Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2022 – 02:13 AM EST

PDB ID	:	1A9X
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:

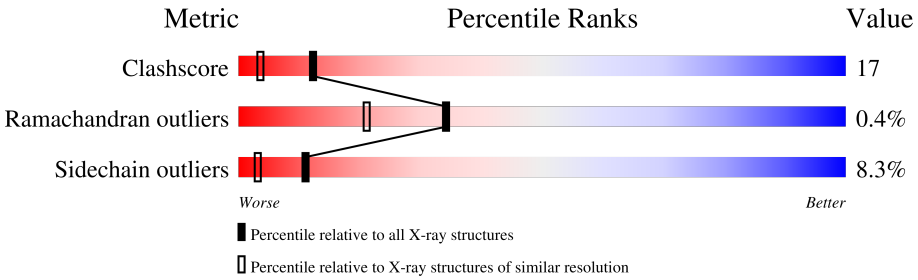
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	60% 31% 7% ••
1	C	1073	61% 29% 7% ••
1	E	1073	60% 30% 7% ••
1	G	1073	55% 33% 9% ••
2	B	379	60% 32% 7%
2	D	379	61% 34% 5% •
2	F	379	61% 34% 5% •
2	H	379	53% 38% 8% •

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	-	-

2 Entry composition (i)

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

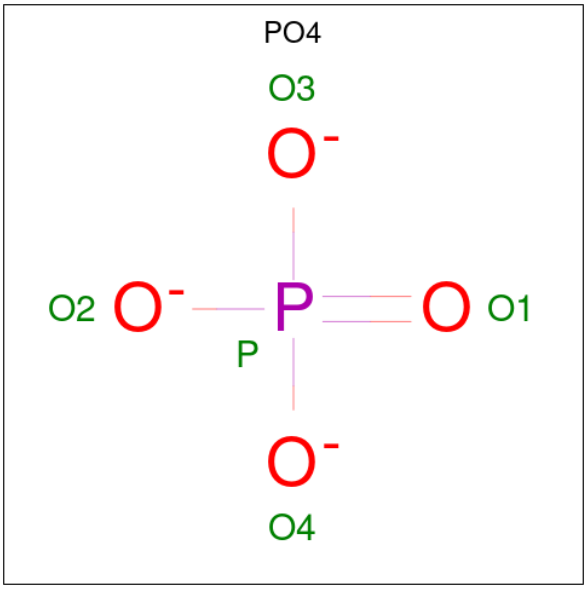
- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN).

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 (three-letter code: PO4) (formula: O_4P).



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

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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 (three-letter code: 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 (three-letter code: 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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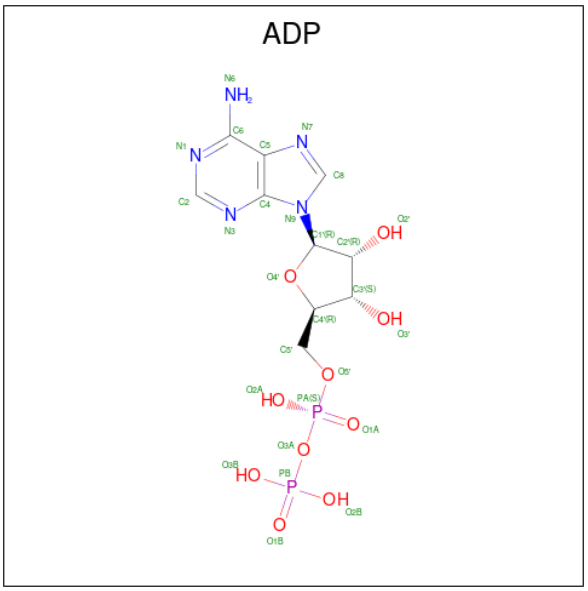
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0
5	E	7	Total K 7 7	0	0
5	F	1	Total K 1 1	0	0
5	G	7	Total K 7 7	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

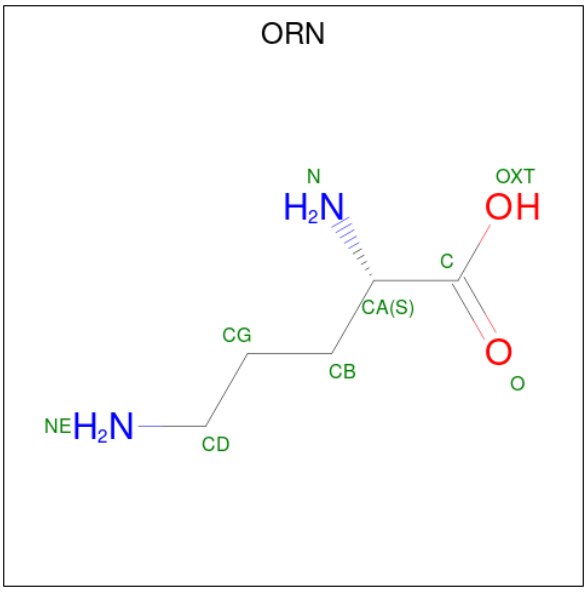
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total Cl 6 6	0	0
6	B	1	Total Cl 1 1	0	0
6	C	6	Total Cl 6 6	0	0
6	D	1	Total Cl 1 1	0	0
6	E	6	Total Cl 6 6	0	0
6	F	1	Total Cl 1 1	0	0
6	G	6	Total Cl 6 6	0	0
6	H	1	Total Cl 1 1	0	0

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



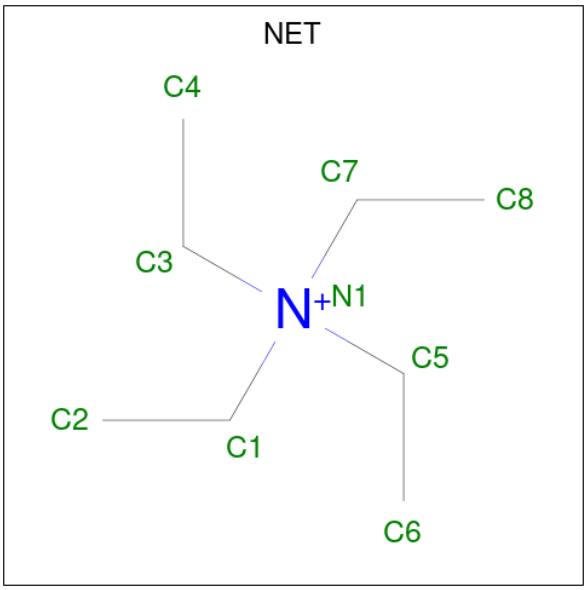
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



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

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



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

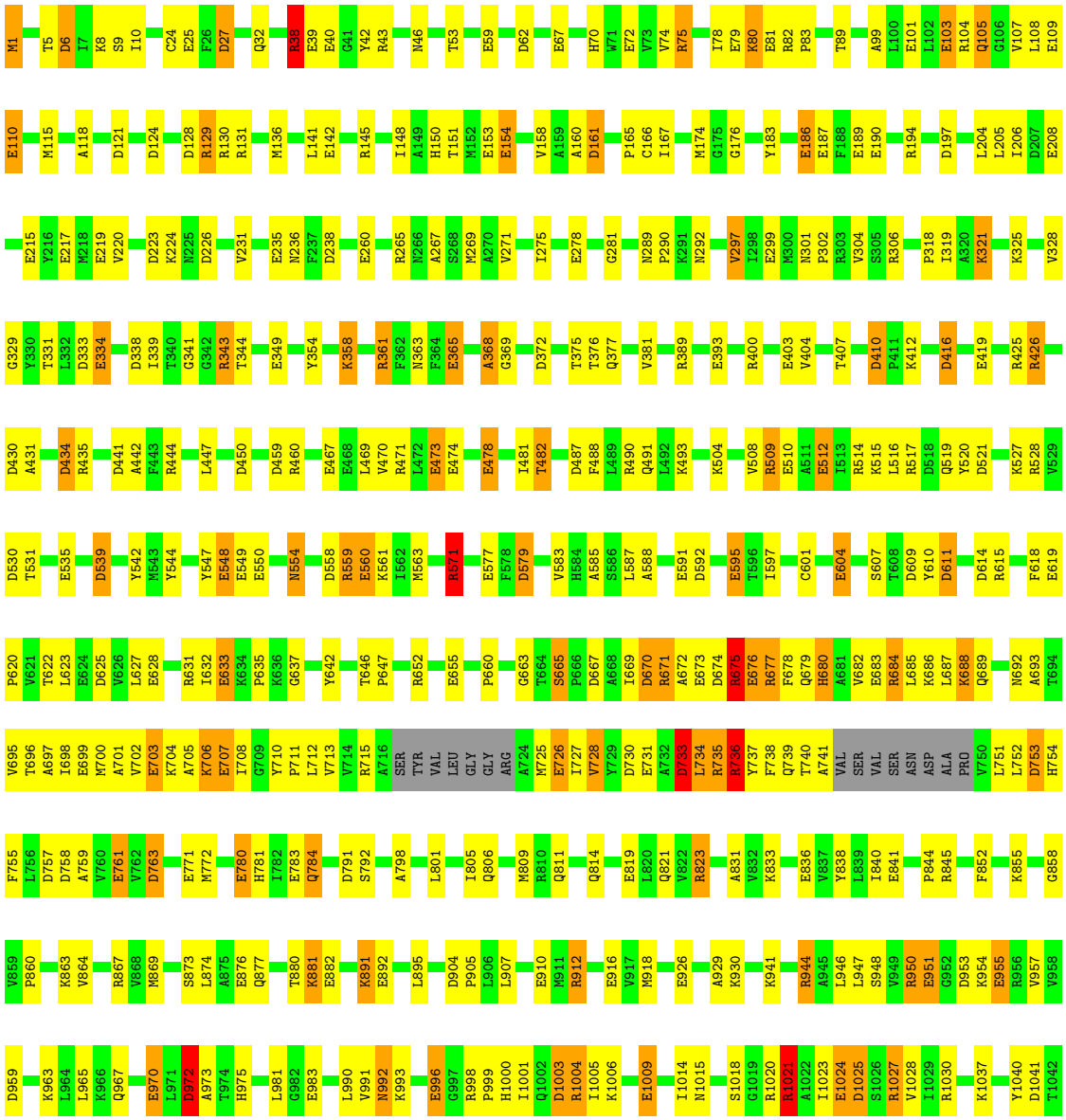
3 Residue-property plots (i)

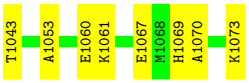
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

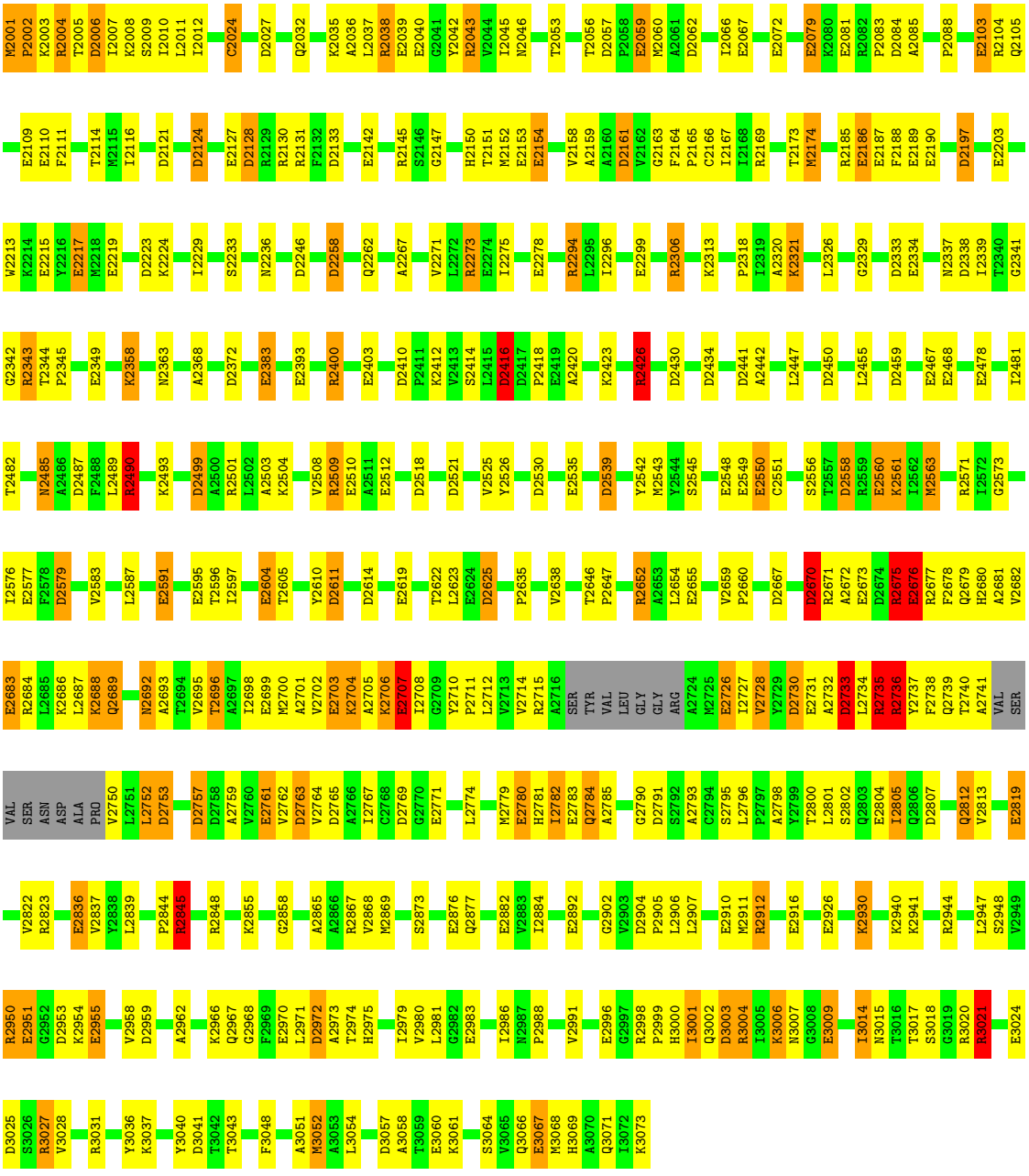
Chain A:





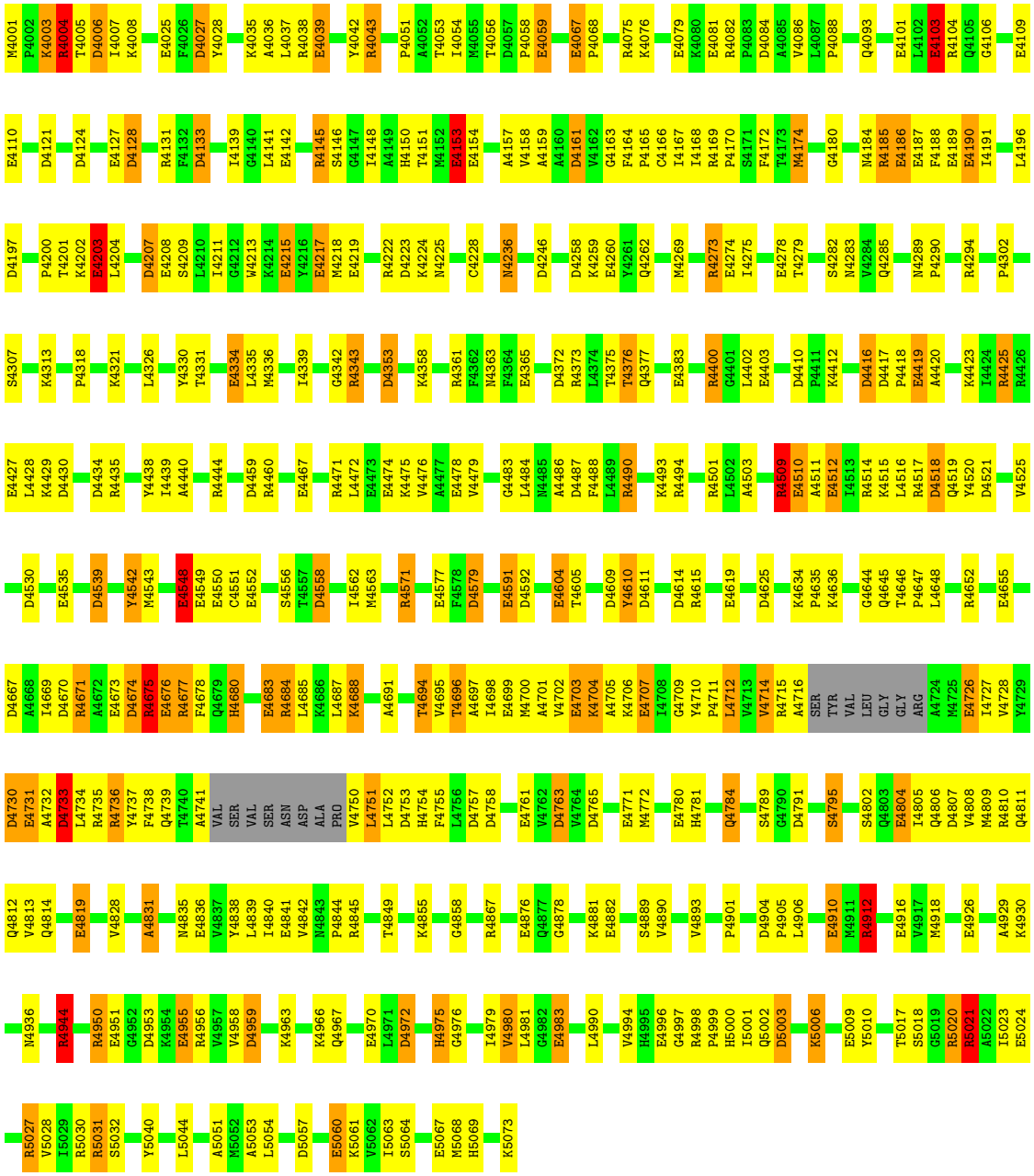
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

