



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:09 PM UTC

PDB ID : 1BXR / pdb_00001bxr
Title : STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE COM-
PLEXED WITH THE ATP ANALOG AMPPNP
Authors : Thoden, J.B.; Wesenberg, G.; Raushel, F.M.; Holden, H.M.
Deposited on : 1998-10-08
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

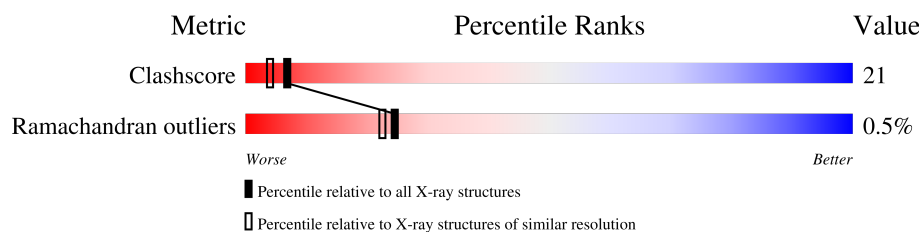
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

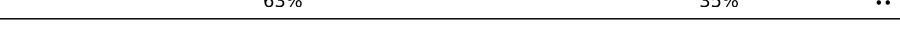
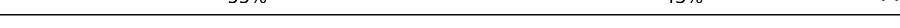
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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)

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	 65% 32% .
1	C	1073	 70% 28% .
1	E	1073	 72% 27% .
1	G	1073	 63% 33% .
2	B	382	 62% 34% ..
2	D	382	 69% 30% ..
2	F	382	 63% 35% ..
2	H	382	 55% 43% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	E	2980	-	-	X	-
8	NET	A	1086	-	-	X	-
8	NET	E	2950	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 48307 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 CARBAMOYL-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1073	Total	C	N	O	S	0	4	0
			8288	5203	1445	1594	46			
1	C	1073	Total	C	N	O	S	0	0	0
			8268	5190	1441	1592	45			
1	E	1073	Total	C	N	O	S	0	3	0
			8284	5199	1445	1595	45			
1	G	1073	Total	C	N	O	S	0	2	0
			8279	5196	1445	1593	45			

- Molecule 2 is a protein called CARBAMOYL-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	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 Mn 3 3	0	0
3	C	4	Total Mn 4 4	0	0
3	E	3	Total Mn 3 3	0	0
3	G	3	Total Mn 3 3	0	0

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

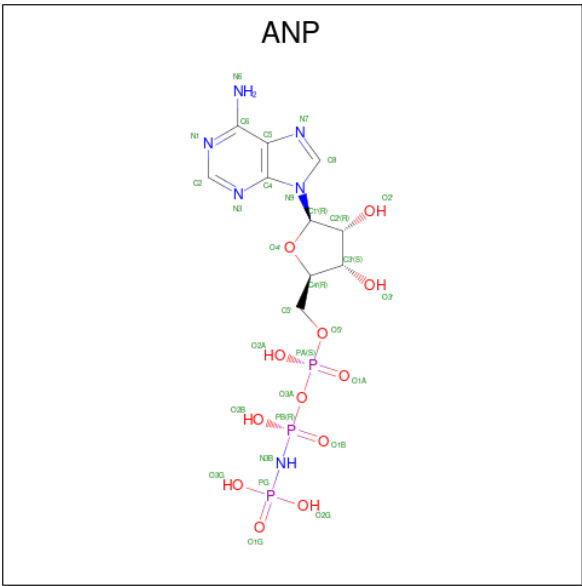
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total K 3 3	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	G	4	Total K 4 4	0	0
4	H	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	2	Total Cl 2 2	0	0
5	G	4	Total Cl 4 4	0	0

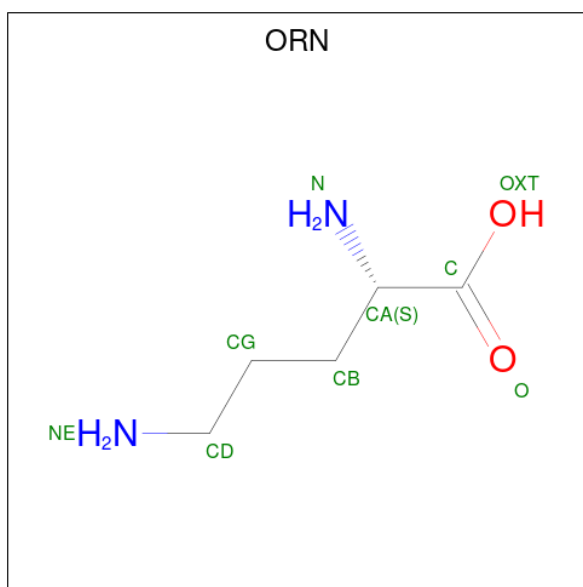
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



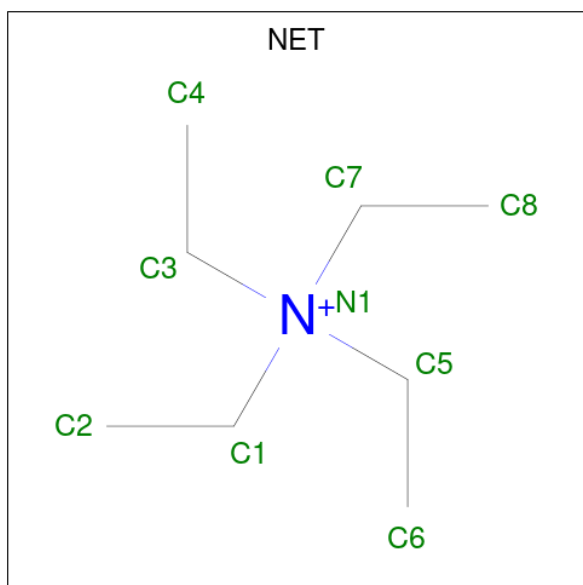
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂).



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

- Molecule 8 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: C₈H₂₀N⁺).



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

- Molecule 9 is water.

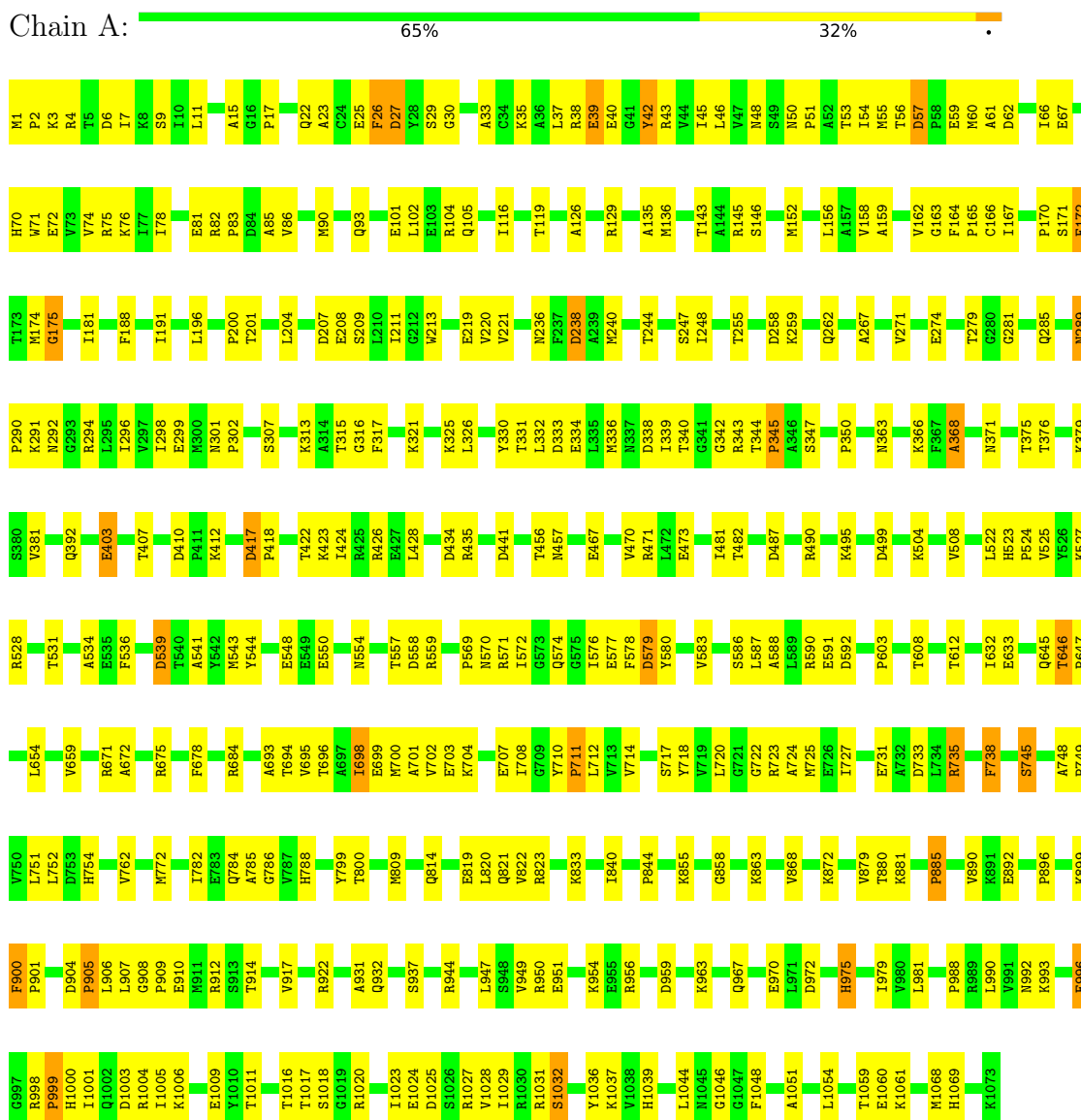
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	677	Total O 677 677	0	0
9	B	169	Total O 169 169	0	0
9	C	624	Total O 624 624	0	0
9	D	234	Total O 234 234	0	0
9	E	650	Total O 650 650	0	0
9	F	193	Total O 193 193	0	0
9	G	530	Total O 530 530	0	0
9	H	165	Total O 165 165	0	0

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.

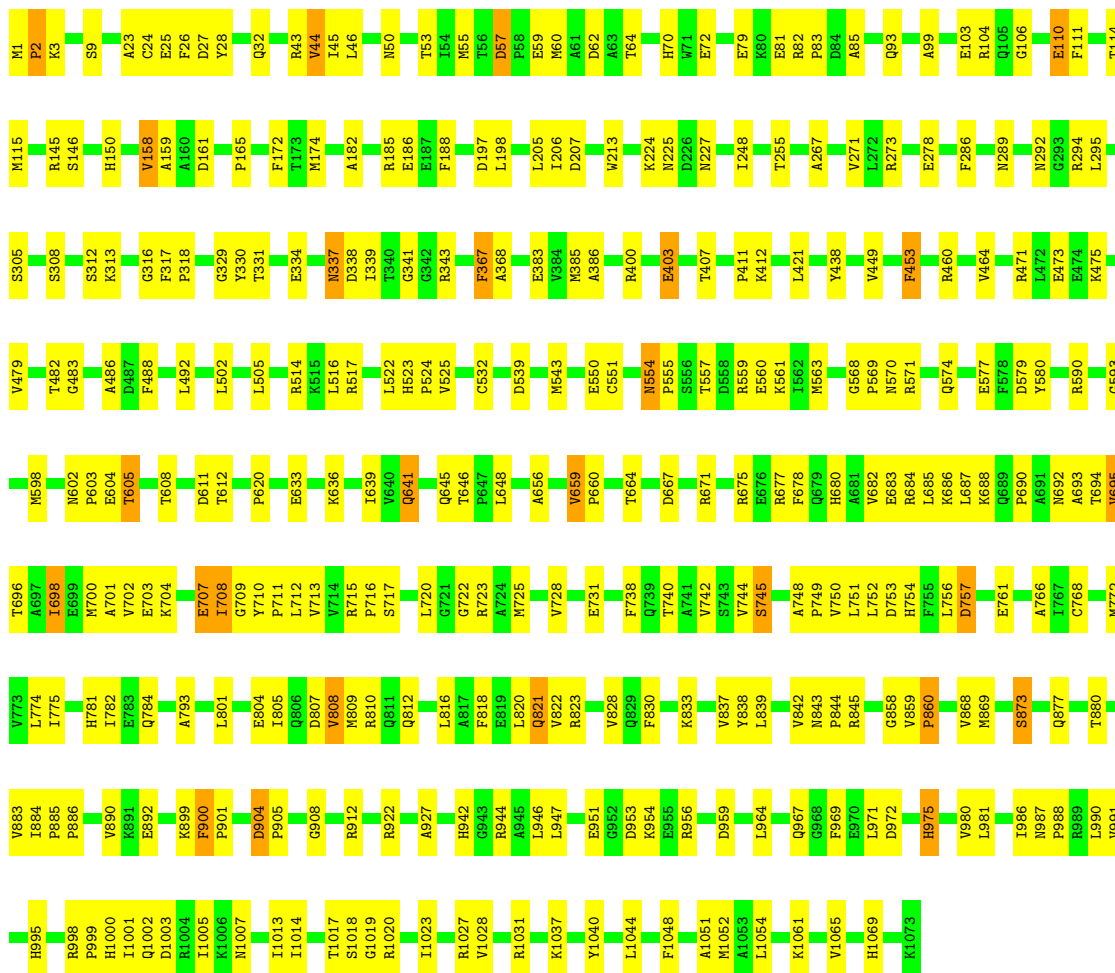
Note EDS was not executed.

• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE



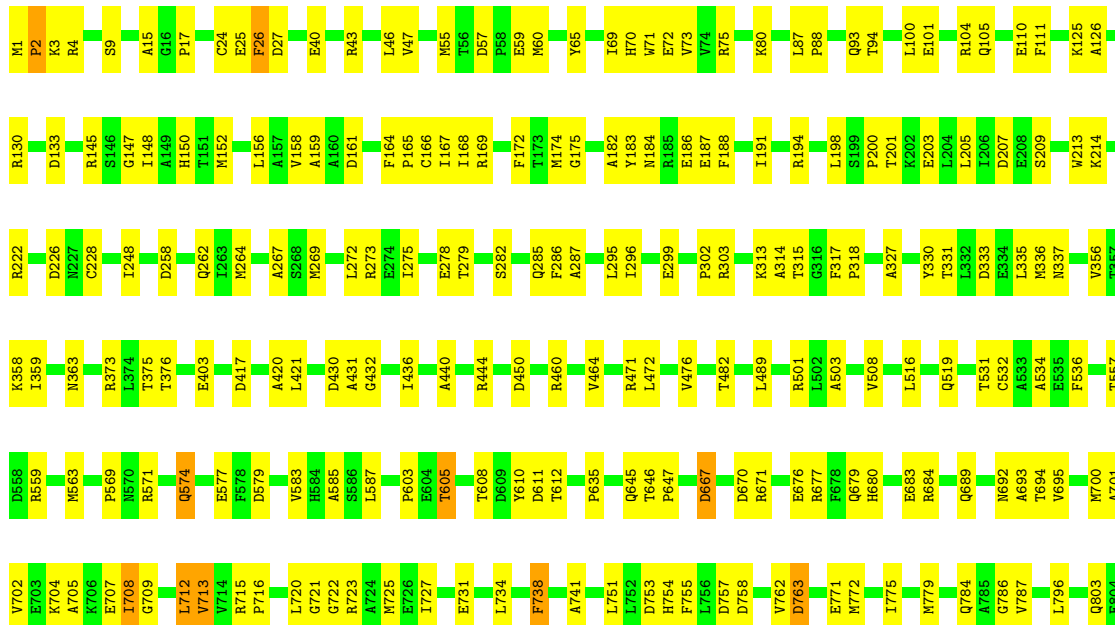
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

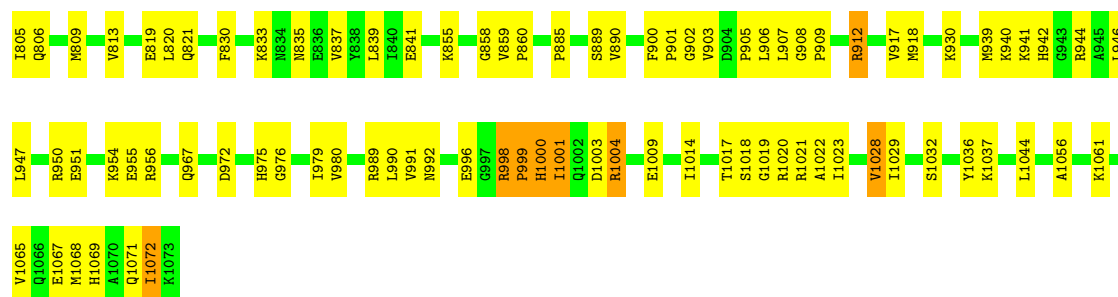




- Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

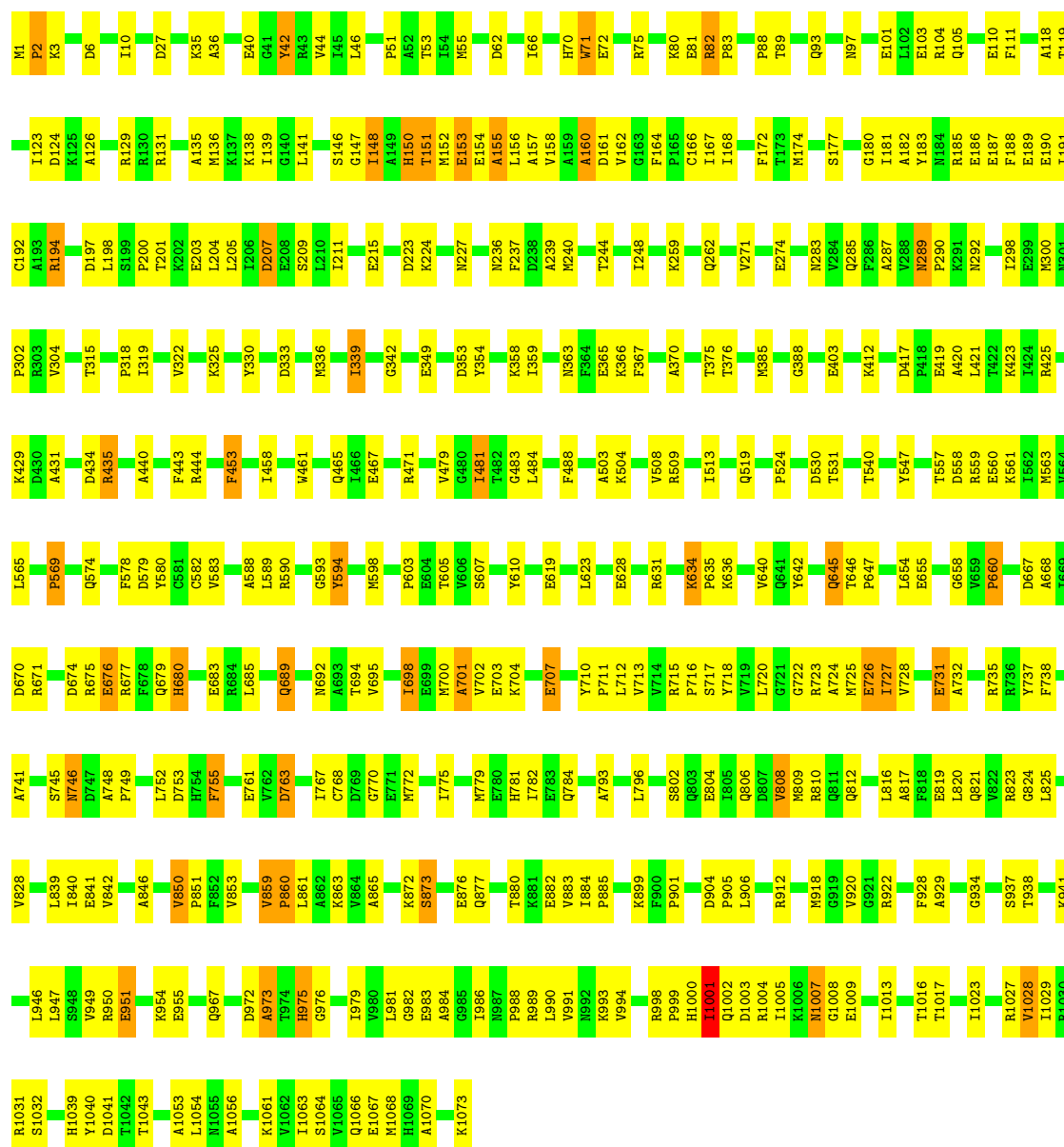
Chain E: 72% 27%





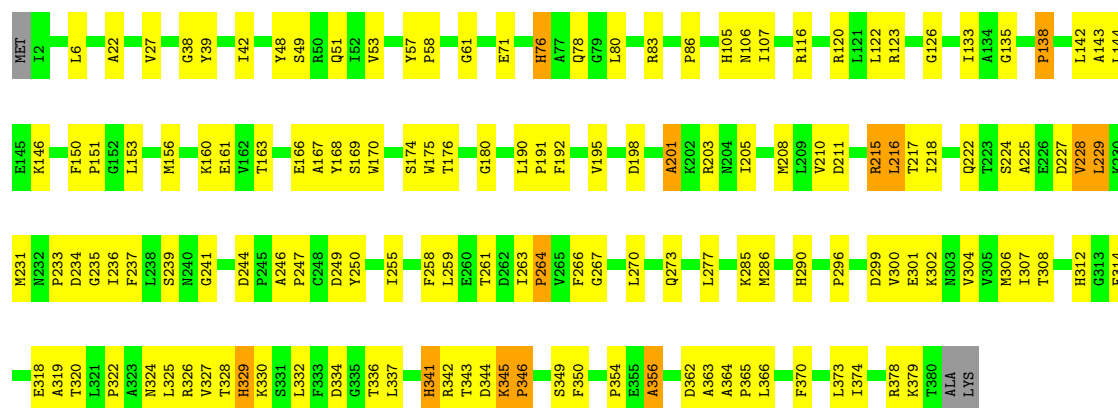
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

Chain G: 63% 33%



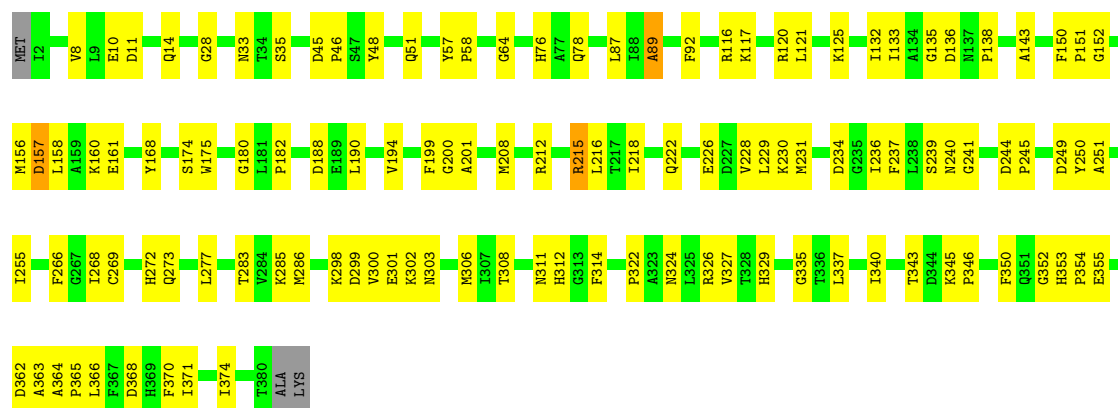
• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain B:



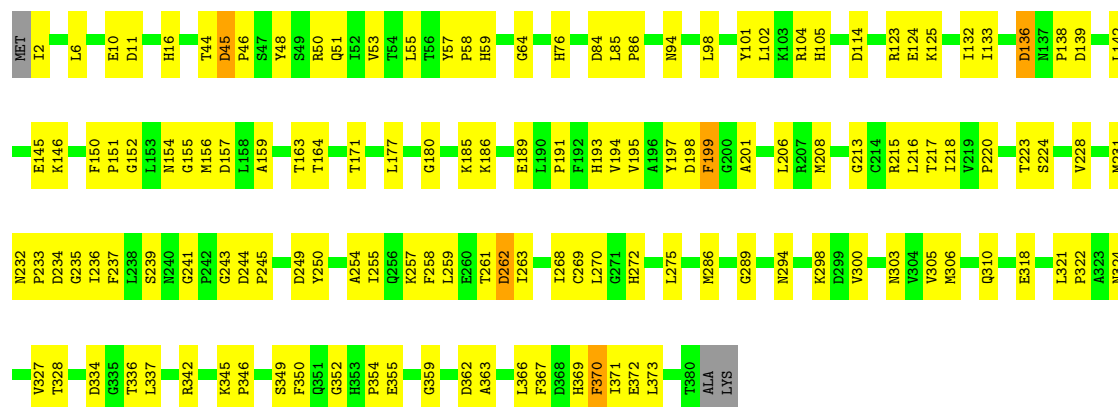
- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain D:



- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain F:



- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain H:



E355	H272	F192	R83	ME1
G359	Q273	H193	P86	I2
A363	L274	V194		A5
A364	L275	V195	F92	L7
P365	A276	A196	R83	V8
L366	L277	D198	N94	L9
F367	A278	F199	H104	E10
D368	S279	G200	R105	
H369	G280	A201	N106	T13
	A281	K202		Q14
		R203	I110	F15
L373	M286	G204	A111	
	F287	I205	D112	T23
T380	G288		I113	
ALA	G289	M208	D114	V27
LYS	H290	L209		G28
	H291	V210	K117	E29
	G292			
	G293	G213		
	N294	R214	A127	F32
	K298	R215	N233	N32
		L216	I132	T34
		T217	I133	S35
	M306	I218	A134	
	L307			Y39
	T308	A225	N137	
	A309		P138	T44
	Q310	V228		D45
	R311	L229	A147	P46
	H312		R148	S47
	G313	N232		Y48
		P233	G152	
	E318	D234		Q51
			M156	T52
	L321	F237	D157	V53
	P322	L238	L158	T54
	A323	S239	A159	L55
	N324	N240	K160	T56
	L325	G241	V161	V57
	R326		V162	P58
	V327	D244	T163	H59
	L328	P245		I60
	H329	D249	Y168	G61
		Y250	M169	N62
	L337		T171	V63
			Q172	
	H341	T253	G173	D69
	R342	A254	I172	E70
	T343	I255	S174	E71
	D344	Q256	M175	S72
	K345	K257	T176	S73
	P346	F258		Q74
	A347	L259	G180	V75
	F348			H76
	S349	P264	A184	A77
	F350	V265	K185	Q78
	Q351	F266		
			L190	V81
			D191	T82

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	151.90Å 164.50Å 332.60Å 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}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48307	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: NET, K, CL, MN, ORN, ANP

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	1.10	5/8435 (0.1%)	1.58	88/11407 (0.8%)
1	C	1.09	2/8399 (0.0%)	1.54	75/11361 (0.7%)
1	E	1.10	7/8427 (0.1%)	1.55	68/11398 (0.6%)
1	G	1.09	7/8418 (0.1%)	1.59	85/11386 (0.7%)
2	B	0.99	0/2957	1.52	20/4016 (0.5%)
2	D	1.08	1/2957 (0.0%)	1.55	20/4016 (0.5%)
2	F	1.02	1/2957 (0.0%)	1.52	22/4016 (0.5%)
2	H	1.01	1/2957 (0.0%)	1.56	23/4016 (0.6%)
All	All	1.08	24/45507 (0.1%)	1.56	401/61616 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	F	1	0
All	All	1	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	THR	C-O	-10.77	1.10	1.23
1	A	15	ALA	C-O	-7.80	1.13	1.23
1	G	631	ARG	CZ-NH1	7.78	1.43	1.32
1	E	999	PRO	N-CD	7.26	1.58	1.47
1	E	999	PRO	N-CA	-7.08	1.35	1.47
1	E	279	THR	C-O	-6.98	1.15	1.23
1	E	758	ASP	CG-OD1	6.70	1.38	1.25
2	F	262	ASP	CG-OD2	6.46	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1072	ILE	C-O	-6.41	1.15	1.23
1	G	1007	ASN	CA-C	-6.39	1.41	1.52
1	G	676	GLU	C-O	-5.93	1.16	1.24
1	A	39	GLU	CD-OE1	5.88	1.36	1.25
1	A	879	VAL	CA-C	-5.87	1.48	1.53
1	A	833	LYS	CE-NZ	-5.86	1.31	1.49
1	C	667	ASP	CG-OD1	5.74	1.36	1.25
2	H	10	GLU	CD-OE1	5.71	1.36	1.25
1	G	62	ASP	CG-OD1	5.57	1.35	1.25
1	E	731	GLU	CA-CB	5.51	1.61	1.53
2	D	28	GLY	CA-C	-5.34	1.45	1.51
1	G	153	GLU	CD-OE1	5.31	1.35	1.25
1	G	850	VAL	CA-CB	-5.21	1.51	1.54
1	E	680	HIS	CB-CG	-5.16	1.43	1.50
1	C	110	GLU	CD-OE1	5.04	1.34	1.25
1	G	103	GLU	CD-OE1	5.01	1.34	1.25

