



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 1A9X / pdb_00001a9x
Title : CARBAMOYL PHOSPHATE SYNTHETASE: CAUGHT IN THE ACT OF
GLUTAMINE HYDROLYSIS
Authors : Thoden, J.; Holden, H.
Deposited on : 1998-04-14
Resolution : 1.80 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

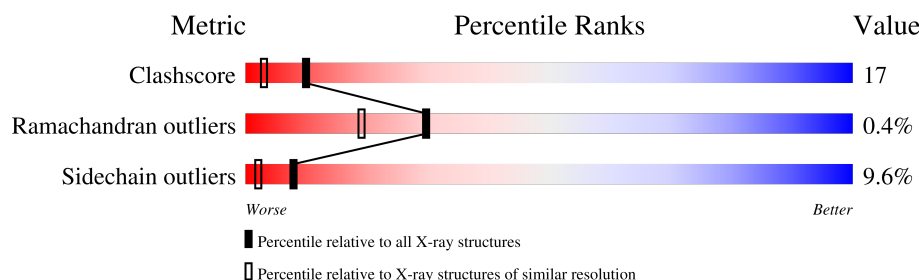
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	63% 30% 5% ..
1	C	1073	62% 29% 6% ..
1	E	1073	63% 30% 5% ..
1	G	1073	56% 34% 8% ..
2	B	379	59% 34% 7% .
2	D	379	63% 30% 7%
2	F	379	61% 32% 6%
2	H	379	52% 39% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	C	3906	-	X	-	-
3	PO4	C	3981	-	X	-	-
3	PO4	C	3982	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 49310 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 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	7	0
			8193	5142	1428	1577	46			
1	C	1058	Total	C	N	O	S	0	7	0
			8198	5144	1432	1577	45			
1	E	1058	Total	C	N	O	S	0	2	0
			8169	5126	1423	1575	45			
1	G	1058	Total	C	N	O	S	0	1	0
			8164	5123	1423	1573	45			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	conflict	UNP P00968
A	716	ALA	PRO	conflict	UNP P00968
C	2046	ASN	LEU	conflict	UNP P00968
C	2716	ALA	PRO	conflict	UNP P00968
E	4046	ASN	LEU	conflict	UNP P00968
E	4716	ALA	PRO	conflict	UNP P00968
G	6046	ASN	LEU	conflict	UNP P00968
G	6716	ALA	PRO	conflict	UNP P00968

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2904	1829	509	556	10			
2	D	379	Total	C	N	O	S	0	0	0
			2902	1828	509	555	10			
2	F	379	Total	C	N	O	S	0	3	0
			2915	1836	510	558	11			
2	H	379	Total	C	N	O	S	0	0	0
			2902	1828	509	555	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1683	GLN	GLU	conflict	UNP P00907
B	1769	CYG	CYS	modified residue	UNP P00907
B	1853	ASN	HIS	engineered mutation	UNP P00907
D	3683	GLN	GLU	conflict	UNP P00907
D	3769	CYG	CYS	modified residue	UNP P00907
D	3853	ASN	HIS	engineered mutation	UNP P00907
F	5683	GLN	GLU	conflict	UNP P00907
F	5769	CYG	CYS	modified residue	UNP P00907
F	5853	ASN	HIS	engineered mutation	UNP P00907
H	7683	GLN	GLU	conflict	UNP P00907
H	7769	CYG	CYS	modified residue	UNP P00907
H	7853	ASN	HIS	engineered mutation	UNP P00907

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total K 7 7	0	0
5	B	1	Total K 1 1	0	0
5	C	7	Total K 7 7	0	0

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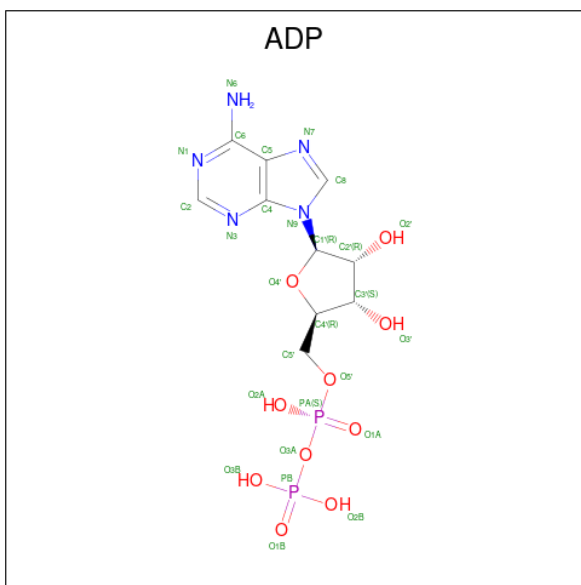
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0
5	E	7	Total K 7 7	0	0
5	F	1	Total K 1 1	0	0
5	G	7	Total K 7 7	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

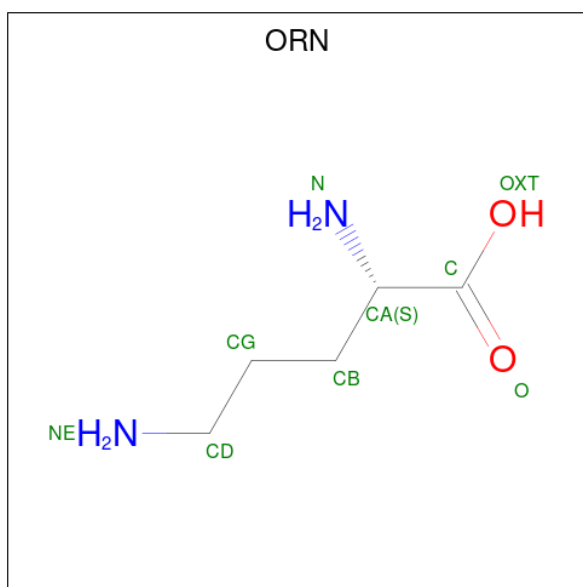
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total Cl 6 6	0	0
6	B	1	Total Cl 1 1	0	0
6	C	6	Total Cl 6 6	0	0
6	D	1	Total Cl 1 1	0	0
6	E	6	Total Cl 6 6	0	0
6	F	1	Total Cl 1 1	0	0
6	G	6	Total Cl 6 6	0	0
6	H	1	Total Cl 1 1	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



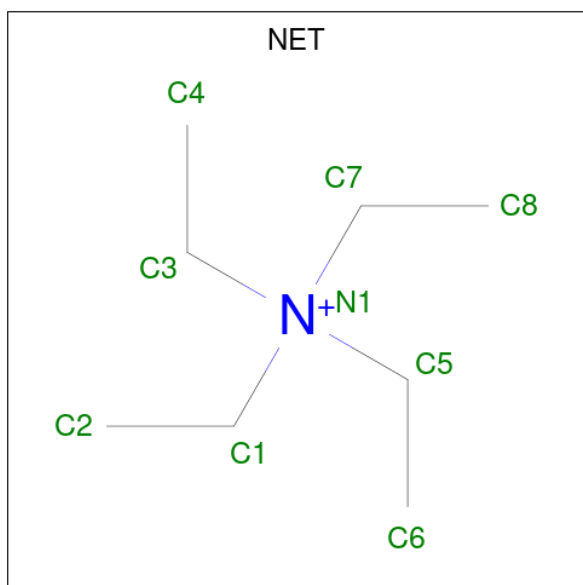
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0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

- Molecule 8 is L-ornithine (CCD ID: ORN) (formula: $\text{C}_5\text{H}_{12}\text{N}_2\text{O}_2$).



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.

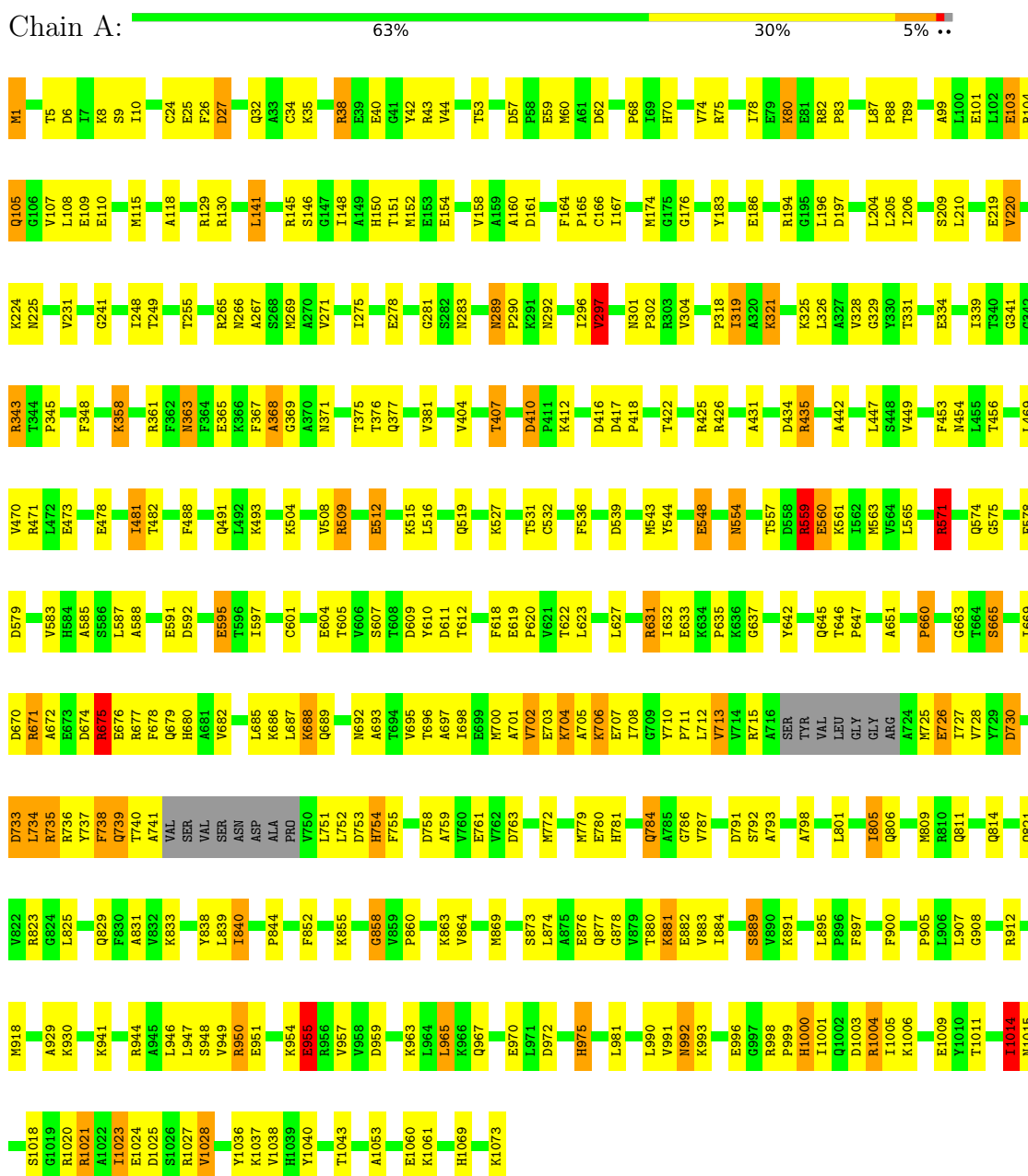
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	904	Total O 904 904	0	0
10	B	256	Total O 256 256	0	0
10	C	897	Total O 897 897	0	0
10	D	330	Total O 330 330	0	0
10	E	900	Total O 900 900	0	0
10	F	276	Total O 276 276	0	0
10	G	733	Total O 733 733	0	0
10	H	232	Total O 232 232	0	0

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.

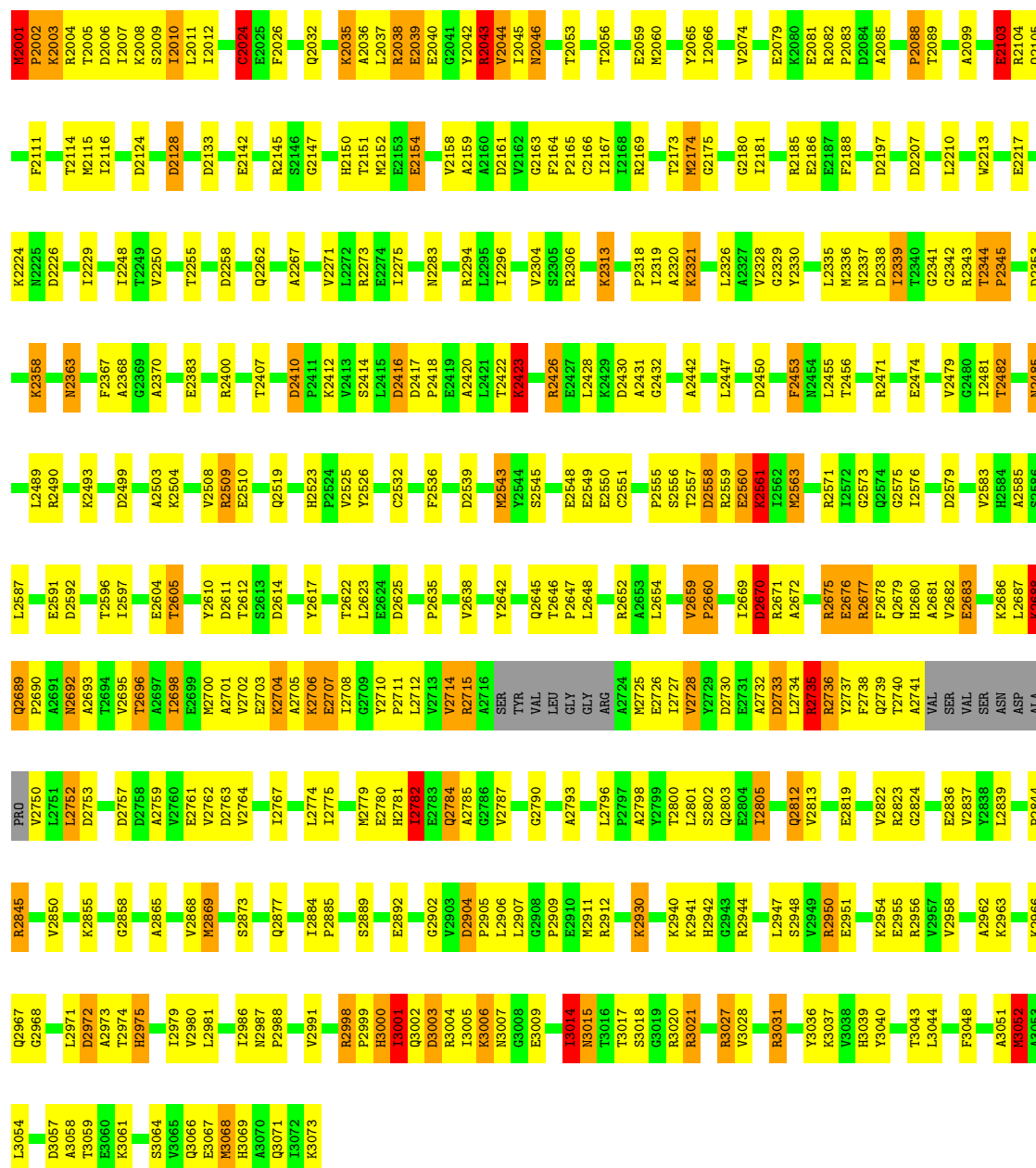
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)



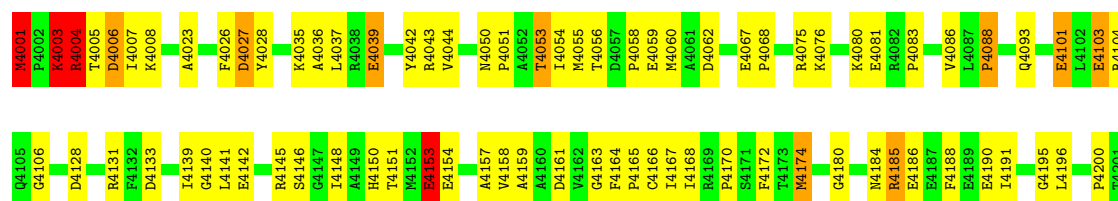
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

Chain C:  62% 29% 6% ..



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

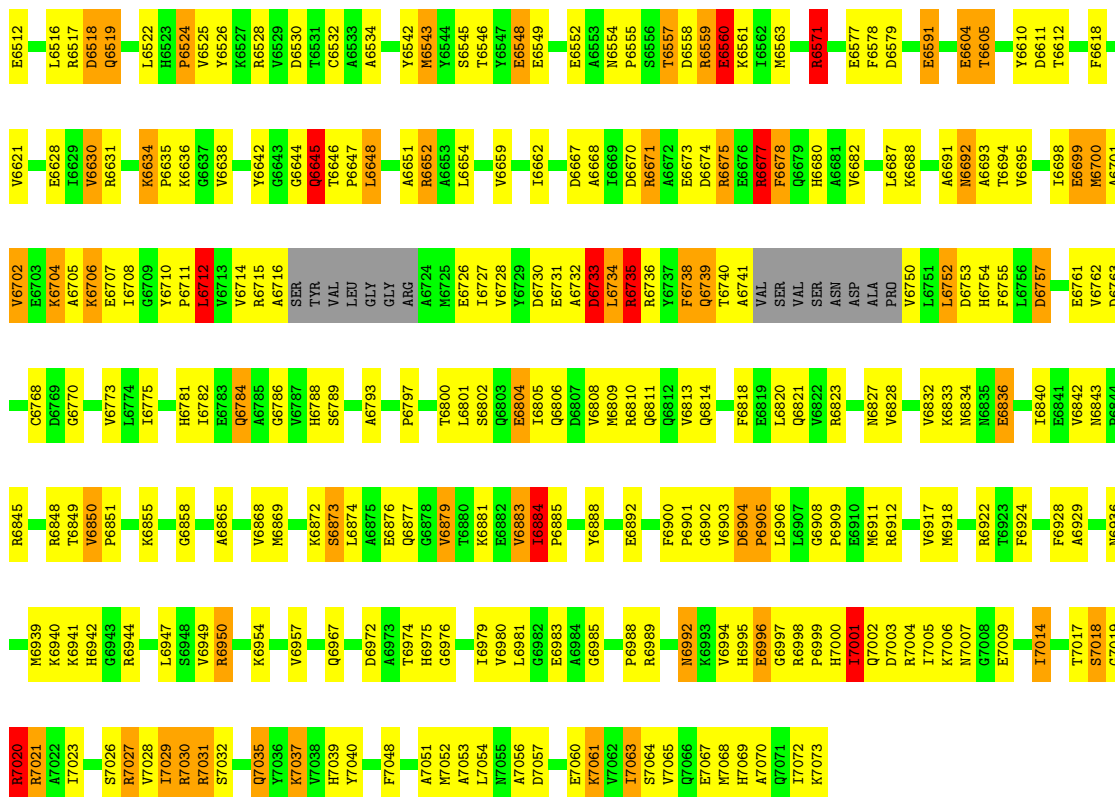
Chain E:  63% 30% 5% ..





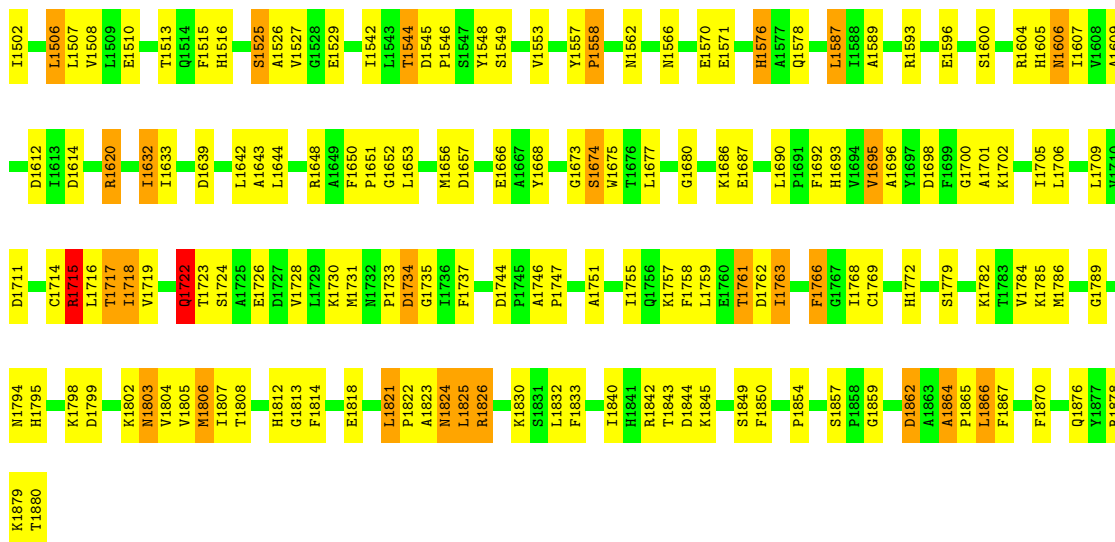
Chain G: 56% 34% 8% ..





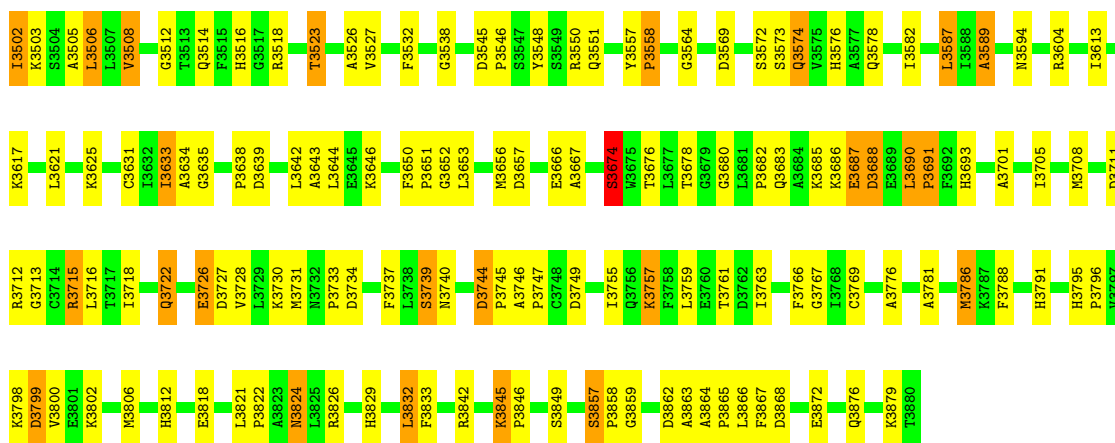
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain B: 59% 34% 7%



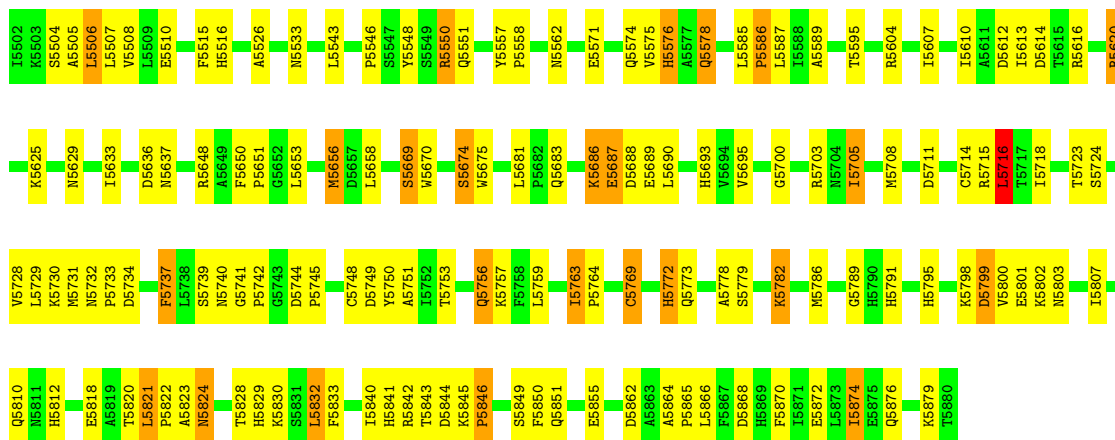
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain D:  63% 30% 7%



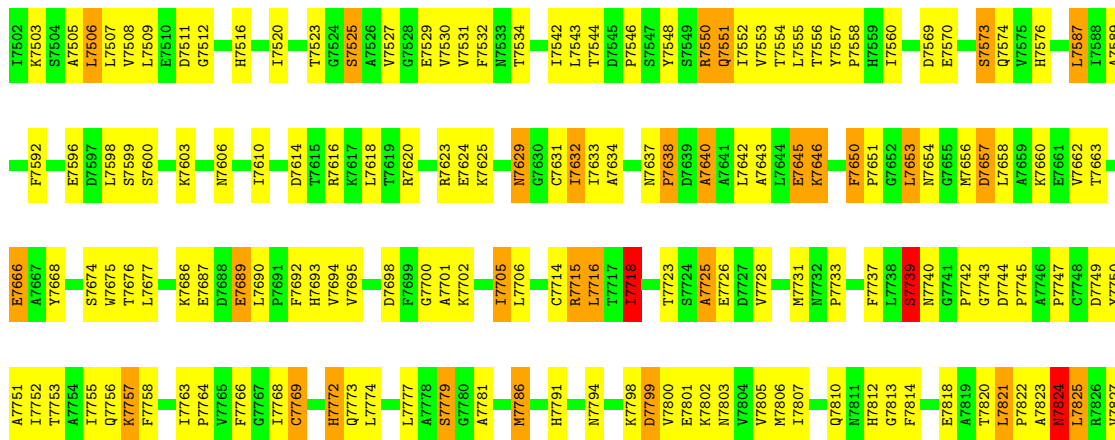
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain F: 61% 32% 6%



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain H: 52% 39% 9%



T7828	H7829	K7830	S7831	L7832	F7833
R7842	T7843	D7844	K7845	P7846	A7847
F7848	S7849	F7850	Q7851	G7852	N7853
P7854	E7855	D7862	A7863	A7864	P7865
L7866	Q7876	Y7877	R7878	K7879	T7880

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.10Å 164.40Å 332.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	92.0 (30.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49310	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: ORN, ADP, K, CL, CYG, MN, NET, 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	1.28	6/8347 (0.1%)	1.76	129/11284 (1.1%)
1	C	1.24	7/8352 (0.1%)	1.73	122/11288 (1.1%)
1	E	1.30	7/8303 (0.1%)	1.77	124/11225 (1.1%)
1	G	1.21	6/8294 (0.1%)	1.73	134/11213 (1.2%)
2	B	1.19	2/2953 (0.1%)	1.71	54/4009 (1.3%)
2	D	1.22	4/2947 (0.1%)	1.71	37/4001 (0.9%)
2	F	1.18	1/2972 (0.0%)	1.67	35/4034 (0.9%)
2	H	1.14	1/2947 (0.0%)	1.74	46/4001 (1.1%)
All	All	1.24	34/45115 (0.1%)	1.74	681/61055 (1.1%)

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	A	1	0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4912	ARG	CZ-NH2	-13.45	1.16	1.33
1	E	4670	ASP	CG-OD2	-11.97	1.02	1.25
1	G	6076	LYS	CE-NZ	-9.93	1.19	1.49
1	G	6757	ASP	CG-OD1	8.73	1.42	1.25
1	G	6905	PRO	CA-C	-7.59	1.45	1.52
1	C	2850	VAL	CA-CB	-7.25	1.50	1.54
1	G	6850	VAL	CA-CB	-6.56	1.50	1.54
1	A	80	LYS	CE-NZ	6.21	1.68	1.49
1	A	779	MET	CA-C	-5.93	1.45	1.52
1	E	4655	GLU	CD-OE1	5.73	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	7072	ILE	C-O	-5.72	1.17	1.24
1	C	2001	MET	SD-CE	5.64	1.93	1.79
1	C	2133	ASP	CG-OD2	5.61	1.36	1.25
1	E	4912	ARG	CZ-NH1	5.59	1.40	1.32
1	A	565	LEU	CA-C	-5.46	1.46	1.52
2	D	3872	GLU	CD-OE1	5.44	1.35	1.25
1	A	1004	ARG	NE-CZ	5.42	1.39	1.33
1	C	2683	GLU	CD-OE1	5.39	1.35	1.25
2	F	5533	ASN	C-O	-5.32	1.18	1.24
1	C	2088	PRO	N-CA	-5.32	1.44	1.47
2	D	3690	LEU	C-O	-5.28	1.20	1.25
1	G	6631	ARG	C-N	-5.24	1.27	1.33
1	E	4771	GLU	CD-OE2	5.23	1.35	1.25
1	E	4819	GLU	CD-OE1	5.22	1.35	1.25
1	E	4652	ARG	NE-CZ	5.17	1.38	1.33
1	C	2782	ILE	CA-CB	-5.07	1.48	1.54
2	B	1545	ASP	CG-OD1	5.06	1.34	1.25
2	B	1693	HIS	CA-C	-5.03	1.47	1.53
2	D	3545	ASP	CG-OD1	5.03	1.34	1.25
1	A	512	GLU	CD-OE1	5.01	1.34	1.25
1	C	2226	ASP	CG-OD1	5.01	1.34	1.25
2	D	3726	GLU	CD-OE1	5.01	1.34	1.25
2	H	7666	GLU	CD-OE2	5.01	1.34	1.25
1	A	454	ASN	N-CA	-5.00	1.40	1.46

