



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:03 PM UTC

PDB ID : 1CS0 / pdb_00001cs0
Title : Crystal structure of carbamoyl phosphate synthetase complexed at CYS269 in the small subunit with the tetrahedral mimic l-glutamate gamma-semialdehyde
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-08-16
Resolution : 2.00 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

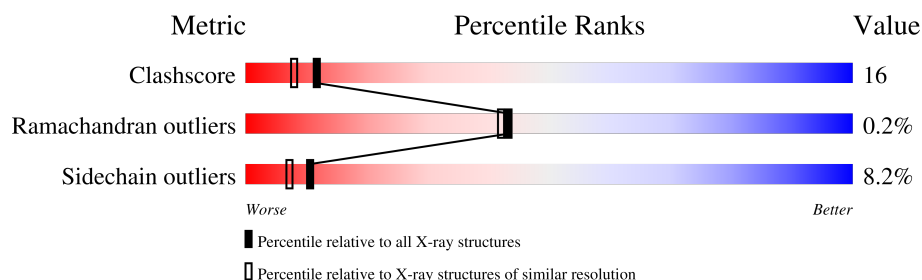
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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% 29% . .
1	C	1073	67% 26% 5% .
1	E	1073	69% 25% . .
1	G	1073	65% 28% 5% .
2	B	382	61% 34% . .
2	D	382	61% 33% 5% .
2	F	382	62% 32% 5% . .
2	H	382	55% 37% 7% .

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 48889 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 SYNTHETASE: LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	3	0
			8169	5128	1422	1574	45			
1	C	1058	Total	C	N	O	S	0	3	0
			8173	5132	1423	1573	45			
1	E	1058	Total	C	N	O	S	0	6	0
			8186	5140	1424	1576	46			
1	G	1058	Total	C	N	O	S	0	3	0
			8175	5132	1425	1572	46			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	D	379	Total	C	N	O	S	0	1	0
			2909	1833	509	557	10			
2	F	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	H	379	Total	C	N	O	S	0	1	0
			2906	1831	509	556	10			

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Mn 3	0	0

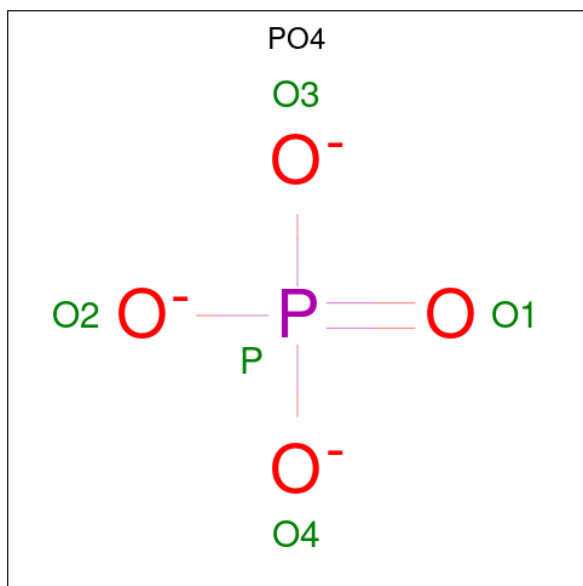
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	K 7	0	0
4	B	1	Total 1	K 1	0	0
4	C	7	Total 7	K 7	0	0
4	D	1	Total 1	K 1	0	0
4	E	8	Total 8	K 8	0	0
4	F	1	Total 1	K 1	0	0
4	G	7	Total 7	K 7	0	0
4	H	1	Total 1	K 1	0	0

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

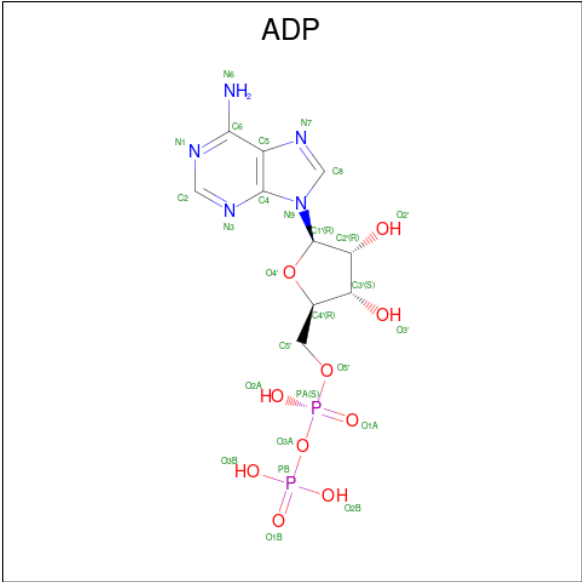
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	Cl 6	0	0
5	B	2	Total 2	Cl 2	0	0
5	C	5	Total 5	Cl 5	0	0
5	D	2	Total 2	Cl 2	0	0
5	E	5	Total 5	Cl 5	0	0
5	F	2	Total 2	Cl 2	0	0
5	G	5	Total 5	Cl 5	0	0
5	H	2	Total 2	Cl 2	0	0

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



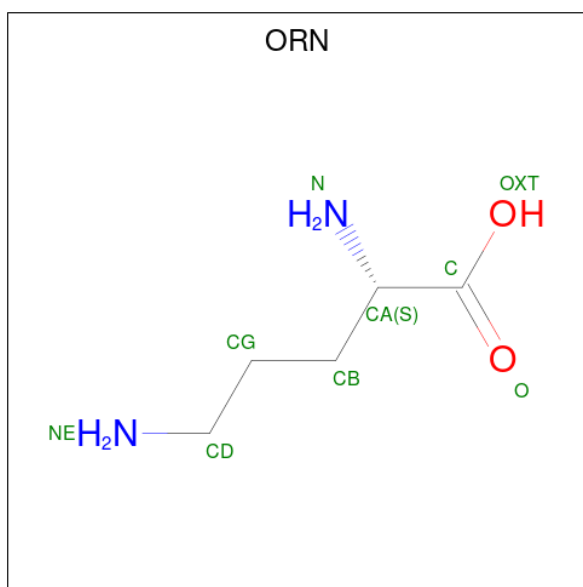
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

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



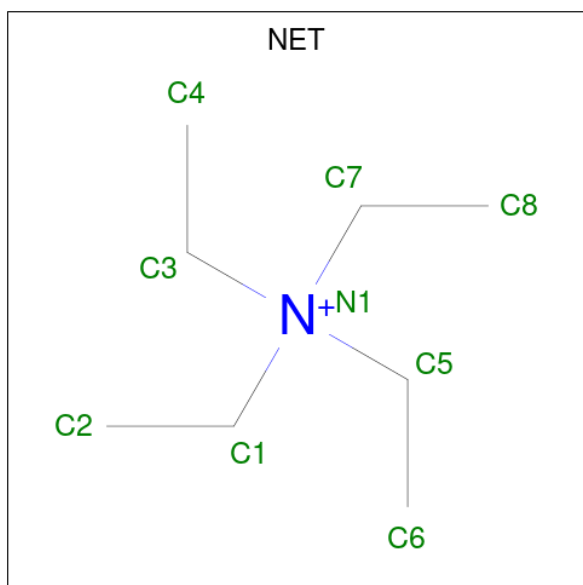
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

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



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

- Molecule 9 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: C₈H₂₀N).



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

- Molecule 10 is water.

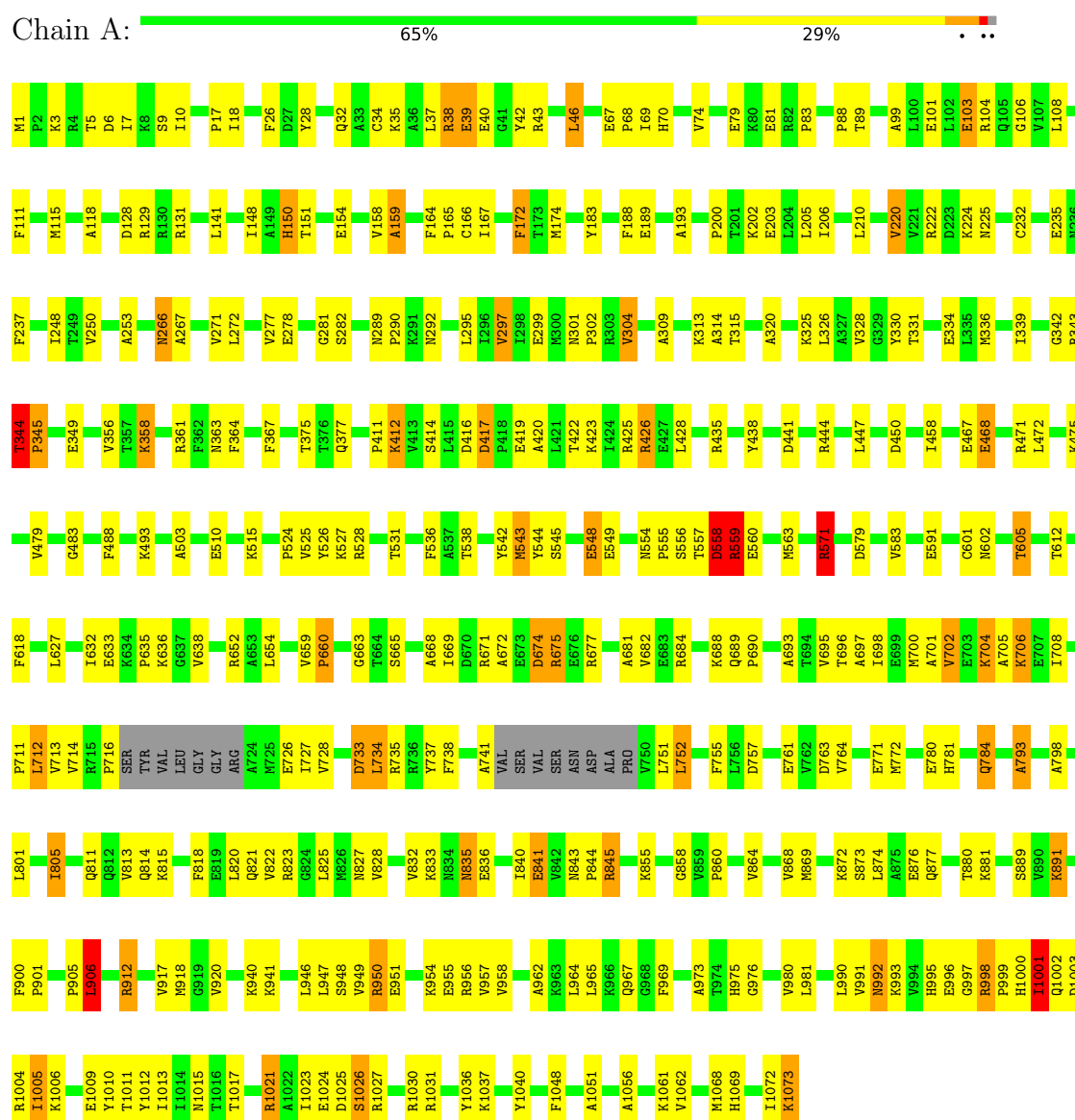
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	869	Total O 869 869	0	0
10	B	213	Total O 213 213	0	0
10	C	784	Total O 784 784	0	0
10	D	275	Total O 275 275	0	0
10	E	864	Total O 864 864	0	0
10	F	235	Total O 235 235	0	0
10	G	743	Total O 743 743	0	0
10	H	193	Total O 193 193	0	0

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.

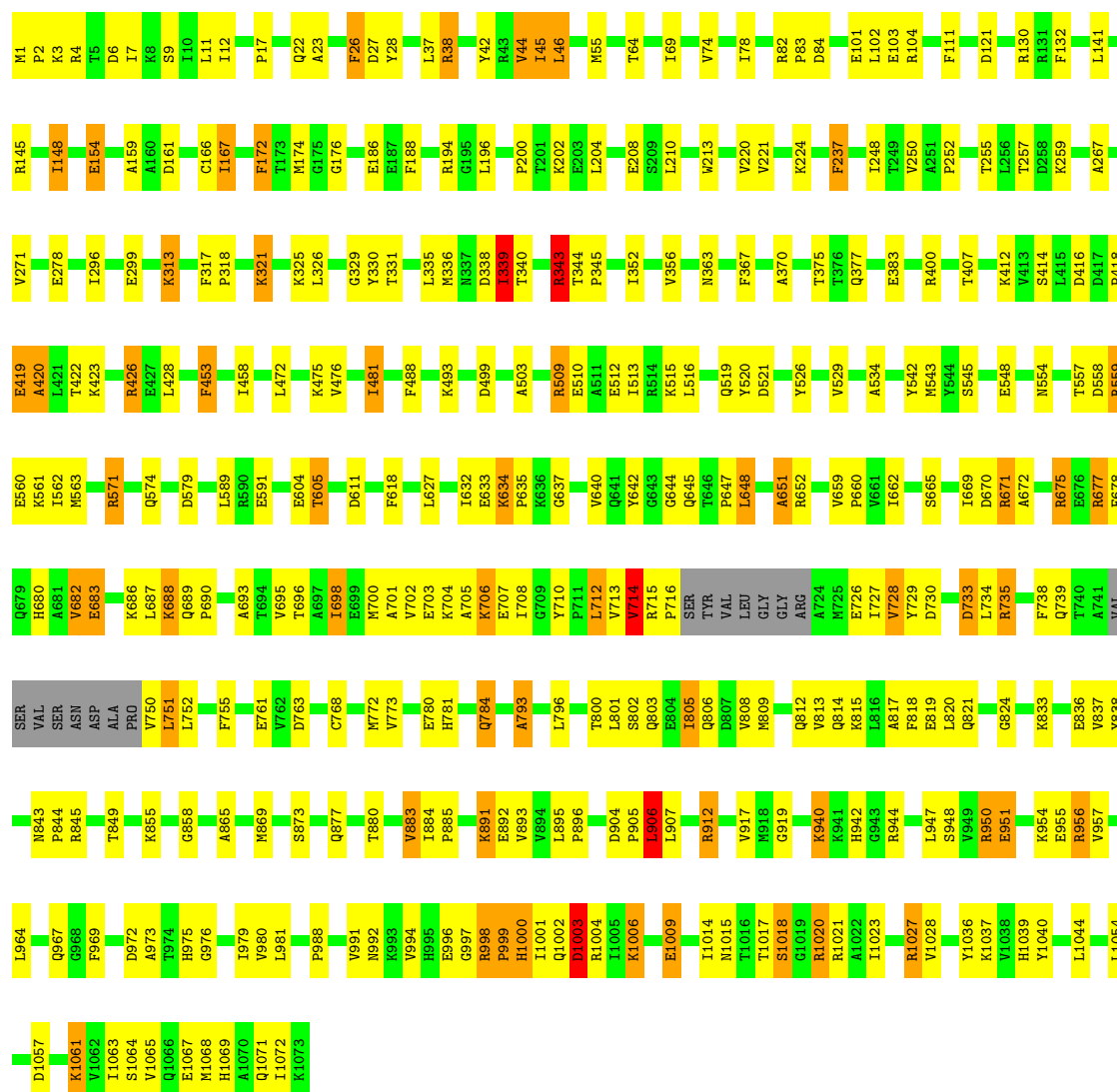
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



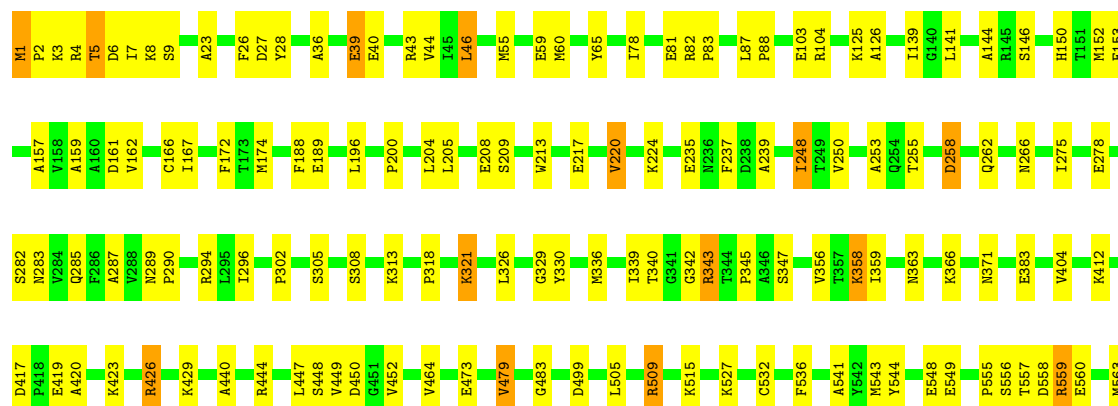
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

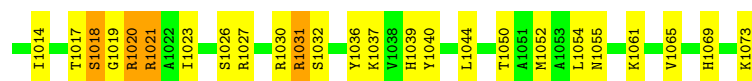
Chain C:  67% 26% 5% .



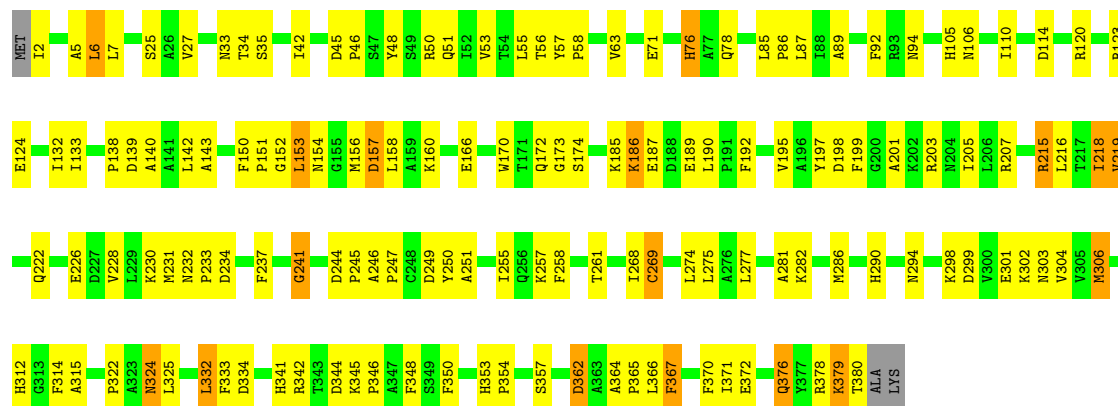
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain E:  69% 25% . .

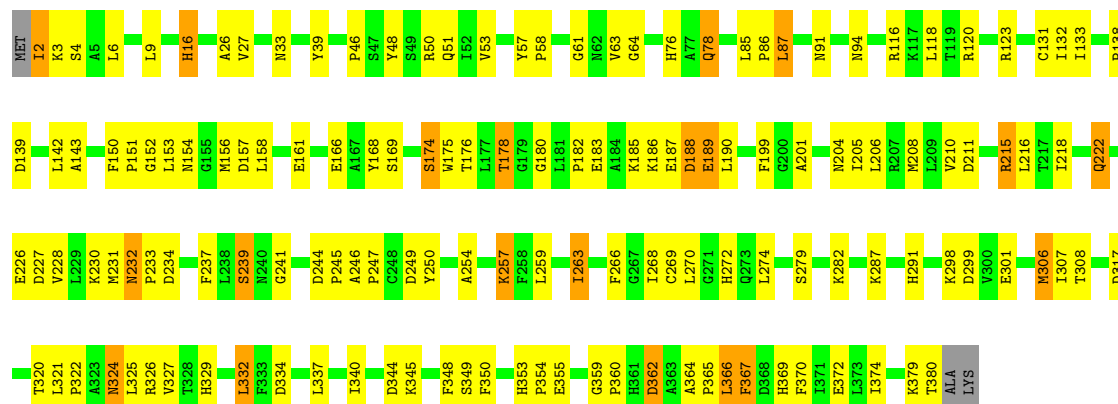




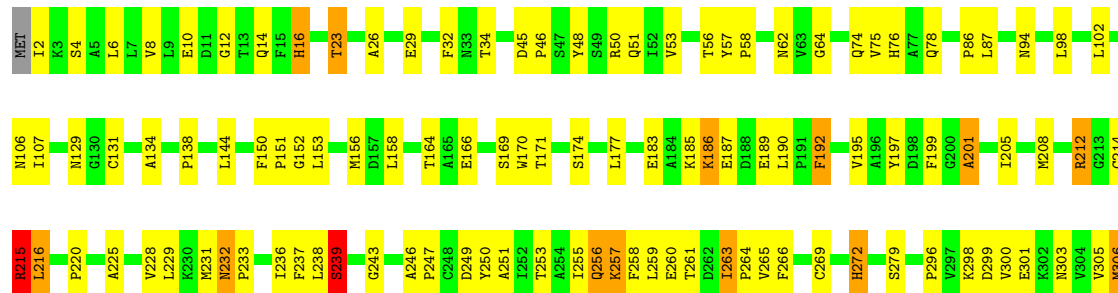
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT



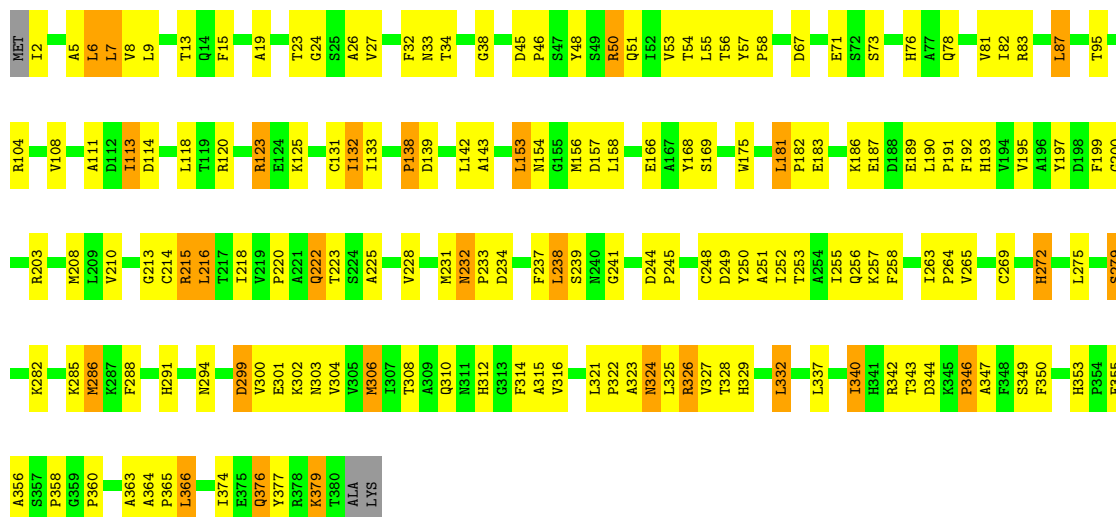
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT





• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 55% 37% 7% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.70Å 163.80Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.7 (30.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48889	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NET, ORN, CYG, K, CL, ADP, PO4

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	1.20	0/8307	1.54	61/11230 (0.5%)
1	C	1.18	1/8311 (0.0%)	1.54	58/11236 (0.5%)
1	E	1.20	0/8336	1.52	70/11267 (0.6%)
1	G	1.17	6/8313 (0.1%)	1.53	57/11237 (0.5%)
2	B	1.10	0/2950	1.53	18/4005 (0.4%)
2	D	1.15	1/2959 (0.0%)	1.52	22/4017 (0.5%)
2	F	1.15	0/2950	1.57	33/4005 (0.8%)
2	H	1.09	0/2956	1.55	25/4013 (0.6%)
All	All	1.17	8/45082 (0.0%)	1.54	344/61010 (0.6%)

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	C	1	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	189	GLU	CD-OE2	7.71	1.40	1.25
1	C	554	ASN	CA-C	-7.06	1.48	1.53
1	G	188	PHE	N-CA	-5.61	1.39	1.46
1	G	110	GLU	C-O	-5.38	1.17	1.24
1	G	39	GLU	CD-OE1	-5.27	1.15	1.25
1	G	1003	ASP	N-CA	-5.21	1.40	1.46
1	G	1002	GLN	CA-C	-5.05	1.46	1.52
1	G	859	VAL	N-CA	-5.04	1.42	1.46

