



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:28 PM UTC

PDB ID : 1CE8 / pdb_00001ce8
Title : CARBAMOYL PHOSPHATE SYNTHETASE FROM ESCHERICHIS COLI
WITH COMPLEXED WITH THE ALLOSTERIC LIGAND IMP
Authors : Thoden, J.B.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-03-18
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

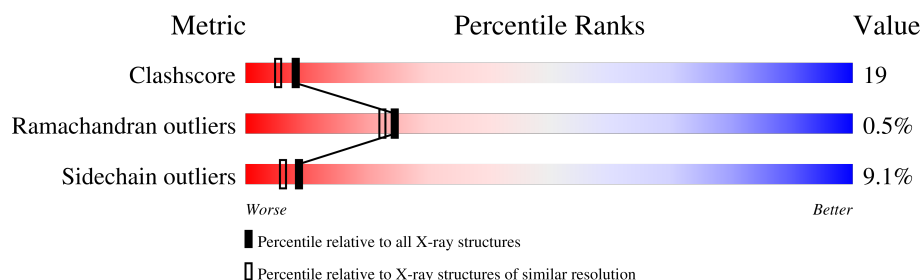
1 Overall quality at a glance

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	1073	63% 31% 5% .
1	C	1073	63% 30% 5% .
1	E	1073	64% 29% 5% .
1	G	1073	53% 37% 8% ..
2	B	382	50% 40% 8% ..
2	D	382	61% 34% . .
2	F	382	53% 39% 7% ..
2	H	382	35% 50% 12% . .

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48888 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 PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	8	0
			8198	5143	1427	1583	45			
1	C	1058	Total	C	N	O	S	0	1	0
			8167	5125	1426	1571	45			
1	E	1058	Total	C	N	O	S	0	12	0
			8232	5165	1444	1578	45			
1	G	1058	Total	C	N	O	S	0	2	0
			8170	5128	1424	1573	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	conflict	UNP P00968
C	46	ASN	LEU	conflict	UNP P00968
E	46	ASN	LEU	conflict	UNP P00968
G	46	ASN	LEU	conflict	UNP P00968

- Molecule 2 is a protein called PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2902	1829	512	551	10			
2	D	379	Total	C	N	O	S	0	1	0
			2899	1828	509	551	11			
2	F	379	Total	C	N	O	S	0	1	0
			2900	1828	510	552	10			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	conflict	UNP P0A6F1
D	183	GLN	GLU	conflict	UNP P0A6F1
F	183	GLN	GLU	conflict	UNP P0A6F1
H	183	GLN	GLU	conflict	UNP P0A6F1

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Mn 3	0	0
3	C	3	Total 3	Mn 3	0	0
3	E	3	Total 3	Mn 3	0	0
3	G	3	Total 3	Mn 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

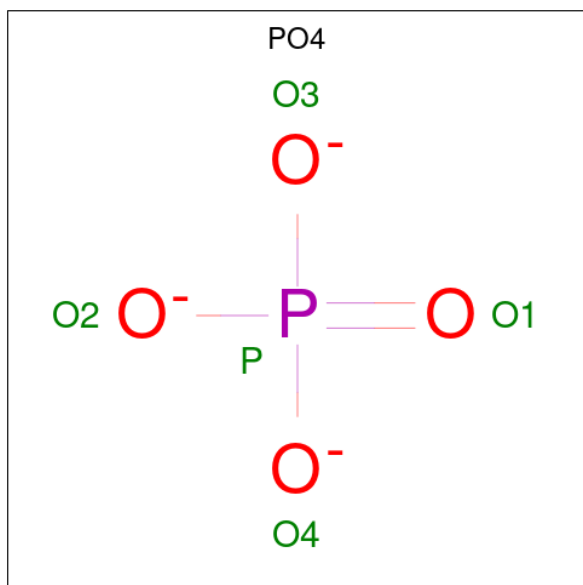
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	Cl 3	0	0

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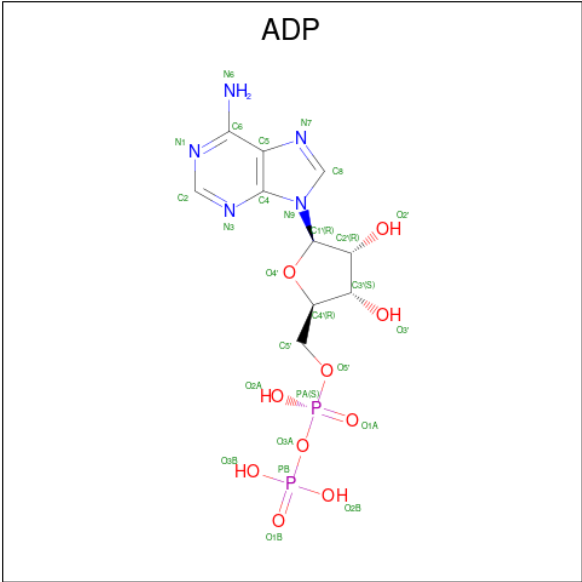
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total	Cl	0	0
			3	3		
5	E	3	Total	Cl	0	0
			3	3		
5	G	3	Total	Cl	0	0
			3	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



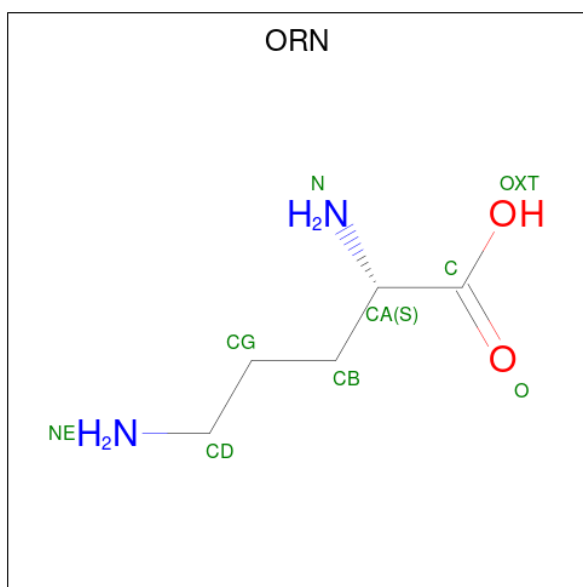
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



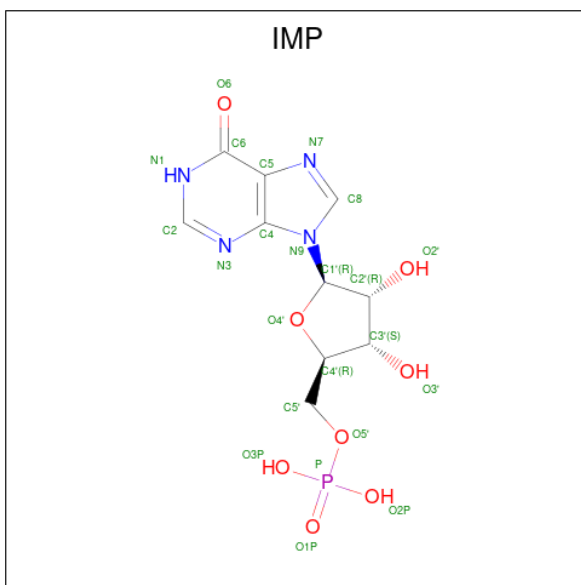
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂).



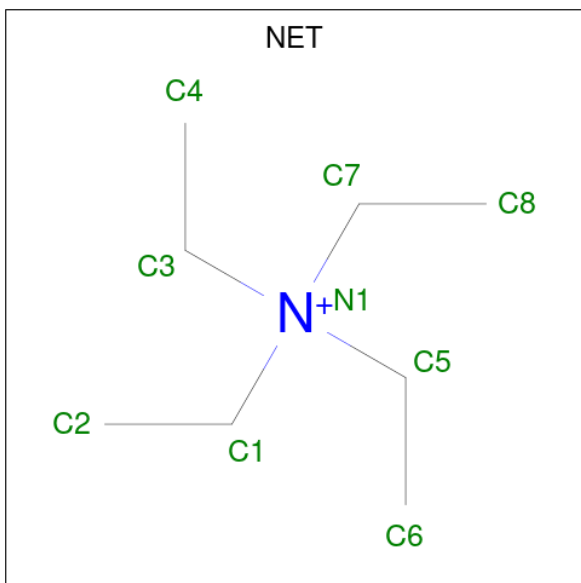
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is INOSINIC ACID (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 10 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N 9 8 1	0	0
10	C	1	Total C N 9 8 1	0	0
10	E	1	Total C N 9 8 1	0	0
10	G	1	Total C N 9 8 1	0	0

- Molecule 11 is water.

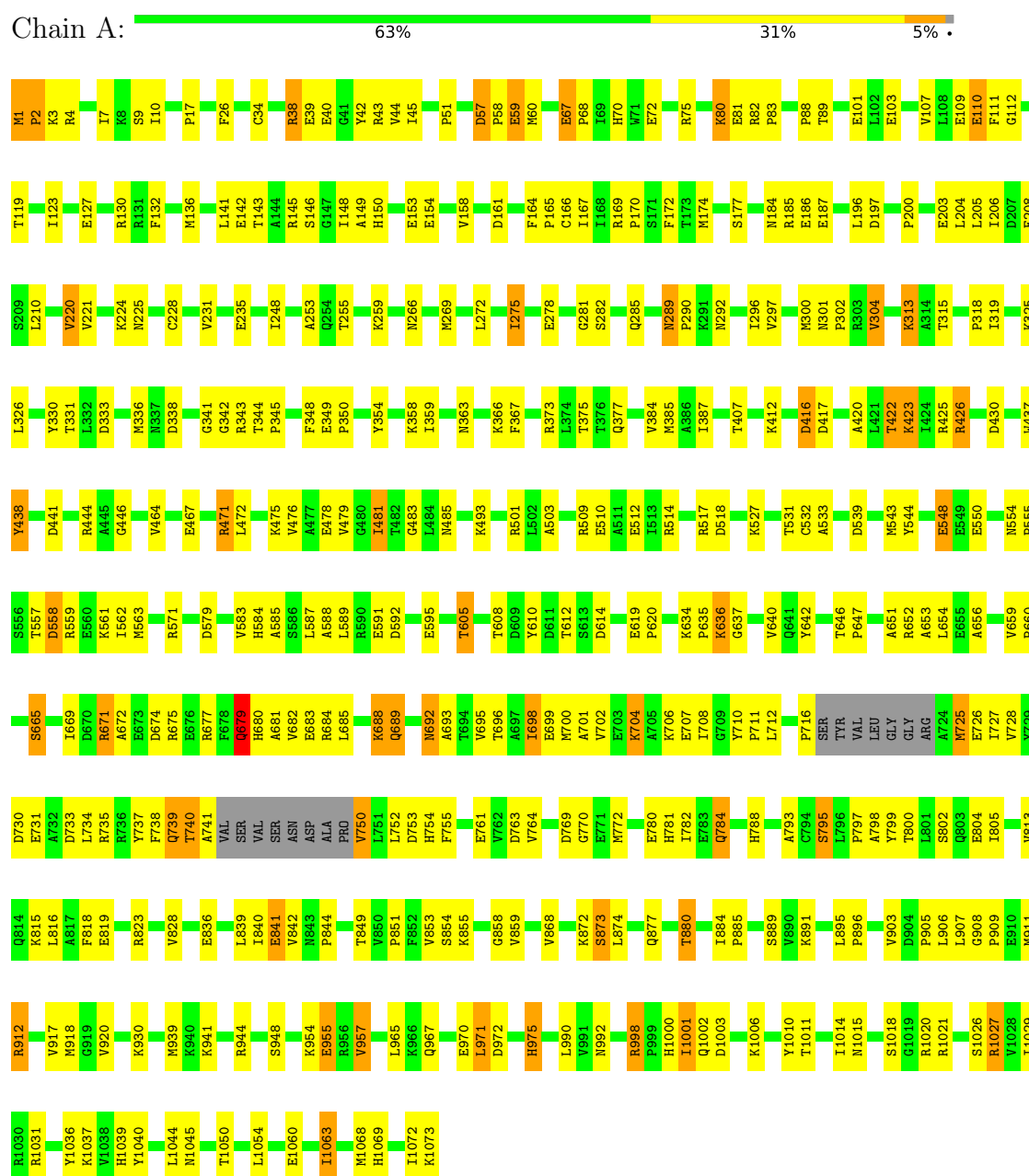
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	842	Total O 842 842	0	0
11	B	190	Total O 190 190	0	0
11	C	732	Total O 732 732	0	0
11	D	193	Total O 193 193	0	0
11	E	939	Total O 939 939	0	0
11	F	233	Total O 233 233	0	0
11	G	743	Total O 743 743	0	0
11	H	165	Total O 165 165	0	0

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.

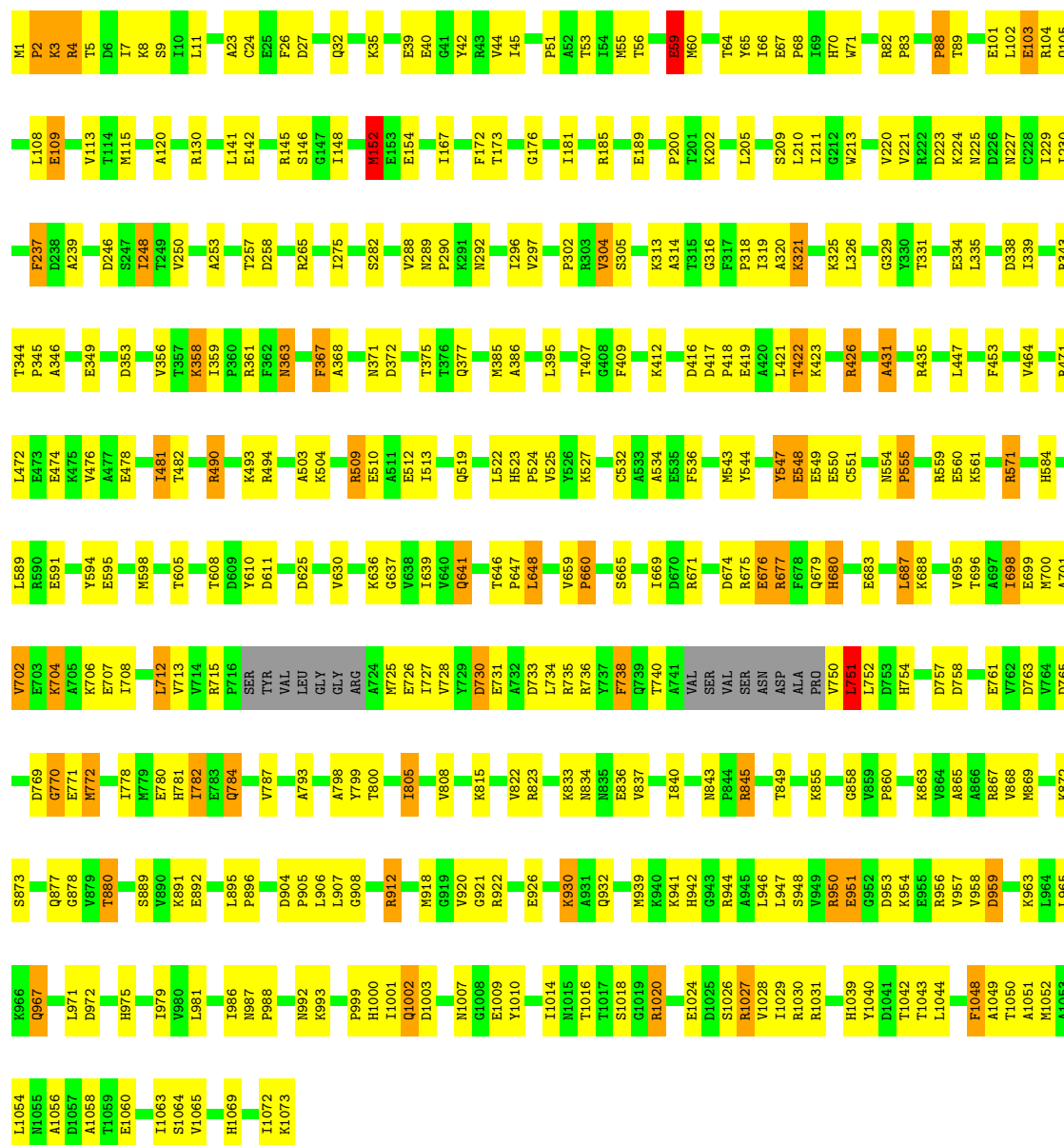
Note EDS was not executed.

• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)



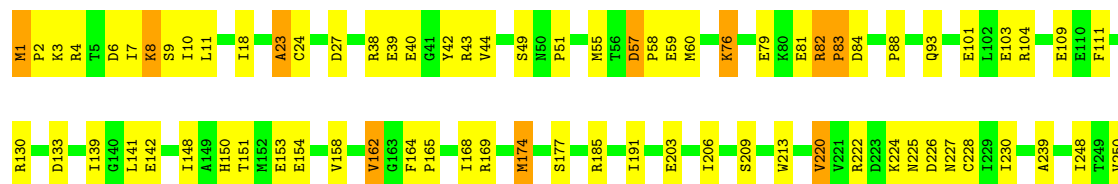
• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

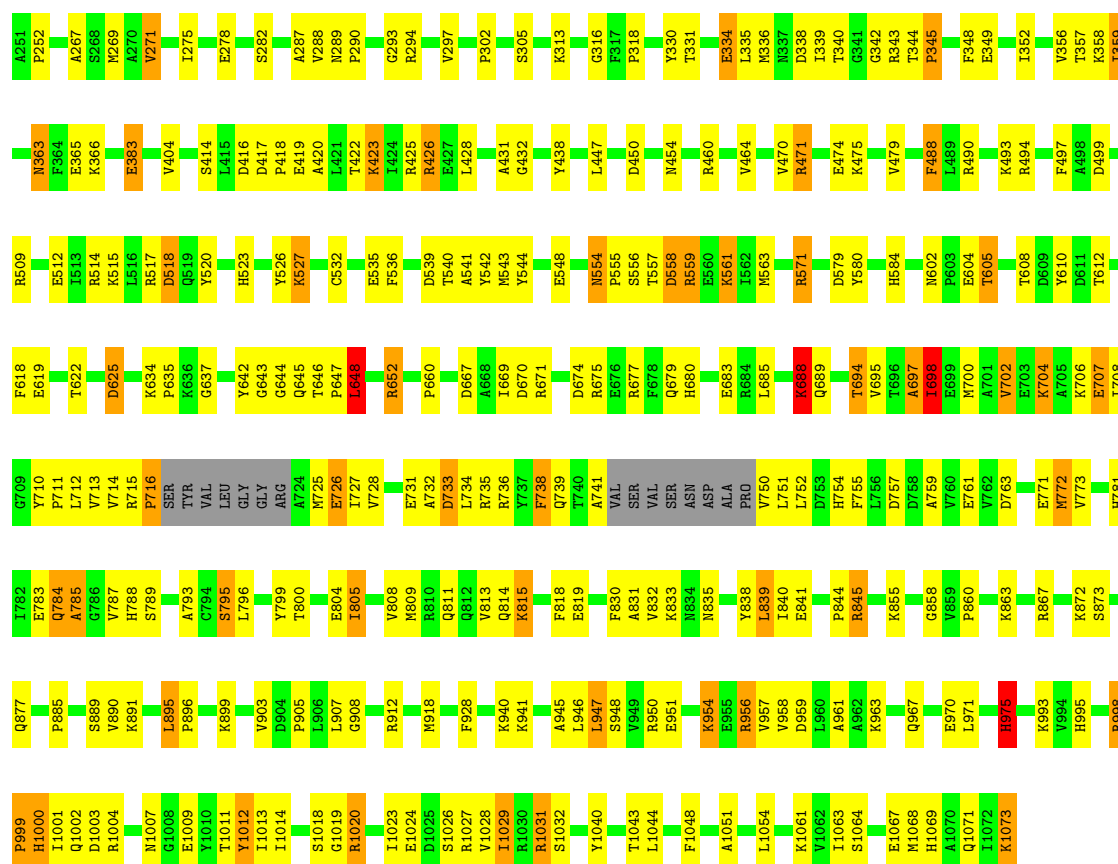
Chain C:  63% 30% 5% •



• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

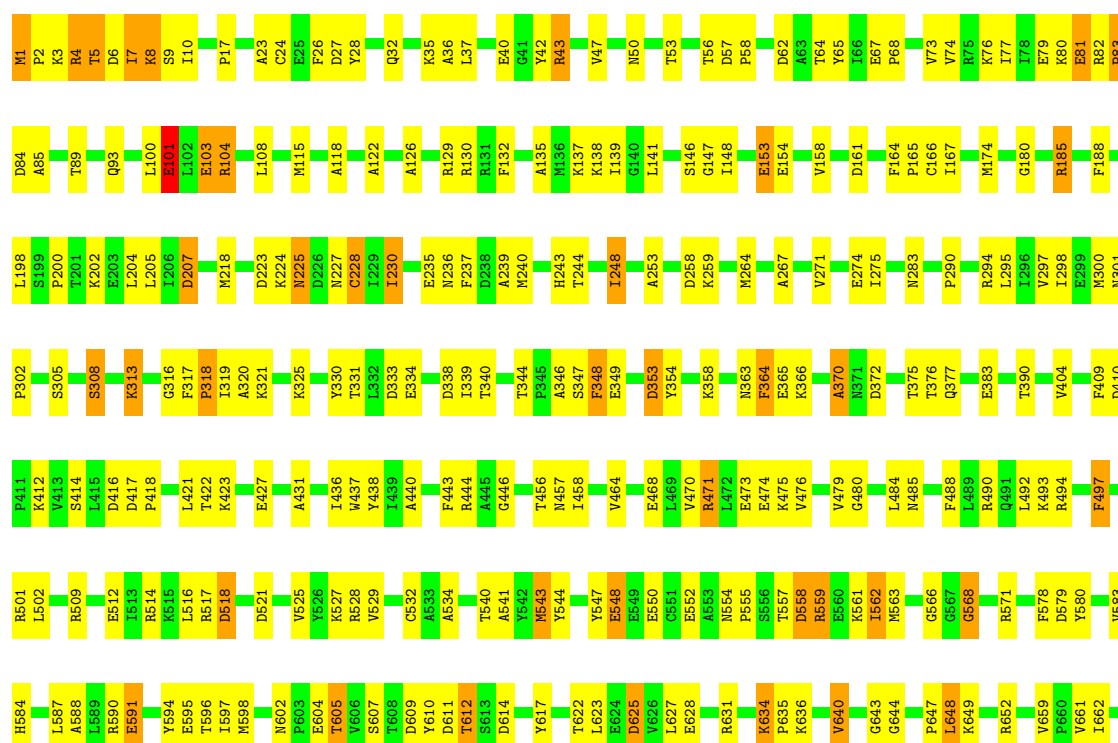
Chain E:  64% 29% 5% •

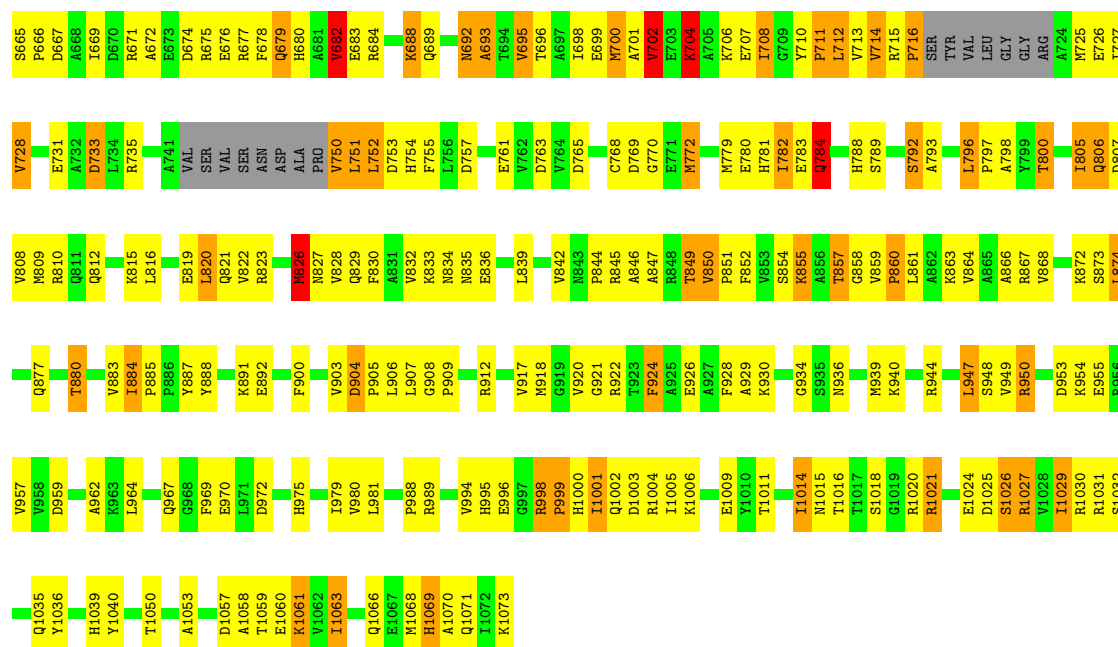




• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

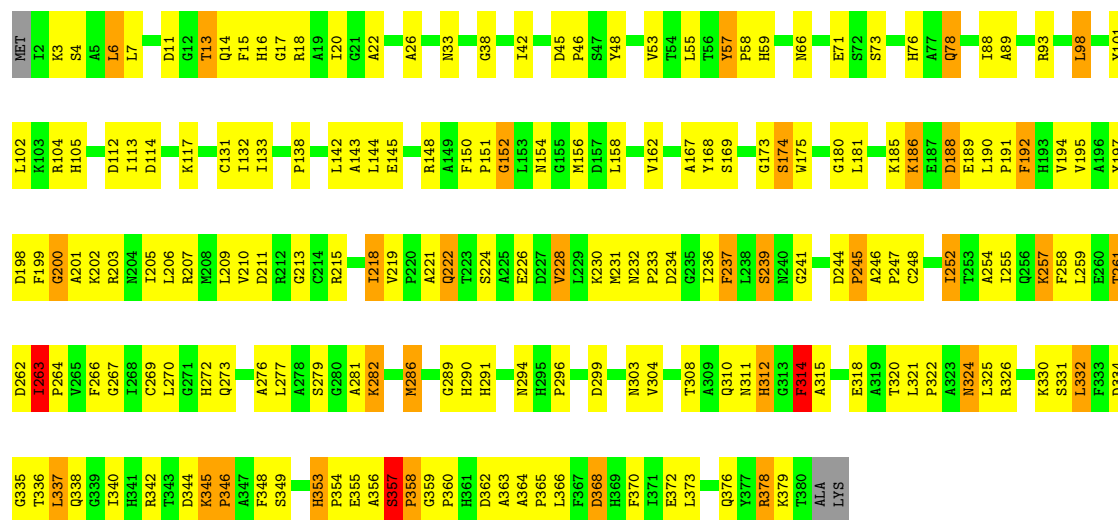
Chain G: 53% 37% 8% ..





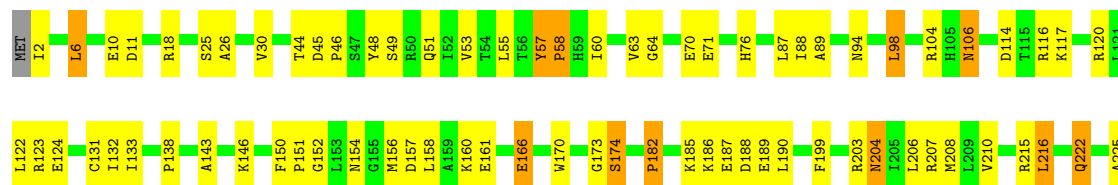
• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

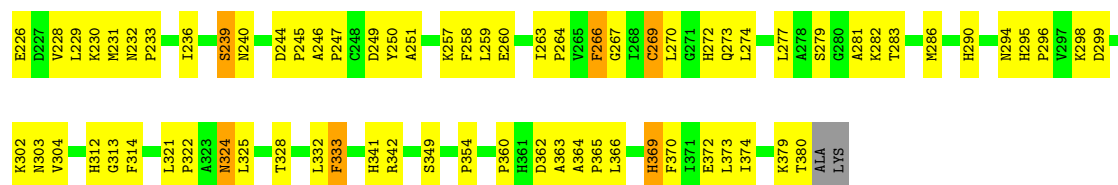
Chain B: 50% 40% 8% ..



• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

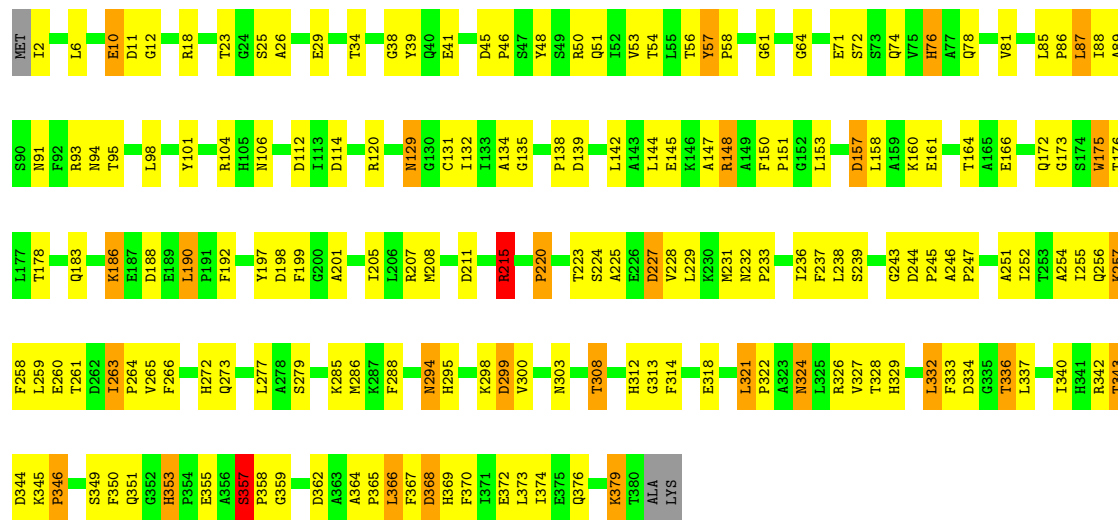
Chain D: 61% 34% ..





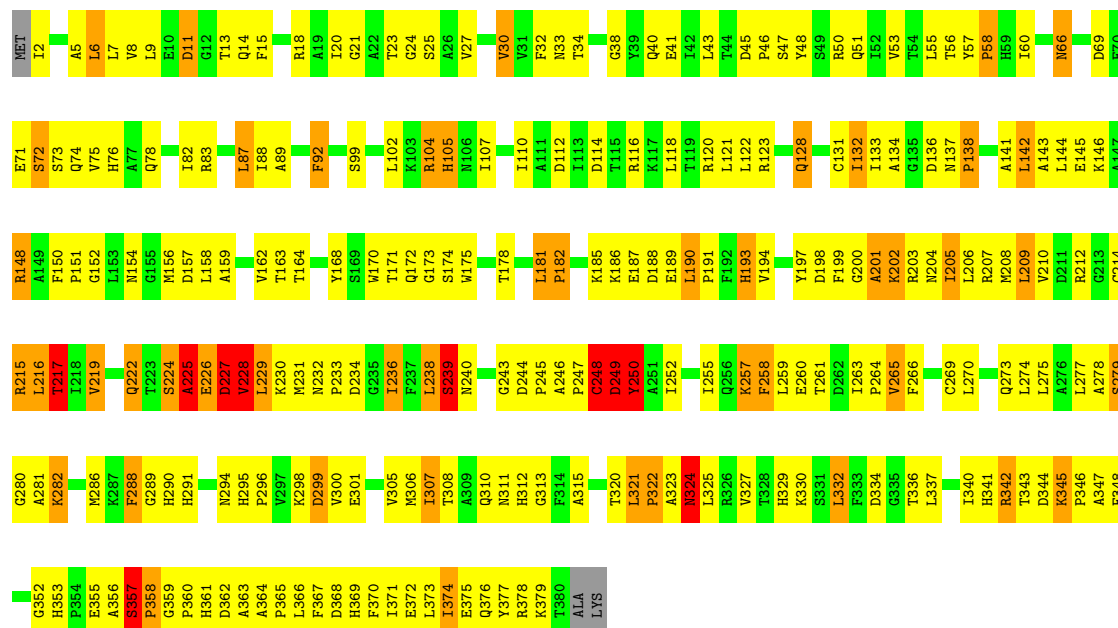
• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain F: 53% 39% 7% ..



• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain H: 35% 50% 12% ..