Chain C:



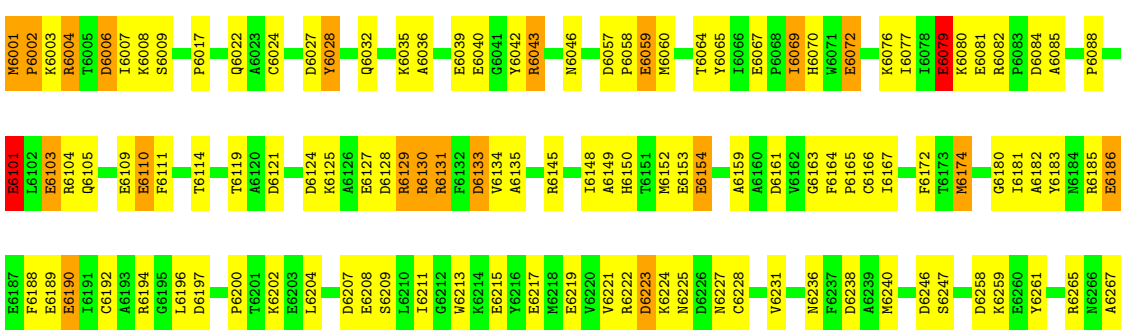
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

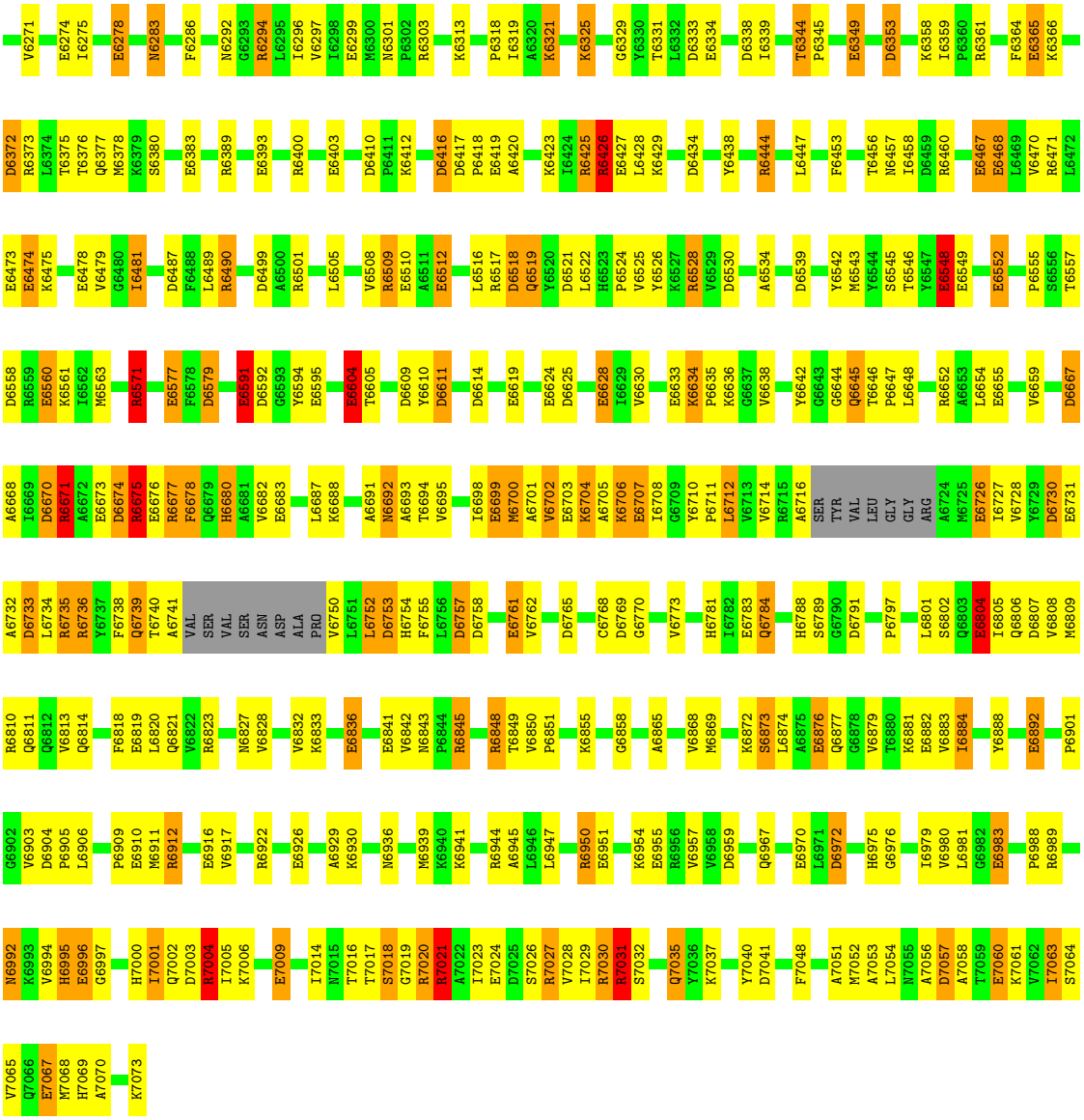
Chain E:



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

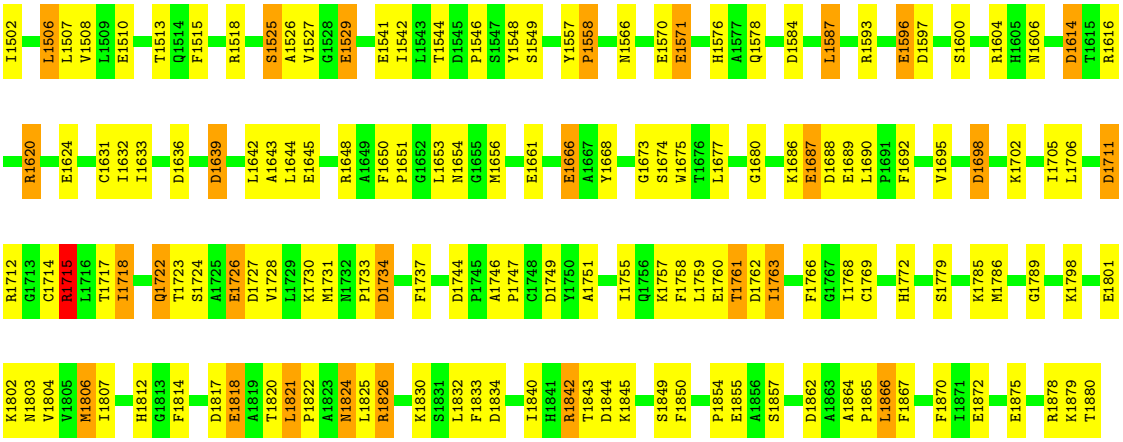
Chain G:





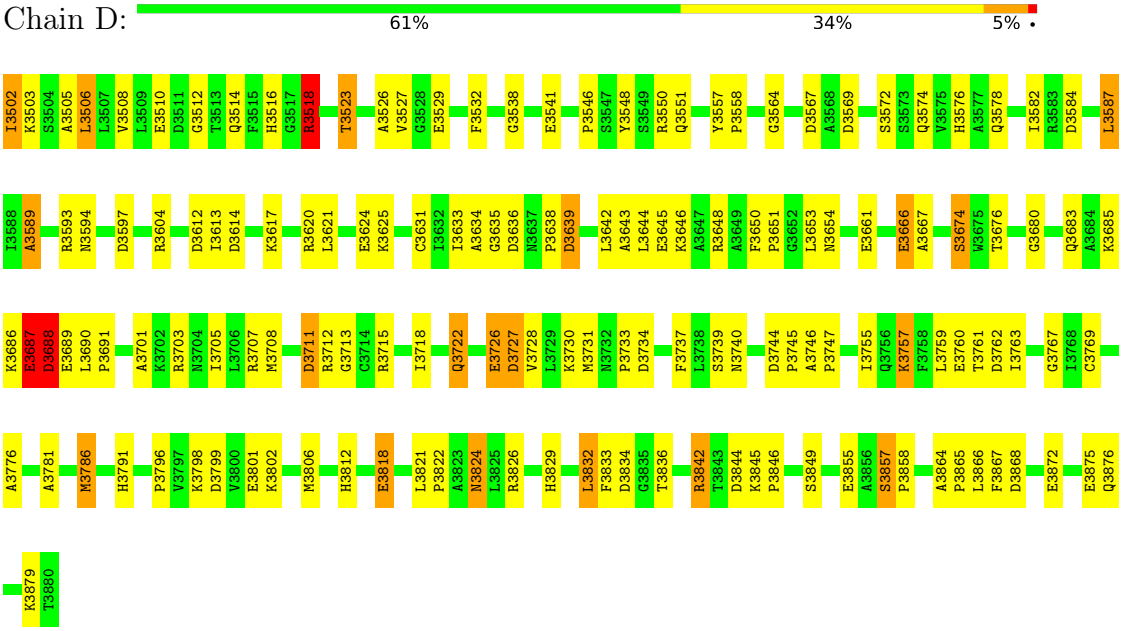
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain B:



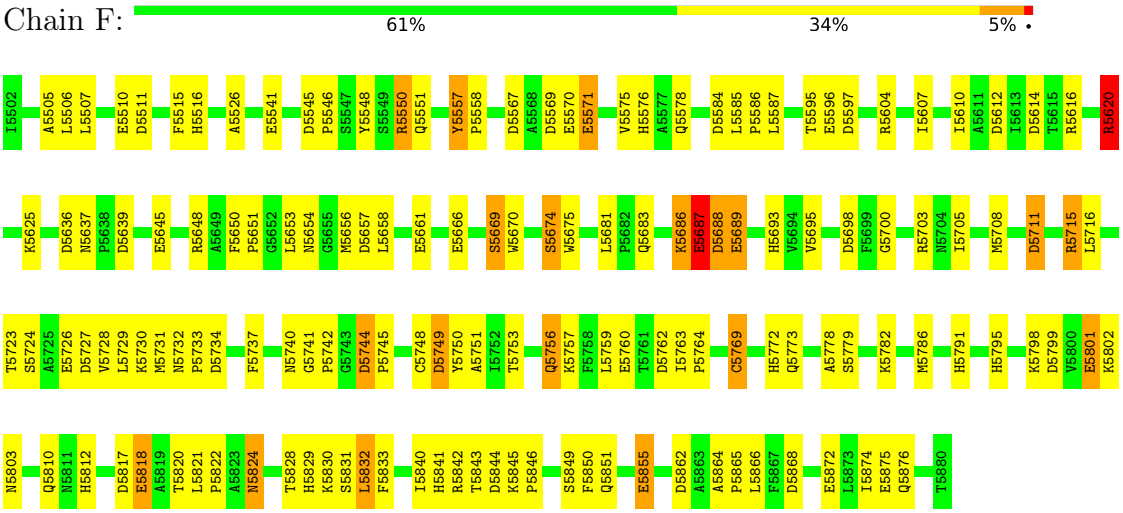
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain D:



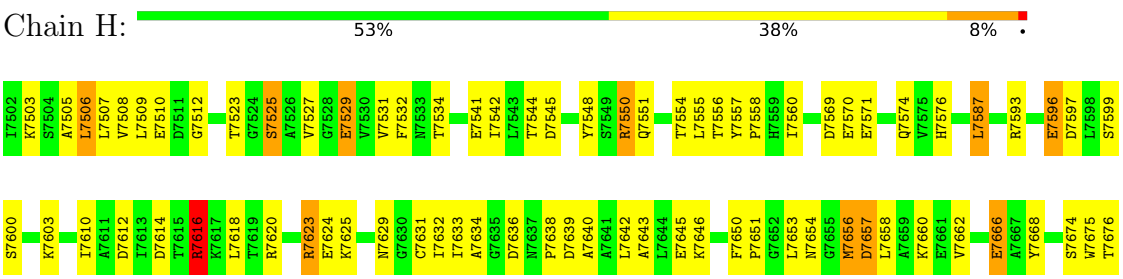
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

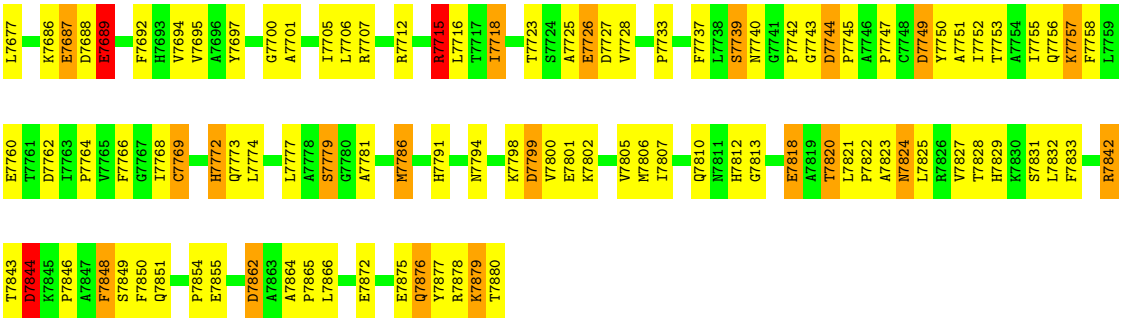
Chain F:



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain H:




L7677 K7686 E7687 D7688 E7689 F7692 H7693 V7694 V7695 A7696 Y7697 G7700 A7701 I7705 L7706 R7707 R7712 R7715 L7716 T7717 I7718 T7723 S7724 A7725 E7726 D7727 V7728 P7733 F7737 L7738 S7739 N7740 G7741 P7742 G7743 D7744 P7745 A7746 P7747 C7748 D7749 Y7750 A7751 I7752 T7753 A7754 I7755 Q7756 K7757 F7758 L7759
E7760 T7761 D7762 I7763 P7764 V7765 F7766 G7767 I7768 C7769 H7772 Q7773 L7774 L7777 A7778 S7779 G7780 A7781 M7786 H7791 N7794 K7798 D7799 V7800 E7801 K7802 V7805 M7806 I7807 Q7810 N7811 H7812 G7813 E7818 A7819 T7820 L7821 P7822 A7823 N7824 L7825 R7826 V7827 T7828 H7829 K7830 S7831 L7832 F7833 R7842
T7843 D7844 K7845 P7846 A7847 F7848 S7849 F7850 Q7851 P7854 E7855 D7862 A7863 A7864 P7865 L7866 E7872 E7875 Q7876 Y7877 R7878 K7879 T7880