All (401) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	ASP	CB-CA-C	9.72	126.26	110.90
1	E	680	HIS	CA-CB-CG	-9.34	104.46	113.80
1	E	999	PRO	N-CA-C	-8.93	88.89	112.10
1	A	612	THR	N-CA-C	8.74	120.42	111.07
1	A	712	LEU	N-CA-CB	-8.63	95.47	111.52
1	C	908	GLY	CA-C-N	8.57	128.31	119.56
1	C	908	GLY	C-N-CA	8.57	128.31	119.56
1	G	162	VAL	N-CA-C	8.53	120.34	110.62
1	E	908	GLY	CA-C-N	8.50	128.23	119.56
1	E	908	GLY	C-N-CA	8.50	128.23	119.56
1	A	26	PHE	CA-CB-CG	-8.39	105.41	113.80
2	F	199	PHE	CA-CB-CG	-8.17	105.63	113.80
1	E	557	THR	CA-C-N	8.14	131.40	120.65
1	E	557	THR	C-N-CA	8.14	131.40	120.65
1	E	999	PRO	N-CA-CB	8.03	111.44	102.60
1	A	57	ASP	CA-CB-CG	-7.96	104.64	112.60
1	E	998	ARG	CA-C-O	-7.93	110.79	120.54
1	G	185	ARG	N-CA-C	7.81	119.88	111.36
1	A	557	THR	CA-C-N	7.78	130.92	120.65
1	A	557	THR	C-N-CA	7.78	130.92	120.65
1	A	172	PHE	CA-CB-CG	-7.71	106.09	113.80
1	C	339	ILE	N-CA-C	7.70	118.47	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	THR	N-CA-C	-7.69	103.24	114.39
1	A	539	ASP	N-CA-CB	7.57	121.62	110.56
2	B	105	HIS	CA-CB-CG	-7.57	106.23	113.80
1	E	738	PHE	N-CA-C	7.57	119.31	111.14
2	F	372	GLU	CB-CG-CD	-7.52	99.82	112.60
2	H	359	GLY	CA-C-N	7.49	127.54	119.90
2	H	359	GLY	C-N-CA	7.49	127.54	119.90
1	C	659	VAL	N-CA-C	7.49	117.12	108.96
1	C	554	ASN	O-C-N	7.44	124.95	121.53
1	C	605	THR	N-CA-C	7.42	122.11	110.17
2	D	215	ARG	CB-CA-C	7.41	121.93	109.48
1	E	612	THR	N-CA-C	7.41	119.35	111.28
1	G	1001	ILE	CA-C-N	7.35	130.45	120.38
1	G	1001	ILE	C-N-CA	7.35	130.45	120.38
1	A	580	TYR	N-CA-CB	-7.27	99.44	110.12
1	A	1039	HIS	CA-CB-CG	-7.19	106.61	113.80
2	H	105	HIS	CA-CB-CG	-7.18	106.62	113.80
1	E	605	THR	N-CA-C	7.16	121.24	110.14
1	G	605	THR	N-CA-C	7.15	121.23	110.14
1	G	155	ALA	N-CA-C	-7.15	103.18	110.97
1	A	908	GLY	CA-C-N	7.14	126.77	119.56
1	A	908	GLY	C-N-CA	7.14	126.77	119.56
1	G	726	GLU	N-CA-CB	-7.14	98.21	111.13
2	F	114	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	27	ASP	N-CA-C	-7.09	103.56	111.28
1	A	23	ALA	N-CA-C	7.07	119.26	109.29
1	C	557	THR	CA-C-N	7.07	130.62	120.79
1	C	557	THR	C-N-CA	7.07	130.62	120.79
1	A	733	ASP	N-CA-C	-7.02	103.71	111.36
1	G	1039	HIS	CA-CB-CG	-7.02	106.78	113.80
2	B	106	ASN	CA-CB-CG	-6.98	105.62	112.60
1	A	678	PHE	CA-CB-CG	-6.97	106.83	113.80
1	E	536	PHE	CA-CB-CG	-6.97	106.83	113.80
1	E	786	GLY	N-CA-C	-6.95	106.20	114.48
1	C	793	ALA	N-CA-C	-6.95	101.17	110.55
1	G	283	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	885	PRO	CA-C-N	6.90	126.50	119.19
1	A	885	PRO	C-N-CA	6.90	126.50	119.19
1	G	1028	VAL	N-CA-C	6.88	117.64	110.62
2	D	190	LEU	CA-C-N	6.82	126.29	118.85
2	D	190	LEU	C-N-CA	6.82	126.29	118.85
2	F	10	GLU	CB-CA-C	-6.80	99.12	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	180	GLY	N-CA-C	-6.75	103.27	112.52
1	G	289	ASN	CA-C-N	6.74	126.44	119.56
1	G	289	ASN	C-N-CA	6.74	126.44	119.56
1	E	557	THR	N-CA-C	-6.67	106.09	114.56
1	G	435	ARG	N-CA-C	6.65	120.26	111.75
1	G	634	LYS	CA-C-N	6.64	126.61	120.03
1	G	634	LYS	C-N-CA	6.64	126.61	120.03
1	G	569	PRO	CB-CA-C	-6.63	102.75	111.23
1	A	67	GLU	O-C-N	6.62	127.50	121.80
1	G	731	GLU	CA-C-N	6.59	129.95	120.79
1	G	731	GLU	C-N-CA	6.59	129.95	120.79
1	A	339	ILE	N-CA-C	6.58	121.36	111.89
1	E	1028	VAL	N-CA-C	6.52	117.20	110.36
1	E	209	SER	N-CA-C	6.50	120.10	109.76
1	E	1072	ILE	N-CA-C	6.50	116.60	107.37
1	C	339	ILE	N-CA-CB	6.49	119.36	110.54
1	A	536	PHE	CA-CB-CG	-6.48	107.32	113.80
1	G	88	PRO	CB-CA-C	-6.48	102.79	109.92
1	E	574	GLN	CB-CA-C	-6.47	102.84	112.09
2	H	369	HIS	CA-CB-CG	-6.42	107.38	113.80
1	G	619	GLU	N-CA-C	6.42	118.57	108.55
1	E	432	GLY	N-CA-C	-6.42	103.96	112.81
2	D	234	ASP	N-CA-C	-6.41	104.94	112.89
1	E	26	PHE	CA-CB-CG	-6.41	107.39	113.80
2	B	341	HIS	CA-CB-CG	-6.38	107.42	113.80
1	C	738	PHE	N-CA-C	6.38	119.18	111.40
2	F	11	ASP	CA-CB-CG	6.37	118.97	112.60
1	C	757	ASP	CA-CB-CG	6.36	118.96	112.60
1	E	133	ASP	CA-CB-CG	-6.33	106.27	112.60
1	C	559	ARG	N-CA-C	6.33	119.06	109.95
1	E	771	GLU	N-CA-C	-6.32	106.11	113.88
1	A	403	GLU	CB-CA-C	-6.29	103.77	111.82
1	A	1048	PHE	CA-CB-CG	-6.28	107.52	113.80
1	C	407	THR	N-CA-C	-6.28	105.56	113.72
1	E	175	GLY	N-CA-C	-6.27	106.58	115.30
1	C	554	ASN	CA-C-N	6.27	126.22	119.76
1	C	554	ASN	C-N-CA	6.27	126.22	119.76
1	A	698	ILE	N-CA-C	6.25	116.93	110.36
1	G	370	ALA	N-CA-C	6.25	119.53	110.28
1	A	949	VAL	N-CA-C	6.24	118.87	109.20
1	G	645	GLN	CB-CG-CD	6.24	123.21	112.60
1	A	238	ASP	CA-CB-CG	-6.23	106.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	559	ARG	N-CA-CB	6.23	120.06	110.60
1	A	738	PHE	N-CA-C	6.22	117.72	111.07
1	A	572	ILE	CA-C-N	-6.21	116.05	123.44
1	A	572	ILE	C-N-CA	-6.21	116.05	123.44
1	G	594	TYR	CA-C-N	-6.21	113.92	122.30
1	G	594	TYR	C-N-CA	-6.21	113.92	122.30
1	C	680	HIS	CA-CB-CG	-6.20	107.60	113.80
1	C	620	PRO	N-CA-CB	6.17	108.80	103.31
1	A	1025	ASP	CA-CB-CG	6.17	118.77	112.60
1	G	186	GLU	CA-C-N	6.17	128.83	120.44
1	G	186	GLU	C-N-CA	6.17	128.83	120.44
1	A	220	VAL	CB-CA-C	-6.15	101.35	110.82
1	G	885	PRO	CA-C-N	6.14	125.87	119.05
1	G	885	PRO	C-N-CA	6.14	125.87	119.05
1	G	150	HIS	N-CA-C	-6.14	105.74	113.72
2	H	184	ALA	N-CA-C	6.13	118.18	108.67
1	C	172	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	786	GLY	N-CA-C	-6.11	107.04	113.58
1	G	763	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	209	SER	N-CA-C	6.10	119.19	109.24
1	C	904	ASP	O-C-N	6.10	126.17	121.23
1	A	422	THR	CB-CA-C	6.08	121.19	110.85
1	A	745	SER	N-CA-C	6.08	120.30	113.01
1	A	558	ASP	CB-CA-C	-6.07	101.62	110.96
1	G	44	VAL	N-CA-C	6.06	116.84	107.99
1	A	557	THR	CA-C-O	6.05	125.65	118.69
2	D	157	ASP	CA-CB-CG	6.04	118.64	112.60
2	H	148	ARG	CA-C-N	6.03	129.48	120.31
2	H	148	ARG	C-N-CA	6.03	129.48	120.31
1	E	450	ASP	CA-CB-CG	6.03	118.63	112.60
2	H	112	ASP	N-CA-C	6.02	119.92	112.58
1	A	248	ILE	N-CA-C	-5.99	100.99	108.89
1	C	557	THR	N-CA-C	-5.97	106.33	113.97
1	C	57	ASP	CA-CB-CG	-5.97	106.63	112.60
1	G	151	THR	CA-CB-OG1	5.97	118.55	109.60
1	G	689	GLN	CB-CA-C	5.97	117.41	109.65
1	A	592	ASP	CA-CB-CG	5.96	118.56	112.60
2	F	157	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	900	PHE	CA-C-N	5.95	126.10	119.32
1	A	900	PHE	C-N-CA	5.95	126.10	119.32
1	C	44	VAL	N-CA-C	5.95	116.67	107.99
1	G	207	ASP	N-CA-C	5.94	119.39	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	900	PHE	CA-C-N	5.93	126.08	119.32
1	C	900	PHE	C-N-CA	5.93	126.08	119.32
1	C	255	THR	N-CA-C	5.93	119.82	112.59
1	G	285	GLN	N-CA-CB	5.93	120.33	110.85
1	G	194	ARG	CA-C-N	5.92	126.40	119.94
1	G	194	ARG	C-N-CA	5.92	126.40	119.94
1	C	818	PHE	CA-CB-CG	-5.91	107.89	113.80
2	H	308	THR	N-CA-C	5.90	118.67	109.52
1	G	634	LYS	O-C-N	5.90	124.24	121.53
1	E	755	PHE	N-CA-C	5.88	118.73	109.96
1	G	850	VAL	CA-C-O	5.87	123.17	118.71
1	C	486	ALA	N-CA-C	5.87	118.43	111.33
1	A	417	ASP	CA-C-N	5.86	126.00	119.32
1	A	417	ASP	C-N-CA	5.86	126.00	119.32
1	E	559	ARG	N-CA-C	5.86	118.39	109.95
1	C	23	ALA	N-CA-C	5.85	118.35	109.63
1	G	148	ILE	N-CA-CB	5.85	118.63	110.56
1	A	317	PHE	CA-C-N	5.85	127.15	119.84
1	A	317	PHE	C-N-CA	5.85	127.15	119.84
1	A	735	ARG	NE-CZ-NH2	-5.85	113.94	119.20
1	G	793	ALA	N-CA-C	-5.85	101.02	110.32
1	A	1011	THR	N-CA-CB	5.85	119.24	110.65
1	A	718	TYR	N-CA-C	5.84	119.48	111.54
1	A	1005	ILE	CB-CA-C	-5.83	104.38	112.02
2	F	177	LEU	CA-C-N	5.83	128.02	120.44
2	F	177	LEU	C-N-CA	5.83	128.02	120.44
1	A	175	GLY	N-CA-C	-5.83	105.93	114.90
1	C	338	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	904	ASP	CA-C-N	5.81	127.10	119.84
1	C	904	ASP	C-N-CA	5.81	127.10	119.84
1	A	646	THR	CA-CB-CG2	-5.81	100.62	110.50
1	G	660	PRO	N-CA-CB	5.80	106.47	102.35
1	A	59	GLU	CG-CD-OE1	-5.80	105.06	118.40
2	H	132	ILE	CB-CA-C	-5.79	102.01	110.81
2	H	198	ASP	CA-CB-CG	5.79	118.39	112.60
1	E	713	VAL	N-CA-C	5.76	115.90	107.37
1	G	698	ILE	CB-CA-C	-5.76	104.61	111.81
1	E	763	ASP	CA-CB-CG	5.76	118.36	112.60
1	E	775	ILE	N-CA-CB	5.75	118.06	111.39
2	B	76	HIS	CA-CB-CG	-5.75	108.05	113.80
1	E	285	GLN	N-CA-CB	5.75	120.05	110.85
1	G	808	VAL	CB-CA-C	-5.75	104.28	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	42	TYR	CA-C-N	-5.74	115.38	122.84
1	G	42	TYR	C-N-CA	-5.74	115.38	122.84
1	E	841	GLU	N-CA-C	5.74	115.97	107.88
1	G	209	SER	N-CA-C	5.73	118.88	109.76
1	G	928	PHE	CA-CB-CG	-5.73	108.07	113.80
2	F	53	VAL	N-CA-C	5.71	116.80	108.58
1	C	227	ASN	N-CA-C	-5.70	101.19	110.20
1	E	667	ASP	CA-CB-CG	-5.69	106.91	112.60
2	B	216	LEU	N-CA-C	5.69	119.33	110.17
1	G	746	ASN	CA-CB-CG	5.68	118.28	112.60
1	A	39	GLU	CB-CG-CD	-5.68	102.95	112.60
1	C	403	GLU	CB-CA-C	-5.65	103.95	111.63
2	D	10	GLU	CB-CA-C	-5.64	101.78	110.81
1	A	129	ARG	N-CA-C	5.64	117.11	111.07
1	G	319	ILE	N-CA-C	5.64	116.09	110.23
1	G	631	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	C	337	ASN	CA-C-N	5.62	130.12	121.19
1	C	337	ASN	C-N-CA	5.62	130.12	121.19
2	H	264	PRO	N-CA-CB	5.62	108.53	103.19
1	G	82	ARG	CG-CD-NE	-5.61	99.66	112.00
1	E	363	ASN	CA-CB-CG	5.61	118.21	112.60
2	F	220	PRO	N-CA-CB	5.61	108.23	103.35
1	E	317	PHE	CA-C-N	5.60	126.84	119.84
1	E	317	PHE	C-N-CA	5.60	126.84	119.84
1	G	239	ALA	N-CA-C	5.59	117.12	110.19
1	C	695	VAL	N-CA-C	5.58	117.70	108.99
1	A	285	GLN	CB-CG-CD	-5.58	103.12	112.60
1	C	26	PHE	N-CA-CB	5.58	118.89	110.30
1	G	727	ILE	N-CA-CB	5.57	118.16	111.31
2	B	356	ALA	CB-CA-C	-5.56	110.15	116.54
2	F	45	ASP	CA-C-N	5.55	125.91	119.47
2	F	45	ASP	C-N-CA	5.55	125.91	119.47
1	E	24	CYS	N-CA-C	5.54	118.84	111.75
1	E	754	HIS	CA-CB-CG	-5.54	108.26	113.80
2	B	329	HIS	N-CA-C	5.54	117.68	108.99
1	E	787	VAL	N-CA-CB	5.52	118.63	111.67
1	G	484	LEU	N-CA-C	5.52	118.17	108.56
1	C	453	PHE	CA-CB-CG	-5.51	108.28	113.80
2	B	201	ALA	N-CA-C	5.51	118.44	110.28
1	C	524	PRO	CB-CA-C	-5.50	103.74	110.95
1	A	350	PRO	N-CA-CB	5.50	108.45	103.33
1	A	146	SER	N-CA-C	5.49	118.81	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	559	ARG	O-C-N	5.49	129.01	122.20
1	C	667	ASP	CA-CB-CG	-5.49	107.11	112.60
1	E	885	PRO	CA-C-N	5.49	125.97	120.04
1	E	885	PRO	C-N-CA	5.49	125.97	120.04
1	E	998	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	C	745	SER	N-CA-C	5.48	119.07	112.38
1	C	543	MET	N-CA-C	5.48	118.50	109.85
1	A	840	ILE	CB-CA-C	-5.47	105.34	111.80
2	F	132	ILE	CB-CA-C	-5.47	102.68	110.83
1	G	443	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	499	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	578	PHE	CB-CA-C	5.45	121.71	110.31
1	E	705	ALA	N-CA-C	5.45	119.10	112.23
1	C	185	ARG	N-CA-C	5.45	117.92	111.33
1	C	995	HIS	CA-C-N	5.45	131.94	121.54
1	C	995	HIS	C-N-CA	5.45	131.94	121.54
1	C	995	HIS	CA-CB-CG	5.45	119.25	113.80
1	E	532	CYS	N-CA-C	5.44	119.07	111.56
2	B	345	LYS	N-CA-C	5.44	117.73	109.41
2	B	308	THR	N-CA-C	5.44	117.67	109.41
1	C	150	HIS	N-CA-C	-5.44	106.56	114.12
1	E	88	PRO	CB-CA-C	-5.44	102.59	111.56
2	H	106	ASN	CA-CB-CG	-5.43	107.17	112.60
2	F	359	GLY	CA-C-N	5.43	125.37	119.78
2	F	359	GLY	C-N-CA	5.43	125.37	119.78
1	C	158	VAL	CB-CA-C	-5.43	104.91	112.02
1	C	659	VAL	CA-C-N	5.43	126.62	119.84
1	C	659	VAL	C-N-CA	5.43	126.62	119.84
2	D	266	PHE	CA-C-N	-5.43	117.43	121.61
2	D	266	PHE	C-N-CA	-5.43	117.43	121.61
1	C	207	ASP	CA-CB-CG	5.42	118.02	112.60
2	D	136	ASP	CA-C-N	-5.42	116.49	123.16
2	D	136	ASP	C-N-CA	-5.42	116.49	123.16
1	A	714	VAL	CB-CA-C	-5.42	104.37	111.25
1	A	15	ALA	CA-C-O	-5.41	113.02	119.35
2	D	188	ASP	CA-CB-CG	-5.40	107.20	112.60
2	F	50	ARG	CB-CA-C	5.40	122.54	110.76
1	C	523	HIS	CA-C-N	5.40	125.37	120.03
1	C	523	HIS	C-N-CA	5.40	125.37	120.03
1	G	557	THR	CA-C-N	5.38	131.82	121.54
1	G	557	THR	C-N-CA	5.38	131.82	121.54
1	C	411	PRO	N-CA-CB	5.38	108.36	103.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	TYR	CA-C-N	-5.37	113.50	121.24
1	A	42	TYR	C-N-CA	-5.37	113.50	121.24
1	A	996	GLU	N-CA-C	5.37	118.29	111.69
2	F	372	GLU	CB-CA-C	-5.37	101.72	110.85
2	B	241	GLY	CA-C-N	5.37	125.83	120.52
2	B	241	GLY	C-N-CA	5.37	125.83	120.52
1	C	248	ILE	N-CA-C	-5.36	100.86	108.58
1	G	755	PHE	CA-CB-CG	-5.36	108.44	113.80
1	C	991	VAL	CB-CA-C	5.36	119.26	110.69
2	H	13	THR	N-CA-CB	5.36	117.83	109.85
1	E	337	ASN	CA-C-N	5.33	127.74	120.54
1	E	337	ASN	C-N-CA	5.33	127.74	120.54
1	G	453	PHE	CA-CB-CG	-5.33	108.47	113.80
1	G	488	PHE	CA-CB-CG	-5.33	108.47	113.80
1	G	481	ILE	CB-CA-C	5.33	120.02	111.29
1	A	345	PRO	CB-CA-C	-5.32	103.98	110.95
2	B	53	VAL	N-CA-C	5.32	115.92	108.89
1	C	24	CYS	N-CA-C	5.32	118.56	111.75
2	D	132	ILE	CB-CA-C	-5.32	102.76	110.63
2	D	311	ASN	CA-CB-CG	-5.31	107.29	112.60
1	G	339	ILE	N-CA-C	5.31	119.89	112.50
1	G	136	MET	CA-C-O	5.31	126.18	120.55
1	G	559	ARG	CA-C-N	5.31	129.46	122.30
1	G	559	ARG	C-N-CA	5.31	129.46	122.30
1	G	51	PRO	CB-CA-C	-5.30	103.94	111.68
1	C	667	ASP	CB-CG-OD1	-5.30	106.22	118.40
2	D	236	ILE	CA-C-N	-5.30	115.00	122.94
2	D	236	ILE	C-N-CA	-5.30	115.00	122.94
1	E	501	ARG	N-CA-C	-5.28	105.60	111.36
2	F	370	PHE	N-CA-C	-5.28	105.21	110.97
1	G	631	ARG	NH1-CZ-NH2	5.28	126.17	119.30
1	E	611	ASP	CA-C-N	5.28	127.35	120.28
1	E	611	ASP	C-N-CA	5.28	127.35	120.28
1	C	612	THR	N-CA-C	5.27	117.71	111.33
1	E	912	ARG	CD-NE-CZ	-5.27	117.02	124.40
2	H	157	ASP	CA-CB-CG	5.27	117.87	112.60
2	B	166	GLU	N-CA-CB	5.26	119.16	110.69
1	E	248	ILE	N-CA-C	-5.26	102.06	109.21
1	A	711	PRO	N-CA-CB	5.26	108.38	102.60
1	C	641	GLN	N-CA-C	5.26	119.69	113.28
2	H	29	GLU	CA-C-N	-5.25	116.19	122.90
2	H	29	GLU	C-N-CA	-5.25	116.19	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	ILE	N-CA-C	-5.24	105.97	110.74
2	B	86	PRO	N-CA-CB	5.24	107.72	103.32
1	E	1004	ARG	NE-CZ-NH1	5.24	126.73	121.50
1	G	160	ALA	N-CA-C	-5.24	106.04	112.90
1	C	987	ASN	CB-CA-C	-5.23	105.21	110.65
2	B	215	ARG	CB-CA-C	5.23	118.76	109.72
1	C	959	ASP	CA-CB-CG	-5.23	107.37	112.60
1	C	971	LEU	N-CA-C	5.23	118.08	109.72
1	C	27	ASP	N-CA-C	-5.22	106.42	112.89
1	G	680	HIS	N-CA-CB	-5.21	102.43	110.20
2	H	53	VAL	N-CA-C	5.21	116.21	108.23
2	H	168	TYR	N-CA-C	5.21	115.42	108.38
1	C	782	ILE	N-CA-C	-5.21	106.00	110.74
2	D	92	PHE	CA-CB-CG	-5.21	108.59	113.80
2	F	124	GLU	N-CA-C	5.20	118.09	111.69
1	C	611	ASP	CA-C-N	5.20	127.50	120.38
1	C	611	ASP	C-N-CA	5.20	127.50	120.38
2	F	369	HIS	CA-CB-CG	-5.19	108.61	113.80
1	A	289	ASN	CA-C-N	5.18	125.48	119.47
1	A	289	ASN	C-N-CA	5.18	125.48	119.47
1	G	701	ALA	CA-C-N	5.18	127.28	120.60
1	G	701	ALA	C-N-CA	5.18	127.28	120.60
1	E	194	ARG	CA-C-N	5.18	125.70	120.00
1	E	194	ARG	C-N-CA	5.18	125.70	120.00
1	A	255	THR	N-CA-C	5.18	119.09	112.26
2	B	379	LYS	N-CA-C	-5.17	105.82	111.82
1	C	316	GLY	N-CA-C	-5.17	107.99	115.27
2	F	16	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	675	ARG	N-CA-C	5.16	117.64	111.71
1	G	973	ALA	N-CA-CB	5.16	119.27	110.71
1	G	123	ILE	CB-CA-C	-5.16	105.28	111.88
1	C	860	PRO	N-CA-CB	5.15	106.38	102.36
1	A	1046	GLY	N-CA-C	-5.15	106.53	112.50
2	H	92	PHE	CA-CB-CG	-5.15	108.65	113.80
1	E	1001	ILE	CA-C-N	5.15	127.49	120.54
1	E	1001	ILE	C-N-CA	5.15	127.49	120.54
2	D	308	THR	N-CA-C	5.14	117.97	109.85
1	E	712	LEU	N-CA-CB	-5.13	102.62	111.55
1	A	554	ASN	O-C-N	5.13	123.89	121.53
2	D	11	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	4	ARG	N-CA-C	5.12	117.71	110.50
1	E	1004	ARG	N-CA-C	5.11	116.85	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ARG	N-CA-C	5.11	119.80	111.37
1	G	1001	ILE	N-CA-CB	-5.10	102.81	111.23
2	H	137	ASN	O-C-N	5.10	125.36	121.23
2	B	264	PRO	N-CA-CB	5.10	108.08	103.34
1	E	1021	ARG	N-CA-C	5.10	116.92	111.36
1	A	289	ASN	O-C-N	5.09	125.36	121.23
1	C	728	VAL	CB-CA-C	5.09	118.16	110.98
1	G	680	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	G	951	GLU	N-CA-CB	5.09	118.38	109.72
1	A	905	PRO	N-CA-CB	5.09	106.15	102.79
1	A	785	ALA	N-CA-C	-5.08	102.86	110.23
1	A	999	PRO	N-CA-CB	5.08	108.19	102.60
1	E	585	ALA	N-CA-C	-5.08	105.74	111.28
1	E	1000	HIS	CA-CB-CG	-5.08	108.72	113.80
1	E	998	ARG	N-CA-C	-5.08	103.14	110.40
1	A	407	THR	N-CA-C	-5.07	107.12	113.72
1	C	532	CYS	N-CA-C	5.07	119.20	112.30
1	E	87	LEU	CA-C-O	5.07	123.62	119.36
1	A	579	ASP	CA-C-O	5.07	125.87	120.24
2	D	353	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	1032	SER	N-CA-CB	5.07	117.66	110.16
1	G	976	GLY	N-CA-C	5.07	119.01	112.83
1	E	1001	ILE	CB-CA-C	5.07	118.36	111.88
1	G	197	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	316	GLY	N-CA-C	-5.05	108.30	115.43
1	G	718	TYR	N-CA-C	5.05	118.41	111.54
1	E	431	ALA	N-CA-C	5.04	117.61	110.10
1	A	191	ILE	N-CA-CB	5.04	116.44	110.55
1	A	727	ILE	N-CA-CB	5.03	116.74	111.00
2	D	89	ALA	N-CA-C	-5.03	101.51	109.96
1	C	367	PHE	CA-CB-CG	-5.03	108.77	113.80
1	G	580	TYR	N-CA-CB	-5.03	102.73	110.12
1	A	102	LEU	N-CA-C	-5.03	105.88	111.36
2	B	192	PHE	N-CA-C	5.03	117.02	110.43
1	E	1072	ILE	O-C-N	-5.03	117.07	122.45
1	C	830	PHE	CB-CA-C	-5.03	99.91	109.66
2	H	147	ALA	CA-C-N	5.02	127.26	120.38
2	H	147	ALA	C-N-CA	5.02	127.26	120.38
1	C	808	VAL	CB-CA-C	-5.01	105.45	112.02
2	B	138	PRO	N-CA-CB	5.01	108.00	103.34
1	G	859	VAL	CA-C-N	5.01	126.10	119.84
1	G	859	VAL	C-N-CA	5.01	126.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1068	MET	CB-CA-C	-5.00	103.02	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	50	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1008	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8288	0	8332	283	0
1	C	8268	0	8308	262	0
1	E	8284	0	8321	224	0
1	G	8279	0	8320	356	0
2	B	2895	0	2863	122	0
2	D	2895	0	2863	74	0
2	F	2895	0	2863	104	0
2	H	2895	0	2863	132	0
3	A	3	0	0	0	0
3	C	4	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	G	4	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	2	0
5	G	4	0	0	0	0
6	A	62	0	26	3	0
6	C	62	0	26	1	0
6	E	62	0	25	5	0
6	G	62	0	26	4	0
7	A	9	0	11	1	0
7	C	9	0	11	1	0
7	E	9	0	11	1	0
7	G	9	0	11	1	0
8	A	9	0	20	6	0
8	C	9	0	20	4	0
8	E	9	0	20	4	0
8	G	9	0	20	4	0
9	A	677	0	0	20	0
9	B	169	0	0	1	0
9	C	624	0	0	21	0
9	D	234	0	0	2	0
9	E	650	0	0	15	0
9	F	193	0	0	5	0
9	G	530	0	0	21	0
9	H	165	0	0	6	0
All	All	48307	0	44960	1547	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1547) 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:C:574:GLN:NE2	1:C:645:GLN:H	1.44	1.13
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.32	1.12
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.12	1.10
1:C:574:GLN:HE22	1:C:645:GLN:N	1.51	1.09
2:F:228:VAL:HA	2:F:231:MET:HE3	1.35	1.07
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.31	1.07
1:G:994:VAL:HG23	1:G:1001:ILE:HD11	1.32	1.05
2:F:324:ASN:HD22	2:F:324:ASN:N	1.54	1.03
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.39	0.99
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.27	0.99
2:H:324:ASN:H	2:H:324:ASN:HD22	1.08	0.98
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.29	0.96
1:C:784:GLN:HE21	1:C:784:GLN:H	1.11	0.96
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.47	0.95
1:C:954:LYS:HG2	1:C:980:VAL:HG21	1.48	0.95
2:F:286:MET:HE3	2:F:289:GLY:HA2	1.45	0.95
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.45	0.95
2:D:324:ASN:HD22	2:D:324:ASN:N	1.58	0.95
1:G:152:MET:HE1	1:G:189:GLU:HA	1.47	0.95
1:C:784:GLN:H	1:C:784:GLN:NE2	1.65	0.94
1:E:130:ARG:HG3	1:E:148:ILE:HG13	1.49	0.94
1:G:1029:ILE:H	1:G:1029:ILE:HD12	1.32	0.93
1:E:71:TRP:CH2	1:E:105:GLN:HG2	2.03	0.93
1:E:676:GLU:HB2	1:E:694:THR:HG21	1.50	0.93
2:F:327:VAL:HG13	2:F:337:LEU:HD11	1.51	0.93
1:A:992:ASN:ND2	1:A:996:GLU:HB2	1.84	0.93
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.84	0.92
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.34	0.92
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.49	0.92
1:G:828:VAL:HG13	1:G:842:VAL:HG22	1.52	0.92
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.82	0.92
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.53	0.91
2:D:324:ASN:H	2:D:324:ASN:ND2	1.61	0.91
1:A:574:GLN:NE2	1:A:645:GLN:H	1.68	0.90
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.51	0.90
2:F:324:ASN:ND2	2:F:324:ASN:H	1.66	0.90
8:A:1086:NET:H42	8:A:1086:NET:H22	1.53	0.89
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.37	0.89
1:E:147:GLY:HA3	1:E:158:VAL:HG11	1.55	0.89
2:B:150:PHE:CD1	2:B:151:PRO:HD2	2.08	0.88
1:E:574:GLN:HE22	1:E:645:GLN:H	0.96	0.88
1:A:993:LYS:HB2	1:A:996:GLU:HG3	1.56	0.88
1:C:684:ARG:HH11	1:C:684:ARG:HG3	1.39	0.88
1:G:147:GLY:HA3	1:G:158:VAL:HG11	1.53	0.88
2:H:327:VAL:HG13	2:H:337:LEU:HD11	1.55	0.87
1:A:784:GLN:NE2	1:A:784:GLN:H	1.73	0.87
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.05	0.87
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.55	0.87
1:A:574:GLN:HE22	1:A:645:GLN:H	1.22	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
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.88	0.86
1:G:1:MET:HG3	1:G:2:PRO:HD2	1.55	0.86
2:F:150:PHE:CD1	2:F:151:PRO:HD2	2.10	0.85
1:G:685:LEU:HD11	1:G:819:GLU:CB	2.07	0.85
1:G:574:GLN:NE2	1:G:645:GLN:HB2	1.91	0.84
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.60	0.84
1:G:772:MET:SD	1:G:880:THR:HG22	2.17	0.84
1:E:574:GLN:NE2	1:E:645:GLN:H	1.75	0.83
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.13	0.83
1:A:695:VAL:HG12	1:A:738:PHE:CZ	2.12	0.83
1:A:993:LYS:HB2	1:A:996:GLU:CG	2.08	0.83
1:C:403:GLU:CD	1:C:646:THR:HG21	2.04	0.83
1:E:784:GLN:NE2	1:E:784:GLN:H	1.76	0.82
1:A:4:ARG:NH2	1:A:7:ILE:HD11	1.94	0.82
1:C:571:ARG:HD2	1:C:574:GLN:HB2	1.62	0.81
1:A:723:ARG:NH1	1:A:724:ALA:H	1.78	0.81
1:G:403:GLU:CD	1:G:646:THR:HG21	2.04	0.81
8:C:1950:NET:H42	8:C:1950:NET:H22	1.61	0.81
1:C:922:ARG:HE	1:C:1061:LYS:HD3	1.44	0.81
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.61	0.81
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.95	0.81
1:C:574:GLN:HE21	1:C:720:LEU:HD21	1.43	0.81
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.16	0.80
2:F:324:ASN:HD22	2:F:324:ASN:H	0.85	0.80
1:G:110:GLU:HG2	1:G:111:PHE:CE1	2.15	0.80
1:E:784:GLN:H	1:E:784:GLN:HE21	1.29	0.80
1:G:147:GLY:HA3	1:G:158:VAL:CG1	2.10	0.80
1:A:694:THR:HG23	1:A:749:PRO:HB2	1.64	0.80
1:A:1017:THR:HG21	1:A:1023:ILE:CA	2.13	0.79
1:G:168:ILE:HD13	1:G:191:ILE:HG21	1.64	0.79
1:G:967:GLN:HG2	1:G:1054:LEU:HD13	1.63	0.79
2:F:201:ALA:HB2	2:F:239:SER:CB	2.14	0.78
1:C:716:PRO:HD2	1:C:725:MET:HG2	1.66	0.78
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.32	0.78
1:G:861:LEU:HD21	9:G:4404:HOH:O	1.83	0.78
2:D:324:ASN:HD22	2:D:324:ASN:H	0.81	0.78
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.66	0.77
2:H:324:ASN:H	2:H:324:ASN:ND2	1.81	0.77
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.13	0.77
1:E:1020:ARG:HB2	9:E:3584:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:GLY:O	2:D:156:MET:HE3	1.85	0.77
8:G:3950:NET:H22	8:G:3950:NET:H42	1.65	0.77
1:E:1:MET:HG3	1:E:2:PRO:HD2	1.66	0.77
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.66	0.76
1:C:716:PRO:HG2	1:C:723:ARG:O	1.85	0.76
1:E:991:VAL:CG2	1:E:1001:ILE:HG23	2.15	0.76
2:F:262:ASP:HB2	9:F:2830:HOH:O	1.84	0.76
1:A:72:GLU:O	1:A:75:ARG:HB3	1.85	0.76
2:F:85:LEU:HD12	2:F:86:PRO:HD2	1.68	0.76
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.68	0.76
1:A:574:GLN:NE2	1:A:645:GLN:HB2	1.98	0.76
2:B:318:GLU:OE1	2:B:330:LYS:HE3	1.86	0.76
1:E:1029:ILE:H	1:E:1029:ILE:HD12	1.51	0.75
1:A:695:VAL:HG12	1:A:738:PHE:HZ	1.49	0.75
2:B:341:HIS:ND1	2:B:342:ARG:N	2.35	0.75
2:H:201:ALA:HB2	2:H:239:SER:CB	2.17	0.75
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.21	0.75
1:E:991:VAL:HG21	1:E:1001:ILE:HG23	1.68	0.75
1:A:403:GLU:OE1	1:A:646:THR:HG21	1.86	0.75
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.67	0.75
8:A:1086:NET:H82	8:A:1086:NET:H62	1.68	0.75
1:C:998:ARG:HG2	1:C:998:ARG:HH11	1.51	0.75
1:C:1027:ARG:HH21	1:C:1031:ARG:HH11	1.35	0.74
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.69	0.74
1:G:1001:ILE:HD12	1:G:1002:GLN:HB2	1.69	0.74
1:C:313:LYS:HE2	1:C:608:THR:O	1.88	0.74
2:H:255:ILE:HG22	2:H:259:LEU:CD1	2.19	0.73
1:A:344:THR:HB	1:A:345:PRO:HD2	1.70	0.73
1:E:286:PHE:CD1	1:E:295:LEU:HD11	2.23	0.73
2:B:324:ASN:HD22	2:B:325:LEU:N	1.86	0.73
1:C:772:MET:SD	1:C:880:THR:HG22	2.28	0.73
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.71	0.73
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.71	0.73
1:A:85:ALA:HB1	1:A:116:ILE:HG12	1.70	0.73
1:A:694:THR:HG23	1:A:749:PRO:CB	2.19	0.73
1:E:46:LEU:HD13	1:E:55:MET:HE2	1.71	0.73
1:G:403:GLU:OE2	1:G:646:THR:HG21	1.89	0.73
1:A:267:ALA:O	1:A:271:VAL:HG23	1.89	0.72
1:G:574:GLN:HE21	1:G:645:GLN:HB2	1.54	0.72
2:F:318:GLU:O	2:F:321:LEU:HB2	1.89	0.72
2:B:324:ASN:HD22	2:B:325:LEU:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:713:VAL:HG22	1:G:727:ILE:CG1	2.19	0.72
1:C:951:GLU:O	1:C:954:LYS:HB2	1.89	0.72
1:E:105:GLN:HG3	9:E:3514:HOH:O	1.89	0.72
2:B:235:GLY:HA3	2:B:374:ILE:HD11	1.71	0.71
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.73	0.71
1:E:679:GLN:HA	1:E:689:GLN:HE22	1.54	0.71
1:G:700:MET:SD	1:G:703:GLU:HG2	2.31	0.71
1:G:479:VAL:CG2	1:G:483:GLY:HA3	2.19	0.71
2:D:215:ARG:HH11	2:D:215:ARG:HG3	1.54	0.71
1:E:482:THR:HB	9:E:3533:HOH:O	1.89	0.71
1:G:574:GLN:NE2	1:G:645:GLN:H	1.89	0.71
1:A:772[B]:MET:HE1	1:A:880:THR:HB	1.73	0.71
1:G:574:GLN:HG3	1:G:720:LEU:HD11	1.73	0.71
1:A:1017:THR:CG2	1:A:1023:ILE:HG13	2.21	0.70
2:B:27:VAL:O	2:B:78:GLN:HG2	1.91	0.70
2:F:2:ILE:HD11	9:F:2530:HOH:O	1.91	0.70
1:G:75:ARG:HG2	1:G:75:ARG:HH11	1.55	0.70
1:E:1000:HIS:H	1:E:1000:HIS:CD2	2.09	0.70
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.20	0.70
2:H:215:ARG:HH11	2:H:215:ARG:HG3	1.55	0.70
1:E:954:LYS:HG2	1:E:980:VAL:HG21	1.74	0.70
1:G:922:ARG:HE	1:G:1061:LYS:HD3	1.56	0.70
1:G:828:VAL:HG13	1:G:842:VAL:CG2	2.22	0.70
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.27	0.69
1:G:726:GLU:HG3	1:G:737:TYR:CG	2.26	0.69
1:G:152:MET:CE	1:G:189:GLU:HA	2.21	0.69
2:H:8:VAL:HG22	2:H:14:GLN:HG2	1.74	0.69
1:E:574:GLN:HE22	1:E:645:GLN:N	1.81	0.69
1:E:951:GLU:O	1:E:954:LYS:HB2	1.92	0.69
2:B:153:LEU:HA	2:B:156:MET:HE3	1.73	0.69
1:G:951:GLU:HA	1:G:954:LYS:HD2	1.73	0.69
2:H:255:ILE:HG22	2:H:259:LEU:HD12	1.74	0.69
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.74	0.69
1:C:1027:ARG:HH21	1:C:1031:ARG:NH1	1.89	0.69
2:B:142:LEU:O	2:B:146:LYS:HG3	1.92	0.69
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.75	0.69
2:F:334:ASP:OD1	2:F:336:THR:HG23	1.93	0.69
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.75	0.69
1:G:1029:ILE:H	1:G:1029:ILE:CD1	2.06	0.69
2:H:324:ASN:O	2:H:342:ARG:HD2	1.92	0.69
1:A:57:ASP:O	1:A:60:MET:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:ASP:O	1:E:583:VAL:HG23	1.93	0.68
1:C:473:GLU:HG2	1:C:505:LEU:CD1	2.23	0.68
1:E:889:SER:HB3	1:E:918:MET:HE3	1.76	0.68
2:H:171:THR:O	2:H:185:LYS:HB2	1.92	0.68
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.74	0.68
1:G:481:ILE:HG21	1:G:508:VAL:HG11	1.75	0.68
1:E:1017:THR:HG21	1:E:1023:ILE:HA	1.75	0.68
1:G:172:PHE:CB	1:G:200:PRO:HG2	2.23	0.68
2:H:345:LYS:HB3	2:H:346:PRO:HD2	1.75	0.68
1:C:471:ARG:HD2	9:C:4389:HOH:O	1.92	0.68
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.75	0.68
1:G:695:VAL:CG1	1:G:701:ALA:HB2	2.17	0.68
1:G:1001:ILE:HD12	1:G:1002:GLN:N	2.08	0.68
1:E:976:GLY:O	1:E:980:VAL:HG23	1.94	0.68
2:H:286:MET:HE1	2:H:312:HIS:ND1	2.09	0.68
1:E:992:ASN:HB3	1:E:996:GLU:HB3	1.75	0.68
1:G:579:ASP:O	1:G:583:VAL:HG23	1.93	0.68
1:E:166:CYS:C	1:E:167:ILE:HD12	2.19	0.68
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.12	0.67
1:C:693:ALA:HB3	1:C:708:ILE:HD11	1.76	0.67
1:C:473:GLU:HG2	1:C:505:LEU:HD11	1.75	0.67
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.23	0.67
1:E:80:LYS:HB2	9:E:3512:HOH:O	1.94	0.67
1:G:119:THR:HG23	9:G:4481:HOH:O	1.94	0.67
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.09	0.67
1:E:110:GLU:HG2	1:E:111:PHE:CD2	2.28	0.67
1:G:704:LYS:O	1:G:707:GLU:HB2	1.94	0.67
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.75	0.67
2:F:145:GLU:HG3	9:F:2667:HOH:O	1.94	0.67
1:A:46:LEU:HG	1:A:46:LEU:O	1.94	0.67
1:C:816:LEU:HD11	1:C:839:LEU:HD21	1.74	0.67
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.30	0.67
1:C:828:VAL:HG22	1:C:842:VAL:HG13	1.76	0.67
1:E:1017:THR:HG22	1:E:1018:SER:N	2.10	0.67
1:G:640:VAL:O	1:G:647:PRO:HB2	1.94	0.67
1:G:1041:ASP:HA	7:G:3920:ORN:O	1.94	0.67
1:A:695:VAL:CG1	1:A:701:ALA:HB2	2.22	0.67
1:G:955:GLU:HB2	9:G:4511:HOH:O	1.93	0.67
2:B:300:VAL:HG22	2:B:328:THR:O	1.95	0.66
1:C:694:THR:HG23	1:C:749:PRO:HB2	1.77	0.66
1:E:172:PHE:CB	1:E:200:PRO:HG2	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1000:HIS:O	1:G:1003:ASP:HB2	1.94	0.66
1:A:906:LEU:HD12	1:A:907:LEU:N	2.09	0.66
1:A:1004:ARG:HH22	1:G:983:GLU:HG2	1.58	0.66
2:D:286:MET:HE1	2:D:312:HIS:ND1	2.10	0.66
1:E:93:GLN:HB2	1:E:174:MET:HG2	1.76	0.66
2:H:83:ARG:HD2	2:H:83:ARG:O	1.95	0.66
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.42	0.66
1:C:50:ASN:ND2	1:C:53:THR:HG23	2.11	0.66
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.31	0.66
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.76	0.66
1:A:172:PHE:CB	1:A:200:PRO:HG2	2.19	0.66
2:B:306:MET:HB2	2:B:362:ASP:HB3	1.77	0.66
1:G:300:MET:HG3	1:G:300:MET:O	1.95	0.66
1:G:812:GLN:O	1:G:816:LEU:HG	1.95	0.66
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.31	0.66
1:C:740:THR:O	1:C:744:VAL:HG13	1.96	0.66
1:E:946:LEU:C	1:E:947:LEU:HD12	2.21	0.66
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.31	0.66
1:A:43:ARG:NH2	1:A:81:GLU:OE1	2.28	0.66
1:G:676:GLU:HB2	1:G:694:THR:HG21	1.76	0.66
1:A:51:PRO:O	1:A:855:LYS:NZ	2.29	0.66
1:A:863:LYS:HE2	9:A:1712:HOH:O	1.95	0.66
1:G:71:TRP:CZ3	1:G:105:GLN:HG2	2.31	0.66
1:G:694:THR:HG23	1:G:749:PRO:CB	2.24	0.66
1:G:1001:ILE:O	1:G:1005:ILE:HG13	1.96	0.66
2:F:324:ASN:N	2:F:324:ASN:ND2	2.31	0.65
1:G:872:LYS:HG2	1:G:877:GLN:HG3	1.77	0.65
1:G:906:LEU:O	1:G:912:ARG:NH2	2.29	0.65
1:A:35:LYS:O	1:A:39:GLU:HG3	1.96	0.65
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.32	0.65
1:E:313:LYS:NZ	1:E:603:PRO:O	2.29	0.65
1:A:101:GLU:OE1	1:A:104:ARG:NE	2.30	0.65
2:F:193:HIS:N	2:F:234:ASP:OD2	2.29	0.65
2:B:350:PHE:HD2	2:B:354:PRO:HD3	1.61	0.65
2:D:150:PHE:CD1	2:D:151:PRO:HD2	2.30	0.65
1:G:810:ARG:HH11	1:G:810:ARG:HG3	1.60	0.65
2:F:261:THR:OG1	2:F:263:ILE:HG13	1.97	0.65
1:A:583:VAL:HG12	1:A:587:LEU:HD22	1.79	0.65
2:B:264:PRO:HB3	2:B:373:LEU:HB3	1.79	0.65
1:G:367:PHE:CE1	1:G:912:ARG:HG2	2.31	0.65
1:C:742:VAL:HA	1:C:745:SER:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:THR:HG21	1:A:1023:ILE:HG13	1.79	0.65
1:C:784:GLN:HE21	1:C:784:GLN:N	1.91	0.65
1:C:998:ARG:HG2	1:C:998:ARG:NH1	2.08	0.65
1:E:335:LEU:C	1:E:336:MET:HE2	2.22	0.64
1:E:569:PRO:O	1:E:571:ARG:NH1	2.30	0.64
1:G:168:ILE:HG23	1:G:204:LEU:HD22	1.78	0.64
1:G:667:ASP:OD1	1:G:677:ARG:NH2	2.30	0.64
1:A:410:ASP:OD2	1:A:504:LYS:NZ	2.30	0.64
1:G:679:GLN:HG3	1:G:689:GLN:NE2	2.13	0.64
1:G:702:VAL:HG21	1:G:735:ARG:NH1	2.13	0.64
2:H:23:THR:HG23	2:H:134:ALA:O	1.97	0.64
2:B:38:GLY:O	2:B:42:ILE:HD12	1.98	0.64
1:C:946:LEU:C	1:C:947:LEU:HD12	2.22	0.64
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.79	0.64
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.97	0.64
1:A:722:GLY:C	1:A:725:MET:HG3	2.23	0.64
1:G:129:ARG:HB3	1:G:205:LEU:HD22	1.78	0.64
1:A:698:ILE:O	1:A:702:VAL:HG23	1.97	0.64
1:C:822:VAL:O	1:C:823:ARG:HD3	1.97	0.64
1:C:964:LEU:O	1:C:969:PHE:HB2	1.97	0.64
1:A:772[B]:MET:HE1	1:A:880:THR:CB	2.26	0.64
2:H:71:GLU:O	2:H:203:ARG:HG3	1.98	0.64
1:C:953:ASP:HB3	1:C:1044:LEU:CD2	2.20	0.64
1:E:1004:ARG:HD3	1:E:1009[B]:GLU:OE2	1.98	0.64
1:C:944:ARG:NH1	1:C:972:ASP:OD1	2.30	0.63
1:E:722:GLY:N	6:E:2910:ANP:O1B	2.29	0.63
2:F:228:VAL:HA	2:F:231:MET:CE	2.22	0.63
1:E:403:GLU:HG3	1:E:569:PRO:HD2	1.80	0.63
1:E:403:GLU:OE2	1:E:646:THR:HG21	1.99	0.63
1:G:731:GLU:CD	1:G:732:ALA:H	2.06	0.63
1:G:89:THR:O	1:G:304:VAL:HG22	1.98	0.63
1:A:166:CYS:C	1:A:167:ILE:HD12	2.23	0.63
1:C:698:ILE:O	1:C:702:VAL:HG23	1.99	0.63
1:G:1066:GLN:HB2	9:G:4018:HOH:O	1.99	0.63
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.81	0.63
1:E:71:TRP:CZ3	1:E:105:GLN:HG2	2.33	0.63
2:H:269:CYS:O	2:H:272:HIS:HB3	1.98	0.63
1:A:27:ASP:OD1	1:A:53:THR:HB	1.98	0.63
1:E:184:ASN:OD1	1:E:186:GLU:HB3	1.99	0.63
2:F:199:PHE:O	2:F:241:GLY:HA3	1.98	0.63
1:C:678:PHE:CE1	1:C:842:VAL:HG23	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:504:LYS:NZ	9:G:4453:HOH:O	2.32	0.63
2:H:327:VAL:HG13	2:H:337:LEU:CD1	2.26	0.63
1:A:417:ASP:OD2	1:A:423:LYS:NZ	2.31	0.63
2:F:224:SER:O	2:F:228:VAL:HG23	1.98	0.63
1:A:175:GLY:N	6:A:1083:ANP:O1G	2.26	0.62
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.34	0.62
1:C:64:THR:O	1:C:1065:VAL:HG23	1.98	0.62
2:F:254:ALA:O	2:F:257:LYS:HB2	1.98	0.62
1:G:403:GLU:HG3	1:G:569:PRO:HD2	1.82	0.62
2:B:273:GLN:O	2:B:277:LEU:HG	1.99	0.62
1:C:278:GLU:HG2	9:C:4561:HOH:O	1.99	0.62
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.82	0.62
1:A:22:GLN:CD	8:A:1086:NET:H41	2.25	0.62
1:A:39:GLU:OE2	9:A:1380:HOH:O	2.16	0.62
1:C:722:GLY:N	6:C:1910:ANP:O1B	2.30	0.62
1:C:951:GLU:HA	1:C:954:LYS:CD	2.26	0.62
1:G:166:CYS:C	1:G:167:ILE:HD12	2.23	0.62
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.35	0.62
2:B:324:ASN:ND2	2:B:324:ASN:N	2.38	0.62
1:E:258:ASP:O	1:E:262:GLN:HG2	1.99	0.62
1:A:313:LYS:HE2	1:A:608:THR:O	1.99	0.62
1:A:375:THR:OG1	1:A:376:THR:N	2.32	0.62
1:G:994:VAL:HG22	1:G:1000:HIS:ND1	2.15	0.62
1:E:168:ILE:HD13	1:E:191:ILE:CG2	2.30	0.62
1:C:9:SER:OG	1:C:83:PRO:HA	2.00	0.62
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.82	0.62
1:E:152:MET:O	1:E:156:LEU:HG	2.00	0.62
1:G:563:MET:CE	1:G:635:PRO:HG3	2.30	0.62
1:E:1019:GLY:O	1:E:1023:ILE:HD12	2.00	0.61
1:G:712:LEU:HG	1:G:753:ASP:O	2.00	0.61
1:A:583:VAL:HG12	1:A:587:LEU:CD2	2.30	0.61
2:B:299:ASP:OD2	2:B:302:LYS:HD2	2.00	0.61
1:G:147:GLY:CA	1:G:158:VAL:HG11	2.28	0.61
1:A:868:VAL:HA	1:A:872:LYS:O	2.00	0.61
2:B:345:LYS:HB3	2:B:346:PRO:CD	2.31	0.61
1:C:1017:THR:HG21	1:C:1023:ILE:CA	2.28	0.61
1:G:675:ARG:HG3	1:G:717:SER:OG	2.01	0.61
1:G:763:ASP:HB3	1:G:779:MET:HE3	1.81	0.61
2:H:152:GLY:O	2:H:156:MET:HE3	2.00	0.61
1:G:767:ILE:HG23	1:G:824:GLY:O	2.01	0.61
2:H:324:ASN:HA	2:H:343:THR:OG1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:GLU:HG3	1:G:153:GLU:O	1.99	0.61
1:A:1017:THR:HG22	1:A:1018:SER:N	2.15	0.61
1:C:574:GLN:NE2	1:C:720:LEU:HD21	2.15	0.61
2:D:116:ARG:O	2:D:120:ARG:HG3	2.01	0.61
1:E:3:LYS:HB3	1:E:330:TYR:CZ	2.35	0.61
1:A:62:ASP:OD1	1:A:62:ASP:N	2.31	0.61
1:G:318:PRO:HG3	1:G:610:TYR:OH	2.00	0.61
1:C:873:SER:O	1:C:877:GLN:HG3	2.00	0.61
1:C:953:ASP:CB	1:C:1044:LEU:HD22	2.23	0.61
2:F:218:ILE:HD13	2:F:218:ILE:N	2.16	0.61
1:G:679:GLN:HA	1:G:689:GLN:HE22	1.66	0.61
1:G:685:LEU:HD11	1:G:819:GLU:HB2	1.81	0.61
1:C:892:GLU:OE2	7:C:1920:ORN:NE	2.30	0.61
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.65	0.61
2:D:168:TYR:CE2	2:D:218:ILE:HG13	2.35	0.61
1:E:375:THR:OG1	1:E:376:THR:N	2.30	0.61
1:G:181:ILE:HD11	1:G:376:THR:HG23	1.81	0.61
1:A:482:THR:HB	9:A:1595:HOH:O	2.00	0.60
2:F:286:MET:CE	2:F:289:GLY:HA2	2.27	0.60
1:G:190:GLU:O	1:G:194:ARG:NH1	2.33	0.60
1:G:710:TYR:HB3	1:G:711:PRO:HA	1.83	0.60
1:A:50:ASN:ND2	1:A:53:THR:HG23	2.16	0.60
1:C:686:LYS:HA	9:C:4403:HOH:O	2.01	0.60
1:C:956:ARG:NH2	9:C:4548:HOH:O	2.33	0.60
2:F:194:VAL:N	2:F:215:ARG:O	2.30	0.60
1:E:944:ARG:NH1	1:E:972:ASP:OD1	2.29	0.60
1:G:223:ASP:CG	1:G:227:ASN:HB2	2.26	0.60
2:H:249:ASP:OD1	2:H:250:TYR:N	2.30	0.60
1:G:471:ARG:HD2	9:G:4379:HOH:O	2.01	0.60
2:B:255:ILE:HA	2:B:258:PHE:HD2	1.67	0.60
1:C:403:GLU:OE1	1:C:646:THR:HG21	2.00	0.60
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.16	0.60
1:A:42:TYR:N	9:A:1112:HOH:O	2.35	0.60
1:E:150:HIS:CD2	1:E:203:GLU:HB2	2.37	0.60
2:H:253:THR:HG22	2:H:254:ALA:N	2.16	0.60
2:B:326:ARG:HG3	2:B:326:ARG:O	2.00	0.60
1:G:695:VAL:HG12	1:G:738:PHE:CZ	2.37	0.60
2:B:174:SER:HB2	2:B:211:ASP:OD2	2.02	0.60
1:C:990:LEU:HD13	1:E:990:LEU:HD22	1.83	0.60
2:D:199:PHE:O	2:D:241:GLY:HA3	2.01	0.60
1:G:1:MET:CG	1:G:2:PRO:HD2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ARG:HG3	2:B:215:ARG:HH11	1.67	0.59
2:B:228:VAL:HG12	2:B:229:LEU:N	2.16	0.59
1:C:639:ILE:HD13	1:C:869:MET:HE3	1.83	0.59
1:C:694:THR:HG23	1:C:749:PRO:CB	2.32	0.59
1:C:883:VAL:O	1:C:884:ILE:HD13	2.02	0.59
1:E:168:ILE:CD1	1:E:191:ILE:HG21	2.32	0.59
1:G:479:VAL:HG23	1:G:483:GLY:HA3	1.84	0.59
1:A:799:TYR:CD2	1:A:800:THR:HG22	2.37	0.59
1:G:685:LEU:HD11	1:G:819:GLU:HG2	1.83	0.59
1:C:400:ARG:HD3	9:C:4133:HOH:O	2.02	0.59
1:E:695:VAL:CG1	1:E:701:ALA:HB2	2.24	0.59
2:B:324:ASN:ND2	2:B:325:LEU:N	2.50	0.59
1:C:807:ASP:OD1	1:C:810:ARG:NH1	2.34	0.59
1:E:712:LEU:C	1:E:712:LEU:HD23	2.28	0.59
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.03	0.59
1:E:15:ALA:HB3	5:E:2980:CL:CL	2.40	0.59
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.83	0.59
1:G:40:GLU:OE2	1:G:325:LYS:HE2	2.01	0.59
1:G:333:ASP:N	1:G:333:ASP:OD1	2.31	0.59
1:G:1001:ILE:CG1	1:G:1002:GLN:H	2.15	0.59
1:C:698:ILE:HD12	1:C:698:ILE:N	2.18	0.59
1:E:757:ASP:O	1:E:833:LYS:NZ	2.30	0.59
1:G:118:ALA:HA	9:G:4481:HOH:O	2.03	0.59
1:E:906:LEU:O	1:E:912:ARG:NH2	2.36	0.59
1:G:1001:ILE:CD1	1:G:1002:GLN:H	2.16	0.59
8:A:1086:NET:H82	8:A:1086:NET:C6	2.27	0.59
1:E:700:MET:O	1:E:704:LYS:HB2	2.03	0.59
1:A:967:GLN:HG2	1:A:1054:LEU:HD13	1.85	0.59
1:E:472:LEU:O	1:E:476:VAL:HG23	2.02	0.59
1:G:138:LYS:HE2	9:G:4301:HOH:O	2.02	0.59
1:G:574:GLN:CG	1:G:720:LEU:HD11	2.33	0.59
1:G:685:LEU:HD11	1:G:819:GLU:CG	2.33	0.59
1:A:699:GLU:OE2	1:A:735:ARG:NH2	2.34	0.59
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.85	0.59
2:D:370:PHE:O	2:D:374:ILE:HG13	2.03	0.59
1:A:993:LYS:CB	1:A:996:GLU:HG3	2.32	0.58
1:A:1000:HIS:HD2	1:A:1003:ASP:HB2	1.66	0.58
2:B:144:LEU:HD12	2:B:144:LEU:O	2.03	0.58
1:C:820:LEU:O	1:C:821:GLN:HB2	2.00	0.58
2:F:272:HIS:HA	2:F:349:SER:CB	2.32	0.58
1:G:148:ILE:HG22	1:G:150:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:CYS:HB2	1:A:207:ASP:O	2.02	0.58
1:E:683:GLU:OE1	1:E:683:GLU:HA	2.03	0.58
1:E:222:ARG:NH2	1:E:226:ASP:OD1	2.35	0.58
1:E:991:VAL:HG21	1:E:1001:ILE:CG2	2.33	0.58
1:A:577:GLU:H	1:A:577:GLU:CD	2.11	0.58
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.28	0.58
1:G:403:GLU:OE1	1:G:646:THR:HG21	2.03	0.58
1:G:715:ARG:HA	1:G:725:MET:HG2	1.85	0.58
2:B:48:TYR:O	2:B:51:GLN:HB2	2.04	0.58
2:B:267:GLY:O	2:B:349:SER:HB2	2.03	0.58
1:C:337:ASN:OD1	9:C:4485:HOH:O	2.17	0.58
2:H:277:LEU:HD23	2:H:281:ALA:O	2.03	0.58
2:H:7:LEU:HB3	2:H:15:PHE:HB2	1.85	0.58
1:E:17:PRO:HG3	1:E:917:VAL:CG1	2.33	0.58
1:G:1007:ASN:HB2	1:G:1009:GLU:HG3	1.86	0.58
2:H:193:HIS:O	2:H:234:ASP:HB2	2.04	0.58
2:B:324:ASN:ND2	2:B:324:ASN:H	1.99	0.58
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.32	0.58
2:B:215:ARG:HH11	2:B:215:ARG:CG	2.17	0.58
1:E:574:GLN:HE21	1:E:720:LEU:CD2	2.13	0.58
2:H:78:GLN:NE2	9:H:3324:HOH:O	2.36	0.58
2:D:158:LEU:HD23	2:D:161:GLU:HG3	1.86	0.57
2:B:218:ILE:HD13	2:B:218:ILE:N	2.18	0.57
2:B:228:VAL:O	2:B:231:MET:HG3	2.03	0.57
8:C:1950:NET:H42	8:C:1950:NET:C2	2.27	0.57
1:A:3:LYS:HB3	1:A:330:TYR:CZ	2.39	0.57
2:D:208:MET:O	2:D:212:ARG:HG3	2.05	0.57
2:D:368:ASP:HB2	9:D:1592:HOH:O	2.05	0.57
2:B:190:LEU:HB2	2:B:215:ARG:HB3	1.86	0.57
1:C:110:GLU:O	1:C:110:GLU:HG2	2.03	0.57
1:C:675:ARG:HD2	1:C:716:PRO:O	2.04	0.57
1:G:151:THR:O	1:G:155:ALA:N	2.29	0.57
1:A:25:GLU:OE1	1:A:25:GLU:N	2.33	0.57
1:A:814:GLN:NE2	9:A:1315:HOH:O	2.36	0.57
1:C:93:GLN:HB2	1:C:174:MET:HE3	1.86	0.57
1:C:1019:GLY:O	1:C:1023:ILE:HD12	2.04	0.57
1:G:784:GLN:HE22	1:G:1043:THR:HB	1.69	0.57
1:A:574:GLN:HE21	1:A:720:LEU:HD21	1.70	0.57
1:G:1029:ILE:HD12	1:G:1029:ILE:N	2.11	0.57
1:A:704:LYS:O	1:A:707:GLU:HB2	2.05	0.57
1:C:3:LYS:NZ	9:C:4567:HOH:O	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:ASN:C	1:C:571:ARG:HG3	2.29	0.57
2:D:174:SER:O	2:D:182:PRO:HD3	2.03	0.57
2:D:286:MET:HE1	2:D:312:HIS:CE1	2.39	0.57
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.04	0.57
1:G:10:ILE:HD11	1:G:42:TYR:CD1	2.40	0.57
1:G:82:ARG:N	1:G:83:PRO:HD3	2.18	0.57
2:H:201:ALA:HA	2:H:240:ASN:OD1	2.03	0.57
1:E:471:ARG:HD2	9:E:3384:HOH:O	2.03	0.57
1:A:76:LYS:HD2	1:A:1059:THR:O	2.04	0.57
1:A:959:ASP:O	1:A:963:LYS:HG3	2.05	0.57
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.87	0.57
1:G:628:GLU:OE1	9:G:4185:HOH:O	2.17	0.56
1:G:820:LEU:O	1:G:821:GLN:HB2	2.05	0.56
2:H:156:MET:HG2	2:H:158:LEU:HG	1.87	0.56
2:B:225:ALA:O	2:B:228:VAL:HB	2.05	0.56
1:G:683:GLU:OE1	1:G:683:GLU:HA	2.05	0.56
1:G:1004:ARG:O	1:G:1009:GLU:HB2	2.04	0.56
1:A:164:PHE:HB3	1:A:165:PRO:HA	1.87	0.56
1:C:560:GLU:OE2	1:C:636:LYS:HE3	2.05	0.56
1:E:164:PHE:HB3	1:E:165:PRO:HA	1.88	0.56
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.69	0.56
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.05	0.56
2:F:306:MET:HB3	2:F:362:ASP:HB3	1.88	0.56
1:A:975:HIS:HD1	1:G:975:HIS:HD1	0.70	0.56
2:F:191:PRO:HD2	2:F:213:GLY:O	2.05	0.56
2:H:364:ALA:N	2:H:365:PRO:HD2	2.20	0.56
1:C:717:SER:HB3	1:C:748:ALA:HB3	1.88	0.56
1:E:684:ARG:HD3	1:E:819:GLU:OE2	2.04	0.56
1:G:157:ALA:O	1:G:160:ALA:HB3	2.06	0.56
1:G:194:ARG:NH1	1:G:194:ARG:HB2	2.20	0.56
1:G:579:ASP:OD1	1:G:607:SER:HB3	2.06	0.56
1:A:26:PHE:O	1:A:30:GLY:N	2.30	0.56
1:E:727:ILE:HG13	1:E:909:PRO:HG3	1.86	0.56
1:E:1029:ILE:HD12	1:E:1029:ILE:N	2.20	0.56
1:A:559:ARG:NH2	9:A:1677:HOH:O	2.28	0.56
2:D:355:GLU:OE1	2:D:355:GLU:N	2.33	0.56
1:A:583:VAL:O	1:A:587:LEU:HD22	2.05	0.56
1:C:975:HIS:HE2	1:E:992:ASN:ND2	2.04	0.56
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.70	0.56
1:G:151:THR:H	1:G:154:GLU:HB2	1.71	0.56
2:H:254:ALA:O	2:H:257:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:272:HIS:HA	2:H:349:SER:HB2	1.87	0.56
2:F:59:HIS:ND1	2:F:84:ASP:OD2	2.34	0.56
1:G:167:ILE:HD12	1:G:167:ILE:N	2.21	0.56
1:G:336:MET:HB3	1:G:342:GLY:HA2	1.88	0.56
2:H:255:ILE:O	2:H:259:LEU:HD12	2.06	0.56
1:A:1061:LYS:HG3	9:A:1389:HOH:O	2.06	0.56
2:D:306:MET:HB2	2:D:362:ASP:HB3	1.87	0.55
2:F:171:THR:O	2:F:185:LYS:HB2	2.05	0.55
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.36	0.55
1:G:949:VAL:O	1:G:954:LYS:HE3	2.06	0.55
1:G:1017:THR:CG2	1:G:1023:ILE:HG13	2.36	0.55
1:A:196:LEU:HG	1:A:204:LEU:HD11	1.88	0.55
1:A:534:ALA:O	2:B:123:ARG:HD3	2.06	0.55
1:A:1060:GLU:HB3	9:A:1350:HOH:O	2.05	0.55
2:D:222:GLN:HE21	2:D:222:GLN:H	1.55	0.55
1:E:579:ASP:OD2	1:E:605:THR:HB	2.05	0.55
1:G:259:LYS:HE2	2:H:69:ASP:OD1	2.06	0.55
1:A:26:PHE:HA	1:A:29:SER:HB2	1.87	0.55
1:E:172:PHE:HB3	1:E:200:PRO:CG	2.26	0.55
1:A:922:ARG:HH21	1:A:1061:LYS:HB3	1.71	0.55
1:A:1001:ILE:HD13	1:A:1029:ILE:HG13	1.88	0.55
1:C:313:LYS:NZ	1:C:603:PRO:O	2.40	0.55
1:E:998:ARG:CG	1:E:998:ARG:HH11	2.19	0.55
2:H:275:LEU:HD23	2:H:349:SER:OG	2.07	0.55
2:D:285:LYS:HG3	2:D:314:PHE:CE2	2.42	0.55
1:G:784:GLN:HE21	1:G:784:GLN:H	1.55	0.55
1:A:588:ALA:HB2	1:A:863:LYS:HG2	1.87	0.55
1:A:654:LEU:O	1:A:659:VAL:HG23	2.07	0.55
1:C:225:ASN:ND2	1:C:331:THR:HG21	2.22	0.55
1:C:343:ARG:NH2	1:C:539:ASP:OD2	2.40	0.55
1:C:990:LEU:HD23	1:E:979:ILE:HG12	1.87	0.55
1:G:93:GLN:HB2	1:G:174:MET:CG	2.36	0.55
1:G:698:ILE:O	1:G:702:VAL:N	2.30	0.55
1:C:698:ILE:HD12	1:C:698:ILE:H	1.72	0.55
1:G:941:LYS:NZ	1:G:1056:ALA:O	2.38	0.55
2:H:193:HIS:HA	2:H:215:ARG:HG2	1.89	0.55
1:C:690:PRO:HG3	1:C:756:LEU:HD11	1.89	0.55
1:E:169:ARG:O	1:E:205:LEU:N	2.38	0.55
1:C:751:LEU:O	1:C:752:LEU:HD12	2.07	0.54
2:D:226:GLU:O	2:D:230:LYS:HG3	2.07	0.54
1:E:930:LYS:HE3	9:E:3016:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:998:ARG:HA	1:G:999:PRO:C	2.30	0.54
1:A:403:GLU:CD	1:A:646:THR:HG21	2.32	0.54
1:C:574:GLN:NE2	1:C:645:GLN:HB2	2.22	0.54
2:D:8:VAL:HG22	2:D:14:GLN:HG2	1.89	0.54
1:A:4:ARG:CZ	1:A:7:ILE:HD11	2.37	0.54
2:B:286:MET:HE2	2:B:314:PHE:C	2.31	0.54
1:C:678:PHE:O	1:C:682:VAL:HG23	2.06	0.54
1:E:75:ARG:HG2	1:E:75:ARG:HH11	1.72	0.54
2:F:6:LEU:HD22	2:F:138:PRO:HB2	1.89	0.54
1:G:782:ILE:HD12	1:G:782:ILE:N	2.22	0.54
2:D:33:ASN:OD1	2:D:35:SER:HB2	2.07	0.54
1:G:674:ASP:O	1:G:677:ARG:HB2	2.07	0.54
1:C:1051:ALA:O	1:C:1054:LEU:HB2	2.07	0.54
1:E:168:ILE:HD11	1:E:182:ALA:HB2	1.90	0.54
1:E:1004:ARG:HD3	1:E:1009[A]:GLU:OE2	2.06	0.54
2:B:144:LEU:HD12	2:B:144:LEU:C	2.30	0.54
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.42	0.54
1:C:43:ARG:NH2	1:C:81:GLU:OE1	2.29	0.54
1:C:956:ARG:NH2	1:C:1048:PHE:CD2	2.75	0.54
1:C:1027:ARG:NE	1:C:1031:ARG:HD3	2.22	0.54
1:A:82:ARG:N	1:A:83:PRO:HD3	2.23	0.54
1:E:950:ARG:HD3	9:E:3431:HOH:O	2.06	0.54
1:G:6:ASP:N	1:G:6:ASP:OD1	2.36	0.54
1:G:70:HIS:CE1	1:G:72:GLU:HB2	2.42	0.54
1:G:676:GLU:O	1:G:680:HIS:ND1	2.35	0.54
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.42	0.54