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	152.10Å 163.90Å 331.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.0 (30.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.193 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48888	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: MN, CL, ADP, IMP, PO4, ORN, NET, K

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	1.13	1/8356 (0.0%)	1.59	58/11295 (0.5%)
1	C	1.13	1/8297 (0.0%)	1.60	84/11216 (0.7%)
1	E	1.16	0/8406	1.64	109/11358 (1.0%)
1	G	1.14	2/8304 (0.0%)	1.71	125/11225 (1.1%)
2	B	1.07	2/2968 (0.1%)	1.67	36/4030 (0.9%)
2	D	1.10	1/2965 (0.0%)	1.62	30/4026 (0.7%)
2	F	1.13	6/2966 (0.2%)	1.68	41/4028 (1.0%)
2	H	1.20	6/2957 (0.2%)	1.77	59/4016 (1.5%)
All	All	1.14	19/45219 (0.0%)	1.65	542/61194 (0.9%)

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
2	B	0	2
2	H	0	2
All	All	0	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	227	ASP	CG-OD2	11.08	1.46	1.25
2	F	148	ARG	N-CA	-8.66	1.35	1.46
1	G	850	VAL	CA-CB	-7.80	1.50	1.54
1	A	841	GLU	CD-OE1	-7.56	1.10	1.25
2	H	324	ASN	CA-CB	7.52	1.64	1.53
2	H	226	GLU	N-CA	-6.08	1.38	1.46
2	H	225	ALA	C-N	6.05	1.41	1.33
1	C	959	ASP	CG-OD2	5.89	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	148	ARG	CA-C	5.50	1.60	1.52
2	F	336	THR	CB-OG1	-5.48	1.34	1.43
2	F	157	ASP	CG-OD2	-5.46	1.15	1.25
2	D	166	GLU	CD-OE2	5.45	1.35	1.25
2	B	312	HIS	CE1-NE2	-5.41	1.27	1.32
1	G	807	ASP	CG-OD1	5.38	1.35	1.25
2	B	359	GLY	N-CA	5.25	1.51	1.44
2	F	368	ASP	CG-OD1	5.21	1.35	1.25
2	F	359	GLY	N-CA	5.17	1.51	1.44
2	H	359	GLY	N-CA	5.16	1.51	1.44
2	H	249	ASP	CA-CB	5.03	1.61	1.53

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	357	SER	O-C-N	-17.94	100.69	121.32
2	H	357	SER	O-C-N	-16.69	102.13	121.32
2	F	357	SER	O-C-N	-16.68	102.14	121.32
1	G	50	ASN	CA-C-O	10.57	126.16	119.29
1	C	338	ASP	CA-CB-CG	10.04	122.64	112.60
1	G	885	PRO	O-C-N	9.97	125.89	121.31
1	A	605	THR	N-CA-C	9.93	124.99	110.59
2	F	353	HIS	CA-CB-CG	-9.77	104.03	113.80
1	G	57	ASP	CA-C-N	9.56	131.79	119.84
1	G	57	ASP	C-N-CA	9.56	131.79	119.84
1	C	154	GLU	CB-CG-CD	9.56	128.85	112.60
2	B	314	PHE	CB-CA-C	-9.17	93.61	109.65
1	G	137	LYS	N-CA-C	-9.16	100.99	110.97
2	F	148	ARG	N-CA-CB	-9.08	96.68	110.20
2	D	157	ASP	CA-CB-CG	8.98	121.58	112.60
1	C	676	GLU	CA-C-N	8.89	132.19	120.28
1	C	676	GLU	C-N-CA	8.89	132.19	120.28
1	C	605	THR	N-CA-C	8.82	123.57	110.52
1	C	44	VAL	N-CA-C	8.73	120.74	107.99
2	B	353	HIS	CA-CB-CG	-8.62	105.18	113.80
1	C	1039	HIS	CA-CB-CG	-8.58	105.22	113.80
1	G	348	PHE	CA-CB-CG	-8.55	105.25	113.80
1	E	557	THR	CA-C-N	8.54	132.67	120.79
1	E	557	THR	C-N-CA	8.54	132.67	120.79
2	H	299	ASP	N-CA-C	-8.48	95.52	108.67
1	G	23	ALA	N-CA-C	8.46	121.21	109.29
1	G	319	ILE	N-CA-C	8.40	119.17	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	345	LYS	N-CA-C	8.32	117.71	108.14
2	B	188	ASP	CA-CB-CG	8.28	120.88	112.60
2	B	286	MET	CG-SD-CE	-8.25	82.75	100.90
1	G	605	THR	N-CA-C	8.13	123.02	110.42
1	C	782	ILE	N-CA-C	-8.05	102.85	110.42
2	H	322	PRO	N-CA-C	-8.03	97.95	110.95
1	G	782	ILE	N-CA-C	-7.98	103.48	110.74
1	G	793	ALA	N-CA-C	-7.98	100.59	110.41
1	C	23	ALA	N-CA-C	7.98	120.54	109.29
2	B	312	HIS	CG-CD2-NE2	-7.95	99.25	107.20
2	F	190	LEU	CA-C-N	7.86	127.15	118.97
2	F	190	LEU	C-N-CA	7.86	127.15	118.97
1	G	431	ALA	CA-C-N	7.86	131.32	122.67
1	G	431	ALA	C-N-CA	7.86	131.32	122.67
1	C	942	HIS	CA-CB-CG	-7.82	105.98	113.80
1	G	543	MET	N-CA-C	7.79	122.17	109.85
1	E	787	VAL	N-CA-CB	7.79	121.27	111.46
2	H	190	LEU	CA-C-N	7.76	128.16	119.32
2	H	190	LEU	C-N-CA	7.76	128.16	119.32
1	G	928	PHE	CA-CB-CG	-7.73	106.07	113.80
1	G	532	CYS	N-CA-C	7.71	121.51	112.72
1	A	289	ASN	CA-C-N	7.62	127.33	119.56
1	A	289	ASN	C-N-CA	7.62	127.33	119.56
1	E	82[A]	ARG	CA-C-O	7.58	125.70	120.47
1	E	82[B]	ARG	CA-C-O	7.58	125.70	120.47
2	D	266	PHE	CA-C-N	-7.55	115.79	121.61
2	D	266	PHE	C-N-CA	-7.55	115.79	121.61
1	G	885	PRO	N-CA-CB	7.50	107.39	103.19
1	G	1070	ALA	N-CA-C	-7.44	103.11	111.07
2	F	353	HIS	CB-CA-C	-7.42	100.70	110.34
1	G	248	ILE	N-CA-C	-7.39	99.16	109.21
1	C	367	PHE	CA-CB-CG	-7.36	106.44	113.80
1	E	999	PRO	N-CA-CB	7.32	110.65	102.60
1	E	1007	ASN	CA-CB-CG	-7.30	105.30	112.60
1	G	1039	HIS	CA-CB-CG	-7.30	106.50	113.80
1	A	88	PRO	CB-CA-C	-7.28	101.91	109.92
2	F	372	GLU	CB-CA-C	-7.25	99.39	110.92
1	G	594	TYR	CB-CA-C	-7.22	97.19	109.83
1	E	248	ILE	N-CA-C	-7.22	99.39	109.21
1	C	676	GLU	N-CA-C	7.12	118.69	111.07
1	A	716	PRO	N-CA-CB	7.11	110.82	103.00
1	C	248	ILE	N-CA-C	-7.11	98.34	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	76	HIS	CA-CB-CG	-7.11	106.69	113.80
1	E	998	ARG	CB-CA-C	7.11	119.82	109.09
1	A	210	LEU	N-CA-C	-7.10	102.65	112.30
1	C	730	ASP	CA-CB-CG	7.08	119.68	112.60
2	H	307	ILE	N-CA-C	-7.07	98.25	108.36
2	F	129	ASN	CA-CB-CG	-7.04	105.56	112.60
1	G	443	PHE	CA-CB-CG	-7.04	106.76	113.80
1	A	571	ARG	CD-NE-CZ	-7.02	114.58	124.40
1	G	806	GLN	N-CA-C	-6.99	103.66	111.28
1	G	188	PHE	CA-CB-CG	-6.98	106.82	113.80
1	A	793	ALA	N-CA-C	-6.98	101.13	110.55
2	H	321	LEU	O-C-N	6.97	127.76	121.35
1	E	345	PRO	CB-CA-C	-6.96	100.04	110.20
1	G	353	ASP	CA-CB-CG	6.95	119.55	112.60
1	G	716	PRO	N-CA-CB	6.95	110.64	103.00
1	G	1011	THR	N-CA-C	-6.95	105.35	114.31
1	C	417	ASP	CB-CA-C	6.92	117.85	110.17
2	F	57	TYR	CA-CB-CG	-6.89	101.49	113.90
2	H	228	VAL	CB-CA-C	-6.88	104.69	111.30
1	E	230	ILE	N-CA-CB	6.88	119.86	111.60
2	H	198	ASP	CA-CB-CG	6.88	119.47	112.60
1	G	578	PHE	CA-CB-CG	-6.87	106.93	113.80
2	B	358	PRO	O-C-N	-6.85	116.29	122.93
2	D	239	SER	N-CA-C	6.83	119.15	110.33
1	C	808	VAL	CB-CA-C	-6.83	102.79	112.22
1	C	1028	VAL	N-CA-C	6.83	118.40	110.62
1	E	488	PHE	CA-CB-CG	-6.82	106.98	113.80
1	C	787	VAL	N-CA-C	-6.82	98.03	107.99
1	E	908	GLY	CA-C-N	6.82	126.96	119.87
1	E	908	GLY	C-N-CA	6.82	126.96	119.87
1	E	339	ILE	N-CA-C	6.82	121.86	113.00
1	G	850	VAL	N-CA-C	6.80	121.17	112.67
1	G	998	ARG	N-CA-C	6.78	120.63	109.58
1	E	316	GLY	N-CA-C	-6.78	105.74	115.64
2	H	215	ARG	N-CA-C	-6.76	99.01	109.76
2	F	215	ARG	N-CA-CB	6.74	121.29	110.16
1	E	57	ASP	CA-C-N	6.71	127.25	119.47
1	E	57	ASP	C-N-CA	6.71	127.25	119.47
1	G	7	ILE	N-CA-C	6.68	117.51	107.75
1	A	417	ASP	CA-C-N	6.66	126.29	119.56
1	A	417	ASP	C-N-CA	6.66	126.29	119.56
2	F	53	VAL	N-CA-C	6.65	118.40	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	190	LEU	CA-C-O	6.62	124.75	119.59
1	G	57	ASP	CA-CB-CG	6.61	119.21	112.60
1	E	625	ASP	CA-CB-CG	-6.61	105.99	112.60
1	C	625	ASP	CA-CB-CG	-6.60	106.00	112.60
1	E	532	CYS	N-CA-C	6.59	121.26	112.30
2	D	89	ALA	N-CA-C	-6.56	98.93	109.96
1	E	688	LYS	N-CA-C	6.56	119.61	107.99
1	C	305	SER	N-CA-C	6.56	116.71	108.45
1	A	248	ILE	N-CA-C	-6.56	99.14	108.58
1	C	407	THR	N-CA-C	-6.56	103.69	112.94
1	A	739	GLN	CA-C-N	6.55	128.96	120.44
1	A	739	GLN	C-N-CA	6.55	128.96	120.44
2	F	201	ALA	N-CA-C	6.55	119.73	110.23
1	E	605	THR	N-CA-C	6.55	120.57	110.42
2	D	174	SER	N-CA-C	6.53	118.98	110.43
2	H	193	HIS	N-CA-CB	6.52	120.79	110.55
1	G	230	ILE	N-CA-CB	6.51	119.55	111.41
1	A	612	THR	N-CA-C	6.51	120.32	112.38
1	E	520	TYR	CB-CA-C	-6.50	99.58	110.56
1	A	67	GLU	O-C-N	6.49	125.86	121.71
2	F	10	GLU	CB-CG-CD	-6.48	101.58	112.60
1	A	1011	THR	N-CA-C	-6.48	105.12	114.12
1	E	697	ALA	CA-C-N	6.47	131.48	121.19
1	E	697	ALA	C-N-CA	6.47	131.48	121.19
1	C	987	ASN	CB-CA-C	-6.47	103.92	110.65
1	G	26	PHE	CA-CB-CG	-6.47	107.33	113.80
1	A	407	THR	N-CA-C	-6.45	103.84	112.94
1	A	57	ASP	CA-C-O	6.43	125.48	119.76
1	A	338	ASP	N-CA-C	6.42	118.86	111.02
2	H	53	VAL	N-CA-C	6.42	118.05	108.23
1	E	999	PRO	N-CA-C	-6.41	95.44	112.10
2	F	89	ALA	N-CA-C	-6.40	99.21	109.96
1	A	1060	GLU	N-CA-C	6.40	118.13	111.03
1	A	558	ASP	N-CA-C	6.38	118.81	111.02
1	G	806	GLN	CA-C-O	6.37	127.31	120.55
1	C	959	ASP	CA-CB-CG	-6.37	106.23	112.60
1	G	885	PRO	N-CA-C	6.36	116.57	110.47
1	C	904	ASP	CA-C-N	6.35	127.78	119.84
1	C	904	ASP	C-N-CA	6.35	127.78	119.84
1	C	88	PRO	CB-CA-C	-6.35	102.94	109.92
1	E	431	ALA	N-CA-C	6.32	119.15	110.24
1	G	588	ALA	N-CA-C	6.31	117.85	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	555	PRO	N-CA-CB	6.31	108.62	103.32
1	E	558	ASP	N-CA-C	6.29	118.69	111.02
2	H	45	ASP	CA-C-O	-6.29	114.67	119.32
2	D	260	GLU	N-CA-C	-6.28	105.75	113.41
1	E	27	ASP	N-CA-C	-6.28	103.97	111.69
2	H	188	ASP	CA-CB-CG	6.27	118.87	112.60
2	H	358	PRO	O-C-N	-6.27	116.85	122.93
1	G	370	ALA	N-CA-C	6.27	119.34	110.50
2	F	18	ARG	N-CA-C	6.26	119.11	108.90
1	E	450	ASP	CA-CB-CG	6.25	118.86	112.60
2	B	53	VAL	N-CA-C	6.25	117.79	108.23
2	D	362	ASP	N-CA-C	6.22	118.86	111.33
1	C	584	HIS	CA-CB-CG	-6.21	107.59	113.80
1	G	757	ASP	CA-CB-CG	-6.20	106.40	112.60
1	C	453	PHE	CA-CB-CG	-6.20	107.60	113.80
1	E	735	ARG	O-C-N	6.20	128.71	122.08
2	H	225	ALA	CB-CA-C	-6.20	98.61	110.57
1	C	319	ILE	N-CA-C	6.17	116.83	110.36
2	F	112	ASP	N-CA-C	6.16	120.10	112.58
2	H	182	PRO	CB-CA-C	-6.16	102.91	110.98
2	B	112	ASP	CA-CB-CG	6.16	118.76	112.60
1	G	101	GLU	CB-CG-CD	6.15	123.06	112.60
1	A	26	PHE	CA-CB-CG	-6.14	107.66	113.80
1	E	738	PHE	CA-CB-CG	-6.14	107.66	113.80
2	H	138	PRO	N-CA-CB	6.14	108.72	103.19
1	C	173	THR	N-CA-CB	6.13	122.22	111.55
1	E	543	MET	N-CA-C	6.13	119.16	110.14
1	E	357	THR	CA-C-N	-6.12	113.75	122.94
1	E	357	THR	C-N-CA	-6.12	113.75	122.94
1	C	152	MET	N-CA-CB	6.12	119.64	110.22
1	G	476	VAL	CB-CA-C	-6.12	104.05	111.88
1	A	319	ILE	N-CA-C	6.12	116.78	110.36
1	C	660	PRO	CB-CA-C	-6.11	104.78	113.09
1	A	196	LEU	N-CA-C	-6.11	104.53	111.07
1	E	716	PRO	N-CA-CB	6.11	109.72	103.00
2	F	260	GLU	N-CA-C	-6.11	104.53	112.23
1	A	438	TYR	CA-CB-CG	-6.11	102.91	113.90
1	C	363	ASN	CA-CB-CG	6.10	118.70	112.60
1	G	857	THR	N-CA-C	6.10	120.79	113.23
1	C	751	LEU	N-CA-C	6.09	119.57	109.46
1	A	1045	ASN	CA-C-N	6.08	126.57	119.94
1	A	1045	ASN	C-N-CA	6.08	126.57	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	788	HIS	CA-CB-CG	-6.08	107.72	113.80
2	H	227	ASP	CB-CG-OD2	-6.07	104.43	118.40
1	E	707	GLU	CA-C-N	6.07	128.43	120.60
1	E	707	GLU	C-N-CA	6.07	128.43	120.60
1	C	67	GLU	O-C-N	6.07	125.59	121.71
2	B	312	HIS	ND1-CG-CD2	6.07	112.17	106.10
1	A	559	ARG	N-CA-C	6.06	118.67	109.95
1	G	994	VAL	N-CA-CB	6.06	116.98	110.62
1	G	298	ILE	N-CA-C	6.05	117.08	111.45
1	A	44	VAL	N-CA-C	6.05	116.82	107.99
1	E	993	LYS	N-CA-C	-6.05	102.97	110.41
1	G	819	GLU	N-CA-C	6.04	117.87	111.28
2	H	66	ASN	CA-C-N	6.04	128.69	120.54
2	H	66	ASN	C-N-CA	6.04	128.69	120.54
2	H	228	VAL	N-CA-C	-6.03	107.01	111.90
2	F	288	PHE	CB-CA-C	6.02	118.39	109.29
1	C	971	LEU	N-CA-C	6.02	119.35	109.72
1	A	971	LEU	N-CA-C	6.01	119.28	109.24
1	E	1012	TYR	N-CA-C	5.99	118.26	108.55
1	C	993	LYS	N-CA-C	-5.99	102.62	110.53
1	C	738	PHE	CA-CB-CG	-5.99	107.81	113.80
2	H	217	THR	CB-CA-C	5.97	120.35	110.74
2	F	346	PRO	N-CA-CB	5.96	106.75	102.28
1	G	27	ASP	N-CA-C	-5.95	104.18	112.45
1	G	541	ALA	CB-CA-C	-5.94	103.61	111.74
2	H	249	ASP	CB-CG-OD1	-5.94	104.74	118.40
1	E	220	VAL	CB-CA-C	-5.94	101.68	110.82
1	C	70	HIS	CA-CB-CG	-5.93	107.87	113.80
1	G	695	VAL	N-CA-C	5.92	118.23	108.99
1	C	246	ASP	CA-CB-CG	5.92	118.52	112.60
1	E	612	THR	N-CA-C	5.92	118.69	111.82
1	A	588	ALA	N-CA-C	5.92	117.53	111.14
1	A	880	THR	N-CA-CB	-5.92	103.17	110.98
1	E	1048	PHE	CA-CB-CG	-5.92	107.88	113.80
1	E	793	ALA	N-CA-C	-5.91	102.57	110.55
2	B	312	HIS	CE1-NE2-CD2	5.91	114.91	109.00
1	E	338	ASP	CA-CB-CG	5.89	118.50	112.60
1	G	305	SER	N-CA-C	5.89	115.79	108.19
1	E	619	GLU	N-CA-C	5.89	117.74	108.55
1	E	928	PHE	CA-CB-CG	-5.88	107.92	113.80
2	B	57	TYR	CA-CB-CG	-5.87	103.33	113.90
1	G	866	ALA	N-CA-C	-5.87	104.57	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	688	LYS	N-CA-C	5.87	118.29	108.96
1	A	1039	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	1020	ARG	N-CA-C	5.86	117.34	111.07
2	B	372	GLU	N-CA-CB	-5.85	101.22	109.94
1	G	139	ILE	N-CA-C	5.84	117.11	111.91
2	F	95	THR	N-CA-CB	5.84	118.67	110.90
1	G	364	PHE	N-CA-C	5.84	118.39	111.33
1	G	711	PRO	N-CA-CB	5.82	109.00	102.60
1	E	885	PRO	N-CA-CB	5.82	106.25	103.22
2	B	98	LEU	N-CA-C	5.82	118.09	111.11
1	E	971	LEU	N-CA-C	5.82	119.03	109.72
1	C	660	PRO	N-CA-CB	5.82	106.48	102.35
2	H	181	LEU	CA-C-O	5.81	123.94	119.46
1	C	543	MET	N-CA-C	5.80	118.51	109.52
2	H	58	PRO	N-CA-C	5.79	121.59	113.53
1	C	109	GLU	CA-C-N	5.79	128.31	120.38
1	C	109	GLU	C-N-CA	5.79	128.31	120.38
2	H	229	LEU	N-CA-C	-5.78	106.07	113.01
1	E	998	ARG	N-CA-C	5.78	117.97	110.40
1	A	557	THR	CA-C-N	5.77	128.81	120.79
1	A	557	THR	C-N-CA	5.77	128.81	120.79
2	H	132	ILE	CB-CA-C	-5.77	102.24	110.83
2	F	148	ARG	CA-C-O	5.76	126.64	120.24
1	E	239	ALA	N-CA-C	5.76	117.33	110.19
1	A	422	THR	CB-CA-C	5.75	120.63	110.85
1	C	559	ARG	N-CA-C	5.75	118.60	109.81
1	A	782	ILE	N-CA-C	-5.74	105.03	110.42
2	H	105	HIS	CA-CB-CG	-5.73	108.07	113.80
1	E	209	SER	N-CA-C	5.73	118.88	109.76
2	D	98	LEU	N-CA-C	5.73	117.98	111.11
1	E	82[A]	ARG	NE-CZ-NH2	-5.73	114.05	119.20
1	E	82[B]	ARG	NE-CZ-NH2	-5.73	114.05	119.20
1	G	283	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	620	PRO	N-CA-CB	5.72	108.66	103.34
1	E	704	LYS	N-CA-C	-5.72	105.05	111.28
1	C	549	GLU	N-CA-C	5.71	118.61	111.24
2	F	357	SER	CA-C-N	-5.71	113.67	120.13
2	F	357	SER	C-N-CA	-5.71	113.67	120.13
1	G	1015	ASN	CA-C-N	-5.71	113.68	122.87
1	G	1015	ASN	C-N-CA	-5.71	113.68	122.87
1	E	499	ASP	CB-CA-C	-5.71	101.32	110.79
1	A	908	GLY	CA-C-N	5.70	125.80	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	908	GLY	C-N-CA	5.70	125.80	119.87
1	E	334	GLU	CB-CA-C	-5.70	97.99	109.55
2	H	181	LEU	CA-C-N	5.69	125.60	119.85
2	H	181	LEU	C-N-CA	5.69	125.60	119.85
1	G	3	LYS	N-CA-C	5.69	119.19	110.20
2	F	368	ASP	CA-CB-CG	-5.67	106.93	112.60
1	C	316	GLY	N-CA-C	-5.66	107.44	115.43
1	E	698	ILE	N-CA-CB	-5.66	97.87	111.23
2	B	368	ASP	CA-CB-CG	-5.65	106.95	112.60
1	G	904	ASP	O-C-N	5.65	125.81	121.23
1	C	27	ASP	N-CA-C	-5.65	105.11	112.23
1	A	417	ASP	CA-CB-CG	5.63	118.23	112.60
2	B	362	ASP	N-CA-C	5.63	118.15	111.33
1	G	634	LYS	CA-C-N	5.63	125.94	119.92
1	G	634	LYS	C-N-CA	5.63	125.94	119.92
1	E	83	PRO	CB-CA-C	-5.62	103.74	111.21
1	G	625	ASP	CA-CB-CG	-5.62	106.98	112.60
1	C	532	CYS	N-CA-C	5.62	119.31	111.56
1	A	584	HIS	CA-CB-CG	-5.61	108.19	113.80
1	G	122	ALA	N-CA-C	-5.61	105.07	111.07
1	G	609	ASP	N-CA-C	-5.61	100.15	109.46
1	C	595	GLU	N-CA-C	-5.60	100.06	108.96
1	E	404	VAL	N-CA-C	-5.59	106.86	112.17
1	E	785	ALA	CA-C-N	-5.59	115.53	123.08
1	E	785	ALA	C-N-CA	-5.59	115.53	123.08
2	B	263	ILE	N-CA-CB	5.58	115.27	110.08
1	A	557	THR	N-CA-C	-5.58	106.63	113.50
1	G	612	THR	N-CA-C	5.58	118.13	111.71
2	D	53	VAL	N-CA-C	5.58	116.77	108.23
2	F	294	ASN	N-CA-CB	-5.58	102.23	111.49
1	E	1011	THR	N-CA-C	-5.58	105.25	113.61
1	C	253	ALA	N-CA-C	-5.57	102.77	110.35
1	E	558	ASP	CA-CB-CG	5.57	118.17	112.60
2	H	299	ASP	CA-CB-CG	5.57	118.17	112.60
2	H	359	GLY	CA-C-N	5.56	125.83	119.83
2	H	359	GLY	C-N-CA	5.56	125.83	119.83
1	C	431	ALA	N-CA-C	5.55	118.28	110.23
2	B	360	PRO	N-CA-CB	5.54	108.25	103.31
1	G	924	PHE	CA-CB-CG	-5.54	108.25	113.80
2	H	11	ASP	CA-CB-CG	5.54	118.14	112.60
1	E	44	VAL	N-CA-C	5.53	116.27	108.36
1	C	237	PHE	N-CA-C	-5.53	105.17	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	207	ASP	CA-CB-CG	5.53	118.12	112.60
1	E	497	PHE	N-CA-C	5.52	118.33	110.10
1	E	287	ALA	CA-C-N	-5.52	115.91	123.14
1	E	287	ALA	C-N-CA	-5.52	115.91	123.14
1	C	1072	ILE	N-CA-C	5.51	116.51	108.58
1	E	895	LEU	CA-C-N	5.50	126.56	120.45
1	E	895	LEU	C-N-CA	5.50	126.56	120.45
1	G	887	TYR	CA-CB-CG	-5.50	103.99	113.90
1	G	1071	GLN	CA-C-N	-5.50	115.50	122.43
1	G	1071	GLN	C-N-CA	-5.50	115.50	122.43
2	B	89	ALA	N-CA-C	-5.50	100.74	109.59
2	B	152	GLY	N-CA-C	-5.49	106.73	111.95
1	C	770	GLY	CA-C-O	5.49	124.86	119.04
1	G	228	CYS	N-CA-C	5.49	118.40	109.24
2	B	22	ALA	N-CA-C	5.48	117.16	110.41
2	F	239	SER	N-CA-C	5.48	116.99	110.19
1	G	566	GLY	O-C-N	-5.48	118.43	122.71
2	D	10	GLU	N-CA-CB	-5.48	100.84	109.78
1	G	89	THR	N-CA-C	5.48	119.60	113.02
2	D	182	PRO	CB-CA-C	-5.48	102.95	111.22
2	D	240	ASN	N-CA-C	-5.48	103.46	110.53
2	F	308	THR	N-CA-C	5.48	117.74	109.41
1	E	571	ARG	CB-CA-C	-5.47	98.68	110.45
1	C	363	ASN	N-CA-CB	-5.46	105.24	111.79
1	G	908	GLY	CA-C-N	5.46	125.93	120.04
1	G	908	GLY	C-N-CA	5.46	125.93	120.04
1	C	547	TYR	CA-CB-CG	-5.45	104.08	113.90
2	F	120	ARG	CD-NE-CZ	5.45	132.03	124.40
2	D	236	ILE	CA-C-N	-5.45	114.77	122.94
2	D	236	ILE	C-N-CA	-5.45	114.77	122.94
1	C	793	ALA	N-CA-C	-5.44	102.43	110.48
1	G	521	ASP	N-CA-C	-5.43	105.29	112.24
1	C	26	PHE	CA-CB-CG	-5.42	108.38	113.80
1	C	536	PHE	CA-CB-CG	-5.42	108.38	113.80
1	C	641	GLN	N-CA-C	5.42	119.77	113.20
1	G	404	VAL	CB-CA-C	-5.42	104.96	111.85
1	C	1048	PHE	CA-CB-CG	-5.42	108.38	113.80
1	A	111	PHE	CA-CB-CG	-5.42	108.38	113.80
2	H	301	GLU	N-CA-C	-5.42	105.06	110.97
2	F	120	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	C	59	GLU	CB-CG-CD	5.41	121.80	112.60
2	D	106	ASN	CA-CB-CG	-5.41	107.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	860	PRO	N-CA-CB	5.40	106.32	102.65
1	A	543	MET	N-CA-C	5.40	118.38	109.85
1	E	642	TYR	CB-CG-CD1	5.40	128.89	120.80
1	G	944	ARG	N-CA-C	5.39	118.03	109.24
2	B	237	PHE	CA-CB-CG	-5.39	108.41	113.80
1	E	432	GLY	O-C-N	-5.38	118.91	123.59
1	E	526	TYR	CA-CB-CG	-5.38	104.22	113.90
2	B	59	HIS	N-CA-C	5.38	117.48	108.23
2	B	221	ALA	N-CA-C	5.38	117.14	111.28
1	G	333	ASP	N-CA-CB	5.38	118.61	110.28
1	E	438	TYR	CB-CG-CD1	5.37	128.86	120.80
2	F	147	ALA	CA-C-N	5.37	129.77	120.58
2	F	147	ALA	C-N-CA	5.37	129.77	120.58
1	G	239	ALA	N-CA-C	5.37	116.85	110.19
1	G	295	LEU	N-CA-C	5.37	117.27	108.52
2	B	105	HIS	CA-CB-CG	-5.37	108.43	113.80
2	B	357	SER	CA-C-N	-5.36	112.58	120.46
2	B	357	SER	C-N-CA	-5.36	112.58	120.46
1	G	796	LEU	C-N-CD	-5.36	108.80	120.60
1	E	602	ASN	CA-C-N	5.36	124.97	119.56
1	E	602	ASN	C-N-CA	5.36	124.97	119.56
1	G	346	ALA	N-CA-C	-5.36	106.79	113.38
1	G	518	ASP	O-C-N	5.36	127.66	122.09
2	H	174	SER	N-CA-C	5.36	117.00	110.41
1	C	371	ASN	N-CA-C	-5.34	101.95	109.96
2	F	299	ASP	N-CA-C	-5.34	97.94	107.98
1	C	908	GLY	CA-C-N	5.34	125.42	119.87
1	C	908	GLY	C-N-CA	5.34	125.42	119.87
1	A	255	THR	N-CA-C	5.33	119.30	112.26
2	D	204	ASN	CA-CB-CG	-5.33	107.27	112.60
2	H	250	TYR	CB-CG-CD2	5.33	128.80	120.80
1	E	227	ASN	N-CA-C	-5.33	102.39	110.28
1	G	541	ALA	N-CA-C	5.32	117.36	110.65
2	H	248	CYS	CA-C-N	5.32	127.67	120.65
2	H	248	CYS	C-N-CA	5.32	127.67	120.65
2	D	216	LEU	N-CA-C	5.32	118.40	109.95
1	C	339	ILE	N-CA-C	5.31	119.54	111.89
1	E	732	ALA	O-C-N	5.31	127.54	122.07
1	A	485	ASN	CA-CB-CG	-5.31	107.29	112.60
2	D	57	TYR	CA-CB-CG	-5.31	104.34	113.90
2	H	258	PHE	N-CA-C	-5.31	105.61	111.71
2	D	379	LYS	N-CA-C	-5.30	105.50	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	965	LEU	N-CA-C	-5.30	105.40	111.07
1	E	975	HIS	CA-CB-CG	-5.30	108.50	113.80
1	G	431	ALA	O-C-N	5.30	129.38	122.87
1	A	1014	ILE	N-CA-CB	5.29	118.57	111.90
2	D	58	PRO	N-CA-C	5.29	122.36	113.78
1	G	557	THR	N-CA-C	-5.29	106.84	113.72
1	E	554	ASN	CA-C-N	5.29	125.23	119.78
1	E	554	ASN	C-N-CA	5.29	125.23	119.78
1	G	704	LYS	CA-C-N	5.29	127.32	120.44
1	G	704	LYS	C-N-CA	5.29	127.32	120.44
1	E	4	ARG	CA-C-N	-5.29	111.79	121.52
1	E	4	ARG	C-N-CA	-5.29	111.79	121.52
1	G	562	ILE	N-CA-CB	5.28	118.50	111.64
1	C	258	ASP	CA-CB-CG	-5.28	107.32	112.60
2	F	157	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	1020	ARG	N-CA-C	5.27	117.45	111.02
1	C	181	ILE	CA-C-N	-5.27	115.67	123.05
1	C	181	ILE	C-N-CA	-5.27	115.67	123.05
2	D	11	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	559[A]	ARG	N-CA-C	5.26	118.25	110.46
1	E	559[B]	ARG	N-CA-C	5.26	118.25	110.46
2	H	353	HIS	CA-CB-CG	-5.26	108.54	113.80
2	B	201	ALA	N-CA-C	5.26	117.86	110.23
1	E	561	LYS	N-CA-C	5.25	118.38	109.76
2	F	114	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	932	GLN	N-CA-C	5.25	117.00	111.28
1	C	68	PRO	N-CA-CB	5.25	107.99	103.27
2	H	239	SER	N-CA-C	5.25	116.70	110.19
2	D	45	ASP	CA-CB-CG	5.25	117.85	112.60
2	H	72	SER	CA-C-N	5.25	127.83	120.28
2	H	72	SER	C-N-CA	5.25	127.83	120.28
2	H	137	ASN	O-C-N	5.25	126.09	121.37
1	G	317	PHE	CA-CB-CG	5.24	119.04	113.80
2	H	228	VAL	CA-CB-CG1	-5.24	101.49	110.40
2	H	30	VAL	CB-CA-C	-5.24	104.41	110.91
2	F	11	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	714	VAL	N-CA-C	5.24	114.28	106.85
1	A	1014	ILE	CB-CA-C	5.23	117.79	110.99
2	D	269	CYS	CB-CA-C	5.23	120.83	110.42
1	E	995	HIS	CA-CB-CG	5.23	119.03	113.80
1	G	422	THR	CB-CA-C	5.22	120.26	110.70
1	G	457	ASN	CA-CB-CG	-5.22	107.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	340	THR	N-CA-C	-5.22	106.22	112.59
2	D	369	HIS	CA-C-O	5.21	125.94	120.42
2	H	89	ALA	N-CA-C	-5.21	100.68	109.07
2	F	263	ILE	CA-C-N	5.21	126.64	120.23
2	F	263	ILE	C-N-CA	5.21	126.64	120.23
1	G	949	VAL	N-CA-C	5.21	117.27	109.20
1	C	304	VAL	N-CA-C	-5.20	104.33	110.21
2	F	362	ASP	N-CA-C	5.20	117.69	111.71
2	B	346	PRO	N-CA-CB	5.20	106.29	102.81
1	A	885	PRO	N-CA-CB	5.19	108.12	103.08
1	E	454	ASN	CA-CB-CG	-5.19	107.41	112.60
1	E	271	VAL	N-CA-C	5.18	115.40	110.42
1	C	338	ASP	CB-CA-C	-5.18	102.68	110.92
1	C	555	PRO	N-CA-CB	5.18	107.86	103.35
1	G	970	GLU	CA-C-N	-5.18	114.68	122.81
1	G	970	GLU	C-N-CA	-5.18	114.68	122.81
1	G	682	VAL	N-CA-C	-5.18	105.66	110.53
1	G	308	SER	N-CA-C	-5.17	105.64	111.28
1	G	146	SER	N-CA-C	5.16	115.86	108.74
1	G	826	MET	N-CA-CB	5.16	119.55	111.56
1	E	726	GLU	N-CA-C	5.16	118.00	109.85
2	H	288	PHE	N-CA-CB	5.16	119.20	110.49
2	D	166	GLU	N-CA-CB	5.15	118.78	111.05
1	G	597	ILE	N-CA-CB	-5.15	105.42	111.90
2	D	58	PRO	N-CA-CB	5.14	108.76	103.15
1	E	518	ASP	CA-C-N	5.14	127.17	120.28
1	E	518	ASP	C-N-CA	5.14	127.17	120.28
1	G	83	PRO	N-CA-CB	5.14	108.07	103.19
1	G	590	ARG	N-CA-C	-5.14	105.57	111.07
2	B	17	GLY	CA-C-O	-5.13	117.11	121.78
1	G	225	ASN	CA-CB-CG	-5.13	107.47	112.60
2	H	136	ASP	CA-C-N	-5.13	116.85	123.16
2	H	136	ASP	C-N-CA	-5.13	116.85	123.16
1	G	1069	HIS	CA-CB-CG	-5.12	108.68	113.80
1	C	154	GLU	CA-C-O	5.12	126.38	120.90
1	A	200	PRO	N-CA-CB	5.12	108.59	103.48
2	D	124	GLU	N-CA-C	5.11	116.93	111.36
1	C	102	LEU	CA-C-O	5.11	125.97	120.55
1	C	210	LEU	N-CA-C	-5.11	105.35	112.30
1	E	39	GLU	CB-CA-C	-5.11	102.63	110.81
1	G	497	PHE	CA-CB-CG	-5.11	108.69	113.80
1	E	305	SER	N-CA-C	5.11	114.98	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	GLU	CB-CA-C	-5.10	102.32	110.79
1	E	557	THR	N-CA-C	-5.10	107.61	113.88
1	A	698	ILE	N-CA-C	5.10	115.53	110.23
1	C	239	ALA	N-CA-C	5.10	116.51	110.19
1	G	316	GLY	N-CA-C	-5.09	107.66	115.00
1	A	1010	TYR	N-CA-C	5.09	118.05	109.95
1	E	787	VAL	N-CA-C	-5.09	100.42	107.80
1	E	348	PHE	CA-CB-CG	-5.09	108.71	113.80
1	G	485	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	G	62	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	957	VAL	N-CA-C	5.08	115.81	110.62
2	B	308	THR	N-CA-C	5.08	117.14	109.41
1	A	304	VAL	N-CA-C	-5.08	104.51	110.05
1	E	648	LEU	O-C-N	-5.07	116.74	122.12
1	G	880	THR	N-CA-CB	-5.07	103.31	110.81
2	H	141	ALA	N-CA-C	5.07	116.81	111.28
1	C	314	ALA	N-CA-C	5.06	116.88	111.36
1	E	359	ILE	N-CA-C	5.06	113.63	107.61
1	G	571	ARG	CB-CA-C	-5.06	99.61	111.09
2	F	220	PRO	CB-CA-C	5.06	117.70	111.23
1	G	80	LYS	N-CA-C	5.05	118.60	112.23
1	G	132	PHE	CA-CB-CG	-5.05	108.75	113.80
1	E	23	ALA	N-CA-C	5.05	121.55	110.80
1	E	527	LYS	N-CA-C	-5.04	102.32	110.14
1	G	47	VAL	N-CA-CB	5.04	118.37	111.41
1	G	81	GLU	O-C-N	5.04	129.25	122.49
2	H	92	PHE	CA-CB-CG	-5.04	108.76	113.80
1	C	372	ASP	N-CA-C	5.04	118.74	112.59
1	G	518	ASP	CA-C-N	5.04	127.53	120.28
1	G	518	ASP	C-N-CA	5.04	127.53	120.28
1	G	597	ILE	N-CA-C	5.04	115.29	107.28
2	H	112	ASP	CA-C-N	-5.04	115.77	122.77
2	H	112	ASP	C-N-CA	-5.04	115.77	122.77
1	G	559	ARG	N-CA-C	5.03	117.02	110.53
2	D	372	GLU	CA-C-N	5.03	127.33	120.54
2	D	372	GLU	C-N-CA	5.03	127.33	120.54
1	E	954	LYS	CA-C-O	5.03	125.78	120.10
1	G	784	GLN	N-CA-C	5.03	116.60	110.41
2	H	249	ASP	O-C-N	5.02	127.25	122.03
1	E	895	LEU	O-C-N	5.02	126.44	121.57
2	H	164	THR	N-CA-C	5.01	117.17	110.35
1	A	619	GLU	N-CA-C	5.01	116.37	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	568	GLY	CA-C-N	5.01	124.77	119.76
1	G	568	GLY	C-N-CA	5.01	124.77	119.76
2	B	174	SER	N-CA-C	5.01	117.14	110.53
1	E	542	TYR	N-CA-CB	-5.01	101.99	110.46
1	G	318	PRO	CB-CA-C	-5.01	104.45	112.27
1	G	999	PRO	N-CA-CB	5.01	108.11	102.60
2	B	132	ILE	CB-CA-C	-5.01	103.37	110.83
2	B	200	GLY	CA-C-N	5.01	127.82	120.71
2	B	200	GLY	C-N-CA	5.01	127.82	120.71
2	B	353	HIS	CB-CA-C	-5.01	103.83	110.34
1	G	484	LEU	N-CA-C	5.00	117.35	109.39