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4001	MET	CA-C-N	-10.46	106.77	119.84
1	E	4001	MET	C-N-CA	-10.46	106.77	119.84
1	G	6560	GLU	N-CA-CB	10.44	127.44	110.42
1	A	417	ASP	CA-CB-CG	10.34	122.94	112.60
1	G	6884	ILE	CB-CA-C	9.62	120.22	111.08
1	A	605	THR	N-CA-C	9.59	124.50	110.59
1	C	2367	PHE	CA-CB-CG	-9.50	104.30	113.80
1	E	4782	ILE	N-CA-C	-9.47	102.12	110.74
2	D	3674	SER	N-CA-C	9.43	122.97	110.53
1	A	367	PHE	CA-CB-CG	-9.12	104.68	113.80
2	H	7657	ASP	CA-CB-CG	9.08	121.68	112.60
1	C	2885	PRO	O-C-N	8.95	125.36	121.15
1	G	6885	PRO	N-CA-CB	8.91	108.18	103.19
1	G	6578	PHE	CA-CB-CG	-8.87	104.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2885	PRO	N-CA-CB	8.87	107.83	103.22
1	A	543	MET	N-CA-C	8.78	123.13	109.52
2	B	1657	ASP	CA-CB-CG	8.68	121.28	112.60
1	C	2782	ILE	N-CA-C	-8.68	102.84	110.74
1	G	6319	ILE	N-CA-C	8.68	119.47	110.36
2	B	1803	ASN	CA-CB-CG	-8.63	103.97	112.60
1	E	4652	ARG	NE-CZ-NH2	-8.61	111.45	119.20
1	C	2884	ILE	N-CA-CB	8.55	123.19	111.21
1	G	6928	PHE	CA-CB-CG	-8.52	105.28	113.80
1	A	559	ARG	N-CA-C	8.50	123.31	110.14
1	E	4026	PHE	CA-CB-CG	-8.32	105.48	113.80
2	D	3862	ASP	N-CA-C	8.24	122.30	111.75
1	C	2824	GLY	N-CA-C	-8.18	103.30	111.56
1	G	6763	ASP	CA-CB-CG	8.17	120.77	112.60
1	E	4004	ARG	CA-C-N	-8.16	108.72	122.11
1	E	4004	ARG	C-N-CA	-8.16	108.72	122.11
2	F	5574	GLN	N-CA-C	8.16	120.00	108.74
1	A	248	ILE	N-CA-C	-8.06	98.25	109.21
1	A	908	GLY	CA-C-N	8.06	127.78	119.56
1	A	908	GLY	C-N-CA	8.06	127.78	119.56
1	A	328	VAL	CA-C-N	-8.00	110.76	123.31
1	A	328	VAL	C-N-CA	-8.00	110.76	123.31
2	F	5739	SER	N-CA-C	7.99	120.09	110.19
1	E	4559	ARG	N-CA-C	7.98	122.51	110.14
1	C	2558	ASP	N-CA-CB	-7.98	98.35	110.16
1	G	7039	HIS	CA-CB-CG	-7.97	105.83	113.80
1	A	536	PHE	CA-CB-CG	-7.96	105.84	113.80
2	D	3589	ALA	N-CA-C	-7.94	96.74	109.76
1	G	6557	THR	N-CA-C	-7.91	104.16	113.88
1	G	6612	THR	N-CA-C	7.90	120.79	111.71
1	A	726	GLU	N-CA-CB	7.87	125.17	111.39
1	E	4584	HIS	CA-CB-CG	-7.87	105.93	113.80
1	E	4912	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	G	6733	ASP	CA-CB-CG	7.86	120.46	112.60
1	E	4735	ARG	O-C-N	7.85	130.48	122.08
1	G	6559	ARG	N-CA-C	7.82	121.63	110.14
1	E	4543	MET	N-CA-CB	-7.80	99.35	111.05
2	F	5576	HIS	CA-CB-CG	-7.77	106.03	113.80
1	E	4906	LEU	N-CA-CB	-7.77	97.31	110.83
1	G	6026	PHE	CA-CB-CG	-7.72	106.08	113.80
1	C	2557	THR	CA-C-N	7.70	131.22	120.29
1	C	2557	THR	C-N-CA	7.70	131.22	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6044	VAL	N-CA-C	7.69	118.95	107.80
1	C	2328	VAL	CA-C-N	-7.67	114.31	123.44
1	C	2328	VAL	C-N-CA	-7.67	114.31	123.44
1	A	675	ARG	CB-CA-C	-7.67	98.02	110.74
1	C	3001	ILE	N-CA-CB	-7.66	98.60	111.23
1	A	196	LEU	N-CA-C	-7.65	102.94	111.28
1	E	4670	ASP	CA-CB-CG	7.64	120.24	112.60
1	G	6651	ALA	N-CA-C	7.64	120.34	111.02
2	F	5716	LEU	N-CA-C	7.63	122.09	109.95
1	G	6027	ASP	N-CA-C	-7.63	102.30	111.69
1	C	2906	LEU	N-CA-CB	-7.57	97.65	110.83
1	G	6225	ASN	CA-CB-CG	-7.57	105.03	112.60
1	E	5060	GLU	N-CA-C	7.55	119.30	111.14
1	G	7007	ASN	CA-CB-CG	-7.53	105.07	112.60
2	D	3734	ASP	N-CA-C	-7.53	102.75	112.23
1	E	4754	HIS	CA-CB-CG	-7.49	106.31	113.80
1	E	4039	GLU	N-CA-CB	-7.47	98.70	110.28
1	A	363	ASN	CA-CB-CG	7.42	120.02	112.60
1	A	730	ASP	CA-CB-CG	7.40	120.00	112.60
1	E	4334	GLU	CB-CG-CD	-7.38	100.06	112.60
2	B	1516	HIS	CA-C-N	-7.37	116.49	122.16
2	B	1516	HIS	C-N-CA	-7.37	116.49	122.16
1	C	2210	LEU	N-CA-C	-7.36	102.29	112.30
1	A	839	LEU	CA-C-N	-7.34	115.54	122.66
1	A	839	LEU	C-N-CA	-7.34	115.54	122.66
2	F	5714	CYS	N-CA-C	7.32	120.44	109.25
1	C	2248	ILE	N-CA-C	-7.30	99.25	108.89
2	D	3657	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	660	PRO	N-CA-CB	7.23	107.56	102.65
1	E	4248	ILE	N-CA-C	-7.23	99.38	109.21
1	G	6407	THR	N-CA-C	-7.21	102.79	113.61
1	A	241	GLY	N-CA-C	-7.20	105.13	114.85
2	H	7693	HIS	CA-CB-CG	-7.19	106.61	113.80
2	D	3845	LYS	O-C-N	7.18	126.89	121.65
1	E	4625	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	557	THR	CA-C-N	7.13	130.14	120.44
1	A	557	THR	C-N-CA	7.13	130.14	120.44
1	C	2605	THR	N-CA-C	7.12	121.00	110.46
2	D	3799	ASP	CA-CB-CG	7.12	119.72	112.60
1	E	4338	ASP	CA-CB-CG	7.11	119.71	112.60
1	A	571	ARG	CD-NE-CZ	-7.09	114.48	124.40
2	F	5633	ILE	N-CA-CB	7.08	120.85	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2026	PHE	CA-CB-CG	-7.06	106.74	113.80
2	D	3795	HIS	CA-C-O	7.04	123.87	119.29
1	A	26	PHE	CA-CB-CG	-7.02	106.78	113.80
2	B	1674[A]	SER	N-CA-C	7.01	120.01	110.55
2	B	1674[B]	SER	N-CA-C	7.01	120.01	110.55
1	E	4557	THR	CA-C-N	7.00	132.54	120.58
1	E	4557	THR	C-N-CA	7.00	132.54	120.58
2	H	7553	VAL	N-CA-C	6.98	118.92	108.23
2	F	5846	PRO	CB-CA-C	-6.97	103.76	112.89
1	A	560	GLU	N-CA-CB	6.95	121.84	110.17
1	E	4153	GLU	CB-CA-C	6.94	121.78	110.88
1	E	4707	GLU	CA-C-N	6.94	129.55	120.60
1	E	4707	GLU	C-N-CA	6.94	129.55	120.60
1	E	4279	THR	N-CA-C	6.90	122.09	107.67
1	E	4283	ASN	CA-CB-CG	6.90	119.50	112.60
1	G	6905	PRO	CB-CA-C	-6.89	103.72	113.09
2	H	7650	PHE	CA-C-O	6.88	126.21	119.75
2	F	5874	ILE	CB-CA-C	-6.87	102.74	112.22
2	H	7698	ASP	CA-CB-CG	6.87	119.47	112.60
1	C	2283	ASN	CA-CB-CG	6.86	119.46	112.60
1	G	6339	ILE	N-CA-C	6.85	121.91	113.00
2	H	7803	ASN	CA-CB-CG	-6.85	105.75	112.60
1	C	2432	GLY	N-CA-C	-6.83	103.39	112.81
1	E	4453	PHE	CA-CB-CG	-6.82	106.98	113.80
1	A	713	VAL	CB-CA-C	-6.81	104.00	112.45
2	B	1864	ALA	CA-C-O	6.80	124.59	118.33
1	C	2181	ILE	CA-C-N	-6.80	113.61	123.00
1	C	2181	ILE	C-N-CA	-6.80	113.61	123.00
1	G	6207	ASP	N-CA-C	6.77	120.19	109.50
1	G	6243	HIS	CA-CB-CG	-6.75	107.05	113.80
2	F	5656	MET	N-CA-C	6.74	119.73	108.20
1	E	4339	ILE	N-CA-C	6.74	121.47	112.04
1	C	2536	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	1000	HIS	CA-CB-CG	-6.71	107.09	113.80
1	G	6161	ASP	CA-CB-CG	-6.68	105.92	112.60
2	B	1862	ASP	N-CA-C	6.68	119.41	111.33
1	G	6367	PHE	CA-CB-CG	-6.67	107.13	113.80
1	C	2660	PRO	N-CA-CB	6.65	107.17	102.65
1	C	2304	VAL	N-CA-C	-6.65	102.69	110.21
1	C	2532	CYS	N-CA-C	6.65	121.06	112.41
1	C	2103	GLU	CB-CG-CD	-6.63	101.33	112.60
1	C	2024	CYS	N-CA-C	6.60	120.44	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6712	LEU	N-CA-C	6.60	120.27	109.85
1	G	6908	GLY	CA-C-N	6.60	126.73	119.87
1	G	6908	GLY	C-N-CA	6.60	126.73	119.87
1	G	6605	THR	N-CA-C	6.59	120.35	110.14
1	E	4209	SER	N-CA-C	6.59	119.84	109.96
1	C	2714	VAL	N-CA-C	6.58	116.09	106.55
2	D	3739	SER	N-CA-C	6.58	118.81	110.33
1	G	6239	ALA	N-CA-C	6.56	118.33	110.19
1	E	4363	ASN	CA-CB-CG	6.56	119.16	112.60
2	F	5690	LEU	CA-C-N	6.55	125.99	118.85
2	F	5690	LEU	C-N-CA	6.55	125.99	118.85
1	G	6248	ILE	N-CA-C	-6.55	100.31	109.21
2	D	3574	GLN	N-CA-C	6.54	117.21	108.38
2	F	5589	ALA	N-CA-C	-6.54	99.64	110.17
1	E	4318	PRO	N-CA-CB	6.51	107.08	102.65
1	G	6557	THR	CA-C-N	6.50	130.57	120.82
1	G	6557	THR	C-N-CA	6.50	130.57	120.82
1	A	197	ASP	N-CA-CB	6.50	119.43	110.01
2	B	1716	LEU	N-CA-C	6.49	119.58	109.52
1	A	44	VAL	N-CA-C	6.49	117.25	108.17
1	A	612	THR	N-CA-C	6.48	120.44	112.54
1	E	4750	VAL	CA-C-N	6.48	129.91	120.71
1	E	4750	VAL	C-N-CA	6.48	129.91	120.71
1	G	6353	ASP	CA-CB-CG	6.46	119.06	112.60
2	H	7606	ASN	CA-CB-CG	-6.46	106.14	112.60
2	H	7690	LEU	CA-C-N	6.46	127.91	119.84
2	H	7690	LEU	C-N-CA	6.46	127.91	119.84
1	G	6678	PHE	N-CA-CB	-6.45	100.71	110.07
1	A	557	THR	CA-C-O	6.45	126.00	118.90
2	F	5737	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	793	ALA	N-CA-C	-6.42	101.88	110.55
1	E	4532	CYS	N-CA-C	6.42	121.03	112.30
1	E	4062	ASP	CA-CB-CG	-6.41	106.19	112.60
1	G	6735	ARG	O-C-N	6.40	129.00	122.09
1	G	6297	VAL	N-CA-CB	6.39	117.49	110.53
1	A	371	ASN	N-CA-C	-6.38	100.20	109.59
1	G	6549	GLU	N-CA-C	6.38	120.93	111.04
2	H	7799	ASP	N-CA-C	-6.38	96.77	107.99
1	E	4571	ARG	CB-CA-C	-6.37	96.76	110.45
1	G	6652	ARG	CA-C-O	6.37	127.30	120.55
1	G	7001	ILE	N-CA-CB	-6.37	100.73	111.23
1	G	6618	PHE	CA-CB-CG	-6.36	107.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1700	GLY	CA-C-N	6.36	129.78	120.82
2	B	1700	GLY	C-N-CA	6.36	129.78	120.82
1	G	6532	CYS	N-CA-CB	-6.36	102.32	111.54
2	H	7520	ILE	N-CA-C	-6.35	106.94	113.10
2	H	7714	CYS	N-CA-C	6.35	119.30	109.07
1	E	4239	ALA	N-CA-C	6.35	118.06	110.19
1	A	164	PHE	CA-CB-CG	-6.34	107.46	113.80
1	A	949	VAL	N-CA-C	6.34	118.88	108.99
2	D	3693	HIS	CA-CB-CG	-6.34	107.46	113.80
1	E	5001	ILE	N-CA-CB	-6.33	103.97	110.62
1	E	4620	PRO	CA-C-N	-6.33	115.70	121.65
1	E	4620	PRO	C-N-CA	-6.33	115.70	121.65
2	H	7824	ASN	N-CA-C	-6.32	105.94	113.21
1	G	6904	ASP	CA-CB-CG	6.32	118.92	112.60
2	B	1544	THR	N-CA-C	6.31	120.00	112.93
2	B	1859	GLY	CA-C-N	6.31	126.28	119.78
2	B	1859	GLY	C-N-CA	6.31	126.28	119.78
1	A	210	LEU	N-CA-C	-6.29	103.74	112.30
1	A	283	ASN	CA-CB-CG	6.29	118.89	112.60
1	C	3052	MET	CB-CA-C	-6.28	100.76	110.81
2	F	5636	ASP	N-CA-C	6.28	118.68	111.02
1	C	2670	ASP	CA-CB-CG	-6.27	106.33	112.60
2	F	5868	ASP	CA-CB-CG	-6.27	106.33	112.60
2	D	3766	PHE	CA-C-N	-6.27	117.75	122.33
2	D	3766	PHE	C-N-CA	-6.27	117.75	122.33
1	E	4023	ALA	N-CA-C	6.25	124.11	110.80
2	B	1612	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	999	PRO	N-CA-CB	6.24	109.46	102.60
1	C	2869	MET	N-CA-CB	6.23	119.28	110.12
1	C	3031	ARG	N-CA-CB	6.22	119.03	110.01
1	A	631	ARG	CB-CA-C	-6.22	100.86	110.81
1	C	2338	ASP	N-CA-C	6.22	118.61	111.02
1	A	680	HIS	CB-CA-C	-6.22	100.28	110.85
1	E	4605	THR	N-CA-C	6.21	119.27	110.14
1	C	2612	THR	N-CA-C	6.20	120.11	112.54
1	G	6317	PHE	CA-CB-CG	6.19	119.99	113.80
1	G	6738	PHE	CA-CB-CG	-6.19	107.61	113.80
2	D	3523	THR	CA-C-N	-6.18	111.77	121.97
2	D	3523	THR	C-N-CA	-6.18	111.77	121.97
2	H	7632	ILE	CB-CA-C	-6.18	101.62	110.83
1	C	2690	PRO	N-CA-CB	6.18	109.08	103.34
1	G	6532	CYS	N-CA-C	6.17	120.07	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7573	SER	CA-C-N	-6.16	112.62	122.53
2	H	7573	SER	C-N-CA	-6.16	112.62	122.53
1	A	532	CYS	N-CA-C	6.16	120.05	111.56
1	G	6210	LEU	N-CA-C	-6.15	103.93	112.30
1	C	2422	THR	CB-CA-C	6.15	121.95	110.70
1	E	4255	THR	N-CA-C	6.14	120.37	112.26
1	G	6885	PRO	O-C-N	6.14	124.13	121.31
2	B	1606	ASN	CA-CB-CG	-6.14	106.46	112.60
2	H	7569	ASP	N-CA-CB	6.13	119.02	110.56
1	A	975	HIS	N-CA-C	6.13	123.85	110.80
1	C	2523	HIS	CA-C-N	-6.12	114.46	120.52
1	C	2523	HIS	C-N-CA	-6.12	114.46	120.52
1	A	858	GLY	CA-C-N	-6.12	116.65	123.02
1	A	858	GLY	C-N-CA	-6.12	116.65	123.02
1	E	4027	ASP	N-CA-C	-6.12	104.17	111.69
1	E	4543	MET	N-CA-C	6.12	119.17	109.81
1	G	6782	ILE	N-CA-C	-6.11	105.18	110.74
1	G	6900	PHE	N-CA-CB	-6.11	102.85	110.79
2	F	5879	LYS	N-CA-C	-6.09	104.64	111.28
1	A	578	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	609	ASP	N-CA-C	-6.09	99.32	109.24
1	C	2559	ARG	N-CA-C	6.08	119.56	110.14
1	E	4635	PRO	CB-CA-C	-6.08	103.28	111.12
1	G	6543	MET	N-CA-C	6.08	118.94	109.52
1	C	3003	ASP	CA-CB-CG	6.08	118.67	112.60
1	A	592	ASP	CA-CB-CG	6.06	118.66	112.60
2	B	1766	PHE	CA-C-N	-6.05	118.00	122.18
2	B	1766	PHE	C-N-CA	-6.05	118.00	122.18
1	G	6328	VAL	CA-C-N	-6.05	113.80	123.31
1	G	6328	VAL	C-N-CA	-6.05	113.80	123.31
1	C	2417	ASP	CA-C-O	6.05	123.22	119.29
1	C	2803	GLN	N-CA-C	-6.05	104.69	111.28
2	H	7739	SER	N-CA-C	6.04	117.85	110.41
1	C	2735	ARG	N-CA-C	-6.04	104.38	110.97
1	A	955	GLU	CB-CA-C	-6.03	101.37	110.90
1	A	146	SER	N-CA-C	6.03	116.05	108.45
1	A	557	THR	N-CA-C	-6.03	105.74	114.12
1	C	2557	THR	CA-C-O	6.02	125.61	118.69
1	A	87	LEU	CA-C-O	6.01	125.22	119.99
2	D	3715	ARG	N-CA-C	-6.01	99.91	109.76
1	G	6018	ILE	CB-CA-C	-6.01	102.38	111.33
1	C	2423	LYS	N-CA-C	-6.01	104.65	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2255	THR	N-CA-C	6.00	120.18	112.26
1	A	1023	ILE	CB-CA-C	-6.00	104.04	112.14
1	G	6132	PHE	CA-C-O	6.00	127.11	120.63
1	A	204	LEU	CB-CA-C	-6.00	96.85	109.38
1	A	319	ILE	N-CA-C	5.98	116.45	110.23
1	A	651	ALA	N-CA-C	5.98	118.31	111.02
1	A	998	ARG	N-CA-C	5.98	119.24	110.10
1	G	6309	ALA	CA-C-O	5.96	126.87	120.55
1	A	209	SER	N-CA-C	5.96	119.11	110.28
1	G	6571	ARG	CD-NE-CZ	-5.96	116.06	124.40
2	F	5629	ASN	CA-CB-CG	-5.96	106.64	112.60
1	G	6504	LYS	CB-CA-C	-5.93	100.94	110.79
1	G	6132	PHE	CA-CB-CG	-5.93	107.87	113.80
1	C	2345	PRO	CB-CA-C	-5.92	101.98	110.75
1	C	3057	ASP	N-CA-CB	5.92	120.01	110.65
1	E	4571	ARG	CA-CB-CG	5.92	125.95	114.10
2	B	1620	ARG	CG-CD-NE	-5.91	99.00	112.00
1	G	6283	ASN	CA-CB-CG	5.90	118.50	112.60
2	F	5648	ARG	CD-NE-CZ	-5.90	116.14	124.40
1	C	2003	LYS	N-CA-CB	5.90	118.71	109.69
1	G	6186	GLU	CA-C-N	5.90	128.10	120.44
1	G	6186	GLU	C-N-CA	5.90	128.10	120.44
1	A	726	GLU	CB-CA-C	5.89	120.94	110.16
2	F	5807	ILE	N-CA-C	-5.89	100.10	108.58
1	E	4560	GLU	N-CA-C	-5.89	100.24	109.25
1	G	6230	ILE	CB-CA-C	-5.88	102.92	110.98
1	E	4714	VAL	N-CA-CB	5.88	118.66	111.60
1	C	2353	ASP	CA-CB-CG	5.87	118.47	112.60
1	E	4712	LEU	N-CA-CB	-5.86	100.70	111.37
1	A	825	LEU	N-CA-C	5.86	118.46	110.55
2	B	1558	PRO	N-CA-CB	5.85	109.52	103.15
1	A	88	PRO	CB-CA-C	-5.84	101.92	111.56
1	C	2972	ASP	N-CA-CB	5.84	120.67	111.20
1	A	791	ASP	CA-CB-CG	-5.83	106.77	112.60
1	E	4771	GLU	N-CA-C	-5.83	106.20	113.55
1	G	6443	PHE	CA-CB-CG	-5.83	107.97	113.80
2	D	3744	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	2154	GLU	N-CA-C	-5.82	104.84	111.07
1	E	4509	ARG	CB-CA-C	-5.81	98.76	109.46
1	C	2173	THR	N-CA-CB	5.80	120.65	111.43
1	C	3039	HIS	CA-CB-CG	-5.79	108.01	113.80
1	A	738	PHE	CA-CB-CG	-5.79	108.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2793	ALA	N-CA-C	-5.79	102.73	110.55
2	F	5504	SER	N-CA-C	5.79	119.04	110.48
1	C	2431	ALA	N-CA-C	5.78	118.70	110.10
2	B	1696	ALA	N-CA-C	5.77	118.35	109.07
1	E	4345	PRO	CB-CA-C	-5.75	101.80	110.20
1	C	2669	ILE	N-CA-C	-5.75	104.90	110.42
2	B	1709	LEU	N-CA-C	-5.75	104.93	111.14
1	G	6167	ILE	CA-C-N	-5.74	115.66	123.12
1	G	6167	ILE	C-N-CA	-5.74	115.66	123.12
1	E	4249	THR	CA-C-N	-5.73	114.55	122.69
1	E	4249	THR	C-N-CA	-5.73	114.55	122.69
1	E	4694	THR	N-CA-CB	5.71	119.48	110.23
2	B	1589	ALA	N-CA-C	-5.71	100.40	109.76
1	A	882	GLU	CA-C-N	-5.70	115.74	122.93
1	A	882	GLU	C-N-CA	-5.70	115.74	122.93
2	H	7718	ILE	N-CA-CB	5.70	117.50	111.00
2	B	1795	HIS	N-CA-C	5.70	117.85	109.42
1	E	4224	LYS	N-CA-C	5.70	118.26	111.71
1	E	4554	ASN	CB-CA-C	-5.69	107.16	111.20
1	G	6062	ASP	CA-CB-CG	-5.69	106.91	112.60
1	E	4536	PHE	CA-CB-CG	-5.68	108.12	113.80
2	D	3868	ASP	CA-CB-CG	-5.68	106.92	112.60
2	H	7786	MET	CG-SD-CE	-5.68	88.41	100.90
2	B	1632	ILE	CB-CA-C	-5.67	102.39	110.83
1	G	6345	PRO	CB-CA-C	-5.67	101.55	110.96
1	A	965	LEU	N-CA-C	-5.66	105.03	111.14
2	H	7592	PHE	CA-CB-CG	-5.66	108.14	113.80
1	E	4678	PHE	N-CA-CB	-5.66	101.51	109.94
1	A	34	CYS	N-CA-CB	5.65	118.20	110.01
2	B	1735	GLY	CA-C-N	-5.65	115.09	122.94
2	B	1735	GLY	C-N-CA	-5.65	115.09	122.94
1	G	6054	ILE	N-CA-C	-5.65	105.01	110.72
1	G	6734	LEU	N-CA-C	5.65	118.17	111.33
1	G	6840	ILE	N-CA-C	5.65	115.88	110.74
2	H	7530	VAL	CB-CA-C	-5.65	103.91	110.91
1	A	786	GLY	N-CA-C	-5.64	107.76	114.48
1	A	840	ILE	N-CA-C	-5.64	107.33	111.90
2	B	1715	ARG	N-CA-C	-5.64	99.23	108.76
2	D	3690	LEU	CA-C-N	5.63	125.16	119.19
2	D	3690	LEU	C-N-CA	5.63	125.16	119.19
1	A	754	HIS	CA-CB-CG	-5.63	108.17	113.80
1	E	4371	ASN	N-CA-C	-5.63	101.95	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5000	HIS	CA-CB-CG	-5.63	108.17	113.80
1	G	6834	ASN	CB-CA-C	-5.63	103.89	111.89
2	B	1794	ASN	CA-CB-CG	-5.63	106.97	112.60
2	B	1805	VAL	N-CA-C	5.63	117.10	108.71
1	G	6142	GLU	N-CA-C	5.62	119.09	110.20
1	A	27	ASP	N-CA-CB	5.62	118.48	110.16
1	A	1038	VAL	CB-CA-C	-5.62	103.94	110.91
2	F	5586	PRO	CA-C-N	5.62	127.74	120.44
2	F	5586	PRO	C-N-CA	5.62	127.74	120.44
1	A	278	GLU	CB-CA-C	-5.62	99.94	109.38
2	D	3859	GLY	CA-C-N	5.62	125.56	119.78
2	D	3859	GLY	C-N-CA	5.62	125.56	119.78
1	C	3000	HIS	CA-CB-CG	-5.61	108.19	113.80
2	H	7862	ASP	N-CA-C	5.61	118.11	111.33
2	B	1576	HIS	CA-CB-CG	-5.60	108.20	113.80
1	C	2592	ASP	CA-C-N	-5.60	114.74	122.63
1	C	2592	ASP	C-N-CA	-5.60	114.74	122.63
1	E	4044	VAL	N-CA-C	5.60	116.36	108.36
2	H	7716	LEU	N-CA-C	5.59	118.67	109.72
1	G	6294	ARG	CD-NE-CZ	-5.59	116.58	124.40
1	A	671	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	793	ALA	CA-C-N	-5.58	112.71	121.87
1	A	793	ALA	C-N-CA	-5.58	112.71	121.87
1	C	2787	VAL	N-CA-C	-5.58	99.11	107.37
1	C	2942	HIS	CA-CB-CG	-5.58	108.22	113.80
1	E	4334	GLU	CB-CA-C	-5.58	98.22	109.55
1	E	4712	LEU	N-CA-C	5.58	118.32	109.50
1	G	6489	LEU	CA-C-O	5.58	126.47	120.55
1	A	348	PHE	CA-CB-CG	-5.58	108.22	113.80
1	E	4711	PRO	CA-C-N	-5.57	113.94	122.62
1	E	4711	PRO	C-N-CA	-5.57	113.94	122.62
2	F	5823	ALA	N-CA-C	5.57	119.17	112.38
1	G	6631	ARG	CA-C-N	-5.57	112.61	121.02
1	G	6631	ARG	C-N-CA	-5.57	112.61	121.02
1	E	5069	HIS	CA-CB-CG	-5.57	108.23	113.80
1	E	4211	ILE	CA-C-N	-5.56	114.34	122.46
1	E	4211	ILE	C-N-CA	-5.56	114.34	122.46
1	E	4940	LYS	CA-C-N	-5.56	113.93	122.60
1	E	4940	LYS	C-N-CA	-5.56	113.93	122.60
1	A	998	ARG	C-N-CD	-5.56	108.38	120.60
1	E	4965	LEU	N-CA-C	-5.55	105.31	111.36
2	H	7624	GLU	N-CA-C	5.55	117.14	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	619	GLU	N-CA-C	5.55	117.21	108.55
1	A	225	ASN	CA-CB-CG	-5.54	107.06	112.60
1	G	6150	HIS	CA-CB-CG	-5.53	108.27	113.80
1	A	739	GLN	O-C-N	5.53	128.00	122.08
1	E	4334	GLU	CA-CB-CG	5.52	125.15	114.10
1	C	2450	ASP	CA-C-N	5.52	125.95	119.94
1	C	2450	ASP	C-N-CA	5.52	125.95	119.94
2	B	1701	ALA	N-CA-C	5.51	118.31	110.10
1	C	2003	LYS	N-CA-C	5.51	118.31	110.10
1	C	2407	THR	N-CA-C	-5.51	105.35	113.61
2	F	5870	PHE	N-CA-C	-5.51	105.19	111.14
1	C	2575	GLY	N-CA-C	5.51	120.48	112.55
1	G	6163	GLY	O-C-N	5.51	128.00	122.77
1	E	4683	GLU	N-CA-C	-5.50	104.32	111.02
2	F	5807	ILE	CA-C-N	-5.49	113.59	122.82
2	F	5807	ILE	C-N-CA	-5.49	113.59	122.82
1	C	2417	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	2560	GLU	N-CA-CB	5.49	119.42	110.37
1	G	6949	VAL	N-CA-C	5.49	117.55	108.99
1	C	2313	LYS	N-CA-C	-5.48	105.39	111.36
2	B	1799	ASP	N-CA-C	-5.48	100.18	108.67
2	B	1825	LEU	CA-C-N	-5.48	114.49	122.65
2	B	1825	LEU	C-N-CA	-5.48	114.49	122.65
1	E	4278	GLU	CA-C-N	-5.48	114.81	123.24
1	E	4278	GLU	C-N-CA	-5.48	114.81	123.24
1	G	6918	MET	CA-C-N	-5.47	118.33	122.33
1	G	6918	MET	C-N-CA	-5.47	118.33	122.33
1	A	735	ARG	O-C-N	5.47	127.93	122.08
1	G	6786	GLY	N-CA-C	-5.47	107.73	113.58
1	E	4712	LEU	CA-C-N	-5.46	115.77	122.93
1	E	4712	LEU	C-N-CA	-5.46	115.77	122.93
1	A	410	ASP	CA-CB-CG	-5.46	107.14	112.60
2	H	7637	ASN	CA-CB-CG	5.46	118.06	112.60
1	E	4713	VAL	N-CA-CB	5.46	118.23	111.41
2	H	7589	ALA	N-CA-C	-5.46	100.81	109.76
1	E	4906	LEU	N-CA-C	5.45	118.29	109.40
1	A	249	THR	CA-C-N	-5.45	114.95	122.69
1	A	249	THR	C-N-CA	-5.45	114.95	122.69
1	A	574	GLN	CB-CA-C	-5.45	103.08	111.74
1	A	1060	GLU	N-CA-C	5.45	116.90	111.07
2	B	1762	ASP	CA-CB-CG	-5.44	107.16	112.60
1	C	2074	VAL	N-CA-C	-5.44	105.22	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3569	ASP	N-CA-CB	5.44	118.07	110.56
2	F	5772	HIS	CA-CB-CG	5.44	119.24	113.80
2	B	1605	HIS	CA-CB-CG	-5.43	108.37	113.80
1	A	595	GLU	N-CA-C	-5.43	100.32	108.96
2	B	1607	ILE	N-CA-C	5.43	116.13	108.36
1	G	6043	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	C	2659	VAL	N-CA-C	5.43	114.07	109.02
1	C	2987	ASN	CB-CA-C	-5.43	103.29	110.34
2	D	3633	ILE	N-CA-CB	5.42	118.89	111.41
1	A	141	LEU	N-CA-C	-5.42	101.33	109.95
1	G	6757	ASP	CA-CB-CG	-5.42	107.18	112.60
2	D	3682	PRO	CB-CA-C	-5.41	103.13	110.60
1	C	2082	ARG	CA-C-O	5.41	124.64	120.48
1	C	2363	ASN	CA-CB-CG	5.41	118.01	112.60
1	C	2319	ILE	N-CA-C	5.41	115.61	110.42
1	C	2519	GLN	CB-CG-CD	-5.40	103.42	112.60
1	E	4793	ALA	N-CA-C	-5.40	102.49	110.48
1	C	2688	LYS	N-CA-C	5.40	117.54	108.96
1	G	6338	ASP	CA-CB-CG	5.39	117.99	112.60
1	G	6124	ASP	CA-CB-CG	-5.39	107.21	112.60
1	A	289	ASN	CA-CB-CG	-5.38	107.22	112.60
2	H	7543	LEU	CB-CA-C	-5.38	101.86	110.79
2	H	7640	ALA	CA-C-N	5.38	127.80	120.54
2	H	7640	ALA	C-N-CA	5.38	127.80	120.54
1	G	6524	PRO	CB-CA-C	-5.38	103.10	111.22
1	A	758	ASP	N-CA-C	5.37	118.75	111.17
2	D	3749	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	739	GLN	CA-C-N	5.36	127.91	120.29
1	A	739	GLN	C-N-CA	5.36	127.91	120.29
2	D	3508	VAL	N-CA-CB	5.36	119.34	111.52
2	B	1734	ASP	CA-CB-CG	-5.36	107.24	112.60
1	C	2561	LYS	N-CA-C	5.36	118.79	110.17
1	A	367	PHE	CB-CA-C	-5.35	103.98	111.85
2	H	7640	ALA	O-C-N	5.35	127.81	122.08
2	B	1553	VAL	N-CA-C	5.34	116.41	108.23
1	G	6404	VAL	N-CA-CB	5.34	118.89	111.94
1	G	6557	THR	CA-C-O	5.34	125.27	119.24
1	G	6699	GLU	CA-C-N	5.34	127.74	120.54
1	G	6699	GLU	C-N-CA	5.34	127.74	120.54
1	C	2453	PHE	CA-CB-CG	-5.33	108.47	113.80
1	C	2128	ASP	CA-CB-CG	5.33	117.93	112.60
1	E	4548	GLU	N-CA-CB	5.33	119.30	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6160	ALA	N-CA-C	-5.33	105.64	111.82
2	B	1562	ASN	CA-C-N	-5.33	114.40	122.76
2	B	1562	ASN	C-N-CA	-5.33	114.40	122.76
1	A	1014	ILE	CB-CA-C	5.32	117.91	110.99
1	C	2344	THR	CA-C-N	5.32	125.79	120.52
1	C	2344	THR	C-N-CA	5.32	125.79	120.52
1	C	3014	ILE	N-CA-CB	5.32	118.60	111.90
1	A	407	THR	N-CA-C	-5.32	106.18	113.30
1	E	4588	ALA	N-CA-C	5.32	116.76	111.07
1	E	4441	ASP	N-CA-C	-5.31	105.57	111.36
1	E	4785	ALA	CA-C-N	-5.31	117.67	123.30
1	E	4785	ALA	C-N-CA	-5.31	117.67	123.30
2	H	7511	ASP	CA-CB-CG	5.31	117.91	112.60
1	E	4279	THR	CB-CA-C	-5.31	104.50	112.09
1	C	2775	ILE	N-CA-CB	5.30	116.71	110.82
1	C	3005	ILE	CA-C-O	5.30	126.79	121.17
1	E	4659	VAL	CA-C-O	5.30	124.91	119.82
1	C	2044	VAL	N-CA-C	5.30	115.48	107.80
2	D	3786	MET	CG-SD-CE	-5.29	89.25	100.90
1	G	6518	ASP	CA-C-N	5.29	128.14	120.79
1	G	6518	ASP	C-N-CA	5.29	128.14	120.79
1	A	345	PRO	CB-CA-C	-5.28	102.84	111.56
1	C	2456	THR	N-CA-C	5.28	119.78	113.23
1	C	2909	PRO	N-CA-CB	5.28	108.38	103.41
2	H	7638	PRO	N-CA-CB	5.28	108.80	103.25
1	E	4993	LYS	N-CA-C	-5.28	103.92	110.41
2	F	5799	ASP	CA-CB-CG	5.28	117.88	112.60
2	H	7598	LEU	N-CA-C	5.28	117.72	111.33
1	E	4360	PRO	N-CA-CB	5.28	108.24	103.33
1	G	6302	PRO	CB-CA-C	-5.28	105.98	112.89
1	A	449	VAL	N-CA-C	-5.27	105.24	110.62
1	C	2549	GLU	N-CA-C	5.27	119.21	111.04
1	E	4088	PRO	CB-CA-C	-5.27	102.86	111.56
1	C	3015	ASN	CA-CB-CG	5.26	117.86	112.60
2	F	5612	ASP	N-CA-C	5.26	119.00	112.58
1	C	2082	ARG	CB-CA-C	5.26	115.58	111.00
2	D	3788	PHE	CB-CA-C	5.26	117.23	109.29
2	D	3845	LYS	CA-C-N	5.26	126.41	119.84
2	D	3845	LYS	C-N-CA	5.26	126.41	119.84
1	E	4883	VAL	CB-CA-C	-5.26	104.39	110.91
2	F	5562	ASN	CA-CB-CG	5.26	117.86	112.60
1	G	6518	ASP	O-C-N	5.26	127.48	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5021	ARG	N-CA-CB	5.25	117.58	109.91
1	A	1028	VAL	N-CA-C	5.25	117.61	111.05
2	D	3691	PRO	CA-C-N	-5.25	113.69	122.92
2	D	3691	PRO	C-N-CA	-5.25	113.69	122.92
1	C	2998	ARG	O-C-N	5.24	126.31	121.80
1	G	6404	VAL	N-CA-C	-5.24	106.32	111.88
1	A	876	GLU	N-CA-CB	5.24	118.29	110.22
2	D	3505	ALA	N-CA-CB	5.24	121.26	111.52
1	A	878	GLY	CA-C-N	-5.24	117.99	122.96
1	A	878	GLY	C-N-CA	-5.24	117.99	122.96
1	C	2255	THR	CA-C-N	-5.24	115.34	122.93
1	C	2255	THR	C-N-CA	-5.24	115.34	122.93
1	C	2410	ASP	CA-CB-CG	-5.24	107.36	112.60
1	G	6996	GLU	CA-C-N	-5.24	113.05	121.32
1	G	6996	GLU	C-N-CA	-5.24	113.05	121.32
1	A	68	PRO	N-CA-CB	5.23	107.90	103.19
2	F	5578	GLN	N-CA-CB	-5.23	102.28	110.44
1	A	1011	THR	N-CA-C	-5.23	106.85	114.12
1	G	6064	THR	CA-C-N	-5.23	115.69	123.11
1	G	6064	THR	C-N-CA	-5.23	115.69	123.11
1	C	2046	ASN	CA-CB-CG	5.23	117.83	112.60
1	E	4860	PRO	N-CA-CB	5.23	106.55	102.73
1	E	4951	GLU	CB-CA-C	-5.23	102.45	110.81
1	E	4512	GLU	CB-CG-CD	-5.22	103.72	112.60
1	G	6918	MET	CB-CA-C	5.22	119.70	109.35
1	C	2175	GLY	N-CA-C	-5.22	107.78	115.30
1	C	2585	ALA	CA-C-O	5.22	126.09	120.55
1	C	3001	ILE	CA-CB-CG2	5.22	119.37	110.50
1	G	7020	ARG	N-CA-CB	5.22	117.89	110.06
2	B	1620	ARG	CB-CG-CD	-5.21	99.31	111.30
1	E	4140	GLY	N-CA-C	5.21	122.55	115.30
2	F	5508	VAL	N-CA-CB	5.21	118.60	111.41
1	G	6057	ASP	CA-C-N	5.21	125.26	119.32
1	G	6057	ASP	C-N-CA	5.21	125.26	119.32
1	E	4677	ARG	CA-C-O	5.21	126.29	120.82
2	B	1744	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	1823	ALA	N-CA-C	5.21	117.70	111.71
1	C	2229	ILE	CB-CA-C	-5.20	101.40	110.71
1	E	5038	VAL	CB-CA-C	-5.20	103.76	110.84
1	C	2975	HIS	N-CA-C	5.20	121.88	110.80
1	G	6231	VAL	CB-CA-C	-5.20	105.27	112.24
1	A	829	GLN	CA-CB-CG	-5.20	103.71	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1808	THR	N-CA-C	5.19	116.87	109.14
1	C	2180	GLY	CA-C-N	-5.19	116.75	123.19
1	C	2180	GLY	C-N-CA	-5.19	116.75	123.19
2	B	1695	VAL	CB-CA-C	-5.19	103.87	110.98
1	C	2430	ASP	CA-CB-CG	-5.19	107.41	112.60
1	C	2971	LEU	CB-CA-C	-5.18	99.47	109.37
1	E	4959	ASP	CA-CB-CG	-5.18	107.42	112.60
2	H	7725	ALA	CA-C-N	5.18	127.99	120.79
2	H	7725	ALA	C-N-CA	5.18	127.99	120.79
1	A	266	ASN	CA-CB-CG	5.17	117.77	112.60
1	E	4919	GLY	N-CA-C	-5.17	101.88	111.04
1	G	6554	ASN	N-CA-CB	5.17	118.91	111.51
1	C	2555	PRO	N-CA-CB	5.17	107.85	103.35
1	A	900	PHE	CB-CA-C	-5.17	103.67	111.27
1	A	456	THR	N-CA-C	5.17	119.85	113.50
1	G	6558	ASP	CA-CB-CG	5.17	117.77	112.60
1	G	6735	ARG	N-CA-C	-5.17	105.56	111.14
1	E	4880	THR	N-CA-CB	-5.16	103.76	110.88
1	G	6662	ILE	CA-C-O	-5.16	117.60	121.68
1	E	4896	PRO	N-CA-C	5.16	120.04	114.68
2	H	7629	ASN	N-CA-C	-5.16	103.59	110.55
1	G	6185	ARG	N-CA-C	5.16	116.90	111.28
1	G	6630	VAL	CA-C-N	5.16	127.50	120.54
1	G	6630	VAL	C-N-CA	5.16	127.50	120.54
2	B	1715	ARG	CA-C-N	-5.15	114.50	122.59
2	B	1715	ARG	C-N-CA	-5.15	114.50	122.59
1	C	2558	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	2715	ARG	CB-CA-C	-5.15	101.25	109.75
1	E	4524	PRO	CB-CA-C	-5.15	103.45	111.22
1	A	897	PHE	N-CA-C	5.15	118.34	111.75
1	C	2207	ASP	N-CA-C	5.15	117.96	109.72
2	B	1722	GLN	N-CA-C	5.14	119.27	113.15
2	H	7663	THR	CA-C-N	5.14	128.17	120.87
2	H	7663	THR	C-N-CA	5.14	128.17	120.87
1	G	6883	VAL	CA-C-N	-5.14	117.60	123.25
1	G	6883	VAL	C-N-CA	-5.14	117.60	123.25
2	F	5862	ASP	N-CA-C	5.14	117.55	111.33
1	G	6237	PHE	N-CA-C	-5.14	105.59	111.14
1	A	453	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	255	THR	N-CA-C	5.13	118.57	112.72
1	A	194	ARG	N-CA-C	5.12	117.26	111.11
1	A	62	ASP	N-CA-C	5.12	117.99	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2039	GLU	CB-CA-C	-5.12	101.98	110.68
1	A	57	ASP	CA-C-O	5.12	125.45	120.23
2	B	1657	ASP	N-CA-CB	5.11	118.34	110.21
1	C	3014	ILE	CB-CA-C	5.11	117.64	110.99
1	E	4714	VAL	N-CA-C	5.11	114.65	106.88
1	C	2370	ALA	N-CA-C	5.11	117.70	110.50
2	H	7865	PRO	N-CA-CB	5.11	108.21	103.41
1	E	4050	ASN	CA-C-N	5.11	124.80	119.64
1	E	4050	ASN	C-N-CA	5.11	124.80	119.64
1	G	6974	THR	N-CA-C	-5.11	103.66	110.55
1	C	2089	THR	N-CA-C	5.10	119.19	112.92
1	E	4083	PRO	CB-CA-C	-5.10	104.30	110.98
1	A	787	VAL	N-CA-C	-5.10	100.41	107.80
1	A	418	PRO	CA-C-N	-5.09	114.60	122.49
1	A	418	PRO	C-N-CA	-5.09	114.60	122.49
1	A	575	GLY	N-CA-C	5.09	119.88	112.55
1	G	6985	GLY	CA-C-N	-5.09	116.19	123.11
1	G	6985	GLY	C-N-CA	-5.09	116.19	123.11
1	C	2904	ASP	CA-C-O	5.09	123.38	119.46
1	G	6677	ARG	CA-C-N	5.08	127.35	120.44
1	G	6677	ARG	C-N-CA	5.08	127.35	120.44
1	C	2642	TYR	CB-CA-C	-5.08	101.59	110.17
1	E	4297	VAL	N-CA-CB	5.08	116.25	110.72
1	G	6003	LYS	N-CA-C	5.08	117.66	110.10
1	G	6942	HIS	CA-CB-CG	-5.08	108.72	113.80
1	G	6793	ALA	N-CA-C	-5.07	103.70	110.55
1	G	6316	GLY	N-CA-C	-5.07	108.32	115.32
1	A	509	ARG	CB-CA-C	-5.07	100.13	109.46
1	E	4039	GLU	CB-CA-C	-5.07	100.94	110.67
2	D	3795	HIS	N-CA-C	5.07	117.54	108.47
2	H	7552	ILE	N-CA-CB	-5.07	105.28	111.21
1	C	2035	LYS	CA-C-O	5.07	125.92	120.55
1	E	4523	HIS	N-CA-CB	-5.06	101.81	110.72
1	A	297	VAL	CA-CB-CG1	-5.06	101.79	110.40
1	A	435	ARG	N-CA-CB	5.06	118.03	109.78
1	C	2043	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	456	THR	CA-C-N	-5.06	115.86	124.31
1	A	456	THR	C-N-CA	-5.06	115.86	124.31
2	D	3716	LEU	N-CA-C	5.06	117.99	109.95
1	E	4080	LYS	N-CA-C	5.06	116.87	111.36
1	G	6257	THR	N-CA-C	-5.06	103.72	110.55
2	H	7878	ARG	CA-C-N	5.06	127.76	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7878	ARG	C-N-CA	5.06	127.76	120.38
1	E	4471	ARG	CA-C-O	-5.05	115.51	120.82
1	E	4971	LEU	N-CA-C	5.05	117.64	109.40
2	B	1609	ALA	CA-C-O	5.05	126.66	120.60
1	C	2549	GLU	CA-C-O	5.05	126.19	120.89
2	D	3558	PRO	N-CA-CB	5.05	108.66	103.15
1	E	4003	LYS	CA-C-N	5.05	131.19	121.54
1	E	4003	LYS	C-N-CA	5.05	131.19	121.54
1	E	4006	ASP	CA-C-N	-5.05	116.56	123.12
1	E	4006	ASP	C-N-CA	-5.05	116.56	123.12
2	B	1545	ASP	CA-CB-CG	5.05	117.65	112.60
2	H	7516	HIS	CA-C-N	-5.05	115.82	121.83
2	H	7516	HIS	C-N-CA	-5.05	115.82	121.83
2	H	7546	PRO	N-CA-CB	5.04	108.84	103.39
1	E	4316	GLY	N-CA-C	-5.04	108.36	115.32
2	B	1510	GLU	N-CA-CB	-5.04	101.98	110.49
1	A	883	VAL	CB-CA-C	-5.04	103.99	110.84
2	F	5799	ASP	N-CA-C	-5.03	99.13	107.99
1	C	2065	TYR	N-CA-C	5.03	116.89	107.99
1	G	6227	ASN	N-CA-C	-5.03	103.41	110.50
1	A	889	SER	CA-C-N	-5.02	115.97	122.94
1	A	889	SER	C-N-CA	-5.02	115.97	122.94
1	G	6348	PHE	CA-CB-CG	-5.02	108.78	113.80
1	C	2889	SER	CA-C-N	-5.02	116.14	123.06
1	C	2889	SER	C-N-CA	-5.02	116.14	123.06
1	E	4970	GLU	N-CA-C	-5.02	102.09	110.17
1	E	4558	ASP	N-CA-CB	-5.01	102.73	110.20
1	G	6343	ARG	CA-CB-CG	-5.01	104.08	114.10
1	G	6645	GLN	N-CA-C	5.01	116.74	111.28
1	A	219	GLU	CB-CA-C	-5.01	102.08	110.19
1	A	897	PHE	CA-CB-CG	5.01	118.81	113.80
2	F	5543	LEU	N-CA-C	5.01	117.39	111.33
1	G	6902	GLY	CA-C-N	-5.00	114.58	122.64
1	G	6902	GLY	C-N-CA	-5.00	114.58	122.64
1	G	6924	PHE	CA-CB-CG	-5.00	108.80	113.80
1	A	103	GLU	CA-C-N	5.00	127.25	120.65
1	A	103	GLU	C-N-CA	5.00	127.25	120.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	GLU	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	8193	0	8225	267	0
1	C	8198	0	8230	263	0
1	E	8169	0	8194	267	0
1	G	8164	0	8193	345	0
2	B	2904	0	2868	104	0
2	D	2902	0	2867	90	0
2	F	2915	0	2876	95	0
2	H	2902	0	2868	136	0
3	A	20	0	0	0	0
3	C	20	0	0	1	0
3	E	15	0	0	0	0
3	G	20	0	0	1	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
4	E	3	0	0	0	0
4	G	3	0	0	0	0
5	A	7	0	0	0	0
5	B	1	0	0	0	0
5	C	7	0	0	0	0
5	D	1	0	0	0	0
5	E	7	0	0	0	0
5	F	1	0	0	0	0
5	G	7	0	0	0	0
5	H	1	0	0	0	0
6	A	6	0	0	0	0
6	B	1	0	0	0	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	6	0	0	2	0
6	H	1	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	54	0	24	1	0
7	G	54	0	24	4	0
8	A	9	0	11	1	0
8	C	9	0	11	3	0
8	E	9	0	11	1	0
8	G	9	0	11	1	0
9	A	9	0	20	1	0
9	C	9	0	20	0	0
9	E	9	0	20	2	0
9	G	9	0	20	0	0
10	A	904	0	0	34	0
10	B	256	0	0	2	0
10	C	897	0	0	26	0
10	D	330	0	0	8	1
10	E	900	0	0	29	0
10	F	276	0	0	7	0
10	G	733	0	0	26	0
10	H	232	0	0	6	1
All	All	49310	0	44541	1551	1