1:C:890:VAL:HG23	1:C:927:ALA:HB1	1.89	0.54
1:E:264:MET:O	1:E:267:ALA:HB3	2.08	0.54
1:E:715:ARG:NH1	1:E:753:ASP:OD2	2.40	0.54
1:G:922:ARG:NE	1:G:1061:LYS:HD3	2.21	0.54
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.42	0.54
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.72	0.54
1:G:588:ALA:HB2	1:G:863:LYS:HG2	1.90	0.54
1:A:345:PRO:HG3	2:B:332:LEU:HB3	1.89	0.54
1:A:693:ALA:HB3	1:A:708:ILE:HD11	1.90	0.54
2:B:324:ASN:HA	2:B:343:THR:OG1	2.07	0.54
1:E:159:ALA:HB2	1:E:188:PHE:CZ	2.43	0.54
1:E:563:MET:CE	1:E:635:PRO:HG3	2.38	0.54
1:G:784:GLN:H	1:G:784:GLN:NE2	2.06	0.54
1:G:839:LEU:HD12	1:G:840:ILE:N	2.23	0.54
2:B:286:MET:HE2	2:B:314:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:868:VAL:HG23	1:C:877:GLN:HE22	1.73	0.53
2:F:201:ALA:CB	2:F:239:SER:HB2	2.36	0.53
1:G:741:ALA:O	1:G:745:SER:HB2	2.08	0.53
1:A:74:VAL:O	1:A:78:ILE:HG13	2.08	0.53
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.42	0.53
1:A:956:ARG:HB2	1:A:1044:LEU:HD23	1.90	0.53
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.89	0.53
1:E:26:PHE:HB2	5:E:2980:CL:CL	2.46	0.53
1:E:583:VAL:O	1:E:587:LEU:HD22	2.07	0.53
1:E:967:GLN:HG3	1:E:967:GLN:O	2.07	0.53
2:F:186:LYS:O	2:F:189:GLU:N	2.30	0.53
2:B:135:GLY:O	2:B:138:PRO:HD3	2.08	0.53
2:B:225:ALA:HA	2:B:258:PHE:CZ	2.44	0.53
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.08	0.53
1:C:146:SER:CB	1:C:205:LEU:HD11	2.38	0.53
1:E:796:LEU:HD23	1:E:796:LEU:C	2.33	0.53
2:F:249:ASP:OD1	2:F:250:TYR:N	2.39	0.53
1:A:947:LEU:N	1:A:947:LEU:HD12	2.22	0.53
2:B:334:ASP:CG	2:B:336:THR:HG23	2.33	0.53
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.24	0.53
1:A:321:LYS:NZ	1:A:338:ASP:OD2	2.29	0.53
2:B:255:ILE:HA	2:B:258:PHE:CD2	2.44	0.53
1:C:590:ARG:O	1:C:593:GLY:N	2.32	0.53
2:D:215:ARG:HH11	2:D:215:ARG:CG	2.21	0.53
1:E:174:MET:HE2	1:E:303:ARG:NH2	2.22	0.53
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.08	0.53
1:G:211:ILE:HG13	6:G:3900:ANP:H2	1.91	0.53
1:G:698:ILE:O	1:G:702:VAL:HG23	2.09	0.53
2:H:208:MET:SD	2:H:355:GLU:HA	2.49	0.53
2:H:232:ASN:N	2:H:233:PRO:HD3	2.22	0.53
2:B:300:VAL:HG23	2:B:301:GLU:N	2.23	0.53
1:G:290:PRO:O	2:H:92:PHE:HB3	2.08	0.53
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.39	0.53
1:A:70:HIS:ND1	1:A:72:GLU:HB2	2.23	0.53
1:G:796:LEU:HD23	1:G:796:LEU:C	2.34	0.53
1:A:152:MET:O	1:A:156:LEU:HG	2.08	0.53
1:C:368:ALA:HB3	9:C:4425:HOH:O	2.09	0.53
2:D:327:VAL:HG13	2:D:337:LEU:CD1	2.39	0.53
1:E:299:GLU:HB2	9:E:3103:HOH:O	2.09	0.53
2:F:300:VAL:HG22	2:F:328:THR:O	2.08	0.53
1:G:126:ALA:CB	1:G:302:PRO:HG3	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:THR:HG22	1:A:1023:ILE:HG13	1.90	0.53
1:C:684:ARG:HH11	1:C:684:ARG:CG	2.17	0.53
2:B:168:TYR:O	2:B:218:ILE:N	2.32	0.52
1:A:54:ILE:O	1:A:57:ASP:N	2.41	0.52
1:A:892:GLU:OE1	7:A:1085:ORN:NE	2.40	0.52
1:G:873:SER:OG	1:G:876:GLU:HG3	2.09	0.52
2:H:277:LEU:O	2:H:280:GLY:N	2.39	0.52
1:C:482:THR:HB	9:C:4517:HOH:O	2.10	0.52
1:E:762:VAL:HG12	1:E:763:ASP:N	2.24	0.52
1:E:947:LEU:HD12	1:E:947:LEU:N	2.25	0.52
2:F:46:PRO:HA	2:F:76:HIS:CG	2.44	0.52
1:G:561:LYS:O	1:G:636:LYS:N	2.40	0.52
1:G:720:LEU:C	1:G:720:LEU:HD12	2.35	0.52
1:A:164:PHE:HA	1:A:165:PRO:C	2.35	0.52
1:C:421:LEU:HB3	1:G:421:LEU:HB3	1.92	0.52
2:F:244:ASP:OD1	2:F:245:PRO:HD2	2.10	0.52
1:G:158:VAL:O	1:G:161:ASP:HB3	2.09	0.52
2:B:116:ARG:O	2:B:120:ARG:HG3	2.09	0.52
2:B:286:MET:HE1	2:B:312:HIS:CE1	2.43	0.52
2:D:157:ASP:CG	2:D:160:LYS:HG2	2.35	0.52
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.09	0.52
1:A:723:ARG:NH1	1:A:910:GLU:OE1	2.43	0.52
1:A:772[B]:MET:CE	1:A:880:THR:HG22	2.39	0.52
1:E:183:TYR:HB2	1:E:187:GLU:OE1	2.09	0.52
1:E:264:MET:HE2	1:E:286:PHE:CB	2.39	0.52
1:E:991:VAL:HG22	1:E:1001:ILE:HG23	1.88	0.52
1:G:519:GLN:NE2	9:G:4492:HOH:O	2.43	0.52
1:G:703:GLU:HG3	1:G:704:LYS:N	2.22	0.52
1:G:722:GLY:HA2	1:G:725:MET:SD	2.49	0.52
2:H:313:GLY:HA3	9:H:3476:HOH:O	2.09	0.52
1:G:904:ASP:CG	1:G:1027:ARG:HG3	2.35	0.52
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.90	0.52
1:C:698:ILE:H	1:C:698:ILE:CD1	2.23	0.52
1:E:516:LEU:O	1:E:519:GLN:HB3	2.09	0.52
1:G:679:GLN:HG3	1:G:689:GLN:HE22	1.73	0.52
1:A:143:THR:HA	1:A:296:ILE:HG23	1.91	0.52
1:C:403:GLU:OE2	1:C:646:THR:HG21	2.08	0.52
1:C:479:VAL:HB	1:C:483:GLY:HA3	1.92	0.52
1:C:951:GLU:CA	1:C:954:LYS:HD2	2.34	0.52
1:E:40:GLU:OE1	1:E:40:GLU:HA	2.10	0.52
1:G:425:ARG:NH1	9:G:4363:HOH:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:HIS:ND1	1:C:72:GLU:HB2	2.24	0.52
1:C:692:ASN:HB3	1:C:753:ASP:HA	1.91	0.52
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.92	0.52
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.91	0.51
1:A:1061:LYS:HA	9:A:1389:HOH:O	2.09	0.51
1:C:145:ARG:HH12	1:C:161:ASP:CG	2.18	0.51
1:E:671:ARG:NH2	1:E:819:GLU:O	2.43	0.51
1:G:166:CYS:SG	1:G:182:ALA:HB3	2.50	0.51
1:G:590:ARG:O	1:G:593:GLY:N	2.42	0.51
2:B:244:ASP:HB3	2:B:247:PRO:CD	2.40	0.51
1:C:99:ALA:HB1	1:C:115:MET:HE2	1.92	0.51
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.91	0.51
1:E:126:ALA:CB	1:E:302:PRO:HG3	2.40	0.51
1:E:164:PHE:HA	1:E:165:PRO:C	2.35	0.51
2:F:275:LEU:HD23	2:F:349:SER:HB3	1.92	0.51
2:H:46:PRO:HG2	2:H:200:GLY:O	2.11	0.51
2:H:172:GLN:HG2	2:H:173:GLY:N	2.25	0.51
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.46	0.51
1:A:57:ASP:OD1	1:A:855:LYS:HE3	2.10	0.51
1:A:700:MET:SD	1:A:703:GLU:HG2	2.51	0.51
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.11	0.51
1:E:684:ARG:NH1	1:E:684:ARG:HG3	2.24	0.51
2:F:236:ILE:HG22	2:F:237:PHE:N	2.24	0.51
1:G:191:ILE:HG22	1:G:192:CYS:N	2.25	0.51
1:A:331:THR:O	1:A:334:GLU:HB2	2.11	0.51
1:A:772[B]:MET:HE1	1:A:880:THR:HG22	1.92	0.51
1:C:709:GLY:O	1:C:754:HIS:HD2	1.94	0.51
1:G:859:VAL:O	1:G:861:LEU:N	2.43	0.51
1:A:11:LEU:HD12	1:A:45:ILE:O	2.10	0.51
1:A:343:ARG:NH2	1:A:539:ASP:OD1	2.38	0.51
1:A:956:ARG:HB2	1:A:1044:LEU:CD2	2.40	0.51
1:C:146:SER:HB2	1:C:205:LEU:CD1	2.37	0.51
1:C:742:VAL:HG22	1:C:750:VAL:HG21	1.92	0.51
1:C:805:ILE:CD1	1:C:837:VAL:HG22	2.40	0.51
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.16	0.51
1:A:896:PRO:HG3	1:A:914:THR:HG23	1.93	0.51
1:C:722:GLY:HA2	1:C:725:MET:SD	2.50	0.51
1:G:712:LEU:HB3	1:G:728:VAL:HG23	1.92	0.51
2:H:27:VAL:O	2:H:78:GLN:HG2	2.10	0.51
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.40	0.51
1:C:103:GLU:HG3	1:C:104:ARG:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:286:MET:HE3	2:H:289:GLY:HA2	1.91	0.51
2:D:249:ASP:OD1	2:D:250:TYR:N	2.44	0.51
1:E:1029:ILE:H	1:E:1029:ILE:CD1	2.21	0.51
1:E:1065:VAL:O	1:E:1068:MET:HB2	2.10	0.51
6:E:2910:ANP:O3'	9:E:3414:HOH:O	2.19	0.51
2:H:114:ASP:O	2:H:117:LYS:HB3	2.10	0.51
1:A:731:GLU:O	1:A:735:ARG:HG3	2.11	0.51
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.41	0.51
2:D:78:GLN:NE2	2:D:78:GLN:HA	2.25	0.51
1:E:315:THR:O	1:E:531:THR:HG22	2.11	0.51
1:G:412:LYS:HE2	1:G:434:ASP:OD2	2.11	0.51
1:G:582:CYS:HB3	1:G:598:MET:HE1	1.93	0.51
1:A:426:ARG:C	1:A:426:ARG:HD3	2.36	0.50
2:B:302:LYS:HB2	2:B:304:VAL:HG13	1.92	0.50
1:C:1028:VAL:HG12	9:C:4605:HOH:O	2.11	0.50
1:E:721:GLY:N	6:E:2910:ANP:O1G	2.30	0.50
2:H:215:ARG:HG3	2:H:215:ARG:NH1	2.23	0.50
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.12	0.50
1:A:333:ASP:OD1	1:A:333:ASP:N	2.42	0.50
1:C:554:ASN:N	1:C:555:PRO:HD3	2.26	0.50
1:E:168:ILE:HD13	1:E:191:ILE:HG21	1.89	0.50
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.46	0.50
2:F:159:ALA:O	2:F:163:THR:HG22	2.11	0.50
2:F:269:CYS:O	2:F:272:HIS:HB3	2.11	0.50
1:G:259:LYS:HD3	2:H:175:TRP:CE3	2.47	0.50
1:G:417:ASP:OD2	1:G:423:LYS:NZ	2.42	0.50
1:A:910:GLU:O	1:A:912[A]:ARG:HD3	2.11	0.50
1:E:25:GLU:OE1	1:E:25:GLU:N	2.28	0.50
1:G:810:ARG:HG3	1:G:810:ARG:NH1	2.26	0.50
1:G:899:LYS:O	1:G:901:PRO:HD3	2.12	0.50
1:A:70:HIS:O	1:A:74:VAL:HG23	2.11	0.50
1:A:574:GLN:HE22	1:A:645:GLN:HB2	1.73	0.50
2:B:150:PHE:CG	2:B:151:PRO:HD2	2.46	0.50
1:C:146:SER:HA	1:C:206:ILE:O	2.11	0.50
2:D:135:GLY:O	2:D:138:PRO:HD3	2.11	0.50
2:D:326:ARG:O	2:D:340:ILE:HA	2.12	0.50
1:G:950:ARG:HD3	9:G:4425:HOH:O	2.11	0.50
2:B:205:ILE:HG21	2:B:237:PHE:CE2	2.46	0.50
1:E:956:ARG:HB2	1:E:1044:LEU:HD21	1.94	0.50
2:F:6:LEU:HD23	2:F:6:LEU:O	2.11	0.50
2:F:310:GLN:NE2	2:F:352:GLY:HA3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:ILE:O	2:F:268:ILE:HG22	2.11	0.50
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.46	0.50
2:H:176:THR:O	2:H:180:GLY:N	2.41	0.50
1:A:1004:ARG:O	1:A:1009:GLU:HB2	2.11	0.50
1:A:1028:VAL:O	1:A:1032:SER:OG	2.29	0.50
1:G:994:VAL:HG22	1:G:1000:HIS:CE1	2.46	0.50
2:H:9:LEU:N	2:H:9:LEU:HD23	2.25	0.50
2:H:273:GLN:HE21	2:H:351:GLN:HE22	1.60	0.50
1:A:900:PHE:N	1:A:901:PRO:HD3	2.26	0.50
1:C:403:GLU:HG3	1:C:569:PRO:HD2	1.94	0.50
1:C:460:ARG:O	1:C:464:VAL:HG22	2.12	0.50
1:G:168:ILE:HD11	1:G:188:PHE:CD1	2.47	0.50
1:G:431:ALA:HB2	1:G:435:ARG:CZ	2.41	0.50
1:G:982:GLY:HA2	1:G:986:ILE:O	2.12	0.50
1:A:181:ILE:HD11	1:A:376:THR:HG23	1.94	0.50
2:B:249:ASP:OD1	2:B:250:TYR:N	2.45	0.50
1:G:349:GLU:O	2:H:294:ASN:HB2	2.12	0.50
1:C:294:ARG:NH1	9:C:4348:HOH:O	2.43	0.49
1:G:589:LEU:O	1:G:594:TYR:HB2	2.12	0.49
1:G:947:LEU:HD12	1:G:947:LEU:N	2.27	0.49
2:F:232:ASN:N	2:F:233:PRO:HD3	2.27	0.49
1:G:1001:ILE:HD12	1:G:1002:GLN:CB	2.41	0.49
1:A:1:MET:HB3	1:A:2:PRO:HD2	1.94	0.49
1:A:993:LYS:N	1:A:996:GLU:HG3	2.27	0.49
1:G:481:ILE:HG21	1:G:508:VAL:CG1	2.42	0.49
1:G:825:LEU:HG	1:G:865:ALA:CB	2.41	0.49
1:A:467:GLU:O	1:A:471:ARG:HG2	2.13	0.49
2:B:327:VAL:HG13	2:B:337:LEU:CD1	2.42	0.49
1:G:46:LEU:O	1:G:46:LEU:HG	2.12	0.49
2:H:272:HIS:HA	2:H:349:SER:CB	2.42	0.49
1:C:688:LYS:HE2	1:C:838:TYR:CE2	2.47	0.49
1:C:998:ARG:HA	1:C:999:PRO:C	2.37	0.49
1:C:1017:THR:HG22	1:C:1018:SER:N	2.27	0.49
1:E:313:LYS:HE2	1:E:608:THR:O	2.13	0.49
1:E:327:ALA:HB2	9:E:3520:HOH:O	2.12	0.49
1:E:941:LYS:NZ	1:E:1056:ALA:O	2.30	0.49
2:H:160:LYS:HG3	2:H:161:GLU:HG2	1.94	0.49
1:A:570:ASN:C	1:A:571:ARG:HG3	2.37	0.49
1:A:586:SER:O	1:A:590:ARG:HB2	2.13	0.49
1:C:692:ASN:HA	1:C:708:ILE:HD13	1.95	0.49
1:C:768:CYS:HA	1:C:772:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:922:ARG:HH21	1:C:1061:LYS:CB	2.25	0.49
2:F:206:LEU:HB3	2:F:216:LEU:CD1	2.43	0.49
1:G:152:MET:HB2	9:G:4034:HOH:O	2.13	0.49
1:G:716:PRO:HD2	1:G:725:MET:CG	2.42	0.49
1:A:1027:ARG:HH21	1:A:1031:ARG:HH11	1.59	0.49
2:B:246:ALA:HB3	2:B:247:PRO:CD	2.41	0.49
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.93	0.49
1:G:712:LEU:HD11	1:G:752:LEU:HB3	1.94	0.49
2:H:225:ALA:O	2:H:228:VAL:HB	2.12	0.49
1:A:219:GLU:OE2	1:A:307:SER:HB2	2.12	0.49
2:B:356:ALA:HB3	9:B:1123:HOH:O	2.12	0.49
1:E:130:ARG:CG	1:E:148:ILE:HG13	2.33	0.49
1:E:712:LEU:HD23	1:E:713:VAL:N	2.27	0.49
1:E:906:LEU:CD2	1:E:1023:ILE:HG23	2.43	0.49
1:G:860:PRO:HB2	1:G:863:LYS:HD2	1.94	0.49
1:A:174:MET:HA	6:A:1083:ANP:O1B	2.13	0.49
1:A:899:LYS:C	1:A:901:PRO:HD3	2.37	0.49
1:C:44:VAL:N	1:C:62:ASP:OD2	2.30	0.49
1:E:692:ASN:HB3	1:E:753:ASP:OD1	2.13	0.49
1:E:784:GLN:HE21	1:E:784:GLN:N	2.02	0.49
2:F:259:LEU:O	2:F:345:LYS:HE3	2.12	0.49
1:G:698:ILE:H	1:G:698:ILE:HG13	1.47	0.49
1:G:929:ALA:HB2	1:G:1053:ALA:HB1	1.93	0.49
1:A:710:TYR:CB	1:A:711:PRO:HA	2.33	0.49
1:A:762:VAL:HG11	1:A:809:MET:HE1	1.94	0.49
1:C:1001:ILE:HD12	1:C:1002:GLN:HB2	1.94	0.49
1:E:695:VAL:HG11	1:E:701:ALA:CA	2.42	0.49
1:G:365:GLU:HG2	1:G:366:LYS:N	2.27	0.49
1:G:716:PRO:HD2	1:G:725:MET:HG3	1.95	0.49
1:A:366:LYS:O	1:A:912[B]:ARG:NH1	2.46	0.48
1:A:820:LEU:O	1:A:821:GLN:HB2	2.13	0.48
1:A:890:VAL:HG12	1:A:931:ALA:CB	2.43	0.48
1:C:1027:ARG:NH2	1:C:1031:ARG:HH11	2.08	0.48
2:F:199:PHE:HB3	2:F:270:LEU:HD23	1.95	0.48
2:H:46:PRO:HA	2:H:76:HIS:CG	2.48	0.48
1:A:46:LEU:HD13	1:A:55:MET:HE2	1.94	0.48
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.27	0.48
1:G:767:ILE:HD13	1:G:865:ALA:HB2	1.94	0.48
1:G:853:VAL:CG1	1:G:861:LEU:HD11	2.43	0.48
1:A:574:GLN:HE21	1:A:645:GLN:HB2	1.74	0.48
1:C:574:GLN:CG	1:C:720:LEU:HD11	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:LYS:O	1:E:287:ALA:HA	2.13	0.48
2:F:2:ILE:C	2:F:2:ILE:HD12	2.36	0.48
2:F:194:VAL:O	2:F:216:LEU:HA	2.13	0.48
1:A:1051:ALA:O	1:A:1054:LEU:HB2	2.13	0.48
1:C:331:THR:OG1	1:C:334:GLU:HG3	2.12	0.48
1:C:805:ILE:HD11	1:C:837:VAL:CG2	2.43	0.48
2:D:201:ALA:HB2	2:D:239:SER:CB	2.43	0.48
1:G:722:GLY:N	6:G:3910:ANP:O1B	2.39	0.48
1:G:1028:VAL:O	1:G:1032:SER:OG	2.30	0.48
1:A:998:ARG:HA	1:A:999:PRO:C	2.38	0.48
1:C:704:LYS:O	1:C:707:GLU:HB2	2.14	0.48
1:C:805:ILE:HD11	1:C:837:VAL:HG22	1.94	0.48
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.61	0.48
2:H:51:GLN:O	2:H:78:GLN:N	2.39	0.48
1:E:712:LEU:HG	1:E:753:ASP:O	2.14	0.48
1:C:671:ARG:HG2	1:C:677:ARG:NH1	2.28	0.48
2:F:142:LEU:O	2:F:146:LYS:HG3	2.14	0.48
1:A:671:ARG:NH2	1:A:819:GLU:O	2.47	0.48
2:B:163:THR:OG1	2:B:198:ASP:O	2.30	0.48
2:B:244:ASP:HB3	2:B:247:PRO:CG	2.44	0.48
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.32	0.48
2:D:121:LEU:HD11	2:D:125:LYS:HD2	1.96	0.48
2:D:228:VAL:O	2:D:231:MET:HG3	2.14	0.48
2:D:251:ALA:O	2:D:255:ILE:HG13	2.13	0.48
2:F:370:PHE:O	2:F:373:LEU:N	2.46	0.48
1:G:839:LEU:HD12	1:G:840:ILE:H	1.79	0.48
2:H:34:THR:HA	2:H:56:THR:OG1	2.13	0.48
1:A:145:ARG:HB2	1:A:208:GLU:CD	2.39	0.48
1:A:970:GLU:HG3	9:A:1524:HOH:O	2.12	0.48
1:E:708:ILE:HG22	1:E:709:GLY:N	2.27	0.48
2:H:46:PRO:HB2	2:H:200:GLY:O	2.14	0.48
1:A:213:TRP:HH2	1:A:294:ARG:HD3	1.78	0.48
8:A:1086:NET:H42	8:A:1086:NET:C2	2.29	0.48
2:B:249:ASP:OD1	2:B:249:ASP:N	2.46	0.48
1:C:224:LYS:HE2	1:C:329:GLY:O	2.14	0.48
2:D:244:ASP:OD1	2:D:245:PRO:HD2	2.14	0.48
2:F:354:PRO:HA	2:F:363:ALA:HB3	1.96	0.48
1:G:181:ILE:CD1	1:G:376:THR:HG23	2.44	0.48
1:G:271:VAL:HG12	1:G:300:MET:CE	2.44	0.48
1:G:972:ASP:HB3	1:G:991:VAL:HG11	1.95	0.48
2:B:58:PRO:HA	2:B:83:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ASP:CG	2:B:378:ARG:HH11	2.21	0.47
2:B:261:THR:OG1	2:B:263:ILE:HG13	2.14	0.47
1:C:449:VAL:HG12	1:C:460:ARG:HG2	1.97	0.47
1:E:725:MET:HE1	6:E:2910:ANP:O3A	2.14	0.47
2:H:318:GLU:O	2:H:321:LEU:HB2	2.13	0.47
1:A:541:ALA:HB1	1:A:543:MET:HE2	1.96	0.47
2:B:270:LEU:HD12	2:B:273:GLN:OE1	2.14	0.47
1:C:514:ARG:HD3	9:C:4176:HOH:O	2.14	0.47
1:C:517:ARG:HB3	1:C:522:LEU:O	2.14	0.47
1:C:820:LEU:HD23	1:C:820:LEU:HA	1.46	0.47
2:D:175:TRP:HA	2:D:180:GLY:O	2.13	0.47
2:F:46:PRO:HA	2:F:76:HIS:CD2	2.49	0.47
1:G:101:GLU:OE1	1:G:104:ARG:NH2	2.45	0.47
1:G:419:GLU:O	1:G:423:LYS:HG3	2.14	0.47
1:G:565:LEU:N	1:G:565:LEU:HD23	2.25	0.47
1:G:912:ARG:NE	9:G:4346:HOH:O	2.30	0.47
1:G:937:SER:OG	1:G:938:THR:N	2.48	0.47
1:G:993:LYS:NZ	9:G:4423:HOH:O	2.47	0.47
1:G:1063:ILE:CD1	1:G:1068:MET:HG3	2.43	0.47
1:C:312:SER:HA	1:C:317:PHE:O	2.14	0.47
1:C:412:LYS:HG2	1:C:438:TYR:CZ	2.50	0.47
1:C:516:LEU:HD12	1:C:516:LEU:HA	1.72	0.47
2:F:55:LEU:HA	2:F:55:LEU:HD23	1.59	0.47
2:H:54:THR:HA	2:H:81:VAL:HB	1.95	0.47
2:H:342:ARG:NE	2:H:344:ASP:OD1	2.47	0.47
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.48	0.47
1:C:639:ILE:HD13	1:C:869:MET:CE	2.43	0.47
1:G:27:ASP:OD1	1:G:53:THR:HB	2.13	0.47
1:G:804:GLU:O	1:G:808:VAL:HG23	2.14	0.47
2:H:171:THR:OG1	2:H:185:LYS:O	2.29	0.47
1:C:46:LEU:HD13	1:C:55:MET:HE2	1.94	0.47
1:C:967:GLN:HG2	1:C:1054:LEU:CD1	2.19	0.47
1:E:57:ASP:OD1	1:E:855:LYS:HE3	2.15	0.47
1:E:145:ARG:HH12	1:E:161:ASP:CG	2.23	0.47
1:G:623:LEU:HD12	1:G:654:LEU:CD2	2.44	0.47
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.96	0.47
1:C:106:GLY:HA2	9:C:4569:HOH:O	2.13	0.47
1:C:145:ARG:NH1	1:C:161:ASP:OD2	2.48	0.47
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.97	0.47
1:G:358:LYS:HG2	1:G:359:ILE:N	2.28	0.47
1:A:9:SER:OG	1:A:83:PRO:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HA	1:A:281:GLY:HA2	1.97	0.47
1:A:1004:ARG:HH22	1:G:983:GLU:CG	2.27	0.47
2:B:302:LYS:C	2:B:304:VAL:HG13	2.39	0.47
1:C:383:GLU:OE2	9:C:4593:HOH:O	2.20	0.47
1:C:574:GLN:HE22	1:C:645:GLN:H	0.67	0.47
1:C:1061:LYS:NZ	9:C:4430:HOH:O	2.48	0.47
2:D:212:ARG:CG	2:D:212:ARG:HH11	2.27	0.47
1:E:70:HIS:CE1	1:E:72:GLU:HB2	2.50	0.47
1:E:715:ARG:HA	1:E:725:MET:HG2	1.96	0.47
1:E:998:ARG:HH11	1:E:998:ARG:HG2	1.80	0.47
2:F:163:THR:OG1	2:F:164:THR:N	2.48	0.47
1:G:1061:LYS:NZ	9:G:4418:HOH:O	2.38	0.47
8:G:3950:NET:H23	8:G:3950:NET:H83	1.97	0.47
1:A:291:LYS:HD2	9:A:1552:HOH:O	2.15	0.47
1:A:588:ALA:O	1:A:591:GLU:HB2	2.15	0.47
1:C:904:ASP:HA	1:C:905:PRO:HD3	1.72	0.47
1:E:587:LEU:HD12	1:E:587:LEU:HA	1.77	0.47
2:F:104:ARG:HG2	2:F:105:HIS:CD2	2.50	0.47
1:G:685:LEU:HD11	1:G:819:GLU:HB3	1.92	0.47
2:H:255:ILE:C	2:H:259:LEU:HD12	2.38	0.47
1:A:525:VAL:HG22	1:A:548:GLU:H	1.78	0.47
1:C:700:MET:CE	1:C:703:GLU:HG2	2.45	0.47
1:C:899:LYS:C	1:C:901:PRO:HD3	2.40	0.47
1:C:1020:ARG:HA	1:C:1020:ARG:HD2	1.69	0.47
1:E:314:ALA:HB1	1:E:356:VAL:HG21	1.97	0.47
2:F:298:LYS:HE2	2:F:303:ASN:OD1	2.15	0.47
1:G:215:GLU:HG3	1:G:240:MET:SD	2.55	0.47
1:G:353:ASP:OD1	1:G:353:ASP:N	2.48	0.47
1:A:315:THR:O	1:A:531:THR:HG22	2.15	0.47
2:B:201:ALA:HB2	2:B:239:SER:CB	2.45	0.47
1:E:955:GLU:HB2	9:E:3611:HOH:O	2.14	0.47
1:E:1001:ILE:H	1:E:1001:ILE:HG13	1.46	0.47
1:G:859:VAL:HG12	1:G:861:LEU:HD23	1.97	0.47
2:H:264:PRO:HB3	2:H:373:LEU:HB3	1.95	0.47
1:A:788:HIS:HD2	1:A:909:PRO:O	1.98	0.46
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.50	0.46
1:C:568:GLY:O	1:C:602:ASN:HB2	2.14	0.46
1:E:534:ALA:O	2:F:123:ARG:HD3	2.14	0.46
1:G:503:ALA:HB2	1:G:513:ILE:HG13	1.97	0.46
1:G:560:GLU:OE2	1:G:636:LYS:HE3	2.15	0.46
1:G:973:ALA:O	1:G:990:LEU:HD12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:325:LEU:HD23	2:H:342:ARG:HD2	1.97	0.46
1:A:579:ASP:O	1:A:583:VAL:HG23	2.15	0.46
1:G:563:MET:HE3	1:G:563:MET:HB2	1.77	0.46
1:A:932:GLN:O	1:A:937:SER:HB3	2.15	0.46
1:C:731:GLU:H	1:C:731:GLU:HG3	1.38	0.46
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.44	0.46
1:A:990:LEU:HG	1:G:979:ILE:HD11	1.96	0.46
1:C:723:ARG:HA	1:C:723:ARG:HD2	1.72	0.46
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.60	0.46
1:G:124:ASP:OD2	1:G:131:ARG:NH1	2.46	0.46
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.79	0.46
1:C:577:GLU:O	1:C:580:TYR:HB3	2.15	0.46
2:D:298:LYS:O	2:D:329:HIS:HA	2.15	0.46
1:G:146:SER:HB3	1:G:207:ASP:OD1	2.16	0.46
1:G:802:SER:O	1:G:806:GLN:HG3	2.15	0.46
2:H:72:SER:OG	2:H:74:GLN:O	2.33	0.46
2:H:253:THR:O	2:H:256:GLN:HB2	2.15	0.46
1:A:434:ASP:HB2	9:A:1457:HOH:O	2.14	0.46
1:E:69:ILE:O	1:E:69:ILE:HG22	2.16	0.46
1:A:684:ARG:HH11	1:A:684:ARG:CG	2.29	0.46
1:A:1020:ARG:HA	1:A:1020:ARG:HD2	1.64	0.46
1:C:57:ASP:HB3	1:C:59:GLU:OE1	2.15	0.46
1:C:801:LEU:HD23	1:C:801:LEU:HA	1.80	0.46
2:D:45:ASP:HB3	2:D:48:TYR:HD2	1.81	0.46
1:E:27:ASP:OD1	1:E:55:MET:HB3	2.15	0.46
1:E:583:VAL:HG12	1:E:587:LEU:HD22	1.97	0.46
2:F:305:VAL:HG12	2:F:306:MET:N	2.31	0.46
1:G:172:PHE:CD2	1:G:201:THR:HG23	2.51	0.46
1:G:720:LEU:HD12	1:G:720:LEU:O	2.16	0.46
2:H:44:THR:O	2:H:46:PRO:HD3	2.15	0.46
2:H:163:THR:OG1	2:H:198:ASP:O	2.30	0.46
1:A:325:LYS:O	1:A:330:TYR:HB2	2.15	0.46
1:C:482:THR:HG22	1:C:483:GLY:N	2.29	0.46
1:C:698:ILE:C	1:C:702:VAL:HG23	2.41	0.46
1:E:9:SER:HA	1:E:43:ARG:O	2.16	0.46
1:E:489:LEU:HD22	1:E:516:LEU:HD23	1.97	0.46
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.46	0.46
1:G:46:LEU:HD13	1:G:55:MET:HE2	1.98	0.46
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.79	0.46
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.15	0.46
2:H:57:TYR:CE1	2:H:58:PRO:HD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:OD1	1:A:244:THR:HG22	2.14	0.46
1:A:951:GLU:HA	1:A:954:LYS:CD	2.46	0.46
1:C:602:ASN:ND2	1:C:605:THR:CG2	2.79	0.46
2:D:215:ARG:CG	2:D:215:ARG:NH1	2.78	0.46
2:D:229:LEU:HA	2:D:229:LEU:HD23	1.77	0.46
2:D:273:GLN:O	2:D:277:LEU:HG	2.15	0.46
1:G:574:GLN:HE22	1:G:645:GLN:HB2	1.78	0.46
1:G:899:LYS:C	1:G:901:PRO:HD3	2.41	0.46
2:H:190:LEU:HD21	2:H:210:VAL:HG13	1.97	0.46
2:H:350:PHE:HB2	2:H:366:LEU:CD2	2.46	0.46
1:A:82:ARG:N	1:A:83:PRO:CD	2.79	0.46
1:A:471:ARG:HG3	9:A:1484:HOH:O	2.15	0.46
1:C:267:ALA:O	1:C:271:VAL:HG23	2.16	0.46
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.98	0.46
1:E:1036:TYR:C	1:E:1037:LYS:HG2	2.41	0.46
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.51	0.46
1:G:172:PHE:CD2	1:G:201:THR:CG2	2.99	0.46
1:G:746:ASN:C	1:G:748:ALA:H	2.24	0.46
1:A:299:GLU:HB2	9:A:1200:HOH:O	2.16	0.45
1:A:299:GLU:OE2	1:A:301:ASN:ND2	2.48	0.45
1:A:490:ARG:HA	1:A:522:LEU:HD21	1.98	0.45
1:A:1003:ASP:OD1	1:A:1006:LYS:NZ	2.40	0.45
1:A:1017:THR:CG2	1:A:1018:SER:N	2.78	0.45
2:B:71:GLU:C	2:B:203:ARG:HG3	2.41	0.45
1:C:550:GLU:HB2	2:D:117:LYS:HG3	1.97	0.45
1:C:712:LEU:HD23	1:C:712:LEU:C	2.41	0.45
1:C:1007:ASN:HB3	9:C:4604:HOH:O	2.16	0.45
2:D:194:VAL:O	2:D:216:LEU:HA	2.16	0.45
2:D:212:ARG:CG	2:D:212:ARG:NH1	2.79	0.45
2:D:371:ILE:O	2:D:374:ILE:HB	2.16	0.45
1:E:222:ARG:HD3	1:E:278:GLU:HA	1.97	0.45
1:E:820:LEU:O	1:E:821:GLN:HB2	2.16	0.45
1:E:1017:THR:CG2	1:E:1018:SER:N	2.79	0.45
2:F:217:THR:C	2:F:218:ILE:HD13	2.40	0.45
1:G:524:PRO:HD3	1:G:547:TYR:OH	2.17	0.45
1:A:822:VAL:C	1:A:823:ARG:HG2	2.41	0.45
1:C:82:ARG:N	1:C:83:PRO:CD	2.79	0.45
1:G:262:GLN:OE1	1:G:262:GLN:HA	2.15	0.45
1:G:782:ILE:N	1:G:782:ILE:CD1	2.80	0.45
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.33	0.45
8:G:3950:NET:H83	9:G:4270:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HB3	1:A:347:SER:HB3	1.98	0.45
1:A:708:ILE:CG2	1:A:754:HIS:HB2	2.46	0.45
2:B:133:ILE:CG2	2:B:138:PRO:HB3	2.46	0.45
2:B:224:SER:OG	2:B:227:ASP:OD2	2.34	0.45
1:E:100:LEU:HA	1:E:100:LEU:HD12	1.52	0.45
1:E:460:ARG:O	1:E:464:VAL:HG22	2.16	0.45
1:E:716:PRO:HG2	1:E:723:ARG:O	2.15	0.45
1:E:999:PRO:HA	1:E:1003:ASP:OD2	2.16	0.45
1:G:339:ILE:HG22	1:G:540:THR:HG21	1.96	0.45
1:G:385:MET:HB2	1:G:603:PRO:HG3	1.98	0.45
1:E:125:LYS:HD3	1:E:275:ILE:HA	1.97	0.45
1:G:151:THR:N	1:G:154:GLU:HB2	2.31	0.45
1:G:918:MET:HE2	1:G:920:VAL:CG2	2.46	0.45
1:G:982:GLY:C	1:G:984:ALA:H	2.24	0.45
1:A:456:THR:O	1:A:457:ASN:HB2	2.15	0.45
1:A:990:LEU:HD23	1:G:979:ILE:CD1	2.46	0.45
2:B:160:LYS:HG3	2:B:161:GLU:HG2	1.98	0.45
2:B:263:ILE:HG13	2:B:263:ILE:H	1.57	0.45
2:B:350:PHE:CG	2:B:366:LEU:CD2	3.00	0.45
1:C:82:ARG:HA	1:C:82:ARG:HD2	1.64	0.45
1:C:579:ASP:OD1	1:C:605:THR:HB	2.17	0.45
1:C:1017:THR:HG22	1:C:1018:SER:H	1.81	0.45
1:E:1:MET:CG	1:E:2:PRO:HD2	2.42	0.45
1:E:272:LEU:HD11	1:E:282:SER:HB2	1.99	0.45
1:E:720:LEU:C	1:E:720:LEU:HD12	2.41	0.45
1:E:1067:GLU:O	1:E:1071:GLN:HG3	2.16	0.45
1:G:240:MET:HE3	6:G:3900:ANP:C4	2.46	0.45
1:G:363:ASN:ND2	1:G:365:GLU:OE2	2.49	0.45
1:G:677:ARG:O	1:G:680:HIS:HB2	2.17	0.45
2:H:306:MET:CE	2:H:329:HIS:CD2	3.00	0.45
2:H:324:ASN:ND2	2:H:324:ASN:N	2.42	0.45
1:A:979:ILE:HD13	1:G:990:LEU:HB3	1.97	0.45
1:E:1017:THR:CG2	1:E:1018:SER:H	2.29	0.45
1:G:35:LYS:HD2	9:G:4283:HOH:O	2.16	0.45
1:G:318:PRO:O	1:G:322:VAL:HG23	2.16	0.45
1:G:645:GLN:HG2	1:G:720:LEU:HG	1.98	0.45
1:G:711:PRO:HG2	1:G:755:PHE:HB3	1.98	0.45
2:H:286:MET:CE	2:H:312:HIS:ND1	2.80	0.45
1:A:71:TRP:CH2	1:A:105:GLN:HG2	2.51	0.45
1:C:213:TRP:N	1:C:213:TRP:CD1	2.84	0.45
1:C:843:ASN:O	1:C:845:ARG:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:ASP:OD2	2:D:302:LYS:HD2	2.16	0.45
1:E:695:VAL:HG12	1:E:738:PHE:CZ	2.51	0.45
2:F:367:PHE:O	2:F:370:PHE:HB3	2.17	0.45
1:G:167:ILE:N	1:G:167:ILE:CD1	2.80	0.45
2:H:168:TYR:O	2:H:217:THR:HA	2.16	0.45
2:H:191:PRO:HD2	2:H:213:GLY:O	2.17	0.45
2:H:210:VAL:HG22	2:H:214:CYS:O	2.16	0.45
2:H:287:LYS:HD2	9:H:3198:HOH:O	2.17	0.45
2:B:6:LEU:HD22	2:B:138:PRO:HB2	1.99	0.45
2:B:168:TYR:O	2:B:217:THR:HA	2.17	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:710:TYR:HB3	1:C:711:PRO:HA	1.98	0.45
2:D:364:ALA:N	2:D:365:PRO:CD	2.79	0.45
1:C:224:LYS:NZ	9:C:3987:HOH:O	2.48	0.45
1:C:525:VAL:HG12	1:C:551:CYS:HB2	1.98	0.45
1:C:685:LEU:HD23	1:C:685:LEU:HA	1.84	0.45
1:E:574:GLN:HG2	1:E:720:LEU:HD11	1.98	0.45
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.99	0.45
1:E:989:ARG:NH2	1:E:1009[B]:GLU:OE1	2.42	0.45
2:F:235:GLY:HA2	2:F:263:ILE:HG22	1.98	0.45
1:G:354:TYR:HB2	1:G:388:GLY:O	2.16	0.45
1:G:440:ALA:O	1:G:444:ARG:HG3	2.17	0.45
1:G:1063:ILE:HG12	1:G:1064:SER:N	2.32	0.45
1:A:37:LEU:O	1:A:40:GLU:N	2.49	0.45
1:E:421:LEU:HD23	1:E:421:LEU:HA	1.71	0.45
2:F:197:TYR:OH	2:F:228:VAL:HG21	2.18	0.45
1:G:36:ALA:O	1:G:40:GLU:HG2	2.16	0.45
1:A:6:ASP:C	1:A:7:ILE:HG13	2.42	0.44
1:A:722:GLY:CA	1:A:725:MET:HG3	2.46	0.44
1:E:3:LYS:CB	1:E:330:TYR:CE1	3.00	0.44
8:E:2950:NET:H23	8:E:2950:NET:H71	1.63	0.44
1:G:289:ASN:HB3	1:G:292:ASN:OD1	2.16	0.44
1:G:713:VAL:HG12	1:G:715:ARG:HG2	1.99	0.44
1:G:1067:GLU:O	1:G:1070:ALA:HB3	2.18	0.44
1:A:417:ASP:HA	1:A:418:PRO:HD3	1.80	0.44
2:B:22:ALA:N	2:B:107:ILE:O	2.46	0.44
2:B:49:SER:HA	2:B:76:HIS:O	2.18	0.44
1:C:656:ALA:HA	9:C:4594:HOH:O	2.17	0.44
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.46	0.44
1:C:757:ASP:O	1:C:833:LYS:HE3	2.17	0.44
1:C:804:GLU:O	1:C:808:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:VAL:HA	2:D:231:MET:HE2	1.99	0.44
1:E:174:MET:CE	1:E:303:ARG:NH2	2.81	0.44
2:F:98:LEU:O	2:F:101:TYR:HB3	2.18	0.44
2:F:125:LYS:HB2	9:F:2666:HOH:O	2.17	0.44
1:G:467:GLU:O	1:G:471:ARG:HG2	2.17	0.44
1:G:702:VAL:HG21	1:G:735:ARG:HH12	1.82	0.44
1:G:990:LEU:HD12	1:G:990:LEU:HA	1.77	0.44
1:A:159:ALA:HB2	1:A:188:PHE:CE1	2.51	0.44
1:A:163:GLY:O	1:A:166:CYS:HB3	2.17	0.44
1:A:956:ARG:HG3	9:A:1626:HOH:O	2.17	0.44
1:C:50:ASN:ND2	1:C:53:THR:CG2	2.80	0.44
1:C:698:ILE:O	1:C:701:ALA:N	2.49	0.44
2:D:64:GLY:N	2:D:89:ALA:HB1	2.32	0.44
1:E:168:ILE:HD13	1:E:191:ILE:HG22	2.00	0.44
2:F:236:ILE:CG2	2:F:237:PHE:N	2.80	0.44
1:G:139:ILE:HG13	1:G:141:LEU:HG	1.99	0.44
1:G:147:GLY:HA3	1:G:158:VAL:HG13	1.96	0.44
1:G:530:ASP:O	1:G:531:THR:OG1	2.31	0.44
1:G:642:TYR:CE1	1:G:825:LEU:HD12	2.52	0.44
1:G:692:ASN:HB3	1:G:753:ASP:OD1	2.16	0.44
2:H:275:LEU:O	2:H:275:LEU:HG	2.15	0.44
2:H:337:LEU:HD12	2:H:337:LEU:HA	1.69	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:975:HIS:ND1	1:G:975:HIS:ND1	2.32	0.44
1:A:1006:LYS:HB3	1:A:1006:LYS:HE3	1.57	0.44
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.82	0.44
1:C:713:VAL:HG12	1:C:715:ARG:HG2	1.99	0.44
1:A:947:LEU:N	1:A:947:LEU:CD1	2.81	0.44
1:A:993:LYS:H	1:A:996:GLU:HG3	1.82	0.44
2:B:169:SER:HA	2:B:216:LEU:O	2.18	0.44
1:E:331:THR:OG1	1:E:333:ASP:OD1	2.29	0.44
2:F:45:ASP:OD1	2:F:46:PRO:HD2	2.18	0.44
2:F:136:ASP:O	2:F:138:PRO:HD3	2.18	0.44
2:F:142:LEU:HA	2:F:142:LEU:HD12	1.79	0.44
1:G:75:ARG:HG2	1:G:75:ARG:NH1	2.26	0.44
1:G:75:ARG:NH1	1:G:75:ARG:CG	2.81	0.44
1:G:946:LEU:HB3	1:G:1013:ILE:HG12	1.99	0.44
2:H:354:PRO:HB3	2:H:363:ALA:O	2.17	0.44
1:A:158:VAL:O	1:A:162:VAL:HG22	2.17	0.44
1:A:167:ILE:HD12	1:A:167:ILE:N	2.32	0.44
1:A:340:THR:O	1:A:343:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ARG:NH1	1:A:910:GLU:OE2	2.50	0.44
2:B:266:PHE:HB2	2:B:370:PHE:CD1	2.53	0.44
2:B:290:HIS:HB2	2:B:312:HIS:CD2	2.53	0.44
1:C:905:PRO:HB2	1:C:1040:TYR:OH	2.17	0.44
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.98	0.44
1:G:710:TYR:HA	1:G:711:PRO:C	2.43	0.44
1:G:839:LEU:HD13	1:G:839:LEU:HA	1.61	0.44
2:H:266:PHE:CD1	2:H:348:PHE:CZ	3.06	0.44
1:A:172:PHE:HB3	1:A:200:PRO:CG	2.22	0.44
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.99	0.44
8:A:1086:NET:H22	8:A:1086:NET:C4	2.38	0.44
1:C:158:VAL:HG11	1:C:206:ILE:HB	1.99	0.44
2:D:286:MET:CE	2:D:312:HIS:ND1	2.78	0.44
2:H:274:LEU:HD23	2:H:274:LEU:HA	1.82	0.44
2:H:275:LEU:HD22	2:H:349:SER:HB3	2.00	0.44
1:A:45:ILE:HD13	1:A:81:GLU:HB3	2.00	0.44
1:A:717:SER:HB2	1:A:748:ALA:HB3	1.99	0.44
1:A:981:LEU:HD12	1:A:988:PRO:HG3	2.00	0.44
2:B:208:MET:C	2:B:211:ASP:HB2	2.43	0.44
2:B:215:ARG:CG	2:B:215:ARG:NH1	2.80	0.44
1:E:264:MET:HE2	1:E:286:PHE:HB2	2.00	0.44
1:E:890:VAL:O	1:E:918:MET:HA	2.17	0.44
2:F:232:ASN:N	2:F:233:PRO:CD	2.80	0.44
1:G:93:GLN:HG3	1:G:97:ASN:ND2	2.33	0.44
1:G:668:ALA:O	1:G:671:ARG:HB2	2.18	0.44
1:G:882:GLU:OE2	1:G:884:ILE:HD11	2.17	0.44
2:H:324:ASN:O	2:H:342:ARG:HA	2.18	0.44
1:A:403:GLU:HG3	1:A:569:PRO:HD2	1.98	0.44
1:A:487:ASP:HA	1:A:490:ARG:HH12	1.83	0.44
1:A:632:ILE:HG13	1:A:633:GLU:N	2.32	0.44
1:C:385:MET:HB2	1:C:603:PRO:HG3	2.00	0.44
2:D:237:PHE:HE1	2:D:268:ILE:HD12	1.77	0.44
2:F:237:PHE:CE1	2:F:268:ILE:HD12	2.52	0.44
1:G:994:VAL:CG2	1:G:1001:ILE:HD11	2.23	0.44
1:A:944:ARG:NH1	1:A:972:ASP:OD1	2.51	0.43
1:C:1001:ILE:O	1:C:1005:ILE:HG13	2.18	0.43
1:E:166:CYS:HB2	1:E:207:ASP:O	2.18	0.43
2:F:259:LEU:CD1	2:F:342:ARG:NH1	2.80	0.43
1:G:375:THR:OG1	1:G:376:THR:N	2.49	0.43
2:H:83:ARG:O	2:H:112:ASP:HA	2.18	0.43
1:A:298:ILE:O	1:A:299:GLU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:TYR:CZ	2:B:61:GLY:HA2	2.53	0.43
2:B:205:ILE:HD13	2:B:237:PHE:HZ	1.83	0.43
2:B:354:PRO:HB3	2:B:363:ALA:O	2.18	0.43
1:C:981:LEU:HD12	1:C:988:PRO:HG3	2.00	0.43
1:C:1044:LEU:HD12	1:C:1044:LEU:HA	1.82	0.43
1:E:198:LEU:HD12	1:E:198:LEU:HA	1.74	0.43
1:E:763:ASP:HB3	1:E:779:MET:HE3	1.99	0.43
1:E:1017:THR:HG21	1:E:1023:ILE:CA	2.44	0.43
1:G:174:MET:O	1:G:177:SER:OG	2.30	0.43
1:G:726:GLU:HG3	1:G:737:TYR:CD2	2.53	0.43
2:H:199:PHE:O	2:H:241:GLY:HA3	2.18	0.43
1:A:48:ASN:O	1:A:66:ILE:HA	2.18	0.43
1:A:371:ASN:O	1:A:379:LYS:NZ	2.47	0.43
2:B:229:LEU:CD2	2:B:263:ILE:HD11	2.48	0.43
2:B:334:ASP:OD1	2:B:336:THR:HG23	2.19	0.43
1:C:45:ILE:HD13	1:C:83:PRO:HB3	1.99	0.43
2:D:194:VAL:HB	2:D:216:LEU:HD23	2.00	0.43
2:D:335:GLY:HA2	9:D:1770:HOH:O	2.18	0.43
1:G:655:GLU:HB2	9:G:4206:HOH:O	2.18	0.43
1:G:860:PRO:CB	1:G:863:LYS:HD2	2.47	0.43
2:H:33:ASN:OD1	2:H:35:SER:HB2	2.18	0.43
1:A:313:LYS:NZ	1:A:603:PRO:O	2.44	0.43
1:A:368:ALA:HB3	9:A:1521:HOH:O	2.18	0.43
1:A:717:SER:CB	1:A:748:ALA:HB3	2.47	0.43
1:A:731:GLU:HB3	9:A:1738:HOH:O	2.17	0.43
1:A:922:ARG:HE	1:A:1061:LYS:HD3	1.83	0.43
1:A:1004:ARG:NH2	1:G:983:GLU:HG2	2.30	0.43
2:B:259:LEU:O	2:B:345:LYS:HE3	2.17	0.43
1:C:693:ALA:HB2	1:C:708:ILE:HD11	1.94	0.43
1:E:101:GLU:OE1	1:E:104[A]:ARG:NH2	2.48	0.43
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.53	0.43
1:E:830:PHE:CE1	1:E:839:LEU:HD13	2.53	0.43
1:E:991:VAL:HG22	1:E:992:ASN:N	2.33	0.43
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.48	0.43
1:A:574:GLN:HG2	1:A:720:LEU:HD21	1.99	0.43
1:C:922:ARG:NE	1:C:1061:LYS:HD3	2.23	0.43
1:E:358:LYS:HG2	1:E:359:ILE:N	2.33	0.43
2:H:5:ALA:HA	2:H:133:ILE:O	2.18	0.43
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.58	0.43
1:A:126:ALA:HB3	1:A:302:PRO:HG3	2.01	0.43
1:A:412:LYS:NZ	9:A:1241:HOH:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLU:CD	2:B:120:ARG:HH21	2.27	0.43
1:C:25:GLU:OE1	1:C:604:GLU:OE2	2.37	0.43
1:C:766:ALA:HB1	1:C:774:LEU:O	2.19	0.43
1:C:990:LEU:HD23	1:E:979:ILE:CD1	2.49	0.43
2:D:352:GLY:O	2:D:354:PRO:HD3	2.18	0.43
1:E:859:VAL:HA	1:E:860:PRO:HD3	1.85	0.43
2:F:44:THR:O	2:F:46:PRO:HD3	2.18	0.43
2:F:195:VAL:HG11	2:F:228:VAL:HG13	2.00	0.43
1:G:148:ILE:CG2	1:G:150:HIS:NE2	2.81	0.43
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.34	0.43
2:H:83:ARG:HD2	2:H:83:ARG:C	2.44	0.43
2:H:290:HIS:HB3	2:H:310:GLN:HB3	1.99	0.43
1:A:880:THR:O	1:A:881[B]:LYS:HD2	2.19	0.43
1:A:1017:THR:HG21	1:A:1023:ILE:CG1	2.48	0.43
2:B:264:PRO:HG3	2:B:373:LEU:O	2.18	0.43
1:C:197:ASP:OD2	1:C:1037:LYS:NZ	2.36	0.43
1:C:712:LEU:HG	1:C:753:ASP:O	2.19	0.43
1:C:975:HIS:HE2	1:E:992:ASN:HD21	1.67	0.43
2:D:120:ARG:HH11	2:D:120:ARG:HD2	1.69	0.43
1:G:820:LEU:HA	1:G:820:LEU:HD23	1.52	0.43
1:A:951:GLU:O	1:A:954:LYS:HB2	2.19	0.43
2:B:170:TRP:HD1	2:B:210:VAL:HG21	1.81	0.43
1:C:317:PHE:HA	1:C:318:PRO:HD3	1.94	0.43
1:C:602:ASN:ND2	1:C:605:THR:HG23	2.33	0.43
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.49	0.43
1:E:1018:SER:O	1:E:1022:ALA:HB3	2.19	0.43
2:F:164:THR:N	2:F:198:ASP:OD2	2.51	0.43
1:G:425:ARG:O	1:G:429:LYS:HB2	2.19	0.43
1:G:717:SER:CB	1:G:748:ALA:HB3	2.48	0.43
1:A:170:PRO:HA	1:A:204:LEU:HA	2.01	0.43
1:C:28:TYR:O	1:C:32:GLN:HG3	2.19	0.43
1:C:475:LYS:HG2	1:C:488:PHE:CZ	2.54	0.43
1:E:646:THR:HB	1:E:647:PRO:HD3	2.01	0.43
1:A:38:ARG:HH11	1:A:61:ALA:CA	2.32	0.43
1:A:86:VAL:O	1:A:86:VAL:HG13	2.17	0.43
1:A:171:SER:O	1:A:172:PHE:HB2	2.18	0.43
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.49	0.43
1:C:165:PRO:HA	1:C:182:ALA:O	2.19	0.43
1:C:198:LEU:HD12	1:C:198:LEU:HA	1.77	0.43
1:E:228:CYS:SG	1:E:269:MET:HG2	2.59	0.43
1:E:692:ASN:HB2	1:E:751:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ALA:HB1	1:G:274:GLU:HG2	2.00	0.43
2:H:232:ASN:HD22	2:H:232:ASN:HA	1.39	0.43
1:A:326:LEU:HA	1:A:326:LEU:HD12	1.85	0.42
1:A:528:ARG:HG2	1:A:543:MET:HG2	2.01	0.42
1:C:884:ILE:HD13	1:C:884:ILE:HA	1.73	0.42
1:C:885:PRO:HA	1:C:886:PRO:HD3	1.90	0.42
1:G:723:ARG:O	1:G:724:ALA:HB3	2.19	0.42
1:G:775:ILE:HD13	1:G:775:ILE:HA	1.82	0.42
2:H:217:THR:C	2:H:218:ILE:HD13	2.43	0.42
1:A:722:GLY:HA2	1:A:725:MET:HG3	2.00	0.42
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.90	0.42
1:C:574:GLN:HG2	1:C:720:LEU:HD11	2.02	0.42
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.19	0.42
1:E:436:ILE:HG22	9:E:3065:HOH:O	2.19	0.42
1:E:702:VAL:HG22	1:E:734:LEU:HD23	2.01	0.42
1:E:1061:LYS:NZ	9:E:3425:HOH:O	2.48	0.42
1:G:164:PHE:HB3	1:G:183:TYR:O	2.19	0.42
1:G:623:LEU:HD12	1:G:654:LEU:HD23	2.01	0.42
2:H:265:VAL:O	2:H:347:ALA:HA	2.18	0.42
1:A:481:ILE:HD12	1:A:508:VAL:HG11	2.02	0.42
1:A:998:ARG:HG2	1:A:998:ARG:HH11	1.84	0.42
1:C:421:LEU:HD23	1:C:421:LEU:HA	1.86	0.42
1:C:693:ALA:N	1:C:708:ILE:HD11	2.34	0.42
2:D:269:CYS:O	2:D:272:HIS:HB3	2.19	0.42
1:E:803:GLN:O	1:E:806:GLN:HB2	2.19	0.42
2:F:255:ILE:HA	2:F:258:PHE:HD2	1.83	0.42
1:G:93:GLN:HG3	1:G:97:ASN:HD21	1.84	0.42
1:G:287:ALA:HB2	1:G:298:ILE:HD11	2.01	0.42
2:H:171:THR:HB	2:H:185:LYS:HB2	2.01	0.42
1:A:172:PHE:CD2	1:A:201:THR:CG2	3.02	0.42
1:A:696:THR:O	1:A:696:THR:HG23	2.19	0.42
1:C:186:GLU:HB2	9:C:4321:HOH:O	2.18	0.42
1:C:453:PHE:CD1	1:C:453:PHE:C	2.98	0.42
1:C:986:ILE:O	1:C:988:PRO:HD3	2.19	0.42
2:D:46:PRO:HA	2:D:76:HIS:CG	2.54	0.42
1:E:440:ALA:O	1:E:444:ARG:HG3	2.18	0.42
1:E:900:PHE:HA	1:E:901:PRO:HD2	1.83	0.42
2:F:208:MET:SD	2:F:355:GLU:HA	2.59	0.42
2:F:286:MET:HE3	2:F:289:GLY:CA	2.33	0.42
1:G:198:LEU:HA	1:G:198:LEU:HD12	1.80	0.42
1:G:224:LYS:NZ	9:G:3992:HOH:O	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:658:GLY:O	1:G:660:PRO:HD3	2.19	0.42
1:G:809:MET:HE3	1:G:809:MET:HB2	1.79	0.42
1:A:412:LYS:N	1:A:441:ASP:OD2	2.32	0.42
1:A:490:ARG:NH1	1:A:490:ARG:HB3	2.35	0.42
1:C:79:GLU:HA	1:C:111:PHE:CE2	2.54	0.42
1:C:563:MET:HE3	1:C:563:MET:HB2	1.73	0.42
1:C:1000:HIS:O	1:C:1003:ASP:HB2	2.19	0.42
1:G:675:ARG:HD2	1:G:716:PRO:O	2.20	0.42
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.23	0.42
2:H:46:PRO:HD3	2:H:72:SER:HB3	2.01	0.42
1:A:136:MET:HE2	1:A:136:MET:N	2.35	0.42
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.89	0.42
1:A:392:GLN:OE1	1:A:495:LYS:HD3	2.19	0.42
1:C:701:ALA:HB1	1:C:752:LEU:HD21	2.01	0.42
1:E:725:MET:HE1	6:E:2910:ANP:PB	2.60	0.42
1:E:907:LEU:HD11	7:E:2920:ORN:HD3	2.01	0.42
1:A:93:GLN:H	1:A:174:MET:HE3	1.84	0.42
2:B:167:ALA:HA	2:B:218:ILE:O	2.19	0.42
2:B:176:THR:O	2:B:180:GLY:N	2.45	0.42
1:C:2:PRO:HB2	1:C:3:LYS:H	1.72	0.42
1:C:305:SER:H	1:C:308:SER:HB3	1.85	0.42
2:D:200:GLY:O	2:D:240:ASN:ND2	2.52	0.42
1:G:768:CYS:HB2	1:G:817:ALA:HB1	2.02	0.42
1:G:1001:ILE:CG1	1:G:1002:GLN:N	2.80	0.42
1:A:135:ALA:HB1	1:A:274:GLU:CG	2.49	0.42
2:D:300:VAL:HG23	2:D:301:GLU:N	2.33	0.42
2:D:302:LYS:O	2:D:303:ASN:HB3	2.19	0.42
1:E:1017:THR:CG2	1:E:1023:ILE:HG13	2.49	0.42
1:E:1028:VAL:HG13	1:E:1029:ILE:HD12	2.01	0.42
1:A:574:GLN:NE2	1:A:720:LEU:HD21	2.32	0.42
1:A:890:VAL:HG12	1:A:931:ALA:HB2	2.01	0.42
1:C:3:LYS:HB3	1:C:330:TYR:CE2	2.55	0.42
1:C:482:THR:HG22	9:C:4511:HOH:O	2.19	0.42
1:C:922:ARG:HH21	1:C:1061:LYS:CG	2.33	0.42
1:E:939:MET:HE3	1:E:940:LYS:O	2.20	0.42
1:E:1028:VAL:O	1:E:1032:SER:OG	2.30	0.42
2:F:123:ARG:NH2	9:F:2627:HOH:O	2.53	0.42
2:F:237:PHE:CZ	2:F:268:ILE:HD12	2.53	0.42
1:G:755:PHE:CE1	6:G:3910:ANP:H2	2.54	0.42
1:G:981:LEU:CD1	1:G:988:PRO:HG3	2.41	0.42
2:H:32:PHE:O	2:H:291:HIS:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:SER:HB2	2:H:325:LEU:HD11	2.00	0.42
2:H:298:LYS:O	2:H:329:HIS:HA	2.19	0.42
1:A:33:ALA:HB2	1:A:90:MET:HE3	2.02	0.42
1:A:885:PRO:HG2	9:A:1623:HOH:O	2.19	0.42
2:B:264:PRO:HG2	2:B:374:ILE:HG12	2.02	0.42
2:B:332:LEU:HA	2:B:332:LEU:HD12	1.79	0.42
1:C:774:LEU:HD12	1:C:775:ILE:N	2.35	0.42
1:C:784:GLN:NE2	1:C:784:GLN:N	2.49	0.42
1:C:859:VAL:HA	1:C:860:PRO:HD3	1.92	0.42
2:D:350:PHE:HB2	2:D:366:LEU:HD22	2.01	0.42
2:F:249:ASP:OD1	2:F:249:ASP:N	2.53	0.42
1:G:82:ARG:NH1	1:G:111:PHE:HE2	2.18	0.42
1:G:187:GLU:O	1:G:191:ILE:HD12	2.20	0.42
1:G:623:LEU:CD1	1:G:654:LEU:HD23	2.50	0.42
2:H:244:ASP:OD1	2:H:245:PRO:HD2	2.20	0.42
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.20	0.41
1:C:488:PHE:O	1:C:492:LEU:HG	2.20	0.41
1:C:890:VAL:HG23	1:C:927:ALA:CB	2.50	0.41
1:E:577:GLU:CD	1:E:577:GLU:H	2.28	0.41
8:E:2950:NET:H12	8:E:2950:NET:H43	1.71	0.41
2:F:321:LEU:HA	2:F:321:LEU:HD12	1.80	0.41
1:G:183:TYR:N	1:G:187:GLU:OE1	2.43	0.41
1:G:671:ARG:NH2	1:G:819:GLU:O	2.53	0.41
1:G:984:ALA:HB2	9:G:4514:HOH:O	2.20	0.41
2:H:138:PRO:HA	9:H:3552:HOH:O	2.20	0.41
1:A:238:ASP:HB2	1:A:247:SER:HB3	2.02	0.41
1:A:981:LEU:CD1	1:A:988:PRO:HG3	2.50	0.41
2:B:307:ILE:O	2:B:362:ASP:HB2	2.19	0.41
1:C:85:ALA:HA	1:C:114:THR:O	2.20	0.41
1:C:367:PHE:CE1	1:C:912:ARG:HG2	2.56	0.41
1:E:94:THR:OG1	8:E:2950:NET:H71	2.20	0.41
1:G:574:GLN:HG2	1:G:720:LEU:HD21	2.01	0.41
1:G:1001:ILE:HD12	1:G:1002:GLN:CA	2.50	0.41
2:H:205:ILE:HG21	2:H:237:PHE:CZ	2.56	0.41
1:A:745:SER:O	1:A:748:ALA:HB3	2.20	0.41
1:A:1000:HIS:CD2	1:A:1003:ASP:CB	3.03	0.41
1:C:502:LEU:HA	1:C:502:LEU:HD23	1.77	0.41
1:G:453:PHE:HD1	1:G:458:ILE:O	2.03	0.41
1:G:816:LEU:HD11	1:G:839:LEU:HD21	2.02	0.41
1:G:883:VAL:O	1:G:884:ILE:HD13	2.20	0.41
1:A:240:MET:HE3	1:A:240:MET:HB3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:OD1	1:A:381:VAL:HG21	2.21	0.41
1:A:723:ARG:NH1	1:A:910:GLU:CD	2.78	0.41
2:B:277:LEU:HA	2:B:277:LEU:HD23	1.78	0.41
2:B:285:LYS:CG	2:B:314:PHE:CE1	3.02	0.41
1:C:900:PHE:N	1:C:901:PRO:HD3	2.35	0.41
1:E:148:ILE:HD13	1:E:148:ILE:HA	1.93	0.41
1:E:172:PHE:CD2	1:E:201:THR:HG23	2.55	0.41
1:E:503:ALA:HB1	1:E:508:VAL:O	2.20	0.41
8:E:2950:NET:H31	8:E:2950:NET:H63	1.66	0.41
2:F:98:LEU:HG	2:F:102:LEU:HD11	2.01	0.41
1:G:675:ARG:NH2	1:G:841:GLU:OE1	2.54	0.41
1:G:949:VAL:HB	1:G:1016:THR:OG1	2.20	0.41
1:G:982:GLY:C	1:G:984:ALA:N	2.78	0.41
2:H:158:LEU:HD23	2:H:158:LEU:HA	1.76	0.41
1:A:145:ARG:HB2	1:A:208:GLU:OE2	2.20	0.41
2:B:80:LEU:HD12	2:B:80:LEU:HA	1.85	0.41
2:B:208:MET:HA	2:B:211:ASP:HB2	2.01	0.41
1:G:3:LYS:CB	1:G:330:TYR:CE2	3.04	0.41
1:G:642:TYR:OH	1:G:865:ALA:HB3	2.21	0.41
1:G:679:GLN:O	1:G:679:GLN:HG2	2.20	0.41
1:G:717:SER:HB3	1:G:748:ALA:HB3	2.03	0.41
1:G:981:LEU:HA	1:G:981:LEU:HD23	1.78	0.41
1:G:1064:SER:OG	1:G:1066:GLN:HB2	2.21	0.41
2:H:354:PRO:HB2	2:H:367:PHE:CE2	2.56	0.41
1:A:136:MET:HE2	1:A:136:MET:HA	2.02	0.41
1:A:347:SER:O	2:B:296:PRO:HB3	2.21	0.41
1:A:1017:THR:HG22	1:A:1018:SER:H	1.83	0.41
2:B:299:ASP:HA	2:B:329:HIS:CD2	2.55	0.41
2:B:350:PHE:CD1	2:B:366:LEU:HD21	2.55	0.41
1:C:809:MET:HG2	1:C:837:VAL:HG11	2.02	0.41
1:C:1000:HIS:CD2	1:C:1000:HIS:H	2.39	0.41
1:G:66:ILE:O	1:G:66:ILE:HG22	2.20	0.41
1:G:194:ARG:NH1	1:G:194:ARG:CB	2.84	0.41
2:H:2:ILE:O	2:H:2:ILE:HG13	2.20	0.41
2:H:60:ILE:O	2:H:86:PRO:HD2	2.21	0.41
1:A:904:ASP:HA	1:A:905:PRO:HD3	1.87	0.41
2:B:222:GLN:HE21	2:B:222:GLN:H	1.69	0.41
1:C:695:VAL:HG12	1:C:696:THR:N	2.34	0.41
1:E:772:MET:HE3	9:E:3588:HOH:O	2.21	0.41
1:E:998:ARG:CG	1:E:998:ARG:NH1	2.81	0.41
1:G:172:PHE:CE2	1:G:201:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:412:LYS:HE2	1:G:434:ASP:CG	2.46	0.41
1:G:578:PHE:HE1	1:G:846:ALA:O	2.03	0.41
1:G:698:ILE:O	1:G:701:ALA:HB3	2.20	0.41
2:H:169:SER:HA	2:H:216:LEU:O	2.20	0.41
1:A:424:ILE:O	1:A:428:LEU:HD13	2.21	0.41
1:C:828:VAL:HG13	1:C:842:VAL:HG22	2.03	0.41
1:C:942:HIS:CD2	1:C:942:HIS:C	2.99	0.41
1:E:667:ASP:OD1	1:E:677:ARG:NH2	2.42	0.41
2:H:342:ARG:HH21	2:H:344:ASP:CG	2.27	0.41
1:A:38:ARG:NH1	1:A:61:ALA:C	2.79	0.41
1:A:119:THR:H	1:A:119:THR:HG23	1.56	0.41
1:A:470:VAL:O	1:A:473:GLU:HB2	2.21	0.41
1:A:523:HIS:HB3	1:A:524:PRO:HD2	2.02	0.41
1:A:576:ILE:HD13	1:A:576:ILE:HG21	1.85	0.41
1:A:646:THR:CB	1:A:647:PRO:HD3	2.51	0.41
1:A:751:LEU:HG	1:A:752:LEU:N	2.36	0.41
2:B:122:LEU:O	2:B:126:GLY:N	2.53	0.41
1:C:648:LEU:HD12	1:C:648:LEU:HA	1.89	0.41
1:C:659:VAL:HA	1:C:660:PRO:HD3	1.84	0.41
1:C:720:LEU:O	1:C:720:LEU:HD12	2.21	0.41
1:C:900:PHE:HA	1:C:901:PRO:HD2	1.68	0.41
1:E:47:VAL:HA	1:E:65:TYR:O	2.21	0.41
1:E:516:LEU:HD12	1:E:516:LEU:HA	1.91	0.41
1:E:942:HIS:CD2	1:E:942:HIS:C	2.98	0.41
2:F:154:ASN:HD22	2:F:155:GLY:N	2.19	0.41
1:G:152:MET:O	1:G:156:LEU:HG	2.21	0.41
1:G:634:LYS:N	1:G:635:PRO:HD3	2.36	0.41
1:G:770:GLY:CA	1:G:823:ARG:CZ	2.98	0.41
1:G:1000:HIS:O	1:G:1000:HIS:HD2	2.04	0.41
1:G:1073:LYS:HD3	1:G:1073:LYS:HA	1.78	0.41
8:G:3950:NET:H63	8:G:3950:NET:H31	1.57	0.41
2:H:225:ALA:HB1	2:H:258:PHE:CE1	2.56	0.41
2:H:292:GLY:HA3	9:H:3478:HOH:O	2.21	0.41
1:A:258:ASP:O	1:A:262:GLN:HG2	2.21	0.41
1:A:574:GLN:HG3	1:A:720:LEU:HD11	2.02	0.41
1:A:1000:HIS:NE2	1:A:1003:ASP:OD2	2.54	0.41
2:B:236:ILE:HG22	2:B:237:PHE:N	2.36	0.41
1:C:598:MET:HE2	1:C:598:MET:HB2	1.81	0.41
1:C:659:VAL:CG1	1:C:660:PRO:HD2	2.51	0.41
1:E:903:VAL:O	1:E:905:PRO:HD3	2.21	0.41
2:F:223:THR:HG22	2:F:228:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:255:ILE:HA	2:F:258:PHE:CD2	2.56	0.41
1:G:80:LYS:HG2	1:G:81:GLU:HG2	2.01	0.41
1:G:315:THR:O	1:G:531:THR:HG22	2.20	0.41
1:G:461:TRP:O	1:G:465:GLN:HG3	2.21	0.41
1:G:828:VAL:CG1	1:G:842:VAL:HG22	2.38	0.41
2:H:209:LEU:HD23	2:H:209:LEU:HA	1.91	0.41
2:H:341:HIS:ND1	2:H:347:ALA:O	2.54	0.41
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.56	0.40
1:A:1069:HIS:ND1	9:A:1644:HOH:O	2.37	0.40
1:C:286:PHE:CD1	1:C:295:LEU:HD11	2.55	0.40
1:C:683:GLU:O	1:C:686:LYS:N	2.53	0.40
8:C:1950:NET:H83	8:C:1950:NET:H11	1.76	0.40
1:E:70:HIS:O	1:E:73:VAL:N	2.54	0.40
1:E:1072:ILE:HG22	9:E:3630:HOH:O	2.20	0.40
2:F:294:ASN:OD1	2:F:294:ASN:N	2.54	0.40
1:G:679:GLN:CB	1:G:689:GLN:HE22	2.34	0.40
1:G:679:GLN:CG	1:G:689:GLN:HE22	2.32	0.40
1:A:904:ASP:OD1	1:A:905:PRO:HD2	2.20	0.40
1:A:950:ARG:HG3	1:A:1016:THR:OG1	2.20	0.40
1:A:951:GLU:HA	1:A:954:LYS:HD2	2.04	0.40
1:A:990:LEU:HB3	1:G:979:ILE:HD13	2.04	0.40
2:B:344:ASP:OD1	2:B:345:LYS:N	2.54	0.40
2:B:363:ALA:C	2:B:365:PRO:HD2	2.46	0.40
1:C:561:LYS:NZ	1:C:633:GLU:O	2.51	0.40
8:C:1950:NET:H63	8:C:1950:NET:H31	1.90	0.40
1:E:1:MET:HG3	1:E:2:PRO:CD	2.44	0.40
2:F:152:GLY:O	2:F:156:MET:HE3	2.20	0.40
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.36	0.40
2:H:127:ALA:HB2	9:H:3532:HOH:O	2.21	0.40
1:A:82:ARG:HD2	1:A:82:ARG:HA	1.48	0.40
1:A:172:PHE:CD2	1:A:201:THR:HG23	2.56	0.40
2:B:346:PRO:HB2	2:B:373:LEU:HD13	2.03	0.40
1:C:273:ARG:HD2	9:C:4089:HOH:O	2.22	0.40
2:D:201:ALA:HB2	2:D:239:SER:HB2	2.03	0.40
1:E:273:ARG:HH11	1:E:273:ARG:HD2	1.72	0.40
1:E:373:ARG:NH1	1:E:430:ASP:O	2.47	0.40
1:E:809:MET:O	1:E:813:VAL:HG23	2.21	0.40
1:G:148:ILE:HG23	1:G:203:GLU:HG3	2.02	0.40
1:G:236:ASN:OD1	1:G:244:THR:HG22	2.22	0.40
1:G:1001:ILE:HG13	1:G:1002:GLN:H	1.86	0.40
2:H:63:VAL:O	2:H:94:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:255:ILE:CG2	2:H:259:LEU:HD11	2.48	0.40
1:A:56:THR:O	1:A:855:LYS:HE2	2.22	0.40
2:B:319:ALA:C	2:B:320:THR:HG23	2.46	0.40
1:C:385:MET:HG2	1:C:386:ALA:N	2.36	0.40
1:C:684:ARG:HG3	1:C:684:ARG:NH1	2.16	0.40
1:C:843:ASN:HA	1:C:844:PRO:HD3	1.84	0.40
2:D:324:ASN:HA	2:D:343:THR:OG1	2.21	0.40
2:F:275:LEU:HD23	2:F:349:SER:CB	2.51	0.40
1:G:1:MET:CB	1:G:2:PRO:HD2	2.51	0.40
2:H:225:ALA:O	2:H:229:LEU:HD12	2.22	0.40
2:H:342:ARG:HD2	2:H:342:ARG:HA	1.76	0.40
1:A:4:ARG:CZ	1:A:7:ILE:CD1	3.00	0.40
1:A:211:ILE:HG13	6:A:1083:ANP:H2	2.04	0.40
1:C:1:MET:CB	1:C:2:PRO:HD2	2.52	0.40
1:C:641:GLN:NE2	1:C:664:THR:O	2.55	0.40
1:C:715:ARG:HA	1:C:716:PRO:HD2	2.00	0.40
2:D:363:ALA:O	2:D:366:LEU:HB2	2.21	0.40
1:E:716:PRO:HB3	1:E:741:ALA:O	2.21	0.40
2:F:371:ILE:HD13	2:F:371:ILE:HA	1.88	0.40
1:G:825:LEU:HG	1:G:865:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1051/1073 (98%)	988 (94%)	61 (6%)	2 (0%)	43	44
1	C	1071/1073 (100%)	1009 (94%)	54 (5%)	8 (1%)	18	15
1	E	1074/1073 (100%)	1020 (95%)	48 (4%)	6 (1%)	21	18
1	G	1073/1073 (100%)	993 (92%)	72 (7%)	8 (1%)	18	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	377/382 (99%)	350 (93%)	23 (6%)	4 (1%)	11	8
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	377/382 (99%)	361 (96%)	14 (4%)	2 (0%)	24	22
2	H	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
All	All	5777/5820 (99%)	5442 (94%)	305 (5%)	30 (0%)	24	22