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	314	PHE	Mainchain
2	B	357	SER	Peptide
2	H	250	TYR	Sidechain
2	H	357	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8198	0	8215	279	1
1	C	8167	0	8201	257	0
1	E	8232	0	8274	256	0
1	G	8170	0	8204	358	0
2	B	2902	0	2872	154	0
2	D	2899	0	2868	98	0
2	F	2900	0	2867	122	1
2	H	2895	0	2863	241	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	0	0	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
5	E	3	0	0	1	0
5	G	3	0	0	2	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	1	0
7	E	54	0	24	5	0
7	G	54	0	24	4	0
8	A	18	0	22	4	0
8	C	18	0	22	3	0
8	E	18	0	21	4	0
8	G	18	0	22	4	0
9	A	23	0	11	0	0
9	C	23	0	11	1	0
9	E	23	0	11	2	0
9	G	23	0	11	1	0
10	A	9	0	20	0	0
10	C	9	0	20	0	0
10	E	9	0	20	3	0
10	G	9	0	20	1	0
11	A	842	0	0	26	1
11	B	190	0	0	3	0
11	C	732	0	0	12	0
11	D	193	0	0	3	0
11	E	939	0	0	30	0
11	F	233	0	0	5	1
11	G	743	0	0	20	0
11	H	165	0	0	4	0
All	All	48888	0	44671	1732	2

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 19.

