



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 AM UTC

PDB ID : 1A49 / pdb_00001a49
Title : BIS MG-ATP-K-OXALATE COMPLEX OF PYRUVATE KINASE
Authors : Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.
Deposited on : 1998-02-12
Resolution : 2.10 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

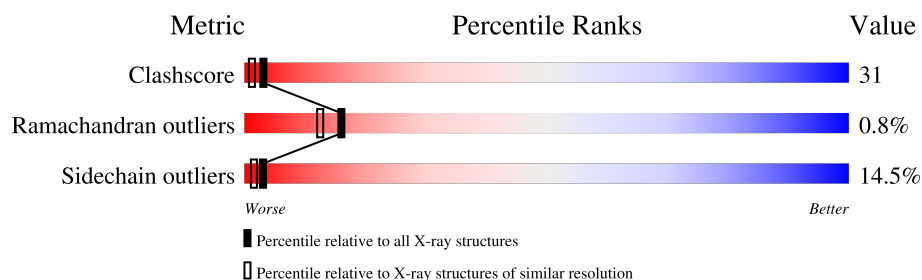
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	
1	B	530	
1	C	530	
1	D	530	
1	E	530	
1	F	530	
1	G	530	
1	H	530	

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	-
3	OXL	F	4133	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34001 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 POTASSIUM ION (CCD ID: K) (formula: K).

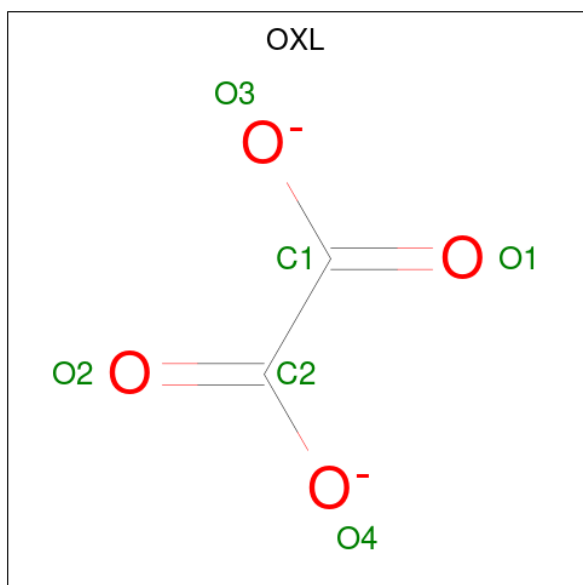
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	F	1	Total	K	0	0
			1	1		

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

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

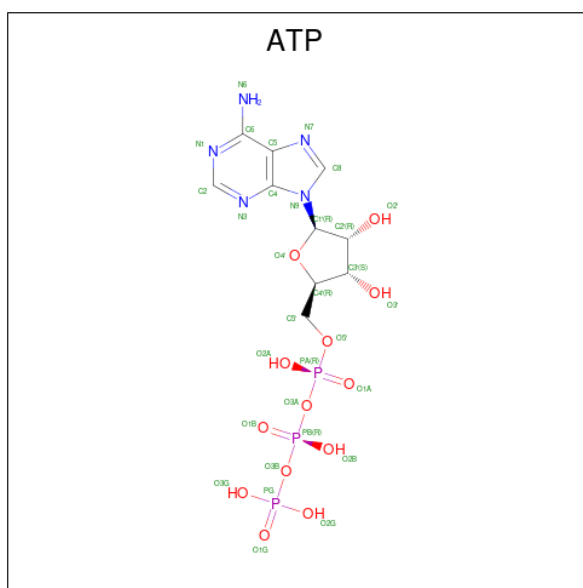


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

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

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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	195	Total	O	0	0
			195	195		
6	B	270	Total	O	0	0
			270	270		
6	C	178	Total	O	0	0
			178	178		
6	D	272	Total	O	0	0
			272	272		
6	E	279	Total	O	0	0
			279	279		
6	F	197	Total	O	0	0
			197	197		
6	G	228	Total	O	0	0
			228	228		
6	H	302	Total	O	0	0
			302	302		

3 Residue-property plots

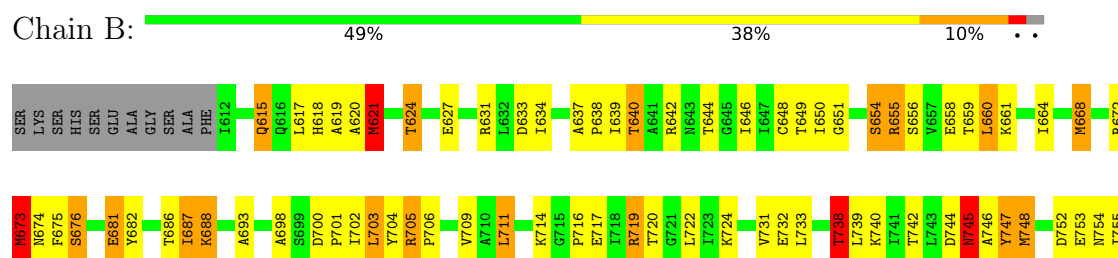
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

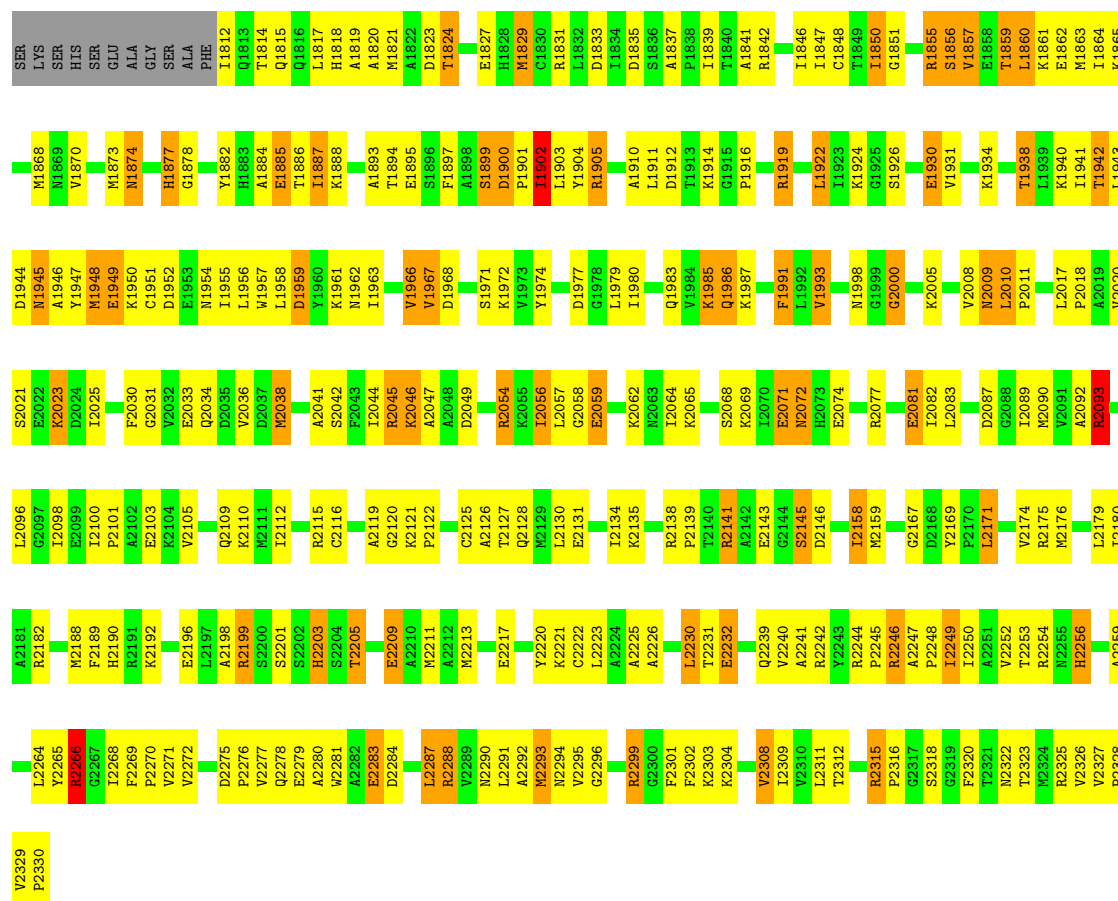
• Molecule 1: PYRUVATE KINASE



• Molecule 1: PYRUVATE KINASE

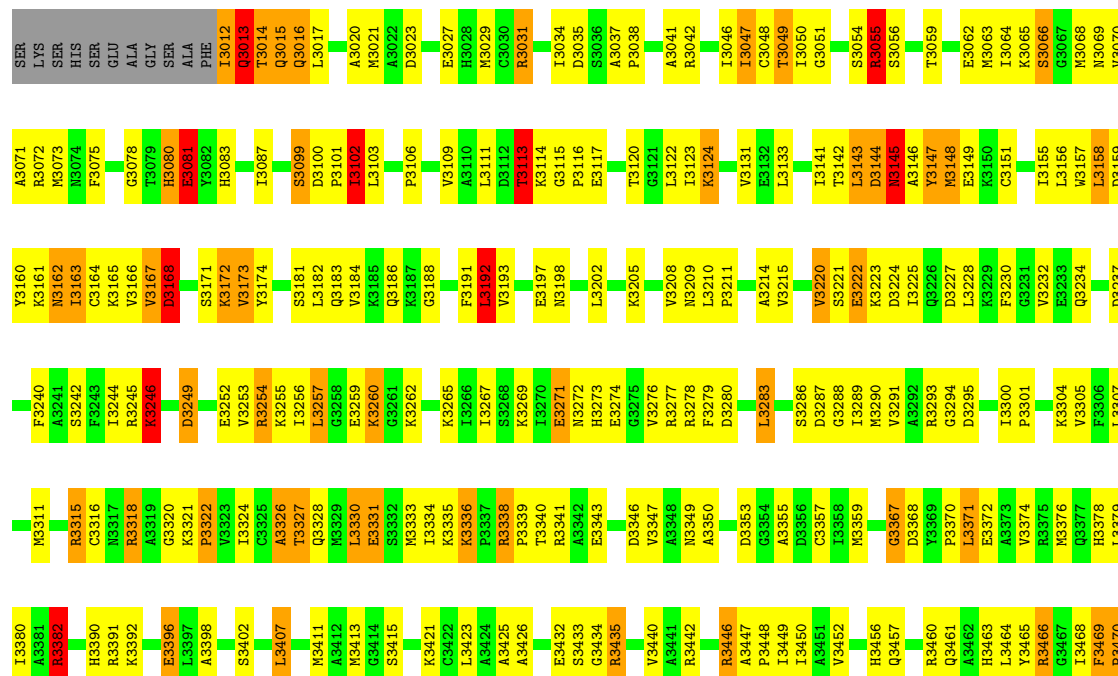


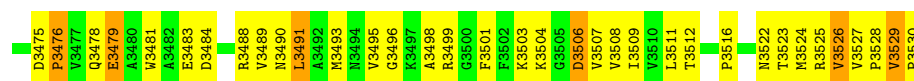




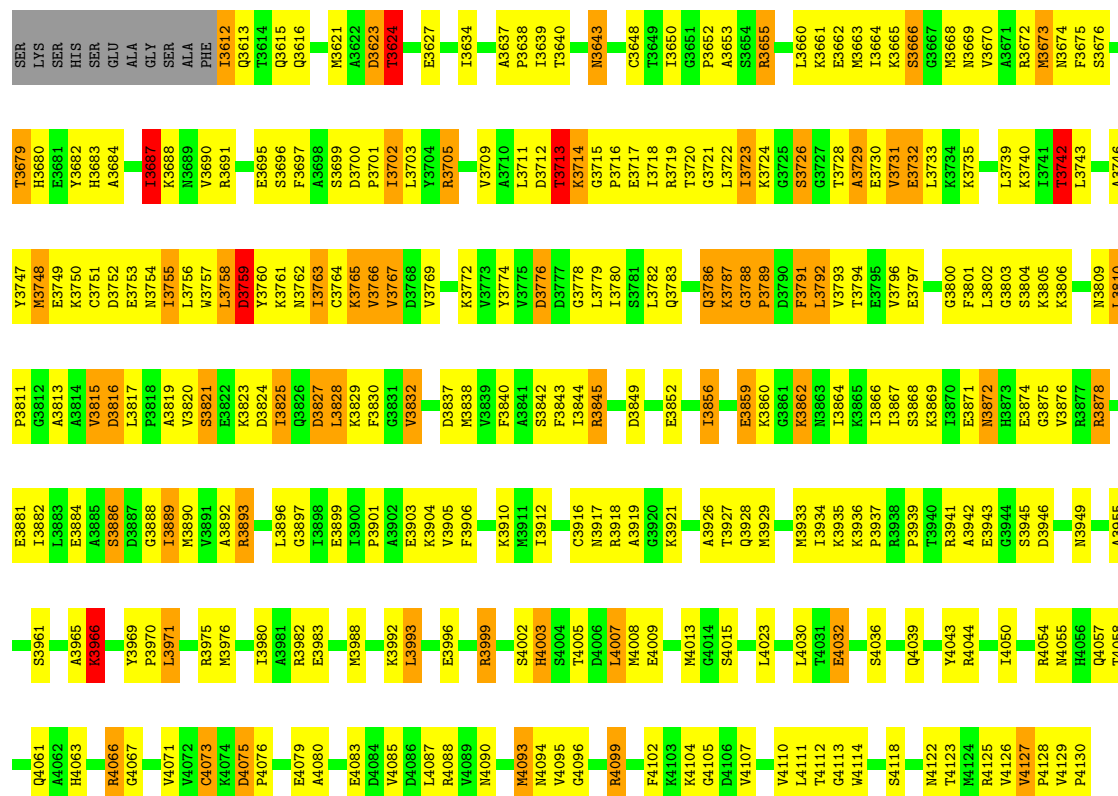
● Molecule 1: PYRUVATE KINASE

Chain E: 45% 41% 10% 10%

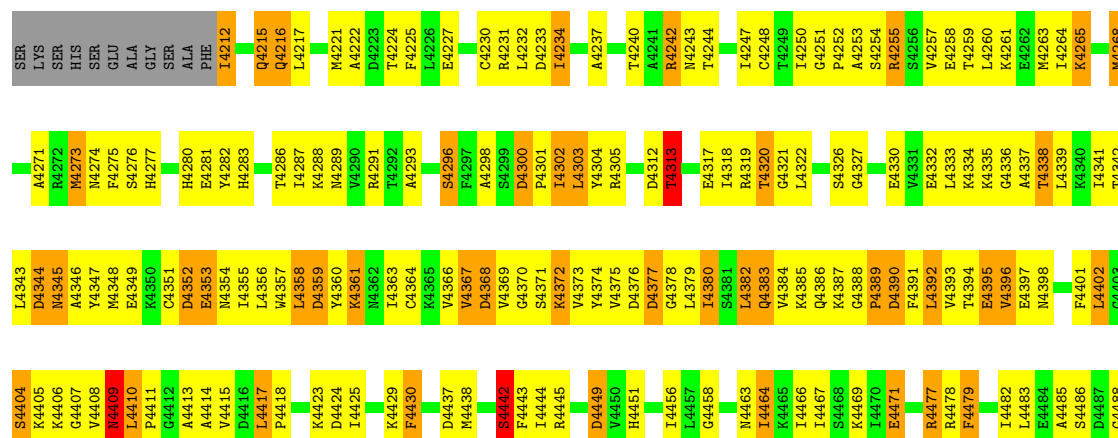


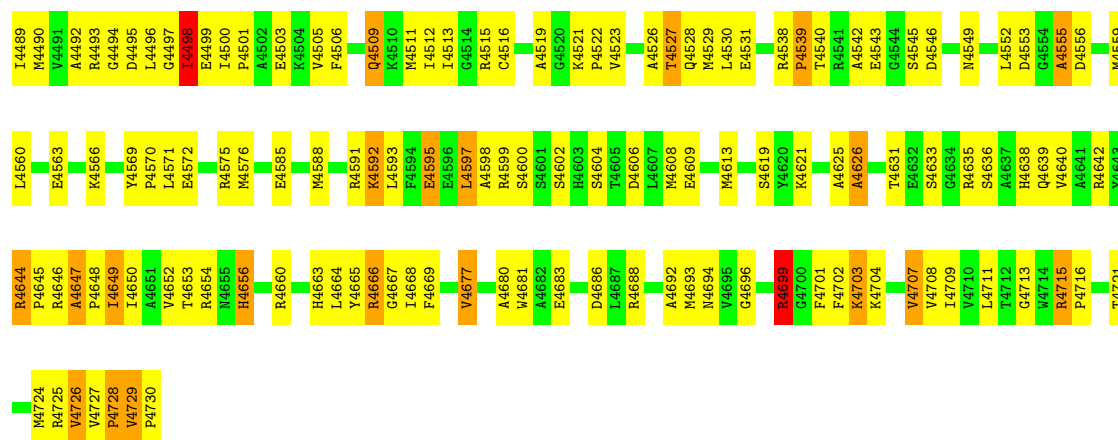


Molecule 1: PYRUVATE KINASE



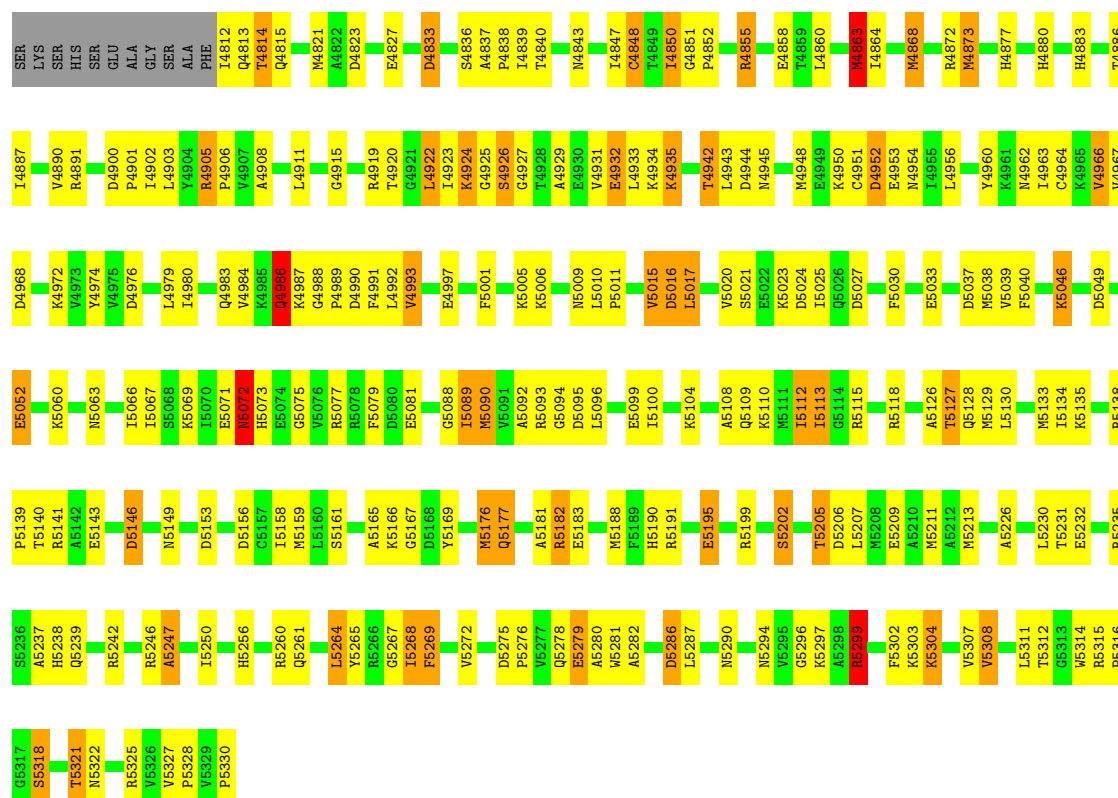
Molecule 1: PYRUVATE KINASE





• Molecule 1: PYRUVATE KINASE

Chain H: 53% 36% 8% ..



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 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (30.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: K, OXL, MG, ATP

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	1.76	42/4041 (1.0%)	1.52	35/5452 (0.6%)
1	B	1.80	63/4041 (1.6%)	1.51	25/5452 (0.5%)
1	C	1.71	40/4041 (1.0%)	1.54	35/5452 (0.6%)
1	D	1.80	48/4041 (1.2%)	1.47	25/5452 (0.5%)
1	E	1.78	40/4041 (1.0%)	1.53	25/5452 (0.5%)
1	F	1.70	36/4041 (0.9%)	1.47	28/5452 (0.5%)
1	G	1.77	48/4041 (1.2%)	1.53	32/5452 (0.6%)
1	H	1.78	50/4041 (1.2%)	1.46	25/5452 (0.5%)
All	All	1.76	367/32328 (1.1%)	1.50	230/43616 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	H	1	0
All	All	1	2

All (367) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1561	SER	CA-C	-12.63	1.46	1.52
1	G	4644	ARG	C-O	-9.80	1.19	1.23
1	A	158	LEU	CA-C	-9.78	1.40	1.52
1	D	2315	ARG	N-CA	-8.70	1.37	1.45
1	B	1092	ALA	C-N	-8.44	1.21	1.33
1	B	955	ALA	C-O	-8.21	1.13	1.23
1	B	738	THR	CA-C	-8.10	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1402	LEU	N-CA	-8.06	1.36	1.46
1	G	4707	VAL	CA-C	-8.04	1.43	1.52
1	E	3246	LYS	CA-C	-8.02	1.42	1.52
1	E	3173	VAL	CA-CB	-7.91	1.44	1.54
1	C	1629	VAL	CA-C	-7.86	1.43	1.52
1	A	305	VAL	C-O	7.84	1.33	1.24
1	E	3338	ARG	NE-CZ	7.66	1.41	1.33
1	H	4863	MET	C-N	-7.65	1.24	1.33
1	B	1069	PHE	CA-CB	7.63	1.63	1.53
1	E	3367	GLY	N-CA	7.48	1.54	1.45
1	D	1874	ASN	CA-C	-7.47	1.43	1.52
1	G	4626	ALA	CA-C	-7.45	1.43	1.52
1	A	450	ILE	CA-C	-7.40	1.44	1.52
1	F	4050	ILE	CA-C	-7.39	1.45	1.53
1	D	2256	HIS	CA-C	-7.33	1.43	1.52
1	H	4993	VAL	CA-C	-7.30	1.43	1.52
1	H	5247	ALA	CA-C	-7.26	1.44	1.53
1	F	3687	ILE	CA-CB	-7.26	1.46	1.54
1	C	1374	TYR	CA-C	-7.24	1.44	1.52
1	E	3470	PRO	N-CA	-7.22	1.38	1.47
1	A	442	ARG	CA-CB	-7.20	1.41	1.53
1	G	4252	PRO	CA-C	-7.20	1.41	1.52
1	C	1599	ARG	NE-CZ	7.18	1.41	1.33
1	C	1264	ILE	CA-CB	-7.14	1.46	1.54
1	G	4409	ASN	CA-C	-7.12	1.43	1.52
1	E	3173	VAL	CA-C	-7.10	1.43	1.52
1	D	2115	ARG	C-N	7.08	1.43	1.33
1	D	2266	ARG	NE-CZ	-7.06	1.25	1.33
1	G	4595	GLU	CD-OE1	7.06	1.38	1.25
1	C	1500	ILE	CA-C	-7.00	1.46	1.52
1	D	1950	LYS	N-CA	-6.92	1.36	1.46
1	A	468	ILE	CA-CB	-6.90	1.46	1.54
1	F	3966	LYS	N-CA	-6.90	1.37	1.46
1	H	4952	ASP	CA-C	-6.85	1.44	1.52
1	C	1666	ARG	CD-NE	-6.84	1.36	1.46
1	B	765	LYS	C-O	-6.80	1.16	1.24
1	H	5017	LEU	C-N	-6.79	1.25	1.33
1	D	2071	GLU	N-CA	-6.70	1.40	1.46
1	H	4838	PRO	CA-C	-6.69	1.45	1.52
1	F	3971	LEU	C-N	-6.66	1.25	1.34
1	A	426	ALA	N-CA	-6.66	1.38	1.46
1	B	777	ASP	CA-C	-6.65	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	SER	CA-C	-6.64	1.44	1.52
1	E	3174	TYR	CA-C	-6.64	1.44	1.52
1	H	5166	LYS	N-CA	-6.63	1.38	1.46
1	B	681	GLU	CD-OE2	6.62	1.38	1.25
1	D	2158	ILE	CA-CB	-6.61	1.44	1.54
1	F	3828	LEU	N-CA	-6.59	1.38	1.46
1	D	2250	ILE	CA-C	-6.59	1.44	1.52
1	G	4713	GLY	CA-C	6.58	1.56	1.52
1	A	428	ILE	N-CA	-6.56	1.38	1.46
1	C	1417	LEU	CA-C	-6.56	1.45	1.53
1	E	3434	GLY	C-N	-6.53	1.25	1.33
1	D	2220	TYR	N-CA	-6.52	1.38	1.46
1	A	270	ILE	CA-C	-6.50	1.44	1.52
1	B	881	GLU	C-O	6.50	1.31	1.24
1	F	3827	ASP	C-N	-6.49	1.25	1.33
1	B	975	ARG	CA-C	-6.48	1.44	1.52
1	F	4127	VAL	C-N	-6.48	1.25	1.33
1	D	1930	GLU	CA-C	-6.46	1.44	1.52
1	B	803	GLY	CA-C	6.45	1.60	1.52
1	C	1697	LYS	C-N	6.43	1.42	1.34
1	D	1949	GLU	C-N	-6.43	1.24	1.33
1	G	4688	ARG	N-CA	-6.42	1.38	1.46
1	B	681	GLU	CA-C	6.42	1.61	1.52
1	B	1027	LEU	C-O	6.42	1.31	1.24
1	H	4864	ILE	N-CA	-6.41	1.39	1.46
1	G	4497	GLY	C-N	6.41	1.39	1.33
1	H	5039	VAL	N-CA	-6.40	1.39	1.46
1	F	3732	GLU	CA-C	-6.38	1.45	1.52
1	B	798	ASN	N-CA	-6.38	1.38	1.46
1	A	372	GLU	N-CA	-6.37	1.38	1.46
1	B	624	THR	CA-C	-6.36	1.44	1.52
1	D	2272	VAL	CA-C	-6.35	1.47	1.53
1	H	5017	LEU	CA-C	-6.29	1.45	1.52
1	D	2087	ASP	C-O	-6.28	1.15	1.24
1	B	627	GLU	CD-OE2	6.27	1.37	1.25
1	F	3993	LEU	C-N	-6.26	1.25	1.33
1	H	4813	GLN	C-N	-6.24	1.25	1.33
1	E	3489	VAL	CA-CB	-6.22	1.47	1.54
1	A	389	PHE	N-CA	6.21	1.54	1.46
1	D	2138	ARG	NE-CZ	6.21	1.39	1.33
1	B	1095	VAL	CA-CB	-6.19	1.47	1.54
1	G	4283	HIS	CG-ND1	6.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1949	GLU	CA-C	-6.18	1.45	1.52
1	B	621	MET	CA-C	-6.18	1.43	1.52
1	B	711	LEU	CA-C	-6.16	1.45	1.52
1	G	4486	SER	CA-C	-6.16	1.44	1.53
1	E	3184	VAL	C-O	6.16	1.29	1.23
1	A	473	CYS	N-CA	-6.16	1.38	1.46
1	H	4880	HIS	N-CA	-6.16	1.39	1.46
1	H	5072	ASN	C-O	6.15	1.30	1.23
1	B	919	ALA	C-N	-6.15	1.25	1.33
1	A	282	ILE	CA-CB	-6.13	1.47	1.54
1	B	895	ASP	CA-C	-6.13	1.44	1.52
1	H	5169	TYR	CA-CB	6.12	1.60	1.53
1	A	310	LYS	CA-C	-6.12	1.45	1.52
1	H	4984	VAL	CA-CB	-6.12	1.46	1.53
1	H	5250	ILE	CA-C	-6.12	1.45	1.52
1	F	4085	VAL	CA-C	6.11	1.60	1.52
1	D	1974	TYR	CA-C	-6.08	1.45	1.52
1	F	3860	LYS	N-CA	-6.08	1.38	1.46
1	G	4232	LEU	N-CA	-6.08	1.38	1.46
1	D	1835	ASP	CA-C	-6.07	1.43	1.52
1	A	245	ARG	C-N	-6.05	1.25	1.33
1	A	70	VAL	C-O	6.03	1.30	1.24
1	G	4553	ASP	C-O	-6.02	1.16	1.24
1	A	27	GLU	CD-OE2	6.01	1.36	1.25
1	F	3797	GLU	CD-OE1	6.01	1.36	1.25
1	H	4905	ARG	CA-C	-5.99	1.47	1.52
1	B	908	ALA	CA-C	-5.99	1.45	1.52
1	F	4095	VAL	CA-CB	-5.98	1.47	1.54
1	G	4650	ILE	CA-CB	-5.98	1.47	1.53
1	H	5113	ILE	C-O	5.97	1.30	1.24
1	H	5095	ASP	C-O	-5.97	1.17	1.24
1	D	1859	THR	CA-CB	-5.97	1.44	1.53
1	C	1401	PHE	CA-C	-5.96	1.45	1.52
1	B	1028	ILE	CA-CB	-5.96	1.47	1.54
1	E	3215	VAL	N-CA	-5.96	1.39	1.46
1	G	4644	ARG	N-CA	5.93	1.50	1.46
1	A	225	ILE	CA-CB	-5.93	1.47	1.54
1	A	140	LYS	N-CA	-5.93	1.39	1.46
1	G	4287	ILE	CA-CB	-5.92	1.47	1.54
1	G	4726	VAL	N-CA	-5.89	1.39	1.46
1	G	4650	ILE	CA-C	-5.87	1.46	1.52
1	B	758	LEU	CA-C	-5.87	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	4864	ILE	CA-CB	-5.87	1.47	1.54
1	H	5138	ARG	NE-CZ	5.86	1.39	1.33
1	F	4023	LEU	CA-C	-5.85	1.45	1.53
1	G	4396	VAL	N-CA	-5.85	1.39	1.46
1	F	3616	GLN	CA-CB	5.84	1.62	1.53
1	H	5232	GLU	N-CA	-5.84	1.38	1.46
1	F	3903	GLU	CD-OE1	5.84	1.36	1.25
1	B	839	VAL	N-CA	-5.83	1.39	1.46
1	C	1358	LEU	N-CA	5.83	1.53	1.45
1	D	2054	ARG	NE-CZ	5.81	1.39	1.33
1	G	4291	ARG	CD-NE	5.79	1.54	1.46
1	D	2250	ILE	CA-CB	-5.79	1.47	1.53
1	B	874	GLU	CD-OE1	5.78	1.36	1.25
1	D	2069	LYS	N-CA	-5.78	1.39	1.46
1	A	117	GLU	CA-C	-5.78	1.45	1.52
1	H	4814	THR	N-CA	-5.78	1.39	1.46
1	F	3637	ALA	C-N	5.77	1.40	1.33
1	E	3078	GLY	CA-C	5.77	1.59	1.52
1	E	3378	HIS	C-O	-5.75	1.17	1.24
1	H	5325	ARG	CA-C	-5.75	1.45	1.52
1	G	4398	ASN	CA-CB	5.75	1.67	1.53
1	H	4966	VAL	CA-CB	-5.75	1.48	1.54
1	H	5169	TYR	C-N	-5.74	1.26	1.34
1	G	4477	ARG	NE-CZ	5.74	1.39	1.33
1	A	503	LYS	CA-C	-5.73	1.45	1.52
1	B	1093	MET	N-CA	-5.73	1.39	1.46
1	C	1694	ASN	CA-C	-5.72	1.45	1.52
1	H	5090	MET	N-CA	-5.72	1.39	1.46
1	D	2120	GLY	CA-C	5.72	1.59	1.51
1	F	4073	CYS	CA-C	-5.72	1.45	1.52
1	B	955	ALA	CA-C	-5.71	1.45	1.52
1	C	1410	LEU	C-N	-5.71	1.26	1.33
1	B	681	GLU	CA-CB	5.71	1.62	1.53
1	A	383	GLU	N-CA	-5.71	1.39	1.46
1	D	2072	ASN	CA-C	-5.70	1.45	1.52
1	E	3064	ILE	CA-CB	-5.69	1.47	1.54
1	E	3013	GLN	C-N	-5.68	1.26	1.33
1	E	3063	MET	C-N	-5.68	1.26	1.33
1	H	5238	HIS	N-CA	5.68	1.53	1.46
1	B	633	ASP	CG-OD1	5.68	1.36	1.25
1	E	3114	LYS	CA-C	-5.68	1.45	1.53
1	G	4543	GLU	N-CA	-5.68	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	779	LEU	CA-C	-5.67	1.45	1.52
1	E	3491	LEU	N-CA	-5.67	1.39	1.46
1	B	989	PHE	CA-C	5.66	1.59	1.53
1	H	5231	THR	C-N	-5.65	1.25	1.33
1	A	371	LEU	C-N	-5.65	1.26	1.34
1	A	529	VAL	N-CA	-5.64	1.41	1.46
1	B	798	ASN	CA-C	-5.62	1.45	1.53
1	H	4990	ASP	CA-C	-5.62	1.45	1.52
1	D	2045	ARG	CA-CB	-5.61	1.46	1.54
1	G	4356	LEU	N-CA	-5.61	1.39	1.46
1	A	300	ILE	C-N	-5.60	1.27	1.33
1	G	4377	ASP	CA-CB	5.59	1.61	1.53
1	B	1032	GLU	CA-C	-5.59	1.45	1.52
1	D	2074	GLU	CA-C	-5.58	1.45	1.52
1	H	5176	MET	N-CA	-5.58	1.39	1.46
1	B	1004	SER	N-CA	-5.58	1.39	1.46
1	E	3066	SER	CA-C	5.58	1.60	1.52
1	G	4216	GLN	C-O	5.58	1.31	1.24
1	E	3338	ARG	CA-C	5.57	1.57	1.52
1	C	1606	ASP	CA-C	5.57	1.59	1.52
1	A	529	VAL	CA-C	-5.57	1.48	1.53
1	F	4071	VAL	CA-C	-5.57	1.45	1.52
1	A	117	GLU	CD-OE1	5.56	1.35	1.25
1	F	3999	ARG	NE-CZ	5.56	1.39	1.33
1	C	1312	ASP	C-N	-5.55	1.26	1.33
1	G	4686	ASP	CG-OD1	5.55	1.35	1.25
1	B	964	THR	C-N	-5.55	1.26	1.33
1	A	217	LEU	CA-C	-5.54	1.46	1.52
1	F	3876	VAL	CA-CB	-5.53	1.47	1.54
1	G	4485	ALA	CA-C	-5.53	1.45	1.52
1	B	655	ARG	C-N	-5.53	1.26	1.33
1	C	1627	LEU	CA-C	-5.52	1.45	1.52
1	E	3192	LEU	CA-C	-5.52	1.45	1.52
1	A	527	VAL	C-O	5.51	1.28	1.24
1	B	758	LEU	C-O	-5.51	1.17	1.23
1	E	3116	PRO	N-CA	-5.50	1.40	1.47
1	A	427	LEU	C-N	-5.50	1.26	1.33
1	A	520	PHE	C-N	-5.49	1.25	1.33
1	H	5195	GLU	CD-OE1	5.49	1.35	1.25
1	C	1666	ARG	NE-CZ	-5.49	1.27	1.33
1	D	2038	MET	CA-C	-5.49	1.45	1.52
1	A	371	LEU	C-O	-5.49	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	3919	ALA	CA-C	-5.48	1.45	1.52
1	H	5279	GLU	CD-OE2	5.48	1.35	1.25
1	C	1690	ASN	N-CA	-5.47	1.39	1.46
1	H	5089	ILE	C-N	-5.47	1.26	1.33
1	A	450	ILE	CA-CB	-5.46	1.47	1.53
1	E	3254	ARG	N-CA	-5.46	1.39	1.46
1	D	2009	ASN	CA-C	-5.45	1.46	1.52
1	F	3664	ILE	CA-CB	-5.45	1.48	1.54
1	H	5104	LYS	C-N	-5.45	1.27	1.33
1	D	2000	GLY	N-CA	5.44	1.52	1.45
1	C	1656	HIS	CA-C	-5.43	1.45	1.52
1	A	525	ARG	CA-C	-5.42	1.46	1.52
1	C	1466	ILE	N-CA	-5.42	1.39	1.46
1	H	4993	VAL	N-CA	-5.42	1.39	1.46
1	B	1082	ALA	CA-C	-5.42	1.45	1.52
1	B	896	LEU	N-CA	-5.42	1.39	1.46
1	C	1292	THR	CA-CB	5.42	1.61	1.53
1	F	4075	ASP	CA-C	-5.42	1.46	1.53
1	D	1900	ASP	CA-C	-5.41	1.47	1.52
1	C	1361	LYS	N-CA	5.40	1.53	1.46
1	C	1690	ASN	CA-C	-5.40	1.45	1.52
1	A	148	MET	N-CA	-5.39	1.39	1.46
1	D	1979	LEU	N-CA	5.39	1.52	1.46
1	C	1555	ALA	CA-C	-5.38	1.46	1.52
1	E	3081	GLU	CD-OE2	5.38	1.35	1.25
1	G	4281	GLU	CA-C	5.38	1.59	1.52
1	G	4451	HIS	CA-C	-5.38	1.46	1.52
1	A	475	ASP	CA-C	-5.38	1.47	1.53
1	G	4479	PHE	C-N	-5.38	1.27	1.33
1	F	3859	GLU	C-N	-5.37	1.26	1.34
1	H	4962	ASN	CA-C	-5.37	1.45	1.52
1	G	4512	ILE	CA-CB	-5.36	1.48	1.54
1	G	4556	ASP	CG-OD2	5.36	1.35	1.25
1	E	3240	PHE	CA-C	-5.35	1.46	1.52
1	E	3490	ASN	CA-C	-5.35	1.45	1.52
1	F	3901	PRO	CA-C	-5.35	1.45	1.52
1	H	4986	GLN	N-CA	-5.35	1.39	1.45
1	B	991	ARG	CA-C	-5.34	1.45	1.52
1	G	4271	ALA	C-N	-5.34	1.25	1.33
1	D	2059	GLU	CA-C	-5.33	1.45	1.52
1	C	1486	SER	CA-C	-5.33	1.46	1.52
1	G	4509	GLN	C-N	-5.32	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	3670	VAL	CA-C	5.31	1.59	1.52
1	B	789	PRO	CA-C	-5.31	1.47	1.52
1	E	3214	ALA	C-N	-5.31	1.25	1.33
1	H	5016	ASP	CA-CB	5.31	1.62	1.53
1	D	2199	ARG	N-CA	-5.29	1.39	1.46
1	H	5099	GLU	CD-OE2	5.29	1.35	1.25
1	H	5156	ASP	CG-OD2	5.28	1.35	1.25
1	C	1394	THR	C-N	-5.28	1.26	1.33
1	G	4549	ASN	N-CA	-5.28	1.39	1.46
1	H	4890	VAL	C-N	-5.28	1.26	1.33
1	F	3912	ILE	CA-CB	-5.28	1.48	1.54
1	B	808	VAL	CA-C	-5.27	1.46	1.52
1	B	912	ILE	CA-C	-5.27	1.46	1.52
1	D	2125	CYS	C-N	-5.26	1.26	1.33
1	G	4410	LEU	CA-C	-5.26	1.46	1.52
1	H	4868	MET	CA-C	-5.25	1.45	1.52
1	E	3148	MET	N-CA	-5.25	1.39	1.46
1	C	1283	HIS	ND1-CE1	5.25	1.37	1.32
1	B	644	THR	CB-OG1	-5.25	1.35	1.43
1	C	1378	GLY	C-N	-5.25	1.27	1.33
1	H	5072	ASN	CA-C	-5.24	1.46	1.52
1	D	2138	ARG	CZ-NH1	5.24	1.40	1.32
1	F	3776	ASP	CG-OD1	5.24	1.35	1.25
1	E	3523	THR	N-CA	-5.24	1.39	1.46
1	F	3917	ASN	C-O	-5.24	1.18	1.24
1	D	1877	HIS	CB-CG	5.22	1.57	1.50
1	B	1033	SER	N-CA	-5.22	1.39	1.46
1	E	3080	HIS	CA-C	-5.22	1.46	1.52
1	G	4376	ASP	N-CA	-5.21	1.39	1.46
1	C	1590	HIS	C-N	-5.21	1.27	1.33
1	B	747	TYR	C-N	-5.20	1.26	1.33
1	B	769	VAL	CA-C	-5.20	1.46	1.52
1	D	1857	VAL	N-CA	-5.20	1.40	1.46
1	A	107	VAL	CA-C	-5.20	1.46	1.52
1	C	1317	GLU	CD-OE2	5.20	1.35	1.25
1	B	1069	PHE	CA-C	5.20	1.59	1.52
1	C	1583	GLU	N-CA	-5.19	1.40	1.46
1	E	3065	LYS	C-N	-5.19	1.25	1.33
1	G	4555	ALA	C-O	-5.19	1.17	1.23
1	H	5052	GLU	N-CA	-5.18	1.40	1.46
1	H	5181	ALA	N-CA	-5.17	1.40	1.46
1	C	1466	ILE	CA-C	-5.17	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	761	LYS	CA-C	-5.16	1.45	1.52
1	B	924	ILE	CA-CB	-5.16	1.48	1.54
1	E	3476	PRO	N-CA	-5.16	1.40	1.47
1	F	3840	PHE	CA-CB	5.16	1.60	1.52
1	G	4430	PHE	CA-C	5.16	1.59	1.52
1	B	840	PHE	CA-CB	5.15	1.59	1.53
1	H	5161	SER	CA-C	5.15	1.55	1.52
1	C	1379	LEU	N-CA	-5.15	1.40	1.46
1	C	1390	ASP	CG-OD2	5.14	1.35	1.25
1	D	2112	ILE	CA-CB	-5.14	1.48	1.54
1	E	3255	LYS	N-CA	5.14	1.52	1.46
1	B	1083	GLU	N-CA	-5.14	1.40	1.46
1	F	3889	ILE	CA-C	-5.14	1.46	1.52
1	E	3311	MET	C-N	-5.14	1.27	1.33
1	C	1411	PRO	N-CA	-5.13	1.41	1.47
1	E	3396	GLU	CD-OE1	5.13	1.35	1.25
1	A	244	ILE	CA-CB	-5.12	1.48	1.54
1	B	673	MET	CA-C	-5.12	1.46	1.52
1	F	4128	PRO	N-CA	-5.12	1.41	1.47
1	G	4464	ILE	CA-CB	-5.12	1.48	1.54
1	C	1290	VAL	CA-CB	-5.12	1.48	1.54
1	D	2109	GLN	CA-C	-5.12	1.46	1.52
1	D	1850	ILE	CA-CB	-5.11	1.47	1.54
1	D	2171	LEU	C-N	-5.10	1.27	1.33
1	B	1001	SER	C-O	-5.10	1.17	1.23
1	B	899	GLU	CD-OE2	5.09	1.35	1.25
1	D	2074	GLU	C-N	-5.09	1.27	1.33
1	C	1582	ARG	C-N	-5.09	1.27	1.33
1	H	5146	ASP	CG-OD1	5.09	1.35	1.25
1	A	249	ASP	CG-OD2	5.08	1.35	1.25
1	A	328	GLN	C-N	-5.08	1.27	1.33
1	G	4277	HIS	N-CA	5.08	1.52	1.45
1	A	222	GLU	CD-OE2	5.08	1.35	1.25
1	E	3249	ASP	C-N	-5.08	1.27	1.33
1	B	1026	ALA	CA-C	-5.08	1.46	1.52
1	D	2232	GLU	CA-C	-5.08	1.46	1.52
1	G	4466	ILE	N-CA	-5.08	1.40	1.46
1	F	3889	ILE	C-O	-5.07	1.18	1.23
1	H	4833	ASP	CG-OD1	5.07	1.34	1.25
1	B	1099	ARG	C-N	-5.07	1.26	1.33
1	D	1926	SER	N-CA	5.07	1.52	1.45
1	E	3291	VAL	C-N	5.07	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4563	GLU	CA-C	-5.07	1.45	1.52
1	F	3866	ILE	CA-C	-5.07	1.46	1.52
1	A	191	PHE	CA-C	-5.06	1.46	1.52
1	B	761	LYS	N-CA	-5.06	1.40	1.46
1	D	2217	GLU	C-O	-5.05	1.18	1.24
1	G	4300	ASP	CA-C	5.05	1.59	1.52
1	C	1416	ASP	CG-OD1	5.05	1.34	1.25
1	B	755	ILE	CA-C	-5.05	1.46	1.52
1	G	4291	ARG	C-N	-5.04	1.27	1.33
1	D	2199	ARG	C-N	-5.04	1.26	1.33
1	B	997	LEU	N-CA	-5.04	1.40	1.46
1	H	5069	LYS	CA-CB	5.04	1.60	1.53
1	C	1328	THR	N-CA	-5.04	1.39	1.45
1	E	3331	GLU	CD-OE2	5.03	1.34	1.25
1	B	1113	GLY	CA-C	5.03	1.57	1.52
1	F	4007	LEU	CA-C	-5.03	1.46	1.52
1	B	1072	VAL	N-CA	-5.03	1.40	1.46
1	D	2198	ALA	C-N	-5.02	1.27	1.33
1	D	1900	ASP	CG-OD1	5.01	1.34	1.25
1	E	3047	ILE	CA-CB	-5.01	1.48	1.54
1	E	3529	VAL	CA-C	-5.01	1.49	1.53
1	G	4424	ASP	C-O	5.01	1.29	1.24
1	B	634	ILE	CA-C	-5.01	1.45	1.52
1	G	4231	ARG	NE-CZ	-5.01	1.27	1.33