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	975	HIS
2	F	136	ASP
1	G	975	HIS
2	B	346	PRO
1	C	707	GLU
1	C	975	HIS
1	E	835	ASN
1	G	558	ASP
1	G	873	SER
1	G	1001	ILE
1	A	368	ALA
2	B	191	PRO
1	C	2	PRO
1	C	708	ILE
1	C	873	SER
1	E	708	ILE
2	F	243	GLY
1	G	707	GLU
2	B	229	LEU
1	C	821	GLN
1	E	2	PRO
1	E	707	GLU
1	E	975	HIS
1	G	71	TRP
1	G	860	PRO
1	C	341	GLY
1	C	698	ILE
1	G	2	PRO
1	E	902	GLY
2	B	228	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 62 ligands modelled in this entry, 46 are monoatomic - leaving 16 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
6	ANP	C	1900	3	33,33,33	1.36	6 (18%)	45,52,52	1.25	3 (6%)
6	ANP	A	1083	3	33,33,33	1.64	6 (18%)	45,52,52	1.34	5 (11%)
7	ORN	E	2920	-	7,8,8	0.89	0	6,9,9	1.17	1 (16%)
8	NET	A	1086	-	8,8,8	0.81	0	10,10,10	0.51	0
8	NET	C	1950	-	8,8,8	0.71	0	10,10,10	0.72	0
8	NET	G	3950	-	8,8,8	0.72	0	10,10,10	0.59	0
6	ANP	A	1084	3	33,33,33	1.53	6 (18%)	45,52,52	1.23	4 (8%)
7	ORN	G	3920	-	7,8,8	0.76	0	6,9,9	1.09	1 (16%)
6	ANP	E	2900	3	33,33,33	1.40	6 (18%)	45,52,52	1.27	4 (8%)
6	ANP	E	2910	3	33,33,33	1.46	5 (15%)	45,52,52	1.22	3 (6%)
6	ANP	G	3910	3	33,33,33	1.42	8 (24%)	45,52,52	1.40	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ANP	C	1910	3	33,33,33	1.56	7 (21%)	45,52,52	1.37	7 (15%)
7	ORN	A	1085	-	7,8,8	0.84	0	6,9,9	1.54	1 (16%)
8	NET	E	2950	-	8,8,8	0.64	0	10,10,10	0.62	0
7	ORN	C	1920	-	7,8,8	0.93	0	6,9,9	1.06	1 (16%)
6	ANP	G	3900	3	33,33,33	1.40	6 (18%)	45,52,52	1.33	5 (11%)

