091:LEU:HD12	2.01	0.60
1:C:1522:PRO:HA	1:C:1556:ASP:OD2	2.00	0.60
1:E:3073:MET:HE3	1:E:3087:ILE:HG12	1.82	0.60
1:E:3113:THR:HG21	6:E:6221:HOH:O	2.00	0.60
1:F:3661:LYS:O	1:F:3665:LYS:HG3	2.00	0.60
1:C:1715:ARG:HB3	1:C:1716:PRO:HD2	1.83	0.60
1:E:3122:LEU:HB2	1:E:3149:GLU:HA	1.83	0.60
1:E:3506:ASP:O	1:E:3529:VAL:HG23	2.01	0.60
1:F:3702:ILE:HG22	1:F:3703:LEU:CD1	2.31	0.60
1:A:49:THR:OG1	1:A:72:ARG:HD3	2.02	0.60
1:B:619:ALA:HA	1:B:631:ARG:HD2	1.83	0.60
1:B:1115:ARG:HB3	1:B:1116:PRO:CD	2.32	0.60
1:C:1327:GLY:HA2	1:C:1404:SER:HB2	1.84	0.60
1:F:3903:GLU:OE1	1:F:3903:GLU:N	2.29	0.60
1:G:4471:GLU:OE1	1:G:4495:ASP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:MET:HE3	1:A:326:ALA:CB	2.31	0.60
1:A:301:PRO:HG2	1:A:304:LYS:CD	2.30	0.60
1:F:3672:ARG:O	1:F:3673:MET:HE3	2.01	0.60
1:F:3786:GLN:O	1:F:3793:VAL:N	2.28	0.60
1:F:4075:ASP:HB3	1:F:4076:PRO:HD2	1.84	0.60
1:G:4313:THR:HG21	6:G:6257:HOH:O	2.02	0.60
1:A:47:ILE:CG2	1:A:359:MET:HG3	2.31	0.60
1:B:1065:TYR:CB	1:B:1068:ILE:HD12	2.30	0.60
1:C:1257:VAL:CG2	1:C:1292:THR:HG22	2.31	0.60
1:E:3160:TYR:HE2	1:E:3166:VAL:HG21	1.67	0.60
1:A:237:ASP:OD1	1:A:460:ARG:NH1	2.34	0.60
1:F:3655:ARG:HD2	1:F:3682:TYR:CZ	2.37	0.60
1:G:4323:ILE:H	1:G:4404:SER:HB3	1.67	0.60
1:B:1080:ALA:HB3	1:B:1083:GLU:CD	2.27	0.59
1:C:1728:PRO:O	1:C:1730:PRO:HD3	2.02	0.59
1:H:4855:ARG:NH2	1:H:4885:GLU:HB3	2.17	0.59
1:F:3928:GLN:NE2	1:H:5140:THR:HB	2.17	0.59
1:B:990:HIS:H	1:B:990:HIS:CD2	2.20	0.59
1:C:1493:ARG:NH1	1:C:1527:THR:O	2.36	0.59
1:D:2315:ARG:HB3	1:D:2316:PRO:HD2	1.84	0.59
1:E:3339:PRO:HG3	1:E:3376:MET:HG2	1.84	0.59
1:G:4492:ALA:HB1	3:G:4733:OXL:C2	2.32	0.59
1:E:3237:ASP:OD1	1:E:3460:ARG:HD2	2.02	0.59
1:A:225:ILE:HG23	1:A:256:ILE:HG21	1.83	0.59
1:F:3928:GLN:HE22	1:H:5140:THR:HA	1.68	0.59
1:G:4255:ARG:HD2	1:G:4282:TYR:OH	2.02	0.59
1:B:890:MET:HE3	1:B:892:ALA:HA	1.85	0.59
1:C:1713:GLY:HA2	1:C:1722:ASN:OD1	2.03	0.59
1:D:2083:LEU:O	1:D:2121:LYS:NZ	2.34	0.59
1:F:3752:ASP:OD2	1:F:3754:ASN:HB2	2.02	0.59
1:F:3904:LYS:HD3	1:H:5183:GLU:CD	2.28	0.59
1:A:51:GLY:C	1:A:55:ARG:HG3	2.26	0.59
1:A:293:ARG:O	1:C:1541:ARG:NE	2.31	0.59
1:C:1341:ILE:HB	1:C:1392:LEU:HB2	1.83	0.59
1:D:1857:VAL:O	1:D:1861:LYS:HG3	2.02	0.59
1:E:3328:GLN:HE22	1:G:4540:THR:HA	1.67	0.59
1:F:3722:LEU:HD12	1:F:3749:GLU:OE1	2.03	0.59
1:G:4493:ARG:NH2	1:G:4546:ASP:OD1	2.35	0.59
1:B:639:ILE:O	1:B:982:ARG:HD2	2.03	0.59
1:D:1902:ILE:HG22	1:D:1903:LEU:HD21	1.83	0.59
1:E:3341:ARG:N	1:G:4528:GLN:NE2	2.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4333:LEU:HG	1:G:4402:LEU:HD23	1.83	0.59
1:G:4681:TRP:CD2	1:G:4716:PRO:HD3	2.38	0.59
1:C:1491:VAL:HG23	1:C:1524:ILE:O	2.03	0.59
1:E:3481:TRP:CD1	1:E:3516:PRO:HD3	2.37	0.59
1:F:3638:PRO:HG3	1:F:3983:GLU:CD	2.28	0.59
1:F:3726:SER:HB3	1:F:3729:ALA:CB	2.30	0.59
1:F:3872:ASN:HD22	1:F:3875:GLY:H	1.50	0.59
1:G:4348:MET:HG2	1:G:4357:TRP:CZ2	2.37	0.59
1:G:4467:ILE:HD12	1:G:4488:GLY:HA3	1.84	0.59
1:G:4479:PHE:HZ	1:G:4483:LEU:HD22	1.67	0.59
1:G:4681:TRP:CG	1:G:4716:PRO:HD3	2.38	0.59
1:H:5281:TRP:CG	1:H:5316:PRO:HD3	2.37	0.59
1:B:886:SER:O	1:B:921:LYS:HE2	2.03	0.58
1:D:2176:MET:HE3	1:D:2176:MET:CA	2.28	0.58
1:E:3433:SER:OG	1:E:3435:ARG:HB3	2.03	0.58
1:F:3719:ARG:O	1:F:3759:ASP:HB2	2.02	0.58
1:G:4654:ARG:HD2	6:G:6523:HOH:O	2.03	0.58
1:H:5106:PHE:O	1:H:5110:LYS:HG3	2.02	0.58
1:A:134:LYS:O	1:A:196:VAL:HB	2.03	0.58
1:A:268:SER:HB2	1:A:289:ILE:CD1	2.33	0.58
1:A:341:ARG:NE	1:C:1493:ARG:O	2.30	0.58
1:E:3421:LYS:HD3	1:F:4013:MET:SD	2.43	0.58
1:F:3742:THR:N	1:F:3756:LEU:O	2.31	0.58
1:F:3859:GLU:O	1:F:3862:LYS:HG3	2.04	0.58
1:H:5188:MET:HE2	6:H:6225:HOH:O	2.02	0.58
1:A:181:SER:C	1:A:182:LEU:HD23	2.28	0.58
1:D:1902:ILE:C	1:D:1903:LEU:HD23	2.28	0.58
1:E:3068:MET:HE2	1:E:3071:ALA:HA	1.85	0.58
1:A:141:ILE:HA	1:A:156:LEU:O	2.03	0.58
1:A:407:LEU:HD21	1:B:1107:VAL:HG21	1.84	0.58
1:D:2122:PRO:HG3	1:D:2265:TYR:CE2	2.38	0.58
1:F:3717:GLU:OE2	1:F:3719:ARG:NH2	2.35	0.58
1:F:3928:GLN:NE2	1:H:5141:ARG:N	2.49	0.58
1:G:4273:MET:HE2	1:G:4286:THR:HG22	1.85	0.58
1:G:4477:ARG:HH21	1:G:4478:ARG:HH11	1.51	0.58
1:B:648:CYS:CB	1:B:668:MET:HE3	2.27	0.58
1:C:1360:TYR:HE2	1:C:1366:VAL:CG1	2.15	0.58
1:F:3715:GLY:O	1:F:3717:GLU:N	2.36	0.58
1:H:5275:ASP:HB3	1:H:5276:PRO:HD2	1.85	0.58
1:C:1453:VAL:HG12	1:C:1457:LEU:HD22	1.86	0.58
1:E:3142:THR:HG22	1:E:3143:LEU:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3328:GLN:NE2	1:G:4540:THR:HB	2.18	0.58
1:G:4383:GLN:O	1:G:4394:THR:HG22	2.04	0.58
1:H:4852:PRO:HD2	1:H:5165:ALA:O	2.04	0.58
1:A:141:ILE:N	1:A:192:LEU:O	2.30	0.58
1:A:326:ALA:HB1	1:A:359:MET:CE	2.28	0.58
1:D:1855:ARG:HD3	6:D:7309:HOH:O	2.02	0.58
1:E:3068:MET:HE2	1:E:3071:ALA:CA	2.33	0.58
1:F:3726:SER:HB2	1:F:3729:ALA:HB2	1.85	0.58
1:G:4498:ILE:HD13	1:G:4498:ILE:H	1.69	0.58
1:H:5311:LEU:HD22	1:H:5321:THR:HG23	1.86	0.58
1:A:511:LEU:CD2	1:A:521:THR:HG23	2.34	0.58
1:B:658:GLU:HG2	6:B:7720:HOH:O	2.04	0.58
1:C:1326:SER:HB3	1:C:1329:ALA:HB2	1.86	0.58
1:E:3016:GLN:NE2	6:E:6183:HOH:O	2.36	0.58
1:G:4494:GLY:N	1:G:4527:THR:HG21	2.18	0.58
1:A:48:CYS:CB	1:A:68:MET:HE2	2.34	0.58
1:G:4251:GLY:O	1:G:4255:ARG:HG3	2.04	0.58
1:A:329:MET:O	1:A:343:GLU:HB3	2.04	0.57
1:B:731:VAL:O	1:B:801:PHE:HA	2.04	0.57
1:C:1347:TYR:HD2	1:C:1355:ILE:HG21	1.65	0.57
1:C:1422:GLU:O	1:C:1425:ILE:HB	2.04	0.57
1:C:1478:ARG:O	1:C:1482:ILE:HG13	2.04	0.57
1:E:3019:ALA:HB2	1:E:3031:ARG:HB2	1.86	0.57
1:F:4085:VAL:O	1:F:4089:VAL:HG23	2.04	0.57
1:G:4273:MET:HE2	1:G:4286:THR:CG2	2.34	0.57
1:G:4302:ILE:HD12	1:G:4694:ASN:CB	2.33	0.57
1:G:4336:GLY:HA2	1:G:4395:GLU:CD	2.29	0.57
1:A:49:THR:HG22	1:A:365:ALA:HB2	1.84	0.57
1:C:1714:TRP:HD1	1:C:1715:ARG:HE	1.53	0.57
1:G:4391:PHE:HE1	1:G:4393:VAL:HG23	1.69	0.57
1:H:5038:MET:CE	1:H:5264:LEU:HD22	2.34	0.57
1:A:290:MET:HG3	1:A:324:ILE:HB	1.86	0.57
1:B:745:ASN:ND2	1:B:757:TRP:HE1	2.02	0.57
1:H:4967:VAL:O	1:H:4987:LYS:NZ	2.36	0.57
1:A:487:LEU:HD23	1:A:487:LEU:C	2.29	0.57
1:A:514:TRP:H	1:A:522:ASN:ND2	1.92	0.57
1:E:3142:THR:HG21	1:E:3144:ASP:HB3	1.85	0.57
1:F:3660:LEU:HD13	1:F:3690:VAL:HA	1.87	0.57
1:A:172:LYS:HE3	1:A:197:GLU:OE2	2.04	0.57
1:B:716:PRO:HG2	1:B:843:PHE:HB3	1.87	0.57
1:B:1028:ILE:HD13	1:B:1092:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1714:TRP:CE3	1:D:2325:ARG:HD3	2.39	0.57
1:C:1533:MET:HA	1:C:1536:LYS:O	2.04	0.57
1:D:2093:ARG:HD3	1:D:2126:ALA:O	2.05	0.57
1:E:3316:CYS:O	1:E:3320:GLY:N	2.36	0.57
1:E:3390:HIS:HD2	6:E:6368:HOH:O	1.87	0.57
1:H:5314:TRP:O	1:H:5315:ARG:HG2	2.05	0.57
1:A:399:ARG:NH2	1:C:1223:ASP:OD2	2.38	0.57
1:G:4274:ASN:HA	1:G:4312:ASP:HB3	1.87	0.57
1:A:518:SER:HB2	6:A:7635:HOH:O	2.05	0.57
1:C:1378:GLY:CA	1:C:1498:ILE:HG13	2.34	0.57
1:D:1887:ILE:HD13	1:D:1887:ILE:N	2.19	0.57
1:E:3144:ASP:HB3	1:E:3147:TYR:HD2	1.70	0.57
1:G:4457:LEU:HD12	1:G:4466:ILE:HD11	1.85	0.57
1:G:4666:ARG:HG3	1:G:4667:GLY:N	2.19	0.57
1:B:673:MET:CE	1:B:686:THR:HG22	2.34	0.57
1:B:740:LYS:HE2	1:B:742:THR:CG2	2.35	0.57
1:B:953:ASP:O	1:D:1829:MET:HE1	2.03	0.57
1:C:1318:ILE:CG2	1:C:1408:VAL:HB	2.35	0.57
1:C:1537:PRO:HG2	1:C:1538:ARG:NH2	2.19	0.57
1:D:1842:ARG:NH1	1:D:1846:ILE:HG13	2.19	0.57
1:E:3440:VAL:HG12	1:E:3449:ILE:CD1	2.35	0.57
1:F:3663:MET:HE3	1:F:3668:MET:HE3	1.85	0.57
1:A:191:PHE:CE2	1:A:193:VAL:HG23	2.38	0.57
1:B:971:LEU:O	1:B:975:ARG:HD2	2.04	0.57
1:D:1855:ARG:NH2	1:D:1885:GLU:HB3	2.20	0.57
1:E:3041:ALA:HB2	1:E:3501:PHE:CE1	2.39	0.57
1:E:3160:TYR:CE2	1:E:3162:ASN:HB3	2.40	0.57
1:F:3723:ILE:HG12	1:F:3804:SER:OG	2.05	0.57
1:A:133:LEU:N	1:A:200:GLY:O	2.35	0.56
1:D:1958:LEU:HD21	1:D:2008:VAL:HG21	1.87	0.56
1:F:4104:LYS:HG3	1:F:4130:PRO:C	2.30	0.56
1:G:4302:ILE:HD12	1:G:4694:ASN:HB2	1.85	0.56
1:A:86:THR:HG22	1:A:87:ILE:N	2.20	0.56
1:A:144:ASP:HB3	1:A:147:TYR:HD1	1.70	0.56
1:A:503:LYS:O	1:A:506:ASP:HB2	2.05	0.56
1:B:1057:GLN:O	1:B:1061:GLN:HG3	2.05	0.56
1:F:3739:LEU:HD21	1:F:3756:LEU:HB2	1.87	0.56
1:G:4336:GLY:N	1:G:4396:VAL:O	2.37	0.56
1:C:1452:GLU:O	1:C:1455:LYS:HB3	2.04	0.56
1:D:1910:ALA:HB2	1:D:2038:MET:CG	2.35	0.56
1:D:2191:ARG:HD2	1:D:2191:ARG:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4133:OXL:O1	6:F:6293:HOH:O	2.17	0.56
1:G:4408:VAL:CG1	1:G:4410:LEU:HD11	2.35	0.56
1:A:375:ARG:O	1:A:378:HIS:HB3	2.06	0.56
1:D:1952:ASP:OD1	1:D:1955:ILE:N	2.35	0.56
1:E:3091:ARG:O	1:E:3095:GLU:HG2	2.06	0.56
1:E:3198:ASN:ND2	6:E:6391:HOH:O	2.37	0.56
1:E:3272:ASN:OD1	1:E:3274:GLU:HB3	2.05	0.56
1:F:3711:LEU:HD23	1:F:3711:LEU:O	2.05	0.56
1:H:4920:THR:HB	1:H:4956:LEU:HD11	1.87	0.56
1:A:111:LEU:HD23	1:A:111:LEU:C	2.30	0.56
1:A:351:VAL:O	1:A:466:ARG:NH2	2.37	0.56
1:E:3230:PHE:CE1	1:E:3234:GLN:HG3	2.40	0.56
1:E:3245:ARG:CB	1:E:3274:GLU:HG2	2.30	0.56
1:E:3276:VAL:HG11	1:G:4234:ILE:HD13	1.86	0.56
1:F:3724:LYS:C	1:F:3726:SER:H	2.14	0.56
1:G:4344:ASP:OD1	1:G:4346:ALA:HB3	2.04	0.56
1:A:18:HIS:O	1:A:21:MET:HB2	2.06	0.56
1:C:1363:ILE:HA	1:C:1366:VAL:HG12	1.86	0.56
1:C:1471:GLU:HB2	1:C:1495:ASP:HB2	1.88	0.56
1:G:4358:LEU:HD21	1:G:4363:ILE:HD12	1.88	0.56
1:G:4630:LEU:HD12	1:G:4712:THR:HG22	1.87	0.56
1:A:328:GLN:NE2	1:C:1541:ARG:N	2.50	0.56
1:A:435:ARG:HA	1:A:438:HIS:CD2	2.41	0.56
1:B:1028:ILE:HD13	1:B:1092:ALA:HB1	1.87	0.56
1:D:1847:ILE:HG12	1:D:1870:VAL:HB	1.87	0.56
1:D:2038:MET:HE2	1:D:2264:LEU:HD11	1.87	0.56
1:E:3158:LEU:HD11	1:E:3208:VAL:HG21	1.87	0.56
1:G:4611:MET:HE1	1:G:4724:MET:HB2	1.87	0.56
1:A:172:LYS:HE3	1:A:197:GLU:CD	2.30	0.56
1:A:336:LYS:HB3	1:A:337:PRO:HD2	1.88	0.56
1:C:1343:LEU:HD23	1:C:1361:LYS:HA	1.88	0.56
1:D:2278:GLN:HB2	1:D:2284:ASP:HB2	1.88	0.56
1:H:5028:LEU:HD22	1:H:5057:LEU:HD21	1.87	0.56
1:A:141:ILE:HD11	1:A:194:THR:HG21	1.88	0.56
1:A:269:LYS:HE2	1:A:271:GLU:OE2	2.05	0.56
1:A:333:MET:HE2	1:A:373:ALA:HA	1.87	0.56
1:C:1685:VAL:O	1:C:1689:VAL:HG23	2.06	0.56
1:D:1910:ALA:CB	1:D:2038:MET:HG3	2.36	0.56
1:E:3074:ASN:HA	1:E:3112:ASP:HB3	1.88	0.56
1:F:3802:LEU:HD12	1:F:3803:GLY:N	2.21	0.56
1:F:3810:LEU:HB3	1:F:3813:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4221:MET:HA	1:G:4221:MET:HE3	1.88	0.56
1:G:4379:LEU:HD12	1:G:4379:LEU:O	2.06	0.56
1:G:4646:ARG:HB3	6:G:6223:HOH:O	2.06	0.56
1:A:295:ASP:O	1:A:298:ILE:HG22	2.06	0.56
1:B:928:GLN:NE2	1:D:2141:ARG:HH11	2.04	0.56
1:E:3411:MET:HE2	1:E:3522:ASN:C	2.31	0.56
1:F:3756:LEU:HD12	1:F:3757:TRP:N	2.21	0.56
1:F:3829:LYS:HE2	1:F:3856:ILE:HG23	1.87	0.56
1:F:3961:SER:HB2	6:F:6395:HOH:O	2.06	0.56
1:F:4093:MET:CE	1:F:4129:VAL:HG22	2.36	0.56
1:G:4322:LEU:C	1:G:4351:CYS:HB2	2.31	0.56
1:H:4860:LEU:HD13	1:H:4890:VAL:HA	1.88	0.56
1:H:4873:MET:HG3	1:H:4887:ILE:HD11	1.87	0.56
1:B:1091:LEU:HD12	1:B:1091:LEU:C	2.31	0.55
1:C:1243:ASN:H	1:C:1585:GLU:CD	2.13	0.55
1:C:1572:GLU:OE1	1:C:1572:GLU:N	2.40	0.55
1:D:1848:CYS:SG	1:D:1868:MET:HB2	2.46	0.55
1:D:2038:MET:CE	1:D:2264:LEU:HD11	2.37	0.55
1:G:4379:LEU:HG	1:G:4380:ILE:HG12	1.88	0.55
1:G:4715:ARG:CB	1:G:4716:PRO:HD2	2.36	0.55
1:H:5118:ARG:HD2	6:H:6689:HOH:O	2.04	0.55
1:H:5281:TRP:CD1	1:H:5316:PRO:HD3	2.41	0.55
1:A:408:MET:SD	1:A:520:PHE:HD2	2.29	0.55
1:A:417:GLU:OE2	1:B:1013:MET:HE2	2.07	0.55
1:A:510:VAL:HG12	1:A:512:THR:HG23	1.87	0.55
1:B:934:ILE:HG22	1:B:935:LYS:HD3	1.88	0.55
1:E:3506:ASP:O	1:E:3528:PRO:HA	2.06	0.55
1:G:4386:GLN:HB2	1:G:4393:VAL:HB	1.87	0.55
1:B:928:GLN:NE2	1:D:2141:ARG:HG2	2.22	0.55
1:C:1374:TYR:O	1:C:1408:VAL:HA	2.05	0.55
1:D:2109:GLN:O	1:D:2113:ILE:HG13	2.05	0.55
1:F:3650:ILE:HG12	1:F:3673:MET:HE1	1.88	0.55
1:G:4388:GLY:HA3	1:G:4391:PHE:CZ	2.40	0.55
1:H:5092:ALA:HB1	3:H:5333:OXL:C2	2.37	0.55
1:A:141:ILE:CD1	1:A:194:THR:HG21	2.37	0.55
1:A:328:GLN:NE2	1:C:1540:THR:HB	2.22	0.55
1:C:1484:GLU:HG3	6:C:6549:HOH:O	2.06	0.55
1:F:3893:ARG:HH22	1:F:3946:ASP:CG	2.14	0.55
1:G:4248:CYS:CB	1:G:4268:MET:HE3	2.33	0.55
1:A:525:ARG:HB2	1:A:525:ARG:HH11	1.71	0.55
1:B:1087:LEU:HD23	1:B:1087:LEU:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1322:LEU:HD12	1:C:1349:GLU:CG	2.31	0.55
1:D:2176:MET:HE2	1:D:2180:ILE:HG13	1.88	0.55
1:G:4222:ALA:CB	1:G:4227:GLU:HG2	2.37	0.55
1:G:4729:VAL:CG1	1:G:4730:PRO:HD2	2.36	0.55
1:A:60:LEU:O	1:A:63:MET:N	2.39	0.55
1:C:1262:GLU:OE2	1:C:1265:LYS:HE3	2.06	0.55
1:E:3191:PHE:CE2	1:E:3193:VAL:HG23	2.36	0.55
1:E:3324:ILE:HG12	1:E:3357:CYS:HB2	1.89	0.55
1:H:4974:TYR:CE2	1:H:5011:PRO:HG3	2.42	0.55
1:H:5314:TRP:HD1	1:H:5315:ARG:HG3	1.69	0.55
1:A:181:SER:O	1:A:182:LEU:HD23	2.06	0.55
1:A:511:LEU:HB3	1:A:521:THR:CG2	2.36	0.55
1:C:1661:GLN:O	1:C:1664:LEU:HB2	2.06	0.55
1:D:2252:VAL:HG21	1:D:2292:ALA:HB2	1.87	0.55
1:F:3941:ARG:NH2	1:H:5094:GLY:O	2.37	0.55
1:H:5245:PRO:HG2	1:H:5249:ILE:HD11	1.88	0.55
1:A:238:MET:CE	1:A:464:LEU:HD22	2.36	0.55
1:B:706:PRO:O	1:B:1063:HIS:HE1	1.88	0.55
1:B:999:ARG:NH1	1:D:1823:ASP:HB2	2.21	0.55
1:C:1280:HIS:NE2	1:C:1427:ASP:OD1	2.36	0.55
1:D:1902:ILE:CG1	1:D:2295:VAL:HG22	2.34	0.55
1:D:2045:ARG:HG2	1:D:2072:ASN:HD21	1.72	0.55
1:E:3376:MET:HE3	1:E:3379:LEU:HB2	1.89	0.55
1:G:4571:LEU:O	1:G:4575:ARG:HG3	2.07	0.55
1:B:1127:VAL:HG12	1:B:1128:PRO:N	2.20	0.55
1:C:1345:ASN:C	1:C:1347:TYR:H	2.15	0.55
1:C:1431:GLY:O	1:C:1436:VAL:HG22	2.07	0.55
1:D:2090:MET:HE1	3:D:2333:OXL:O1	2.07	0.55
1:E:3160:TYR:HB3	1:E:3163:ILE:HG22	1.89	0.55
1:F:3711:LEU:HD23	1:F:3711:LEU:C	2.31	0.55
1:G:4729:VAL:HG13	1:G:4730:PRO:HD2	1.88	0.55
1:B:617:LEU:O	1:B:621:MET:HG2	2.07	0.54
1:B:1067:GLY:HA3	6:B:7611:HOH:O	2.06	0.54
1:C:1532:SER:OG	1:C:1540:THR:HG23	2.07	0.54
1:D:2281:TRP:CH2	1:D:2316:PRO:HA	2.42	0.54
1:E:3495:VAL:O	1:E:3498:ALA:HB3	2.07	0.54
1:D:1985:LYS:HB2	1:D:1993:VAL:O	2.07	0.54
1:E:3192:LEU:HD22	1:E:3192:LEU:N	2.22	0.54
1:E:3525:ARG:HD3	1:F:4114:TRP:CE3	2.42	0.54
1:H:4877:HIS:O	1:H:4883:HIS:NE2	2.37	0.54
1:H:4920:THR:O	1:H:5005:LYS:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5239:GLN:OE1	1:H:5242:ARG:HD3	2.06	0.54
1:A:296:LEU:O	1:A:300:ILE:HG12	2.06	0.54
1:A:393:LEU:HG	1:A:397:LEU:HD22	1.88	0.54
1:E:3167:VAL:HG22	1:E:3171:SER:CB	2.37	0.54
1:G:4564:THR:HA	1:G:4570:PRO:HB3	1.89	0.54
1:E:3160:TYR:HB3	1:E:3163:ILE:CG2	2.37	0.54
1:F:4055:ASN:HB3	1:F:4058:THR:HB	1.89	0.54
1:F:4096:GLY:HA3	1:F:4102:PHE:CZ	2.42	0.54
1:G:4691:LEU:O	1:G:4695:VAL:HG23	2.08	0.54
1:A:144:ASP:HB3	1:A:147:TYR:CD1	2.43	0.54
1:A:145:ASN:C	1:A:147:TYR:H	2.15	0.54
1:A:451:ALA:HB2	1:A:468:ILE:CG2	2.37	0.54
1:B:1103:LYS:HG3	1:B:1106:ASP:OD2	2.07	0.54
1:C:1477:ARG:NH2	1:C:1478:ARG:NH1	2.47	0.54
1:D:2135:LYS:O	1:D:2169:TYR:HE2	1.91	0.54
1:D:2275:ASP:HB2	1:D:2287:LEU:HD21	1.89	0.54
1:G:4217:LEU:O	1:G:4221:MET:HG2	2.07	0.54
1:A:79:THR:OG1	1:A:81:GLU:N	2.40	0.54
1:A:163:ILE:HA	1:A:166:VAL:HB	1.89	0.54
1:A:294:GLY:CA	1:A:327:THR:HG21	2.37	0.54
1:B:1031:THR:CG2	1:B:1034:GLY:HA2	2.38	0.54
1:C:1434:GLN:OE1	1:C:1434:GLN:HA	2.08	0.54
1:F:3755:ILE:O	1:F:3755:ILE:HG12	2.07	0.54
1:G:4628:ILE:HD13	1:G:4692:ALA:CB	2.37	0.54
1:A:489:VAL:O	1:A:493:MET:HG2	2.07	0.54
1:B:686:THR:O	1:B:690:VAL:HG23	2.08	0.54
1:B:788:GLY:HA3	1:B:791:PHE:CE1	2.42	0.54
1:C:1255:ARG:HH22	1:C:1285:GLU:HB3	1.71	0.54
1:E:3221:SER:O	1:E:3224:ASP:HB2	2.07	0.54
1:E:3259:GLU:O	1:E:3262:LYS:HG2	2.08	0.54
1:F:3845:ARG:CG	1:F:3874:GLU:HB3	2.38	0.54
1:C:1681:TRP:CH2	1:C:1716:PRO:HA	2.43	0.54
1:D:2252:VAL:CG2	1:D:2292:ALA:HB2	2.38	0.54
1:E:3493:MET:CE	1:E:3530:PRO:HD2	2.17	0.54
1:F:3663:MET:HE2	1:F:3668:MET:HE3	1.87	0.54
1:G:4483:LEU:O	1:G:4521:LYS:NZ	2.40	0.54
1:G:4652:VAL:HG21	1:G:4692:ALA:HB2	1.89	0.54
1:H:4887:ILE:HD13	1:H:4887:ILE:N	2.22	0.54
1:A:511:LEU:HD22	1:A:521:THR:CG2	2.37	0.54
1:A:514:TRP:N	1:A:522:ASN:HD21	1.93	0.54
1:D:1980:ILE:HD11	1:D:2000:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3407:LEU:HG	1:F:4126:VAL:HG11	1.90	0.54
1:F:3910:LYS:NZ	1:H:5149:ASN:HD21	2.06	0.54
1:A:432:GLU:O	1:A:458:THR:HG21	2.08	0.54
1:B:624:THR:HB	1:D:2196:GLU:CD	2.33	0.54
1:B:654:SER:HA	1:B:659:THR:HG21	1.90	0.54
1:C:1213:GLN:OE1	1:C:1213:GLN:HA	2.08	0.54
1:C:1326:SER:HB3	1:C:1329:ALA:HB3	1.90	0.54
1:C:1347:TYR:HE2	1:C:1355:ILE:CD1	2.21	0.54
1:C:1561:SER:HB2	6:C:6410:HOH:O	2.07	0.54
1:D:1940:LYS:HE3	1:D:1991:PHE:CG	2.43	0.54
1:D:2296:GLY:HA3	1:D:2302:PHE:CZ	2.43	0.54
1:E:3080:HIS:HE1	1:E:3227:ASP:OD1	1.91	0.54
1:G:4212:ILE:HD13	1:G:4233:ASP:OD2	2.08	0.54
1:G:4437:ASP:OD1	1:G:4660:ARG:HD2	2.08	0.54
1:A:333:MET:HE1	1:A:373:ALA:HA	1.88	0.53
1:D:1833:ASP:HA	6:D:6995:HOH:O	2.07	0.53
1:E:3524:MET:HE3	1:F:4124:MET:HE3	1.90	0.53
1:G:4257:VAL:HG23	1:G:4289:ASN:HB3	1.90	0.53
1:A:224:ASP:O	1:A:228:LEU:HG	2.08	0.53
1:C:1421:SER:O	1:C:1424:ASP:HB2	2.09	0.53
1:D:1958:LEU:CD1	1:D:1963:ILE:HD13	2.38	0.53
1:D:2008:VAL:HG12	1:D:2010:LEU:CD2	2.38	0.53
1:G:4451:HIS:O	1:G:4455:LYS:HG2	2.08	0.53
1:H:5133:MET:CE	1:H:5139:PRO:HB3	2.29	0.53
1:A:87:ILE:HG22	1:A:91:ARG:HD2	1.91	0.53
1:B:618:HIS:CE1	1:B:631:ARG:HD3	2.43	0.53
1:C:1348:MET:HA	1:C:1357:TRP:CG	2.44	0.53
1:C:1518:ARG:HD2	6:C:6442:HOH:O	2.07	0.53
1:C:1571:LEU:O	1:C:1575:ARG:HG3	2.08	0.53
1:F:3867:ILE:HD13	1:F:3867:ILE:N	2.24	0.53
1:F:3939:PRO:HG3	1:F:3976:MET:HG2	1.90	0.53
1:G:4270:VAL:HG22	1:G:4308:ALA:HB3	1.90	0.53
1:A:57:VAL:HG23	1:A:89:ASN:CG	2.33	0.53
1:B:716:PRO:HG2	1:B:843:PHE:CB	2.38	0.53
1:C:1611:MET:SD	1:D:2326:VAL:HG23	2.49	0.53
1:D:1839:ILE:O	1:D:2182:ARG:HD2	2.09	0.53
1:D:2176:MET:HA	1:D:2176:MET:CE	2.31	0.53
1:D:2288:ARG:O	1:D:2291:LEU:HB3	2.08	0.53
1:E:3306:PHE:HA	6:E:7081:HOH:O	2.08	0.53
1:C:1362:ASN:ND2	1:C:1365:LYS:HB2	2.24	0.53
1:C:1516:CYS:HB3	1:C:1521:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5130:LEU:HD23	1:H:5143:GLU:HB3	1.88	0.53
1:A:172:LYS:HE3	1:A:197:GLU:OE1	2.09	0.53
1:C:1250:ILE:HD13	1:C:1250:ILE:N	2.24	0.53
1:F:3642:ARG:HB2	1:F:3982:ARG:HG3	1.91	0.53
1:G:4333:LEU:C	1:G:4334:LYS:HG2	2.33	0.53
1:G:4661:GLN:O	1:G:4664:LEU:HB2	2.09	0.53
1:H:4923:ILE:O	1:H:4925:GLY:N	2.42	0.53
1:C:1650:ILE:HD12	1:C:1669:PHE:HB2	1.90	0.53
1:F:3732:GLU:HB2	1:F:3801:PHE:CE1	2.44	0.53
1:G:4531:GLU:O	1:G:4534:ILE:HD12	2.09	0.53
1:A:188:GLY:HA3	1:A:191:PHE:CD1	2.43	0.53
1:A:209:ASN:C	1:A:210:LEU:HD13	2.33	0.53
1:C:1293:ALA:O	1:C:1296:SER:OG	2.26	0.53
1:G:4363:ILE:HG23	1:G:4364:CYS:N	2.23	0.53
1:A:178:GLY:O	1:C:1538:ARG:NH1	2.42	0.53
1:A:353:ASP:HB3	1:C:1229:MET:HE1	1.91	0.53
1:B:804:SER:O	1:B:806:LYS:HD3	2.09	0.53
1:B:928:GLN:HB2	1:D:2141:ARG:HB2	1.91	0.53
1:C:1376:ASP:CG	1:C:1406:LYS:HE2	2.32	0.53
1:D:2064:ILE:HD11	6:D:7350:HOH:O	2.09	0.53
1:D:2281:TRP:CD1	1:D:2316:PRO:HD3	2.44	0.53
1:F:3683:HIS:O	1:F:3687:ILE:HG13	2.09	0.53
1:A:27:GLU:O	1:A:31:ARG:HG3	2.08	0.53
1:A:102:ILE:HG22	1:A:103:LEU:CD1	2.39	0.53
1:A:454:ARG:CG	1:A:473:CYS:HB3	2.39	0.53
1:C:1532:SER:O	1:C:1534:ILE:N	2.40	0.53
1:C:1555:ALA:O	1:C:1666:ARG:NH1	2.35	0.53
1:D:1987:LYS:HA	1:D:1992:LEU:HD23	1.90	0.53
1:F:4066:ARG:HG3	1:F:4067:GLY:N	2.22	0.53
1:H:5073:HIS:CE1	1:H:5100:ILE:HG22	2.44	0.53
1:B:815:VAL:HG21	1:B:843:PHE:HE2	1.73	0.52
1:C:1379:LEU:HG	1:C:1380:ILE:HG12	1.90	0.52
1:E:3024:THR:HB	1:G:4596:GLU:CD	2.34	0.52
1:G:4445:ARG:N	1:G:4449:ASP:OD2	2.29	0.52
1:A:425:ALA:HB1	1:A:502:PHE:HB3	1.92	0.52
1:B:720:THR:HG22	1:B:758:LEU:HD21	1.90	0.52
1:C:1255:ARG:NH2	1:C:1285:GLU:HB3	2.23	0.52
1:C:1675:ASP:CB	1:C:1676:PRO:HD2	2.38	0.52
1:F:3653:ALA:CB	1:F:3966:LYS:HA	2.39	0.52
1:G:4276:SER:HB3	1:G:4319:ARG:NE	2.20	0.52
1:G:4452:GLU:O	1:G:4456:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:VAL:HG22	6:B:6888:HOH:O	2.08	0.52
1:G:4260:LEU:HD23	1:G:4263:MET:HG3	1.91	0.52
1:H:4945:ASN:HB3	1:H:4948:MET:CE	2.40	0.52
1:A:87:ILE:O	1:A:91:ARG:HG3	2.10	0.52
1:B:890:MET:CE	1:B:892:ALA:HB2	2.36	0.52
1:C:1323:ILE:HG21	1:C:1331:VAL:HG23	1.91	0.52
1:C:1428:LEU:HD12	1:C:1456:ILE:HG21	1.90	0.52
1:C:1532:SER:C	1:C:1534:ILE:H	2.17	0.52
1:E:3113:THR:HG22	1:E:3242:SER:H	1.74	0.52
1:E:3133:LEU:HD22	1:E:3202:LEU:HB2	1.92	0.52
1:G:4274:ASN:OD1	1:G:4276:SER:HB2	2.10	0.52
1:C:1372:LYS:HA	1:C:1382:LEU:O	2.10	0.52
1:C:1472:ASN:HD22	1:C:1475:GLY:H	1.57	0.52
1:D:1860:LEU:HB3	1:D:1893:ALA:CB	2.39	0.52
1:H:4843:ASN:HB3	1:H:5267:GLY:CA	2.39	0.52
1:A:334:ILE:HG23	1:A:367:GLY:HA2	1.92	0.52
1:E:3017:LEU:O	1:E:3020:ALA:HB3	2.10	0.52
1:F:4075:ASP:HB2	1:F:4087:LEU:HD21	1.91	0.52
1:G:4608:MET:SD	1:G:4721:THR:HG22	2.49	0.52
1:B:1054:ARG:HG2	1:B:1073:CYS:HB3	1.91	0.52
1:F:3926:ALA:HB1	1:F:3959:MET:HE2	1.90	0.52
1:A:63:MET:HE1	1:A:364:THR:HB	1.92	0.52
1:A:283:LEU:C	1:A:283:LEU:HD22	2.33	0.52
1:A:454:ARG:NH2	1:A:484:ASP:OD2	2.42	0.52
1:B:847:ALA:N	1:B:881:GLU:OE1	2.30	0.52
1:C:1326:SER:CB	1:C:1329:ALA:HB2	2.40	0.52
1:C:1431:GLY:HA2	1:C:1434:GLN:HB2	1.92	0.52
1:C:1621:LYS:NZ	1:D:2201:SER:O	2.43	0.52
1:D:2230:LEU:HD22	1:D:2312:THR:HG22	1.91	0.52
1:H:4847:ILE:HG21	1:H:5159:MET:CE	2.37	0.52
1:H:4932:GLU:OE1	1:H:4934:LYS:HG2	2.10	0.52
1:A:210:LEU:HB3	1:A:213:ALA:HB2	1.92	0.52
1:A:292:ALA:HB1	3:A:533:OXL:C2	2.39	0.52
1:A:480:ALA:HB3	1:A:483:GLU:HB2	1.90	0.52
1:B:731:VAL:CG1	1:B:753:GLU:HB3	2.40	0.52
1:D:2280:ALA:HB3	1:D:2283:GLU:HG3	1.90	0.52
1:E:3496:GLY:O	1:E:3501:PHE:N	2.37	0.52
1:H:4851:GLY:HA3	1:H:5165:ALA:O	2.10	0.52
1:A:123:ILE:O	1:A:129:ALA:HB3	2.10	0.52
1:A:308:ALA:O	1:A:312:ILE:HG13	2.10	0.52
1:C:1252:PRO:HD2	1:C:1565:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3145:ASN:HD22	1:E:3145:ASN:N	2.08	0.52
1:F:3673:MET:HE3	1:F:3673:MET:N	2.25	0.52
1:G:4333:LEU:N	1:G:4333:LEU:HD23	2.25	0.52
1:G:4522:PRO:HG3	1:G:4665:TYR:CE2	2.44	0.52
1:A:176:ASP:HB3	1:A:179:LEU:HB3	1.92	0.51
1:A:300:ILE:HB	1:A:301:PRO:HD2	1.91	0.51
1:A:493:MET:HE2	1:A:529:VAL:HG13	1.91	0.51
1:D:2046:LYS:HB3	1:D:2081:GLU:OE2	2.10	0.51
1:D:2094:GLY:CA	1:D:2127:THR:HG21	2.39	0.51
1:F:3971:LEU:O	1:F:3975:ARG:HG3	2.10	0.51
1:A:69:ASN:HB3	1:A:463:HIS:CE1	2.44	0.51
1:A:456:HIS:CD2	1:A:456:HIS:N	2.79	0.51
1:C:1687:LEU:HG	1:C:1688:ARG:N	2.24	0.51
1:D:1958:LEU:CD2	1:D:2008:VAL:HG21	2.40	0.51
1:E:3453:THR:CG2	1:E:3459:ALA:HB2	2.40	0.51
1:H:4988:GLY:HA3	1:H:4991:PHE:CE2	2.45	0.51
1:F:3894:GLY:CA	1:F:3927:THR:HG21	2.41	0.51
1:H:5096:LEU:O	1:H:5100:ILE:HG12	2.11	0.51
1:A:126:SER:CB	1:A:129:ALA:HB2	2.28	0.51
1:A:293:ARG:HD3	1:A:326:ALA:O	2.11	0.51
1:A:392:LYS:O	1:A:396:GLU:HG3	2.11	0.51
1:B:756:LEU:HD13	1:B:758:LEU:HD21	1.92	0.51
1:C:1367:VAL:O	1:C:1387:LYS:NZ	2.36	0.51
1:C:1531:GLU:OE1	1:C:1531:GLU:HA	2.10	0.51
1:H:5130:LEU:CD1	1:H:5133:MET:HE3	2.39	0.51
1:A:252:GLU:O	1:A:255:LYS:N	2.42	0.51
1:B:656:SER:O	1:B:660:LEU:HB2	2.10	0.51
1:D:1954:ASN:O	1:D:1955:ILE:HG13	2.09	0.51
1:D:2083:LEU:HD21	1:D:2119:ALA:CB	2.41	0.51
1:D:2141:ARG:HG2	1:D:2141:ARG:NH1	2.21	0.51
1:D:2225:ALA:HB1	1:D:2302:PHE:HB3	1.93	0.51
1:E:3068:MET:CE	1:E:3071:ALA:HB2	2.40	0.51
1:G:4322:LEU:HD22	1:G:4326:SER:C	2.36	0.51
1:B:931:GLU:HA	1:B:931:GLU:OE1	2.11	0.51
1:D:1854:SER:O	1:D:1860:LEU:HD13	2.09	0.51
1:D:1966:VAL:O	1:D:1966:VAL:HG23	2.10	0.51
1:E:3164:CYS:O	1:E:3187:LYS:CE	2.59	0.51
1:E:3300:ILE:HB	1:E:3301:PRO:HD2	1.92	0.51
1:F:3783:GLN:O	1:F:3794:THR:HA	2.11	0.51
1:G:4379:LEU:HD12	1:G:4379:LEU:C	2.35	0.51
1:A:283:LEU:HD22	1:A:283:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:VAL:HG11	1:A:499:ARG:HH11	1.75	0.51
1:C:1227:GLU:O	1:C:1231:ARG:HG3	2.10	0.51
1:C:1429:LYS:HB3	6:C:7020:HOH:O	2.11	0.51
1:D:1902:ILE:O	1:D:1903:LEU:HD23	2.11	0.51
1:D:1952:ASP:OD1	1:D:1954:ASN:N	2.42	0.51
1:F:3699:SER:O	1:F:3701:PRO:HD3	2.11	0.51
1:F:3881:GLU:HG3	1:F:3882:ILE:N	2.25	0.51
1:G:4370:GLY:N	1:G:4384:VAL:O	2.31	0.51
1:H:5015:VAL:HG11	1:H:5017:LEU:HD12	1.92	0.51
1:A:53:ALA:HB2	1:A:366:LYS:HA	1.91	0.51
1:A:186:GLN:HB2	1:A:193:VAL:HB	1.93	0.51
1:B:614:THR:O	1:B:617:LEU:HG	2.11	0.51
1:C:1696:GLY:HA3	1:C:1702:PHE:CZ	2.46	0.51
1:F:4075:ASP:HB3	1:F:4076:PRO:CD	2.41	0.51
1:A:24:THR:HB	1:C:1596:GLU:CD	2.35	0.51
1:A:162:ASN:N	1:A:162:ASN:HB2	2.24	0.51
1:A:173:VAL:N	1:A:182:LEU:O	2.30	0.51
1:C:1247:ILE:HB	1:C:1559:MET:HG3	1.92	0.51
1:E:3100:ASP:C	1:E:3102:ILE:H	2.18	0.51
1:F:3739:LEU:HD21	1:F:3756:LEU:CB	2.41	0.51