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3168	ASP	CA-CB-CG	11.91	124.51	112.60
1	B	758	LEU	CA-C-N	10.36	134.16	120.28
1	B	758	LEU	C-N-CA	10.36	134.16	120.28
1	G	4368	ASP	CA-CB-CG	8.98	121.58	112.60
1	E	3490	ASN	CA-CB-CG	-8.89	103.71	112.60
1	A	222	GLU	N-CA-C	-8.70	101.88	111.36
1	B	759	ASP	CB-CA-C	-8.63	96.46	110.79
1	G	4300	ASP	CA-C-N	8.43	128.55	119.28
1	G	4300	ASP	C-N-CA	8.43	128.55	119.28
1	G	4352	ASP	N-CA-C	8.31	118.86	107.73
1	C	1328	THR	N-CA-C	-8.30	103.34	113.97
1	F	3687	ILE	CB-CA-C	-8.08	101.54	111.88
1	H	5153	ASP	CA-CB-CG	7.94	120.54	112.60
1	A	37	ALA	N-CA-C	7.86	119.97	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5015	VAL	CA-C-N	7.71	132.94	120.60
1	H	5015	VAL	C-N-CA	7.71	132.94	120.60
1	F	3742	THR	N-CA-C	7.50	120.85	109.23
1	A	163	ILE	O-C-N	7.44	131.87	122.57
1	B	1115	ARG	CB-CA-C	7.39	120.72	109.56
1	H	5318	SER	N-CA-C	-7.34	104.36	113.38
1	B	1127	VAL	C-N-CD	-7.33	94.97	125.00
1	B	668	MET	CG-SD-CE	-7.31	84.82	100.90
1	C	1645	PRO	CB-CA-C	-7.25	101.46	110.95
1	A	75	PHE	CA-CB-CG	-7.16	106.64	113.80
1	E	3066	SER	CB-CA-C	7.14	123.44	109.72
1	A	191	PHE	CA-CB-CG	-7.12	106.68	113.80
1	C	1663	HIS	CA-CB-CG	-7.08	106.72	113.80
1	B	759	ASP	N-CA-C	6.97	118.88	111.28
1	H	5205	THR	CA-CB-OG1	6.91	119.97	109.60
1	A	220	VAL	N-CA-C	6.80	116.70	106.42
1	B	759	ASP	N-CA-CB	-6.74	100.22	110.12
1	A	280	ASP	CA-CB-CG	6.71	119.31	112.60
1	G	4677	VAL	N-CA-C	6.68	117.65	108.84
1	A	527	VAL	O-C-N	6.67	125.89	121.69
1	F	4090	ASN	N-CA-C	6.61	118.49	111.28
1	G	4377	ASP	CA-CB-CG	6.59	119.19	112.60
1	E	3279	PHE	CA-CB-CG	-6.56	107.24	113.80
1	C	1647	ALA	CA-C-N	6.54	126.30	119.76
1	C	1647	ALA	C-N-CA	6.54	126.30	119.76
1	G	4361	LYS	N-CA-C	6.48	119.34	111.82
1	E	3382	ARG	N-CA-CB	6.42	120.23	110.28
1	C	1275	PHE	CA-CB-CG	-6.41	107.39	113.80
1	D	1902	ILE	CB-CA-C	6.37	116.61	110.63
1	F	3763	ILE	N-CA-C	6.36	117.04	110.36
1	G	4415	VAL	CB-CA-C	6.35	117.64	111.23
1	A	190	ASP	CA-CB-CG	6.31	118.91	112.60
1	D	1919	ARG	CD-NE-CZ	6.31	133.23	124.40
1	B	1126	VAL	N-CA-CB	6.30	118.55	110.99
1	G	4498	ILE	N-CA-CB	6.28	121.85	110.86
1	F	3816	ASP	N-CA-CB	6.28	120.84	110.42
1	G	4237	ALA	N-CA-C	6.24	118.67	109.50
1	C	1368	ASP	CA-CB-CG	6.21	118.81	112.60
1	D	2093	ARG	N-CA-C	6.20	118.84	111.71
1	F	3624	THR	N-CA-CB	-6.20	101.16	111.20
1	G	4498	ILE	CB-CA-C	-6.18	104.44	111.55
1	G	4255	ARG	N-CA-C	6.16	118.79	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3293	ARG	N-CA-C	6.14	118.77	111.71
1	F	4127	VAL	N-CA-C	6.10	114.19	109.19
1	G	4647	ALA	CA-C-N	6.09	125.85	119.76
1	G	4647	ALA	C-N-CA	6.09	125.85	119.76
1	C	1300	ASP	CA-C-N	6.07	125.77	119.82
1	C	1300	ASP	C-N-CA	6.07	125.77	119.82
1	E	3168	ASP	N-CA-CB	6.07	119.83	110.60
1	C	1313	THR	N-CA-CB	-6.07	101.68	110.36
1	F	3788	GLY	C-N-CD	-6.06	100.15	125.00
1	E	3305	VAL	N-CA-C	6.06	116.72	110.36
1	E	3055	ARG	N-CA-C	6.05	117.88	111.28
1	E	3322	PRO	N-CA-CB	6.04	108.56	103.25
1	G	4390	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	654	SER	CA-C-N	6.03	129.19	120.38
1	B	654	SER	C-N-CA	6.03	129.19	120.38
1	G	4415	VAL	N-CA-C	6.03	115.52	106.42
1	H	4905	ARG	CA-C-N	-6.00	113.76	119.76
1	H	4905	ARG	C-N-CA	-6.00	113.76	119.76
1	G	4539	PRO	CB-CA-C	-5.97	102.21	111.22
1	F	3843	PHE	N-CA-C	5.93	119.61	111.54
1	B	777	ASP	CB-CA-C	-5.93	103.47	111.89
1	H	4837	ALA	N-CA-C	5.92	117.12	109.72
1	B	633	ASP	N-CA-C	5.91	118.03	108.34
1	F	4090	ASN	N-CA-CB	5.89	118.78	110.12
1	D	2098	ILE	N-CA-C	-5.88	107.08	112.96
1	F	4003	HIS	CA-CB-CG	-5.87	107.93	113.80
1	F	3758	LEU	CA-C-N	5.83	130.55	120.58
1	F	3758	LEU	C-N-CA	5.83	130.55	120.58
1	H	5290	ASN	CA-CB-CG	-5.82	106.78	112.60
1	D	2105	VAL	N-CA-C	5.80	116.54	110.62
1	A	279	PHE	CA-CB-CG	-5.78	108.02	113.80
1	C	1527	THR	N-CA-C	5.77	123.09	110.80
1	A	508	VAL	N-CA-CB	-5.75	101.16	111.92
1	C	1360	TYR	N-CA-C	5.75	118.73	107.57
1	C	1484	GLU	N-CA-CB	5.73	118.54	110.12
1	F	3819	ALA	N-CA-C	-5.73	104.95	111.14
1	C	1666	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	G	4501	PRO	N-CA-CB	5.72	108.42	103.27
1	D	1919	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	C	1389	PRO	CA-C-N	5.71	130.25	120.71
1	C	1389	PRO	C-N-CA	5.71	130.25	120.71
1	H	5294	ASN	CA-CB-CG	-5.71	106.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	4927	GLY	N-CA-C	-5.70	105.69	115.61
1	F	3759	ASP	CB-CA-C	-5.68	100.30	110.70
1	B	1127	VAL	N-CA-C	5.67	115.42	109.01
1	C	1501	PRO	N-CA-CB	5.63	108.21	103.25
1	D	2042	SER	N-CA-C	5.63	118.01	110.35
1	H	5079	PHE	CA-CB-CG	-5.62	108.19	113.80
1	C	1377	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	353	ASP	N-CA-CB	5.60	118.36	110.12
1	C	1237	ALA	N-CA-C	5.59	116.94	109.83
1	E	3168	ASP	CB-CA-C	-5.59	100.80	111.48
1	D	2309	ILE	N-CA-CB	5.59	116.81	110.72
1	C	1701	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	324	ILE	CA-C-N	-5.58	115.35	122.77
1	A	324	ILE	C-N-CA	-5.58	115.35	122.77
1	G	4644	ARG	CB-CA-C	-5.58	106.15	111.00
1	A	276	VAL	N-CA-CB	5.56	116.68	110.62
1	A	293	ARG	N-CA-C	5.53	119.29	112.54
1	F	3815	VAL	N-CA-C	5.53	115.22	107.37
1	C	1553	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	402	SER	N-CA-C	5.51	119.50	112.34
1	F	3759	ASP	CA-CB-CG	5.50	118.10	112.60
1	F	3791	PHE	CA-CB-CG	-5.50	108.31	113.80
1	F	3901	PRO	N-CA-CB	5.49	108.19	103.31
1	A	112	ASP	CA-C-N	5.49	128.89	120.82
1	A	112	ASP	C-N-CA	5.49	128.89	120.82
1	H	5205	THR	OG1-CB-CG2	5.47	120.25	109.30
1	A	116	PRO	N-CA-CB	5.47	106.23	102.35
1	B	872	ASN	CA-CB-CG	5.45	118.05	112.60
1	F	3961	SER	CA-C-O	5.45	122.88	119.77
1	A	495	VAL	N-CA-C	5.44	115.64	110.42
1	E	3049	THR	CA-C-N	-5.44	116.08	122.93
1	E	3049	THR	C-N-CA	-5.44	116.08	122.93
1	H	4906	PRO	N-CA-CB	5.43	108.39	103.34
1	B	901	PRO	N-CA-CB	5.43	108.16	103.27
1	H	4872	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	245	ARG	CA-C-O	5.42	124.78	118.77
1	F	3713	THR	N-CA-CB	-5.41	102.38	110.17
1	C	1326	SER	CA-C-N	-5.41	115.78	123.08
1	C	1326	SER	C-N-CA	-5.41	115.78	123.08
1	A	467	GLY	CA-C-N	-5.40	115.62	122.37
1	A	467	GLY	C-N-CA	-5.40	115.62	122.37
1	D	1977	ASP	CA-CB-CG	5.40	118.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLY	C-N-CD	-5.40	102.87	125.00
1	A	336	LYS	CA-C-N	5.39	124.91	119.19
1	A	336	LYS	C-N-CA	5.39	124.91	119.19
1	H	5205	THR	CA-CB-CG2	5.39	119.67	110.50
1	A	472	VAL	N-CA-CB	5.38	116.39	110.53
1	G	4728	PRO	CB-CA-C	-5.37	102.69	111.56
1	E	3113	THR	N-CA-CB	-5.37	102.68	110.36
1	A	192	LEU	N-CA-CB	5.37	121.50	111.52
1	D	2189	PHE	CA-C-N	5.36	127.46	120.28
1	D	2189	PHE	C-N-CA	5.36	127.46	120.28
1	C	1602	SER	N-CA-C	5.35	117.80	111.33
1	A	313	ILE	N-CA-CB	5.35	116.81	110.55
1	D	1855	ARG	CB-CA-C	-5.35	100.74	110.63
1	F	3643	ASN	N-CA-C	5.35	119.52	112.89
1	G	4414	ALA	CA-C-N	-5.35	117.88	122.96
1	G	4414	ALA	C-N-CA	-5.35	117.88	122.96
1	D	1993	VAL	CB-CA-C	-5.34	104.50	110.96
1	G	4313	THR	N-CA-CB	-5.34	102.18	110.29
1	H	5299	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	D	1905	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	H	4915	GLY	CA-C-N	5.33	125.09	119.76
1	H	4915	GLY	C-N-CA	5.33	125.09	119.76
1	H	5090	MET	CG-SD-CE	-5.32	89.19	100.90
1	F	4099	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	1099	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	G	4410	LEU	O-C-N	5.29	126.09	121.17
1	A	499	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	2299	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	495	VAL	N-CA-CB	5.27	116.72	110.55
1	F	3705	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	E	3210	LEU	CA-C-N	5.27	126.42	119.84
1	E	3210	LEU	C-N-CA	5.27	126.42	119.84
1	E	3499	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	C	1305	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	919	ALA	CA-C-O	5.25	125.63	119.28
1	C	1699	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	D	1938	THR	N-CA-CB	5.24	119.17	110.63
1	G	4699	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	D	1991	PHE	CA-CB-CG	-5.24	108.56	113.80
1	F	3712	ASP	CA-C-N	5.23	129.14	120.94
1	F	3712	ASP	C-N-CA	5.23	129.14	120.94
1	C	1264	ILE	CB-CA-C	-5.22	105.29	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1534	ILE	N-CA-C	-5.20	104.47	111.44
1	C	1726	VAL	CB-CA-C	5.19	118.08	110.98
1	D	1919	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	705	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	E	3144	ASP	N-CA-C	5.18	116.61	109.15
1	E	3147	TYR	CA-CB-CG	-5.17	104.60	113.90
1	H	5079	PHE	N-CA-C	5.17	117.31	111.11
1	G	4531	GLU	N-CA-C	5.16	117.31	111.11
1	E	3102	ILE	CA-C-O	5.16	125.02	119.91
1	H	5272	VAL	N-CA-CB	5.14	116.13	110.53
1	E	3434	GLY	CA-C-O	5.14	124.49	119.04
1	A	113	THR	N-CA-C	5.13	116.91	110.24
1	H	5127	THR	N-CA-C	5.13	121.73	110.80
1	G	4505	VAL	N-CA-C	5.13	117.46	111.05
1	A	326	ALA	N-CA-C	5.12	117.46	109.52
1	E	3220	VAL	CB-CA-C	-5.12	104.33	110.99
1	D	2272	VAL	N-CA-C	5.12	114.64	107.37
1	H	5066	ILE	N-CA-C	5.12	114.94	107.37
1	B	705	ARG	CA-C-N	5.12	124.88	119.76
1	B	705	ARG	C-N-CA	5.12	124.88	119.76
1	D	2139	PRO	CB-CA-C	-5.11	103.19	110.75
1	E	3210	LEU	C-N-CD	-5.11	104.05	125.00
1	D	2308	VAL	N-CA-CB	-5.10	102.49	111.93
1	D	2232	GLU	N-CA-CB	5.10	117.80	110.40
1	D	2249	ILE	CA-C-N	-5.10	116.25	122.93
1	D	2249	ILE	C-N-CA	-5.10	116.25	122.93
1	G	4344	ASP	N-CA-C	5.09	116.99	108.23
1	G	4519	ALA	CA-C-N	-5.09	115.13	122.00
1	G	4519	ALA	C-N-CA	-5.09	115.13	122.00
1	G	4442	SER	N-CA-C	5.09	117.81	110.28
1	H	4976	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	770	GLY	CA-C-N	-5.06	113.68	122.64
1	B	770	GLY	C-N-CA	-5.06	113.68	122.64
1	E	3326	ALA	N-CA-C	5.05	116.86	109.24
1	F	3791	PHE	N-CA-C	5.04	115.80	108.14
1	C	1667	GLY	CA-C-N	-5.04	114.71	121.66
1	C	1667	GLY	C-N-CA	-5.04	114.71	121.66
1	F	3637	ALA	N-CA-C	5.04	116.18	109.93
1	B	681	GLU	CB-CA-C	5.04	119.15	110.79
1	C	1424	ASP	N-CA-C	-5.03	104.88	111.02
1	C	1505	VAL	N-CA-C	5.03	115.75	110.62
1	C	1697	LYS	CA-C-N	5.03	127.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1697	LYS	C-N-CA	5.03	127.53	120.28
1	E	3075	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	476	PRO	N-CA-CB	5.01	107.98	103.33
1	B	1092	ALA	CA-C-O	5.01	125.55	119.49
1	D	2203	HIS	CA-CB-CG	-5.01	108.79	113.80
1	G	4645	PRO	CB-CA-C	-5.00	103.67	111.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	5205	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	759	ASP	Mainchain
1	C	1599	ARG	Mainchain

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	4055	339	2
1	B	3978	0	4056	224	1
1	C	3978	0	4055	326	3
1	D	3978	0	4055	262	5
1	E	3978	0	4056	240	14
1	F	3978	0	4055	252	2
1	G	3978	0	4055	287	2
1	H	3978	0	4055	199	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1	0	0	0	0
3	A	6	0	0	2	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0
3	E	6	0	0	0	0
3	F	6	0	0	3	0
3	G	6	0	0	1	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	3	0
5	C	31	0	12	3	0
5	D	31	0	12	1	0
5	E	31	0	12	0	0
5	F	31	0	12	0	0
5	G	31	0	12	1	0
6	A	195	0	0	11	0
6	B	270	0	0	16	0
6	C	178	0	0	11	0
6	D	272	0	0	21	0
6	E	279	0	0	15	0
6	F	197	0	0	9	0
6	G	228	0	0	7	0
6	H	302	0	0	13	3
All	All	34001	0	32514	2022	25

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 31.