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
6	ANP	C	1900	3	-	2/18/38/38	0/3/3/3
6	ANP	A	1083	3	-	3/18/38/38	0/3/3/3
7	ORN	E	2920	-	-	7/8/8/8	-
8	NET	A	1086	-	-	6/12/12/12	-
8	NET	C	1950	-	-	3/12/12/12	-
8	NET	G	3950	-	-	6/12/12/12	-
6	ANP	A	1084	3	-	3/18/38/38	0/3/3/3
7	ORN	G	3920	-	-	5/8/8/8	-
6	ANP	E	2900	3	-	3/18/38/38	0/3/3/3
6	ANP	E	2910	3	-	5/18/38/38	0/3/3/3
6	ANP	G	3910	3	-	4/18/38/38	0/3/3/3
6	ANP	C	1910	3	-	3/18/38/38	0/3/3/3
7	ORN	A	1085	-	-	4/8/8/8	-
8	NET	E	2950	-	-	12/12/12/12	-
7	ORN	C	1920	-	-	7/8/8/8	-
6	ANP	G	3900	3	-	2/18/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1083	ANP	PG-O1G	5.31	1.54	1.46
6	C	1910	ANP	PB-O1B	4.29	1.52	1.46
6	E	2910	ANP	PB-O1B	4.26	1.52	1.46
6	A	1084	ANP	PB-O1B	4.22	1.52	1.46
6	A	1084	ANP	PG-O1G	3.73	1.51	1.46
6	E	2900	ANP	PG-O1G	3.58	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3910	ANP	C6-N6	-3.51	1.25	1.34
6	A	1083	ANP	PB-O1B	3.49	1.51	1.46
6	C	1910	ANP	C6-N6	-3.37	1.25	1.34
6	A	1084	ANP	C6-N6	-3.35	1.25	1.34
6	E	2910	ANP	C6-N6	-3.29	1.25	1.34
6	E	2910	ANP	PG-O1G	3.25	1.51	1.46
6	G	3900	ANP	PB-O1B	3.19	1.51	1.46
6	A	1083	ANP	PG-O2G	-3.16	1.48	1.56
6	C	1900	ANP	C6-N6	-3.12	1.26	1.34
6	C	1900	ANP	PG-O1G	3.07	1.50	1.46
6	A	1083	ANP	C6-N6	-3.04	1.26	1.34
6	G	3900	ANP	C6-N6	-3.04	1.26	1.34
6	E	2900	ANP	PB-O1B	3.01	1.50	1.46
6	C	1910	ANP	PG-O1G	2.98	1.50	1.46
6	E	2900	ANP	C6-N6	-2.97	1.26	1.34
6	G	3910	ANP	PB-O1B	2.93	1.50	1.46
6	C	1900	ANP	PB-O1B	2.81	1.50	1.46
6	C	1910	ANP	PG-O2G	-2.57	1.50	1.56
6	G	3910	ANP	PB-O2B	-2.56	1.50	1.56
6	G	3900	ANP	C2-N1	2.53	1.38	1.33
6	A	1084	ANP	PG-O2G	-2.48	1.50	1.56
6	C	1900	ANP	PG-O2G	-2.48	1.50	1.56
6	G	3900	ANP	PG-O2G	-2.47	1.50	1.56
6	E	2910	ANP	PB-O2B	-2.47	1.50	1.56
6	C	1910	ANP	PB-O2B	-2.45	1.50	1.56
6	E	2900	ANP	PG-O2G	-2.44	1.50	1.56
6	C	1910	ANP	C4-N9	2.44	1.42	1.37
6	A	1083	ANP	C2-N1	2.42	1.38	1.33
6	G	3910	ANP	PA-O3A	2.35	1.62	1.59
6	G	3900	ANP	PG-O1G	2.32	1.49	1.46
6	E	2900	ANP	PB-O2B	-2.31	1.50	1.56
6	G	3910	ANP	PG-O1G	2.31	1.49	1.46
6	E	2910	ANP	C2-N1	2.30	1.38	1.33
6	A	1084	ANP	PB-O2B	-2.25	1.50	1.56
6	A	1083	ANP	PB-O2B	-2.23	1.50	1.56
6	C	1900	ANP	C2-N1	2.23	1.37	1.33
6	G	3900	ANP	PA-O3A	2.21	1.61	1.59
6	E	2900	ANP	C2-N1	2.19	1.37	1.33
6	A	1084	ANP	C2-N1	2.14	1.37	1.33
6	G	3910	ANP	C2-N1	2.10	1.37	1.33
6	G	3910	ANP	PG-O2G	-2.10	1.51	1.56
6	G	3910	ANP	C2-N3	-2.08	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1910	ANP	C2-N1	2.04	1.37	1.33
6	C	1900	ANP	PB-O2B	-2.02	1.51	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3910	ANP	C2-N1-C6	4.73	126.51	118.73
6	G	3900	ANP	C2-N1-C6	4.73	126.50	118.73
6	A	1083	ANP	C2-N1-C6	4.70	126.44	118.73
6	E	2910	ANP	C2-N1-C6	4.58	126.26	118.73
6	E	2900	ANP	C2-N1-C6	4.47	126.08	118.73
6	C	1900	ANP	C2-N1-C6	4.46	126.05	118.73
6	C	1910	ANP	C2-N1-C6	4.13	125.52	118.73
6	A	1084	ANP	C2-N1-C6	4.13	125.51	118.73
6	G	3910	ANP	N3-C2-N1	-3.75	122.90	128.58
6	E	2910	ANP	N3-C2-N1	-3.59	123.14	128.58
6	C	1900	ANP	N3-C2-N1	-3.51	123.27	128.58
6	E	2900	ANP	N3-C2-N1	-3.49	123.29	128.58
6	A	1083	ANP	N3-C2-N1	-3.16	123.79	128.58
6	A	1084	ANP	O1B-PB-N3B	-2.99	107.37	111.77
6	G	3900	ANP	N3-C2-N1	-2.94	124.13	128.58
6	A	1083	ANP	C5-C6-N1	-2.88	110.20	117.51
6	A	1084	ANP	N3-C2-N1	-2.84	124.28	128.58
7	A	1085	ORN	OXT-C-O	-2.82	117.68	124.08
7	E	2920	ORN	OXT-C-O	-2.81	117.71	124.08
6	C	1910	ANP	N3-C2-N1	-2.75	124.42	128.58
6	G	3900	ANP	C5-C6-N1	-2.70	110.66	117.51
7	G	3920	ORN	OXT-C-O	-2.51	118.38	124.08
7	C	1920	ORN	OXT-C-O	-2.51	118.39	124.08
6	G	3910	ANP	C5-C6-N1	-2.51	111.15	117.51
6	G	3910	ANP	N6-C6-N1	2.49	123.93	118.38
6	C	1910	ANP	C5-C6-N1	-2.40	111.42	117.51
6	E	2900	ANP	C5-C6-N1	-2.40	111.43	117.51
6	C	1910	ANP	C6-C5-C4	2.39	120.44	117.18
6	C	1910	ANP	O4'-C1'-N9	2.37	112.64	108.09
6	G	3900	ANP	O2G-PG-O1G	-2.37	107.51	113.45
6	A	1083	ANP	C6-C5-C4	2.33	120.36	117.18
6	A	1084	ANP	C5-C6-N1	-2.30	111.67	117.51
6	E	2910	ANP	C5-C6-N1	-2.28	111.73	117.51
6	C	1900	ANP	C5-C6-N1	-2.26	111.78	117.51
6	G	3900	ANP	C5-C6-N6	2.25	128.84	123.29
6	C	1910	ANP	O3'-C3'-C2'	2.19	118.83	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3910	ANP	O2G-PG-O1G	-2.15	108.05	113.45
6	C	1910	ANP	O2G-PG-O1G	-2.14	108.08	113.45
6	A	1083	ANP	C3'-C2'-C1'	2.12	105.47	101.46
6	E	2900	ANP	C3'-C2'-C1'	2.07	105.37	101.46