1:F:3809:ASN:C	1:F:3811:PRO:HD3	2.36	0.51
1:F:3821:SER:O	1:F:3824:ASP:HB2	2.11	0.51
1:F:4104:LYS:HA	1:F:4129:VAL:O	2.11	0.51
1:H:4974:TYR:HB2	1:H:5009:ASN:HB2	1.92	0.51
1:A:210:LEU:HB2	1:A:213:ALA:HB3	1.93	0.51
1:A:411:MET:HG2	1:A:521:THR:O	2.11	0.51
1:C:1302:ILE:HA	1:C:1695:VAL:HG22	1.93	0.51
1:D:2042:SER:HA	1:D:2069:LYS:HE2	1.91	0.51
1:D:2304:LYS:HG3	1:D:2330:PRO:O	2.09	0.51
1:G:4636:SER:O	1:G:4639:GLN:HB2	2.11	0.51
1:H:5115:ARG:NH2	6:H:6799:HOH:O	2.44	0.51
1:A:34:ILE:HD13	1:C:1476:VAL:HG11	1.93	0.50
1:A:122:LEU:CD2	1:A:204:SER:HB3	2.21	0.50
1:C:1360:TYR:CE2	1:C:1366:VAL:HG11	2.44	0.50
1:D:2240:VAL:HG12	1:D:2249:ILE:HD11	1.92	0.50
1:E:3160:TYR:CD2	1:E:3163:ILE:N	2.79	0.50
1:G:4241:ALA:HB2	1:G:4701:PHE:CE1	2.46	0.50
1:G:4387:LYS:HG3	1:G:4392:LEU:HD11	1.93	0.50
1:G:4444:ILE:HD12	1:G:4449:ASP:HB2	1.93	0.50
1:G:4493:ARG:NH1	1:G:4529:MET:HG2	2.26	0.50
1:A:330:LEU:HD22	1:A:377:GLN:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1343:LEU:HD23	1:C:1361:LYS:HD3	1.93	0.50
1:C:1612:ALA:O	1:C:1616:VAL:HG23	2.11	0.50
1:C:1665:TYR:N	1:C:1665:TYR:CD1	2.80	0.50
1:F:3762:ASN:OD1	1:F:3765:LYS:HD3	2.11	0.50
1:H:5023:LYS:NZ	1:H:5027:ASP:OD2	2.30	0.50
1:A:330:LEU:CD2	1:A:377:GLN:HG3	2.42	0.50
1:E:3274:GLU:O	1:E:3278:ARG:HG3	2.12	0.50
1:H:5130:LEU:CG	1:H:5133:MET:HE3	2.41	0.50
1:A:57:VAL:HG22	1:A:89:ASN:CB	2.42	0.50
1:C:1715:ARG:HB3	1:C:1716:PRO:CD	2.40	0.50
1:E:3022:ALA:HB1	1:E:3027:GLU:HB3	1.94	0.50
1:E:3198:ASN:HD21	1:G:4538:ARG:HH22	1.58	0.50
1:F:3688:LYS:HG2	6:F:7588:HOH:O	2.11	0.50
1:F:3893:ARG:HA	1:F:3896:LEU:HB3	1.92	0.50
1:A:520:PHE:N	1:A:520:PHE:CD1	2.79	0.50
1:E:3068:MET:HE2	1:E:3071:ALA:HB2	1.93	0.50
1:G:4345:ASN:O	1:G:4348:MET:HG3	2.10	0.50
1:G:4474:GLU:O	1:G:4478:ARG:HG3	2.11	0.50
1:H:4945:ASN:O	1:H:4948:MET:HB2	2.11	0.50
1:B:911:MET:HE2	6:D:7520:HOH:O	2.12	0.50
1:C:1272:ARG:NE	1:C:1312:ASP:OD2	2.41	0.50
1:C:1671:VAL:CG1	1:C:1691:LEU:HD21	2.39	0.50
1:F:3634:ILE:HG23	6:F:6928:HOH:O	2.11	0.50
1:C:1654:ARG:HG2	1:C:1673:CYS:O	2.12	0.50
1:D:1861:LYS:O	1:D:1865:LYS:HG3	2.12	0.50
1:D:2190:HIS:HD2	6:D:6448:HOH:O	1.94	0.50
1:E:3398:ALA:CB	1:E:3413:MET:HE1	2.42	0.50
1:G:4243:ASN:CB	1:G:4667:GLY:HA2	2.41	0.50
1:G:4250:ILE:CB	1:G:4273:MET:HE3	2.26	0.50
1:G:4504:LYS:O	1:G:4507:LEU:HB2	2.12	0.50
1:G:4621:LYS:O	1:G:4621:LYS:HD2	2.12	0.50
1:A:57:VAL:HG11	1:A:92:THR:HG22	1.94	0.50
1:A:343:GLU:O	1:A:347:VAL:HG23	2.11	0.50
1:A:456:HIS:CD2	1:A:456:HIS:H	2.27	0.50
1:B:720:THR:HG22	1:B:758:LEU:HD23	1.89	0.50
1:D:2057:LEU:HB2	6:D:7479:HOH:O	2.11	0.50
1:E:3135:LYS:HA	1:E:3196:VAL:HG12	1.93	0.50
1:G:4276:SER:CB	1:G:4319:ARG:HH21	2.24	0.50
1:G:4377:ASP:C	1:G:4498:ILE:HD12	2.36	0.50
1:G:4647:ALA:HB1	1:G:4648:PRO:HD2	1.92	0.50
1:D:2192:LYS:HB2	6:D:7514:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2206:ASP:HB3	1:D:2209:GLU:OE1	2.12	0.50
1:E:3456:HIS:N	1:E:3456:HIS:CD2	2.79	0.50
1:F:3910:LYS:HZ2	1:H:5149:ASN:HD21	1.58	0.50
1:A:123:ILE:HD11	1:A:202:LEU:CD2	2.42	0.49
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.93	0.49
1:B:1056:HIS:H	1:B:1056:HIS:CD2	2.30	0.49
1:C:1247:ILE:HG23	1:C:1270:VAL:HB	1.94	0.49
1:C:1363:ILE:HA	1:C:1366:VAL:CG1	2.42	0.49
1:D:2113:ILE:HD13	1:D:2155:ALA:HB2	1.93	0.49
1:G:4391:PHE:CE1	1:G:4393:VAL:HG23	2.47	0.49
1:H:5133:MET:HE1	1:H:5176:MET:HG2	1.93	0.49
1:A:191:PHE:O	1:A:192:LEU:HD13	2.11	0.49
1:A:391:ARG:HD3	6:A:6393:HOH:O	2.10	0.49
1:A:409:GLU:O	1:A:413:MET:HG3	2.12	0.49
1:A:451:ALA:HB2	1:A:468:ILE:HG23	1.94	0.49
1:A:469:PHE:N	1:A:469:PHE:CD1	2.81	0.49
1:C:1421:SER:N	1:C:1424:ASP:HB2	2.27	0.49
1:D:1916:PRO:HG3	1:D:2045:ARG:NH2	2.27	0.49
1:F:3899:GLU:HB3	6:F:7535:HOH:O	2.11	0.49
1:F:4104:LYS:HB2	1:F:4130:PRO:O	2.12	0.49
1:G:4243:ASN:HB3	1:G:4667:GLY:HA2	1.92	0.49
1:G:4522:PRO:HG3	1:G:4665:TYR:CZ	2.48	0.49
1:A:75:PHE:CE1	1:A:111:LEU:HG	2.47	0.49
1:B:941:ARG:N	1:D:2128:GLN:NE2	2.59	0.49
1:C:1492:ALA:HB1	3:C:1733:OXL:C2	2.42	0.49
1:E:3209:ASN:O	1:E:3211:PRO:HD3	2.12	0.49
1:F:3955:ALA:O	1:F:4066:ARG:NH1	2.38	0.49
1:F:4122:ASN:OD1	1:F:4122:ASN:N	2.45	0.49
1:G:4322:LEU:HD22	1:G:4326:SER:O	2.12	0.49
1:G:4351:CYS:O	1:G:4352:ASP:HB3	2.11	0.49
1:G:4625:ALA:HB1	1:G:4702:PHE:HB3	1.94	0.49
1:C:1428:LEU:CD1	1:C:1456:ILE:HB	2.40	0.49
1:G:4222:ALA:HB1	1:G:4227:GLU:HB3	1.95	0.49
1:G:4410:LEU:HD12	1:G:4410:LEU:N	2.24	0.49
1:G:4611:MET:CE	1:G:4724:MET:HB2	2.41	0.49
1:G:4725:ARG:HD3	1:H:5314:TRP:CE3	2.47	0.49
1:H:5133:MET:CE	1:H:5139:PRO:HG3	2.41	0.49
1:A:453:THR:CG2	1:A:459:ALA:HB2	2.42	0.49
1:C:1287:ILE:O	1:C:1290:VAL:HB	2.11	0.49
1:C:1342:THR:O	1:C:1357:TRP:HA	2.11	0.49
1:C:1479:PHE:CE1	1:C:1489:ILE:HD12	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1958:LEU:HD12	1:D:1963:ILE:HD13	1.94	0.49
1:E:3073:MET:CE	1:E:3109:VAL:HG13	2.42	0.49
1:E:3167:VAL:HG22	1:E:3171:SER:HB2	1.95	0.49
1:A:240:PHE:HB3	1:A:269:LYS:HD2	1.94	0.49
1:B:928:GLN:HE22	1:D:2141:ARG:HH11	1.58	0.49
1:B:1078:GLN:HA	1:B:1078:GLN:HE21	1.78	0.49
1:C:1656:HIS:HB3	1:C:1660:ARG:HH21	1.78	0.49
1:D:1940:LYS:HE3	1:D:1991:PHE:CB	2.43	0.49
1:D:2110:LYS:NZ	6:D:6361:HOH:O	2.44	0.49
1:E:3322:PRO:HG3	1:E:3465:TYR:CE2	2.47	0.49
1:F:3717:GLU:HG3	1:F:3843:PHE:HE2	1.78	0.49
1:F:3890:MET:HE1	3:F:4133:OXL:O1	2.12	0.49
1:G:4372:LYS:HE2	1:G:4397:GLU:OE1	2.13	0.49
1:H:4979:LEU:HD12	1:H:4979:LEU:O	2.13	0.49
1:A:64:ILE:CD1	1:A:94:THR:HA	2.42	0.49
1:B:781:SER:HB3	1:B:798:ASN:HB2	1.94	0.49
1:C:1335:LYS:HG3	1:C:1336:GLY:N	2.28	0.49
1:G:4377:ASP:HA	1:G:4498:ILE:HD11	1.95	0.49
1:G:4443:PHE:O	1:G:4445:ARG:HG3	2.12	0.49
1:G:4570:PRO:O	1:G:4574:VAL:HG23	2.12	0.49
1:H:5130:LEU:HD13	1:H:5133:MET:HE1	1.91	0.49
1:C:1356:LEU:HD12	1:C:1356:LEU:C	2.38	0.49
1:G:4506:PHE:HB2	6:G:7537:HOH:O	2.13	0.49
1:G:4645:PRO:HD2	6:G:7272:HOH:O	2.13	0.49
1:H:5296:GLY:HA3	1:H:5302:PHE:CZ	2.48	0.49
1:A:215:VAL:CG2	1:A:217:LEU:HD12	2.43	0.49
1:A:235:ASP:OD1	1:A:235:ASP:O	2.30	0.49
1:B:1009:GLU:O	1:B:1013:MET:HG3	2.13	0.49
1:D:1877:HIS:CE1	5:D:2335:ATP:H2'	2.48	0.49
1:D:2009:ASN:C	1:D:2010:LEU:HD22	2.38	0.49
1:G:4631:THR:O	1:G:4653:THR:OG1	2.29	0.49
1:G:4714:TRP:HA	1:G:4714:TRP:CE3	2.48	0.49
1:H:4942:THR:CG2	1:H:4944:ASP:H	2.11	0.49
1:B:1008:MET:O	1:B:1008:MET:HE3	2.12	0.49
1:C:1347:TYR:HE2	1:C:1355:ILE:HD12	1.78	0.49
1:C:1357:TRP:CE3	1:C:1358:LEU:N	2.81	0.49
1:C:1479:PHE:CZ	1:C:1483:LEU:HG	2.48	0.49
1:C:1601:SER:OG	1:D:2221:LYS:NZ	2.46	0.49
1:D:2203:HIS:ND1	1:D:2203:HIS:N	2.61	0.49
1:E:3376:MET:HE3	1:E:3376:MET:CA	2.32	0.49
1:E:3391:ARG:O	1:E:3395:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4845:GLY:N	6:H:6157:HOH:O	2.45	0.49
1:A:93:ALA:O	1:A:96:SER:HB3	2.13	0.48
1:C:1294:THR:HG22	1:C:1295:GLU:OE1	2.12	0.48
1:C:1706:ASP:O	1:C:1728:PRO:HA	2.12	0.48
1:C:1724:MET:HE3	1:D:2324:MET:HE3	1.95	0.48
1:D:1937:ALA:O	1:D:1996:VAL:HG23	2.13	0.48
1:E:3242:SER:HA	1:E:3269:LYS:HE2	1.95	0.48
1:G:4503:GLU:OE1	1:G:4503:GLU:N	2.41	0.48
1:H:4821:MET:HA	1:H:4821:MET:HE3	1.94	0.48
1:A:47:ILE:HB	1:A:359:MET:HG3	1.94	0.48
1:C:1628:ILE:HD13	1:C:1692:ALA:HB3	1.95	0.48
1:D:1945:ASN:HD21	1:D:1961:LYS:HZ1	1.58	0.48
1:D:2009:ASN:C	1:D:2011:PRO:HD3	2.37	0.48
1:E:3283:LEU:O	1:E:3283:LEU:HD22	2.12	0.48
1:E:3415:SER:HA	1:E:3524:MET:HE2	1.95	0.48
1:F:3662:GLU:O	1:F:3666:SER:OG	2.29	0.48
1:G:4334:LYS:O	1:G:4337:ALA:HB3	2.13	0.48
1:A:77:HIS:CE1	5:A:535:ATP:H3'	2.49	0.48
1:C:1609:GLU:HB3	1:D:2221:LYS:HE2	1.95	0.48
1:E:3163:ILE:O	1:E:3163:ILE:HG23	2.13	0.48
1:F:3694:THR:HG22	1:F:3704:TYR:OH	2.12	0.48
1:F:3817:LEU:HD22	1:F:3818:PRO:HD2	1.95	0.48
1:F:3933:MET:HA	1:F:3936:LYS:O	2.13	0.48
1:E:3028:HIS:HE1	6:E:6278:HOH:O	1.96	0.48
1:E:3273:HIS:CE1	1:E:3300:ILE:HG22	2.49	0.48
1:F:3623:ASP:OD1	1:F:3623:ASP:N	2.45	0.48
1:F:3731:VAL:HG13	1:F:3732:GLU:N	2.29	0.48
1:F:3789:PRO:HD2	1:F:3791:PHE:CE1	2.48	0.48
1:F:3845:ARG:HG2	1:F:3874:GLU:CB	2.43	0.48
1:G:4322:LEU:HB2	1:G:4349:GLU:HA	1.94	0.48
1:H:4843:ASN:H	1:H:5185:GLU:CD	2.22	0.48
1:H:5238:HIS:NE2	6:H:7259:HOH:O	2.34	0.48
1:A:237:ASP:O	1:A:461:GLN:NE2	2.45	0.48
1:B:870:ILE:HG21	1:B:912:ILE:HD11	1.95	0.48
1:E:3083:HIS:O	1:E:3087:ILE:HG13	2.14	0.48
1:F:3820:VAL:HG21	1:F:3852:GLU:HB3	1.95	0.48
1:H:4868:MET:HE2	1:H:4871:ALA:HA	1.94	0.48
1:H:5015:VAL:HG12	1:H:5017:LEU:H	1.78	0.48
1:A:80:HIS:CE1	1:A:230:PHE:HB2	2.48	0.48
1:C:1308:ALA:HB1	1:C:1438:MET:HE3	1.95	0.48
1:E:3142:THR:CG2	1:E:3144:ASP:H	1.99	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3294:GLY:CA	1:E:3327:THR:HG21	2.44	0.48
1:E:3509:ILE:HD13	1:E:3526:VAL:HG23	1.93	0.48
1:F:3815:VAL:O	1:F:3817:LEU:N	2.46	0.48
1:F:3817:LEU:HD23	1:F:3817:LEU:HA	1.51	0.48
1:H:4900:ASP:OD2	1:H:4903:LEU:HG	2.14	0.48
1:A:50:ILE:HD13	1:A:50:ILE:N	2.29	0.48
1:A:77:HIS:CD2	5:A:535:ATP:H2'	2.49	0.48
1:A:216:ASP:OD1	1:A:216:ASP:O	2.32	0.48
1:A:322:PRO:HG3	1:A:465:TYR:CE2	2.48	0.48
1:B:700:ASP:O	1:B:703:LEU:N	2.46	0.48
1:C:1630:LEU:HD22	1:C:1712:THR:HG22	1.95	0.48
1:C:1671:VAL:HG12	1:C:1691:LEU:CD2	2.41	0.48
1:D:1817:LEU:HA	1:D:1820:ALA:CB	2.44	0.48
1:E:3146:ALA:O	1:E:3150:LYS:HD2	2.14	0.48
1:E:3179:LEU:HB2	6:E:6658:HOH:O	2.12	0.48
1:G:4257:VAL:CG2	1:G:4289:ASN:HB3	2.44	0.48
1:A:47:ILE:HG22	1:A:359:MET:HG3	1.94	0.48
1:A:89:ASN:HD22	1:A:89:ASN:N	2.11	0.48
1:C:1421:SER:HB2	1:C:1424:ASP:H	1.79	0.48
1:C:1727:VAL:HG13	1:C:1728:PRO:HD2	1.96	0.48
1:D:2188:MET:HE3	1:D:2190:HIS:CE1	2.49	0.48
1:E:3062:GLU:OE1	1:E:3062:GLU:HA	2.12	0.48
1:H:5275:ASP:HB3	1:H:5276:PRO:CD	2.43	0.48
1:B:1015:SER:HA	1:B:1124:MET:HE2	1.95	0.48
1:C:1294:THR:HG22	1:C:1295:GLU:N	2.29	0.48
1:C:1360:TYR:HD2	1:C:1363:ILE:CB	2.27	0.48
1:C:1611:MET:HG3	1:C:1721:THR:O	2.14	0.48
1:D:1819:ALA:HA	1:D:1831:ARG:HD2	1.95	0.48
1:D:1942:THR:O	1:D:1957:TRP:HA	2.14	0.48
1:E:3019:ALA:HA	1:E:3031:ARG:CD	2.44	0.48
1:E:3181:SER:O	1:E:3197:GLU:HB2	2.14	0.48
1:F:3721:GLY:CA	1:F:3757:TRP:HE3	2.26	0.48
1:A:57:VAL:CG1	1:A:92:THR:HG22	2.44	0.47
1:A:139:LEU:HD21	1:A:156:LEU:HB2	1.95	0.47
1:A:328:GLN:HE22	1:C:1540:THR:CA	2.26	0.47
1:B:873:HIS:ND1	1:B:900:ILE:HG22	2.29	0.47
1:B:923:VAL:HG22	1:B:924:ILE:N	2.29	0.47
1:C:1276:SER:HB3	1:C:1319:ARG:NH1	2.28	0.47
1:G:4599:ARG:O	1:G:4602:SER:HB3	2.14	0.47
1:H:5293:MET:O	1:H:5297:LYS:HD3	2.14	0.47
1:A:245:ARG:HG2	1:A:274:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ARG:HD2	6:B:6993:HOH:O	2.14	0.47
1:B:924:ILE:HG12	1:B:957:CYS:HB2	1.95	0.47
1:C:1445:ARG:HB3	1:C:1474:GLU:CD	2.39	0.47
1:C:1666:ARG:HG3	1:C:1667:GLY:N	2.28	0.47
1:D:2281:TRP:CZ2	1:D:2316:PRO:HA	2.49	0.47
1:F:3787:LYS:HB3	1:F:3792:LEU:HD11	1.94	0.47
1:G:4275:PHE:HE2	1:G:4280:HIS:CD2	2.32	0.47
1:G:4524:ILE:HG12	1:G:4557:CYS:HB2	1.96	0.47
1:G:4681:TRP:NE1	1:G:4715:ARG:HA	2.28	0.47
1:H:5279:GLU:HG3	1:H:5280:ALA:N	2.30	0.47
1:A:409:GLU:HB3	1:B:1021:LYS:HE2	1.95	0.47
1:C:1360:TYR:CD2	1:C:1363:ILE:HB	2.46	0.47
1:C:1391:PHE:O	1:C:1392:LEU:HD13	2.14	0.47
1:C:1588:MET:SD	1:C:1666:ARG:NH2	2.87	0.47
1:D:2190:HIS:NE2	1:D:2246:ARG:HG3	2.29	0.47
1:E:3331:GLU:HA	1:E:3331:GLU:OE1	2.14	0.47
1:F:3752:ASP:OD1	1:F:3755:ILE:N	2.45	0.47
1:F:3786:GLN:HB3	1:F:3793:VAL:HB	1.95	0.47
1:F:3889:ILE:HG22	1:F:3890:MET:N	2.29	0.47
1:H:5039:VAL:HG23	1:H:5064:ILE:CG2	2.45	0.47
1:C:1277:HIS:NE2	5:C:1735:ATP:H3'	2.29	0.47
1:C:1318:ILE:HG22	1:C:1408:VAL:HB	1.95	0.47
1:C:1417:LEU:HB3	1:C:1418:PRO:HD2	1.95	0.47
1:E:3108:ALA:HB2	1:E:3460:ARG:O	2.13	0.47
1:F:3916:CYS:HB3	1:F:3921:LYS:O	2.15	0.47
1:G:4322:LEU:HA	1:G:4404:SER:HB3	1.95	0.47
1:H:5188:MET:CE	1:H:5190:HIS:NE2	2.78	0.47
1:A:454:ARG:HG2	1:A:473:CYS:O	2.15	0.47
1:B:762:ASN:ND2	6:B:6065:HOH:O	2.47	0.47
1:C:1252:PRO:HG3	5:C:1735:ATP:C2	2.50	0.47
1:C:1356:LEU:HD12	1:C:1357:TRP:N	2.30	0.47
1:E:3478:GLN:HB2	1:E:3484:ASP:CB	2.44	0.47
1:F:3893:ARG:HD3	1:F:3926:ALA:O	2.14	0.47
1:H:5067:ILE:HD12	1:H:5088:GLY:HA3	1.97	0.47
1:A:398:ALA:CB	1:A:413:MET:HE1	2.45	0.47
1:A:515:ARG:HB3	1:A:516:PRO:HD2	1.97	0.47
1:F:3988:MET:SD	1:F:4066:ARG:NH2	2.88	0.47
1:A:79:THR:H	1:A:82:TYR:HB3	1.78	0.47
1:A:123:ILE:HD11	1:A:202:LEU:CG	2.45	0.47
1:A:334:ILE:HG12	1:A:362:GLY:O	2.15	0.47
1:A:407:LEU:HD12	1:A:407:LEU:HA	1.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:PHE:CD1	1:B:711:LEU:HG	2.50	0.47
1:B:774:TYR:CE2	1:B:811:PRO:HG3	2.50	0.47
1:C:1320:THR:HG22	1:C:1358:LEU:CD1	2.44	0.47
1:C:1323:ILE:C	1:C:1324:LYS:HG3	2.40	0.47
1:C:1376:ASP:N	1:C:1407:GLY:O	2.46	0.47
1:D:1859:THR:O	1:D:1862:GLU:N	2.47	0.47
1:E:3252:GLU:HG2	6:E:7072:HOH:O	2.15	0.47
1:E:3425:ALA:HB1	1:E:3502:PHE:HB3	1.97	0.47
1:F:3629:MET:O	1:H:5111:MET:HA	2.14	0.47
1:F:3646:ILE:HG23	1:F:3977:GLN:NE2	2.30	0.47
1:F:3717:GLU:CD	1:F:3719:ARG:HE	2.22	0.47
1:G:4471:GLU:O	1:G:4499:GLU:HG3	2.14	0.47
1:G:4680:ALA:HB3	1:G:4683:GLU:CD	2.40	0.47
1:G:4686:ASP:O	1:G:4690:ASN:HB2	2.15	0.47
1:H:5135:LYS:HB2	6:H:6479:HOH:O	2.14	0.47
1:B:772:LYS:HE2	1:B:783:GLN:HG3	1.97	0.47
1:C:1650:ILE:HD13	1:C:1650:ILE:N	2.29	0.47
1:C:1681:TRP:CZ2	1:C:1716:PRO:HA	2.50	0.47
1:D:1945:ASN:ND2	1:D:1961:LYS:NZ	2.57	0.47
1:D:2088:GLY:O	1:D:2089:ILE:HD13	2.15	0.47
1:E:3304:LYS:O	1:E:3307:LEU:HB2	2.14	0.47
1:F:3872:ASN:ND2	1:F:3875:GLY:H	2.12	0.47
1:F:4055:ASN:O	1:F:4058:THR:HB	2.15	0.47
1:G:4222:ALA:HB1	1:G:4227:GLU:HG2	1.96	0.47
1:G:4339:LEU:CD1	1:G:4354:ASN:HA	2.43	0.47
1:G:4501:PRO:HG2	1:G:4504:LYS:HD2	1.96	0.47
1:A:29:MET:HE2	1:C:1510:LYS:CB	2.44	0.47
1:A:79:THR:HG1	1:A:81:GLU:HB3	1.80	0.47
1:A:172:LYS:HA	1:A:182:LEU:O	2.15	0.47
1:A:338:ARG:HG3	1:A:338:ARG:NH1	2.30	0.47
1:D:1812:ILE:HD13	1:D:1833:ASP:OD2	2.14	0.47
1:D:1851:GLY:C	1:D:1855:ARG:HG3	2.39	0.47
1:D:2206:ASP:HB3	1:D:2209:GLU:HB2	1.96	0.47
1:D:2291:LEU:O	1:D:2291:LEU:HD12	2.14	0.47
1:E:3142:THR:HG21	1:E:3144:ASP:CB	2.45	0.47
1:F:3675:PHE:CZ	1:F:3683:HIS:CD2	3.03	0.47
1:G:4417:LEU:HD12	1:G:4417:LEU:HA	1.51	0.47
1:B:660:LEU:HB3	1:B:693:ALA:CB	2.45	0.47
1:D:2127:THR:O	1:D:2128:GLN:HB2	2.14	0.47
1:E:3113:THR:HG23	1:E:3114:LYS:N	2.29	0.47
1:E:3343:GLU:O	1:E:3347:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3665:LYS:HE2	1:F:3697:PHE:HE2	1.80	0.47
1:F:3679:THR:OG1	1:F:3681:GLU:N	2.47	0.47
1:F:3889:ILE:CG2	1:F:3890:MET:N	2.78	0.47
1:G:4385:LYS:HB2	1:G:4393:VAL:O	2.15	0.47
1:C:1452:GLU:HG2	1:C:1455:LYS:NZ	2.30	0.46
1:D:1976:ASP:HB2	1:D:2006:LYS:HG3	1.98	0.46
1:D:2295:VAL:O	1:D:2299:ARG:HG3	2.16	0.46
1:E:3019:ALA:CB	1:E:3031:ARG:HB2	2.45	0.46
1:E:3055:ARG:NH2	1:E:3082:TYR:O	2.47	0.46
1:F:3659:THR:O	1:F:3663:MET:HG2	2.15	0.46
1:G:4321:GLY:N	1:G:4357:TRP:O	2.48	0.46
1:H:5327:VAL:CG1	1:H:5328:PRO:HD2	2.41	0.46
1:C:1313:THR:O	1:C:1442:SER:OG	2.31	0.46
1:C:1319:ARG:HB2	1:C:1359:ASP:OD2	2.15	0.46
1:D:2188:MET:CE	1:D:2266:ARG:HH21	2.28	0.46
1:F:3928:GLN:HE21	1:H:5140:THR:HB	1.79	0.46
1:G:4560:LEU:HD23	1:G:4560:LEU:HA	1.79	0.46
1:H:4922:LEU:HB3	1:H:4926:SER:O	2.15	0.46
1:C:1591:ARG:O	1:C:1595:GLU:HG3	2.15	0.46
1:D:1911:LEU:C	1:D:1911:LEU:HD23	2.40	0.46
1:E:3382:ARG:NH1	6:E:6629:HOH:O	2.47	0.46
1:E:3425:ALA:O	1:E:3426:ALA:HB2	2.15	0.46
1:G:4323:ILE:HA	1:G:4351:CYS:HB2	1.98	0.46
1:H:4860:LEU:O	1:H:4863:MET:HB2	2.15	0.46
1:A:163:ILE:O	1:A:163:ILE:CG2	2.52	0.46
1:A:439:GLN:O	1:A:442:ARG:HG2	2.15	0.46
1:B:739:LEU:HD12	1:B:754:ASN:O	2.14	0.46
1:B:774:TYR:HB2	1:B:809:ASN:HB2	1.98	0.46
1:C:1253:ALA:HB1	6:C:7310:HOH:O	2.14	0.46
1:E:3055:ARG:NH2	1:E:3085:GLU:HB3	2.31	0.46
1:G:4428:LEU:HD12	1:G:4456:ILE:HG21	1.95	0.46
1:H:5038:MET:HE1	1:H:5264:LEU:HD22	1.97	0.46
1:A:289:ILE:CG2	1:A:290:MET:N	2.78	0.46
1:C:1257:VAL:HG12	1:C:1258:GLU:N	2.31	0.46
1:C:1263:MET:HA	1:C:1266:SER:HB2	1.97	0.46
1:C:1707:VAL:HG12	1:C:1708:VAL:N	2.31	0.46
1:D:2209:GLU:O	1:D:2213:MET:HG3	2.16	0.46
1:G:4409:ASN:ND2	6:G:6819:HOH:O	2.40	0.46
1:H:5231:THR:HG21	1:H:5234:GLY:HA2	1.97	0.46
1:H:5256:HIS:H	1:H:5256:HIS:CD2	2.34	0.46
1:A:114:LYS:HB2	6:A:6007:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:7662:HOH:O	1:C:1536:LYS:HE2	2.15	0.46
1:B:815:VAL:CB	1:B:817:LEU:HD12	2.38	0.46
1:C:1524:ILE:HG12	1:C:1557:CYS:HB2	1.96	0.46
1:D:2089:ILE:CG2	1:D:2090:MET:N	2.79	0.46
1:F:3906:PHE:HB2	6:F:6288:HOH:O	2.15	0.46
1:F:4009:GLU:OE2	1:F:4043:TYR:OH	2.28	0.46
1:F:4080:ALA:O	1:F:4083:GLU:HB2	2.16	0.46
1:G:4569:TYR:HB3	1:G:4572:GLU:HB2	1.97	0.46
1:H:4824:THR:OG1	1:H:4827:GLU:HB2	2.15	0.46
1:A:203:GLY:HA3	1:A:206:LYS:CE	2.45	0.46
1:B:1106:ASP:O	1:B:1129:VAL:HG23	2.16	0.46
1:C:1529:MET:O	1:C:1543:GLU:HB3	2.15	0.46
1:D:1884:ALA:HB2	1:D:2030:PHE:HZ	1.80	0.46
1:E:3220:VAL:HG11	1:E:3225:ILE:HD11	1.98	0.46
1:E:3333:MET:SD	1:E:3339:PRO:HD3	2.56	0.46
1:F:3763:ILE:HG23	1:F:3764:CYS:N	2.31	0.46
1:G:4410:LEU:CD1	1:G:4410:LEU:N	2.79	0.46
1:G:4494:GLY:HA3	1:G:4527:THR:HG21	1.96	0.46
1:G:4628:ILE:HD13	1:G:4692:ALA:HB3	1.98	0.46
1:A:131:VAL:HG22	6:A:7655:HOH:O	2.15	0.46
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.74	0.46
1:B:698:ALA:HA	1:B:704:TYR:CD1	2.51	0.46
1:B:1109:ILE:HD13	1:B:1126:VAL:HG22	1.91	0.46
1:C:1226:LEU:O	1:C:1229:MET:HB2	2.16	0.46
1:C:1260:LEU:HD13	1:C:1290:VAL:HA	1.97	0.46
1:E:3306:PHE:HB2	6:E:7081:HOH:O	2.14	0.46
1:F:3641:ALA:CB	1:F:4048:PRO:HG3	2.46	0.46
1:G:4593:LEU:HG	1:G:4597:LEU:HD22	1.97	0.46
1:H:5265:TYR:CD1	1:H:5265:TYR:N	2.84	0.46
1:A:162:ASN:ND2	1:A:165:LYS:HD3	2.31	0.46
1:A:432:GLU:OE1	1:A:454:ARG:HB2	2.15	0.46
1:B:949:ASN:HD21	1:D:2110:LYS:NZ	2.14	0.46
1:C:1456:ILE:N	1:C:1456:ILE:CD1	2.79	0.46
1:D:2103:GLU:OE1	1:D:2103:GLU:N	2.38	0.46
1:D:2176:MET:O	1:D:2180:ILE:HG13	2.16	0.46
1:E:3116:PRO:HD2	1:E:3243:PHE:HB2	1.97	0.46
1:E:3311:MET:SD	1:E:3315:ARG:HD3	2.56	0.46
1:A:252:GLU:O	1:A:255:LYS:HB3	2.16	0.46
1:D:1922:LEU:O	1:D:1951:CYS:HB2	2.16	0.46
1:D:2054:ARG:HD2	1:D:2066:ILE:HD12	1.97	0.46
1:E:3103:LEU:HD12	1:E:3103:LEU:HA	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3167:VAL:O	1:E:3187:LYS:HE3	2.16	0.46
1:E:3172:LYS:HE3	1:E:3183:GLN:CB	2.42	0.46
1:E:3173:VAL:HB	1:E:3182:LEU:HB2	1.97	0.46
1:F:3649:THR:HG22	1:F:3965:ALA:HB2	1.97	0.46
1:F:3929:MET:O	1:F:3943:GLU:HG2	2.15	0.46
1:A:118:ILE:HG21	1:A:208:VAL:HB	1.95	0.45
1:A:141:ILE:HG23	1:A:156:LEU:O	2.17	0.45
1:A:279:PHE:CD2	1:A:311:MET:HE1	2.51	0.45
1:C:1335:LYS:CG	1:C:1336:GLY:N	2.79	0.45
1:C:1339:LEU:HD12	1:C:1354:ASN:O	2.16	0.45
1:C:1381:SER:O	1:C:1397:GLU:HB3	2.16	0.45
1:E:3188:GLY:HA3	1:E:3191:PHE:CD1	2.51	0.45
1:F:3650:ILE:CG1	1:F:3673:MET:HE1	2.46	0.45
1:H:4889:ASN:ND2	6:H:6193:HOH:O	2.48	0.45
1:A:471:VAL:O	1:A:471:VAL:HG12	2.16	0.45
1:B:815:VAL:HG21	1:B:843:PHE:CE2	2.52	0.45
1:C:1655:ASN:HB3	1:C:1658:THR:HB	1.99	0.45
1:E:3168:ASP:O	1:E:3171:SER:HB2	2.15	0.45
1:E:3333:MET:O	1:E:3369:TYR:HB2	2.16	0.45
1:G:4376:ASP:OD2	1:G:4406:LYS:HD2	2.16	0.45
1:A:79:THR:OG1	1:A:81:GLU:HB3	2.15	0.45
1:B:731:VAL:HG11	1:B:753:GLU:HB3	1.97	0.45
1:B:1101:PHE:CD1	1:B:1101:PHE:N	2.84	0.45
1:B:1114:TRP:CD1	1:B:1115:ARG:CD	2.99	0.45
1:C:1352:ASP:OD1	1:C:1354:ASN:HB2	2.16	0.45
1:E:3350:ALA:O	1:E:3353:ASP:HB2	2.15	0.45
1:E:3465:TYR:N	1:E:3465:TYR:CD1	2.83	0.45
1:F:3721:GLY:CA	1:F:3757:TRP:CE3	2.99	0.45
1:G:4348:MET:HA	1:G:4357:TRP:CE3	2.51	0.45
1:H:4918:ILE:CD1	1:H:5010:LEU:HD22	2.46	0.45
1:H:4923:ILE:C	1:H:4925:GLY:H	2.25	0.45
1:H:5130:LEU:CB	1:H:5133:MET:HE3	2.43	0.45
1:H:5230:LEU:HG	1:H:5312:THR:HG22	1.98	0.45
1:H:5231:THR:O	1:H:5253:THR:HB	2.16	0.45
1:B:704:TYR:HD2	6:B:6584:HOH:O	1.99	0.45
1:C:1275:PHE:N	1:C:1275:PHE:CD1	2.83	0.45
1:G:4251:GLY:C	1:G:4255:ARG:HG3	2.41	0.45
1:H:4926:SER:HB3	1:H:4929:ALA:N	2.21	0.45
1:H:5046:LYS:O	1:H:5049:ASP:HB2	2.16	0.45
1:H:5226:ALA:HA	1:H:5247:ALA:HB1	1.98	0.45
1:H:5244:ARG:NE	6:H:6931:HOH:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLN:NE2	1:C:1540:THR:CA	2.80	0.45
1:B:619:ALA:HB2	1:B:631:ARG:HB3	1.98	0.45
1:B:731:VAL:CG1	1:B:732:GLU:N	2.80	0.45
1:B:890:MET:HE1	3:B:1133:OXL:O1	2.17	0.45
1:C:1250:ILE:HG12	1:C:1271:ALA:HB1	1.97	0.45
1:C:1347:TYR:CE2	1:C:1355:ILE:CD1	3.00	0.45
1:C:1406:LYS:HA	1:C:1406:LYS:HD2	1.47	0.45
1:F:4057:GLN:O	1:F:4061:GLN:HG3	2.15	0.45
1:A:63:MET:HG3	1:A:371:LEU:CD2	2.47	0.45
1:A:290:MET:HE3	1:A:326:ALA:HB3	1.97	0.45
1:A:333:MET:HA	1:A:336:LYS:O	2.16	0.45
1:A:341:ARG:H	1:C:1528:GLN:NE2	2.14	0.45
1:B:731:VAL:HG12	1:B:732:GLU:N	2.31	0.45
1:B:843:PHE:CD2	1:B:845:ARG:NE	2.85	0.45
1:C:1212:ILE:O	1:C:1212:ILE:HG22	2.15	0.45
1:C:1677:VAL:HG12	1:C:1678:GLN:N	2.32	0.45
1:D:2188:MET:SD	1:D:2266:ARG:NH2	2.89	0.45
1:E:3156:LEU:HD23	1:E:3156:LEU:HA	1.70	0.45
1:F:3756:LEU:HD12	1:F:3756:LEU:C	2.41	0.45
1:A:55:ARG:NH2	1:A:85:GLU:HB3	2.31	0.45
1:A:245:ARG:HE	1:A:245:ARG:HB2	1.50	0.45
1:A:316:CYS:O	1:A:320:GLY:N	2.50	0.45
1:C:1597:LEU:HD12	1:C:1597:LEU:HA	1.68	0.45
1:C:1656:HIS:HB3	1:C:1660:ARG:NH2	2.32	0.45
1:D:1874:ASN:OD1	1:D:1876:SER:HB2	2.16	0.45
1:E:3162:ASN:HD21	1:E:3165:LYS:HE2	1.81	0.45
1:F:3676:SER:HA	1:F:3714:LYS:HG3	1.97	0.45
1:F:3933:MET:HE3	1:F:3937:PRO:O	2.17	0.45
1:G:4342:THR:HG21	1:G:4347:TYR:HD2	1.79	0.45
1:H:5023:LYS:HG2	1:H:5027:ASP:OD2	2.17	0.45
1:A:113:THR:HG23	1:A:114:LYS:N	2.32	0.45
1:A:133:LEU:N	1:A:133:LEU:CD1	2.79	0.45
1:B:672:ARG:HH11	1:B:672:ARG:HD3	1.67	0.45
1:C:1215:GLN:CD	1:C:1239:ILE:HG23	2.42	0.45
1:C:1472:ASN:O	1:C:1476:VAL:HG23	2.17	0.45
1:D:1878:GLY:HA2	6:D:6136:HOH:O	2.16	0.45
1:E:3340:THR:HB	1:G:4528:GLN:HE21	1.81	0.45
1:F:3824:ASP:O	1:F:3827:ASP:HB2	2.17	0.45
1:F:3829:LYS:CE	1:F:3856:ILE:HG23	2.46	0.45
1:F:3893:ARG:NH2	1:F:3946:ASP:OD1	2.50	0.45
1:F:3894:GLY:HA3	1:F:3927:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3897:GLY:HA2	1:F:3905:VAL:CG2	2.47	0.45
1:H:4990:ASP:OD1	1:H:4991:PHE:HD2	2.00	0.45
1:A:140:LYS:HE2	1:A:191:PHE:HB2	1.98	0.45
1:A:192:LEU:N	1:A:192:LEU:CD2	2.76	0.45
1:A:452:VAL:HG11	1:A:488:ARG:HB3	1.98	0.45
1:B:640:THR:O	1:B:982:ARG:NH1	2.41	0.45
1:B:857:LEU:HD12	1:B:866:ILE:HD11	1.99	0.45
1:B:997:LEU:O	1:B:1000:SER:OG	2.29	0.45
1:B:1104:LYS:HA	1:B:1129:VAL:HG12	1.97	0.45
1:C:1395:GLU:HB2	6:C:7744:HOH:O	2.16	0.45
1:C:1488:GLY:C	1:C:1489:ILE:HG12	2.42	0.45
1:C:1518:ARG:HB3	6:C:6442:HOH:O	2.16	0.45
1:C:1539:PRO:HG3	1:C:1576:MET:HG2	1.98	0.45
1:D:1814:THR:CG2	1:D:1815:GLN:N	2.80	0.45
1:D:1856:SER:O	1:D:1860:LEU:HB2	2.17	0.45
1:E:3049:THR:HA	1:E:3072:ARG:O	2.17	0.45
1:E:3379:LEU:HD12	1:E:3379:LEU:HA	1.85	0.45
1:F:3806:LYS:HA	1:F:3806:LYS:HD2	1.59	0.45
1:F:3941:ARG:NE	1:H:5093:ARG:O	2.50	0.45
1:G:4212:ILE:HG22	1:G:4213:GLN:O	2.17	0.45
1:H:5242:ARG:NH2	6:H:7238:HOH:O	2.29	0.45
1:A:156:LEU:CD2	1:A:157:TRP:N	2.80	0.45
1:B:1115:ARG:HB3	1:B:1116:PRO:HD3	1.98	0.45
1:C:1322:LEU:CD1	1:C:1349:GLU:HG2	2.35	0.45
1:C:1351:CYS:O	1:C:1352:ASP:HB3	2.17	0.45
1:C:1373:VAL:HG13	1:C:1410:LEU:HD11	1.99	0.45
1:C:1639:GLN:OE1	1:C:1642:ARG:HD3	2.16	0.45
1:C:1704:LYS:HD2	1:C:1730:PRO:O	2.17	0.45
1:D:2025:ILE:HD12	1:D:2056:ILE:HG13	1.98	0.45
1:D:2175:ARG:HG3	1:D:2175:ARG:H	1.43	0.45
1:E:3012:ILE:CG2	1:E:3013:GLN:N	2.79	0.45
1:E:3068:MET:HE2	1:E:3071:ALA:CB	2.47	0.45
1:F:3837:ASP:HB3	1:F:4061:GLN:HG2	1.99	0.45
1:F:3878:ARG:O	1:F:3881:GLU:HG2	2.16	0.45
1:F:3922:PRO:HB3	1:F:4064:LEU:O	2.17	0.45
1:G:4255:ARG:NE	1:G:4282:TYR:CZ	2.85	0.45
1:G:4613:MET:SD	1:H:5221:LYS:HE2	2.57	0.45
1:H:4960:TYR:CD2	1:H:4963:ILE:HB	2.52	0.45
1:H:4960:TYR:OH	1:H:5016:ASP:HB2	2.16	0.45
1:A:131:VAL:HG13	1:A:133:LEU:CD1	2.47	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:HA	1:A:269:LYS:HB2	1.98	0.44
1:A:293:ARG:NH2	1:A:346:ASP:OD1	2.44	0.44
1:A:300:ILE:HB	1:A:301:PRO:CD	2.48	0.44
1:B:655:ARG:HD2	1:B:682:TYR:OH	2.17	0.44
1:B:1030:LEU:HD12	1:B:1030:LEU:N	2.32	0.44
1:D:1841:ALA:CB	1:D:2248:PRO:HG3	2.47	0.44
1:D:1848:CYS:SG	1:D:1868:MET:HE3	2.57	0.44
1:F:3719:ARG:HD3	1:F:3807:GLY:HA2	1.99	0.44
1:A:267:ILE:N	1:A:267:ILE:CD1	2.79	0.44
1:B:744:ASP:C	1:B:746:ALA:H	2.25	0.44
1:C:1287:ILE:CG2	1:C:1291:ARG:NH1	2.80	0.44
1:C:1482:ILE:O	1:C:1486:SER:OG	2.34	0.44
1:C:1664:LEU:HD12	1:C:1664:LEU:HA	1.77	0.44