All (2022) 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:499:ARG:NH2	6:A:6596:HOH:O	1.57	1.36
1:D:1850:ILE:HD11	1:D:1868:MET:HE1	1.17	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3493:MET:HE2	1:E:3530:PRO:HD2	1.23	1.14
1:C:1693:MET:HE2	1:C:1729:VAL:HG22	1.25	1.11
1:E:3048:CYS:HB2	1:E:3068:MET:HE3	1.32	1.10
1:E:3142:THR:HG22	1:E:3144:ASP:H	1.05	1.10
1:H:4850:ILE:HD11	1:H:4868:MET:HE1	1.13	1.10
1:G:4250:ILE:HD11	1:G:4268:MET:HE1	1.23	1.09
1:G:4250:ILE:HB	1:G:4273:MET:HE3	1.36	1.08
1:H:4848:CYS:HB2	1:H:4868:MET:HE3	1.32	1.08
1:C:1248:CYS:HB2	1:C:1268:MET:HE3	1.08	1.07
1:G:4665:TYR:HB2	1:G:4668:ILE:HD12	1.36	1.07
1:C:1678:GLN:HB2	1:C:1684:ASP:HB2	1.31	1.06
1:F:3624:THR:HG22	1:F:3627:GLU:H	1.21	1.05
1:D:1848:CYS:HB2	1:D:1868:MET:HE3	1.39	1.03
1:E:3376:MET:HA	1:E:3376:MET:HE3	1.41	1.03
1:A:122:LEU:HD23	1:A:204:SER:HB3	1.41	1.02
1:H:5133:MET:HE2	1:H:5139:PRO:HB3	1.40	1.02
1:G:4367:VAL:HG22	1:G:4371:SER:HB3	1.42	1.01
1:D:1850:ILE:HB	1:D:1873:MET:HE3	1.44	0.97
1:B:928:GLN:NE2	1:D:2141:ARG:H	1.63	0.96
1:D:2044:ILE:HG22	1:D:2082:ILE:HD12	1.47	0.96
1:G:4680:ALA:HB3	1:G:4683:GLU:HG3	1.48	0.96
1:F:3941:ARG:H	1:H:5128:GLN:HE21	1.13	0.95
1:B:703:LEU:HD23	1:B:1099:ARG:NH2	1.82	0.95
1:C:1257:VAL:HG21	1:C:1292:THR:HG22	1.48	0.94
1:F:3648:CYS:HB2	1:F:3668:MET:HE2	1.48	0.94
1:A:191:PHE:HE2	1:A:193:VAL:HG23	1.32	0.93
1:A:431:THR:HG21	1:A:434:GLY:HA2	1.49	0.93
1:A:160:TYR:HD2	1:A:163:ILE:HB	1.30	0.92
1:B:648:CYS:HB2	1:B:668:MET:HE3	1.52	0.92
1:E:3160:TYR:HD2	1:E:3163:ILE:HB	1.34	0.92
1:B:815:VAL:HB	1:B:817:LEU:HD12	1.51	0.92
1:F:3743:LEU:HD11	1:F:3761:LYS:HA	1.51	0.91
1:G:4593:LEU:HD21	1:G:4644:ARG:HG3	1.53	0.91
1:E:3050:ILE:HD11	1:E:3068:MET:HE1	1.52	0.91
1:G:4479:PHE:CZ	1:G:4483:LEU:HD22	2.06	0.90
1:C:1479:PHE:HE1	1:C:1489:ILE:HD12	1.35	0.90
1:C:1322:LEU:HD12	1:C:1349:GLU:HG2	1.53	0.90
1:H:5133:MET:HE2	1:H:5139:PRO:CB	2.00	0.89
1:G:4389:PRO:HD2	1:G:4391:PHE:CE2	2.08	0.89
1:H:5020:VAL:HG13	1:H:5024:ASP:HB2	1.55	0.89
1:A:328:GLN:NE2	1:C:1541:ARG:H	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1526:ALA:HB1	1:C:1559:MET:HE2	1.55	0.89
1:A:514:TRP:H	1:A:522:ASN:HD21	1.17	0.88
1:B:650:ILE:HD11	1:B:668:MET:HE1	1.56	0.88
1:G:4408:VAL:HG12	1:G:4410:LEU:HD11	1.56	0.88
1:A:141:ILE:HG21	1:A:158:LEU:HD22	1.56	0.88
1:E:3142:THR:HG22	1:E:3144:ASP:N	1.88	0.87
1:C:1693:MET:CE	1:C:1729:VAL:HG22	2.04	0.87
1:H:5015:VAL:HG11	1:H:5017:LEU:HD12	1.57	0.87
1:C:1319:ARG:H	1:C:1359:ASP:HB2	1.39	0.86
1:G:4408:VAL:HG12	1:G:4410:LEU:CD1	2.06	0.86
1:F:3928:GLN:NE2	1:H:5141:ARG:H	1.74	0.86
1:B:976:MET:HE3	1:B:980:ILE:HG13	1.58	0.85
1:E:3191:PHE:HE1	1:E:3193:VAL:HG23	1.39	0.85
1:G:4276:SER:HB3	1:G:4319:ARG:HE	1.41	0.85
1:A:126:SER:HB3	1:A:129:ALA:HB2	1.57	0.85
1:B:648:CYS:HB2	1:B:668:MET:CE	2.06	0.85
1:A:120:THR:HG22	1:A:205:LYS:N	1.90	0.85
1:A:48:CYS:HB2	1:A:68:MET:HE2	1.57	0.85
1:A:118:ILE:CG2	1:A:208:VAL:HB	2.06	0.85
1:C:1248:CYS:CB	1:C:1268:MET:HE3	2.03	0.85
1:H:5327:VAL:HG13	1:H:5328:PRO:HD2	1.58	0.85
1:F:3650:ILE:HD11	1:F:3668:MET:HE1	1.56	0.84
1:C:1477:ARG:NH2	1:C:1478:ARG:HH11	1.75	0.84
1:F:3941:ARG:H	1:H:5128:GLN:NE2	1.73	0.84
1:H:5130:LEU:HD13	1:H:5133:MET:HE3	1.60	0.84
1:A:73:MET:HE2	1:A:86:THR:HG21	1.58	0.84
1:D:1850:ILE:HD11	1:D:1868:MET:CE	2.05	0.84
1:A:103:LEU:HD11	1:A:498:ALA:HB1	1.59	0.83
1:A:225:ILE:HG23	1:A:256:ILE:CG2	2.08	0.83
1:D:2304:LYS:HG3	1:D:2330:PRO:C	2.02	0.83
1:C:1248:CYS:HB2	1:C:1268:MET:CE	2.02	0.83
1:D:1902:ILE:HG13	1:D:2295:VAL:HG22	1.61	0.83
1:D:1824:THR:HG22	1:D:1827:GLU:HB2	1.60	0.83
1:D:2201:SER:HA	1:D:2203:HIS:CE1	2.13	0.83
1:H:4942:THR:HG23	1:H:4944:ASP:H	1.39	0.83
1:D:1824:THR:HG23	1:D:1827:GLU:H	1.43	0.83
1:C:1250:ILE:HB	1:C:1273:MET:HE3	1.59	0.82
1:F:3726:SER:CB	1:F:3729:ALA:HB2	2.08	0.82
1:B:1104:LYS:HB3	1:B:1130:PRO:C	2.04	0.82
1:A:160:TYR:O	1:A:163:ILE:HG22	1.79	0.82
1:D:1899:SER:O	1:D:1901:PRO:HD3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3890:MET:HE3	1:F:3926:ALA:CB	2.08	0.82
1:A:431:THR:CG2	1:A:434:GLY:HA2	2.08	0.82
1:H:5130:LEU:HD13	1:H:5133:MET:CE	2.09	0.82
1:E:3493:MET:CE	1:E:3529:VAL:HG13	2.10	0.82
1:G:4248:CYS:HB2	1:G:4268:MET:HE3	1.62	0.82
1:D:2176:MET:HE3	1:D:2176:MET:HA	1.60	0.82
1:E:3186:GLN:HB3	1:E:3193:VAL:HB	1.60	0.82
1:H:4873:MET:HG3	1:H:4887:ILE:HD11	1.61	0.82
1:F:3624:THR:CG2	1:F:3627:GLU:H	1.92	0.82
1:B:720:THR:HG22	1:B:758:LEU:CD2	2.10	0.81
1:A:328:GLN:HE21	1:C:1541:ARG:H	1.25	0.81
1:D:1824:THR:HG22	1:D:1827:GLU:CB	2.10	0.81
1:D:2176:MET:CE	1:D:2179:LEU:HB2	2.10	0.81
1:E:3050:ILE:HD11	1:E:3068:MET:CE	2.10	0.81
1:E:3493:MET:HE2	1:E:3530:PRO:CD	2.06	0.81
1:C:1442:SER:HA	1:C:1469:LYS:HD3	1.63	0.81
1:B:1109:ILE:CD1	1:B:1126:VAL:HG22	2.10	0.81
1:E:3160:TYR:O	1:E:3163:ILE:HG22	1.80	0.81
1:F:3949:ASN:HD21	1:H:5110:LYS:NZ	1.79	0.81
1:G:4367:VAL:HG22	1:G:4371:SER:CB	2.11	0.81
1:A:118:ILE:HG22	1:A:208:VAL:HB	1.63	0.80
1:A:277:ARG:NH2	1:A:278:ARG:NH1	2.30	0.80
1:F:3776:ASP:HB3	1:F:3779:LEU:HB3	1.64	0.80
1:G:4305:ARG:HD3	1:G:4699:ARG:NH1	1.96	0.80
1:C:1678:GLN:HB2	1:C:1684:ASP:CB	2.11	0.80
1:G:4333:LEU:HG	1:G:4402:LEU:HD23	1.62	0.80
1:E:3106:PRO:HG2	1:E:3470:PRO:HB2	1.63	0.80
1:G:4322:LEU:HD23	1:G:4404:SER:CB	2.12	0.80
1:C:1273:MET:HE2	1:C:1286:THR:HG22	1.63	0.80
1:H:4850:ILE:HD11	1:H:4868:MET:CE	2.07	0.80
1:F:3803:GLY:HA3	1:F:3806:LYS:HE2	1.64	0.80
1:A:69:ASN:HB3	1:A:463:HIS:ND1	1.98	0.79
1:D:1905:ARG:NH1	1:D:2299:ARG:HH21	1.79	0.79
1:E:3162:ASN:HD21	1:E:3165:LYS:HD3	1.47	0.79
1:E:3191:PHE:C	1:E:3192:LEU:HD22	2.07	0.79
1:E:3341:ARG:H	1:G:4528:GLN:HE21	1.30	0.79
1:F:3648:CYS:HB2	1:F:3668:MET:CE	2.13	0.79
1:F:3726:SER:HB3	1:F:3729:ALA:HB2	1.62	0.79
1:A:73:MET:HE2	1:A:86:THR:CG2	2.11	0.79
1:A:120:THR:HG22	1:A:205:LYS:H	1.44	0.79
1:C:1409:ASN:O	1:C:1411:PRO:HD3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3158:LEU:HD11	1:E:3208:VAL:HG21	1.64	0.79
1:A:63:MET:HE2	1:A:68:MET:CE	2.13	0.79
1:B:928:GLN:HE21	1:D:2141:ARG:H	1.27	0.79
1:A:327:THR:HG22	1:A:328:GLN:HG3	1.63	0.79
1:A:391:ARG:O	1:A:395:GLU:HG3	1.83	0.79
1:C:1343:LEU:CD2	1:C:1361:LYS:HA	2.12	0.79
1:A:411:MET:HE2	1:A:522:ASN:C	2.07	0.78
1:G:4680:ALA:HB3	1:G:4683:GLU:CG	2.14	0.78
1:D:1945:ASN:HD21	1:D:1961:LYS:NZ	1.80	0.78
1:H:4848:CYS:HB2	1:H:4868:MET:CE	2.10	0.78
1:H:5133:MET:HE1	1:H:5176:MET:HG2	1.65	0.78
1:A:191:PHE:CE2	1:A:193:VAL:HG23	2.17	0.78
1:H:5133:MET:HE2	1:H:5139:PRO:CG	2.12	0.78
1:H:5311:LEU:HB3	1:H:5321:THR:CG2	2.13	0.78
1:G:4313:THR:CG2	1:G:4442:SER:H	1.97	0.78
1:C:1259:THR:O	1:C:1263:MET:HG3	1.83	0.78
1:G:4313:THR:HG22	1:G:4442:SER:H	1.47	0.78
1:B:897:GLY:HA3	1:D:2141:ARG:HE	1.49	0.77
1:C:1534:ILE:HG23	1:C:1567:GLY:HA2	1.67	0.77
1:C:1479:PHE:CE1	1:C:1489:ILE:HD12	2.19	0.77
1:G:4339:LEU:HD11	1:G:4354:ASN:CA	2.15	0.77
1:H:5090:MET:HE3	1:H:5126:ALA:CB	2.14	0.77
1:H:4905:ARG:NH2	1:H:5299:ARG:HD3	1.99	0.77
1:D:1824:THR:CG2	1:D:1827:GLU:H	1.96	0.77
1:D:1848:CYS:HB2	1:D:1868:MET:CE	2.13	0.77
1:E:3509:ILE:CD1	1:E:3526:VAL:HG23	2.14	0.77
1:H:4926:SER:HB3	1:H:4929:ALA:H	1.48	0.77
1:B:759:ASP:HB3	6:B:6599:HOH:O	1.85	0.77
1:G:4216:GLN:HE22	1:G:4233:ASP:H	1.33	0.77
1:C:1257:VAL:HG21	1:C:1292:THR:CG2	2.15	0.77
1:A:288:GLY:O	1:A:289:ILE:HD13	1.84	0.77
1:B:989:PHE:CE2	1:B:992:LYS:HD2	2.20	0.76
1:C:1347:TYR:CD2	1:C:1355:ILE:HG21	2.19	0.76
1:H:4952:ASP:HB2	1:H:4953:GLU:OE1	1.85	0.76
1:C:1376:ASP:OD2	1:C:1406:LYS:HE2	1.84	0.76
1:C:1477:ARG:HH22	1:C:1478:ARG:HH11	1.34	0.76
1:D:2284:ASP:O	1:D:2288:ARG:HG3	1.86	0.76
1:G:4369:VAL:HA	1:G:4384:VAL:HG12	1.67	0.76
1:A:47:ILE:HG22	1:A:359:MET:HG3	1.66	0.76
1:A:181:SER:C	1:A:182:LEU:HD23	2.10	0.76
1:C:1477:ARG:HH22	1:C:1478:ARG:NH1	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3724:LYS:HG3	6:F:7473:HOH:O	1.85	0.76
1:D:2038:MET:CE	1:D:2264:LEU:HD11	2.16	0.76
1:A:47:ILE:CG2	1:A:359:MET:HG3	2.16	0.76
1:C:1602:SER:HB2	1:D:1821:MET:HE1	1.67	0.76
1:H:4945:ASN:HB3	1:H:4948:MET:HE2	1.67	0.76
1:C:1286:THR:O	1:C:1290:VAL:HG23	1.86	0.76
1:F:3663:MET:CE	1:F:3668:MET:HE3	2.15	0.76
1:C:1472:ASN:ND2	1:C:1475:GLY:H	1.82	0.75
1:E:3341:ARG:H	1:G:4528:GLN:NE2	1.83	0.75
1:G:4257:VAL:O	1:G:4261:LYS:HG3	1.86	0.75
1:A:131:VAL:CG1	1:A:202:LEU:HD23	2.15	0.75
1:D:2141:ARG:HG2	1:D:2141:ARG:HH11	1.50	0.75
1:E:3481:TRP:CG	1:E:3516:PRO:HD3	2.21	0.75
1:A:50:ILE:HB	1:A:73:MET:CE	2.15	0.75
1:C:1493:ARG:HD3	1:C:1526:ALA:O	1.86	0.75
1:C:1723:THR:HG23	1:D:2325:ARG:HG3	1.68	0.75
1:F:3752:ASP:OD1	1:F:3755:ILE:HD13	1.87	0.75
1:G:4704:LYS:HG2	1:G:4730:PRO:C	2.10	0.75
1:E:3113:THR:HG22	1:E:3242:SER:H	1.52	0.75
1:E:3493:MET:CE	1:E:3530:PRO:HD2	2.12	0.75
1:E:3479:GLU:HG3	6:E:6695:HOH:O	1.85	0.75
1:F:3845:ARG:HG2	1:F:3874:GLU:HB3	1.66	0.75
1:G:4715:ARG:HB3	1:G:4716:PRO:HD2	1.67	0.75
1:D:1958:LEU:CD2	1:D:2008:VAL:HG21	2.16	0.75
1:D:2201:SER:HA	1:D:2203:HIS:HE1	1.51	0.75
1:G:4360:TYR:HE2	1:G:4366:VAL:HG21	1.52	0.75
1:B:815:VAL:HG22	6:B:6919:HOH:O	1.86	0.75
1:E:3246:LYS:HD2	1:E:3249:ASP:OD1	1.87	0.75
1:G:4438:MET:HA	1:G:4464:ILE:HG23	1.68	0.75
1:B:651:GLY:O	1:B:655:ARG:HG3	1.86	0.75
1:C:1404:SER:O	1:C:1406:LYS:HD3	1.86	0.74
1:C:1428:LEU:HD13	1:C:1456:ILE:HB	1.69	0.74
1:A:113:THR:CG2	1:A:242:SER:H	2.00	0.74
1:B:1011:MET:HE2	1:B:1122:ASN:C	2.12	0.74
1:C:1678:GLN:HA	1:C:1678:GLN:NE2	2.02	0.74
1:F:3949:ASN:HD21	1:H:5110:LYS:HZ1	1.32	0.74
1:C:1406:LYS:HE3	5:C:1735:ATP:O3'	1.87	0.74
1:G:4371:SER:H	1:G:4384:VAL:HB	1.51	0.74
1:D:2295:VAL:HG12	1:D:2299:ARG:HD2	1.68	0.74
1:H:4850:ILE:CD1	1:H:4868:MET:HE1	2.06	0.74
1:E:3160:TYR:CD2	1:E:3163:ILE:HB	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4248:CYS:HB2	1:G:4268:MET:CE	2.18	0.74
1:A:515:ARG:HD2	6:A:6021:HOH:O	1.86	0.74
1:C:1368:ASP:HB3	6:C:7539:HOH:O	1.88	0.74
1:F:3663:MET:HE3	1:F:3668:MET:HE3	1.67	0.74
6:B:6064:HOH:O	1:D:1824:THR:HG21	1.86	0.74
1:C:1728:PRO:O	1:C:1730:PRO:HD3	1.88	0.74
1:B:815:VAL:HB	1:B:817:LEU:CD1	2.17	0.73
1:B:1087:LEU:HD23	1:B:1088:ARG:N	2.03	0.73
1:D:1986:GLN:HB3	1:D:1993:VAL:HB	1.70	0.73
1:G:4305:ARG:HH22	1:G:4663:HIS:HE1	1.36	0.73
1:B:823:LYS:HE3	1:B:827:ASP:OD2	1.88	0.73
1:E:3402:SER:HB2	1:F:3621:MET:HE1	1.70	0.73
1:F:3732:GLU:HB2	1:F:3801:PHE:CD1	2.22	0.73
1:G:4498:ILE:HD13	1:G:4498:ILE:N	2.02	0.73
1:C:1671:VAL:HG12	1:C:1691:LEU:HD21	1.70	0.73
1:G:4348:MET:HA	1:G:4357:TRP:CD2	2.24	0.73
1:C:1343:LEU:HD13	1:C:1390:ASP:O	1.89	0.73
1:F:3750:LYS:O	1:F:3755:ILE:HD11	1.88	0.73
1:H:5209:GLU:O	1:H:5213:MET:HG3	1.88	0.73
1:B:991:ARG:O	1:B:995:GLU:HG3	1.88	0.73
1:C:1422:GLU:O	1:C:1425:ILE:HB	1.88	0.73
1:D:2038:MET:HE2	1:D:2264:LEU:HD11	1.71	0.73
1:F:3672:ARG:C	1:F:3673:MET:HE3	2.14	0.73
1:H:5020:VAL:HG11	1:H:5025:ILE:HG12	1.70	0.73
1:A:326:ALA:HB1	1:A:359:MET:HE2	1.71	0.73
1:B:976:MET:HE3	1:B:980:ILE:CG1	2.18	0.73
1:D:2176:MET:HE3	1:D:2179:LEU:HB2	1.69	0.73
1:F:3650:ILE:CD1	1:F:3668:MET:HE1	2.19	0.73
1:C:1665:TYR:HB2	1:C:1668:ILE:HD12	1.70	0.73
1:E:3316:CYS:HB3	1:E:3321:LYS:O	1.89	0.73
1:F:3723:ILE:HA	1:F:3751:CYS:O	1.89	0.73
1:A:399:ARG:NH2	1:C:1223:ASP:HB2	2.04	0.73
1:A:14:THR:HG23	1:A:15:GLN:HB2	1.69	0.73
1:C:1291:ARG:O	1:C:1295:GLU:HG2	1.89	0.73
1:G:4680:ALA:CB	1:G:4683:GLU:HG3	2.18	0.73
1:G:4681:TRP:CD2	1:G:4716:PRO:HD3	2.24	0.73
1:D:1873:MET:HE2	1:D:1886:THR:HG22	1.70	0.72
1:F:3892:ALA:HB1	3:F:4133:OXL:C2	2.19	0.72
1:B:938:ARG:HH22	1:D:1998:ASN:HD21	1.37	0.72
1:G:4250:ILE:HB	1:G:4273:MET:CE	2.17	0.72
1:B:1091:LEU:O	1:B:1095:VAL:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1850:ILE:CD1	1:D:1868:MET:HE1	2.09	0.72
1:H:4873:MET:HE3	1:H:4887:ILE:HD13	1.72	0.72
1:A:93:ALA:O	1:A:96:SER:HB3	1.89	0.72
1:C:1313:THR:HG22	1:C:1442:SER:H	1.53	0.72
1:D:2265:TYR:HB2	1:D:2268:ILE:HD12	1.70	0.72
1:F:3739:LEU:HD21	1:F:3756:LEU:HB2	1.71	0.72
1:F:3763:ILE:O	1:F:3767:VAL:HG13	1.90	0.72
1:A:102:ILE:HG22	1:A:103:LEU:CD1	2.20	0.72
1:E:3493:MET:HE1	1:E:3529:VAL:HG13	1.72	0.72
1:F:3740:LYS:HE2	1:F:3791:PHE:CD2	2.24	0.72
1:A:167:VAL:HG21	1:A:184:VAL:HG21	1.72	0.72
1:C:1257:VAL:CG2	1:C:1292:THR:HG22	2.19	0.72
1:A:503:LYS:O	1:A:506:ASP:HB2	1.89	0.71
1:H:5108:ALA:O	1:H:5112:ILE:HG13	1.88	0.71
1:B:703:LEU:CD2	1:B:1099:ARG:NH2	2.54	0.71
1:C:1250:ILE:HD11	1:C:1268:MET:HE1	1.71	0.71
1:G:4647:ALA:HB1	1:G:4648:PRO:HD2	1.72	0.71
1:A:484:ASP:O	1:A:487:LEU:HB3	1.91	0.71
1:F:4008:MET:HG3	1:F:4039:GLN:HG2	1.71	0.71
1:A:421:LYS:HE2	1:B:1013:MET:SD	2.30	0.71
1:A:511:LEU:HD22	1:A:521:THR:HG23	1.71	0.71
1:F:3890:MET:HE3	1:F:3926:ALA:HB3	1.71	0.71
1:A:18:HIS:O	1:A:21:MET:HB2	1.91	0.71
1:A:48:CYS:CB	1:A:68:MET:HE2	2.20	0.71
1:A:55:ARG:HD2	1:A:82:TYR:CZ	2.26	0.71
1:D:1839:ILE:O	1:D:2182:ARG:HD2	1.90	0.71
1:G:4322:LEU:CD2	1:G:4327:GLY:HA2	2.20	0.71
1:E:3172:LYS:HE2	1:E:3197:GLU:OE1	1.91	0.71
1:A:481:TRP:O	1:A:485:VAL:HG23	1.90	0.70
1:E:3099:SER:O	1:E:3101:PRO:HD3	1.91	0.70
1:E:3300:ILE:HB	1:E:3301:PRO:HD2	1.73	0.70
1:G:4243:ASN:HB3	1:G:4667:GLY:HA2	1.71	0.70
1:A:225:ILE:HG23	1:A:256:ILE:HG21	1.74	0.70
1:H:5090:MET:HE3	1:H:5126:ALA:HB3	1.72	0.70
1:C:1323:ILE:HG22	1:C:1324:LYS:HG3	1.73	0.70
1:A:231:GLY:O	1:A:236:VAL:HG13	1.92	0.70
1:B:1093:MET:HE2	1:B:1129:VAL:HG22	1.73	0.70
1:H:5311:LEU:HB3	1:H:5321:THR:HG21	1.74	0.70
1:D:1910:ALA:HB2	1:D:2038:MET:HG3	1.73	0.70
1:E:3276:VAL:HG11	1:G:4234:ILE:HD13	1.73	0.70
1:A:145:ASN:O	1:A:148:MET:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1814:THR:HG22	1:D:1815:GLN:HG3	1.72	0.70
1:F:3723:ILE:HD11	1:F:3803:GLY:O	1.91	0.70
1:F:4093:MET:HE2	1:F:4129:VAL:HG22	1.72	0.70
1:G:4322:LEU:HD23	1:G:4404:SER:HB3	1.71	0.70
1:E:3432:GLU:HA	1:E:3432:GLU:OE1	1.91	0.70
1:F:3650:ILE:HD11	1:F:3668:MET:CE	2.22	0.70
1:G:4509:GLN:O	1:G:4513:ILE:HG13	1.92	0.70
1:H:4963:ILE:O	1:H:4967:VAL:HG22	1.92	0.70
1:C:1387:LYS:HB3	1:C:1392:LEU:HD12	1.74	0.69
1:G:4339:LEU:HD11	1:G:4354:ASN:HA	1.72	0.69
1:A:192:LEU:HD22	1:A:192:LEU:N	2.07	0.69
1:B:705:ARG:NE	1:B:1099:ARG:HH12	1.90	0.69
1:E:3027:GLU:O	1:E:3031:ARG:HG3	1.92	0.69
1:F:3928:GLN:HE21	1:H:5141:ARG:H	1.39	0.69
1:H:4848:CYS:CB	1:H:4868:MET:HE3	2.15	0.69
1:A:126:SER:HB3	1:A:129:ALA:CB	2.22	0.69
1:G:4409:ASN:C	1:G:4410:LEU:HD12	2.17	0.69
1:C:1343:LEU:HD21	1:C:1361:LYS:HA	1.74	0.69
1:D:2176:MET:HE2	1:D:2180:ILE:HG13	1.74	0.69
1:F:3740:LYS:HE2	1:F:3791:PHE:CG	2.27	0.69
1:E:3142:THR:CG2	1:E:3144:ASP:H	1.97	0.69
1:A:51:GLY:O	1:A:55:ARG:HG3	1.91	0.69
1:A:413:MET:SD	1:B:1021:LYS:HD3	2.32	0.69
1:C:1609:GLU:O	1:C:1613:MET:HG3	1.93	0.69
1:B:650:ILE:CD1	1:B:668:MET:HE1	2.22	0.69
1:C:1678:GLN:CB	1:C:1684:ASP:HB2	2.18	0.69
1:D:1902:ILE:HG22	1:D:1903:LEU:CD2	2.23	0.69
1:H:4873:MET:CG	1:H:4887:ILE:HD11	2.22	0.69
1:A:160:TYR:CD2	1:A:163:ILE:HB	2.20	0.69
1:F:3752:ASP:CG	1:F:3754:ASN:H	2.00	0.69
1:D:1814:THR:HG23	1:D:1837:ALA:O	1.91	0.69
1:D:1851:GLY:O	1:D:1855:ARG:HG3	1.93	0.69
1:E:3245:ARG:HB3	1:E:3274:GLU:HG2	1.75	0.69
1:E:3253:VAL:HG12	1:E:3257:LEU:CD2	2.23	0.69
1:H:4942:THR:CG2	1:H:4944:ASP:H	2.06	0.69
1:F:3890:MET:HE2	1:F:3892:ALA:HB2	1.74	0.68
1:A:225:ILE:HG23	1:A:256:ILE:HG23	1.73	0.68
1:E:3371:LEU:HB2	6:E:6194:HOH:O	1.93	0.68
1:H:5191:ARG:O	1:H:5195:GLU:HG3	1.93	0.68
1:A:172:LYS:HE3	1:A:197:GLU:OE1	1.92	0.68
1:B:705:ARG:CZ	1:B:1099:ARG:HH12	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3652:PRO:HD2	1:F:3965:ALA:O	1.93	0.68
1:G:4409:ASN:C	1:G:4411:PRO:HD3	2.19	0.68
1:G:4469:LYS:HD2	1:G:4490:MET:SD	2.33	0.68
1:H:4964:CYS:HB2	6:H:6481:HOH:O	1.93	0.68
1:E:3051:GLY:O	1:E:3055:ARG:HG3	1.94	0.68
1:G:4273:MET:HE2	1:G:4286:THR:CG2	2.23	0.68
1:H:4815:GLN:HG3	1:H:4839:ILE:HG23	1.74	0.68
1:H:4847:ILE:HG21	1:H:5159:MET:CE	2.24	0.68
1:C:1326:SER:HB3	1:C:1329:ALA:CB	2.24	0.68
1:G:4332:GLU:HA	1:G:4401:PHE:HA	1.76	0.68
1:C:1270:VAL:HG22	1:C:1308:ALA:HB3	1.75	0.68
1:C:1500:ILE:HB	1:C:1501:PRO:HD2	1.75	0.68
1:A:55:ARG:HD2	1:A:82:TYR:OH	1.93	0.68
1:B:703:LEU:CD2	1:B:1099:ARG:HH21	2.07	0.68
1:C:1423:LYS:O	1:C:1426:GLN:HB3	1.93	0.68
1:G:4305:ARG:NH2	1:G:4663:HIS:HE1	1.91	0.68
1:E:3252:GLU:O	1:E:3256:ILE:HG12	1.92	0.68
1:H:4843:ASN:HB3	1:H:5267:GLY:CA	2.22	0.67
1:D:2281:TRP:CG	1:D:2316:PRO:HD3	2.29	0.67
1:F:3733:LEU:HD11	1:F:3802:LEU:HD22	1.76	0.67
1:B:703:LEU:HD23	1:B:1099:ARG:HH21	1.58	0.67
1:E:3481:TRP:CD1	1:E:3516:PRO:HD3	2.29	0.67
1:G:4255:ARG:HD2	1:G:4282:TYR:OH	1.95	0.67
1:D:1855:ARG:NH2	1:D:1885:GLU:HG2	2.09	0.67
1:D:2044:ILE:CG2	1:D:2082:ILE:HD12	2.24	0.67
1:D:2171:LEU:O	1:D:2175:ARG:HG3	1.95	0.67
1:F:3828:LEU:O	1:F:3832:VAL:HG23	1.94	0.67
1:F:4104:LYS:HG3	1:F:4130:PRO:C	2.19	0.67
1:G:4585:GLU:HA	1:G:4588:MET:HE2	1.76	0.67
1:A:122:LEU:HD23	1:A:204:SER:CB	2.22	0.67
1:C:1322:LEU:HB2	1:C:1349:GLU:HA	1.76	0.67
1:A:328:GLN:HE22	1:C:1540:THR:HA	1.60	0.67
1:C:1251:GLY:O	1:C:1255:ARG:HG3	1.94	0.67
1:D:2291:LEU:O	1:D:2295:VAL:HG23	1.93	0.67
1:D:1848:CYS:CB	1:D:1868:MET:HE3	2.21	0.67
1:H:4850:ILE:HD13	1:H:4850:ILE:N	2.10	0.67
1:C:1273:MET:HE2	1:C:1286:THR:CG2	2.25	0.67
1:D:1850:ILE:CB	1:D:1873:MET:HE3	2.20	0.67
1:D:1958:LEU:HD21	1:D:2008:VAL:HG21	1.75	0.67
1:B:1109:ILE:HD12	1:B:1126:VAL:HG22	1.75	0.67
1:F:4093:MET:CE	1:F:4129:VAL:HG22	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:HB3	1:A:463:HIS:CE1	2.30	0.67
1:B:618:HIS:CE1	1:B:631:ARG:HD3	2.30	0.67
1:E:3254:ARG:NH2	1:E:3287:ASP:OD2	2.28	0.67
1:G:4322:LEU:HD22	1:G:4326:SER:O	1.95	0.67
1:C:1305:ARG:NE	1:C:1699:ARG:NH2	2.43	0.66
1:C:1370:GLY:O	1:C:1383:GLN:NE2	2.28	0.66
1:E:3050:ILE:CD1	1:E:3068:MET:HE1	2.25	0.66
1:F:4113:GLY:HA2	1:F:4122:ASN:OD1	1.95	0.66
1:A:191:PHE:HE2	1:A:193:VAL:CG2	2.08	0.66
1:A:238:MET:HE1	1:A:464:LEU:HD22	1.75	0.66
1:B:1078:GLN:NE2	1:B:1078:GLN:HA	2.09	0.66
1:C:1362:ASN:ND2	1:C:1365:LYS:HD2	2.10	0.66
1:D:2030:PHE:CE1	1:D:2034:GLN:HG3	2.30	0.66
1:D:2239:GLN:O	1:D:2242:ARG:HG2	1.95	0.66
1:E:3392:LYS:O	1:E:3396:GLU:HG3	1.96	0.66
1:F:3722:LEU:O	1:F:3751:CYS:N	2.25	0.66
1:B:928:GLN:NE2	1:D:2141:ARG:N	2.41	0.66
1:G:4243:ASN:HB3	1:G:4667:GLY:CA	2.25	0.66
1:H:4968:ASP:OD1	6:H:7656:HOH:O	2.11	0.66
1:C:1339:LEU:HD12	1:C:1340:LYS:H	1.61	0.66
1:A:167:VAL:CG2	1:A:184:VAL:HG21	2.25	0.66
1:E:3192:LEU:HD22	1:E:3192:LEU:N	2.11	0.66
1:A:15:GLN:HG3	1:A:39:ILE:HG23	1.77	0.66
1:G:4681:TRP:CG	1:G:4716:PRO:HD3	2.31	0.66
1:A:144:ASP:HB3	1:A:147:TYR:HD1	1.61	0.66
1:B:873:HIS:O	1:B:877:ARG:HG3	1.96	0.66
1:C:1250:ILE:HB	1:C:1273:MET:CE	2.26	0.66
1:C:1421:SER:O	1:C:1424:ASP:HB2	1.96	0.66
1:E:3145:ASN:O	1:E:3148:MET:HB2	1.96	0.66
1:G:4479:PHE:HZ	1:G:4483:LEU:HD22	1.60	0.66
1:H:4920:THR:HB	1:H:4956:LEU:HD11	1.77	0.66
1:D:1919:ARG:H	1:D:1959:ASP:HB2	1.61	0.66
1:E:3372:GLU:OE1	1:E:3372:GLU:N	2.29	0.66
1:F:3687:ILE:HD13	1:F:3709:VAL:HG11	1.77	0.66
1:H:5311:LEU:HD22	1:H:5321:THR:HG23	1.77	0.66
1:B:938:ARG:HH22	1:D:1998:ASN:ND2	1.94	0.65
1:C:1250:ILE:HD11	1:C:1268:MET:CE	2.27	0.65
1:G:4555:ALA:O	1:G:4666:ARG:NH1	2.30	0.65
1:C:1327:GLY:HA2	1:C:1404:SER:CB	2.26	0.65
1:G:4388:GLY:HA3	1:G:4391:PHE:CE2	2.32	0.65
1:A:99:SER:O	1:A:101:PRO:HD3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:928:GLN:NE2	1:D:2141:ARG:HH11	1.94	0.65
1:D:2280:ALA:HB3	1:D:2283:GLU:HG3	1.78	0.65
1:E:3167:VAL:HG22	1:E:3171:SER:CB	2.26	0.65
1:F:3612:ILE:N	6:F:7480:HOH:O	2.29	0.65
1:F:4075:ASP:HB3	1:F:4076:PRO:HD2	1.79	0.65
1:H:5015:VAL:HG11	1:H:5017:LEU:CD1	2.26	0.65
1:A:340:THR:OG1	1:A:343:GLU:HG3	1.97	0.65
1:C:1456:ILE:HD13	1:C:1456:ILE:N	2.10	0.65
1:D:1902:ILE:C	1:D:1903:LEU:HD23	2.22	0.65
1:D:2033:GLU:HG3	6:D:6683:HOH:O	1.95	0.65
1:F:3731:VAL:O	1:F:3802:LEU:N	2.29	0.65
1:E:3330:LEU:HD12	1:E:3343:GLU:HB3	1.77	0.65
1:A:131:VAL:HG12	1:A:202:LEU:HD23	1.76	0.65
1:A:221:SER:HB2	1:A:224:ASP:CG	2.22	0.65
1:C:1255:ARG:HD2	1:C:1282:TYR:CZ	2.31	0.65
1:F:3669:ASN:HB3	1:F:4063:HIS:CD2	2.31	0.65
1:A:141:ILE:O	1:A:191:PHE:HB2	1.96	0.65
1:A:486:ASP:O	1:A:490:ASN:ND2	2.29	0.65
1:C:1343:LEU:HD23	1:C:1361:LYS:HA	1.77	0.65
1:H:5023:LYS:NZ	1:H:5027:ASP:OD2	2.28	0.65
1:A:23:ASP:HB2	6:A:7647:HOH:O	1.97	0.65
1:C:1647:ALA:HB1	1:C:1648:PRO:HD2	1.79	0.65
1:F:3802:LEU:HD12	1:F:3803:GLY:N	2.12	0.65
1:G:4273:MET:HE2	1:G:4286:THR:HG22	1.79	0.65
1:C:1511:MET:O	1:C:1515:ARG:HG3	1.97	0.65
1:E:3160:TYR:HD2	1:E:3163:ILE:CB	2.06	0.65
1:E:3012:ILE:HG22	1:E:3013:GLN:N	2.12	0.64
1:G:4345:ASN:O	1:G:4348:MET:HG3	1.97	0.64
1:A:172:LYS:HE3	1:A:197:GLU:CD	2.22	0.64
1:E:3457:GLN:O	1:E:3461:GLN:HG3	1.96	0.64
1:A:454:ARG:NH2	1:A:484:ASP:OD2	2.30	0.64
1:E:3188:GLY:HA3	1:E:3191:PHE:CE2	2.32	0.64
1:F:3726:SER:HB2	1:F:3729:ALA:HB2	1.78	0.64
1:G:4360:TYR:CE2	1:G:4366:VAL:HG21	2.32	0.64
1:H:4979:LEU:HD12	1:H:4979:LEU:O	1.96	0.64
1:C:1431:GLY:O	1:C:1436:VAL:HG22	1.97	0.64
1:F:3928:GLN:HE22	1:H:5140:THR:HA	1.62	0.64
1:A:280:ASP:OD1	1:A:315:ARG:NH1	2.30	0.64
1:A:478:GLN:HB2	1:A:484:ASP:HB2	1.80	0.64
1:B:1027:LEU:HD23	1:B:1109:ILE:HB	1.80	0.64
1:C:1345:ASN:O	1:C:1348:MET:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3376:MET:HE2	1:E:3380:ILE:HG13	1.80	0.64
1:F:3624:THR:HG22	1:F:3627:GLU:N	2.04	0.64
1:F:3766:VAL:HG13	1:F:3813:ALA:HB1	1.78	0.64
1:G:4302:ILE:HD12	1:G:4694:ASN:CB	2.28	0.64
1:A:221:SER:HB2	1:A:224:ASP:H	1.62	0.64
1:B:740:LYS:HE2	1:B:742:THR:HG22	1.78	0.64
1:B:1054:ARG:HD2	6:B:7433:HOH:O	1.98	0.64
1:C:1363:ILE:O	1:C:1367:VAL:HG12	1.96	0.64
1:D:1873:MET:HE2	1:D:1886:THR:CG2	2.28	0.64
1:E:3068:MET:HE2	1:E:3071:ALA:HA	1.78	0.64
1:F:3732:GLU:HB2	1:F:3801:PHE:CE1	2.33	0.64
1:F:3743:LEU:CD1	1:F:3761:LYS:HA	2.24	0.64
1:G:4341:ILE:HB	1:G:4392:LEU:HB2	1.78	0.64
1:F:3715:GLY:O	1:F:3717:GLU:N	2.30	0.64
1:G:4493:ARG:HD3	1:G:4526:ALA:O	1.98	0.64
1:A:263:ASN:HB2	6:A:6418:HOH:O	1.98	0.64
1:B:639:ILE:O	1:B:982:ARG:HD2	1.98	0.64
1:G:4379:LEU:HD12	1:G:4379:LEU:O	1.97	0.64
1:B:971:LEU:O	1:B:975:ARG:HD2	1.98	0.63
1:D:2245:PRO:HD2	6:D:6587:HOH:O	1.98	0.63
1:E:3253:VAL:HG12	1:E:3257:LEU:HD23	1.80	0.63
1:F:3856:ILE:HD13	1:F:3856:ILE:N	2.12	0.63
1:G:4251:GLY:O	1:G:4255:ARG:HG3	1.98	0.63
1:C:1661:GLN:O	1:C:1664:LEU:HB2	1.98	0.63
1:H:4923:ILE:O	1:H:4925:GLY:N	2.32	0.63
1:C:1531:GLU:N	1:C:1543:GLU:OE2	2.31	0.63
1:D:1905:ARG:CZ	1:D:2299:ARG:HH21	2.10	0.63
1:H:5109:GLN:O	1:H:5113:ILE:HG13	1.98	0.63
1:A:223:LYS:O	1:A:226:GLN:HB2	1.98	0.63
1:B:1103:LYS:HG3	1:B:1106:ASP:OD2	1.99	0.63
1:E:3041:ALA:HB2	1:E:3501:PHE:CE1	2.33	0.63
1:B:871:GLU:HG2	1:B:892:ALA:HB3	1.79	0.63
1:D:2141:ARG:HG2	1:D:2141:ARG:NH1	2.10	0.63
1:F:3787:LYS:HB3	1:F:3792:LEU:HD12	1.81	0.63
1:G:4243:ASN:CB	1:G:4667:GLY:HA2	2.28	0.63
1:C:1715:ARG:HB3	1:C:1716:PRO:HD2	1.80	0.63
1:G:4322:LEU:O	1:G:4351:CYS:HB2	1.99	0.63
1:H:5275:ASP:OD2	1:H:5287:LEU:HD21	1.97	0.63
1:A:49:THR:HG22	1:A:365:ALA:HB2	1.80	0.63
1:E:3402:SER:CB	1:F:3621:MET:HE1	2.28	0.63
1:A:113:THR:HG22	1:A:242:SER:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4591:ARG:NH1	1:G:4592:LYS:HD2	2.14	0.63
1:A:181:SER:O	1:A:182:LEU:HD23	1.99	0.63
1:C:1382:LEU:HD21	1:C:1396:VAL:HG22	1.81	0.63
1:F:3941:ARG:NH2	1:H:5094:GLY:O	2.30	0.63
1:G:4410:LEU:O	1:G:4413:ALA:HB3	1.99	0.63
1:H:5311:LEU:HB3	1:H:5321:THR:HG23	1.81	0.63
1:E:3448:PRO:HB3	1:E:3469:PHE:CE1	2.34	0.62
1:A:84:ALA:HB2	1:A:230:PHE:HZ	1.64	0.62
1:A:160:TYR:HD2	1:A:163:ILE:CB	2.07	0.62
1:A:188:GLY:HA3	1:A:191:PHE:CE1	2.34	0.62
1:B:731:VAL:CG1	1:B:753:GLU:HB3	2.29	0.62
1:B:1091:LEU:O	1:B:1091:LEU:HD12	2.00	0.62
1:C:1685:VAL:O	1:C:1689:VAL:HG23	2.00	0.62
1:D:1855:ARG:HD2	1:D:1882:TYR:OH	1.99	0.62
1:D:1941:ILE:HA	1:D:1956:LEU:O	1.99	0.62
1:E:3113:THR:HG21	6:E:6225:HOH:O	1.99	0.62
1:A:113:THR:HG22	1:A:242:SER:HB2	1.80	0.62
1:A:134:LYS:O	1:A:196:VAL:HB	1.99	0.62
1:B:624:THR:HB	1:D:2196:GLU:CD	2.25	0.62
1:B:740:LYS:HE2	1:B:742:THR:CG2	2.28	0.62
1:C:1326:SER:HB3	1:C:1329:ALA:HB3	1.82	0.62
1:C:1360:TYR:HE2	1:C:1366:VAL:HG11	1.62	0.62
1:E:3068:MET:HE2	1:E:3071:ALA:CA	2.30	0.62
1:G:4257:VAL:HG23	1:G:4289:ASN:HB3	1.81	0.62
1:G:4322:LEU:C	1:G:4351:CYS:HB2	2.23	0.62
1:H:5092:ALA:HB1	3:H:5333:OXL:C2	2.29	0.62
1:F:3723:ILE:N	1:F:3723:ILE:HD13	2.14	0.62
1:A:113:THR:HG21	1:A:242:SER:H	1.63	0.62
1:A:399:ARG:HD2	6:C:6758:HOH:O	1.99	0.62
1:B:953:ASP:O	1:D:1829:MET:HE1	2.00	0.62
1:B:999:ARG:HH12	1:D:1823:ASP:CB	2.11	0.62
1:G:4293:ALA:O	1:G:4296:SER:HB3	1.99	0.62
1:B:999:ARG:HH12	1:D:1823:ASP:HB2	1.65	0.62
1:D:2281:TRP:CD1	1:D:2316:PRO:HD3	2.34	0.62
1:H:4905:ARG:HH22	1:H:5299:ARG:HD3	1.62	0.62
1:C:1453:VAL:HG12	1:C:1457:LEU:HD22	1.82	0.62
1:E:3014:THR:HG23	1:E:3015:GLN:HB2	1.82	0.62
1:F:3752:ASP:OD1	1:F:3755:ILE:N	2.31	0.62
1:D:1945:ASN:ND2	1:D:1961:LYS:NZ	2.48	0.62
1:E:3083:HIS:O	1:E:3087:ILE:HG13	2.00	0.62
1:E:3481:TRP:HB2	1:E:3516:PRO:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1339:LEU:HD12	1:C:1340:LYS:N	2.15	0.62
1:H:4847:ILE:HG21	1:H:5159:MET:HE2	1.82	0.62
1:C:1255:ARG:HD2	1:C:1282:TYR:OH	1.99	0.61
1:E:3172:LYS:HE3	1:E:3183:GLN:HB2	1.81	0.61
1:H:5275:ASP:HB3	1:H:5276:PRO:HD2	1.82	0.61
1:H:5281:TRP:CD1	1:H:5316:PRO:HD3	2.35	0.61
1:H:5130:LEU:HB3	1:H:5133:MET:HE3	1.81	0.61
1:A:439:GLN:O	1:A:442:ARG:HG2	2.01	0.61
1:B:866:ILE:O	1:B:887:ASP:HB2	2.00	0.61
1:B:1003:HIS:HB2	6:B:7042:HOH:O	1.99	0.61
1:F:3999:ARG:HH12	1:H:4823:ASP:HB2	1.65	0.61
1:C:1362:ASN:ND2	1:C:1365:LYS:HB2	2.16	0.61
1:G:4302:ILE:HD12	1:G:4694:ASN:HB2	1.82	0.61
1:F:3928:GLN:NE2	1:H:5140:THR:HB	2.15	0.61
1:F:3999:ARG:NH1	1:H:4823:ASP:HB2	2.15	0.61
1:G:4370:GLY:N	1:G:4384:VAL:O	2.28	0.61
1:C:1272:ARG:NE	1:C:1312:ASP:OD2	2.31	0.61
1:G:4305:ARG:HD3	1:G:4699:ARG:CZ	2.31	0.61
1:A:29:MET:CE	1:C:1510:LYS:HB3	2.31	0.61
1:A:237:ASP:OD1	1:A:460:ARG:NH1	2.31	0.61
1:C:1317:GLU:OE1	1:C:1319:ARG:NH1	2.33	0.61
1:D:2045:ARG:C	1:D:2046:LYS:HG3	2.25	0.61
1:G:4471:GLU:HA	1:G:4496:LEU:HB2	1.82	0.61
1:B:873:HIS:CE1	1:B:900:ILE:HG22	2.36	0.61
1:C:1280:HIS:NE2	1:C:1427:ASP:OD1	2.30	0.61
1:A:246:LYS:HG3	1:A:248:ALA:HB3	1.83	0.61
1:A:510:VAL:HG12	1:A:512:THR:HG23	1.83	0.61
1:B:739:LEU:HD12	1:B:754:ASN:C	2.26	0.61
1:C:1382:LEU:CD2	1:C:1396:VAL:HG22	2.31	0.61
1:H:5133:MET:HE2	1:H:5139:PRO:HG3	1.82	0.61
1:C:1385:LYS:HB2	1:C:1393:VAL:O	2.01	0.61
1:C:1532:SER:HB2	1:C:1543:GLU:OE1	2.01	0.61
1:E:3465:TYR:HB2	1:E:3468:ILE:HD12	1.83	0.61
1:G:4387:LYS:HG3	1:G:4392:LEU:HD11	1.82	0.61
1:D:1952:ASP:OD1	1:D:1954:ASN:N	2.33	0.60
1:D:2064:ILE:HD11	6:D:7414:HOH:O	2.01	0.60
1:H:5067:ILE:HD12	1:H:5088:GLY:HA3	1.83	0.60
1:A:456:HIS:H	1:A:456:HIS:CD2	2.18	0.60
1:B:714:LYS:NZ	1:B:717:GLU:OE2	2.35	0.60
1:B:1114:TRP:C	1:B:1115:ARG:HG3	2.26	0.60
1:C:1378:GLY:HA3	1:C:1498:ILE:HG13	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3638:PRO:HG3	1:F:3983:GLU:CD	2.26	0.60
1:B:731:VAL:HG11	1:B:753:GLU:HB3	1.82	0.60
1:E:3073:MET:HE3	1:E:3087:ILE:HG12	1.81	0.60
1:G:4498:ILE:HD13	1:G:4498:ILE:H	1.67	0.60
1:B:617:LEU:O	1:B:621:MET:HG2	2.01	0.60
1:B:941:ARG:H	1:D:2128:GLN:NE2	1.99	0.60
1:D:1902:ILE:HG22	1:D:1903:LEU:HD21	1.82	0.60
1:F:3720:THR:HG22	1:F:3721:GLY:O	2.02	0.60
1:G:4333:LEU:N	1:G:4333:LEU:HD23	2.15	0.60
1:A:48:CYS:SG	1:A:68:MET:HE2	2.42	0.60
1:A:310:LYS:NZ	1:A:353:ASP:OD1	2.35	0.60
1:C:1493:ARG:NH1	1:C:1527:THR:O	2.35	0.60
1:D:2241:ALA:O	1:D:2244:ARG:NH1	2.34	0.60
1:E:3367:GLY:HA3	6:E:7134:HOH:O	2.00	0.60
1:G:4725:ARG:HD3	1:H:5314:TRP:CE3	2.37	0.60
1:B:722:LEU:HA	1:B:804:SER:HB3	1.84	0.60
1:C:1362:ASN:HD22	1:C:1365:LYS:HD2	1.67	0.60
1:D:1914:LYS:NZ	1:D:2023:LYS:HD3	2.17	0.60
1:H:4945:ASN:HB3	1:H:4948:MET:CE	2.32	0.60
1:H:5130:LEU:CD1	1:H:5133:MET:HE3	2.31	0.60
1:A:141:ILE:CG2	1:A:158:LEU:HD22	2.30	0.60
1:A:292:ALA:HB1	3:A:533:OXL:C2	2.32	0.60
1:E:3411:MET:SD	1:F:4126:VAL:HG23	2.41	0.60
1:G:4348:MET:HG2	1:G:4357:TRP:CZ2	2.37	0.60
1:H:4923:ILE:HD12	1:H:4931:VAL:HG23	1.83	0.60
1:A:29:MET:HE2	1:C:1510:LYS:HB3	1.84	0.60
1:A:300:ILE:HB	1:A:301:PRO:HD2	1.84	0.60
1:G:4344:ASP:OD2	1:G:4346:ALA:HB3	2.00	0.60
1:A:63:MET:HE2	1:A:68:MET:HE1	1.82	0.59
1:A:209:ASN:C	1:A:210:LEU:HD13	2.27	0.59
1:D:2044:ILE:HG22	1:D:2082:ILE:CD1	2.27	0.59
1:G:4322:LEU:HA	1:G:4404:SER:HB3	1.84	0.59
1:G:4385:LYS:HB2	1:G:4393:VAL:O	2.02	0.59
1:C:1472:ASN:HD21	1:C:1475:GLY:H	1.45	0.59
1:H:5130:LEU:HD23	1:H:5143:GLU:HB3	1.84	0.59
1:C:1459:GLU:O	1:C:1462:LYS:HG2	2.03	0.59
1:G:4704:LYS:HE2	1:G:4730:PRO:O	2.02	0.59
1:A:113:THR:CG2	1:A:242:SER:HB2	2.32	0.59
1:B:1031:THR:HG21	1:B:1034:GLY:HA2	1.84	0.59
1:B:1080:ALA:HB3	1:B:1083:GLU:CD	2.27	0.59
1:C:1714:TRP:HD1	1:C:1715:ARG:HE	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3966:LYS:O	1:F:3966:LYS:HG2	1.99	0.59
1:A:49:THR:OG1	1:A:72:ARG:HD3	2.02	0.59
1:E:3426:ALA:HA	1:E:3447:ALA:HB1	1.84	0.59
1:F:3757:TRP:C	1:F:3758:LEU:HD23	2.27	0.59
1:G:4388:GLY:HA3	1:G:4391:PHE:CZ	2.37	0.59
1:G:4633:SER:OG	1:G:4635:ARG:HG3	2.02	0.59
1:E:3237:ASP:OD1	1:E:3460:ARG:HD2	2.03	0.59
1:A:130:GLU:HA	1:A:202:LEU:O	2.02	0.59
1:B:934:ILE:HG23	1:B:967:GLY:HA2	1.85	0.59
1:D:2141:ARG:HD3	6:D:6362:HOH:O	2.02	0.59
1:D:2252:VAL:HG21	1:D:2292:ALA:HB2	1.83	0.59
1:E:3113:THR:CG2	1:E:3242:SER:H	2.14	0.59
1:B:720:THR:HA	1:B:758:LEU:HD23	1.85	0.59
1:B:1114:TRP:CD1	1:B:1115:ARG:HG3	2.38	0.59
1:C:1305:ARG:HE	1:C:1699:ARG:NH2	2.01	0.59
1:C:1366:VAL:HG22	1:C:1413:ALA:HB1	1.84	0.59
1:C:1509:GLN:HG2	1:C:1513:ILE:HD12	1.84	0.59
1:C:1599:ARG:NH1	1:D:1823:ASP:HB3	2.17	0.59
1:C:1714:TRP:CE3	1:D:2325:ARG:HD3	2.38	0.59
1:G:4333:LEU:C	1:G:4334:LYS:HG2	2.26	0.59
1:B:1099:ARG:HB3	1:B:1101:PHE:CE1	2.37	0.59
1:E:3315:ARG:NH1	1:G:4230:CYS:O	2.29	0.59
1:A:506:ASP:O	1:A:529:VAL:HG23	2.03	0.58
1:B:1127:VAL:HG12	1:B:1128:PRO:N	2.16	0.58
1:D:2090:MET:HE2	1:D:2092:ALA:HB2	1.84	0.58
1:E:3269:LYS:HE2	1:E:3271:GLU:OE2	2.03	0.58
1:C:1313:THR:CG2	1:C:1442:SER:H	2.16	0.58
1:C:1442:SER:CA	1:C:1469:LYS:HD3	2.32	0.58
1:A:147:TYR:HA	1:A:150:LYS:HB2	1.86	0.58
1:B:844:ILE:HG13	1:B:868:SER:HB3	1.84	0.58
1:D:1817:LEU:O	1:D:1820:ALA:HB3	2.03	0.58
1:F:4075:ASP:CB	1:F:4087:LEU:HD21	2.33	0.58
1:D:2126:ALA:HB1	1:D:2159:MET:HE2	1.86	0.58
1:C:1727:VAL:HG13	1:C:1728:PRO:HD2	1.85	0.58
1:A:238:MET:CE	1:A:464:LEU:HD22	2.33	0.58
1:C:1360:TYR:HE2	1:C:1366:VAL:CG1	2.15	0.58
1:D:2278:GLN:HB2	1:D:2284:ASP:HB2	1.85	0.58
1:E:3326:ALA:HB1	1:E:3359:MET:HE2	1.84	0.58
1:E:3376:MET:HE3	1:E:3376:MET:CA	2.26	0.58
1:H:5015:VAL:HG12	1:H:5017:LEU:H	1.69	0.58
1:A:144:ASP:HB3	1:A:147:TYR:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:HB2	1:A:468:ILE:HG23	1.85	0.58
1:B:1087:LEU:HD23	1:B:1087:LEU:C	2.29	0.58
1:C:1345:ASN:C	1:C:1347:TYR:H	2.12	0.58
1:C:1615:SER:HA	1:C:1724:MET:HE2	1.84	0.58
1:D:1910:ALA:CB	1:D:2038:MET:HG3	2.34	0.58
1:H:5281:TRP:CG	1:H:5316:PRO:HD3	2.38	0.58
1:A:173:VAL:HG13	1:A:210:LEU:HD11	1.85	0.58
1:B:1125:ARG:HD2	6:B:7774:HOH:O	2.03	0.58
1:G:4322:LEU:HD23	1:G:4404:SER:HB2	1.85	0.58
1:E:3440:VAL:HG12	1:E:3449:ILE:CD1	2.33	0.58