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1083	ANP	PB-N3B-PG-O1G
6	A	1083	ANP	PG-N3B-PB-O1B
6	A	1083	ANP	PG-N3B-PB-O3A
6	A	1084	ANP	PB-N3B-PG-O1G
6	A	1084	ANP	PG-N3B-PB-O1B
6	C	1900	ANP	PB-N3B-PG-O1G
6	C	1900	ANP	PG-N3B-PB-O1B
6	C	1910	ANP	PB-N3B-PG-O1G
6	C	1910	ANP	PG-N3B-PB-O1B
6	C	1910	ANP	PG-N3B-PB-O3A
6	E	2900	ANP	PB-N3B-PG-O1G
6	E	2900	ANP	PG-N3B-PB-O1B
6	E	2900	ANP	PG-N3B-PB-O3A
6	E	2910	ANP	PB-N3B-PG-O1G
6	E	2910	ANP	PG-N3B-PB-O1B
6	E	2910	ANP	PG-N3B-PB-O3A
6	E	2910	ANP	C5'-O5'-PA-O2A
6	G	3900	ANP	PB-N3B-PG-O1G
6	G	3900	ANP	PG-N3B-PB-O1B
6	G	3910	ANP	PB-N3B-PG-O1G
6	G	3910	ANP	PG-N3B-PB-O1B
6	G	3910	ANP	C5'-O5'-PA-O2A
6	G	3910	ANP	C5'-O5'-PA-O3A
7	A	1085	ORN	C-CA-CB-CG
7	C	1920	ORN	N-CA-CB-CG
7	C	1920	ORN	C-CA-CB-CG
7	E	2920	ORN	N-CA-CB-CG
7	E	2920	ORN	C-CA-CB-CG
7	E	2920	ORN	O-C-CA-N
7	G	3920	ORN	C-CA-CB-CG
8	G	3950	NET	C4-C3-N1-C1
8	A	1086	NET	C4-C3-N1-C1
8	E	2950	NET	C4-C3-N1-C1