1:D:1855:ARG:HD2	1:D:1882:TYR:CZ	2.52	0.44
1:E:3328:GLN:NE2	1:G:4540:THR:HA	2.30	0.44
1:F:3941:ARG:N	1:H:5128:GLN:NE2	2.55	0.44
1:G:4303:LEU:HA	1:G:4303:LEU:HD22	1.78	0.44
1:H:5285:VAL:O	1:H:5289:VAL:HG23	2.17	0.44
1:A:52:PRO:HD2	1:A:365:ALA:O	2.17	0.44
1:A:481:TRP:HB2	1:A:516:PRO:HG3	2.00	0.44
1:B:724:LYS:HE2	1:B:752:ASP:HB3	2.00	0.44
1:B:1129:VAL:HA	1:B:1130:PRO:HD2	1.71	0.44
1:C:1268:MET:HE2	1:C:1271:ALA:HA	1.98	0.44
1:C:1425:ILE:O	1:C:1428:LEU:HB2	2.18	0.44
1:D:2205:THR:O	1:D:2205:THR:HG23	2.17	0.44
1:E:3126:SER:HB3	1:E:3129:ALA:CB	2.46	0.44
1:E:3209:ASN:O	1:E:3210:LEU:HD23	2.17	0.44
1:E:3396:GLU:CD	1:G:4224:THR:HB	2.42	0.44
1:E:3453:THR:HG21	1:E:3459:ALA:HB2	2.00	0.44
1:E:3456:HIS:CD2	1:E:3456:HIS:H	2.35	0.44
1:F:3700:ASP:HA	1:F:3701:PRO:HD2	1.83	0.44
1:F:3774:TYR:CE2	1:F:3811:PRO:HG2	2.52	0.44
1:F:3838:MET:HA	1:F:3864:ILE:CG2	2.46	0.44
1:F:4031:THR:HG21	1:F:4034:GLY:HA2	1.99	0.44
1:H:4847:ILE:HD13	1:H:5159:MET:HE3	1.99	0.44
1:A:130:GLU:HG3	1:A:201:PHE:HB3	1.99	0.44
1:A:406:ASP:OD1	1:A:407:LEU:N	2.51	0.44
1:A:503:LYS:O	1:A:529:VAL:HB	2.18	0.44
1:B:809:ASN:C	1:B:810:LEU:HD13	2.43	0.44
1:B:975:ARG:O	1:B:978:HIS:HB3	2.17	0.44
1:D:1959:ASP:HB3	6:D:7764:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3245:ARG:HB3	1:E:3274:GLU:CG	2.38	0.44
1:E:3293:ARG:HB3	1:G:4541:ARG:HG3	1.98	0.44
1:E:3469:PHE:CD1	1:E:3469:PHE:N	2.86	0.44
1:F:3687:ILE:O	1:F:3691:ARG:HG3	2.18	0.44
1:F:4008:MET:HE2	1:F:4036:SER:O	2.17	0.44
1:G:4488:GLY:C	1:G:4489:ILE:HG12	2.41	0.44
1:G:4711:LEU:HB3	1:G:4721:THR:OG1	2.17	0.44
1:H:4931:VAL:HG12	1:H:4932:GLU:H	1.82	0.44
1:A:209:ASN:HB3	1:A:299:GLU:OE2	2.16	0.44
1:B:647:ILE:HG12	1:B:670:VAL:HB	2.00	0.44
1:B:748:MET:HB2	1:B:757:TRP:CD2	2.52	0.44
1:B:1028:ILE:HG13	1:B:1108:VAL:HG11	2.00	0.44
1:C:1250:ILE:HG21	1:C:1286:THR:CG2	2.47	0.44
1:C:1276:SER:HB3	1:C:1319:ARG:HD2	2.00	0.44
1:C:1283:HIS:O	1:C:1287:ILE:HG12	2.18	0.44
1:D:1817:LEU:C	1:D:1820:ALA:HB3	2.42	0.44
1:D:1887:ILE:CG2	1:D:1891:ARG:NH1	2.80	0.44
1:D:2044:ILE:CG1	1:D:2068:SER:HB3	2.44	0.44
1:D:2192:LYS:HD2	6:D:7514:HOH:O	2.16	0.44
1:E:3205:LYS:HG2	6:E:6937:HOH:O	2.18	0.44
1:F:3713:THR:HG22	1:F:3842:SER:HB2	1.99	0.44
1:F:4105:GLY:N	1:F:4129:VAL:O	2.40	0.44
1:G:4444:ILE:HG23	1:G:4449:ASP:HB2	1.99	0.44
1:G:4693:MET:CE	1:G:4729:VAL:HG22	2.46	0.44
1:H:5010:LEU:HB3	1:H:5013:ALA:HB3	1.99	0.44
1:B:882:ILE:O	1:B:886:SER:OG	2.31	0.44
1:C:1249:THR:C	1:C:1250:ILE:HD13	2.43	0.44
1:C:1358:LEU:HD12	1:C:1358:LEU:HA	1.71	0.44
1:C:1445:ARG:HG2	1:C:1474:GLU:HB3	1.98	0.44
1:C:1650:ILE:CD1	1:C:1669:PHE:HB2	2.47	0.44
1:F:3842:SER:HA	1:F:3869:LYS:HD3	1.99	0.44
1:F:4032:GLU:OE1	1:F:4054:ARG:N	2.40	0.44
1:G:4363:ILE:CG2	1:G:4364:CYS:N	2.79	0.44
1:G:4368:ASP:O	1:G:4384:VAL:HG11	2.18	0.44
1:H:4868:MET:HE2	1:H:4870:VAL:O	2.17	0.44
1:H:5089:ILE:CG2	1:H:5090:MET:N	2.80	0.44
1:A:277:ARG:NH2	1:A:278:ARG:CZ	2.81	0.44
1:A:338:ARG:HG3	1:A:338:ARG:HH11	1.83	0.44
1:B:904:LYS:HB3	1:D:1834:ILE:HG22	1.99	0.44
1:B:935:LYS:HA	1:B:935:LYS:HD2	1.75	0.44
1:C:1287:ILE:HG22	1:C:1291:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1345:ASN:HD21	1:C:1361:LYS:NZ	2.16	0.44
1:C:1534:ILE:HG23	1:C:1567:GLY:CA	2.41	0.44
1:E:3346:ASP:CG	1:G:4542:ALA:HA	2.43	0.44
1:F:3735:LYS:HG2	1:F:3736:GLY:N	2.33	0.44
1:H:4855:ARG:HD3	6:H:7187:HOH:O	2.18	0.44
1:H:5179:LEU:HA	1:H:5179:LEU:HD23	1.79	0.44
1:B:1114:TRP:C	1:B:1115:ARG:HG3	2.43	0.44
1:C:1341:ILE:HD12	1:C:1394:THR:CG2	2.46	0.44
1:C:1446:LYS:HE2	6:C:7626:HOH:O	2.18	0.44
1:C:1457:LEU:HD23	1:C:1466:ILE:HD11	2.00	0.44
1:D:2030:PHE:CE1	1:D:2034:GLN:CG	3.00	0.44
1:D:2126:ALA:O	1:D:2127:THR:HB	2.18	0.44
1:E:3114:LYS:HD3	6:E:6705:HOH:O	2.17	0.44
1:E:3294:GLY:HA3	1:E:3327:THR:HG21	2.00	0.44
1:E:3376:MET:HA	1:E:3376:MET:CE	2.31	0.44
1:F:4029:VAL:O	1:F:4051:ALA:HA	2.18	0.44
1:G:4319:ARG:O	1:G:4359:ASP:HB2	2.16	0.44
1:G:4337:ALA:O	1:G:4396:VAL:N	2.34	0.44
1:G:4628:ILE:HD13	1:G:4692:ALA:HB1	1.98	0.44
1:G:4652:VAL:CG2	1:G:4692:ALA:HB2	2.47	0.44
1:A:47:ILE:CB	1:A:359:MET:HG3	2.48	0.44
1:B:843:PHE:CE2	1:B:845:ARG:HD3	2.52	0.44
1:B:992:LYS:O	1:B:996:GLU:HG3	2.18	0.44
1:C:1602:SER:HB2	1:D:1821:MET:CE	2.43	0.44
1:C:1699:ARG:HD3	1:C:1701:PHE:CE2	2.53	0.44
1:F:3872:ASN:ND2	6:F:6201:HOH:O	2.50	0.44
1:F:3890:MET:HE2	1:F:3892:ALA:CA	2.47	0.44
1:G:4364:CYS:O	1:G:4387:LYS:HE3	2.17	0.44
1:A:48:CYS:SG	1:A:68:MET:HE2	2.58	0.43
1:B:738:THR:CG2	1:B:739:LEU:N	2.79	0.43
1:B:988:MET:SD	1:B:1066:ARG:NH2	2.91	0.43
1:D:2320:PHE:CE2	1:D:2322:ASN:HB3	2.53	0.43
1:E:3220:VAL:CG1	1:E:3225:ILE:HD13	2.46	0.43
1:B:637:ALA:HA	1:B:638:PRO:HD3	1.79	0.43
1:B:1061:GLN:O	1:B:1064:LEU:HB2	2.18	0.43
1:C:1679:GLU:HG3	1:C:1680:ALA:N	2.32	0.43
1:D:1914:LYS:HD3	6:D:7805:HOH:O	2.17	0.43
1:E:3113:THR:CG2	1:E:3242:SER:H	2.30	0.43
1:E:3278:ARG:O	1:E:3282:ILE:HG13	2.19	0.43
1:E:3398:ALA:HB1	1:E:3413:MET:HE1	2.00	0.43
1:G:4302:ILE:HD12	1:G:4694:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4931:VAL:HG12	1:H:4932:GLU:N	2.33	0.43
1:H:5049:ASP:O	1:H:5053:VAL:HG23	2.18	0.43
1:A:191:PHE:C	1:A:192:LEU:HD22	2.43	0.43
1:A:246:LYS:CG	1:A:248:ALA:HB3	2.46	0.43
1:A:333:MET:HE2	1:A:373:ALA:CA	2.48	0.43
1:D:1991:PHE:CD1	1:D:1991:PHE:C	2.96	0.43
1:D:2020:VAL:HG11	1:D:2025:ILE:HD11	1.99	0.43
1:E:3254:ARG:HH22	1:E:3287:ASP:CG	2.26	0.43
1:F:3842:SER:HB3	1:F:3843:PHE:CD2	2.53	0.43
1:F:3931:GLU:O	1:F:3934:ILE:HG13	2.18	0.43
1:G:4322:LEU:HD21	1:G:4327:GLY:HA2	1.99	0.43
1:G:4387:LYS:HA	1:G:4392:LEU:CD1	2.48	0.43
1:G:4552:LEU:HD12	1:G:4552:LEU:HA	1.70	0.43
1:H:4911:LEU:HD23	1:H:4911:LEU:C	2.42	0.43
1:H:5237:ALA:HB1	1:H:5268:ILE:HD13	2.00	0.43
1:A:176:ASP:HB3	1:A:179:LEU:CB	2.48	0.43
1:A:221:SER:CB	1:A:224:ASP:H	2.25	0.43
1:D:2192:LYS:HE3	1:D:2196:GLU:OE2	2.18	0.43
1:E:3253:VAL:HG12	1:E:3257:LEU:HD23	1.96	0.43
1:E:3300:ILE:HB	1:E:3301:PRO:CD	2.49	0.43
1:E:3366:LYS:HG2	5:E:3535:ATP:H1'	2.00	0.43
1:F:3717:GLU:OE2	1:F:3719:ARG:NE	2.49	0.43
1:A:132:GLU:HA	1:A:201:PHE:HA	2.01	0.43
1:B:779:LEU:HA	1:B:779:LEU:HD23	1.69	0.43
1:B:825:ILE:O	1:B:829:LYS:HG3	2.19	0.43
1:B:941:ARG:HG2	1:D:2128:GLN:NE2	2.33	0.43
1:C:1636:SER:O	1:C:1640:VAL:HG23	2.18	0.43
1:D:1874:ASN:HA	1:D:1912:ASP:HB3	2.00	0.43
1:D:2017:LEU:HB3	1:D:2018:PRO:HD2	2.00	0.43
1:E:3013:GLN:HB3	1:E:3014:THR:H	1.54	0.43
1:F:3732:GLU:HA	1:F:3800:GLY:O	2.18	0.43
1:F:4065:TYR:CD1	1:F:4065:TYR:N	2.85	0.43
1:G:4316:PRO:HG2	1:G:4443:PHE:CB	2.49	0.43
1:H:5072:ASN:ND2	1:H:5075:GLY:H	2.16	0.43
1:H:5275:ASP:OD2	1:H:5287:LEU:HD21	2.18	0.43
1:A:464:LEU:HD13	1:A:464:LEU:HA	1.68	0.43
1:B:668:MET:HE2	1:B:671:ALA:HA	2.01	0.43
1:C:1272:ARG:HE	1:C:1312:ASP:CG	2.26	0.43
1:C:1274:ASN:O	1:C:1283:HIS:NE2	2.51	0.43
1:D:1855:ARG:NH2	1:D:1885:GLU:CG	2.80	0.43
1:F:3723:ILE:HG12	1:F:3723:ILE:H	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4986:GLN:HG2	1:H:4993:VAL:CG2	2.49	0.43
1:H:5130:LEU:CD2	1:H:5133:MET:HE3	2.47	0.43
1:H:5256:HIS:O	1:H:5260:ARG:HG3	2.19	0.43
1:A:181:SER:O	1:A:197:GLU:HB2	2.18	0.43
1:C:1239:ILE:O	1:C:1582:ARG:HD3	2.19	0.43
1:C:1494:GLY:CA	1:C:1527:THR:HG21	2.48	0.43
1:D:1968:ASP:O	1:D:1971:SER:HB2	2.18	0.43
1:D:2020:VAL:HG11	1:D:2025:ILE:CD1	2.49	0.43
1:E:3144:ASP:HB3	1:E:3147:TYR:CD2	2.51	0.43
1:E:3244:ILE:HD13	1:E:3244:ILE:HA	1.78	0.43
1:E:3266:ILE:HG21	1:E:3266:ILE:HD13	1.72	0.43
1:F:3650:ILE:HB	1:F:3673:MET:HE2	2.01	0.43
1:F:3867:ILE:HA	1:F:3888:GLY:O	2.18	0.43
1:G:4640:VAL:CG1	1:G:4649:ILE:HD13	2.49	0.43
1:A:181:SER:H	1:A:198:ASN:HD21	1.66	0.43
1:B:663:MET:HE1	1:B:964:THR:CG2	2.48	0.43
1:B:770:GLY:HA2	1:B:783:GLN:HE21	1.83	0.43
1:B:928:GLN:HE21	1:D:2141:ARG:HB2	1.83	0.43
1:B:938:ARG:NH2	1:D:1978:GLY:O	2.47	0.43
1:C:1218:HIS:CD2	1:C:1231:ARG:HD3	2.53	0.43
1:C:1465:LYS:HA	1:C:1487:ASP:OD2	2.18	0.43
1:E:3351:VAL:HG13	1:E:3466:ARG:NH2	2.34	0.43
1:F:3673:MET:HE3	1:F:3673:MET:CA	2.48	0.43
1:F:3700:ASP:OD2	1:F:3703:LEU:HD13	2.19	0.43
1:F:3956:ASP:HB3	1:F:4064:LEU:O	2.18	0.43
1:F:4093:MET:HE1	1:F:4108:VAL:HG21	2.01	0.43
1:G:4532:SER:OG	1:G:4543:GLU:OE1	2.29	0.43
1:H:4941:ILE:HA	1:H:4956:LEU:O	2.18	0.43
1:B:844:ILE:HG13	1:B:868:SER:CB	2.47	0.43
1:B:845:ARG:O	1:B:846:LYS:HB3	2.17	0.43
1:C:1235:ASP:HA	6:C:7739:HOH:O	2.17	0.43
1:C:1323:ILE:CG2	1:C:1324:LYS:HG3	2.45	0.43
1:D:2094:GLY:HA3	1:D:2127:THR:HG21	2.01	0.43
1:E:3144:ASP:C	1:E:3146:ALA:H	2.26	0.43
1:E:3341:ARG:N	1:G:4528:GLN:HE21	2.00	0.43
1:F:3714:LYS:HG2	1:F:3717:GLU:OE1	2.18	0.43
1:F:3735:LYS:HG3	1:F:3797:GLU:O	2.19	0.43
1:F:3802:LEU:HD12	1:F:3802:LEU:C	2.44	0.43
1:G:4260:LEU:HD23	1:G:4260:LEU:HA	1.89	0.43
1:A:29:MET:CE	1:C:1510:LYS:HB3	2.47	0.43
1:A:145:ASN:C	1:A:147:TYR:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:HB2	6:A:7561:HOH:O	2.19	0.43
1:B:617:LEU:O	1:B:620:ALA:HB3	2.18	0.43
1:B:928:GLN:HE21	1:D:2141:ARG:CB	2.32	0.43
1:D:1880:HIS:ND1	1:D:2030:PHE:CD2	2.87	0.43
1:D:2291:LEU:HD12	1:D:2291:LEU:C	2.44	0.43
1:E:3143:LEU:HD12	1:E:3143:LEU:HA	1.55	0.43
1:F:3642:ARG:HB2	1:F:3982:ARG:CG	2.48	0.43
1:F:3857:LEU:HD23	1:F:3857:LEU:HA	1.91	0.43
1:G:4470:ILE:HG21	1:G:4476:VAL:HG22	2.01	0.43
1:H:4941:ILE:CD1	1:H:4994:THR:HG21	2.49	0.43
1:A:75:PHE:N	1:A:75:PHE:CD1	2.87	0.42
1:A:425:ALA:O	1:A:448:PRO:HD2	2.19	0.42
1:B:719:ARG:HH11	1:B:719:ARG:CG	2.32	0.42
1:B:879:PHE:CZ	1:B:883:LEU:HG	2.54	0.42
1:C:1471:GLU:HA	1:C:1496:LEU:HB2	2.00	0.42
1:D:2047:ALA:HB2	1:D:2081:GLU:HG3	2.00	0.42
1:G:4250:ILE:HB	1:G:4273:MET:CE	2.27	0.42
1:G:4259:THR:O	1:G:4263:MET:HG2	2.19	0.42
1:G:4652:VAL:HA	1:G:4671:VAL:O	2.19	0.42
1:H:4966:VAL:O	6:H:7456:HOH:O	2.21	0.42
1:H:5245:PRO:CG	1:H:5249:ILE:HD11	2.48	0.42
1:A:98:ALA:HA	1:A:104:TYR:CD1	2.54	0.42
1:A:522:ASN:HD22	1:A:522:ASN:N	2.10	0.42
1:B:615:GLN:O	1:B:615:GLN:HG2	2.18	0.42
1:D:2139:PRO:HD2	6:D:7610:HOH:O	2.20	0.42
1:E:3141:ILE:HA	1:E:3156:LEU:O	2.19	0.42
1:E:3172:LYS:HA	1:E:3182:LEU:O	2.19	0.42
1:E:3172:LYS:HA	1:E:3172:LYS:HD2	1.42	0.42
1:F:3906:PHE:O	1:F:3910:LYS:HG3	2.19	0.42
1:F:4030:LEU:HD22	1:F:4052:VAL:HB	2.00	0.42
1:G:4330:GLU:HA	1:G:4402:LEU:O	2.18	0.42
1:G:4526:ALA:O	1:G:4527:THR:HB	2.19	0.42
1:A:507:VAL:CG1	1:A:508:VAL:N	2.79	0.42
1:B:615:GLN:HA	6:B:6399:HOH:O	2.19	0.42
1:B:700:ASP:OD2	1:B:703:LEU:HB2	2.19	0.42
1:B:969:TYR:HD1	1:B:972:GLU:OE1	2.02	0.42
1:D:1986:GLN:HE21	1:D:1986:GLN:HB2	1.50	0.42
1:D:2093:ARG:HH22	1:D:2146:ASP:CG	2.27	0.42
1:D:2281:TRP:CG	1:D:2316:PRO:HD3	2.54	0.42
1:F:3622:ALA:O	1:F:3991:ARG:NH2	2.52	0.42
1:F:4081:TRP:O	1:F:4085:VAL:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4409:ASN:O	1:G:4411:PRO:HD3	2.18	0.42
1:G:4522:PRO:HD3	1:G:4665:TYR:CE2	2.54	0.42
1:G:4656:HIS:N	1:G:4656:HIS:ND1	2.65	0.42
1:H:5063:ASN:HB2	6:H:7226:HOH:O	2.18	0.42
1:D:1875:PHE:CD1	1:D:1911:LEU:HG	2.54	0.42
1:D:2083:LEU:HD21	1:D:2119:ALA:HB2	2.02	0.42
1:E:3109:VAL:N	1:E:3237:ASP:OD2	2.40	0.42
1:E:3514:TRP:N	1:E:3522:ASN:OD1	2.41	0.42
1:F:3864:ILE:CG2	1:F:3865:LYS:N	2.82	0.42
1:G:4276:SER:OG	1:G:4317:GLU:OE2	2.29	0.42
1:G:4369:VAL:HA	1:G:4384:VAL:HG12	2.00	0.42
1:H:5139:PRO:HG3	1:H:5176:MET:HG2	2.01	0.42
1:A:38:PRO:HD3	1:A:383:GLU:OE2	2.19	0.42
1:A:174:TYR:HA	1:A:180:ILE:O	2.19	0.42
1:A:246:LYS:HG3	1:A:248:ALA:CB	2.48	0.42
1:A:411:MET:HE1	1:B:1125:ARG:HA	2.00	0.42
1:A:525:ARG:HA	1:B:1122:ASN:O	2.18	0.42
1:B:838:MET:HG3	1:B:840:PHE:CE1	2.53	0.42
1:B:926:ALA:O	1:B:927:THR:HB	2.19	0.42
1:C:1347:TYR:CE2	1:C:1355:ILE:HD12	2.55	0.42
1:D:1887:ILE:N	1:D:1887:ILE:CD1	2.79	0.42
1:D:2311:LEU:HA	1:D:2323:THR:O	2.19	0.42
1:E:3131:VAL:HG12	1:E:3202:LEU:HB3	2.02	0.42
1:E:3133:LEU:HD12	1:E:3133:LEU:HA	1.71	0.42
1:E:3206:LYS:HE3	6:E:6233:HOH:O	2.19	0.42
1:H:4948:MET:HE2	1:H:4948:MET:HB2	1.63	0.42
1:C:1382:LEU:HD22	1:C:1394:THR:OG1	2.19	0.42
1:C:1447:ALA:HB2	1:C:1481:GLU:O	2.20	0.42
1:C:1534:ILE:HA	6:C:7028:HOH:O	2.20	0.42
1:C:1718:SER:C	1:C:1720:PHE:H	2.26	0.42
1:D:2089:ILE:HG22	1:D:2090:MET:N	2.35	0.42
1:E:3050:ILE:CG1	1:E:3068:MET:HE1	2.50	0.42
1:E:3115:GLY:O	1:E:3117:GLU:N	2.52	0.42
1:E:3178:GLY:HA3	1:E:3298:ILE:HD13	2.01	0.42
1:F:3764:CYS:N	6:F:7596:HOH:O	2.44	0.42
1:G:4325:GLY:N	1:G:4349:GLU:O	2.52	0.42
1:H:4923:ILE:HA	1:H:4951:CYS:O	2.19	0.42
1:H:4933:LEU:HD23	1:H:4933:LEU:HA	1.83	0.42
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.59	0.42
1:A:229:LYS:O	1:A:233:GLU:HG3	2.20	0.42
1:B:640:THR:HA	1:B:982:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ALA:O	1:B:896:LEU:HB2	2.19	0.42
1:C:1249:THR:OG1	1:C:1561:SER:HA	2.19	0.42
1:C:1320:THR:HA	1:C:1358:LEU:CD1	2.50	0.42
1:C:1503:GLU:OE1	1:C:1503:GLU:N	2.38	0.42
1:C:1703:LYS:O	1:C:1729:VAL:HB	2.20	0.42
1:D:1818:HIS:CD2	1:D:1831:ARG:HD3	2.54	0.42
1:D:2271:VAL:HG11	1:D:2291:LEU:HG	2.02	0.42
1:D:2315:ARG:CB	1:D:2316:PRO:HD2	2.47	0.42
1:E:3430:LEU:HD21	1:E:3488:ARG:HB2	2.01	0.42
1:E:3493:MET:HE1	1:E:3529:VAL:CG1	2.36	0.42
1:F:3783:GLN:HG2	1:F:3784:VAL:N	2.35	0.42
1:F:4081:TRP:O	1:F:4085:VAL:HG23	2.20	0.42
1:G:4275:PHE:HB2	1:G:4312:ASP:O	2.20	0.42
1:G:4316:PRO:HG2	1:G:4443:PHE:HB2	2.01	0.42
1:G:4516:CYS:HB3	1:G:4521:LYS:O	2.19	0.42
1:G:4726:VAL:HG23	1:H:5211:MET:SD	2.60	0.42
1:C:1250:ILE:CD1	1:C:1268:MET:HE1	2.45	0.42
1:C:1334:LYS:HE3	1:C:1334:LYS:HB3	1.72	0.42
1:C:1457:LEU:HA	1:C:1457:LEU:HD12	1.51	0.42
1:D:1922:LEU:HD12	1:D:1949:GLU:CD	2.45	0.42
1:D:2256:HIS:N	1:D:2256:HIS:CD2	2.87	0.42
1:F:3739:LEU:HG	1:F:3740:LYS:N	2.34	0.42
1:F:3774:TYR:HB3	1:F:3778:GLY:HA2	2.02	0.42
1:G:4625:ALA:O	1:G:4648:PRO:HD2	2.20	0.42
1:H:4841:ALA:HB2	1:H:5301:PHE:CE1	2.54	0.42
1:H:4991:PHE:C	1:H:4992:LEU:HG	2.44	0.42
1:H:5010:LEU:HB3	1:H:5013:ALA:CB	2.50	0.42
1:H:5193:LEU:HD21	6:H:6931:HOH:O	2.20	0.42
1:A:148:MET:HB3	1:A:148:MET:HE3	1.60	0.42
1:A:182:LEU:HD22	1:A:196:VAL:HA	2.01	0.42
1:D:1985:LYS:HD3	1:D:1985:LYS:HA	1.87	0.42
1:E:3016:GLN:HG3	6:E:6528:HOH:O	2.20	0.42
1:E:3225:ILE:CD1	1:E:3256:ILE:HD12	2.45	0.42
1:E:3292:ALA:HB1	3:E:3533:OXL:C2	2.49	0.42
1:F:3740:LYS:O	1:F:3755:ILE:HA	2.20	0.42
1:G:4680:ALA:O	1:G:4683:GLU:HB2	2.19	0.42
1:H:4974:TYR:CD2	1:H:5011:PRO:HG3	2.55	0.42
1:H:5111:MET:O	1:H:5115:ARG:HG3	2.20	0.42
1:A:163:ILE:O	1:A:163:ILE:HG12	2.19	0.42
1:A:328:GLN:HE21	1:C:1540:THR:HB	1.82	0.42
1:B:664:ILE:HG22	1:B:665:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:PRO:HG2	1:B:843:PHE:HD2	1.79	0.42
1:B:733:LEU:N	1:B:800:GLY:O	2.40	0.42
1:C:1258:GLU:O	1:C:1258:GLU:HG2	2.20	0.42
1:C:1727:VAL:HA	1:C:1728:PRO:HD3	1.85	0.42
1:D:1879:THR:H	1:D:1882:TYR:HB3	1.85	0.42
1:E:3164:CYS:O	1:E:3187:LYS:HE3	2.19	0.42
1:E:3220:VAL:CG1	1:E:3225:ILE:CD1	2.95	0.42
1:F:3964:THR:HA	1:F:3970:PRO:HB3	2.01	0.42
1:G:4221:MET:HE3	1:G:4221:MET:CA	2.49	0.42
1:G:4341:ILE:HB	1:G:4392:LEU:CB	2.46	0.42
1:G:4391:PHE:CD1	1:G:4391:PHE:C	2.98	0.42
1:G:4459:GLU:O	1:G:4459:GLU:HG3	2.20	0.42
1:G:4696:GLY:HA3	1:G:4702:PHE:CZ	2.54	0.42
1:H:5304:LYS:HA	1:H:5329:VAL:HG12	2.02	0.42
1:A:162:ASN:O	1:A:164:CYS:N	2.43	0.41
1:A:181:SER:HB3	1:A:198:ASN:ND2	2.35	0.41
1:A:294:GLY:HA3	1:A:327:THR:HG21	2.02	0.41
1:B:1035:ARG:HD3	6:B:7457:HOH:O	2.19	0.41
1:D:1967:VAL:HG13	1:D:1968:ASP:N	2.34	0.41
1:D:2020:VAL:CG1	1:D:2025:ILE:HD11	2.50	0.41
1:D:2056:ILE:HD13	1:D:2056:ILE:N	2.35	0.41
1:D:2086:SER:O	1:D:2121:LYS:NZ	2.46	0.41
1:E:3157:TRP:CH2	1:E:3159:ASP:HB3	2.55	0.41
1:F:3735:LYS:HA	1:F:3796:VAL:HG12	2.02	0.41
1:F:3830:PHE:O	1:F:3834:GLN:N	2.45	0.41
1:G:4471:GLU:HA	1:G:4496:LEU:HB2	2.01	0.41
1:G:4696:GLY:O	1:G:4701:PHE:N	2.49	0.41
1:H:5244:ARG:HH11	1:H:5244:ARG:HD3	1.57	0.41
1:A:301:PRO:HG2	1:A:304:LYS:CE	2.50	0.41
1:A:431:THR:HG23	1:A:434:GLY:HA2	1.97	0.41
1:B:747:TYR:CD1	1:B:747:TYR:N	2.89	0.41
1:C:1727:VAL:HG12	1:C:1728:PRO:N	2.34	0.41
1:D:1855:ARG:HH22	1:D:1885:GLU:HG2	1.81	0.41
1:D:2008:VAL:HG12	1:D:2010:LEU:HD21	2.00	0.41
1:E:3228:LEU:CD1	1:E:3256:ILE:HG21	2.50	0.41
1:E:3289:ILE:HG22	1:E:3290:MET:N	2.35	0.41
1:E:3493:MET:HE1	1:E:3529:VAL:HA	2.02	0.41
1:F:3774:TYR:HE2	1:F:3811:PRO:HG2	1.84	0.41
1:G:4321:GLY:CA	1:G:4357:TRP:HE3	2.32	0.41
1:G:4529:MET:O	1:G:4543:GLU:HG2	2.20	0.41
1:G:4630:LEU:CD1	1:G:4712:THR:HG22	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5076:VAL:O	1:H:5079:PHE:HB2	2.20	0.41
1:H:5276:PRO:O	1:H:5278:GLN:OE1	2.38	0.41
1:A:42:ARG:HB2	1:A:378:HIS:CE1	2.55	0.41
1:B:774:TYR:HB3	1:B:778:GLY:HA2	2.03	0.41
1:B:791:PHE:CD2	1:B:791:PHE:C	2.98	0.41
1:B:1128:PRO:O	1:B:1130:PRO:HD3	2.20	0.41
1:G:4522:PRO:HB3	1:G:4664:LEU:O	2.20	0.41
1:A:118:ILE:HG12	1:A:160:TYR:HB2	2.01	0.41
1:A:316:CYS:SG	1:A:323:VAL:HB	2.60	0.41
1:B:655:ARG:O	1:B:660:LEU:HD22	2.20	0.41
1:C:1273:MET:HG2	1:C:1287:ILE:HD11	2.01	0.41
1:C:1285:GLU:O	1:C:1288:LYS:HB3	2.20	0.41
1:C:1472:ASN:HD21	1:C:1475:GLY:H	1.61	0.41
1:E:3220:VAL:O	1:E:3220:VAL:HG12	2.12	0.41
1:F:3942:ALA:HB2	1:H:5146:ASP:OD2	2.20	0.41
1:G:4377:ASP:O	1:G:4498:ILE:HD12	2.20	0.41
1:G:4382:LEU:HA	1:G:4382:LEU:HD12	1.65	0.41
1:A:223:LYS:HA	1:A:226:GLN:CD	2.45	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.71	0.41
1:A:428:ILE:HD13	1:A:428:ILE:HG21	1.77	0.41
1:B:889:ILE:HG22	1:B:890:MET:N	2.36	0.41
1:C:1345:ASN:O	1:C:1347:TYR:N	2.53	0.41
1:D:1833:ASP:HB3	1:D:1836:SER:HB2	2.03	0.41
1:D:2254:ARG:NH1	1:D:2277:VAL:HG22	2.35	0.41
1:F:3724:LYS:O	1:F:3726:SER:N	2.47	0.41
1:G:4693:MET:HE2	1:G:4729:VAL:CG2	2.49	0.41
1:H:5081:GLU:HG2	6:H:6308:HOH:O	2.20	0.41
1:A:336:LYS:HA	1:A:337:PRO:HD3	1.92	0.41
1:B:618:HIS:ND1	1:B:631:ARG:HD3	2.36	0.41
1:B:1088:ARG:O	1:B:1091:LEU:HB3	2.20	0.41
1:B:1111:LEU:C	1:B:1112:THR:HG23	2.46	0.41
1:C:1346:ALA:C	1:C:1347:TYR:CD1	2.99	0.41
1:C:1693:MET:HG2	1:C:1730:PRO:HD2	2.01	0.41
1:D:1900:ASP:OD2	1:D:1903:LEU:HG	2.21	0.41
1:D:1958:LEU:HD23	1:D:1958:LEU:HA	1.83	0.41
1:D:2046:LYS:NZ	1:D:2049:ASP:OD1	2.35	0.41
1:D:2065:LYS:HD3	1:D:2065:LYS:HA	1.76	0.41
1:D:2239:GLN:O	1:D:2242:ARG:HG2	2.20	0.41
1:E:3048:CYS:SG	1:E:3068:MET:HB2	2.61	0.41
1:E:3334:ILE:HA	6:E:7083:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3928:GLN:NE2	1:H:5140:THR:CA	2.84	0.41
1:F:3992:LYS:O	1:F:3996:GLU:HG3	2.19	0.41
1:F:3993:LEU:HD21	1:F:4044:ARG:HG3	2.02	0.41
1:G:4248:CYS:SG	1:G:4268:MET:HB2	2.61	0.41
1:G:4323:ILE:HD13	1:G:4351:CYS:CB	2.47	0.41
1:G:4609:GLU:HB3	1:H:5221:LYS:HE3	2.03	0.41
1:G:4660:ARG:HD2	1:G:4660:ARG:HH11	1.64	0.41
1:H:4941:ILE:CD1	1:H:4994:THR:CG2	2.98	0.41
1:A:57:VAL:O	1:A:57:VAL:HG12	2.20	0.41
1:A:302:ALA:C	1:A:304:LYS:H	2.29	0.41
1:B:1127:VAL:CG1	1:B:1128:PRO:N	2.82	0.41
1:C:1303:LEU:HA	1:C:1305:ARG:HH21	1.86	0.41
1:C:1483:LEU:HA	1:C:1483:LEU:HD23	1.78	0.41
1:C:1515:ARG:O	1:C:1518:ARG:HB3	2.21	0.41
1:C:1598:ALA:CB	1:C:1613:MET:HE1	2.51	0.41
1:D:1947:TYR:CD1	1:D:1947:TYR:N	2.89	0.41
1:E:3160:TYR:HD2	1:E:3163:ILE:CA	2.33	0.41
1:G:4251:GLY:O	1:G:4255:ARG:N	2.52	0.41
1:G:4621:LYS:HE2	1:H:5209:GLU:HB3	2.03	0.41
1:H:4843:ASN:HB3	1:H:5267:GLY:N	2.36	0.41
1:A:74:ASN:HA	1:A:112:ASP:HB3	2.02	0.41
1:A:88:LYS:NZ	1:A:88:LYS:HB3	2.35	0.41
1:A:114:LYS:HG2	1:A:117:GLU:OE2	2.21	0.41
1:A:269:LYS:HE2	1:A:269:LYS:HB3	1.89	0.41
1:B:922:PRO:HB3	1:B:1064:LEU:O	2.21	0.41
1:B:1114:TRP:HD1	1:B:1115:ARG:HD2	1.86	0.41
1:C:1472:ASN:HD22	1:C:1472:ASN:C	2.29	0.41
1:D:1932:GLU:HG3	1:D:2001:PHE:CZ	2.55	0.41
1:D:2223:LEU:HD23	1:D:2223:LEU:HA	1.89	0.41
1:E:3024:THR:HB	1:G:4596:GLU:HG2	2.03	0.41
1:E:3366:LYS:HE2	1:E:3366:LYS:HB2	1.94	0.41
1:F:3866:ILE:C	1:F:3867:ILE:HD13	2.45	0.41
1:G:4721:THR:HG23	1:G:4721:THR:O	2.20	0.41
1:H:4821:MET:HE3	1:H:4821:MET:CA	2.49	0.41
1:H:5211:MET:HE3	1:H:5211:MET:HB3	1.93	0.41
1:A:50:ILE:HB	1:A:73:MET:HE3	2.00	0.41
1:A:215:VAL:HG21	1:A:217:LEU:HD12	2.01	0.41
1:A:461:GLN:O	1:A:464:LEU:HB2	2.21	0.41
1:B:651:GLY:C	1:B:655:ARG:HG3	2.46	0.41
1:B:718:ILE:CD1	1:B:810:LEU:HD22	2.51	0.41
1:B:866:ILE:HD13	1:B:866:ILE:HG21	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:LYS:H	1:B:1104:LYS:HG2	1.42	0.41
1:C:1410:LEU:HD12	1:C:1410:LEU:HA	1.81	0.41
1:C:1628:ILE:HD13	1:C:1692:ALA:CB	2.51	0.41
1:C:1647:ALA:HB1	1:C:1648:PRO:HD2	2.02	0.41
1:C:1701:PHE:HD1	1:C:1701:PHE:HA	1.52	0.41
1:D:1817:LEU:HA	1:D:1820:ALA:HB2	2.03	0.41
1:D:1819:ALA:O	1:D:1828:HIS:ND1	2.50	0.41
1:D:1855:ARG:HH22	1:D:1885:GLU:HB3	1.85	0.41
1:D:1875:PHE:CE1	1:D:1911:LEU:HG	2.56	0.41
1:D:2167:GLY:HA3	6:D:6414:HOH:O	2.20	0.41
1:D:2295:VAL:HG12	1:D:2299:ARG:HG3	2.01	0.41
1:E:3228:LEU:HD12	1:E:3256:ILE:HG21	2.03	0.41
1:E:3366:LYS:HG2	5:E:3535:ATP:C1'	2.51	0.41
1:E:3463:HIS:CE1	1:E:3470:PRO:HG2	2.56	0.41
1:F:3632:LEU:HD23	1:F:3632:LEU:HA	1.90	0.41
1:F:3731:VAL:HG12	1:F:3802:LEU:CB	2.42	0.41
1:F:3788:GLY:HA3	1:F:3791:PHE:CE1	2.55	0.41
1:G:4277:HIS:HE1	1:G:4405:LYS:O	2.04	0.41
1:G:4621:LYS:HG2	1:H:5210:ALA:HA	2.03	0.41
1:H:4960:TYR:HD2	1:H:4963:ILE:HB	1.86	0.41
1:H:5089:ILE:HG22	1:H:5090:MET:N	2.35	0.41
1:H:5199:ARG:O	1:H:5202:SER:OG	2.29	0.41
1:A:490:ASN:HA	1:A:493:MET:HG3	2.03	0.41
1:C:1428:LEU:HD23	1:C:1428:LEU:HA	1.78	0.41
1:D:1986:GLN:O	1:D:1992:LEU:HA	2.21	0.41
1:F:4127:VAL:HA	1:F:4128:PRO:HD3	1.68	0.41
1:G:4275:PHE:HZ	1:G:4430:PHE:CE2	2.39	0.41
1:G:4302:ILE:HG23	1:G:4695:VAL:HA	2.03	0.41
1:G:4305:ARG:HA	1:G:4306:PRO:HD2	2.00	0.41
1:G:4429:LYS:HE2	1:G:4456:ILE:O	2.20	0.41
1:H:5193:LEU:HD21	1:H:5244:ARG:HG3	2.03	0.41
1:A:77:HIS:NE2	5:A:535:ATP:H2'	2.37	0.40
1:A:306:PHE:CD1	1:A:306:PHE:C	2.99	0.40
1:B:838:MET:SD	1:B:1064:LEU:HD21	2.62	0.40
1:C:1720:PHE:CZ	1:C:1722:ASN:HB3	2.56	0.40
1:D:2093:ARG:NH1	1:D:2127:THR:O	2.55	0.40
1:E:3119:ARG:O	1:E:3158:LEU:HD12	2.21	0.40
1:E:3142:THR:CG2	1:E:3144:ASP:CB	3.00	0.40
1:F:3733:LEU:HB3	1:F:3796:VAL:HG21	2.03	0.40
1:H:4988:GLY:HA3	1:H:4991:PHE:CZ	2.55	0.40
1:A:146:ALA:C	1:A:147:TYR:CD1	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:O	1:A:262:LYS:HG2	2.22	0.40
1:A:293:ARG:HA	1:A:296:LEU:HB3	2.03	0.40
1:A:349:ASN:HD21	1:C:1510:LYS:NZ	2.20	0.40
1:A:493:MET:CE	1:A:529:VAL:HG13	2.51	0.40
1:B:700:ASP:HA	1:B:701:PRO:HD2	1.89	0.40
1:B:845:ARG:O	1:B:878:ARG:HD3	2.21	0.40
1:B:851:HIS:CE1	1:B:885:ALA:HB1	2.56	0.40
1:C:1250:ILE:CG2	1:C:1286:THR:CG2	2.99	0.40
1:C:1261:LYS:HG3	1:C:1293:ALA:HB1	2.04	0.40
1:D:1873:MET:HG2	1:D:1887:ILE:HD11	2.02	0.40
1:E:3100:ASP:C	1:E:3102:ILE:N	2.79	0.40
1:E:3398:ALA:CB	1:E:3413:MET:CE	3.00	0.40
1:G:4212:ILE:HD12	1:G:4235:ASP:HB2	2.04	0.40
1:G:4377:ASP:HA	1:G:4498:ILE:CD1	2.51	0.40
1:A:106:PRO:C	1:A:107:VAL:HG23	2.46	0.40
1:B:934:ILE:HG23	1:B:967:GLY:CA	2.50	0.40
1:C:1276:SER:CB	1:C:1319:ARG:NH1	2.84	0.40
1:C:1300:ASP:OD2	1:C:1303:LEU:HG	2.21	0.40
1:C:1378:GLY:HA3	1:C:1498:ILE:CG1	2.49	0.40
1:C:1445:ARG:HB3	1:C:1474:GLU:OE1	2.22	0.40
1:C:1569:TYR:HB3	1:C:1572:GLU:HB2	2.03	0.40
1:D:1873:MET:CE	1:D:1886:THR:HG22	2.45	0.40
1:D:2027:ASP:O	1:D:2030:PHE:HB3	2.21	0.40
1:D:2188:MET:CE	1:D:2266:ARG:NH2	2.85	0.40
1:G:4276:SER:HB3	1:G:4319:ARG:HH21	1.86	0.40
1:G:4483:LEU:O	1:G:4483:LEU:HD12	2.21	0.40
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.95	0.40
1:A:238:MET:CE	1:A:464:LEU:CD2	2.99	0.40
1:B:716:PRO:HG2	1:B:843:PHE:CG	2.56	0.40
1:B:751:CYS:HB3	1:B:756:LEU:HD23	2.03	0.40
1:B:910:LYS:HB3	1:D:1829:MET:HG2	2.04	0.40
1:B:922:PRO:HG3	1:B:1065:TYR:CE2	2.55	0.40
1:C:1374:TYR:HE2	1:C:1411:PRO:HG2	1.86	0.40
1:D:2041:ALA:O	1:D:2044:ILE:HG12	2.22	0.40
1:F:3928:GLN:NE2	1:H:5141:ARG:HG2	2.36	0.40
1:H:4848:CYS:SG	1:H:4868:MET:HB2	2.61	0.40
1:H:5283:GLU:HA	1:H:5286:ASP:HB2	2.04	0.40
1:A:328:GLN:HE21	1:C:1541:ARG:N	2.07	0.40
1:C:1215:GLN:CG	1:C:1239:ILE:HG23	2.51	0.40
1:C:1387:LYS:CB	1:C:1392:LEU:CD1	3.00	0.40
1:C:1677:VAL:CG1	1:C:1678:GLN:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2130:LEU:HD23	1:D:2143:GLU:HB3	2.04	0.40
1:E:3527:VAL:HA	1:E:3528:PRO:HD3	1.82	0.40
1:F:3655:ARG:CZ	1:F:3682:TYR:CE2	3.04	0.40
1:F:3675:PHE:CE1	1:F:3683:HIS:CD2	3.09	0.40
1:F:3719:ARG:H	1:F:3759:ASP:HB2	1.87	0.40
1:F:3741:ILE:HA	1:F:3756:LEU:O	2.22	0.40
1:G:4327:GLY:HA2	1:G:4404:SER:OG	2.22	0.40