1:F:4032:GLU:OE1	1:F:4054:ARG:N	2.30	0.58
1:H:5096:LEU:O	1:H:5100:ILE:HG12	2.04	0.58
1:H:5133:MET:CE	1:H:5139:PRO:HB3	2.23	0.58
1:E:3142:THR:HG22	1:E:3143:LEU:N	2.18	0.58
1:E:3475:ASP:HB3	1:E:3476:PRO:HD2	1.86	0.58
1:F:3731:VAL:HG12	1:F:3802:LEU:HB3	1.85	0.58
1:F:3859:GLU:O	1:F:3862:LYS:HG3	2.04	0.58
1:C:1313:THR:HG21	6:C:6158:HOH:O	2.03	0.57
1:C:1484:GLU:HG3	6:C:6559:HOH:O	2.04	0.57
1:D:1887:ILE:HD13	1:D:1887:ILE:N	2.19	0.57
1:D:2145:SER:HB2	6:D:6669:HOH:O	2.04	0.57
1:E:3407:LEU:HG	1:F:4126:VAL:HG11	1.86	0.57
1:G:4342:THR:HG21	1:G:4347:TYR:CD2	2.39	0.57
1:A:487:LEU:HD23	1:A:487:LEU:C	2.29	0.57
1:B:1015:SER:HA	1:B:1124:MET:HE2	1.85	0.57
1:C:1492:ALA:HB1	3:C:1733:OXL:C2	2.34	0.57
1:F:3660:LEU:HD13	1:F:3690:VAL:HA	1.86	0.57
1:G:4391:PHE:HE1	1:G:4393:VAL:HG23	1.68	0.57
1:H:4851:GLY:O	1:H:4855:ARG:HG2	2.04	0.57
1:H:5314:TRP:CD1	1:H:5315:ARG:HG3	2.39	0.57
1:G:4389:PRO:HD2	1:G:4391:PHE:HE2	1.65	0.57
1:C:1376:ASP:N	1:C:1407:GLY:O	2.34	0.57
1:B:745:ASN:ND2	1:B:757:TRP:HE1	2.01	0.57
1:B:1103:LYS:N	1:B:1106:ASP:OD2	2.30	0.57
1:E:3080:HIS:HE1	1:E:3227:ASP:OD1	1.86	0.57
1:E:3493:MET:HE1	1:E:3529:VAL:HA	1.86	0.57
1:G:4593:LEU:HG	1:G:4597:LEU:HD22	1.85	0.57
1:A:439:GLN:OE1	1:A:439:GLN:HA	2.04	0.57
1:A:503:LYS:NZ	6:A:7773:HOH:O	2.36	0.57
1:B:976:MET:HE2	1:B:980:ILE:HD11	1.86	0.57
1:D:2190:HIS:HD2	6:D:6458:HOH:O	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3838:MET:HA	1:F:3864:ILE:HG23	1.85	0.57
1:G:4409:ASN:O	1:G:4410:LEU:HD12	2.05	0.57
1:H:4843:ASN:HB3	1:H:5267:GLY:N	2.19	0.57
1:A:241:ALA:O	1:A:244:ILE:HG12	2.03	0.57
1:B:928:GLN:HE22	1:D:2141:ARG:HH11	1.52	0.57
1:C:1322:LEU:CD1	1:C:1349:GLU:HG2	2.30	0.57
1:G:4321:GLY:HA3	1:G:4357:TRP:HE3	1.69	0.57
1:E:3355:ALA:O	1:E:3466:ARG:NH1	2.38	0.57
1:A:77:HIS:CD2	5:A:535:ATP:H2'	2.39	0.57
1:A:122:LEU:HB2	1:A:149:GLU:HA	1.85	0.57
1:A:330:LEU:HD22	1:A:377:GLN:HG3	1.86	0.57
1:D:1877:HIS:CE1	5:D:2335:ATP:H2'	2.40	0.57
1:F:3623:ASP:OD1	1:F:3623:ASP:N	2.36	0.57
1:G:4322:LEU:HD21	1:G:4327:GLY:HA2	1.84	0.57
1:G:4384:VAL:HA	1:G:4394:THR:HG22	1.85	0.57
1:H:4920:THR:O	1:H:5005:LYS:HA	2.04	0.57
1:A:372:GLU:HA	1:A:375:ARG:HD2	1.87	0.57
1:B:774:TYR:CE2	1:B:811:PRO:HG3	2.40	0.57
1:C:1633:SER:OG	1:C:1635:ARG:HG3	2.04	0.57
1:G:4369:VAL:HA	1:G:4384:VAL:CG1	2.35	0.57
1:A:398:ALA:CB	1:A:413:MET:HE1	2.34	0.56
1:E:3167:VAL:HG22	1:E:3171:SER:HB2	1.86	0.56
1:E:3259:GLU:O	1:E:3262:LYS:HG2	2.05	0.56
1:F:3726:SER:HB3	1:F:3729:ALA:CB	2.34	0.56
1:F:3802:LEU:HD12	1:F:3803:GLY:H	1.70	0.56
1:A:163:ILE:HG23	1:A:163:ILE:O	2.06	0.56
1:C:1242:ARG:HB2	1:C:1578:HIS:CE1	2.40	0.56
1:C:1366:VAL:CG2	1:C:1413:ALA:HB1	2.35	0.56
1:C:1373:VAL:N	1:C:1382:LEU:O	2.33	0.56
1:D:2295:VAL:CG1	1:D:2299:ARG:HD2	2.35	0.56
1:F:3748:MET:HG3	1:F:3757:TRP:CE2	2.39	0.56
1:G:4625:ALA:HB1	1:G:4702:PHE:HB3	1.87	0.56
1:A:86:THR:HG22	1:A:87:ILE:N	2.19	0.56
1:B:706:PRO:O	1:B:1063:HIS:HE1	1.88	0.56
1:C:1343:LEU:HD23	1:C:1361:LYS:CD	2.35	0.56
1:E:3382:ARG:HH11	1:E:3382:ARG:CG	2.19	0.56
1:D:1842:ARG:NH1	1:D:1846:ILE:HG13	2.19	0.56
1:D:2008:VAL:HG12	1:D:2010:LEU:CD2	2.36	0.56
1:C:1611:MET:SD	1:D:2326:VAL:HG23	2.46	0.56
1:E:3390:HIS:HD2	6:E:6377:HOH:O	1.87	0.56
1:G:4336:GLY:HA2	1:G:4395:GLU:CD	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LEU:HD21	1:B:1107:VAL:HG21	1.87	0.56
1:D:1911:LEU:C	1:D:1911:LEU:HD23	2.31	0.56
1:F:3717:GLU:CD	1:F:3719:ARG:HE	2.13	0.56
1:F:3872:ASN:HD22	1:F:3875:GLY:H	1.54	0.56
1:A:133:LEU:HD13	1:A:133:LEU:N	2.20	0.56
1:B:648:CYS:CB	1:B:668:MET:HE3	2.32	0.56
1:C:1261:LYS:HG3	1:C:1293:ALA:HB1	1.87	0.56
1:F:3787:LYS:HB3	1:F:3792:LEU:CD1	2.36	0.56
1:G:4276:SER:HB3	1:G:4319:ARG:NE	2.16	0.56
1:G:4729:VAL:HG12	1:G:4730:PRO:HD2	1.88	0.56
1:H:5020:VAL:HG12	1:H:5021:SER:O	2.05	0.56
1:D:1819:ALA:HA	1:D:1831:ARG:HD2	1.87	0.56
1:D:2135:LYS:O	1:D:2169:TYR:HE2	1.89	0.56
1:G:4665:TYR:CB	1:G:4668:ILE:HD12	2.22	0.56
1:F:3928:GLN:HE21	1:H:5140:THR:HB	1.69	0.56
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.41	0.56
1:A:511:LEU:HB3	1:A:521:THR:CG2	2.36	0.56
1:C:1318:ILE:CG2	1:C:1408:VAL:HB	2.36	0.56
1:C:1363:ILE:HA	1:C:1366:VAL:HG12	1.88	0.55
1:D:1958:LEU:HD22	1:D:2008:VAL:HG21	1.85	0.55
1:E:3163:ILE:O	1:E:3163:ILE:HG12	2.04	0.55
1:B:1054:ARG:HG2	1:B:1073:CYS:HB3	1.89	0.55
1:C:1374:TYR:O	1:C:1408:VAL:HA	2.05	0.55
1:C:1452:GLU:O	1:C:1455:LYS:HB3	2.06	0.55
1:D:1815:GLN:CG	1:D:1839:ILE:HG23	2.36	0.55
1:G:4320:THR:O	1:G:4405:LYS:HA	2.05	0.55
1:D:1954:ASN:O	1:D:1955:ILE:HG13	2.06	0.55
1:B:804:SER:O	1:B:806:LYS:HD3	2.06	0.55
1:C:1360:TYR:HD2	1:C:1363:ILE:HB	1.71	0.55
1:G:4275:PHE:HE2	1:G:4280:HIS:CD2	2.24	0.55
1:A:108:ALA:HB2	1:A:460:ARG:HB3	1.89	0.55
1:A:123:ILE:HD11	1:A:202:LEU:CD2	2.37	0.55
1:B:934:ILE:HG22	1:B:935:LYS:HD3	1.88	0.55
1:C:1345:ASN:O	1:C:1347:TYR:N	2.39	0.55
1:C:1675:ASP:HB3	1:C:1676:PRO:HD2	1.87	0.55
1:E:3343:GLU:O	1:E:3347:VAL:HG23	2.07	0.55
1:F:3679:THR:OG1	1:F:3680:HIS:N	2.38	0.55
1:G:4444:ILE:HD12	1:G:4449:ASP:HB2	1.88	0.55
1:G:4640:VAL:CG1	1:G:4649:ILE:HD13	2.37	0.55
1:A:14:THR:HG23	1:A:15:GLN:N	2.22	0.55
1:A:416:VAL:HG22	1:A:445:PRO:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:PRO:HG2	1:B:843:PHE:CD2	2.41	0.55
1:B:731:VAL:O	1:B:801:PHE:HA	2.07	0.55
1:B:928:GLN:NE2	1:D:2141:ARG:HG2	2.21	0.55
1:E:3160:TYR:CE2	1:E:3162:ASN:HB3	2.42	0.55
1:E:3333:MET:HA	1:E:3336:LYS:O	2.07	0.55
1:E:3339:PRO:HG3	1:E:3376:MET:HG2	1.89	0.55
1:F:3643:ASN:HB3	1:F:4067:GLY:HA2	1.89	0.55
1:A:131:VAL:HG11	1:A:202:LEU:HD23	1.89	0.55
1:A:328:GLN:NE2	1:C:1540:THR:HB	2.22	0.55
1:A:411:MET:HE2	1:A:522:ASN:O	2.07	0.55
1:C:1681:TRP:CH2	1:C:1716:PRO:HA	2.42	0.55
1:D:1934:LYS:HG3	6:D:7630:HOH:O	2.07	0.55
1:F:3825:ILE:O	1:F:3829:LYS:HG2	2.06	0.55
1:F:3893:ARG:HH22	1:F:3946:ASP:CG	2.14	0.55
1:F:3971:LEU:O	1:F:3975:ARG:HG3	2.07	0.55
1:G:4221:MET:HE1	1:H:5202:SER:HB2	1.88	0.55
1:C:1244:THR:N	1:C:1585:GLU:OE2	2.31	0.55
1:A:111:LEU:HD23	1:A:111:LEU:C	2.31	0.55
1:C:1243:ASN:H	1:C:1585:GLU:CD	2.14	0.55
1:C:1532:SER:OG	1:C:1540:THR:HG23	2.07	0.55
1:E:3493:MET:CE	1:E:3529:VAL:HA	2.37	0.55
1:G:4217:LEU:O	1:G:4221:MET:HG2	2.06	0.55
1:G:4729:VAL:CG1	1:G:4730:PRO:HD2	2.36	0.55
1:A:295:ASP:O	1:A:298:ILE:HG22	2.06	0.54
1:A:333:MET:CE	1:A:373:ALA:HA	2.37	0.54
1:B:654:SER:O	1:B:660:LEU:HD13	2.07	0.54
1:C:1650:ILE:HD13	1:C:1650:ILE:N	2.23	0.54
1:H:4960:TYR:OH	1:H:5016:ASP:HB2	2.07	0.54
1:A:63:MET:HE2	1:A:68:MET:HE3	1.90	0.54
1:A:145:ASN:C	1:A:147:TYR:H	2.15	0.54
1:A:290:MET:HE2	1:A:292:ALA:HB2	1.90	0.54
1:D:2116:CYS:HB3	1:D:2121:LYS:O	2.07	0.54
1:E:3122:LEU:HB2	1:E:3149:GLU:HA	1.89	0.54
1:H:5239:GLN:OE1	1:H:5242:ARG:HD3	2.08	0.54
1:B:1115:ARG:HB3	1:B:1116:PRO:CD	2.37	0.54
1:C:1533:MET:HA	1:C:1536:LYS:O	2.07	0.54
1:E:3324:ILE:HG12	1:E:3357:CYS:HB2	1.89	0.54
1:A:514:TRP:H	1:A:522:ASN:ND2	1.96	0.54
1:B:656:SER:O	1:B:660:LEU:HB2	2.07	0.54
1:B:687:ILE:HD13	1:B:709:VAL:HG11	1.89	0.54
1:A:133:LEU:N	1:A:200:GLY:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:MET:HG2	1:A:336:LYS:O	2.08	0.54
1:B:720:THR:HG22	1:B:758:LEU:HD23	1.89	0.54
1:C:1431:GLY:HA2	1:C:1434:GLN:HB2	1.90	0.54
1:D:2054:ARG:NH2	1:D:2062:LYS:O	2.39	0.54
1:D:2275:ASP:HB2	1:D:2287:LEU:HD21	1.89	0.54
1:A:252:GLU:O	1:A:255:LYS:N	2.40	0.54
1:E:3222:GLU:HG2	1:E:3223:LYS:N	2.22	0.54
1:E:3376:MET:HA	1:E:3376:MET:CE	2.27	0.54
1:F:4066:ARG:HG3	1:F:4067:GLY:N	2.22	0.54
1:G:4437:ASP:OD1	1:G:4660:ARG:HD2	2.08	0.54
1:A:221:SER:CB	1:A:224:ASP:H	2.20	0.54
1:A:453:THR:CG2	1:A:459:ALA:HB2	2.37	0.54
1:F:3928:GLN:NE2	1:H:5141:ARG:N	2.51	0.54
1:C:1341:ILE:HB	1:C:1392:LEU:HB2	1.90	0.54
1:C:1421:SER:HB2	1:C:1424:ASP:H	1.72	0.54
1:E:3382:ARG:NH1	6:E:6645:HOH:O	2.37	0.54
1:F:3788:GLY:N	1:F:3791:PHE:O	2.28	0.54
1:D:2093:ARG:HD3	1:D:2126:ALA:O	2.07	0.54
1:E:3123:ILE:HD13	1:E:3151:CYS:HB2	1.88	0.54
1:E:3160:TYR:HB3	1:E:3163:ILE:CG2	2.37	0.54
1:G:4477:ARG:NH2	1:G:4478:ARG:NH1	2.55	0.54
1:H:5040:PHE:CE2	1:H:5159:MET:HE1	2.43	0.54
1:A:123:ILE:HD11	1:A:202:LEU:HG	1.90	0.54
1:B:619:ALA:HA	1:B:631:ARG:HD2	1.90	0.54
1:B:1104:LYS:HA	1:B:1129:VAL:HG12	1.89	0.54
1:G:4339:LEU:CD1	1:G:4354:ASN:HA	2.37	0.54
1:C:1287:ILE:O	1:C:1290:VAL:HB	2.08	0.53
1:E:3301:PRO:HG2	1:E:3304:LYS:HD2	1.89	0.53
1:G:4300:ASP:OD2	1:G:4303:LEU:HB2	2.07	0.53
1:G:4391:PHE:CE1	1:G:4393:VAL:HG23	2.43	0.53
1:H:4900:ASP:OD2	1:H:4903:LEU:HG	2.08	0.53
1:A:409:GLU:O	1:A:413:MET:HG3	2.07	0.53
1:B:1091:LEU:HD12	1:B:1091:LEU:C	2.33	0.53
1:C:1671:VAL:CG1	1:C:1691:LEU:HD21	2.37	0.53
1:F:3824:ASP:O	1:F:3827:ASP:HB2	2.08	0.53
1:H:4952:ASP:OD1	1:H:4954:ASN:N	2.32	0.53
1:H:5073:HIS:O	1:H:5077:ARG:HG3	2.08	0.53
1:B:740:LYS:HE3	1:B:791:PHE:HB2	1.90	0.53
1:B:745:ASN:HD22	1:B:745:ASN:N	2.07	0.53
1:B:825:ILE:HG22	1:B:829:LYS:NZ	2.23	0.53
1:C:1213:GLN:OE1	1:C:1213:GLN:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1430:PHE:O	1:C:1434:GLN:HG2	2.09	0.53
1:G:4669:PHE:CZ	1:G:4699:ARG:HD2	2.43	0.53
1:A:203:GLY:HA3	1:A:206:LYS:HE2	1.91	0.53
1:A:268:SER:HB2	1:A:289:ILE:CD1	2.39	0.53
1:A:310:LYS:NZ	1:C:1549:ASN:HD21	2.05	0.53
1:C:1255:ARG:NH2	1:C:1282:TYR:O	2.40	0.53
1:H:4883:HIS:O	1:H:4887:ILE:HG12	2.09	0.53
1:H:5275:ASP:HB3	1:H:5276:PRO:CD	2.38	0.53
1:A:24:THR:HB	1:C:1596:GLU:CD	2.33	0.53
1:A:141:ILE:HA	1:A:156:LEU:O	2.08	0.53
1:A:172:LYS:HE3	1:A:197:GLU:OE2	2.08	0.53
1:B:748:MET:HB2	1:B:757:TRP:CE2	2.44	0.53
1:B:976:MET:CE	1:B:980:ILE:HD11	2.38	0.53
1:C:1715:ARG:HB3	1:C:1716:PRO:CD	2.37	0.53
1:D:2009:ASN:C	1:D:2010:LEU:HD22	2.34	0.53
1:E:3068:MET:CE	1:E:3071:ALA:HB2	2.37	0.53
1:E:3493:MET:HE3	1:E:3529:VAL:HG13	1.88	0.53
1:C:1255:ARG:HH22	1:C:1285:GLU:HB3	1.72	0.53
1:C:1378:GLY:CA	1:C:1498:ILE:HG13	2.39	0.53
1:C:1421:SER:N	1:C:1424:ASP:HB2	2.23	0.53
1:C:1706:ASP:O	1:C:1728:PRO:HA	2.08	0.53
1:D:2320:PHE:CE2	1:D:2322:ASN:HB3	2.44	0.53
1:E:3017:LEU:O	1:E:3020:ALA:HB3	2.07	0.53
1:F:3787:LYS:HA	1:F:3792:LEU:HD12	1.90	0.53
1:H:5242:ARG:NH2	6:H:7298:HOH:O	2.31	0.53
1:A:162:ASN:O	1:A:164:CYS:N	2.42	0.53
1:B:703:LEU:CG	1:B:1099:ARG:HH21	2.21	0.53
1:C:1347:TYR:HE2	1:C:1355:ILE:CD1	2.21	0.53
1:C:1383:GLN:HG2	1:C:1385:LYS:HE2	1.91	0.53
1:C:1593:LEU:CD1	1:C:1597:LEU:HD22	2.39	0.53
1:C:1650:ILE:CD1	1:C:1669:PHE:HB2	2.38	0.53
1:E:3506:ASP:O	1:E:3528:PRO:HA	2.09	0.53
1:H:4931:VAL:HG11	1:H:4953:GLU:OE1	2.08	0.53
1:H:5015:VAL:CG1	1:H:5017:LEU:HG	2.39	0.53
1:B:654:SER:HA	1:B:659:THR:HG21	1.91	0.53
1:E:3115:GLY:O	1:E:3117:GLU:N	2.41	0.53
1:E:3495:VAL:O	1:E:3498:ALA:HB3	2.09	0.53
1:B:941:ARG:H	1:D:2128:GLN:HE21	1.57	0.53
1:D:2281:TRP:CH2	1:D:2316:PRO:HA	2.44	0.53
1:F:3717:GLU:OE2	1:F:3719:ARG:NH2	2.40	0.53
1:F:3752:ASP:OD2	1:F:3754:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4257:VAL:CG2	1:G:4289:ASN:HB3	2.39	0.53
1:A:141:ILE:N	1:A:192:LEU:O	2.33	0.53
1:D:2083:LEU:HD21	1:D:2119:ALA:CB	2.39	0.53
1:G:4319:ARG:O	1:G:4359:ASP:HB2	2.09	0.53
1:G:4591:ARG:O	1:G:4595:GLU:HG3	2.09	0.53
1:H:5327:VAL:CG1	1:H:5328:PRO:HD2	2.36	0.53
1:A:322:PRO:HG3	1:A:465:TYR:CE2	2.43	0.52
1:D:2269:PHE:N	1:D:2269:PHE:CD1	2.76	0.52
1:E:3054:SER:HA	1:E:3059:THR:HG21	1.92	0.52
1:E:3168:ASP:O	1:E:3171:SER:HB2	2.09	0.52
1:E:3260:LYS:HG3	1:E:3260:LYS:O	2.08	0.52
1:F:3634:ILE:HG23	6:F:6961:HOH:O	2.09	0.52
1:G:4321:GLY:N	1:G:4357:TRP:O	2.42	0.52
1:G:4339:LEU:HD11	1:G:4354:ASN:C	2.34	0.52
1:H:5038:MET:CE	1:H:5264:LEU:HD22	2.39	0.52
1:A:454:ARG:HG2	1:A:473:CYS:HB3	1.91	0.52
1:C:1477:ARG:NH2	1:C:1478:ARG:NH1	2.46	0.52
1:D:2122:PRO:HG3	1:D:2265:TYR:CE2	2.44	0.52
1:E:3433:SER:OG	1:E:3435:ARG:HB3	2.10	0.52
1:F:3650:ILE:HB	1:F:3673:MET:HE2	1.92	0.52
1:F:3758:LEU:HD23	1:F:3758:LEU:N	2.24	0.52
1:C:1539:PRO:HD2	6:C:7859:HOH:O	2.08	0.52
1:D:2083:LEU:O	1:D:2121:LYS:NZ	2.39	0.52
1:E:3440:VAL:HG12	1:E:3449:ILE:HD11	1.91	0.52
1:F:3665:LYS:HE2	1:F:3697:PHE:HE2	1.75	0.52
1:H:4953:GLU:H	1:H:4953:GLU:CD	2.11	0.52
1:A:27:GLU:O	1:A:31:ARG:HG3	2.09	0.52
1:A:173:VAL:N	1:A:182:LEU:O	2.30	0.52
1:A:191:PHE:CD2	1:A:192:LEU:N	2.78	0.52
1:A:328:GLN:NE2	1:C:1541:ARG:N	2.49	0.52
1:A:333:MET:HE1	1:A:373:ALA:HA	1.91	0.52
1:E:3160:TYR:HB3	1:E:3163:ILE:HG22	1.90	0.52
1:E:3335:LYS:HE3	6:E:6947:HOH:O	2.08	0.52
1:F:3742:THR:N	1:F:3756:LEU:O	2.35	0.52
1:G:4255:ARG:NE	1:G:4282:TYR:CZ	2.78	0.52
1:G:4443:PHE:O	1:G:4445:ARG:HG3	2.09	0.52
1:H:5046:LYS:O	1:H:5049:ASP:HB2	2.09	0.52
1:A:48:CYS:HB2	1:A:68:MET:CE	2.33	0.52
1:D:1847:ILE:HG12	1:D:1870:VAL:HB	1.90	0.52
1:E:3328:GLN:HE22	1:G:4540:THR:HA	1.74	0.52
1:F:3731:VAL:O	1:F:3801:PHE:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3890:MET:HE2	1:F:3892:ALA:CB	2.38	0.52
1:F:3893:ARG:HA	1:F:3896:LEU:HB3	1.91	0.52
1:G:4408:VAL:CG1	1:G:4410:LEU:HD11	2.33	0.52
1:A:456:HIS:CD2	1:A:456:HIS:N	2.78	0.52
1:C:1372:LYS:HA	1:C:1382:LEU:O	2.10	0.52
1:H:4847:ILE:HG21	1:H:5159:MET:HE3	1.92	0.52
1:A:89:ASN:HD22	1:A:89:ASN:N	2.08	0.52
1:A:525:ARG:HB2	1:A:525:ARG:HH11	1.75	0.52
1:C:1343:LEU:HD23	1:C:1361:LYS:HD2	1.91	0.52
1:E:3209:ASN:O	1:E:3211:PRO:HD3	2.10	0.52
1:H:5226:ALA:HA	1:H:5247:ALA:HB1	1.92	0.52
1:A:50:ILE:HD13	1:A:50:ILE:N	2.25	0.52
1:G:4363:ILE:HG23	1:G:4364:CYS:N	2.25	0.52
1:H:4923:ILE:C	1:H:4925:GLY:H	2.18	0.52
1:C:1687:LEU:O	1:C:1690:ASN:HB2	2.09	0.52
1:D:1824:THR:HG22	1:D:1827:GLU:HB3	1.90	0.52
1:A:57:VAL:HG23	1:A:89:ASN:CG	2.35	0.52
1:B:838:MET:SD	1:B:1064:LEU:HD21	2.50	0.52
1:B:1024:ALA:HA	1:B:1107:VAL:HG12	1.92	0.52
1:C:1352:ASP:OD1	1:C:1354:ASN:N	2.29	0.52
1:C:1376:ASP:CG	1:C:1406:LYS:HE2	2.35	0.52
1:C:1681:TRP:CZ2	1:C:1716:PRO:HA	2.45	0.52
1:D:1860:LEU:HB3	1:D:1893:ALA:CB	2.40	0.52
1:A:181:SER:O	1:A:197:GLU:HB2	2.09	0.51
1:B:739:LEU:HD12	1:B:754:ASN:O	2.10	0.51
1:E:3073:MET:CE	1:E:3109:VAL:HG13	2.40	0.51
1:G:4344:ASP:O	1:G:4346:ALA:N	2.43	0.51
1:H:5314:TRP:O	1:H:5315:ARG:HG2	2.10	0.51
1:A:51:GLY:C	1:A:55:ARG:HG3	2.35	0.51
1:C:1335:LYS:HG3	1:C:1336:GLY:N	2.24	0.51
1:H:4851:GLY:HA3	1:H:5165:ALA:O	2.10	0.51
1:A:454:ARG:HH22	1:A:484:ASP:CG	2.18	0.51
1:B:924:ILE:HG12	1:B:957:CYS:HB2	1.91	0.51
1:E:3042:ARG:CZ	1:E:3046:ILE:HD12	2.40	0.51
1:E:3068:MET:HE2	1:E:3071:ALA:HB2	1.92	0.51
1:A:283:LEU:O	1:A:283:LEU:HD22	2.11	0.51
1:B:658:GLU:HG2	6:B:7821:HOH:O	2.11	0.51
1:B:720:THR:O	1:B:805:LYS:HA	2.11	0.51
1:B:999:ARG:NH1	1:D:1823:ASP:HB2	2.25	0.51
1:B:1028:ILE:HG13	1:B:1108:VAL:HG11	1.93	0.51
1:C:1522:PRO:HA	1:C:1556:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2047:ALA:HB2	1:D:2081:GLU:HG3	1.91	0.51
1:F:3675:PHE:CZ	1:F:3683:HIS:CD2	2.99	0.51
1:G:4276:SER:OG	1:G:4317:GLU:OE2	2.29	0.51
1:G:4571:LEU:O	1:G:4575:ARG:HG3	2.10	0.51
1:A:210:LEU:HB3	1:A:213:ALA:CB	2.41	0.51
1:A:293:ARG:HD3	1:A:326:ALA:O	2.09	0.51
1:B:969:TYR:HB3	1:B:972:GLU:HB2	1.92	0.51
1:C:1639:GLN:OE1	1:C:1642:ARG:HD3	2.10	0.51
1:D:1945:ASN:HD21	1:D:1961:LYS:HZ3	1.55	0.51
1:E:3456:HIS:H	1:E:3456:HIS:CD2	2.28	0.51
1:F:3674:ASN:OD1	1:F:3676:SER:HB2	2.11	0.51
1:F:3774:TYR:HB3	1:F:3778:GLY:HA2	1.92	0.51
1:F:3889:ILE:HG22	1:F:3890:MET:N	2.26	0.51
1:G:4503:GLU:OE1	1:G:4503:GLU:N	2.39	0.51
1:A:437:ALA:HB1	1:A:468:ILE:HD13	1.92	0.51
1:E:3162:ASN:ND2	1:E:3165:LYS:HD3	2.20	0.51
1:E:3191:PHE:CE1	1:E:3193:VAL:HG23	2.32	0.51
1:E:3341:ARG:N	1:G:4528:GLN:NE2	2.56	0.51
1:E:3509:ILE:HD12	1:E:3526:VAL:HG23	1.90	0.51
1:F:3717:GLU:OE2	1:F:3719:ARG:NE	2.43	0.51
1:F:3764:CYS:SG	1:F:3792:LEU:HD13	2.51	0.51
1:G:4305:ARG:NH2	1:G:4663:HIS:CE1	2.77	0.51
1:G:4322:LEU:HD22	1:G:4326:SER:C	2.35	0.51
1:B:1065:TYR:HB2	1:B:1068:ILE:HD12	1.93	0.51
1:E:3221:SER:O	1:E:3224:ASP:HB2	2.09	0.51
1:G:4305:ARG:HH22	1:G:4663:HIS:CE1	2.22	0.51
1:A:245:ARG:HG2	1:A:274:GLU:HB3	1.93	0.51
1:B:703:LEU:HG	1:B:1099:ARG:HH21	1.75	0.51
1:C:1427:ASP:O	1:C:1430:PHE:HB3	2.11	0.51
1:C:1686:ASP:O	1:C:1690:ASN:ND2	2.44	0.51
1:D:1940:LYS:HB3	1:D:1955:ILE:HG12	1.93	0.51
1:D:1952:ASP:OD1	1:D:1955:ILE:N	2.40	0.51
1:F:3904:LYS:HD3	1:H:5183:GLU:CD	2.36	0.51
1:A:411:MET:HG2	1:A:521:THR:O	2.11	0.51
1:E:3230:PHE:CE1	1:E:3234:GLN:HG3	2.46	0.51
1:E:3456:HIS:CD2	1:E:3456:HIS:N	2.79	0.51
1:F:4057:GLN:O	1:F:4061:GLN:HG3	2.11	0.51
1:G:4494:GLY:CA	1:G:4527:THR:HG21	2.41	0.51
1:A:75:PHE:CE1	1:A:111:LEU:HG	2.45	0.51
1:A:122:LEU:HD12	1:A:149:GLU:HG2	1.92	0.51
1:A:318:ARG:HD2	6:A:6148:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:NH2	1:C:1223:ASP:OD2	2.44	0.51
1:A:451:ALA:HB2	1:A:468:ILE:CG2	2.41	0.51
1:C:1347:TYR:O	1:C:1350:LYS:N	2.31	0.51
1:D:2192:LYS:HE3	1:D:2196:GLU:OE2	2.11	0.51
1:E:3392:LYS:NZ	1:G:4225:PHE:HB2	2.26	0.51
1:A:303:GLU:OE2	1:C:1579:LEU:HG	2.11	0.50
1:C:1652:VAL:CG1	1:C:1691:LEU:HD23	2.41	0.50
1:F:3890:MET:HE1	3:F:4133:OXL:O3	2.10	0.50
1:F:4096:GLY:HA3	1:F:4102:PHE:CZ	2.46	0.50
1:G:4319:ARG:HH11	1:G:4407:GLY:CA	2.24	0.50
1:E:3469:PHE:CD1	1:E:3469:PHE:N	2.79	0.50
1:F:3752:ASP:C	1:F:3754:ASN:H	2.19	0.50
1:H:4847:ILE:CG2	1:H:5159:MET:HE2	2.41	0.50
1:A:102:ILE:C	1:A:103:LEU:HD12	2.37	0.50
1:A:120:THR:HG22	1:A:205:LYS:CA	2.41	0.50
1:B:926:ALA:O	1:B:927:THR:HB	2.12	0.50
1:D:1959:ASP:HB3	6:D:7872:HOH:O	2.12	0.50
1:D:2211:MET:HE2	1:D:2322:ASN:C	2.36	0.50
1:E:3172:LYS:HE2	1:E:3197:GLU:CD	2.36	0.50
1:F:3688:LYS:HE3	6:F:7669:HOH:O	2.10	0.50
1:F:3722:LEU:HB2	1:F:3749:GLU:HA	1.93	0.50
1:F:3829:LYS:HE2	1:F:3856:ILE:HG23	1.93	0.50
1:A:118:ILE:HG21	1:A:208:VAL:HB	1.91	0.50
1:C:1357:TRP:CE3	1:C:1358:LEU:N	2.79	0.50
1:C:1360:TYR:CE2	1:C:1366:VAL:HG11	2.44	0.50
1:D:1905:ARG:NH1	1:D:2299:ARG:NH2	2.55	0.50
1:F:3976:MET:O	1:F:3980:ILE:HG13	2.11	0.50
1:G:4492:ALA:HB1	3:G:4733:OXL:C2	2.41	0.50
1:H:5130:LEU:HD13	1:H:5133:MET:HE1	1.90	0.50
1:A:83:HIS:O	1:A:87:ILE:HG13	2.12	0.50
1:B:941:ARG:HG2	1:D:2128:GLN:NE2	2.27	0.50
1:F:3615:GLN:NE2	6:F:7151:HOH:O	2.44	0.50
1:F:3724:LYS:C	1:F:3726:SER:H	2.20	0.50
1:F:3869:LYS:HE2	1:F:3871:GLU:OE2	2.10	0.50
1:H:4986:GLN:HG2	1:H:4993:VAL:CG2	2.42	0.50
1:A:57:VAL:HG22	1:A:89:ASN:CB	2.42	0.50
1:A:315:ARG:HD3	1:A:318:ARG:HH12	1.77	0.50
1:C:1255:ARG:NH2	1:C:1285:GLU:HB3	2.26	0.50
1:C:1326:SER:HB3	1:C:1329:ALA:HB2	1.91	0.50
1:E:3228:LEU:O	1:E:3232:VAL:HG23	2.10	0.50
1:F:3612:ILE:O	1:F:3612:ILE:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3722:LEU:HD12	1:F:3749:GLU:OE1	2.12	0.50
1:F:3810:LEU:HB3	1:F:3813:ALA:HB3	1.92	0.50
1:F:4075:ASP:HB2	1:F:4087:LEU:HD21	1.92	0.50
1:G:4377:ASP:HA	1:G:4498:ILE:HD11	1.94	0.50
1:B:788:GLY:HA3	1:B:791:PHE:CE1	2.46	0.50
1:D:1945:ASN:HD21	1:D:1961:LYS:HZ1	1.57	0.50
1:D:1966:VAL:HG23	1:D:1966:VAL:O	2.12	0.50
1:D:1967:VAL:HG12	1:D:1987:LYS:HE3	1.94	0.50
1:F:3655:ARG:HD2	1:F:3682:TYR:CZ	2.47	0.50
1:F:3662:GLU:O	1:F:3666:SER:OG	2.29	0.50
1:F:4003:HIS:HB2	6:F:7655:HOH:O	2.11	0.50
1:G:4652:VAL:HG21	1:G:4692:ALA:HB2	1.93	0.50
1:H:4974:TYR:CE2	1:H:5011:PRO:HG3	2.47	0.50
1:D:2190:HIS:NE2	1:D:2246:ARG:HG3	2.26	0.50
1:H:5020:VAL:HG13	1:H:5024:ASP:CB	2.34	0.50
1:A:102:ILE:HG22	1:A:103:LEU:HD12	1.94	0.50
1:A:290:MET:HE3	1:A:326:ALA:CB	2.42	0.50
1:B:673:MET:HE3	1:B:686:THR:HG22	1.94	0.50
1:B:1078:GLN:HA	1:B:1078:GLN:HE21	1.77	0.50
1:B:1114:TRP:HE1	1:B:1115:ARG:HE	1.59	0.50
1:C:1270:VAL:HG13	1:C:1308:ALA:HB3	1.94	0.50
1:C:1572:GLU:OE1	1:C:1572:GLU:N	2.42	0.50
1:C:1675:ASP:CB	1:C:1676:PRO:HD2	2.40	0.50
1:E:3522:ASN:O	1:F:4125:ARG:HG2	2.12	0.50
1:F:4009:GLU:OE2	1:F:4043:TYR:OH	2.28	0.50
1:G:4379:LEU:HG	1:G:4380:ILE:HG12	1.94	0.50
1:G:4467:ILE:HD12	1:G:4488:GLY:HA3	1.94	0.50
1:H:4974:TYR:HB2	1:H:5009:ASN:HB2	1.93	0.50
1:A:353:ASP:HB3	1:C:1229:MET:HE1	1.94	0.49
1:A:393:LEU:HG	1:A:397:LEU:HD22	1.93	0.49
1:D:2203:HIS:ND1	1:D:2203:HIS:N	2.60	0.49
1:F:3675:PHE:CE1	1:F:3683:HIS:CD2	3.00	0.49
1:G:4222:ALA:CB	1:G:4227:GLU:HG2	2.42	0.49
1:G:4506:PHE:HB2	6:G:7616:HOH:O	2.12	0.49
1:G:4711:LEU:HB3	1:G:4721:THR:OG1	2.12	0.49
1:D:2293:MET:HG2	1:D:2330:PRO:HD2	1.94	0.49
1:E:3181:SER:O	1:E:3197:GLU:HB2	2.13	0.49
1:G:4302:ILE:HD12	1:G:4694:ASN:HB3	1.93	0.49
1:G:4352:ASP:OD1	1:G:4354:ASN:N	2.37	0.49
1:G:4703:LYS:O	1:G:4729:VAL:HB	2.13	0.49
1:B:827:ASP:O	1:B:830:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5314:TRP:HD1	1:H:5315:ARG:HG3	1.77	0.49
1:B:618:HIS:ND1	1:B:631:ARG:HD3	2.26	0.49
1:C:1287:ILE:HG22	1:C:1291:ARG:HD2	1.94	0.49
1:D:1902:ILE:CG1	1:D:2295:VAL:HG22	2.38	0.49
1:D:2046:LYS:HB3	1:D:2081:GLU:OE2	2.13	0.49
1:D:2103:GLU:OE1	1:D:2103:GLU:N	2.35	0.49
1:F:3815:VAL:O	1:F:3817:LEU:N	2.45	0.49
1:G:4334:LYS:O	1:G:4337:ALA:HB3	2.12	0.49
1:G:4696:GLY:HA3	1:G:4702:PHE:CZ	2.46	0.49
1:A:432:GLU:O	1:A:458:THR:HG21	2.11	0.49
1:B:700:ASP:O	1:B:703:LEU:N	2.45	0.49
1:B:762:ASN:ND2	6:B:6065:HOH:O	2.46	0.49
1:C:1323:ILE:CG2	1:C:1324:LYS:HG3	2.41	0.49
1:C:1348:MET:HA	1:C:1357:TRP:CG	2.48	0.49
1:D:1940:LYS:HE3	1:D:1991:PHE:CB	2.43	0.49
1:F:3721:GLY:CA	1:F:3757:TRP:HE3	2.25	0.49
1:A:87:ILE:HG22	1:A:91:ARG:HD2	1.93	0.49
1:A:120:THR:CG2	1:A:206:LYS:H	2.26	0.49
1:A:514:TRP:N	1:A:522:ASN:HD21	1.99	0.49
1:C:1247:ILE:HB	1:C:1559:MET:HG3	1.92	0.49
1:D:2225:ALA:HB1	1:D:2302:PHE:HB3	1.95	0.49
1:E:3162:ASN:OD1	1:E:3165:LYS:HE2	2.13	0.49
1:A:21:MET:HE1	1:B:1002:SER:HB2	1.94	0.49
1:A:113:THR:HG21	1:A:242:SER:N	2.26	0.49
1:B:1031:THR:CG2	1:B:1034:GLY:HA2	2.42	0.49
1:C:1260:LEU:O	1:C:1264:ILE:HG13	2.12	0.49
1:C:1417:LEU:HB3	1:C:1418:PRO:HD2	1.93	0.49
1:D:1861:LYS:O	1:D:1865:LYS:HG3	2.11	0.49
1:E:3252:GLU:HG2	6:E:7122:HOH:O	2.12	0.49
1:F:3786:GLN:O	1:F:3793:VAL:N	2.29	0.49
1:F:3899:GLU:HB3	6:F:7614:HOH:O	2.11	0.49
1:H:4833:ASP:HB3	1:H:4836:SER:HB2	1.95	0.49
1:H:4873:MET:CG	1:H:4887:ILE:CD1	2.90	0.49
1:H:4923:ILE:HA	1:H:4951:CYS:O	2.12	0.49
1:H:5093:ARG:NH2	1:H:5129:MET:HG2	2.28	0.49
1:A:113:THR:HG22	1:A:242:SER:H	1.77	0.49
1:D:1940:LYS:HE3	1:D:1991:PHE:CG	2.48	0.49
1:F:3672:ARG:O	1:F:3673:MET:HE3	2.12	0.49
1:F:3680:HIS:NE2	1:F:3827:ASP:OD1	2.30	0.49
1:G:4212:ILE:HD13	1:G:4233:ASP:OD2	2.12	0.49
1:D:1855:ARG:HH22	1:D:1885:GLU:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1884:ALA:HB2	1:D:2030:PHE:HZ	1.78	0.49
1:E:3328:GLN:HE21	1:G:4540:THR:HB	1.77	0.49
1:H:5130:LEU:CG	1:H:5133:MET:HE3	2.43	0.49
1:A:123:ILE:HD11	1:A:202:LEU:HD21	1.95	0.49
1:D:1814:THR:CG2	1:D:1815:GLN:N	2.76	0.49
1:E:3168:ASP:HB3	6:E:6720:HOH:O	2.13	0.49
1:G:4320:THR:HG22	1:G:4406:LYS:H	1.77	0.49
1:G:4396:VAL:O	1:G:4396:VAL:HG12	2.11	0.49
1:G:4445:ARG:O	1:G:4478:ARG:HD3	2.13	0.49
1:A:328:GLN:HE21	1:C:1541:ARG:N	2.02	0.48
1:A:511:LEU:CD2	1:A:521:THR:HG23	2.42	0.48
1:D:1958:LEU:HD13	1:D:1963:ILE:HD12	1.94	0.48
1:D:2083:LEU:HD21	1:D:2119:ALA:HB2	1.95	0.48
1:E:3157:TRP:CH2	1:E:3159:ASP:HB3	2.48	0.48
1:F:3691:ARG:O	1:F:3695:GLU:HG2	2.12	0.48
1:G:4358:LEU:HD21	1:G:4363:ILE:HD12	1.95	0.48
1:H:5063:ASN:HB2	6:H:7909:HOH:O	2.12	0.48
1:A:388:MET:HB2	1:A:390:HIS:CE1	2.48	0.48
1:A:509:ILE:HD13	1:A:526:VAL:HG22	1.93	0.48
1:C:1305:ARG:HG3	1:C:1699:ARG:HH21	1.77	0.48
1:C:1657:GLN:O	1:C:1661:GLN:HG3	2.14	0.48
1:E:3289:ILE:HG22	1:E:3290:MET:N	2.27	0.48
1:A:57:VAL:HG22	1:A:89:ASN:HA	1.94	0.48
1:A:79:THR:H	1:A:82:TYR:HB3	1.78	0.48
1:A:118:ILE:HG12	1:A:160:TYR:HB2	1.94	0.48
1:C:1351:CYS:O	1:C:1352:ASP:HB3	2.13	0.48
1:C:1479:PHE:CZ	1:C:1483:LEU:HG	2.48	0.48
1:D:1942:THR:HG22	1:D:1944:ASP:H	1.78	0.48
1:D:2230:LEU:HD22	1:D:2312:THR:HG22	1.95	0.48
1:E:3145:ASN:HD22	1:E:3145:ASN:N	2.11	0.48
1:G:4379:LEU:HD12	1:G:4379:LEU:C	2.37	0.48
1:H:5072:ASN:ND2	1:H:5075:GLY:H	2.10	0.48
1:A:240:PHE:HB3	1:A:269:LYS:HD2	1.95	0.48
1:B:747:TYR:N	1:B:747:TYR:CD1	2.81	0.48
1:C:1472:ASN:HD22	1:C:1472:ASN:C	2.21	0.48
1:E:3100:ASP:C	1:E:3102:ILE:H	2.22	0.48
1:G:4313:THR:HG21	6:G:6263:HOH:O	2.12	0.48
1:G:4319:ARG:H	1:G:4359:ASP:HB2	1.78	0.48
1:G:4646:ARG:HB3	6:G:6227:HOH:O	2.12	0.48
1:G:4709:ILE:HG23	1:G:4724:MET:SD	2.53	0.48
1:H:4945:ASN:CB	1:H:4948:MET:HE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:MET:O	1:A:343:GLU:HB3	2.14	0.48
1:A:495:VAL:CG1	1:A:499:ARG:HG3	2.44	0.48
1:C:1532:SER:C	1:C:1534:ILE:H	2.20	0.48
1:D:1855:ARG:NH2	1:D:1885:GLU:HB3	2.29	0.48
1:D:2008:VAL:HG12	1:D:2010:LEU:HD21	1.95	0.48
1:F:3941:ARG:N	1:H:5128:GLN:NE2	2.52	0.48
1:H:4815:GLN:OE1	1:H:5246:ARG:HD3	2.14	0.48
1:H:5188:MET:HE2	6:H:6229:HOH:O	2.13	0.48
1:C:1588:MET:SD	1:C:1666:ARG:NH2	2.87	0.48
1:C:1652:VAL:HG13	1:C:1691:LEU:HD23	1.94	0.48
1:E:3068:MET:HE2	1:E:3071:ALA:CB	2.44	0.48
1:F:3955:ALA:O	1:F:4066:ARG:NH1	2.40	0.48
1:G:4275:PHE:HB2	1:G:4312:ASP:O	2.14	0.48
1:A:240:PHE:N	1:A:240:PHE:CD1	2.81	0.48
1:E:3173:VAL:HB	1:E:3182:LEU:HB2	1.94	0.48
1:E:3457:GLN:HB2	1:E:3460:ARG:NH1	2.29	0.48
1:G:4383:GLN:O	1:G:4394:THR:HG22	2.14	0.48
1:H:5282:ALA:O	1:H:5286:ASP:HB2	2.14	0.48
1:A:49:THR:HB	1:A:361:SER:HA	1.95	0.48
1:A:57:VAL:HG22	1:A:89:ASN:CA	2.42	0.48
1:A:113:THR:HG23	1:A:114:LYS:N	2.29	0.48
1:B:1015:SER:HB3	1:B:1109:ILE:HG21	1.96	0.48
1:D:2011:PRO:HB3	6:D:7715:HOH:O	2.14	0.48
1:E:3160:TYR:CD2	1:E:3163:ILE:N	2.81	0.48
1:G:4288:LYS:HE2	6:G:7504:HOH:O	2.13	0.48
1:H:4873:MET:CE	1:H:4887:ILE:HD13	2.43	0.48
1:A:334:ILE:HG23	1:A:367:GLY:HA2	1.96	0.48
1:A:425:ALA:HB1	1:A:502:PHE:HB3	1.96	0.48
1:B:1114:TRP:NE1	1:B:1115:ARG:HE	2.11	0.48
1:C:1250:ILE:CD1	1:C:1268:MET:HE1	2.43	0.48
1:D:2046:LYS:N	1:D:2082:ILE:HD11	2.28	0.48
1:E:3172:LYS:HD2	1:E:3172:LYS:HA	1.40	0.48
1:G:4251:GLY:C	1:G:4255:ARG:HG3	2.39	0.48
1:H:4988:GLY:HA3	1:H:4991:PHE:CE2	2.49	0.48
1:A:283:LEU:HD22	1:A:283:LEU:C	2.38	0.48
1:B:651:GLY:C	1:B:655:ARG:HG3	2.39	0.48
1:B:720:THR:HG22	1:B:758:LEU:HD21	1.90	0.48
1:C:1247:ILE:HG23	1:C:1270:VAL:HB	1.96	0.48
1:C:1287:ILE:HG21	1:C:1291:ARG:NH1	2.28	0.48
1:C:1356:LEU:HD12	1:C:1357:TRP:N	2.29	0.48
1:C:1530:LEU:O	1:C:1563:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1718:SER:C	1:C:1720:PHE:H	2.20	0.48
1:D:2296:GLY:HA3	1:D:2302:PHE:CZ	2.49	0.48
1:F:3988:MET:SD	1:F:4066:ARG:NH2	2.87	0.48
1:H:5135:LYS:HB2	6:H:6489:HOH:O	2.13	0.48
1:A:469:PHE:N	1:A:469:PHE:CD1	2.82	0.47
1:A:489:VAL:O	1:A:493:MET:HG2	2.14	0.47
1:B:724:LYS:HE2	1:B:752:ASP:HB3	1.96	0.47
1:C:1258:GLU:O	1:C:1258:GLU:HG2	2.13	0.47
1:D:1899:SER:OG	1:D:1900:ASP:N	2.46	0.47
1:E:3350:ALA:O	1:E:3353:ASP:HB2	2.13	0.47
1:F:3655:ARG:HD2	1:F:3682:TYR:OH	2.14	0.47
1:F:3910:LYS:NZ	1:H:5149:ASN:HD21	2.12	0.47
1:G:4715:ARG:CB	1:G:4716:PRO:HD2	2.35	0.47
1:B:617:LEU:O	1:B:620:ALA:HB3	2.14	0.47
1:B:758:LEU:HD22	1:B:808:VAL:HG21	1.96	0.47
1:C:1300:ASP:OD1	1:C:1303:LEU:HD12	2.14	0.47
1:C:1342:THR:O	1:C:1357:TRP:HA	2.14	0.47
1:C:1347:TYR:HD2	1:C:1355:ILE:HG21	1.77	0.47
1:C:1630:LEU:HD22	1:C:1712:THR:HG22	1.95	0.47
1:D:2134:ILE:HG23	1:D:2167:GLY:HA2	1.97	0.47
1:D:2188:MET:SD	1:D:2266:ARG:NH2	2.87	0.47
1:F:3893:ARG:HD3	1:F:3926:ALA:O	2.14	0.47
1:G:4704:LYS:HA	1:G:4729:VAL:O	2.13	0.47
1:A:289:ILE:CG2	1:A:290:MET:N	2.77	0.47
1:B:950:ALA:O	1:B:953:ASP:HB2	2.13	0.47
1:B:1028:ILE:HG13	1:B:1108:VAL:CG1	2.44	0.47
1:D:1833:ASP:HA	6:D:7034:HOH:O	2.12	0.47
1:F:3699:SER:O	1:F:3701:PRO:HD3	2.14	0.47
1:A:292:ALA:HB1	3:A:533:OXL:C1	2.44	0.47
1:B:745:ASN:HD22	1:B:757:TRP:HE1	1.63	0.47
1:B:972:GLU:OE1	1:B:972:GLU:N	2.43	0.47
1:C:1428:LEU:CD1	1:C:1456:ILE:HB	2.43	0.47
1:D:2190:HIS:CD2	1:D:2246:ARG:HG3	2.49	0.47
1:E:3023:ASP:HA	1:E:3391:ARG:NH2	2.29	0.47
1:G:4608:MET:HE1	1:G:4721:THR:CG2	2.44	0.47
1:G:4640:VAL:HG12	1:G:4649:ILE:HD13	1.97	0.47
1:A:60:LEU:O	1:A:63:MET:N	2.47	0.47
1:B:640:THR:O	1:B:982:ARG:HD3	2.15	0.47
1:B:988:MET:SD	1:B:1066:ARG:NH2	2.87	0.47
1:B:1114:TRP:HE1	1:B:1115:ARG:NE	2.13	0.47
1:B:1118:SER:HB2	6:B:6107:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3331:GLU:HA	1:E:3331:GLU:OE1	2.13	0.47
1:G:4336:GLY:N	1:G:4396:VAL:O	2.47	0.47
1:B:1129:VAL:HA	1:B:1130:PRO:HD2	1.69	0.47
1:C:1275:PHE:N	1:C:1275:PHE:CD1	2.81	0.47
1:C:1318:ILE:HG22	1:C:1408:VAL:HB	1.96	0.47
1:C:1441:ALA:O	1:C:1469:LYS:HG3	2.15	0.47
1:D:2256:HIS:N	1:D:2256:HIS:CD2	2.82	0.47
1:A:392:LYS:HE2	1:A:396:GLU:OE2	2.14	0.47
1:A:522:ASN:HD22	1:A:522:ASN:N	2.12	0.47
1:B:776:ASP:O	1:B:779:LEU:HG	2.14	0.47
1:B:859:GLU:HG3	6:B:7831:HOH:O	2.14	0.47
1:B:904:LYS:NZ	6:B:7033:HOH:O	2.47	0.47
1:C:1252:PRO:HG3	5:C:1735:ATP:C2	2.50	0.47
1:C:1326:SER:CB	1:C:1329:ALA:HB2	2.44	0.47
1:C:1360:TYR:HD2	1:C:1363:ILE:CB	2.28	0.47
1:C:1650:ILE:HD12	1:C:1669:PHE:HB2	1.97	0.47
1:C:1707:VAL:HG12	1:C:1708:VAL:N	2.28	0.47
1:D:2072:ASN:HB2	6:D:6557:HOH:O	2.14	0.47
1:D:2176:MET:HE3	1:D:2176:MET:CA	2.40	0.47
1:D:2311:LEU:HA	1:D:2323:THR:O	2.15	0.47
1:E:3141:ILE:O	1:E:3191:PHE:HB2	2.15	0.47
1:F:3783:GLN:O	1:F:3794:THR:HA	2.15	0.47
1:F:3872:ASN:ND2	1:F:3875:GLY:H	2.10	0.47
1:F:3929:MET:O	1:F:3943:GLU:HG2	2.15	0.47
1:F:4080:ALA:O	1:F:4083:GLU:HB2	2.15	0.47
1:G:4370:GLY:HA2	1:G:4383:GLN:NE2	2.29	0.47
1:H:4877:HIS:O	1:H:4883:HIS:NE2	2.45	0.47
1:H:4887:ILE:O	1:H:4891:ARG:HG3	2.14	0.47
1:H:5199:ARG:O	1:H:5202:SER:OG	2.30	0.47
1:C:1343:LEU:N	1:C:1343:LEU:HD12	2.30	0.47
1:C:1688:ARG:O	1:C:1691:LEU:HB3	2.14	0.47
1:C:1704:LYS:HD2	1:C:1730:PRO:O	2.14	0.47
1:C:1727:VAL:CG1	1:C:1728:PRO:HD2	2.45	0.47
1:D:1902:ILE:O	1:D:1903:LEU:HD23	2.15	0.47
1:D:2315:ARG:HB3	1:D:2316:PRO:HD2	1.97	0.47
1:E:3245:ARG:CB	1:E:3274:GLU:HG2	2.45	0.47
1:F:3721:GLY:CA	1:F:3757:TRP:CE3	2.98	0.47
1:A:141:ILE:HG23	1:A:156:LEU:O	2.15	0.47
1:B:719:ARG:HH11	1:B:719:ARG:CG	2.27	0.47
1:D:2252:VAL:HG22	1:D:2271:VAL:HB	1.96	0.47
1:E:3111:LEU:C	1:E:3111:LEU:HD23	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3713:THR:HG22	1:F:3842:SER:H	1.80	0.47
1:G:4483:LEU:HD13	1:G:4489:ILE:HG13	1.96	0.47
1:B:655:ARG:HD2	1:B:682:TYR:OH	2.14	0.47
1:B:719:ARG:HH11	1:B:719:ARG:HG3	1.79	0.47
1:B:740:LYS:HE3	1:B:791:PHE:CB	2.44	0.47
1:C:1555:ALA:O	1:C:1666:ARG:NH1	2.39	0.47
1:E:3049:THR:HA	1:E:3072:ARG:O	2.14	0.47
1:F:3889:ILE:CG2	1:F:3890:MET:N	2.78	0.47
1:H:4922:LEU:HB3	1:H:4926:SER:O	2.15	0.47
1:F:3661:LYS:O	1:F:3665:LYS:HG3	2.14	0.46
1:F:3733:LEU:HD12	1:F:3780:ILE:HG21	1.96	0.46
1:G:4363:ILE:CG2	1:G:4364:CYS:N	2.78	0.46
1:H:4843:ASN:HB3	1:H:5267:GLY:HA2	1.96	0.46
1:H:5094:GLY:HA3	6:H:6869:HOH:O	2.13	0.46
1:H:5115:ARG:NH2	6:H:6821:HOH:O	2.48	0.46
1:A:50:ILE:HB	1:A:73:MET:HE3	1.94	0.46
1:B:910:LYS:HB3	1:D:1829:MET:HG2	1.97	0.46
1:D:2205:THR:O	1:D:2205:THR:HG23	2.15	0.46
1:E:3023:ASP:HB3	1:F:3999:ARG:NH2	2.30	0.46
1:E:3318:ARG:HD2	6:E:6699:HOH:O	2.14	0.46
1:F:3688:LYS:HG2	6:F:7669:HOH:O	2.15	0.46
1:F:3933:MET:HA	1:F:3936:LYS:O	2.15	0.46
1:G:4275:PHE:HZ	1:G:4430:PHE:CE2	2.34	0.46
1:G:4516:CYS:HB3	1:G:4521:LYS:O	2.15	0.46
1:G:4638:HIS:HD2	6:G:7226:HOH:O	1.99	0.46
1:G:4639:GLN:NE2	1:G:4639:GLN:HA	2.27	0.46
1:A:407:LEU:HD12	1:A:407:LEU:HA	1.51	0.46
1:C:1250:ILE:HG12	1:C:1271:ALA:HB1	1.98	0.46
1:D:1894:THR:HG22	1:D:1904:TYR:HE1	1.79	0.46
1:F:3756:LEU:HD12	1:F:3757:TRP:N	2.30	0.46
1:G:4608:MET:HE2	1:G:4636:SER:O	2.16	0.46