All (1732) 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:130[B]:ARG:NH2	1:A:130[B]:ARG:CZ	1.70	1.49
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.26	1.16
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.06	1.12
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.13	1.06
1:A:130[B]:ARG:CZ	1:A:130[B]:ARG:NH1	2.18	1.05
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.39	1.04
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.04
2:H:227:ASP:HA	2:H:230:LYS:HD2	1.41	1.02
1:A:554:ASN:HD22	8:A:5014:ORN:HD3	1.19	1.01
1:E:784:GLN:H	1:E:784:GLN:NE2	1.58	0.99
2:H:236:ILE:HD12	2:H:263:ILE:HG21	1.43	0.98
1:G:554:ASN:HD22	8:G:5074:ORN:HD3	1.30	0.97
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.80	0.95
2:D:222:GLN:H	2:D:222:GLN:HE21	1.05	0.94
1:A:682:VAL:HG11	1:A:689:GLN:HE21	1.33	0.93
2:B:261:THR:HG21	2:B:263:ILE:HG13	1.49	0.92
2:H:286:MET:HE2	2:H:315:ALA:HB2	1.47	0.92
1:A:710:TYR:HA	1:A:712:LEU:HD12	1.50	0.92
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.50	0.92
1:G:1001:ILE:HD13	1:G:1029:ILE:HB	1.51	0.91
1:G:1027:ARG:NH1	1:G:1031:ARG:HD2	1.85	0.91
1:E:715:ARG:HG3	1:E:725:MET:HE3	1.53	0.91
2:H:324:ASN:HD22	2:H:324:ASN:H	1.17	0.90
1:G:708:ILE:HG23	1:G:754:HIS:HB2	1.52	0.90
1:G:1063:ILE:HD13	1:G:1068:MET:HG3	1.51	0.90
1:E:571:ARG:HH21	1:E:645[B]:GLN:HE21	1.16	0.89
1:A:554:ASN:ND2	8:A:5014:ORN:HD3	1.87	0.89
1:G:1001:ILE:CD1	1:G:1029:ILE:HB	2.03	0.89
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.54	0.89
2:F:150:PHE:CD1	2:F:151:PRO:HD2	2.09	0.88
2:H:322:PRO:CB	2:H:324:ASN:HD21	1.85	0.88
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.08	0.88
2:D:286[A]:MET:HE1	2:D:312:HIS:ND1	1.89	0.88
1:A:784:GLN:HE21	1:A:784:GLN:H	1.21	0.87
2:H:342:ARG:HG3	2:H:342:ARG:HH11	1.39	0.87
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.54	0.87
2:H:150:PHE:CD1	2:H:151:PRO:HD2	2.09	0.87
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.90	0.86
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.10	0.85
1:E:728:VAL:CG1	1:E:733:ASP:HB3	2.04	0.85
2:F:322:PRO:HG2	2:F:324:ASN:HD21	1.39	0.84
2:H:38:GLY:HA3	2:H:358:PRO:HB3	1.58	0.84
2:D:228:VAL:HA	2:D:231:MET:HE2	1.59	0.84
2:B:261:THR:HG22	2:B:263:ILE:H	1.43	0.83
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.13	0.83
2:F:228:VAL:HA	2:F:231:MET:HE3	1.60	0.83
10:E:5053:NET:H22	10:E:5053:NET:H42	1.61	0.83
1:G:708:ILE:CG2	1:G:712:LEU:HD11	2.08	0.83
1:E:1001:ILE:CD1	1:E:1029:ILE:HB	2.09	0.82
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.61	0.82
1:E:784:GLN:H	1:E:784:GLN:HE21	1.25	0.82
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.62	0.81
2:H:324:ASN:HD22	2:H:324:ASN:N	1.75	0.81
2:H:7:LEU:HD23	2:H:15:PHE:CD1	2.16	0.81
2:B:322:PRO:HG2	2:B:324:ASN:HD21	1.46	0.81
2:B:286:MET:HE2	2:B:315:ALA:HB2	1.64	0.80
2:B:261:THR:CG2	2:B:263:ILE:H	1.95	0.80
1:E:1001:ILE:HG13	1:E:1002:GLN:N	1.95	0.80
1:C:784:GLN:H	1:C:784:GLN:HE21	1.31	0.79
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.65	0.79
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.65	0.79
2:H:286:MET:HE1	2:H:312:HIS:ND1	1.97	0.79
2:H:228:VAL:HG11	2:H:258:PHE:CE1	2.18	0.79
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.65	0.78
1:C:59:GLU:HG3	1:C:60:MET:HE2	1.64	0.78
2:F:215:ARG:HG3	2:F:215:ARG:HH11	1.49	0.78
2:D:152:GLY:O	2:D:156:MET:HE3	1.84	0.78
2:F:236:ILE:HB	2:F:265:VAL:HG22	1.64	0.78
1:E:6:ASP:OD1	1:E:7:ILE:HG13	1.83	0.78
1:A:225:ASN:ND2	1:A:331:THR:HG21	1.99	0.78
2:B:152:GLY:O	2:B:156:MET:HE3	1.84	0.78
1:A:784:GLN:H	1:A:784:GLN:NE2	1.80	0.78
1:G:939:MET:HE2	1:G:1050:THR:CG2	2.14	0.77
2:H:236:ILE:HD12	2:H:263:ILE:CG2	2.14	0.77
2:D:370:PHE:O	2:D:374:ILE:HG13	1.84	0.77
1:E:679:GLN:O	1:E:683:GLU:HG3	1.84	0.77
1:E:1020:ARG:HH21	1:E:1023:ILE:HG21	1.50	0.77
1:G:769:ASP:HB3	1:G:874:LEU:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.68	0.76
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.12	0.76
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.85	0.76
2:H:321:LEU:HD23	2:H:325:LEU:O	1.86	0.76
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.51	0.76
1:A:313:LYS:HE2	1:A:608:THR:O	1.84	0.76
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.68	0.76
1:C:845:ARG:HG3	1:C:845:ARG:HH11	1.50	0.76
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.14	0.76
1:E:872:LYS:HD3	1:E:877:GLN:HG2	1.67	0.76
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.20	0.76
2:F:300:VAL:HG22	2:F:328:THR:O	1.87	0.75
2:B:228:VAL:HA	2:B:231:MET:HE3	1.67	0.75
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.67	0.75
1:G:480:GLY:HA3	11:G:5615:HOH:O	1.87	0.75
1:E:76:LYS:HE3	11:E:5750:HOH:O	1.86	0.75
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.68	0.75
1:E:1020:ARG:NH2	1:E:1023:ILE:HG21	2.02	0.75
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.51	0.75
2:H:152:GLY:O	2:H:156:MET:HE3	1.87	0.75
1:C:318:PRO:HG3	1:C:610:TYR:OH	1.87	0.75
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.67	0.74
1:E:79:GLU:O	1:E:82[B]:ARG:NH1	2.18	0.74
1:E:151:THR:OG1	1:E:154:GLU:HG3	1.87	0.74
1:C:873:SER:O	1:C:877:GLN:HG3	1.86	0.74
2:F:286:MET:HE1	2:F:312:HIS:ND1	2.03	0.74
2:D:222:GLN:HE21	2:D:222:GLN:N	1.85	0.74
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.68	0.74
1:G:708:ILE:HG22	1:G:712:LEU:HD11	1.69	0.74
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.23	0.73
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.87	0.73
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.87	0.73
1:A:130[B]:ARG:NH1	1:A:130[B]:ARG:HD2	2.03	0.73
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.70	0.73
2:H:367:PHE:O	2:H:371:ILE:HG12	1.88	0.73
2:H:209:LEU:HD22	2:H:216:LEU:CD2	2.18	0.73
1:E:905:PRO:HB2	1:E:1040:TYR:OH	1.89	0.72
2:H:186:LYS:O	2:H:189:GLU:HB2	1.89	0.72
1:A:318:PRO:HG3	1:A:610:TYR:OH	1.88	0.72
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.72	0.72
1:G:4:ARG:HD3	1:G:7:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLY:HA3	2:B:358:PRO:HB3	1.69	0.72
1:A:130[B]:ARG:NH2	1:A:130[B]:ARG:NE	2.38	0.72
1:E:873:SER:O	1:E:877:GLN:HG3	1.89	0.72
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.54	0.72
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.71	0.72
2:H:32:PHE:O	2:H:291:HIS:HB2	1.90	0.71
1:G:318:PRO:HG3	1:G:610:TYR:OH	1.90	0.71
1:G:763:ASP:HB3	1:G:779:MET:HE3	1.72	0.71
2:H:74:GLN:HB3	11:H:3855:HOH:O	1.90	0.71
2:H:313:GLY:HA3	11:H:3579:HOH:O	1.90	0.71
1:G:784:GLN:NE2	1:G:784:GLN:H	1.87	0.71
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.15	0.71
2:H:369:HIS:O	2:H:373:LEU:HG	1.90	0.71
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.90	0.71
1:A:1054:LEU:HD23	11:A:5359:HOH:O	1.90	0.71
1:G:810:ARG:HG3	1:G:810:ARG:HH11	1.54	0.71
2:H:275:LEU:O	2:H:279:SER:HB2	1.91	0.71
2:B:286:MET:HE2	2:B:315:ALA:CB	2.21	0.71
1:E:715:ARG:CG	1:E:725:MET:HE3	2.20	0.71
1:G:921:GLY:HA3	1:G:926:GLU:HB3	1.72	0.71
1:A:550:GLU:HB2	2:B:117:LYS:HD2	1.72	0.71
2:B:322:PRO:HB2	2:B:324:ASN:ND2	2.05	0.70
1:E:563:MET:CE	1:E:635:PRO:HG3	2.21	0.70
2:H:205:ILE:HG12	2:H:355:GLU:HG3	1.74	0.70
1:E:335:LEU:C	1:E:336:MET:HE2	2.16	0.70
1:C:975:HIS:HD1	1:E:975:HIS:HD1	0.81	0.70
2:F:322:PRO:CG	2:F:324:ASN:HD21	2.03	0.70
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.21	0.70
1:A:1069:HIS:HA	1:A:1072:ILE:HD12	1.74	0.70
2:H:342:ARG:HB2	2:H:347:ALA:HB3	1.74	0.70
1:E:313:LYS:HE2	1:E:608:THR:O	1.91	0.70
1:G:218:MET:HE3	1:G:264:MET:SD	2.31	0.70
1:A:475:LYS:O	1:A:479:VAL:HG22	1.92	0.70
1:A:873:SER:O	1:A:877:GLN:HG3	1.91	0.70
1:C:696:THR:HB	1:C:700:MET:SD	2.32	0.70
1:E:139:ILE:HD11	1:E:141:LEU:HD12	1.72	0.70
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.55	0.70
1:E:150:HIS:ND1	11:E:5507:HOH:O	2.25	0.69
1:C:482:THR:HG23	11:C:5556:HOH:O	1.92	0.69
1:E:685:LEU:HD22	1:E:815:LYS:HB3	1.72	0.69
1:C:860:PRO:HB2	1:C:863:LYS:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.93	0.69
2:H:41:GLU:HB3	2:H:358:PRO:HD3	1.74	0.69
2:H:173:GLY:O	2:H:207:ARG:HG2	1.92	0.69
1:G:860:PRO:O	1:G:864:VAL:HG23	1.92	0.69
2:F:313:GLY:HA3	11:F:3076:HOH:O	1.92	0.69
1:A:426:ARG:C	1:A:426:ARG:HD2	2.18	0.69
1:E:1026:SER:O	1:E:1029:ILE:HG22	1.93	0.69
1:G:365:GLU:HG2	1:G:366:LYS:N	2.07	0.69
1:G:784:GLN:H	1:G:784:GLN:HE21	1.40	0.69
2:H:193:HIS:NE2	2:H:217:THR:HB	2.08	0.69
1:A:358:LYS:HE3	11:A:5399:HOH:O	1.92	0.69
1:E:222[B]:ARG:NH2	1:E:278:GLU:HG2	2.07	0.69
2:H:369:HIS:CE1	2:H:373:LEU:HD21	2.28	0.69
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.20	0.69
1:A:1:MET:HB3	1:A:224:LYS:CE	2.23	0.68
2:B:173:GLY:O	2:B:207:ARG:HG2	1.93	0.68
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.08	0.68
2:H:222:GLN:H	2:H:222:GLN:HE21	1.41	0.68
1:G:873:SER:O	1:G:877:GLN:HG3	1.93	0.68
2:H:361:HIS:HA	11:H:3881:HOH:O	1.93	0.68
1:A:702:VAL:HG13	1:A:731:GLU:HG3	1.76	0.68
1:G:1021:ARG:HG2	1:G:1021:ARG:HH11	1.58	0.68
2:F:279:SER:O	2:F:322:PRO:HG3	1.94	0.68
1:A:467:GLU:O	1:A:471:ARG:HG2	1.92	0.68
1:C:930:LYS:HE3	11:C:5088:HOH:O	1.93	0.68
1:E:728:VAL:HG13	1:E:733:ASP:CB	2.08	0.68
2:B:255:ILE:HA	2:B:258:PHE:HD2	1.59	0.68
1:C:59:GLU:CG	1:C:60:MET:HE2	2.23	0.68
1:E:554:ASN:HD22	8:E:5054:ORN:HD3	1.59	0.68
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.09	0.68
1:A:59:GLU:CG	1:A:60:MET:HE2	2.24	0.68
2:D:215:ARG:HG3	2:D:215:ARG:HH11	1.59	0.68
2:H:341:HIS:CD2	2:H:348:PHE:HB3	2.28	0.68
2:H:363:ALA:C	2:H:365:PRO:HD2	2.19	0.68
1:C:865:ALA:O	1:C:869:MET:HG3	1.94	0.67
1:G:708:ILE:HG21	1:G:712:LEU:HD11	1.75	0.67
2:B:46:PRO:HA	2:B:76:HIS:CG	2.30	0.67
1:E:1001:ILE:HG13	1:E:1002:GLN:H	1.56	0.67
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.77	0.67
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.12	0.67
1:G:154:GLU:O	1:G:158:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:699:GLU:HA	1:G:702:VAL:CG2	2.24	0.67
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.76	0.67
1:C:313:LYS:HE2	1:C:608:THR:O	1.94	0.67
1:E:751:LEU:O	1:E:752:LEU:HD12	1.94	0.67
2:B:353:HIS:HB3	2:B:355:GLU:OE1	1.95	0.67
1:G:947:LEU:HD12	1:G:947:LEU:N	2.09	0.67
2:H:83:ARG:HD2	2:H:83:ARG:O	1.95	0.67
1:E:891:LYS:NZ	11:E:5694:HOH:O	2.28	0.67
2:F:369:HIS:O	2:F:373:LEU:HG	1.95	0.67
2:F:370:PHE:O	2:F:374:ILE:HG13	1.94	0.67
2:B:186:LYS:O	2:B:189:GLU:HB2	1.95	0.66
2:F:324:ASN:N	2:F:324:ASN:HD22	1.90	0.66
1:C:679:GLN:O	1:C:683:GLU:HG3	1.95	0.66
1:E:158:VAL:HG11	1:E:206:ILE:HB	1.77	0.66
1:E:667:ASP:OD1	1:E:677:ARG:NH2	2.28	0.66
1:G:525:VAL:HG22	1:G:548:GLU:H	1.60	0.66
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.59	0.66
1:G:1057:ASP:HB3	1:G:1060:GLU:HB2	1.77	0.66
1:A:1063:ILE:HD13	1:A:1068:MET:HG3	1.78	0.66
1:G:509:ARG:HB2	1:G:512:GLU:HG3	1.77	0.66
1:C:698:ILE:HD12	1:C:698:ILE:H	1.61	0.66
1:E:652[B]:ARG:HG3	11:E:5628:HOH:O	1.94	0.66
2:F:23:THR:HG23	2:F:134:ALA:O	1.96	0.66
2:H:342:ARG:HG3	2:H:342:ARG:NH1	2.06	0.66
1:A:145:ARG:HH12	1:A:161:ASP:CG	2.04	0.66
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.78	0.66
1:E:998:ARG:HB3	1:E:999:PRO:HA	1.78	0.66
2:H:263:ILE:HG12	2:H:377:TYR:OH	1.96	0.66
1:G:17:PRO:HG3	1:G:917:VAL:CG1	2.26	0.66
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.18	0.66
1:G:464:VAL:HG21	2:H:88:ILE:HG12	1.78	0.65
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.23	0.65
2:H:40:GLN:NE2	2:H:66:ASN:O	2.28	0.65
2:B:299:ASP:O	2:B:303:ASN:N	2.30	0.65
2:F:322:PRO:HB2	2:F:324:ASN:ND2	2.12	0.65
1:G:559:ARG:HH11	1:G:595:GLU:HA	1.61	0.65
1:A:696:THR:HB	1:A:700:MET:SD	2.36	0.65
1:A:708:ILE:CG2	1:A:754:HIS:HB2	2.26	0.65
1:G:43:ARG:NH2	1:G:81:GLU:OE1	2.30	0.65
1:G:666:PRO:HA	1:G:669:ILE:HD12	1.79	0.65
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:THR:CG2	2:B:263:ILE:HG13	2.25	0.65
1:E:947:LEU:HD12	1:E:947:LEU:N	2.12	0.65
1:G:833:LYS:O	1:G:836:GLU:HB2	1.96	0.65
1:G:930:LYS:NZ	1:G:1058:ALA:O	2.30	0.65
2:H:266:PHE:HB2	2:H:370:PHE:CD1	2.31	0.65
2:B:353:HIS:HB3	2:B:355:GLU:CD	2.22	0.65
1:E:863:LYS:HE2	11:E:5733:HOH:O	1.95	0.65
2:H:247:PRO:O	2:H:249:ASP:N	2.30	0.65
1:A:112:GLY:HA2	11:A:5423:HOH:O	1.95	0.65
1:G:648:LEU:HD13	1:G:845:ARG:HD3	1.78	0.65
2:H:60:ILE:HB	2:H:82:ILE:HD13	1.79	0.65
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.78	0.65
2:B:190:LEU:O	2:B:215[B]:ARG:NH2	2.29	0.65
1:E:784:GLN:HE21	1:E:784:GLN:N	1.94	0.65
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.77	0.65
1:C:321:LYS:NZ	1:C:611:ASP:OD2	2.29	0.65
1:G:1027:ARG:HH11	1:G:1031:ARG:HD2	1.60	0.65
2:H:123:ARG:HA	2:H:288:PHE:CD2	2.32	0.65
2:H:321:LEU:HD23	2:H:325:LEU:HB3	1.79	0.65
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.43	0.64
1:A:9:SER:OG	1:A:83:PRO:HA	1.98	0.64
1:C:523:HIS:HB3	1:C:524:PRO:HD2	1.78	0.64
1:C:715:ARG:NH2	7:C:5027:ADP:O1A	2.30	0.64
2:F:38:GLY:HA3	2:F:358:PRO:HB3	1.80	0.64
1:C:784:GLN:H	1:C:784:GLN:NE2	1.95	0.64
1:E:417:ASP:OD2	1:E:423:LYS:NZ	2.30	0.64
1:G:223:ASP:CG	1:G:227:ASN:HB2	2.23	0.64
1:C:422:THR:HG22	1:C:423:LYS:HG3	1.79	0.64
2:D:182:PRO:HB2	11:D:1950:HOH:O	1.96	0.64
2:D:286[A]:MET:HE2	2:D:314:PHE:C	2.22	0.64
1:G:331:THR:OG1	1:G:334:GLU:HG3	1.97	0.64
1:A:844:PRO:HD2	11:A:5463:HOH:O	1.97	0.64
1:C:1026:SER:O	1:C:1029:ILE:HG22	1.97	0.64
1:E:1000:HIS:CD2	1:E:1002:GLN:HB3	2.33	0.64
1:G:1027:ARG:HH12	1:G:1031:ARG:HD2	1.63	0.64
1:A:671:ARG:HD3	11:A:5564:HOH:O	1.98	0.64
2:B:272:HIS:ND1	2:B:349:SER:OG	2.30	0.64
1:C:708:ILE:CG2	1:C:754:HIS:HB2	2.27	0.64
2:F:205:ILE:HG21	2:F:237:PHE:CZ	2.32	0.64
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.15	0.64
1:A:228:CYS:SG	1:A:269:MET:HG2	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:715:ARG:NH2	7:E:5047:ADP:O1A	2.29	0.64
1:E:959:ASP:O	1:E:963:LYS:HG3	1.97	0.64
2:F:252:ILE:O	2:F:256:GLN:HG3	1.97	0.64
2:H:334:ASP:OD1	2:H:336:THR:HG23	1.98	0.64
1:E:1073:LYS:N	1:E:1073:LYS:HD2	2.13	0.64
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.80	0.63
1:E:903:VAL:O	1:E:905:PRO:HD3	1.99	0.63
1:E:998:ARG:CB	1:E:999:PRO:HA	2.27	0.63
1:E:685:LEU:HD11	1:E:819:GLU:HG2	1.81	0.63
2:B:335:GLY:HA2	11:B:5198:HOH:O	1.96	0.63
1:E:8:LYS:HE3	11:E:5452:HOH:O	1.99	0.63
2:H:324:ASN:O	2:H:342:ARG:HD2	1.98	0.63
2:H:264:PRO:HD3	2:H:377:TYR:CD1	2.34	0.63
1:C:704:LYS:O	1:C:707:GLU:HB2	1.98	0.63
2:F:225:ALA:O	2:F:229:LEU:HG	1.98	0.63
2:B:45:ASP:HB3	2:B:48:TYR:HD2	1.64	0.63
1:C:1024:GLU:HG3	11:C:5748:HOH:O	1.98	0.63
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.79	0.63
2:F:322:PRO:HG2	2:F:324:ASN:ND2	2.13	0.63
1:G:769:ASP:CB	1:G:874:LEU:HD12	2.29	0.63
1:G:954:LYS:O	1:G:957:VAL:HG12	1.99	0.63
1:A:154:GLU:HA	11:A:5142:HOH:O	1.99	0.63
1:A:289:ASN:OD1	1:A:290:PRO:HD2	1.98	0.63
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.33	0.63
1:E:535:GLU:HG2	1:E:536:PHE:CE2	2.34	0.62
1:E:571:ARG:HH21	1:E:645[B]:GLN:NE2	1.94	0.62
2:F:46:PRO:HA	2:F:76:HIS:CG	2.33	0.62
1:E:267:ALA:O	1:E:271:VAL:HG23	1.99	0.62
2:D:228:VAL:HA	2:D:231:MET:CE	2.30	0.62
1:G:883:VAL:C	1:G:884:ILE:HG12	2.23	0.62
1:A:930:LYS:HE3	11:A:5068:HOH:O	1.99	0.62
1:G:130:ARG:HG3	1:G:148:ILE:HG13	1.81	0.62
2:H:248:CYS:O	2:H:252:ILE:HG13	1.99	0.62
2:B:218:ILE:HD13	2:B:218:ILE:N	2.13	0.62
2:B:273:GLN:NE2	2:B:314:PHE:O	2.32	0.62
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.81	0.62
1:C:1:MET:HA	1:C:224:LYS:CE	2.30	0.62
1:C:426:ARG:HD3	1:C:426:ARG:C	2.24	0.62
1:C:698:ILE:HG13	1:C:738:PHE:CD2	2.34	0.62
1:A:1026:SER:O	1:A:1029:ILE:HG22	1.99	0.62
2:B:255:ILE:HA	2:B:258:PHE:CD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ASN:ND2	1:E:365:GLU:OE2	2.31	0.62
1:G:715:ARG:NH2	7:G:5067:ADP:O1A	2.32	0.62
2:H:41:GLU:HB2	2:H:358:PRO:HG3	1.80	0.62
1:E:563:MET:HE1	1:E:635:PRO:HG3	1.82	0.62
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.45	0.62
2:H:224:SER:OG	2:H:226:GLU:HB2	1.99	0.62
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.35	0.61
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.64	0.61
2:H:34:THR:HA	2:H:56:THR:OG1	2.00	0.61
1:A:654:LEU:O	1:A:659:VAL:HG23	2.00	0.61
1:C:353:ASP:OD2	2:D:116:ARG:HD2	1.99	0.61
1:C:695:VAL:CG1	1:C:701:ALA:HB2	2.21	0.61
1:E:418:PRO:HD2	11:E:5587:HOH:O	2.00	0.61
1:E:795:SER:HB2	1:E:890:VAL:HG22	1.82	0.61
1:G:805:ILE:HG22	1:G:806:GLN:N	2.15	0.61
1:C:698:ILE:HD12	1:C:698:ILE:N	2.16	0.61
1:G:596:THR:O	1:G:614:ASP:HB2	2.01	0.61
2:B:71:GLU:O	2:B:203:ARG:HG3	1.99	0.61
2:D:286[A]:MET:HE3	2:D:313:GLY:C	2.25	0.61
2:H:281:ALA:HA	2:H:320:THR:O	2.01	0.61
1:A:426:ARG:HD3	11:A:5504:HOH:O	2.00	0.61
2:B:299:ASP:HB3	2:B:304:VAL:HG22	1.81	0.61
1:E:941[A]:LYS:NZ	11:E:5448:HOH:O	2.32	0.61
2:F:364:ALA:N	2:F:365:PRO:HD2	2.15	0.61
1:E:460:ARG:HG3	11:E:5326:HOH:O	2.01	0.61
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.00	0.61
1:G:678:PHE:CZ	1:G:842:VAL:HG23	2.35	0.61
1:G:699:GLU:HA	1:G:702:VAL:HG21	1.82	0.61
2:H:193:HIS:O	2:H:234:ASP:HB2	2.01	0.61
1:C:1001:ILE:HD13	1:C:1029:ILE:HB	1.83	0.61
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.36	0.61
1:G:1:MET:HG3	1:G:225:ASN:HD21	1.66	0.61
1:G:704:LYS:O	1:G:707:GLU:HB2	2.01	0.61
1:G:998:ARG:HA	1:G:999:PRO:C	2.26	0.61
2:H:266:PHE:HD2	2:H:370:PHE:CD2	2.18	0.61
2:B:202:LYS:NZ	2:B:356:ALA:O	2.27	0.61
2:D:222:GLN:H	2:D:222:GLN:NE2	1.88	0.61
1:C:863:LYS:O	1:C:867:ARG:HG3	2.00	0.60
1:E:43:ARG:NH2	1:E:81:GLU:OE1	2.29	0.60
1:A:682:VAL:HG11	1:A:689:GLN:NE2	2.11	0.60
1:A:998:ARG:HG2	1:A:1003:ASP:OD2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ILE:HD13	1:A:1029:ILE:HB	1.82	0.60
1:C:35:LYS:O	1:C:39:GLU:HB2	2.00	0.60
1:G:9:SER:N	1:G:84:ASP:OD2	2.32	0.60
1:G:24:CYS:HB2	1:G:604:GLU:HB3	1.84	0.60
1:G:950:ARG:HG3	1:G:1016:THR:OG1	2.02	0.60
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.36	0.60
2:H:240:ASN:HA	2:H:270:LEU:H	1.67	0.60
2:H:374:ILE:O	2:H:377:TYR:HB3	2.01	0.60
2:F:34:THR:HA	2:F:56:THR:OG1	2.01	0.60
2:H:33:ASN:HA	2:H:291:HIS:O	2.01	0.60
2:B:150:PHE:CD1	2:B:151:PRO:HD2	2.37	0.60
1:E:757:ASP:O	1:E:833:LYS:NZ	2.35	0.60
1:G:67:GLU:HB3	1:G:68:PRO:HD2	1.82	0.60
1:G:644:GLY:O	1:G:647:PRO:HD2	2.01	0.60
2:H:197:TYR:HA	2:H:219:VAL:HG22	1.84	0.60
2:H:365:PRO:HA	2:H:368:ASP:OD2	2.01	0.60
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.84	0.60
1:G:780:GLU:OE2	1:G:800:THR:HG23	2.02	0.60
2:H:144:LEU:O	2:H:148:ARG:HG3	2.01	0.60
1:A:583:VAL:O	1:A:587:LEU:HG	2.00	0.60
1:E:1:MET:HA	1:E:224:LYS:CE	2.32	0.60
1:G:40:GLU:HG2	1:G:325:LYS:HE2	1.84	0.60
2:B:11:ASP:OD1	2:B:13:THR:HB	2.02	0.59
2:D:26:ALA:O	2:D:131:CYS:HA	2.02	0.59
1:G:417:ASP:OD2	1:G:423:LYS:NZ	2.28	0.59
2:H:73:SER:HA	2:H:203:ARG:NH2	2.16	0.59
2:H:286:MET:HB2	2:H:313:GLY:O	2.03	0.59
1:A:679:GLN:O	1:A:683:GLU:HG3	2.03	0.59
1:C:142:GLU:HG2	1:C:296:ILE:HG12	1.84	0.59
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.37	0.59
2:D:298:LYS:HB2	2:D:332:LEU:HD11	1.84	0.59
2:F:324:ASN:HD22	2:F:324:ASN:H	1.50	0.59
2:H:199:PHE:HE2	2:H:238:LEU:HB3	1.67	0.59
2:H:344:ASP:C	2:H:345:LYS:HG2	2.25	0.59
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.03	0.59
1:G:1:MET:CG	1:G:225:ASN:HD21	2.15	0.59
2:H:46:PRO:HG2	2:H:201:ALA:O	2.03	0.59
2:H:322:PRO:O	2:H:325:LEU:N	2.35	0.59
1:A:698:ILE:O	1:A:702:VAL:HG23	2.03	0.59
1:A:710:TYR:HA	1:A:712:LEU:CD1	2.26	0.59
1:E:757:ASP:HB2	11:E:5978:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:LEU:O	2:H:146:LYS:HG3	2.02	0.59
2:H:228:VAL:HG11	2:H:258:PHE:CZ	2.38	0.59
2:H:263:ILE:HA	2:H:377:TYR:CE1	2.38	0.59
1:A:1000:HIS:CD2	1:A:1002:GLN:HB3	2.38	0.59
2:B:192:PHE:O	2:B:215[B]:ARG:HG2	2.03	0.59
2:B:205:ILE:O	2:B:209:LEU:HG	2.02	0.59
2:B:365:PRO:HA	2:B:368:ASP:OD2	2.02	0.59
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.37	0.59
1:G:623:LEU:O	1:G:627:LEU:HG	2.03	0.59
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.03	0.59
2:H:208:MET:SD	2:H:355:GLU:HA	2.42	0.59
1:A:349:GLU:O	2:B:294:ASN:HB2	2.02	0.58
1:A:682:VAL:CG1	1:A:689:GLN:HE21	2.10	0.58
2:H:142:LEU:O	2:H:142:LEU:HD12	2.03	0.58
1:A:130[B]:ARG:NH1	1:A:130[B]:ARG:CD	2.66	0.58
2:B:326:ARG:O	2:B:326:ARG:HG3	2.01	0.58
1:E:1004:ARG:O	1:E:1009[B]:GLU:HG3	2.03	0.58
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.38	0.58
1:G:998:ARG:CB	1:G:999:PRO:HA	2.33	0.58
2:H:226:GLU:C	2:H:228:VAL:H	2.11	0.58
1:A:59:GLU:CD	1:A:60:MET:HE2	2.28	0.58
2:B:322:PRO:CG	2:B:324:ASN:HD21	2.15	0.58
1:G:423:LYS:HB3	11:G:5599:HOH:O	2.04	0.58
1:G:698:ILE:O	1:G:702:VAL:HG23	2.03	0.58
2:H:249:ASP:N	2:H:249:ASP:OD1	2.28	0.58
1:E:130:ARG:HG3	1:E:148:ILE:HG13	1.85	0.58
1:E:954:LYS:NZ	9:E:5052:IMP:O3P	2.29	0.58
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.85	0.58
1:A:735:ARG:O	1:A:738:PHE:N	2.36	0.58
1:C:728:VAL:HG13	1:C:733:ASP:HB3	1.86	0.58
1:G:550:GLU:OE1	2:H:120:ARG:NH2	2.30	0.58
1:G:563:MET:CE	1:G:635:PRO:HG3	2.34	0.58
1:G:751:LEU:O	1:G:752:LEU:HD13	2.03	0.58
1:G:765:ASP:OD1	1:G:827:ASN:ND2	2.30	0.58
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.35	0.58
2:F:224:SER:OG	2:F:227:ASP:HB2	2.02	0.58
2:F:334:ASP:OD1	2:F:336:THR:HG23	2.03	0.58
2:H:78:GLN:HA	2:H:78:GLN:NE2	2.19	0.58
1:A:780:GLU:HG2	1:A:799:TYR:CE1	2.38	0.58
1:G:167:ILE:N	1:G:167:ILE:HD12	2.19	0.58
1:G:225:ASN:ND2	1:G:331:THR:HG21	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ASP:HB3	1:A:677:ARG:HB2	1.85	0.57
2:B:296:PRO:HB2	2:B:332:LEU:HB2	1.86	0.57
1:C:561:LYS:HE2	11:C:5569:HOH:O	2.04	0.57
1:E:704:LYS:O	1:E:707:GLU:HB2	2.04	0.57
1:G:223:ASP:OD1	1:G:227:ASN:HB2	2.04	0.57
2:B:66:ASN:HB3	2:B:93:ARG:O	2.04	0.57
1:C:951:GLU:O	1:C:954:LYS:HB2	2.04	0.57
2:H:236:ILE:CD1	2:H:263:ILE:HG21	2.28	0.57
2:D:244:ASP:OD1	2:D:245:PRO:HD2	2.05	0.57
1:G:710:TYR:HB3	1:G:711:PRO:HA	1.86	0.57
2:B:232:ASN:N	2:B:233:PRO:HD3	2.20	0.57
2:B:279:SER:O	2:B:322:PRO:HG3	2.04	0.57
2:H:133:ILE:CG2	2:H:138:PRO:HB3	2.34	0.57
1:C:730:ASP:OD1	1:C:733:ASP:HB2	2.04	0.57
2:D:150:PHE:CD1	2:D:151:PRO:HD2	2.39	0.57
1:G:9:SER:OG	1:G:83:PRO:HA	2.04	0.57
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.85	0.57
1:G:769:ASP:CG	1:G:874:LEU:HD12	2.30	0.57
1:C:906:LEU:HD13	1:C:1030:ARG:CD	2.34	0.57
2:H:244:ASP:OD1	2:H:245:PRO:HD2	2.05	0.57
1:A:740:THR:HG22	1:A:741:ALA:N	2.20	0.57
1:G:166:CYS:C	1:G:167:ILE:HD12	2.29	0.57
2:H:228:VAL:HA	2:H:231:MET:CE	2.35	0.57
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.87	0.57
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.85	0.57
2:B:324:ASN:O	2:B:342:ARG:HD2	2.05	0.57
1:E:153:GLU:HB3	11:E:5512:HOH:O	2.05	0.57
1:G:591:GLU:O	1:G:591:GLU:HG3	2.04	0.57
1:G:679:GLN:HG2	1:G:683:GLU:OE1	2.04	0.57
1:G:708:ILE:CG2	1:G:754:HIS:HB2	2.28	0.57
1:G:490:ARG:HD3	11:G:5750:HOH:O	2.04	0.57
1:G:716:PRO:HA	1:G:750:VAL:HG22	1.85	0.57
1:E:726:GLU:HG2	1:E:727:ILE:N	2.19	0.57
2:H:232:ASN:N	2:H:233:PRO:HD3	2.19	0.57
2:H:342:ARG:NH2	2:H:344:ASP:OD2	2.37	0.57
1:A:51:PRO:HG3	1:A:918:MET:HB2	1.86	0.56
1:E:1:MET:CA	1:E:224:LYS:HZ1	2.18	0.56
1:G:118:ALA:HA	11:G:5712:HOH:O	2.05	0.56
1:G:998:ARG:HB3	1:G:999:PRO:HA	1.87	0.56
1:G:704:LYS:O	1:G:708:ILE:HD12	2.05	0.56
1:C:51:PRO:HG3	1:C:918:MET:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ILE:H	1:C:698:ILE:CD1	2.18	0.56
2:F:157:ASP:OD2	11:F:3087:HOH:O	2.17	0.56
2:F:164:THR:O	2:F:220:PRO:HG3	2.06	0.56
2:F:215:ARG:HG3	2:F:215:ARG:NH1	2.18	0.56
2:D:71:GLU:O	2:D:203:ARG:HG3	2.05	0.56
2:H:286:MET:N	2:H:313:GLY:O	2.27	0.56
1:A:412:LYS:HG2	1:A:438:TYR:CZ	2.41	0.56
1:G:185:ARG:NH2	11:G:5523:HOH:O	2.38	0.56
1:E:644:GLY:O	1:E:647:PRO:HD2	2.06	0.56
1:G:548:GLU:HG2	2:H:114:ASP:CG	2.30	0.56
1:G:682:VAL:HG11	1:G:689:GLN:HE21	1.71	0.56
1:A:651:ALA:HB3	11:A:5560:HOH:O	2.05	0.56
1:A:954:LYS:O	1:A:957:VAL:HG12	2.06	0.56
1:C:525:VAL:HB	1:C:551:CYS:HA	1.87	0.56
1:C:757:ASP:O	1:C:833:LYS:HE3	2.05	0.56
1:G:79:GLU:O	1:G:82:ARG:NE	2.38	0.56
1:G:267:ALA:O	1:G:271:VAL:HG23	2.05	0.56
1:G:410:ASP:OD1	1:G:501:ARG:NH1	2.39	0.56
1:C:481:ILE:O	1:C:481:ILE:HG13	2.06	0.56
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.06	0.56
2:H:206:LEU:O	2:H:210:VAL:HG23	2.06	0.56
1:C:548:GLU:OE2	2:D:114:ASP:HA	2.06	0.56
1:E:716:PRO:HA	1:E:750:VAL:HG22	1.87	0.56
1:A:1:MET:HB3	1:A:224:LYS:HE3	1.87	0.56
1:C:9:SER:OG	1:C:83:PRO:HA	2.06	0.56
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.86	0.56
1:C:954:LYS:O	1:C:957:VAL:HG12	2.06	0.56
1:E:82[B]:ARG:HE	1:E:111:PHE:HD1	1.52	0.56
1:E:228:CYS:SG	1:E:269:MET:HE2	2.46	0.56
1:C:349:GLU:O	2:D:294:ASN:HB2	2.06	0.55
1:C:494:ARG:HG3	1:C:547:TYR:HB3	1.88	0.55
1:C:967:GLN:HG3	1:C:1054:LEU:CD1	2.33	0.55
1:G:559:ARG:HD2	1:G:595:GLU:HB2	1.89	0.55
1:G:698:ILE:HD12	1:G:698:ILE:N	2.20	0.55
2:H:322:PRO:HD2	2:H:325:LEU:HD12	1.89	0.55
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.36	0.55
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.31	0.55
1:A:514:ARG:HD3	11:A:5539:HOH:O	2.06	0.55
2:B:45:ASP:HB3	2:B:48:TYR:CD2	2.41	0.55
1:G:850:VAL:O	1:G:854:SER:N	2.37	0.55
1:A:970:GLU:O	1:A:971:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ASP:HB3	2:B:304:VAL:CG2	2.37	0.55
1:C:630:VAL:HG11	1:C:659:VAL:HG22	1.87	0.55
1:E:38:ARG:HG2	11:E:5462:HOH:O	2.06	0.55
1:E:998:ARG:HA	1:E:999:PRO:C	2.26	0.55
1:G:28:TYR:CE1	1:G:313:LYS:HE3	2.41	0.55
1:G:907:LEU:HD11	8:G:5071:ORN:HD3	1.89	0.55
2:B:185:LYS:NZ	11:B:5146:HOH:O	2.39	0.55
2:B:290:HIS:NE2	2:B:334:ASP:OD2	2.36	0.55
1:E:1020:ARG:HH21	1:E:1023:ILE:CG2	2.19	0.55
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.88	0.55
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.88	0.55
2:F:286:MET:HE2	2:F:314:PHE:C	2.31	0.55
1:A:184:ASN:OD1	1:A:187:GLU:HG3	2.07	0.55
1:C:845:ARG:HG3	1:C:845:ARG:NH1	2.21	0.55
1:G:436:ILE:HG22	11:G:5277:HOH:O	2.07	0.55
1:G:554:ASN:ND2	8:G:5074:ORN:HD3	2.12	0.55
1:E:336:MET:HB3	1:E:342:GLY:HA2	1.88	0.55
2:F:41:GLU:HB3	2:F:358:PRO:HD3	1.88	0.55
1:G:417:ASP:OD1	1:G:418:PRO:HD2	2.06	0.55
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.37	0.55
2:H:252:ILE:HD13	2:H:277:LEU:HB3	1.89	0.55
2:F:173:GLY:C	2:F:207:ARG:HG2	2.32	0.54
1:G:10:ILE:HD12	1:G:42:TYR:HB3	1.89	0.54
1:G:135:ALA:HB1	1:G:274:GLU:CG	2.37	0.54
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.88	0.54
2:H:265:VAL:HG12	2:H:347:ALA:HA	1.89	0.54
1:A:730:ASP:OD1	1:A:733:ASP:HB2	2.07	0.54
2:B:286:MET:CE	2:B:315:ALA:HB2	2.34	0.54
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.07	0.54
1:E:228:CYS:O	1:E:269:MET:HE1	2.07	0.54
1:G:153:GLU:HB3	11:G:5520:HOH:O	2.05	0.54