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 17.

All (1551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:CE	1:A:80:LYS:NZ	1.68	1.53
1:E:4001:MET:HB3	10:E:6618:HOH:O	1.38	1.21
2:F:5687:GLU:HG2	2:F:5715:ARG:HD2	1.21	1.13
1:C:2695:VAL:HG21	1:C:2701:ALA:HA	1.30	1.12
1:G:6695:VAL:HG11	1:G:6701:ALA:HB2	1.24	1.12
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.35	1.08
1:C:2728:VAL:HG12	1:C:2733:ASP:HB3	1.35	1.06
1:C:2695:VAL:HG11	1:C:2701:ALA:HB2	1.36	1.06
2:H:7633:ILE:HD12	2:H:7643:ALA:HB2	1.37	1.06
1:G:6674:ASP:HB3	1:G:6677:ARG:HB2	1.38	1.05
1:E:4714:VAL:HG13	1:E:4752:LEU:HD12	1.42	1.01
1:E:4695:VAL:HG21	1:E:4752:LEU:HD22	1.42	1.01
2:H:7506:LEU:HD11	2:H:7508:VAL:HG23	1.44	0.99
2:D:3728:VAL:HA	2:D:3731:MET:HE3	1.42	0.99
2:B:1695:VAL:HG23	2:B:1733:PRO:HB3	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6784:GLN:H	1:G:6784:GLN:HE21	0.96	0.94
2:F:5824:ASN:HD22	2:F:5824:ASN:H	1.08	0.93
1:G:6784:GLN:H	1:G:6784:GLN:NE2	1.65	0.93
1:G:6698:ILE:HD12	1:G:6698:ILE:H	1.34	0.93
2:D:3687:GLU:HG2	2:D:3715:ARG:HD2	1.50	0.92
1:C:2784:GLN:H	1:C:2784:GLN:HE21	1.15	0.91
1:A:784:GLN:HE21	1:A:784:GLN:H	0.96	0.91
1:A:784:GLN:H	1:A:784:GLN:NE2	1.68	0.90
2:H:7822:PRO:HB2	2:H:7824:ASN:ND2	1.87	0.90
2:H:7786:MET:HE1	2:H:7812:HIS:CE1	2.07	0.90
1:E:4695:VAL:HG11	1:E:4701:ALA:HB2	1.54	0.89
2:B:1687:GLU:HG2	2:B:1715:ARG:HD2	1.52	0.89
1:E:4728:VAL:HG13	1:E:4733:ASP:HB3	1.54	0.89
1:G:6728:VAL:CG1	1:G:6733:ASP:HB3	2.03	0.88
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.53	0.88
2:D:3728:VAL:HA	2:D:3731:MET:CE	2.03	0.88
2:B:1728:VAL:HA	2:B:1731:MET:HE2	1.53	0.87
1:G:6670:ASP:HB3	1:G:6677:ARG:HH21	1.38	0.87
1:E:4994:VAL:HG13	1:E:5000:HIS:CE1	2.10	0.87
1:G:6994:VAL:HG13	1:G:7000:HIS:CE1	2.10	0.87
1:E:4889:SER:HB3	1:E:4918:MET:HE3	1.55	0.86
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.38	0.86
1:A:481:ILE:HD12	1:A:508:VAL:HG11	1.57	0.86
1:C:2710:TYR:HB3	1:C:2711:PRO:HA	1.56	0.86
2:F:5687:GLU:CG	2:F:5715:ARG:HD2	2.05	0.86
2:B:1728:VAL:HA	2:B:1731:MET:CE	2.06	0.85
2:D:3687:GLU:CG	2:D:3715:ARG:HD2	2.05	0.85
1:C:2509:ARG:HH11	1:C:2509:ARG:HB2	1.42	0.85
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.59	0.84
2:H:7715:ARG:HH11	2:H:7715:ARG:HG3	1.42	0.84
1:E:4059:GLU:HG2	1:E:4060:MET:HE2	1.60	0.84
2:H:7824:ASN:HD22	2:H:7824:ASN:N	1.74	0.84
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.06	0.84
1:G:6714:VAL:HG22	1:G:6752:LEU:HD12	1.57	0.84
1:E:4228:CYS:SG	1:E:4269:MET:HG2	2.18	0.83
2:H:7557:TYR:CD1	2:H:7558:PRO:HD2	2.13	0.83
2:H:7506:LEU:HD11	2:H:7508:VAL:CG2	2.08	0.83
2:H:7822:PRO:HB2	2:H:7824:ASN:HD21	1.41	0.83
2:B:1506:LEU:HD12	2:B:1507:LEU:N	1.94	0.82
2:D:3727:ASP:HA	2:D:3730:LYS:HD2	1.60	0.82
2:F:5695:VAL:HG23	2:F:5733:PRO:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2761:GLU:HG2	1:C:2781:HIS:CE1	2.13	0.82
2:D:3824:ASN:HD22	2:D:3824:ASN:H	1.28	0.81
2:F:5759:LEU:HD13	2:F:5842:ARG:NH1	1.95	0.81
2:H:7824:ASN:HD22	2:H:7824:ASN:H	1.23	0.81
1:A:726:GLU:HG3	1:A:727:ILE:H	1.45	0.81
1:C:2004:ARG:HD3	1:C:2007:ILE:HD12	1.62	0.81
1:G:6710:TYR:HB3	1:G:6711:PRO:HA	1.62	0.81
2:H:7786:MET:HE1	2:H:7812:HIS:ND1	1.95	0.81
2:F:5822:PRO:HB2	2:F:5824:ASN:ND2	1.96	0.81
1:E:4059:GLU:CG	1:E:4060:MET:HE2	2.12	0.80
2:H:7650:PHE:CD1	2:H:7651:PRO:HD2	2.17	0.80
1:G:7063:ILE:HD13	1:G:7068:MET:HG3	1.63	0.80
1:C:2573:GLY:HA3	10:C:4806:HOH:O	1.81	0.79
1:C:2845:ARG:HH11	1:C:2845:ARG:HG3	1.47	0.79
1:G:6712:LEU:CD2	1:G:6752:LEU:HG	2.12	0.79
1:E:4001:MET:N	1:E:4224:LYS:HZ1	1.81	0.79
2:D:3786:MET:HE1	2:D:3812:HIS:CE1	2.17	0.78
2:B:1557:TYR:CD1	2:B:1558:PRO:HD2	2.18	0.78
1:E:4003:LYS:HB3	1:E:4330:TYR:CE1	2.18	0.78
1:E:4936:ASN:HB2	10:E:6008:HOH:O	1.82	0.78
1:C:2784:GLN:H	1:C:2784:GLN:NE2	1.81	0.78
1:G:6064:THR:O	1:G:7065:VAL:HG23	1.83	0.78
1:E:4695:VAL:CG2	1:E:4752:LEU:HD22	2.14	0.78
1:A:151:THR:OG1	1:A:154:GLU:HG3	1.84	0.77
1:C:2944:ARG:HD3	1:C:2972:ASP:OD1	1.85	0.77
1:C:2975:HIS:HD1	1:E:4975:HIS:HD1	0.82	0.77
1:G:6028:TYR:CE1	1:G:6313:LYS:HE3	2.19	0.77
9:A:1950:NET:H42	9:A:1950:NET:H22	1.66	0.77
1:G:6714:VAL:HG22	1:G:6752:LEU:CD1	2.14	0.77
1:E:4282:SER:OG	1:E:4302:PRO:HA	1.84	0.77
1:G:6695:VAL:HG11	1:G:6701:ALA:CB	2.10	0.77
1:A:99:ALA:HB1	1:A:115:MET:HE1	1.67	0.76
1:C:2563:MET:HE3	1:C:2635:PRO:HG3	1.67	0.76
1:E:4035:LYS:O	1:E:4039:GLU:HB2	1.86	0.76
1:E:4695:VAL:HG21	1:E:4752:LEU:CD2	2.15	0.76
1:G:7000:HIS:HD2	1:G:7003:ASP:H	1.32	0.76
2:D:3652:GLY:O	2:D:3656:MET:HE3	1.85	0.76
2:H:7876:GLN:HG2	10:H:619:HOH:O	1.85	0.76
1:A:343:ARG:HD2	10:A:2208:HOH:O	1.86	0.76
1:C:2670:ASP:HB3	1:C:2677:ARG:HH21	1.50	0.76
1:G:6981:LEU:HD12	1:G:6988:PRO:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6059:GLU:OE2	1:G:6060:MET:HE2	1.85	0.75
1:G:6475:LYS:O	1:G:6479:VAL:HG13	1.87	0.75
1:G:6858:GLY:HA2	1:G:7069:HIS:CE1	2.21	0.75
1:A:944:ARG:HD3	1:A:972:ASP:OD1	1.86	0.75
1:A:1001:ILE:O	1:A:1005:ILE:HG13	1.86	0.75
2:B:1506:LEU:HD11	2:B:1508:VAL:CG2	2.16	0.75
1:G:7064:SER:OG	1:G:7067:GLU:HG3	1.86	0.75
1:G:6294:ARG:NH1	6:G:7931:CL:CL	2.55	0.75
1:A:831:ALA:HB2	1:A:840:ILE:HD11	1.68	0.74
1:G:6728:VAL:HG13	1:G:6733:ASP:HB3	1.69	0.74
1:G:6784:GLN:HE21	1:G:6784:GLN:N	1.78	0.74
2:F:5822:PRO:HB2	2:F:5824:ASN:HD21	1.52	0.74
1:E:4967:GLN:HG2	1:E:5054:LEU:HD13	1.67	0.74
1:E:4335:LEU:O	1:E:4336:MET:HE2	1.88	0.74
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.53	0.74
1:E:4697:ALA:O	1:E:4700:MET:HB3	1.87	0.74
2:H:7824:ASN:O	2:H:7842:ARG:HD2	1.88	0.74
1:C:2675:ARG:H	1:C:2675:ARG:HD2	1.52	0.74
1:E:4151:THR:OG1	1:E:4154:GLU:HG3	1.87	0.74
1:G:6022:GLN:HG3	1:G:6174:MET:HE1	1.70	0.74
1:G:6936:ASN:HB2	10:G:22:HOH:O	1.86	0.74
1:G:6702:VAL:O	1:G:6706:LYS:HD3	1.88	0.73
1:G:6873:SER:O	1:G:6877:GLN:HG3	1.87	0.73
1:G:6994:VAL:HG13	1:G:7000:HIS:ND1	2.02	0.73
1:A:873:SER:O	1:A:877:GLN:HG3	1.87	0.73
2:H:7633:ILE:HD12	2:H:7643:ALA:CB	2.17	0.73
1:G:7001:ILE:HG21	1:G:7029:ILE:HD13	1.70	0.73
1:A:675:ARG:O	1:A:679:GLN:HG3	1.88	0.73
1:G:6339:ILE:HD12	1:G:6530:ASP:HA	1.71	0.73
1:A:129:ARG:HB3	1:A:205:LEU:HD22	1.70	0.73
2:B:1824:ASN:HD22	2:B:1824:ASN:N	1.87	0.73
1:A:784:GLN:HE21	1:A:784:GLN:N	1.80	0.73
1:C:2336:MET:HE3	10:C:4201:HOH:O	1.88	0.73
1:C:2675:ARG:H	1:C:2675:ARG:CD	2.02	0.73
1:A:471:ARG:HD2	10:A:2730:HOH:O	1.89	0.73
2:H:7574:GLN:HG3	2:H:7576:HIS:NE2	2.04	0.73
1:A:734:LEU:HD12	1:A:734:LEU:O	1.89	0.72
1:C:2966[A]:LYS:HE3	10:C:4594:HOH:O	1.88	0.72
1:C:2687:LEU:HD13	1:C:2812:GLN:CG	2.18	0.72
1:E:4003:LYS:HB2	1:E:4042:TYR:OH	1.89	0.72
1:A:947[B]:LEU:HD12	1:A:1014:ILE:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2695:VAL:HG21	1:C:2701:ALA:CA	2.13	0.72
1:E:4674:ASP:HB3	1:E:4677:ARG:HG3	1.71	0.72
1:C:2679:GLN:O	1:C:2683:GLU:HG3	1.89	0.72
2:B:1690:LEU:HD22	2:B:1714:CYS:O	1.88	0.72
1:E:4001:MET:O	1:E:4334:GLU:OE2	2.08	0.72
1:E:4001:MET:N	10:E:6621:HOH:O	2.23	0.72
1:G:6738:PHE:O	1:G:6741:ALA:HB3	1.90	0.72
1:G:7026:SER:HB2	1:G:7030:ARG:HH12	1.55	0.72
1:A:186:GLU:HB2	10:A:2505:HOH:O	1.89	0.71
2:B:1506:LEU:HD11	2:B:1508:VAL:HG22	1.72	0.71
1:E:4688:LYS:HD3	1:E:4838:TYR:CE2	2.25	0.71
2:H:7824:ASN:ND2	2:H:7824:ASN:H	1.86	0.71
1:C:3064:SER:O	1:C:3068:MET:HG3	1.90	0.71
2:B:1652:GLY:O	2:B:1656:MET:HE3	1.90	0.71
2:F:5734:ASP:HB3	2:F:5874:ILE:CG2	2.21	0.71
1:C:2973:ALA:O	1:C:2991:VAL:HG12	1.89	0.71
1:C:2998:ARG:HB3	1:C:2999:PRO:HA	1.73	0.71
2:F:5604:ARG:HA	10:F:2667:HOH:O	1.91	0.70
1:G:6563:MET:HE3	1:G:6635:PRO:HG3	1.73	0.70
1:G:6698:ILE:H	1:G:6698:ILE:CD1	2.04	0.70
2:D:3786:MET:HE1	2:D:3812:HIS:ND1	2.07	0.70
1:G:7000:HIS:CD2	1:G:7003:ASP:H	2.09	0.70
1:A:708:ILE:HG23	1:A:754:HIS:HB2	1.73	0.70
2:D:3633:ILE:HD12	2:D:3643:ALA:HB2	1.72	0.70
2:D:3642:LEU:O	2:D:3642:LEU:HD12	1.92	0.70
1:G:6873:SER:OG	1:G:6876:GLU:HG3	1.92	0.70
1:A:698:ILE:O	1:A:702:VAL:HG23	1.92	0.70
1:A:697:ALA:O	1:A:700:MET:HB3	1.92	0.69
1:C:2224:LYS:HE2	1:C:2329:GLY:O	1.91	0.69
1:G:6318:PRO:HG3	1:G:6610:TYR:OH	1.92	0.69
2:H:7764:PRO:HA	2:H:7846:PRO:HB2	1.72	0.69
1:G:6702:VAL:HG11	1:G:6735:ARG:NH2	2.06	0.69
1:A:1020:ARG:HH21	1:A:1023:ILE:HG21	1.56	0.69
1:E:4703:GLU:O	1:E:4706:LYS:HB2	1.92	0.69
2:H:7772:HIS:HB2	2:H:7849:SER:HB2	1.74	0.69
1:E:4994:VAL:HG13	1:E:5000:HIS:ND1	2.07	0.69
1:A:80:LYS:NZ	1:A:80:LYS:CD	2.55	0.69
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.74	0.69
2:B:1786:MET:HE3	2:B:1789:GLY:HA2	1.72	0.69
1:C:2677:ARG:O	1:C:2680:HIS:HB2	1.93	0.69
1:G:6259:LYS:HD3	2:H:7675:TRP:CE3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2321:LYS:NZ	1:C:2611:ASP:OD2	2.25	0.68
2:H:7799:ASP:OD2	2:H:7802:LYS:HD2	1.92	0.68
1:C:2482:THR:HB	10:C:4742:HOH:O	1.93	0.68
2:D:3715:ARG:HG3	2:D:3715:ARG:HH11	1.57	0.68
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.74	0.68
1:A:726:GLU:HG3	1:A:727:ILE:N	2.08	0.68
1:C:2416:ASP:O	1:C:2418:PRO:HD3	1.94	0.68
1:E:4004:ARG:HA	10:E:6625:HOH:O	1.93	0.68
2:H:7531:VAL:HG12	10:H:929:HOH:O	1.92	0.68
1:C:2043:ARG:NH2	1:C:2081:GLU:OE1	2.27	0.68
1:C:2714:VAL:HG11	1:C:2737:TYR:CE2	2.29	0.68
1:E:4335:LEU:C	1:E:4336:MET:HE2	2.19	0.68
2:D:3726:GLU:O	2:D:3730:LYS:HG3	1.92	0.68
1:A:59:GLU:CG	1:A:60:MET:HE2	2.24	0.67
1:A:710:TYR:CD2	1:A:712:LEU:HD13	2.29	0.67
2:D:3722:GLN:HE21	2:D:3722:GLN:H	1.42	0.67
1:G:6159:ALA:HB2	1:G:6188:PHE:CE1	2.29	0.67
1:A:738:PHE:O	1:A:741:ALA:HB3	1.93	0.67
1:G:6375:THR:HG23	1:G:6377:GLN:H	1.59	0.67
1:A:698:ILE:HD12	1:A:698:ILE:H	1.59	0.67
1:G:6757:ASP:O	1:G:6833:LYS:HE3	1.95	0.67
1:G:6954:LYS:O	1:G:6980:VAL:HG11	1.94	0.67
2:F:5669:SER:HA	2:F:5716:LEU:O	1.95	0.67
2:F:5824:ASN:HD22	2:F:5824:ASN:N	1.87	0.67
2:B:1698:ASP:HB2	2:B:1718:ILE:CG2	2.25	0.66
1:G:6079:GLU:HB2	1:G:6111:PHE:CE2	2.30	0.66
1:G:6509:ARG:HB2	1:G:6512:GLU:OE2	1.95	0.66
1:A:434:ASP:HB2	10:A:2524:HOH:O	1.94	0.66
2:H:7694:VAL:HB	2:H:7716:LEU:HD23	1.75	0.66
1:G:7063:ILE:HD13	1:G:7068:MET:CG	2.25	0.66
1:G:6001:MET:HA	1:G:6224:LYS:CE	2.26	0.66
1:A:519:GLN:NE2	10:A:2758:HOH:O	2.28	0.66
1:A:1021:ARG:HG3	1:A:1021:ARG:HH11	1.60	0.66
1:C:2032:GLN:OE1	1:C:2320:ALA:HB3	1.96	0.66
1:E:4944:ARG:HG2	1:E:5010:TYR:CD1	2.30	0.66
1:G:6712:LEU:HD21	1:G:6752:LEU:HG	1.77	0.66
1:C:2059:GLU:HG2	1:C:2060:MET:CE	2.25	0.66
1:G:6734:LEU:HD12	1:G:6734:LEU:O	1.95	0.66
1:G:6471:ARG:HD2	10:G:4256:HOH:O	1.94	0.66
1:G:6728:VAL:HG12	1:G:6733:ASP:HB3	1.76	0.66
1:C:2698:ILE:HD12	1:C:2698:ILE:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4730:ASP:OD1	1:E:4733:ASP:HB2	1.96	0.66
1:E:4944:ARG:HG2	1:E:5010:TYR:HD1	1.60	0.66
2:F:5845:LYS:HB3	2:F:5846:PRO:HD2	1.77	0.66
1:G:6806:GLN:O	1:G:6810:ARG:HG3	1.95	0.66
1:G:6043:ARG:NH1	10:G:838:HOH:O	2.23	0.65
2:H:7800:VAL:HG22	2:H:7828:THR:O	1.96	0.65
1:A:990:LEU:HD23	1:G:6979:ILE:CD1	2.27	0.65
1:C:2726:GLU:HG2	1:C:2727:ILE:H	1.60	0.65
1:E:4736:ARG:NH2	1:E:5020:ARG:HG2	2.12	0.65
1:G:7001:ILE:HG22	1:G:7002:GLN:N	2.11	0.65
2:H:7801:GLU:OE2	2:H:7828:THR:HG22	1.96	0.65
2:D:3776:ALA:HB1	2:D:3781:ALA:HB3	1.77	0.65
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.43	0.65
1:C:2687:LEU:HD13	1:C:2812:GLN:HG2	1.78	0.65
1:E:4959:ASP:OD2	1:E:4963:LYS:NZ	2.30	0.65
2:B:1824:ASN:HD22	2:B:1824:ASN:H	1.44	0.65
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.79	0.65
2:B:1772:HIS:ND1	2:B:1849:SER:OG	2.30	0.65
1:G:6057:ASP:HB3	1:G:6059:GLU:OE2	1.97	0.65
2:D:3824:ASN:HD22	2:D:3824:ASN:N	1.95	0.64
1:E:4375:THR:OG1	1:E:4376:THR:N	2.30	0.64
1:E:4733:ASP:O	1:E:4736:ARG:HB3	1.97	0.64
1:A:715:ARG:HG3	1:A:725:MET:HG2	1.78	0.64
2:D:3557:TYR:CD1	2:D:3558:PRO:HD2	2.33	0.64
1:C:2712:LEU:HD23	1:C:2752:LEU:HG	1.79	0.64
1:E:4714:VAL:HG13	1:E:4752:LEU:CD1	2.21	0.64
1:C:2400:ARG:HD3	10:C:4233:HOH:O	1.96	0.64
2:H:7715:ARG:HG3	2:H:7715:ARG:NH1	2.06	0.64
1:G:6159:ALA:HB2	1:G:6188:PHE:CZ	2.32	0.64
1:A:811:GLN:HG2	10:A:2834:HOH:O	1.97	0.64
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.28	0.64
1:C:2728:VAL:HG11	1:C:2734:LEU:HA	1.80	0.64
2:D:3691:PRO:HD2	2:D:3713:GLY:O	1.97	0.64
1:G:6353:ASP:OD2	2:H:7616:ARG:HD2	1.97	0.64
1:G:6172:PHE:HB3	1:G:6200:PRO:HG2	1.80	0.64
2:H:7548:TYR:HA	2:H:7551:GLN:NE2	2.13	0.64
1:G:7017:THR:HG21	1:G:7023:ILE:HA	1.79	0.63
2:H:7686:LYS:O	2:H:7689:GLU:HB2	1.98	0.63
2:D:3715:ARG:HG3	2:D:3715:ARG:NH1	2.12	0.63
1:E:4734:LEU:HD12	1:E:4734:LEU:O	1.97	0.63
1:G:6167:ILE:N	1:G:6167:ILE:HD12	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3728:VAL:O	2:D:3731:MET:HG3	1.99	0.63
1:C:2426:ARG:HD3	1:C:2426:ARG:C	2.24	0.63
1:G:6164:PHE:HA	1:G:6165:PRO:C	2.23	0.63
2:F:5557:TYR:CD1	2:F:5558:PRO:HD2	2.32	0.63
1:G:6001:MET:HA	1:G:6224:LYS:HE3	1.79	0.63
1:G:6209:SER:OG	1:G:6211:ILE:HG13	1.99	0.63
1:G:6427:GLU:HG3	1:G:6438:TYR:CE2	2.33	0.63
2:H:7769:CYG:HO2	2:H:7812:HIS:HB2	1.64	0.63
2:H:7850:PHE:CD1	2:H:7866:LEU:HD21	2.34	0.63
2:B:1650:PHE:CD1	2:B:1651:PRO:HD2	2.34	0.63
1:G:6668:ALA:HA	10:G:398:HOH:O	1.99	0.63
1:A:43:ARG:NH1	10:A:2620:HOH:O	2.31	0.63
1:G:6563:MET:CE	1:G:6635:PRO:HG3	2.29	0.63
1:C:2550:GLU:OE1	2:D:3617:LYS:HG3	1.99	0.62
1:E:4003:LYS:HB3	1:E:4330:TYR:CZ	2.34	0.62
1:E:5000:HIS:HD2	1:E:5003:ASP:H	1.47	0.62
2:F:5732:ASN:N	2:F:5733:PRO:HD3	2.14	0.62
1:G:6110:GLU:HG2	1:G:6111:PHE:CD1	2.34	0.62
1:G:6646:THR:HB	1:G:6647:PRO:HD3	1.80	0.62
1:G:6726:GLU:HG3	1:G:6727:ILE:N	2.13	0.62
1:C:2509:ARG:HB2	1:C:2509:ARG:NH1	2.13	0.62
2:F:5674:SER:HB2	2:F:5711:ASP:OD2	1.99	0.62
2:B:1726:GLU:N	2:B:1726:GLU:OE1	2.30	0.62
1:G:6223:ASP:OD2	1:G:6227:ASN:HB2	1.99	0.62
1:G:7026:SER:CB	1:G:7030:ARG:HH12	2.11	0.62
1:A:1037:LYS:HA	10:A:2859:HOH:O	1.99	0.62
1:C:2009:SER:OG	1:C:2083:PRO:HA	1.99	0.62
2:F:5749:ASP:OD1	2:F:5750:TYR:N	2.32	0.62
2:F:5764:PRO:HG2	2:F:5874:ILE:HA	1.81	0.62
1:A:563:MET:CE	1:A:635:PRO:HG3	2.29	0.62
1:G:6420:ALA:HA	1:G:6423:LYS:HD2	1.81	0.62
2:H:7791:HIS:HA	2:H:7810:GLN:O	1.99	0.62
1:E:4289:ASN:OD1	1:E:4290:PRO:HD2	2.00	0.62
1:E:4698:ILE:HD12	1:E:4698:ILE:N	2.15	0.62
1:E:4998:ARG:HA	1:E:4999:PRO:C	2.24	0.62
1:E:5001:ILE:HG22	1:E:5002:GLN:N	2.13	0.62
2:H:7779:SER:OG	2:H:7842:ARG:HD3	1.99	0.62
2:B:1722:GLN:HE21	2:B:1722:GLN:H	1.47	0.62
2:F:5818:GLU:O	2:F:5821:LEU:HB2	1.98	0.62
1:C:2103:GLU:HG3	1:C:2104:ARG:N	2.12	0.62
1:C:2907:LEU:HD11	8:C:3920:ORN:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2954:LYS:HB3	1:C:2980:VAL:HG21	1.82	0.62
2:H:7824:ASN:HA	2:H:7843:THR:OG1	1.99	0.62
1:C:2001:MET:HA	1:C:2224:LYS:NZ	2.15	0.61
1:C:3027:ARG:HG3	1:C:3027:ARG:HH11	1.65	0.61
2:H:7506:LEU:CD1	2:H:7508:VAL:HG23	2.26	0.61
1:A:40:GLU:OE2	1:A:325:LYS:NZ	2.32	0.61
1:G:6733:ASP:O	1:G:6736:ARG:HB3	2.00	0.61
1:G:7051:ALA:HA	1:G:7054:LEU:HD12	1.81	0.61
1:C:2670:ASP:HB3	1:C:2677:ARG:NH2	2.14	0.61
1:C:2698:ILE:HD12	1:C:2698:ILE:N	2.16	0.61
1:C:3000:HIS:HD2	1:C:3003:ASP:H	1.45	0.61
2:H:7757:LYS:HE2	10:H:586:HOH:O	2.00	0.61
1:A:365:GLU:OE1	1:A:365:GLU:N	2.30	0.61
1:E:4698:ILE:HD12	1:E:4698:ILE:H	1.65	0.61
1:G:6339:ILE:CD1	1:G:6530:ASP:HA	2.30	0.61
1:G:7037:LYS:HE3	10:G:76:HOH:O	1.99	0.61
2:H:7726:GLU:OE2	2:H:7757:LYS:HE3	1.99	0.61
2:H:7844:ASP:OD1	2:H:7844:ASP:N	2.30	0.61
2:D:3755:ILE:O	2:D:3759:LEU:HG	1.99	0.61
1:E:4440:ALA:O	1:E:4444:ARG:HG3	2.00	0.61
2:H:7813:GLY:HA3	10:H:483:HOH:O	2.00	0.61
1:A:693:ALA:HB2	1:A:708:ILE:HD11	1.83	0.61
1:G:6768:CYS:HB2	1:G:6773:VAL:HG22	1.82	0.61
1:G:7021:ARG:HG3	1:G:7021:ARG:HH11	1.65	0.61
1:C:2967:GLN:HG2	1:C:3054:LEU:HD13	1.83	0.61
1:C:3067:GLU:HG3	10:C:4439:HOH:O	2.00	0.61
1:E:4784:GLN:H	1:E:4784:GLN:NE2	1.99	0.61
1:A:698:ILE:HD12	1:A:698:ILE:N	2.15	0.61
1:C:2646:THR:HB	1:C:2647:PRO:HD3	1.82	0.61
1:E:5027:ARG:HE	1:E:5031:ARG:HH11	1.49	0.61
1:G:6828:VAL:HG22	1:G:6842:VAL:HG13	1.82	0.61
1:G:6833:LYS:O	1:G:6836:GLU:HB2	2.01	0.61
1:A:715:ARG:NH1	10:A:2845:HOH:O	2.28	0.61
1:A:941:LYS:HE3	10:A:2879:HOH:O	2.01	0.61
1:C:2504:LYS:HE2	10:C:4756:HOH:O	2.01	0.61
2:H:7542:ILE:HG23	2:H:7548:TYR:CE2	2.35	0.61
1:E:4142:GLU:OE2	1:E:4294:ARG:NH2	2.34	0.60
1:E:4893:VAL:HG22	8:E:5920:ORN:HD2	1.83	0.60
1:C:2006:ASP:OD1	1:C:2006:ASP:N	2.32	0.60
1:C:2147:GLY:HA3	1:C:2158:VAL:CG1	2.32	0.60
1:E:4795:SER:HB2	1:E:4890:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7850:PHE:CG	2:H:7866:LEU:HD21	2.35	0.60
1:A:442:ALA:HB1	1:A:447:LEU:HD12	1.82	0.60
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.31	0.60
1:C:2105:GLN:HA	1:C:2105:GLN:NE2	2.16	0.60
1:C:2676:GLU:O	1:C:2680:HIS:ND1	2.29	0.60
1:E:4648:LEU:CD2	1:E:4845:ARG:HD3	2.30	0.60
2:H:7695:VAL:HG23	2:H:7733:PRO:HB3	1.82	0.60
1:A:993:LYS:NZ	10:A:2399:HOH:O	2.34	0.60
1:E:5017:THR:CG2	1:E:5023:ILE:HG13	2.32	0.60
1:E:5057:ASP:HB3	1:E:5060:GLU:HB2	1.84	0.60
1:C:2858:GLY:HA2	1:C:3069:HIS:CE1	2.37	0.60
1:C:2930:LYS:HE3	10:C:4381:HOH:O	2.01	0.60
1:C:2981:LEU:HD12	1:C:2988:PRO:HG3	1.84	0.60
1:G:6400:ARG:HD3	10:G:274:HOH:O	2.00	0.60
1:A:160:ALA:HB2	10:A:2669:HOH:O	2.01	0.60
2:B:1850:PHE:HB2	2:B:1866:LEU:HD22	1.84	0.60
1:G:6868:VAL:HG23	1:G:6877:GLN:HE22	1.66	0.60
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.32	0.60
1:A:860:PRO:O	1:A:864:VAL:HG23	2.01	0.60
1:A:6:ASP:OD1	1:A:6:ASP:N	2.35	0.60
1:A:737:TYR:O	1:A:741:ALA:N	2.29	0.60
2:D:3564:GLY:HA3	2:D:3594:ASN:OD1	2.01	0.60
2:F:5620:ARG:HD2	10:F:3115:HOH:O	2.01	0.60
1:G:6043:ARG:NH2	1:G:6081:GLU:OE1	2.29	0.60
1:G:6678:PHE:O	1:G:6682:VAL:HG23	2.02	0.60
1:E:4966:LYS:HB3	10:E:6859:HOH:O	2.01	0.59
2:H:7818:GLU:OE2	2:H:7827:VAL:HG21	2.01	0.59
1:E:4358:LYS:HE3	10:E:6526:HOH:O	2.02	0.59
1:G:6196:LEU:HG	1:G:6204:LEU:HD11	1.83	0.59
1:G:7017:THR:HG21	1:G:7023:ILE:HG12	1.84	0.59
1:A:646:THR:HB	1:A:647:PRO:HD3	1.84	0.59
1:C:2873:SER:O	1:C:2877:GLN:HG3	2.03	0.59
1:E:4509:ARG:HB2	1:E:4512:GLU:OE2	2.02	0.59
1:E:4648:LEU:HD21	1:E:4845:ARG:HD3	1.84	0.59
1:G:6119:THR:HG23	10:G:656:HOH:O	2.02	0.59
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.21	0.59
1:A:1020:ARG:HG3	1:A:1024:GLU:OE2	2.01	0.59