1:A:409:GLU:HB3	1:B:1021:LYS:HE2	1.97	0.46
1:E:3069:ASN:HB3	1:E:3463:HIS:CD2	2.50	0.46
1:G:4253:ALA:HB2	1:G:4566:LYS:HA	1.97	0.46
1:G:4276:SER:CB	1:G:4319:ARG:HH21	2.28	0.46
1:H:4908:ALA:HB2	1:H:5260:ARG:HB3	1.98	0.46
1:H:4952:ASP:OD1	1:H:4954:ASN:HB2	2.15	0.46
1:B:889:ILE:HG22	1:B:890:MET:N	2.31	0.46
1:B:928:GLN:NE2	1:D:2141:ARG:NH1	2.62	0.46
1:E:3050:ILE:CG1	1:E:3068:MET:HE1	2.46	0.46
1:E:3328:GLN:NE2	1:G:4540:THR:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4030:LEU:HG	1:F:4112:THR:HG22	1.97	0.46
1:H:5134:ILE:HG23	1:H:5167:GLY:HA2	1.96	0.46
1:A:77:HIS:NE2	5:A:535:ATP:H2'	2.31	0.46
1:A:279:PHE:CD2	1:A:311:MET:HE1	2.51	0.46
1:A:318:ARG:HD3	6:A:6437:HOH:O	2.16	0.46
1:A:435:ARG:HA	1:A:438:HIS:CD2	2.50	0.46
1:C:1249:THR:OG1	1:C:1561:SER:HA	2.16	0.46
1:D:2192:LYS:HB2	6:D:7588:HOH:O	2.14	0.46
1:E:3142:THR:HG21	1:E:3144:ASP:HB3	1.98	0.46
1:E:3273:HIS:CE1	1:E:3300:ILE:HG22	2.51	0.46
1:B:845:ARG:O	1:B:846:LYS:HB3	2.14	0.46
1:B:871:GLU:O	1:B:899:GLU:HG3	2.16	0.46
1:B:881:GLU:HG3	1:B:882:ILE:N	2.31	0.46
1:C:1260:LEU:HD13	1:C:1290:VAL:HA	1.97	0.46
1:C:1609:GLU:HB3	1:D:2221:LYS:HE2	1.98	0.46
1:D:2089:ILE:CG2	1:D:2090:MET:N	2.79	0.46
1:E:3370:PRO:O	1:E:3374:VAL:HG23	2.16	0.46
1:E:3491:LEU:HD12	1:E:3491:LEU:HA	1.72	0.46
1:F:3992:LYS:O	1:F:3996:GLU:HG3	2.15	0.46
1:F:4075:ASP:HB3	1:F:4076:PRO:CD	2.45	0.46
1:G:4264:ILE:HG22	1:G:4265:LYS:N	2.28	0.46
1:G:4348:MET:HA	1:G:4357:TRP:CE3	2.49	0.46
1:G:4368:ASP:O	1:G:4371:SER:HB2	2.15	0.46
1:H:4935:LYS:HE3	1:H:4997:GLU:O	2.16	0.46
1:H:5265:TYR:CD1	1:H:5265:TYR:N	2.84	0.46
1:A:120:THR:O	1:A:205:LYS:HA	2.16	0.46
1:A:188:GLY:HA3	1:A:191:PHE:CD1	2.50	0.46
1:B:1114:TRP:NE1	1:B:1115:ARG:NE	2.64	0.46
1:C:1409:ASN:C	1:C:1411:PRO:HD3	2.41	0.46
1:D:2232:GLU:HB3	6:D:7100:HOH:O	2.14	0.46
1:F:3743:LEU:HD13	1:F:3743:LEU:HA	1.82	0.46
1:G:4274:ASN:ND2	5:G:4735:ATP:O3G	2.40	0.46
1:G:4656:HIS:N	1:G:4656:HIS:ND1	2.62	0.46
1:H:5230:LEU:HG	1:H:5312:THR:HG22	1.98	0.46
1:A:12:ILE:O	1:A:12:ILE:HG22	2.14	0.46
1:A:174:TYR:HA	1:A:180:ILE:O	2.16	0.46
1:A:495:VAL:HG12	1:A:499:ARG:HG3	1.97	0.46
1:B:673:MET:N	1:B:673:MET:SD	2.88	0.46
1:A:77:HIS:CE1	5:A:535:ATP:H3'	2.51	0.46
1:C:1327:GLY:HA2	1:C:1404:SER:HB2	1.95	0.46
1:E:3012:ILE:CG2	1:E:3013:GLN:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3789:PRO:HD2	1:F:3791:PHE:CE1	2.51	0.46
1:F:4110:VAL:HG21	1:F:4127:VAL:HG21	1.98	0.46
1:G:4250:ILE:CB	1:G:4273:MET:HE3	2.27	0.46
1:G:4522:PRO:HG3	1:G:4665:TYR:CE2	2.51	0.46
1:H:4873:MET:CE	1:H:4886:THR:HG22	2.46	0.46
1:H:4967:VAL:O	1:H:4987:LYS:NZ	2.36	0.46
1:B:642:ARG:CZ	1:B:646:ILE:HD12	2.46	0.45
1:B:1114:TRP:CD1	1:B:1115:ARG:CD	2.99	0.45
1:C:1305:ARG:NE	1:C:1699:ARG:HH21	2.14	0.45
1:C:1655:ASN:HB3	1:C:1658:THR:HB	1.98	0.45
1:F:3820:VAL:HG21	1:F:3852:GLU:HB3	1.98	0.45
1:F:4054:ARG:HG2	1:F:4073:CYS:HB3	1.97	0.45
1:H:5030:PHE:O	1:H:5033:GLU:HB2	2.15	0.45
1:A:42:ARG:HB2	1:A:378:HIS:CE1	2.51	0.45
1:A:132:GLU:HA	1:A:201:PHE:HA	1.98	0.45
1:B:958:ILE:HG13	1:B:977:GLN:NE2	2.30	0.45
1:C:1347:TYR:CE2	1:C:1355:ILE:CD1	2.98	0.45
1:E:3475:ASP:HB3	1:E:3476:PRO:CD	2.45	0.45
1:F:4105:GLY:N	1:F:4129:VAL:O	2.39	0.45
1:G:4631:THR:O	1:G:4653:THR:OG1	2.29	0.45
1:H:4966:VAL:HB	6:H:7523:HOH:O	2.14	0.45
1:H:5182:ARG:NH1	6:H:7313:HOH:O	2.47	0.45
1:B:674:ASN:OD1	1:B:676:SER:HB2	2.16	0.45
1:B:774:TYR:HB3	1:B:778:GLY:HA2	1.99	0.45
1:C:1287:ILE:CG2	1:C:1291:ARG:NH1	2.80	0.45
1:D:2009:ASN:O	1:D:2010:LEU:HD22	2.15	0.45
1:D:2281:TRP:CD2	1:D:2316:PRO:HD3	2.50	0.45
1:E:3283:LEU:HD22	1:E:3321:LYS:HD2	1.99	0.45
1:G:4647:ALA:CB	1:G:4648:PRO:HD2	2.38	0.45
1:A:514:TRP:CE3	1:B:1125:ARG:HD3	2.52	0.45
1:C:1687:LEU:HG	1:C:1688:ARG:N	2.29	0.45
1:D:2301:PHE:N	1:D:2301:PHE:CD1	2.84	0.45
1:E:3316:CYS:O	1:E:3320:GLY:N	2.50	0.45
1:E:3440:VAL:CG1	1:E:3449:ILE:HD13	2.46	0.45
1:E:3493:MET:HE1	1:E:3529:VAL:CG1	2.45	0.45
1:E:3503:LYS:O	1:E:3506:ASP:HB2	2.16	0.45
1:F:3766:VAL:CG1	1:F:3813:ALA:HB1	2.45	0.45
1:G:4318:ILE:HG23	1:G:4360:TYR:HB2	1.98	0.45
1:G:4493:ARG:NH2	1:G:4546:ASP:OD1	2.50	0.45
1:H:5133:MET:CE	1:H:5139:PRO:HG3	2.46	0.45
1:B:1080:ALA:HB3	1:B:1083:GLU:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1914:LYS:HZ2	1:D:2023:LYS:HD3	1.80	0.45
1:D:2231:THR:O	1:D:2253:THR:HB	2.16	0.45
1:G:4248:CYS:CB	1:G:4268:MET:HE3	2.39	0.45
1:G:4358:LEU:CD2	1:G:4363:ILE:HD12	2.47	0.45
1:G:4511:MET:O	1:G:4515:ARG:HG3	2.16	0.45
1:H:5296:GLY:HA3	1:H:5302:PHE:CZ	2.52	0.45
1:A:408:MET:SD	1:A:520:PHE:HD2	2.40	0.45
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.98	0.45
1:C:1272:ARG:HE	1:C:1312:ASP:CG	2.22	0.45
1:C:1305:ARG:HE	1:C:1699:ARG:CZ	2.30	0.45
1:C:1532:SER:O	1:C:1534:ILE:N	2.49	0.45
1:F:3928:GLN:HE22	1:H:5140:THR:CA	2.29	0.45
1:G:4666:ARG:HG3	1:G:4667:GLY:N	2.30	0.45
1:A:123:ILE:HD11	1:A:202:LEU:CG	2.47	0.45
1:A:267:ILE:N	1:A:267:ILE:CD1	2.80	0.45
1:C:1318:ILE:HG12	1:C:1360:TYR:HB2	1.98	0.45
1:E:3440:VAL:HG12	1:E:3449:ILE:HD13	1.97	0.45
1:F:3809:ASN:C	1:F:3811:PRO:HD3	2.42	0.45
1:G:4364:CYS:O	1:G:4387:LYS:HE3	2.17	0.45
1:G:4602:SER:HB2	1:H:4821:MET:HE1	1.99	0.45
1:G:4608:MET:SD	1:G:4721:THR:HG22	2.56	0.45
1:H:5211:MET:HE2	1:H:5322:ASN:C	2.42	0.45
1:A:14:THR:CG2	1:A:15:GLN:HB2	2.43	0.45
1:A:480:ALA:HB3	1:A:483:GLU:HB2	1.99	0.45
1:B:928:GLN:HB2	1:D:2141:ARG:HB2	1.98	0.45
1:E:3103:LEU:HD12	1:E:3103:LEU:HA	1.58	0.45
1:E:3415:SER:HA	1:E:3524:MET:HE2	1.98	0.45
1:F:3748:MET:HG3	1:F:3757:TRP:CZ2	2.51	0.45
1:F:3928:GLN:NE2	1:H:5140:THR:CB	2.79	0.45
1:G:4248:CYS:SG	1:G:4268:MET:HB2	2.56	0.45
1:G:4729:VAL:HA	1:G:4730:PRO:HD3	1.70	0.45
1:A:103:LEU:CD1	1:A:103:LEU:N	2.80	0.45
1:A:180:ILE:CG2	1:A:182:LEU:HD21	2.47	0.45
1:A:330:LEU:CD2	1:A:377:GLN:HG3	2.46	0.45
1:B:1111:LEU:C	1:B:1112:THR:HG23	2.42	0.45
1:C:1302:ILE:HA	1:C:1695:VAL:HG22	1.98	0.45
1:C:1335:LYS:CG	1:C:1336:GLY:N	2.80	0.45
1:D:1910:ALA:HB2	1:D:2038:MET:CG	2.42	0.45
1:E:3425:ALA:O	1:E:3426:ALA:HB2	2.16	0.45
1:F:3928:GLN:NE2	1:H:5140:THR:CA	2.80	0.45
1:G:4477:ARG:HD3	6:G:7521:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4621:LYS:O	1:G:4621:LYS:HD2	2.17	0.45
1:A:310:LYS:HZ1	1:C:1549:ASN:HD21	1.63	0.45
1:B:675:PHE:CD1	1:B:711:LEU:HG	2.52	0.45
1:B:825:ILE:CG2	1:B:829:LYS:NZ	2.80	0.45
1:B:844:ILE:HG13	1:B:868:SER:CB	2.47	0.45
1:C:1632:GLU:OE1	1:C:1654:ARG:HB2	2.17	0.45
1:D:1916:PRO:HG3	1:D:2045:ARG:NH2	2.32	0.45
1:D:2065:LYS:HA	1:D:2065:LYS:HD3	1.75	0.45
1:F:3684:ALA:HB2	1:F:3830:PHE:HZ	1.82	0.45
1:F:4111:LEU:HD23	1:F:4123:THR:O	2.17	0.45
1:G:4410:LEU:N	1:G:4411:PRO:HD3	2.31	0.45
1:G:4636:SER:O	1:G:4639:GLN:HB2	2.17	0.45
1:G:4680:ALA:HB3	1:G:4683:GLU:CD	2.42	0.45
1:A:180:ILE:HG22	1:A:182:LEU:HD21	1.99	0.44
1:A:209:ASN:O	1:A:210:LEU:HD13	2.17	0.44
1:B:838:MET:HE1	1:B:1064:LEU:HD22	1.99	0.44
1:B:992:LYS:O	1:B:996:GLU:HG3	2.17	0.44
1:C:1274:ASN:O	1:C:1283:HIS:NE2	2.50	0.44
1:C:1664:LEU:HD12	1:C:1664:LEU:HA	1.78	0.44
1:F:3705:ARG:NE	1:F:4099:ARG:NH2	2.65	0.44
1:H:5279:GLU:HG3	1:H:5280:ALA:N	2.32	0.44
1:A:300:ILE:HB	1:A:301:PRO:CD	2.46	0.44
1:A:507:VAL:CG1	1:A:508:VAL:N	2.79	0.44
1:B:660:LEU:HB3	1:B:693:ALA:CB	2.47	0.44
1:B:843:PHE:CE2	1:B:845:ARG:HD3	2.51	0.44
1:C:1429:LYS:HB3	6:C:7061:HOH:O	2.17	0.44
1:C:1707:VAL:CG1	1:C:1708:VAL:N	2.80	0.44
1:D:1948:MET:HA	1:D:1957:TRP:CG	2.52	0.44
1:D:2291:LEU:O	1:D:2291:LEU:HD12	2.17	0.44
1:D:2327:VAL:HG12	1:D:2328:PRO:O	2.18	0.44
1:E:3015:GLN:OE1	1:E:3446:ARG:HD3	2.17	0.44
1:E:3277:ARG:NE	6:E:7207:HOH:O	2.49	0.44
1:G:4471:GLU:O	1:G:4499:GLU:HG3	2.17	0.44
1:G:4471:GLU:OE1	1:G:4495:ASP:HB2	2.17	0.44
1:A:520:PHE:N	1:A:520:PHE:CD1	2.86	0.44
1:B:866:ILE:C	1:B:867:ILE:HD13	2.43	0.44
1:B:1127:VAL:CG1	1:B:1128:PRO:N	2.79	0.44
1:C:1314:LYS:HE3	1:C:1427:ASP:OD2	2.17	0.44
1:C:1319:ARG:NE	1:C:1405:LYS:O	2.43	0.44
1:D:1968:ASP:O	1:D:1971:SER:HB2	2.17	0.44
1:E:3244:ILE:HD13	1:E:3244:ILE:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3720:THR:CG2	1:F:3721:GLY:N	2.80	0.44
1:F:3764:CYS:HB2	6:F:7678:HOH:O	2.17	0.44
1:F:3886:SER:O	1:F:3921:LYS:HE2	2.17	0.44
1:A:131:VAL:O	1:A:201:PHE:HA	2.17	0.44
1:A:522:ASN:HD22	1:A:522:ASN:H	1.64	0.44
1:C:1379:LEU:HG	1:C:1380:ILE:HG12	2.00	0.44
1:D:1863:MET:HE3	1:D:2174:VAL:HG21	2.00	0.44
1:D:1947:TYR:CD1	1:D:1947:TYR:N	2.86	0.44
1:E:3415:SER:HB3	1:E:3509:ILE:HG21	1.98	0.44
1:E:3452:VAL:HG11	1:E:3488:ARG:HB3	1.98	0.44
1:F:3719:ARG:H	1:F:3759:ASP:HB2	1.82	0.44
1:G:4242:ARG:HD2	1:G:4244:THR:O	2.18	0.44
1:G:4516:CYS:CB	1:G:4523:VAL:HB	2.47	0.44
1:H:4979:LEU:HD21	6:H:7671:HOH:O	2.17	0.44
1:H:5089:ILE:HG22	1:H:5090:MET:N	2.31	0.44
1:A:50:ILE:HD11	1:A:68:MET:HE1	1.98	0.44
1:A:328:GLN:NE2	1:C:1540:THR:CA	2.80	0.44
1:A:369:TYR:N	1:A:370:PRO:CD	2.81	0.44
1:B:1009:GLU:O	1:B:1013:MET:HG3	2.17	0.44
1:D:2031:GLY:O	1:D:2036:VAL:HG13	2.17	0.44
1:E:3191:PHE:C	1:E:3191:PHE:CD1	2.96	0.44
1:E:3450:ILE:HD11	1:E:3501:PHE:HD2	1.83	0.44
1:F:3774:TYR:CE2	1:F:3811:PRO:HG2	2.52	0.44
1:F:3774:TYR:HE2	1:F:3811:PRO:HG2	1.81	0.44
1:F:4008:MET:CG	1:F:4039:GLN:HG2	2.43	0.44
1:A:259:GLU:O	1:A:262:LYS:HG2	2.18	0.44
1:D:2089:ILE:HG22	1:D:2090:MET:N	2.33	0.44
1:D:2288:ARG:O	1:D:2291:LEU:HB3	2.18	0.44
1:F:3893:ARG:NH2	1:F:3946:ASP:OD1	2.50	0.44
1:G:4333:LEU:CG	1:G:4402:LEU:HD23	2.38	0.44
1:G:4444:ILE:HD13	1:G:4444:ILE:HA	1.77	0.44
1:A:409:GLU:OE1	1:A:443:TYR:OH	2.36	0.44
1:B:615:GLN:O	1:B:615:GLN:HG2	2.17	0.44
1:B:949:ASN:HD21	1:D:2110:LYS:NZ	2.16	0.44
1:D:2222:CYS:O	1:D:2223:LEU:HB2	2.16	0.44
1:F:4122:ASN:OD1	1:F:4122:ASN:N	2.42	0.44
1:H:4919:ARG:HA	1:H:5006:LYS:O	2.18	0.44
1:H:5049:ASP:O	1:H:5052:GLU:HB2	2.17	0.44
1:H:5089:ILE:CG2	1:H:5090:MET:N	2.79	0.44
1:H:5328:PRO:O	1:H:5330:PRO:HD3	2.18	0.44
1:A:75:PHE:N	1:A:75:PHE:CD1	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:HG2	1:A:117:GLU:OE2	2.17	0.44
1:A:302:ALA:C	1:A:304:LYS:H	2.25	0.44
1:A:515:ARG:HB3	1:A:516:PRO:HD2	1.99	0.44
1:B:990:HIS:HD2	6:B:6334:HOH:O	2.00	0.44
1:C:1621:LYS:NZ	1:D:2201:SER:O	2.51	0.44
1:D:1873:MET:CE	1:D:1886:THR:HG22	2.42	0.44
1:D:2017:LEU:HB3	1:D:2018:PRO:HD2	1.98	0.44
1:E:3349:ASN:HB3	6:E:6204:HOH:O	2.18	0.44
1:G:4373:VAL:O	1:G:4382:LEU:HB2	2.17	0.44
1:H:4933:LEU:HD23	1:H:4933:LEU:HA	1.71	0.44
1:A:172:LYS:HA	1:A:182:LEU:O	2.18	0.44
1:A:246:LYS:HG3	6:A:7641:HOH:O	2.18	0.44
1:B:825:ILE:HG22	1:B:829:LYS:HZ2	1.81	0.44
1:B:1124:MET:HG2	1:B:1125:ARG:N	2.32	0.44
1:C:1603:HIS:CG	1:C:1604:SER:N	2.86	0.44
1:D:1874:ASN:HA	1:D:1912:ASP:HB3	2.00	0.44
1:D:2044:ILE:HG13	1:D:2068:SER:HB3	2.00	0.44
1:D:2056:ILE:HD13	1:D:2056:ILE:N	2.32	0.44
1:F:3821:SER:O	1:F:3824:ASP:HB2	2.18	0.44
1:G:4338:THR:HG23	1:G:4339:LEU:N	2.32	0.44
1:G:4529:MET:O	1:G:4530:LEU:HD23	2.18	0.44
1:H:4960:TYR:CD2	1:H:4963:ILE:HB	2.53	0.44
1:B:990:HIS:HE1	6:B:6944:HOH:O	2.01	0.43
1:C:1310:ALA:HB1	1:C:1440:PHE:CZ	2.53	0.43
1:C:1588:MET:HE3	6:C:7860:HOH:O	2.18	0.43
1:D:1895:GLU:C	1:D:1897:PHE:H	2.26	0.43
1:E:3163:ILE:O	1:E:3163:ILE:HG23	2.17	0.43
1:F:3716:PRO:HB3	1:F:3817:LEU:HB3	2.00	0.43
1:G:4222:ALA:HB1	1:G:4227:GLU:HG2	2.00	0.43
1:A:57:VAL:HG22	1:A:89:ASN:HB3	2.00	0.43
1:B:873:HIS:HE1	1:B:899:GLU:O	2.01	0.43
1:B:970:PRO:O	1:B:974:VAL:HG23	2.17	0.43
1:C:1534:ILE:HG23	1:C:1567:GLY:CA	2.41	0.43
1:D:1980:ILE:HD11	1:D:2000:GLY:HA3	1.98	0.43
1:E:3012:ILE:HD12	1:E:3035:ASP:HB3	1.98	0.43
1:E:3304:LYS:O	1:E:3307:LEU:HB2	2.18	0.43
1:F:3755:ILE:O	1:F:3755:ILE:HG12	2.13	0.43
1:F:3897:GLY:HA2	1:F:3905:VAL:CG2	2.49	0.43
1:G:4274:ASN:HA	1:G:4312:ASP:HB3	2.00	0.43
1:H:4860:LEU:O	1:H:4863:MET:HB2	2.18	0.43
1:H:5130:LEU:CB	1:H:5133:MET:HE3	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:CD2	1:A:163:ILE:N	2.85	0.43
1:A:301:PRO:HG2	1:A:304:LYS:HD2	2.00	0.43
1:C:1382:LEU:HD23	1:C:1396:VAL:HA	1.99	0.43
1:C:1445:ARG:HB3	1:C:1474:GLU:OE1	2.18	0.43
1:D:1856:SER:O	1:D:1860:LEU:HB2	2.18	0.43
1:D:2046:LYS:HB2	6:D:7884:HOH:O	2.18	0.43
1:D:2057:LEU:HB2	6:D:7550:HOH:O	2.18	0.43
1:G:4313:THR:HG22	1:G:4442:SER:N	2.26	0.43
1:G:4522:PRO:HD3	1:G:4665:TYR:CE2	2.53	0.43
1:A:91:ARG:O	1:A:95:GLU:HG2	2.17	0.43
1:A:145:ASN:C	1:A:147:TYR:N	2.76	0.43
1:A:456:HIS:H	1:A:456:HIS:HD2	1.65	0.43
1:B:990:HIS:H	1:B:990:HIS:CD2	2.35	0.43
1:B:997:LEU:O	1:B:1000:SER:OG	2.29	0.43
1:B:1077:VAL:HG12	1:B:1078:GLN:O	2.18	0.43
1:C:1347:TYR:CE2	1:C:1355:ILE:HD13	2.53	0.43
1:C:1428:LEU:HD12	1:C:1456:ILE:HG21	2.00	0.43
1:E:3334:ILE:HA	6:E:7134:HOH:O	2.16	0.43
1:F:4008:MET:HE2	1:F:4036:SER:O	2.18	0.43
1:H:4932:GLU:HG3	1:H:5001:PHE:CZ	2.54	0.43
1:A:49:THR:O	1:A:365:ALA:HB2	2.18	0.43
1:B:688:LYS:HE3	6:B:7688:HOH:O	2.17	0.43
1:B:779:LEU:HD23	1:B:779:LEU:HA	1.78	0.43
1:C:1343:LEU:HD23	1:C:1361:LYS:HD3	2.01	0.43
1:D:1983:GLN:HG2	1:D:1985:LYS:HE2	2.01	0.43
1:E:3120:THR:O	1:E:3205:LYS:HA	2.18	0.43
1:E:3272:ASN:OD1	1:E:3274:GLU:N	2.52	0.43
1:F:3906:PHE:O	1:F:3910:LYS:HG3	2.18	0.43
1:F:3942:ALA:HB2	1:H:5146:ASP:OD2	2.19	0.43
1:G:4621:LYS:HE2	1:H:5209:GLU:HB3	2.00	0.43
1:H:5130:LEU:HD22	1:H:5133:MET:HE3	1.99	0.43
1:B:700:ASP:O	1:B:702:ILE:N	2.51	0.43
1:C:1322:LEU:HD23	1:C:1322:LEU:HA	1.65	0.43
1:D:2100:ILE:HB	1:D:2101:PRO:HD2	2.01	0.43
1:F:3676:SER:HA	1:F:3714:LYS:HG3	2.01	0.43
1:F:3820:VAL:HB	1:F:3852:GLU:OE1	2.18	0.43
1:G:4300:ASP:HA	1:G:4301:PRO:HD3	1.81	0.43
1:G:4339:LEU:HA	1:G:4339:LEU:HD12	1.32	0.43
1:G:4619:SER:N	1:G:4709:ILE:HD11	2.34	0.43
1:A:245:ARG:HD3	1:A:272:ASN:HD21	1.84	0.43
1:C:1368:ASP:O	1:C:1371:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1612:ALA:O	1:C:1616:VAL:HG23	2.19	0.43
1:D:1855:ARG:NH2	1:D:1885:GLU:CG	2.79	0.43
1:D:2252:VAL:CG2	1:D:2292:ALA:HB2	2.48	0.43
1:E:3257:LEU:HD13	1:E:3257:LEU:HA	1.86	0.43
1:E:3461:GLN:O	1:E:3464:LEU:HB2	2.19	0.43
1:G:4660:ARG:HD2	1:G:4660:ARG:HH11	1.66	0.43
1:G:4681:TRP:NE1	1:G:4715:ARG:HA	2.33	0.43
1:H:5130:LEU:HD22	1:H:5133:MET:CE	2.49	0.43
1:H:5242:ARG:NE	6:H:7298:HOH:O	2.50	0.43
1:H:5307:VAL:CG1	1:H:5308:VAL:N	2.82	0.43
1:A:119:ARG:HD3	1:A:207:GLY:HA2	2.00	0.43
1:A:182:LEU:HD23	1:A:182:LEU:N	2.26	0.43
1:A:192:LEU:N	1:A:192:LEU:CD2	2.79	0.43
1:A:228:LEU:O	1:A:232:VAL:HG23	2.19	0.43
1:C:1366:VAL:HG22	1:C:1366:VAL:O	2.18	0.43
1:C:1457:LEU:HA	1:C:1457:LEU:HD12	1.53	0.43
1:C:1654:ARG:HG2	1:C:1673:CYS:O	2.19	0.43
1:E:3288:GLY:C	1:E:3289:ILE:HG12	2.42	0.43
1:F:3933:MET:HE2	1:F:3933:MET:HB3	1.93	0.43
1:G:4498:ILE:N	1:G:4498:ILE:CD1	2.80	0.43
1:A:29:MET:HE3	1:C:1510:LYS:HB3	2.00	0.43
1:A:167:VAL:CG2	1:A:168:ASP:N	2.80	0.43
1:C:1263:MET:HA	1:C:1266:SER:HB2	2.00	0.43
1:C:1410:LEU:HD12	1:C:1410:LEU:HA	1.79	0.43
1:C:1539:PRO:HG3	1:C:1576:MET:HG2	2.00	0.43
1:D:1859:THR:O	1:D:1862:GLU:N	2.51	0.43
1:D:2275:ASP:HA	1:D:2276:PRO:HD3	1.88	0.43
1:G:4298:ALA:HA	1:G:4304:TYR:CD1	2.54	0.43
1:H:5015:VAL:CG1	1:H:5017:LEU:H	2.31	0.43
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.89	0.43
1:B:698:ALA:HA	1:B:704:TYR:CD1	2.54	0.43
1:B:764:CYS:O	1:B:787:LYS:NZ	2.39	0.43
1:C:1268:MET:HE2	1:C:1271:ALA:HA	2.00	0.43
1:C:1322:LEU:HD12	1:C:1349:GLU:CG	2.37	0.43
1:C:1339:LEU:HD12	1:C:1354:ASN:O	2.19	0.43
1:C:1387:LYS:HB3	1:C:1392:LEU:CD1	2.46	0.43
1:D:1878:GLY:HA2	6:D:6138:HOH:O	2.18	0.43
1:D:1902:ILE:HG22	1:D:1903:LEU:HD23	2.00	0.43
1:E:3016:GLN:NE2	6:E:6187:HOH:O	2.52	0.43
1:F:3817:LEU:HD23	1:F:3817:LEU:HA	1.59	0.43
1:A:74:ASN:HA	1:A:112:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:O	1:A:147:TYR:N	2.51	0.42
1:A:291:VAL:HG12	1:A:293:ARG:HG3	2.00	0.42
1:A:493:MET:HE1	1:A:529:VAL:HG22	2.00	0.42
1:B:744:ASP:C	1:B:746:ALA:H	2.27	0.42
1:C:1305:ARG:HE	1:C:1699:ARG:HH21	1.65	0.42
1:D:2020:VAL:CG1	1:D:2025:ILE:HD11	2.48	0.42
1:D:2021:SER:O	1:D:2025:ILE:HG12	2.19	0.42
1:D:2304:LYS:HG3	1:D:2330:PRO:O	2.17	0.42
1:E:3507:VAL:CG1	1:E:3508:VAL:N	2.78	0.42
1:F:3739:LEU:HD21	1:F:3756:LEU:CB	2.43	0.42
1:F:3890:MET:HE2	1:F:3892:ALA:CA	2.49	0.42
1:H:5304:LYS:HB2	1:H:5330:PRO:O	2.19	0.42
1:A:238:MET:CE	1:A:464:LEU:CD2	2.97	0.42
1:A:376:MET:O	1:A:380:ILE:HG13	2.18	0.42
1:A:493:MET:HE2	1:A:529:VAL:HG13	2.01	0.42
1:B:880:ASP:HB2	6:B:7833:HOH:O	2.19	0.42
1:C:1720:PHE:CZ	1:C:1722:ASN:HB3	2.54	0.42
1:D:2046:LYS:NZ	1:D:2049:ASP:OD1	2.37	0.42
1:D:2265:TYR:HB2	1:D:2268:ILE:CD1	2.44	0.42
1:G:4260:LEU:HA	1:G:4263:MET:HG3	2.00	0.42
1:G:4372:LYS:NZ	1:G:4397:GLU:OE1	2.50	0.42
1:G:4640:VAL:HG12	1:G:4649:ILE:CD1	2.48	0.42
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.47	0.42
1:C:1305:ARG:NH1	6:C:7519:HOH:O	2.52	0.42
1:C:1649:ILE:C	1:C:1650:ILE:HD13	2.43	0.42
1:E:3144:ASP:O	1:E:3146:ALA:N	2.52	0.42
1:E:3186:GLN:CB	1:E:3193:VAL:HB	2.39	0.42
1:E:3191:PHE:HE1	1:E:3193:VAL:CG2	2.22	0.42
1:F:3867:ILE:HA	1:F:3888:GLY:O	2.19	0.42
1:G:4217:LEU:HD23	1:G:4217:LEU:HA	1.86	0.42
1:G:4313:THR:HG21	1:G:4442:SER:H	1.81	0.42
1:G:4322:LEU:HB2	1:G:4349:GLU:HA	2.01	0.42
1:G:4560:LEU:HA	1:G:4560:LEU:HD23	1.70	0.42
1:G:4569:TYR:HB3	1:G:4572:GLU:HB2	2.01	0.42
1:H:5256:HIS:H	1:H:5256:HIS:CD2	2.37	0.42
1:A:25:PHE:O	1:A:28:HIS:HB3	2.20	0.42
1:A:57:VAL:O	1:A:61:LYS:HG3	2.19	0.42
1:A:425:ALA:O	1:A:448:PRO:HD2	2.19	0.42
1:B:637:ALA:HA	1:B:638:PRO:HD3	1.83	0.42
1:D:2188:MET:HE3	1:D:2190:HIS:CE1	2.54	0.42
1:E:3144:ASP:HB3	1:E:3147:TYR:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3162:ASN:HD22	1:E:3162:ASN:HA	1.59	0.42
1:F:3735:LYS:HA	1:F:3796:VAL:HG12	2.01	0.42
1:F:3881:GLU:HG3	1:F:3882:ILE:N	2.34	0.42
1:H:4948:MET:HE2	1:H:4948:MET:HB2	1.75	0.42
1:H:5158:ILE:HD12	1:H:5177:GLN:HG2	2.02	0.42
1:H:5188:MET:CE	1:H:5190:HIS:NE2	2.83	0.42
1:B:738:THR:CG2	1:B:739:LEU:N	2.78	0.42
1:C:1445:ARG:HB3	1:C:1474:GLU:CD	2.44	0.42
1:E:3198:ASN:HD21	1:G:4538:ARG:HH22	1.67	0.42
1:E:3398:ALA:CB	1:E:3413:MET:HE1	2.50	0.42
1:F:3726:SER:HB3	1:F:3729:ALA:N	2.34	0.42
1:H:4843:ASN:CB	1:H:5267:GLY:HA2	2.48	0.42
1:A:328:GLN:HE21	1:C:1540:THR:HB	1.84	0.42
1:B:935:LYS:HA	1:B:935:LYS:HD2	1.70	0.42
1:C:1345:ASN:C	1:C:1347:TYR:N	2.74	0.42
1:C:1687:LEU:HA	1:C:1690:ASN:HD22	1.85	0.42
1:D:1818:HIS:CD2	1:D:1831:ARG:HD3	2.54	0.42
1:D:1863:MET:HG3	1:D:2171:LEU:CD2	2.49	0.42
1:D:1958:LEU:CD1	1:D:1963:ILE:HD12	2.50	0.42
1:D:2071:GLU:HB3	1:D:2092:ALA:HB3	2.01	0.42
1:D:2096:LEU:O	1:D:2100:ILE:HG12	2.19	0.42
1:E:3254:ARG:HH22	1:E:3287:ASP:CG	2.28	0.42
1:F:3675:PHE:CE2	1:F:3683:HIS:HD2	2.37	0.42
1:F:3756:LEU:HD12	1:F:3756:LEU:C	2.42	0.42
1:G:4300:ASP:OD1	1:G:4301:PRO:HD2	2.20	0.42
1:G:4337:ALA:O	1:G:4395:GLU:HA	2.19	0.42
1:G:4374:TYR:HB3	1:G:4378:GLY:HA2	2.02	0.42
1:G:4387:LYS:HA	1:G:4392:LEU:CD1	2.50	0.42
1:A:146:ALA:C	1:A:147:TYR:CD1	2.98	0.42
1:A:439:GLN:OE1	1:A:442:ARG:HD3	2.18	0.42
1:B:815:VAL:HG21	1:B:843:PHE:HE2	1.85	0.42
1:C:1305:ARG:CG	1:C:1699:ARG:HH21	2.33	0.42
1:C:1406:LYS:HA	1:C:1406:LYS:HD2	1.40	0.42
1:C:1417:LEU:HA	1:C:1418:PRO:HD3	1.78	0.42
1:E:3457:GLN:HB2	1:E:3460:ARG:HH12	1.84	0.42
1:F:3743:LEU:HD12	1:F:3761:LYS:HG2	2.01	0.42
1:G:4273:MET:HE2	1:G:4286:THR:HG21	2.02	0.42
1:G:4303:LEU:HD22	1:G:4303:LEU:HA	1.78	0.42
1:G:4377:ASP:C	1:G:4498:ILE:HD12	2.45	0.42
1:H:5261:GLN:O	1:H:5264:LEU:HB2	2.20	0.42
1:A:210:LEU:HB3	1:A:213:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1363:ILE:HA	1:C:1366:VAL:CG1	2.48	0.42
1:C:1575:ARG:O	1:C:1578:HIS:HB3	2.20	0.42
1:D:1841:ALA:CB	1:D:2248:PRO:HG3	2.50	0.42
1:D:1991:PHE:CD1	1:D:1991:PHE:C	2.98	0.42
1:D:2291:LEU:HD12	1:D:2291:LEU:C	2.44	0.42
1:E:3062:GLU:OE1	1:E:3062:GLU:HA	2.19	0.42
1:E:3103:LEU:HG	1:E:3103:LEU:O	2.20	0.42
1:E:3271:GLU:OE1	1:E:3295:ASP:HB2	2.20	0.42
1:E:3300:ILE:HB	1:E:3301:PRO:CD	2.46	0.42
1:E:3402:SER:OG	1:F:3621:MET:HE1	2.18	0.42
1:G:4391:PHE:CD1	1:G:4391:PHE:C	2.98	0.42
1:G:4701:PHE:HD1	1:G:4701:PHE:HA	1.63	0.42
1:H:4873:MET:HG3	1:H:4887:ILE:CD1	2.38	0.42
1:H:4923:ILE:C	1:H:4925:GLY:N	2.78	0.42
1:A:168:ASP:O	1:A:169:VAL:C	2.63	0.42
1:A:328:GLN:HE22	1:C:1540:THR:CA	2.30	0.42
1:A:375:ARG:O	1:A:378:HIS:HB3	2.20	0.42
1:B:733:LEU:HD11	1:B:802:LEU:HD22	2.02	0.42
1:B:791:PHE:CD2	1:B:791:PHE:C	2.97	0.42
1:D:1857:VAL:O	1:D:1861:LYS:HG3	2.19	0.42
1:E:3496:GLY:O	1:E:3501:PHE:N	2.46	0.42
1:G:4259:THR:O	1:G:4263:MET:HG2	2.19	0.42
1:G:4341:ILE:N	1:G:4392:LEU:O	2.46	0.42
1:H:5269:PHE:N	1:H:5269:PHE:CD1	2.88	0.42
1:A:224:ASP:O	1:A:228:LEU:HG	2.20	0.42
1:B:846:LYS:N	1:B:846:LYS:HD2	2.35	0.42
1:D:1922:LEU:O	1:D:1951:CYS:HB2	2.19	0.42
1:E:3145:ASN:HD21	1:E:3161:LYS:NZ	2.17	0.42
1:E:3396:GLU:CD	1:G:4224:THR:HB	2.45	0.42
1:F:3639:ILE:O	1:F:3982:ARG:HD2	2.20	0.42
1:G:4335:LYS:C	1:G:4337:ALA:H	2.28	0.42
1:G:4417:LEU:HD12	1:G:4417:LEU:HA	1.71	0.42
1:G:4539:PRO:HG3	1:G:4576:MET:HG2	2.01	0.42
1:A:225:ILE:H	1:A:225:ILE:HG13	1.64	0.41
1:A:238:MET:HE2	1:A:238:MET:HB3	1.85	0.41
1:C:1346:ALA:C	1:C:1347:TYR:CD1	2.98	0.41
1:C:1713:GLY:HA2	1:C:1722:ASN:OD1	2.20	0.41
1:D:1894:THR:HG22	1:D:1904:TYR:CE1	2.55	0.41
1:D:1900:ASP:OD2	1:D:1903:LEU:HG	2.20	0.41
1:D:2090:MET:HE1	3:D:2333:OXL:O3	2.20	0.41
1:D:2293:MET:CG	1:D:2330:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3280:ASP:HB2	6:E:6959:HOH:O	2.20	0.41
1:E:3511:LEU:C	1:E:3512:THR:HG23	2.45	0.41
1:F:3872:ASN:HD22	1:F:3872:ASN:C	2.28	0.41
1:F:3928:GLN:NE2	1:H:5140:THR:HA	2.33	0.41
1:F:3993:LEU:HD21	1:F:4044:ARG:HG3	2.02	0.41
1:G:4339:LEU:N	1:G:4394:THR:O	2.40	0.41
1:H:4942:THR:CG2	1:H:4944:ASP:N	2.79	0.41
1:A:244:ILE:HD13	1:A:244:ILE:HA	1.86	0.41
1:A:277:ARG:NH2	1:A:278:ARG:CZ	2.83	0.41
1:A:284:GLU:HA	6:A:6607:HOH:O	2.20	0.41
1:A:478:GLN:HB2	1:A:484:ASP:CB	2.50	0.41
1:C:1288:LYS:HD3	6:C:7421:HOH:O	2.19	0.41
1:C:1647:ALA:HB1	1:C:1648:PRO:CD	2.49	0.41
1:D:2041:ALA:O	1:D:2044:ILE:HG12	2.20	0.41
1:E:3225:ILE:HD12	1:E:3256:ILE:HD12	2.02	0.41
1:E:3411:MET:SD	1:F:4126:VAL:CG2	3.08	0.41
1:F:3733:LEU:N	1:F:3800:GLY:O	2.48	0.41
1:G:4247:ILE:HB	1:G:4559:MET:HG3	2.02	0.41
1:H:4943:LEU:HD23	1:H:4943:LEU:HA	1.85	0.41
1:B:866:ILE:HD13	1:B:866:ILE:HG21	1.77	0.41
1:B:1111:LEU:HD21	1:B:1124:MET:HB2	2.01	0.41
1:D:2130:LEU:HD23	1:D:2143:GLU:HB3	2.01	0.41
1:D:2158:ILE:H	1:D:2158:ILE:HG12	1.71	0.41
1:E:3165:LYS:O	1:E:3165:LYS:HG3	2.20	0.41
1:E:3192:LEU:N	1:E:3192:LEU:CD2	2.80	0.41
1:E:3274:GLU:O	1:E:3278:ARG:HG3	2.20	0.41
1:F:3746:ALA:HB3	1:F:3747:TYR:CD1	2.55	0.41
1:G:4726:VAL:HG23	1:H:5211:MET:SD	2.60	0.41
1:H:5081:GLU:HG2	6:H:6315:HOH:O	2.21	0.41
1:A:90:VAL:HG12	1:A:91:ARG:N	2.34	0.41
1:A:122:LEU:HD22	1:A:126:SER:C	2.45	0.41
1:B:879:PHE:CZ	1:B:883:LEU:HG	2.55	0.41
1:C:1218:HIS:O	1:C:1231:ARG:NH1	2.45	0.41
1:C:1360:TYR:CD2	1:C:1363:ILE:HB	2.52	0.41
1:C:1465:LYS:HA	1:C:1487:ASP:OD2	2.20	0.41
1:C:1516:CYS:HB3	1:C:1521:LYS:O	2.20	0.41
1:C:1599:ARG:NH1	1:D:1823:ASP:CG	2.78	0.41
1:D:1851:GLY:O	1:D:1855:ARG:N	2.54	0.41
1:D:2030:PHE:CE1	1:D:2034:GLN:CG	3.03	0.41
1:E:3220:VAL:O	1:E:3220:VAL:HG12	2.18	0.41
1:F:3849:ASP:OD1	1:F:3849:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4410:LEU:N	1:G:4411:PRO:CD	2.82	0.41
1:H:4900:ASP:O	1:H:4902:ILE:N	2.54	0.41
1:A:176:ASP:HB3	1:A:179:LEU:CB	2.51	0.41
1:A:246:LYS:CG	1:A:248:ALA:HB3	2.50	0.41
1:B:1011:MET:HE2	1:B:1122:ASN:O	2.21	0.41
6:B:6588:HOH:O	1:D:2131:GLU:HB3	2.20	0.41
1:C:1338:THR:HG22	1:C:1339:LEU:N	2.35	0.41
1:C:1599:ARG:HG3	6:D:6052:HOH:O	2.20	0.41
1:C:1609:GLU:HG2	1:C:1643:TYR:OH	2.19	0.41
1:E:3047:ILE:HG12	1:E:3070:VAL:HB	2.01	0.41
1:E:3423:LEU:HD12	1:F:4005:THR:HG21	2.01	0.41
1:F:3760:TYR:HE2	1:F:3766:VAL:HG21	1.85	0.41
1:G:4215:GLN:HB3	1:G:4217:LEU:HG	2.01	0.41
1:G:4639:GLN:O	1:G:4642:ARG:HG2	2.19	0.41
1:A:148:MET:HE3	1:A:148:MET:HB3	1.60	0.41
1:A:210:LEU:CB	1:A:213:ALA:HB3	2.50	0.41
1:B:617:LEU:HD23	1:B:617:LEU:HA	1.89	0.41
1:B:889:ILE:CG2	1:B:890:MET:N	2.83	0.41
1:C:1287:ILE:O	1:C:1290:VAL:N	2.53	0.41
1:C:1428:LEU:HD23	1:C:1428:LEU:HA	1.82	0.41
1:D:2226:ALA:HA	1:D:2247:ALA:HB1	2.03	0.41
1:E:3172:LYS:HA	1:E:3182:LEU:O	2.20	0.41
1:E:3272:ASN:OD1	1:E:3274:GLU:HB3	2.20	0.41
1:F:3700:ASP:OD2	1:F:3703:LEU:HD13	2.21	0.41
1:F:3718:ILE:C	1:F:3719:ARG:HG2	2.45	0.41
1:F:3746:ALA:HB3	1:F:3747:TYR:CE1	2.54	0.41
1:F:3936:LYS:HA	1:F:3937:PRO:HD3	1.90	0.41
1:G:4478:ARG:O	1:G:4482:ILE:HG13	2.21	0.41
1:G:4669:PHE:HZ	1:G:4699:ARG:HD2	1.85	0.41
1:B:731:VAL:HG12	1:B:732:GLU:N	2.35	0.41
1:B:1087:LEU:CD2	1:B:1088:ARG:N	2.79	0.41
1:C:1391:PHE:O	1:C:1392:LEU:HD13	2.21	0.41
1:C:1500:ILE:HB	1:C:1501:PRO:CD	2.49	0.41
1:D:1864:ILE:HD13	1:D:1864:ILE:HG21	1.79	0.41
1:D:2271:VAL:HG11	1:D:2291:LEU:HG	2.03	0.41
1:E:3346:ASP:CG	1:G:4542:ALA:HA	2.46	0.41
1:G:4429:LYS:HE2	1:G:4456:ILE:O	2.21	0.41
1:A:454:ARG:CG	1:A:473:CYS:HB3	2.50	0.41
1:A:518:SER:HB2	6:A:7722:HOH:O	2.21	0.41
1:B:781:SER:HB3	1:B:798:ASN:HB2	2.03	0.41
1:C:1409:ASN:ND2	6:C:6568:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1526:ALA:CB	1:C:1559:MET:HE2	2.37	0.41
1:C:1605:THR:HG22	6:D:6122:HOH:O	2.20	0.41
1:C:1708:VAL:CG1	1:C:1709:ILE:N	2.81	0.41
1:D:1814:THR:HG22	1:D:1815:GLN:N	2.35	0.41
1:D:2294:ASN:HD22	1:D:2294:ASN:HA	1.71	0.41
1:E:3209:ASN:C	1:E:3211:PRO:HD3	2.45	0.41
1:F:3653:ALA:HB2	1:F:3966:LYS:HA	2.03	0.41
1:F:3752:ASP:C	1:F:3754:ASN:N	2.78	0.41
1:F:4007:LEU:HA	1:F:4007:LEU:HD23	1.64	0.41
1:G:4319:ARG:H	1:G:4359:ASP:CB	2.33	0.41
1:G:4727:VAL:HA	1:G:4728:PRO:HD3	1.92	0.41
1:H:5067:ILE:HD12	1:H:5088:GLY:CA	2.51	0.41
1:A:47:ILE:HG22	1:A:359:MET:CG	2.42	0.41
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.43	0.41
1:A:133:LEU:N	1:A:133:LEU:CD1	2.84	0.41
1:A:173:VAL:HG13	1:A:210:LEU:CD1	2.49	0.41
1:A:176:ASP:O	1:A:179:LEU:HB2	2.21	0.41
1:A:191:PHE:CG	1:A:192:LEU:N	2.82	0.41
1:A:306:PHE:CD1	1:A:306:PHE:C	2.99	0.41
1:A:511:LEU:HD22	1:A:521:THR:CG2	2.44	0.41
1:B:700:ASP:C	1:B:702:ILE:N	2.79	0.41
1:B:790:ASP:O	1:B:790:ASP:OD1	2.38	0.41
1:B:1054:ARG:HD2	1:B:1054:ARG:HH11	1.64	0.41
1:C:1334:LYS:HB3	1:C:1334:LYS:HE3	1.82	0.41
1:C:1421:SER:O	1:C:1425:ILE:HG13	2.21	0.41
1:C:1608:MET:HE2	1:C:1636:SER:O	2.20	0.41
1:D:1947:TYR:C	1:D:1949:GLU:N	2.78	0.41
1:E:3037:ALA:HA	1:E:3038:PRO:HD3	1.91	0.41
1:E:3143:LEU:HD12	1:E:3143:LEU:HA	1.65	0.41
1:E:3289:ILE:CG2	1:E:3290:MET:N	2.84	0.41
1:F:3702:ILE:CD1	1:F:4094:ASN:HB2	2.50	0.41
1:F:3791:PHE:CD2	1:F:3791:PHE:C	2.99	0.41
1:F:3844:ILE:HG13	1:F:3868:SER:HB3	2.03	0.41
1:F:3869:LYS:NZ	3:F:4133:OXL:O1	2.45	0.41
1:F:4030:LEU:N	1:F:4030:LEU:HD23	2.35	0.41
1:G:4320:THR:HG23	1:G:4321:GLY:N	2.35	0.41
1:G:4344:ASP:C	1:G:4346:ALA:N	2.79	0.41
1:G:4463:ASN:HD22	1:G:4463:ASN:HA	1.62	0.41
1:G:4626:ALA:HA	1:G:4647:ALA:HB1	2.03	0.41
1:H:4945:ASN:O	1:H:4948:MET:HB2	2.21	0.41
1:H:5237:ALA:HB1	1:H:5268:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1535:LYS:HA	1:C:1535:LYS:HD3	1.91	0.41
1:C:1579:LEU:HA	1:C:1579:LEU:HD12	1.81	0.41
1:C:1720:PHE:CE2	1:C:1722:ASN:HB3	2.56	0.41
1:D:1819:ALA:HB2	1:D:1831:ARG:HB2	2.03	0.41
1:D:2209:GLU:O	1:D:2213:MET:HG3	2.21	0.41
1:D:2329:VAL:HA	1:D:2330:PRO:HD3	1.90	0.41
1:F:3650:ILE:HG13	1:F:3673:MET:HE1	2.03	0.41
1:F:3837:ASP:HB3	1:F:4061:GLN:HG2	2.03	0.41
1:F:3878:ARG:O	1:F:3881:GLU:HG2	2.20	0.41
1:F:4030:LEU:HD13	1:F:4088:ARG:HB2	2.03	0.41
1:F:4099:ARG:HA	1:F:4099:ARG:HD3	1.84	0.41
1:G:4250:ILE:HD11	1:G:4268:MET:CE	2.18	0.41
1:G:4374:TYR:HA	1:G:4380:ILE:O	2.20	0.41
1:G:4625:ALA:CB	1:G:4702:PHE:HB3	2.51	0.41
1:G:4726:VAL:CG2	1:H:5211:MET:SD	3.09	0.41
1:H:4986:GLN:HG2	1:H:4993:VAL:HB	2.02	0.41
1:A:302:ALA:C	1:A:304:LYS:N	2.79	0.40
1:B:673:MET:CE	1:B:686:THR:HG22	2.51	0.40
1:B:825:ILE:O	1:B:829:LYS:HG3	2.21	0.40
1:B:942:ALA:HB1	1:D:2146:ASP:HB2	2.03	0.40
1:C:1656:HIS:N	1:C:1656:HIS:CD2	2.88	0.40
1:D:2192:LYS:CG	6:D:7588:HOH:O	2.69	0.40
1:E:3068:MET:CE	1:E:3071:ALA:HA	2.47	0.40
1:E:3142:THR:CG2	1:E:3143:LEU:N	2.84	0.40
1:E:3145:ASN:ND2	1:E:3161:LYS:NZ	2.69	0.40
1:E:3335:LYS:HE2	1:E:3368:ASP:OD2	2.20	0.40
1:E:3398:ALA:CB	1:E:3413:MET:CE	2.99	0.40
1:E:3421:LYS:HD3	1:F:4013:MET:SD	2.61	0.40
1:F:3711:LEU:HD23	1:F:3711:LEU:C	2.45	0.40
1:F:3788:GLY:HA3	1:F:3791:PHE:CZ	2.57	0.40
1:F:3842:SER:HA	1:F:3869:LYS:HD3	2.03	0.40
1:G:4275:PHE:CE2	1:G:4280:HIS:CD2	3.06	0.40
1:G:4402:LEU:HA	1:G:4402:LEU:HD22	1.77	0.40
1:H:4847:ILE:CG2	1:H:5159:MET:CE	2.97	0.40
1:H:5020:VAL:CG1	1:H:5025:ILE:CG1	2.99	0.40
1:A:57:VAL:CG2	1:A:89:ASN:CB	3.00	0.40
6:A:7332:HOH:O	1:C:1542:ALA:HB3	2.20	0.40
1:B:673:MET:HE3	1:B:686:THR:CG2	2.51	0.40
1:C:1215:GLN:HA	6:C:6142:HOH:O	2.21	0.40
1:C:1294:THR:C	1:C:1296:SER:H	2.29	0.40
1:C:1371:SER:O	1:C:1383:GLN:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2240:VAL:HG12	1:D:2249:ILE:CD1	2.51	0.40
1:E:3294:GLY:HA3	1:E:3327:THR:HG21	2.04	0.40
1:G:4598:ALA:HB1	1:G:4613:MET:HE1	2.03	0.40
1:G:4654:ARG:HH11	1:G:4654:ARG:HD2	1.77	0.40
1:H:5037:ASP:OD1	1:H:5260:ARG:HD2	2.20	0.40
1:A:47:ILE:CB	1:A:359:MET:HG3	2.51	0.40
1:A:216:ASP:O	1:A:216:ASP:OD1	2.39	0.40
1:A:235:ASP:OD1	1:A:235:ASP:O	2.39	0.40
1:C:1429:LYS:O	1:C:1433:GLU:HG2	2.21	0.40
1:C:1456:ILE:N	1:C:1456:ILE:CD1	2.79	0.40
1:D:2254:ARG:HD2	6:D:7101:HOH:O	2.20	0.40
1:E:3068:MET:CE	1:E:3071:ALA:CB	2.99	0.40
1:E:3340:THR:HB	1:G:4528:GLN:HE21	1.86	0.40
1:E:3478:GLN:HB2	1:E:3484:ASP:HB2	2.02	0.40
1:F:3650:ILE:CG1	1:F:3673:MET:CE	2.99	0.40
1:F:4055:ASN:O	1:F:4058:THR:HB	2.21	0.40
1:G:4353:GLU:H	1:G:4353:GLU:HG2	1.44	0.40
1:G:4570:PRO:HD2	6:G:6548:HOH:O	2.19	0.40
1:G:4608:MET:HG3	1:G:4639:GLN:HG3	2.04	0.40
1:A:451:ALA:CB	1:A:468:ILE:CG2	2.99	0.40
1:C:1250:ILE:CG2	1:C:1286:THR:CG2	3.00	0.40
1:C:1277:HIS:NE2	5:C:1735:ATP:H3'	2.36	0.40
1:C:1357:TRP:CD2	1:C:1358:LEU:N	2.90	0.40
1:C:1482:ILE:O	1:C:1486:SER:OG	2.38	0.40
1:D:1944:ASP:C	1:D:1946:ALA:N	2.80	0.40
1:D:2311:LEU:HD23	1:D:2323:THR:O	2.20	0.40
1:H:4911:LEU:HD23	1:H:4911:LEU:C	2.45	0.40
1:H:5275:ASP:CB	1:H:5276:PRO:CD	2.99	0.40
1:A:398:ALA:HB1	1:A:413:MET:HE1	2.03	0.40
1:A:454:ARG:CZ	1:A:477:VAL:HG22	2.51	0.40
1:B:649:THR:OG1	1:B:672:ARG:NH1	2.50	0.40
1:B:976:MET:HE3	1:B:980:ILE:CD1	2.50	0.40
1:B:1128:PRO:O	1:B:1130:PRO:HD3	2.22	0.40
1:D:1850:ILE:CG1	1:D:1873:MET:HE3	2.50	0.40
1:D:2093:ARG:NH2	1:D:2146:ASP:OD1	2.55	0.40
1:D:2246:ARG:HD3	6:D:6077:HOH:O	2.22	0.40
1:D:2259:ALA:HB1	1:D:2270:PRO:HB2	2.02	0.40
1:E:3287:ASP:O	1:E:3322:PRO:HD2	2.21	0.40
1:E:3392:LYS:HZ1	1:G:4225:PHE:HB2	1.86	0.40
1:E:3525:ARG:HD3	1:F:4114:TRP:CE3	2.57	0.40
1:F:3650:ILE:HG23	1:F:3650:ILE:HD12	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3702:ILE:HD12	1:F:4094:ASN:HB3	2.03	0.40
1:F:3721:GLY:N	1:F:3757:TRP:HE3	2.19	0.40
1:F:3916:CYS:HB3	1:F:3921:LYS:O	2.22	0.40
1:F:3939:PRO:HG3	1:F:3976:MET:HG2	2.03	0.40
1:F:3969:TYR:N	1:F:3970:PRO:CD	2.83	0.40
1:G:4339:LEU:HD11	1:G:4353:GLU:C	2.47	0.40
1:G:4363:ILE:O	1:G:4366:VAL:HB	2.21	0.40
1:G:4417:LEU:HA	1:G:4418:PRO:HD3	1.89	0.40
1:G:4493:ARG:HH22	1:G:4546:ASP:CG	2.29	0.40
1:G:4606:ASP:O	1:G:4609:GLU:HB2	2.22	0.40
1:H:4852:PRO:HD2	1:H:5165:ALA:O	2.21	0.40