1:A:646:THR:HB	1:A:647:PRO:HD3	1.89	0.54
1:C:1027:ARG:HD3	1:C:1031:ARG:HD3	1.88	0.54
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.88	0.54
1:A:702:VAL:CG1	1:A:731:GLU:HG3	2.37	0.54
2:B:228:VAL:O	2:B:231:MET:HB2	2.07	0.54
2:F:251:ALA:O	2:F:255:ILE:HD12	2.07	0.54
1:G:1026:SER:O	1:G:1029:ILE:HG22	2.07	0.54
2:H:345:LYS:HB3	2:H:346:PRO:HD2	1.88	0.54
1:A:343:ARG:NH2	1:A:539:ASP:OD2	2.40	0.54
1:C:490:ARG:HG3	1:C:522:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:GLU:O	1:E:422:THR:HB	2.07	0.54
1:G:32:GLN:OE1	1:G:320:ALA:HB3	2.08	0.54
1:G:710:TYR:OH	1:G:731:GLU:HA	2.08	0.54
2:H:259:LEU:HD22	2:H:342:ARG:NH1	2.22	0.54
1:A:367:PHE:HB3	1:A:903:VAL:HG21	1.88	0.54
2:D:44:THR:HG21	2:D:70:GLU:HG2	1.89	0.54
1:E:559[A]:ARG:NH1	11:E:5624:HOH:O	2.37	0.54
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.26	0.54
1:A:45:ILE:HD13	1:A:81:GLU:HB3	1.90	0.54
1:A:75:ARG:HD2	1:A:107:VAL:HG22	1.90	0.54
1:A:315:THR:O	1:A:531:THR:HG22	2.08	0.54
1:A:764:VAL:HG11	1:A:813:VAL:HG21	1.88	0.54
1:A:955:GLU:HB2	11:A:5594:HOH:O	2.07	0.54
1:C:1000:HIS:CD2	1:C:1002:GLN:HB3	2.43	0.54
1:G:259:LYS:HE2	2:H:69:ASP:OD1	2.07	0.54
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.42	0.54
2:H:46:PRO:HD3	2:H:72:SER:HB3	1.90	0.54
2:H:321:LEU:CD2	2:H:325:LEU:HB3	2.37	0.54
1:A:143:THR:HA	1:A:296:ILE:HG23	1.89	0.54
1:A:186:GLU:HB2	11:A:5469:HOH:O	2.08	0.54
1:A:637:GLY:HA2	1:A:660:PRO:O	2.08	0.54
1:E:561:LYS:HB2	1:E:635:PRO:HA	1.89	0.54
2:F:324:ASN:O	2:F:342:ARG:HD2	2.07	0.54
1:A:906:LEU:O	1:A:912:ARG:NH2	2.30	0.54
1:C:104:ARG:HG3	1:C:104:ARG:HH11	1.73	0.54
2:H:364:ALA:N	2:H:365:PRO:HD2	2.23	0.54
1:A:554:ASN:HD22	8:A:5014:ORN:CD	2.05	0.53
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.42	0.53
1:E:907:LEU:HD11	8:E:5051:ORN:HD3	1.89	0.53
8:E:5051:ORN:HB3	11:E:5697:HOH:O	2.07	0.53
1:G:559:ARG:HH12	1:G:614:ASP:CG	2.16	0.53
1:G:782:ILE:N	1:G:782:ILE:HD12	2.21	0.53
1:G:1027:ARG:HH11	1:G:1027:ARG:HG2	1.73	0.53
1:C:4:ARG:CD	1:C:7:ILE:HD12	2.37	0.53
1:E:648:LEU:HD13	1:E:845:ARG:HD3	1.91	0.53
2:F:342:ARG:NE	2:F:344:ASP:OD1	2.39	0.53
1:G:712:LEU:HD12	1:G:754:HIS:HA	1.90	0.53
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.90	0.53
1:C:920:VAL:O	1:C:930:LYS:HD3	2.08	0.53
1:E:554:ASN:HD22	8:E:5054:ORN:CD	2.22	0.53
1:G:58:PRO:HA	1:G:1066:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:266:PHE:CD2	2:H:370:PHE:CD2	2.97	0.53
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.39	0.53
2:B:324:ASN:HD22	2:B:325:LEU:N	2.06	0.53
1:C:282:SER:OG	1:C:302:PRO:HA	2.09	0.53
1:C:421:LEU:HD22	1:G:421:LEU:HD13	1.90	0.53
1:C:699:GLU:HA	1:C:702:VAL:HG23	1.91	0.53
1:E:59:GLU:OE2	1:E:60:MET:HE2	2.09	0.53
1:G:852:PHE:CE1	1:G:918:MET:HE3	2.44	0.53
1:G:863:LYS:HE2	11:G:5696:HOH:O	2.07	0.53
2:H:173:GLY:C	2:H:207:ARG:HG2	2.33	0.53
1:A:146:SER:HB2	1:A:205:LEU:HD11	1.91	0.53
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.43	0.53
1:E:358:LYS:HG2	1:E:359:ILE:N	2.22	0.53
2:F:41:GLU:HB2	2:F:358:PRO:HG3	1.90	0.53
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.89	0.53
1:E:313:LYS:HE2	1:E:608:THR:C	2.33	0.53
1:G:103:GLU:HB2	1:G:108:LEU:HD12	1.90	0.53
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.09	0.53
2:H:355:GLU:OE1	2:H:355:GLU:N	2.33	0.53
1:A:868:VAL:HA	1:A:872:LYS:O	2.08	0.53
2:B:226:GLU:O	2:B:230:LYS:HG3	2.09	0.53
1:C:419:GLU:O	1:C:422:THR:HG22	2.08	0.53
1:C:941:LYS:NZ	1:C:1056:ALA:O	2.33	0.53
2:D:174:SER:O	2:D:182:PRO:HD3	2.08	0.53
1:E:509:ARG:HH11	1:E:512:GLU:HG3	1.73	0.53
2:B:71:GLU:C	2:B:203:ARG:HG3	2.33	0.53
1:C:213:TRP:CZ3	1:C:296:ILE:HD12	2.43	0.53
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.09	0.53
1:E:343:ARG:NH1	1:E:539:ASP:OD2	2.37	0.53
1:G:308:SER:HB3	11:G:5484:HOH:O	2.08	0.53
1:G:698:ILE:O	1:G:701:ALA:HB3	2.08	0.53
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.31	0.53
1:C:104:ARG:NH2	11:C:5648:HOH:O	2.35	0.53
1:G:53:THR:O	1:G:855:LYS:NZ	2.42	0.53
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.43	0.53
1:A:1:MET:H2	1:A:2:PRO:CD	2.22	0.52
1:A:167:ILE:HD12	1:A:167:ILE:N	2.24	0.52
1:A:275:ILE:HD13	1:A:275:ILE:N	2.23	0.52
2:B:244:ASP:OD1	2:B:245:PRO:HD2	2.09	0.52
1:E:772:MET:HA	1:E:818:PHE:HZ	1.74	0.52
1:G:344:THR:OG1	11:G:5810:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:805:ILE:O	1:G:808:VAL:N	2.42	0.52
2:H:228:VAL:HG12	2:H:229:LEU:N	2.15	0.52
2:H:274:LEU:O	2:H:277:LEU:N	2.39	0.52
1:A:1:MET:N	1:A:2:PRO:HD3	2.24	0.52
1:A:585:ALA:HB2	1:A:642:TYR:CE2	2.43	0.52
2:B:73:SER:HA	2:B:203:ARG:NH2	2.24	0.52
2:B:337:LEU:HD12	2:B:338:GLN:N	2.25	0.52
1:C:115:MET:HE1	1:C:120:ALA:HB2	1.91	0.52
1:C:822:VAL:O	1:C:823:ARG:HD3	2.10	0.52
1:E:335:LEU:O	1:E:336:MET:HE2	2.08	0.52
2:F:173:GLY:O	2:F:207:ARG:HG2	2.08	0.52
2:F:286:MET:HE2	2:F:314:PHE:O	2.09	0.52
1:G:135:ALA:HB1	1:G:274:GLU:HG2	1.90	0.52
1:A:712:LEU:O	1:A:727:ILE:HA	2.09	0.52
2:F:186:LYS:HB3	2:F:188:ASP:OD1	2.09	0.52
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.92	0.52
2:H:224:SER:C	2:H:226:GLU:H	2.16	0.52
1:A:939:MET:HE2	1:A:1050:THR:CG2	2.40	0.52
2:D:225:ALA:O	2:D:228:VAL:HB	2.10	0.52
2:D:277:LEU:CD2	2:D:283:THR:HG23	2.35	0.52
1:C:907:LEU:HD11	8:C:5031:ORN:HD3	1.92	0.52
2:D:173:GLY:C	2:D:207:ARG:HG2	2.35	0.52
2:F:299:ASP:O	2:F:303:ASN:N	2.42	0.52
2:F:318:GLU:HA	2:F:321:LEU:HD13	1.91	0.52
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.44	0.52
1:G:679:GLN:O	1:G:682:VAL:HB	2.09	0.52
1:G:833:LYS:O	1:G:834:ASN:HB2	2.08	0.52
2:H:257:LYS:O	2:H:260:GLU:HB2	2.09	0.52
2:H:342:ARG:CB	2:H:347:ALA:HB3	2.37	0.52
1:A:446:GLY:O	1:E:447:LEU:HD23	2.10	0.52
1:A:680:HIS:HB3	11:A:5749:HOH:O	2.09	0.52
1:G:929:ALA:HB2	1:G:1053:ALA:HB1	1.90	0.52
2:D:259:LEU:HD13	2:D:342:ARG:NH1	2.25	0.52
2:F:232:ASN:N	2:F:233:PRO:HD3	2.25	0.52
1:A:849:THR:O	1:A:853:VAL:HG23	2.10	0.52
1:A:907:LEU:HD11	8:A:5011:ORN:HD3	1.92	0.52
2:B:71:GLU:OE2	2:B:357:SER:OG	2.27	0.52
1:E:571:ARG:NH2	1:E:645[B]:GLN:HE21	1.98	0.52
2:F:364:ALA:O	2:F:367:PHE:HB2	2.09	0.52
1:G:436:ILE:HG23	1:G:437:TRP:CE3	2.45	0.52
1:G:796:LEU:C	1:G:796:LEU:HD23	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:290:HIS:ND1	2:H:312:HIS:NE2	2.57	0.52
1:A:420:ALA:HA	1:A:423:LYS:HD2	1.92	0.52
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.91	0.52
2:F:144:LEU:O	2:F:148:ARG:HB2	2.10	0.52
2:H:259:LEU:HD22	2:H:342:ARG:HH12	1.75	0.52
2:H:295:HIS:O	2:H:308:THR:N	2.39	0.52
1:A:708:ILE:HG23	1:A:754:HIS:HB2	1.91	0.52
1:E:799:TYR:HD1	1:E:799:TYR:H	1.57	0.52
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.58	0.52
2:F:285:LYS:NZ	11:F:3075:HOH:O	2.43	0.52
1:G:634:LYS:N	1:G:635:PRO:HD3	2.25	0.52
1:G:863:LYS:O	1:G:867:ARG:HG3	2.09	0.52
1:G:939:MET:HE2	1:G:1050:THR:HG22	1.92	0.52
1:A:708:ILE:HG22	1:A:754:HIS:HB2	1.91	0.51
2:B:286:MET:SD	2:B:289:GLY:HA2	2.50	0.51
1:C:648:LEU:HD13	1:C:845:ARG:HD2	1.92	0.51
1:C:1001:ILE:HG13	1:C:1002:GLN:H	1.75	0.51
1:E:554:ASN:N	1:E:555:PRO:HD3	2.25	0.51
1:E:680:HIS:HB3	11:E:5910:HOH:O	2.09	0.51
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.92	0.51
1:A:1:MET:HB3	1:A:224:LYS:HE2	1.92	0.51
1:E:698:ILE:CD1	1:E:698:ILE:N	2.74	0.51
1:G:230:ILE:H	1:G:349:GLU:HG2	1.75	0.51
1:C:331:THR:OG1	1:C:334:GLU:OE2	2.29	0.51
1:C:560:GLU:OE2	1:C:636:LYS:NZ	2.30	0.51
1:A:493:LYS:HE2	1:A:517:ARG:HD3	1.93	0.51
1:C:946:LEU:C	1:C:947:LEU:HD12	2.36	0.51
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.40	0.51
1:E:669:ILE:HA	1:E:844:PRO:HG2	1.93	0.51
1:G:1001:ILE:O	1:G:1005:ILE:HG13	2.11	0.51
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.92	0.51
1:A:682:VAL:HG21	1:A:689:GLN:NE2	2.25	0.51
1:A:698:ILE:N	1:A:698:ILE:HD12	2.25	0.51
1:C:209:SER:OG	1:C:211:ILE:HG13	2.10	0.51
1:C:805:ILE:CD1	1:C:837:VAL:HG23	2.40	0.51
1:E:82[B]:ARG:NE	1:E:111:PHE:CD1	2.78	0.51
1:G:58:PRO:HA	1:G:1066:GLN:HE21	1.75	0.51
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.92	0.51
2:H:60:ILE:HB	2:H:82:ILE:CD1	2.40	0.51
1:E:213:TRP:CZ3	1:E:289:ASN:HB2	2.46	0.51
1:E:784:GLN:NE2	1:E:784:GLN:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1001:ILE:HD12	1:E:1029:ILE:HB	1.90	0.51
2:F:135:GLY:O	2:F:138:PRO:HD3	2.10	0.51
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.40	0.51
1:G:692:ASN:HD22	1:G:692:ASN:N	2.08	0.51
1:G:796:LEU:HD23	1:G:797:PRO:N	2.26	0.51
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.40	0.51
1:A:941:LYS:HG2	1:A:1054:LEU:HD22	1.92	0.51
1:G:643:GLY:HA3	1:G:647:PRO:HG3	1.93	0.51
1:E:24:CYS:HB2	1:E:604:GLU:HB3	1.93	0.51
1:E:101:GLU:OE1	1:E:104:ARG:NH2	2.38	0.51
1:E:755:PHE:CE1	7:E:5047:ADP:C2	2.99	0.51
2:F:350:PHE:CG	2:F:366:LEU:HD21	2.46	0.51
1:G:828:VAL:CG1	1:G:839:LEU:HD11	2.40	0.51
1:A:10:ILE:CD1	1:A:42:TYR:HB3	2.41	0.51
1:A:10:ILE:HD12	1:A:42:TYR:HB3	1.93	0.51
1:A:692:ASN:N	1:A:692:ASN:ND2	2.59	0.51
1:C:734:LEU:O	1:C:734:LEU:HD12	2.11	0.51
1:C:878:GLY:HA2	11:C:5590:HOH:O	2.10	0.51
1:E:470:VAL:O	1:E:474:GLU:HG3	2.11	0.51
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.46	0.51
1:G:830:PHE:CE1	1:G:839:LEU:HD13	2.46	0.51
2:H:202:LYS:NZ	2:H:356:ALA:O	2.40	0.51
2:B:191:PRO:HD2	2:B:213:GLY:O	2.11	0.51
1:G:667:ASP:O	1:G:677:ARG:NH2	2.44	0.51
1:A:89:THR:O	1:A:304:VAL:HG22	2.12	0.50
1:A:164:PHE:HB3	1:A:165:PRO:HA	1.92	0.50
1:A:710:TYR:CD2	1:A:712:LEU:HD13	2.46	0.50
1:C:959:ASP:O	1:C:963:LYS:HG3	2.11	0.50
1:C:986:ILE:O	1:C:988:PRO:HD3	2.12	0.50
2:F:259:LEU:O	2:F:345:LYS:HE3	2.11	0.50
1:G:699:GLU:HA	1:G:702:VAL:HG23	1.93	0.50
1:A:737:TYR:O	1:A:740:THR:HB	2.11	0.50
1:A:804:GLU:HB3	11:A:5774:HOH:O	2.10	0.50
1:A:918:MET:HE2	1:A:920:VAL:HG22	1.94	0.50
1:C:464:VAL:HG21	2:D:88:ILE:HG12	1.92	0.50
1:E:493:LYS:HE2	1:E:517:ARG:HD3	1.91	0.50
1:G:158:VAL:O	1:G:161:ASP:HB3	2.10	0.50
1:G:692:ASN:HD22	1:G:692:ASN:H	1.60	0.50
1:G:698:ILE:H	1:G:698:ILE:CD1	2.24	0.50
1:A:75:ARG:HG2	1:A:75:ARG:HH11	1.75	0.50
1:A:659:VAL:CG1	1:A:660:PRO:HD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ILE:HG22	2:B:138:PRO:HB3	1.93	0.50
1:E:514:ARG:HD3	11:E:5606:HOH:O	2.10	0.50
2:H:46:PRO:HA	2:H:76:HIS:CG	2.46	0.50
1:A:132:PHE:O	1:A:136:MET:HG2	2.11	0.50
1:A:665:SER:O	1:A:669:ILE:HG13	2.12	0.50
2:B:26:ALA:O	2:B:131:CYS:HA	2.11	0.50
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.46	0.50
1:E:1:MET:O	1:E:334:GLU:OE2	2.29	0.50
1:G:349:GLU:O	2:H:294:ASN:HB2	2.11	0.50
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.93	0.50
1:G:710:TYR:HA	1:G:711:PRO:C	2.37	0.50
1:G:755:PHE:CE1	7:G:5067:ADP:C2	2.99	0.50
1:G:868:VAL:HA	1:G:872:LYS:O	2.11	0.50
1:A:561:LYS:HE3	11:A:5830:HOH:O	2.10	0.50
1:A:563:MET:SD	1:A:635:PRO:HG3	2.52	0.50
1:A:671:ARG:NH2	1:A:819:GLU:O	2.45	0.50
2:B:192:PHE:O	2:B:215[A]:ARG:HG2	2.10	0.50
1:E:523:HIS:HB2	11:E:5996:HOH:O	2.12	0.50
1:E:863:LYS:O	1:E:867:ARG:HG3	2.11	0.50
2:F:272:HIS:HA	2:F:349:SER:CB	2.41	0.50
2:H:255:ILE:HA	2:H:258:PHE:CD2	2.47	0.50
1:A:755:PHE:CE1	7:A:5007:ADP:C2	3.00	0.50
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.50
1:E:18:ILE:HD12	1:E:23:ALA:HA	1.93	0.50
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.41	0.50
1:G:470:VAL:O	1:G:474:GLU:HG3	2.12	0.50
1:G:692:ASN:H	1:G:692:ASN:ND2	2.10	0.50
1:G:845:ARG:NH1	1:G:846:ALA:O	2.44	0.50
1:A:344:THR:HB	1:A:345:PRO:HD2	1.92	0.50
1:A:813:VAL:HG22	1:A:828:VAL:HG21	1.93	0.50
2:D:215:ARG:HG3	2:D:215:ARG:NH1	2.25	0.50
1:E:945:ALA:HA	1:E:1012:TYR:O	2.11	0.50
2:F:45:ASP:HB3	2:F:48:TYR:HD2	1.77	0.50
1:G:339:ILE:HG22	1:G:540:THR:OG1	2.12	0.50
1:G:812:GLN:O	1:G:816:LEU:HD12	2.11	0.50
1:E:150:HIS:HB2	11:E:5507:HOH:O	2.11	0.50
2:F:273:GLN:HE21	2:F:351:GLN:HE22	1.59	0.50
1:A:150:HIS:NE2	1:A:203:GLU:HG3	2.26	0.50
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.94	0.50
1:A:348:PHE:HB3	2:B:296:PRO:HG3	1.94	0.50
1:A:412:LYS:HG2	1:A:438:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:SER:O	1:A:1015:ASN:HA	2.11	0.50
1:C:64:THR:O	1:C:1065:VAL:HG23	2.11	0.50
2:D:328:THR:HG21	2:D:341:HIS:HB2	1.93	0.50
2:H:123:ARG:HA	2:H:288:PHE:CE2	2.47	0.50
2:H:281:ALA:C	2:H:282:LYS:HG2	2.37	0.50
2:H:290:HIS:HB3	2:H:310:GLN:CB	2.42	0.50
1:A:548:GLU:HG2	2:B:114:ASP:CG	2.37	0.49
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.93	0.49
1:C:152:MET:HG3	1:C:152:MET:O	2.10	0.49
1:E:814:GLN:NE2	11:E:5378:HOH:O	2.45	0.49
1:G:672:ALA:HB3	1:G:844:PRO:HG3	1.92	0.49
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.47	0.49
2:H:277:LEU:HD23	2:H:281:ALA:O	2.12	0.49
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.42	0.49
1:A:698:ILE:CD1	1:A:698:ILE:H	2.24	0.49
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.12	0.49
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.93	0.49
1:G:68:PRO:HB3	1:G:934:GLY:CA	2.41	0.49
1:G:427:GLU:HG3	1:G:438:TYR:CE2	2.47	0.49
2:H:162:VAL:HG23	2:H:200:GLY:HA3	1.95	0.49
2:H:348:PHE:HZ	2:H:370:PHE:HB2	1.77	0.49
1:A:423:LYS:NZ	11:A:5823:HOH:O	2.45	0.49
2:B:228:VAL:HA	2:B:231:MET:CE	2.40	0.49
1:E:759:ALA:O	1:E:784:GLN:HB2	2.12	0.49
1:A:679:GLN:HA	1:A:689:GLN:HE22	1.77	0.49
1:C:554:ASN:N	1:C:555:PRO:HD3	2.27	0.49
2:D:173:GLY:O	2:D:207:ARG:HG2	2.13	0.49
2:D:185:LYS:HE2	2:D:189:GLU:HB3	1.95	0.49
1:E:18:ILE:HD12	1:E:23:ALA:C	2.37	0.49
1:E:796:LEU:C	1:E:796:LEU:HD23	2.38	0.49
1:G:939:MET:HE2	1:G:1050:THR:HG21	1.92	0.49
2:H:23:THR:HG22	2:H:24:GLY:N	2.27	0.49
2:H:290:HIS:HB3	2:H:310:GLN:HB3	1.95	0.49
1:A:285:GLN:HB3	11:A:5606:HOH:O	2.12	0.49
2:B:337:LEU:HD12	2:B:338:GLN:H	1.78	0.49
1:C:89:THR:O	1:C:304:VAL:HG22	2.13	0.49
1:C:103:GLU:HB2	1:C:108:LEU:HD12	1.93	0.49
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.76	0.49
1:E:509:ARG:HH11	1:E:512:GLU:CG	2.25	0.49
1:E:715:ARG:HB2	1:E:751:LEU:HB2	1.94	0.49
2:F:223:THR:HG22	2:F:228:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:ALA:O	2:H:163:THR:HB	2.13	0.49
2:B:236:ILE:HD13	2:B:258:PHE:CE1	2.48	0.49
1:C:220:VAL:HG12	1:C:221:VAL:N	2.26	0.49
1:C:734:LEU:HD12	1:C:734:LEU:C	2.36	0.49
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.12	0.49
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.93	0.49
1:C:554:ASN:OD1	8:C:5034:ORN:HD3	2.12	0.49
2:F:300:VAL:HG22	2:F:328:THR:C	2.37	0.49
1:G:563:MET:HE1	1:G:635:PRO:HG3	1.95	0.49
2:H:142:LEU:HD12	2:H:142:LEU:C	2.36	0.49
2:H:266:PHE:HB2	2:H:370:PHE:CE1	2.47	0.49
2:H:305:VAL:HG12	2:H:306:MET:N	2.28	0.49
2:H:342:ARG:CG	2:H:347:ALA:HB3	2.43	0.49
2:B:7:LEU:HD23	2:B:15:PHE:CD1	2.47	0.49
1:C:265:ARG:NH1	2:D:360:PRO:HB3	2.28	0.49
1:C:490:ARG:CZ	1:C:490:ARG:HB3	2.28	0.49
2:D:199:PHE:HB3	2:D:270:LEU:HD23	1.95	0.49
1:E:49:SER:O	1:E:51:PRO:HD3	2.13	0.49
1:E:426:ARG:C	1:E:426:ARG:HD3	2.37	0.49
1:E:652[B]:ARG:NH2	11:E:5846:HOH:O	2.45	0.49
1:E:1001:ILE:HD13	1:E:1029:ILE:HB	1.92	0.49
1:G:148:ILE:HD13	1:G:204:LEU:O	2.12	0.49
1:G:755:PHE:CD1	7:G:5067:ADP:C2	3.00	0.49
2:H:172:GLN:O	2:H:207:ARG:HA	2.12	0.49
2:H:228:VAL:HG11	2:H:258:PHE:HE1	1.74	0.49
2:H:342:ARG:NE	2:H:344:ASP:OD1	2.46	0.49
1:C:637:GLY:HA2	1:C:660:PRO:O	2.12	0.49
1:C:676:GLU:O	1:C:680:HIS:HB2	2.12	0.49
1:C:1003:ASP:O	1:C:1007:ASN:ND2	2.45	0.49
1:E:420:ALA:HA	1:E:423:LYS:HG3	1.95	0.49
1:E:799:TYR:CD2	1:E:800:THR:HG23	2.48	0.49
1:G:5:THR:O	1:G:8:LYS:NZ	2.41	0.49
2:H:334:ASP:CG	2:H:336:THR:HG23	2.37	0.49
1:C:1:MET:HA	1:C:224:LYS:NZ	2.28	0.49
1:C:40:GLU:HA	1:C:40:GLU:OE1	2.12	0.49
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.95	0.49
1:E:677:ARG:O	1:E:680:HIS:HB2	2.12	0.49
2:F:286:MET:HE3	2:F:313:GLY:C	2.37	0.49
1:G:534:ALA:O	2:H:123:ARG:NH1	2.43	0.49
1:G:780:GLU:OE1	1:G:798:ALA:HB1	2.13	0.49
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1021:ARG:HD2	1:G:1025:ASP:OD2	2.12	0.49
2:H:286:MET:HE1	2:H:312:HIS:CE1	2.48	0.49
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.94	0.48
1:A:1027:ARG:O	1:A:1031:ARG:HG3	2.13	0.48
1:C:770:GLY:HA2	1:C:823:ARG:NH1	2.28	0.48
2:D:298:LYS:CB	2:D:332:LEU:HD11	2.42	0.48
2:D:321:LEU:HG	2:D:325:LEU:HB3	1.95	0.48
1:G:579:ASP:OD2	1:G:605:THR:HB	2.13	0.48
2:H:48:TYR:CE2	2:H:311:ASN:ND2	2.82	0.48
2:H:71:GLU:C	2:H:203:ARG:HG3	2.37	0.48
2:H:327:VAL:HG13	2:H:337:LEU:HD11	1.95	0.48
1:A:70:HIS:ND1	1:A:72:GLU:HB2	2.28	0.48
1:A:636:LYS:HE3	11:A:5551:HOH:O	2.13	0.48
2:D:190:LEU:HB2	2:D:215:ARG:HB3	1.96	0.48
1:E:941[B]:LYS:HE3	1:E:1054:LEU:O	2.13	0.48
1:G:198:LEU:O	1:G:200:PRO:HD3	2.13	0.48
1:G:370:ALA:HB2	1:G:900:PHE:HB3	1.96	0.48
1:C:66:ILE:HG21	1:C:918:MET:HB3	1.95	0.48
1:C:361:ARG:CZ	1:C:571:ARG:HG2	2.43	0.48
1:C:708:ILE:HG23	1:C:754:HIS:HB2	1.96	0.48
2:H:263:ILE:HG12	2:H:377:TYR:CZ	2.48	0.48
2:F:86:PRO:HA	11:F:2588:HOH:O	2.13	0.48
1:G:73:VAL:O	1:G:77:ILE:HG13	2.13	0.48
2:H:255:ILE:HG22	2:H:278:ALA:CB	2.42	0.48
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.40	0.48
1:G:659:VAL:O	1:G:661:VAL:HG23	2.13	0.48
1:C:250:VAL:HA	1:C:356:VAL:O	2.14	0.48
1:C:288:VAL:O	1:C:290:PRO:HD3	2.14	0.48
1:C:975:HIS:O	1:C:979:ILE:HG12	2.13	0.48
1:E:9:SER:OG	1:E:83:PRO:HA	2.13	0.48
2:F:85:LEU:HD12	2:F:86:PRO:HD2	1.95	0.48
1:G:768:CYS:HB3	1:G:822:VAL:HG12	1.96	0.48
1:A:851:PRO:O	1:A:854:SER:HB2	2.13	0.48
2:B:222:GLN:H	2:B:222:GLN:HE21	1.61	0.48
1:C:225:ASN:ND2	1:C:331:THR:HG21	2.28	0.48
1:C:780:GLU:OE1	1:C:799:TYR:N	2.46	0.48
1:E:349:GLU:O	2:F:294:ASN:HB2	2.14	0.48
1:E:667:ASP:O	1:E:677:ARG:NH2	2.46	0.48
2:F:98:LEU:O	2:F:101:TYR:HB3	2.13	0.48
1:G:688:LYS:NZ	1:G:836:GLU:OE1	2.44	0.48
1:A:1:MET:N	1:A:2:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:MET:HA	1:A:818:PHE:HZ	1.78	0.48
2:B:364:ALA:N	2:B:365:PRO:HD2	2.29	0.48
1:C:257:THR:HG22	2:D:63:VAL:HG21	1.96	0.48
1:E:809:MET:O	1:E:813:VAL:HG23	2.12	0.48
1:E:1028:VAL:O	1:E:1032:SER:HB2	2.14	0.48
2:F:379:LYS:HB3	2:F:379:LYS:HE2	1.46	0.48
1:G:64:THR:CB	1:G:1066:GLN:HE22	2.25	0.48
2:B:218:ILE:HG22	2:B:219:VAL:N	2.28	0.48
2:D:206:LEU:O	2:D:210:VAL:HG23	2.13	0.48
2:D:246:ALA:HB3	2:D:247:PRO:HD3	1.96	0.48
1:E:1:MET:C	1:E:224:LYS:HZ1	2.21	0.48
1:A:107:VAL:O	1:A:110:GLU:HB2	2.14	0.48
1:C:101:GLU:O	1:C:105:GLN:HG2	2.13	0.48
1:C:992:ASN:O	1:C:1000:HIS:HA	2.14	0.48
2:D:225:ALA:O	2:D:229:LEU:HG	2.14	0.48
2:D:295:HIS:CE1	2:D:333:PHE:HD2	2.31	0.48
1:G:964:LEU:O	1:G:969:PHE:HB2	2.14	0.48
2:H:8:VAL:HG22	2:H:14:GLN:HG2	1.96	0.48
2:H:194:VAL:O	2:H:216:LEU:HA	2.13	0.48
1:A:464:VAL:HG21	2:B:88:ILE:HG12	1.96	0.47
2:B:252:ILE:HD13	2:B:277:LEU:HB3	1.95	0.47
1:C:868:VAL:HA	1:C:872:LYS:O	2.14	0.47
1:E:946:LEU:C	1:E:947:LEU:HD12	2.39	0.47
1:E:1063:ILE:HG12	1:E:1064:SER:N	2.27	0.47
2:F:332:LEU:HD12	2:F:332:LEU:HA	1.65	0.47
1:G:68:PRO:HB3	1:G:934:GLY:HA2	1.96	0.47
2:H:228:VAL:HA	2:H:231:MET:HE3	1.94	0.47
1:A:692:ASN:N	1:A:692:ASN:HD22	2.13	0.47
2:D:369:HIS:O	2:D:373:LEU:HG	2.14	0.47
1:E:164:PHE:HB3	1:E:165:PRO:HA	1.96	0.47
1:G:552:GLU:OE2	2:H:116:ARG:NE	2.36	0.47
2:H:286:MET:SD	2:H:289:GLY:HA2	2.54	0.47
2:H:343:THR:OG1	2:H:344:ASP:N	2.46	0.47
1:A:43:ARG:NH1	11:A:5640:HOH:O	2.46	0.47
1:A:738:PHE:HZ	1:A:750:VAL:HG11	1.80	0.47
2:B:261:THR:CG2	2:B:262:ASP:N	2.78	0.47
2:B:325:LEU:HD23	2:B:325:LEU:HA	1.77	0.47
1:C:229:ILE:HG13	1:C:229:ILE:O	2.14	0.47
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.95	0.47
1:G:93:GLN:HG2	5:G:5076:CL:CL	2.51	0.47
1:G:676:GLU:O	1:G:680:HIS:ND1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.31	0.47
1:A:45:ILE:HD13	1:A:81:GLU:CB	2.43	0.47
1:A:221:VAL:HA	1:A:281:GLY:HA2	1.97	0.47
2:B:363:ALA:C	2:B:365:PRO:HD2	2.39	0.47
1:C:375:THR:HG23	1:C:377:GLN:H	1.79	0.47
1:C:554:ASN:ND2	11:C:5322:HOH:O	2.47	0.47
2:D:226:GLU:O	2:D:230:LYS:HG3	2.14	0.47
1:E:958:VAL:O	1:E:961:ALA:HB3	2.15	0.47
1:G:36:ALA:HB1	1:G:325:LYS:HE3	1.96	0.47
2:H:73:SER:HA	2:H:203:ARG:HH22	1.79	0.47
1:A:119:THR:O	1:A:123:ILE:HG13	2.14	0.47
2:D:364:ALA:N	2:D:365:PRO:HD2	2.30	0.47
1:E:158:VAL:O	1:E:162:VAL:HG13	2.15	0.47
1:G:138:LYS:HE2	11:G:5508:HOH:O	2.15	0.47
1:A:478:GLU:HG3	11:A:5534:HOH:O	2.13	0.47
2:B:269:CYS:O	2:B:272:HIS:HB3	2.14	0.47
1:E:340:THR:O	1:E:343:ARG:HB2	2.15	0.47
1:G:847:ALA:C	1:G:849:THR:H	2.23	0.47
2:H:25:SER:HA	2:H:132:ILE:O	2.14	0.47
1:A:653:ALA:O	1:A:656:ALA:HB3	2.15	0.47
2:B:142:LEU:O	2:B:145:GLU:HB3	2.15	0.47
2:B:261:THR:HG23	2:B:262:ASP:N	2.30	0.47
1:E:670:ASP:HB2	11:E:5438:HOH:O	2.15	0.47
1:E:785:ALA:HB1	7:E:5047:ADP:C2	2.49	0.47
1:G:330:TYR:HD1	1:G:334:GLU:OE1	1.97	0.47
1:G:347:SER:O	1:G:348:PHE:HB3	2.15	0.47
1:G:959:ASP:O	1:G:962:ALA:HB3	2.14	0.47
2:H:20:ILE:O	2:H:99:SER:OG	2.28	0.47
2:H:57:TYR:CE1	2:H:58:PRO:HD2	2.47	0.47
2:H:157:ASP:CG	2:H:250:TYR:HH	2.22	0.47
2:H:280:GLY:HA3	2:H:322:PRO:HG3	1.95	0.47
1:A:45:ILE:CD1	1:A:81:GLU:HB3	2.44	0.47
2:B:264:PRO:HB3	2:B:373:LEU:HB3	1.95	0.47
2:B:266:PHE:HB3	2:B:370:PHE:CD1	2.50	0.47
2:B:331:SER:O	2:B:335:GLY:HA2	2.15	0.47
2:D:354:PRO:HB3	2:D:363:ALA:O	2.15	0.47
1:E:10:ILE:HG22	1:E:11:LEU:N	2.30	0.47
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.45	0.47
2:F:342:ARG:HD2	2:F:342:ARG:HA	1.69	0.47
1:G:290:PRO:O	2:H:92:PHE:HB3	2.15	0.47
1:G:659:VAL:O	1:G:661:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:209:LEU:HB3	2:H:216:LEU:HD21	1.97	0.47
1:A:698:ILE:HG22	1:A:699:GLU:N	2.30	0.47
1:A:802:SER:O	1:A:805:ILE:HG22	2.14	0.47
2:B:197:TYR:HB3	2:B:199:PHE:CZ	2.50	0.47
2:D:133:ILE:HD12	2:D:143:ALA:CB	2.28	0.47
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.50	0.47
2:F:272:HIS:HA	2:F:349:SER:HB2	1.96	0.47
1:G:810:ARG:HG3	1:G:810:ARG:NH1	2.22	0.47
1:G:1004:ARG:HA	1:G:1009:GLU:HG3	1.96	0.47
2:H:190:LEU:HB2	2:H:215:ARG:HB3	1.96	0.47
2:H:322:PRO:C	2:H:324:ASN:ND2	2.73	0.47
1:C:176:GLY:HA3	1:C:377:GLN:HA	1.96	0.46
1:C:695:VAL:CG1	1:C:700:MET:HB3	2.37	0.46
2:H:290:HIS:ND1	2:H:312:HIS:CE1	2.84	0.46
1:A:975:HIS:HD1	1:G:975:HIS:HD1	0.72	0.46
2:D:270:LEU:O	2:D:274:LEU:HG	2.15	0.46
1:E:946:LEU:HB3	1:E:1013:ILE:HG12	1.96	0.46
1:E:1067:GLU:O	1:E:1071:GLN:HG3	2.15	0.46
2:F:29:GLU:HA	2:F:129:ASN:HA	1.97	0.46
1:G:141:LEU:HB3	1:G:297:VAL:HG21	1.97	0.46
2:H:370:PHE:O	2:H:374:ILE:HG13	2.15	0.46
1:A:441:ASP:OD1	1:A:444:ARG:NH1	2.44	0.46
1:C:490:ARG:HG3	1:C:522:LEU:CD1	2.45	0.46
1:C:534:ALA:HB1	2:D:120:ARG:HG2	1.97	0.46
1:C:769:ASP:OD1	1:C:771:GLU:HB3	2.16	0.46
1:E:76:LYS:NZ	11:E:5748:HOH:O	2.42	0.46
1:E:805:ILE:HD12	1:E:832:VAL:HG11	1.97	0.46
1:G:7:ILE:HD13	1:G:85:ALA:HB2	1.95	0.46
1:G:164:PHE:HB3	1:G:165:PRO:HA	1.97	0.46
1:G:1021:ARG:HH11	1:G:1021:ARG:CG	2.27	0.46
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.67	0.46
2:H:361:HIS:N	2:H:361:HIS:CD2	2.80	0.46
1:A:1:MET:HA	1:A:224:LYS:NZ	2.30	0.46
1:A:166:CYS:C	1:A:167:ILE:HD12	2.40	0.46
2:D:246:ALA:N	2:D:247:PRO:HD2	2.30	0.46
2:D:272:HIS:HA	2:D:349:SER:CB	2.46	0.46
2:D:296:PRO:HB2	2:D:332:LEU:HB2	1.97	0.46
1:E:130:ARG:HD2	11:E:5490:HOH:O	2.16	0.46
1:E:169:ARG:NH1	7:E:5040:ADP:O2A	2.45	0.46
1:E:643:GLY:HA3	1:E:647:PRO:HG3	1.97	0.46
2:F:41:GLU:CB	2:F:358:PRO:HG3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:TRP:CG	2:F:176:THR:N	2.84	0.46
1:G:1:MET:N	1:G:2:PRO:CD	2.79	0.46
1:G:74:VAL:O	1:G:77:ILE:N	2.48	0.46
1:G:763:ASP:HB3	1:G:779:MET:CE	2.43	0.46
1:G:783:GLU:HB2	1:G:792:SER:HB3	1.98	0.46
1:G:883:VAL:O	1:G:884:ILE:HG12	2.15	0.46
1:A:57:ASP:HA	1:A:58:PRO:HD3	1.78	0.46
1:A:472:LEU:O	1:A:476:VAL:HG23	2.16	0.46
1:A:679:GLN:HG2	1:A:689:GLN:OE1	2.14	0.46
2:B:206:LEU:O	2:B:210:VAL:HG23	2.16	0.46
1:E:9:SER:OG	1:E:84:ASP:N	2.46	0.46
1:E:1063:ILE:HD13	1:E:1068:MET:HG3	1.97	0.46
1:G:10:ILE:HD13	1:G:37:LEU:HD13	1.96	0.46
1:G:640:VAL:O	1:G:640:VAL:HG23	2.14	0.46
2:H:298:LYS:O	2:H:329:HIS:HA	2.14	0.46
1:A:164:PHE:HA	1:A:165:PRO:C	2.39	0.46
1:A:503:ALA:HB2	1:A:510:GLU:HA	1.98	0.46
1:A:728:VAL:HB	1:A:733:ASP:HB3	1.98	0.46
1:A:780:GLU:HB3	1:A:798:ALA:HA	1.97	0.46
1:E:490[B]:ARG:NH1	1:E:494:ARG:HD2	2.31	0.46
1:G:236:ASN:OD1	1:G:244:THR:HG22	2.15	0.46
1:G:554:ASN:N	1:G:555:PRO:HD3	2.31	0.46
1:E:420:ALA:O	1:E:423:LYS:HG3	2.16	0.46
1:E:799:TYR:CD1	1:E:799:TYR:N	2.83	0.46
1:G:580:TYR:CE1	1:G:584:HIS:CE1	3.04	0.46
1:G:628:GLU:OE1	1:G:628:GLU:HA	2.15	0.46
1:A:130[B]:ARG:HE	1:A:130[B]:ARG:HB3	1.38	0.46
1:C:921:GLY:HA3	1:C:926:GLU:HB3	1.98	0.46
2:D:225:ALA:HA	2:D:258:PHE:CZ	2.50	0.46
1:E:222[A]:ARG:NE	1:E:226:ASP:OD1	2.39	0.46
2:H:168:TYR:CD1	2:H:168:TYR:N	2.83	0.46
1:A:693:ALA:HB3	1:A:708:ILE:HD11	1.98	0.46
1:A:698:ILE:N	1:A:698:ILE:CD1	2.79	0.46
2:B:246:ALA:N	2:B:247:PRO:CD	2.79	0.46
1:C:1001:ILE:HG13	1:C:1002:GLN:N	2.31	0.46
1:G:695:VAL:CG1	1:G:696:THR:N	2.79	0.46
2:H:181:LEU:HA	2:H:182:PRO:HD3	1.73	0.46
1:A:127:GLU:HB2	1:A:172:PHE:CE1	2.51	0.46
1:A:141:LEU:HB3	1:A:297:VAL:HG21	1.98	0.46
1:C:947:LEU:HD12	1:C:947:LEU:N	2.31	0.46
1:E:252:PRO:HD3	1:E:352:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.46
1:E:947:LEU:N	1:E:947:LEU:CD1	2.79	0.46
1:G:93:GLN:HB3	10:G:5073:NET:H22	1.96	0.46
1:G:301:ASN:HA	1:G:302:PRO:HD3	1.81	0.46
1:G:698:ILE:HD12	1:G:698:ILE:H	1.80	0.46
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.63	0.46
1:C:527:LYS:NZ	1:C:550:GLU:O	2.48	0.45
1:C:930:LYS:NZ	1:C:1058:ALA:O	2.48	0.45
1:C:948:SER:OG	9:C:5032:IMP:H8	2.16	0.45
1:E:509:ARG:NH1	1:E:512:GLU:CG	2.80	0.45
1:E:509:ARG:NH1	1:E:512:GLU:HG3	2.31	0.45
1:E:750:VAL:O	1:E:750:VAL:HG12	2.16	0.45
1:G:129:ARG:HB3	1:G:205:LEU:HD22	1.96	0.45
1:G:698:ILE:N	1:G:698:ILE:CD1	2.79	0.45
1:G:768:CYS:O	1:G:822:VAL:O	2.34	0.45
1:A:423:LYS:HB3	11:A:5517:HOH:O	2.15	0.45
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.99	0.45
1:A:780:GLU:HG2	1:A:799:TYR:HE1	1.81	0.45
2:D:186:LYS:HB2	2:D:189:GLU:CD	2.40	0.45
2:F:322:PRO:CB	2:F:324:ASN:ND2	2.79	0.45
1:G:805:ILE:C	1:G:808:VAL:H	2.23	0.45
2:H:21:GLY:HA3	2:H:107:ILE:O	2.17	0.45
2:H:209:LEU:HD23	2:H:214:CYS:SG	2.56	0.45
1:A:231:VAL:O	1:A:350:PRO:HG2	2.16	0.45
2:B:98:LEU:O	2:B:102:LEU:HG	2.17	0.45
2:B:282:LYS:HG2	2:B:320:THR:HG21	1.97	0.45
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.16	0.45
1:C:782:ILE:N	1:C:782:ILE:HD12	2.31	0.45
1:C:868:VAL:HG23	1:C:877:GLN:HE22	1.81	0.45
1:E:1:MET:HA	1:E:224:LYS:NZ	2.31	0.45
1:E:580:TYR:CE1	1:E:584:HIS:CE1	3.05	0.45
1:G:860:PRO:HB2	1:G:863:LYS:HB2	1.99	0.45
1:A:272:LEU:HD11	1:A:282:SER:HB2	1.98	0.45
1:A:481:ILE:O	1:A:481:ILE:HG13	2.17	0.45
1:A:816:LEU:HD11	1:A:839:LEU:HD21	1.99	0.45
1:C:674:ASP:HB3	1:C:677:ARG:HB2	1.98	0.45
2:D:49:SER:HA	2:D:76:HIS:O	2.17	0.45
1:E:708:ILE:CG2	1:E:754:HIS:HB2	2.47	0.45
2:F:12:GLY:HA2	2:F:144:LEU:CD1	2.47	0.45
2:F:172:GLN:HG2	2:F:173:GLY:N	2.26	0.45