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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	1.11	77/8347 (0.9%)	1.53	140/11284 (1.2%)
1	C	1.10	72/8352 (0.9%)	1.48	121/11288 (1.1%)
1	E	1.13	70/8303 (0.8%)	1.55	137/11225 (1.2%)
1	G	1.08	79/8294 (1.0%)	1.49	125/11213 (1.1%)
2	B	0.97	20/2953 (0.7%)	1.39	32/4009 (0.8%)
2	D	1.01	16/2947 (0.5%)	1.42	40/4001 (1.0%)
2	F	0.98	18/2972 (0.6%)	1.42	36/4034 (0.9%)
2	H	0.95	15/2947 (0.5%)	1.45	39/4001 (1.0%)
All	All	1.07	367/45115 (0.8%)	1.49	670/61055 (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 (367) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4912	ARG	CZ-NH2	-13.14	1.16	1.33
1	G	6076	LYS	CE-NZ	-11.79	1.19	1.49
1	E	4670	ASP	CG-OD2	-9.89	1.02	1.25
1	E	4655	GLU	CD-OE1	9.63	1.36	1.25
2	D	3872	GLU	CD-OE1	9.12	1.35	1.25
1	C	2683	GLU	CD-OE1	9.04	1.35	1.25
1	E	4771	GLU	CD-OE2	8.76	1.35	1.25
1	E	4819	GLU	CD-OE1	8.74	1.35	1.25
1	A	512	GLU	CD-OE1	8.38	1.34	1.25
2	D	3726	GLU	CD-OE1	8.38	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	7666	GLU	CD-OE2	8.38	1.34	1.25
1	C	2403	GLU	CD-OE2	8.26	1.34	1.25
2	D	3666	GLU	CD-OE2	8.18	1.34	1.25
1	A	110	GLU	CD-OE1	8.08	1.34	1.25
1	C	2655	GLU	CD-OE2	8.04	1.34	1.25
1	G	6673	GLU	CD-OE1	7.78	1.34	1.25
2	B	1645	GLU	CD-OE1	7.77	1.34	1.25
1	A	771	GLU	CD-OE1	7.75	1.34	1.25
1	G	6474	GLU	CD-OE1	7.73	1.34	1.25
1	A	655	GLU	CD-OE2	7.59	1.33	1.25
1	A	761	GLU	CD-OE1	7.58	1.33	1.25
1	A	80	LYS	CE-NZ	7.58	1.68	1.49
1	E	4215	GLU	CD-OE1	7.47	1.33	1.25
1	A	217	GLU	CD-OE2	7.46	1.33	1.25
1	A	478	GLU	CD-OE1	7.45	1.33	1.25
1	E	4676	GLU	CD-OE2	7.41	1.33	1.25
1	E	4110	GLU	CD-OE1	7.40	1.33	1.25
1	G	6577	GLU	CD-OE1	7.40	1.33	1.25
1	G	7024	GLU	CD-OE1	7.39	1.33	1.25
2	B	1666	GLU	CD-OE2	7.38	1.33	1.25
1	A	549	GLU	CD-OE2	7.36	1.33	1.25
2	B	1818	GLU	CD-OE2	7.36	1.33	1.25
1	E	4703	GLU	CD-OE1	7.35	1.33	1.25
1	C	2109	GLU	CD-OE1	7.33	1.33	1.25
2	H	7726	GLU	CD-OE1	7.27	1.33	1.25
1	A	703	GLU	CD-OE2	7.25	1.33	1.25
1	E	4217	GLU	CD-OE2	7.25	1.33	1.25
1	C	2535	GLU	CD-OE1	7.22	1.33	1.25
1	G	6757	ASP	CG-OD1	7.21	1.42	1.25
1	G	6882	GLU	CD-OE2	7.18	1.33	1.25
1	C	3009[A]	GLU	CD-OE1	7.16	1.33	1.25
1	C	3009[B]	GLU	CD-OE1	7.16	1.33	1.25
1	C	2127	GLU	CD-OE1	7.15	1.33	1.25
1	G	6876	GLU	CD-OE2	7.11	1.33	1.25
1	E	4910	GLU	CD-OE2	7.11	1.33	1.25
1	G	6334	GLU	CD-OE2	7.08	1.33	1.25
1	A	1024	GLU	CD-OE1	7.05	1.33	1.25
1	C	2059	GLU	CD-OE1	7.04	1.33	1.25
1	E	4186	GLU	CD-OE2	7.01	1.33	1.25
1	G	7009	GLU	CD-OE1	7.00	1.33	1.25
1	C	2549	GLU	CD-OE2	6.99	1.33	1.25
1	C	3024	GLU	CD-OE1	6.99	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	6707	GLU	CD-OE2	6.99	1.33	1.25
1	C	2955	GLU	CD-OE1	6.94	1.33	1.25
2	F	5541	GLU	CD-OE1	6.86	1.33	1.25
1	G	6604	GLU	CD-OE1	6.85	1.33	1.25
1	A	403	GLU	CD-OE2	6.84	1.33	1.25
1	C	2676	GLU	CD-OE1	6.84	1.33	1.25
1	E	4260	GLU	CD-OE1	6.83	1.33	1.25
1	G	6731	GLU	CD-OE2	6.82	1.33	1.25
1	E	4683	GLU	CD-OE1	6.80	1.33	1.25
1	A	72	GLU	CD-OE2	6.80	1.33	1.25
1	A	699	GLU	CD-OE1	6.78	1.33	1.25
1	E	4535	GLU	CD-OE1	6.77	1.33	1.25
1	C	2186	GLU	CD-OE2	6.77	1.33	1.25
2	F	5801	GLU	CD-OE1	6.76	1.33	1.25
1	A	1067	GLU	CD-OE1	6.76	1.33	1.25
2	B	1726	GLU	CD-OE1	6.76	1.33	1.25
1	C	2996	GLU	CD-OE2	6.76	1.33	1.25
1	G	6916	GLU	CD-OE2	6.75	1.33	1.25
1	C	2876[A]	GLU	CD-OE1	6.74	1.33	1.25
1	C	2876[B]	GLU	CD-OE1	6.74	1.33	1.25
1	G	6683	GLU	CD-OE1	6.72	1.33	1.25
1	C	2187	GLU	CD-OE2	6.71	1.33	1.25
1	A	604	GLU	CD-OE1	6.70	1.33	1.25
1	E	4153	GLU	CD-OE1	6.69	1.33	1.25
1	C	2882	GLU	CD-OE2	6.69	1.33	1.25
1	E	4707	GLU	CD-OE2	6.68	1.33	1.25
1	E	4996	GLU	CD-OE2	6.67	1.32	1.25
1	A	186	GLU	CD-OE2	6.67	1.32	1.25
1	C	2926	GLU	CD-OE1	6.66	1.32	1.25
1	G	6467	GLU	CD-OE1	6.65	1.32	1.25
2	H	7571	GLU	CD-OE2	6.65	1.32	1.25
1	E	4190	GLU	CD-OE1	6.64	1.32	1.25
2	F	5666	GLU	CD-OE2	6.64	1.32	1.25
1	C	2910	GLU	CD-OE2	6.63	1.32	1.25
1	C	2478	GLU	CD-OE1	6.62	1.32	1.25
1	A	419	GLU	CD-OE1	6.62	1.32	1.25
1	G	6110	GLU	CD-OE1	6.62	1.32	1.25
2	B	1872	GLU	CD-OE2	6.60	1.32	1.25
1	C	2604	GLU	CD-OE1	6.60	1.32	1.25
1	G	6549	GLU	CD-OE2	6.60	1.32	1.25
1	C	2703	GLU	CD-OE1	6.58	1.32	1.25
1	G	6699	GLU	CD-OE1	6.57	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5596	GLU	CD-OE2	6.56	1.32	1.25
2	D	3818	GLU	CD-OE2	6.55	1.32	1.25
1	G	6783	GLU	CD-OE1	6.54	1.32	1.25
1	E	4427	GLU	CD-OE2	6.53	1.32	1.25
2	B	1687	GLU	CD-OE1	6.53	1.32	1.25
1	C	2467	GLU	CD-OE1	6.52	1.32	1.25
1	C	2707	GLU	CD-OE2	6.52	1.32	1.25
1	G	6419	GLU	CD-OE1	6.51	1.32	1.25
1	A	1009[A]	GLU	CD-OE1	6.51	1.32	1.25
1	A	1009[B]	GLU	CD-OE1	6.51	1.32	1.25
1	G	6079	GLU	CD-OE2	6.50	1.32	1.25
1	G	6841	GLU	CD-OE2	6.50	1.32	1.25
1	A	260	GLU	CD-OE2	6.49	1.32	1.25
1	E	5009[A]	GLU	CD-OE1	6.49	1.32	1.25
1	E	5009[B]	GLU	CD-OE1	6.49	1.32	1.25
1	C	2591	GLU	CD-OE1	6.49	1.32	1.25
1	G	6996	GLU	CD-OE2	6.49	1.32	1.25
1	C	2153	GLU	CD-OE2	6.49	1.32	1.25
1	G	6926	GLU	CD-OE1	6.48	1.32	1.25
1	E	4109	GLU	CD-OE1	6.48	1.32	1.25
1	G	6726	GLU	CD-OE1	6.48	1.32	1.25
1	E	4951	GLU	CD-OE1	6.47	1.32	1.25
1	A	393	GLU	CD-OE1	6.45	1.32	1.25
1	E	4208	GLU	CD-OE1	6.45	1.32	1.25
1	E	4591	GLU	CD-OE1	6.45	1.32	1.25
1	E	4059	GLU	CD-OE1	6.44	1.32	1.25
2	D	3855	GLU	CD-OE1	6.42	1.32	1.25
1	E	4067	GLU	CD-OE1	6.42	1.32	1.25
2	F	5872	GLU	CD-OE1	6.42	1.32	1.25
1	A	926	GLU	CD-OE1	6.41	1.32	1.25
1	A	535	GLU	CD-OE1	6.41	1.32	1.25
1	E	4403	GLU	CD-OE2	6.40	1.32	1.25
1	A	910	GLU	CD-OE2	6.40	1.32	1.25
2	F	5726	GLU	CD-OE1	6.39	1.32	1.25
2	H	7541	GLU	CD-OE1	6.38	1.32	1.25
1	G	6153	GLU	CD-OE2	6.37	1.32	1.25
1	A	153	GLU	CD-OE1	6.36	1.32	1.25
1	G	6892	GLU	CD-OE2	6.36	1.32	1.25
1	G	6703	GLU	CD-OE1	6.36	1.32	1.25
1	A	299	GLU	CD-OE2	6.35	1.32	1.25
1	C	2951	GLU	CD-OE1	6.33	1.32	1.25
1	A	707	GLU	CD-OE1	6.32	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	GLU	CD-OE1	6.32	1.32	1.25
1	A	560	GLU	CD-OE1	6.32	1.32	1.25
1	C	2726	GLU	CD-OE1	6.32	1.32	1.25
1	G	6186	GLU	CD-OE2	6.32	1.32	1.25
1	G	6804	GLU	CD-OE2	6.32	1.32	1.25
2	F	5661	GLU	CD-OE2	6.31	1.32	1.25
1	C	2393	GLU	CD-OE1	6.31	1.32	1.25
1	C	2804	GLU	CD-OE1	6.29	1.32	1.25
1	G	6278	GLU	CD-OE2	6.29	1.32	1.25
2	D	3645	GLU	CD-OE1	6.29	1.32	1.25
1	E	4550	GLU	CD-OE2	6.29	1.32	1.25
1	E	5024	GLU	CD-OE1	6.27	1.32	1.25
1	A	683	GLU	CD-OE2	6.26	1.32	1.25
1	C	2699	GLU	CD-OE1	6.26	1.32	1.25
1	E	4876	GLU	CD-OE2	6.26	1.32	1.25
1	E	4836	GLU	CD-OE2	6.26	1.32	1.25
1	C	2761	GLU	CD-OE1	6.25	1.32	1.25
1	C	2203	GLU	CD-OE2	6.24	1.32	1.25
1	A	474	GLU	CD-OE1	6.24	1.32	1.25
1	A	633	GLU	CD-OE1	6.23	1.32	1.25
1	C	2836	GLU	CD-OE1	6.23	1.32	1.25
2	H	7818	GLU	CD-OE2	6.22	1.32	1.25
1	E	4955	GLU	CD-OE2	6.21	1.32	1.25
1	C	3067	GLU	CD-OE1	6.20	1.32	1.25
1	C	2882	GLU	CD-OE1	-6.20	1.18	1.25
2	H	7872	GLU	CD-OE1	6.18	1.32	1.25
1	E	4699	GLU	CD-OE1	6.18	1.32	1.25
1	G	6478	GLU	CD-OE2	6.17	1.32	1.25
1	G	6190	GLU	CD-OE1	6.17	1.32	1.25
1	A	876	GLU	CD-OE2	6.16	1.32	1.25
1	E	4926	GLU	CD-OE1	6.15	1.32	1.25
1	G	6217	GLU	CD-OE2	6.15	1.32	1.25
1	C	2079	GLU	CD-OE1	6.14	1.32	1.25
1	E	4619	GLU	CD-OE1	6.13	1.32	1.25
1	C	2067	GLU	CD-OE1	6.13	1.32	1.25
1	G	6393	GLU	CD-OE1	6.13	1.32	1.25
1	E	4365	GLU	CD-OE1	6.12	1.32	1.25
1	G	6403	GLU	CD-OE2	6.12	1.32	1.25
1	C	2190	GLU	CD-OE1	6.11	1.32	1.25