1:E:4001:MET:HA	1:E:4224:LYS:HE2	1.84	0.59
1:G:6695:VAL:HG21	1:G:6701:ALA:HA	1.84	0.59
1:A:959:ASP:O	1:A:963:LYS:HG3	2.03	0.59
2:B:1864:ALA:HB3	2:B:1865:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2151:THR:OG1	1:C:2154:GLU:HB2	2.02	0.59
1:E:4695:VAL:HG11	1:E:4701:ALA:CB	2.29	0.59
2:H:7779:SER:OG	2:H:7842:ARG:NH1	2.30	0.59
1:A:698:ILE:H	1:A:698:ILE:CD1	2.16	0.59
2:D:3574:GLN:HB2	10:D:4036:HOH:O	2.02	0.59
2:D:3701:ALA:HB2	2:D:3739:SER:CB	2.33	0.59
1:G:6648:LEU:CD2	1:G:6845:ARG:HD3	2.33	0.59
1:G:6734:LEU:HD11	1:G:6738:PHE:CE2	2.38	0.59
2:B:1705:ILE:HG21	2:B:1737:PHE:CZ	2.38	0.59
1:G:6129:ARG:NH2	7:G:7900:ADP:O3B	2.30	0.59
1:G:6534:ALA:O	2:H:7623:ARG:HD3	2.02	0.59
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.03	0.59
1:C:2059:GLU:HG2	1:C:2060:MET:HE2	1.84	0.59
2:H:7749:ASP:OD1	2:H:7750:TYR:N	2.35	0.59
1:A:751:LEU:O	1:A:752:LEU:HD12	2.02	0.59
1:C:2974:THR:CG2	1:C:3001:ILE:HD11	2.32	0.59
2:D:3523:THR:HG23	2:D:3634:ALA:O	2.03	0.59
1:G:6470:VAL:O	1:G:6474:GLU:HG3	2.03	0.59
1:G:6667:ASP:CG	1:G:6677:ARG:HH22	2.11	0.59
1:G:6905:PRO:HB2	1:G:7040:TYR:OH	2.03	0.59
1:G:6929:ALA:HB2	1:G:7053:ALA:HB1	1.85	0.59
2:H:7779:SER:O	2:H:7822:PRO:HG3	2.03	0.59
1:C:2294:ARG:NH1	10:C:4151:HOH:O	2.25	0.59
1:C:2344:THR:HB	1:C:2345:PRO:HD2	1.84	0.59
1:E:4511:ALA:O	1:E:4515:LYS:HG3	2.03	0.59
1:G:6426:ARG:HD3	1:G:6426:ARG:C	2.28	0.59
1:G:6809:MET:O	1:G:6813:VAL:HG23	2.02	0.58
2:H:7725:ALA:HA	2:H:7758:PHE:CZ	2.38	0.58
1:C:2024:CYS:HB3	1:C:2576:ILE:HD12	1.85	0.58
1:C:2958:VAL:HG13	1:C:2986:ILE:HD12	1.85	0.58
1:G:6065:TYR:OH	1:G:6080:LYS:HE2	2.02	0.58
1:C:2504:LYS:HD3	10:C:4760:HOH:O	2.02	0.58
1:E:4646:THR:HB	1:E:4647:PRO:HD3	1.84	0.58
2:F:5548:TYR:HA	2:F:5551:GLN:HE21	1.68	0.58
1:C:2343:ARG:NH2	1:C:2539:ASP:OD2	2.30	0.58
1:G:6708:ILE:CG2	1:G:6754:HIS:HB2	2.33	0.58
1:G:6994:VAL:HG23	10:G:458:HOH:O	2.02	0.58
1:C:3021:ARG:HG3	1:C:3021:ARG:HH11	1.67	0.58
1:E:4518:ASP:HB3	10:E:6556:HOH:O	2.02	0.58
2:F:5844:ASP:OD1	2:F:5844:ASP:N	2.30	0.58
2:D:3759:LEU:HD13	2:D:3842:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4412:LYS:HG2	1:E:4438:TYR:CZ	2.39	0.58
1:E:4702:VAL:HG13	1:E:4731:GLU:HG2	1.85	0.58
1:G:6667:ASP:OD1	1:G:6677:ARG:NH2	2.35	0.58
1:G:6802:SER:O	1:G:6805:ILE:HG22	2.03	0.58
2:B:1544:THR:HG21	2:B:1570:GLU:HG2	1.85	0.58
2:B:1639:ASP:HB3	2:B:1642:LEU:HB3	1.86	0.58
2:B:1644:LEU:HD21	2:B:1648:ARG:CZ	2.33	0.58
2:B:1824:ASN:H	2:B:1824:ASN:ND2	1.99	0.58
1:E:4728:VAL:CG1	1:E:4733:ASP:HB3	2.31	0.58
1:G:6591:GLU:O	1:G:6591:GLU:HG3	2.03	0.58
2:H:7723:THR:HG22	2:H:7728:VAL:HG23	1.84	0.58
2:B:1818:GLU:OE1	2:B:1830:LYS:HE3	2.03	0.58
1:C:2726:GLU:HG2	1:C:2727:ILE:N	2.19	0.58
1:E:4343:ARG:NH2	1:E:4539:ASP:OD2	2.31	0.58
2:F:5700:GLY:O	2:F:5740:ASN:ND2	2.37	0.58
2:F:5748:CYS:HB3	2:F:5750:TYR:CZ	2.38	0.58
1:A:905:PRO:HB2	1:A:1040:TYR:OH	2.05	0.57
2:D:3726:GLU:OE1	2:D:3726:GLU:N	2.37	0.57
1:E:4691:ALA:HB3	1:E:4754:HIS:HB2	1.84	0.57
1:E:5028:VAL:O	1:E:5032:SER:HB2	2.04	0.57
1:A:358:LYS:HE3	10:A:2520:HOH:O	2.04	0.57
1:A:675:ARG:CD	1:A:675:ARG:H	2.15	0.57
1:E:5020:ARG:NE	1:E:5020:ARG:HA	2.19	0.57
2:H:7657:ASP:OD1	2:H:7660:LYS:HG2	2.04	0.57
1:A:426:ARG:HD3	1:A:426:ARG:C	2.30	0.57
1:C:3000:HIS:CD2	1:C:3003:ASP:H	2.23	0.57
1:G:6292:ASN:HB2	10:G:222:HOH:O	2.04	0.57
2:B:1718:ILE:HD13	2:B:1718:ILE:N	2.19	0.57
2:B:1786:MET:HE3	2:B:1789:GLY:CA	2.34	0.57
1:C:2695:VAL:HA	1:C:2700:MET:HE2	1.86	0.57
2:D:3687:GLU:HG3	2:D:3715:ARG:HD2	1.84	0.57
2:H:7737:PHE:CE1	2:H:7768:ILE:HD12	2.40	0.57
1:C:2672:ALA:HB3	1:C:2844:PRO:HG3	1.85	0.57
1:C:2698:ILE:H	1:C:2698:ILE:CD1	2.18	0.57
1:C:2726:GLU:CG	1:C:2727:ILE:H	2.18	0.57
1:E:4979:ILE:O	1:E:4983:GLU:HG3	2.05	0.57
1:A:708:ILE:CG2	1:A:754:HIS:HB2	2.34	0.57
2:B:1786:MET:HE1	2:B:1812:HIS:ND1	2.19	0.57
2:D:3548:TYR:HA	2:D:3551:GLN:HE21	1.70	0.57
1:E:4157:ALA:HA	10:E:6503:HOH:O	2.05	0.57
1:G:6954:LYS:HB3	1:G:6980:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1786:MET:CE	2:B:1789:GLY:HA2	2.35	0.57
1:E:4698:ILE:O	1:E:4702:VAL:HG23	2.04	0.57
2:F:5744:ASP:OD1	2:F:5745:PRO:HD2	2.05	0.57
2:F:5786[A]:MET:HE1	2:F:5812:HIS:ND1	2.20	0.57
1:G:6941:LYS:NZ	1:G:7056:ALA:O	2.29	0.57
2:H:7657:ASP:HB2	2:H:7747:PRO:HB2	1.86	0.57
1:G:6698:ILE:HD12	1:G:6698:ILE:N	2.13	0.57
1:G:6733:ASP:HA	1:G:6736:ARG:HH11	1.68	0.57
2:H:7725:ALA:HA	2:H:7758:PHE:CE1	2.39	0.57
1:A:704:LYS:O	1:A:707:GLU:HB2	2.04	0.56
1:C:2563:MET:CE	1:C:2635:PRO:HG3	2.35	0.56
1:E:4180:GLY:HA2	1:E:4376:THR:OG1	2.05	0.56
1:A:954:LYS:O	1:A:957:VAL:HG12	2.05	0.56
1:C:2979:ILE:HG12	1:E:4990:LEU:HD23	1.85	0.56
2:F:5693:HIS:N	2:F:5734:ASP:OD2	2.36	0.56
1:G:6950:ARG:NH1	10:G:912:HOH:O	2.30	0.56
1:A:772[A]:MET:SD	1:A:880:THR:HG22	2.45	0.56
2:D:3687:GLU:HG2	2:D:3715:ARG:CD	2.30	0.56
1:E:4353:ASP:OD2	2:F:5616:ARG:HD2	2.05	0.56
1:A:412:LYS:HD3	10:A:2715:HOH:O	2.05	0.56
1:E:4695:VAL:HA	1:E:4700:MET:HE2	1.86	0.56
1:E:4738:PHE:C	1:E:4741:ALA:HB3	2.30	0.56
1:G:6671:ARG:HG2	1:G:6677:ARG:CZ	2.35	0.56
2:B:1542:ILE:HG23	2:B:1548:TYR:CE2	2.41	0.56
2:F:5550:ARG:HH12	2:F:5650:PHE:HE1	1.51	0.56
1:G:6004:ARG:HD3	1:G:6007:ILE:HD12	1.86	0.56
1:G:6517:ARG:HB3	1:G:6522:LEU:O	2.06	0.56
1:A:410:ASP:OD2	1:A:504:LYS:NZ	2.37	0.56
1:A:738:PHE:HA	1:A:741:ALA:HB2	1.86	0.56
2:H:7550:ARG:NH1	2:H:7650:PHE:HE1	2.03	0.56
1:A:730:ASP:H	1:A:733:ASP:HB2	1.71	0.56
1:E:4150:HIS:CD2	1:E:4203:GLU:HB2	2.41	0.56
2:F:5585:LEU:HD12	2:F:5586:PRO:HD2	1.86	0.56
1:G:6186:GLU:HB2	10:G:705:HOH:O	2.05	0.56
2:H:7554:THR:HG21	2:H:7618:LEU:HD23	1.88	0.56
1:A:99:ALA:HB1	1:A:115:MET:CE	2.35	0.56
1:C:2442:ALA:HB1	1:C:2447:LEU:HD12	1.88	0.56
2:F:5824:ASN:H	2:F:5824:ASN:ND2	1.87	0.56
1:G:6648:LEU:HD22	1:G:6845:ARG:HD3	1.88	0.56
2:D:3798:LYS:NZ	10:D:3956:HOH:O	2.29	0.56
1:E:4687:LEU:HD22	1:E:4812:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4959:ASP:O	1:E:4963:LYS:HG3	2.06	0.56
1:G:6947:LEU:HA	1:G:7014:ILE:HG23	1.88	0.56
1:A:814:GLN:NE2	10:A:2362:HOH:O	2.38	0.55
2:F:5734:ASP:O	2:F:5874:ILE:HG23	2.06	0.55
1:C:2672:ALA:CB	1:C:2844:PRO:HG3	2.36	0.55
1:C:2687:LEU:HD13	1:C:2812:GLN:HG3	1.88	0.55
1:G:6548:GLU:HG2	2:H:7614:ASP:HB2	1.88	0.55
1:A:166:CYS:C	1:A:167:ILE:HD12	2.31	0.55
2:B:1880:THR:HG22	2:B:1880:THR:O	2.06	0.55
2:D:3818:GLU:O	2:D:3821:LEU:HB2	2.05	0.55
1:E:4751:LEU:O	1:E:4752:LEU:HD12	2.06	0.55
1:E:4967:GLN:HB2	10:E:6862:HOH:O	2.07	0.55
1:G:6165:PRO:HA	1:G:6182:ALA:O	2.07	0.55
2:D:3744:ASP:OD1	2:D:3745:PRO:HD2	2.05	0.55
1:A:339:ILE:C	1:A:341:GLY:H	2.13	0.55
1:C:2796:LEU:C	1:C:2796:LEU:HD23	2.32	0.55
2:D:3728:VAL:HG22	2:D:3731:MET:HE3	1.89	0.55
1:E:4944:ARG:HD3	1:E:4972:ASP:CG	2.32	0.55
2:F:5571:GLU:O	2:F:5703:ARG:HG3	2.07	0.55
2:F:5786[A]:MET:HE1	2:F:5812:HIS:CE1	2.41	0.55
1:A:947[B]:LEU:HD12	1:A:1014:ILE:HG22	1.87	0.55
1:G:6101:GLU:HA	1:G:6101:GLU:OE1	2.06	0.55
1:G:7019:GLY:O	1:G:7023:ILE:HG13	2.06	0.55
1:A:416:ASP:N	1:A:416:ASP:OD1	2.30	0.55
1:A:967:GLN:O	1:A:967:GLN:HG3	2.07	0.55
1:C:2358:LYS:HE3	10:C:4513:HOH:O	2.07	0.55
1:C:2998:ARG:CB	1:C:2999:PRO:HA	2.30	0.55
1:E:4705:ALA:HB1	1:E:4710:TYR:CZ	2.41	0.55
1:G:6695:VAL:HG13	1:G:6700:MET:HB3	1.88	0.55
1:G:6770:GLY:HA2	1:G:6823:ARG:NH1	2.22	0.55
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.37	0.55
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.22	0.55
1:C:2079:GLU:HB2	1:C:2111:PHE:CZ	2.42	0.55
2:B:1779:SER:O	2:B:1822:PRO:HG3	2.06	0.55
1:C:2805:ILE:HD13	1:C:2837:VAL:CG2	2.37	0.55
1:E:4003:LYS:O	1:E:4003:LYS:HG3	2.06	0.55
1:E:4425:ARG:HD3	10:E:6254:HOH:O	2.07	0.55
1:G:6349:GLU:O	2:H:7794:ASN:HB2	2.07	0.55
1:G:6947:LEU:HD12	1:G:6947:LEU:N	2.22	0.55
2:H:7534:THR:HA	2:H:7556:THR:OG1	2.07	0.55
2:D:3526:ALA:O	2:D:3631:CYS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4711:PRO:HG2	1:E:4755:PHE:HD2	1.73	0.54
1:G:6710:TYR:HA	1:G:6711:PRO:C	2.30	0.54
2:H:7599:SER:O	2:H:7603:LYS:HG3	2.07	0.54
1:A:363:ASN:OD1	1:A:381:VAL:HG21	2.07	0.54
1:A:736:ARG:O	1:A:740:THR:HG23	2.06	0.54
1:A:930:LYS:HE3	10:A:2385:HOH:O	2.07	0.54
1:C:2675:ARG:HD2	1:C:2675:ARG:N	2.22	0.54
1:C:2948:SER:O	1:C:3015:ASN:HA	2.08	0.54
1:E:4027:ASP:HB2	1:E:4053:THR:HG22	1.89	0.54
2:B:1526:ALA:HB1	2:B:1578:GLN:HG3	1.90	0.54
1:C:2001:MET:HA	1:C:2224:LYS:HZ2	1.72	0.54
1:C:2358:LYS:HD2	1:C:2383:GLU:OE1	2.06	0.54
1:E:4103:GLU:HG3	1:E:4104:ARG:N	2.15	0.54
1:G:6972:ASP:OD1	1:G:6989:ARG:HB3	2.08	0.54
2:B:1802:LYS:O	2:B:1804:VAL:HG13	2.07	0.54
1:E:4704:LYS:O	1:E:4707:GLU:N	2.40	0.54
2:F:5759:LEU:HD13	2:F:5842:ARG:HH12	1.72	0.54
1:G:6874:LEU:HB3	1:G:6879:VAL:O	2.07	0.54
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.23	0.54
2:D:3642:LEU:O	2:D:3646:LYS:HG3	2.07	0.54
1:E:5000:HIS:CD2	1:E:5003:ASP:H	2.25	0.54
1:A:89:THR:O	1:A:304:VAL:HG22	2.08	0.54
1:C:2152:MET:O	1:C:2152:MET:HG3	2.07	0.54
1:C:2736:ARG:O	1:C:2740:THR:HG23	2.08	0.54
1:E:4930:LYS:HE3	10:E:6385:HOH:O	2.07	0.54
1:G:6223:ASP:CG	1:G:6227:ASN:HB2	2.33	0.54
1:G:6412:LYS:HG2	1:G:6438:TYR:CZ	2.42	0.54
2:B:1864:ALA:N	2:B:1865:PRO:HD2	2.22	0.54
1:G:6425:ARG:HD3	10:G:288:HOH:O	2.07	0.54
1:G:6804:GLU:O	1:G:6808:VAL:HG23	2.08	0.54
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.08	0.54
1:C:2659:VAL:HG13	1:C:2660:PRO:HD2	1.90	0.54
2:D:3728:VAL:HG22	2:D:3731:MET:CE	2.38	0.54
2:D:3845:LYS:HB3	2:D:3846:PRO:HD2	1.89	0.54
1:E:4784:GLN:H	1:E:4784:GLN:HE21	1.53	0.54
1:G:6555:PRO:HD2	10:G:893:HOH:O	2.07	0.54
1:E:4153:GLU:HB3	10:E:6500:HOH:O	2.08	0.54
2:F:5723:THR:HG22	2:F:5728:VAL:HG23	1.90	0.54
1:A:1:MET:N	1:A:224:LYS:NZ	2.56	0.54
1:A:583:VAL:O	1:A:587:LEU:HG	2.08	0.54
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2679:GLN:HA	1:C:2689:GLN:HE22	1.72	0.54
1:E:4003:LYS:HD3	1:E:4330:TYR:OH	2.08	0.54
1:E:4185:ARG:O	1:E:4185:ARG:HG2	2.08	0.54
1:A:1021:ARG:HH11	1:A:1021:ARG:CG	2.21	0.53
1:G:6901:PRO:HD2	6:G:7932:CL:CL	2.45	0.53
2:H:7823:ALA:C	2:H:7825:LEU:H	2.15	0.53
1:A:734:LEU:HD12	1:A:734:LEU:C	2.31	0.53
1:C:2420:ALA:HA	1:C:2423:LYS:HD2	1.89	0.53
1:C:2490:ARG:HD3	10:C:4546:HOH:O	2.08	0.53
1:C:2941:LYS:HE2	1:C:3054:LEU:O	2.07	0.53
2:D:3688:ASP:OD1	2:D:3688:ASP:N	2.40	0.53
1:E:4435:ARG:O	1:E:4439:ILE:HG13	2.08	0.53
1:G:6762:VAL:CG2	1:G:6801:LEU:HD11	2.38	0.53
1:G:6873:SER:HG	1:G:6876:GLU:HG3	1.73	0.53
2:B:1785:LYS:HG3	2:B:1814:PHE:CE1	2.43	0.53
1:E:4738:PHE:O	1:E:4741:ALA:HB3	2.09	0.53
1:G:6358:LYS:HE3	10:G:720:HOH:O	2.08	0.53
1:G:6528:ARG:HG2	1:G:6543:MET:HG2	1.90	0.53
2:H:7818:GLU:O	2:H:7821:LEU:HB2	2.09	0.53
1:A:692:ASN:HB3	1:A:753:ASP:CG	2.33	0.53
2:F:5824:ASN:O	2:F:5842:ARG:HD2	2.08	0.53
1:G:6130:ARG:HG3	1:G:6148:ILE:HG13	1.90	0.53
2:H:7505:ALA:HB3	2:H:7610:ILE:HG13	1.91	0.53
1:A:907:LEU:HD11	8:A:1920:ORN:HD3	1.91	0.53
1:A:167:ILE:HD12	1:A:167:ILE:N	2.23	0.53
1:A:561:LYS:HE2	1:A:595:GLU:OE1	2.08	0.53
2:B:1698:ASP:HB2	2:B:1718:ILE:HG22	1.89	0.53
1:E:4343:ARG:HD2	10:E:6211:HOH:O	2.08	0.53
1:G:6579:ASP:OD2	1:G:6605:THR:HB	2.09	0.53
1:G:6710:TYR:CB	1:G:6711:PRO:HA	2.30	0.53
2:H:7744:ASP:OD1	2:H:7745:PRO:HD2	2.09	0.53
1:G:6674:ASP:O	1:G:6677:ARG:N	2.40	0.53
1:G:6947:LEU:HG	1:G:7014:ILE:HG21	1.89	0.53
1:G:7070:ALA:HA	10:G:810:HOH:O	2.08	0.53
2:H:7668:TYR:CE2	2:H:7718:ILE:HG12	2.44	0.53
1:A:990:LEU:HD23	1:G:6979:ILE:HD13	1.90	0.53
1:C:2683:GLU:O	1:C:2686:LYS:N	2.36	0.53
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.23	0.53
1:A:692:ASN:HB3	1:A:753:ASP:OD2	2.09	0.53
2:B:1786:MET:HE1	2:B:1812:HIS:CE1	2.44	0.53
1:C:2951:GLU:HA	1:C:2954:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4579:ASP:OD2	1:E:4605:THR:HB	2.09	0.53
1:E:4998:ARG:HB3	1:E:4999:PRO:HA	1.91	0.53
1:G:6181:ILE:HD11	1:G:6376:THR:HG23	1.91	0.53
2:B:1746:ALA:HB3	2:B:1747:PRO:HD3	1.91	0.53
2:H:7675:TRP:CZ2	2:H:7677:LEU:HA	2.44	0.53
1:A:1:MET:HB3	1:A:334:GLU:OE2	2.09	0.52
1:E:4697:ALA:HB3	1:E:4700:MET:HB2	1.90	0.52
1:E:5027:ARG:O	1:E:5031:ARG:HG3	2.10	0.52
2:F:5798:LYS:O	2:F:5829:HIS:HA	2.09	0.52
2:F:5799:ASP:OD2	2:F:5802:LYS:HD2	2.09	0.52
1:A:59:GLU:HG3	1:A:60:MET:HE2	1.92	0.52
2:D:3722:GLN:NE2	10:D:4205:HOH:O	2.30	0.52
2:F:5595:THR:HG21	10:F:2627:HOH:O	2.07	0.52
1:G:6671:ARG:HG2	1:G:6677:ARG:HD2	1.91	0.52
1:G:6699:GLU:O	1:G:6702:VAL:HG23	2.09	0.52
2:H:7772:HIS:HA	2:H:7849:SER:HB2	1.91	0.52
1:A:806:GLN:HA	1:A:809:MET:HE3	1.91	0.52
1:G:7057:ASP:HB3	1:G:7060:GLU:HB2	1.90	0.52
1:A:24:CYS:HB2	1:A:604:GLU:HB3	1.92	0.52
1:C:2011:LEU:HA	1:C:2045:ILE:O	2.10	0.52
1:C:2059:GLU:HG2	1:C:2060:MET:HE3	1.90	0.52
1:C:2166:CYS:C	1:C:2167:ILE:HD12	2.34	0.52
1:C:2739:GLN:HG2	1:C:2740:THR:N	2.23	0.52
1:C:2892:GLU:OE1	8:C:3920:ORN:NE	2.37	0.52
2:F:5550:ARG:NH1	2:F:5650:PHE:HE1	2.08	0.52
1:G:6467:GLU:OE1	10:G:295:HOH:O	2.19	0.52
1:A:821[A]:GLN:NE2	1:A:823:ARG:NH2	2.57	0.52
1:E:4259:LYS:HD3	2:F:5675:TRP:CE3	2.44	0.52
1:E:4704:LYS:NZ	1:E:4707:GLU:OE1	2.30	0.52
2:D:3512:GLY:HA2	2:D:3644:LEU:HD13	1.91	0.52
1:E:4318:PRO:HG3	1:E:4610:TYR:OH	2.09	0.52
1:E:5063:ILE:HD13	1:E:5068:MET:HG3	1.90	0.52
1:A:738:PHE:HA	1:A:741:ALA:CB	2.39	0.52
1:E:4058:PRO:HD2	1:E:4059:GLU:OE1	2.09	0.52
1:E:4101:GLU:HA	1:E:4101:GLU:OE1	2.09	0.52
1:G:6954:LYS:HE2	1:G:6976:GLY:C	2.34	0.52
1:G:7017:THR:HG21	1:G:7023:ILE:CA	2.39	0.52
2:H:7657:ASP:CG	2:H:7660:LYS:HG2	2.34	0.52
1:A:946:LEU:C	1:A:947[B]:LEU:HD13	2.34	0.52
1:C:2703:GLU:O	1:C:2706:LYS:HB2	2.10	0.52
1:G:6728:VAL:HG11	1:G:6734:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7027:ARG:O	1:G:7031:ARG:HG3	2.10	0.52
2:H:7645:GLU:HG2	10:H:936:HOH:O	2.09	0.52
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.92	0.52
2:B:1557:TYR:CE1	2:B:1558:PRO:HD2	2.44	0.52
1:E:4710:TYR:CD2	1:E:4712:LEU:HD13	2.45	0.52
1:G:6906:LEU:HB2	1:G:7030:ARG:HE	1.75	0.52
2:H:7506:LEU:HD21	2:H:7640:ALA:HA	1.92	0.52
1:A:772[B]:MET:HE3	10:A:2818:HOH:O	2.09	0.52
2:D:3635:GLY:O	2:D:3638:PRO:HD3	2.10	0.52
1:E:4417:ASP:HB3	1:E:4420:ALA:HB2	1.92	0.52
1:E:4710:TYR:HB3	1:E:4711:PRO:HA	1.91	0.52
1:G:6701:ALA:O	1:G:6705:ALA:N	2.31	0.52
1:A:674:ASP:HB3	1:A:677:ARG:HB2	1.90	0.51
1:C:2482:THR:HG22	10:C:4743:HOH:O	2.09	0.51
1:E:4004:ARG:N	10:E:6624:HOH:O	2.43	0.51
1:G:6365:GLU:HG2	1:G:6366:LYS:N	2.24	0.51
1:G:6670:ASP:HB3	1:G:6677:ARG:NH2	2.17	0.51
1:A:130:ARG:HB2	1:A:148:ILE:HG13	1.92	0.51
1:C:2343:ARG:HD2	10:C:4204:HOH:O	2.10	0.51
1:C:2455:LEU:HG	10:C:4264:HOH:O	2.11	0.51
1:C:2974:THR:HG21	1:C:3001:ILE:HD11	1.91	0.51
1:E:4164:PHE:HA	1:E:4165:PRO:C	2.35	0.51
1:E:4715:ARG:O	1:E:4751:LEU:HB2	2.10	0.51
2:F:5745:PRO:HG3	2:F:5773:GLN:OE1	2.10	0.51
1:G:6286:PHE:CE2	1:G:6297:VAL:HG22	2.45	0.51
1:G:6525:VAL:HG22	1:G:6546:THR:O	2.09	0.51
2:H:7694:VAL:HB	2:H:7716:LEU:CD2	2.41	0.51
1:E:4738:PHE:HA	1:E:4741:ALA:HB3	1.92	0.51
2:F:5506:LEU:HD13	2:F:5516:HIS:CE1	2.45	0.51
2:F:5656:MET:SD	2:F:5658:LEU:HD21	2.51	0.51
1:G:6064:THR:HG22	1:G:7065:VAL:HG21	1.91	0.51
1:G:6164:PHE:HB3	1:G:6165:PRO:HA	1.92	0.51
1:G:6473:GLU:HG2	1:G:6505:LEU:HD11	1.91	0.51
1:C:2003:LYS:HB2	1:C:2042:TYR:OH	2.10	0.51
1:C:2009:SER:C	1:C:2010:ILE:HG13	2.36	0.51
2:D:3746:ALA:HB3	2:D:3747:PRO:HD3	1.91	0.51
2:D:3746:ALA:N	2:D:3747:PRO:HD2	2.25	0.51
1:E:4703:GLU:HA	1:E:4706:LYS:HD3	1.93	0.51
2:B:1722:GLN:H	2:B:1722:GLN:NE2	2.07	0.51
1:E:4685:LEU:HD11	1:E:4819:GLU:CB	2.40	0.51
1:E:4730:ASP:H	1:E:4733:ASP:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6001:MET:N	1:G:6224:LYS:HZ1	2.08	0.51
1:G:6481:ILE:HD13	1:G:6508:VAL:HG11	1.91	0.51
1:A:321:LYS:NZ	1:A:611:ASP:OD2	2.39	0.51
1:C:2099:ALA:HB1	1:C:2115:MET:HE2	1.93	0.51
1:C:2705:ALA:HB1	1:C:2710:TYR:CZ	2.46	0.51
9:E:5950:NET:H62	10:E:6004:HOH:O	2.11	0.51
1:A:563:MET:HA	1:A:597:ILE:O	2.11	0.51
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.75	0.51
2:B:1766:PHE:HB2	2:B:1870:PHE:CD1	2.45	0.51
1:C:2503:ALA:HB2	1:C:2510:GLU:HA	1.92	0.51
1:E:4259:LYS:HD3	2:F:5675:TRP:CD2	2.46	0.51
1:E:4709:GLY:O	1:E:4712:LEU:HD12	2.10	0.51
1:E:4814:GLN:NE2	10:E:6362:HOH:O	2.43	0.51
2:F:5507:LEU:HB3	2:F:5515:PHE:HB2	1.92	0.51
1:G:6024:CYS:HB2	1:G:6604:GLU:HB2	1.93	0.51
2:B:1751:ALA:O	2:B:1755:ILE:HG13	2.10	0.51
1:C:2010:ILE:HD12	1:C:2042:TYR:HB3	1.92	0.51
2:D:3572:SER:HB2	10:D:4012:HOH:O	2.10	0.51
2:D:3650:PHE:CD1	2:D:3651:PRO:HD2	2.46	0.51
1:G:6180:GLY:HA2	1:G:6376:THR:OG1	2.11	0.51
1:G:6692:ASN:HB3	1:G:6753:ASP:OD2	2.10	0.51
1:A:103:GLU:HG2	1:A:108:LEU:HD12	1.93	0.51
1:C:2147:GLY:HA3	1:C:2158:VAL:HG13	1.93	0.51
1:C:2761:GLU:HB3	1:C:2781:HIS:ND1	2.26	0.51
1:E:4417:ASP:OD2	1:E:4423:LYS:NZ	2.31	0.51
1:E:4680:HIS:O	1:E:4683:GLU:HB2	2.11	0.51
2:F:5686:LYS:N	2:F:5689:GLU:OE2	2.42	0.51
1:G:6892:GLU:OE1	8:G:7920:ORN:NE	2.42	0.51
1:A:955:GLU:HB3	10:A:2860:HOH:O	2.10	0.51
2:B:1506:LEU:HD11	2:B:1508:VAL:HG23	1.90	0.51
1:C:2004:ARG:HD3	1:C:2007:ILE:CD1	2.37	0.51
1:E:4163:GLY:O	1:E:4166:CYS:HB3	2.11	0.51
2:D:3705:ILE:HG21	2:D:3737:PHE:CE2	2.46	0.50
1:E:4043:ARG:NH2	1:E:4081:GLU:OE1	2.35	0.50
1:G:6730:ASP:OD1	1:G:6733:ASP:HB2	2.12	0.50
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.41	0.50
1:A:710:TYR:HB3	1:A:711:PRO:CA	2.35	0.50
1:C:2335:LEU:O	1:C:2336:MET:HE2	2.11	0.50
1:G:6004:ARG:CD	1:G:6007:ILE:HD12	2.41	0.50
1:G:6104:ARG:HD3	10:G:87:HOH:O	2.10	0.50
1:G:6883:VAL:C	1:G:6884:ILE:HG12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5681:LEU:HD12	10:F:2629:HOH:O	2.10	0.50
1:G:6028:TYR:CZ	1:G:6313:LYS:HE3	2.46	0.50
1:G:7026:SER:HB2	1:G:7030:ARG:NH1	2.24	0.50
1:A:881:LYS:O	10:A:2581:HOH:O	2.20	0.50
1:E:4196:LEU:HG	1:E:4204:LEU:HD11	1.94	0.50
1:E:4698:ILE:H	1:E:4698:ILE:CD1	2.25	0.50
1:G:6820:LEU:C	1:G:6821:GLN:HG2	2.36	0.50
2:H:7525:SER:HA	2:H:7632:ILE:O	2.11	0.50
2:H:7705:ILE:HG21	2:H:7737:PHE:CE2	2.47	0.50
2:H:7800:VAL:HG22	2:H:7828:THR:C	2.35	0.50
1:C:2339:ILE:C	1:C:2341:GLY:H	2.19	0.50
1:E:4001:MET:N	10:E:6620:HOH:O	2.44	0.50
1:E:4001:MET:HA	1:E:4224:LYS:CE	2.41	0.50
2:H:7529:GLU:HA	2:H:7629:ASN:HA	1.93	0.50
2:H:7751:ALA:O	2:H:7755:ILE:HG13	2.12	0.50