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	885	PRO	N-CA-CB	11.69	109.73	103.19
1	E	557	THR	CA-C-N	10.26	134.20	120.65
1	E	557	THR	C-N-CA	10.26	134.20	120.65
1	C	557	THR	CA-C-N	9.62	133.72	120.63
1	C	557	THR	C-N-CA	9.62	133.72	120.63
1	C	1039	HIS	CA-CB-CG	-9.59	104.21	113.80
1	C	998	ARG	N-CA-C	9.58	119.36	108.25
1	C	367	PHE	CA-CB-CG	-9.18	104.62	113.80
1	E	584	HIS	CA-CB-CG	-9.12	104.68	113.80
2	H	299	ASP	N-CA-C	-8.80	96.48	109.15
1	C	554	ASN	CB-CA-C	-8.64	103.49	111.00
1	G	319	ILE	N-CA-C	8.15	118.24	110.42
1	G	605	THR	N-CA-C	8.08	122.31	110.59
1	A	367	PHE	CA-CB-CG	-8.08	105.72	113.80
1	A	468	GLU	CG-CD-OE2	-8.03	99.93	118.40
1	G	716	PRO	N-CA-CB	7.98	111.78	103.00
1	C	1003	ASP	CA-CB-CG	7.96	120.56	112.60
2	B	76	HIS	CA-CB-CG	-7.91	105.89	113.80
1	E	23	ALA	N-CA-C	7.90	120.43	109.29
1	A	605	THR	N-CA-C	7.86	121.16	110.55
1	C	558	ASP	N-CA-CB	-7.79	98.68	109.98
1	G	188	PHE	CA-CB-CG	-7.78	106.02	113.80
2	B	106	ASN	CA-CB-CG	-7.77	104.83	112.60
1	A	1025	ASP	CA-CB-CG	7.76	120.36	112.60
2	F	346	PRO	N-CA-CB	7.71	107.65	102.25
2	F	353	HIS	CA-CB-CG	-7.70	106.11	113.80
1	E	793	ALA	N-CA-C	-7.62	100.26	110.55
1	E	885	PRO	N-CA-CB	7.61	107.18	103.22
2	F	239	SER	N-CA-C	7.59	119.60	110.19
1	C	23	ALA	N-CA-C	7.42	119.76	109.29
1	C	605	THR	N-CA-C	7.42	121.35	110.59
1	E	557	THR	N-CA-C	-7.38	103.86	114.12
1	E	884	ILE	CA-C-N	7.31	124.93	119.66
1	E	884	ILE	C-N-CA	7.31	124.93	119.66
1	A	716	PRO	N-CA-CB	7.31	111.04	103.00
2	B	105	HIS	CA-CB-CG	-7.30	106.50	113.80
1	G	27	ASP	N-CA-C	-7.30	102.71	111.69
1	C	132	PHE	CA-CB-CG	-7.29	106.51	113.80
1	A	559	ARG	N-CA-C	7.25	120.34	110.55
1	C	453	PHE	CA-CB-CG	-7.19	106.61	113.80
1	G	928	PHE	CA-CB-CG	-7.19	106.61	113.80
2	H	303	ASN	CA-CB-CG	-7.17	105.43	112.60
2	F	16	HIS	CA-CB-CG	-7.15	106.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	PHE	CA-CB-CG	-7.12	106.67	113.80
1	E	161	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	172	PHE	CA-CB-CG	-7.00	106.80	113.80
1	G	885	PRO	O-C-N	6.97	124.52	121.31
1	A	993	LYS	N-CA-C	-6.92	101.40	110.53
1	C	44	VAL	N-CA-C	6.89	117.79	107.80
1	A	417	ASP	CA-CB-CG	6.84	119.44	112.60
2	D	157	ASP	CA-CB-CG	6.83	119.43	112.60
1	C	942	HIS	CA-CB-CG	-6.80	107.00	113.80
1	A	889	SER	CA-C-N	-6.79	113.69	123.06
1	A	889	SER	C-N-CA	-6.79	113.69	123.06
1	E	305	SER	N-CA-C	6.74	117.14	108.24
1	G	793	ALA	N-CA-C	-6.69	101.52	110.55
1	G	44	VAL	N-CA-C	6.63	117.67	107.99
1	A	468	GLU	CG-CD-OE1	6.63	133.65	118.40
1	G	578	PHE	CA-CB-CG	-6.60	107.20	113.80
2	B	362	ASP	N-CA-C	6.58	119.29	111.33
1	G	557	THR	CA-C-N	6.58	134.10	121.54
1	G	557	THR	C-N-CA	6.58	134.10	121.54
1	G	353	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	558	ASP	N-CA-C	6.54	118.10	110.97
1	C	210	LEU	N-CA-C	-6.52	103.43	112.30
1	G	316	GLY	N-CA-C	-6.51	106.33	115.32
2	B	157	ASP	CA-CB-CG	6.51	119.11	112.60
1	E	782	ILE	N-CA-C	-6.50	104.83	110.74
1	A	1010	TYR	N-CA-C	6.49	120.62	110.17
1	C	255	THR	N-CA-C	6.49	120.51	112.59
1	G	132	PHE	CA-CB-CG	-6.48	107.32	113.80
2	D	263	ILE	N-CA-CB	6.47	116.10	110.08
2	F	303	ASN	CA-CB-CG	-6.46	106.14	112.60
1	A	557	THR	CA-C-N	6.44	133.84	121.54
1	A	557	THR	C-N-CA	6.44	133.84	121.54
1	A	26	PHE	CA-CB-CG	-6.43	107.37	113.80
1	E	1000	HIS	CA-CB-CG	-6.41	107.39	113.80
1	C	1003	ASP	N-CA-CB	6.41	119.64	110.16
1	E	811	GLN	CB-CG-CD	-6.39	101.74	112.60
1	C	338	ASP	CA-CB-CG	6.37	118.97	112.60
1	G	443	PHE	CA-CB-CG	-6.34	107.46	113.80
1	G	364	PHE	N-CA-C	6.34	119.00	111.71
2	B	201	ALA	N-CA-C	6.32	119.52	110.10
1	G	26	PHE	CA-CB-CG	-6.32	107.48	113.80
2	D	86	PRO	CB-CA-C	-6.30	103.33	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	GLU	CB-CA-C	-6.29	98.25	110.46
1	A	906	LEU	N-CA-CB	-6.29	100.78	110.85
1	C	1000	HIS	CA-CB-CG	-6.28	107.52	113.80
1	G	994	VAL	N-CA-C	6.28	116.44	110.53
1	A	536	PHE	CA-CB-CG	-6.28	107.52	113.80
2	D	299	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	525	VAL	N-CA-CB	6.26	119.48	112.34
1	G	900	PHE	CA-C-N	6.24	125.98	119.05
1	G	900	PHE	C-N-CA	6.24	125.98	119.05
1	A	557	THR	CA-C-O	6.22	125.62	118.97
1	G	1007	ASN	CA-CB-CG	-6.21	106.39	112.60
1	A	435	ARG	N-CA-C	6.17	118.52	111.11
1	A	266	ASN	CA-CB-CG	6.17	118.77	112.60
1	E	248	ILE	N-CA-C	-6.14	99.53	108.87
1	A	949	VAL	N-CA-C	6.09	118.50	108.99
2	F	192	PHE	N-CA-C	6.09	119.97	110.17
1	E	499	ASP	CA-CB-CG	6.09	118.69	112.60
2	H	272	HIS	CA-CB-CG	6.08	119.88	113.80
2	H	182	PRO	CB-CA-C	-6.08	103.45	111.23
2	D	369	HIS	CA-CB-CG	-6.06	107.74	113.80
1	A	304	VAL	N-CA-C	-6.01	103.50	110.05
1	E	971	LEU	N-CA-C	6.01	119.26	109.59
1	A	364	PHE	CA-CB-CG	-5.99	107.81	113.80
2	H	346	PRO	N-CA-CB	5.99	106.44	102.25
2	D	239	SER	N-CA-C	5.99	117.77	110.41
1	E	339	ILE	N-CA-C	5.98	121.20	113.07
1	E	619	GLU	O-C-N	5.98	125.54	121.71
1	C	339	ILE	N-CA-C	5.97	120.49	111.89
2	F	174	SER	N-CA-C	5.96	118.24	110.43
1	A	998	ARG	N-CA-C	5.96	115.80	108.11
2	D	174	SER	N-CA-C	5.96	117.74	110.41
1	C	370	ALA	N-CA-C	5.95	118.89	110.50
2	D	359	GLY	CA-C-N	5.95	125.89	119.76
2	D	359	GLY	C-N-CA	5.95	125.89	119.76
1	E	894	VAL	N-CA-CB	5.94	119.61	111.41
2	H	232	ASN	CA-C-N	5.93	126.39	119.99
2	H	232	ASN	C-N-CA	5.93	126.39	119.99
1	G	1001	ILE	N-CA-C	5.93	119.35	111.17
1	E	712	LEU	N-CA-C	5.93	119.06	109.40
2	B	53	VAL	N-CA-C	5.92	117.10	108.58
2	D	353	HIS	CA-CB-CG	-5.91	107.89	113.80
2	F	129	ASN	CA-CB-CG	-5.91	106.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	ASP	N-CA-CB	-5.91	100.51	110.49
1	E	555	PRO	N-CA-CB	5.90	108.49	103.35
1	E	239	ALA	N-CA-C	5.88	117.48	110.19
2	B	89	ALA	N-CA-C	-5.87	100.13	109.76
2	H	181	LEU	CA-C-N	5.87	125.82	119.78
2	H	181	LEU	C-N-CA	5.87	125.82	119.78
2	D	367	PHE	CA-CB-CG	-5.87	107.93	113.80
2	F	237	PHE	CA-CB-CG	-5.87	107.94	113.80
2	H	53	VAL	N-CA-C	5.86	116.74	108.36
1	A	900	PHE	CA-C-N	5.86	125.53	119.56
1	A	900	PHE	C-N-CA	5.86	125.53	119.56
1	C	26	PHE	CA-CB-CG	-5.85	107.95	113.80
1	E	283	ASN	CA-CB-CG	5.84	118.44	112.60
1	E	557	THR	O-C-N	5.84	129.04	122.27
2	F	4	SER	N-CA-C	5.84	118.73	110.50
2	H	132	ILE	CB-CA-C	-5.83	101.94	110.81
2	D	9	LEU	CA-C-N	5.82	128.36	120.38
2	D	9	LEU	C-N-CA	5.82	128.36	120.38
2	F	368	ASP	CA-CB-CG	-5.82	106.78	112.60
1	C	999	PRO	N-CA-CB	5.80	108.98	102.60
1	C	121	ASP	N-CA-CB	5.78	118.45	110.07
2	F	215	ARG	N-CA-CB	5.78	119.59	110.23
2	F	372	GLU	CA-C-N	5.78	128.02	120.28
2	F	372	GLU	C-N-CA	5.78	128.02	120.28
2	F	32	PHE	CA-CB-CG	5.77	119.57	113.80
1	C	906	LEU	CB-CA-C	5.77	120.38	109.37
2	H	215	ARG	CA-C-N	-5.76	113.63	122.62
2	H	215	ARG	C-N-CA	-5.76	113.63	122.62
1	G	81	GLU	N-CA-C	5.76	119.49	112.23
2	B	332	LEU	N-CA-C	-5.75	106.26	113.28
2	F	214	CYS	N-CA-C	5.75	118.11	108.96
1	E	787	VAL	N-CA-CB	5.75	118.92	111.67
2	D	232	ASN	CA-CB-CG	-5.75	106.85	112.60
2	B	241	GLY	CA-C-N	5.73	125.71	120.21
2	B	241	GLY	C-N-CA	5.73	125.71	120.21
1	A	612	THR	N-CA-C	5.72	119.52	112.54
1	C	339	ILE	N-CA-CB	5.71	122.09	110.78
1	E	255	THR	N-CA-C	5.71	119.56	112.59
1	C	543	MET	N-CA-C	5.71	118.87	109.85
1	E	26	PHE	CA-CB-CG	-5.71	108.09	113.80
1	G	557	THR	CA-C-O	5.70	125.17	118.90
1	C	793	ALA	N-CA-C	-5.68	102.07	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	PHE	CA-CB-CG	-5.67	108.13	113.80
2	H	138	PRO	N-CA-CB	5.66	108.29	103.19
1	E	258	ASP	CA-CB-CG	-5.66	106.94	112.60
2	F	201	ALA	N-CA-C	5.66	118.66	110.28
1	G	210	LEU	N-CA-C	-5.66	104.60	112.30
2	H	264	PRO	N-CA-CB	5.65	108.59	103.34
2	F	299	ASP	N-CA-C	-5.64	98.07	107.99
1	G	435	ARG	N-CA-C	5.63	118.14	111.33
1	A	880	THR	N-CA-CB	-5.63	103.52	111.00
2	B	174	SER	N-CA-C	5.62	117.95	110.53
1	G	3	LYS	N-CA-C	5.62	117.95	110.53
1	A	248	ILE	N-CA-C	-5.62	101.48	108.89
1	A	1001	ILE	N-CA-C	5.61	117.01	110.62
2	B	367	PHE	CA-CB-CG	-5.60	108.20	113.80
1	E	605	THR	N-CA-C	5.59	119.09	110.42
2	H	327	VAL	CB-CA-C	-5.59	104.54	111.08
1	E	885	PRO	O-C-N	5.58	123.77	121.15
2	H	239	SER	N-CA-C	5.58	117.52	110.33
1	A	159	ALA	N-CA-C	-5.57	105.21	111.28
1	C	707	GLU	CA-C-N	5.56	127.77	120.60
1	C	707	GLU	C-N-CA	5.56	127.77	120.60
1	G	23	ALA	N-CA-C	5.55	117.11	109.29
1	E	404	VAL	N-CA-C	-5.54	106.90	112.17
1	E	956	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	E	220	VAL	CB-CA-C	-5.52	102.95	110.90
1	C	237	PHE	N-CA-C	-5.52	104.67	111.40
2	F	53	VAL	N-CA-C	5.52	116.25	108.36
1	C	407	THR	N-CA-C	-5.51	105.34	113.61
1	E	715	ARG	CB-CA-C	-5.51	103.57	109.85
1	E	44	VAL	N-CA-C	5.51	116.03	107.99
1	E	39	GLU	CB-CA-C	-5.50	101.33	110.68
1	E	928	PHE	CA-CB-CG	-5.50	108.30	113.80
1	E	735	ARG	O-C-N	5.49	127.96	122.08
1	A	524	PRO	CB-CA-C	-5.49	103.02	110.60
2	D	4	SER	N-CA-C	5.49	117.96	110.55
1	E	27	ASP	N-CA-C	-5.49	105.38	111.36
1	E	1072	ILE	N-CA-C	5.49	116.14	108.89
1	G	885	PRO	N-CA-C	5.49	115.74	110.47
2	H	220	PRO	N-CA-CB	5.48	108.12	103.35
1	E	532	CYS	N-CA-C	5.48	119.75	112.30
1	E	371	ASN	N-CA-C	-5.47	101.06	109.76
1	A	825	LEU	N-CA-C	5.47	118.57	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	MET	N-CA-C	5.46	117.70	109.41
1	C	651	ALA	N-CA-C	5.45	117.65	111.11
1	A	660	PRO	N-CA-CB	5.44	106.35	102.65
1	E	811	GLN	OE1-CD-NE2	5.44	128.04	122.60
1	A	344	THR	CA-C-N	5.44	125.90	120.52
1	A	344	THR	C-N-CA	5.44	125.90	120.52
1	A	295	LEU	N-CA-C	5.43	117.58	108.73
1	G	559	ARG	CB-CA-C	-5.42	101.07	110.45
1	C	154	GLU	CB-CG-CD	5.42	121.82	112.60
1	C	1057	ASP	CA-CB-CG	5.42	118.02	112.60
1	G	983	GLU	N-CA-CB	5.42	119.54	110.32
2	D	234	ASP	N-CA-C	-5.42	106.17	112.89
1	G	339	ILE	N-CA-C	5.41	120.43	113.07
1	A	345	PRO	CB-CA-C	-5.40	102.75	110.75
1	E	738	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	1011	THR	N-CA-CB	5.39	118.75	110.61
2	H	232	ASN	CA-CB-CG	-5.39	107.20	112.60
1	E	625	ASP	CA-CB-CG	-5.39	107.21	112.60
1	G	370	ALA	N-CA-C	5.37	117.62	110.53
2	F	379	LYS	N-CA-C	-5.36	105.43	111.28
1	E	880	THR	N-CA-CB	-5.36	103.77	110.90
1	C	557	THR	CA-C-O	5.36	125.70	119.32
1	C	683	GLU	CA-C-N	5.36	127.72	120.38
1	C	683	GLU	C-N-CA	5.36	127.72	120.38
1	G	729	TYR	N-CA-C	5.36	119.94	113.41
1	G	1061	LYS	N-CA-C	5.36	118.17	108.69
1	G	558	ASP	N-CA-CB	-5.35	101.44	110.49
1	G	39	GLU	CB-CA-C	-5.35	99.78	110.42
1	A	18	ILE	CB-CA-C	-5.34	103.37	111.33
1	E	707	GLU	CA-C-N	5.34	127.29	120.56
1	E	707	GLU	C-N-CA	5.34	127.29	120.56
1	E	209	SER	N-CA-C	5.34	118.25	109.76
1	E	955	GLU	CB-CA-C	-5.34	101.83	110.79
2	F	374	ILE	CB-CA-C	-5.33	105.09	112.24
1	A	450	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	668	ALA	CA-C-O	5.33	126.20	120.55
1	C	154	GLU	N-CA-C	-5.33	104.72	111.11
1	C	883	VAL	CB-CA-C	-5.33	103.91	111.21
2	H	157	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	150	HIS	O-C-N	5.31	128.02	122.23
1	C	682	VAL	O-C-N	5.31	127.23	121.87
2	D	308	THR	N-CA-C	5.31	117.75	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	ARG	CB-CA-C	5.31	115.62	111.00
1	C	808	VAL	CB-CA-C	-5.31	104.98	112.14
1	G	983	GLU	CB-CG-CD	-5.30	103.58	112.60
2	F	138	PRO	N-CA-CB	5.30	107.89	103.17
2	F	353	HIS	CB-CA-C	-5.30	102.60	110.97
1	A	1068	MET	CB-CA-C	-5.30	102.34	110.81
1	G	830	PHE	CA-CB-CG	5.29	119.09	113.80
2	F	232	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	314	ALA	N-CA-C	5.29	116.73	111.07
1	E	885	PRO	CA-C-O	5.29	124.91	120.73
1	A	1005	ILE	CB-CA-C	-5.29	105.00	112.14
1	C	714	VAL	N-CA-C	5.29	115.24	107.15
1	G	557	THR	N-CA-C	-5.28	106.78	114.12
2	F	272	HIS	CA-CB-CG	5.28	119.08	113.80
1	C	885	PRO	N-CA-CB	5.25	108.17	103.08
2	H	356	ALA	CB-CA-C	-5.25	110.51	116.54
1	E	536	PHE	CA-CB-CG	-5.24	108.56	113.80
2	F	266	PHE	CA-C-N	-5.23	118.57	122.18
2	F	266	PHE	C-N-CA	-5.23	118.57	122.18
2	F	263	ILE	N-CA-C	5.23	114.07	108.95
1	A	557	THR	O-C-N	5.22	128.79	122.48
2	H	67	ASP	CA-CB-CG	5.21	117.81	112.60
1	E	87	LEU	CA-C-O	5.20	123.73	119.36
1	E	825	LEU	N-CA-C	5.20	117.57	110.55
2	F	320	THR	CB-CA-C	-5.20	101.93	110.72
1	E	88	PRO	CB-CA-C	-5.20	102.98	111.56
1	G	96	LEU	N-CA-CB	5.19	118.33	110.28
2	H	308	THR	N-CA-C	5.18	117.55	109.52
1	A	468	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	571	ARG	CD-NE-CZ	-5.18	117.15	124.40
1	G	150	HIS	CA-CB-CG	-5.17	108.62	113.80
2	B	124	GLU	CA-C-N	-5.17	114.00	122.54
2	B	124	GLU	C-N-CA	-5.17	114.00	122.54
1	A	682	VAL	N-CA-C	-5.17	105.46	110.42
1	A	555	PRO	N-CA-CB	5.16	108.24	103.39
2	F	359	GLY	CA-C-N	5.16	125.09	119.78
2	F	359	GLY	C-N-CA	5.16	125.09	119.78
1	A	210	LEU	N-CA-C	-5.15	105.29	112.30
1	A	793	ALA	N-CA-C	-5.15	103.59	110.55
1	C	558	ASP	N-CA-C	5.15	116.75	111.03
1	G	674	ASP	CA-C-N	5.15	127.90	120.38
1	G	674	ASP	C-N-CA	5.15	127.90	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	ARG	N-CA-C	-5.15	106.16	112.90
1	C	998	ARG	O-C-N	5.15	125.41	121.65
1	E	700	MET	N-CA-C	-5.15	105.32	111.03
1	E	82	ARG	CA-C-O	5.14	124.44	120.48
1	E	287	ALA	CA-C-N	-5.13	116.42	123.14
1	E	287	ALA	C-N-CA	-5.13	116.42	123.14
2	D	85	LEU	CA-C-O	5.13	123.67	119.36
2	D	362	ASP	N-CA-C	5.13	118.32	111.75
2	B	379	LYS	N-CA-C	-5.13	106.86	113.01
1	C	278	GLU	CB-CA-C	-5.13	100.77	109.38
1	C	560	GLU	N-CA-C	-5.13	101.41	109.25
1	C	111	PHE	N-CA-C	5.12	118.56	112.72
1	C	248	ILE	N-CA-C	-5.12	102.13	108.89
1	G	612	THR	N-CA-C	5.12	118.78	112.54
1	C	803	GLN	N-CA-C	-5.12	105.60	111.07
1	G	225	ASN	CA-CB-CG	-5.12	107.48	112.60
1	G	453	PHE	CA-CB-CG	-5.11	108.69	113.80
1	G	248	ILE	N-CA-C	-5.11	102.14	108.89
1	E	450	ASP	CA-CB-CG	5.11	117.70	112.60
1	G	880	THR	N-CA-CB	-5.10	104.21	111.00
1	C	27	ASP	CA-C-O	5.10	125.90	120.24
1	G	779	MET	CA-C-N	-5.10	115.68	122.72
1	G	779	MET	C-N-CA	-5.10	115.68	122.72
1	G	971	LEU	N-CA-C	5.10	118.05	109.95
1	E	993	LYS	N-CA-C	-5.09	104.15	110.41
2	H	360	PRO	N-CA-CB	5.08	107.84	103.31
1	C	420	ALA	N-CA-C	5.07	117.20	111.11
1	A	69	ILE	N-CA-C	5.07	111.63	106.21
1	C	27	ASP	N-CA-C	-5.06	105.46	111.69
1	E	1037	LYS	N-CA-C	5.06	118.72	112.24
2	H	326	ARG	N-CA-CB	5.05	118.65	110.41
1	C	716	PRO	N-CA-CB	5.05	108.56	103.00
2	B	353	HIS	CA-CB-CG	-5.05	108.75	113.80
2	F	74	GLN	N-CA-C	5.05	115.71	108.74
1	C	824	GLY	N-CA-C	-5.04	106.47	111.56
2	D	53	VAL	N-CA-C	5.03	115.93	108.23
1	E	345	PRO	CB-CA-C	-5.03	103.31	110.75
2	F	10	GLU	CB-CA-C	-5.02	102.78	110.81
1	G	543	MET	N-CA-C	5.02	117.49	109.81
1	E	716	PRO	N-CA-CB	5.02	108.52	103.00
1	A	801	LEU	N-CA-C	5.02	117.49	109.96
1	E	726	GLU	CB-CG-CD	5.02	121.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	998	ARG	N-CA-C	5.02	116.36	108.23
1	E	786	GLY	N-CA-C	-5.01	108.21	113.58
1	G	878	GLY	N-CA-C	-5.01	106.86	115.08
2	D	16	HIS	CA-C-N	-5.01	118.31	122.16
2	D	16	HIS	C-N-CA	-5.01	118.31	122.16
1	G	953	ASP	CA-CB-CG	5.00	117.60	112.60
1	A	34	CYS	CB-CA-C	-5.00	103.03	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	339	ILE	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8169	0	8201	254	0
1	C	8173	0	8207	265	0
1	E	8186	0	8220	209	0
1	G	8175	0	8210	292	0
2	B	2904	0	2867	95	0
2	D	2909	0	2869	98	0
2	F	2904	0	2867	88	0
2	H	2906	0	2868	129	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	8	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	6	0	0	2	0
5	B	2	0	0	0	0
5	C	5	0	0	2	0
5	D	2	0	0	0	0
5	E	5	0	0	2	0
5	F	2	0	0	0	0
5	G	5	0	0	3	0
5	H	2	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	1	0
7	G	54	0	24	2	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	3	0
8	G	9	0	11	0	0
9	A	9	0	20	2	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	0	0
10	A	869	0	0	27	0
10	B	213	0	0	3	0
10	C	784	0	0	16	0
10	D	275	0	0	6	0
10	E	864	0	0	23	0
10	F	235	0	0	2	0
10	G	743	0	0	26	0
10	H	193	0	0	6	0
All	All	48889	0	44529	1418	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 16.