All (24) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3149:GLU:OE1	1:H:4934:LYS:CE[3_655]	0.67	1.53
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.03	1.17
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.23	0.97
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.38	0.82
1:E:3149:GLU:OE1	1:H:4934:LYS:CD[3_655]	1.43	0.77
1:E:3081:GLU:OE1	1:H:4924:LYS:NZ[3_655]	1.49	0.71
1:E:3149:GLU:OE2	1:H:4934:LYS:NZ[3_655]	1.51	0.69
1:D:1924:LYS:CE	1:H:4858:GLU:OE1[1_455]	1.56	0.64
1:E:3149:GLU:OE1	1:H:4934:LYS:NZ[3_655]	1.56	0.64
1:C:1387:LYS:O	1:H:4987:LYS:CB[3_645]	1.66	0.54
1:D:1948:MET:CE	1:F:3765:LYS:NZ[4_465]	1.67	0.53
1:D:1945:ASN:OD1	1:F:3816:ASP:OD2[4_465]	1.85	0.35
1:E:3149:GLU:OE2	1:H:4934:LYS:CE[3_655]	1.85	0.35
1:E:3124:LYS:C	6:H:6911:HOH:O[3_655]	1.86	0.34
1:C:1386:GLN:CB	1:H:4989:PRO:CD[3_645]	1.87	0.33
1:E:3124:LYS:O	6:H:6911:HOH:O[3_655]	1.88	0.32
1:D:1924:LYS:NZ	1:H:4858:GLU:CD[1_455]	2.00	0.20
1:C:1389:PRO:CG	1:H:4985:LYS:O[3_645]	2.02	0.18
1:E:3149:GLU:CG	1:H:4934:LYS:NZ[3_655]	2.03	0.17
1:A:277:ARG:NH1	1:G:4425:ILE:CD1[4_465]	2.07	0.13
1:A:277:ARG:CZ	1:G:4425:ILE:CD1[4_465]	2.10	0.10
1:C:1387:LYS:O	1:H:4987:LYS:CA[3_645]	2.11	0.09
1:E:3081:GLU:OE1	1:H:4924:LYS:CE[3_655]	2.17	0.03
1:C:1385:LYS:O	1:H:4989:PRO:CG[3_645]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/530 (98%)	476 (92%)	36 (7%)	5 (1%)	12	12
1	B	517/530 (98%)	485 (94%)	30 (6%)	2 (0%)	30	34
1	C	517/530 (98%)	464 (90%)	42 (8%)	11 (2%)	5	4
1	D	517/530 (98%)	487 (94%)	27 (5%)	3 (1%)	21	24
1	E	517/530 (98%)	484 (94%)	26 (5%)	7 (1%)	9	7
1	F	517/530 (98%)	486 (94%)	27 (5%)	4 (1%)	16	17
1	G	517/530 (98%)	487 (94%)	27 (5%)	3 (1%)	21	24
1	H	517/530 (98%)	485 (94%)	27 (5%)	5 (1%)	12	12
All	All	4136/4240 (98%)	3854 (93%)	242 (6%)	40 (1%)	12	12