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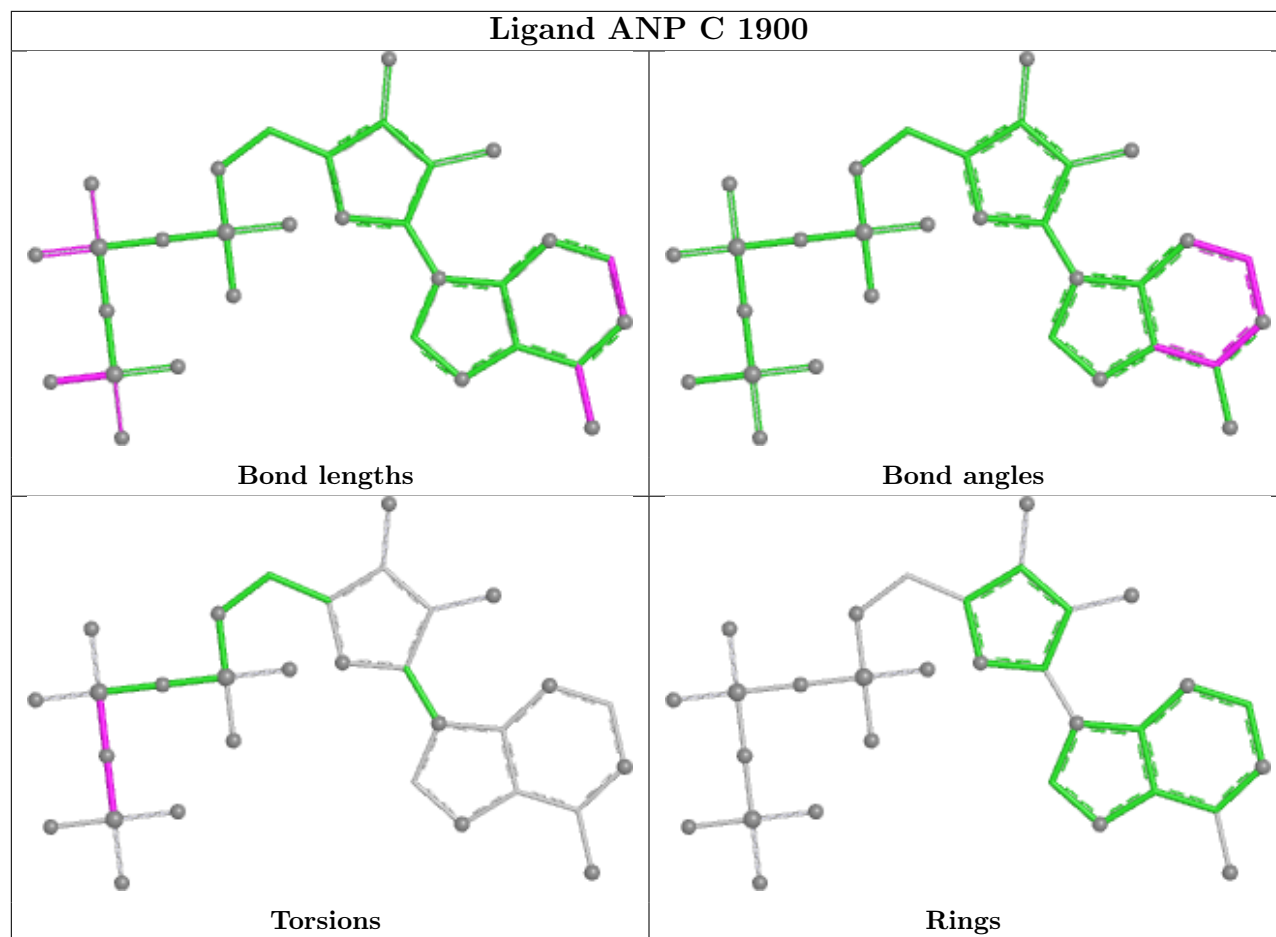
Mol	Chain	Res	Type	Atoms
8	A	1086	NET	C8-C7-N1-C5
8	A	1086	NET	C8-C7-N1-C3
8	E	2950	NET	C4-C3-N1-C5
8	A	1086	NET	C8-C7-N1-C1
8	E	2950	NET	C4-C3-N1-C7
8	A	1086	NET	C4-C3-N1-C7
8	A	1086	NET	C4-C3-N1-C5
8	G	3950	NET	C4-C3-N1-C7
8	G	3950	NET	C4-C3-N1-C5
8	E	2950	NET	C8-C7-N1-C3
8	C	1950	NET	C4-C3-N1-C7
8	C	1950	NET	C4-C3-N1-C5
8	E	2950	NET	C8-C7-N1-C1
8	E	2950	NET	C2-C1-N1-C5
7	E	2920	ORN	OXT-C-CA-N
7	E	2920	ORN	CA-CB-CG-CD
8	C	1950	NET	C4-C3-N1-C1
8	E	2950	NET	C8-C7-N1-C5
8	E	2950	NET	C2-C1-N1-C3
8	E	2950	NET	C2-C1-N1-C7
8	E	2950	NET	C6-C5-N1-C1
7	C	1920	ORN	CA-CB-CG-CD
7	G	3920	ORN	CA-CB-CG-CD
8	G	3950	NET	C6-C5-N1-C7
8	G	3950	NET	C6-C5-N1-C3
8	E	2950	NET	C6-C5-N1-C7
8	G	3950	NET	C6-C5-N1-C1
8	E	2950	NET	C6-C5-N1-C3
7	A	1085	ORN	O-C-CA-N
7	C	1920	ORN	O-C-CA-N
7	C	1920	ORN	NE-CD-CG-CB
6	A	1084	ANP	PG-N3B-PB-O3A
6	E	2910	ANP	C5'-O5'-PA-O3A
7	C	1920	ORN	OXT-C-CA-N
7	E	2920	ORN	O-C-CA-CB
7	A	1085	ORN	NE-CD-CG-CB
7	E	2920	ORN	NE-CD-CG-CB
7	G	3920	ORN	NE-CD-CG-CB
7	G	3920	ORN	O-C-CA-N
7	C	1920	ORN	O-C-CA-CB
7	A	1085	ORN	N-CA-CB-CG
7	G	3920	ORN	N-CA-CB-CG