All (1418) 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)
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.21	1.15
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.30	1.14
2:F:228:VAL:HA	2:F:231:MET:HE2	1.27	1.08
2:H:228:VAL:HA	2:H:231:MET:HE3	1.32	1.08
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.35	1.08
2:B:286:MET:HE2	2:B:315:ALA:HB2	1.14	1.08
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.35	1.05
1:G:1027[B]:ARG:HE	1:G:1031:ARG:HD3	1.17	1.05
1:E:559:ARG:HG3	1:E:559:ARG:HH11	1.19	1.02
1:A:472:LEU:HG	10:A:5510:HOH:O	1.59	1.01
2:B:228:VAL:HA	2:B:231:MET:HE2	1.42	1.01
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.26	1.00
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.44	0.99
1:C:814:GLN:HG3	1:C:818:PHE:HE2	1.30	0.96
2:D:78:GLN:HA	2:D:78:GLN:HE21	1.32	0.94
1:E:784:GLN:H	1:E:784:GLN:HE21	1.07	0.94
1:A:1:MET:HB2	1:A:224:LYS:HZ2	1.32	0.94
1:G:784:GLN:H	1:G:784:GLN:HE21	0.96	0.94
1:A:784:GLN:HE21	1:A:784:GLN:H	1.15	0.93
1:C:38:ARG:HG3	1:C:38:ARG:HH11	1.34	0.92
1:C:784:GLN:H	1:C:784:GLN:HE21	1.16	0.92
2:H:54:THR:HG21	2:H:118:LEU:HD23	1.51	0.92
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.49	0.92
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.50	0.92
1:A:713:VAL:HG23	1:A:755:PHE:HB2	1.53	0.91
2:B:286:MET:HE1	2:B:312:HIS:ND1	1.86	0.91
1:G:784:GLN:H	1:G:784:GLN:NE2	1.68	0.90
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.53	0.90
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.52	0.90
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.88	0.88
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.55	0.88
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.03	0.88
1:G:1001:ILE:HD12	1:G:1002:GLN:N	1.89	0.88
1:E:1:MET:H3	1:E:224:LYS:HE3	1.40	0.87
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.10	0.87
1:C:814:GLN:HG3	1:C:818:PHE:CE2	2.10	0.87
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.09	0.87
1:A:784:GLN:H	1:A:784:GLN:NE2	1.72	0.86
1:A:1:MET:HB2	1:A:224:LYS:NZ	1.90	0.86
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.04	0.86
2:B:286:MET:HE1	2:B:312:HIS:CE1	2.11	0.85
1:E:714:VAL:HG13	1:E:752:LEU:CD1	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:950:ARG:HD3	5:G:5087:CL:CL	2.14	0.85
1:G:663:GLY:CA	1:G:869:MET:HG2	2.07	0.85
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.40	0.85
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.56	0.85
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.93	0.84
1:G:1:MET:HB2	1:G:224:LYS:NZ	1.92	0.84
2:B:324:ASN:HD22	2:B:324:ASN:N	1.74	0.83
1:G:76:LYS:HE3	10:G:5232:HOH:O	1.78	0.83
1:E:784:GLN:H	1:E:784:GLN:NE2	1.77	0.83
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.59	0.83
1:G:1027[B]:ARG:NE	1:G:1031:ARG:HD3	1.93	0.82
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.61	0.82
2:B:286:MET:HE2	2:B:315:ALA:CB	2.06	0.82
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.60	0.82
1:G:682:VAL:HG13	1:G:687:LEU:HB2	1.61	0.82
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.61	0.81
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.63	0.81
2:H:50:ARG:HG3	2:H:158:LEU:HD11	1.61	0.81
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.62	0.81
1:G:901:PRO:HD2	5:G:5085:CL:CL	2.17	0.81
2:B:324:ASN:ND2	2:B:324:ASN:H	1.78	0.80
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.62	0.80
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.65	0.79
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.48	0.79
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.12	0.79
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.98	0.79
2:D:226:GLU:O	2:D:230:LYS:HG3	1.83	0.79
2:H:286:MET:HE1	2:H:312:HIS:CE1	2.19	0.78
2:B:324:ASN:HD22	2:B:324:ASN:H	1.31	0.78
2:H:324:ASN:O	2:H:342:ARG:HD2	1.84	0.78
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.64	0.78
1:G:873:SER:O	1:G:877:GLN:HG3	1.83	0.78
1:G:939:MET:HE2	1:G:1050:THR:CG2	2.13	0.78
1:C:784:GLN:H	1:C:784:GLN:NE2	1.82	0.78
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.66	0.78
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.45	0.78
1:E:684:ARG:HG3	1:E:684:ARG:HH11	1.49	0.78
1:G:726:GLU:HG3	1:G:727:ILE:N	1.99	0.77
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.65	0.77
1:G:563:MET:CE	1:G:635:PRO:HG3	2.12	0.77
2:B:269:CYG:N1	10:B:5022:HOH:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.66	0.77
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.46	0.77
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.65	0.77
1:G:967:GLN:HG3	1:G:1054:LEU:HD13	1.67	0.77
2:H:248:CYS:O	2:H:252:ILE:HG13	1.84	0.76
1:E:1:MET:N	1:E:224:LYS:HE3	2.00	0.76
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.12	0.76
1:G:472:LEU:O	1:G:476:VAL:HG23	1.85	0.76
2:B:226:GLU:O	2:B:230:LYS:HG3	1.85	0.75
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.21	0.75
2:H:322:PRO:HG2	2:H:324:ASN:HD21	1.49	0.75
2:H:346:PRO:HG3	10:H:3959:HOH:O	1.87	0.75
1:G:784:GLN:HE21	1:G:784:GLN:N	1.80	0.75
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.16	0.75
1:E:714:VAL:HG13	1:E:752:LEU:HD11	1.67	0.75
2:D:228:VAL:HA	2:D:231:MET:HE3	1.68	0.75
1:A:873:SER:O	1:A:877:GLN:HG3	1.86	0.75
2:D:133:ILE:HG22	2:D:138:PRO:HB3	1.69	0.74
1:A:726:GLU:HG3	1:A:727:ILE:H	1.51	0.74
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.21	0.74
1:A:726:GLU:HG3	1:A:727:ILE:N	2.02	0.74
2:B:152:GLY:O	2:B:156:MET:HE3	1.88	0.74
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.23	0.74
1:A:1001:ILE:HD12	1:A:1002:GLN:N	2.03	0.74
1:A:38:ARG:HG3	1:A:38:ARG:NH1	1.98	0.74
1:C:145:ARG:HH12	1:C:161:ASP:CG	1.95	0.74
1:C:1004:ARG:HB3	1:C:1009[A]:GLU:HG3	1.68	0.74
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.22	0.74
2:F:322:PRO:HB2	2:F:324:ASN:ND2	2.03	0.74
1:A:563:MET:CE	1:A:635:PRO:HG3	2.18	0.73
2:F:225:ALA:O	2:F:229:LEU:HG	1.88	0.73
1:G:482:THR:HB	10:G:5525:HOH:O	1.87	0.73
1:C:726:GLU:HG3	1:C:727:ILE:N	2.03	0.73
2:F:236:ILE:HB	2:F:265:VAL:HG22	1.70	0.73
1:A:734:LEU:HD12	1:A:734:LEU:O	1.87	0.73
1:C:773:VAL:HG23	1:C:818:PHE:CZ	2.24	0.73
1:C:780:GLU:HG3	1:C:801:LEU:HD11	1.71	0.73
1:E:912:ARG:HD2	10:E:5689:HOH:O	1.88	0.73
1:G:70:HIS:CE1	1:G:72:GLU:HG3	2.23	0.73
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.17	0.73
2:D:206:LEU:O	2:D:210:VAL:HG23	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.03	0.72
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.71	0.72
1:G:225:ASN:ND2	1:G:331:THR:HG21	2.05	0.72
1:G:663:GLY:HA3	1:G:869:MET:HG2	1.72	0.72
1:G:998:ARG:HA	1:G:999:PRO:C	2.13	0.72
2:H:34:THR:HA	2:H:56:THR:OG1	1.89	0.72
1:A:954:LYS:O	1:A:957:VAL:HG12	1.89	0.72
1:G:475:LYS:O	1:G:479:VAL:HG13	1.89	0.72
1:C:154:GLU:OE1	10:C:2077:HOH:O	2.06	0.72
2:D:78:GLN:HA	2:D:78:GLN:NE2	2.05	0.72
2:D:233:PRO:HG2	2:D:263:ILE:CD1	2.20	0.71
1:C:559:ARG:HG3	1:C:559:ARG:HH11	1.54	0.71
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.70	0.71
1:C:998:ARG:HG2	1:C:999:PRO:HA	1.71	0.71
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.21	0.71
1:G:64:THR:O	1:G:1065:VAL:HG23	1.91	0.71
1:G:698:ILE:HD12	1:G:698:ILE:H	1.56	0.71
2:B:228:VAL:HA	2:B:231:MET:CE	2.21	0.71
1:G:809:MET:O	1:G:813:VAL:HG23	1.90	0.71
1:E:1:MET:HB2	1:E:224:LYS:HZ2	1.54	0.71
1:A:1001:ILE:HD12	1:A:1002:GLN:H	1.57	0.70
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.27	0.70
1:G:954:LYS:O	1:G:957:VAL:HG12	1.92	0.70
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.19	0.70
1:E:224:LYS:HE2	1:E:329:GLY:O	1.91	0.70
1:E:726:GLU:HG3	1:E:727:ILE:N	2.07	0.70
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.72	0.70
1:C:648:LEU:HD13	1:C:845:ARG:HD2	1.73	0.70
1:G:490:ARG:HD3	10:G:5702:HOH:O	1.90	0.70
1:A:700:MET:O	1:A:704:LYS:HB2	1.92	0.70
1:E:714:VAL:HG13	1:E:752:LEU:HD12	1.73	0.70
1:G:733:ASP:HA	1:G:736:ARG:HH11	1.56	0.70
1:G:878:GLY:O	10:G:5645:HOH:O	2.09	0.70
2:H:186:LYS:O	2:H:189:GLU:HB2	1.92	0.70
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.22	0.69
2:F:6:LEU:HD13	2:F:16:HIS:CE1	2.27	0.69
1:G:2:PRO:HB2	10:G:5791:HOH:O	1.92	0.69
1:C:726:GLU:HG3	1:C:727:ILE:H	1.57	0.69
1:A:151:THR:OG1	1:A:154:GLU:HG3	1.93	0.69
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.75	0.69
1:C:991[A]:VAL:HG11	1:C:1004:ARG:HE	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1004:ARG:CB	1:C:1009[A]:GLU:HG3	2.23	0.69
1:A:675:ARG:CD	1:A:675:ARG:H	2.02	0.69
1:G:427:GLU:HG3	1:G:438:TYR:CE1	2.28	0.69
1:E:998:ARG:HA	1:E:999:PRO:C	2.18	0.68
1:C:648:LEU:CD1	1:C:845:ARG:HD2	2.24	0.68
1:G:344:THR:HB	1:G:345:PRO:HD2	1.75	0.68
2:D:222:GLN:H	2:D:222:GLN:HE21	1.42	0.68
1:E:684:ARG:HG3	1:E:684:ARG:NH1	2.07	0.68
1:E:955:GLU:HB2	10:E:5928:HOH:O	1.93	0.68
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.76	0.68
1:E:1001:ILE:HD12	1:E:1002:GLN:N	2.09	0.68
2:B:286:MET:CE	2:B:315:ALA:HB2	2.08	0.68
1:C:1009[B]:GLU:HG3	10:C:1999:HOH:O	1.93	0.68
2:B:186:LYS:O	2:B:189:GLU:HB2	1.94	0.67
1:G:828:VAL:HG22	1:G:842:VAL:HG13	1.76	0.67
2:B:71:GLU:O	2:B:203:ARG:HG3	1.93	0.67
1:C:509:ARG:HD3	10:C:1979:HOH:O	1.94	0.67
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.76	0.67
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.27	0.67
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.28	0.67
2:H:95:THR:HG21	10:H:3945:HOH:O	1.94	0.67
1:C:416:ASP:O	1:C:418:PRO:HD3	1.94	0.67
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.08	0.67
1:A:698:ILE:HD12	1:A:698:ILE:H	1.60	0.67
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.29	0.67
1:E:950:ARG:HD3	5:E:5062:CL:CL	2.32	0.67
1:G:548:GLU:HG2	2:H:114:ASP:CG	2.18	0.67
1:G:475:LYS:NZ	10:G:5514:HOH:O	2.27	0.67
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.76	0.67
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.76	0.67
1:E:417:ASP:OD1	1:E:423:LYS:NZ	2.27	0.67
1:C:973:ALA:O	1:C:991[B]:VAL:HG12	1.95	0.67
2:H:300:VAL:HG22	2:H:328:THR:O	1.95	0.67
2:H:322:PRO:HB2	2:H:324:ASN:ND2	2.10	0.67
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.06	0.67
2:D:152:GLY:O	2:D:156:MET:HE3	1.95	0.67
2:F:322:PRO:HG2	2:F:324:ASN:HD21	1.58	0.67
1:A:315:THR:O	1:A:531:THR:HG22	1.95	0.66
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.25	0.66
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.95	0.66
1:A:997:GLY:O	1:A:998:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.03	0.66
1:E:698:ILE:HG13	1:E:738:PHE:CD1	2.30	0.66
1:C:1004:ARG:CA	1:C:1009[A]:GLU:HG3	2.26	0.66
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.57	0.66
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.11	0.66
2:D:174:SER:O	2:D:182:PRO:HD3	1.96	0.66
1:A:471:ARG:HD2	10:A:5515:HOH:O	1.95	0.66
1:C:559:ARG:NH2	10:C:1994:HOH:O	2.28	0.66
2:D:228:VAL:O	2:D:231:MET:HG3	1.96	0.66
1:E:726:GLU:HG3	1:E:727:ILE:H	1.60	0.66
1:G:423:LYS:HB3	10:G:5480:HOH:O	1.95	0.66
2:H:50:ARG:HG3	2:H:158:LEU:CD1	2.25	0.66
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.76	0.66
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.78	0.66
1:C:975:HIS:O	1:C:979:ILE:HG12	1.96	0.65
1:C:1061:LYS:HG2	10:C:1883:HOH:O	1.96	0.65
1:E:734:LEU:HD12	1:E:734:LEU:O	1.96	0.65
1:G:682:VAL:CG1	1:G:687:LEU:HB2	2.26	0.65
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.77	0.65
2:H:232:ASN:N	2:H:233:PRO:HD3	2.10	0.65
1:C:865:ALA:O	1:C:869:MET:HG3	1.96	0.65
1:E:976:GLY:O	1:E:980:VAL:HG23	1.97	0.65
1:G:663:GLY:HA2	1:G:869:MET:HG2	1.79	0.65
1:G:224:LYS:NZ	10:G:5173:HOH:O	2.28	0.65
2:H:275:LEU:HD23	2:H:349:SER:OG	1.96	0.65
1:A:224:LYS:NZ	10:A:5169:HOH:O	2.29	0.65
1:A:814:GLN:NE2	10:A:5628:HOH:O	2.29	0.65
1:A:1001:ILE:O	1:A:1005:ILE:HG13	1.97	0.65
1:C:954:LYS:HG2	1:C:980:VAL:HG21	1.79	0.65
2:F:34:THR:HA	2:F:56:THR:OG1	1.97	0.65
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.78	0.65
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.78	0.65
1:G:701:ALA:O	1:G:705:ALA:N	2.29	0.65
1:C:780:GLU:HG3	1:C:801:LEU:CD1	2.27	0.65
1:A:38:ARG:NH2	10:A:5735:HOH:O	2.29	0.65
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.77	0.65
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.26	0.64
1:C:802:SER:OG	1:C:805:ILE:HB	1.96	0.64
1:C:734:LEU:O	1:C:734:LEU:HD12	1.96	0.64
1:E:728:VAL:CG1	1:E:733:ASP:HB3	2.27	0.64
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:SER:HB2	1:G:205:LEU:HD11	1.79	0.64
2:H:322:PRO:CG	2:H:324:ASN:HD21	2.10	0.64
2:D:233:PRO:HG2	2:D:263:ILE:HD13	1.79	0.64
1:G:698:ILE:HD12	1:G:698:ILE:N	2.12	0.64
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.30	0.64
1:C:509:ARG:NH1	1:C:512:GLU:OE1	2.30	0.64
1:C:954:LYS:O	1:C:957:VAL:HG12	1.98	0.64
2:F:195:VAL:HG21	2:F:231:MET:HE3	1.79	0.64
2:B:46:PRO:HA	2:B:76:HIS:CG	2.33	0.64
1:E:559:ARG:NH1	10:E:5798:HOH:O	2.29	0.64
1:E:897:PHE:HB3	10:E:5859:HOH:O	1.98	0.64
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.97	0.64
1:E:6:ASP:OD2	1:E:6:ASP:N	2.30	0.64
1:A:528:ARG:HG2	1:A:543:MET:HG2	1.78	0.64
1:A:189:GLU:HB3	10:A:5919:HOH:O	1.98	0.63
1:C:812:GLN:NE2	10:C:1654:HOH:O	2.31	0.63
2:F:324:ASN:O	2:F:342:ARG:HD2	1.98	0.63
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.32	0.63
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.33	0.63
2:H:249:ASP:OD2	2:H:249:ASP:N	2.31	0.63
1:C:1:MET:HB2	1:C:224:LYS:NZ	2.14	0.63
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.33	0.63
1:G:6:ASP:N	1:G:6:ASP:OD2	2.29	0.63
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.80	0.63
1:G:963:LYS:HE3	1:G:1052[B]:MET:HE3	1.81	0.63
1:G:734:LEU:HD12	1:G:734:LEU:O	1.97	0.63
1:A:698:ILE:O	1:A:702:VAL:HG23	1.99	0.63
1:E:998:ARG:CB	1:E:999:PRO:HA	2.27	0.63
1:G:318:PRO:HG3	1:G:610:TYR:OH	1.99	0.63
1:E:1027:ARG:HE	1:E:1031:ARG:HE	1.45	0.62
1:G:340:THR:O	1:G:343:ARG:NE	2.31	0.62
1:G:947:LEU:HD12	1:G:947:LEU:N	2.12	0.62
1:C:698:ILE:HD12	1:C:698:ILE:H	1.64	0.62
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.81	0.62
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.14	0.62
2:H:142:LEU:HD12	2:H:142:LEU:O	1.97	0.62
1:G:833:LYS:O	1:G:836:GLU:HB2	1.98	0.62
2:D:78:GLN:NE2	10:D:1778:HOH:O	2.31	0.62
1:A:632:ILE:HG13	1:A:633:GLU:N	2.14	0.62
1:E:1001:ILE:HD13	1:E:1029:ILE:HG13	1.81	0.62
1:G:994:VAL:HG22	1:G:1000:HIS:CG	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:698:ILE:O	1:E:702:VAL:HG23	2.00	0.62
1:G:680:HIS:O	1:G:683:GLU:HB2	1.99	0.62
1:G:963:LYS:HE2	10:G:5691:HOH:O	1.99	0.62
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.98	0.62
2:B:173:GLY:O	2:B:207:ARG:HG2	2.00	0.62
1:E:772[B]:MET:HE3	10:E:5821:HOH:O	1.99	0.62
1:G:224:LYS:HE2	1:G:329:GLY:O	1.98	0.62
1:C:519[A]:GLN:NE2	10:C:1959:HOH:O	2.33	0.62
1:C:675:ARG:H	1:C:675:ARG:CD	2.09	0.62
1:E:1021:ARG:HH11	1:E:1021:ARG:CG	2.13	0.62
1:G:1017:THR:HG22	1:G:1018:SER:N	2.14	0.62
2:H:363:ALA:C	2:H:365:PRO:HD2	2.24	0.62
1:A:266:ASN:ND2	10:A:5382:HOH:O	2.30	0.61
1:G:343:ARG:HG3	1:G:344:THR:HG23	1.82	0.61
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.81	0.61
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.30	0.61
1:C:677:ARG:O	1:C:680:HIS:HB2	2.00	0.61
1:C:713:VAL:HG23	1:C:755:PHE:HB2	1.82	0.61
1:G:1021:ARG:CG	1:G:1021:ARG:HH11	2.14	0.61
1:C:991[A]:VAL:HG11	1:C:1004:ARG:NE	2.15	0.61
1:E:43:ARG:NH1	10:E:5867:HOH:O	2.24	0.61
2:F:300:VAL:HG22	2:F:328:THR:O	2.01	0.61
2:H:78:GLN:NE2	10:H:3934:HOH:O	2.29	0.61
1:G:939:MET:HE2	1:G:1050:THR:HG22	1.81	0.61
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.81	0.61
2:H:71:GLU:O	2:H:203:ARG:HG3	2.00	0.61
1:E:559:ARG:HG3	1:E:559:ARG:NH1	1.99	0.61
1:E:967:GLN:HG3	1:E:1054:LEU:HD13	1.82	0.61
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.65	0.61
2:H:168:TYR:CE1	2:H:218:ILE:HB	2.36	0.61
2:D:46:PRO:HA	2:D:76:HIS:CG	2.35	0.61
1:A:780:GLU:OE2	1:A:798:ALA:HB1	2.00	0.61
1:E:669:ILE:O	1:E:673:GLU:HG2	2.01	0.61
1:E:873:SER:O	1:E:877:GLN:HG3	2.01	0.61
2:H:322:PRO:HG2	2:H:324:ASN:ND2	2.15	0.61
1:A:344:THR:HB	1:A:345:PRO:HD2	1.82	0.61
1:C:698:ILE:HD12	1:C:698:ILE:N	2.16	0.61
1:C:998:ARG:CG	1:C:999:PRO:HA	2.30	0.61
1:A:891:LYS:NZ	10:A:5624:HOH:O	2.34	0.60
2:B:185:LYS:HD2	2:B:190:LEU:HD21	1.82	0.60
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASP:OD2	1:C:6:ASP:N	2.30	0.60
1:E:1061[A]:LYS:NZ	10:E:5637:HOH:O	2.29	0.60
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.46	0.60
1:G:637:GLY:HA2	1:G:660:PRO:HB2	1.83	0.60
1:G:671:ARG:NH2	1:G:819:GLU:O	2.34	0.60
1:G:1001:ILE:HD12	1:G:1002:GLN:HB2	1.82	0.60
1:A:698:ILE:H	1:A:698:ILE:CD1	2.14	0.60
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.31	0.60
1:C:991[A]:VAL:CG1	1:C:1004:ARG:HE	2.14	0.60
1:G:321:LYS:NZ	1:G:611:ASP:OD1	2.31	0.60
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.84	0.60
1:G:667:ASP:OD2	1:G:677:ARG:NH2	2.34	0.60
1:G:1021:ARG:HH11	1:G:1021:ARG:HG2	1.67	0.60
2:D:334:ASP:HB3	10:D:1431:HOH:O	2.00	0.60
1:G:964:LEU:O	1:G:969:PHE:HB2	2.02	0.60
1:A:1004:ARG:O	1:A:1009[B]:GLU:HG2	2.01	0.60
1:C:145:ARG:NH1	1:C:161:ASP:OD1	2.33	0.60
1:E:1061[B]:LYS:NZ	10:E:5860:HOH:O	2.30	0.60
1:A:425:ARG:HD3	10:A:5482:HOH:O	2.01	0.60
1:A:950:ARG:HD3	5:A:5015:CL:CL	2.39	0.60
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.23	0.60
1:C:892:GLU:OE1	8:C:5033:ORN:NE	2.34	0.60
1:E:4:ARG:HA	10:E:5150:HOH:O	2.02	0.60
1:E:1021:ARG:HH11	1:E:1021:ARG:HG2	1.65	0.60
2:F:212:ARG:HG3	2:F:212:ARG:HH11	1.67	0.60
1:A:1021:ARG:HG3	1:A:1021:ARG:HH11	1.67	0.60
1:C:1061:LYS:HE2	10:C:1737:HOH:O	2.02	0.60
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.37	0.60
1:G:956:ARG:HB3	1:G:1044:LEU:HD21	1.84	0.60
2:H:322:PRO:HD2	2:H:325:LEU:HD12	1.84	0.60
2:B:286:MET:HE3	2:B:314:PHE:C	2.26	0.60
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.84	0.60
1:E:930:LYS:HE3	10:E:5202:HOH:O	2.02	0.60
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.67	0.59
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.83	0.59
1:C:997:GLY:O	1:C:998:ARG:HG3	2.02	0.59
1:G:704:LYS:O	1:G:708:ILE:HD12	2.01	0.59
2:B:139:ASP:OD2	2:B:142:LEU:HB2	2.01	0.59
2:D:189:GLU:OE2	10:D:2123:HOH:O	2.17	0.59
1:A:278:GLU:HG2	10:A:5759:HOH:O	2.02	0.59
2:B:299:ASP:OD1	2:B:302:LYS:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:187:GLU:OE2	2:F:215:ARG:NH1	2.36	0.59
1:E:703:GLU:O	1:E:706:LYS:HB2	2.02	0.59
2:B:251:ALA:O	2:B:255:ILE:HD12	2.01	0.59
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.37	0.59
1:G:65:TYR:OH	1:G:80:LYS:HE2	2.03	0.59
2:F:232:ASN:N	2:F:233:PRO:HD3	2.17	0.59
2:D:306:MET:HE1	2:D:366:LEU:HD11	1.84	0.59
1:G:946:LEU:C	1:G:947:LEU:HD12	2.28	0.59
1:A:698:ILE:HD12	1:A:698:ILE:N	2.17	0.59
1:C:561:LYS:NZ	1:C:633:GLU:O	2.30	0.58
1:C:671:ARG:NH2	1:C:819:GLU:O	2.36	0.58
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.32	0.58
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.03	0.58
1:E:926:GLU:HB2	10:E:5838:HOH:O	2.02	0.58
1:C:689:GLN:HG2	1:C:690:PRO:HD2	1.85	0.58
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.68	0.58
10:G:5445:HOH:O	2:H:87:LEU:HD13	2.04	0.58
1:A:28:TYR:O	1:A:32:GLN:HG3	2.04	0.58
1:C:883:VAL:O	1:C:884:ILE:HD13	2.04	0.58
1:C:906:LEU:O	1:C:912:ARG:NH2	2.29	0.58
1:E:473:GLU:HG2	1:E:505:LEU:HD11	1.85	0.58
2:B:371:ILE:HG13	10:B:5233:HOH:O	2.04	0.58
1:A:906:LEU:O	1:A:912:ARG:NH2	2.32	0.58
1:A:973:ALA:C	1:A:991:VAL:HG12	2.29	0.58
1:A:560:GLU:HB3	1:A:636:LYS:HD2	1.85	0.58
1:A:998:ARG:HA	1:A:999:PRO:C	2.25	0.57
1:C:947:LEU:HG	1:C:1014:ILE:HG21	1.84	0.57
1:G:734:LEU:HD12	1:G:734:LEU:C	2.29	0.57
2:H:364:ALA:N	2:H:365:PRO:HD2	2.18	0.57
1:E:645[B]:GLN:HG3	1:E:649:LYS:HE3	1.86	0.57
1:A:106:GLY:HA2	10:A:5910:HOH:O	2.04	0.57
1:C:325:LYS:O	1:C:330:TYR:HB2	2.04	0.57
1:E:282:SER:OG	1:E:302:PRO:HA	2.04	0.57
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.19	0.57
2:F:306:MET:HB3	2:F:362:ASP:HB3	1.85	0.57
1:G:267:ALA:O	1:G:271:VAL:HG23	2.04	0.57
1:G:713:VAL:HG23	1:G:755:PHE:HB2	1.86	0.57
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.85	0.57
1:C:11:LEU:HA	1:C:45:ILE:O	2.04	0.57
1:C:375:THR:HG23	1:C:377:GLN:H	1.68	0.57
1:C:563:MET:CE	1:C:635:PRO:HG3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:998:ARG:HB3	1:E:999:PRO:HA	1.87	0.57
1:A:325:LYS:O	1:A:330:TYR:HB2	2.05	0.57
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.05	0.57
1:E:734:LEU:HD12	1:E:734:LEU:C	2.30	0.57
1:A:784:GLN:HE21	1:A:784:GLN:N	1.95	0.57
2:F:8:VAL:HG22	2:F:14:GLN:HG2	1.86	0.57
1:A:150:HIS:N	1:A:154:GLU:OE2	2.37	0.57
1:A:412:LYS:NZ	10:A:5488:HOH:O	2.37	0.57
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.86	0.56
1:A:813:VAL:HG22	1:A:828:VAL:HG21	1.86	0.56
1:C:726:GLU:OE1	1:C:1020:ARG:HD3	2.04	0.56
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.39	0.56
2:H:302:LYS:HD2	10:H:3986:HOH:O	2.03	0.56
1:A:193:ALA:HA	10:A:5203:HOH:O	2.05	0.56
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.87	0.56
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.51	0.56
1:C:698:ILE:H	1:C:698:ILE:CD1	2.19	0.56
2:D:322:PRO:HD2	2:D:325:LEU:HD12	1.88	0.56
1:E:336:MET:HB3	1:E:342:GLY:HA2	1.87	0.56
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.88	0.56
1:G:427:GLU:HG3	1:G:438:TYR:CD1	2.40	0.56
1:A:166:CYS:C	1:A:167:ILE:HD12	2.31	0.56
1:E:809:MET:O	1:E:813:VAL:HG23	2.05	0.56
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.36	0.56
2:F:324:ASN:N	2:F:324:ASN:HD22	2.03	0.56
1:G:675:ARG:CD	1:G:675:ARG:H	2.19	0.56
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.70	0.56
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.36	0.56
1:C:426:ARG:HD3	1:C:426:ARG:C	2.30	0.56
1:C:710:TYR:HB3	1:C:729:TYR:O	2.05	0.56
1:E:646:THR:HB	1:E:647:PRO:HD3	1.87	0.56
1:E:669:ILE:HA	1:E:844:PRO:HG2	1.87	0.56
1:G:526:TYR:O	1:G:552:GLU:HB2	2.04	0.56
1:C:1:MET:HB2	1:C:224:LYS:HZ2	1.69	0.56
2:H:46:PRO:HA	2:H:76:HIS:CG	2.41	0.56
1:A:559:ARG:HG3	1:A:559:ARG:HH11	1.71	0.56
1:C:559:ARG:HG3	1:C:559:ARG:NH1	2.18	0.56
1:C:905:PRO:HB2	1:C:1040:TYR:OH	2.05	0.56
1:G:294:ARG:HD2	5:G:5084:CL:CL	2.43	0.56
1:G:340:THR:O	1:G:343:ARG:HG2	2.06	0.56
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1004:ARG:HA	1:C:1009[A]:GLU:HG3	1.88	0.56
1:A:973:ALA:O	1:A:991:VAL:HG12	2.06	0.55
2:D:26:ALA:O	2:D:131:CYS:HA	2.06	0.55
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.41	0.55
1:A:426:ARG:HD3	1:A:426:ARG:C	2.31	0.55
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.30	0.55
1:C:715:ARG:HB2	1:C:751:LEU:HB2	1.87	0.55
1:E:46:LEU:C	1:E:46:LEU:HD22	2.32	0.55
1:E:549:GLU:HG2	10:E:5908:HOH:O	2.06	0.55
2:F:171:THR:HG22	2:F:215:ARG:HB2	1.87	0.55
1:G:259:LYS:HD3	2:H:175:TRP:CE3	2.41	0.55
1:C:420:ALA:HA	1:C:423:LYS:HD2	1.87	0.55