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1337	ALA
1	C	1533	MET
1	F	3729	ALA
1	F	3789	PRO
1	G	4389	PRO
1	H	4924	LYS
1	A	221	SER
1	C	1532	SER
1	D	2058	GLY
1	E	3013	GLN
1	E	3164	CYS
1	E	3506	ASP
1	F	3730	GLU
1	A	171	SER
1	C	1320	THR
1	G	4345	ASN
1	A	327	THR

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Mol	Chain	Res	Type
1	B	927	THR
1	C	1346	ALA
1	E	3145	ASN
1	F	3927	THR
1	A	390	HIS
1	C	1389	PRO
1	C	1527	THR
1	D	2127	THR
1	G	4458	GLY
1	H	5092	ALA
1	A	260	LYS
1	C	1371	SER
1	D	1963	ILE
1	E	3211	PRO
1	E	3327	THR
1	H	4901	PRO
1	H	5127	THR
1	H	5317	GLY
1	B	1128	PRO
1	C	1728	PRO
1	E	3258	GLY
1	C	1363	ILE
1	C	1410	LEU

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	426/434 (98%)	342 (80%)	84 (20%)	1	1
1	B	426/434 (98%)	369 (87%)	57 (13%)	4	3
1	C	426/434 (98%)	341 (80%)	85 (20%)	1	1
1	D	426/434 (98%)	375 (88%)	51 (12%)	5	4
1	E	426/434 (98%)	361 (85%)	65 (15%)	3	2
1	F	426/434 (98%)	358 (84%)	68 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	426/434 (98%)	358 (84%)	68 (16%)	2	2
1	H	426/434 (98%)	377 (88%)	49 (12%)	5	5
All	All	3408/3472 (98%)	2881 (84%)	527 (16%)	2	2