1	E	4761	GLU	CD-OE1	6.11	1.32	1.25
1	A	951	GLU	CD-OE2	6.11	1.32	1.25
1	E	4970	GLU	CD-OE1	6.11	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4419	GLU	CD-OE1	6.10	1.32	1.25
1	E	4804	GLU	CD-OE2	6.10	1.32	1.25
1	A	79	GLU	CD-OE1	6.08	1.32	1.25
1	A	676	GLU	CD-OE2	6.08	1.32	1.25
1	C	2334	GLU	CD-OE2	6.08	1.32	1.25
2	D	3689	GLU	CD-OE2	6.08	1.32	1.25
1	A	731	GLU	CD-OE1	6.07	1.32	1.25
2	H	7687	GLU	CD-OE2	6.07	1.32	1.25
2	B	1510	GLU	CD-OE1	6.07	1.32	1.25
1	E	4203	GLU	CD-OE1	6.06	1.32	1.25
1	A	334	GLU	CD-OE2	6.05	1.32	1.25
1	C	2731	GLU	CD-OE1	6.04	1.32	1.25
2	B	1541	GLU	CD-OE1	6.03	1.32	1.25
1	C	2819	GLU	CD-OE1	6.02	1.32	1.25
1	G	6970	GLU	CD-OE1	6.02	1.32	1.25
1	E	4673	GLU	CD-OE1	6.02	1.32	1.25
1	G	6219	GLU	CD-OE1	6.02	1.32	1.25
1	C	2278	GLU	CD-OE2	6.00	1.32	1.25
1	A	996	GLU	CD-OE2	6.00	1.32	1.25
1	C	2040	GLU	CD-OE1	6.00	1.32	1.25
2	F	5687	GLU	CD-OE2	5.98	1.32	1.25
1	C	2771	GLU	CD-OE2	5.97	1.32	1.25
1	E	4187	GLU	CD-OE2	5.96	1.32	1.25
2	F	5571	GLU	CD-OE2	5.95	1.32	1.25
1	G	6836	GLU	CD-OE1	5.95	1.32	1.25
2	H	7529	GLU	CD-OE2	5.92	1.32	1.25
1	G	6154	GLU	CD-OE1	5.92	1.32	1.25
1	C	2916	GLU	CD-OE2	5.91	1.32	1.25
1	G	6955	GLU	CD-OE1	5.91	1.32	1.25
1	E	4549	GLU	CD-OE2	5.89	1.32	1.25
1	A	970	GLU	CD-OE1	5.89	1.32	1.25
1	E	4731	GLU	CD-OE1	5.89	1.32	1.25
2	B	1760	GLU	CD-OE2	5.88	1.32	1.25
1	E	4983	GLU	CD-OE2	5.88	1.32	1.25
1	C	2072	GLU	CD-OE2	5.87	1.32	1.25
1	E	4219	GLU	CD-OE1	5.87	1.32	1.25
1	G	6365	GLU	CD-OE1	5.87	1.32	1.25
1	C	2110	GLU	CD-OE1	5.87	1.32	1.25
1	G	6761	GLU	CD-OE1	5.87	1.32	1.25
1	C	2217	GLU	CD-OE2	5.86	1.32	1.25
1	G	7067	GLU	CD-OE1	5.84	1.32	1.25
1	A	983	GLU	CD-OE2	5.84	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	6072	GLU	CD-OE2	5.83	1.32	1.25
1	C	2673	GLU	CD-OE1	5.83	1.32	1.25
1	E	4548	GLU	CD-OE2	-5.82	1.19	1.25
1	A	673	GLU	CD-OE1	5.82	1.32	1.25
1	A	59	GLU	CD-OE1	5.81	1.32	1.25
1	G	6468	GLU	CD-OE1	5.81	1.32	1.25
1	E	4726	GLU	CD-OE1	5.80	1.32	1.25
1	E	4039	GLU	CD-OE1	5.80	1.32	1.25
2	B	1661	GLU	CD-OE2	5.79	1.32	1.25
1	E	4912	ARG	CZ-NH1	5.79	1.40	1.33
1	A	467	GLU	CD-OE1	5.78	1.32	1.25
1	G	6189	GLU	CD-OE2	5.78	1.32	1.25
1	G	6512	GLU	CD-OE1	5.77	1.32	1.25
1	A	154	GLU	CD-OE1	5.76	1.31	1.25
1	A	628	GLU	CD-OE1	5.75	1.31	1.25
2	D	3541	GLU	CD-OE1	5.75	1.31	1.25
1	G	6595	GLU	CD-OE1	5.75	1.31	1.25
2	B	1689	GLU	CD-OE2	5.73	1.31	1.25
2	B	1624	GLU	CD-OE1	5.72	1.31	1.25
1	A	836	GLU	CD-OE2	5.71	1.31	1.25
1	A	190	GLU	CD-OE1	5.70	1.31	1.25
1	G	6127	GLU	CD-OE1	5.70	1.31	1.25
2	H	7689	GLU	CD-OE1	5.70	1.31	1.25
1	G	6983	GLU	CD-OE2	5.69	1.31	1.25
1	E	4780	GLU	CD-OE1	5.67	1.31	1.25
1	E	4510	GLU	CD-OE1	5.66	1.31	1.25
1	E	5060	GLU	CD-OE2	5.66	1.31	1.25
2	D	3687	GLU	CD-OE1	5.65	1.31	1.25
1	A	619	GLU	CD-OE1	5.65	1.31	1.25
2	H	7510	GLU	CD-OE1	5.65	1.31	1.25
1	A	215	GLU	CD-OE1	5.64	1.31	1.25
1	G	6109	GLU	CD-OE2	5.64	1.31	1.25
1	E	4841	GLU	CD-OE2	5.64	1.31	1.25
2	F	5689	GLU	CD-OE2	5.63	1.31	1.25
2	H	7624	GLU	CD-OE1	5.62	1.31	1.25
1	E	4189	GLU	CD-OE2	5.62	1.31	1.25
1	C	2983	GLU	CD-OE2	5.61	1.31	1.25
1	E	4604	GLU	CD-OE1	5.60	1.31	1.25
1	C	2349	GLU	CD-OE2	5.60	1.31	1.25
1	A	819	GLU	CD-OE1	5.59	1.31	1.25
1	A	550	GLU	CD-OE1	5.59	1.31	1.25
1	A	892	GLU	CD-OE2	5.59	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1875	GLU	CD-OE2	5.58	1.31	1.25
1	C	2383	GLU	CD-OE1	-5.58	1.19	1.25
1	G	6208	GLU	CD-OE1	5.56	1.31	1.25
1	C	2550	GLU	CD-OE2	5.56	1.31	1.25
1	G	6059	GLU	CD-OE1	5.55	1.31	1.25
1	C	2619	GLU	CD-OE1	5.55	1.31	1.25
1	C	3060	GLU	CD-OE2	5.55	1.31	1.25
1	G	6215	GLU	CD-OE1	5.55	1.31	1.25
1	A	510	GLU	CD-OE1	5.54	1.31	1.25
1	G	6103	GLU	CD-OE1	5.54	1.31	1.25
1	E	4474	GLU	CD-OE1	5.54	1.31	1.25
2	H	7875	GLU	CD-OE2	5.54	1.31	1.25
2	B	1855	GLU	CD-OE1	5.53	1.31	1.25
2	D	3875	GLU	CD-OE2	5.51	1.31	1.25
2	F	5875	GLU	CD-OE2	5.51	1.31	1.25
1	G	6560	GLU	CD-OE1	5.50	1.31	1.25
1	E	4467	GLU	CD-OE1	5.50	1.31	1.25
1	G	6349	GLU	CD-OE2	5.50	1.31	1.25
1	A	189	GLU	CG-CD	-5.49	1.43	1.51
1	C	2783	GLU	CD-OE1	5.49	1.31	1.25
1	A	783	GLU	CD-OE1	5.49	1.31	1.25
1	G	6510	GLU	CD-OE1	5.48	1.31	1.25
1	G	7060	GLU	CD-OE1	5.47	1.31	1.25
1	G	6383	GLU	CD-OE2	5.47	1.31	1.25
1	E	4079	GLU	CD-OE1	5.47	1.31	1.25
2	D	3624	GLU	CD-OE1	5.46	1.31	1.25
1	E	4771	GLU	CD-OE1	-5.46	1.19	1.25
1	G	6624	GLU	CD-OE1	5.46	1.31	1.25
1	A	1060	GLU	CD-OE2	5.46	1.31	1.25
1	E	4103	GLU	CD-OE1	5.46	1.31	1.25
1	A	187	GLU	CD-OE2	5.44	1.31	1.25
1	A	142	GLU	CD-OE2	5.44	1.31	1.25
1	C	2219	GLU	CD-OE1	5.43	1.31	1.25
2	D	3801	GLU	CD-OE1	5.43	1.31	1.25
1	G	6591	GLU	CD-OE1	5.43	1.31	1.25
1	C	2299	GLU	CD-OE2	5.42	1.31	1.25
1	C	2512	GLU	CD-OE2	5.41	1.31	1.25
1	A	473	GLU	CD-OE1	5.40	1.31	1.25
1	G	6619	GLU	CD-OE1	5.40	1.31	1.25
1	E	4127	GLU	CD-OE1	5.39	1.31	1.25
1	G	6628	GLU	CD-OE1	5.39	1.31	1.25
1	E	4552	GLU	CD-OE2	5.39	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	GLU	CD-OE1	5.38	1.31	1.25
1	G	6655	GLU	CD-OE1	5.38	1.31	1.25
1	G	6819	GLU	CD-OE1	5.37	1.31	1.25
1	A	81	GLU	CD-OE1	5.36	1.31	1.25
1	A	595	GLU	CD-OE1	5.35	1.31	1.25
1	C	2215	GLU	CD-OE1	5.35	1.31	1.25
1	E	4882	GLU	CD-OE2	5.35	1.31	1.25
2	F	5855	GLU	CD-OE1	5.34	1.31	1.25
1	E	4274	GLU	CD-OE1	5.34	1.31	1.25
2	H	7624	GLU	CD-OE2	-5.34	1.19	1.25
2	B	1596	GLU	CD-OE2	5.33	1.31	1.25
1	A	577	GLU	CD-OE1	5.33	1.31	1.25
1	A	349	GLU	CD-OE2	5.32	1.31	1.25
1	C	2560	GLU	CD-OE1	5.31	1.31	1.25
1	C	2970	GLU	CD-OE2	5.31	1.31	1.25
2	B	1529	GLU	CD-OE1	-5.30	1.19	1.25
2	D	3760	GLU	CD-OE2	5.30	1.31	1.25
2	B	1571	GLU	CD-OE2	5.30	1.31	1.25
1	A	916	GLU	CD-OE2	5.29	1.31	1.25
1	G	6059	GLU	CD-OE2	-5.29	1.19	1.25
1	E	4383	GLU	CD-OE2	5.28	1.31	1.25
2	B	1855	GLU	CD-OE2	-5.27	1.19	1.25
1	C	2595	GLU	CD-OE1	5.27	1.31	1.25
1	E	4512	GLU	CD-OE1	5.27	1.31	1.25
1	C	2189	GLU	CD-OE2	5.26	1.31	1.25
1	G	6039	GLU	CD-OE1	5.26	1.31	1.25
1	C	2203	GLU	CD-OE1	-5.25	1.19	1.25
2	H	7760	GLU	CD-OE2	5.25	1.31	1.25
2	F	5760	GLU	CD-OE2	5.25	1.31	1.25
1	A	219	GLU	CD-OE1	5.24	1.31	1.25
2	F	5570	GLU	CD-OE1	5.23	1.31	1.25
2	F	5855	GLU	CD-OE2	-5.22	1.20	1.25
1	G	6633	GLU	CD-OE1	5.21	1.31	1.25
2	B	1801	GLU	CD-OE1	5.21	1.31	1.25
1	A	235	GLU	CD-OE1	5.20	1.31	1.25
1	C	2577	GLU	CD-OE1	5.19	1.31	1.25
2	F	5818	GLU	CD-OE2	5.18	1.31	1.25
1	A	103	GLU	CD-OE1	5.18	1.31	1.25
2	B	1529	GLU	CD-OE2	5.17	1.31	1.25
1	C	2780	GLU	CD-OE1	5.17	1.31	1.25
1	G	6101	GLU	CD-OE1	5.15	1.31	1.25
1	A	365	GLU	CD-OE1	5.14	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLU	CD-OE1	5.14	1.31	1.25
1	G	6676	GLU	CD-OE2	5.14	1.31	1.25
1	C	2154	GLU	CD-OE2	-5.13	1.20	1.25
2	F	5645[A]	GLU	CD-OE1	5.13	1.31	1.25
2	F	5645[B]	GLU	CD-OE1	5.13	1.31	1.25
1	A	841	GLU	CD-OE2	5.11	1.31	1.25
1	A	780	GLU	CD-OE2	-5.11	1.20	1.25
1	A	882	GLU	CD-OE1	-5.10	1.20	1.25
1	G	6349	GLU	CD-OE1	-5.10	1.20	1.25
1	G	6548	GLU	CD-OE1	5.08	1.31	1.25
1	G	6910	GLU	CD-OE2	5.08	1.31	1.25
2	D	3661	GLU	CD-OE2	5.08	1.31	1.25
1	A	67	GLU	CD-OE1	5.08	1.31	1.25
1	G	6067	GLU	CD-OE1	5.07	1.31	1.25
2	H	7596	GLU	CD-OE2	5.06	1.31	1.25
1	G	6552	GLU	CD-OE2	5.05	1.31	1.25
1	C	2468	GLU	CD-OE1	5.04	1.31	1.25
2	D	3510	GLU	CD-OE2	5.04	1.31	1.25
2	D	3529	GLU	CD-OE1	5.04	1.31	1.25
1	A	726	GLU	CD-OE1	5.01	1.31	1.25
1	G	6951	GLU	CD-OE1	5.01	1.31	1.25