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.07	0.55
1:E:784:GLN:HE21	1:E:784:GLN:N	1.91	0.55
2:D:139:ASP:OD2	2:D:142:LEU:HB2	2.05	0.55
1:E:426:ARG:C	1:E:426:ARG:HD3	2.31	0.55
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.87	0.55
2:F:298:LYS:O	2:F:329:HIS:HA	2.07	0.55
1:G:726:GLU:HG3	1:G:727:ILE:H	1.71	0.55
1:G:548:GLU:HG2	2:H:114:ASP:OD1	2.07	0.55
2:B:367:PHE:O	2:B:370:PHE:HB3	2.07	0.55
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.07	0.55
1:C:976:GLY:O	1:C:979:ILE:HB	2.07	0.55
2:D:178:THR:HB	10:D:1823:HOH:O	2.07	0.55
2:D:307:ILE:HG22	2:D:360:PRO:HG2	1.88	0.55
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.53	0.55
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.42	0.54
2:B:277:LEU:HD23	2:B:281:ALA:O	2.07	0.54
1:C:634:LYS:HG3	10:C:2090:HOH:O	2.07	0.54
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.88	0.54
2:D:367:PHE:O	2:D:370:PHE:HB3	2.06	0.54
1:C:751:LEU:C	1:C:752:LEU:HD12	2.32	0.54
1:E:440:ALA:O	1:E:444:ARG:HG3	2.07	0.54
1:G:308:SER:HB3	10:G:5356:HOH:O	2.06	0.54
1:G:840:ILE:O	1:G:841:GLU:HB3	2.07	0.54
2:H:32:PHE:O	2:H:291:HIS:HB2	2.06	0.54
1:E:59:GLU:CG	1:E:60:MET:HE2	2.38	0.54
1:E:166:CYS:C	1:E:167:ILE:HD12	2.32	0.54
2:H:323:ALA:C	2:H:325:LEU:H	2.16	0.54
1:A:101:GLU:OE2	1:A:101:GLU:HA	2.08	0.54
1:C:873:SER:O	1:C:877:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:ASN:HA	2:D:291:HIS:O	2.07	0.54
1:G:906:LEU:O	1:G:912:ARG:NH2	2.29	0.54
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.22	0.54
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.89	0.54
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.89	0.54
1:A:976:GLY:O	1:A:980:VAL:HG23	2.08	0.54
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.89	0.54
1:A:675:ARG:H	1:A:675:ARG:HD3	1.69	0.54
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.72	0.54
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.89	0.54
1:G:734:LEU:O	1:G:737:TYR:HB3	2.08	0.54
2:H:46:PRO:HG2	2:H:200:GLY:O	2.08	0.54
1:A:411:PRO:HG3	10:A:5493:HOH:O	2.07	0.54
1:A:515:LYS:HG3	10:A:5845:HOH:O	2.07	0.54
1:A:734:LEU:HD12	1:A:734:LEU:C	2.30	0.54
2:F:379:LYS:HZ3	2:F:379:LYS:HB2	1.72	0.54
2:D:204:ASN:ND2	2:D:355:GLU:O	2.35	0.54
1:G:698:ILE:H	1:G:698:ILE:CD1	2.19	0.54
1:G:940:LYS:HG3	1:G:1011:THR:HB	1.90	0.54
1:A:956:ARG:HA	10:A:5872:HOH:O	2.08	0.54
1:C:994:VAL:HG22	1:C:1000:HIS:CG	2.43	0.54
1:G:679:GLN:HG2	1:G:683:GLU:OE2	2.08	0.54
1:G:845:ARG:NH1	10:G:5598:HOH:O	2.41	0.54
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.73	0.54
1:C:257:THR:HG23	2:D:91:ASN:ND2	2.23	0.53
1:A:6:ASP:OD2	1:A:6:ASP:N	2.37	0.53
1:C:954:LYS:CG	1:C:980:VAL:HG21	2.38	0.53
1:E:648:LEU:CD2	1:E:845:ARG:HD3	2.38	0.53
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.38	0.53
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.89	0.53
1:C:708:ILE:CG2	1:C:712:LEU:HD11	2.38	0.53
1:G:1:MET:HB2	1:G:224:LYS:HZ1	1.73	0.53
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.44	0.53
2:B:34:THR:HA	2:B:56:THR:OG1	2.08	0.53
1:G:420:ALA:HA	1:G:423:LYS:HD2	1.91	0.53
1:C:46:LEU:C	1:C:46:LEU:HD22	2.34	0.53
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.22	0.53
1:E:1017:THR:HG22	1:E:1018:SER:N	2.24	0.53
2:H:324:ASN:N	2:H:324:ASN:HD22	2.05	0.53
1:C:805:ILE:HD13	1:C:837:VAL:CG2	2.39	0.53
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:550:GLU:CD	2:H:120:ARG:HH21	2.16	0.53
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.91	0.53
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.91	0.53
2:H:374:ILE:O	2:H:377:TYR:HB3	2.09	0.53
1:A:10:ILE:HD13	1:A:37:LEU:HD13	1.89	0.53
1:C:809:MET:O	1:C:813:VAL:HG23	2.09	0.53
1:E:953:ASP:O	1:E:955:GLU:N	2.42	0.53
1:A:695:VAL:CG2	1:A:752:LEU:HD22	2.39	0.53
1:A:654:LEU:O	1:A:659:VAL:HG23	2.08	0.52
1:C:82:ARG:HD3	10:C:1225:HOH:O	2.08	0.52
1:C:512:GLU:OE1	1:C:515:LYS:NZ	2.40	0.52
1:E:675:ARG:CD	1:E:675:ARG:H	2.21	0.52
1:E:730:ASP:O	1:E:733:ASP:HB2	2.08	0.52
1:G:864:VAL:O	1:G:868:VAL:HG23	2.09	0.52
2:D:185:LYS:HD2	2:D:190:LEU:HD21	1.91	0.52
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.09	0.52
2:H:350:PHE:HB2	2:H:366:LEU:CD2	2.39	0.52
2:H:132:ILE:HG22	2:H:133:ILE:N	2.25	0.52
2:B:306:MET:HB3	2:B:362:ASP:HB3	1.91	0.52
2:F:78:GLN:NE2	10:F:2837:HOH:O	2.43	0.52
1:C:130:ARG:HB2	1:C:148:ILE:HD12	1.90	0.52
1:C:1068:MET:O	1:C:1071:GLN:HB2	2.09	0.52
1:G:485:ASN:HB2	10:G:5526:HOH:O	2.08	0.52
1:G:712:LEU:HD23	1:G:752:LEU:HG	1.92	0.52
1:A:948:SER:O	1:A:1015:ASN:HA	2.09	0.52
2:B:120:ARG:HD2	10:B:5060:HOH:O	2.09	0.52
1:E:153:GLU:HB2	10:E:5278:HOH:O	2.09	0.52
1:E:757:ASP:O	1:E:833:LYS:NZ	2.30	0.52
1:G:167:ILE:N	1:G:167:ILE:HD12	2.25	0.52
1:G:714:VAL:HG13	1:G:752:LEU:HD12	1.92	0.52
1:G:954:LYS:O	1:G:980:VAL:HG11	2.10	0.52
1:G:1001:ILE:HD12	1:G:1002:GLN:CA	2.40	0.52
2:H:82:ILE:O	2:H:111:ALA:HA	2.10	0.52
2:D:279:SER:O	2:D:322:PRO:HG3	2.09	0.52
1:A:998:ARG:HG2	1:A:999:PRO:HA	1.92	0.52
1:E:1004:ARG:HD3	1:E:1009[B]:GLU:OE2	2.08	0.52
1:A:128:ASP:CG	1:A:131:ARG:HG3	2.35	0.52
2:B:350:PHE:HB2	2:B:366:LEU:HD23	1.92	0.52
2:D:199:PHE:O	2:D:241:GLY:HA3	2.10	0.52
1:G:29:SER:HB3	1:G:304:VAL:HG21	1.92	0.52
1:G:733:ASP:O	1:G:736:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:355:GLU:OE2	2:H:355:GLU:N	2.34	0.52
1:A:912:ARG:NH1	10:A:5099:HOH:O	2.42	0.52
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.40	0.52
1:G:185:ARG:O	1:G:188:PHE:HB3	2.10	0.52
1:G:344:THR:HB	1:G:345:PRO:CD	2.40	0.52
2:H:54:THR:HG21	2:H:118:LEU:CD2	2.31	0.52
2:H:218:ILE:N	2:H:218:ILE:HD13	2.25	0.52
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.45	0.51
1:C:686:LYS:O	1:C:687:LEU:HD23	2.10	0.51
1:C:734:LEU:HD12	1:C:734:LEU:C	2.35	0.51
2:D:176:THR:O	2:D:180:GLY:N	2.34	0.51
1:E:448:SER:O	1:E:452:VAL:HG23	2.10	0.51
1:E:698:ILE:O	1:E:701:ALA:HB3	2.09	0.51
2:F:185:LYS:HD2	2:F:190:LEU:HD21	1.92	0.51
1:G:525:VAL:HG22	1:G:548:GLU:H	1.74	0.51
2:H:251:ALA:O	2:H:255:ILE:HG13	2.10	0.51
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.40	0.51
1:A:272:LEU:HD11	1:A:282:SER:HB2	1.92	0.51
2:B:218:ILE:HD13	2:B:218:ILE:N	2.25	0.51
1:C:964:LEU:O	1:C:969:PHE:HB2	2.10	0.51
1:E:146:SER:HB2	1:E:205:LEU:HD11	1.92	0.51
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.45	0.51
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.28	0.51
1:A:339:ILE:HD11	1:A:531:THR:HG23	1.92	0.51
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.29	0.51
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.74	0.51
1:C:336:MET:HG3	10:C:1423:HOH:O	2.10	0.51
2:D:6:LEU:HD13	2:D:16:HIS:CE1	2.45	0.51
2:F:195:VAL:HG21	2:F:231:MET:CE	2.40	0.51
1:G:17:PRO:HG3	1:G:917:VAL:CG1	2.40	0.51
1:G:36:ALA:HB1	1:G:325:LYS:HE3	1.91	0.51
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.25	0.51
1:E:509:ARG:HH22	1:E:515:LYS:HZ3	1.56	0.51
1:E:997:GLY:O	1:E:998:ARG:HG3	2.10	0.51
1:A:88:PRO:HB3	1:A:99:ALA:HB2	1.91	0.51
2:D:2:ILE:HD12	2:D:3:LYS:N	2.25	0.51
1:G:769:ASP:OD2	1:G:769:ASP:N	2.39	0.51
1:A:35:LYS:O	1:A:39:GLU:HG3	2.10	0.51
1:A:417:ASP:HB3	1:A:420:ALA:HB2	1.92	0.51
1:A:548:GLU:OE1	2:B:114:ASP:HA	2.11	0.51
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:698:ILE:HG23	1:E:738:PHE:CD2	2.45	0.51
1:C:1036:TYR:C	1:C:1037:LYS:HG2	2.35	0.51
2:D:2:ILE:HD12	2:D:3:LYS:H	1.75	0.51
1:E:509:ARG:NH2	1:E:515:LYS:NZ	2.59	0.51
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.57	0.51
2:F:212:ARG:HH11	2:F:212:ARG:CG	2.23	0.51
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.26	0.51
2:H:153:LEU:HA	2:H:156:MET:HE3	1.93	0.51
1:A:563:MET:HB3	1:A:638:VAL:HG13	1.93	0.51
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.15	0.51
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.41	0.51
1:C:948:SER:O	1:C:1015:ASN:HA	2.10	0.51
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.46	0.51
2:F:272:HIS:HA	2:F:349:SER:CB	2.41	0.51
2:H:279:SER:O	2:H:322:PRO:HG3	2.11	0.51
1:A:103:GLU:HB3	10:A:5725:HOH:O	2.11	0.51
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.37	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.92	0.51
1:C:992:ASN:ND2	1:C:996:GLU:HB3	2.25	0.51
1:C:998:ARG:CB	1:C:999:PRO:HA	2.41	0.51
2:F:324:ASN:HD22	2:F:324:ASN:H	1.57	0.51
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.93	0.51
1:G:29:SER:CB	1:G:304:VAL:HG21	2.41	0.51
2:H:81:VAL:CG1	2:H:113:ILE:HD11	2.41	0.51
2:H:324:ASN:HA	2:H:343:THR:OG1	2.10	0.51
1:E:1027:ARG:HE	1:E:1031:ARG:NE	2.09	0.51
1:A:992:ASN:HB2	1:A:999:PRO:O	2.12	0.50
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.38	0.50
1:C:78:ILE:O	1:C:82:ARG:N	2.35	0.50
2:F:272:HIS:HA	2:F:349:SER:HB2	1.93	0.50
2:H:195:VAL:O	2:H:237:PHE:N	2.30	0.50
2:H:222:GLN:H	2:H:222:GLN:HE21	1.58	0.50
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.45	0.50
2:F:45:ASP:HB3	2:F:48:TYR:HD2	1.75	0.50
1:A:141:LEU:HB3	1:A:297:VAL:HG21	1.92	0.50
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.92	0.50
1:C:714:VAL:HG21	1:C:728:VAL:HG21	1.93	0.50
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.26	0.50
1:G:730:ASP:H	1:G:733:ASP:HB2	1.76	0.50
1:A:860:PRO:O	1:A:864:VAL:HG23	2.11	0.50
1:A:964:LEU:O	1:A:969:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.42	0.50
1:G:1019:GLY:O	1:G:1023:ILE:HG13	2.11	0.50
2:H:353:HIS:HB3	2:H:355:GLU:CD	2.37	0.50
1:C:224:LYS:HE2	1:C:329:GLY:O	2.09	0.50
1:C:637:GLY:HA2	1:C:660:PRO:O	2.10	0.50
2:D:118:LEU:O	2:D:118:LEU:HD12	2.12	0.50
1:G:735:ARG:O	1:G:738:PHE:HB2	2.12	0.50
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.93	0.50
1:E:907:LEU:HD11	8:E:5056:ORN:HD3	1.93	0.50
2:F:354:PRO:HB3	2:F:363:ALA:O	2.11	0.50
1:A:941:LYS:NZ	1:A:1056:ALA:O	2.30	0.50
2:D:186:LYS:H	2:D:189:GLU:CD	2.20	0.50
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.30	0.50
2:F:322:PRO:CG	2:F:324:ASN:HD21	2.24	0.50
1:A:412:LYS:HD2	10:A:5822:HOH:O	2.10	0.50
1:C:796:LEU:HD23	1:C:796:LEU:C	2.37	0.50
1:G:802:SER:OG	1:G:805:ILE:HB	2.12	0.50
1:C:186:GLU:HA	10:C:1915:HOH:O	2.12	0.50
1:E:785:ALA:HB1	7:E:5052:ADP:N3	2.27	0.50
2:F:369:HIS:O	2:F:373:LEU:HG	2.12	0.50
2:H:199:PHE:O	2:H:241:GLY:HA3	2.11	0.50
2:B:45:ASP:O	2:B:76:HIS:HB2	2.11	0.49
2:B:290:HIS:NE2	2:B:334:ASP:OD1	2.40	0.49
1:E:103:GLU:HG3	1:E:104:ARG:N	2.24	0.49
1:E:702:VAL:HG11	1:E:735:ARG:NH2	2.27	0.49
2:H:208:MET:SD	2:H:355:GLU:HA	2.52	0.49
1:A:1:MET:N	1:A:224:LYS:HE3	2.27	0.49
1:A:79:GLU:HA	1:A:111:PHE:CE2	2.47	0.49
2:B:33:ASN:HB3	2:B:55:LEU:HD23	1.94	0.49
1:C:383:GLU:OE2	1:C:604:GLU:OE1	2.30	0.49
2:D:63:VAL:O	2:D:94:ASN:HB2	2.12	0.49
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.47	0.49
2:F:257:LYS:O	2:F:260:GLU:HB2	2.11	0.49
2:H:123:ARG:HA	2:H:288:PHE:CD2	2.48	0.49
1:A:414:SER:OG	1:A:416:ASP:OD2	2.29	0.49
1:C:690:PRO:HD2	10:C:1875:HOH:O	2.12	0.49
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.48	0.49
2:F:201:ALA:HB2	2:F:239:SER:CB	2.43	0.49
2:B:27:VAL:O	2:B:78:GLN:HG2	2.12	0.49
2:B:185:LYS:CD	2:B:190:LEU:HD21	2.42	0.49
1:E:941:LYS:HE2	10:E:5839:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ARG:N	1:G:83:PRO:HD3	2.28	0.49
1:G:349:GLU:O	2:H:294:ASN:HB2	2.13	0.49
2:H:286:MET:HE2	2:H:315:ALA:HB2	1.94	0.49
1:A:423:LYS:NZ	10:A:5472:HOH:O	2.35	0.49
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.25	0.49
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.42	0.49
1:C:78:ILE:HG23	1:C:83:PRO:HD2	1.93	0.49
1:G:891:LYS:NZ	10:G:5618:HOH:O	2.46	0.49
2:F:75:VAL:HG11	2:F:107:ILE:HG13	1.94	0.49
1:G:103:GLU:HG3	1:G:104:ARG:N	2.26	0.49
1:E:509:ARG:HH22	1:E:515:LYS:NZ	2.11	0.49
1:G:1001:ILE:O	1:G:1005:ILE:HG13	2.12	0.49
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.24	0.49
1:A:164:PHE:HA	1:A:165:PRO:C	2.38	0.49
1:A:220:VAL:O	1:A:281:GLY:HA2	2.12	0.49
1:C:1064:SER:O	1:C:1068:MET:HG3	2.12	0.49
1:G:1030:ARG:HH11	1:G:1030:ARG:HG3	1.78	0.49
2:H:6:LEU:HD12	2:H:7:LEU:N	2.28	0.49
1:A:713:VAL:HG22	1:A:727:ILE:HG12	1.95	0.49
2:B:344:ASP:OD2	2:B:344:ASP:N	2.38	0.49
2:D:201:ALA:HB2	2:D:239:SER:CB	2.43	0.49
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.43	0.49
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.12	0.49
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.94	0.49
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.95	0.49
8:E:5056:ORN:HB3	10:E:5079:HOH:O	2.11	0.49
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.13	0.49
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.95	0.48
1:E:78:ILE:HG23	1:E:83:PRO:HD2	1.95	0.48
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.76	0.48
1:A:689:GLN:HG2	1:A:690:PRO:HD2	1.95	0.48
1:C:640:VAL:HG21	1:C:651:ALA:HB2	1.94	0.48
1:E:659:VAL:CG1	1:E:660:PRO:HD2	2.43	0.48
2:B:234:ASP:CG	2:B:378:ARG:HH11	2.20	0.48
1:E:125:LYS:NZ	10:E:5739:HOH:O	2.46	0.48
1:G:755:PHE:CD1	7:G:5077:ADP:C2	3.01	0.48
2:H:9:LEU:HD12	2:H:13:THR:HB	1.95	0.48
2:H:38:GLY:HA3	2:H:358:PRO:HB3	1.96	0.48
2:F:263:ILE:HG23	2:F:264:PRO:HD2	1.95	0.48
2:F:341:HIS:CD2	2:F:348:PHE:HB3	2.47	0.48
1:G:318:PRO:HG3	1:G:610:TYR:HH	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ALA:O	1:A:684:ARG:HB3	2.13	0.48
2:F:152:GLY:O	2:F:156:MET:HE3	2.14	0.48
1:G:17:PRO:HG3	1:G:917:VAL:HG13	1.96	0.48
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.96	0.48
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.66	0.48
1:A:267:ALA:O	1:A:271:VAL:HG23	2.13	0.48
1:C:237:PHE:CE2	1:C:458:ILE:HD13	2.49	0.48
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	1.96	0.48
1:E:947:LEU:HD12	1:E:947:LEU:N	2.28	0.48
1:G:36:ALA:O	1:G:40:GLU:HG2	2.13	0.48
1:G:569:PRO:O	1:G:571:ARG:HD2	2.14	0.48
1:G:780:GLU:OE2	1:G:798:ALA:HB1	2.14	0.48
1:A:665:SER:O	1:A:669:ILE:HG13	2.14	0.48
1:A:868:VAL:HA	1:A:872:LYS:O	2.14	0.48
2:B:232:ASN:N	2:B:233:PRO:HD3	2.28	0.48
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.96	0.48
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.49	0.48
1:C:526:TYR:CE1	1:C:545:SER:HB3	2.48	0.48
1:C:1004:ARG:O	1:C:1009[A]:GLU:HG2	2.13	0.48
1:E:563:MET:CE	1:E:635:PRO:HG3	2.43	0.48
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.44	0.48
1:G:645:GLN:HE21	1:G:649:LYS:HE3	1.79	0.48
1:G:708:ILE:CG2	1:G:754:HIS:HB2	2.44	0.48
1:A:167:ILE:HD12	1:A:167:ILE:N	2.28	0.48
2:B:228:VAL:O	2:B:231:MET:HB2	2.14	0.48
1:C:944:ARG:HD3	1:C:972:ASP:OD1	2.13	0.48
2:F:26:ALA:O	2:F:131:CYS:HA	2.13	0.48
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.49	0.48
1:C:22:GLN:HG3	1:C:26:PHE:CE2	2.48	0.48
1:C:74:VAL:HG11	1:C:102:LEU:HD11	1.95	0.48
1:C:994:VAL:HG23	1:C:1001:ILE:HD11	1.95	0.48
1:C:1027:ARG:HG3	1:C:1027:ARG:NH1	2.29	0.48
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.89	0.48
2:H:5:ALA:HB2	2:H:19:ALA:HB2	1.95	0.48
1:A:344:THR:HB	1:A:345:PRO:CD	2.43	0.48
1:C:267:ALA:O	1:C:271:VAL:HG23	2.14	0.48
1:C:680:HIS:HA	1:C:683:GLU:OE2	2.14	0.48
1:G:128:ASP:CG	1:G:131:ARG:HG3	2.39	0.48
1:G:640:VAL:HG21	1:G:651:ALA:HB2	1.96	0.48
2:H:169:SER:HA	2:H:216:LEU:O	2.14	0.48
2:H:299:ASP:OD1	2:H:302:LYS:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:O	1:A:304:VAL:HG22	2.14	0.47
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.43	0.47
1:A:772:MET:HG3	1:A:874:LEU:HD12	1.96	0.47
1:C:637:GLY:HA2	1:C:660:PRO:HB2	1.96	0.47
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.96	0.47
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.15	0.47
2:B:376:GLN:O	2:B:376:GLN:HG3	2.14	0.47
1:C:213:TRP:CZ3	1:C:296:ILE:HD12	2.49	0.47
1:G:1000:HIS:CD2	1:G:1002:GLN:H	2.32	0.47
1:A:1027:ARG:O	1:A:1031:ARG:HG3	2.14	0.47
1:A:1048:PHE:O	1:A:1051:ALA:HB3	2.13	0.47
1:C:101:GLU:OE2	1:C:104:ARG:NH2	2.42	0.47
1:C:419:GLU:O	1:C:423:LYS:HG3	2.14	0.47
1:C:579:ASP:OD1	1:C:605:THR:HB	2.14	0.47
1:E:196:LEU:HG	1:E:204:LEU:HD11	1.97	0.47
1:E:1027:ARG:NE	1:E:1031:ARG:HE	2.11	0.47
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.38	0.47
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.95	0.47
2:B:342:ARG:NH2	2:B:344:ASP:OD1	2.39	0.47
1:E:9:SER:OG	1:E:83:PRO:HA	2.15	0.47
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.97	0.47
1:G:426:ARG:HD3	1:G:426:ARG:C	2.39	0.47
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.96	0.47
1:A:764:VAL:O	1:A:827:ASN:HA	2.13	0.47
1:C:820:LEU:O	1:C:821:GLN:HB2	2.14	0.47
1:E:308:SER:HB3	10:E:5336:HOH:O	2.14	0.47
2:B:6:LEU:HD21	2:B:140:ALA:HA	1.96	0.47
2:B:199:PHE:O	2:B:241:GLY:HA3	2.13	0.47
1:C:772:MET:SD	1:C:880:THR:HG22	2.55	0.47
1:E:152:MET:SD	1:E:189:GLU:HG2	2.55	0.47
1:E:710:TYR:HB3	1:E:729:TYR:O	2.14	0.47
1:G:874:LEU:HD22	1:G:879:VAL:O	2.15	0.47
1:A:32:GLN:OE1	1:A:320:ALA:HB3	2.15	0.47
1:A:1001:ILE:CD1	1:A:1002:GLN:N	2.77	0.47
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.49	0.47
2:D:142:LEU:HD12	2:D:142:LEU:O	2.15	0.47
2:F:246:ALA:N	2:F:247:PRO:HD2	2.30	0.47
1:G:755:PHE:CE1	7:G:5077:ADP:C2	3.02	0.47
2:H:6:LEU:CD1	2:H:8:VAL:HG23	2.32	0.47
2:H:316:VAL:CG1	2:H:337:LEU:HD23	2.45	0.47
1:A:475:LYS:NZ	10:A:5519:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.50	0.47
2:D:350:PHE:HB2	2:D:366:LEU:HD22	1.97	0.47
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.50	0.47
1:E:340:THR:O	1:E:343:ARG:HB2	2.15	0.47
1:E:678:PHE:O	1:E:681:ALA:N	2.48	0.47
1:G:436:ILE:HG23	1:G:437:TRP:CE3	2.50	0.47
1:A:5:THR:C	1:A:7:ILE:H	2.23	0.47
1:C:196:LEU:HG	1:C:204:LEU:HD11	1.97	0.47
1:C:400:ARG:HD3	10:C:1475:HOH:O	2.15	0.47
1:C:669:ILE:HA	1:C:844:PRO:HG2	1.97	0.47
1:E:258:ASP:O	1:E:262:GLN:HG2	2.14	0.47
1:E:698:ILE:CD1	1:E:698:ILE:N	2.78	0.47
1:G:76:LYS:HA	1:G:76:LYS:HD2	1.69	0.47
1:G:803:GLN:HG3	1:G:807:ASP:OD1	2.15	0.47
1:G:1001:ILE:HD12	1:G:1002:GLN:CB	2.44	0.47
1:A:669:ILE:HA	1:A:844:PRO:HG2	1.97	0.46
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.95	0.46
2:B:268:ILE:HD13	2:B:354:PRO:HD2	1.96	0.46
1:C:998:ARG:HA	1:C:999:PRO:C	2.40	0.46
1:E:608:THR:HB	1:E:618:PHE:CE2	2.50	0.46
1:G:503:ALA:HB1	1:G:508:VAL:O	2.15	0.46
1:G:951:GLU:OE1	1:G:954:LYS:HD2	2.14	0.46
1:G:1030:ARG:HG3	1:G:1030:ARG:NH1	2.30	0.46
1:A:232:CYS:HA	10:A:5363:HOH:O	2.16	0.46
2:D:158:LEU:O	2:D:161:GLU:HB2	2.14	0.46
1:E:318:PRO:HB2	1:E:321:LYS:HB2	1.97	0.46
1:E:358:LYS:HG2	1:E:359:ILE:N	2.30	0.46
1:E:695:VAL:HG21	1:E:701:ALA:CA	2.40	0.46
2:F:279:SER:O	2:F:322:PRO:HG3	2.15	0.46
1:C:12:ILE:HD11	1:C:37:LEU:HD12	1.97	0.46
1:E:4:ARG:HD3	1:E:7:ILE:HD12	1.96	0.46
1:A:151:THR:HB	10:A:5297:HOH:O	2.15	0.46
1:A:663:GLY:CA	1:A:869:MET:HG2	2.45	0.46
1:C:644:GLY:O	1:C:647:PRO:HD2	2.16	0.46
1:C:858:GLY:HA2	1:C:1069:HIS:NE2	2.30	0.46
1:C:1017:THR:HG22	1:C:1018:SER:N	2.31	0.46
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.51	0.46
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.50	0.46
1:A:358:LYS:HE3	10:A:5372:HOH:O	2.15	0.46
2:B:133:ILE:HG22	2:B:138:PRO:HB3	1.98	0.46
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.34	0.46
1:A:250:VAL:HA	1:A:356:VAL:O	2.16	0.46
1:A:663:GLY:HA2	1:A:869:MET:HG2	1.97	0.46
1:A:901:PRO:HD2	5:A:5013:CL:CL	2.52	0.46
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.97	0.46
1:G:1017:THR:HG22	1:G:1018:SER:H	1.78	0.46
1:G:1039:HIS:HA	10:G:5663:HOH:O	2.15	0.46
1:A:503:ALA:HB2	1:A:510:GLU:HA	1.97	0.46
1:A:814:GLN:HG3	1:A:818:PHE:CE2	2.51	0.46
1:A:998:ARG:CB	1:A:999:PRO:HA	2.43	0.46
1:C:38:ARG:HG3	1:C:38:ARG:NH1	2.12	0.46
2:D:39:TYR:CZ	2:D:61:GLY:HA2	2.51	0.46
2:D:133:ILE:CG2	2:D:138:PRO:HB3	2.42	0.46
2:D:205:ILE:HG13	2:D:355:GLU:HG3	1.98	0.46
1:E:1036:TYR:C	1:E:1037:LYS:HG2	2.40	0.46
2:F:246:ALA:HB3	2:F:247:PRO:HD3	1.96	0.46
1:G:5:THR:C	1:G:7:ILE:H	2.22	0.46
1:G:676:GLU:O	1:G:680:HIS:ND1	2.48	0.46
2:B:157:ASP:CG	2:B:160:LYS:HG2	2.41	0.46
2:D:249:ASP:OD2	2:D:250:TYR:N	2.49	0.46
1:E:157:ALA:HB3	10:E:5280:HOH:O	2.15	0.46
1:E:579:ASP:OD1	1:E:605:THR:HB	2.16	0.46
2:F:324:ASN:HA	2:F:343:THR:OG1	2.16	0.46
1:G:713:VAL:HG22	1:G:727:ILE:HG12	1.98	0.46
1:C:559:ARG:HH11	1:C:559:ARG:CG	2.26	0.46
1:C:991[B]:VAL:CG2	1:C:992:ASN:N	2.79	0.46
1:E:217:GLU:HG2	1:E:285:GLN:HG2	1.98	0.46
1:E:541:ALA:HB1	1:E:543:MET:HE2	1.98	0.46
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.98	0.46
1:G:213:TRP:CZ3	1:G:296:ILE:HD12	2.51	0.46
1:A:701:ALA:O	1:A:705:ALA:N	2.47	0.46
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.79	0.46
1:G:128:ASP:OD1	1:G:130:ARG:HB3	2.16	0.46
1:G:702:VAL:O	1:G:705:ALA:HB3	2.17	0.46
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.98	0.45
1:A:542:TYR:HE1	1:A:618:PHE:HB2	1.82	0.45
1:C:708:ILE:HG22	1:C:712:LEU:HD11	1.97	0.45
1:C:730:ASP:H	1:C:733:ASP:HB2	1.80	0.45
2:H:142:LEU:HD12	2:H:142:LEU:C	2.40	0.45
2:H:376:GLN:O	2:H:376:GLN:HG3	2.16	0.45
1:C:695:VAL:HG11	1:C:701:ALA:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:VAL:O	2:D:78:GLN:HG2	2.16	0.45
1:E:479:VAL:CG2	1:E:483:GLY:HA3	2.46	0.45
1:E:751:LEU:O	1:E:752:LEU:HD12	2.16	0.45
1:E:1068:MET:O	1:E:1071:GLN:HB2	2.16	0.45
2:F:169:SER:HA	2:F:216:LEU:O	2.15	0.45
2:F:353:HIS:CD2	2:F:353:HIS:N	2.84	0.45
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.46	0.45
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.31	0.45
1:G:963:LYS:CE	1:G:1052[B]:MET:HE3	2.44	0.45
2:H:312:HIS:HD2	10:H:3239:HOH:O	1.98	0.45
1:A:659:VAL:HG13	1:A:660:PRO:HD2	1.97	0.45
1:C:475:LYS:HD3	1:C:488:PHE:CZ	2.51	0.45
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.47	0.45
1:C:950:ARG:HD3	5:C:5039:CL:CL	2.53	0.45
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.98	0.45
1:G:456:THR:O	1:G:457:ASN:HB2	2.17	0.45
2:H:54:THR:CG2	2:H:118:LEU:HD23	2.36	0.45
1:A:412:LYS:HG2	1:A:438:TYR:CE1	2.51	0.45
1:A:695:VAL:HG21	1:A:752:LEU:HD22	1.99	0.45
2:B:85:LEU:HD12	2:B:86:PRO:HD2	1.98	0.45
2:B:325:LEU:HD23	2:B:325:LEU:HA	1.80	0.45
1:C:194:ARG:NH2	10:C:1870:HOH:O	2.49	0.45
2:F:253:THR:O	2:F:256:GLN:HB2	2.16	0.45
2:H:265:VAL:O	2:H:347:ALA:HA	2.17	0.45
1:A:467:GLU:O	1:A:471:ARG:HG2	2.15	0.45
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.98	0.45
2:B:364:ALA:N	2:B:365:PRO:HD2	2.31	0.45
1:C:975:HIS:HD1	1:E:975:HIS:HD1	0.79	0.45
2:D:259:LEU:HD23	2:D:259:LEU:HA	1.84	0.45
2:D:344:ASP:OD2	2:D:344:ASP:N	2.43	0.45
1:E:150:HIS:HE1	10:E:5882:HOH:O	2.00	0.45
1:E:726:GLU:OE1	1:E:1020:ARG:HD3	2.16	0.45
9:E:5057:NET:H22	9:E:5057:NET:H42	1.97	0.45
2:F:208:MET:O	2:F:212:ARG:HG3	2.17	0.45
1:G:329:GLY:HA2	10:G:5173:HOH:O	2.17	0.45
1:G:947:LEU:N	1:G:947:LEU:CD1	2.79	0.45
2:H:275:LEU:HD23	2:H:349:SER:CB	2.47	0.45
1:A:70:HIS:O	1:A:74:VAL:HG23	2.17	0.45
1:A:1031:ARG:HE	1:A:1031:ARG:HB3	1.61	0.45
1:C:768:CYS:HB2	1:C:773:VAL:HG22	1.98	0.45
1:E:648:LEU:HD21	1:E:845:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:854:SER:HA	1:E:859:VAL:O	2.17	0.45