There are no ring outliers.

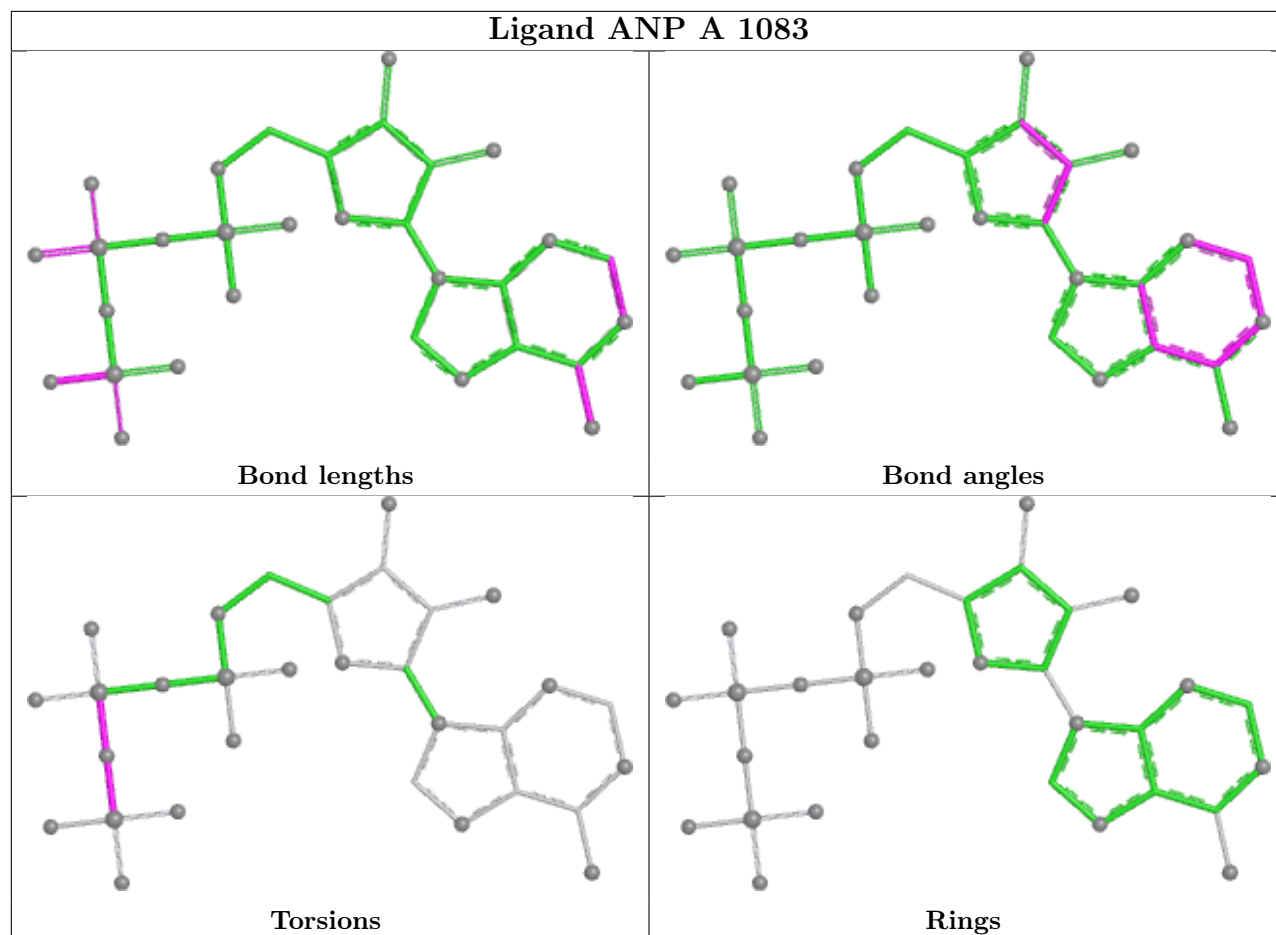
13 monomers are involved in 35 short contacts:

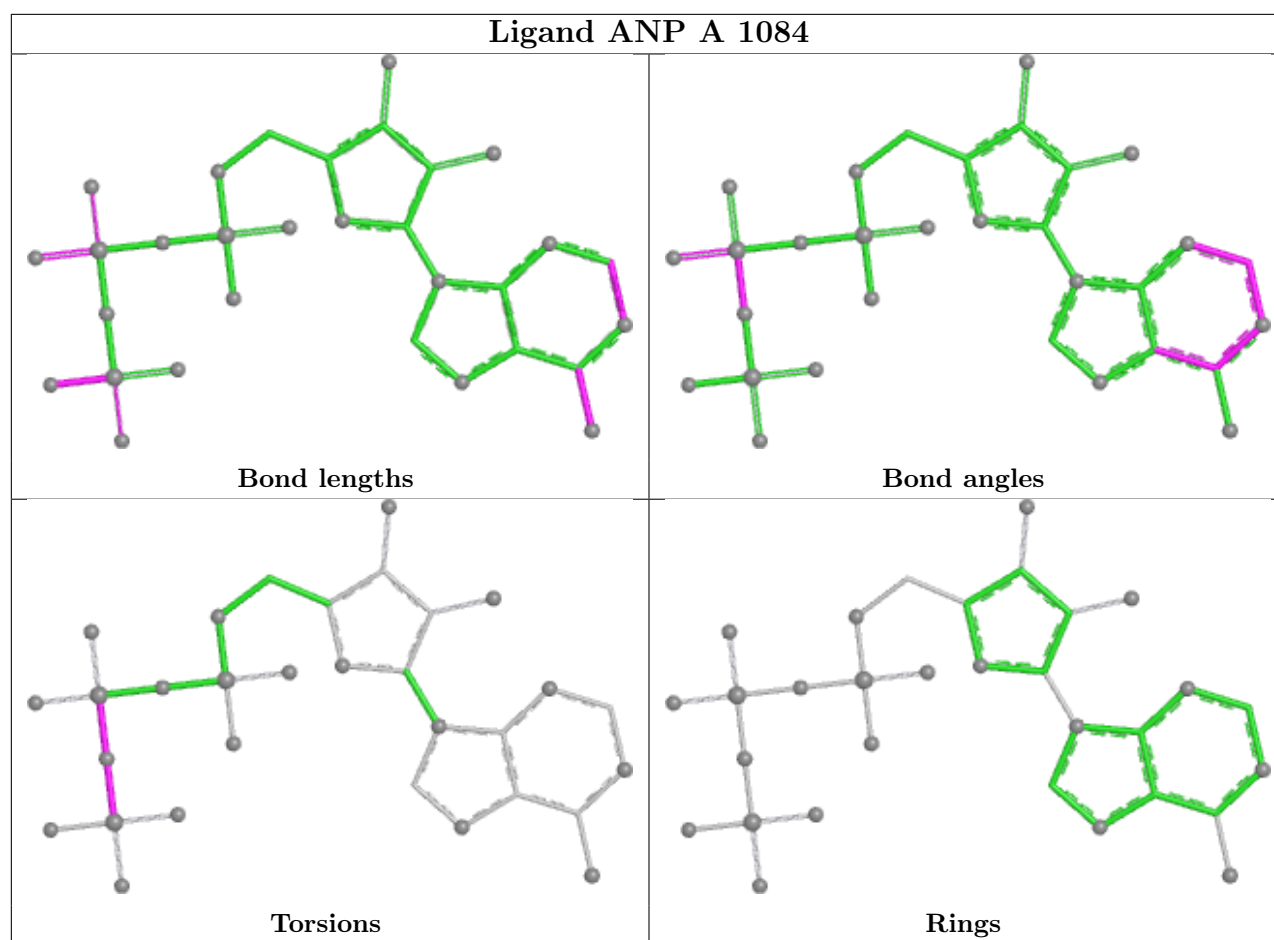
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1083	ANP	3	0
7	E	2920	ORN	1	0
8	A	1086	NET	6	0
8	C	1950	NET	4	0
8	G	3950	NET	4	0
7	G	3920	ORN	1	0
6	E	2910	ANP	5	0
6	G	3910	ANP	2	0
6	C	1910	ANP	1	0
7	A	1085	ORN	1	0
8	E	2950	NET	4	0
7	C	1920	ORN	1	0
6	G	3900	ANP	2	0

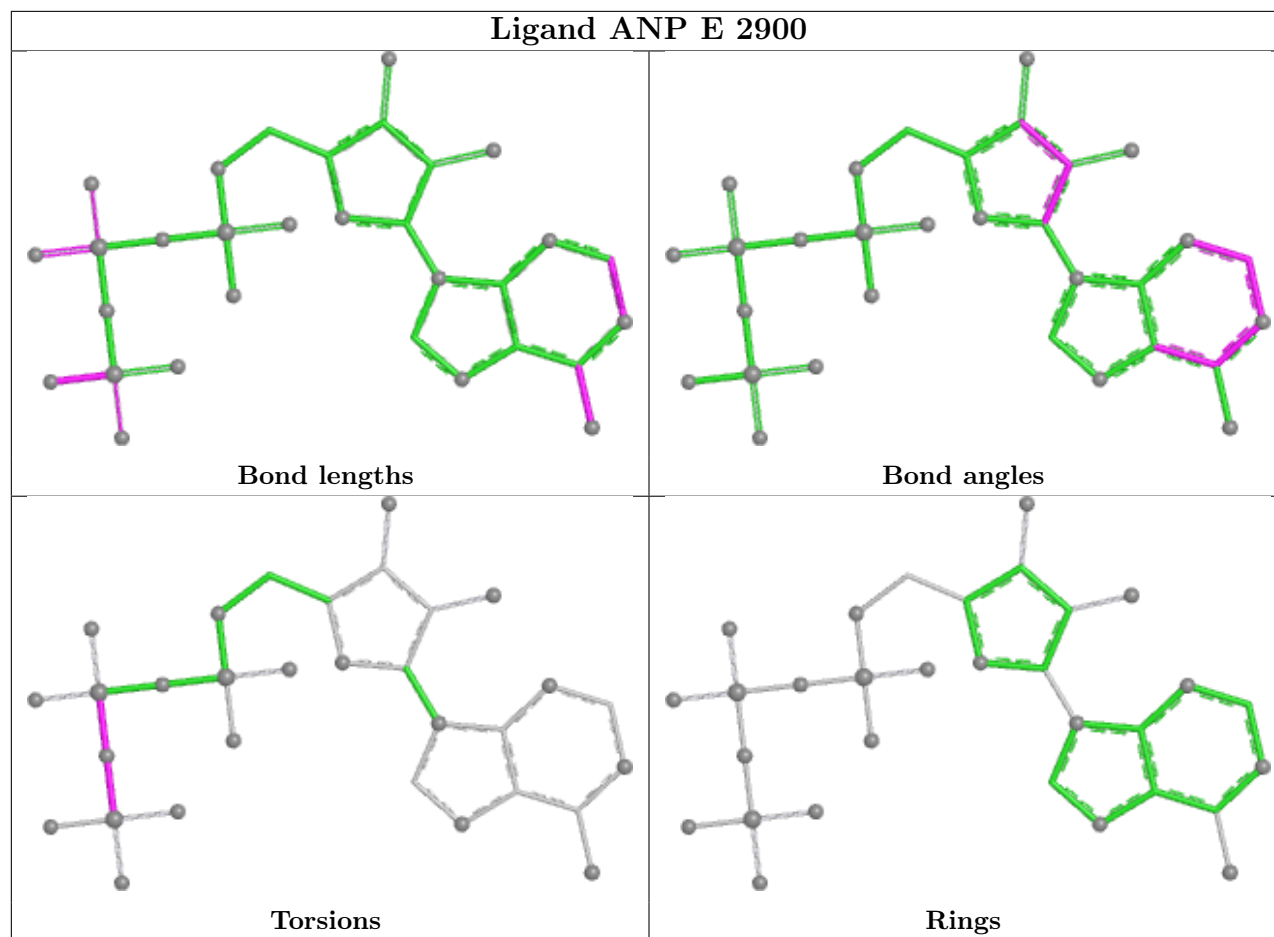
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

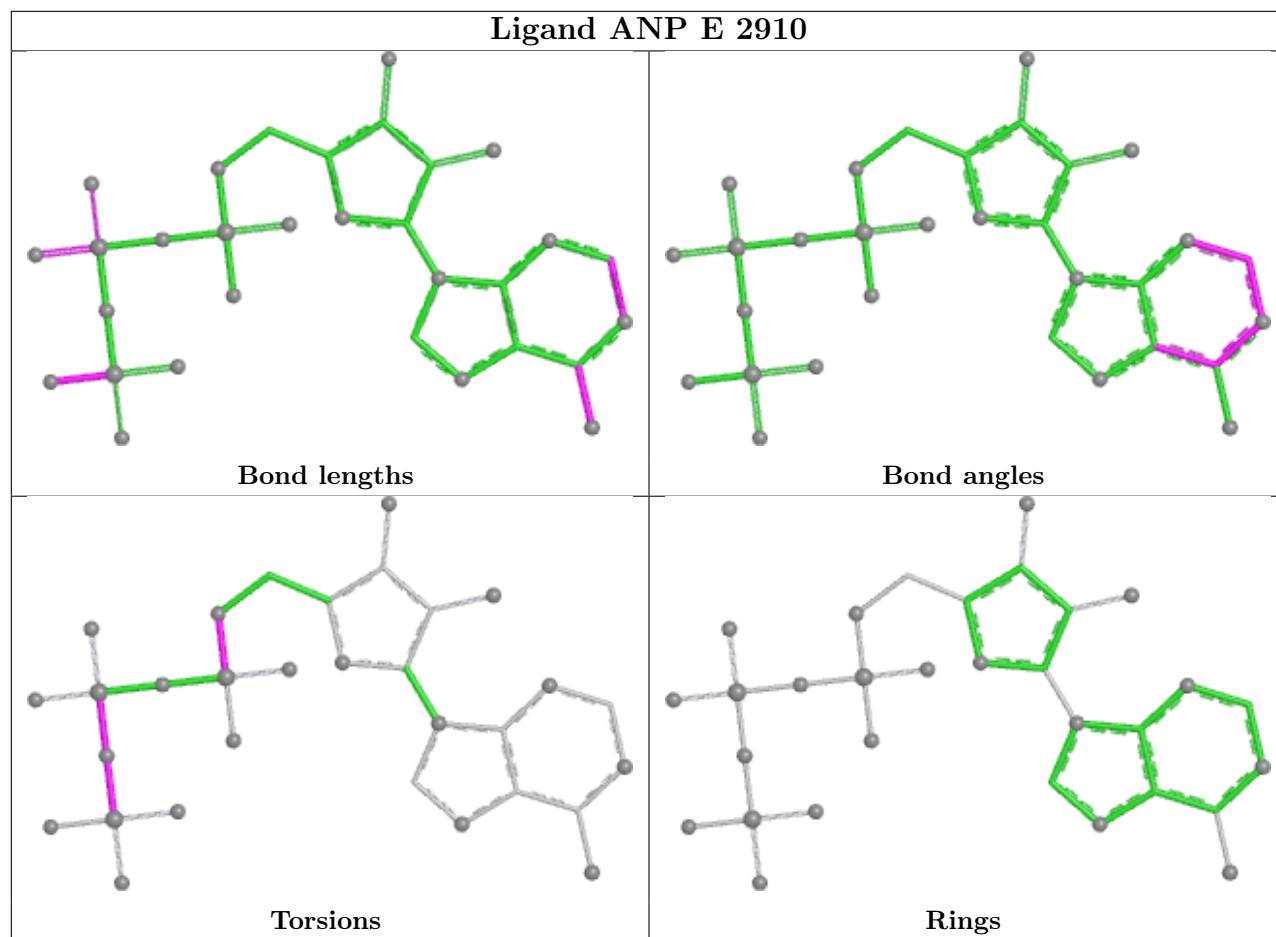


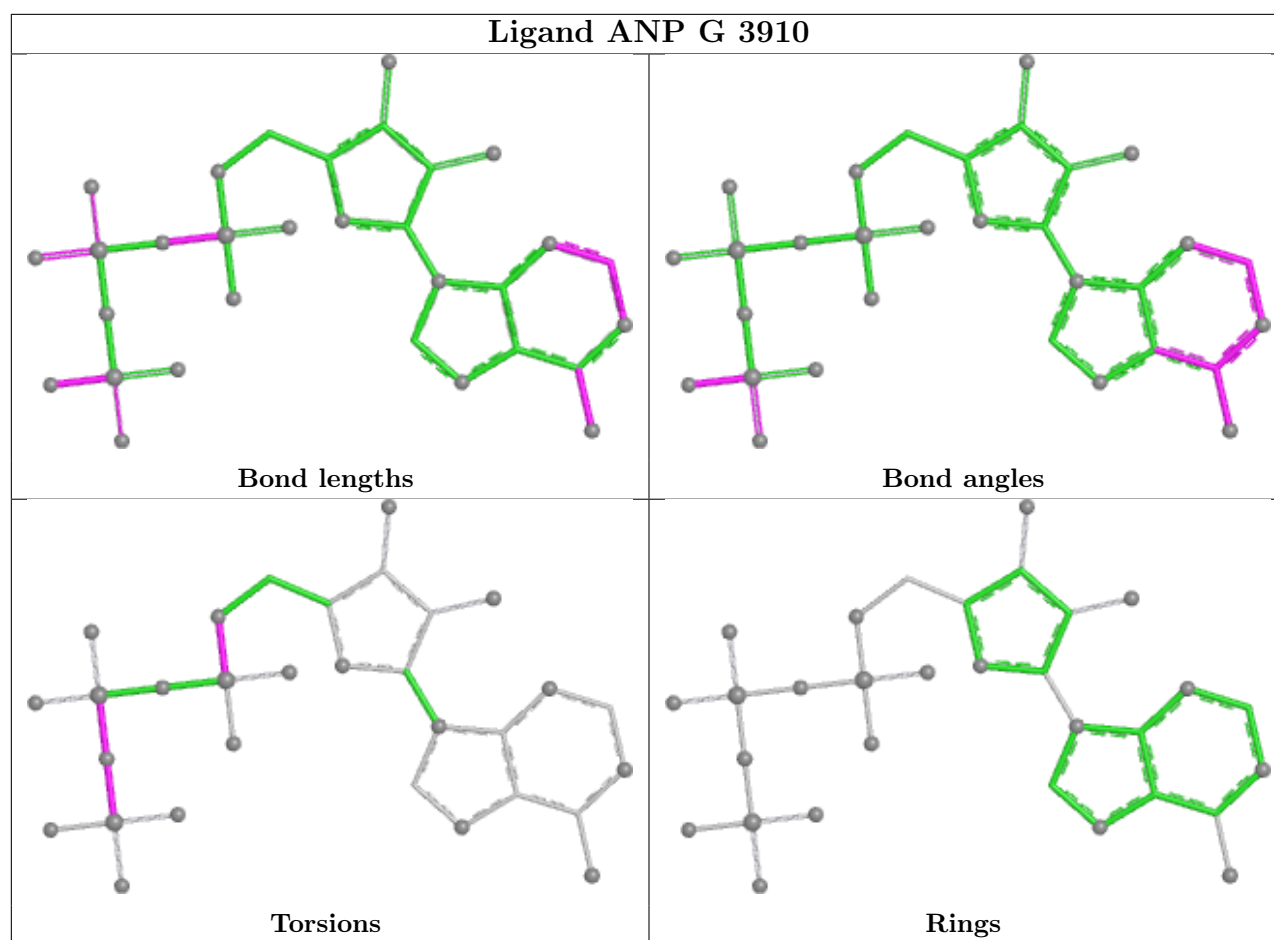
Ligand ANP A 1083

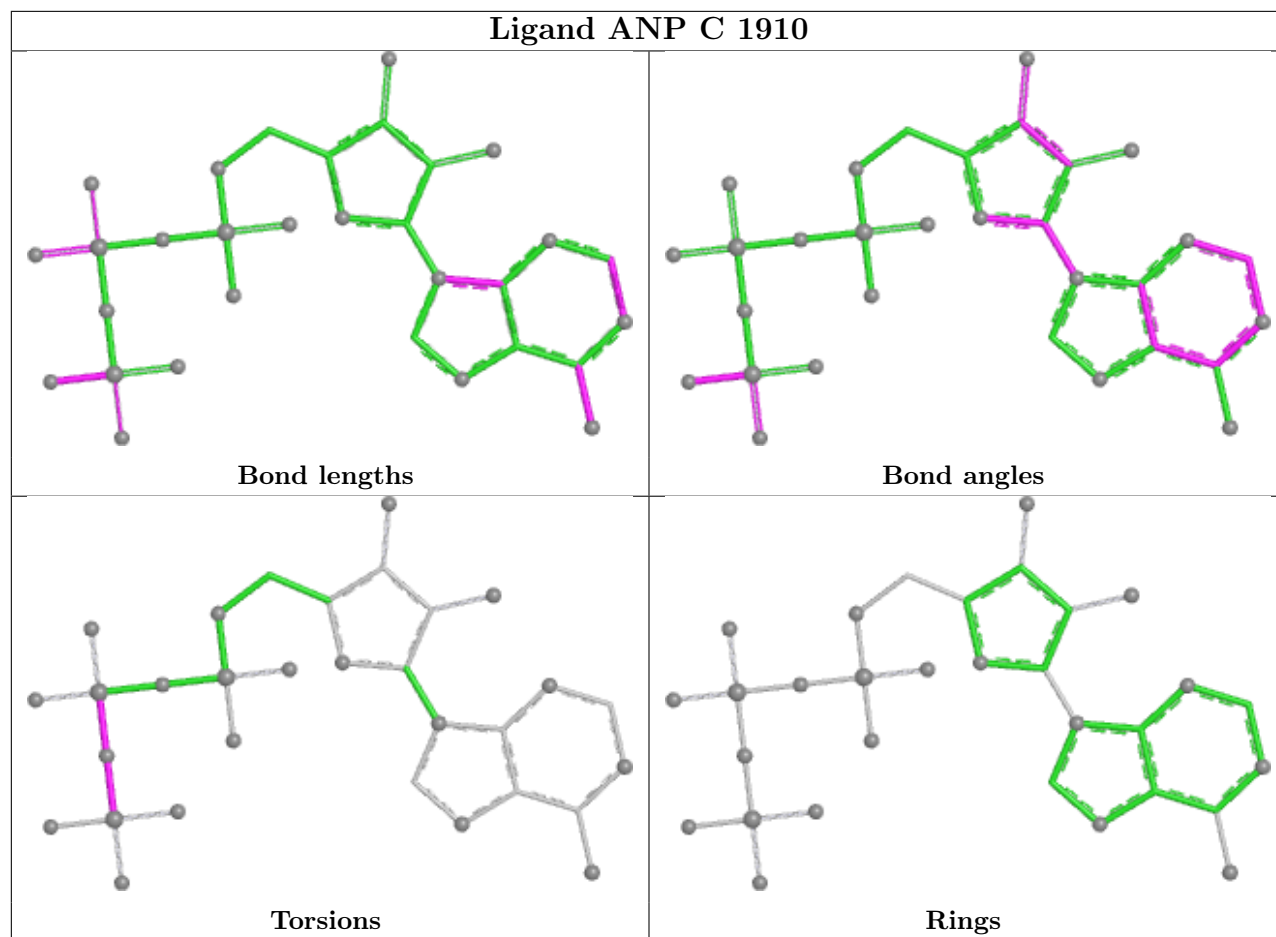


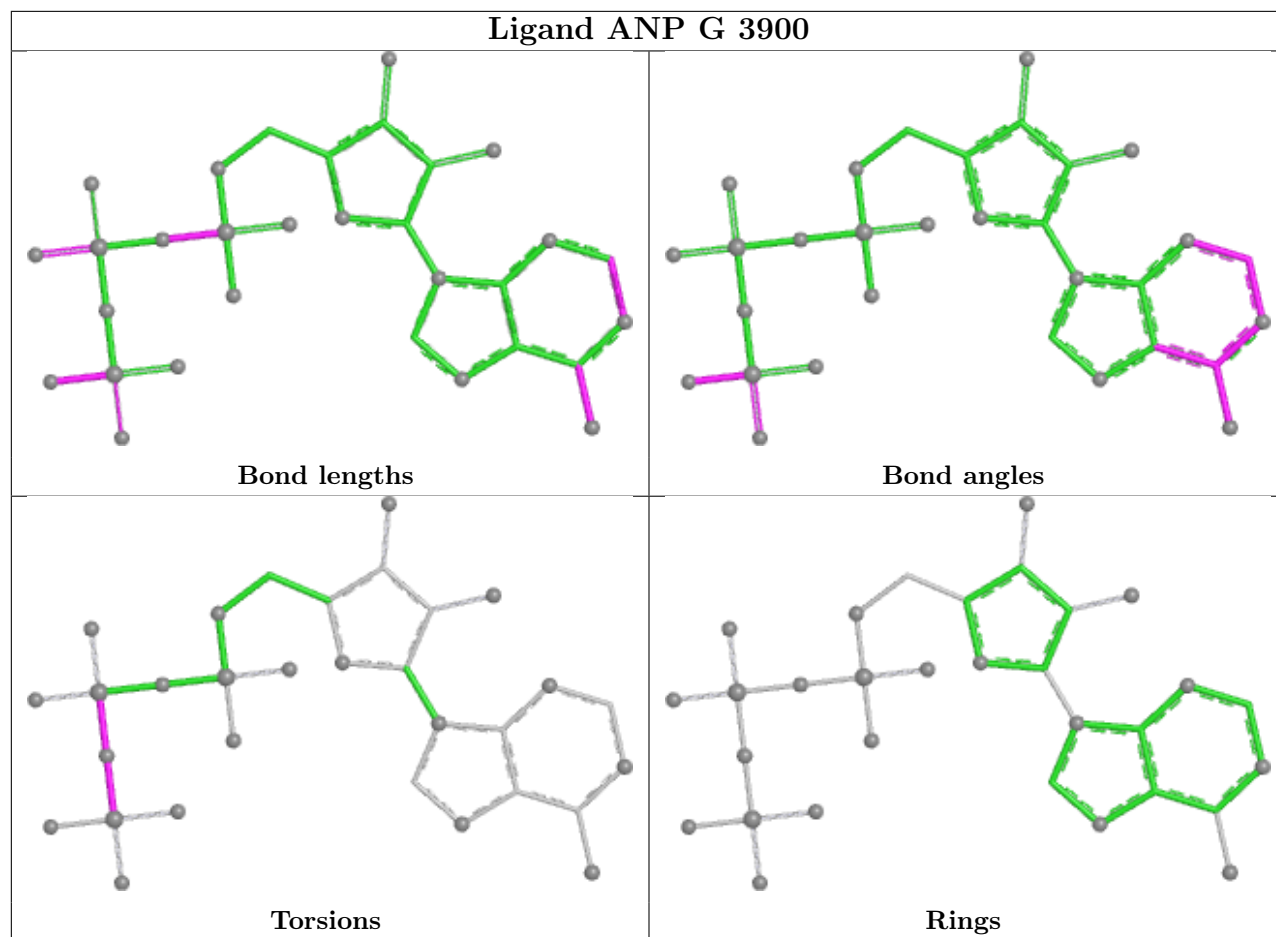












5.7 Other polymers [i](#)

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.