All (670) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4652	ARG	NE-CZ-NH2	-17.70	111.45	120.30
1	E	4912	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	C	2043	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	A	671	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	A	671	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	G	6043	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	A	912	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	944	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	C	2043	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	G	6265	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	E	4161	ASP	CB-CG-OD1	-10.98	108.42	118.30
1	E	4082	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	E	4161	ASP	CB-CG-OD2	10.58	127.82	118.30
1	E	4867	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	912	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	G	6460	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	C	3021	ARG	NE-CZ-NH1	10.19	125.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	6124	ASP	CB-CG-OD1	-10.08	109.23	118.30
1	E	4652	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	E	4670	ASP	CB-CG-OD1	-9.87	109.41	118.30
1	C	2736	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	194	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	G	6043	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	E	4912	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	C	2736	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	C	2400	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	G	6757	ASP	CB-CG-OD2	9.53	126.88	118.30
1	E	4043	ARG	NE-CZ-NH2	-9.49	115.56	120.30
2	D	3711	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	E	4753	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	684	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	G	6560	GLU	N-CA-CB	9.36	127.44	110.60
1	C	2343	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	G	6848	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	G	6084	ASP	CB-CG-OD1	-9.29	109.94	118.30
2	H	7688	ASP	CB-CG-OD2	9.28	126.65	118.30
1	C	2273	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	C	2490	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	C	2867	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	G	6757	ASP	CB-CG-OD1	-9.04	110.17	118.30
1	A	670	ASP	CB-CG-OD1	-9.01	110.19	118.30
1	A	400	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	6	ASP	CB-CG-OD1	-8.84	110.34	118.30
1	A	460	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	C	2579	ASP	CB-CG-OD1	-8.82	110.36	118.30
2	B	1711	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	G	6845	ARG	NE-CZ-NH1	8.79	124.69	120.30
2	D	3834	ASP	CB-CG-OD1	-8.75	110.43	118.30
2	F	5639	ASP	CB-CG-OD1	8.64	126.07	118.30
1	G	6944	ARG	NE-CZ-NH2	-8.63	115.98	120.30
2	B	1597	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	E	4169	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	823	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	G	6444	ARG	NE-CZ-NH2	-8.60	116.00	120.30
2	F	5597	ASP	CB-CG-OD2	-8.55	110.61	118.30
1	E	4410	ASP	CB-CG-OD2	-8.55	110.61	118.30
1	A	677	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	C	2441	ASP	CB-CG-OD1	-8.50	110.65	118.30
1	A	1021	ARG	NE-CZ-NH1	8.49	124.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4027	ASP	CB-CG-OD2	8.49	125.94	118.30
1	A	736	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	C	2670	ASP	CB-CG-OD1	-8.46	110.68	118.30
1	E	4579	ASP	CB-CG-OD2	8.46	125.92	118.30
1	C	2530	ASP	CB-CG-OD1	8.44	125.89	118.30
1	A	667	ASP	CB-CG-OD2	8.43	125.89	118.30
1	A	1030	ARG	NE-CZ-NH1	8.43	124.51	120.30
2	D	3593	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	579	ASP	CB-CG-OD1	-8.42	110.72	118.30
1	A	791	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	G	6614	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	E	4169	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	C	2333	ASP	CB-CG-OD1	8.28	125.75	118.30
1	C	2769	ASP	CB-CG-OD1	-8.28	110.85	118.30
2	H	7636	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	A	625	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	609	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	E	4343	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	F	5597	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	459	ASP	CB-CG-OD1	-8.22	110.91	118.30
1	A	517	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	G	6912	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	C	2441	ASP	CB-CG-OD2	8.13	125.61	118.30
1	E	4514	ARG	NE-CZ-NH2	-8.13	116.24	120.30
2	D	3842	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	E	4434	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	A	726	GLU	N-CA-CB	8.09	125.17	110.60
1	E	4400	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	F	5817	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	G	6121	ASP	CB-CG-OD2	8.04	125.54	118.30
1	G	6753	ASP	CB-CG-OD2	-8.03	111.07	118.30
2	H	7623	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	G	6667	ASP	CB-CG-OD1	-8.03	111.07	118.30
2	F	5744	ASP	CB-CG-OD1	-8.02	111.09	118.30
1	E	4128	ASP	CB-CG-OD2	-7.98	111.12	118.30
2	D	3505	ALA	N-CA-CB	7.97	121.26	110.10
1	G	6128	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	611	ASP	CB-CG-OD2	7.94	125.44	118.30
1	A	625	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	G	6246	ASP	CB-CG-OD2	7.90	125.41	118.30
1	C	2912	ARG	NE-CZ-NH2	-7.89	116.36	120.30
2	B	1616	ARG	NE-CZ-NH2	-7.88	116.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	867	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	C	2459	ASP	CB-CG-OD1	-7.86	111.23	118.30
1	G	6434	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	A	736	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	670	ASP	CB-CG-OD2	7.80	125.32	118.30
1	C	2959	ASP	CB-CG-OD2	-7.79	111.28	118.30
1	E	4082	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	E	4128	ASP	CB-CG-OD1	7.76	125.29	118.30
1	A	1004	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	G	6444	ARG	NE-CZ-NH1	7.73	124.17	120.30
2	H	7545	ASP	CB-CG-OD2	7.69	125.22	118.30
1	C	2579	ASP	CB-CG-OD2	7.68	125.21	118.30
2	F	5636	ASP	CB-CG-OD1	-7.67	111.40	118.30
2	F	5868	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	A	611	ASP	CB-CG-OD1	-7.64	111.42	118.30
1	C	2124	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	A	579	ASP	CB-CG-OD2	7.62	125.16	118.30
1	E	4614	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	C	2006	ASP	CB-CG-OD1	-7.58	111.48	118.30
1	G	6121	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	C	2972	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	E	4373	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	G	6625	ASP	CB-CG-OD2	7.52	125.07	118.30
1	G	6161	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	G	6614	ASP	CB-CG-OD2	7.51	125.06	118.30
2	D	3639	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	G	6084	ASP	CB-CG-OD2	7.44	125.00	118.30
1	E	4959	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	539	ASP	CB-CG-OD1	-7.43	111.61	118.30
2	D	3597	ASP	CB-CG-OD2	7.43	124.98	118.30
1	E	4400	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	H	7715	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	E	4038	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	E	4736	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	1030	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	E	4674	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	G	6006[A]	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	G	6006[B]	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	A	194	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	H	7786	MET	CG-SD-CE	-7.37	88.41	100.20
1	C	2294	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	4625	ASP	CB-CG-OD1	-7.36	111.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	6416	ASP	CB-CG-OD1	-7.32	111.71	118.30
2	H	7597	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	E	5003	ASP	CB-CG-OD1	-7.30	111.73	118.30
2	H	7593	ARG	NE-CZ-NH1	7.29	123.95	120.30
2	D	3639	ASP	CB-CG-OD1	7.29	124.86	118.30
2	F	5868	ASP	CB-CG-OD2	7.28	124.86	118.30
1	E	4807	ASP	CB-CG-OD1	-7.28	111.75	118.30
2	B	1842	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	459	ASP	CB-CG-OD2	7.27	124.85	118.30
1	A	124	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	C	3057	ASP	CB-CG-OD2	7.26	124.84	118.30
1	A	131	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	G	6670	ASP	CB-CG-OD1	-7.26	111.77	118.30
2	H	7639	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	2161	ASP	CB-CG-OD1	-7.24	111.78	118.30
1	A	27	ASP	CB-CG-OD2	7.24	124.81	118.30
1	E	4530	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	E	4517	ARG	NE-CZ-NH1	7.23	123.92	120.30
2	B	1636	ASP	CB-CG-OD1	-7.23	111.79	118.30
2	H	7844	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	609	ASP	CB-CG-OD1	7.23	124.80	118.30
1	E	4373	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	E	4353	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	223	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	G	6082	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	C	2499	ASP	CB-CG-OD2	7.16	124.74	118.30
2	F	5511	ASP	CB-CG-OD2	7.16	124.74	118.30
2	D	3762	ASP	CB-CG-OD2	-7.15	111.87	118.30
2	H	7712	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	416	ASP	CB-CG-OD2	7.12	124.71	118.30
2	H	7762	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	2753	ASP	CB-CG-OD2	-7.10	111.91	118.30
2	B	1727	ASP	CB-CG-OD2	-7.09	111.92	118.30
2	D	3834	ASP	CB-CG-OD2	7.06	124.66	118.30
1	E	4579	ASP	CB-CG-OD1	-7.05	111.95	118.30
2	F	5639	ASP	CB-CG-OD2	-7.04	111.96	118.30
2	D	3711	ASP	CB-CG-OD1	7.04	124.64	118.30
2	D	3597	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	E	4223	ASP	CB-CG-OD1	7.03	124.62	118.30
1	G	6499	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	A	204	LEU	CB-CA-C	-7.03	96.85	110.20
1	E	4004	ARG	NE-CZ-NH1	7.00	123.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4425	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	E	4197	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	2333	ASP	CB-CG-OD2	-6.98	112.02	118.30
2	D	3569	ASP	CB-CG-OD2	6.97	124.58	118.30
1	E	4614	ASP	CB-CG-OD2	6.97	124.58	118.30
1	G	6972	ASP	CB-CG-OD2	-6.96	112.04	118.30
2	F	5567	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	G	6128	ASP	CB-CG-OD1	6.95	124.56	118.30
2	B	1820	THR	CA-CB-CG2	-6.94	102.68	112.40
2	H	7749	ASP	CB-CG-OD2	6.93	124.54	118.30
1	E	4246	ASP	CB-CG-OD2	6.93	124.54	118.30
2	D	3612	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	C	2625	ASP	CB-CG-OD2	6.92	124.53	118.30
1	E	4084	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	C	2539	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	223	ASP	CB-CG-OD1	6.91	124.52	118.30
1	E	4959	ASP	CB-CG-OD1	6.91	124.52	118.30
1	G	6972	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	400	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	6	ASP	CB-CG-OD2	6.89	124.50	118.30
1	G	6460	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	E	4490	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	F	5727	ASP	CB-CG-OD2	-6.88	112.11	118.30
2	H	7636	ASP	CB-CG-OD2	6.88	124.49	118.30
1	G	6959	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	361	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	444	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	E	4807	ASP	CB-CG-OD2	6.85	124.47	118.30
1	G	6736	ARG	NE-CZ-NH1	6.85	123.73	120.30
2	D	3786	MET	CG-SD-CE	-6.84	89.25	100.20
2	D	3518	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	2084	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	E	4571	ARG	CB-CA-C	-6.82	96.76	110.40
1	C	2558	ASP	N-CA-CB	-6.81	98.35	110.60
1	E	4353	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	G	6027	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	129	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	G	6944	ARG	NE-CZ-NH1	6.79	123.69	120.30
2	F	5762	ASP	CB-CG-OD1	6.78	124.40	118.30
1	E	4625	ASP	CB-CG-OD2	6.78	124.40	118.30
1	E	4684	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	E	4410	ASP	CB-CG-OD1	6.78	124.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	6579	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	E	4006	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	E	4416	ASP	CB-CG-OD1	-6.75	112.23	118.30
2	F	5711	ASP	CB-CG-OD2	-6.74	112.24	118.30
2	H	7727	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	C	2128	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	161	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	1041	ASP	CB-CG-OD2	6.71	124.34	118.30
2	H	7844	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	G	6501	ARG	NE-CZ-NH2	-6.69	116.95	120.30
2	D	3703	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	G	6667	ASP	CB-CG-OD2	6.68	124.32	118.30
2	D	3612	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	410	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	G	6197	ASP	CB-CG-OD1	6.66	124.30	118.30
1	C	2652	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	G	6609	ASP	CB-CG-OD1	6.63	124.26	118.30
1	G	6912	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	517	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	C	2124	ASP	CB-CG-OD2	6.61	124.25	118.30
1	E	4039	GLU	N-CA-CB	-6.61	98.70	110.60
1	G	6416	ASP	CB-CG-OD2	6.61	124.25	118.30
1	E	4542	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	G	6959	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	E	4459	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	A	530	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	2434	ASP	CB-CG-OD2	-6.57	112.39	118.30
2	H	7842	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	G	6753	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	615	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	845	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	E	4765	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	904	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	G	6027	ASP	CB-CG-OD1	-6.55	112.41	118.30
2	H	7657	ASP	CB-CG-OD2	6.55	124.19	118.30
1	C	2426	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	4906	LEU	N-CA-CB	-6.54	97.31	110.40
1	C	3041	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	G	6353	ASP	CB-CG-OD2	6.53	124.18	118.30
1	C	2733	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	E	4027	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	E	4944	ARG	NE-CZ-NH1	6.52	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	571	ARG	CD-NE-CZ	-6.51	114.48	123.60
1	C	2670	ASP	CB-CG-OD2	6.50	124.15	118.30
1	G	7021	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	G	6372	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	2416	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	E	4471	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	G	6133	ASP	CB-CG-OD1	-6.45	112.49	118.30
1	G	6410	ASP	CB-CG-OD1	6.45	124.11	118.30
1	G	6373	ARG	NE-CZ-NH2	-6.45	117.08	120.30
2	D	3842	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	416	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	C	2959	ASP	CB-CG-OD1	6.44	124.10	118.30
1	C	2769	ASP	CB-CG-OD2	6.44	124.10	118.30
2	F	5817	ASP	CB-CG-OD2	6.43	124.09	118.30
1	G	6006[A]	ASP	CB-CG-OD2	6.43	124.09	118.30
1	G	6006[B]	ASP	CB-CG-OD2	6.43	124.09	118.30
1	G	6258	ASP	CB-CG-OD1	6.42	124.08	118.30
1	G	6571	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	675	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	E	4430	ASP	CB-CG-OD1	-6.41	112.54	118.30
1	G	6487	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	G	6518	ASP	CB-CG-OD1	-6.39	112.54	118.30
1	A	757	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	G	6246	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	C	2906	LEU	N-CA-CB	-6.37	97.65	110.40
1	A	372	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	2518	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	F	5762	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	G	6671	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	H	7597	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	2953	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	A	121	ASP	CB-CG-OD1	-6.34	112.59	118.30
2	B	1636	ASP	CB-CG-OD2	6.34	124.01	118.30
1	C	2062	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	C	2130	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	791	ASP	CB-CG-OD1	6.32	123.99	118.30
2	B	1727	ASP	CB-CG-OD1	6.32	123.98	118.30
1	A	441	ASP	CB-CG-OD2	6.31	123.98	118.30
1	E	4944	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	H	7616	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	E	4530	ASP	CB-CG-OD1	6.30	123.97	118.30
1	E	4207	ASP	CB-CG-OD1	-6.29	112.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2372	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	E	4518	ASP	CB-CG-OD2	6.28	123.95	118.30
2	D	3614	ASP	CB-CG-OD2	6.28	123.95	118.30
1	G	6197	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	G	6425	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	E	4758[A]	ASP	CB-CG-OD2	6.27	123.94	118.30
1	E	4758[B]	ASP	CB-CG-OD2	6.27	123.94	118.30
1	C	2426	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	E	4487	ASP	CB-CG-OD1	6.26	123.94	118.30
1	G	6042	TYR	CB-CG-CD2	-6.26	117.24	121.00
2	D	3727	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	D	3868	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	E	4543	MET	N-CA-CB	-6.25	99.35	110.60
1	A	560	GLU	N-CA-CB	6.25	121.84	110.60
1	C	2667	ASP	CB-CG-OD1	-6.25	112.68	118.30
2	H	7612	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	C	2161	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	867	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	460	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	D	3762	ASP	CB-CG-OD1	6.21	123.89	118.30
1	E	4810	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	B	1712	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	675	ARG	CB-CA-C	-6.19	98.02	110.40
2	D	3620	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	226	ASP	CB-CG-OD1	-6.18	112.73	118.30
2	H	7623	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	D	3620	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	D	3707	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	E	4671	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	D	3636	ASP	CB-CG-OD2	6.14	123.82	118.30
2	B	1749	ASP	CB-CG-OD1	-6.12	112.79	118.30
2	H	7762	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	136	MET	CG-SD-CE	6.11	109.97	100.20
2	H	7862	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	1597	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	1620	ARG	CG-CD-NE	-6.10	99.00	111.80
1	E	4334	GLU	CB-CA-C	-6.09	98.22	110.40
1	G	6161	ASP	CB-CG-OD2	6.09	123.78	118.30
1	G	6675	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	G	6625	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	A	823	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	H	7569	ASP	CB-CG-OD1	-6.08	112.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4133	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	487	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	2972	ASP	CB-CG-OD1	6.08	123.77	118.30
1	G	6223	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	297	VAL	CA-CB-CG1	-6.07	101.79	110.90
1	G	6848	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	2133	ASP	CB-CG-OD1	6.07	123.76	118.30
1	E	4674	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	444	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	E	4273	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	H	7593	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	E	4201	THR	CA-CB-CG2	-6.05	103.93	112.40
2	F	5584	ASP	CB-CG-OD2	-6.05	112.86	118.30
2	B	1834	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	C	3041	ASP	CB-CG-OD2	6.04	123.74	118.30
2	D	3614	ASP	CB-CG-OD1	-6.03	112.87	118.30
2	F	5657	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	124	ASP	CB-CG-OD2	6.03	123.72	118.30
2	F	5749	ASP	CB-CG-OD2	6.03	123.72	118.30
2	F	5727	ASP	CB-CG-OD1	6.02	123.72	118.30
1	G	6791	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	G	6807	ASP	CB-CG-OD1	-6.01	112.89	118.30
2	H	7707	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	2121	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	735	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	128	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	1025	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	4972	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	B	1749	ASP	CB-CG-OD2	5.98	123.69	118.30
1	C	2763	ASP	CB-CG-OD1	-5.98	112.91	118.30
1	G	6129	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	E	4471	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	E	4757	ASP	CB-CG-OD1	-5.97	112.92	118.30
2	F	5749	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	614	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	A	197	ASP	CB-CG-OD1	5.94	123.65	118.30
2	B	1817	ASP	CB-CG-OD2	5.93	123.64	118.30
2	D	3727	ASP	CB-CG-OD1	5.93	123.64	118.30
2	F	5862	ASP	CB-CG-OD1	-5.93	112.97	118.30
1	G	6410	ASP	CB-CG-OD2	-5.93	112.97	118.30
2	D	3836	THR	CA-CB-CG2	-5.92	104.11	112.40
1	A	1003	ASP	CB-CG-OD1	-5.92	112.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	6609	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	D	3567	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	C	2372	ASP	CB-CG-OD1	5.90	123.61	118.30
1	G	7016	THR	CA-CB-CG2	-5.89	104.15	112.40
1	C	2343	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	E	4765	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	C	2791	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	A	430	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	2487	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	C	2530	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	E	4372	ASP	CB-CG-OD1	5.87	123.58	118.30
1	G	6791	ASP	CB-CG-OD1	5.87	123.58	118.30
2	B	1711	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	2518	ASP	CB-CG-OD1	5.86	123.57	118.30
1	E	4558	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	G	6521	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	C	2625	ASP	CB-CG-OD1	-5.83	113.05	118.30
2	B	1715	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	H	7545	ASP	CB-CG-OD1	-5.83	113.06	118.30
1	A	75	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	4043	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	4671	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	4509	ARG	CB-CA-C	-5.82	98.76	110.40
1	G	6490	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	4494	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	4763	ASP	CB-CG-OD1	-5.81	113.07	118.30
2	B	1817	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	C	2131	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	G	6389	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	B	1698	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	2084	ASP	CB-CG-OD2	5.79	123.51	118.30
1	G	6303	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	H	7744	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	953	ASP	CB-CG-OD2	5.78	123.50	118.30
1	E	4694	THR	CA-CB-CG2	-5.78	104.31	112.40
2	F	5620	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	434	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	E	4372	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	758	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	C	2757	ASP	CB-CG-OD2	5.75	123.47	118.30
1	G	6730	ASP	CB-CG-OD2	5.74	123.47	118.30
2	B	1734	ASP	CB-CG-OD2	-5.73	113.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	G	6258	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	A	410	ASP	CB-CG-OD2	5.71	123.44	118.30
2	F	5698	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	4571	ARG	CA-CB-CG	5.70	125.95	113.40
1	A	490[A]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	490[B]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	4434	ASP	CB-CG-OD1	5.70	123.43	118.30
2	B	1698	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	B	1584	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	4153	GLU	CB-CA-C	5.69	121.78	110.40
1	A	128	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	E	4733	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	972	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	E	4279	THR	CA-CB-CG2	-5.67	104.47	112.40
1	G	6426	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	H	7639	ASP	CB-CG-OD1	5.66	123.40	118.30
1	G	6333	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	E	4758[A]	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	E	4758[B]	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	C	2971	LEU	CB-CA-C	-5.65	99.47	110.20
1	C	2459	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	38	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	2735	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	2197	ASP	CB-CG-OD1	5.63	123.36	118.30
2	D	3636	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	A	161	ASP	CB-CG-OD2	5.63	123.36	118.30
1	E	4133	ASP	CB-CG-OD2	5.62	123.36	118.30
1	G	6425	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	F	5688	ASP	CB-CG-OD2	5.61	123.35	118.30
2	H	7612	ASP	CB-CG-OD2	5.61	123.35	118.30
1	G	6730	ASP	CB-CG-OD1	-5.61	113.25	118.30
2	B	1744	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	2611	ASP	CB-CG-OD2	5.61	123.35	118.30
2	H	7820	THR	CA-CB-CG2	-5.61	104.55	112.40
1	C	2972	ASP	N-CA-CB	5.59	120.67	110.60
2	D	3734	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	614	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	2246	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	C	3003	ASP	CB-CG-OD2	5.58	123.32	118.30