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.97	0.45
1:G:223:ASP:OD2	1:G:227:ASN:HB2	2.17	0.45
1:G:936:ASN:HB2	10:G:5133:HOH:O	2.15	0.45
2:H:286:MET:HE1	2:H:312:HIS:HE1	1.77	0.45
2:H:353:HIS:CD2	2:H:353:HIS:N	2.85	0.45
1:A:835:ASN:ND2	10:A:5879:HOH:O	2.44	0.45
2:B:350:PHE:CG	2:B:366:LEU:CD2	3.00	0.45
1:C:814:GLN:CG	1:C:818:PHE:HE2	2.16	0.45
1:E:781:HIS:HE1	1:E:789:SER:CB	2.30	0.45
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.52	0.45
1:G:400:ARG:HB3	10:G:5451:HOH:O	2.16	0.45
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.46	0.45
1:A:349:GLU:O	2:B:294:ASN:HB2	2.17	0.45
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.76	0.45
1:A:947:LEU:N	1:A:947:LEU:HD12	2.31	0.45
2:B:258:PHE:O	2:B:261:THR:OG1	2.34	0.45
1:C:481:ILE:O	1:C:481:ILE:HG13	2.16	0.45
1:C:773:VAL:HG23	1:C:818:PHE:CE2	2.51	0.45
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.56	0.45
1:E:728:VAL:HG11	1:E:734:LEU:HA	1.98	0.45
2:F:186:LYS:O	2:F:189:GLU:HB2	2.16	0.45
1:G:361:ARG:CZ	1:G:571:ARG:HG2	2.47	0.45
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.98	0.45
2:B:275:LEU:HD12	2:B:275:LEU:O	2.17	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:167:ILE:HD12	1:C:167:ILE:N	2.32	0.45
1:C:950:ARG:H	1:C:950:ARG:HG3	1.45	0.45
1:C:1006:LYS:HB2	1:C:1036:TYR:CZ	2.52	0.45
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.98	0.45
2:F:338:GLN:HA	2:F:351:GLN:HB3	1.99	0.45
1:G:772:MET:HE1	1:G:880:THR:O	2.17	0.45
2:H:210:VAL:HA	2:H:214:CYS:O	2.17	0.45
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.17	0.45
1:C:69:ILE:O	1:C:69:ILE:HG22	2.16	0.45
1:C:509:ARG:HH11	1:C:509:ARG:HB2	1.81	0.45
1:C:698:ILE:N	1:C:698:ILE:CD1	2.79	0.45
2:D:215:ARG:HG3	2:D:215:ARG:HH11	1.82	0.45
1:E:278:GLU:HG2	10:E:5895:HOH:O	2.16	0.45
1:E:1017:THR:CG2	1:E:1018:SER:N	2.80	0.45
1:G:517:ARG:HG2	1:G:522:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:CD1	1:A:738:PHE:CE2	2.99	0.44
1:A:805:ILE:HD12	1:A:832:VAL:CG1	2.47	0.44
1:A:822:VAL:C	1:A:823:ARG:HG2	2.42	0.44
1:C:675:ARG:H	1:C:675:ARG:HD3	1.82	0.44
2:D:222:GLN:H	2:D:222:GLN:NE2	2.12	0.44
1:G:947:LEU:HG	1:G:1014:ILE:CG2	2.47	0.44
1:G:1004:ARG:O	1:G:1009:GLU:HB2	2.17	0.44
1:A:1037:LYS:HA	10:A:5721:HOH:O	2.18	0.44
1:C:145:ARG:HB2	1:C:208:GLU:OE1	2.17	0.44
1:C:472:LEU:O	1:C:476:VAL:HG23	2.17	0.44
1:E:250:VAL:HA	1:E:356:VAL:O	2.17	0.44
1:G:637:GLY:HA2	1:G:660:PRO:O	2.17	0.44
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.17	0.44
1:A:1073:LYS:HD2	1:A:1073:LYS:N	2.31	0.44
1:C:499:ASP:HA	1:C:513:ILE:HG21	1.98	0.44
1:C:883:VAL:CG1	1:C:884:ILE:N	2.80	0.44
1:E:1:MET:H3	1:E:224:LYS:CE	2.20	0.44
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.44
1:G:704:LYS:O	1:G:707:GLU:HB2	2.17	0.44
1:A:579:ASP:O	1:A:583:VAL:HG23	2.17	0.44
1:A:712:LEU:O	1:A:727:ILE:HA	2.17	0.44
2:B:232:ASN:N	2:B:233:PRO:CD	2.80	0.44
2:D:168:TYR:O	2:D:218:ILE:N	2.42	0.44
2:D:190:LEU:HB2	2:D:215:ARG:HB3	1.99	0.44
2:D:270:LEU:O	2:D:274:LEU:HG	2.17	0.44
1:E:795:SER:HB2	1:E:890:VAL:HG22	1.99	0.44
2:B:172:GLN:O	2:B:207:ARG:HA	2.17	0.44
1:C:9:SER:OG	1:C:84:ASP:N	2.45	0.44
1:C:64:THR:O	1:C:1065:VAL:HG23	2.17	0.44
1:C:907:LEU:HD11	8:C:5033:ORN:HD3	1.98	0.44
1:E:213:TRP:HH2	1:E:294:ARG:HD3	1.81	0.44
1:E:814:GLN:NE2	10:E:5604:HOH:O	2.49	0.44
2:F:344:ASP:OD2	2:F:344:ASP:N	2.45	0.44
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.99	0.44
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.53	0.44
2:D:120:ARG:HD2	10:D:1583:HOH:O	2.18	0.44
1:E:659:VAL:HG13	1:E:660:PRO:HD2	2.00	0.44
2:F:305:VAL:HG12	2:F:306:MET:N	2.32	0.44
1:G:222:ARG:HD3	1:G:277:VAL:O	2.18	0.44
1:G:402:LEU:O	1:G:403:GLU:HB2	2.18	0.44
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.20	0.44
2:D:332:LEU:HD12	2:D:332:LEU:HA	1.70	0.44
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.00	0.44
1:G:773:VAL:HG23	1:G:818:PHE:CZ	2.53	0.44
2:H:306:MET:CE	2:H:329:HIS:CD2	3.01	0.44
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.52	0.44
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.47	0.44
1:A:737:TYR:CE1	1:A:741:ALA:HB2	2.53	0.44
1:A:843:ASN:HB3	1:A:845:ARG:HD2	1.99	0.44
1:C:331:THR:O	1:C:335:LEU:HG	2.17	0.44
1:C:633:GLU:O	1:C:634:LYS:HB2	2.18	0.44
1:C:714:VAL:HG23	1:C:728:VAL:HG23	2.00	0.44
1:E:652:ARG:NH2	1:E:667:ASP:OD2	2.44	0.44
1:G:59:GLU:HG2	1:G:60:MET:HE2	1.99	0.44
1:G:273:ARG:HD2	10:G:5275:HOH:O	2.18	0.44
1:G:735:ARG:O	1:G:738:PHE:N	2.51	0.44
1:A:309:ALA:O	1:A:313:LYS:HG2	2.18	0.44
1:A:556[A]:SER:HB2	1:A:558:ASP:HB2	1.99	0.44
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.18	0.44
1:C:340:THR:O	1:C:343:ARG:HB2	2.17	0.44
1:C:703:GLU:O	1:C:706:LYS:HB2	2.18	0.44
1:C:833:LYS:O	1:C:836:GLU:HB2	2.18	0.44
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.48	0.44
2:F:23:THR:HG23	2:F:134:ALA:O	2.17	0.44
1:G:425:ARG:NH1	10:G:5479:HOH:O	2.47	0.44
1:G:671:ARG:CG	1:G:677:ARG:NH1	2.79	0.44
2:H:332:LEU:HA	2:H:332:LEU:HD12	1.53	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.79	0.44
1:C:773:VAL:HG21	1:C:817:ALA:HB3	2.00	0.43
2:D:364:ALA:N	2:D:365:PRO:HD2	2.33	0.43
1:E:793:ALA:HA	1:E:891:LYS:O	2.17	0.43
1:E:892:GLU:OE1	8:E:5056:ORN:NE	2.50	0.43
2:F:342:ARG:HD2	2:F:342:ARG:HA	1.77	0.43
1:G:436:ILE:HG22	10:G:5368:HOH:O	2.16	0.43
1:G:550:GLU:OE2	2:H:120:ARG:NH2	2.45	0.43
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.72	0.43
1:G:938:THR:OG1	1:G:1037:LYS:O	2.30	0.43
1:A:697:ALA:HB3	1:A:700:MET:HB2	1.99	0.43
1:A:998:ARG:CG	1:A:999:PRO:HA	2.47	0.43
1:C:534:ALA:HB1	2:D:120:ARG:HG2	2.00	0.43
2:D:298:LYS:O	2:D:329:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:LEU:HD22	1:E:845:ARG:HD3	2.00	0.43
1:A:693:ALA:HB2	1:A:708:ILE:HD11	2.00	0.43
1:A:698:ILE:O	1:A:701:ALA:HB3	2.18	0.43
1:A:1026:SER:HB2	1:A:1030:ARG:HH12	1.83	0.43
1:C:688:LYS:HD2	1:C:838:TYR:CE1	2.54	0.43
2:D:272:HIS:HA	2:D:349:SER:CB	2.49	0.43
2:F:62:ASN:OD1	2:F:86:PRO:HG3	2.18	0.43
2:H:26:ALA:HB2	2:H:108:VAL:HB	2.00	0.43
2:H:33:ASN:HB3	2:H:55:LEU:HD23	1.99	0.43
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.99	0.43
1:A:419:GLU:O	1:A:423:LYS:HG3	2.19	0.43
2:B:63:VAL:O	2:B:94:ASN:HB2	2.18	0.43
2:B:249:ASP:OD2	2:B:250:TYR:N	2.51	0.43
1:C:991[B]:VAL:HG22	1:C:992:ASN:N	2.32	0.43
1:E:139:ILE:HD11	1:E:141:LEU:HD12	2.00	0.43
1:E:1001:ILE:HG13	1:E:1002:GLN:H	1.82	0.43
1:E:1005:ILE:HG21	1:E:1032:SER:HB3	2.00	0.43
2:H:222:GLN:HA	2:H:250:TYR:CD1	2.54	0.43
2:B:153:LEU:HD12	2:B:153:LEU:HA	1.84	0.43
2:D:188:ASP:OD2	2:D:188:ASP:N	2.47	0.43
1:E:864:VAL:O	1:E:868:VAL:HG23	2.19	0.43
2:F:177:LEU:HB3	10:F:2347:HOH:O	2.18	0.43
1:G:475:LYS:NZ	10:G:5513:HOH:O	2.43	0.43
2:H:253:THR:O	2:H:256:GLN:HB2	2.18	0.43
1:A:946:LEU:C	1:A:947:LEU:HD12	2.43	0.43
1:C:17:PRO:HG3	1:C:917:VAL:HG13	2.01	0.43
1:C:695:VAL:CG1	1:C:700:MET:HB3	2.45	0.43
2:D:116:ARG:O	2:D:120:ARG:HG3	2.18	0.43
1:E:235:GLU:HB2	1:E:253:ALA:HA	2.01	0.43
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.54	0.43
2:H:199:PHE:HE2	2:H:238:LEU:HB3	1.84	0.43
1:A:344:THR:CB	1:A:345:PRO:HD2	2.48	0.43
1:A:601:CYS:HA	1:A:618:PHE:CE1	2.53	0.43
1:A:728:VAL:HG11	1:A:734:LEU:HA	2.00	0.43
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.34	0.43
1:A:1004:ARG:HB3	1:A:1009[B]:GLU:HG3	2.00	0.43
1:C:166:CYS:C	1:C:167:ILE:HD12	2.43	0.43
1:C:671:ARG:HG2	1:C:677:ARG:NH1	2.33	0.43
2:D:370:PHE:O	2:D:374:ILE:HG13	2.19	0.43
1:E:358:LYS:HE3	10:E:5353:HOH:O	2.18	0.43
1:E:560:GLU:OE1	1:E:636:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:249:ASP:OD2	2:F:250:TYR:N	2.50	0.43
1:G:986:ILE:O	1:G:988:PRO:HD3	2.18	0.43
1:A:602:ASN:CG	1:A:605:THR:HG23	2.44	0.43
1:A:793:ALA:HA	1:A:891:LYS:O	2.19	0.43
1:A:992:ASN:O	1:A:1000:HIS:HA	2.19	0.43
2:B:268:ILE:HD13	2:B:268:ILE:HG21	1.73	0.43
1:C:678:PHE:O	1:C:682:VAL:HG23	2.18	0.43
1:E:509:ARG:NH2	1:E:515:LYS:HZ3	2.17	0.43
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.99	0.43
1:A:1061:LYS:HG2	1:A:1062:VAL:N	2.34	0.43
1:C:423:LYS:HG3	1:C:423:LYS:H	1.52	0.43
1:C:642:TYR:OH	1:C:865:ALA:HB3	2.18	0.43
1:E:5:THR:O	1:E:8:LYS:NZ	2.52	0.43
2:H:286:MET:CE	2:H:312:HIS:ND1	2.82	0.43
2:H:322:PRO:CB	2:H:324:ASN:ND2	2.80	0.43
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.83	0.43
2:B:244:ASP:O	2:B:247:PRO:HD2	2.19	0.43
1:C:176:GLY:HA3	1:C:377:GLN:HA	2.01	0.43
2:F:29:GLU:HB3	2:F:51:GLN:HG2	2.00	0.43
2:F:229:LEU:N	2:F:229:LEU:HD23	2.33	0.43
1:A:1:MET:H3	1:A:224:LYS:HE3	1.84	0.42
1:A:995:HIS:CD2	1:A:995:HIS:H	2.36	0.42
1:C:252:PRO:HD3	1:C:352:ILE:HD11	2.01	0.42
2:D:78:GLN:HE21	2:D:78:GLN:CA	2.10	0.42
1:E:40:GLU:OE2	1:E:330:TYR:OH	2.28	0.42
1:E:347:SER:O	2:F:296:PRO:HB3	2.19	0.42
1:G:69:ILE:O	1:G:69:ILE:HG22	2.19	0.42
1:G:165:PRO:HA	1:G:182:ALA:O	2.19	0.42
1:G:681:ALA:O	1:G:685:LEU:HG	2.19	0.42
1:G:998:ARG:CB	1:G:999:PRO:HA	2.47	0.42
1:A:237:PHE:CE2	1:A:458:ILE:HD13	2.54	0.42
1:A:339:ILE:O	1:A:538:THR:OG1	2.36	0.42
1:A:375:THR:HG23	1:A:377:GLN:H	1.84	0.42
1:A:559:ARG:HG3	1:A:559:ARG:NH1	2.32	0.42
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.54	0.42
1:C:419:GLU:HB3	1:C:423:LYS:HE3	2.00	0.42
1:C:637:GLY:HA3	1:C:662:ILE:HG23	2.01	0.42
2:D:6:LEU:O	2:D:132:ILE:HA	2.18	0.42
2:D:326:ARG:O	2:D:340:ILE:HA	2.18	0.42
1:G:1017:THR:CG2	1:G:1018:SER:N	2.80	0.42
2:H:324:ASN:O	2:H:342:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:MET:HE2	1:A:920:VAL:HG22	2.01	0.42
2:B:5:ALA:HB3	2:B:110:ILE:HG13	2.01	0.42
1:C:571:ARG:HD3	1:C:574:GLN:HB2	2.02	0.42
1:E:689:GLN:HG2	1:E:690:PRO:HD2	2.01	0.42
1:E:1001:ILE:CG1	1:E:1002:GLN:N	2.82	0.42
1:E:1004:ARG:NH1	1:E:1009[A]:GLU:OE1	2.45	0.42
2:F:6:LEU:HD13	2:F:16:HIS:ND1	2.33	0.42
2:F:186:LYS:HB2	2:F:189:GLU:OE2	2.20	0.42
1:G:158:VAL:O	1:G:161:ASP:HB3	2.19	0.42
1:G:534:ALA:HB1	2:H:120:ARG:HG2	2.01	0.42
1:G:994:VAL:HG22	1:G:1000:HIS:ND1	2.34	0.42
2:H:310:GLN:OE1	2:H:312:HIS:NE2	2.53	0.42
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.84	0.42
1:A:958:VAL:HG22	1:A:981:LEU:HD23	2.01	0.42
1:C:701:ALA:O	1:C:705:ALA:HB2	2.19	0.42
1:C:793:ALA:HA	1:C:891:LYS:O	2.20	0.42
1:C:994:VAL:HG23	1:C:1001:ILE:CD1	2.49	0.42
1:C:1063:ILE:HG13	1:C:1067:GLU:OE2	2.20	0.42
2:F:170:TRP:HB3	2:F:216:LEU:HD12	2.00	0.42
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.40	0.42
1:A:3:LYS:HA	1:A:328:VAL:O	2.19	0.42
1:A:698:ILE:CD1	1:A:698:ILE:N	2.80	0.42
1:C:703:GLU:HA	1:C:703:GLU:OE2	2.19	0.42
1:C:940:LYS:HA	5:C:5038:CL:CL	2.56	0.42
2:F:46:PRO:HA	2:F:76:HIS:CG	2.54	0.42
1:G:1:MET:HB3	1:G:2:PRO:HD2	2.01	0.42
1:G:904:ASP:HA	1:G:905:PRO:HD3	1.91	0.42
1:A:674:ASP:HB3	1:A:677:ARG:HB2	2.01	0.42
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.92	0.42
1:C:259:LYS:HD3	2:D:175:TRP:CE3	2.55	0.42
1:C:919:GLY:HA2	10:C:1219:HOH:O	2.18	0.42
1:C:991[A]:VAL:HG12	1:C:1004:ARG:HH21	1.83	0.42
1:E:65:TYR:OH	1:E:81:GLU:OE1	2.29	0.42
1:E:855:LYS:HD2	1:E:855:LYS:HA	1.77	0.42
1:E:901:PRO:HD2	5:E:5060:CL:CL	2.57	0.42
1:E:1028:VAL:CG1	1:E:1029:ILE:N	2.82	0.42
2:H:193:HIS:O	2:H:234:ASP:HB2	2.19	0.42
2:H:344:ASP:OD2	2:H:344:ASP:N	2.29	0.42
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.88	0.42
1:A:726:GLU:CG	1:A:727:ILE:N	2.79	0.42
1:C:698:ILE:O	1:C:702:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:VAL:HG21	1:E:464:VAL:HG12	2.01	0.42
1:E:702:VAL:O	1:E:706:LYS:HD3	2.19	0.42
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.54	0.42
1:G:370:ALA:HB2	1:G:900:PHE:HB3	2.00	0.42
1:G:827:ASN:N	1:G:843:ASN:O	2.50	0.42
1:G:1055:ASN:HB2	10:G:5826:HOH:O	2.20	0.42
2:H:190:LEU:HA	2:H:190:LEU:HD23	1.82	0.42
1:A:558:ASP:HB3	1:A:559:ARG:H	1.46	0.42
1:A:814:GLN:CG	1:A:818:PHE:CE2	3.02	0.42
1:C:809:MET:HG2	1:C:837:VAL:HG11	2.01	0.42
1:C:892:GLU:HG3	1:C:893:VAL:N	2.35	0.42
1:C:973:ALA:C	1:C:991[B]:VAL:HG12	2.44	0.42
2:D:169:SER:HA	2:D:216:LEU:O	2.20	0.42
2:D:208:MET:SD	2:D:355:GLU:HA	2.59	0.42
1:E:1:MET:HG3	1:E:2:PRO:HD2	2.01	0.42
1:E:688:LYS:HD2	1:E:838:TYR:CE1	2.55	0.42
2:F:164:THR:O	2:F:220:PRO:HB3	2.20	0.42
1:G:423:LYS:H	1:G:423:LYS:HG3	1.53	0.42
1:G:736:ARG:NH1	1:G:736:ARG:HB3	2.35	0.42
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.92	0.42
2:H:191:PRO:HD2	2:H:213:GLY:O	2.20	0.42
2:B:170:TRP:HB3	2:B:216:LEU:HD12	2.02	0.42
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.89	0.42
1:C:687:LEU:HD11	1:C:812:GLN:HG2	2.02	0.42
1:C:751:LEU:O	1:C:752:LEU:HD12	2.20	0.42
2:D:317:ASP:OD1	2:D:320:THR:HG23	2.20	0.42
2:D:350:PHE:HB2	2:D:366:LEU:CD2	2.50	0.42
1:E:765:ASP:OD2	1:E:827:ASN:HB2	2.20	0.42
1:G:40:GLU:HG2	1:G:325:LYS:HE2	2.02	0.42
1:G:397:LYS:NZ	1:G:619:GLU:OE1	2.49	0.42
1:A:813:VAL:HG22	1:A:828:VAL:CG2	2.48	0.42
1:C:22:GLN:HG3	1:C:26:PHE:HE2	1.84	0.42
1:C:542:TYR:HE1	1:C:618:PHE:HB2	1.85	0.42
1:C:562:ILE:HG21	1:C:589:LEU:HD13	2.02	0.42
2:D:246:ALA:N	2:D:247:PRO:HD2	2.35	0.42
2:F:187:GLU:C	2:F:189:GLU:H	2.27	0.42
1:G:646:THR:HB	1:G:647:PRO:HD3	2.01	0.42
1:G:775:ILE:HD13	1:G:775:ILE:HA	1.71	0.42
1:G:1000:HIS:HD2	1:G:1002:GLN:H	1.66	0.42
1:G:1017:THR:HG21	1:G:1023:ILE:HA	2.01	0.42
2:H:316:VAL:HG12	2:H:337:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ASN:HD22	1:A:835:ASN:HA	1.63	0.41
1:A:992:ASN:ND2	1:A:996:GLU:CB	2.78	0.41
1:C:957:VAL:O	1:C:957:VAL:HG22	2.20	0.41
1:E:698:ILE:N	1:E:698:ILE:HD12	2.35	0.41
1:E:1028:VAL:HG13	1:E:1029:ILE:N	2.34	0.41
1:G:728:VAL:HG11	1:G:734:LEU:N	2.35	0.41
1:G:947:LEU:HG	1:G:1014:ILE:HG21	2.02	0.41
1:A:695:VAL:HA	1:A:700:MET:HE2	2.03	0.41
1:A:805:ILE:HD12	1:A:832:VAL:HG11	2.01	0.41
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.45	0.41
1:E:695:VAL:CG1	1:E:696:THR:N	2.82	0.41
1:G:361:ARG:HG3	1:G:361:ARG:HH11	1.85	0.41
1:G:698:ILE:O	1:G:702:VAL:HG23	2.20	0.41
1:A:129:ARG:HB3	1:A:205:LEU:HD22	2.02	0.41
1:A:990:LEU:HG	1:A:991:VAL:N	2.36	0.41
1:C:734:LEU:HD11	1:C:738:PHE:HE2	1.74	0.41
2:D:208:MET:O	2:D:211:ASP:HB2	2.19	0.41
2:D:254:ALA:O	2:D:257:LYS:HB2	2.19	0.41
1:E:655[B]:GLU:HG2	10:E:5790:HOH:O	2.19	0.41
1:E:702:VAL:CG1	1:E:731:GLU:HG3	2.49	0.41
1:G:102:LEU:HD23	1:G:102:LEU:HA	1.95	0.41
1:G:700:MET:O	1:G:704:LYS:HB2	2.21	0.41
1:C:167:ILE:N	1:C:167:ILE:CD1	2.83	0.41
2:D:364:ALA:N	2:D:365:PRO:CD	2.82	0.41
2:F:251:ALA:O	2:F:255:ILE:HD12	2.21	0.41
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.51	0.41
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.50	0.41
1:A:681:ALA:HA	1:A:684:ARG:HB3	2.02	0.41
1:A:833:LYS:O	1:A:836:GLU:HB2	2.20	0.41
1:A:965:LEU:HA	1:A:965:LEU:HD23	1.68	0.41
1:C:520:TYR:O	1:C:521:ASP:HB3	2.20	0.41
1:C:670:ASP:HB3	1:C:677:ARG:NH2	2.35	0.41
1:C:1027:ARG:HG3	1:C:1027:ARG:HH11	1.85	0.41
2:D:344:ASP:O	2:D:345:LYS:HG2	2.21	0.41
2:F:357:SER:HA	2:F:358:PRO:HA	1.89	0.41
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.53	0.41
1:G:885:PRO:HA	1:G:886:PRO:HD3	1.89	0.41
1:G:1001:ILE:CD1	1:G:1002:GLN:N	2.74	0.41
2:H:190:LEU:HD13	2:H:215:ARG:HA	2.01	0.41
2:H:279:SER:OG	2:H:342:ARG:HD3	2.19	0.41
1:A:159:ALA:HB2	1:A:188:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.51	0.41
1:A:941:LYS:HE3	10:A:5890:HOH:O	2.20	0.41
1:C:493:LYS:HA	1:C:493:LYS:HD2	1.83	0.41
1:C:516:LEU:HA	1:C:516:LEU:HD12	1.75	0.41
1:C:805:ILE:HG22	1:C:806:GLN:N	2.36	0.41
2:D:87:LEU:HB2	10:D:1948:HOH:O	2.20	0.41
2:D:123:ARG:O	2:D:287:LYS:HE2	2.21	0.41
1:E:781:HIS:CE1	1:E:789:SER:HA	2.55	0.41
1:G:423:LYS:NZ	10:G:5476:HOH:O	2.44	0.41
1:G:762:VAL:HG21	1:G:809:MET:HE1	2.02	0.41
1:A:104:ARG:HH11	1:A:104:ARG:HG3	1.85	0.41
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.20	0.41
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.55	0.41
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.92	0.41
2:B:277:LEU:HD23	2:B:277:LEU:HA	1.95	0.41
1:C:317:PHE:CD1	1:C:317:PHE:C	2.99	0.41
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.36	0.41
2:D:46:PRO:HA	2:D:76:HIS:CD2	2.56	0.41
2:D:118:LEU:HD12	2:D:118:LEU:C	2.46	0.41
2:D:158:LEU:HD23	2:D:158:LEU:HA	1.92	0.41
2:D:227:ASP:O	2:D:230:LYS:HB2	2.21	0.41
1:E:447:LEU:HD23	1:E:447:LEU:HA	1.98	0.41
1:E:671:ARG:NH2	1:E:819:GLU:O	2.54	0.41
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.82	0.41
2:H:120:ARG:HD2	10:H:3737:HOH:O	2.21	0.41
1:C:220:VAL:HG12	1:C:221:VAL:N	2.36	0.41
1:E:213:TRP:CZ2	1:E:289:ASN:HB2	2.56	0.41
1:E:775:ILE:HD13	1:E:775:ILE:HA	1.90	0.41
1:G:805:ILE:CD1	1:G:832:VAL:HG13	2.51	0.41
2:H:23:THR:HG22	2:H:24:GLY:N	2.36	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.55	0.41
1:A:17:PRO:HG3	1:A:917:VAL:HG13	2.03	0.41
1:A:702:VAL:O	1:A:706:LYS:HD3	2.21	0.41
1:A:1012:TYR:C	1:A:1013:ILE:HG13	2.45	0.41
9:A:5094:NET:H63	9:A:5094:NET:H31	1.69	0.41
9:A:5094:NET:H82	9:A:5094:NET:H52	1.80	0.41
2:B:378:ARG:C	2:B:380:THR:N	2.79	0.41
1:C:28:TYR:CZ	1:C:313:LYS:HE3	2.56	0.41
1:C:513:ILE:HD13	1:C:513:ILE:HA	1.86	0.41
1:C:730:ASP:OD2	1:C:733:ASP:HB2	2.21	0.41
2:D:204:ASN:O	2:D:208:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.56	0.41
1:E:1:MET:CB	1:E:224:LYS:NZ	2.82	0.41
1:G:1:MET:H3	1:G:224:LYS:HE3	1.85	0.41
1:G:82:ARG:N	1:G:83:PRO:CD	2.84	0.41
1:G:121:ASP:O	1:G:125:LYS:HB2	2.20	0.41
1:G:363:ASN:OD1	1:G:381:VAL:HG21	2.20	0.41
1:G:654:LEU:O	1:G:659:VAL:HB	2.21	0.41
1:G:710:TYR:HB3	1:G:729:TYR:O	2.21	0.41
1:G:1014:ILE:O	1:G:1014:ILE:HG23	2.21	0.41
1:G:1027[B]:ARG:HG2	1:G:1031:ARG:HG3	2.03	0.41
1:G:1032:SER:O	1:G:1036:TYR:HD1	2.03	0.41
2:H:45:ASP:HB3	2:H:48:TYR:HD2	1.85	0.41
2:H:168:TYR:CD1	2:H:168:TYR:N	2.88	0.41
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.55	0.41
2:H:302:LYS:HB2	2:H:304:VAL:HG22	2.02	0.41
1:A:1:MET:HE2	1:A:224:LYS:HZ2	1.86	0.41
1:A:150:HIS:NE2	1:A:203:GLU:HG3	2.36	0.41
1:A:331:THR:O	1:A:334:GLU:HB2	2.21	0.41
2:B:25:SER:HA	2:B:132:ILE:O	2.20	0.41
2:D:266:PHE:HA	2:D:348:PHE:O	2.21	0.41
2:D:327:VAL:HG13	2:D:337:LEU:CD1	2.50	0.41
1:E:891:LYS:HG2	1:E:892:GLU:N	2.36	0.41
1:E:1002:GLN:O	1:E:1006:LYS:HB3	2.20	0.41
1:G:708:ILE:HG23	1:G:754:HIS:HB2	2.03	0.41
1:G:734:LEU:CD1	1:G:738:PHE:CD2	3.04	0.41
1:G:799:TYR:CD2	1:G:799:TYR:N	2.88	0.41
2:H:181:LEU:HD23	2:H:181:LEU:HA	1.90	0.41
1:A:46:LEU:HD22	1:A:46:LEU:C	2.46	0.40
1:A:165:PRO:HB3	1:A:183:TYR:CD1	2.56	0.40
1:A:493:LYS:HD2	1:A:493:LYS:HA	1.80	0.40
1:A:697:ALA:O	1:A:700:MET:HB3	2.21	0.40
1:A:954:LYS:HB3	1:A:980:VAL:HG21	2.03	0.40
1:A:962:ALA:O	1:A:965:LEU:HB2	2.21	0.40
1:C:250:VAL:HA	1:C:356:VAL:O	2.22	0.40
1:C:339:ILE:HD11	1:C:529:VAL:HG12	2.03	0.40
1:C:714:VAL:CG2	1:C:728:VAL:CG2	2.99	0.40
1:C:805:ILE:CD1	1:C:837:VAL:CG2	3.00	0.40
1:C:843:ASN:C	1:C:845:ARG:H	2.29	0.40
1:C:904:ASP:OD1	1:C:906:LEU:HD22	2.21	0.40
2:D:362:ASP:N	2:D:362:ASP:OD2	2.53	0.40
1:E:237:PHE:HB3	1:E:248:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASN:HD22	1:E:266:ASN:HA	1.60	0.40
1:E:711:PRO:HG2	1:E:755:PHE:HD2	1.86	0.40
2:F:98:LEU:O	2:F:102:LEU:HG	2.20	0.40
2:F:158:LEU:HD12	2:F:243:GLY:N	2.36	0.40
1:G:485:ASN:OD1	1:G:487:ASP:HB2	2.21	0.40
2:H:7:LEU:HD23	2:H:15:PHE:CD2	2.56	0.40
2:H:234:ASP:HB3	2:H:374:ILE:CG2	2.51	0.40
2:H:326:ARG:O	2:H:340:ILE:HA	2.21	0.40
1:A:344:THR:CB	1:A:345:PRO:CD	3.00	0.40
2:B:46:PRO:HA	2:B:76:HIS:CB	2.50	0.40
1:C:344:THR:HB	1:C:345:PRO:CD	2.51	0.40
1:C:895:LEU:HA	1:C:896:PRO:HD3	1.91	0.40
1:E:36:ALA:O	1:E:39:GLU:HB2	2.21	0.40
2:F:195:VAL:HG11	2:F:231:MET:HE1	2.02	0.40
2:F:212:ARG:CG	2:F:212:ARG:NH1	2.81	0.40
1:G:375:THR:HG23	1:G:377:GLN:H	1.86	0.40
1:G:426:ARG:NH2	10:G:5760:HOH:O	2.49	0.40
1:G:839:LEU:HA	1:G:839:LEU:HD12	1.69	0.40
1:G:915:GLY:HA2	10:G:5183:HOH:O	2.21	0.40
1:G:1000:HIS:CD2	1:G:1000:HIS:C	2.98	0.40
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.81	0.40
2:H:81:VAL:HG11	2:H:113:ILE:HD11	2.03	0.40
1:A:9:SER:OG	1:A:83:PRO:HA	2.21	0.40
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.16	0.40
2:B:197:TYR:HA	2:B:219:VAL:HG22	2.02	0.40
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.02	0.40
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.56	0.40
1:E:159:ALA:HB2	1:E:188:PHE:CE2	2.56	0.40
1:E:167:ILE:HD12	1:E:167:ILE:N	2.37	0.40
2:F:300:VAL:HG22	2:F:328:THR:C	2.46	0.40
1:G:453:PHE:CD1	1:G:453:PHE:C	2.99	0.40
1:G:712:LEU:O	1:G:727:ILE:HA	2.22	0.40
1:G:858:GLY:O	1:G:860:PRO:HD3	2.22	0.40
1:G:860:PRO:O	1:G:864:VAL:HG23	2.22	0.40
2:H:132:ILE:CG2	2:H:133:ILE:N	2.84	0.40
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.88	0.40
1:A:475:LYS:HE2	1:A:488:PHE:CE2	2.56	0.40
1:C:318:PRO:HB2	1:C:321:LYS:HB2	2.02	0.40
1:C:453:PHE:CD1	1:C:453:PHE:C	2.99	0.40
1:C:708:ILE:HG21	1:C:712:LEU:HD11	2.03	0.40
1:G:51:PRO:HG2	1:G:916:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:ASN:N	1:G:236:ASN:HD22	2.20	0.40
1:G:726:GLU:OE1	1:G:1020:ARG:HD3	2.21	0.40
1:G:733:ASP:HA	1:G:736:ARG:NH1	2.29	0.40
2:H:379:LYS:HE2	2:H:379:LYS:HB3	1.65	0.40
1:A:115:MET:HG2	1:A:118:ALA:O	2.21	0.40
1:A:222:ARG:HD3	1:A:277:VAL:O	2.22	0.40
1:A:441:ASP:OD2	1:A:444:ARG:NH1	2.49	0.40
1:A:820:LEU:O	1:A:821:GLN:HB2	2.21	0.40
1:A:840:ILE:O	1:A:841:GLU:HB3	2.22	0.40
2:B:341:HIS:CD2	2:B:348:PHE:HB3	2.57	0.40
1:C:9:SER:HG	1:C:84:ASP:H	1.65	0.40
1:C:571:ARG:HD3	1:C:571:ARG:N	2.36	0.40
1:C:627:LEU:HA	1:C:627:LEU:HD23	1.87	0.40
1:C:714:VAL:HG21	1:C:728:VAL:CG2	2.52	0.40
1:C:772:MET:HE1	1:C:880:THR:CA	2.51	0.40
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.22	0.40
1:E:693:ALA:HB3	1:E:708:ILE:HD11	2.02	0.40
1:G:481:ILE:O	1:G:481:ILE:HG13	2.21	0.40
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.52	0.40
1:G:1021:ARG:CG	1:G:1021:ARG:NH1	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1055/1073 (98%)	1010 (96%)	43 (4%)	2 (0%)	43	42
1	C	1055/1073 (98%)	999 (95%)	53 (5%)	3 (0%)	36	35
1	E	1058/1073 (99%)	1013 (96%)	42 (4%)	3 (0%)	36	35
1	G	1055/1073 (98%)	1000 (95%)	51 (5%)	4 (0%)	30	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	376/382 (98%)	357 (95%)	19 (5%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	376/382 (98%)	361 (96%)	15 (4%)	0	100	100
2	H	377/382 (99%)	367 (97%)	10 (3%)	0	100	100
All	All	5729/5820 (98%)	5471 (96%)	246 (4%)	12 (0%)	43	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	954	LYS
1	G	739	GLN
1	A	558	ASP
1	C	739	GLN
1	E	738	PHE
1	G	873	SER
1	A	975	HIS
1	C	2	PRO
1	E	675	ARG
1	G	2	PRO
1	G	788	HIS
1	C	698	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	868/878 (99%)	799 (92%)	69 (8%)	11	8
1	C	868/878 (99%)	793 (91%)	75 (9%)	10	6
1	E	871/878 (99%)	806 (92%)	65 (8%)	12	9
1	G	868/878 (99%)	803 (92%)	65 (8%)	12	9
2	B	307/309 (99%)	279 (91%)	28 (9%)	9	6
2	D	308/309 (100%)	283 (92%)	25 (8%)	11	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	307/309 (99%)	280 (91%)	27 (9%)	9	6
2	H	308/309 (100%)	275 (89%)	33 (11%)	6	4
All	All	4705/4748 (99%)	4318 (92%)	387 (8%)	10	7