2:F:295:HIS:O	2:F:308:THR:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:583:VAL:HG13	1:G:612:THR:HG23	1.98	0.45
2:H:87:LEU:HD12	2:H:87:LEU:HA	1.80	0.45
1:A:425:ARG:HD3	11:A:5280:HOH:O	2.16	0.45
1:A:854:SER:HA	1:A:859:VAL:O	2.17	0.45
1:C:906:LEU:HD13	1:C:1030:ARG:HD3	1.99	0.45
1:C:918:MET:HE2	1:C:920:VAL:CG2	2.46	0.45
2:F:46:PRO:HA	2:F:76:HIS:CB	2.47	0.45
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.43	0.45
1:G:726:GLU:HG3	1:G:727:ILE:N	2.32	0.45
1:A:197:ASP:OD2	1:A:1037:LYS:HE3	2.17	0.45
1:A:889:SER:HB3	1:A:918:MET:HE3	1.99	0.45
1:C:950:ARG:HB3	11:C:5613:HOH:O	2.16	0.45
1:C:1049:ALA:HA	1:C:1052:MET:HE3	1.99	0.45
2:F:228:VAL:HG11	2:F:258:PHE:CZ	2.52	0.45
2:F:324:ASN:HA	2:F:343:THR:OG1	2.17	0.45
2:F:350:PHE:CG	2:F:366:LEU:CD2	2.99	0.45
1:G:903:VAL:HG12	1:G:904:ASP:N	2.32	0.45
2:H:258:PHE:C	2:H:260:GLU:H	2.24	0.45
2:B:46:PRO:HG2	2:B:200:GLY:O	2.16	0.45
2:B:181:LEU:HD13	2:B:207:ARG:NH2	2.32	0.45
2:B:190:LEU:HA	2:B:191:PRO:HD3	1.77	0.45
2:B:232:ASN:N	2:B:233:PRO:CD	2.79	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:471:ARG:HH21	1:C:474:GLU:CD	2.25	0.45
1:C:598:MET:HE2	1:C:598:MET:HB2	1.84	0.45
2:D:6:LEU:O	2:D:132:ILE:HA	2.16	0.45
2:D:46:PRO:HA	2:D:76:HIS:CG	2.51	0.45
2:D:264:PRO:HB3	2:D:373:LEU:HB3	1.98	0.45
1:E:830:PHE:CE1	1:E:839:LEU:CD1	2.99	0.45
1:G:258:ASP:OD2	2:H:358:PRO:HA	2.17	0.45
1:G:383:GLU:OE2	1:G:604:GLU:OE2	2.34	0.45
2:H:373:LEU:N	2:H:373:LEU:HD23	2.31	0.45
1:A:142:GLU:CG	1:A:143:THR:N	2.80	0.45
2:B:266:PHE:HB3	2:B:370:PHE:CE1	2.52	0.45
1:C:39:GLU:OE1	1:C:325:LYS:NZ	2.39	0.45
1:C:782:ILE:N	1:C:782:ILE:CD1	2.79	0.45
2:D:324:ASN:N	2:D:324:ASN:HD22	2.14	0.45
1:E:1061:LYS:HE3	11:E:5652:HOH:O	2.16	0.45
10:E:5053:NET:H42	10:E:5053:NET:C2	2.32	0.45
1:G:716:PRO:HA	1:G:750:VAL:CG2	2.47	0.45
1:G:725:MET:HG3	1:G:909:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.82	0.45
2:H:51:GLN:O	2:H:78:GLN:N	2.46	0.45
2:H:225:ALA:O	2:H:229:LEU:HG	2.17	0.45
1:A:412:LYS:HD3	1:A:437:TRP:HB2	1.99	0.45
2:B:322:PRO:HG2	2:B:324:ASN:ND2	2.25	0.45
2:D:269:CYS:O	2:D:272:HIS:HB3	2.16	0.45
1:E:695:VAL:HA	1:E:700:MET:HE2	1.99	0.45
2:F:91:ASN:OD1	2:F:93:ARG:HB2	2.17	0.45
2:F:334:ASP:CG	2:F:336:THR:HG23	2.42	0.45
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.98	0.45
1:G:1020:ARG:O	1:G:1024:GLU:HG3	2.17	0.45
2:H:170:TRP:HB3	2:H:216:LEU:HD12	1.98	0.45
2:H:290:HIS:CB	2:H:310:GLN:HB3	2.47	0.45
2:B:162:VAL:HG12	2:B:162:VAL:O	2.17	0.45
1:C:695:VAL:CG1	1:C:696:THR:N	2.80	0.45
1:C:735:ARG:HG2	1:C:735:ARG:HH11	1.82	0.45
1:C:992:ASN:HB2	1:C:999:PRO:O	2.16	0.45
1:C:1027:ARG:HG3	1:C:1027:ARG:NH1	2.32	0.45
2:F:244:ASP:OD1	2:F:245:PRO:HD2	2.17	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.80	0.45
1:G:471:ARG:HD2	11:G:5606:HOH:O	2.17	0.45
1:G:494:ARG:HG3	1:G:547:TYR:CB	2.47	0.45
1:G:816:LEU:O	1:G:820:LEU:HD12	2.17	0.45
2:H:290:HIS:HB2	2:H:312:HIS:NE2	2.32	0.45
1:A:366:LYS:NZ	1:A:911:MET:O	2.44	0.44
2:B:45:ASP:O	2:B:76:HIS:HB2	2.17	0.44
1:C:1:MET:N	1:C:2:PRO:CD	2.79	0.44
1:C:735:ARG:HG2	1:C:735:ARG:NH1	2.31	0.44
1:E:282:SER:OG	1:E:302:PRO:HA	2.17	0.44
1:G:6:ASP:N	1:G:6:ASP:OD1	2.49	0.44
1:G:325:LYS:HB3	1:G:330:TYR:CD2	2.52	0.44
1:G:859:VAL:O	1:G:861:LEU:N	2.50	0.44
2:H:27:VAL:HG22	2:H:131:CYS:CB	2.42	0.44
2:H:75:VAL:O	2:H:75:VAL:HG12	2.17	0.44
2:H:322:PRO:O	2:H:324:ASN:N	2.49	0.44
2:H:327:VAL:HG11	2:H:330:LYS:HD2	1.98	0.44
1:A:726:GLU:HG3	1:A:727:ILE:H	1.82	0.44
2:B:286:MET:HE3	2:B:314:PHE:CA	2.48	0.44
2:B:324:ASN:HD22	2:B:324:ASN:N	2.15	0.44
2:D:204:ASN:O	2:D:208:MET:HG3	2.17	0.44
1:E:250:VAL:HA	1:E:356:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:840:ILE:O	1:E:841:GLU:HB3	2.17	0.44
2:H:327:VAL:HG13	2:H:337:LEU:CD1	2.48	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:1:MET:H2	1:A:2:PRO:HD3	1.80	0.44
2:B:276:ALA:O	2:B:281:ALA:HB3	2.17	0.44
2:B:318:GLU:HA	2:B:321:LEU:HD13	1.98	0.44
1:C:784:GLN:HA	11:C:5592:HOH:O	2.16	0.44
1:C:944:ARG:O	1:C:1010:TYR:HA	2.17	0.44
1:C:1044:LEU:HD12	1:C:1044:LEU:HA	1.76	0.44
2:D:228:VAL:O	2:D:231:MET:HB2	2.17	0.44
2:D:322:PRO:HD2	2:D:325:LEU:HD12	1.98	0.44
1:E:956:ARG:CB	1:E:1044:LEU:HD21	2.48	0.44
1:G:375:THR:HG23	1:G:377:GLN:H	1.82	0.44
2:H:322:PRO:C	2:H:324:ASN:HD22	2.25	0.44
1:E:1:MET:N	1:E:2:PRO:CD	2.80	0.44
1:E:225:ASN:ND2	1:E:331:THR:HG21	2.33	0.44
1:E:697:ALA:HB3	1:E:700:MET:HB2	2.00	0.44
1:G:224:LYS:HG2	11:G:5551:HOH:O	2.18	0.44
1:G:456:THR:HB	1:G:458:ILE:HG13	1.99	0.44
1:G:543:MET:HE1	1:G:617:TYR:CZ	2.53	0.44
1:G:712:LEU:HD12	1:G:712:LEU:HA	1.74	0.44
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.60	0.44
2:H:217:THR:HG21	2:H:231:MET:SD	2.58	0.44
1:A:585:ALA:HB2	1:A:642:TYR:CD2	2.52	0.44
1:A:788:HIS:HD2	1:A:909:PRO:O	2.00	0.44
1:C:358:LYS:HG2	1:C:359:ILE:N	2.32	0.44
1:C:726:GLU:OE2	1:C:1020:ARG:HD2	2.17	0.44
1:E:652[B]:ARG:NH1	11:E:5630:HOH:O	2.51	0.44
2:F:164:THR:N	2:F:198:ASP:OD2	2.51	0.44
2:F:208:MET:O	2:F:211:ASP:HB2	2.17	0.44
2:F:337:LEU:HD21	2:F:340:ILE:CG2	2.47	0.44
1:G:318:PRO:HG3	1:G:610:TYR:HH	1.81	0.44
2:H:23:THR:HG23	2:H:134:ALA:O	2.16	0.44
1:C:493:LYS:HD2	1:C:493:LYS:HA	1.72	0.44
1:C:1000:HIS:NE2	1:C:1002:GLN:HB3	2.32	0.44
1:E:561:LYS:HE3	11:E:5895:HOH:O	2.16	0.44
1:E:1027:ARG:HG2	1:E:1031:ARG:HG3	1.99	0.44
1:G:235:GLU:HB2	1:G:253:ALA:HA	1.99	0.44
2:H:30:VAL:HG12	2:H:122:LEU:HD11	2.00	0.44
1:A:259:LYS:NZ	11:A:5677:HOH:O	2.51	0.44
1:A:358:LYS:HG2	1:A:359:ILE:N	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:LEU:HD12	1:C:712:LEU:HA	1.77	0.44
1:C:726:GLU:CG	1:C:727:ILE:N	2.80	0.44
1:E:425:ARG:HD3	11:E:5322:HOH:O	2.18	0.44
1:E:948:SER:OG	9:E:5052:IMP:H5'2	2.17	0.44
2:F:54:THR:HA	2:F:81:VAL:HB	2.00	0.44
2:F:160:LYS:HE3	2:F:161:GLU:OE2	2.18	0.44
2:F:246:ALA:N	2:F:247:PRO:HD2	2.33	0.44
1:G:409:PHE:O	1:G:444:ARG:NH2	2.46	0.44
1:G:440:ALA:O	1:G:444:ARG:HG3	2.18	0.44
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.24	0.44
1:G:763:ASP:CB	1:G:779:MET:HE3	2.45	0.44
1:A:313:LYS:HA	1:A:313:LYS:HD2	1.78	0.44
1:A:992:ASN:ND2	1:G:975:HIS:NE2	2.66	0.44
2:B:13:THR:HG22	2:B:15:PHE:CE1	2.53	0.44
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.52	0.44
2:B:71:GLU:HG3	2:B:202:LYS:HE3	2.00	0.44
1:C:423:LYS:HG3	1:C:423:LYS:H	1.43	0.44
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.81	0.44
2:H:270:LEU:HA	2:H:273:GLN:OE1	2.17	0.44
2:B:175:TRP:CD1	2:B:180:GLY:HA2	2.52	0.44
2:B:188:ASP:OD1	2:B:189:GLU:N	2.51	0.44
2:B:248:CYS:O	2:B:252:ILE:HG13	2.18	0.44
1:G:103:GLU:HA	1:G:108:LEU:HD12	1.99	0.44
1:G:1027:ARG:NH1	1:G:1027:ARG:HG2	2.32	0.44
2:H:48:TYR:CZ	2:H:311:ASN:ND2	2.86	0.44
1:A:145:ARG:HB3	1:A:208:GLU:CD	2.42	0.43
1:A:634:LYS:N	1:A:635:PRO:HD3	2.33	0.43
2:B:277:LEU:HD23	2:B:281:ALA:O	2.18	0.43
2:B:342:ARG:NE	2:B:344:ASP:OD1	2.33	0.43
1:C:59:GLU:HG3	1:C:60:MET:CE	2.42	0.43
1:C:335:LEU:HB2	1:C:346:ALA:HB3	2.00	0.43
1:C:698:ILE:N	1:C:698:ILE:CD1	2.80	0.43
1:C:922:ARG:NH2	1:C:1060:GLU:OE1	2.40	0.43
1:C:1042:THR:N	8:C:5031:ORN:O	2.44	0.43
1:E:475:LYS:HD3	1:E:488:PHE:CZ	2.53	0.43
1:E:713:VAL:CG1	1:E:725:MET:HE2	2.48	0.43
2:H:83:ARG:HD2	2:H:83:ARG:C	2.42	0.43
2:H:310:GLN:HE22	2:H:352:GLY:CA	2.31	0.43
1:A:10:ILE:HD11	1:A:42:TYR:CD2	2.52	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.90	0.43
1:A:373:ARG:NH1	1:A:430:ASP:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:GLU:OE2	1:A:1020:ARG:HD2	2.17	0.43
1:C:105:GLN:HA	1:C:105:GLN:NE2	2.33	0.43
1:G:56:THR:OG1	1:G:855:LYS:NZ	2.29	0.43
1:G:822:VAL:HG11	1:G:826:MET:SD	2.58	0.43
1:G:953:ASP:OD2	1:G:1016:THR:OG1	2.30	0.43
1:A:220:VAL:O	1:A:281:GLY:HA2	2.18	0.43
1:A:509:ARG:O	1:A:512:GLU:HB2	2.18	0.43
1:A:532:CYS:O	1:A:533:ALA:HB3	2.18	0.43
2:B:46:PRO:HA	2:B:76:HIS:CB	2.47	0.43
2:B:254:ALA:O	2:B:257:LYS:HB2	2.18	0.43
2:B:324:ASN:HD22	2:B:324:ASN:C	2.26	0.43
1:E:57:ASP:HA	1:E:58:PRO:HD3	1.67	0.43
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.53	0.43
1:G:699:GLU:CA	1:G:702:VAL:HG23	2.48	0.43
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.99	0.43
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.99	0.43
2:D:267:GLY:O	2:D:349:SER:HB2	2.18	0.43
1:E:213:TRP:CH2	1:E:289:ASN:HB2	2.52	0.43
1:E:1004:ARG:HA	1:E:1009[B]:GLU:HG3	2.00	0.43
2:F:266:PHE:HB2	2:F:370:PHE:CD1	2.53	0.43
1:G:543:MET:CE	1:G:617:TYR:CZ	3.02	0.43
2:H:171:THR:HB	2:H:185:LYS:O	2.19	0.43
2:B:138:PRO:HA	11:B:5177:HOH:O	2.18	0.43
2:B:199:PHE:O	2:B:241:GLY:HA3	2.19	0.43
1:C:1:MET:N	1:C:2:PRO:HD2	2.33	0.43
1:C:130:ARG:HG3	1:C:148:ILE:HG13	2.00	0.43
1:C:472:LEU:O	1:C:476:VAL:HG23	2.18	0.43
1:E:1:MET:N	1:E:2:PRO:HD2	2.33	0.43
1:E:733:ASP:O	1:E:736:ARG:HB3	2.18	0.43
2:F:158:LEU:HD12	2:F:243:GLY:N	2.34	0.43
1:G:475:LYS:O	1:G:479:VAL:HG13	2.19	0.43
1:G:920:VAL:O	1:G:930:LYS:HD3	2.19	0.43
1:A:527:LYS:HB2	1:A:544:TYR:CE1	2.54	0.43
2:B:259:LEU:HD23	2:B:259:LEU:HA	1.78	0.43
2:B:286:MET:CE	2:B:314:PHE:C	2.91	0.43
1:G:700:MET:CE	1:G:704:LYS:HD3	2.49	0.43
1:G:857:THR:OG1	1:G:859:VAL:HB	2.18	0.43
2:H:232:ASN:N	2:H:233:PRO:CD	2.82	0.43
1:A:185:ARG:NH2	11:A:5455:HOH:O	2.49	0.43
1:A:579:ASP:OD2	1:A:605:THR:HB	2.18	0.43
2:B:181:LEU:HA	2:B:181:LEU:HD23	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1051:ALA:O	1:E:1054:LEU:HB2	2.19	0.43
2:F:26:ALA:O	2:F:131:CYS:HA	2.18	0.43
2:F:57:TYR:CD1	2:F:58:PRO:CD	3.00	0.43
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.83	0.43
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.49	0.43
1:G:906:LEU:HD13	1:G:1030:ARG:HD3	1.99	0.43
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.54	0.43
1:C:202:LYS:O	1:C:202:LYS:HG2	2.18	0.43
1:C:648:LEU:HD13	1:C:845:ARG:CD	2.49	0.43
1:C:958:VAL:HG13	1:C:986:ILE:HD12	2.01	0.43
2:D:364:ALA:N	2:D:365:PRO:CD	2.82	0.43
1:E:941[B]:LYS:HE2	11:E:5448:HOH:O	2.19	0.43
1:E:951:GLU:OE1	1:E:951:GLU:HA	2.17	0.43
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.54	0.43
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.01	0.43
2:F:353:HIS:ND1	2:F:355:GLU:OE2	2.48	0.43
1:G:339:ILE:HG22	1:G:540:THR:CB	2.49	0.43
1:G:364:PHE:CE1	1:G:372:ASP:HA	2.54	0.43
1:G:922:ARG:CZ	1:G:1061:LYS:HD2	2.48	0.43
1:G:936:ASN:HB2	11:G:5111:HOH:O	2.17	0.43
1:G:995:HIS:CE1	1:G:996:GLU:HG3	2.53	0.43
2:H:342:ARG:HH11	2:H:342:ARG:CG	2.20	0.43
1:A:4:ARG:CZ	1:A:7:ILE:HD11	2.48	0.43
1:A:59:GLU:HG2	1:A:60:MET:HE2	2.01	0.43
1:A:164:PHE:CB	1:A:165:PRO:HA	2.48	0.43
1:A:384:VAL:HG22	1:A:385:MET:N	2.34	0.43
1:A:589:LEU:HA	1:A:592:ASP:HB2	2.01	0.43
1:A:659:VAL:HG12	1:A:660:PRO:HD2	2.00	0.43
2:B:185:LYS:HD3	2:B:190:LEU:HD21	2.01	0.43
1:C:1031:ARG:HE	1:C:1031:ARG:HB3	1.50	0.43
2:D:186:LYS:H	2:D:189:GLU:CD	2.26	0.43
1:E:804:GLU:O	1:E:808:VAL:HG23	2.18	0.43
1:G:5:THR:CG2	1:G:6:ASP:N	2.82	0.43
2:H:199:PHE:CE2	2:H:238:LEU:HB3	2.50	0.43
2:H:286:MET:HE2	2:H:315:ALA:CB	2.35	0.43
1:A:158:VAL:O	1:A:161:ASP:HB3	2.19	0.43
2:B:175:TRP:HB2	2:B:181:LEU:CD2	2.48	0.43
2:B:266:PHE:HA	2:B:348:PHE:O	2.19	0.43
1:C:416:ASP:O	1:C:418:PRO:HD3	2.19	0.43
1:C:509:ARG:O	1:C:512:GLU:HB2	2.19	0.43
1:G:390:THR:HB	11:G:5332:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:548:GLU:HG2	2:H:114:ASP:OD2	2.18	0.43
1:G:1014:ILE:HG23	1:G:1014:ILE:O	2.19	0.43
1:A:142:GLU:HG2	1:A:143:THR:N	2.33	0.42
1:A:169:ARG:HA	1:A:170:PRO:HD3	1.81	0.42
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.90	0.42
1:C:66:ILE:CG2	1:C:918:MET:HB3	2.49	0.42
1:C:101:GLU:HA	1:C:101:GLU:OE1	2.19	0.42
1:C:680:HIS:HA	1:C:683:GLU:OE2	2.18	0.42
1:C:712:LEU:HD12	1:C:754:HIS:HA	2.01	0.42
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.34	0.42
2:D:25:SER:HA	2:D:132:ILE:O	2.19	0.42
1:E:150:HIS:NE2	1:E:203:GLU:HG3	2.34	0.42
1:E:755:PHE:CD1	7:E:5047:ADP:C2	3.07	0.42
2:F:318:GLU:O	2:F:318:GLU:HG2	2.18	0.42
2:H:360:PRO:C	2:H:362:ASP:H	2.26	0.42
1:A:685:LEU:HA	1:A:685:LEU:HD23	1.77	0.42
1:A:769:ASP:OD2	1:A:874:LEU:HB2	2.19	0.42
1:C:769:ASP:C	1:C:771:GLU:H	2.26	0.42
1:C:772:MET:HE1	1:C:880:THR:HG22	2.01	0.42
1:E:751:LEU:C	1:E:752:LEU:HD12	2.45	0.42
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.54	0.42
2:F:324:ASN:N	2:F:324:ASN:ND2	2.63	0.42
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.54	0.42
1:G:502:LEU:HA	1:G:502:LEU:HD23	1.67	0.42
1:G:688:LYS:HE3	1:G:836:GLU:CD	2.44	0.42
1:G:695:VAL:HG12	1:G:696:THR:N	2.34	0.42
1:G:850:VAL:HB	1:G:851:PRO:CD	2.49	0.42
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.86	0.42
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.19	0.42
1:E:1:MET:CA	1:E:224:LYS:NZ	2.81	0.42
1:E:697:ALA:HA	1:E:698:ILE:HD13	2.02	0.42
2:F:229:LEU:HA	2:F:229:LEU:HD23	1.68	0.42
2:F:342:ARG:HB3	2:F:345:LYS:H	1.84	0.42
1:G:17:PRO:HG3	1:G:917:VAL:HG13	2.01	0.42
1:G:103:GLU:HG3	1:G:104:ARG:N	2.31	0.42
1:G:674:ASP:HB3	1:G:677:ARG:HB2	2.02	0.42
1:G:1063:ILE:CD1	1:G:1068:MET:HG3	2.36	0.42
2:H:337:LEU:HD12	2:H:337:LEU:HA	1.58	0.42
1:A:695:VAL:HG11	1:A:701:ALA:N	2.35	0.42
1:A:755:PHE:CD1	7:A:5007:ADP:C2	3.08	0.42
2:B:199:PHE:HB3	2:B:270:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:740:THR:H	1:C:740:THR:HG23	1.52	0.42
1:E:563:MET:HE2	1:E:563:MET:HB2	1.80	0.42
1:E:644:GLY:O	1:E:648:LEU:HB2	2.19	0.42
2:F:365:PRO:HA	2:F:368:ASP:OD2	2.19	0.42
1:G:53:THR:OG1	1:G:56:THR:HG23	2.19	0.42
1:G:354:TYR:OH	1:G:529:VAL:HG13	2.19	0.42
1:G:810:ARG:NH1	1:G:810:ARG:CG	2.79	0.42
2:H:121:LEU:C	2:H:121:LEU:HD12	2.44	0.42
2:B:344:ASP:OD2	2:B:345:LYS:HG2	2.19	0.42
1:C:534:ALA:O	2:D:123:ARG:HD3	2.20	0.42
1:C:868:VAL:HG23	1:C:877:GLN:NE2	2.35	0.42
1:C:939:MET:HE2	1:C:1050:THR:CG2	2.49	0.42
1:E:471:ARG:HH21	1:E:474:GLU:CD	2.28	0.42
1:E:637:GLY:HA2	1:E:660:PRO:O	2.20	0.42
1:E:895:LEU:HA	1:E:896:PRO:HD3	1.81	0.42
1:G:82:ARG:N	1:G:83:PRO:HD3	2.33	0.42
1:G:622:THR:OG1	1:G:625:ASP:OD2	2.28	0.42
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.80	0.42
1:A:493:LYS:HD2	1:A:493:LYS:HA	1.73	0.42
1:C:780:GLU:OE1	1:C:798:ALA:HB1	2.20	0.42
2:D:249:ASP:OD1	2:D:250:TYR:N	2.53	0.42
1:E:1019:GLY:O	1:E:1023:ILE:HD12	2.19	0.42
2:F:50:ARG:H	2:F:78[B]:GLN:NE2	2.18	0.42
2:F:245:PRO:C	2:F:247:PRO:HD2	2.44	0.42
1:G:294:ARG:HD2	5:G:5077:CL:CL	2.57	0.42
1:G:809:MET:HB3	1:G:830:PHE:CE2	2.55	0.42
1:G:891:LYS:HG2	1:G:892:GLU:N	2.29	0.42
2:H:71:GLU:OE2	2:H:204:ASN:HB2	2.20	0.42
2:H:118:LEU:O	2:H:121:LEU:HB3	2.20	0.42
2:H:199:PHE:HD2	2:H:239:SER:O	2.03	0.42
2:H:227:ASP:O	2:H:231:MET:HE2	2.20	0.42
1:A:681:ALA:O	1:A:685:LEU:HG	2.19	0.42
1:A:700:MET:O	1:A:704:LYS:HB2	2.19	0.42
2:B:342:ARG:HD2	2:B:342:ARG:HA	1.76	0.42
1:C:713:VAL:O	1:C:713:VAL:HG12	2.19	0.42
1:C:770:GLY:CA	1:C:823:ARG:NH1	2.82	0.42
2:D:299:ASP:O	2:D:303:ASN:N	2.50	0.42
1:E:93:GLN:HG2	5:E:5056:CL:CL	2.57	0.42
1:E:142:GLU:OE2	1:E:294:ARG:NH2	2.53	0.42
2:F:273:GLN:O	2:F:277:LEU:HG	2.19	0.42
2:F:333:PHE:HD1	2:F:333:PHE:HA	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:534:ALA:HB1	2:H:120:ARG:HG2	2.02	0.42
2:H:78:GLN:NE2	2:H:78:GLN:CA	2.80	0.42
2:H:280:GLY:CA	2:H:322:PRO:HG3	2.50	0.42
1:A:9:SER:HA	1:A:43:ARG:O	2.20	0.42
1:A:278[A]:GLU:HG2	11:A:5637:HOH:O	2.20	0.42
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.81	0.42
2:B:286:MET:CE	2:B:315:ALA:N	2.83	0.42
1:C:32:GLN:OE1	1:C:320:ALA:HB3	2.19	0.42
1:C:956:ARG:NH2	1:C:1048:PHE:CD2	2.88	0.42
2:D:132:ILE:HD13	2:D:132:ILE:HG21	1.84	0.42
1:E:622:THR:OG1	1:E:625:ASP:OD2	2.33	0.42
1:G:65:TYR:CG	1:G:77:ILE:HD13	2.55	0.42
1:G:100:LEU:N	1:G:100:LEU:HD12	2.35	0.42
1:G:243:HIS:CD2	7:G:5060:ADP:H5'2	2.55	0.42
1:G:494:ARG:HG3	1:G:547:TYR:HB2	2.02	0.42
2:H:322:PRO:C	2:H:324:ASN:N	2.78	0.42
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.50	0.42
1:C:237:PHE:HB3	1:C:248:ILE:O	2.19	0.42
2:D:245:PRO:HG3	2:D:273:GLN:OE1	2.20	0.42
1:E:493:LYS:HA	1:E:493:LYS:HD2	1.86	0.42
1:E:708:ILE:HG23	1:E:754:HIS:HB2	2.01	0.42
2:F:298:LYS:O	2:F:329:HIS:HA	2.20	0.42
1:G:780:GLU:CD	1:G:800:THR:HG23	2.44	0.42
1:G:782:ILE:N	1:G:782:ILE:CD1	2.83	0.42
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.35	0.42
1:A:341:GLY:C	1:A:343:ARG:H	2.28	0.42
1:A:375:THR:HG23	1:A:377:GLN:H	1.85	0.42
1:A:646:THR:HB	1:A:647:PRO:CD	2.49	0.42
1:C:167:ILE:HD12	1:C:167:ILE:N	2.35	0.42
1:C:699:GLU:HA	1:C:702:VAL:CG2	2.49	0.42
2:D:133:ILE:HG22	2:D:138:PRO:HB3	2.02	0.42
1:E:103:GLU:HG2	11:E:5484:HOH:O	2.19	0.42
1:E:694:THR:CG2	1:E:695:VAL:N	2.80	0.42
2:F:71:GLU:O	2:F:72:SER:HB3	2.20	0.42
2:H:9:LEU:HD12	2:H:13:THR:HB	2.02	0.42
1:A:148:ILE:CG2	1:A:149:ALA:N	2.82	0.41
1:A:501:ARG:HH11	1:A:501:ARG:HD2	1.73	0.41
1:A:688:LYS:HE3	1:A:836:GLU:OE2	2.19	0.41
1:A:770:GLY:CA	1:A:823:ARG:CZ	2.98	0.41
2:B:78:GLN:NE2	2:B:78:GLN:HA	2.35	0.41
1:C:494:ARG:HA	1:C:547:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:GLU:HG3	1:C:727:ILE:H	1.85	0.41
1:E:164:PHE:HA	1:E:165:PRO:C	2.45	0.41
1:E:383:GLU:OE2	1:E:604:GLU:OE2	2.37	0.41
10:E:5053:NET:H63	10:E:5053:NET:H31	1.83	0.41
2:H:186:LYS:HB2	2:H:189:GLU:HG3	2.01	0.41
2:H:233:PRO:HD2	2:H:263:ILE:HD11	2.01	0.41
1:A:354:TYR:CD1	1:A:387:ILE:HG23	2.56	0.41
1:A:770:GLY:HA2	1:A:823:ARG:CZ	2.50	0.41
2:B:345:LYS:HB3	2:B:346:PRO:HD2	2.02	0.41
1:C:83:PRO:O	1:C:113:VAL:HG22	2.20	0.41
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.00	0.41
1:C:513:ILE:HD12	1:C:513:ILE:HG23	1.75	0.41
1:C:702:VAL:CG1	1:C:731:GLU:HG3	2.50	0.41
1:C:843:ASN:C	1:C:845:ARG:H	2.28	0.41
1:E:694:THR:O	1:E:695:VAL:HG23	2.20	0.41
1:E:783:GLU:HG3	1:E:1043:THR:HG21	2.03	0.41
1:G:108:LEU:HB2	11:G:5174:HOH:O	2.18	0.41
1:G:492:LEU:O	1:G:497:PHE:HD2	2.03	0.41
1:G:680:HIS:O	1:G:684:ARG:N	2.51	0.41
1:A:944:ARG:HD3	1:A:972:ASP:OD1	2.20	0.41
2:B:190:LEU:HD23	2:B:213:GLY:HA2	2.02	0.41
2:B:322:PRO:HD2	2:B:325:LEU:HD12	2.02	0.41
1:C:1:MET:O	1:C:329:GLY:O	2.38	0.41
1:C:11:LEU:HA	1:C:45:ILE:O	2.21	0.41
1:C:71:TRP:CD2	1:C:105:GLN:HG3	2.55	0.41
1:C:504:LYS:HE2	11:C:5562:HOH:O	2.19	0.41
1:C:726:GLU:OE2	1:C:736:ARG:NH2	2.53	0.41
1:C:751:LEU:C	1:C:752:LEU:HD12	2.45	0.41
1:C:891:LYS:HG2	1:C:892:GLU:N	2.35	0.41
2:D:160:LYS:HE3	2:D:161:GLU:OE2	2.20	0.41
1:E:464:VAL:HG21	2:F:88:ILE:HG12	2.01	0.41
1:G:980:VAL:HG13	11:G:5678:HOH:O	2.19	0.41
1:G:1035:GLN:HG2	1:G:1036:TYR:CD2	2.55	0.41
2:H:295:HIS:HA	2:H:296:PRO:HD3	1.87	0.41
1:A:170:PRO:HG2	1:A:177:SER:O	2.20	0.41
1:C:834:ASN:C	1:C:836:GLU:H	2.28	0.41
2:D:279:SER:O	2:D:322:PRO:HG3	2.20	0.41
1:E:40:GLU:OE1	1:E:330:TYR:OH	2.30	0.41
2:F:45:ASP:HB3	2:F:48:TYR:CD2	2.54	0.41
1:G:135:ALA:HB1	1:G:274:GLU:HG3	2.01	0.41
1:G:321:LYS:NZ	1:G:611:ASP:OD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:470:VAL:O	1:G:473:GLU:HB2	2.21	0.41
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.34	0.41
2:H:30:VAL:HB	2:H:128:GLN:O	2.20	0.41
1:A:59:GLU:OE2	1:A:60:MET:HE2	2.20	0.41
1:A:82:ARG:N	1:A:83:PRO:CD	2.84	0.41
1:A:712:LEU:HD23	1:A:752:LEU:HG	2.03	0.41
1:A:795:SER:OG	1:A:797:PRO:O	2.35	0.41
2:B:190:LEU:HB2	2:B:215[B]:ARG:HB3	2.02	0.41
2:B:245:PRO:C	2:B:247:PRO:HD2	2.46	0.41
2:B:267:GLY:O	2:B:349:SER:HB2	2.20	0.41
1:C:223:ASP:CG	1:C:227:ASN:HB2	2.45	0.41
1:C:646:THR:HB	1:C:647:PRO:HD3	2.02	0.41
2:D:87:LEU:HA	2:D:87:LEU:HD23	1.69	0.41
1:E:168:ILE:HD12	1:E:191:ILE:HG21	2.01	0.41
1:E:889:SER:OG	1:E:918:MET:HE3	2.20	0.41
2:F:87:LEU:HA	2:F:87:LEU:HD12	1.74	0.41
2:F:322:PRO:CB	2:F:324:ASN:HD21	2.32	0.41
1:G:101:GLU:HG3	11:G:5486:HOH:O	2.20	0.41
1:G:514:ARG:HG3	1:G:517:ARG:NH2	2.35	0.41
1:G:692:ASN:N	1:G:692:ASN:ND2	2.64	0.41
1:G:924:PHE:CD2	1:G:924:PHE:C	2.98	0.41
2:H:342:ARG:HD2	2:H:342:ARG:HA	1.77	0.41
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.50	0.41
1:A:130[B]:ARG:HD2	1:A:130[B]:ARG:HH11	1.81	0.41
1:A:895:LEU:HA	1:A:896:PRO:HD3	1.86	0.41
1:A:1044:LEU:HD12	1:A:1044:LEU:HA	1.98	0.41
2:B:33:ASN:HB3	2:B:55:LEU:HD23	2.03	0.41
2:B:324:ASN:ND2	2:B:324:ASN:C	2.79	0.41
1:C:230:ILE:HG13	1:C:265:ARG:HG3	2.03	0.41
1:C:431:ALA:HB2	1:C:435:ARG:HD3	2.02	0.41
1:C:895:LEU:HA	1:C:896:PRO:HD3	1.88	0.41
2:D:232:ASN:N	2:D:233:PRO:HD3	2.35	0.41
1:E:773:VAL:HG21	1:E:814:GLN:HA	2.02	0.41
1:G:598:MET:HE3	1:G:607:SER:HB2	2.03	0.41
1:G:763:ASP:OD1	1:G:829:GLN:HG2	2.20	0.41
2:H:128:GLN:NE2	11:H:4033:HOH:O	2.49	0.41
2:H:197:TYR:OH	2:H:228:VAL:HG21	2.21	0.41
1:A:634:LYS:N	1:A:635:PRO:CD	2.84	0.41
1:A:710:TYR:CB	1:A:711:PRO:HA	2.47	0.41
1:A:725:MET:SD	1:A:909:PRO:HB2	2.60	0.41
2:B:291:HIS:HA	2:B:310:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.89	0.41
1:C:213:TRP:CH2	1:C:289:ASN:HB2	2.56	0.41
1:C:639:ILE:HG23	1:C:641:GLN:OE1	2.21	0.41
1:E:10:ILE:HD12	1:E:42:TYR:HB3	2.03	0.41
1:E:1004:ARG:CA	1:E:1009[B]:GLU:HG3	2.50	0.41
1:E:1031:ARG:HE	1:E:1031:ARG:HB3	1.76	0.41
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.28	0.41
8:G:5074:ORN:OXT	2:H:120:ARG:NH1	2.54	0.41
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.71	0.41
2:H:296:PRO:HA	2:H:306:MET:O	2.21	0.41
1:A:80:LYS:O	1:A:80:LYS:HG2	2.20	0.41
2:B:101:TYR:O	2:B:104:ARG:HB3	2.19	0.41
1:C:145[A]:ARG:NH2	11:C:5474:HOH:O	2.53	0.41
1:C:423:LYS:HE3	11:C:5542:HOH:O	2.21	0.41
1:C:447:LEU:HD23	1:G:446:GLY:O	2.20	0.41
2:D:120:ARG:HD2	11:D:1337:HOH:O	2.20	0.41
2:D:250:TYR:CD2	2:D:251:ALA:N	2.89	0.41
1:E:579:ASP:OD2	1:E:605:THR:HB	2.21	0.41
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.29	0.41
2:F:298:LYS:NZ	11:F:2405:HOH:O	2.45	0.41
1:G:240:MET:HE3	1:G:240:MET:HB3	1.93	0.41
1:G:259:LYS:HD3	2:H:175:TRP:CE3	2.56	0.41
1:G:634:LYS:N	1:G:635:PRO:CD	2.81	0.41
1:G:680:HIS:O	1:G:683:GLU:HB2	2.21	0.41
1:G:852:PHE:HE1	1:G:918:MET:HG3	1.85	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CE2	2.56	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CZ	2.55	0.41
1:A:170:PRO:HA	1:A:204:LEU:HD23	2.03	0.41
1:A:828:VAL:HG13	1:A:842:VAL:HG22	2.03	0.41
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.87	0.41
2:B:236:ILE:HD13	2:B:258:PHE:CD1	2.56	0.41
2:B:246:ALA:HB3	2:B:247:PRO:CD	2.49	0.41
2:B:334:ASP:CG	2:B:336:THR:HG23	2.46	0.41
2:B:354:PRO:HA	2:B:363:ALA:HB3	2.03	0.41
1:C:220:VAL:C	1:C:221:VAL:HG23	2.46	0.41
1:C:385:MET:HG2	1:C:386:ALA:N	2.35	0.41
1:C:395:LEU:HD21	1:C:409:PHE:HZ	1.86	0.41
1:C:589:LEU:O	1:C:594:TYR:HB2	2.21	0.41
1:C:665:SER:O	1:C:669:ILE:HG13	2.21	0.41
1:C:944:ARG:HB3	1:C:1009:GLU:O	2.20	0.41
1:C:1001:ILE:HD13	1:C:1029:ILE:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:LEU:HD13	2:D:60:ILE:HD12	2.01	0.41
2:D:170:TRP:CD1	2:D:170:TRP:C	2.98	0.41
1:E:289:ASN:O	1:E:293:GLY:N	2.51	0.41
1:E:710:TYR:HB3	1:E:711:PRO:HA	2.03	0.41
1:E:738:PHE:O	1:E:741:ALA:HB3	2.21	0.41
2:F:254:ALA:O	2:F:257:LYS:HB2	2.21	0.41
1:G:115:MET:HE3	1:G:115:MET:HB2	1.92	0.41
1:G:147:GLY:HA3	1:G:158:VAL:HG13	2.03	0.41
1:G:468:GLU:OE1	2:H:87:LEU:HD21	2.20	0.41
1:G:772:MET:HE2	1:G:772:MET:HB3	1.62	0.41
1:G:888:TYR:O	1:G:920:VAL:HA	2.20	0.41
2:H:33:ASN:HB3	2:H:55:LEU:HD23	2.03	0.41
2:H:48:TYR:HA	2:H:51:GLN:NE2	2.35	0.41
2:H:48:TYR:O	2:H:51:GLN:HB2	2.21	0.41
2:H:225:ALA:HA	2:H:258:PHE:CE1	2.56	0.41
2:H:290:HIS:O	2:H:311:ASN:HA	2.21	0.41
1:C:494:ARG:HG3	1:C:547:TYR:CB	2.51	0.41
1:C:765:ASP:OD2	1:C:849:THR:OG1	2.31	0.41
1:C:1000:HIS:CD2	1:C:1000:HIS:C	2.99	0.41
2:D:302:LYS:HB2	2:D:304:VAL:HG22	2.02	0.41
1:E:608:THR:HB	1:E:618:PHE:CE2	2.56	0.41
1:E:648:LEU:CD1	1:E:845:ARG:HD3	2.51	0.41
1:G:65:TYR:OH	1:G:81:GLU:OE2	2.34	0.41
1:G:339:ILE:HG12	11:G:5306:HOH:O	2.20	0.41
1:G:493:LYS:HA	1:G:493:LYS:HD2	1.69	0.41
1:G:568:GLY:O	1:G:602:ASN:HB2	2.21	0.41
1:G:1063:ILE:O	1:G:1063:ILE:HG23	2.21	0.41
2:H:233:PRO:HG2	2:H:263:ILE:CD1	2.51	0.41
1:A:34:CYS:O	1:A:38:ARG:HB3	2.21	0.40
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.22	0.40
2:B:48:TYR:CZ	2:B:311:ASN:ND2	2.89	0.40
2:B:167:ALA:O	2:B:168:TYR:HB3	2.20	0.40
1:C:65:TYR:CE1	1:C:1063:ILE:C	2.99	0.40
1:E:288:VAL:O	1:E:290:PRO:HD3	2.21	0.40
1:E:540:THR:HG22	1:E:541:ALA:N	2.35	0.40
2:F:25:SER:HA	2:F:132:ILE:O	2.21	0.40
1:G:76:LYS:HE2	1:G:1059:THR:O	2.21	0.40
1:G:224:LYS:NZ	11:G:5093:HOH:O	2.52	0.40
1:G:516:LEU:HA	1:G:516:LEU:HD12	1.73	0.40
2:B:237:PHE:CZ	2:B:239:SER:HA	2.56	0.40
1:C:152:MET:SD	1:C:189:GLU:HA	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:GLU:HB3	2:D:117:LYS:HB2	2.04	0.40
1:C:770:GLY:HA3	1:C:823:ARG:CZ	2.51	0.40
1:E:688:LYS:HD3	1:E:838:TYR:CE2	2.56	0.40
1:G:1021:ARG:HG2	1:G:1021:ARG:NH1	2.32	0.40
2:H:32:PHE:CD1	2:H:32:PHE:C	3.00	0.40
2:H:43:LEU:HB3	2:H:75:VAL:HG13	2.03	0.40
2:H:307:ILE:O	2:H:362:ASP:HB2	2.20	0.40
1:A:266:ASN:ND2	11:A:5484:HOH:O	2.54	0.40
2:B:6:LEU:HD12	2:B:16:HIS:ND1	2.36	0.40
2:B:144:LEU:HD21	2:B:148:ARG:HH21	1.85	0.40
2:B:174:SER:HB2	2:B:211:ASP:OD2	2.21	0.40
2:B:246:ALA:N	2:B:247:PRO:HD2	2.36	0.40
2:B:286:MET:HE1	2:B:312:HIS:ND1	2.36	0.40
1:C:82:ARG:HA	1:C:82:ARG:HD2	1.78	0.40
1:C:431:ALA:HB2	1:C:435:ARG:CZ	2.51	0.40
1:C:953:ASP:OD2	1:C:1016:THR:OG1	2.38	0.40
2:D:158:LEU:HA	2:D:158:LEU:HD23	1.79	0.40
1:E:93:GLN:HB2	1:E:174:MET:HG2	2.04	0.40
1:E:830:PHE:CD1	1:E:839:LEU:CD1	3.04	0.40
1:E:838:TYR:CD1	1:E:838:TYR:N	2.89	0.40
1:G:563:MET:HE3	1:G:563:MET:HB2	1.96	0.40
1:G:948:SER:OG	9:G:5072:IMP:H5'2	2.22	0.40
1:G:1026:SER:HB2	1:G:1030:ARG:NH1	2.32	0.40
1:A:595:GLU:HA	1:A:614:ASP:OD2	2.21	0.40
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.36	0.40
1:C:53:THR:OG1	1:C:56:THR:HG23	2.22	0.40
1:C:367:PHE:CE1	1:C:912:ARG:HG2	2.57	0.40
1:C:554:ASN:N	1:C:555:PRO:CD	2.85	0.40
1:C:687:LEU:HD12	1:C:687:LEU:HA	1.83	0.40
1:C:889:SER:HB3	1:C:918:MET:HE3	2.02	0.40
1:C:1051:ALA:O	1:C:1054:LEU:HB2	2.21	0.40
2:D:30:VAL:HG12	2:D:122:LEU:HD11	2.04	0.40
2:D:281:ALA:HB2	2:D:321:LEU:HD12	2.03	0.40
1:E:177:SER:OG	1:E:899:LYS:NZ	2.54	0.40
1:E:344:THR:HB	1:E:345:PRO:HD2	2.03	0.40
1:G:847:ALA:O	1:G:850:VAL:HG23	2.21	0.40
2:H:73:SER:CA	2:H:203:ARG:NH2	2.85	0.40
2:H:102:LEU:HD23	2:H:102:LEU:HA	1.89	0.40
2:B:190:LEU:HB2	2:B:215[A]:ARG:HB3	2.03	0.40
1:C:944:ARG:HD3	1:C:972:ASP:OD1	2.21	0.40
1:C:1027:ARG:O	1:C:1031:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:LEU:O	2:D:98:LEU:HD12	2.22	0.40
2:D:173:GLY:O	2:D:182:PRO:HG2	2.22	0.40
2:D:290:HIS:HA	11:D:1444:HOH:O	2.22	0.40
1:E:101:GLU:OE1	1:E:101:GLU:HA	2.22	0.40
1:E:420:ALA:HA	1:E:423:LYS:HD2	2.04	0.40
1:E:646:THR:HB	1:E:647:PRO:HD3	2.01	0.40
1:E:648:LEU:HD12	11:E:5366:HOH:O	2.21	0.40
1:G:237:PHE:HB3	1:G:248:ILE:O	2.22	0.40
2:H:60:ILE:HG13	2:H:82:ILE:CG2	2.51	0.40
2:H:121:LEU:HD12	2:H:121:LEU:O	2.21	0.40
2:H:305:VAL:CG1	2:H:306:MET:N	2.85	0.40