2	H	7749	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	E	4791	ASP	CB-CG-OD2	-5.57	113.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1021	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	B	1688	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	333	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	998	ARG	C-N-CD	-5.56	108.38	120.60
1	G	6765	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	E	5021	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	592	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	520	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	A	490[A]	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	490[B]	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	E	4121	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	G	6028	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	C	2450	ASP	CB-CG-OD1	-5.53	113.32	118.30
2	D	3518	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	3025	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	4501	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	728	VAL	CA-CB-CG2	-5.52	102.62	110.90
2	F	5612	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	4025	GLU	CG-CD-OE2	5.51	129.33	118.30
1	G	6344	THR	CA-CB-CG2	-5.50	104.69	112.40
1	G	6579	ASP	CB-CG-OD2	5.50	123.25	118.30
2	F	5636	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	328	VAL	C-N-CA	-5.50	110.76	122.30
1	G	6678	PHE	N-CA-CB	-5.49	100.71	110.60
1	C	2543	MET	CG-SD-CE	5.49	108.99	100.20
1	E	4609	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	G	6183	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	62	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	2848	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	4121	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	482	THR	CA-CB-CG2	-5.47	104.73	112.40
1	A	514	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	G	6611	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	733	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	C	2912	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	4953	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	G	6130	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	F	5744	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	521	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	C	2173	THR	N-CA-CB	5.45	120.65	110.30
1	C	2258	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	226	ASP	CB-CG-OD2	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	7848	PHE	CB-CG-CD1	5.44	124.61	120.80
2	F	5545	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	4592	ASP	CB-CG-OD2	5.43	123.19	118.30
2	H	7727	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	2521	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	G	6594	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	C	3003	ASP	CB-CG-OD1	-5.42	113.43	118.30
1	C	2027	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	121	ASP	CB-CG-OD2	5.41	123.17	118.30
1	E	4124	ASP	CB-CG-OD1	5.40	123.16	118.30
1	E	4667	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	G	6261	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	A	430	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	G	6571	ARG	CD-NE-CZ	-5.39	116.06	123.60
1	A	904	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	2884	ILE	N-CA-CB	5.39	123.19	110.80
1	E	4730	ASP	CB-CG-OD1	-5.38	113.45	118.30
2	H	7862	ASP	CB-CG-OD1	-5.38	113.45	118.30
2	F	5569	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	344	THR	CA-CB-CG2	-5.38	104.87	112.40
1	C	3004[A]	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	3004[B]	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	G	6487	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	2501	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	E	4615	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	E	5003	ASP	CB-CG-OD2	5.35	123.12	118.30
1	C	2733	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	2807	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	G	7057	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	4334	GLU	CA-CB-CG	5.34	125.15	113.40
1	A	592	ASP	CB-CG-OD2	5.33	123.10	118.30
2	F	5648	ARG	CD-NE-CZ	-5.33	116.14	123.60
1	G	6131	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	2233	SER	N-CA-CB	5.32	118.48	110.50
2	F	5688	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	E	4610	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	G	6758	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	3001	ILE	N-CA-CB	-5.31	98.60	110.80
1	C	2400	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	2807	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	4791	ASP	CB-CG-OD1	5.29	123.06	118.30
1	G	6223	ASP	CB-CG-OD1	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5711	ASP	CB-CG-OD1	5.28	123.06	118.30
2	D	3589	ALA	N-CA-C	-5.28	96.74	111.00
1	E	4487	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	G	6426	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	726	GLU	CB-CA-C	5.27	120.94	110.40
2	H	7799	ASP	N-CA-C	-5.27	96.77	111.00
2	B	1518	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	389	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	2258	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	E	4831	ALA	N-CA-CB	5.26	117.47	110.10
1	C	2845	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	H	7877	TYR	CB-CG-CD2	5.26	124.16	121.00
1	C	2684	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	7004	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	3025	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	E	4361	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	G	7031	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	4460	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	4334	GLU	CB-CG-CD	-5.24	100.06	114.20
1	E	4521	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	E	4539	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	G	6592	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	G	6674	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	C	2795	SER	N-CA-CB	-5.23	102.65	110.50
1	C	3057	ASP	N-CA-CB	5.23	120.01	110.60
1	A	278	GLU	CB-CA-C	-5.23	99.94	110.40
1	C	2430	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	D	3844	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	343	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	6765	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	2299	GLU	CG-CD-OE2	-5.21	107.87	118.30
1	E	4402	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	E	4004	ARG	C-N-CA	-5.19	108.72	121.70
1	G	6333	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	528	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	B	1558	PRO	N-CA-CB	5.19	109.52	103.30
1	G	6558	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	G	6945	ALA	CB-CA-C	-5.19	102.32	110.10
1	E	4757	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	1762	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	E	4218	MET	CG-SD-CE	5.17	108.47	100.20
1	G	6528	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	547	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	A	763	ASP	CB-CA-C	-5.16	100.08	110.40
1	E	4197	ASP	CB-CG-OD1	5.16	122.94	118.30
1	G	6758	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	753	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	999	PRO	N-CA-CB	5.14	109.46	103.30
2	D	3567	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	509	ARG	CB-CA-C	-5.13	100.13	110.40
1	E	4904	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	1025	ASP	CB-CG-OD1	-5.13	113.68	118.30
2	F	5557	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	D	3584	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	C	2128	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	G	7041	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	G	7021	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	944	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	2765	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	2057	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	6518	ASP	CB-CG-OD2	5.12	122.91	118.30
2	H	7697	TYR	CB-CG-CD1	-5.11	117.93	121.00
2	F	5584	ASP	CB-CG-OD1	5.11	122.90	118.30
1	E	4459	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	2229	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	667	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	C	2765	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	C	2006	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	306	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	G	6338	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	C	2223	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	D	3688	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	G	6539	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	C	2730	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	C	2539	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	763	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	2338	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	450	ASP	CB-CG-OD1	-5.07	113.73	118.30
1	E	4611	ASP	CB-CG-OD1	-5.07	113.73	118.30
1	E	4810	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	3057	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	680	HIS	CB-CA-C	-5.06	100.28	110.40
2	B	1639	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	C	2953	ASP	CB-CG-OD2	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2121	ASP	CB-CG-OD1	-5.06	113.75	118.30
2	B	1639	ASP	CB-CG-OD1	5.05	122.85	118.30
1	E	4678	PHE	N-CA-CB	-5.05	101.51	110.60
1	A	758	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	973	ALA	N-CA-CB	5.04	117.15	110.10
2	B	1614	ASP	CB-CG-OD1	-5.04	113.77	118.30
2	F	5545	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	G	6378	MET	CG-SD-CE	5.03	108.24	100.20
1	A	354	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	238	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	2793	ALA	N-CA-CB	5.02	117.13	110.10
1	E	4124	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	G	6294	ARG	CD-NE-CZ	-5.02	116.58	123.60
1	G	6769	ASP	CB-CG-OD1	-5.02	113.79	118.30
1	A	372	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	652	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	D	3523	THR	C-N-CA	-5.01	111.77	122.30
1	C	2675	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	1070	ALA	CB-CA-C	5.01	117.61	110.10
2	B	1616	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	E	4376	THR	CA-CB-CG2	-5.00	105.39	112.40
1	C	2667	ASP	CB-CG-OD2	5.00	122.80	118.30
1	E	4145	ARG	NE-CZ-NH1	5.00	122.80	120.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8193	0	8225	260	0
1	C	8198	0	8230	251	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	8169	0	8194	264	0
1	G	8164	0	8193	340	0
2	B	2904	0	2868	99	0
2	D	2902	0	2867	88	0
2	F	2915	0	2876	93	0
2	H	2902	0	2868	135	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	904	0	0	32	0
10	B	256	0	0	2	0
10	C	897	0	0	24	0
10	D	330	0	0	8	1
10	E	900	0	0	28	0
10	F	276	0	0	7	0
10	G	733	0	0	27	0
10	H	232	0	0	6	1
All	All	49310	0	44541	1515	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 (1515) 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:B:1695:VAL:HG23	2:B:1733:PRO:HB3	1.47	0.95
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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:F:5822:PRO:HB2	2:F:5824:ASN:ND2	1.96	0.81
1:C:2059:GLU:HG2	1:C:2060:MET:HE3	1.62	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:A:563:MET:HE3	1:A:635:PRO:HG3	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:3728:VAL:HA	2:D:3731:MET:HE3	1.65	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
2:B:1728:VAL:HA	2:B:1731:MET:HE2	1.67	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: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: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
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: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:6936:ASN:HB2	10:G:22:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2675:ARG:H	1:C:2675:ARG:CD	2.02	0.73
2:D:3728:VAL:HA	2:D:3731:MET:HE2	1.69	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
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: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:6698:ILE:H	1:G:6698:ILE:CD1	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:5824:ASN:H	2:F:5824:ASN:ND2	1.87	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:4001:MET:N	1:E:4224:LYS:HZ1	1.91	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: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
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
2:D:3726:GLU:O	2:D:3730:LYS:HG3	1.92	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:3728:VAL:HG22	2:D:3731:MET:HE3	1.78	0.63
2:D:3728:VAL:O	2:D:3731:MET:HG3	1.99	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:E:5001:ILE:HG22	1:E:5002:GLN:N	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:6563:MET:HE3	1:G:6635:PRO:HG3	1.83	0.60
1:C:2006:ASP:OD1	1:C:2006:ASP:N	2.32	0.60
1:C:2105:GLN:HA	1:C:2105:GLN:NE2	2.16	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
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: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:A:99:ALA:HB1	1:A:115:MET:HE2	1.82	0.60
1:E:4966:LYS:HB3	10:E:6859:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1824:ASN:H	2:B:1824:ASN:ND2	1.99	0.59
2:B:1864:ALA:HB3	2:B:1865:PRO:HD3	1.85	0.59
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
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: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:4417:ASP:OD2	1:E:4423:LYS:NZ	2.31	0.59
1:E:4511:ALA:O	1:E:4515:LYS:HG3	2.03	0.59
1:G:6809:MET:O	1:G:6813:VAL:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2426:ARG:HD3	1:C:2426:ARG:C	2.24	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
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
1:E:4998:ARG:HA	1:E:4999:PRO:C	2.24	0.58
2:B:1644:LEU:HD21	2:B:1648:ARG:CZ	2.33	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
1:C:2563:MET:HE3	1:C:2635:PRO:HG3	1.85	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:C:3000:HIS:CD2	1:C:3003:ASP:H	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:7824:ASN:ND2	2:H:7824:ASN:N	2.45	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: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
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
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:G:6101:GLU:HA	1:G:6101:GLU:OE1	2.06	0.56
1:A:412:LYS:HD3	10:A:2715:HOH:O	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:HB1	1:A:115:MET:CE	2.35	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:C:2442:ALA:HB1	1:C:2447:LEU:HD12	1.88	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
1:E:4959:ASP:O	1:E:4963:LYS:HG3	2.06	0.56
1:G:6164:PHE:HA	1:G:6165:PRO:C	2.23	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
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
2:F:5571:GLU:O	2:F:5703:ARG:HG3	2.07	0.55
1:A:947[B]:LEU:HD12	1:A:1014:ILE:HG22	1.87	0.55
1:G:6001:MET:N	1:G:6224:LYS:HZ1	2.04	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:4704:LYS:NZ	1:E:4707:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:4711:PRO:HG2	1:E:4755:PHE:HD2	1.73	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:G:6667:ASP:CG	1:G:6677:ARG:HH22	2.11	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:6412:LYS:HG2	1:G:6438:TYR:CZ	2.42	0.54
1:G:6426:ARG:HD3	1:G:6426:ARG:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASN:HB3	1:A:753:ASP:OD2	2.09	0.53
1:C:2951:GLU:HA	1:C:2954:LYS:HD2	1.91	0.53
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
1:A:426:ARG:HD3	1:A:426:ARG:C	2.30	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:C:2059:GLU:CG	1:C:2060:MET:HE3	2.36	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: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: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
2:B:1728:VAL:HA	2:B:1731:MET:HE1	1.88	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:4889:SER:HB3	1:E:4918:MET:CE	2.40	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:7017:THR:HG21	1:G:7023:ILE:CA	2.39	0.52
1:C:2703:GLU:O	1:C:2706:LYS:HB2	2.10	0.52
2:D:3786:MET:HE2	2:D:3812:HIS:ND1	2.25	0.52
1:G:6728:VAL:HG11	1:G:6734:LEU:N	2.25	0.52
1:G:7027:ARG:O	1:G:7031:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:4738:PHE:C	1:E:4741:ALA:HB3	2.30	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: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:A:375:THR:OG1	1:A:376:THR:N	2.42	0.51
1:C:2003:LYS:HB2	1:C:2042:TYR:OH	2.10	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
1:G:6022:GLN:HG3	1:G:6174:MET:CE	2.41	0.51
1:G:6481:ILE:HD13	1:G:6508:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:NZ	1:A:611:ASP:OD2	2.39	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
2:B:1786:MET:HE3	2:B:1789:GLY:HA2	1.92	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: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:166:CYS:C	1:A:167:ILE:HD12	2.31	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: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:C:2796:LEU:C	1:C:2796:LEU:HD23	2.32	0.50
1:E:4944:ARG:HD3	1:E:4972:ASP:CG	2.32	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:339:ILE:C	1:A:341:GLY:H	2.13	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
1:G:6710:TYR:HA	1:G:6711:PRO:C	2.30	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: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
1:C:2930:LYS:NZ	1:C:3058:ALA:O	2.43	0.50
2:D:3796:PRO:HB2	2:D:3832:LEU:HB2	1.92	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
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:E:4726:GLU:HG2	1:E:4727:ILE:N	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:548:GLU:HG2	2:B:1614:ASP:HB2	1.93	0.49
1:A:685:LEU:O	1:A:686:LYS:HB2	2.12	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:E:4889:SER:HB3	1:E:4918:MET:HE3	1.95	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
1:G:6223:ASP:CG	1:G:6227:ASN:HB2	2.33	0.49
1:G:6240:MET:HE3	7:G:7900:ADP:C4	2.47	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:A:734:LEU:HD12	1:A:734:LEU:C	2.31	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
2:H:7805:VAL:HG12	2:H:7806:MET:N	2.26	0.49
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.13	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:4563:MET:HE3	1:E:4635:PRO:HG3	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1844:ASP:OD1	2:B:1844:ASP:N	2.42	0.49
1:C:2197:ASP:OD2	1:C:3037:LYS:NZ	2.31	0.49
1:C:2975:HIS:CE1	1:E:4975:HIS:HD1	2.24	0.49
2:H:7823:ALA:C	2:H:7825:LEU:H	2.15	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
1:C:2004:ARG:CD	1:C:2007:ILE:HD12	2.37	0.48
1:C:2167:ILE:N	1:C:2167:ILE:HD12	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: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:A:692:ASN:HB3	1:A:753:ASP:CG	2.33	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
2:H:7653:LEU:HA	2:H:7656:MET:HE3	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:2166:CYS:C	1:C:2167:ILE:HD12	2.34	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:6022:GLN:HG3	1:G:6174:MET:HE1	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:7657:ASP:CG	2:H:7660:LYS:HG2	2.34	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
2:D:3824:ASN:H	2:D:3824:ASN:ND2	2.04	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
1:A:946:LEU:C	1:A:947[B]:LEU:HD13	2.34	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:4164:PHE:HA	1:E:4165:PRO:C	2.35	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
1:G:6954:LYS:HE2	1:G:6976:GLY:C	2.34	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
2:H:7786:MET:CE	2:H:7812:HIS:ND1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:224:LYS:HZ1	2.12	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
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: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: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: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:2009:SER:C	1:C:2010:ILE:HG13	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:3786:MET:CE	2:D:3812:HIS:ND1	2.78	0.46
2:F:5708:MET:SD	2:F:5855:GLU:HA	2.55	0.46
1:C:2802:SER:OG	1:C:2805:ILE:HB	2.16	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: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: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:G:6883:VAL:C	1:G:6884:ILE:HG12	2.37	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:A:806:GLN:HA	1:A:809:MET:HE2	1.98	0.45
1:C:2563:MET:HE2	1:C:2563:MET:HB2	1.84	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
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: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:C:2339:ILE:C	1:C:2341:GLY:H	2.19	0.45
2:D:3786:MET:CE	2:D:3812:HIS:CE1	3.00	0.45
1:G:6654:LEU:HD22	1:G:6659:VAL:HG21	1.98	0.45
1:G:6820:LEU:C	1:G:6821:GLN:HG2	2.36	0.45
1:G:7000:HIS:NE2	1:G:7002:GLN:HB3	2.31	0.45
2:H:7800:VAL:HG22	2:H:7828:THR:C	2.35	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: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: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
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:E:4103:GLU:CG	1:E:4104:ARG:N	2.80	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:B:1786:MET:CE	2:B:1812:HIS:ND1	2.80	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: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
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
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
1:A:508:VAL:HB	1:A:512:GLU:CD	2.38	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
2:B:1695:VAL:CG2	2:B:1733:PRO:HB3	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1675:TRP:CD1	2:B:1680:GLY:HA2	2.53	0.44
2:B:1734:ASP:CG	2:B:1878:ARG:HH11	2.21	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
2:B:1786:MET:HE1	2:B:1812:HIS:O	2.18	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: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
1:G:6152:MET:HE1	1:G:6192:CYS:HB2	2.00	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:E:4335:LEU:O	1:E:4336:MET:HE1	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5670:TRP:HB3	2:F:5716:LEU:HB2	1.99	0.43
1:G:7001:ILE:HG21	1:G:7029:ILE:CD1	2.46	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
2:H:7786:MET:CE	2:H:7812:HIS:CE1	3.02	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
1:G:6563:MET:HE1	1:G:6635:PRO:HG3	2.01	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: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:2710:TYR:HA	1:C:2711:PRO:C	2.39	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
1:A:27:ASP:OD1	1:A:53:THR:HB	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4685:LEU:HD11	1:E:4819:GLU:HG2	2.01	0.43
2:F:5786[A]:MET:HE1	2:F:5812:HIS:CE1	2.53	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
2:F:5786[A]:MET:HE1	2:F:5812:HIS:ND1	2.34	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
1:G:7017:THR:CG2	1:G:7018:SER:N	2.82	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
2:B:1728:VAL:CA	2:B:1731:MET:HE2	2.45	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
1:E:5006:LYS:O	1:E:5006:LYS:HG3	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ARG:O	1:A:1027:ARG:HG2	2.17	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
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:C:2998:ARG:HA	1:C:2999:PRO:C	2.39	0.42
2:D:3824:ASN:N	2:D:3824:ASN:ND2	2.66	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:7786:MET:HE1	2:H:7812:HIS:CE1	2.55	0.42
1:A:579:ASP:OD1	1:A:607:SER:OG	2.30	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: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
2:H:7548:TYR:O	2:H:7551:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:2563:MET:HE3	1:C:2563:MET:HB3	1.80	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:4086:VAL:HG13	1:E:4086:VAL:O	2.19	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: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:4839:LEU:HA	1:E:4839:LEU:HD12	1.58	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2164:PHE:HA	1:C:2165:PRO:C	2.40	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:4001:MET:N	1:E:4224:LYS:NZ	2.65	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
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:E:5061:LYS:HB2	10:E:6869:HOH:O	2.20	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:6930:LYS:NZ	1:G:7058:ALA:O	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:1759:LEU:HD23	2:B:1759:LEU:HA	1.89	0.41
1:C:2152:MET:HE3	1:C:2152:MET:HB2	1.90	0.41
1:C:2762:VAL:CG2	1:C:2801:LEU:HD11	2.50	0.41
1:C:3036:TYR:C	1:C:3037:LYS:HG2	2.40	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: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
2:H:7786:MET:HE1	2:H:7812:HIS:ND1	2.35	0.41
1:A:712:LEU:O	1:A:728:VAL:N	2.53	0.41
1:A:772[B]:MET:HE3	10:A:2818:HOH:O	2.20	0.41
2:B:1651:PRO:HG2	2:B:1656:MET:HE2	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:PRO:C	1:A:712:LEU:HD12	2.42	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:5729:LEU:C	2:F:5731:MET:H	2.22	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
1:G:6699:GLU:C	1:G:6702:VAL:HG23	2.42	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: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:6060:MET:HE1	10:G:638:HOH:O	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1059/1073 (99%)	1010 (95%)	46 (4%)	3 (0%)	41 27
1	C	1059/1073 (99%)	1007 (95%)	49 (5%)	3 (0%)	41 27
1	E	1054/1073 (98%)	1000 (95%)	48 (5%)	6 (1%)	25 12
1	G	1053/1073 (98%)	997 (95%)	50 (5%)	6 (1%)	25 12
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
2	H	376/379 (99%)	360 (96%)	14 (4%)	2 (0%)	29 15
All	All	5733/5808 (99%)	5469 (95%)	244 (4%)	20 (0%)	34 27