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	46	LEU
1	A	103	GLU
1	A	148	ILE
1	A	174	MET
1	A	202	LYS
1	A	220	VAL
1	A	297	VAL
1	A	299	GLU
1	A	326	LEU
1	A	343	ARG
1	A	344	THR
1	A	358	LYS
1	A	363	ASN
1	A	412	LYS
1	A	422	THR
1	A	426	ARG
1	A	428	LEU
1	A	468	GLU
1	A	548	GLU
1	A	549	GLU
1	A	554	ASN
1	A	559	ARG
1	A	571	ARG
1	A	591	GLU
1	A	652	ARG
1	A	671	ARG
1	A	674	ASP
1	A	675	ARG
1	A	688	LYS
1	A	696	THR
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS

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Mol	Chain	Res	Type
1	A	712	LEU
1	A	714	VAL
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	751	LEU
1	A	752	LEU
1	A	757	ASP
1	A	763	ASP
1	A	771	GLU
1	A	784	GLN
1	A	805	ILE
1	A	811	GLN
1	A	815	LYS
1	A	835	ASN
1	A	841	GLU
1	A	845	ARG
1	A	855	LYS
1	A	876	GLU
1	A	881	LYS
1	A	891	LYS
1	A	906	LEU
1	A	912	ARG
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	955	GLU
1	A	967	GLN
1	A	992	ASN
1	A	1001	ILE
1	A	1006	LYS
1	A	1021	ARG
1	A	1026	SER
1	A	1072	ILE
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	7	LEU
2	B	35	SER
2	B	50	ARG
2	B	87	LEU
2	B	123	ARG