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	15	GLN
1	A	50	ILE
1	A	56	SER
1	A	60	LEU
1	A	63	MET
1	A	68	MET
1	A	70	VAL
1	A	79	THR
1	A	86	THR
1	A	88	LYS
1	A	91	ARG
1	A	92	THR
1	A	96	SER
1	A	99	SER
1	A	113	THR
1	A	120	THR
1	A	130	GLU
1	A	131	VAL
1	A	133	LEU
1	A	134	LYS
1	A	138	THR
1	A	148	MET
1	A	153	GLU
1	A	156	LEU
1	A	158	LEU
1	A	162	ASN
1	A	164	CYS
1	A	166	VAL
1	A	167	VAL
1	A	168	ASP
1	A	172	LYS
1	A	173	VAL
1	A	175	VAL

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Mol	Chain	Res	Type
1	A	180	ILE
1	A	185	LYS
1	A	192	LEU
1	A	194	THR
1	A	202	LEU
1	A	206	LYS
1	A	210	LEU
1	A	215	VAL
1	A	223	LYS
1	A	236	VAL
1	A	238	MET
1	A	245	ARG
1	A	246	LYS
1	A	257	LEU
1	A	260	LYS
1	A	264	ILE
1	A	267	ILE
1	A	271	GLU
1	A	278	ARG
1	A	283	LEU
1	A	289	ILE
1	A	293	ARG
1	A	311	MET
1	A	330	LEU
1	A	334	ILE
1	A	358	ILE
1	A	375	ARG
1	A	376	MET
1	A	380	ILE
1	A	382	ARG
1	A	397	LEU
1	A	400	SER
1	A	405	THR
1	A	407	LEU
1	A	411	MET
1	A	423	LEU
1	A	435	ARG
1	A	456	HIS
1	A	464	LEU
1	A	471	VAL
1	A	478	GLN
1	A	479	GLU

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Mol	Chain	Res	Type
1	A	493	MET
1	A	497	LYS
1	A	499	ARG
1	A	508	VAL
1	A	518	SER
1	A	521	THR
1	A	522	ASN
1	A	527	VAL
1	B	615	GLN
1	B	621	MET
1	B	640	THR
1	B	654	SER
1	B	660	LEU
1	B	661	LYS
1	B	664	ILE
1	B	673	MET
1	B	676	SER
1	B	681	GLU
1	B	687	ILE
1	B	702	ILE
1	B	703	LEU
1	B	719	ARG
1	B	748	MET
1	B	756	LEU
1	B	781	SER
1	B	782	LEU
1	B	785	LYS
1	B	786	GLN
1	B	787	LYS
1	B	795	GLU
1	B	798	ASN
1	B	805	LYS
1	B	810	LEU
1	B	817	LEU
1	B	820	VAL
1	B	822	GLU
1	B	829	LYS
1	B	833	GLU
1	B	839	VAL
1	B	846	LYS
1	B	867	ILE
1	B	883	LEU

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Mol	Chain	Res	Type
1	B	886	SER
1	B	921	LYS
1	B	952	LEU
1	B	1027	LEU
1	B	1028	ILE
1	B	1035	ARG
1	B	1039	GLN
1	B	1042	ARG
1	B	1046	ARG
1	B	1058	THR
1	B	1064	LEU
1	B	1066	ARG
1	B	1078	GLN
1	B	1079	GLU
1	B	1086	ASP
1	B	1090	ASN
1	B	1093	MET
1	B	1099	ARG
1	B	1103	LYS
1	B	1104	LYS
1	B	1107	VAL
1	B	1108	VAL
1	B	1125	ARG
1	C	1212	ILE
1	C	1214	THR
1	C	1229	MET
1	C	1240	THR
1	C	1250	ILE
1	C	1254	SER
1	C	1257	VAL
1	C	1273	MET
1	C	1279	THR
1	C	1281	GLU
1	C	1288	LYS
1	C	1292	THR
1	C	1295	GLU
1	C	1302	ILE
1	C	1305	ARG
1	C	1313	THR
1	C	1319	ARG
1	C	1323	ILE
1	C	1328	THR

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Mol	Chain	Res	Type
1	C	1331	VAL
1	C	1334	LYS
1	C	1335	LYS
1	C	1342	THR
1	C	1348	MET
1	C	1355	ILE
1	C	1358	LEU
1	C	1359	ASP
1	C	1363	ILE
1	C	1372	LYS
1	C	1380	ILE
1	C	1390	ASP
1	C	1394	THR
1	C	1395	GLU
1	C	1404	SER
1	C	1405	LYS
1	C	1406	LYS
1	C	1410	LEU
1	C	1415	VAL
1	C	1422	GLU
1	C	1442	SER
1	C	1446	LYS
1	C	1454	ARG
1	C	1456	ILE
1	C	1457	LEU
1	C	1459	GLU
1	C	1462	LYS
1	C	1469	LYS
1	C	1472	ASN
1	C	1477	ARG
1	C	1483	LEU
1	C	1484	GLU
1	C	1486	SER
1	C	1490	MET
1	C	1491	VAL
1	C	1493	ARG
1	C	1498	ILE
1	C	1518	ARG
1	C	1529	MET
1	C	1530	LEU
1	C	1532	SER
1	C	1538	ARG