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 (i)

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%)	814 (93%)	58 (7%)	16 5
1	C	872/877 (99%)	795 (91%)	77 (9%)	10 3
1	E	867/877 (99%)	800 (92%)	67 (8%)	13 4
1	G	866/877 (99%)	786 (91%)	80 (9%)	9 2
2	B	308/307 (100%)	279 (91%)	29 (9%)	8 2
2	D	307/307 (100%)	281 (92%)	26 (8%)	10 3
2	F	310/307 (101%)	284 (92%)	26 (8%)	11 3
2	H	307/307 (100%)	279 (91%)	28 (9%)	9 2
All	All	4709/4736 (99%)	4318 (92%)	391 (8%)	11 3

All (391) 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	46	ASN
1	A	105	GLN
1	A	110	GLU
1	A	174	MET
1	A	236	ASN
1	A	275	ILE
1	A	321	LYS
1	A	358	LYS
1	A	426	ARG
1	A	482	THR
1	A	509	ARG
1	A	542	TYR
1	A	548	GLU
1	A	554[A]	ASN
1	A	554[B]	ASN
1	A	558	ASP
1	A	559	ARG
1	A	560	GLU
1	A	571	ARG
1	A	591	GLU
1	A	665	SER
1	A	671	ARG
1	A	675	ARG
1	A	676	GLU
1	A	680	HIS
1	A	684	ARG
1	A	688	LYS
1	A	696	THR
1	A	706	LYS
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	736	ARG
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	855	LYS
1	A	881	LYS

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Mol	Chain	Res	Type
1	A	891	LYS
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	972	ASP
1	A	992	ASN
1	A	1006	LYS
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	1631	CYS
2	B	1654	ASN
2	B	1666	GLU
2	B	1686	LYS
2	B	1692	PHE
2	B	1715	ARG
2	B	1718	ILE
2	B	1722	GLN
2	B	1757	LYS
2	B	1761	THR
2	B	1763	ILE
2	B	1806	MET
2	B	1821	LEU
2	B	1824	ASN
2	B	1826	ARG
2	B	1832	LEU
2	B	1833	PHE

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Mol	Chain	Res	Type
2	B	1857	SER
2	B	1866	LEU
2	B	1879	LYS
1	C	2001	MET
1	C	2004	ARG
1	C	2005	THR
1	C	2008	LYS
1	C	2024	CYS
1	C	2038	ARG
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	2236	ASN
1	C	2275	ILE
1	C	2306	ARG
1	C	2313	LYS
1	C	2321	LYS
1	C	2326	LEU
1	C	2358	LYS
1	C	2363	ASN
1	C	2412	LYS
1	C	2414	SER
1	C	2416	ASP
1	C	2426	ARG
1	C	2485	ASN
1	C	2490	ARG
1	C	2509	ARG
1	C	2542	TYR
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	2652	ARG
1	C	2670	ASP
1	C	2675	ARG

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Mol	Chain	Res	Type
1	C	2676	GLU
1	C	2688	LYS
1	C	2689	GLN
1	C	2692	ASN
1	C	2696	THR
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
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	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	3052	MET
1	C	3061	LYS
1	C	3073	LYS
2	D	3502	ILE
2	D	3506	LEU
2	D	3518	ARG
2	D	3550	ARG

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Mol	Chain	Res	Type
2	D	3587	LEU
2	D	3604	ARG
2	D	3613	ILE
2	D	3648	ARG
2	D	3653	LEU
2	D	3654	ASN
2	D	3666	GLU
2	D	3674	SER
2	D	3683	GLN
2	D	3686	LYS
2	D	3687	GLU
2	D	3688	ASP
2	D	3722	GLN
2	D	3757	LYS
2	D	3761	THR
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	4004	ARG
1	E	4005	THR
1	E	4008	LYS
1	E	4076	LYS
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	4236	ASN
1	E	4275	ILE
1	E	4278	GLU
1	E	4307	SER
1	E	4321	LYS
1	E	4326	LEU
1	E	4363	ASN

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Mol	Chain	Res	Type
1	E	4416	ASP
1	E	4428	LEU
1	E	4429	LYS
1	E	4478	GLU
1	E	4509	ARG
1	E	4542	TYR
1	E	4548	GLU
1	E	4556	SER
1	E	4558	ASP
1	E	4562	ILE
1	E	4571	ARG
1	E	4591	GLU
1	E	4634	LYS
1	E	4645	GLN
1	E	4671	ARG
1	E	4675	ARG
1	E	4676	GLU
1	E	4677	ARG
1	E	4680	HIS
1	E	4688	LYS
1	E	4696	THR
1	E	4704	LYS
1	E	4712	LEU
1	E	4714	VAL
1	E	4733	ASP
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	4912	ARG
1	E	4944	ARG
1	E	4950	ARG
1	E	4955	GLU
1	E	4980	VAL
1	E	5006	LYS
1	E	5018	SER

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Mol	Chain	Res	Type
1	E	5020	ARG
1	E	5021	ARG
1	E	5027	ARG
1	E	5031	ARG
1	E	5073	LYS
2	F	5510	GLU
2	F	5550	ARG
2	F	5587	LEU
2	F	5620	ARG
2	F	5625	LYS
2	F	5637	ASN
2	F	5653	LEU
2	F	5654	ASN
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	5715	ARG
2	F	5724	SER
2	F	5730	LYS
2	F	5756	GLN
2	F	5757	LYS
2	F	5801	GLU
2	F	5824	ASN
2	F	5830	LYS
2	F	5831	SER
2	F	5832	LEU
2	F	5840	ILE
2	F	5876	GLN
1	G	6001	MET
1	G	6003	LYS
1	G	6004	ARG
1	G	6008	LYS
1	G	6046	ASN
1	G	6079	GLU
1	G	6088	PRO
1	G	6101	GLU
1	G	6103	GLU
1	G	6133	ASP
1	G	6145	ARG

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Mol	Chain	Res	Type
1	G	6174	MET
1	G	6185	ARG
1	G	6202	LYS
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	6325	LYS
1	G	6416	ASP
1	G	6426	ARG
1	G	6428	LEU
1	G	6429	LYS
1	G	6481	ILE
1	G	6490	ARG
1	G	6509	ARG
1	G	6518	ASP
1	G	6519	GLN
1	G	6542	TYR
1	G	6548	GLU
1	G	6557	THR
1	G	6561	LYS
1	G	6571	ARG
1	G	6591	GLU
1	G	6604	GLU
1	G	6634	LYS
1	G	6645	GLN
1	G	6652	ARG
1	G	6671	ARG
1	G	6675	ARG
1	G	6677	ARG
1	G	6680	HIS
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	6733	ASP

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Mol	Chain	Res	Type
1	G	6735	ARG
1	G	6752	LEU
1	G	6784	GLN
1	G	6789	SER
1	G	6804	GLU
1	G	6811	GLN
1	G	6849	THR
1	G	6855	LYS
1	G	6881	LYS
1	G	6884	ILE
1	G	6912	ARG
1	G	6939	MET
1	G	6950	ARG
1	G	6992	ASN
1	G	6995	HIS
1	G	7001	ILE
1	G	7004	ARG
1	G	7018	SER
1	G	7020	ARG
1	G	7021	ARG
1	G	7027	ARG
1	G	7028	VAL
1	G	7030	ARG
1	G	7031	ARG
1	G	7035	GLN
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	7587	LEU
2	H	7616	ARG
2	H	7620	ARG
2	H	7625	LYS
2	H	7654	ASN
2	H	7656	MET
2	H	7666	GLU
2	H	7674	SER
2	H	7687	GLU
2	H	7689	GLU
2	H	7715	ARG

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Mol	Chain	Res	Type
2	H	7718	ILE
2	H	7739	SER
2	H	7757	LYS
2	H	7772	HIS
2	H	7779	SER
2	H	7824	ASN
2	H	7831	SER
2	H	7832	LEU
2	H	7833	PHE
2	H	7844	ASP
2	H	7876	GLN
2	H	7879	LYS
2	H	7880	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
1	A	519	GLN
1	A	679	GLN
1	A	784	GLN
1	A	803	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	1071	GLN
2	B	1654	ASN
2	B	1722	GLN
2	B	1732	ASN
2	B	1824	ASN
2	B	1851	GLN
1	C	2105	GLN
1	C	2266	ASN

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Mol	Chain	Res	Type
1	C	2645	GLN
1	C	2689	GLN
1	C	2692	ASN
1	C	2784	GLN
1	C	2814	GLN
1	C	2835	ASN
1	C	2932	GLN
1	C	2942	HIS
1	C	2987	ASN
1	C	2992	ASN
1	C	2995	HIS
1	C	3000	HIS
1	C	3035	GLN
1	C	3071	GLN
2	D	3514	GLN
2	D	3551	GLN
2	D	3654	ASN
2	D	3722	GLN
2	D	3824	ASN
2	D	3851	GLN
1	E	4105	GLN
1	E	4150	HIS
1	E	4266	ASN
1	E	4457	ASN
1	E	4645	GLN
1	E	4689	GLN
1	E	4784	GLN
1	E	4803	GLN
1	E	4812	GLN
1	E	4814	GLN
1	E	4936	ASN
1	E	4992	ASN
1	E	5000	HIS
1	E	5035	GLN
1	E	5055	ASN
1	E	5071	GLN
2	F	5551	GLN
2	F	5637	ASN
2	F	5654	ASN
2	F	5756	GLN
2	F	5824	ASN
2	F	5851	GLN