All (2) 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:A:130[B]:ARG:NH1	11:F:3079:HOH:O[3_545]	1.65	0.55
2:F:10:GLU:OE1	11:A:5434:HOH:O[3_555]	2.15	0.05

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	1060/1073 (99%)	1010 (95%)	46 (4%)	4 (0%)	30	28
1	C	1053/1073 (98%)	1002 (95%)	48 (5%)	3 (0%)	36	36
1	E	1064/1073 (99%)	1011 (95%)	50 (5%)	3 (0%)	36	36
1	G	1054/1073 (98%)	981 (93%)	67 (6%)	6 (1%)	21	18
2	B	378/382 (99%)	358 (95%)	18 (5%)	2 (0%)	24	22
2	D	378/382 (99%)	362 (96%)	16 (4%)	0	100	100
2	F	378/382 (99%)	360 (95%)	17 (4%)	1 (0%)	36	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	377/382 (99%)	341 (90%)	27 (7%)	9 (2%)	4	2
All	All	5742/5820 (99%)	5425 (94%)	289 (5%)	28 (0%)	24	22

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	357	SER
1	C	368	ALA
2	F	357	SER
2	H	201	ALA
2	H	248	CYS
2	H	323	ALA
2	H	357	SER
1	A	679	GLN
1	C	2	PRO
1	C	698	ILE
1	G	558	ASP
1	G	702	VAL
1	E	975	HIS
1	G	821	GLN
2	H	11	ASP
2	H	243	GLY
2	H	269	CYS
1	A	975	HIS
1	A	1027	ARG
1	G	693	ALA
1	G	788	HIS
2	H	47	SER
2	B	245	PRO
1	E	88	PRO
1	G	860	PRO
2	H	225	ALA
1	A	2	PRO
1	E	702	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	873/878 (99%)	802 (92%)	71 (8%)	11	8
1	C	866/878 (99%)	801 (92%)	65 (8%)	12	10
1	E	877/878 (100%)	804 (92%)	73 (8%)	10	8
1	G	867/878 (99%)	771 (89%)	96 (11%)	6	3
2	B	309/310 (100%)	274 (89%)	35 (11%)	5	3
2	D	309/310 (100%)	290 (94%)	19 (6%)	17	15
2	F	309/310 (100%)	280 (91%)	29 (9%)	8	6
2	H	308/310 (99%)	262 (85%)	46 (15%)	3	1
All	All	4718/4752 (99%)	4284 (91%)	434 (9%)	9	6

All (434) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	38	ARG
1	A	59	GLU
1	A	80	LYS
1	A	103	GLU
1	A	109	GLU
1	A	110	GLU
1	A	153	GLU
1	A	174	MET
1	A	220	VAL
1	A	275	ILE
1	A	300	MET
1	A	313	LYS
1	A	326	LEU
1	A	333	ASP
1	A	363	ASN
1	A	416[A]	ASP
1	A	416[B]	ASP
1	A	422	THR
1	A	423	LYS
1	A	426	ARG
1	A	471	ARG
1	A	481	ILE
1	A	518	ASP
1	A	548	GLU

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Mol	Chain	Res	Type
1	A	558	ASP
1	A	562	ILE
1	A	591	GLU
1	A	636	LYS
1	A	640	VAL
1	A	652	ARG
1	A	665	SER
1	A	671	ARG
1	A	675	ARG
1	A	679	GLN
1	A	684	ARG
1	A	688	LYS
1	A	689	GLN
1	A	692	ASN
1	A	704	LYS
1	A	706	LYS
1	A	707	GLU
1	A	725	MET
1	A	734	LEU
1	A	739	GLN
1	A	740	THR
1	A	750	VAL
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	795	SER
1	A	800	THR
1	A	815	LYS
1	A	840	ILE
1	A	841	GLU
1	A	855	LYS
1	A	873	SER
1	A	880	THR
1	A	884	ILE
1	A	891	LYS
1	A	912	ARG
1	A	955	GLU
1	A	967[A]	GLN
1	A	967[B]	GLN
1	A	998	ARG
1	A	1001	ILE
1	A	1006	LYS

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Mol	Chain	Res	Type
1	A	1018	SER
1	A	1021	ARG
1	A	1063	ILE
1	A	1073	LYS
2	B	3	LYS
2	B	4	SER
2	B	6	LEU
2	B	13	THR
2	B	14	GLN
2	B	18	ARG
2	B	20	ILE
2	B	78	GLN
2	B	113	ILE
2	B	154	ASN
2	B	169	SER
2	B	186	LYS
2	B	192	PHE
2	B	194	VAL
2	B	218	ILE
2	B	222	GLN
2	B	224	SER
2	B	228	VAL
2	B	239	SER
2	B	252	ILE
2	B	257	LYS
2	B	261	THR
2	B	263	ILE
2	B	282	LYS
2	B	324	ASN
2	B	330	LYS
2	B	332	LEU
2	B	337	LEU
2	B	340	ILE
2	B	345	LYS
2	B	357	SER
2	B	366	LEU
2	B	376	GLN
2	B	378	ARG
2	B	379	LYS
1	C	3	LYS
1	C	4	ARG
1	C	5	THR

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Mol	Chain	Res	Type
1	C	8	LYS
1	C	24	CYS
1	C	55	MET
1	C	59	GLU
1	C	88	PRO
1	C	103	GLU
1	C	109	GLU
1	C	152	MET
1	C	185	ARG
1	C	275	ILE
1	C	297	VAL
1	C	321	LYS
1	C	326	LEU
1	C	343	ARG
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	422	THR
1	C	426	ARG
1	C	478	GLU
1	C	481	ILE
1	C	490	ARG
1	C	509	ARG
1	C	519	GLN
1	C	548	GLU
1	C	571	ARG
1	C	591	GLU
1	C	648	LEU
1	C	671	ARG
1	C	675	ARG
1	C	677	ARG
1	C	680	HIS
1	C	687	LEU
1	C	702	VAL
1	C	704	LYS
1	C	706	LYS
1	C	712	LEU
1	C	725	MET
1	C	750	VAL
1	C	751	LEU
1	C	758	ASP
1	C	763	ASP

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Mol	Chain	Res	Type
1	C	772	MET
1	C	778	ILE
1	C	784	GLN
1	C	800	THR
1	C	805	ILE
1	C	815	LYS
1	C	840	ILE
1	C	845	ARG
1	C	855	LYS
1	C	880	THR
1	C	912	ARG
1	C	930	LYS
1	C	950	ARG
1	C	951	GLU
1	C	967	GLN
1	C	1002	GLN
1	C	1018	SER
1	C	1027	ARG
1	C	1064	SER
1	C	1073	LYS
2	D	2	ILE
2	D	6	LEU
2	D	18	ARG
2	D	104	ARG
2	D	106	ASN
2	D	146	LYS
2	D	154	ASN
2	D	166	GLU
2	D	188	ASP
2	D	216	LEU
2	D	222	GLN
2	D	239	SER
2	D	257	LYS
2	D	263	ILE
2	D	282	LYS
2	D	324	ASN
2	D	333	PHE
2	D	366	LEU
2	D	380	THR
1	E	1	MET
1	E	8	LYS
1	E	55	MET

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Mol	Chain	Res	Type
1	E	76	LYS
1	E	109	GLU
1	E	133	ASP
1	E	162	VAL
1	E	174	MET
1	E	185	ARG
1	E	220	VAL
1	E	275	ILE
1	E	297	VAL
1	E	363	ASN
1	E	366	LYS
1	E	383	GLU
1	E	414	SER
1	E	416	ASP
1	E	423	LYS
1	E	426	ARG
1	E	428	LEU
1	E	471	ARG
1	E	479	VAL
1	E	515	LYS
1	E	518	ASP
1	E	548	GLU
1	E	556	SER
1	E	558	ASP
1	E	634[A]	LYS
1	E	634[B]	LYS
1	E	648	LEU
1	E	652[A]	ARG
1	E	652[B]	ARG
1	E	671	ARG
1	E	675	ARG
1	E	688	LYS
1	E	689	GLN
1	E	694	THR
1	E	698	ILE
1	E	702	VAL
1	E	706	LYS
1	E	712	LEU
1	E	731	GLU
1	E	733	ASP
1	E	734	LEU
1	E	739	GLN

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Mol	Chain	Res	Type
1	E	763	ASP
1	E	771[A]	GLU
1	E	771[B]	GLU
1	E	772	MET
1	E	784	GLN
1	E	789	SER
1	E	795	SER
1	E	805	ILE
1	E	811	GLN
1	E	815	LYS
1	E	835	ASN
1	E	839	LEU
1	E	845	ARG
1	E	855	LYS
1	E	912	ARG
1	E	940	LYS
1	E	947	LEU
1	E	950	ARG
1	E	956	ARG
1	E	957	VAL
1	E	967	GLN
1	E	970	GLU
1	E	1000	HIS
1	E	1014	ILE
1	E	1018	SER
1	E	1029	ILE
1	E	1031	ARG
1	E	1073	LYS
2	F	2	ILE
2	F	6	LEU
2	F	74	GLN
2	F	87	LEU
2	F	104	ARG
2	F	106	ASN
2	F	145	GLU
2	F	153	LEU
2	F	166	GLU
2	F	175	TRP
2	F	178	THR
2	F	183	GLN
2	F	186	LYS
2	F	190	LEU

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Mol	Chain	Res	Type
2	F	192	PHE
2	F	215	ARG
2	F	227	ASP
2	F	238	LEU
2	F	257	LYS
2	F	261	THR
2	F	321	LEU
2	F	324	ASN
2	F	326	ARG
2	F	332	LEU
2	F	343	THR
2	F	357	SER
2	F	366	LEU
2	F	376	GLN
2	F	379	LYS
1	G	1	MET
1	G	4	ARG
1	G	5	THR
1	G	8	LYS
1	G	35[A]	LYS
1	G	35[B]	LYS
1	G	43	ARG
1	G	101	GLU
1	G	103	GLU
1	G	104	ARG
1	G	153	GLU
1	G	174	MET
1	G	185	ARG
1	G	202	LYS
1	G	207	ASP
1	G	228	CYS
1	G	275	ILE
1	G	300	MET
1	G	313	LYS
1	G	338	ASP
1	G	353	ASP
1	G	358	LYS
1	G	363	ASN
1	G	412	LYS
1	G	414	SER
1	G	416	ASP
1	G	471	ARG

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Mol	Chain	Res	Type
1	G	518	ASP
1	G	548	GLU
1	G	558	ASP
1	G	561	LYS
1	G	562	ILE
1	G	587	LEU
1	G	591	GLU
1	G	631	ARG
1	G	636	LYS
1	G	640	VAL
1	G	648	LEU
1	G	649	LYS
1	G	652	ARG
1	G	662	ILE
1	G	665	SER
1	G	671	ARG
1	G	675	ARG
1	G	679	GLN
1	G	682	VAL
1	G	688	LYS
1	G	692	ASN
1	G	700	MET
1	G	702	VAL
1	G	704	LYS
1	G	706	LYS
1	G	708	ILE
1	G	712	LEU
1	G	713	VAL
1	G	714	VAL
1	G	728	VAL
1	G	733	ASP
1	G	735	ARG
1	G	750	VAL
1	G	751	LEU
1	G	752	LEU
1	G	753	ASP
1	G	772	MET
1	G	784	GLN
1	G	789	SER
1	G	792	SER
1	G	800	THR
1	G	805	ILE

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Mol	Chain	Res	Type
1	G	815	LYS
1	G	820	LEU
1	G	826	MET
1	G	835	ASN
1	G	849	THR
1	G	855	LYS
1	G	874	LEU
1	G	880	THR
1	G	884	ILE
1	G	912	ARG
1	G	940	LYS
1	G	947	LEU
1	G	950	ARG
1	G	955	GLU
1	G	967	GLN
1	G	1001	ILE
1	G	1006	LYS
1	G	1014	ILE
1	G	1018	SER
1	G	1021	ARG
1	G	1026	SER
1	G	1027	ARG
1	G	1029	ILE
1	G	1032	SER
1	G	1061	LYS
1	G	1063	ILE
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	18	ARG
2	H	50	ARG
2	H	87	LEU
2	H	104	ARG
2	H	128	GLN
2	H	142	LEU
2	H	145	GLU
2	H	148	ARG
2	H	154	ASN
2	H	178	THR
2	H	187	GLU
2	H	202	LYS
2	H	205	ILE

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Mol	Chain	Res	Type
2	H	209	LEU
2	H	212	ARG
2	H	216	LEU
2	H	217	THR
2	H	219	VAL
2	H	222	GLN
2	H	224	SER
2	H	227	ASP
2	H	228	VAL
2	H	236	ILE
2	H	238	LEU
2	H	239	SER
2	H	249	ASP
2	H	257	LYS
2	H	261	THR
2	H	265	VAL
2	H	279	SER
2	H	282	LYS
2	H	300	VAL
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	342	ARG
2	H	357	SER
2	H	366	LEU
2	H	372	GLU
2	H	374	ILE
2	H	375	GLU
2	H	376	GLN
2	H	378	ARG
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	391	GLN
1	A	519	GLN
1	A	554	ASN
1	A	680	HIS
1	A	689	GLN

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Mol	Chain	Res	Type
1	A	692	ASN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	827	ASN
1	A	834	ASN
1	A	835	ASN
1	A	843	ASN
1	A	898	ASN
1	A	936	ASN
1	A	942	HIS
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1071	GLN
2	B	78	GLN
2	B	222	GLN
2	B	232	ASN
2	B	324	ASN
2	B	353	HIS
1	C	105	GLN
1	C	266	ASN
1	C	645	GLN
1	C	692	ASN
1	C	784	GLN
1	C	803	GLN
1	C	812	GLN
1	C	834	ASN
1	C	835	ASN
1	C	898	ASN
1	C	936	ASN
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	78	GLN
2	D	106	ASN
2	D	222	GLN

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Mol	Chain	Res	Type
2	D	256	GLN
2	D	324	ASN
2	D	351	GLN
1	E	105	GLN
1	E	225	ASN
1	E	266	ASN
1	E	337	ASN
1	E	554	ASN
1	E	679	GLN
1	E	692	ASN
1	E	784	GLN
1	E	803	GLN
1	E	814	GLN
1	E	827	ASN
1	E	834	ASN
1	E	835	ASN
1	E	843	ASN
1	E	936	ASN
1	E	942	HIS
1	E	987	ASN
1	E	992	ASN
1	E	995	HIS
1	E	1000	HIS
1	E	1035	GLN
1	E	1039	HIS
1	E	1071	GLN
2	F	51	GLN
2	F	74	GLN
2	F	105	HIS
2	F	154	ASN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	225	ASN
1	G	337	ASN
1	G	457	ASN
1	G	519	GLN
1	G	554	ASN
1	G	679	GLN
1	G	689	GLN
1	G	692	ASN
1	G	784	GLN

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Mol	Chain	Res	Type
1	G	803	GLN
1	G	834	ASN
1	G	898	ASN
1	G	936	ASN
1	G	967	GLN
1	G	987	ASN
1	G	992	ASN
1	G	1055	ASN
1	G	1069	HIS
1	G	1071	GLN
2	H	14	GLN
2	H	51	GLN
2	H	76	HIS
2	H	78	GLN
2	H	105	HIS
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN
2	H	351	GLN
2	H	361	HIS

5.3.3 RNA [i](#)

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 80 ligands modelled in this entry, 52 are monoatomic - leaving 28 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
10	NET	C	5033	-	8,8,8	0.64	0	10,10,10	0.53	0
7	ADP	C	5027	4,3	28,29,29	1.26	3 (10%)	43,45,45	0.90	2 (4%)
8	ORN	C	5031	-	7,8,8	0.91	0	6,9,9	1.05	0
8	ORN	E	5051	-	7,8,8	0.94	0	6,9,9	1.28	1 (16%)
6	PO4	E	5046	4,3	4,4,4	2.90	3 (75%)	6,6,6	0.66	0
9	IMP	A	5012	-	25,25,25	1.56	3 (12%)	37,38,38	1.52	6 (16%)
7	ADP	A	5000	3	28,29,29	1.11	4 (14%)	43,45,45	0.89	2 (4%)
8	ORN	G	5071	-	7,8,8	0.86	1 (14%)	6,9,9	1.10	0
6	PO4	C	5026	4,3	4,4,4	2.59	3 (75%)	6,6,6	0.91	0
8	ORN	A	5011	-	7,8,8	1.21	1 (14%)	6,9,9	1.23	1 (16%)
7	ADP	A	5007	4,3	28,29,29	1.39	2 (7%)	43,45,45	0.99	2 (4%)
9	IMP	E	5052	-	25,25,25	1.37	2 (8%)	37,38,38	2.03	6 (16%)
10	NET	E	5053	-	8,8,8	0.86	0	10,10,10	0.39	0
10	NET	G	5073	-	8,8,8	0.73	0	10,10,10	0.51	0
6	PO4	A	5006	4,3	4,4,4	2.08	2 (50%)	6,6,6	1.33	1 (16%)
7	ADP	E	5040	3	28,29,29	1.13	3 (10%)	43,45,45	0.92	2 (4%)
8	ORN	A	5014	-	7,8,8	1.01	1 (14%)	6,9,9	0.90	0
10	NET	A	5013	-	8,8,8	0.73	0	10,10,10	0.62	0
7	ADP	C	5020	3	28,29,29	1.37	6 (21%)	43,45,45	1.02	4 (9%)
6	PO4	G	5066	4,3	4,4,4	1.86	2 (50%)	6,6,6	1.01	0
8	ORN	G	5074	-	7,8,8	1.09	1 (14%)	6,9,9	0.86	0
7	ADP	E	5047	4,3	28,29,29	1.08	2 (7%)	43,45,45	0.99	3 (6%)
7	ADP	G	5067	4,3	28,29,29	1.17	6 (21%)	43,45,45	1.16	4 (9%)
7	ADP	G	5060	3	28,29,29	1.23	3 (10%)	43,45,45	1.13	2 (4%)
8	ORN	E	5054	-	7,8,8	0.91	0	6,9,9	2.56	3 (50%)
9	IMP	C	5032	-	25,25,25	1.55	2 (8%)	37,38,38	1.44	6 (16%)
9	IMP	G	5072	-	25,25,25	1.30	3 (12%)	37,38,38	1.72	7 (18%)
8	ORN	C	5034	-	7,8,8	1.05	1 (14%)	6,9,9	0.99	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NET	C	5033	-	-	0/12/12/12	-
7	ADP	C	5027	4,3	-	4/16/32/32	0/3/3/3
8	ORN	C	5031	-	-	6/8/8/8	-
8	ORN	E	5051	-	-	5/8/8/8	-
9	IMP	A	5012	-	-	1/10/26/26	0/3/3/3
7	ADP	A	5000	3	-	2/16/32/32	0/3/3/3
8	ORN	G	5071	-	-	6/8/8/8	-
8	ORN	A	5011	-	-	6/8/8/8	-
7	ADP	A	5007	4,3	-	4/16/32/32	0/3/3/3
9	IMP	E	5052	-	-	3/10/26/26	0/3/3/3
10	NET	E	5053	-	-	3/12/12/12	-
10	NET	G	5073	-	-	3/12/12/12	-
7	ADP	E	5040	3	-	2/16/32/32	0/3/3/3
8	ORN	A	5014	-	-	6/8/8/8	-
10	NET	A	5013	-	-	0/12/12/12	-
7	ADP	C	5020	3	-	2/16/32/32	0/3/3/3
8	ORN	G	5074	-	-	4/8/8/8	-
7	ADP	E	5047	4,3	-	3/16/32/32	0/3/3/3
7	ADP	G	5067	4,3	-	2/16/32/32	0/3/3/3
7	ADP	G	5060	3	-	1/16/32/32	0/3/3/3
8	ORN	E	5054	-	-	2/8/8/8	-
9	IMP	C	5032	-	-	1/10/26/26	0/3/3/3
9	IMP	G	5072	-	-	1/10/26/26	0/3/3/3
8	ORN	C	5034	-	-	5/8/8/8	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	5012	IMP	O6-C6	5.93	1.34	1.23
9	C	5032	IMP	O6-C6	5.85	1.34	1.23
7	A	5007	ADP	PA-O3A	-4.66	1.54	1.59
9	E	5052	IMP	O6-C6	4.50	1.32	1.23
9	G	5072	IMP	O6-C6	4.10	1.31	1.23
6	E	5046	PO4	P-O2	-3.92	1.43	1.54
6	C	5026	PO4	P-O4	-3.40	1.44	1.54
6	E	5046	PO4	P-O3	-3.26	1.45	1.54
7	C	5020	ADP	PA-O3A	-3.20	1.56	1.59
7	C	5027	ADP	O3'-C3'	3.09	1.50	1.43
6	C	5026	PO4	P-O2	-3.07	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	5040	ADP	PA-O3A	-3.07	1.56	1.59
7	G	5060	ADP	O3'-C3'	3.06	1.50	1.43
6	A	5006	PO4	P-O2	-3.00	1.45	1.54
9	E	5052	IMP	P-O3P	-2.97	1.43	1.54
7	C	5027	ADP	O2'-C2'	2.81	1.49	1.43
6	E	5046	PO4	P-O4	-2.73	1.46	1.54
7	G	5060	ADP	PA-O3A	-2.70	1.56	1.59
7	C	5020	ADP	O2'-C2'	2.68	1.49	1.43
7	A	5007	ADP	O3'-C3'	2.62	1.49	1.43
7	C	5027	ADP	C2-N1	2.62	1.38	1.33
7	E	5047	ADP	C2-N1	2.60	1.38	1.33
6	G	5066	PO4	P-O2	-2.53	1.47	1.54
6	G	5066	PO4	P-O4	-2.50	1.47	1.54
7	G	5067	ADP	O3'-C3'	2.49	1.49	1.43
7	E	5040	ADP	C2-N3	-2.48	1.29	1.33
7	G	5060	ADP	C2-N3	-2.45	1.29	1.33
9	A	5012	IMP	P-O3P	-2.45	1.45	1.54
9	C	5032	IMP	O3'-C3'	2.43	1.49	1.43
7	C	5020	ADP	O3'-C3'	2.41	1.48	1.43
6	A	5006	PO4	P-O4	-2.40	1.47	1.54
7	A	5000	ADP	O3'-C3'	2.39	1.48	1.43
7	E	5047	ADP	O3'-C3'	2.39	1.48	1.43
7	C	5020	ADP	O4'-C1'	-2.35	1.36	1.42
6	C	5026	PO4	P-O3	-2.35	1.47	1.54
7	G	5067	ADP	C2-N1	2.30	1.38	1.33
8	C	5034	ORN	O-C	2.28	1.28	1.22
7	G	5067	ADP	O4'-C1'	-2.28	1.36	1.42
7	C	5020	ADP	C2-N1	2.25	1.37	1.33
9	G	5072	IMP	O2'-C2'	2.25	1.48	1.43
7	A	5000	ADP	PA-O3A	-2.24	1.57	1.59
8	A	5014	ORN	O-C	2.22	1.28	1.22
7	E	5040	ADP	O3'-C3'	2.21	1.48	1.43
8	A	5011	ORN	O-C	2.19	1.28	1.22
9	G	5072	IMP	O3'-C3'	2.16	1.48	1.43
7	A	5000	ADP	O2'-C2'	2.16	1.48	1.43
8	G	5074	ORN	O-C	2.15	1.28	1.22
9	A	5012	IMP	O3'-C3'	2.11	1.48	1.43
8	G	5071	ORN	O-C	2.05	1.28	1.22
7	G	5067	ADP	O2'-C2'	2.04	1.48	1.43
7	C	5020	ADP	C8-N7	2.04	1.35	1.31
7	G	5067	ADP	PA-O3A	-2.04	1.57	1.59
7	A	5000	ADP	C2-N3	-2.02	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5067	ADP	C8-N7	2.00	1.35	1.31

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	5052	IMP	O3P-P-O5'	-6.43	89.90	106.67
9	E	5052	IMP	C2-N1-C6	-5.42	117.67	125.09
9	G	5072	IMP	C2-N1-C6	-5.00	118.24	125.09
9	A	5012	IMP	C2-N1-C6	-4.72	118.62	125.09
9	E	5052	IMP	C5-C6-N1	4.40	117.10	110.78
9	G	5072	IMP	N1-C2-N3	4.17	130.29	125.50
9	E	5052	IMP	N1-C2-N3	4.15	130.27	125.50
9	G	5072	IMP	C5-C6-N1	4.14	116.74	110.78
9	C	5032	IMP	C2-N1-C6	-4.08	119.50	125.09
7	G	5067	ADP	O3B-PB-O3A	3.91	117.76	104.64
8	E	5054	ORN	CB-CA-N	3.75	119.88	110.12
8	E	5054	ORN	CB-CA-C	3.73	120.34	110.45
9	C	5032	IMP	N1-C2-N3	3.71	129.76	125.50
9	E	5052	IMP	O2'-C2'-C3'	3.70	123.67	111.82
9	A	5012	IMP	N1-C2-N3	3.68	129.73	125.50
9	A	5012	IMP	C5-C6-N1	3.50	115.81	110.78
9	G	5072	IMP	O3P-P-O5'	-3.45	97.67	106.67
7	G	5060	ADP	O3'-C3'-C2'	3.29	122.37	111.82
7	A	5007	ADP	O3B-PB-O3A	3.23	115.46	104.64
7	E	5047	ADP	O2A-PA-O3A	3.08	115.61	107.27
9	C	5032	IMP	O3P-P-O5'	-3.07	98.66	106.67
9	A	5012	IMP	O3'-C3'-C2'	3.04	121.55	111.82
9	G	5072	IMP	O2'-C2'-C3'	2.99	121.40	111.82
7	G	5060	ADP	O2'-C2'-C3'	2.96	121.29	111.82
9	C	5032	IMP	C5-C6-N1	2.84	114.86	110.78
7	E	5040	ADP	O3'-C3'-C2'	2.81	120.82	111.82
7	G	5067	ADP	O2'-C2'-C3'	2.79	120.78	111.82
9	A	5012	IMP	O2P-P-O5'	2.79	113.93	106.67
7	G	5067	ADP	O3'-C3'-C2'	2.76	120.68	111.82
8	A	5011	ORN	CB-CA-C	-2.74	103.18	110.45
7	E	5047	ADP	O2'-C2'-C3'	2.68	120.40	111.82
9	G	5072	IMP	O3'-C3'-C2'	2.60	120.16	111.82
9	E	5052	IMP	O3'-C3'-C2'	2.58	120.10	111.82
7	A	5007	ADP	O2'-C2'-C3'	2.56	120.02	111.82
7	C	5027	ADP	O2'-C2'-C3'	2.48	119.77	111.82
7	G	5067	ADP	O2A-PA-O3A	2.43	113.84	107.27
9	G	5072	IMP	O3P-P-O2P	2.42	116.87	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	5054	ORN	OXT-C-O	-2.41	118.61	124.08
7	E	5047	ADP	O3'-C3'-C2'	2.41	119.54	111.82
9	C	5032	IMP	O3'-C3'-C2'	2.36	119.38	111.82
8	E	5051	ORN	OXT-C-O	-2.36	118.73	124.08
7	C	5020	ADP	O3'-C3'-C2'	2.32	119.25	111.82
7	C	5020	ADP	C5-C6-N6	2.31	129.00	123.29
7	A	5000	ADP	C2'-C3'-C4'	-2.24	98.28	102.61
7	A	5000	ADP	O3B-PB-O3A	-2.23	97.16	104.64
7	E	5040	ADP	C3'-C2'-C1'	2.15	105.53	101.46
7	C	5020	ADP	C2'-C3'-C4'	-2.15	98.45	102.61
6	A	5006	PO4	O4-P-O2	2.12	114.52	107.91
8	C	5034	ORN	OXT-C-O	-2.09	119.34	124.08
9	C	5032	IMP	O2'-C2'-C3'	2.08	118.49	111.82
7	C	5027	ADP	O2A-PA-O3A	2.06	112.85	107.27
9	A	5012	IMP	O3P-P-O5'	-2.05	101.33	106.67
7	C	5020	ADP	N6-C6-N1	-2.01	113.91	118.38

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5007	ADP	PA-O3A-PB-O3B
7	C	5027	ADP	PA-O3A-PB-O3B
7	E	5047	ADP	PA-O3A-PB-O3B
8	A	5011	ORN	N-CA-CB-CG
8	A	5011	ORN	C-CA-CB-CG
8	A	5014	ORN	C-CA-CB-CG
8	A	5014	ORN	NE-CD-CG-CB
8	C	5031	ORN	N-CA-CB-CG
8	C	5031	ORN	C-CA-CB-CG
8	C	5034	ORN	C-CA-CB-CG
8	E	5051	ORN	N-CA-CB-CG
8	E	5051	ORN	C-CA-CB-CG
8	G	5071	ORN	N-CA-CB-CG
8	G	5071	ORN	C-CA-CB-CG
8	G	5074	ORN	N-CA-CB-CG
9	A	5012	IMP	C5'-O5'-P-O2P
9	E	5052	IMP	C5'-O5'-P-O2P
9	E	5052	IMP	C5'-O5'-P-O3P
9	G	5072	IMP	C5'-O5'-P-O2P
10	E	5053	NET	C4-C3-N1-C7
10	E	5053	NET	C4-C3-N1-C5