2:B:1822:PRO:HG2	2:B:1824:ASN:HD21	1.76	0.50
1:C:2035:LYS:O	1:C:2039:GLU:HG3	2.11	0.50
1:C:2930:LYS:NZ	1:C:3058:ALA:O	2.43	0.50
1:E:4516:LEU:O	1:E:4519:GLN:HB3	2.12	0.50
2:F:5753:THR:O	2:F:5756:GLN:HB2	2.12	0.50
1:G:6267:ALA:O	1:G:6271:VAL:HG23	2.11	0.50
2:H:7700:GLY:O	2:H:7740:ASN:ND2	2.45	0.50
1:A:10:ILE:HD12	1:A:42:TYR:HB3	1.93	0.50
1:A:620:PRO:HB2	1:A:622:THR:HG23	1.94	0.50
1:A:688:LYS:HD3	1:A:838:TYR:CE2	2.47	0.50
2:D:3642:LEU:HD12	2:D:3642:LEU:C	2.35	0.50
2:D:3796:PRO:HB2	2:D:3832:LEU:HB2	1.92	0.50
2:F:5786[A]:MET:HE3	2:F:5789:GLY:HA2	1.94	0.50
1:G:6238:ASP:HB2	1:G:6247:SER:HB3	1.93	0.50
2:H:7753:THR:O	2:H:7756:GLN:HB2	2.12	0.50
1:A:35:LYS:NZ	10:A:2322:HOH:O	2.36	0.50
2:B:1818:GLU:O	2:B:1821:LEU:HB2	2.12	0.50
1:G:6642:TYR:OH	1:G:6865:ALA:HB3	2.11	0.50
1:C:2001:MET:O	1:C:2329:GLY:O	2.30	0.50
1:C:2734:LEU:HD12	1:C:2734:LEU:O	2.11	0.50
1:E:4196:LEU:HG	1:E:4204:LEU:CD1	2.42	0.50
1:G:6017:PRO:HG3	1:G:6917:VAL:CG1	2.42	0.50
1:G:6967:GLN:HG3	1:G:6967:GLN:O	2.12	0.50
1:C:2024:CYS:CB	1:C:2576:ILE:HD12	2.42	0.49
2:D:3527:VAL:O	2:D:3578:GLN:HG2	2.12	0.49
1:E:4472:LEU:O	1:E:4476:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:GLY:CA	1:A:869:MET:HG2	2.41	0.49
1:A:755:PHE:CE1	7:A:1910:ADP:C2	2.99	0.49
2:B:1644:LEU:HD21	2:B:1648:ARG:NH1	2.26	0.49
2:B:1826:ARG:HD2	10:B:2179:HOH:O	2.12	0.49
1:E:5017:THR:HG21	1:E:5023:ILE:HG13	1.93	0.49
2:F:5650:PHE:CD1	2:F:5651:PRO:HD2	2.47	0.49
2:H:7799:ASP:HA	2:H:7829:HIS:CD2	2.47	0.49
1:A:508:VAL:HB	1:A:512:GLU:CD	2.38	0.49
1:A:548:GLU:HG2	2:B:1614:ASP:HB2	1.93	0.49
1:A:991:VAL:HB	1:A:1004:ARG:NH1	2.27	0.49
1:C:2761:GLU:OE1	1:C:2785:ALA:HA	2.13	0.49
1:C:2784:GLN:HE22	1:C:3043:THR:HB	1.77	0.49
2:D:3674:SER:OG	2:D:3711:ASP:OD2	2.30	0.49
1:G:6213:TRP:CZ3	1:G:6296:ILE:HD12	2.47	0.49
1:G:6444:ARG:NH2	1:G:6473:GLU:OE1	2.38	0.49
1:G:6740:THR:O	1:G:6741:ALA:O	2.30	0.49
1:G:6868:VAL:HG23	1:G:6877:GLN:NE2	2.27	0.49
1:E:4644:GLY:O	1:E:4647:PRO:HD2	2.12	0.49
1:G:6190:GLU:OE2	1:G:6194:ARG:NH1	2.32	0.49
2:B:1759:LEU:O	2:B:1845:LYS:HD2	2.12	0.49
2:F:5824:ASN:HA	2:F:5843:THR:OG1	2.13	0.49
1:A:426:ARG:HG2	10:A:2726:HOH:O	2.13	0.49
2:B:1527:VAL:O	2:B:1578:GLN:HG2	2.13	0.49
1:C:3068:MET:O	1:C:3071:GLN:HB2	2.11	0.49
1:E:5017:THR:HG21	1:E:5023:ILE:CG1	2.42	0.49
1:E:5021:ARG:HH11	1:E:5021:ARG:CG	2.25	0.49
1:G:6730:ASP:OD1	1:G:6732:ALA:HB3	2.13	0.49
1:G:7030:ARG:HG3	1:G:7030:ARG:HH11	1.77	0.49
1:A:115:MET:HG2	1:A:118:ALA:O	2.12	0.49
1:C:2693:ALA:HB3	1:C:2708:ILE:HD11	1.94	0.49
2:H:7555:LEU:HD12	2:H:7560:ILE:HG21	1.94	0.49
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.13	0.49
1:A:685:LEU:O	1:A:686:LYS:HB2	2.12	0.49
1:C:2001:MET:CB	1:C:2002:PRO:HD3	2.43	0.49
1:C:2623:LEU:HD12	1:C:2654:LEU:HD23	1.94	0.49
2:D:3701:ALA:HA	2:D:3740:ASN:OD1	2.13	0.49
1:E:4726:GLU:HG2	1:E:4727:ILE:N	2.26	0.49
2:F:5505:ALA:HB3	2:F:5610:ILE:HG13	1.94	0.49
1:G:6788:HIS:ND1	1:G:6911:MET:HB2	2.27	0.49
2:H:7656:MET:HG2	2:H:7658:LEU:HG	1.93	0.49
2:H:7805:VAL:HG12	2:H:7806:MET:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2875:HOH:O	1:G:6983:GLU:HG2	2.12	0.49
1:G:6004:ARG:HD3	1:G:6007:ILE:CD1	2.43	0.49
1:G:7017:THR:CG2	1:G:7023:ILE:HG12	2.41	0.49
1:G:7027:ARG:NE	1:G:7031:ARG:HD3	2.27	0.49
2:H:7653:LEU:HA	2:H:7656:MET:HE3	1.94	0.49
2:B:1786:MET:HE2	2:B:1813:GLY:C	2.37	0.49
2:B:1844:ASP:OD1	2:B:1844:ASP:N	2.42	0.49
1:C:2975:HIS:CE1	1:E:4975:HIS:HD1	2.24	0.49
1:A:469:LEU:O	1:A:473:GLU:HG3	2.13	0.48
1:C:2174:MET:HB2	3:C:3906:PO4:O1	2.13	0.48
1:G:6036:ALA:HB1	1:G:6325:LYS:HE3	1.94	0.48
2:B:1734:ASP:CG	2:B:1878:ARG:HH11	2.21	0.48
1:C:2004:ARG:CD	1:C:2007:ILE:HD12	2.37	0.48
1:C:2167:ILE:HD12	1:C:2167:ILE:N	2.28	0.48
1:E:4093:GLN:HB2	1:E:4174:MET:HG2	1.94	0.48
1:E:4417:ASP:OD1	1:E:4418:PRO:HD2	2.12	0.48
1:E:4781:HIS:HE1	1:E:4789:SER:HB3	1.77	0.48
1:E:4809:MET:O	1:E:4813:VAL:HG23	2.13	0.48
1:E:5064:SER:OG	1:E:5067:GLU:HG3	2.14	0.48
1:G:6085:ALA:HA	1:G:6114:THR:O	2.13	0.48
1:C:2036:ALA:HB2	1:C:2321:LYS:HG3	1.95	0.48
1:C:2040:GLU:OE1	1:C:2330:TYR:OH	2.30	0.48
1:C:2150:HIS:N	1:C:2154:GLU:OE1	2.46	0.48
1:C:2525:VAL:HB	1:C:2551:CYS:HA	1.94	0.48
1:E:4958:VAL:HG22	1:E:4981:LEU:HD23	1.95	0.48
1:G:7017:THR:HG21	1:G:7023:ILE:CG1	2.42	0.48
1:A:70:HIS:O	1:A:74:VAL:HG23	2.14	0.48
1:C:2695:VAL:HG11	1:C:2701:ALA:CB	2.26	0.48
1:E:4075:ARG:HH11	1:E:4075:ARG:HG2	1.79	0.48
1:E:4139:ILE:HD11	1:E:4141:LEU:HD12	1.95	0.48
1:E:4944:ARG:HD3	1:E:4972:ASP:OD1	2.14	0.48
1:G:6028:TYR:O	1:G:6032:GLN:HG3	2.13	0.48
1:A:78:ILE:HG23	1:A:83:PRO:HD2	1.95	0.48
1:C:2780:GLU:HB2	1:C:2798:ALA:HA	1.95	0.48
1:E:4734:LEU:O	1:E:4737:TYR:HB3	2.13	0.48
1:G:6163:GLY:O	1:G:6166:CYS:HB3	2.12	0.48
2:B:1705:ILE:HD13	2:B:1768:ILE:HD12	1.94	0.48
1:C:2213:TRP:CZ3	1:C:2296:ILE:HD12	2.49	0.48
1:C:2318:PRO:HG3	1:C:2610:TYR:OH	2.13	0.48
2:D:3767:GLY:O	2:D:3849:SER:HB2	2.14	0.48
2:F:5728:VAL:O	2:F:5731:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1513:THR:HG22	2:B:1515:PHE:CE1	2.48	0.48
1:C:2142:GLU:OE2	1:C:2294:ARG:NH2	2.47	0.48
1:C:2410:ASP:OD1	1:C:2410:ASP:N	2.46	0.48
1:C:2710:TYR:CB	1:C:2711:PRO:HA	2.27	0.48
2:D:3564:GLY:N	2:D:3589:ALA:HB1	2.29	0.48
1:E:4577:GLU:OE2	1:E:4916:GLU:OE2	2.31	0.48
1:E:4669:ILE:HA	1:E:4844:PRO:HG2	1.94	0.48
1:E:4728:VAL:HG11	1:E:4734:LEU:HB2	1.95	0.48
1:E:4737:TYR:O	1:E:4741:ALA:N	2.45	0.48
2:H:7574:GLN:HG3	2:H:7576:HIS:CD2	2.49	0.48
2:H:7737:PHE:HE1	2:H:7768:ILE:HD12	1.79	0.48
1:A:375:THR:OG1	1:A:376:THR:N	2.42	0.48
2:B:1639:ASP:OD2	2:B:1642:LEU:HB2	2.14	0.48
1:C:2104:ARG:NE	10:C:4070:HOH:O	2.42	0.48
1:C:2337:ASN:O	1:C:2342:GLY:HA2	2.14	0.48
2:D:3502:ILE:HG13	2:D:3503:LYS:N	2.27	0.48
1:E:4209:SER:OG	1:E:4211:ILE:HG13	2.13	0.48
1:G:6560:GLU:OE1	1:G:6636:LYS:HD2	2.14	0.48
1:G:6698:ILE:O	1:G:6702:VAL:HG23	2.14	0.48
1:A:710:TYR:CB	1:A:711:PRO:HA	2.28	0.48
1:A:772[A]:MET:HG3	1:A:874:LEU:HD12	1.96	0.48
2:B:1768:ILE:HD13	2:B:1854:PRO:HD2	1.96	0.48
1:C:2845:ARG:HG3	1:C:2845:ARG:NH1	2.18	0.48
1:E:4976:GLY:O	1:E:4980:VAL:HG23	2.13	0.48
1:C:2714:VAL:HG23	1:C:2728:VAL:HG23	1.96	0.48
1:A:702:VAL:O	1:A:706:LYS:HD3	2.13	0.47
1:A:703:GLU:O	1:A:706:LYS:HB2	2.14	0.47
1:C:2710:TYR:HA	1:C:2711:PRO:C	2.39	0.47
1:C:2767:ILE:O	1:C:2774:LEU:N	2.41	0.47
1:E:4400:ARG:HD3	10:E:6240:HOH:O	2.13	0.47
1:E:4831:ALA:HB2	1:E:4840:ILE:HD11	1.95	0.47
1:G:6064:THR:CG2	1:G:7065:VAL:HG21	2.43	0.47
2:H:7855:GLU:OE1	2:H:7855:GLU:N	2.36	0.47
1:A:701:ALA:O	1:A:705:ALA:N	2.38	0.47
1:C:2682:VAL:CG2	1:C:2839:LEU:HD23	2.44	0.47
1:E:4479:VAL:CG2	1:E:4483:GLY:HA3	2.44	0.47
2:F:5798:LYS:HE2	2:F:5803:ASN:OD1	2.14	0.47
1:G:6150:HIS:N	1:G:6154:GLU:OE1	2.35	0.47
1:C:2066:ILE:HG22	1:C:2066:ILE:O	2.14	0.47
1:C:2738:PHE:HA	1:C:2741:ALA:HB3	1.97	0.47
1:E:4929:ALA:HB2	1:E:5053:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6947:LEU:HG	1:G:7014:ILE:CG2	2.44	0.47
1:G:6992:ASN:HA	1:G:6996:GLU:OE1	2.13	0.47
1:A:9:SER:OG	1:A:83:PRO:HA	2.15	0.47
1:A:130:ARG:HB2	1:A:148:ILE:CD1	2.44	0.47
1:A:704:LYS:HD2	1:A:704:LYS:HA	1.77	0.47
2:F:5750:TYR:CD1	2:F:5751:ALA:N	2.82	0.47
1:G:6070:HIS:HE1	1:G:6072:GLU:HG3	1.79	0.47
1:A:601:CYS:HA	1:A:618:PHE:CE1	2.49	0.47
1:C:2526:TYR:CE2	1:C:2545:SER:HB3	2.50	0.47
1:C:2671:ARG:HG2	1:C:2677:ARG:HD2	1.95	0.47
1:E:4674:ASP:O	1:E:4677:ARG:N	2.48	0.47
2:F:5575:VAL:HG11	2:F:5607:ILE:HG13	1.97	0.47
2:F:5578:GLN:HB2	10:F:2646:HOH:O	2.13	0.47
1:G:6194:ARG:HD3	10:G:77:HOH:O	2.13	0.47
1:G:6645:GLN:HB3	10:G:727:HOH:O	2.15	0.47
2:H:7705:ILE:HG22	2:H:7706:LEU:HD23	1.96	0.47
1:A:105:GLN:HE21	1:A:105:GLN:CA	2.19	0.47
1:C:2079:GLU:HA	1:C:2111:PHE:CE2	2.49	0.47
2:D:3705:ILE:HG21	2:D:3737:PHE:CZ	2.50	0.47
1:E:4273:ARG:HD2	10:E:6191:HOH:O	2.14	0.47
1:G:6805:ILE:HD11	1:G:6832:VAL:HG13	1.95	0.47
1:G:7030:ARG:NH1	1:G:7030:ARG:HG3	2.28	0.47
1:A:361:ARG:HG2	1:A:571:ARG:HG3	1.95	0.47
2:B:1673:GLY:HA3	10:B:2166:HOH:O	2.15	0.47
1:C:2186:GLU:HB2	10:C:4498:HOH:O	2.14	0.47
1:C:3001:ILE:HG22	1:C:3002:GLN:N	2.30	0.47
1:E:4145:ARG:HG3	1:E:4145:ARG:HH11	1.80	0.47
1:E:4331:THR:OG1	1:E:4334:GLU:HG3	2.15	0.47
1:E:4905:PRO:HB2	1:E:5040:TYR:OH	2.15	0.47
1:E:5017:THR:HG21	1:E:5023:ILE:HA	1.97	0.47
1:G:6677:ARG:O	1:G:6680:HIS:HB2	2.15	0.47
1:G:6950:ARG:O	1:G:6954:LYS:HG3	2.15	0.47
2:H:7506:LEU:HD12	2:H:7507:LEU:N	2.29	0.47
2:H:7555:LEU:HD23	2:H:7555:LEU:HA	1.61	0.47
2:H:7824:ASN:O	2:H:7842:ARG:HA	2.14	0.47
1:C:2868:VAL:HG23	1:C:2877:GLN:HE22	1.78	0.47
2:H:7781:ALA:HA	2:H:7820:THR:O	2.15	0.47
1:A:488:PHE:O	1:A:491:GLN:HB3	2.15	0.47
1:C:2762:VAL:HG13	1:C:2779:MET:O	2.15	0.47
1:C:2822:VAL:O	1:C:2823:ARG:HD3	2.15	0.47
1:C:3002:GLN:O	1:C:3006:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4548:GLU:HG2	2:F:5614:ASP:HB2	1.97	0.47
1:E:4604:GLU:HG2	10:E:6435:HOH:O	2.13	0.47
1:G:6231:VAL:HG11	1:G:6319:ILE:HD11	1.96	0.47
1:G:6417:ASP:OD1	1:G:6418:PRO:HD2	2.15	0.47
1:G:6704:LYS:O	1:G:6707:GLU:HB3	2.15	0.47
1:G:6941:LYS:HG2	1:G:7054:LEU:HD23	1.96	0.47
2:H:7658:LEU:HD23	2:H:7658:LEU:HA	1.75	0.47
2:H:7773:GLN:HE21	2:H:7851:GLN:HE22	1.62	0.47
1:A:737:TYR:O	1:A:740:THR:OG1	2.31	0.47
1:E:4710:TYR:CE2	1:E:4712:LEU:HD13	2.50	0.47
1:E:4716:ALA:HA	1:E:4750:VAL:HG22	1.96	0.47
1:G:6736:ARG:O	1:G:6739:GLN:HB3	2.14	0.47
1:A:665:SER:O	1:A:669:ILE:HG13	2.15	0.46
1:A:710:TYR:HA	1:A:712:LEU:CD1	2.45	0.46
2:B:1864:ALA:N	2:B:1865:PRO:CD	2.78	0.46
1:C:2543:MET:HE3	1:C:2617:TYR:CE1	2.50	0.46
1:C:2715:ARG:NH2	7:C:3910:ADP:O1A	2.42	0.46
1:C:2954:LYS:O	1:C:2980:VAL:HG11	2.15	0.46
1:E:4336:MET:HB3	1:E:4342:GLY:HA2	1.97	0.46
1:G:6802:SER:O	1:G:6806:GLN:HG3	2.15	0.46
1:A:104:ARG:HD3	10:A:2073:HOH:O	2.15	0.46
1:A:231:VAL:HG11	1:A:319:ILE:HD11	1.97	0.46
1:E:4258:ASP:O	1:E:4262:GLN:HG2	2.15	0.46
1:G:6022:GLN:HG3	1:G:6174:MET:CE	2.41	0.46
1:G:6997:GLY:O	1:G:7000:HIS:HB3	2.15	0.46
2:H:7633:ILE:CD1	2:H:7643:ALA:HB2	2.26	0.46
2:H:7825:LEU:HD21	2:H:7842:ARG:HG2	1.97	0.46
1:C:2053:THR:OG1	1:C:2056:THR:HG23	2.15	0.46
1:C:3027:ARG:HG3	1:C:3027:ARG:NH1	2.28	0.46
1:G:6105:GLN:NE2	10:G:654:HOH:O	2.34	0.46
1:G:6992:ASN:ND2	1:G:6996:GLU:HB2	2.30	0.46
2:B:1726:GLU:O	2:B:1730:LYS:HB2	2.15	0.46
1:C:2688:LYS:HE3	1:C:2836:GLU:HB3	1.98	0.46
2:D:3639:ASP:OD2	2:D:3642:LEU:HB2	2.15	0.46
1:G:6040:GLU:CG	1:G:6325:LYS:HE2	2.45	0.46
1:G:6728:VAL:HG11	1:G:6734:LEU:CA	2.46	0.46
2:H:7557:TYR:CE1	2:H:7558:PRO:HD2	2.48	0.46
1:A:343:ARG:NH2	1:A:539:ASP:OD2	2.43	0.46
1:C:2164:PHE:HA	1:C:2165:PRO:C	2.40	0.46
1:C:2646:THR:HB	1:C:2647:PRO:CD	2.46	0.46
1:C:2819:GLU:OE1	1:C:2819:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5708:MET:SD	2:F:5855:GLU:HA	2.55	0.46
2:H:7786:MET:HE2	2:H:7814:PHE:C	2.40	0.46
1:C:2802:SER:OG	1:C:2805:ILE:HB	2.16	0.46
2:F:5729:LEU:C	2:F:5731:MET:H	2.22	0.46
1:G:6174:MET:HB2	3:G:7906:PO4:O1	2.14	0.46
1:G:7027:ARG:HE	1:G:7031:ARG:HD3	1.79	0.46
2:B:1651:PRO:HG2	2:B:1656:MET:HE1	1.98	0.46
2:D:3518:ARG:HD2	10:D:4127:HOH:O	2.15	0.46
1:E:4636:LYS:HD3	10:E:6332:HOH:O	2.16	0.46
1:G:6035:LYS:NZ	10:G:370:HOH:O	2.39	0.46
1:G:6344:THR:HB	1:G:6345:PRO:HD2	1.97	0.46
1:C:2197:ASP:OD2	1:C:3037:LYS:NZ	2.31	0.46
1:C:2702:VAL:O	1:C:2706:LYS:HD3	2.16	0.46
2:D:3701:ALA:HB2	2:D:3739:SER:OG	2.15	0.46
1:G:6516:LEU:O	1:G:6519:GLN:HB2	2.15	0.46
2:H:7850:PHE:HD2	2:H:7854:PRO:HD3	1.81	0.46
1:A:150:HIS:N	1:A:154:GLU:OE1	2.43	0.46
1:A:726:GLU:CG	1:A:727:ILE:N	2.78	0.46
2:B:1854:PRO:HB2	2:B:1867:PHE:CE2	2.50	0.46
1:C:2962:ALA:O	1:C:2966[A]:LYS:HG2	2.16	0.46
2:D:3546:PRO:HA	2:D:3576:HIS:CG	2.51	0.46
2:D:3799:ASP:OD2	2:D:3802:LYS:HD3	2.15	0.46
1:G:6630:VAL:O	1:G:6634:LYS:N	2.33	0.46
1:G:6708:ILE:HG23	1:G:6754:HIS:HB2	1.98	0.46
1:A:80:LYS:NZ	10:A:2627:HOH:O	2.46	0.46
1:A:331:THR:OG1	1:A:334:GLU:HG3	2.15	0.46
1:A:561:LYS:HG2	1:A:595:GLU:OE1	2.16	0.46
1:E:4910:GLU:HG2	1:E:4912:ARG:HD2	1.98	0.46
2:F:5729:LEU:HD23	2:F:5729:LEU:HA	1.72	0.46
1:G:6130:ARG:O	1:G:6134:VAL:HG23	2.16	0.46
1:G:6321:LYS:NZ	1:G:6611:ASP:OD2	2.42	0.46
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.74	0.45
1:C:2715:ARG:HG2	1:C:2725:MET:HE2	1.99	0.45
1:C:2730:ASP:OD1	1:C:2733:ASP:HB2	2.17	0.45
2:D:3587:LEU:HD12	2:D:3587:LEU:HA	1.49	0.45
2:D:3786:MET:CE	2:D:3812:HIS:ND1	2.78	0.45
1:E:4172:PHE:HB3	1:E:4200:PRO:HG2	1.99	0.45
1:E:4213:TRP:HH2	1:E:4294:ARG:HD3	1.81	0.45
1:E:4738:PHE:CA	1:E:4741:ALA:HB3	2.45	0.45
1:G:6456:THR:O	1:G:6457:ASN:HB2	2.16	0.45
1:G:6716:ALA:HA	1:G:6750:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ASP:OD1	1:A:607:SER:OG	2.30	0.45
1:A:712:LEU:O	1:A:727:ILE:HA	2.17	0.45
1:C:2147:GLY:HA3	1:C:2158:VAL:HG11	1.97	0.45
1:G:6654:LEU:HD22	1:G:6659:VAL:HG21	1.98	0.45
1:G:7000:HIS:NE2	1:G:7002:GLN:HB3	2.31	0.45
1:E:4159:ALA:HB2	1:E:4188:PHE:CZ	2.50	0.45
1:G:6361:ARG:O	1:G:6380:SER:HB2	2.16	0.45
1:G:6827:ASN:N	1:G:6843:ASN:O	2.48	0.45
1:A:682:VAL:HG11	1:A:689:GLN:HB2	1.99	0.45
1:A:711:PRO:C	1:A:712:LEU:HD12	2.42	0.45
1:C:2383:GLU:OE2	1:C:2604:GLU:OE2	2.35	0.45
1:E:4493:LYS:HD2	1:E:4493:LYS:HA	1.66	0.45
1:E:5027:ARG:HE	1:E:5031:ARG:HD3	1.82	0.45
2:F:5773:GLN:HE21	2:F:5851:GLN:HE22	1.63	0.45
1:G:6148:ILE:HD12	1:G:6148:ILE:HG23	1.65	0.45
1:G:6693:ALA:HB2	1:G:6708:ILE:HD11	1.98	0.45
1:G:6699:GLU:C	1:G:6702:VAL:HG23	2.42	0.45
1:G:6728:VAL:HG11	1:G:6734:LEU:HA	1.98	0.45
1:G:6770:GLY:CA	1:G:6823:ARG:NH1	2.79	0.45
2:H:7850:PHE:CG	2:H:7866:LEU:CD2	2.99	0.45
1:A:700:MET:O	1:A:704:LYS:HB2	2.16	0.45
1:A:1020:ARG:O	1:A:1024:GLU:HG3	2.17	0.45
1:E:4694:THR:HG22	1:E:4695:VAL:N	2.32	0.45
1:E:4956:ARG:HB2	1:E:5044:LEU:CD2	2.47	0.45
2:F:5828:THR:HG21	2:F:5841:HIS:HB2	1.98	0.45
1:G:6004:ARG:NE	1:G:6007:ILE:HD12	2.31	0.45
1:G:6644:GLY:O	1:G:6647:PRO:HD2	2.16	0.45
1:G:7000:HIS:O	1:G:7004:ARG:HG3	2.17	0.45
2:H:7807:ILE:O	2:H:7862:ASP:HB2	2.17	0.45
1:C:2712:LEU:O	1:C:2727:ILE:HA	2.17	0.45
1:C:2782:ILE:N	1:C:2782:ILE:CD1	2.79	0.45
2:D:3728:VAL:HA	2:D:3731:MET:HE2	1.93	0.45
1:E:4804:GLU:O	1:E:4808:VAL:HG23	2.16	0.45
1:E:4878:GLY:HA2	10:E:6828:HOH:O	2.16	0.45
2:F:5786[A]:MET:CE	2:F:5812:HIS:ND1	2.80	0.45
1:G:6057:ASP:HA	1:G:6058:PRO:HD3	1.84	0.45
1:G:6704:LYS:HD2	1:G:6704:LYS:HA	1.56	0.45
1:A:25:GLU:OE1	1:A:25:GLU:N	2.42	0.45
1:A:82:ARG:HD2	1:A:82:ARG:HA	1.70	0.45
1:A:675:ARG:CD	1:A:675:ARG:N	2.78	0.45
1:C:2159:ALA:HB2	1:C:2188:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2258:ASP:O	1:C:2262:GLN:HG2	2.16	0.45
1:C:2623:LEU:HD12	1:C:2654:LEU:CD2	2.47	0.45
1:C:2693:ALA:CB	1:C:2708:ILE:HD11	2.47	0.45
1:E:4001:MET:CG	1:E:4225:ASN:HD21	2.30	0.45
1:E:4158:VAL:O	1:E:4161:ASP:HB3	2.16	0.45
1:E:4688:LYS:CD	1:E:4838:TYR:CE2	2.99	0.45
2:F:5734:ASP:HB3	2:F:5874:ILE:HG23	1.97	0.45
2:F:5782:LYS:HB2	2:F:5820:THR:HG21	1.98	0.45
1:G:6125:LYS:HG3	1:G:6131:ARG:CZ	2.47	0.45
1:G:7004:ARG:O	1:G:7009:GLU:HG3	2.17	0.45
2:H:7864:ALA:N	2:H:7865:PRO:CD	2.80	0.45
2:B:1525:SER:HA	2:B:1632:ILE:O	2.17	0.45
1:C:2726:GLU:CG	1:C:2727:ILE:N	2.79	0.45
2:D:3821:LEU:HD12	2:D:3821:LEU:HA	1.73	0.45
1:E:4217:GLU:HG2	1:E:4285:GLN:HG2	1.98	0.45
1:E:4702:VAL:HG11	1:E:4735:ARG:NH2	2.32	0.45
1:G:6148:ILE:CG2	1:G:6149:ALA:N	2.80	0.45
2:H:7658:LEU:HB2	2:H:7742:PRO:HB2	1.99	0.45
1:A:220:VAL:O	1:A:281:GLY:HA2	2.16	0.45
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.17	0.45
2:B:1587:LEU:HD12	2:B:1587:LEU:HA	1.77	0.45
1:C:2998:ARG:HA	1:C:2999:PRO:C	2.39	0.45
1:E:4035:LYS:NZ	10:E:6324:HOH:O	2.46	0.45
1:E:4726:GLU:CG	1:E:4727:ILE:N	2.79	0.45
1:G:6734:LEU:HD11	1:G:6738:PHE:HE2	1.81	0.45
1:A:141:LEU:HB3	1:A:297:VAL:HG21	1.97	0.45
1:A:950:ARG:HD3	10:A:2397:HOH:O	2.17	0.45
1:E:4168:ILE:HG21	1:E:4191:ILE:HG22	1.99	0.45
1:E:4339:ILE:HG21	1:E:4339:ILE:HD13	1.67	0.45
1:E:5063:ILE:HG12	1:E:5064:SER:N	2.32	0.45
1:G:6548:GLU:HG2	2:H:7614:ASP:CB	2.47	0.45
1:G:6905:PRO:HG2	1:G:7030:ARG:HB3	1.99	0.45
2:H:7718:ILE:CD1	2:H:7718:ILE:N	2.79	0.45
2:H:7772:HIS:CB	2:H:7849:SER:HB2	2.45	0.45
1:A:679:GLN:HG2	1:A:689:GLN:OE1	2.17	0.44
1:A:1061:LYS:HE2	10:A:2881:HOH:O	2.16	0.44
2:B:1633:ILE:HD12	2:B:1643:ALA:HB2	1.98	0.44
2:F:5799:ASP:O	2:F:5803:ASN:N	2.47	0.44
2:F:5864:ALA:N	2:F:5865:PRO:CD	2.80	0.44
2:H:7551:GLN:HE21	2:H:7551:GLN:HB2	1.61	0.44
2:B:1728:VAL:HG11	2:B:1758:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3021:ARG:HG3	1:C:3021:ARG:NH1	2.31	0.44
1:C:3036:TYR:C	1:C:3037:LYS:HG2	2.40	0.44
1:G:6167:ILE:N	1:G:6167:ILE:CD1	2.79	0.44
1:G:6224:LYS:NZ	10:G:1:HOH:O	2.50	0.44
1:G:6329:GLY:HA2	10:G:1:HOH:O	2.17	0.44
1:G:6954:LYS:O	1:G:6957:VAL:HG12	2.16	0.44
1:A:698:ILE:N	1:A:698:ILE:CD1	2.79	0.44
2:B:1596:GLU:OE2	2:B:1600:SER:HB3	2.16	0.44
2:B:1644:LEU:CD2	2:B:1648:ARG:NH1	2.80	0.44
2:B:1728:VAL:CA	2:B:1731:MET:HE2	2.38	0.44
1:C:2561:LYS:HD3	1:C:2597:ILE:HD11	2.00	0.44
1:C:2905:PRO:HB2	1:C:3040:TYR:OH	2.17	0.44
1:E:4004:ARG:HD3	1:E:4007:ILE:HD12	1.99	0.44
1:E:4698:ILE:O	1:E:4701:ALA:HB3	2.18	0.44
1:G:6164:PHE:CB	1:G:6165:PRO:HA	2.44	0.44
1:G:6712:LEU:O	1:G:6727:ILE:HA	2.18	0.44
1:A:805:ILE:HG23	1:A:809:MET:HE2	1.99	0.44
2:D:3864:ALA:N	2:D:3865:PRO:CD	2.80	0.44
1:E:4950:ARG:HD3	10:E:6397:HOH:O	2.15	0.44
1:E:5027:ARG:NE	1:E:5031:ARG:HD3	2.33	0.44
1:G:6110:GLU:HG2	1:G:6111:PHE:CE1	2.51	0.44
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.81	0.44
2:D:3733:PRO:HG2	2:D:3763:ILE:HD13	1.99	0.44
1:E:4106:GLY:HA2	10:E:6459:HOH:O	2.17	0.44
2:F:5821:LEU:HA	2:F:5822:PRO:HD2	1.86	0.44
1:G:6069:ILE:HG22	1:G:6069:ILE:O	2.17	0.44
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.42	0.44
2:B:1695:VAL:CG2	2:B:1733:PRO:HB3	2.33	0.44
2:B:1786:MET:CE	2:B:1812:HIS:ND1	2.80	0.44
2:B:1786:MET:HE2	2:B:1814:PHE:N	2.33	0.44
1:C:2163:GLY:O	1:C:2166:CYS:HB3	2.18	0.44
1:C:2950:ARG:HD3	10:C:4393:HOH:O	2.17	0.44
1:C:2975:HIS:HD1	1:E:4975:HIS:CE1	2.28	0.44
1:E:4167:ILE:N	1:E:4167:ILE:HD12	2.31	0.44
1:G:6872:LYS:O	1:G:6877:GLN:NE2	2.47	0.44
1:A:588:ALA:HB2	1:A:863:LYS:HB3	1.99	0.44