All (25) 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]	0.65	1.55
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.12	1.08
1:E:3081:GLU:OE1	1:H:4924:LYS:NZ[3_655]	1.15	1.05
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.22	0.98
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.29	0.91
1:E:3149:GLU:OE1	1:H:4934:LYS:CD[3_655]	1.43	0.77
1:E:3124:LYS:O	6:H:6943:HOH:O[3_655]	1.55	0.65
1:E:3149:GLU:OE2	1:H:4934:LYS:NZ[3_655]	1.58	0.62
1:D:1948:MET:CE	1:F:3765:LYS:NZ[4_465]	1.65	0.55
1:E:3149:GLU:OE1	1:H:4934:LYS:NZ[3_655]	1.68	0.52
1:E:3124:LYS:C	6:H:6943:HOH:O[3_655]	1.72	0.48
1:D:1924:LYS:CE	1:H:4858:GLU:OE1[1_455]	1.74	0.46
1:D:1945:ASN:OD1	1:F:3816:ASP:OD2[4_465]	1.83	0.37
1:E:3149:GLU:OE2	1:H:4934:LYS:CE[3_655]	1.88	0.32
1:E:3081:GLU:OE1	1:H:4924:LYS:CE[3_655]	1.92	0.28
1:C:1387:LYS:O	1:H:4987:LYS:CB[3_645]	1.97	0.23
1:C:1386:GLN:CB	1:H:4989:PRO:CD[3_645]	2.00	0.20
1:D:1924:LYS:NZ	1:H:4858:GLU:CD[1_455]	2.01	0.19
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]	2.08	0.12
1:E:3081:GLU:CD	1:H:4924:LYS:NZ[3_655]	2.10	0.10
1:A:277:ARG:CZ	1:G:4425:ILE:CD1[4_465]	2.11	0.09
1:B:801:PHE:CE2	6:H:7250:HOH:O[1_455]	2.11	0.09
1:C:1385:LYS:O	1:H:4989:PRO:CG[3_645]	2.14	0.06
1:E:3081:GLU:CD	1:H:4924:LYS:CE[3_655]	2.14	0.06