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Mol	Chain	Res	Type
1	C	1558	ILE
1	C	1566	LYS
1	C	1582	ARG
1	C	1583	GLU
1	C	1592	LYS
1	C	1597	LEU
1	C	1599	ARG
1	C	1600	SER
1	C	1607	LEU
1	C	1633	SER
1	C	1642	ARG
1	C	1650	ILE
1	C	1664	LEU
1	C	1666	ARG
1	C	1675	ASP
1	C	1678	GLN
1	C	1679	GLU
1	C	1685	VAL
1	C	1686	ASP
1	C	1687	LEU
1	C	1693	MET
1	C	1708	VAL
1	C	1718	SER
1	C	1723	THR
1	D	1812	ILE
1	D	1814	THR
1	D	1824	THR
1	D	1829	MET
1	D	1848	CYS
1	D	1856	SER
1	D	1860	LEU
1	D	1885	GLU
1	D	1887	ILE
1	D	1899	SER
1	D	1902	ILE
1	D	1924	LYS
1	D	1930	GLU
1	D	1931	VAL
1	D	1938	THR
1	D	1942	THR
1	D	1945	ASN
1	D	1948	MET

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Mol	Chain	Res	Type
1	D	1955	ILE
1	D	1962	ASN
1	D	1966	VAL
1	D	1967	VAL
1	D	1972	LYS
1	D	1985	LYS
1	D	1986	GLN
1	D	1990	ASP
1	D	2046	LYS
1	D	2056	ILE
1	D	2059	GLU
1	D	2068	SER
1	D	2077	ARG
1	D	2081	GLU
1	D	2093	ARG
1	D	2099	GLU
1	D	2113	ILE
1	D	2141	ARG
1	D	2145	SER
1	D	2166	LYS
1	D	2175	ARG
1	D	2205	THR
1	D	2209	GLU
1	D	2213	MET
1	D	2246	ARG
1	D	2266	ARG
1	D	2279	GLU
1	D	2283	GLU
1	D	2288	ARG
1	D	2290	ASN
1	D	2293	MET
1	D	2303	LYS
1	D	2308	VAL
1	E	3012	ILE
1	E	3013	GLN
1	E	3014	THR
1	E	3016	GLN
1	E	3021	MET
1	E	3029	MET
1	E	3034	ILE
1	E	3054	SER
1	E	3055	ARG

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Mol	Chain	Res	Type
1	E	3056	SER
1	E	3066	SER
1	E	3068	MET
1	E	3081	GLU
1	E	3099	SER
1	E	3102	ILE
1	E	3105	ARG
1	E	3113	THR
1	E	3124	LYS
1	E	3131	VAL
1	E	3133	LEU
1	E	3143	LEU
1	E	3145	ASN
1	E	3148	MET
1	E	3155	ILE
1	E	3156	LEU
1	E	3158	LEU
1	E	3162	ASN
1	E	3164	CYS
1	E	3165	LYS
1	E	3166	VAL
1	E	3167	VAL
1	E	3172	LYS
1	E	3192	LEU
1	E	3194	THR
1	E	3222	GLU
1	E	3246	LYS
1	E	3254	ARG
1	E	3257	LEU
1	E	3259	GLU
1	E	3265	LYS
1	E	3267	ILE
1	E	3271	GLU
1	E	3274	GLU
1	E	3283	LEU
1	E	3286	SER
1	E	3315	ARG
1	E	3318	ARG
1	E	3330	LEU
1	E	3335	LYS
1	E	3336	LYS
1	E	3338	ARG

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Mol	Chain	Res	Type
1	E	3366	LYS
1	E	3379	LEU
1	E	3407	LEU
1	E	3432	GLU
1	E	3435	ARG
1	E	3442	ARG
1	E	3446	ARG
1	E	3458	THR
1	E	3466	ARG
1	E	3479	GLU
1	E	3483	GLU
1	E	3504	LYS
1	E	3526	VAL
1	E	3527	VAL
1	F	3612	ILE
1	F	3613	GLN
1	F	3615	GLN
1	F	3623	ASP
1	F	3624	THR
1	F	3640	THR
1	F	3655	ARG
1	F	3666	SER
1	F	3673	MET
1	F	3679	THR
1	F	3687	ILE
1	F	3696	SER
1	F	3705	ARG
1	F	3713	THR
1	F	3714	LYS
1	F	3723	ILE
1	F	3726	SER
1	F	3728	THR
1	F	3731	VAL
1	F	3732	GLU
1	F	3742	THR
1	F	3743	LEU
1	F	3753	GLU
1	F	3755	ILE
1	F	3759	ASP
1	F	3762	ASN
1	F	3765	LYS
1	F	3767	VAL

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Mol	Chain	Res	Type
1	F	3769	VAL
1	F	3772	LYS
1	F	3780	ILE
1	F	3782	LEU
1	F	3786	GLN
1	F	3787	LYS
1	F	3792	LEU
1	F	3804	SER
1	F	3810	LEU
1	F	3821	SER
1	F	3823	LYS
1	F	3832	VAL
1	F	3845	ARG
1	F	3846	LYS
1	F	3855	LYS
1	F	3856	ILE
1	F	3862	LYS
1	F	3865	LYS
1	F	3867	ILE
1	F	3872	ASN
1	F	3878	ARG
1	F	3884	GLU
1	F	3886	SER
1	F	3893	ARG
1	F	3918	ARG
1	F	3934	ILE
1	F	3935	LYS
1	F	3945	SER
1	F	3966	LYS
1	F	3992	LYS
1	F	4002	SER
1	F	4015	SER
1	F	4021	LYS
1	F	4032	GLU
1	F	4066	ARG
1	F	4079	GLU
1	F	4093	MET
1	F	4107	VAL
1	F	4111	LEU
1	F	4118	SER
1	G	4212	ILE
1	G	4213	GLN

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Mol	Chain	Res	Type
1	G	4215	GLN
1	G	4221	MET
1	G	4240	THR
1	G	4254	SER
1	G	4255	ARG
1	G	4258	GLU
1	G	4265	LYS
1	G	4268	MET
1	G	4296	SER
1	G	4303	LEU
1	G	4313	THR
1	G	4320	THR
1	G	4330	GLU
1	G	4338	THR
1	G	4343	LEU
1	G	4353	GLU
1	G	4355	ILE
1	G	4358	LEU
1	G	4359	ASP
1	G	4361	LYS
1	G	4367	VAL
1	G	4371	SER
1	G	4372	LYS
1	G	4375	VAL
1	G	4380	ILE
1	G	4382	LEU
1	G	4383	GLN
1	G	4386	GLN
1	G	4390	ASP
1	G	4392	LEU
1	G	4395	GLU
1	G	4402	LEU
1	G	4404	SER
1	G	4417	LEU
1	G	4422	GLU
1	G	4423	LYS
1	G	4427	ASP
1	G	4442	SER
1	G	4449	ASP
1	G	4471	GLU
1	G	4486	SER
1	G	4493	ARG

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Mol	Chain	Res	Type
1	G	4498	ILE
1	G	4500	ILE
1	G	4517	ASN
1	G	4534	ILE
1	G	4545	SER
1	G	4552	LEU
1	G	4558	ILE
1	G	4576	MET
1	G	4592	LYS
1	G	4597	LEU
1	G	4599	ARG
1	G	4600	SER
1	G	4639	GLN
1	G	4649	ILE
1	G	4656	HIS
1	G	4664	LEU
1	G	4666	ARG
1	G	4677	VAL
1	G	4690	ASN
1	G	4693	MET
1	G	4703	LYS
1	G	4715	ARG
1	G	4718	SER
1	G	4720	PHE
1	H	4812	ILE
1	H	4814	THR
1	H	4827	GLU
1	H	4829	MET
1	H	4844	THR
1	H	4855	ARG
1	H	4863	MET
1	H	4866	SER
1	H	4879	THR
1	H	4887	ILE
1	H	4899	SER
1	H	4922	LEU
1	H	4923	ILE
1	H	4926	SER
1	H	4931	VAL
1	H	4932	GLU
1	H	4934	LYS
1	H	4935	LYS

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Mol	Chain	Res	Type
1	H	4942	THR
1	H	4950	LYS
1	H	4955	ILE
1	H	4969	VAL
1	H	4983	GLN
1	H	4986	GLN
1	H	4992	LEU
1	H	5002	LEU
1	H	5010	LEU
1	H	5025	ILE
1	H	5046	LYS
1	H	5060	LYS
1	H	5067	ILE
1	H	5071	GLU
1	H	5072	ASN
1	H	5112	ILE
1	H	5118	ARG
1	H	5134	ILE
1	H	5182	ARG
1	H	5206	ASP
1	H	5207	LEU
1	H	5235	ARG
1	H	5264	LEU
1	H	5278	GLN
1	H	5286	ASP
1	H	5297	LYS
1	H	5303	LYS
1	H	5304	LYS
1	H	5308	VAL
1	H	5318	SER
1	H	5321	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	89	ASN
1	A	154	ASN
1	A	162	ASN
1	A	198	ASN
1	A	209	ASN
1	A	263	ASN

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Mol	Chain	Res	Type
1	A	273	HIS
1	A	328	GLN
1	A	349	ASN
1	A	377	GLN
1	A	438	HIS
1	A	456	HIS
1	A	457	GLN
1	A	494	ASN
1	A	522	ASN
1	B	643	ASN
1	B	689	ASN
1	B	745	ASN
1	B	762	ASN
1	B	783	GLN
1	B	798	ASN
1	B	826	GLN
1	B	834	GLN
1	B	851	HIS
1	B	863	ASN
1	B	928	GLN
1	B	949	ASN
1	B	977	GLN
1	B	990	HIS
1	B	1003	HIS
1	B	1056	HIS
1	B	1063	HIS
1	B	1078	GLN
1	C	1218	HIS
1	C	1243	ASN
1	C	1345	ASN
1	C	1354	ASN
1	C	1362	ASN
1	C	1409	ASN
1	C	1426	GLN
1	C	1451	HIS
1	C	1463	ASN
1	C	1472	ASN
1	C	1509	GLN
1	C	1528	GLN
1	C	1549	ASN
1	C	1577	GLN
1	C	1590	HIS

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Mol	Chain	Res	Type
1	C	1656	HIS
1	C	1678	GLN
1	D	1815	GLN
1	D	1818	HIS
1	D	1843	ASN
1	D	1889	ASN
1	D	1945	ASN
1	D	1986	GLN
1	D	1998	ASN
1	D	2034	GLN
1	D	2063	ASN
1	D	2073	HIS
1	D	2128	GLN
1	D	2149	ASN
1	D	2177	GLN
1	D	2190	HIS
1	D	2257	GLN
1	D	2294	ASN
1	E	3018	HIS
1	E	3043	ASN
1	E	3080	HIS
1	E	3089	ASN
1	E	3145	ASN
1	E	3162	ASN
1	E	3186	GLN
1	E	3198	ASN
1	E	3263	ASN
1	E	3328	GLN
1	E	3349	ASN
1	E	3390	HIS
1	E	3457	GLN
1	E	3463	HIS
1	F	3613	GLN
1	F	3615	GLN
1	F	3683	HIS
1	F	3689	ASN
1	F	3754	ASN
1	F	3786	GLN
1	F	3798	ASN
1	F	3809	ASN
1	F	3826	GLN
1	F	3851	HIS

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Mol	Chain	Res	Type
1	F	3872	ASN
1	F	3873	HIS
1	F	3928	GLN
1	F	3949	ASN
1	F	3977	GLN
1	F	4063	HIS
1	F	4078	GLN
1	F	4090	ASN
1	G	4215	GLN
1	G	4216	GLN
1	G	4289	ASN
1	G	4345	ASN
1	G	4383	GLN
1	G	4398	ASN
1	G	4409	ASN
1	G	4434	GLN
1	G	4463	ASN
1	G	4509	GLN
1	G	4528	GLN
1	G	4549	ASN
1	G	4577	GLN
1	G	4694	ASN
1	H	4889	ASN
1	H	4986	GLN
1	H	5063	ASN
1	H	5072	ASN
1	H	5128	GLN
1	H	5149	ASN
1	H	5177	GLN
1	H	5256	HIS
1	H	5257	GLN
1	H	5261	GLN
1	H	5263	HIS
1	H	5294	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 22 are monoatomic - leaving 14 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$
5	ATP	F	4135	2,4	32,33,33	2.83	10 (31%)	48,52,52	1.12	5 (10%)
3	OXL	C	1733	4	5,5,5	1.70	2 (40%)	6,6,6	1.99	4 (66%)
3	OXL	D	2333	4	5,5,5	1.65	3 (60%)	6,6,6	2.26	4 (66%)
3	OXL	F	4133	4	5,5,5	1.36	0	6,6,6	1.70	2 (33%)
5	ATP	G	4735	2,4	32,33,33	3.00	9 (28%)	48,52,52	0.92	1 (2%)
3	OXL	G	4733	4	5,5,5	1.38	0	6,6,6	1.71	2 (33%)
3	OXL	H	5333	4	5,5,5	1.68	2 (40%)	6,6,6	2.09	4 (66%)
5	ATP	A	535	2,4	32,33,33	2.14	10 (31%)	48,52,52	1.48	3 (6%)
3	OXL	E	3533	4	5,5,5	1.37	0	6,6,6	1.70	2 (33%)
5	ATP	E	3535	2,4	32,33,33	2.29	7 (21%)	48,52,52	0.86	2 (4%)
3	OXL	A	533	4	5,5,5	1.81	2 (40%)	6,6,6	0.92	0
5	ATP	C	1735	4	32,33,33	2.33	10 (31%)	48,52,52	1.25	6 (12%)
3	OXL	B	1133	4	5,5,5	1.74	2 (40%)	6,6,6	2.09	3 (50%)
5	ATP	D	2335	2,4	32,33,33	2.34	9 (28%)	48,52,52	1.32	7 (14%)

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
5	ATP	F	4135	2,4	-	0/22/38/38	0/3/3/3
3	OXL	C	1733	4	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	D	2333	4	-	4/4/4/4	-
3	OXL	F	4133	4	-	4/4/4/4	-
5	ATP	G	4735	2,4	-	4/22/38/38	0/3/3/3
3	OXL	G	4733	4	-	4/4/4/4	-
3	OXL	H	5333	4	-	4/4/4/4	-
5	ATP	A	535	2,4	-	3/22/38/38	0/3/3/3
3	OXL	E	3533	4	-	4/4/4/4	-
5	ATP	E	3535	2,4	-	4/22/38/38	0/3/3/3
3	OXL	A	533	4	-	4/4/4/4	-
5	ATP	C	1735	4	-	3/22/38/38	0/3/3/3
3	OXL	B	1133	4	-	4/4/4/4	-
5	ATP	D	2335	2,4	-	4/22/38/38	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	4735	ATP	PB-O3B	-12.93	1.45	1.59
5	F	4135	ATP	PB-O3B	-11.19	1.47	1.59
5	E	3535	ATP	PB-O3B	-8.98	1.49	1.59
5	C	1735	ATP	PB-O3B	-8.02	1.50	1.59
5	D	2335	ATP	PB-O3B	-7.89	1.51	1.59
5	G	4735	ATP	PA-O3A	-6.74	1.52	1.59
5	F	4135	ATP	PA-O3A	-5.71	1.53	1.59
5	A	535	ATP	PB-O3B	-5.39	1.53	1.59
5	A	535	ATP	PB-O3A	5.05	1.65	1.59
5	E	3535	ATP	PG-O3G	-5.05	1.36	1.54
5	D	2335	ATP	PG-O3G	-4.96	1.36	1.54
5	C	1735	ATP	PB-O3A	4.93	1.64	1.59
5	D	2335	ATP	PA-O3A	-4.44	1.54	1.59
5	C	1735	ATP	PG-O3G	-4.28	1.38	1.54
5	G	4735	ATP	PG-O3G	-4.20	1.39	1.54
5	F	4135	ATP	C2-N1	4.20	1.41	1.33
5	A	535	ATP	PG-O3G	-4.05	1.39	1.54
5	A	535	ATP	C8-N7	3.97	1.39	1.31
5	F	4135	ATP	PA-O5'	3.96	1.74	1.59
5	E	3535	ATP	PA-O3A	-3.64	1.55	1.59
5	D	2335	ATP	PB-O3A	3.49	1.63	1.59
5	D	2335	ATP	C2-N1	3.35	1.39	1.33
5	A	535	ATP	PA-O3A	-3.33	1.55	1.59
5	F	4135	ATP	PG-O3G	-3.28	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1735	ATP	PA-O3A	-3.24	1.56	1.59
5	C	1735	ATP	PG-O1G	-3.14	1.40	1.50
5	A	535	ATP	PG-O2G	-2.95	1.43	1.54
5	C	1735	ATP	PG-O2G	-2.94	1.43	1.54
5	A	535	ATP	C2-N1	2.93	1.39	1.33
5	E	3535	ATP	PG-O2G	-2.81	1.44	1.54
5	F	4135	ATP	C6-N6	2.81	1.41	1.34
5	D	2335	ATP	PA-O5'	2.79	1.70	1.59
3	A	533	OXL	O3-C1	-2.75	1.23	1.30
5	C	1735	ATP	PA-O5'	2.71	1.70	1.59
5	F	4135	ATP	C2-N3	-2.66	1.29	1.33
3	B	1133	OXL	O4-C2	-2.65	1.23	1.30
5	D	2335	ATP	PG-O2G	-2.62	1.45	1.54
3	H	5333	OXL	O3-C1	-2.61	1.23	1.30
3	A	533	OXL	O4-C2	-2.58	1.23	1.30
5	E	3535	ATP	C2-N3	-2.54	1.29	1.33
5	D	2335	ATP	PG-O1G	-2.50	1.42	1.50
5	G	4735	ATP	O4'-C1'	-2.48	1.36	1.42
5	E	3535	ATP	PA-O5'	2.45	1.69	1.59
5	A	535	ATP	PA-O5'	2.42	1.68	1.59
5	G	4735	ATP	PB-O3A	-2.41	1.56	1.59
5	E	3535	ATP	C2-N1	2.41	1.38	1.33
5	F	4135	ATP	C1'-N9	2.39	1.52	1.46
5	F	4135	ATP	C5-C4	2.36	1.43	1.39
5	G	4735	ATP	C1'-N9	-2.29	1.40	1.46
5	C	1735	ATP	C8-N7	2.29	1.36	1.31
5	A	535	ATP	PG-O1G	-2.27	1.43	1.50
5	F	4135	ATP	PB-O3A	2.22	1.61	1.59
3	D	2333	OXL	O1-C1	2.20	1.28	1.22
3	H	5333	OXL	O4-C2	-2.19	1.24	1.30
3	B	1133	OXL	O3-C1	-2.19	1.24	1.30
3	C	1733	OXL	O3-C1	-2.19	1.24	1.30
5	C	1735	ATP	C2-N3	-2.18	1.30	1.33
3	D	2333	OXL	O3-C1	-2.17	1.24	1.30
3	C	1733	OXL	O4-C2	-2.17	1.24	1.30
5	D	2335	ATP	C4-N3	2.16	1.38	1.34
5	G	4735	ATP	PA-O2A	-2.14	1.45	1.55
5	C	1735	ATP	O4'-C1'	-2.06	1.37	1.42
5	G	4735	ATP	C2-N1	2.04	1.37	1.33
5	A	535	ATP	C2-N3	-2.04	1.30	1.33
5	G	4735	ATP	PG-O1G	-2.02	1.44	1.50
3	D	2333	OXL	O4-C2	-2.00	1.25	1.30

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	535	ATP	O2B-PB-O3B	7.44	127.39	107.27
5	D	2335	ATP	O2G-PG-O1G	4.37	127.86	110.83
5	A	535	ATP	O2G-PG-O1G	3.71	125.28	110.83
5	C	1735	ATP	O2G-PG-O1G	3.64	125.02	110.83
5	D	2335	ATP	O2B-PB-O3B	-3.58	97.60	107.27
5	D	2335	ATP	O2A-PA-O3A	3.36	116.36	107.27
5	D	2335	ATP	O3G-PG-O3B	-3.36	93.36	104.64
3	D	2333	OXL	O4-C2-C1	3.13	118.91	112.83
5	A	535	ATP	O3G-PG-O3B	-3.05	94.42	104.64
3	B	1133	OXL	O3-C1-C2	3.03	118.71	112.83
5	C	1735	ATP	O3G-PG-O3B	-2.91	94.87	104.64
3	D	2333	OXL	O2-C2-C1	-2.87	114.64	120.63
5	C	1735	ATP	O2B-PB-O3A	2.82	114.91	107.27
5	F	4135	ATP	O3B-PB-O1B	-2.82	102.22	110.70
3	G	4733	OXL	O4-C2-C1	2.66	117.99	112.83
3	F	4133	OXL	O4-C2-C1	2.65	117.97	112.83
3	E	3533	OXL	O4-C2-C1	2.65	117.97	112.83
3	H	5333	OXL	O4-C2-C1	2.63	117.93	112.83
3	C	1733	OXL	O1-C1-C2	-2.60	115.20	120.63
3	B	1133	OXL	O4-C2-C1	2.59	117.86	112.83
5	F	4135	ATP	O2B-PB-O3B	2.53	114.10	107.27
3	B	1133	OXL	O1-C1-C2	-2.49	115.43	120.63
3	H	5333	OXL	O1-C1-C2	-2.49	115.45	120.63
3	H	5333	OXL	O3-C1-C2	2.39	117.47	112.83
5	F	4135	ATP	N6-C6-N1	2.36	123.63	118.38
3	D	2333	OXL	O1-C1-C2	-2.31	115.81	120.63
5	G	4735	ATP	O3G-PG-O3B	2.30	112.35	104.64
5	D	2335	ATP	O2G-PG-O3B	-2.28	96.99	104.64
5	C	1735	ATP	C5-C6-N6	2.25	128.85	123.29
5	E	3535	ATP	O2A-PA-O3A	2.24	113.32	107.27
3	H	5333	OXL	O2-C2-C1	-2.20	116.05	120.63
5	D	2335	ATP	C2'-C3'-C4'	-2.17	98.42	102.61
5	C	1735	ATP	N6-C6-N1	-2.15	113.58	118.38
5	C	1735	ATP	O3'-C3'-C2'	2.15	118.71	111.82
3	C	1733	OXL	O2-C2-C1	-2.12	116.22	120.63
3	G	4733	OXL	O2-C2-C1	-2.10	116.26	120.63
3	C	1733	OXL	O3-C1-O1	2.09	128.87	123.90
5	F	4135	ATP	O3G-PG-O3B	2.08	111.62	104.64
3	D	2333	OXL	O3-C1-O1	2.08	128.85	123.90
3	E	3533	OXL	O2-C2-C1	-2.07	116.32	120.63
3	C	1733	OXL	O4-C2-O2	2.07	128.82	123.90
3	F	4133	OXL	O2-C2-C1	-2.05	116.36	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2335	ATP	O4'-C1'-N9	2.03	111.99	108.09
5	E	3535	ATP	O3G-PG-O3B	2.01	111.38	104.64
5	F	4135	ATP	O2A-PA-O3A	2.00	112.69	107.27

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3535	ATP	PB-O3B-PG-O3G
3	A	533	OXL	O3-C1-C2-O4
3	B	1133	OXL	O3-C1-C2-O4
3	C	1733	OXL	O3-C1-C2-O4
3	E	3533	OXL	O3-C1-C2-O4
3	F	4133	OXL	O3-C1-C2-O4
3	G	4733	OXL	O3-C1-C2-O4
5	D	2335	ATP	PB-O3B-PG-O3G
3	D	2333	OXL	O3-C1-C2-O4
3	H	5333	OXL	O3-C1-C2-O4
5	A	535	ATP	PB-O3A-PA-O1A
5	E	3535	ATP	PB-O3A-PA-O1A
3	A	533	OXL	O1-C1-C2-O2
3	H	5333	OXL	O1-C1-C2-O2
3	B	1133	OXL	O1-C1-C2-O2
3	C	1733	OXL	O1-C1-C2-O2
3	D	2333	OXL	O1-C1-C2-O2
3	E	3533	OXL	O1-C1-C2-O2
3	F	4133	OXL	O1-C1-C2-O2
3	G	4733	OXL	O1-C1-C2-O2
5	A	535	ATP	PG-O3B-PB-O1B
5	G	4735	ATP	PA-O3A-PB-O1B
3	A	533	OXL	O1-C1-C2-O4
3	E	3533	OXL	O1-C1-C2-O4
3	E	3533	OXL	O3-C1-C2-O2
3	F	4133	OXL	O1-C1-C2-O4
3	F	4133	OXL	O3-C1-C2-O2
3	G	4733	OXL	O1-C1-C2-O4
3	G	4733	OXL	O3-C1-C2-O2
5	C	1735	ATP	PA-O3A-PB-O2B
5	E	3535	ATP	PA-O3A-PB-O1B
3	A	533	OXL	O3-C1-C2-O2
3	B	1133	OXL	O1-C1-C2-O4
3	B	1133	OXL	O3-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	1733	OXL	O1-C1-C2-O4
3	C	1733	OXL	O3-C1-C2-O2
3	D	2333	OXL	O1-C1-C2-O4
3	H	5333	OXL	O1-C1-C2-O4
3	H	5333	OXL	O3-C1-C2-O2
3	D	2333	OXL	O3-C1-C2-O2
5	D	2335	ATP	PB-O3B-PG-O2G
5	G	4735	ATP	PB-O3B-PG-O2G
5	A	535	ATP	PG-O3B-PB-O2B
5	C	1735	ATP	PB-O3A-PA-O2A
5	G	4735	ATP	PA-O3A-PB-O2B
5	C	1735	ATP	PA-O3A-PB-O1B
5	D	2335	ATP	PB-O3A-PA-O1A
5	D	2335	ATP	PB-O3A-PA-O2A
5	E	3535	ATP	PB-O3A-PA-O2A
5	G	4735	ATP	PB-O3A-PA-O2A