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.51	0.44
2:B:1644:LEU:HD21	2:B:1648:ARG:NH2	2.32	0.44
1:C:2001:MET:N	1:C:2002:PRO:CD	2.79	0.44
1:C:2088:PRO:HD2	1:C:2116:ILE:O	2.18	0.44
1:C:2732:ALA:O	1:C:2736:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2904:ASP:OD1	1:C:2905:PRO:HD2	2.18	0.44
1:E:4680:HIS:HA	1:E:4683:GLU:OE1	2.18	0.44
1:G:6548:GLU:HG2	2:H:7614:ASP:CG	2.41	0.44
2:H:7640:ALA:O	2:H:7643:ALA:HB3	2.18	0.44
1:A:145:ARG:NH1	1:A:161:ASP:O	2.50	0.44
1:A:663:GLY:HA3	1:A:869:MET:HG2	1.99	0.44
2:B:1675:TRP:CD1	2:B:1680:GLY:HA2	2.53	0.44
1:C:2682:VAL:HG22	1:C:2839:LEU:HD23	1.99	0.44
1:G:6814:GLN:HG3	1:G:6818:PHE:CE2	2.53	0.44
1:A:152:MET:HE2	10:A:2117:HOH:O	2.17	0.44
1:C:2702:VAL:HG11	1:C:2735:ARG:NH2	2.33	0.44
1:C:2805:ILE:CD1	1:C:2837:VAL:CG2	2.95	0.44
1:E:4418:PRO:HD2	1:E:4419:GLU:H	1.82	0.44
9:E:5950:NET:H31	9:E:5950:NET:H63	1.72	0.44
2:F:5578:GLN:NE2	10:F:2646:HOH:O	2.30	0.44
1:G:6726:GLU:CG	1:G:6727:ILE:N	2.80	0.44
1:G:6944:ARG:HD3	1:G:6972:ASP:CG	2.42	0.44
1:G:7048:PHE:O	1:G:7052:MET:HG3	2.18	0.44
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.48	0.43
2:B:1546:PRO:HA	2:B:1576:HIS:CG	2.52	0.43
2:B:1668:TYR:CE2	2:B:1718:ILE:HG12	2.52	0.43
1:C:2012:ILE:HD11	1:C:2037:LEU:HD12	1.99	0.43
1:E:4967:GLN:HG3	1:E:4967:GLN:O	2.17	0.43
2:F:5791:HIS:HA	2:F:5810:GLN:O	2.18	0.43
2:H:7642:LEU:O	2:H:7646:LYS:HG3	2.18	0.43
2:H:7676:THR:HB	10:H:569:HOH:O	2.18	0.43
2:B:1759:LEU:HD13	2:B:1842:ARG:NH1	2.33	0.43
1:C:2687:LEU:CD1	1:C:2812:GLN:HG3	2.48	0.43
2:D:3508:VAL:HG22	2:D:3514:GLN:HG2	2.01	0.43
1:E:4006:ASP:OD1	1:E:4006:ASP:N	2.40	0.43
1:E:4067:GLU:HB3	1:E:4068:PRO:HD2	2.00	0.43
1:G:6135:ALA:HB1	1:G:6274:GLU:HG2	2.00	0.43
1:G:6225:ASN:ND2	1:G:6331:THR:HG21	2.34	0.43
1:G:6814:GLN:CG	1:G:6818:PHE:CE2	3.01	0.43
1:A:623:LEU:HD11	1:A:627:LEU:HD11	1.99	0.43
2:B:1706:LEU:N	2:B:1706:LEU:HD23	2.33	0.43
1:E:4128:ASP:HB3	1:E:4131:ARG:HB2	1.99	0.43
1:E:4490:ARG:HB3	10:E:6745:HOH:O	2.18	0.43
1:G:6009:SER:HA	1:G:6043:ARG:HB3	1.99	0.43
1:G:6361:ARG:CZ	1:G:6571:ARG:HG2	2.48	0.43
1:A:733:ASP:O	1:A:736:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1506:LEU:HD12	2:B:1507:LEU:H	1.78	0.43
2:B:1772:HIS:HA	2:B:1849:SER:CB	2.48	0.43
1:E:4712:LEU:CD2	1:E:4752:LEU:HG	2.48	0.43
2:F:5670:TRP:HB3	2:F:5716:LEU:HD12	2.00	0.43
2:F:5670:TRP:HB3	2:F:5716:LEU:HB2	1.99	0.43
1:G:6240:MET:HE3	7:G:7900:ADP:C4	2.53	0.43
1:G:7001:ILE:HG21	1:G:7029:ILE:CD1	2.46	0.43
2:H:7728:VAL:HA	2:H:7731:MET:HE3	2.01	0.43
1:A:948:SER:O	1:A:1015:ASN:HA	2.18	0.43
2:B:1566:ASN:HB3	2:B:1593:ARG:O	2.18	0.43
1:C:2038:ARG:HG2	10:C:4030:HOH:O	2.18	0.43
1:C:2738:PHE:HZ	1:C:2750:VAL:HG11	1.84	0.43
2:D:3822:PRO:HB2	2:D:3824:ASN:ND2	2.34	0.43
1:G:6691:ALA:HB3	1:G:6708:ILE:HG23	1.99	0.43
1:A:801:LEU:O	1:A:806:GLN:NE2	2.51	0.43
1:A:1021:ARG:CG	1:A:1021:ARG:NH1	2.81	0.43
2:B:1506:LEU:O	2:B:1632:ILE:HA	2.18	0.43
2:B:1807:ILE:O	2:B:1862:ASP:HB2	2.17	0.43
1:C:3051:ALA:O	1:C:3054:LEU:HB2	2.18	0.43
1:C:3066:GLN:HB2	10:C:4616:HOH:O	2.18	0.43
1:G:6196:LEU:HD23	1:G:6196:LEU:HA	1.92	0.43
2:H:7523:THR:HG23	2:H:7634:ALA:O	2.19	0.43
1:A:687:LEU:HD23	1:A:687:LEU:HA	1.80	0.43
1:C:2105:GLN:NE2	1:C:2105:GLN:CA	2.79	0.43
1:C:2692:ASN:N	1:C:2692:ASN:ND2	2.66	0.43
1:C:2944:ARG:HD3	1:C:2972:ASP:CG	2.42	0.43
1:E:4674:ASP:CB	1:E:4677:ARG:HG3	2.47	0.43
1:E:4702:VAL:O	1:E:4706:LYS:HD3	2.19	0.43
1:E:4858:GLY:HA2	1:E:5069:HIS:CE1	2.53	0.43
2:F:5772:HIS:HA	2:F:5849:SER:HB2	1.99	0.43
1:G:7005:ILE:HG21	1:G:7032:SER:HB3	2.00	0.43
2:H:7527:VAL:HG22	2:H:7631:CYS:HB2	2.01	0.43
1:A:78:ILE:O	1:A:82:ARG:N	2.49	0.43
1:A:368:ALA:HB3	10:A:2700:HOH:O	2.19	0.43
2:B:1824:ASN:HA	2:B:1843:THR:OG1	2.19	0.43
1:C:2761:GLU:HG2	1:C:2781:HIS:ND1	2.33	0.43
2:D:3532:PHE:O	2:D:3791:HIS:HB2	2.18	0.43
1:E:4146:SER:HB3	1:E:4207:ASP:HA	2.01	0.43
1:E:4375:THR:HG23	1:E:4377:GLN:H	1.84	0.43
1:G:6634:LYS:HG2	10:G:383:HOH:O	2.17	0.43
2:H:7798:LYS:O	2:H:7829:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:OD1	1:A:53:THR:HB	2.19	0.43
1:C:2001:MET:HE3	1:C:2001:MET:HB2	1.97	0.43
2:D:3676:THR:O	2:D:3680:GLY:N	2.51	0.43
1:E:4054:ILE:HD13	1:E:4054:ILE:HA	1.89	0.43
1:E:4680:HIS:O	1:E:4684:ARG:HB2	2.19	0.43
1:E:4685:LEU:HD11	1:E:4819:GLU:HG2	2.01	0.43
1:G:6152:MET:HE1	1:G:6192:CYS:HB2	2.01	0.43
1:G:6509:ARG:HB3	1:G:6512:GLU:HG3	2.00	0.43
1:G:6850:VAL:HB	1:G:6851:PRO:HD3	2.01	0.43
2:H:7774:LEU:HD23	2:H:7774:LEU:HA	1.78	0.43
1:A:9:SER:HA	1:A:43:ARG:O	2.19	0.43
1:A:318:PRO:HG3	1:A:610:TYR:OH	2.19	0.43
1:A:585:ALA:HB2	1:A:642:TYR:CE2	2.53	0.43
1:A:692:ASN:HA	1:A:752:LEU:O	2.19	0.43
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.86	0.43
1:C:2622:THR:OG1	1:C:2625:ASP:OD2	2.34	0.43
2:D:3667:ALA:HA	2:D:3718:ILE:O	2.18	0.43
1:E:4418:PRO:CD	1:E:4419:GLU:H	2.31	0.43
2:F:5705:ILE:HG21	2:F:5737:PHE:CZ	2.54	0.43
1:G:6166:CYS:C	1:G:6167:ILE:HD12	2.44	0.43
1:G:6526:TYR:CE2	1:G:6545:SER:HB3	2.54	0.43
1:G:6682:VAL:CG1	1:G:6687:LEU:HB2	2.48	0.43
1:G:7001:ILE:HD13	1:G:7029:ILE:CD1	2.49	0.43
2:H:7876:GLN:O	2:H:7879:LYS:HB2	2.19	0.43
1:A:176:GLY:HA3	1:A:377:GLN:HA	1.99	0.42
1:A:632:ILE:HG13	1:A:633:GLU:N	2.33	0.42
1:A:670:ASP:HB3	1:A:677:ARG:HH21	1.84	0.42
1:A:698:ILE:O	1:A:701:ALA:HB3	2.19	0.42
1:C:2704:LYS:O	1:C:2707:GLU:HB2	2.19	0.42
1:C:2714:VAL:CG1	1:C:2737:TYR:CE2	3.00	0.42
1:E:4525:VAL:HB	1:E:4551:CYS:HA	1.99	0.42
1:E:4730:ASP:H	1:E:4733:ASP:CB	2.32	0.42
1:E:5051:ALA:O	1:E:5054:LEU:HB2	2.19	0.42
1:A:407:THR:HG21	1:A:504:LYS:HE3	2.00	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.66	0.42
1:C:2306:ARG:NH1	1:C:2306:ARG:HG2	2.34	0.42
1:C:2695:VAL:HG13	1:C:2700:MET:HB3	2.01	0.42
1:C:2865:ALA:O	1:C:2869:MET:HG3	2.19	0.42
2:F:5732:ASN:N	2:F:5733:PRO:CD	2.81	0.42
2:F:5763:ILE:HA	2:F:5764:PRO:HD3	1.92	0.42
1:G:6733:ASP:CA	1:G:6736:ARG:HH11	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6995:HIS:CE1	1:G:6996:GLU:CG	3.01	0.42
2:H:7772:HIS:HA	2:H:7849:SER:CB	2.48	0.42
2:B:1825:LEU:HD22	2:B:1840:ILE:HB	2.02	0.42
1:C:2001:MET:CA	1:C:2224:LYS:NZ	2.80	0.42
1:C:2267:ALA:O	1:C:2271:VAL:HG23	2.20	0.42
1:C:2485:ASN:ND2	1:C:2485:ASN:H	2.17	0.42
2:D:3538:GLY:HA3	2:D:3858:PRO:HB3	2.01	0.42
1:E:4051:PRO:HG3	1:E:4918:MET:HB2	2.01	0.42
1:E:4712:LEU:O	1:E:4727:ILE:HA	2.18	0.42
1:E:5006:LYS:O	1:E:5006:LYS:HG3	2.17	0.42
2:F:5571:GLU:C	2:F:5703:ARG:HG3	2.44	0.42
2:F:5734:ASP:HB3	2:F:5874:ILE:HG21	1.97	0.42
1:G:6671:ARG:CG	1:G:6677:ARG:NH1	2.82	0.42
2:H:7509:LEU:O	2:H:7512:GLY:N	2.38	0.42
2:H:7596:GLU:OE2	2:H:7600:SER:HB3	2.19	0.42
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.54	0.42
2:B:1798:LYS:HE2	2:B:1803:ASN:OD1	2.19	0.42
1:E:4912:ARG:NH2	10:E:6835:HOH:O	2.52	0.42
1:E:5027:ARG:HA	1:E:5030:ARG:NH2	2.35	0.42
1:G:6489:LEU:HA	1:G:6489:LEU:HD12	1.70	0.42
1:G:6755:PHE:CE1	7:G:7910:ADP:C2	3.07	0.42
1:G:6903:VAL:HG12	1:G:6904:ASP:N	2.34	0.42
1:G:6950:ARG:HD3	10:G:446:HOH:O	2.19	0.42
1:G:7000:HIS:CD2	1:G:7002:GLN:HB3	2.54	0.42
1:A:947[A]:LEU:HG	1:A:1014:ILE:CG2	2.49	0.42
1:C:2583:VAL:O	1:C:2587:LEU:HG	2.20	0.42
1:E:4215:GLU:OE2	7:E:5900:ADP:O3'	2.35	0.42
1:E:4236:ASN:N	1:E:4236:ASN:HD22	2.17	0.42
1:E:4997:GLY:O	1:E:5000:HIS:HB3	2.19	0.42
1:E:5054:LEU:HA	1:E:5054:LEU:HD23	1.77	0.42
1:G:7030:ARG:HH11	1:G:7030:ARG:CG	2.31	0.42
2:H:7544:THR:HG21	2:H:7570:GLU:HG2	2.01	0.42
2:H:7853:ASN:HB3	2:H:7855:GLU:CD	2.45	0.42
1:A:759:ALA:HB2	1:A:833:LYS:HB2	2.01	0.42
1:A:784:GLN:HE22	1:A:1043:THR:HB	1.84	0.42
2:B:1571:GLU:OE1	2:B:1702:LYS:HB3	2.18	0.42
1:C:2158:VAL:O	1:C:2161:ASP:HB3	2.20	0.42
1:C:2646:THR:CB	1:C:2647:PRO:HD3	2.47	0.42
1:C:2696:THR:OG1	1:C:2700:MET:SD	2.77	0.42
1:C:2902:GLY:HA2	1:C:3031:ARG:NH1	2.34	0.42
2:D:3806:MET:CE	2:D:3829:HIS:CD2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7548:TYR:O	2:H:7551:GLN:HB2	2.19	0.42
1:A:736:ARG:O	1:A:739:GLN:HB3	2.18	0.42
1:C:2714:VAL:HG21	1:C:2728:VAL:HG21	2.02	0.42
2:D:3674:SER:HB3	10:D:4075:HOH:O	2.19	0.42
2:D:3759:LEU:HB2	10:D:4238:HOH:O	2.18	0.42
2:H:7653:LEU:O	2:H:7656:MET:HB3	2.19	0.42
2:H:7662:VAL:HG11	2:H:7742:PRO:HG3	2.02	0.42
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.92	0.42
2:D:3824:ASN:H	2:D:3824:ASN:ND2	2.04	0.42
2:D:3857:SER:HA	2:D:3858:PRO:HA	1.80	0.42
1:E:4704:LYS:O	1:E:4707:GLU:HB2	2.20	0.42
1:E:4712:LEU:N	1:E:4728:VAL:O	2.44	0.42
1:G:6704:LYS:HD2	1:G:6707:GLU:OE1	2.19	0.42
1:A:75:ARG:HG3	1:A:107:VAL:CG1	2.49	0.42
1:A:713:VAL:O	1:A:713:VAL:HG12	2.20	0.42
1:A:780:GLU:HB3	1:A:798:ALA:HA	2.02	0.42
1:A:821[A]:GLN:HE21	1:A:821[A]:GLN:HB3	1.64	0.42
1:A:929:ALA:HB2	1:A:1053:ALA:HB1	2.02	0.42
2:B:1761:THR:OG1	2:B:1763:ILE:HG13	2.20	0.42
1:C:3027:ARG:O	1:C:3031:ARG:HG3	2.20	0.42
1:E:4170:PRO:HA	1:E:4204:LEU:HA	2.02	0.42
1:E:4486:ALA:HA	1:E:4520:TYR:CE2	2.55	0.42
1:E:4698:ILE:N	1:E:4698:ILE:CD1	2.80	0.42
1:E:4944:ARG:HD2	1:E:5010:TYR:CE1	2.55	0.42
1:E:4998:ARG:CB	1:E:4999:PRO:HA	2.50	0.42
1:E:5021:ARG:HH11	1:E:5021:ARG:HG3	1.85	0.42
1:G:6001:MET:N	1:G:6002:PRO:CD	2.83	0.42
1:G:7000:HIS:CD2	1:G:7000:HIS:C	2.98	0.42
1:G:7021:ARG:HG3	1:G:7021:ARG:NH1	2.33	0.42
1:G:7031:ARG:O	1:G:7035:GLN:HB3	2.20	0.42
1:A:339:ILE:HD11	1:A:531:THR:HG23	2.01	0.42
1:A:361:ARG:NE	1:A:404:VAL:HG12	2.35	0.42
1:A:470:VAL:O	1:A:473:GLU:HB2	2.20	0.42
2:B:1806:MET:HB3	2:B:1862:ASP:HB3	2.02	0.42
1:C:3004[A]:ARG:HD3	1:C:3009[A]:GLU:OE2	2.20	0.42
2:D:3582:ILE:HG21	2:D:3582:ILE:HD13	1.82	0.42
2:D:3712:ARG:CD	2:D:3867:PHE:HB3	2.49	0.42
2:D:3712:ARG:HG3	2:D:3712:ARG:HH11	1.85	0.42
2:D:3833:PHE:HD1	2:D:3833:PHE:HA	1.69	0.42
1:E:4086:VAL:O	1:E:4086:VAL:HG13	2.19	0.42
1:E:4839:LEU:HA	1:E:4839:LEU:HD12	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5741:GLY:O	2:F:5769:CYG:HG12	2.20	0.42
2:F:5832:LEU:HD12	2:F:5832:LEU:HA	1.66	0.42
1:G:6563:MET:HB3	1:G:6638:VAL:HG22	2.01	0.42
1:A:1:MET:O	1:A:329:GLY:O	2.37	0.41
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.82	0.41
1:A:516:LEU:HD12	1:A:516:LEU:HA	1.86	0.41
1:A:792:SER:O	1:A:891:LYS:HE2	2.20	0.41
1:C:2489:LEU:HD12	1:C:2489:LEU:HA	1.88	0.41
1:C:2764:VAL:HG11	1:C:2813:VAL:HG21	2.02	0.41
1:C:2947:LEU:HG	1:C:3014:ILE:HG23	2.01	0.41
2:D:3832:LEU:HD12	2:D:3832:LEU:HA	1.68	0.41
1:E:4503:ALA:HB2	1:E:4510:GLU:HA	2.02	0.41
1:E:4781:HIS:HE1	1:E:4789:SER:CB	2.33	0.41
1:E:4901:PRO:HD2	6:E:5932:CL:CL	2.57	0.41
1:E:5027:ARG:HH21	1:E:5031:ARG:HH11	1.67	0.41
1:G:6222:ARG:HD3	1:G:6278:GLU:HA	2.01	0.41
1:G:6364:PHE:CE1	1:G:6372:ASP:HA	2.55	0.41
1:G:6526:TYR:O	1:G:6552:GLU:N	2.41	0.41
1:G:6998:ARG:HA	1:G:6999:PRO:C	2.45	0.41
1:G:7023:ILE:O	1:G:7026:SER:OG	2.36	0.41
1:A:755:PHE:CD1	7:A:1910:ADP:C2	3.08	0.41
2:B:1825:LEU:HD23	2:B:1825:LEU:HA	1.95	0.41
1:C:2579:ASP:OD2	1:C:2605:THR:HB	2.20	0.41
2:D:3757:LYS:HG2	10:D:4240:HOH:O	2.19	0.41
1:E:4283:ASN:HB2	10:E:6704:HOH:O	2.21	0.41
1:E:4730:ASP:OD1	1:E:4732:ALA:HB3	2.20	0.41
1:E:4889:SER:HB3	1:E:4918:MET:CE	2.40	0.41
2:F:5546:PRO:HA	2:F:5576:HIS:CG	2.55	0.41
1:G:6148:ILE:CG2	1:G:6150:HIS:CE1	3.02	0.41
1:G:6473:GLU:HG2	1:G:6505:LEU:CD1	2.51	0.41
1:G:6805:ILE:HD13	1:G:6832:VAL:HG11	2.02	0.41
1:G:7027:ARG:CD	1:G:7031:ARG:HD3	2.50	0.41
1:A:375:THR:HG23	1:A:377:GLN:H	1.85	0.41
1:A:821[A]:GLN:HE22	1:A:823:ARG:NH2	2.18	0.41
1:A:955:GLU:CB	10:A:2860:HOH:O	2.67	0.41
1:A:992:ASN:ND2	1:A:996:GLU:CB	2.84	0.41
1:A:1020:ARG:O	1:A:1023:ILE:HB	2.20	0.41
1:C:2273:ARG:HD2	10:C:4185:HOH:O	2.19	0.41
1:C:2481:ILE:HD12	1:C:2508:VAL:HG21	2.02	0.41
1:C:2563:MET:HB2	1:C:2563:MET:HE2	1.63	0.41
1:E:5061:LYS:HB2	10:E:6869:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PRO:HB3	1:A:183:TYR:CD1	2.55	0.41
1:A:265:ARG:O	1:A:269:MET:HG3	2.21	0.41
1:A:471:ARG:H	1:A:471:ARG:HG2	1.76	0.41
1:A:675:ARG:N	1:A:675:ARG:HD2	2.35	0.41
1:C:2085:ALA:HA	1:C:2114:THR:O	2.21	0.41
1:C:2493:LYS:NZ	1:C:2499:ASP:OD1	2.50	0.41
1:C:2695:VAL:CG1	1:C:2696:THR:N	2.83	0.41
2:D:3621:LEU:HD11	2:D:3625:LYS:HD3	2.02	0.41
2:F:5526:ALA:HB1	2:F:5578:GLN:HG3	2.02	0.41
1:G:6447:LEU:HD23	1:G:6447:LEU:HA	1.97	0.41
1:G:6714:VAL:HG22	1:G:6752:LEU:HD11	2.00	0.41
2:H:7701:ALA:HB2	2:H:7739:SER:CB	2.50	0.41
2:H:7752:ILE:HD11	2:H:7777:LEU:HD13	2.03	0.41
2:H:7805:VAL:CG1	2:H:7806:MET:N	2.83	0.41
1:A:637:GLY:HA2	1:A:660:PRO:O	2.21	0.41
2:B:1675:TRP:CZ2	2:B:1677:LEU:HA	2.56	0.41
1:C:2733:ASP:O	1:C:2736:ARG:HB3	2.20	0.41
2:D:3685:LYS:HB2	2:D:3690:LEU:HD11	2.02	0.41
1:E:4028:TYR:CZ	1:E:4313:LYS:HE3	2.55	0.41
1:E:4195:GLY:C	1:E:4204:LEU:HD21	2.45	0.41
1:G:7002:GLN:O	1:G:7006:LYS:HB3	2.20	0.41
2:H:7769:CYG:O2	2:H:7812:HIS:HB2	2.19	0.41
1:A:515:LYS:HG3	10:A:2756:HOH:O	2.20	0.41
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.56	0.41
2:B:1717:THR:O	2:B:1717:THR:HG22	2.20	0.41
2:B:1723:THR:HG22	2:B:1724:SER:N	2.36	0.41
1:C:2124:ASP:O	1:C:2128:ASP:HB3	2.21	0.41
1:C:2733:ASP:O	1:C:2736:ARG:NH1	2.54	0.41
8:C:3920:ORN:HG2	10:C:4066:HOH:O	2.21	0.41
1:E:4184:ASN:OD1	1:E:4186:GLU:HB3	2.20	0.41
1:E:4675:ARG:CD	1:E:4675:ARG:H	2.25	0.41
1:G:6427:GLU:HG3	1:G:6438:TYR:CD2	2.55	0.41
1:G:6577:GLU:HG2	1:G:6848:ARG:O	2.19	0.41
1:G:7017:THR:HG22	1:G:7018:SER:N	2.33	0.41
2:H:7825:LEU:HA	2:H:7825:LEU:HD23	1.46	0.41
1:A:559:ARG:HA	10:A:2780:HOH:O	2.19	0.41
2:B:1695:VAL:HG23	2:B:1733:PRO:CB	2.34	0.41
2:B:1768:ILE:HD13	2:B:1768:ILE:HG21	1.82	0.41
2:B:1864:ALA:HB3	2:B:1865:PRO:CD	2.50	0.41
1:C:2169:ARG:HG2	10:C:4634:HOH:O	2.19	0.41
1:E:4036:ALA:O	1:E:4039:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4828:VAL:HG22	1:E:4842:VAL:HG22	2.02	0.41
2:F:5693:HIS:O	2:F:5734:ASP:N	2.47	0.41
2:F:5779:SER:O	2:F:5822:PRO:HG3	2.21	0.41
1:G:6283:ASN:OD1	1:G:6301:ASN:ND2	2.48	0.41
1:G:6468:GLU:OE1	2:H:7587:LEU:HD21	2.20	0.41
1:G:6671:ARG:HG2	1:G:6677:ARG:NH1	2.35	0.41
1:G:6755:PHE:CD1	7:G:7910:ADP:C2	3.09	0.41
1:G:6979:ILE:HD13	1:G:6979:ILE:HA	1.86	0.41
1:G:7020:ARG:HD2	1:G:7020:ARG:HA	1.89	0.41
1:A:954:LYS:C	1:A:957:VAL:HG12	2.46	0.41
1:C:2790:GLY:HA3	1:C:2911:MET:SD	2.61	0.41
1:C:2968:GLY:O	10:C:4591:HOH:O	2.22	0.41
1:G:6358:LYS:HG2	1:G:6359:ILE:N	2.31	0.41
1:G:6761:GLU:HB3	1:G:6781:HIS:ND1	2.36	0.41
1:G:6865:ALA:O	1:G:6869:MET:HG3	2.21	0.41
1:G:6922:ARG:NH1	1:G:7061:LYS:HD2	2.35	0.41
1:A:548:GLU:HG2	2:B:1614:ASP:CB	2.51	0.41
1:A:852:PHE:HE1	1:A:918:MET:HG3	1.86	0.41
1:A:889:SER:HB3	1:A:918:MET:HE3	2.03	0.41
2:B:1759:LEU:HD23	2:B:1759:LEU:HA	1.89	0.41
1:C:2471:ARG:HH21	1:C:2474:GLU:CD	2.28	0.41
1:C:2762:VAL:CG2	1:C:2801:LEU:HD11	2.50	0.41
1:C:2973:ALA:C	1:C:2991:VAL:HG12	2.45	0.41
2:D:3863:ALA:C	2:D:3865:PRO:HD2	2.46	0.41
1:E:4696:THR:N	1:E:4700:MET:SD	2.93	0.41
1:E:4802:SER:O	1:E:4806:GLN:HG3	2.21	0.41
2:F:5687:GLU:HG2	2:F:5715:ARG:CD	2.15	0.41
2:F:5795:HIS:CE1	2:F:5833:PHE:HD2	2.39	0.41
2:F:5824:ASN:ND2	10:F:2746:HOH:O	2.54	0.41
2:F:5845:LYS:HB3	2:F:5846:PRO:CD	2.49	0.41
1:G:6065:TYR:CE1	1:G:6077:ILE:HG23	2.56	0.41
1:G:6300:MET:HE2	1:G:6300:MET:HB2	1.95	0.41
1:G:6710:TYR:CD1	1:G:6710:TYR:N	2.88	0.41
2:H:7650:PHE:HA	2:H:7651:PRO:HD3	1.81	0.41
2:H:7692:PHE:HD1	2:H:7878:ARG:HD2	1.86	0.41
2:H:7766:PHE:HA	2:H:7848:PHE:O	2.21	0.41
1:A:712:LEU:O	1:A:728:VAL:N	2.53	0.41
2:B:1821:LEU:HD12	2:B:1821:LEU:HA	1.81	0.41
1:C:2672:ALA:HB3	1:C:2844:PRO:CG	2.50	0.41
1:C:2759:ALA:O	1:C:2784:GLN:HB2	2.20	0.41
2:F:5620:ARG:HE	2:F:5620:ARG:HB3	1.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6711:PRO:HG2	1:G:6755:PHE:HD2	1.86	0.41
1:G:6770:GLY:HA3	1:G:6823:ARG:CZ	2.51	0.41
1:A:101:GLU:OE1	1:A:104:ARG:NE	2.53	0.40
1:A:516:LEU:HD12	1:A:519:GLN:NE2	2.36	0.40
1:A:710:TYR:HA	1:A:712:LEU:HD12	2.03	0.40
2:B:1731:MET:HE3	2:B:1731:MET:HB2	1.94	0.40
1:C:2423:LYS:NZ	10:C:4717:HOH:O	2.54	0.40
1:C:2596:THR:O	1:C:2614:ASP:HB2	2.22	0.40
1:E:4056:THR:O	1:E:4855:LYS:HE2	2.22	0.40
1:E:4702:VAL:CG1	1:E:4731:GLU:HG2	2.49	0.40
2:F:5658:LEU:HB2	2:F:5742:PRO:HB2	2.01	0.40
2:F:5824:ASN:O	2:F:5842:ARG:HA	2.22	0.40
1:G:6004:ARG:NE	1:G:6007:ILE:CD1	2.84	0.40
1:G:6453:PHE:HD1	1:G:6458:ILE:O	2.04	0.40
2:H:7587:LEU:HD12	2:H:7587:LEU:HA	1.65	0.40
1:A:267:ALA:O	1:A:271:VAL:HG23	2.22	0.40
1:A:425:ARG:HD3	10:A:2251:HOH:O	2.21	0.40
2:B:1650:PHE:HE2	2:B:1653:LEU:HD13	1.87	0.40
1:C:2678:PHE:O	1:C:2681:ALA:N	2.53	0.40
2:D:3708:MET:O	2:D:3711:ASP:HB2	2.21	0.40
1:E:4037:LEU:HD23	1:E:4037:LEU:HA	1.79	0.40
1:E:4145:ARG:HG3	1:E:4145:ARG:NH1	2.37	0.40
1:E:4222:ARG:HH11	1:E:4222:ARG:HD3	1.74	0.40
1:G:6313:LYS:O	1:G:6542:TYR:OH	2.35	0.40
1:G:6481:ILE:CD1	1:G:6508:VAL:HG11	2.50	0.40
1:G:6687:LEU:HD23	1:G:6687:LEU:HA	1.72	0.40
1:G:6727:ILE:HD12	1:G:6909:PRO:HG3	2.02	0.40
1:G:6797:PRO:HD2	1:G:6888:TYR:CD1	2.55	0.40
1:A:431:ALA:HB2	1:A:435:ARG:CZ	2.51	0.40
1:A:678:PHE:O	1:A:682:VAL:HG23	2.21	0.40
1:A:728:VAL:HG11	1:A:734:LEU:HA	2.03	0.40
1:C:2638:VAL:HG21	1:C:2659:VAL:CG1	2.52	0.40
2:D:3506:LEU:HD13	2:D:3516:HIS:CE1	2.56	0.40
1:E:4484:LEU:HD23	1:E:4484:LEU:HA	1.91	0.40
1:E:4648:LEU:HD22	1:E:4845:ARG:HD3	2.03	0.40
1:E:5063:ILE:HD13	1:E:5068:MET:CG	2.52	0.40
1:G:6524:PRO:HD2	1:G:6628:GLU:OE1	2.22	0.40
1:A:627:LEU:O	1:A:631:ARG:HB2	2.22	0.40
1:A:1004:ARG:O	1:A:1009[B]:GLU:HG3	2.22	0.40
2:B:1674[B]:SER:OG	2:B:1711:ASP:OD2	2.31	0.40
1:C:3048:PHE:O	1:C:3052:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4475:LYS:HG2	1:E:4488:PHE:CZ	2.57	0.40
1:G:6004:ARG:HD2	10:G:231:HOH:O	2.21	0.40
1:G:6221:VAL:O	1:G:6228:CYS:HA	2.21	0.40
2:H:7701:ALA:HA	2:H:7740:ASN:OD1	2.20	0.40
2:H:7774:LEU:HD23	2:H:7777:LEU:HD12	2.02	0.40
1:A:32:GLN:NE2	10:A:2519:HOH:O	2.55	0.40
1:A:478:GLU:HG3	10:A:2740:HOH:O	2.21	0.40
1:C:2453:PHE:CD2	1:C:2453:PHE:C	3.00	0.40
2:F:5756:GLN:HE21	2:F:5778:ALA:HA	1.87	0.40
2:F:5850:PHE:CD1	2:F:5866:LEU:HD21	2.56	0.40
1:G:6762:VAL:HG21	1:G:6801:LEU:HD11	2.04	0.40
2:H:7532:PHE:HA	2:H:7554:THR:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:4245:HOH:O	10:H:947:HOH:O[3_554]	2.08	0.12