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%)	480 (93%)	33 (6%)	4 (1%)	16	12
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	12	9
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	12	9
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	21	18
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	12	9
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	16	12
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	16	12
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	21	18
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	16	12

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	PRO
1	C	1533	MET
1	E	3506	ASP
1	F	3729	ALA
1	F	3789	PRO
1	H	4924	LYS
1	A	221	SER
1	C	1346	ALA
1	D	2058	GLY
1	F	3730	GLU
1	G	4345	ASN
1	G	4389	PRO
1	A	164	CYS
1	B	745	ASN
1	D	2277	VAL
1	E	3013	GLN
1	C	1337	ALA

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Mol	Chain	Res	Type
1	E	3145	ASN
1	B	1002	SER
1	C	1527	THR
1	C	1532	SER
1	D	2127	THR
1	E	3327	THR
1	G	4458	GLY
1	A	327	THR
1	B	927	THR
1	B	1128	PRO
1	F	3927	THR
1	G	4527	THR
1	H	4901	PRO
1	H	5127	THR
1	B	701	PRO
1	E	3163	ILE

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%)	346 (81%)	80 (19%)	1	1
1	B	426/434 (98%)	374 (88%)	52 (12%)	5	2
1	C	426/434 (98%)	345 (81%)	81 (19%)	1	1
1	D	426/434 (98%)	375 (88%)	51 (12%)	5	3
1	E	426/434 (98%)	366 (86%)	60 (14%)	3	2
1	F	426/434 (98%)	365 (86%)	61 (14%)	3	1
1	G	426/434 (98%)	364 (85%)	62 (15%)	3	1
1	H	426/434 (98%)	380 (89%)	46 (11%)	6	4
All	All	3408/3472 (98%)	2915 (86%)	493 (14%)	3	1

All (493) 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	60	LEU
1	A	63	MET
1	A	68	MET
1	A	73	MET
1	A	86	THR
1	A	88	LYS
1	A	90	VAL
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	133	LEU
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	163	ILE
1	A	164	CYS
1	A	166	VAL
1	A	167	VAL
1	A	168	ASP
1	A	169	VAL
1	A	172	LYS
1	A	175	VAL
1	A	180	ILE
1	A	190	ASP
1	A	192	LEU
1	A	202	LEU
1	A	206	LYS
1	A	210	LEU
1	A	215	VAL
1	A	245	ARG
1	A	257	LEU
1	A	260	LYS
1	A	264	ILE
1	A	267	ILE

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Mol	Chain	Res	Type
1	A	271	GLU
1	A	278	ARG
1	A	283	LEU
1	A	284	GLU
1	A	289	ILE
1	A	293	ARG
1	A	311	MET
1	A	328	GLN
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	460	ARG
1	A	464	LEU
1	A	469	PHE
1	A	471	VAL
1	A	478	GLN
1	A	479	GLU
1	A	493	MET
1	A	497	LYS
1	A	503	LYS
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	660	LEU
1	B	661	LYS

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Mol	Chain	Res	Type
1	B	664	ILE
1	B	673	MET
1	B	676	SER
1	B	681	GLU
1	B	687	ILE
1	B	688	LYS
1	B	703	LEU
1	B	719	ARG
1	B	738	THR
1	B	745	ASN
1	B	748	MET
1	B	756	LEU
1	B	782	LEU
1	B	785	LYS
1	B	786	GLN
1	B	787	LYS
1	B	798	ASN
1	B	810	LEU
1	B	822	GLU
1	B	839	VAL
1	B	846	LYS
1	B	867	ILE
1	B	883	LEU
1	B	886	SER
1	B	921	LYS
1	B	952	LEU
1	B	1004	SER
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	1086	ASP
1	B	1087	LEU
1	B	1090	ASN
1	B	1093	MET
1	B	1099	ARG
1	B	1103	LYS

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Mol	Chain	Res	Type
1	B	1104	LYS
1	B	1107	VAL
1	B	1108	VAL
1	B	1118	SER
1	B	1125	ARG
1	C	1212	ILE
1	C	1214	THR
1	C	1229	MET
1	C	1250	ILE
1	C	1257	VAL
1	C	1273	MET
1	C	1281	GLU
1	C	1287	ILE
1	C	1288	LYS
1	C	1292	THR
1	C	1295	GLU
1	C	1302	ILE
1	C	1313	THR
1	C	1319	ARG
1	C	1323	ILE
1	C	1328	THR
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	1368	ASP
1	C	1372	LYS
1	C	1380	ILE
1	C	1383	GLN
1	C	1387	LYS
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

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Mol	Chain	Res	Type
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	1464	ILE
1	C	1469	LYS
1	C	1472	ASN
1	C	1483	LEU
1	C	1484	GLU
1	C	1486	SER
1	C	1489	ILE
1	C	1493	ARG
1	C	1498	ILE
1	C	1518	ARG
1	C	1530	LEU
1	C	1532	SER
1	C	1558	ILE
1	C	1566	LYS
1	C	1579	LEU
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	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	1686	ASP
1	C	1687	LEU
1	C	1693	MET
1	C	1708	VAL

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Mol	Chain	Res	Type
1	C	1718	SER
1	C	1723	THR
1	D	1812	ILE
1	D	1824	THR
1	D	1829	MET
1	D	1856	SER
1	D	1860	LEU
1	D	1885	GLU
1	D	1887	ILE
1	D	1888	LYS
1	D	1899	SER
1	D	1902	ILE
1	D	1922	LEU
1	D	1930	GLU
1	D	1931	VAL
1	D	1938	THR
1	D	1942	THR
1	D	1943	LEU
1	D	1945	ASN
1	D	1948	MET
1	D	1959	ASP
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	2005	LYS
1	D	2010	LEU
1	D	2023	LYS
1	D	2046	LYS
1	D	2056	ILE
1	D	2059	GLU
1	D	2077	ARG
1	D	2081	GLU
1	D	2093	ARG
1	D	2141	ARG
1	D	2145	SER
1	D	2199	ARG
1	D	2205	THR
1	D	2209	GLU
1	D	2230	LEU

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Mol	Chain	Res	Type
1	D	2246	ARG
1	D	2266	ARG
1	D	2279	GLU
1	D	2283	GLU
1	D	2287	LEU
1	D	2288	ARG
1	D	2290	ASN
1	D	2293	MET
1	D	2303	LYS
1	D	2308	VAL
1	D	2318	SER
1	E	3012	ILE
1	E	3013	GLN
1	E	3014	THR
1	E	3015	GLN
1	E	3016	GLN
1	E	3021	MET
1	E	3029	MET
1	E	3031	ARG
1	E	3034	ILE
1	E	3055	ARG
1	E	3056	SER
1	E	3066	SER
1	E	3081	GLU
1	E	3099	SER
1	E	3102	ILE
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	3155	ILE
1	E	3156	LEU
1	E	3158	LEU
1	E	3162	ASN
1	E	3164	CYS
1	E	3166	VAL
1	E	3167	VAL
1	E	3168	ASP
1	E	3172	LYS
1	E	3192	LEU

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Mol	Chain	Res	Type
1	E	3202	LEU
1	E	3222	GLU
1	E	3246	LYS
1	E	3257	LEU
1	E	3260	LYS
1	E	3265	LYS
1	E	3267	ILE
1	E	3271	GLU
1	E	3283	LEU
1	E	3286	SER
1	E	3315	ARG
1	E	3318	ARG
1	E	3330	LEU
1	E	3336	LYS
1	E	3338	ARG
1	E	3371	LEU
1	E	3379	LEU
1	E	3382	ARG
1	E	3407	LEU
1	E	3435	ARG
1	E	3442	ARG
1	E	3446	ARG
1	E	3466	ARG
1	E	3469	PHE
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	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	3702	ILE
1	F	3713	THR

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Mol	Chain	Res	Type
1	F	3714	LYS
1	F	3723	ILE
1	F	3726	SER
1	F	3728	THR
1	F	3731	VAL
1	F	3742	THR
1	F	3748	MET
1	F	3753	GLU
1	F	3755	ILE
1	F	3759	ASP
1	F	3762	ASN
1	F	3765	LYS
1	F	3766	VAL
1	F	3767	VAL
1	F	3769	VAL
1	F	3772	LYS
1	F	3782	LEU
1	F	3786	GLN
1	F	3787	LYS
1	F	3792	LEU
1	F	3804	SER
1	F	3805	LYS
1	F	3810	LEU
1	F	3821	SER
1	F	3823	LYS
1	F	3825	ILE
1	F	3832	VAL
1	F	3845	ARG
1	F	3856	ILE
1	F	3862	LYS
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	4002	SER
1	F	4015	SER

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Mol	Chain	Res	Type
1	F	4032	GLU
1	F	4066	ARG
1	F	4079	GLU
1	F	4093	MET
1	F	4107	VAL
1	F	4118	SER
1	G	4212	ILE
1	G	4215	GLN
1	G	4234	ILE
1	G	4240	THR
1	G	4242	ARG
1	G	4254	SER
1	G	4258	GLU
1	G	4265	LYS
1	G	4268	MET
1	G	4273	MET
1	G	4296	SER
1	G	4302	ILE
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	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	4409	ASN

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Mol	Chain	Res	Type
1	G	4417	LEU
1	G	4423	LYS
1	G	4442	SER
1	G	4449	ASP
1	G	4471	GLU
1	G	4498	ILE
1	G	4500	ILE
1	G	4545	SER
1	G	4552	LEU
1	G	4592	LYS
1	G	4597	LEU
1	G	4599	ARG
1	G	4600	SER
1	G	4604	SER
1	G	4649	ILE
1	G	4656	HIS
1	G	4664	LEU
1	G	4666	ARG
1	G	4677	VAL
1	G	4693	MET
1	G	4699	ARG
1	G	4703	LYS
1	G	4707	VAL
1	G	4708	VAL
1	G	4715	ARG
1	G	4729	VAL
1	H	4812	ILE
1	H	4814	THR
1	H	4827	GLU
1	H	4840	THR
1	H	4848	CYS
1	H	4850	ILE
1	H	4855	ARG
1	H	4863	MET
1	H	4873	MET
1	H	4922	LEU
1	H	4926	SER
1	H	4932	GLU
1	H	4935	LYS
1	H	4942	THR
1	H	4950	LYS
1	H	4972	LYS