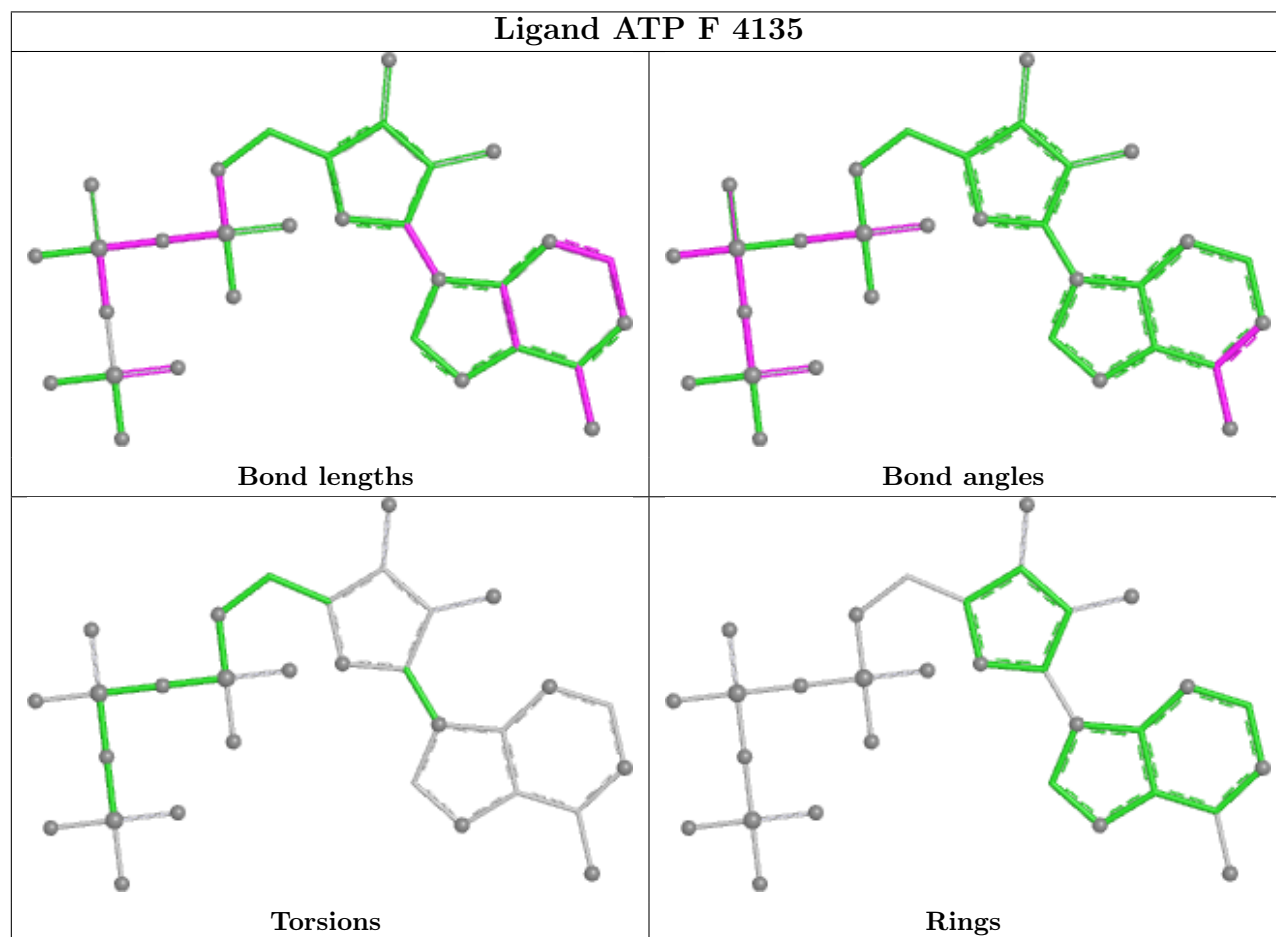
There are no ring outliers.

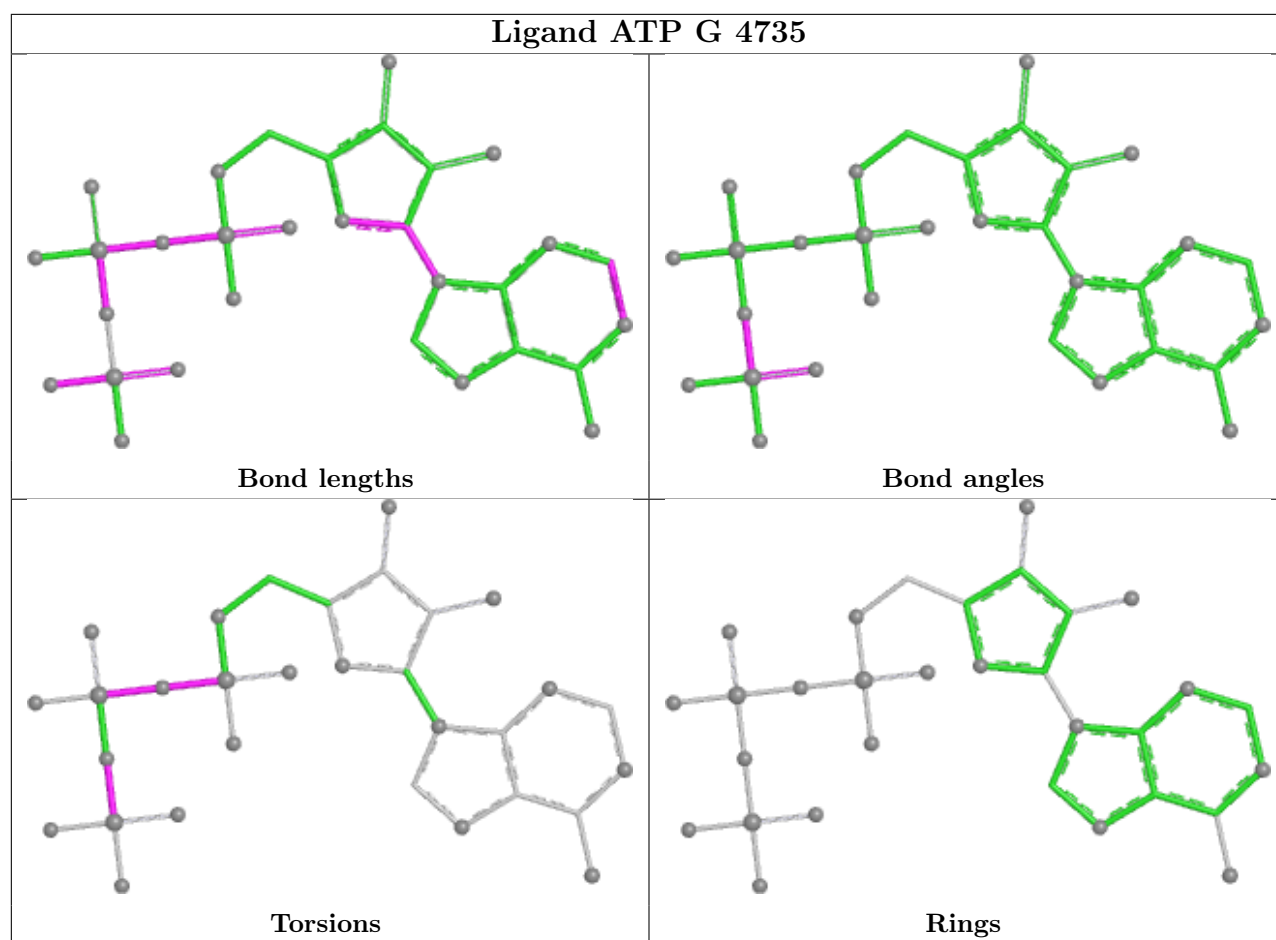
12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1733	OXL	1	0
3	D	2333	OXL	1	0
3	F	4133	OXL	3	0
3	G	4733	OXL	2	0
3	H	5333	OXL	1	0
5	A	535	ATP	4	0
3	E	3533	OXL	1	0
5	E	3535	ATP	2	0
3	A	533	OXL	2	0
5	C	1735	ATP	4	0
3	B	1133	OXL	1	0
5	D	2335	ATP	1	0

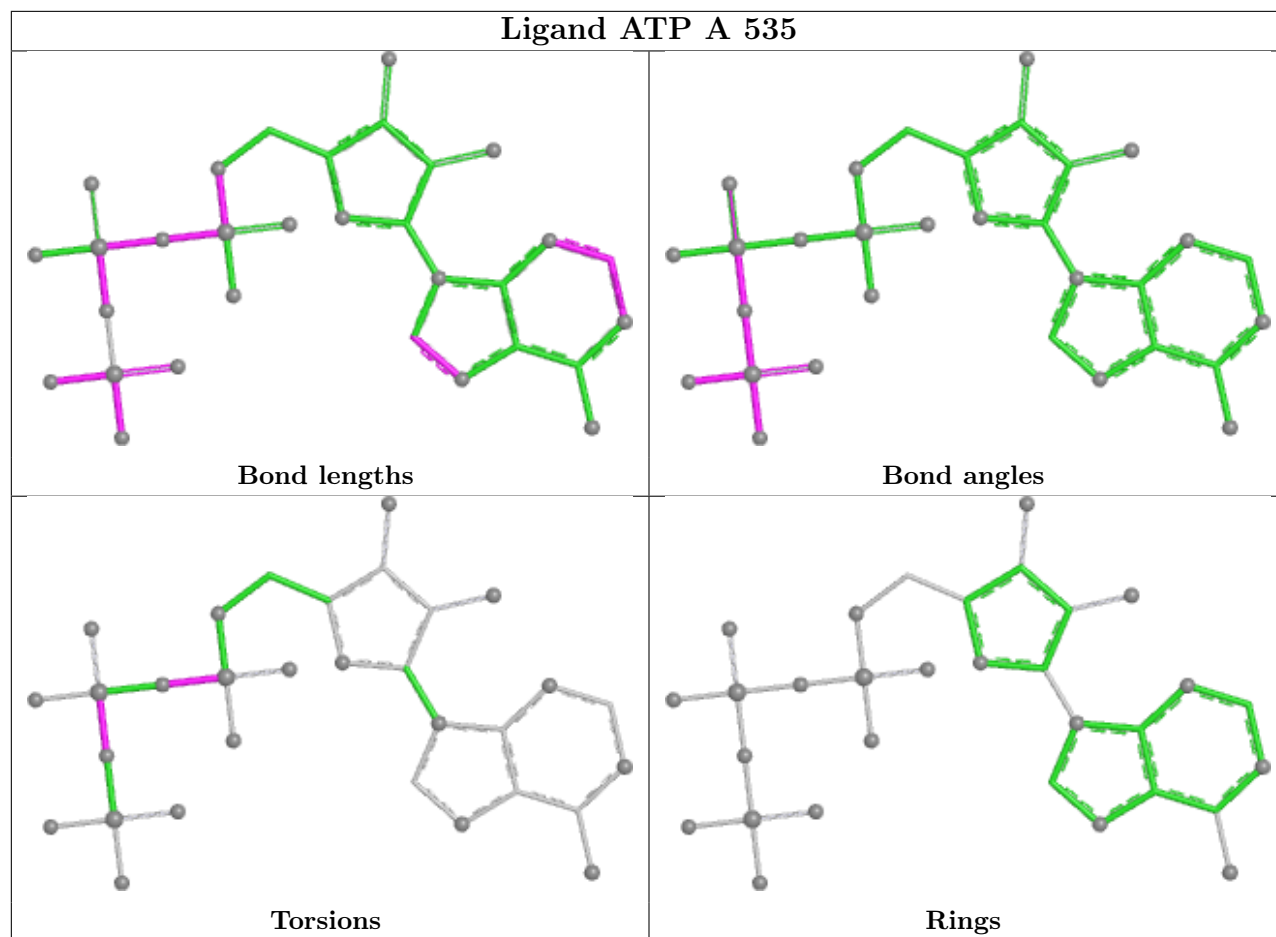
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

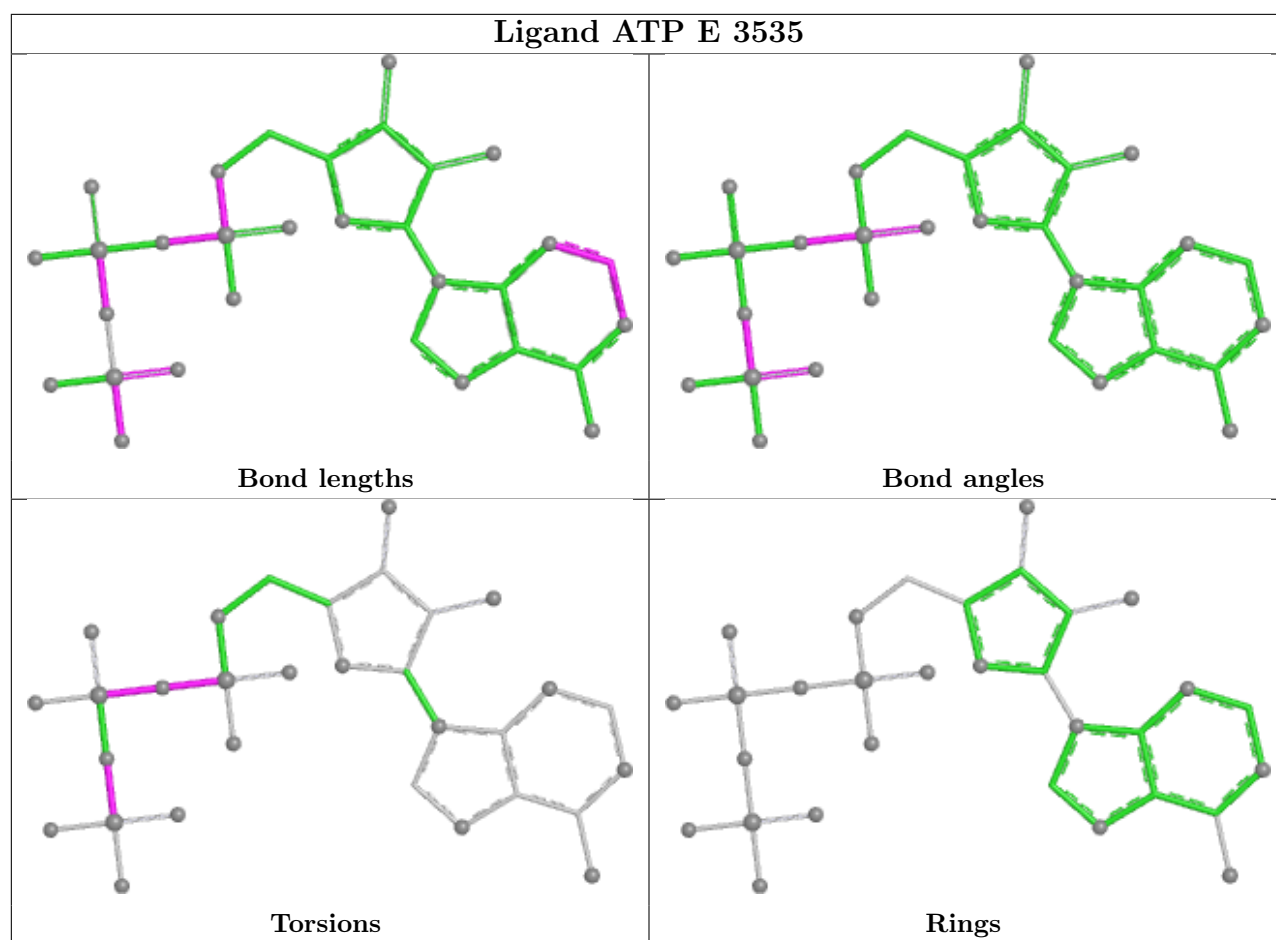
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

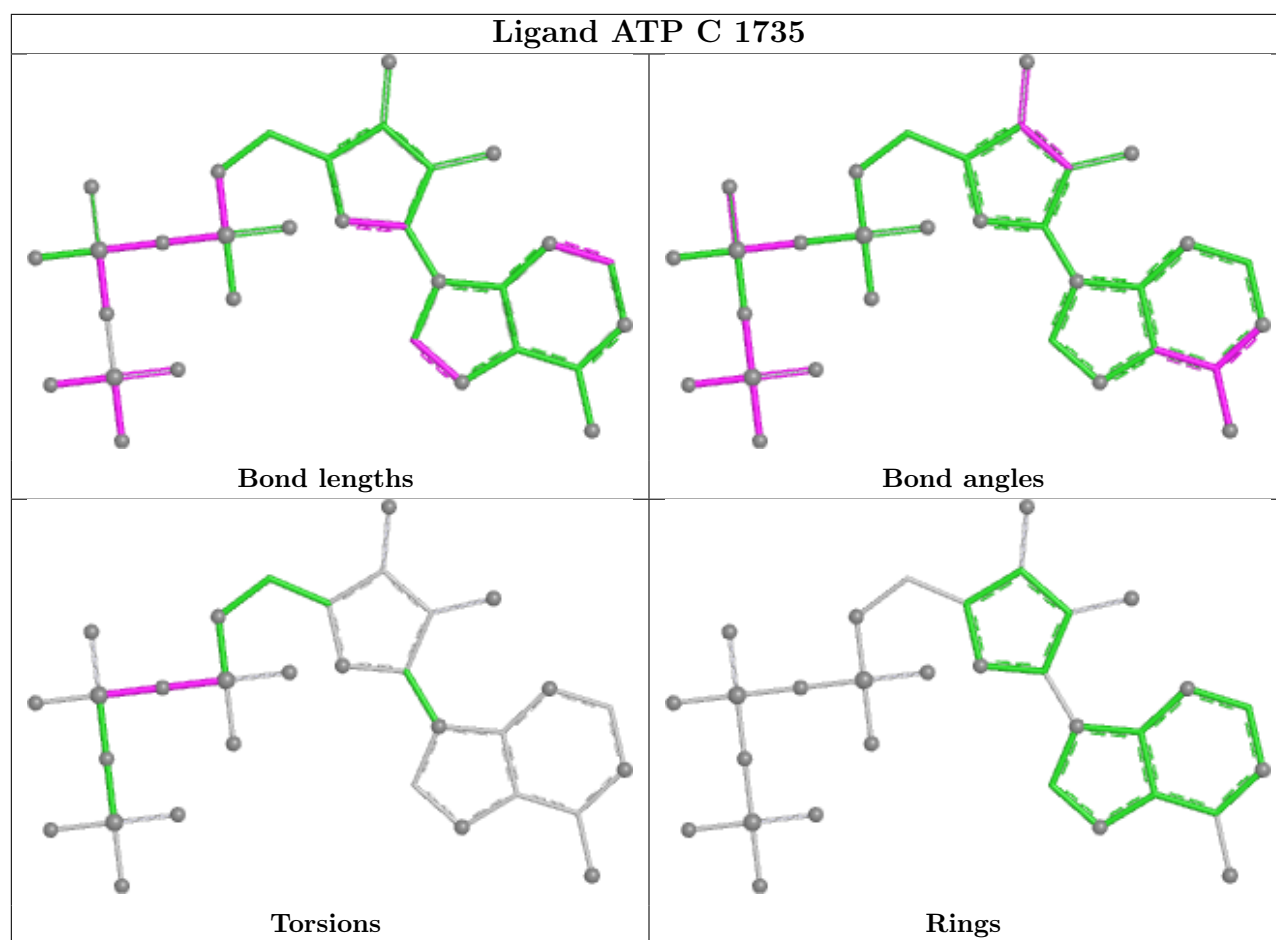


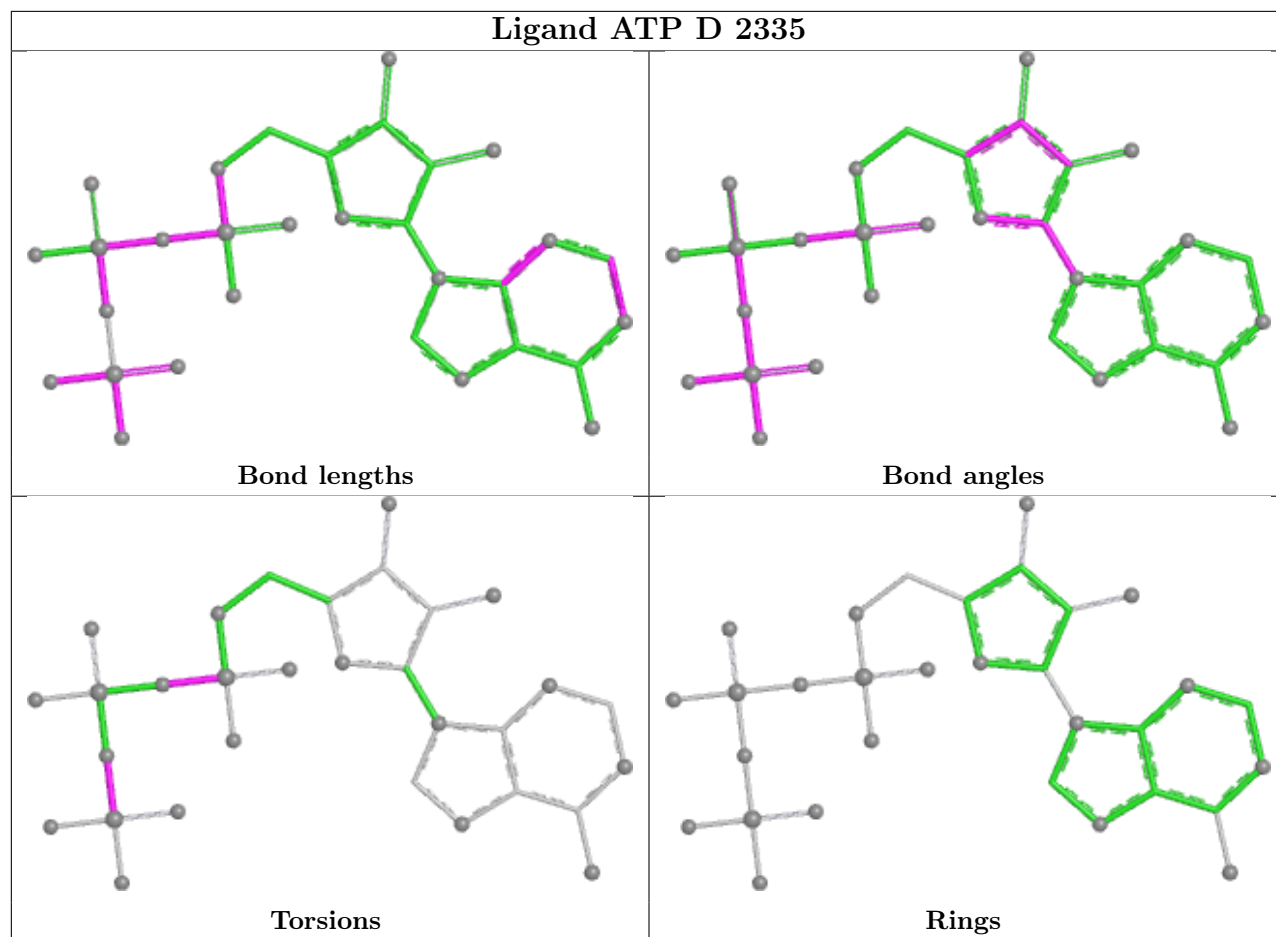


Ligand ATP A 535









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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	241:ALA	C	242:SER	N	1.14

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.