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	1059/1073 (99%)	1010 (95%)	46 (4%)	3 (0%)	36	25
1	C	1059/1073 (99%)	1007 (95%)	49 (5%)	3 (0%)	36	25
1	E	1054/1073 (98%)	1000 (95%)	48 (5%)	6 (1%)	21	11
1	G	1053/1073 (98%)	997 (95%)	50 (5%)	6 (1%)	21	11
2	B	377/379 (100%)	363 (96%)	14 (4%)	0	100	100
2	D	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
2	F	379/379 (100%)	372 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	376/379 (99%)	360 (96%)	14 (4%)	2 (0%)	24	14
All	All	5733/5808 (99%)	5469 (95%)	244 (4%)	20 (0%)	30	25

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ALA
1	E	4004	ARG
1	G	6739	GLN
1	A	975	HIS
1	C	2368	ALA
1	G	6975	HIS
1	E	4003	LYS
1	E	4739	GLN
1	E	4975	HIS
1	A	369	GLY
1	C	2736	ARG
1	G	6675	ARG
2	H	7638	PRO
1	C	2002	PRO
1	E	4088	PRO
1	E	4675	ARG
1	G	6873	SER
2	H	7743	GLY
1	G	6069	ILE
1	G	6002	PRO

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	872/877 (99%)	811 (93%)	61 (7%)	14	4
1	C	872/877 (99%)	780 (89%)	92 (11%)	6	1
1	E	867/877 (99%)	789 (91%)	78 (9%)	9	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	866/877 (99%)	773 (89%)	93 (11%)	6	1
2	B	308/307 (100%)	276 (90%)	32 (10%)	7	2
2	D	307/307 (100%)	281 (92%)	26 (8%)	10	3
2	F	310/307 (101%)	277 (89%)	33 (11%)	6	1
2	H	307/307 (100%)	272 (89%)	35 (11%)	5	1
All	All	4709/4736 (99%)	4259 (90%)	450 (10%)	8	2

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	THR
1	A	8	LYS
1	A	38	ARG
1	A	105	GLN
1	A	109	GLU
1	A	110	GLU
1	A	174	MET
1	A	220	VAL
1	A	275	ILE
1	A	296	ILE
1	A	297	VAL
1	A	321	LYS
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	422	THR
1	A	481	ILE
1	A	482	THR
1	A	509	ARG
1	A	548	GLU
1	A	554[A]	ASN
1	A	554[B]	ASN
1	A	559	ARG
1	A	560	GLU
1	A	571	ARG
1	A	591	GLU
1	A	645	GLN
1	A	665	SER
1	A	671	ARG

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Mol	Chain	Res	Type
1	A	675	ARG
1	A	676	GLU
1	A	688	LYS
1	A	696	THR
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	855	LYS
1	A	881	LYS
1	A	884	ILE
1	A	895	LEU
1	A	912	ARG
1	A	950	ARG
1	A	951	GLU
1	A	955	GLU
1	A	970	GLU
1	A	992	ASN
1	A	1006	LYS
1	A	1014	ILE
1	A	1018	SER
1	A	1021	ARG
1	A	1025	ASP
1	A	1027	ARG
1	A	1028	VAL
1	A	1073	LYS
2	B	1502	ILE
2	B	1506	LEU
2	B	1525	SER
2	B	1529	GLU
2	B	1549	SER
2	B	1587	LEU
2	B	1604	ARG
2	B	1606	ASN
2	B	1620	ARG
2	B	1666	GLU
2	B	1686	LYS

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Mol	Chain	Res	Type
2	B	1692	PHE
2	B	1715	ARG
2	B	1717	THR
2	B	1718	ILE
2	B	1719	VAL
2	B	1722	GLN
2	B	1757	LYS
2	B	1761	THR
2	B	1763	ILE
2	B	1782	LYS
2	B	1784	VAL
2	B	1806	MET
2	B	1821	LEU
2	B	1824	ASN
2	B	1826	ARG
2	B	1832	LEU
2	B	1833	PHE
2	B	1857	SER
2	B	1866	LEU
2	B	1876	GLN
2	B	1879	LYS
1	C	2001	MET
1	C	2005	THR
1	C	2008	LYS
1	C	2010	ILE
1	C	2024	CYS
1	C	2038	ARG
1	C	2043	ARG
1	C	2044	VAL
1	C	2046	ASN
1	C	2103	GLU
1	C	2145	ARG
1	C	2174	MET
1	C	2185	ARG
1	C	2217	GLU
1	C	2250	VAL
1	C	2275	ILE
1	C	2313	LYS
1	C	2321	LYS
1	C	2326	LEU
1	C	2339	ILE
1	C	2358	LYS

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Mol	Chain	Res	Type
1	C	2363	ASN
1	C	2412	LYS
1	C	2414	SER
1	C	2416	ASP
1	C	2423	LYS
1	C	2426	ARG
1	C	2428	LEU
1	C	2479	VAL
1	C	2482	THR
1	C	2485	ASN
1	C	2509	ARG
1	C	2543	MET
1	C	2548	GLU
1	C	2556	SER
1	C	2558	ASP
1	C	2560	GLU
1	C	2561	LYS
1	C	2563	MET
1	C	2571	ARG
1	C	2591	GLU
1	C	2645	GLN
1	C	2648	LEU
1	C	2652	ARG
1	C	2670	ASP
1	C	2675	ARG
1	C	2676	GLU
1	C	2677	ARG
1	C	2688	LYS
1	C	2689	GLN
1	C	2692	ASN
1	C	2696	THR
1	C	2698	ILE
1	C	2704	LYS
1	C	2706	LYS
1	C	2707	GLU
1	C	2728	VAL
1	C	2733	ASP
1	C	2735	ARG
1	C	2752	LEU
1	C	2753	ASP
1	C	2757	ASP
1	C	2763	ASP

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Mol	Chain	Res	Type
1	C	2782	ILE
1	C	2784	GLN
1	C	2800	THR
1	C	2805	ILE
1	C	2812	GLN
1	C	2845	ARG
1	C	2855	LYS
1	C	2912	ARG
1	C	2930	LYS
1	C	2940	LYS
1	C	2950	ARG
1	C	2955	GLU
1	C	2956	ARG
1	C	2963	LYS
1	C	3001	ILE
1	C	3006	LYS
1	C	3014	ILE
1	C	3017	THR
1	C	3018	SER
1	C	3020	ARG
1	C	3021	ARG
1	C	3027	ARG
1	C	3028	VAL
1	C	3044	LEU
1	C	3052	MET
1	C	3059	THR
1	C	3061	LYS
1	C	3068	MET
1	C	3073	LYS
2	D	3502	ILE
2	D	3506	LEU
2	D	3550	ARG
2	D	3573	SER
2	D	3587	LEU
2	D	3604	ARG
2	D	3613	ILE
2	D	3653	LEU
2	D	3666	GLU
2	D	3674	SER
2	D	3678	THR
2	D	3683	GLN
2	D	3686	LYS

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Mol	Chain	Res	Type
2	D	3687	GLU
2	D	3688	ASP
2	D	3722	GLN
2	D	3757	LYS
2	D	3761	THR
2	D	3800	VAL
2	D	3824	ASN
2	D	3826	ARG
2	D	3832	LEU
2	D	3857	SER
2	D	3866	LEU
2	D	3876	GLN
2	D	3879	LYS
1	E	4001	MET
1	E	4004	ARG
1	E	4005	THR
1	E	4008	LYS
1	E	4053	THR
1	E	4055	MET
1	E	4076	LYS
1	E	4101	GLU
1	E	4103	GLU
1	E	4133	ASP
1	E	4148	ILE
1	E	4153	GLU
1	E	4174	MET
1	E	4185	ARG
1	E	4190	GLU
1	E	4202	LYS
1	E	4203	GLU
1	E	4272	LEU
1	E	4275	ILE
1	E	4278	GLU
1	E	4296	ILE
1	E	4321	LYS
1	E	4326	LEU
1	E	4363	ASN
1	E	4428	LEU
1	E	4429	LYS
1	E	4478	GLU
1	E	4509	ARG
1	E	4548	GLU

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Mol	Chain	Res	Type
1	E	4556	SER
1	E	4558	ASP
1	E	4562	ILE
1	E	4571	ARG
1	E	4576	ILE
1	E	4591	GLU
1	E	4634	LYS
1	E	4645	GLN
1	E	4648	LEU
1	E	4671	ARG
1	E	4675	ARG
1	E	4676	GLU
1	E	4677	ARG
1	E	4679	GLN
1	E	4688	LYS
1	E	4696	THR
1	E	4704	LYS
1	E	4712	LEU
1	E	4713	VAL
1	E	4714	VAL
1	E	4733	ASP
1	E	4750	VAL
1	E	4751	LEU
1	E	4763	ASP
1	E	4772	MET
1	E	4784	GLN
1	E	4795	SER
1	E	4805	ILE
1	E	4811	GLN
1	E	4835	ASN
1	E	4849	THR
1	E	4881	LYS
1	E	4884	ILE
1	E	4912	ARG
1	E	4941	LYS
1	E	4944	ARG
1	E	4950	ARG
1	E	4955	GLU
1	E	4980	VAL
1	E	5001	ILE
1	E	5006	LYS
1	E	5017	THR

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Mol	Chain	Res	Type
1	E	5018	SER
1	E	5020	ARG
1	E	5021	ARG
1	E	5027	ARG
1	E	5031	ARG
1	E	5063	ILE
1	E	5073	LYS
2	F	5506	LEU
2	F	5510	GLU
2	F	5550	ARG
2	F	5587	LEU
2	F	5613	ILE
2	F	5620	ARG
2	F	5625	LYS
2	F	5637	ASN
2	F	5653	LEU
2	F	5669	SER
2	F	5674	SER
2	F	5683	GLN
2	F	5686	LYS
2	F	5687	GLU
2	F	5688	ASP
2	F	5705	ILE
2	F	5716	LEU
2	F	5718	ILE
2	F	5724	SER
2	F	5730	LYS
2	F	5756	GLN
2	F	5757	LYS
2	F	5763	ILE
2	F	5782	LYS
2	F	5800	VAL
2	F	5801	GLU
2	F	5821	LEU
2	F	5824	ASN
2	F	5830	LYS
2	F	5832	LEU
2	F	5840	ILE
2	F	5872	GLU
2	F	5876	GLN
1	G	6001	MET
1	G	6003	LYS

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Mol	Chain	Res	Type
1	G	6004	ARG
1	G	6008	LYS
1	G	6055	MET
1	G	6079	GLU
1	G	6088	PRO
1	G	6101	GLU
1	G	6103	GLU
1	G	6133	ASP
1	G	6145	ARG
1	G	6174	MET
1	G	6185	ARG
1	G	6202	LYS
1	G	6206	ILE
1	G	6207	ASP
1	G	6236	ASN
1	G	6275	ILE
1	G	6283	ASN
1	G	6299	GLU
1	G	6321	LYS
1	G	6416	ASP
1	G	6426	ARG
1	G	6428	LEU
1	G	6429	LYS
1	G	6479	VAL
1	G	6481	ILE
1	G	6490	ARG
1	G	6509	ARG
1	G	6518	ASP
1	G	6519	GLN
1	G	6548	GLU
1	G	6557	THR
1	G	6559	ARG
1	G	6560	GLU
1	G	6561	LYS
1	G	6571	ARG
1	G	6591	GLU
1	G	6604	GLU
1	G	6621	VAL
1	G	6634	LYS
1	G	6645	GLN
1	G	6648	LEU
1	G	6652	ARG

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Mol	Chain	Res	Type
1	G	6671	ARG
1	G	6673	GLU
1	G	6675	ARG
1	G	6677	ARG
1	G	6688	LYS
1	G	6692	ASN
1	G	6694	THR
1	G	6700	MET
1	G	6702	VAL
1	G	6704	LYS
1	G	6706	LYS
1	G	6712	LEU
1	G	6715	ARG
1	G	6731	GLU
1	G	6733	ASP
1	G	6735	ARG
1	G	6752	LEU
1	G	6775	ILE
1	G	6784	GLN
1	G	6789	SER
1	G	6800	THR
1	G	6804	GLU
1	G	6811	GLN
1	G	6836	GLU
1	G	6849	THR
1	G	6855	LYS
1	G	6879	VAL
1	G	6881	LYS
1	G	6884	ILE
1	G	6912	ARG
1	G	6939	MET
1	G	6940	LYS
1	G	6950	ARG
1	G	6992	ASN
1	G	7001	ILE
1	G	7014	ILE
1	G	7018	SER
1	G	7020	ARG
1	G	7021	ARG
1	G	7027	ARG
1	G	7028	VAL
1	G	7029	ILE

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Mol	Chain	Res	Type
1	G	7030	ARG
1	G	7031	ARG
1	G	7035	GLN
1	G	7037	LYS
1	G	7061	LYS
1	G	7063	ILE
1	G	7073	LYS
2	H	7503	LYS
2	H	7506	LEU
2	H	7525	SER
2	H	7550	ARG
2	H	7551	GLN
2	H	7573	SER
2	H	7587	LEU
2	H	7620	ARG
2	H	7625	LYS
2	H	7645	GLU
2	H	7646	LYS
2	H	7653	LEU
2	H	7654	ASN
2	H	7666	GLU
2	H	7674	SER
2	H	7687	GLU
2	H	7689	GLU
2	H	7702	LYS
2	H	7705	ILE
2	H	7715	ARG
2	H	7718	ILE
2	H	7739	SER
2	H	7757	LYS
2	H	7763	ILE
2	H	7772	HIS
2	H	7779	SER
2	H	7821	LEU
2	H	7824	ASN
2	H	7825	LEU
2	H	7831	SER
2	H	7832	LEU
2	H	7833	PHE
2	H	7844	ASP
2	H	7876	GLN
2	H	7880	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	519	GLN
1	A	679	GLN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	834	ASN
1	A	835	ASN
1	A	936	ASN
1	A	942	HIS
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1055	ASN
2	B	1551	GLN
2	B	1578	GLN
2	B	1722	GLN
2	B	1732	ASN
2	B	1810	GLN
2	B	1824	ASN
2	B	1838	GLN
2	B	1851	GLN
2	B	1876	GLN
1	C	2046	ASN
1	C	2105	GLN
1	C	2391	GLN
1	C	2689	GLN
1	C	2692	ASN
1	C	2784	GLN
1	C	2803	GLN
1	C	2814	GLN
1	C	2834	ASN
1	C	2835	ASN
1	C	2898	ASN
1	C	2936	ASN
1	C	2942	HIS
1	C	2995	HIS
1	C	3000	HIS
1	C	3035	GLN

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Mol	Chain	Res	Type
1	C	3055	ASN
1	C	3071	GLN
2	D	3516	HIS
2	D	3551	GLN
2	D	3629	ASN
2	D	3654	ASN
2	D	3722	GLN
2	D	3824	ASN
1	E	4105	GLN
1	E	4266	ASN
1	E	4337	ASN
1	E	4457	ASN
1	E	4491	GLN
1	E	4584	HIS
1	E	4784	GLN
1	E	4803	GLN
1	E	4812	GLN
1	E	4814	GLN
1	E	4827	ASN
1	E	4843	ASN
1	E	4936	ASN
1	E	5000	HIS
1	E	5035	GLN
1	E	5039	HIS
1	E	5055	ASN
1	E	5069	HIS
1	E	5071	GLN
2	F	5551	GLN
2	F	5637	ASN
2	F	5756	GLN
2	F	5824	ASN
2	F	5851	GLN
1	G	6105	GLN
1	G	6457	ASN
1	G	6689	GLN
1	G	6692	ASN
1	G	6784	GLN
1	G	6803	GLN
1	G	6814	GLN
1	G	6898	ASN
1	G	6932	GLN
1	G	6936	ASN

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Mol	Chain	Res	Type
1	G	6987	ASN
1	G	6992	ASN
1	G	7002	GLN
1	G	7007	ASN
1	G	7015	ASN
1	G	7035	GLN
1	G	7055	ASN
2	H	7551	GLN
2	H	7578	GLN
2	H	7605	HIS
2	H	7654	ASN
2	H	7722	GLN
2	H	7732	ASN
2	H	7773	GLN
2	H	7824	ASN

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	F	5769	2	12,14,15	3.30	3 (25%)	10,17,19	1.88	2 (20%)
2	CYG	H	7769	2	12,14,15	3.58	4 (33%)	10,17,19	1.92	3 (30%)
2	CYG	B	1769	2	12,14,15	3.57	3 (25%)	10,17,19	2.78	4 (40%)
2	CYG	D	3769	2	12,14,15	3.30	2 (16%)	10,17,19	2.34	4 (40%)

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	F	5769	2	-	0/14/16/18	-
2	CYG	H	7769	2	-	1/14/16/18	-
2	CYG	B	1769	2	-	3/14/16/18	-
2	CYG	D	3769	2	-	3/14/16/18	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1769	CYG	OE2-CD1	11.03	1.38	1.21
2	H	7769	CYG	OE2-CD1	10.56	1.37	1.21
2	D	3769	CYG	OE2-CD1	10.36	1.37	1.21
2	F	5769	CYG	OE2-CD1	9.68	1.36	1.21
2	H	7769	CYG	O1-C1	4.77	1.36	1.22
2	F	5769	CYG	O1-C1	4.42	1.35	1.22
2	B	1769	CYG	O1-C1	4.32	1.34	1.22
2	D	3769	CYG	O1-C1	4.14	1.34	1.22
2	F	5769	CYG	CD1-SG	-3.27	1.68	1.76
2	H	7769	CYG	CD1-SG	-2.99	1.69	1.76
2	H	7769	CYG	O2-C1	2.55	1.38	1.30
2	B	1769	CYG	CG1-CD1	-2.00	1.48	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1769	CYG	OE2-CD1-CG1	-6.28	116.73	123.98
2	D	3769	CYG	OE2-CD1-CG1	-5.38	117.78	123.98
2	H	7769	CYG	CB-SG-CD1	-4.31	94.85	100.76
2	F	5769	CYG	CG1-CD1-SG	4.16	118.35	113.40
2	B	1769	CYG	CB-SG-CD1	3.65	105.78	100.76
2	F	5769	CYG	OE2-CD1-SG	-3.24	118.56	122.68
2	D	3769	CYG	CG1-CD1-SG	3.11	117.11	113.40
2	B	1769	CYG	CG1-CD1-SG	2.87	116.82	113.40
2	B	1769	CYG	OE2-CD1-SG	2.86	126.32	122.68
2	H	7769	CYG	CG1-CD1-SG	2.68	116.59	113.40
2	D	3769	CYG	CB-SG-CD1	2.35	103.99	100.76
2	H	7769	CYG	OE2-CD1-CG1	-2.14	121.51	123.98
2	D	3769	CYG	CG1-CB1-CA1	-2.13	108.98	113.86

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3769	CYG	OE2-CD1-SG-CB
2	B	1769	CYG	CG1-CD1-SG-CB
2	D	3769	CYG	CG1-CD1-SG-CB
2	B	1769	CYG	OE2-CD1-SG-CB
2	B	1769	CYG	N-CA-CB-SG
2	D	3769	CYG	N-CA-CB-SG
2	H	7769	CYG	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5769	CYG	1	0
2	H	7769	CYG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 103 ligands modelled in this entry, 72 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	C	3906	5,4	4,4,4	1.97	3 (75%)	6,6,6	1.33	1 (16%)
3	PO4	A	1980	-	4,4,4	2.11	1 (25%)	6,6,6	1.10	0
7	ADP	C	3910	5,4	28,29,29	1.47	3 (10%)	43,45,45	1.23	5 (11%)
3	PO4	E	5906	5,4	4,4,4	1.99	1 (25%)	6,6,6	0.89	0
3	PO4	E	5980	-	4,4,4	3.44	3 (75%)	6,6,6	1.17	0
3	PO4	E	5981	-	4,4,4	1.40	1 (25%)	6,6,6	0.86	0
3	PO4	C	3981	-	4,4,4	3.96	4 (100%)	6,6,6	1.09	1 (16%)
8	ORN	G	7920	-	7,8,8	1.25	1 (14%)	6,9,9	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NET	E	5950	-	8,8,8	0.83	0	10,10,10	0.56	0
3	PO4	C	3980	-	4,4,4	1.45	0	6,6,6	0.52	0
7	ADP	A	1910	5,4	28,29,29	1.25	2 (7%)	43,45,45	1.27	5 (11%)
3	PO4	G	7981	-	4,4,4	2.77	1 (25%)	6,6,6	1.17	1 (16%)
8	ORN	C	3920	-	7,8,8	1.11	1 (14%)	6,9,9	1.03	1 (16%)
7	ADP	G	7900	4	28,29,29	1.46	4 (14%)	43,45,45	1.24	4 (9%)
8	ORN	E	5920	-	7,8,8	1.17	1 (14%)	6,9,9	0.93	0
3	PO4	C	3982	-	4,4,4	3.14	4 (100%)	6,6,6	1.32	0
3	PO4	A	1906	5,4	4,4,4	1.91	2 (50%)	6,6,6	1.18	1 (16%)
8	ORN	A	1920	-	7,8,8	0.98	0	6,9,9	1.58	1 (16%)
3	PO4	A	1982	-	4,4,4	3.01	3 (75%)	6,6,6	0.76	0
3	PO4	G	7982	-	4,4,4	3.47	3 (75%)	6,6,6	1.43	0
7	ADP	C	3900	4	28,29,29	1.64	4 (14%)	43,45,45	1.00	2 (4%)
7	ADP	E	5900	4	28,29,29	1.73	5 (17%)	43,45,45	1.01	1 (2%)
7	ADP	E	5910	5,4	28,29,29	1.35	3 (10%)	43,45,45	1.10	3 (6%)
7	ADP	A	1900	4	28,29,29	1.43	4 (14%)	43,45,45	1.16	3 (6%)
3	PO4	A	1981	-	4,4,4	2.42	2 (50%)	6,6,6	1.58	1 (16%)
9	NET	A	1950	-	8,8,8	0.85	0	10,10,10	0.52	0
7	ADP	G	7910	5,4	28,29,29	1.69	4 (14%)	43,45,45	1.10	4 (9%)
9	NET	C	3950	-	8,8,8	0.73	0	10,10,10	0.67	0
3	PO4	G	7980	-	4,4,4	3.25	2 (50%)	6,6,6	1.01	0
9	NET	G	7950	-	8,8,8	0.71	0	10,10,10	0.54	0
3	PO4	G	7906	5,4	4,4,4	1.76	1 (25%)	6,6,6	0.71	0