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Mol	Chain	Res	Type	Atoms
10	E	5053	NET	C4-C3-N1-C1
8	A	5011	ORN	OXT-C-CA-N
8	G	5071	ORN	OXT-C-CA-N
8	C	5031	ORN	CA-CB-CG-CD
8	G	5071	ORN	CA-CB-CG-CD
8	A	5014	ORN	OXT-C-CA-N
8	C	5031	ORN	OXT-C-CA-N
8	E	5051	ORN	OXT-C-CA-N
9	E	5052	IMP	C5'-O5'-P-O1P
8	E	5051	ORN	CA-CB-CG-CD
8	A	5011	ORN	O-C-CA-N
8	A	5014	ORN	O-C-CA-N
8	C	5031	ORN	O-C-CA-N
8	E	5051	ORN	O-C-CA-N
8	G	5071	ORN	O-C-CA-N
9	C	5032	IMP	C5'-O5'-P-O2P
7	C	5027	ADP	PA-O3A-PB-O1B
8	G	5074	ORN	C-CA-CB-CG
7	A	5000	ADP	PB-O3A-PA-O1A
7	G	5060	ADP	PB-O3A-PA-O1A
8	C	5034	ORN	NE-CD-CG-CB
8	G	5074	ORN	NE-CD-CG-CB
8	A	5011	ORN	CA-CB-CG-CD
8	C	5034	ORN	N-CA-CB-CG
10	G	5073	NET	C8-C7-N1-C1
8	C	5031	ORN	NE-CD-CG-CB
10	G	5073	NET	C8-C7-N1-C5
7	A	5007	ADP	PB-O3A-PA-O2A
7	E	5047	ADP	PB-O3A-PA-O2A
10	G	5073	NET	C8-C7-N1-C3
8	E	5054	ORN	NE-CD-CG-CB
8	C	5034	ORN	OXT-C-CA-N
8	E	5054	ORN	OXT-C-CA-N
8	A	5014	ORN	CA-CB-CG-CD
8	G	5071	ORN	NE-CD-CG-CB
7	C	5027	ADP	PB-O3A-PA-O2A
7	E	5040	ADP	PB-O3A-PA-O1A
8	A	5011	ORN	NE-CD-CG-CB
7	A	5007	ADP	PA-O3A-PB-O1B
7	C	5020	ADP	PA-O3A-PB-O2B
7	E	5047	ADP	PA-O3A-PB-O2B
8	G	5074	ORN	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
7	C	5020	ADP	PB-O3A-PA-O1A
7	C	5027	ADP	PB-O3A-PA-O1A
7	G	5067	ADP	PB-O3A-PA-O1A
7	G	5067	ADP	PB-O3A-PA-O2A
8	A	5014	ORN	N-CA-CB-CG
8	C	5034	ORN	O-C-CA-N
7	A	5000	ADP	PB-O3A-PA-O2A
7	A	5007	ADP	PB-O3A-PA-O1A
7	E	5040	ADP	PB-O3A-PA-O2A

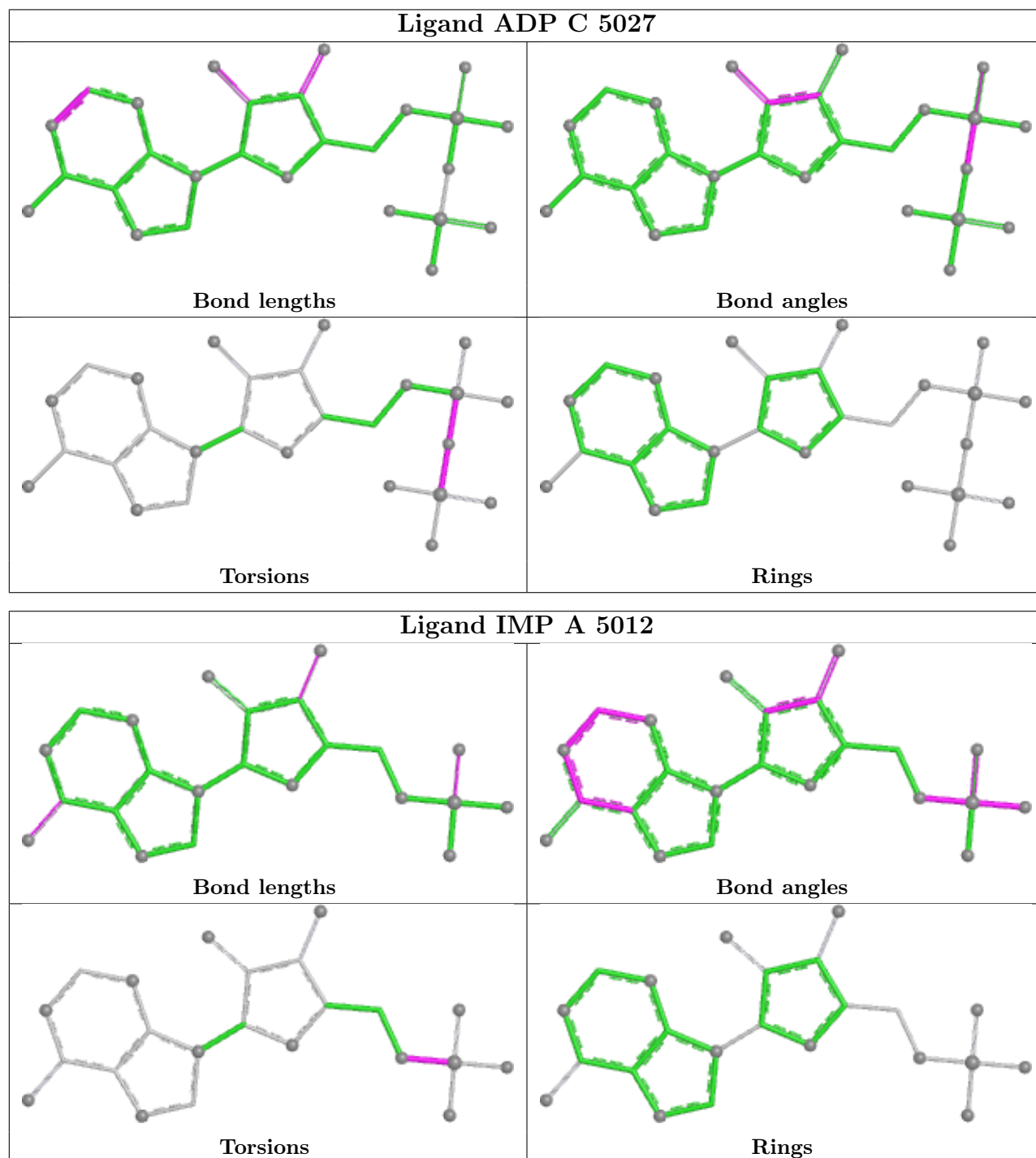
There are no ring outliers.

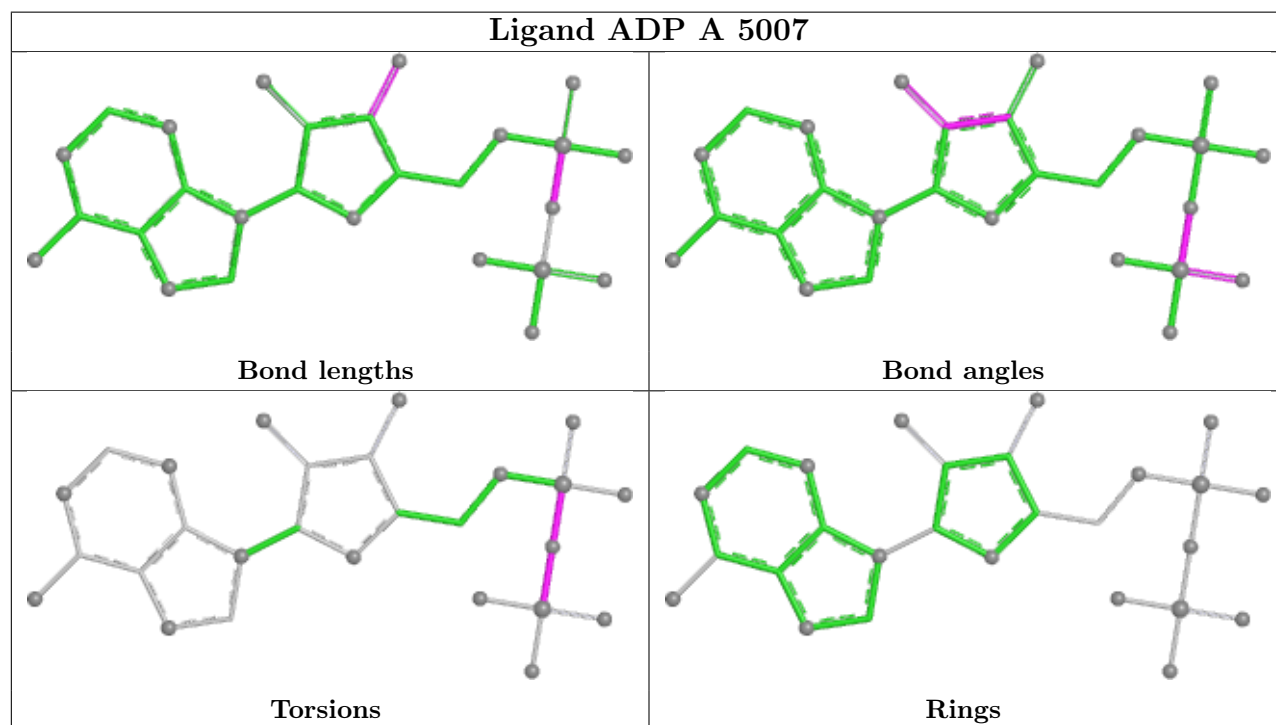
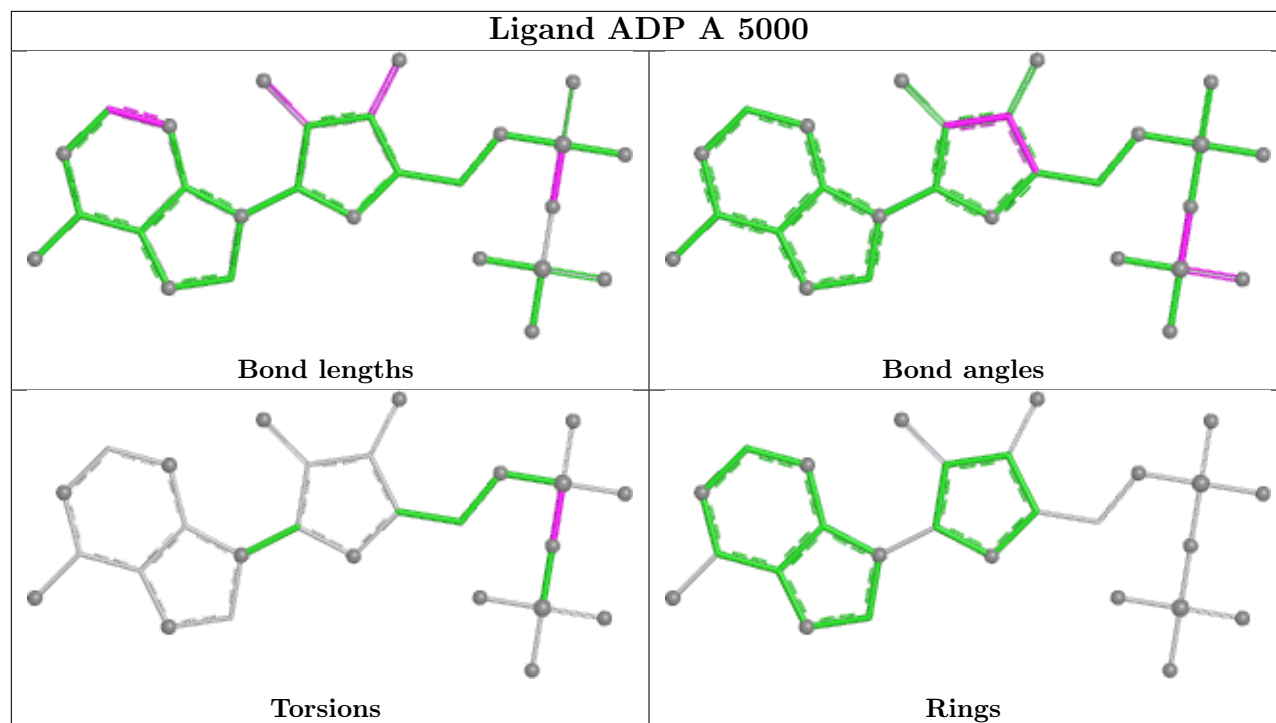
19 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	5027	ADP	1	0
8	C	5031	ORN	2	0
8	E	5051	ORN	2	0
8	G	5071	ORN	1	0
8	A	5011	ORN	1	0
7	A	5007	ADP	2	0
9	E	5052	IMP	2	0
10	E	5053	NET	3	0
10	G	5073	NET	1	0
7	E	5040	ADP	1	0
8	A	5014	ORN	3	0
8	G	5074	ORN	3	0
7	E	5047	ADP	4	0
7	G	5067	ADP	3	0
7	G	5060	ADP	1	0
8	E	5054	ORN	2	0
9	C	5032	IMP	1	0
9	G	5072	IMP	1	0
8	C	5034	ORN	1	0

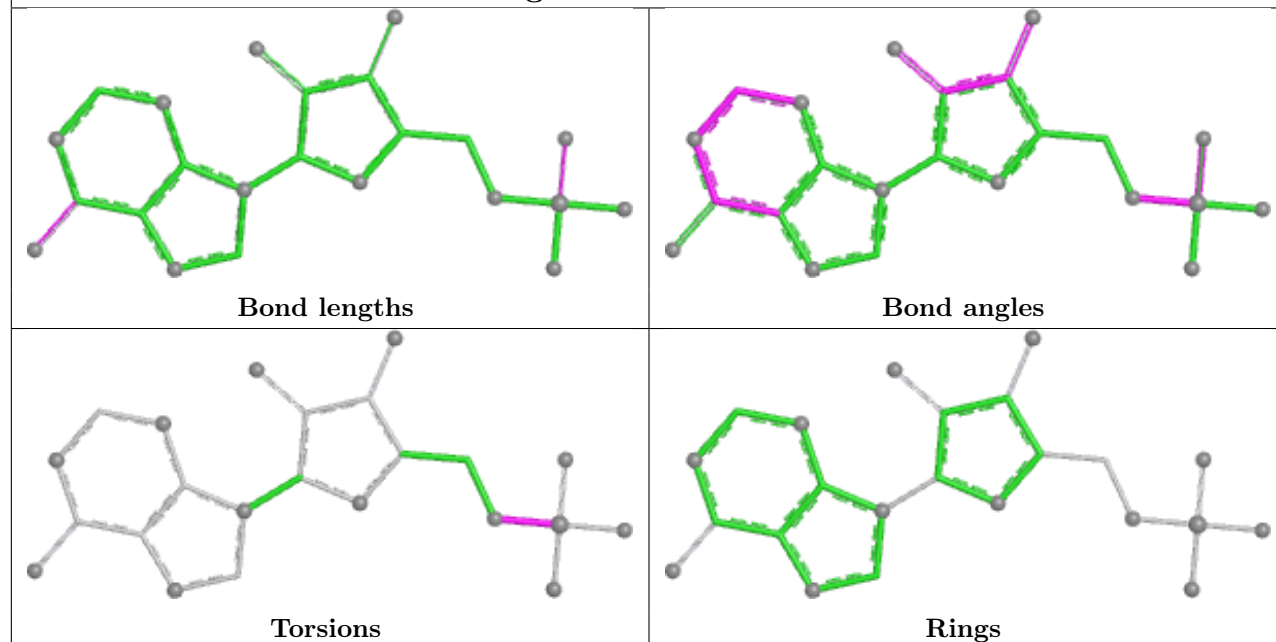
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

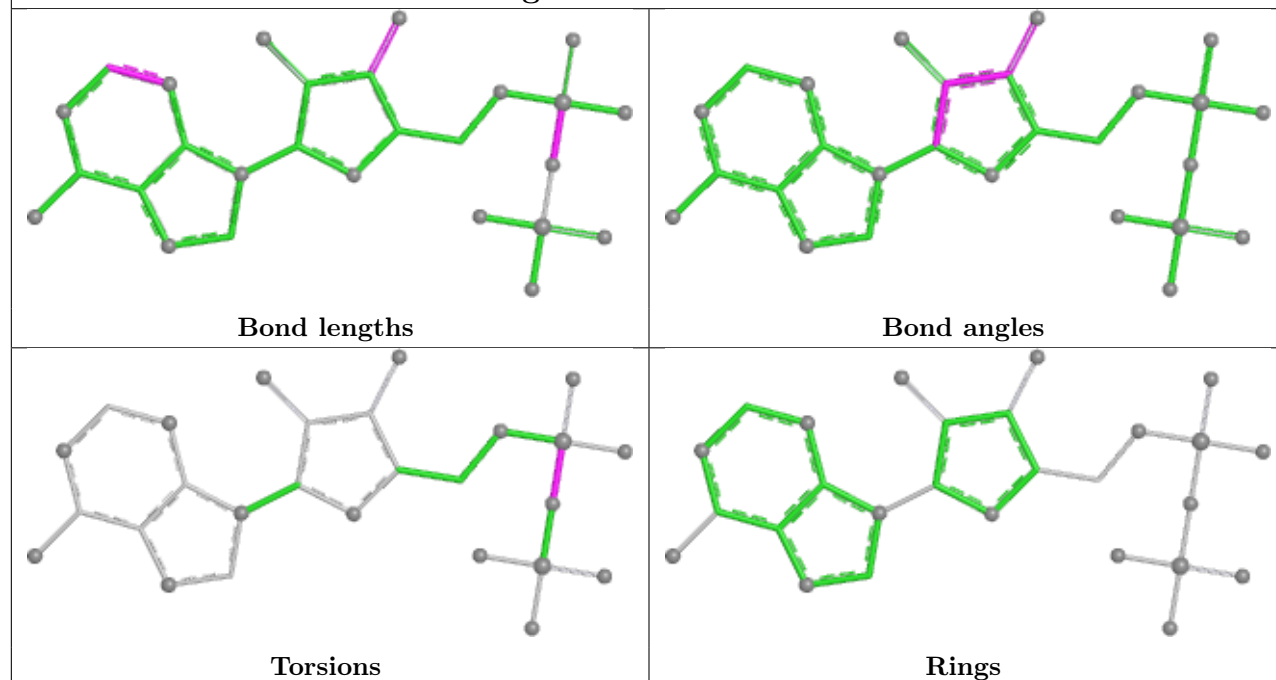




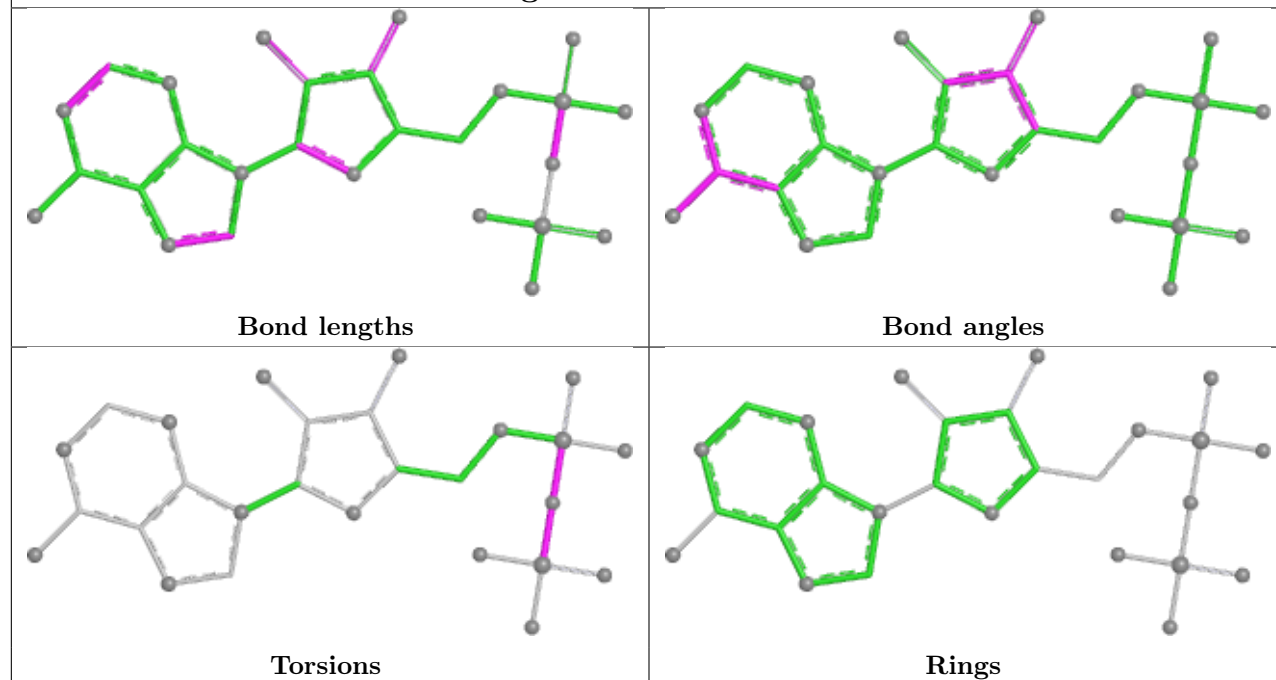
Ligand IMP E 5052



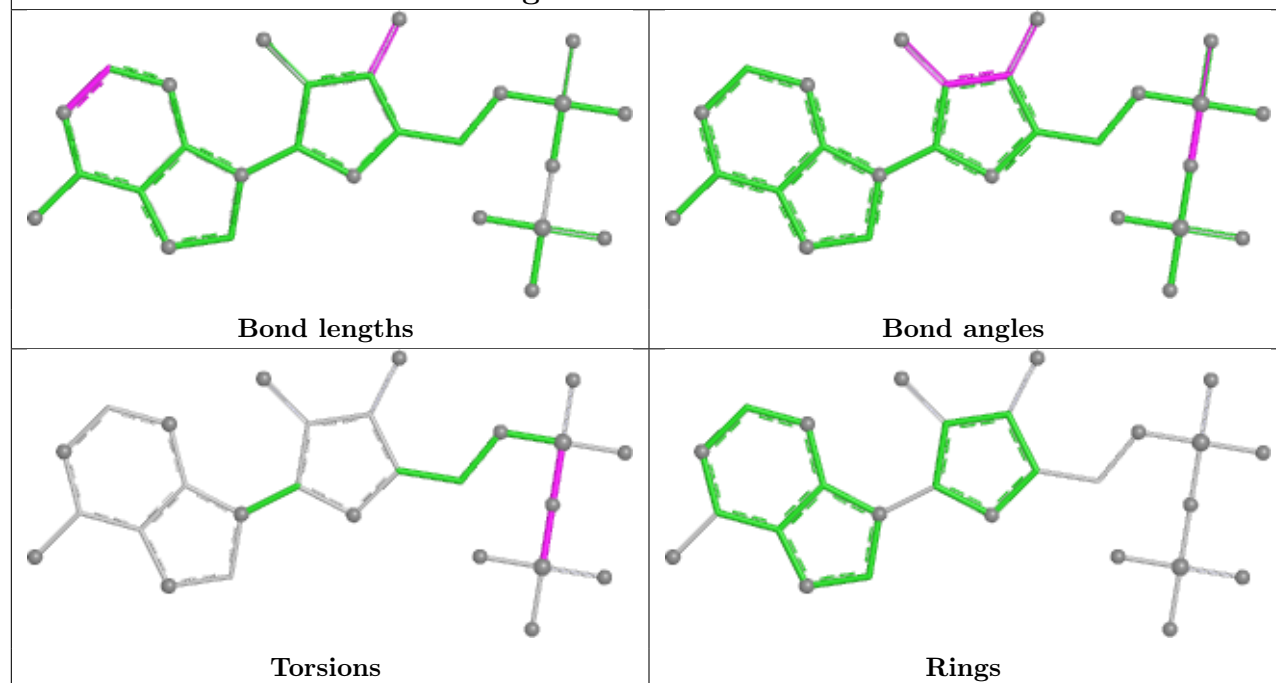
Ligand ADP E 5040



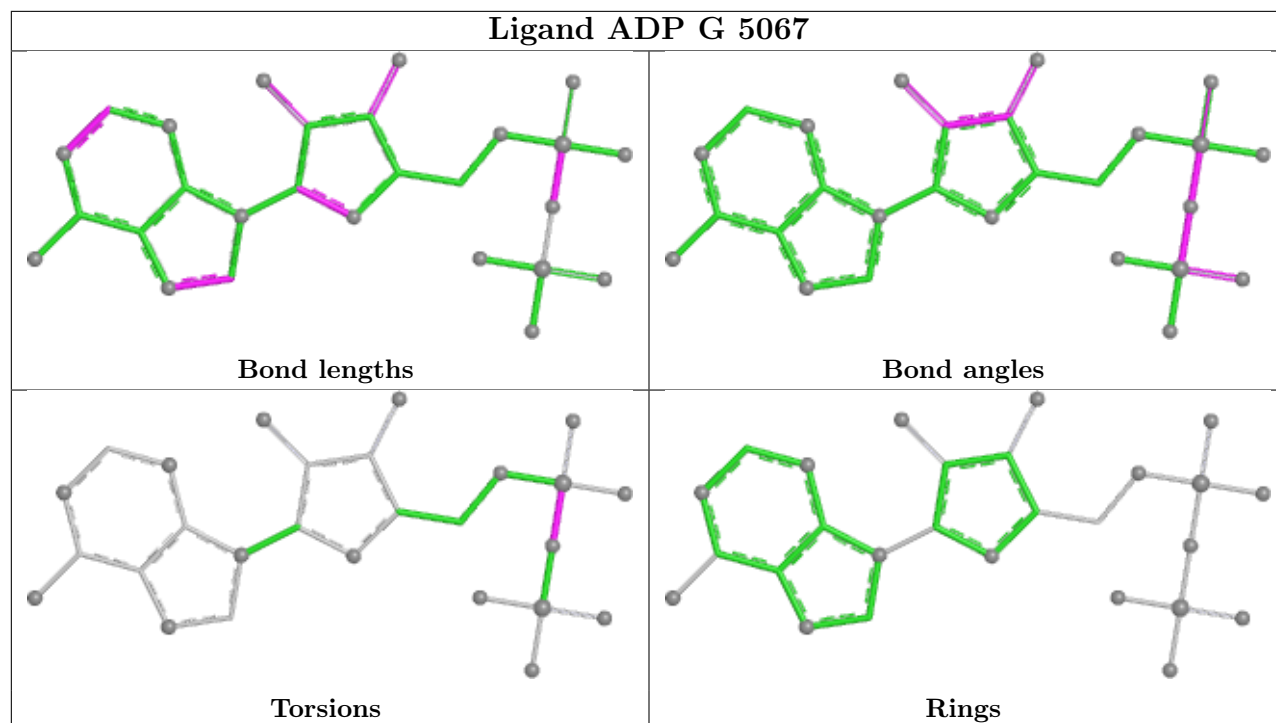
Ligand ADP C 5020



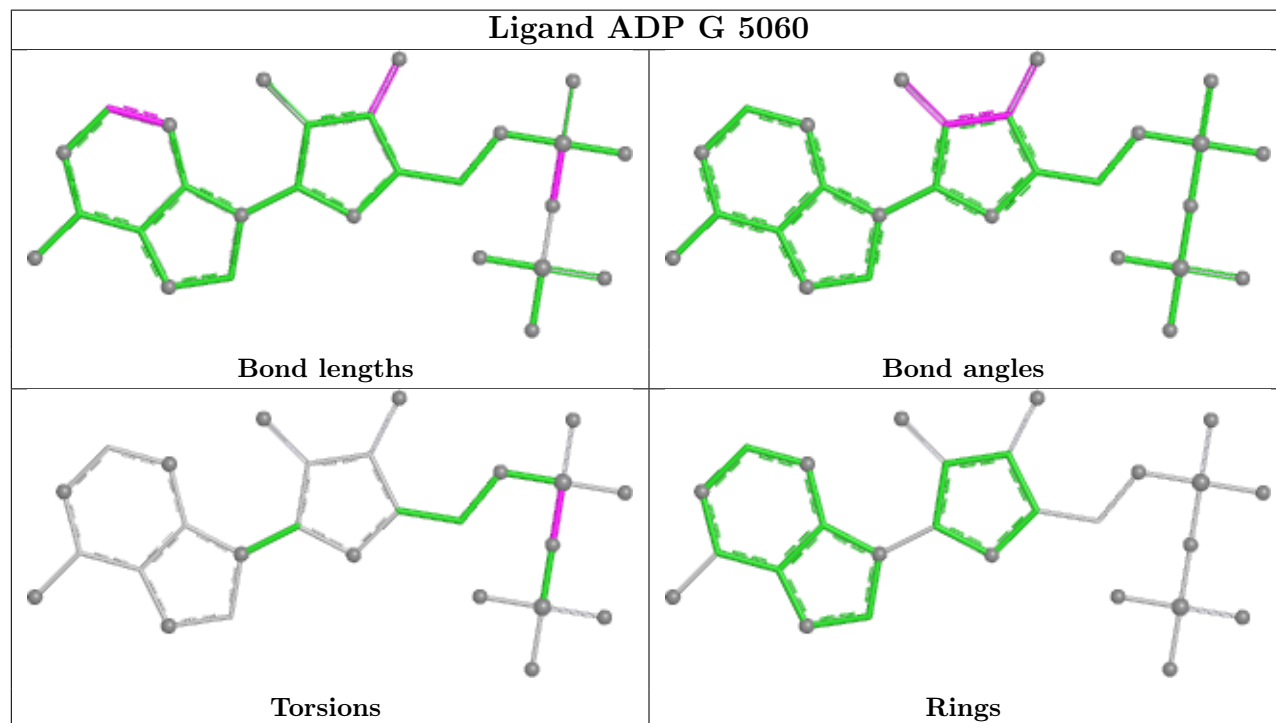
Ligand ADP E 5047

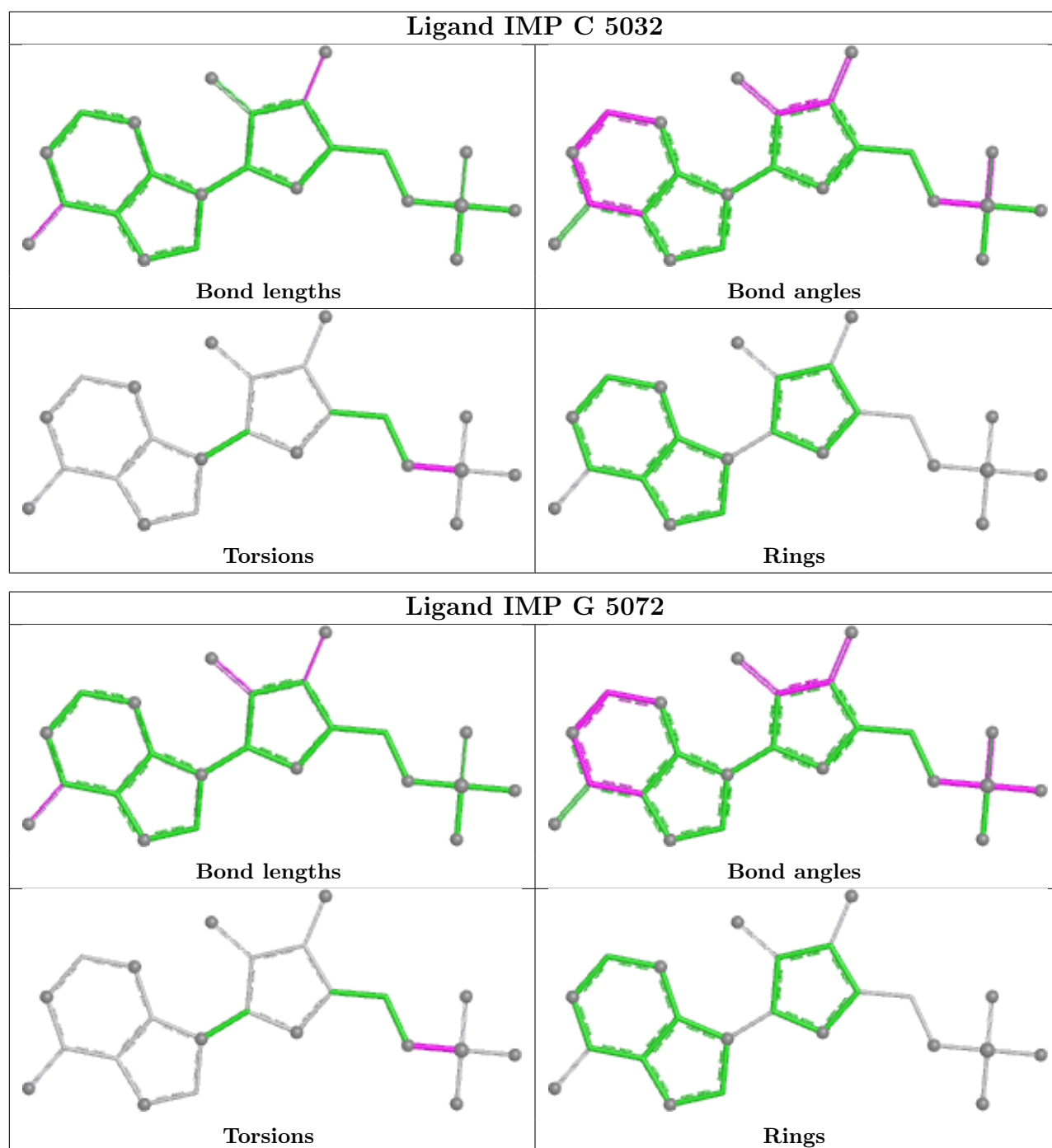


Ligand ADP G 5067



Ligand ADP G 5060





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.