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Mol	Chain	Res	Type
2	B	153	LEU
2	B	154	ASN
2	B	166	GLU
2	B	186	LYS
2	B	192	PHE
2	B	215	ARG
2	B	218	ILE
2	B	219	VAL
2	B	222	GLN
2	B	257	LYS
2	B	282	LYS
2	B	301	GLU
2	B	304	VAL
2	B	306	MET
2	B	324	ASN
2	B	332	LEU
2	B	333	PHE
2	B	357	SER
2	B	372	GLU
2	B	376	GLN
2	B	379	LYS
1	C	38	ARG
1	C	44	VAL
1	C	45	ILE
1	C	46	LEU
1	C	55	MET
1	C	103	GLU
1	C	148	ILE
1	C	167	ILE
1	C	174	MET
1	C	202	LYS
1	C	299	GLU
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	339	ILE
1	C	343	ARG
1	C	363	ASN
1	C	412	LYS
1	C	414	SER
1	C	419	GLU
1	C	422	THR

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Mol	Chain	Res	Type
1	C	426	ARG
1	C	428	LEU
1	C	481	ILE
1	C	509	ARG
1	C	548	GLU
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	632	ILE
1	C	634	LYS
1	C	645	GLN
1	C	648	LEU
1	C	652	ARG
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	677	ARG
1	C	688	LYS
1	C	696	THR
1	C	704	LYS
1	C	706	LYS
1	C	712	LEU
1	C	714	VAL
1	C	728	VAL
1	C	733	ASP
1	C	735	ARG
1	C	750	VAL
1	C	751	LEU
1	C	763	ASP
1	C	784	GLN
1	C	800	THR
1	C	805	ILE
1	C	815	LYS
1	C	849	THR
1	C	855	LYS
1	C	891	LYS
1	C	906	LEU
1	C	912	ARG
1	C	940	LYS
1	C	950	ARG
1	C	951	GLU
1	C	955	GLU

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Mol	Chain	Res	Type
1	C	956	ARG
1	C	1003	ASP
1	C	1006	LYS
1	C	1009[A]	GLU
1	C	1009[B]	GLU
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1027	ARG
1	C	1028	VAL
1	C	1061	LYS
1	C	1072	ILE
2	D	2	ILE
2	D	50	ARG
2	D	78	GLN
2	D	87	LEU
2	D	153	LEU
2	D	154	ASN
2	D	166	GLU
2	D	178	THR
2	D	183	GLU
2	D	188	ASP
2	D	215	ARG
2	D	222	GLN
2	D	232	ASN
2	D	257	LYS
2	D	282	LYS
2	D	301	GLU
2	D	306	MET
2	D	321	LEU
2	D	324	ASN
2	D	332	LEU
2	D	366	LEU
2	D	372[A]	GLU
2	D	372[B]	GLU
2	D	379	LYS
2	D	380	THR
1	E	1	MET
1	E	5	THR
1	E	46	LEU
1	E	55	MET
1	E	162	VAL

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Mol	Chain	Res	Type
1	E	174	MET
1	E	220	VAL
1	E	275	ILE
1	E	321	LYS
1	E	326	LEU
1	E	343	ARG
1	E	358	LYS
1	E	363	ASN
1	E	366	LYS
1	E	412	LYS
1	E	419	GLU
1	E	426	ARG
1	E	429	LYS
1	E	479	VAL
1	E	509	ARG
1	E	548	GLU
1	E	556	SER
1	E	559	ARG
1	E	571	ARG
1	E	591	GLU
1	E	634	LYS
1	E	675	ARG
1	E	677	ARG
1	E	688	LYS
1	E	696	THR
1	E	698	ILE
1	E	702	VAL
1	E	706	LYS
1	E	712	LEU
1	E	714	VAL
1	E	725	MET
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	750	VAL
1	E	751	LEU
1	E	752	LEU
1	E	784	GLN
1	E	795	SER
1	E	805	ILE
1	E	811	GLN
1	E	835	ASN

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Mol	Chain	Res	Type
1	E	845	ARG
1	E	849	THR
1	E	855	LYS
1	E	881	LYS
1	E	906	LEU
1	E	912	ARG
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG
1	E	963	LYS
1	E	967	GLN
1	E	993	LYS
1	E	1020	ARG
1	E	1021	ARG
1	E	1027	ARG
1	E	1031	ARG
1	E	1073	LYS
2	F	2	ILE
2	F	23	THR
2	F	50	ARG
2	F	87	LEU
2	F	106	ASN
2	F	153	LEU
2	F	166	GLU
2	F	183	GLU
2	F	186	LYS
2	F	192	PHE
2	F	205	ILE
2	F	212	ARG
2	F	215	ARG
2	F	216	LEU
2	F	238	LEU
2	F	239	SER
2	F	256	GLN
2	F	257	LYS
2	F	261	THR
2	F	301	GLU
2	F	306	MET
2	F	324	ASN
2	F	331	SER
2	F	332	LEU

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Mol	Chain	Res	Type
2	F	366	LEU
2	F	372	GLU
2	F	379	LYS
1	G	8	LYS
1	G	46	LEU
1	G	55	MET
1	G	76	LYS
1	G	145	ARG
1	G	146	SER
1	G	174	MET
1	G	236	ASN
1	G	297	VAL
1	G	307	SER
1	G	321	LYS
1	G	326	LEU
1	G	423	LYS
1	G	426	ARG
1	G	479	VAL
1	G	481	ILE
1	G	482	THR
1	G	519	GLN
1	G	548	GLU
1	G	559	ARG
1	G	571	ARG
1	G	591	GLU
1	G	631	ARG
1	G	634	LYS
1	G	652	ARG
1	G	671	ARG
1	G	673	GLU
1	G	675	ARG
1	G	684	ARG
1	G	688	LYS
1	G	692	ASN
1	G	696	THR
1	G	702	VAL
1	G	706	LYS
1	G	712	LEU
1	G	714	VAL
1	G	733	ASP
1	G	734	LEU
1	G	735	ARG

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Mol	Chain	Res	Type
1	G	752	LEU
1	G	763	ASP
1	G	778	ILE
1	G	784	GLN
1	G	805	ILE
1	G	815	LYS
1	G	835	ASN
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	869	MET
1	G	884	ILE
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	949	VAL
1	G	950	ARG
1	G	951	GLU
1	G	956	ARG
1	G	966	LYS
1	G	967	GLN
1	G	1018	SER
1	G	1020	ARG
1	G	1021	ARG
1	G	1031	ARG
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	7	LEU
2	H	50	ARG
2	H	73	SER
2	H	87	LEU
2	H	104	ARG
2	H	113	ILE
2	H	123	ARG
2	H	125	LYS
2	H	153	LEU
2	H	154	ASN
2	H	166	GLU
2	H	183	GLU
2	H	192	PHE
2	H	216	LEU

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Mol	Chain	Res	Type
2	H	222	GLN
2	H	223	THR
2	H	238	LEU
2	H	257	LYS
2	H	263	ILE
2	H	279	SER
2	H	282	LYS
2	H	286	MET
2	H	301	GLU
2	H	306	MET
2	H	321	LEU
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	366	LEU
2	H	376	GLN
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	645	GLN
1	A	679	GLN
1	A	689	GLN
1	A	692	ASN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	827	ASN
1	A	835	ASN
1	A	843	ASN
1	A	898	ASN
1	A	936	ASN
1	A	987	ASN
1	A	992	ASN
1	A	995	HIS
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	16	HIS
2	B	51	GLN

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Mol	Chain	Res	Type
2	B	78	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN
1	C	391	GLN
1	C	679	GLN
1	C	689	GLN
1	C	784	GLN
1	C	803	GLN
1	C	827	ASN
1	C	835	ASN
1	C	843	ASN
1	C	936	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1007	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	78	GLN
2	D	222	GLN
2	D	324	ASN
2	D	351	GLN
1	E	105	GLN
1	E	266	ASN
1	E	337	ASN
1	E	391	GLN
1	E	457	ASN
1	E	784	GLN
1	E	803	GLN
1	E	812	GLN
1	E	814	GLN
1	E	827	ASN
1	E	843	ASN
1	E	898	ASN
1	E	936	ASN
1	E	942	HIS

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Mol	Chain	Res	Type
1	E	992	ASN
1	E	1000	HIS
1	E	1015	ASN
1	E	1035	GLN
2	F	51	GLN
2	F	78	GLN
2	F	105	HIS
2	F	154	ASN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	266	ASN
1	G	457	ASN
1	G	645	GLN
1	G	679	GLN
1	G	692	ASN
1	G	784	GLN
1	G	803	GLN
1	G	814	GLN
1	G	827	ASN
1	G	835	ASN
1	G	843	ASN
1	G	898	ASN
1	G	932	GLN
1	G	936	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	78	GLN
2	H	105	HIS
2	H	129	ASN
2	H	154	ASN
2	H	222	GLN
2	H	324	ASN
2	H	351	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CYG	D	269	2	12,14,15	2.88	4 (33%)	10,17,19	4.48	3 (30%)
2	CYG	F	269	2	12,14,15	2.89	5 (41%)	10,17,19	4.48	3 (30%)
2	CYG	H	269	2	12,14,15	2.90	5 (41%)	10,17,19	4.49	3 (30%)
2	CYG	B	269	2	12,14,15	2.88	5 (41%)	10,17,19	4.49	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CYG	D	269	2	-	5/14/16/18	-
2	CYG	F	269	2	-	5/14/16/18	-
2	CYG	H	269	2	-	5/14/16/18	-
2	CYG	B	269	2	-	5/14/16/18	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	CYG	OE2-CD1	7.36	1.32	1.21
2	F	269	CYG	OE2-CD1	7.31	1.32	1.21
2	D	269	CYG	OE2-CD1	7.31	1.32	1.21
2	B	269	CYG	OE2-CD1	7.29	1.32	1.21
2	F	269	CYG	O1-C1	4.67	1.35	1.22
2	B	269	CYG	O1-C1	4.67	1.35	1.22
2	H	269	CYG	O1-C1	4.67	1.35	1.22
2	D	269	CYG	O1-C1	4.66	1.35	1.22
2	H	269	CYG	CD1-SG	-3.74	1.67	1.76
2	F	269	CYG	CD1-SG	-3.73	1.67	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	269	CYG	CD1-SG	-3.72	1.67	1.76
2	D	269	CYG	CD1-SG	-3.71	1.67	1.76
2	D	269	CYG	O2-C1	2.07	1.37	1.30
2	F	269	CYG	O2-C1	2.06	1.37	1.30
2	H	269	CYG	O2-C1	2.05	1.37	1.30
2	B	269	CYG	O2-C1	2.05	1.37	1.30
2	H	269	CYG	CG1-CD1	2.02	1.52	1.50
2	B	269	CYG	CG1-CD1	2.01	1.52	1.50
2	F	269	CYG	CG1-CD1	2.00	1.52	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	269	CYG	OE2-CD1-CG1	-10.49	111.88	123.98
2	B	269	CYG	OE2-CD1-CG1	-10.48	111.89	123.98
2	F	269	CYG	OE2-CD1-CG1	-10.48	111.89	123.98
2	D	269	CYG	OE2-CD1-CG1	-10.45	111.92	123.98
2	D	269	CYG	OE2-CD1-SG	-8.75	111.55	122.68
2	B	269	CYG	OE2-CD1-SG	-8.75	111.56	122.68
2	H	269	CYG	OE2-CD1-SG	-8.74	111.57	122.68
2	F	269	CYG	OE2-CD1-SG	-8.73	111.57	122.68
2	B	269	CYG	CB-SG-CD1	-2.59	97.21	100.76
2	F	269	CYG	CB-SG-CD1	-2.59	97.21	100.76
2	H	269	CYG	CB-SG-CD1	-2.58	97.22	100.76
2	D	269	CYG	CB-SG-CD1	-2.58	97.22	100.76

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	CYG	N-CA-CB-SG
2	B	269	CYG	SG-CD1-CG1-CB1
2	D	269	CYG	N-CA-CB-SG
2	D	269	CYG	SG-CD1-CG1-CB1
2	F	269	CYG	N-CA-CB-SG
2	F	269	CYG	SG-CD1-CG1-CB1
2	H	269	CYG	N-CA-CB-SG
2	H	269	CYG	SG-CD1-CG1-CB1
2	B	269	CYG	CG1-CD1-SG-CB
2	D	269	CYG	CG1-CD1-SG-CB
2	F	269	CYG	CG1-CD1-SG-CB
2	H	269	CYG	CG1-CD1-SG-CB

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Mol	Chain	Res	Type	Atoms
2	B	269	CYG	CA-CB-SG-CD1
2	D	269	CYG	CA-CB-SG-CD1
2	F	269	CYG	CA-CB-SG-CD1
2	H	269	CYG	CA-CB-SG-CD1
2	B	269	CYG	OE2-CD1-SG-CB
2	D	269	CYG	OE2-CD1-SG-CB
2	F	269	CYG	OE2-CD1-SG-CB
2	H	269	CYG	OE2-CD1-SG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	269	CYG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 74 are monoatomic - leaving 21 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	$\# Z > 2$
8	ORN	C	5033	-	7,8,8	1.09	1 (14%)	6,9,9	0.58	0
9	NET	G	5082	-	8,8,8	0.67	0	10,10,10	0.55	0
9	NET	A	5094	-	8,8,8	0.61	0	10,10,10	0.73	0
6	PO4	C	5028	4,3	4,4,4	2.32	3 (75%)	6,6,6	1.11	0
6	PO4	E	5070	-	4,4,4	1.95	2 (50%)	6,6,6	1.01	0
6	PO4	G	5076	4,3	4,4,4	2.17	2 (50%)	6,6,6	0.96	0
7	ADP	C	5023	3	28,29,29	1.71	5 (17%)	43,45,45	0.80	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	G	5077	4,3	28,29,29	1.32	5 (17%)	43,45,45	1.02	3 (6%)
8	ORN	G	5081	-	7,8,8	0.79	0	6,9,9	0.99	0
7	ADP	E	5046	3	28,29,29	1.34	4 (14%)	43,45,45	0.80	1 (2%)
9	NET	E	5057	-	8,8,8	0.87	0	10,10,10	0.41	0
7	ADP	A	5006	4,3	28,29,29	1.38	3 (10%)	43,45,45	0.91	2 (4%)
8	ORN	A	5010	-	7,8,8	1.11	0	6,9,9	1.43	2 (33%)
8	ORN	E	5056	-	7,8,8	0.88	0	6,9,9	0.97	0
7	ADP	C	5029	4,3	28,29,29	1.29	4 (14%)	43,45,45	0.99	3 (6%)
6	PO4	E	5051	4,3	4,4,4	2.70	3 (75%)	6,6,6	0.96	0
7	ADP	G	5071	3	28,29,29	1.47	4 (14%)	43,45,45	1.23	3 (6%)
9	NET	C	5034	-	8,8,8	0.75	0	10,10,10	0.55	0
7	ADP	A	5000	3	28,29,29	1.40	4 (14%)	43,45,45	0.99	1 (2%)
6	PO4	A	5005	4,3	4,4,4	2.04	2 (50%)	6,6,6	1.12	0
7	ADP	E	5052	4,3	28,29,29	1.07	3 (10%)	43,45,45	0.97	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	E	5046	3	-	2/16/32/32	0/3/3/3
8	ORN	C	5033	-	-	6/8/8/8	-
9	NET	E	5057	-	-	0/12/12/12	-
7	ADP	A	5006	4,3	-	4/16/32/32	0/3/3/3
9	NET	G	5082	-	-	0/12/12/12	-
9	NET	A	5094	-	-	8/12/12/12	-
7	ADP	G	5071	3	-	2/16/32/32	0/3/3/3
8	ORN	A	5010	-	-	6/8/8/8	-
7	ADP	E	5052	4,3	-	4/16/32/32	0/3/3/3
8	ORN	E	5056	-	-	6/8/8/8	-
9	NET	C	5034	-	-	0/12/12/12	-
7	ADP	C	5029	4,3	-	4/16/32/32	0/3/3/3
7	ADP	A	5000	3	-	2/16/32/32	0/3/3/3
7	ADP	C	5023	3	-	1/16/32/32	0/3/3/3
7	ADP	G	5077	4,3	-	2/16/32/32	0/3/3/3
8	ORN	G	5081	-	-	6/8/8/8	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5023	ADP	PA-O3A	-6.49	1.52	1.59
7	A	5000	ADP	PA-O3A	-4.35	1.54	1.59
7	E	5046	ADP	PA-O3A	-4.35	1.54	1.59
7	A	5006	ADP	PA-O3A	-4.06	1.55	1.59
6	E	5051	PO4	P-O3	-3.72	1.43	1.54
7	C	5029	ADP	O3'-C3'	3.64	1.52	1.43
7	G	5071	ADP	PA-O3A	-3.61	1.55	1.59
7	G	5071	ADP	O3'-C3'	3.44	1.51	1.43
7	G	5071	ADP	C2-N1	3.26	1.39	1.33
7	G	5077	ADP	PA-O3A	-3.18	1.56	1.59
6	G	5076	PO4	P-O2	-3.12	1.45	1.54
6	E	5051	PO4	P-O2	-2.93	1.46	1.54
6	C	5028	PO4	P-O2	-2.90	1.46	1.54
7	C	5029	ADP	PA-O3A	-2.85	1.56	1.59
7	G	5077	ADP	O2'-C2'	2.84	1.50	1.43
7	C	5023	ADP	C2-N1	2.81	1.38	1.33
6	A	5005	PO4	P-O4	-2.74	1.46	1.54
6	C	5028	PO4	P-O3	-2.56	1.47	1.54
6	C	5028	PO4	P-O4	-2.55	1.47	1.54
6	E	5070	PO4	P-O3	-2.54	1.47	1.54
7	E	5052	ADP	C2-N1	2.51	1.38	1.33
7	C	5029	ADP	O2'-C2'	2.49	1.49	1.43
6	E	5051	PO4	P-O4	-2.48	1.47	1.54
6	G	5076	PO4	P-O4	-2.46	1.47	1.54
7	A	5000	ADP	O4'-C1'	-2.46	1.36	1.42
6	E	5070	PO4	P-O2	-2.42	1.47	1.54
7	G	5077	ADP	C2-N1	2.40	1.38	1.33
7	C	5023	ADP	PA-O2A	-2.38	1.44	1.55
7	A	5006	ADP	C2-N3	-2.38	1.29	1.33
7	A	5000	ADP	C2-N1	2.37	1.38	1.33
7	C	5023	ADP	O2'-C2'	2.30	1.48	1.43
7	A	5006	ADP	O3'-C3'	2.29	1.48	1.43
6	A	5005	PO4	P-O2	-2.24	1.48	1.54
7	A	5000	ADP	O3'-C3'	2.22	1.48	1.43
7	G	5077	ADP	C2-N3	-2.17	1.30	1.33
7	E	5046	ADP	O3'-C3'	2.15	1.48	1.43
7	E	5046	ADP	C2-N1	2.14	1.37	1.33
7	G	5071	ADP	O2'-C2'	2.14	1.48	1.43
8	C	5033	ORN	O-C	2.14	1.28	1.22
7	G	5077	ADP	O3'-C3'	2.13	1.48	1.43
7	E	5046	ADP	O4'-C1'	-2.12	1.37	1.42
7	E	5052	ADP	O3'-C3'	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5029	ADP	C2-N1	2.10	1.37	1.33
7	C	5023	ADP	PB-O2B	-2.08	1.47	1.54
7	E	5052	ADP	PA-O3A	-2.06	1.57	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	5071	ADP	O2'-C2'-C3'	3.97	124.54	111.82
7	G	5077	ADP	O3B-PB-O3A	3.49	116.35	104.64
7	E	5052	ADP	O2A-PA-O3A	3.31	116.22	107.27
7	G	5071	ADP	O3'-C3'-C2'	3.21	122.10	111.82
7	C	5029	ADP	O2A-PA-O3A	3.17	115.83	107.27
7	G	5071	ADP	O3B-PB-O3A	-2.67	95.68	104.64
7	A	5006	ADP	O3B-PB-O3A	2.58	113.30	104.64
7	C	5023	ADP	O2A-PA-O3A	2.52	114.07	107.27
7	G	5077	ADP	O2'-C2'-C3'	2.47	119.75	111.82
7	E	5052	ADP	C2'-C3'-C4'	-2.41	97.96	102.61
7	A	5000	ADP	N6-C6-N1	2.30	123.50	118.38
7	C	5029	ADP	O3'-C3'-C2'	2.30	119.19	111.82
7	E	5052	ADP	O3'-C3'-C2'	2.25	119.03	111.82
7	G	5077	ADP	O3'-C3'-C2'	2.23	118.95	111.82
7	E	5046	ADP	C3'-C2'-C1'	2.12	105.47	101.46
7	C	5029	ADP	O2'-C2'-C3'	2.12	118.61	111.82
7	C	5023	ADP	O3'-C3'-C2'	2.10	118.55	111.82
8	A	5010	ORN	OXT-C-O	-2.10	119.32	124.08
8	A	5010	ORN	CB-CA-C	-2.09	104.91	110.45
7	A	5006	ADP	C2'-C3'-C4'	-2.03	98.69	102.61