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	C	3900	4	-	2/16/32/32	0/3/3/3
7	ADP	G	7900	4	-	0/16/32/32	0/3/3/3
8	ORN	E	5920	-	-	5/8/8/8	-
7	ADP	E	5900	4	-	2/16/32/32	0/3/3/3
7	ADP	E	5910	5,4	-	0/16/32/32	0/3/3/3
7	ADP	A	1900	4	-	2/16/32/32	0/3/3/3
9	NET	A	1950	-	-	3/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	A	1920	-	-	7/8/8/8	-
9	NET	E	5950	-	-	9/12/12/12	-
7	ADP	A	1910	5,4	-	2/16/32/32	0/3/3/3
7	ADP	C	3910	5,4	-	2/16/32/32	0/3/3/3
7	ADP	G	7910	5,4	-	0/16/32/32	0/3/3/3
9	NET	C	3950	-	-	0/12/12/12	-
9	NET	G	7950	-	-	2/12/12/12	-
8	ORN	C	3920	-	-	7/8/8/8	-
8	ORN	G	7920	-	-	6/8/8/8	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	7910	ADP	PA-O3A	-6.77	1.52	1.59
7	C	3900	ADP	PA-O3A	-6.37	1.52	1.59
7	E	5900	ADP	PA-O3A	-6.24	1.52	1.59
3	G	7982	PO4	P-O1	5.73	1.63	1.50
3	C	3981	PO4	P-O1	5.66	1.63	1.50
3	E	5980	PO4	P-O1	5.20	1.62	1.50
3	G	7981	PO4	P-O1	5.11	1.62	1.50
3	G	7980	PO4	P-O1	4.53	1.61	1.50
3	C	3982	PO4	P-O1	4.30	1.60	1.50
3	A	1981	PO4	P-O1	4.07	1.60	1.50
3	G	7980	PO4	P-O4	4.02	1.66	1.54
3	A	1982	PO4	P-O1	3.90	1.59	1.50
7	C	3910	ADP	PA-O3A	-3.82	1.55	1.59
7	A	1900	ADP	PA-O3A	-3.80	1.55	1.59
7	E	5910	ADP	PA-O3A	-3.78	1.55	1.59
3	A	1980	PO4	P-O1	3.57	1.58	1.50
7	C	3910	ADP	O3'-C3'	3.53	1.51	1.43
3	A	1982	PO4	P-O3	3.48	1.64	1.54
3	C	3981	PO4	P-O2	3.43	1.64	1.54
3	E	5980	PO4	P-O4	3.40	1.64	1.54
7	E	5900	ADP	O4'-C1'	-3.34	1.34	1.42
3	C	3982	PO4	P-O2	3.22	1.64	1.54
7	G	7900	ADP	PA-O3A	-3.20	1.56	1.59
7	A	1910	ADP	PA-O3A	-3.16	1.56	1.59
3	C	3981	PO4	P-O4	3.11	1.63	1.54
7	E	5900	ADP	C2-N3	-3.07	1.28	1.33
8	G	7920	ORN	O-C	3.06	1.31	1.22
3	C	3981	PO4	P-O3	3.03	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1900	ADP	O3'-C3'	3.02	1.50	1.43
3	G	7982	PO4	P-O4	2.96	1.63	1.54
3	E	5906	PO4	P-O4	-2.86	1.46	1.54
3	G	7906	PO4	P-O4	-2.84	1.46	1.54
7	E	5910	ADP	O3'-C3'	2.81	1.49	1.43
7	A	1900	ADP	C2-N3	-2.78	1.29	1.33
7	G	7900	ADP	O3'-C3'	2.70	1.49	1.43
8	C	3920	ORN	O-C	2.69	1.30	1.22
3	A	1906	PO4	P-O3	-2.69	1.46	1.54
7	A	1910	ADP	O3'-C3'	2.62	1.49	1.43
3	A	1982	PO4	P-O2	2.62	1.62	1.54
7	G	7910	ADP	O2'-C2'	2.60	1.49	1.43
3	C	3982	PO4	P-O3	2.57	1.62	1.54
7	C	3900	ADP	C2-N1	2.49	1.38	1.33
3	E	5980	PO4	P-O2	2.48	1.61	1.54
7	G	7900	ADP	O2'-C2'	2.47	1.49	1.43
7	C	3900	ADP	O2'-C2'	2.36	1.48	1.43
7	C	3910	ADP	O2'-C2'	2.36	1.48	1.43
3	C	3906	PO4	P-O3	-2.36	1.47	1.54
7	C	3900	ADP	PA-O2A	-2.35	1.44	1.55
7	G	7900	ADP	PB-O2B	-2.33	1.46	1.54
7	A	1900	ADP	PA-O2A	-2.32	1.44	1.55
7	G	7910	ADP	O3'-C3'	2.30	1.48	1.43
3	C	3906	PO4	P-O4	-2.28	1.48	1.54
3	A	1906	PO4	P-O4	-2.24	1.48	1.54
7	E	5900	ADP	O3'-C3'	2.23	1.48	1.43
3	C	3906	PO4	P-O2	-2.19	1.48	1.54
8	E	5920	ORN	O-C	2.17	1.28	1.22
3	A	1981	PO4	P-O2	2.16	1.60	1.54
7	E	5900	ADP	O2'-C2'	2.16	1.48	1.43
7	E	5910	ADP	O2'-C2'	2.08	1.48	1.43
3	G	7982	PO4	P-O3	2.08	1.60	1.54
3	C	3982	PO4	P-O4	2.04	1.60	1.54
3	E	5981	PO4	P-O3	2.03	1.60	1.54
7	G	7910	ADP	C2-N1	2.01	1.37	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1910	ADP	O3B-PB-O3A	4.21	118.76	104.64
7	G	7900	ADP	O2A-PA-O3A	3.63	117.09	107.27
7	C	3910	ADP	O3'-C3'-C2'	3.63	123.45	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	5910	ADP	O2A-PA-O3A	3.48	116.67	107.27
7	A	1900	ADP	C5-C6-N6	3.17	131.13	123.29
7	E	5900	ADP	O3B-PB-O3A	-3.01	94.55	104.64
7	G	7900	ADP	C5-C6-N6	2.85	130.35	123.29
7	C	3910	ADP	O2A-PA-O3A	2.82	114.89	107.27
3	A	1981	PO4	O4-P-O3	2.82	116.68	107.91
7	E	5910	ADP	O3'-C3'-C2'	2.80	120.80	111.82
7	G	7910	ADP	O2'-C2'-C3'	2.77	120.69	111.82
8	A	1920	ORN	OXT-C-O	-2.66	118.05	124.08
7	C	3910	ADP	O2'-C2'-C3'	2.48	119.75	111.82
7	C	3900	ADP	O2A-PA-O3A	2.45	113.90	107.27
3	C	3906	PO4	O4-P-O3	2.44	115.52	107.91
7	A	1900	ADP	O3B-PB-O2B	2.43	116.93	107.80
7	C	3910	ADP	C2'-C1'-N9	2.42	119.31	113.30
7	G	7910	ADP	O2A-PA-O3A	2.37	113.69	107.27
7	A	1900	ADP	O3'-C3'-C2'	2.37	119.41	111.82
7	A	1910	ADP	O3A-PA-O1A	2.35	117.76	110.70
8	C	3920	ORN	OXT-C-O	-2.30	118.86	124.08
7	G	7900	ADP	O3'-C3'-C2'	2.29	119.16	111.82
7	A	1910	ADP	O3B-PB-O2B	-2.26	99.31	107.80
7	C	3900	ADP	O2B-PB-O1B	-2.25	102.06	110.83
7	C	3910	ADP	C3'-C2'-C1'	2.23	105.68	101.46
3	C	3981	PO4	O4-P-O1	-2.20	103.18	110.95
7	A	1910	ADP	C3'-C2'-C1'	2.17	105.57	101.46
7	A	1910	ADP	O3'-C3'-C2'	2.16	118.75	111.82
3	G	7981	PO4	O4-P-O3	2.15	114.61	107.91
7	G	7910	ADP	O3'-C3'-C2'	2.13	118.64	111.82
3	A	1906	PO4	O4-P-O3	2.05	114.28	107.91
7	E	5910	ADP	O2'-C2'-C3'	2.03	118.34	111.82
7	G	7900	ADP	O2'-C2'-C3'	2.02	118.28	111.82
7	G	7910	ADP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1920	ORN	N-CA-CB-CG
8	A	1920	ORN	C-CA-CB-CG
8	C	3920	ORN	N-CA-CB-CG
8	C	3920	ORN	C-CA-CB-CG
8	C	3920	ORN	O-C-CA-N
8	E	5920	ORN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
8	E	5920	ORN	O-C-CA-N
8	G	7920	ORN	N-CA-CB-CG
9	A	1950	NET	C4-C3-N1-C1
9	E	5950	NET	C4-C3-N1-C1
9	A	1950	NET	C4-C3-N1-C7
9	E	5950	NET	C4-C3-N1-C7
9	E	5950	NET	C4-C3-N1-C5
9	A	1950	NET	C4-C3-N1-C5
9	E	5950	NET	C2-C1-N1-C5
9	E	5950	NET	C2-C1-N1-C7
9	E	5950	NET	C2-C1-N1-C3
8	G	7920	ORN	OXT-C-CA-N
8	A	1920	ORN	OXT-C-CA-N
8	C	3920	ORN	OXT-C-CA-N
8	E	5920	ORN	NE-CD-CG-CB
8	A	1920	ORN	CA-CB-CG-CD
8	C	3920	ORN	CA-CB-CG-CD
9	E	5950	NET	C8-C7-N1-C1
9	E	5950	NET	C8-C7-N1-C3
8	G	7920	ORN	CA-CB-CG-CD
8	A	1920	ORN	O-C-CA-N
8	G	7920	ORN	O-C-CA-N
8	G	7920	ORN	C-CA-CB-CG
9	E	5950	NET	C8-C7-N1-C5
7	A	1900	ADP	PB-O3A-PA-O1A
8	G	7920	ORN	NE-CD-CG-CB
8	C	3920	ORN	O-C-CA-CB
7	C	3910	ADP	PA-O3A-PB-O1B
8	A	1920	ORN	O-C-CA-CB
8	E	5920	ORN	O-C-CA-CB
8	E	5920	ORN	OXT-C-CA-N
8	C	3920	ORN	NE-CD-CG-CB
8	A	1920	ORN	NE-CD-CG-CB
7	A	1910	ADP	PB-O3A-PA-O2A
7	E	5900	ADP	PB-O3A-PA-O1A
9	G	7950	NET	C8-C7-N1-C5
9	G	7950	NET	C8-C7-N1-C3
7	A	1910	ADP	PB-O3A-PA-O1A
7	C	3900	ADP	PB-O3A-PA-O1A
7	E	5900	ADP	PB-O3A-PA-O2A
7	C	3910	ADP	C3'-C4'-C5'-O5'
7	A	1900	ADP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
7	C	3900	ADP	PB-O3A-PA-O2A

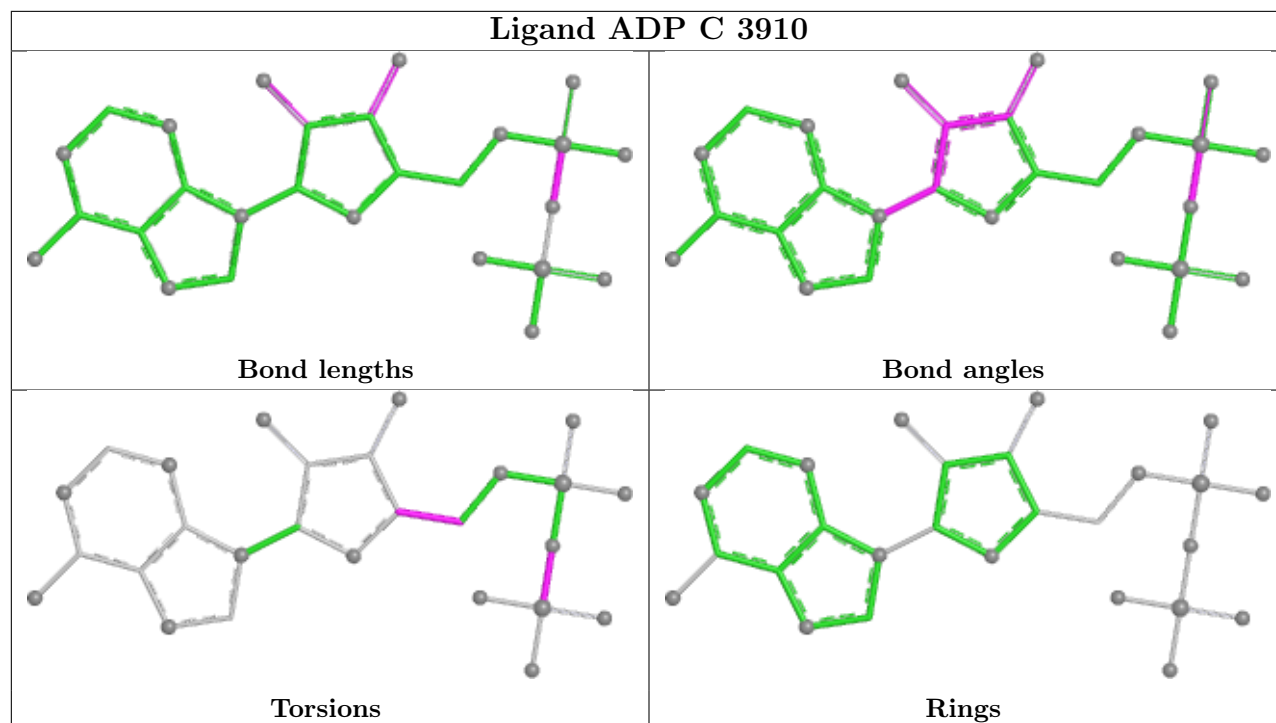
There are no ring outliers.

13 monomers are involved in 19 short contacts:

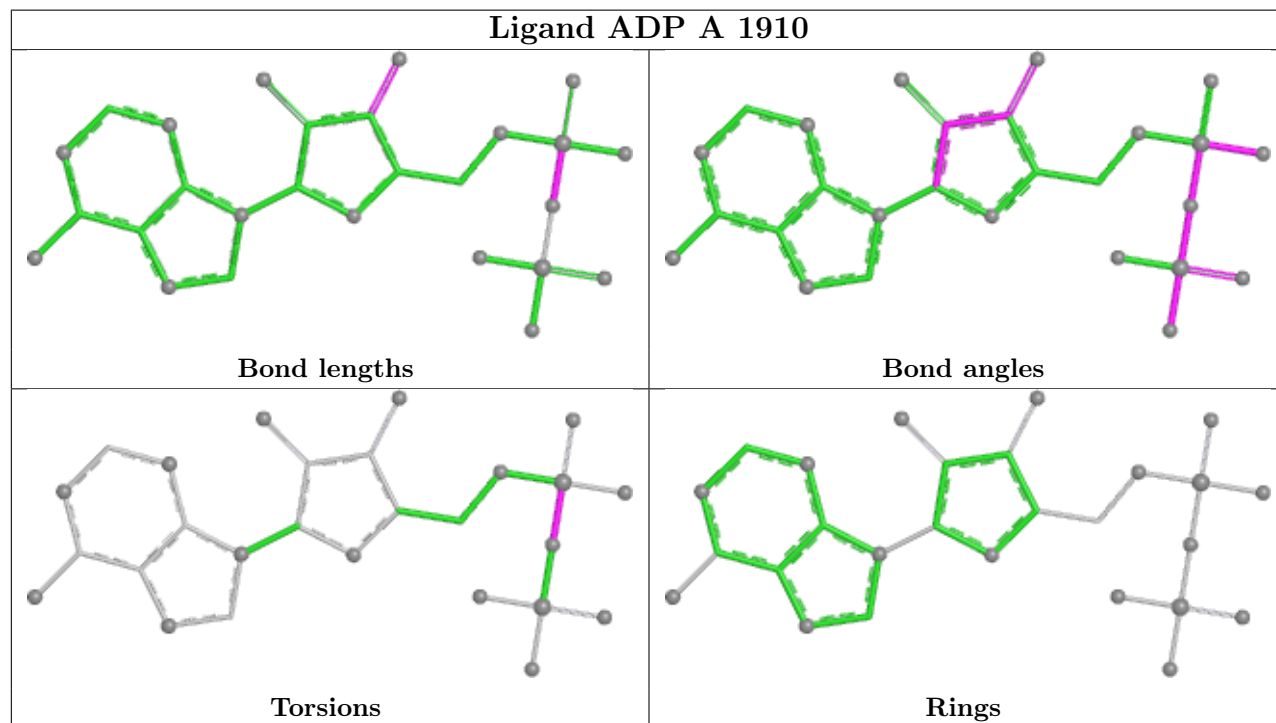
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3906	PO4	1	0
7	C	3910	ADP	1	0
8	G	7920	ORN	1	0
9	E	5950	NET	2	0
7	A	1910	ADP	2	0
8	C	3920	ORN	3	0
7	G	7900	ADP	2	0
8	E	5920	ORN	1	0
8	A	1920	ORN	1	0
7	E	5900	ADP	1	0
9	A	1950	NET	1	0
7	G	7910	ADP	2	0
3	G	7906	PO4	1	0

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.

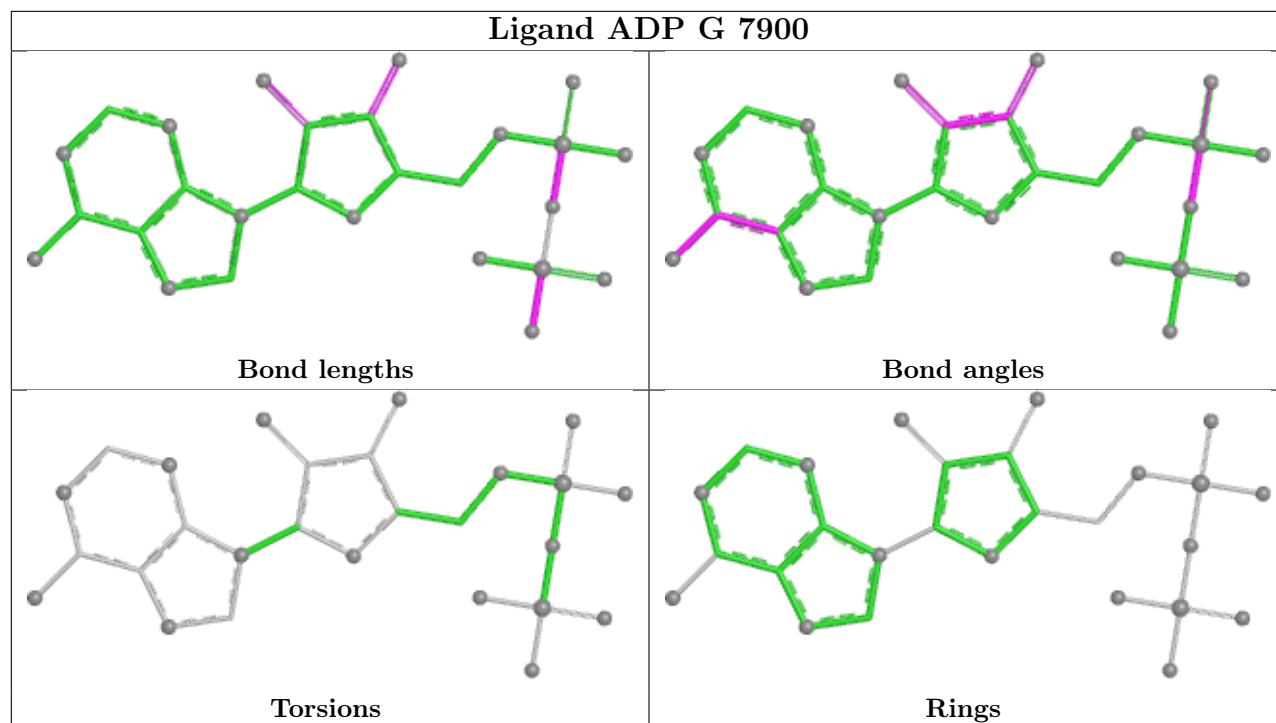
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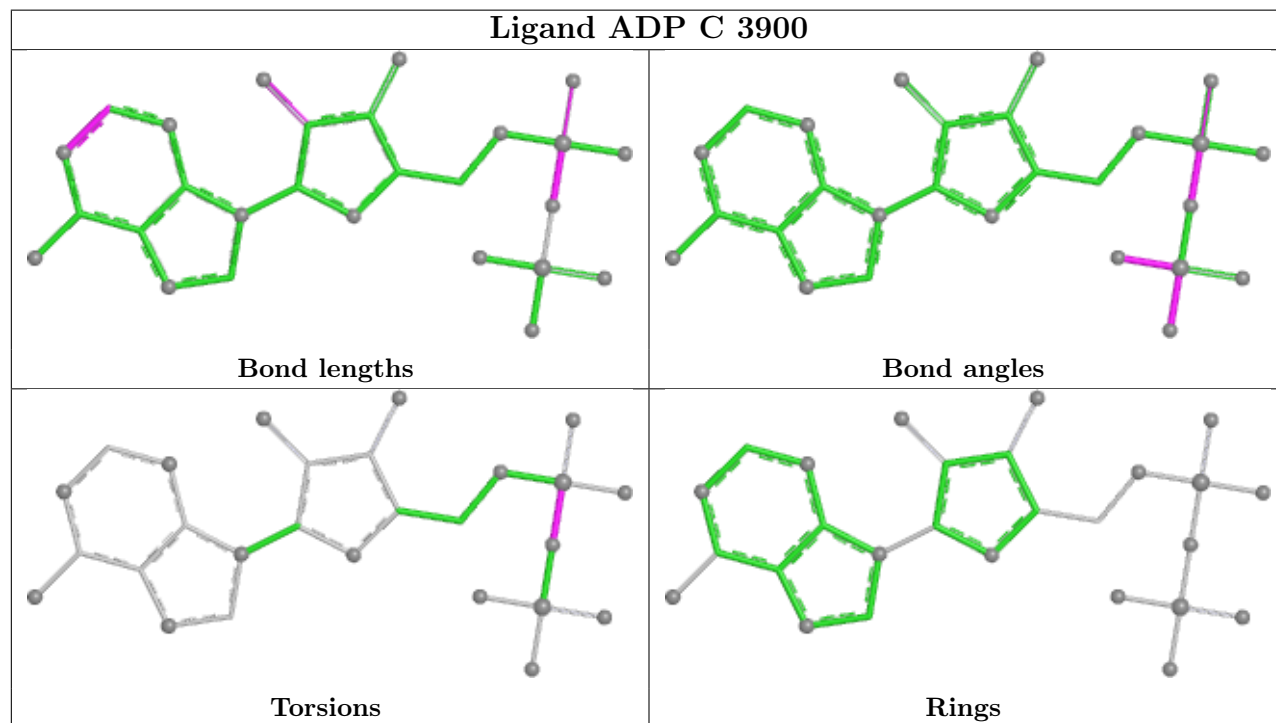
Ligand ADP A 1910

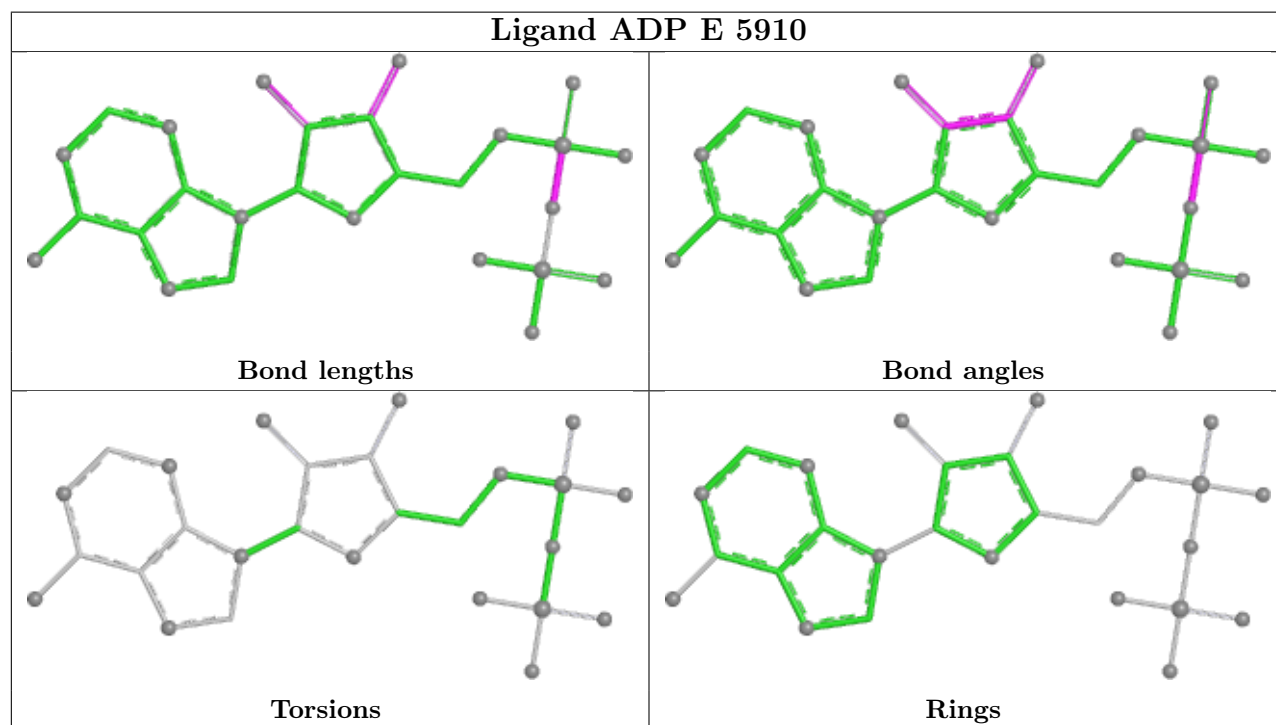
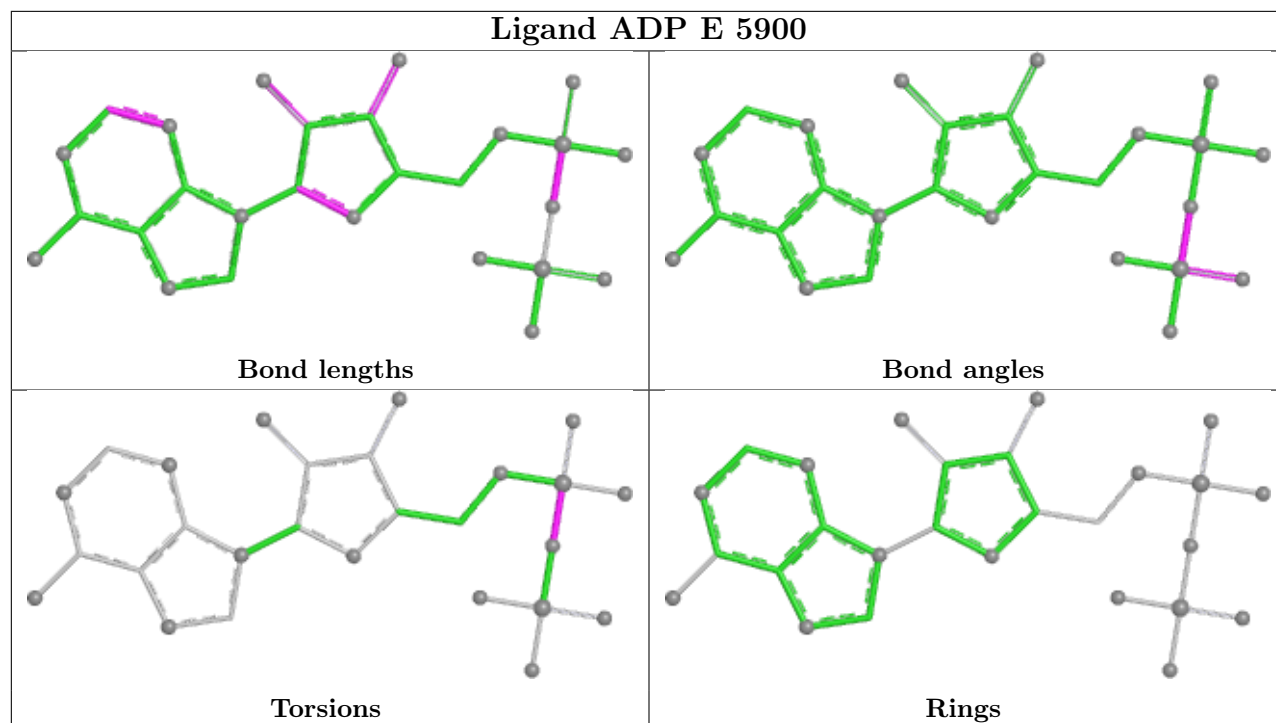


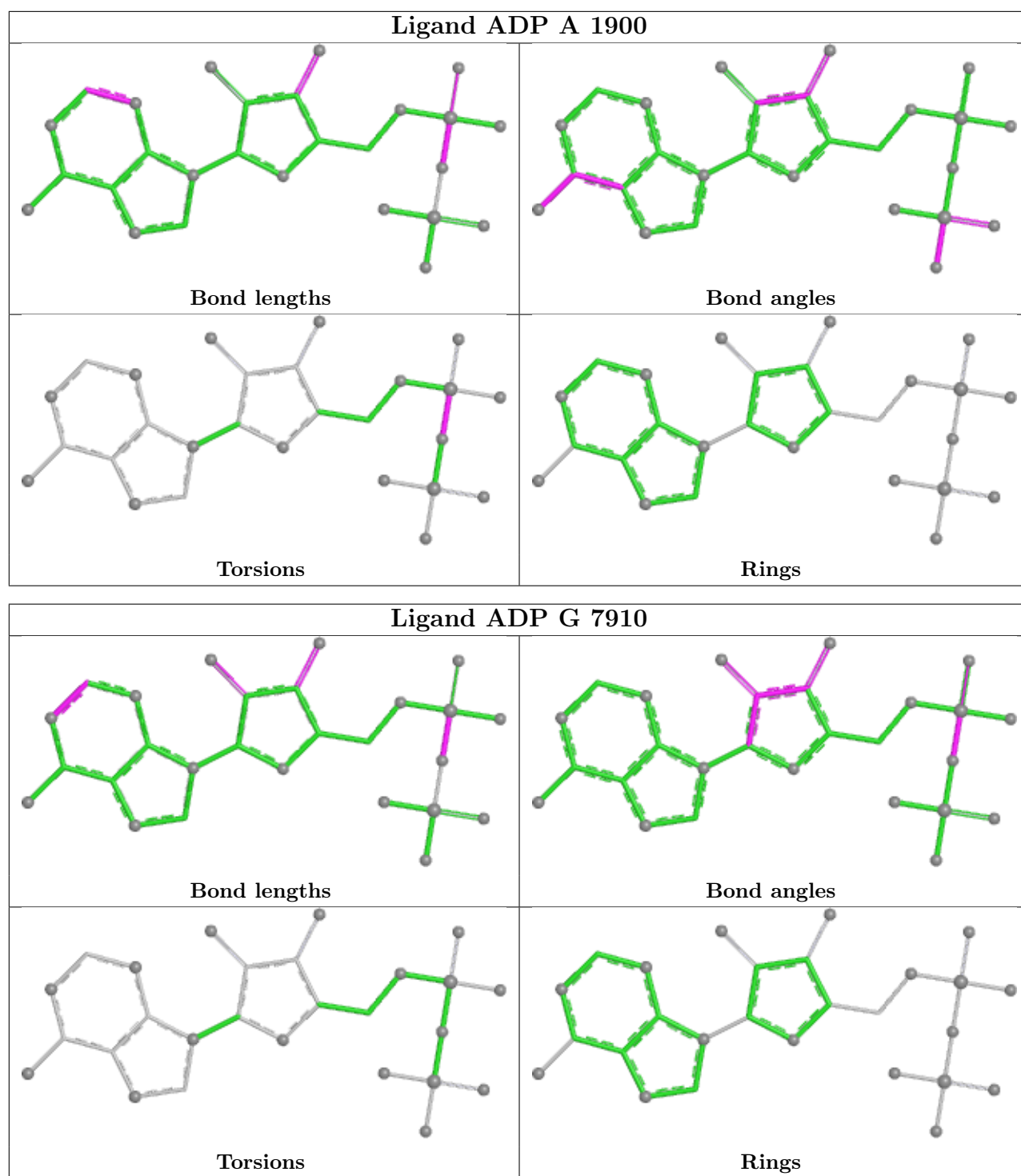
Ligand ADP G 7900



Ligand ADP C 3900







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.