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Mol	Chain	Res	Type
1	H	4980	ILE
1	H	4983	GLN
1	H	4986	GLN
1	H	4992	LEU
1	H	5010	LEU
1	H	5046	LYS
1	H	5060	LYS
1	H	5071	GLU
1	H	5072	ASN
1	H	5112	ILE
1	H	5118	ARG
1	H	5177	GLN
1	H	5182	ARG
1	H	5202	SER
1	H	5205	THR
1	H	5206	ASP
1	H	5207	LEU
1	H	5235	ARG
1	H	5264	LEU
1	H	5268	ILE
1	H	5269	PHE
1	H	5278	GLN
1	H	5286	ASP
1	H	5297	LYS
1	H	5299	ARG
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 (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	89	ASN
1	A	154	ASN
1	A	162	ASN
1	A	198	ASN
1	A	263	ASN
1	A	273	HIS
1	A	317	ASN

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	349	ASN
1	A	377	GLN
1	A	438	HIS
1	A	456	HIS
1	A	478	GLN
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	863	ASN
1	B	928	GLN
1	B	949	ASN
1	B	977	GLN
1	B	990	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	1528	GLN
1	C	1549	ASN
1	C	1577	GLN
1	C	1590	HIS
1	C	1656	HIS
1	C	1678	GLN
1	C	1690	ASN
1	D	1815	GLN
1	D	1818	HIS

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Mol	Chain	Res	Type
1	D	1843	ASN
1	D	1889	ASN
1	D	1945	ASN
1	D	1962	ASN
1	D	1986	GLN
1	D	1998	ASN
1	D	2034	GLN
1	D	2073	HIS
1	D	2128	GLN
1	D	2149	ASN
1	D	2177	GLN
1	D	2190	HIS
1	D	2238	HIS
1	D	2256	HIS
1	D	2257	GLN
1	D	2263	HIS
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	3198	ASN
1	E	3263	ASN
1	E	3328	GLN
1	E	3349	ASN
1	E	3390	HIS
1	E	3463	HIS
1	E	3494	ASN
1	F	3613	GLN
1	F	3615	GLN
1	F	3618	HIS
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	3851	HIS
1	F	3863	ASN
1	F	3872	ASN

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Mol	Chain	Res	Type
1	F	3873	HIS
1	F	3928	GLN
1	F	3949	ASN
1	F	4063	HIS
1	F	4090	ASN
1	F	4094	ASN
1	G	4215	GLN
1	G	4216	GLN
1	G	4243	ASN
1	G	4289	ASN
1	G	4345	ASN
1	G	4383	GLN
1	G	4409	ASN
1	G	4434	GLN
1	G	4463	ASN
1	G	4472	ASN
1	G	4509	GLN
1	G	4528	GLN
1	G	4549	ASN
1	G	4577	GLN
1	G	4694	ASN
1	H	4843	ASN
1	H	4889	ASN
1	H	4986	GLN
1	H	5026	GLN
1	H	5051	HIS
1	H	5063	ASN
1	H	5072	ASN
1	H	5128	GLN
1	H	5149	ASN
1	H	5177	GLN
1	H	5203	HIS
1	H	5256	HIS
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 [i](#)

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$
3	OXL	A	533	4	5,5,5	1.47	1 (20%)	6,6,6	2.38	2 (33%)
3	OXL	H	5333	4	5,5,5	1.26	1 (20%)	6,6,6	1.75	2 (33%)
5	ATP	E	3535	2,4	32,33,33	2.29	7 (21%)	48,52,52	0.86	2 (4%)
3	OXL	C	1733	4	5,5,5	2.15	3 (60%)	6,6,6	1.78	1 (16%)
3	OXL	B	1133	4	5,5,5	1.50	2 (40%)	6,6,6	1.75	2 (33%)
3	OXL	F	4133	4	5,5,5	1.38	0	6,6,6	1.98	4 (66%)
5	ATP	F	4135	2,4	32,33,33	2.83	10 (31%)	48,52,52	1.12	5 (10%)
3	OXL	D	2333	4	5,5,5	1.45	1 (20%)	6,6,6	1.97	3 (50%)
5	ATP	G	4735	2,4	32,33,33	3.00	9 (28%)	48,52,52	0.92	1 (2%)
5	ATP	D	2335	2,4	32,33,33	2.45	9 (28%)	48,52,52	1.21	6 (12%)
3	OXL	G	4733	4	5,5,5	1.41	0	6,6,6	2.00	4 (66%)
3	OXL	E	3533	4	5,5,5	1.39	0	6,6,6	1.99	4 (66%)
5	ATP	C	1735	2,4	32,33,33	3.39	9 (28%)	48,52,52	1.02	4 (8%)
5	ATP	A	535	2,4	32,33,33	2.41	9 (28%)	48,52,52	1.38	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	A	533	4	-	0/4/4/4	-
3	OXL	H	5333	4	-	0/4/4/4	-
5	ATP	E	3535	2,4	-	4/22/38/38	0/3/3/3
3	OXL	C	1733	4	-	0/4/4/4	-
3	OXL	B	1133	4	-	0/4/4/4	-
3	OXL	F	4133	4	-	0/4/4/4	-
5	ATP	F	4135	2,4	-	0/22/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/4/4/4	-
5	ATP	G	4735	2,4	-	4/22/38/38	0/3/3/3
5	ATP	D	2335	2,4	-	4/22/38/38	0/3/3/3
3	OXL	G	4733	4	-	0/4/4/4	-
3	OXL	E	3533	4	-	0/4/4/4	-
5	ATP	C	1735	2,4	-	5/22/38/38	0/3/3/3
5	ATP	A	535	2,4	-	1/22/38/38	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1735	ATP	PB-O3B	-16.43	1.41	1.59
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	D	2335	ATP	PB-O3B	-10.59	1.48	1.59
5	A	535	ATP	PB-O3B	-9.25	1.49	1.59
5	E	3535	ATP	PB-O3B	-8.98	1.49	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	PA-O3A	-5.28	1.53	1.59
5	E	3535	ATP	PG-O3G	-5.05	1.36	1.54
5	D	2335	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	C2-N1	4.11	1.41	1.33
5	F	4135	ATP	PA-O5'	3.96	1.74	1.59
5	C	1735	ATP	PA-O3A	-3.94	1.55	1.59
5	C	1735	ATP	PG-O3G	-3.89	1.40	1.54
5	D	2335	ATP	PA-O3A	-3.75	1.55	1.59
5	A	535	ATP	PG-O3G	-3.67	1.41	1.54
5	E	3535	ATP	PA-O3A	-3.64	1.55	1.59
5	C	1735	ATP	C8-N7	3.35	1.38	1.31
5	C	1735	ATP	C2-N1	3.33	1.39	1.33
5	F	4135	ATP	PG-O3G	-3.28	1.42	1.54
3	C	1733	OXL	O2-C2	3.05	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	C	1735	ATP	PB-O3A	-2.73	1.56	1.59
5	A	535	ATP	PB-O3A	2.68	1.62	1.59
5	F	4135	ATP	C2-N3	-2.66	1.29	1.33
5	C	1735	ATP	C8-N9	-2.60	1.33	1.37
5	E	3535	ATP	C2-N3	-2.54	1.29	1.33
5	C	1735	ATP	O4'-C1'	-2.50	1.36	1.42
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	D	2335	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	A	535	ATP	C4-N3	2.38	1.38	1.34
5	F	4135	ATP	C5-C4	2.36	1.43	1.39
3	C	1733	OXL	O3-C1	-2.36	1.24	1.30
5	D	2335	ATP	C4-N3	2.34	1.38	1.34
3	C	1733	OXL	C2-C1	-2.31	1.50	1.54
5	G	4735	ATP	C1'-N9	-2.29	1.40	1.46
3	B	1133	OXL	O4-C2	-2.28	1.24	1.30
3	A	533	OXL	O4-C2	-2.28	1.24	1.30
3	B	1133	OXL	O3-C1	-2.25	1.24	1.30
5	A	535	ATP	C2-N3	-2.24	1.30	1.33
5	D	2335	ATP	C2'-C1'	-2.23	1.46	1.53
5	F	4135	ATP	PB-O3A	2.22	1.61	1.59
5	D	2335	ATP	PA-O2A	-2.22	1.45	1.55
3	D	2333	OXL	C2-C1	2.21	1.58	1.54
3	H	5333	OXL	O4-C2	-2.19	1.24	1.30
5	D	2335	ATP	PG-O2G	-2.19	1.46	1.54
5	A	535	ATP	PG-O2G	-2.18	1.46	1.54
5	G	4735	ATP	PA-O2A	-2.14	1.45	1.55
5	C	1735	ATP	PG-O2G	-2.10	1.47	1.54
5	D	2335	ATP	C2-N1	2.05	1.37	1.33
5	A	535	ATP	C8-N7	2.04	1.35	1.31
5	G	4735	ATP	C2-N1	2.04	1.37	1.33
5	G	4735	ATP	PG-O1G	-2.02	1.44	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	535	ATP	O2B-PB-O3B	7.42	127.32	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2335	ATP	O2B-PB-O3B	-4.26	95.76	107.27
3	A	533	OXL	O3-C1-C2	4.07	120.72	112.83
3	A	533	OXL	O1-C1-C2	-3.65	113.02	120.63
5	D	2335	ATP	O3G-PG-O3B	3.26	115.58	104.64
5	C	1735	ATP	O2B-PB-O3A	3.02	115.43	107.27
5	F	4135	ATP	O3B-PB-O1B	-2.82	102.22	110.70
3	D	2333	OXL	O3-C1-C2	2.77	118.19	112.83
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	C	1733	OXL	O4-C2-O2	2.65	130.20	123.90
3	E	3533	OXL	O3-C1-C2	2.64	117.95	112.83
3	G	4733	OXL	O3-C1-C2	2.63	117.94	112.83
3	H	5333	OXL	O4-C2-C1	2.63	117.93	112.83
3	F	4133	OXL	O3-C1-C2	2.62	117.91	112.83
3	D	2333	OXL	O1-C1-C2	-2.59	115.24	120.63
5	D	2335	ATP	O2A-PA-O3A	2.55	114.16	107.27
5	F	4135	ATP	O2B-PB-O3B	2.53	114.10	107.27
3	B	1133	OXL	O2-C2-C1	-2.43	115.57	120.63
5	C	1735	ATP	O3G-PG-O3B	2.40	112.68	104.64
3	D	2333	OXL	O4-C2-C1	2.36	117.41	112.83
5	F	4135	ATP	N6-C6-N1	2.36	123.63	118.38
5	G	4735	ATP	O3G-PG-O3B	2.30	112.35	104.64
5	D	2335	ATP	O4'-C1'-N9	2.27	112.44	108.09
5	D	2335	ATP	O2B-PB-O3A	2.24	113.33	107.27
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
3	B	1133	OXL	O4-C2-C1	2.18	117.06	112.83
5	C	1735	ATP	C2'-C3'-C4'	-2.18	98.39	102.61
5	A	535	ATP	O3G-PG-O3B	2.16	111.87	104.64
5	C	1735	ATP	O3B-PB-O1B	-2.10	104.38	110.70
3	G	4733	OXL	O2-C2-C1	-2.10	116.26	120.63
5	F	4135	ATP	O3G-PG-O3B	2.08	111.62	104.64
3	G	4733	OXL	O1-C1-C2	-2.08	116.30	120.63
5	D	2335	ATP	C2'-C3'-C4'	-2.08	98.59	102.61
5	A	535	ATP	O2B-PB-O1B	-2.07	102.80	112.44
3	E	3533	OXL	O1-C1-C2	-2.07	116.31	120.63
3	E	3533	OXL	O2-C2-C1	-2.07	116.32	120.63
3	F	4133	OXL	O1-C1-C2	-2.06	116.34	120.63
3	F	4133	OXL	O2-C2-C1	-2.05	116.36	120.63
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 (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3535	ATP	PB-O3B-PG-O3G
5	C	1735	ATP	PB-O3B-PG-O1G
5	E	3535	ATP	PB-O3A-PA-O1A
5	D	2335	ATP	PB-O3B-PG-O1G
5	C	1735	ATP	PA-O3A-PB-O1B
5	C	1735	ATP	PB-O3A-PA-O1A
5	G	4735	ATP	PA-O3A-PB-O1B
5	D	2335	ATP	PB-O3A-PA-O1A
5	E	3535	ATP	PA-O3A-PB-O1B
5	C	1735	ATP	PB-O3B-PG-O3G
5	D	2335	ATP	PB-O3B-PG-O3G
5	G	4735	ATP	PB-O3B-PG-O2G
5	C	1735	ATP	PB-O3A-PA-O2A
5	G	4735	ATP	PA-O3A-PB-O2B
5	A	535	ATP	PB-O3A-PA-O2A
5	D	2335	ATP	PB-O3A-PA-O2A
5	E	3535	ATP	PB-O3A-PA-O2A
5	G	4735	ATP	PB-O3A-PA-O2A

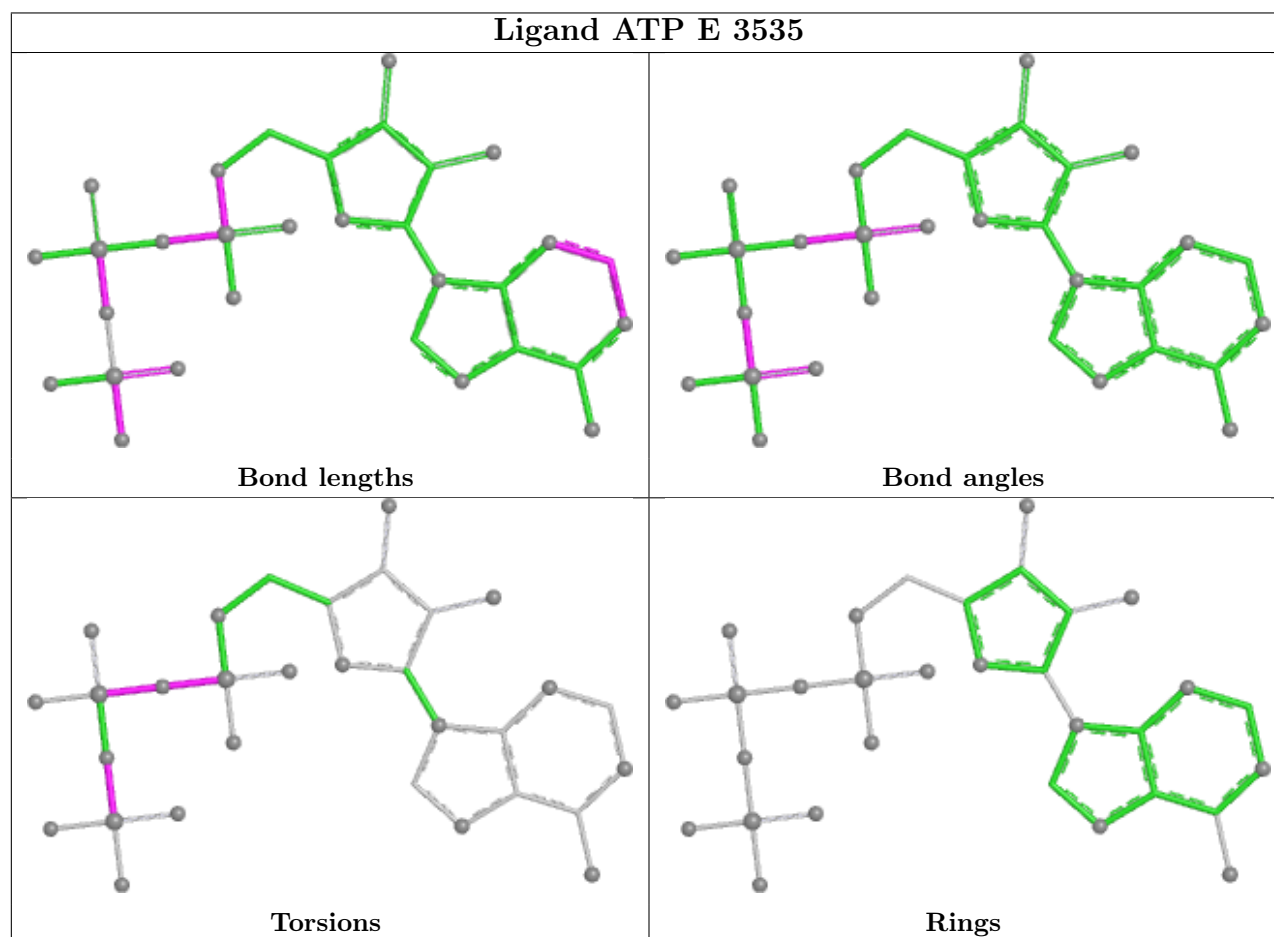
There are no ring outliers.

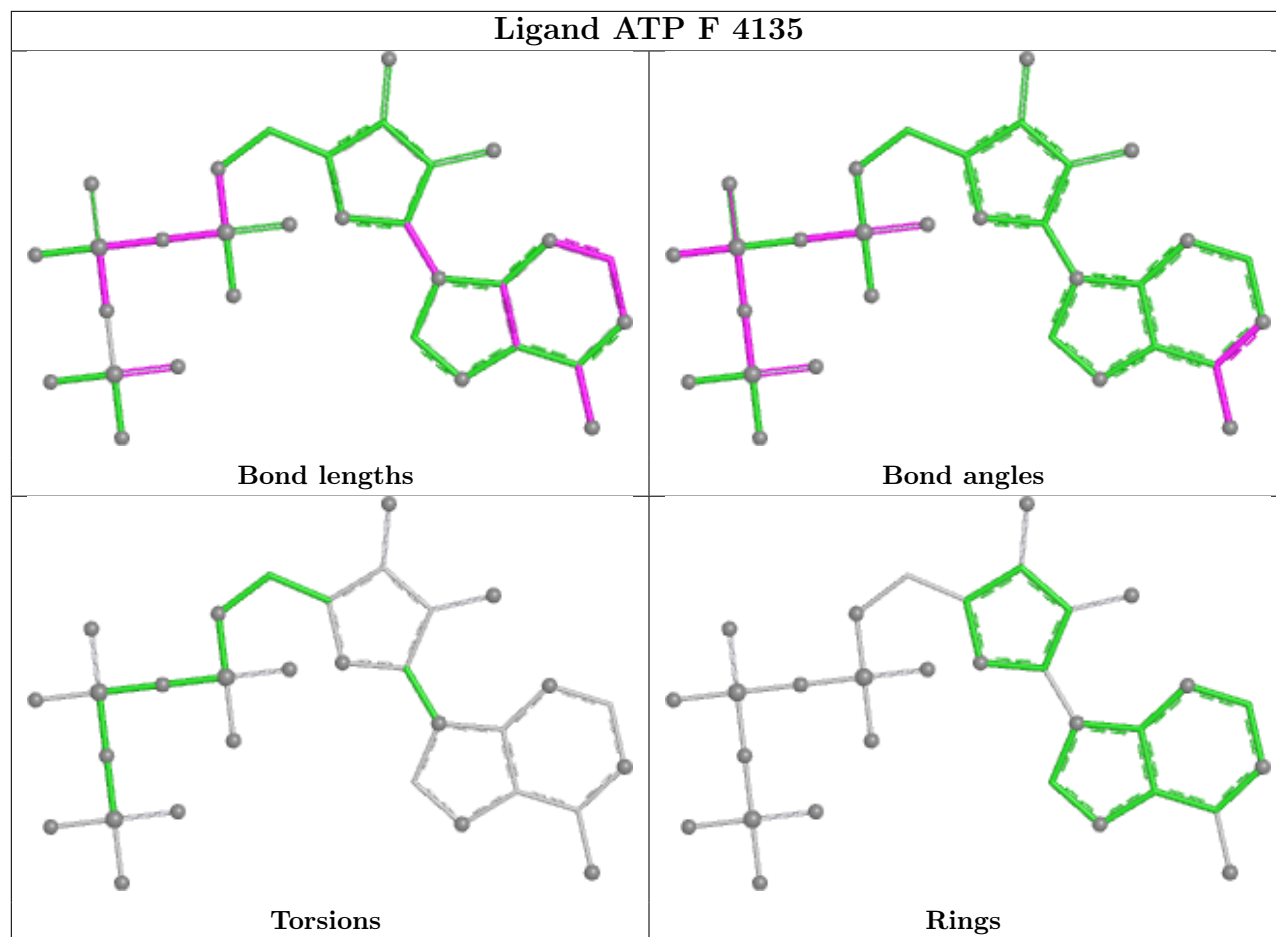
10 monomers are involved in 17 short contacts:

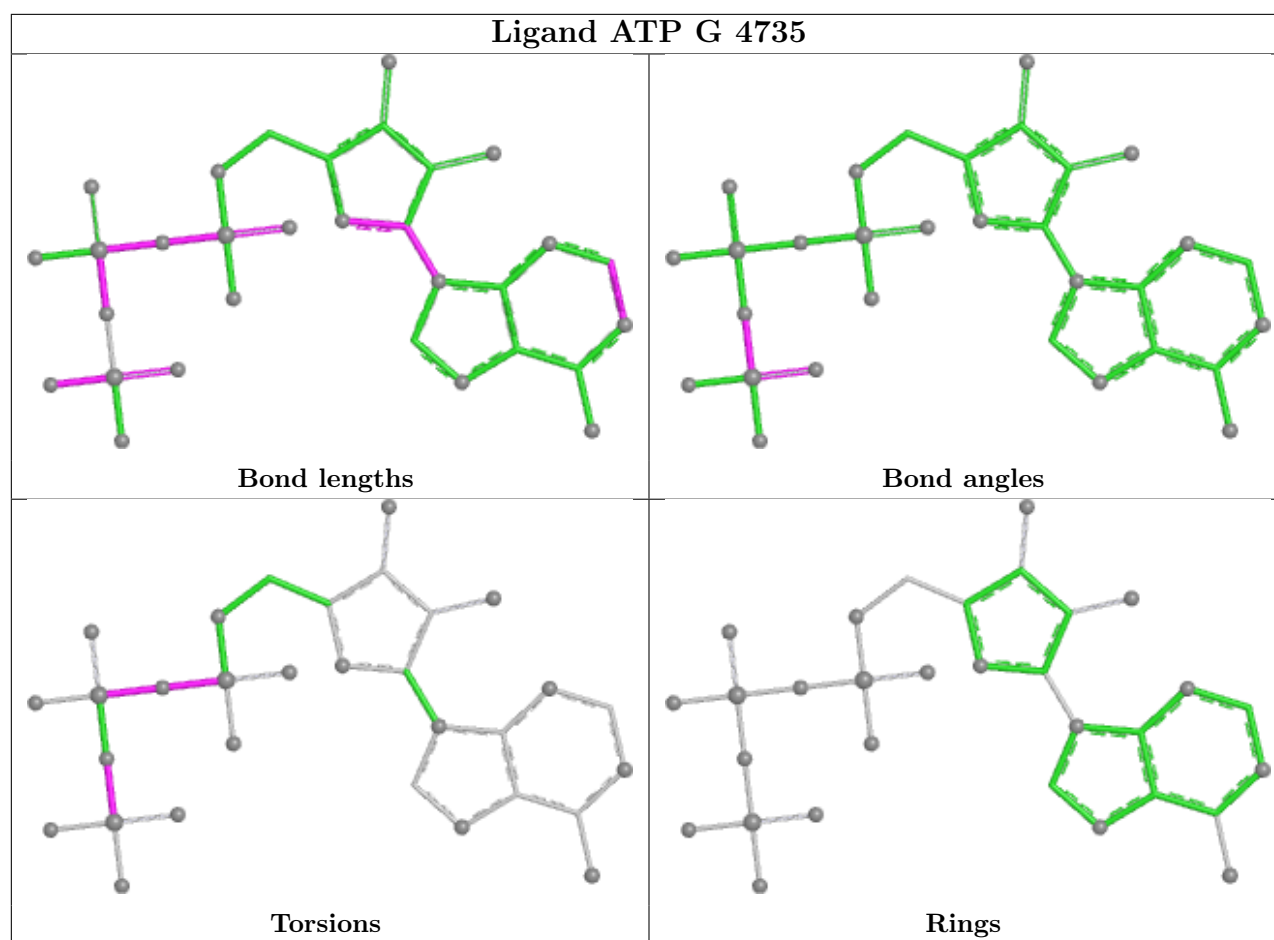
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	533	OXL	2	0
3	H	5333	OXL	1	0
3	C	1733	OXL	1	0
3	F	4133	OXL	3	0
3	D	2333	OXL	1	0
5	G	4735	ATP	1	0
5	D	2335	ATP	1	0
3	G	4733	OXL	1	0
5	C	1735	ATP	3	0
5	A	535	ATP	3	0

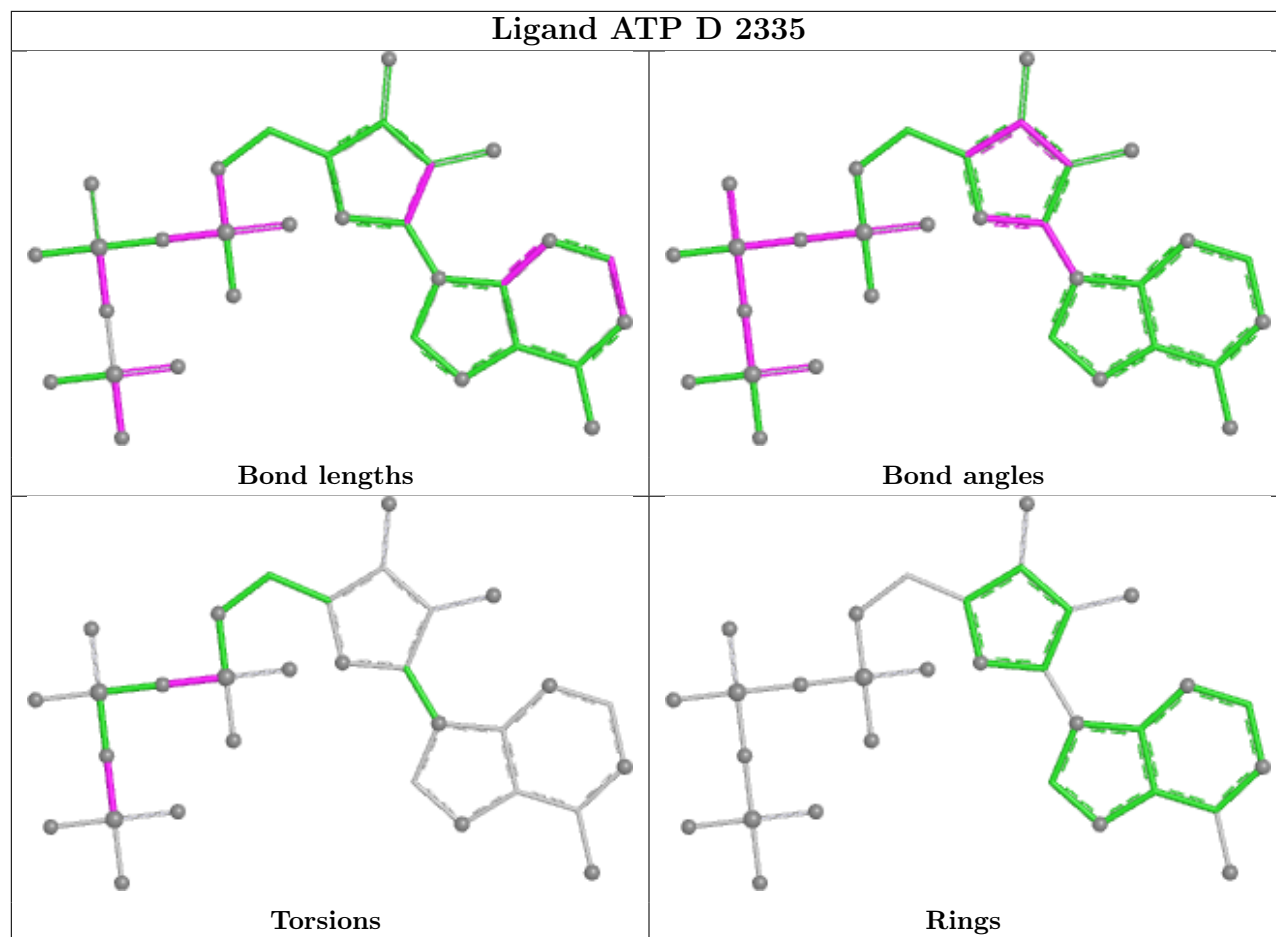
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

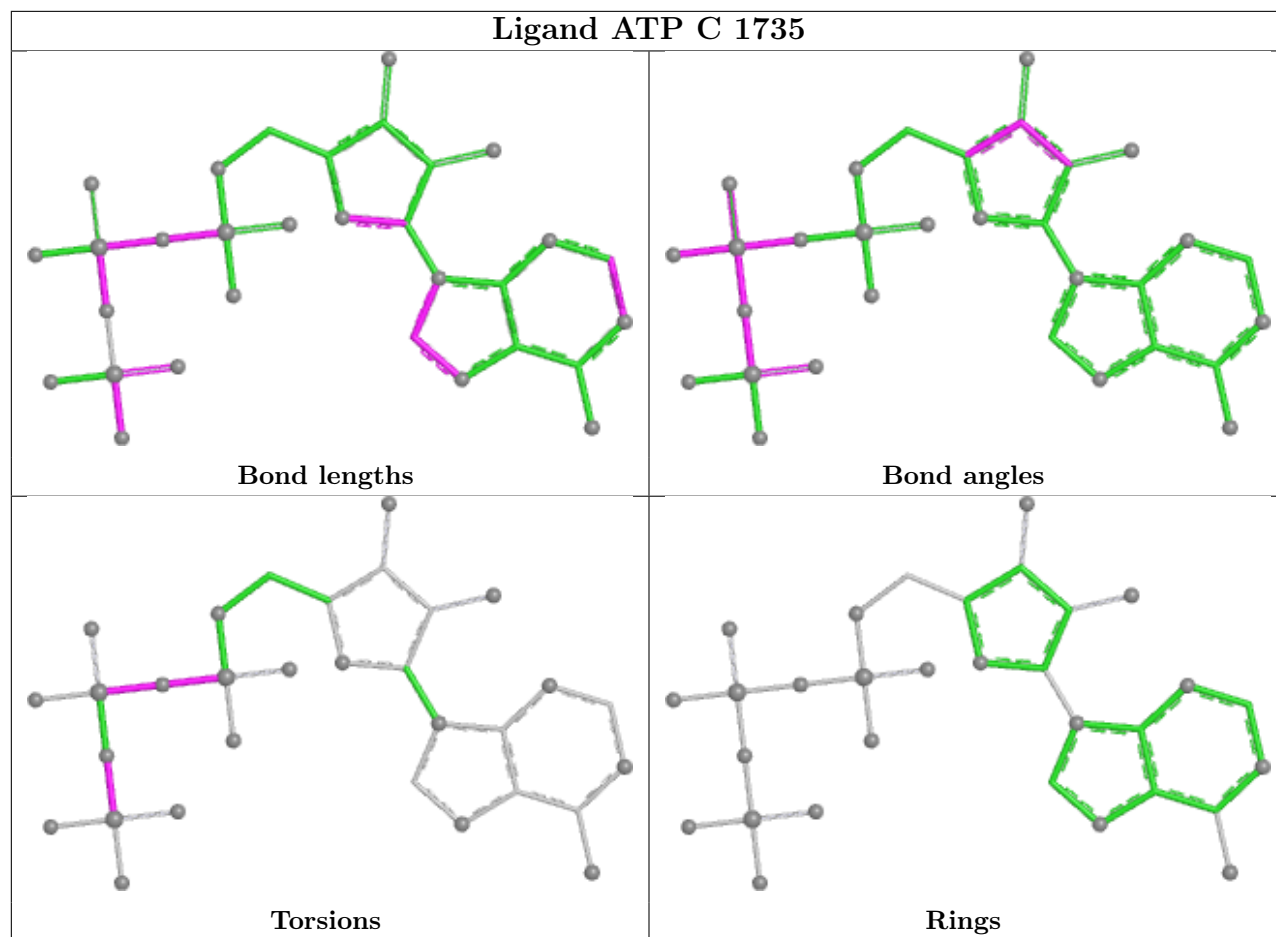
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

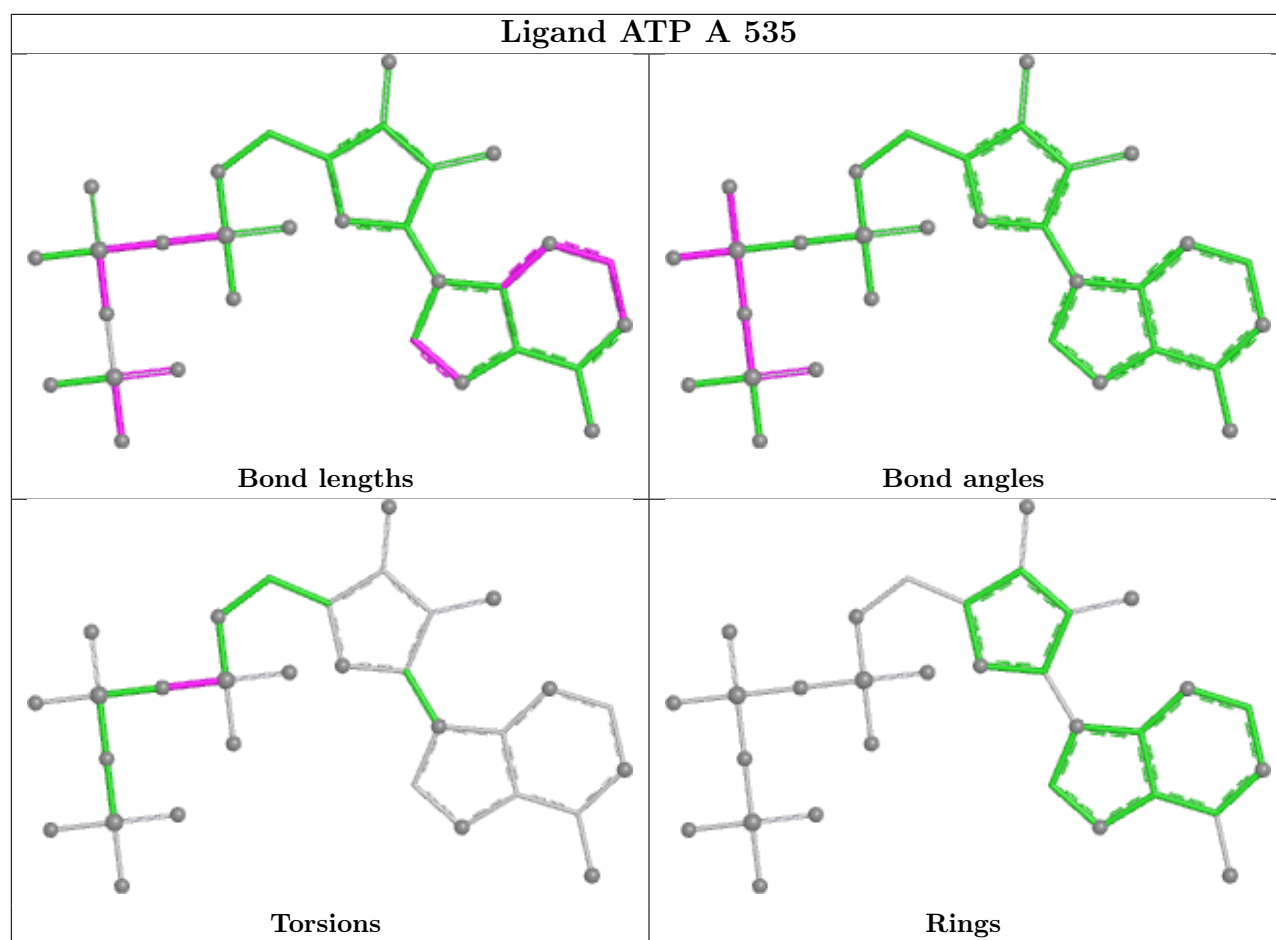












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.