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5006	ADP	PA-O3A-PB-O3B
7	C	5029	ADP	PA-O3A-PB-O3B
7	E	5052	ADP	PA-O3A-PB-O3B
8	A	5010	ORN	N-CA-CB-CG
8	A	5010	ORN	C-CA-CB-CG
8	C	5033	ORN	N-CA-CB-CG
8	C	5033	ORN	C-CA-CB-CG
8	E	5056	ORN	N-CA-CB-CG
8	E	5056	ORN	C-CA-CB-CG
8	G	5081	ORN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
8	G	5081	ORN	C-CA-CB-CG
9	A	5094	NET	C4-C3-N1-C7
8	A	5010	ORN	OXT-C-CA-N
8	E	5056	ORN	CA-CB-CG-CD
9	A	5094	NET	C4-C3-N1-C5
9	A	5094	NET	C4-C3-N1-C1
8	E	5056	ORN	OXT-C-CA-N
8	C	5033	ORN	OXT-C-CA-N
8	A	5010	ORN	CA-CB-CG-CD
8	A	5010	ORN	O-C-CA-N
8	C	5033	ORN	O-C-CA-N
8	E	5056	ORN	O-C-CA-N
9	A	5094	NET	C8-C7-N1-C3
7	C	5029	ADP	PA-O3A-PB-O1B
7	A	5000	ADP	PB-O3A-PA-O1A
7	A	5006	ADP	PB-O3A-PA-O2A
7	C	5023	ADP	PB-O3A-PA-O1A
7	G	5071	ADP	PB-O3A-PA-O1A
8	C	5033	ORN	NE-CD-CG-CB
9	A	5094	NET	C8-C7-N1-C1
7	E	5046	ADP	C5'-O5'-PA-O1A
8	G	5081	ORN	OXT-C-CA-N
8	A	5010	ORN	NE-CD-CG-CB
8	G	5081	ORN	CA-CB-CG-CD
9	A	5094	NET	C8-C7-N1-C5
7	E	5052	ADP	PA-O3A-PB-O1B
8	G	5081	ORN	O-C-CA-N
8	C	5033	ORN	CA-CB-CG-CD
7	C	5029	ADP	PB-O3A-PA-O2A
7	E	5052	ADP	PB-O3A-PA-O2A
7	A	5006	ADP	PA-O3A-PB-O2B
8	E	5056	ORN	NE-CD-CG-CB
9	A	5094	NET	C6-C5-N1-C3
7	A	5006	ADP	PB-O3A-PA-O1A
7	C	5029	ADP	PB-O3A-PA-O1A
7	G	5077	ADP	PB-O3A-PA-O2A
9	A	5094	NET	C6-C5-N1-C1
8	G	5081	ORN	NE-CD-CG-CB
7	A	5000	ADP	PB-O3A-PA-O2A
7	E	5046	ADP	PB-O3A-PA-O2A
7	E	5052	ADP	PB-O3A-PA-O1A
7	G	5071	ADP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
7	G	5077	ADP	PB-O3A-PA-O1A

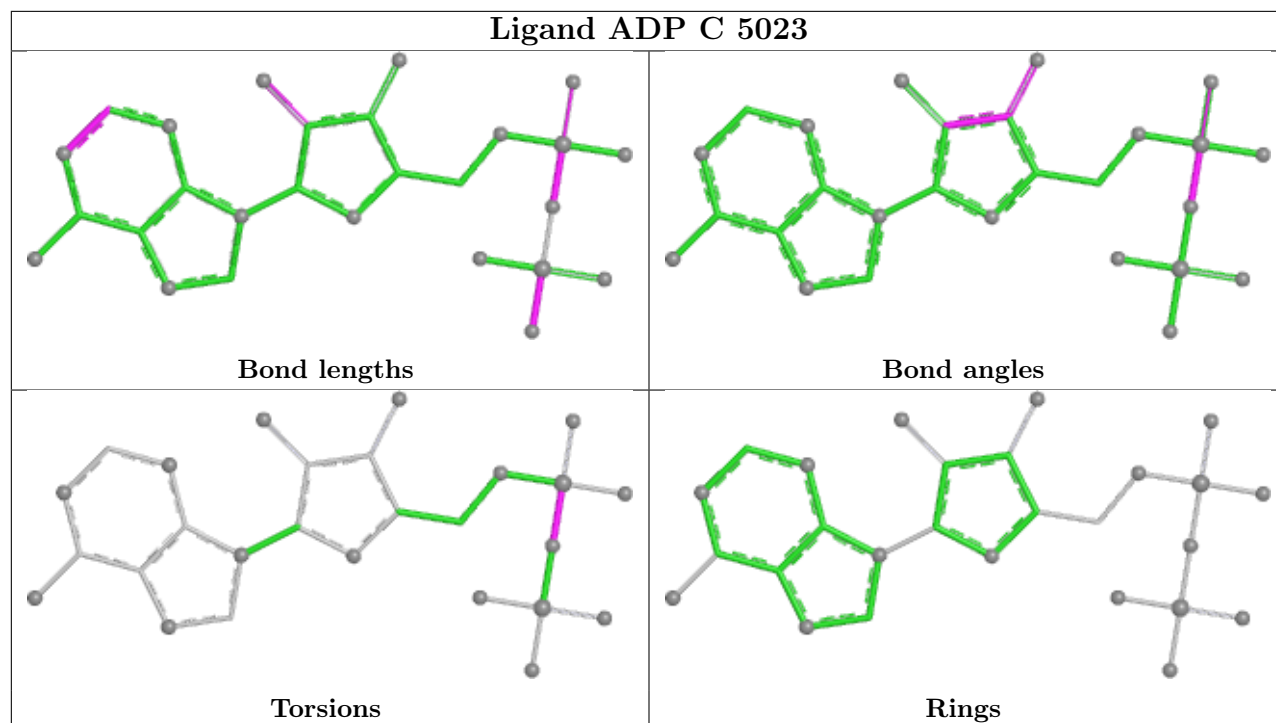
There are no ring outliers.

6 monomers are involved in 11 short contacts:

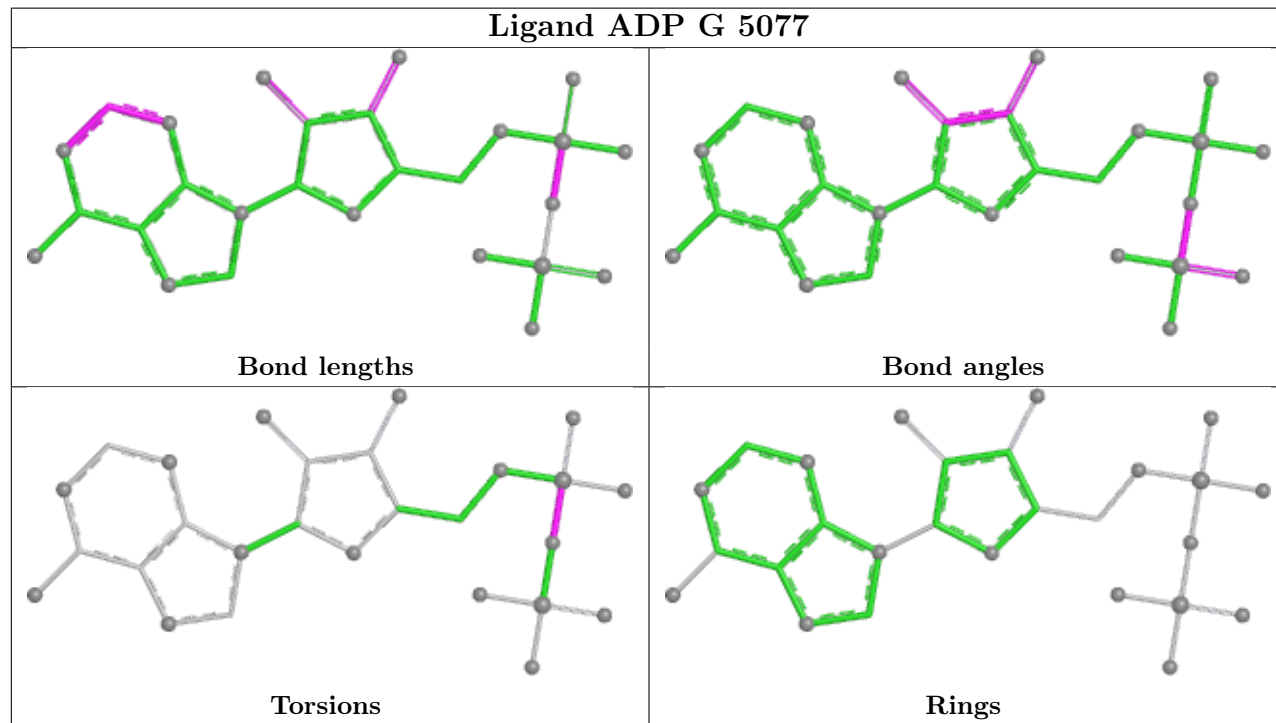
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5033	ORN	2	0
9	A	5094	NET	2	0
7	G	5077	ADP	2	0
9	E	5057	NET	1	0
8	E	5056	ORN	3	0
7	E	5052	ADP	1	0

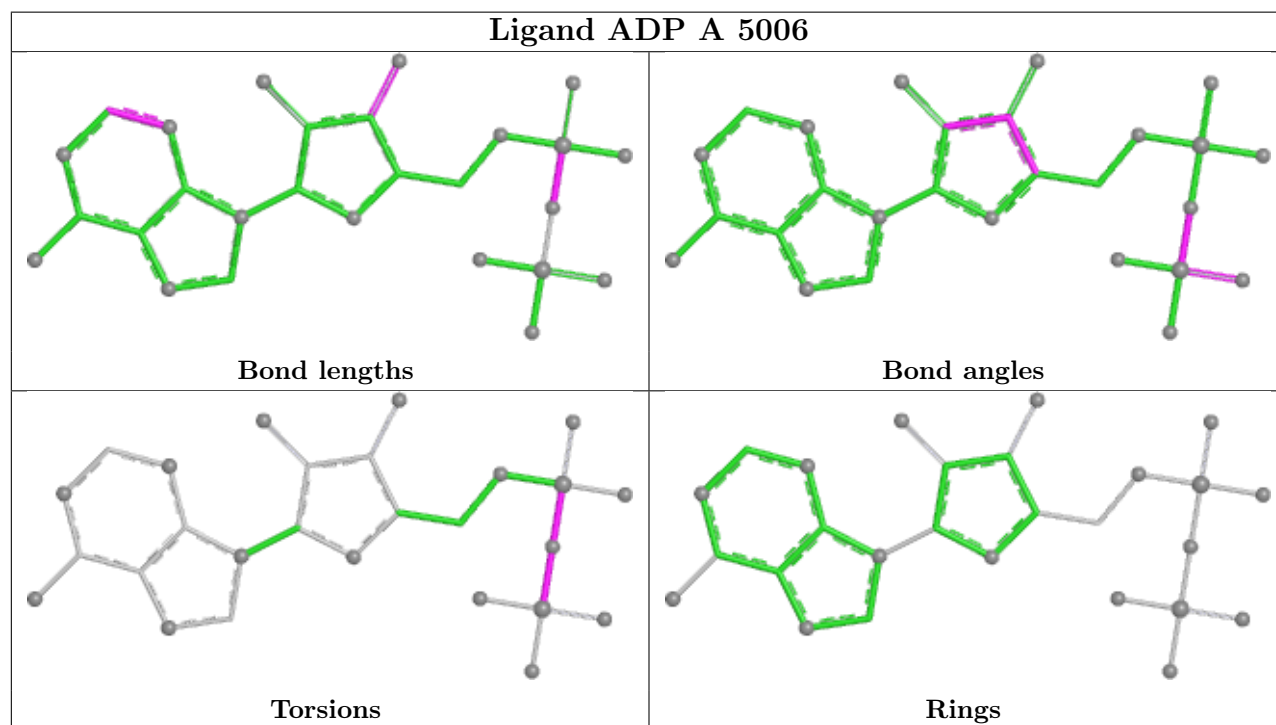
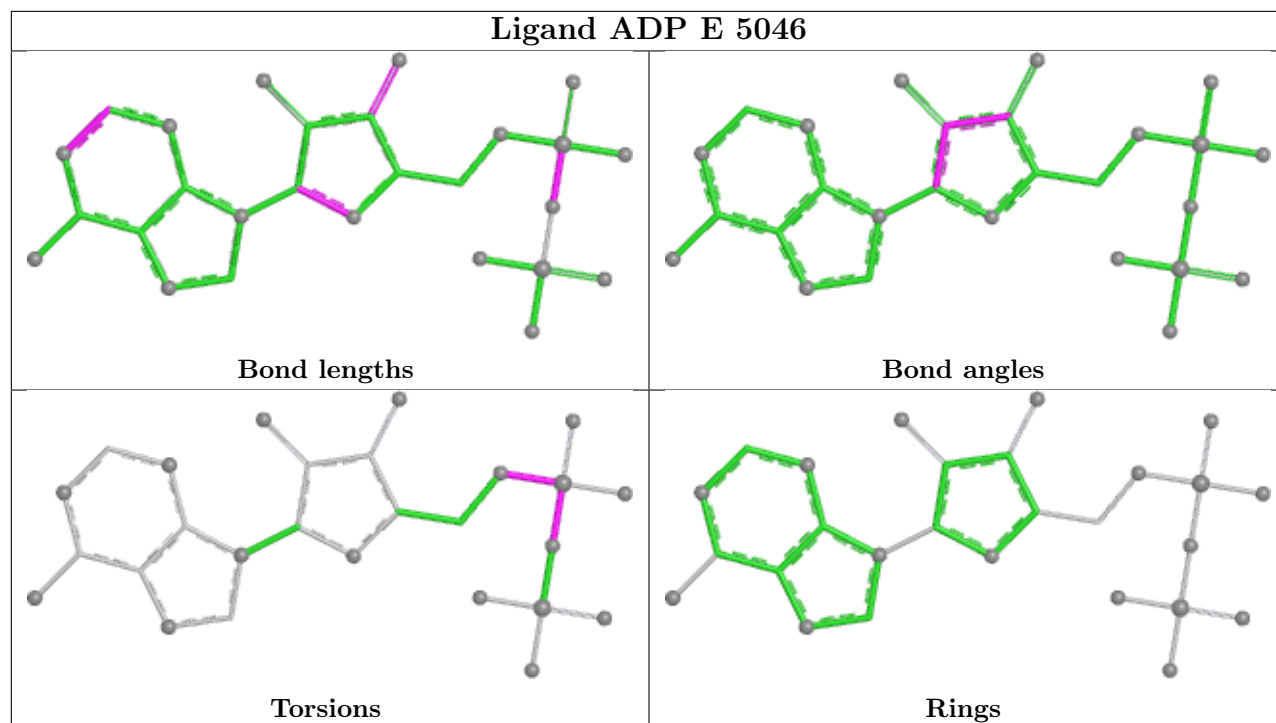
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP C 5023

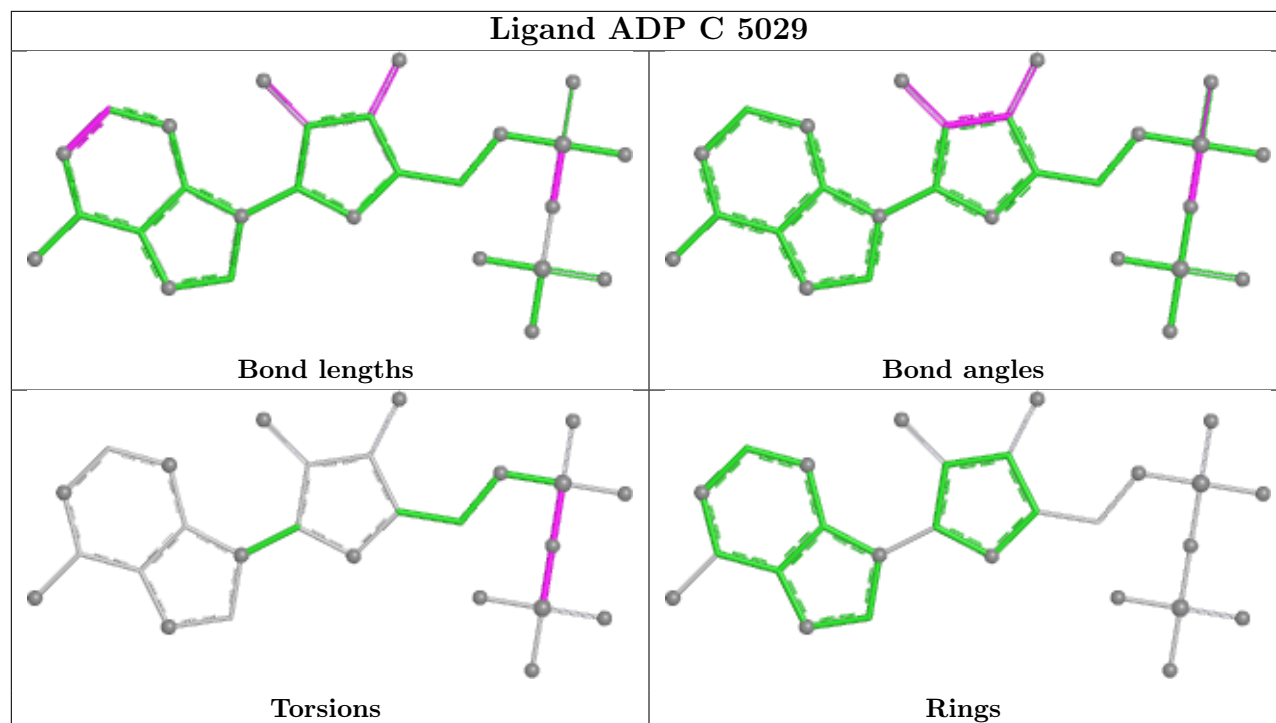


Ligand ADP G 5077

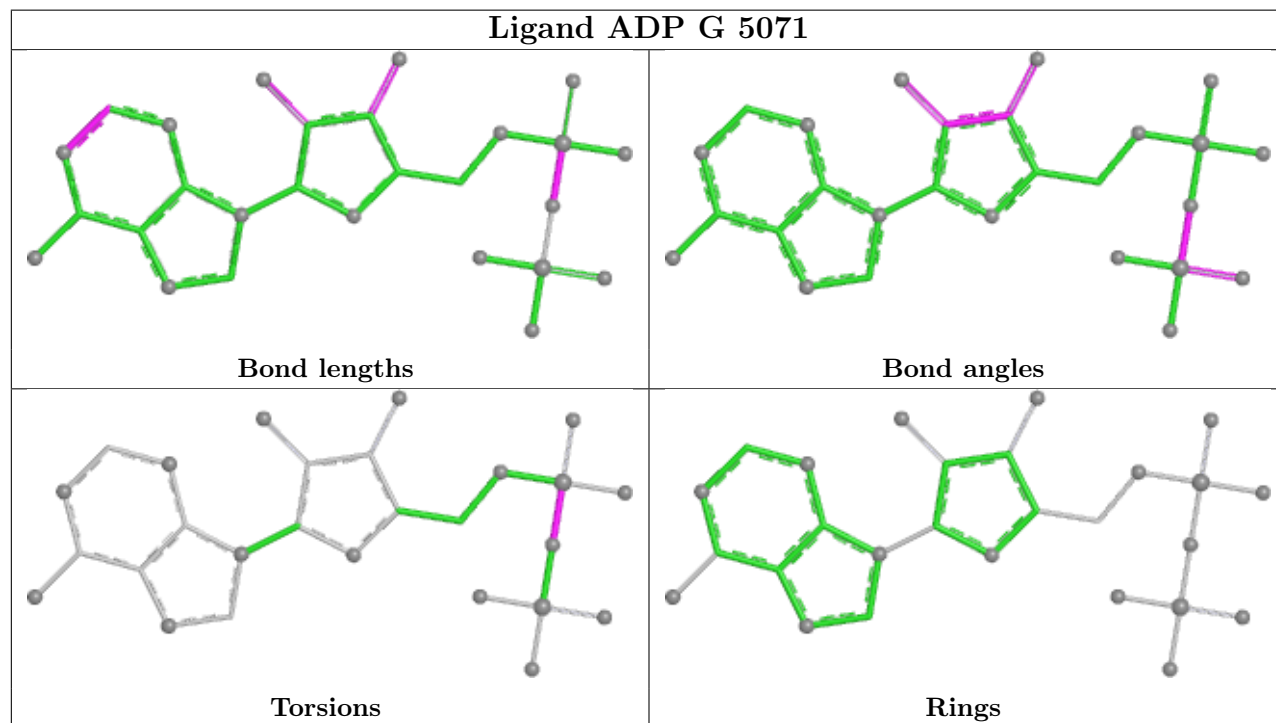


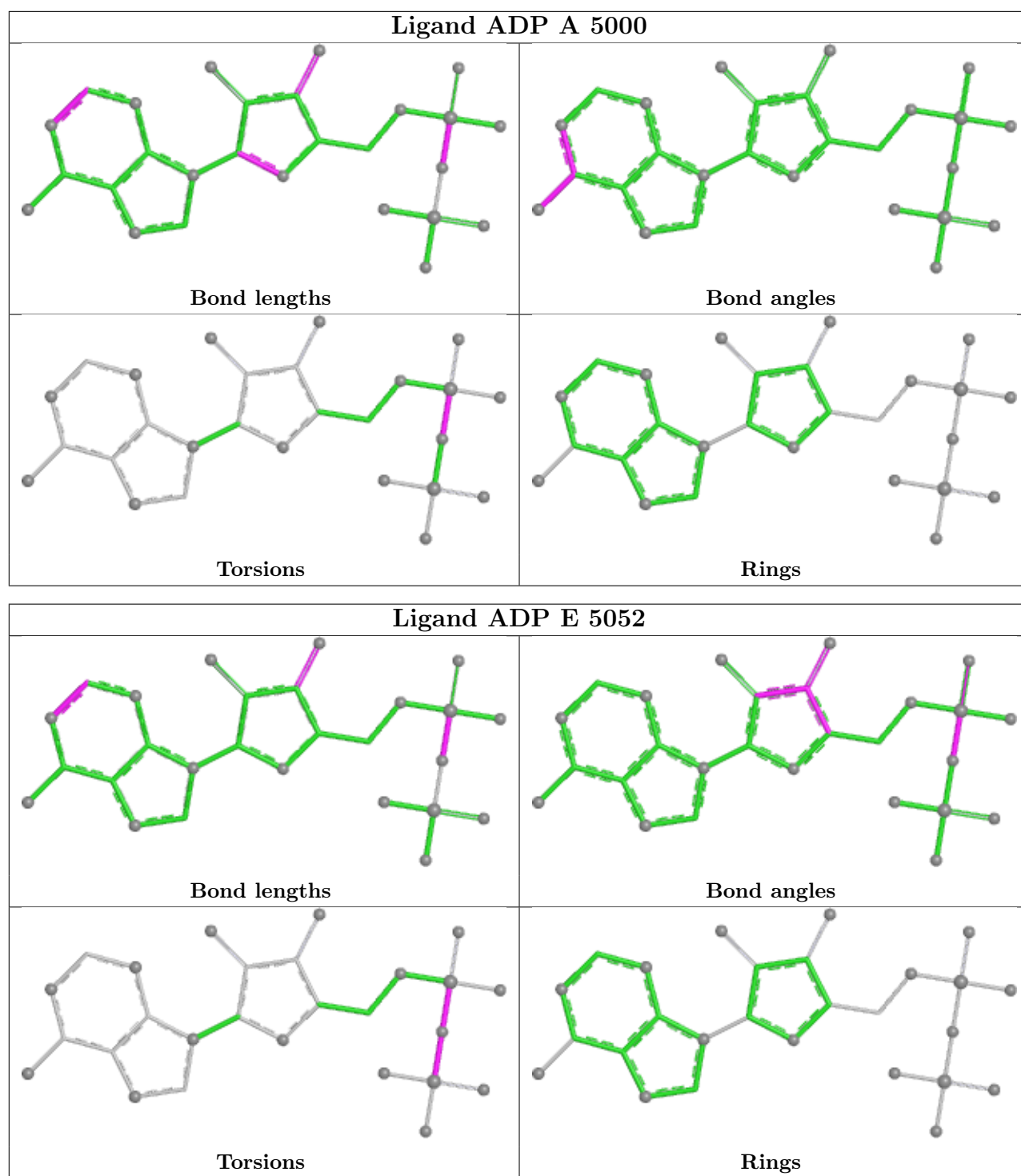


Ligand ADP C 5029



Ligand ADP G 5071





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.