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Mol	Chain	Res	Type
1	G	6105	GLN
1	G	6457	ASN
1	G	6689	GLN
1	G	6784	GLN
1	G	6803	GLN
1	G	6987	ASN
1	G	6992	ASN
1	G	7000	HIS
1	G	7007	ASN
1	G	7035	GLN
1	G	7071	GLN
2	H	7551	GLN
2	H	7578	GLN
2	H	7654	ASN
2	H	7722	GLN
2	H	7732	ASN
2	H	7824	ASN
2	H	7851	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CYG	H	7769	2	12,14,15	3.44	4 (33%)	11,17,19	2.01	4 (36%)
2	CYG	F	5769	2	12,14,15	3.17	3 (25%)	11,17,19	1.93	3 (27%)
2	CYG	B	1769	2	12,14,15	3.43	2 (16%)	11,17,19	2.64	5 (45%)
2	CYG	D	3769	2	12,14,15	3.17	2 (16%)	11,17,19	2.30	5 (45%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1769	CYG	OE2-CD1	10.57	1.38	1.21
2	H	7769	CYG	OE2-CD1	10.13	1.37	1.21
2	D	3769	CYG	OE2-CD1	9.94	1.37	1.21
2	F	5769	CYG	OE2-CD1	9.29	1.36	1.21
2	H	7769	CYG	O1-C1	4.62	1.36	1.22
2	F	5769	CYG	O1-C1	4.28	1.35	1.22
2	B	1769	CYG	O1-C1	4.18	1.34	1.22
2	D	3769	CYG	O1-C1	4.01	1.34	1.22
2	F	5769	CYG	CD1-SG	-3.11	1.68	1.76
2	H	7769	CYG	CD1-SG	-2.83	1.69	1.76
2	H	7769	CYG	O2-C1	2.50	1.38	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1769	CYG	OE2-CD1-CG1	-6.15	116.73	123.99
2	D	3769	CYG	OE2-CD1-CG1	-5.26	117.78	123.99
2	H	7769	CYG	CB-SG-CD1	-4.29	94.85	100.84
2	F	5769	CYG	CG1-CD1-SG	4.21	118.35	113.46
2	B	1769	CYG	CB-SG-CD1	3.54	105.78	100.84
2	D	3769	CYG	CG1-CD1-SG	3.13	117.11	113.46
2	F	5769	CYG	OE2-CD1-SG	-3.12	118.56	122.61
2	B	1769	CYG	CG1-CD1-SG	2.89	116.82	113.46
2	B	1769	CYG	OE2-CD1-SG	2.85	126.32	122.61
2	H	7769	CYG	CG1-CD1-SG	2.69	116.59	113.46
2	H	7769	CYG	O2-C1-CA1	2.36	121.41	113.38
2	F	5769	CYG	O2-C1-CA1	2.25	121.06	113.38
2	D	3769	CYG	CB-SG-CD1	2.25	103.99	100.84
2	B	1769	CYG	O2-C1-CA1	2.14	120.68	113.38
2	H	7769	CYG	OE2-CD1-CG1	-2.10	121.51	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3769	CYG	CG1-CB1-CA1	-2.08	108.98	113.84
2	D	3769	CYG	O2-C1-CA1	2.07	120.44	113.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1769	CYG	OE2-CD1-SG-CB
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	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	H	7769	CYG	2	0
2	F	5769	CYG	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	3980	-	4,4,4	1.40	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	C	3982	-	4,4,4	3.05	3 (75%)	6,6,6	1.27	0
7	ADP	G	7900	4	24,29,29	1.30	4 (16%)	29,45,45	1.69	3 (10%)
8	ORN	C	3920	-	7,8,8	1.09	1 (14%)	8,9,9	1.23	1 (12%)
7	ADP	C	3900	4	24,29,29	1.16	3 (12%)	29,45,45	1.29	3 (10%)
7	ADP	C	3910	5,4	24,29,29	1.29	2 (8%)	29,45,45	1.49	4 (13%)
3	PO4	E	5906	5,4	4,4,4	1.93	1 (25%)	6,6,6	0.85	0
3	PO4	G	7980	-	4,4,4	3.15	2 (50%)	6,6,6	0.96	0
3	PO4	A	1982	-	4,4,4	2.91	3 (75%)	6,6,6	0.73	0
3	PO4	E	5981	-	4,4,4	1.36	0	6,6,6	0.83	0
8	ORN	G	7920	-	7,8,8	1.22	1 (14%)	8,9,9	1.46	1 (12%)
9	NET	E	5950	-	8,8,8	0.79	0	10,10,10	0.53	0
3	PO4	G	7906	5,4	4,4,4	1.69	1 (25%)	6,6,6	0.68	0
8	ORN	A	1920	-	7,8,8	0.95	0	8,9,9	1.61	2 (25%)
3	PO4	E	5980	-	4,4,4	3.34	3 (75%)	6,6,6	1.12	0
3	PO4	C	3981	-	4,4,4	3.84	4 (100%)	6,6,6	1.04	1 (16%)
7	ADP	G	7910	5,4	24,29,29	1.13	2 (8%)	29,45,45	1.32	4 (13%)
8	ORN	E	5920	-	7,8,8	1.14	1 (14%)	8,9,9	0.93	0
7	ADP	E	5910	5,4	24,29,29	1.26	3 (12%)	29,45,45	1.17	4 (13%)
3	PO4	A	1906	5,4	4,4,4	1.84	2 (50%)	6,6,6	1.13	0
7	ADP	E	5900	4	24,29,29	1.46	4 (16%)	29,45,45	1.34	4 (13%)
3	PO4	A	1980	-	4,4,4	2.04	1 (25%)	6,6,6	1.06	0
3	PO4	A	1981	-	4,4,4	2.34	2 (50%)	6,6,6	1.52	1 (16%)
3	PO4	G	7981	-	4,4,4	2.68	1 (25%)	6,6,6	1.12	1 (16%)
3	PO4	G	7982	-	4,4,4	3.36	3 (75%)	6,6,6	1.37	0
3	PO4	C	3906	5,4	4,4,4	1.90	3 (75%)	6,6,6	1.28	1 (16%)
7	ADP	A	1900	4	24,29,29	1.32	4 (16%)	29,45,45	1.81	5 (17%)
9	NET	A	1950	-	8,8,8	0.81	0	10,10,10	0.50	0
9	NET	C	3950	-	8,8,8	0.69	0	10,10,10	0.64	0
9	NET	G	7950	-	8,8,8	0.67	0	10,10,10	0.51	0
7	ADP	A	1910	5,4	24,29,29	1.13	2 (8%)	29,45,45	1.45	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	E	5900	4	-	2/12/32/32	0/3/3/3
8	ORN	C	3920	-	-	7/8/8/8	-
7	ADP	G	7900	4	-	0/12/32/32	0/3/3/3
8	ORN	G	7920	-	-	6/8/8/8	-
9	NET	E	5950	-	-	9/12/12/12	-
7	ADP	G	7910	5,4	-	0/12/32/32	0/3/3/3
7	ADP	C	3900	4	-	1/12/32/32	0/3/3/3
7	ADP	C	3910	5,4	-	2/12/32/32	0/3/3/3
8	ORN	A	1920	-	-	7/8/8/8	-
9	NET	A	1950	-	-	3/12/12/12	-
9	NET	C	3950	-	-	0/12/12/12	-
9	NET	G	7950	-	-	2/12/12/12	-
7	ADP	A	1910	5,4	-	2/12/32/32	0/3/3/3
8	ORN	E	5920	-	-	5/8/8/8	-
7	ADP	E	5910	5,4	-	0/12/32/32	0/3/3/3
7	ADP	A	1900	4	-	1/12/32/32	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7982	PO4	P-O1	5.55	1.63	1.50
3	C	3981	PO4	P-O1	5.48	1.63	1.50
3	E	5980	PO4	P-O1	5.03	1.62	1.50
3	G	7981	PO4	P-O1	4.94	1.62	1.50
7	E	5900	ADP	O4'-C1'	-4.86	1.34	1.41
3	G	7980	PO4	P-O1	4.37	1.61	1.50
3	C	3982	PO4	P-O1	4.14	1.60	1.50
3	A	1981	PO4	P-O1	3.92	1.60	1.50
3	G	7980	PO4	P-O4	3.91	1.66	1.54
3	A	1982	PO4	P-O1	3.75	1.59	1.50
7	C	3910	ADP	O3'-C3'	3.70	1.51	1.43
3	A	1980	PO4	P-O1	3.43	1.58	1.50
3	A	1982	PO4	P-O3	3.38	1.64	1.54
3	C	3981	PO4	P-O2	3.34	1.64	1.54
3	E	5980	PO4	P-O4	3.30	1.64	1.54
7	A	1900	ADP	O3'-C3'	3.17	1.50	1.43
3	C	3982	PO4	P-O2	3.13	1.64	1.54
3	C	3981	PO4	P-O4	3.02	1.63	1.54
8	G	7920	ORN	O-C	2.96	1.31	1.22
3	C	3981	PO4	P-O3	2.95	1.63	1.54
7	E	5910	ADP	O3'-C3'	2.94	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7982	PO4	P-O4	2.88	1.63	1.54
7	G	7900	ADP	O3'-C3'	2.83	1.49	1.43
3	E	5906	PO4	P-O4	-2.76	1.46	1.54
7	A	1910	ADP	O3'-C3'	2.75	1.49	1.43
3	G	7906	PO4	P-O4	-2.74	1.46	1.54
7	G	7910	ADP	O2'-C2'	2.73	1.49	1.43
7	A	1900	ADP	O4'-C1'	-2.63	1.37	1.41
8	C	3920	ORN	O-C	2.61	1.30	1.22
3	A	1906	PO4	P-O3	-2.60	1.46	1.54
7	G	7900	ADP	O2'-C2'	2.59	1.49	1.43
3	A	1982	PO4	P-O2	2.55	1.62	1.54
3	C	3982	PO4	P-O3	2.50	1.62	1.54
7	C	3900	ADP	O2'-C2'	2.48	1.48	1.43
7	C	3910	ADP	O2'-C2'	2.47	1.48	1.43
3	E	5980	PO4	P-O2	2.41	1.61	1.54
7	G	7910	ADP	O3'-C3'	2.41	1.48	1.43
7	C	3900	ADP	C2-N1	2.39	1.38	1.33
7	E	5910	ADP	O4'-C1'	-2.35	1.37	1.41
7	E	5900	ADP	O3'-C3'	2.34	1.48	1.43
7	C	3900	ADP	PA-O2A	-2.31	1.44	1.55
7	A	1900	ADP	PA-O2A	-2.28	1.44	1.55
3	C	3906	PO4	P-O3	-2.27	1.47	1.54
7	E	5900	ADP	O2'-C2'	2.26	1.48	1.43
7	G	7900	ADP	PB-O2B	-2.25	1.46	1.54
7	E	5900	ADP	C2-N3	-2.23	1.28	1.32
7	A	1910	ADP	O4'-C1'	-2.20	1.38	1.41
3	C	3906	PO4	P-O4	-2.20	1.48	1.54
7	E	5910	ADP	O2'-C2'	2.18	1.48	1.43
3	A	1906	PO4	P-O4	-2.16	1.48	1.54
3	C	3906	PO4	P-O2	-2.11	1.48	1.54
3	A	1981	PO4	P-O2	2.10	1.60	1.54
7	G	7900	ADP	O4'-C1'	-2.10	1.38	1.41
8	E	5920	ORN	O-C	2.10	1.28	1.22
7	A	1900	ADP	O2'-C2'	2.08	1.47	1.43
3	G	7982	PO4	P-O3	2.02	1.60	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1900	ADP	C5-C6-N6	7.09	131.13	120.35
7	G	7900	ADP	C5-C6-N6	6.58	130.35	120.35
7	A	1910	ADP	O3B-PB-O3A	4.21	118.76	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	3900	ADP	C5-C6-N6	4.01	126.44	120.35
7	C	3910	ADP	O3'-C3'-C2'	3.59	123.45	111.82
7	E	5900	ADP	C5-C6-N6	3.36	125.45	120.35
7	C	3910	ADP	C5-C6-N6	3.33	125.42	120.35
7	C	3910	ADP	C3'-C2'-C1'	3.12	105.68	100.98
7	A	1910	ADP	C3'-C2'-C1'	3.05	105.57	100.98
7	E	5900	ADP	O3B-PB-O3A	-3.01	94.55	104.64
7	G	7910	ADP	C4-C5-N7	2.97	112.50	109.40
7	A	1900	ADP	C5-C6-N1	-2.97	113.62	120.35
7	G	7910	ADP	C3'-C2'-C1'	2.85	105.26	100.98
8	G	7920	ORN	OXT-C-CA	2.83	123.02	113.38
7	E	5910	ADP	O3'-C3'-C2'	2.77	120.80	111.82
7	G	7910	ADP	O2'-C2'-C3'	2.74	120.69	111.82
3	A	1981	PO4	O4-P-O3	2.71	116.68	107.97
8	A	1920	ORN	OXT-C-O	-2.66	118.05	124.09
7	C	3910	ADP	O2'-C2'-C3'	2.45	119.75	111.82
7	A	1900	ADP	O3B-PB-O2B	2.43	116.93	107.64
7	G	7900	ADP	C5-C6-N1	-2.42	114.86	120.35
3	C	3906	PO4	O4-P-O3	2.35	115.52	107.97
7	A	1900	ADP	O3'-C3'-C2'	2.35	119.41	111.82
7	E	5900	ADP	C3'-C2'-C1'	2.31	104.46	100.98
8	C	3920	ORN	OXT-C-O	-2.30	118.86	124.09
7	G	7900	ADP	O3'-C3'-C2'	2.27	119.16	111.82
7	E	5900	ADP	C5-C6-N1	-2.21	115.34	120.35
7	C	3900	ADP	O2B-PB-O1B	-2.20	102.06	110.68
7	A	1910	ADP	O3B-PB-O2B	-2.18	99.31	107.64
8	A	1920	ORN	OXT-C-CA	2.15	120.72	113.38
7	E	5910	ADP	C5-C6-N1	-2.15	115.48	120.35
7	A	1910	ADP	O3'-C3'-C2'	2.14	118.75	111.82
7	C	3900	ADP	C1'-N9-C4	-2.14	122.89	126.64
3	C	3981	PO4	O4-P-O1	-2.11	103.18	110.89
7	G	7910	ADP	O3'-C3'-C2'	2.11	118.64	111.82
3	G	7981	PO4	O4-P-O3	2.07	114.61	107.97
7	E	5910	ADP	C3'-C2'-C1'	2.05	104.07	100.98
7	A	1900	ADP	C3'-C2'-C1'	2.03	104.03	100.98
7	E	5910	ADP	O2'-C2'-C3'	2.01	118.34	111.82

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1920	ORN	N-CA-CB-CG

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

Continued on next page...

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Mol	Chain	Res	Type	Atoms
7	C	3910	ADP	C3'-C4'-C5'-O5'
7	A	1910	ADP	PB-O3A-PA-O1A
7	C	3900	ADP	PB-O3A-PA-O1A
7	E	5900	ADP	PB-O3A-PA-O2A

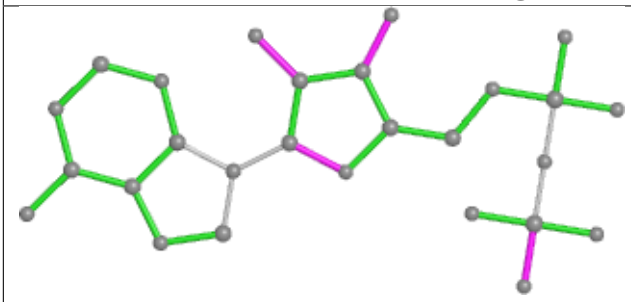
There are no ring outliers.

13 monomers are involved in 19 short contacts:

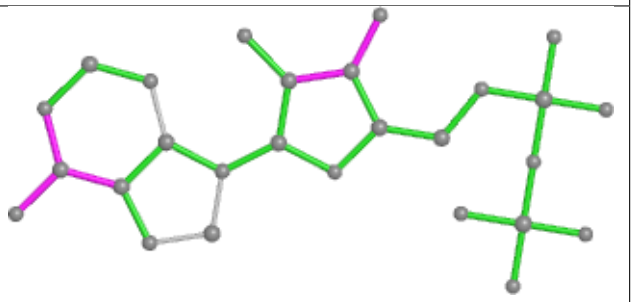
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	7900	ADP	2	0
8	C	3920	ORN	3	0
7	C	3910	ADP	1	0
8	G	7920	ORN	1	0
9	E	5950	NET	2	0
3	G	7906	PO4	1	0
8	A	1920	ORN	1	0
7	G	7910	ADP	2	0
8	E	5920	ORN	1	0
7	E	5900	ADP	1	0
3	C	3906	PO4	1	0
9	A	1950	NET	1	0
7	A	1910	ADP	2	0

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

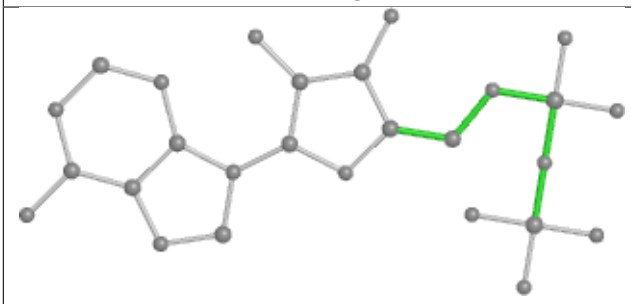
Ligand ADP G 7900



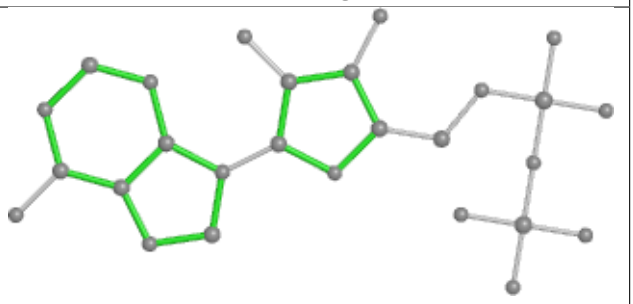
Bond lengths



Bond angles

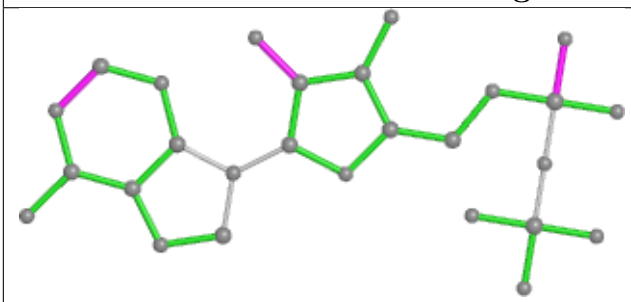


Torsions

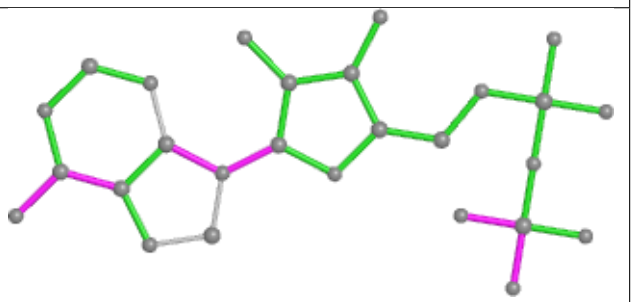


Rings

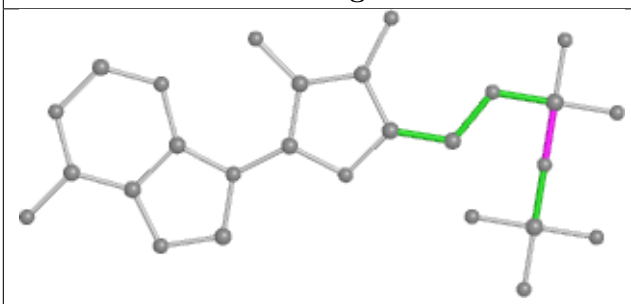
Ligand ADP C 3900



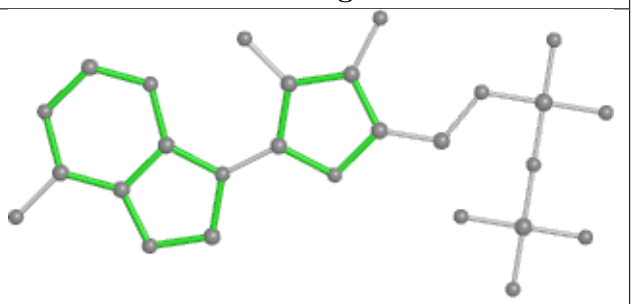
Bond lengths



Bond angles

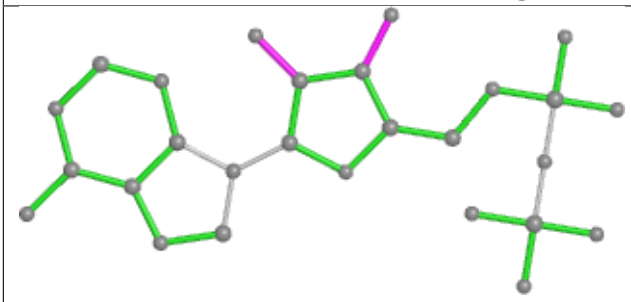


Torsions

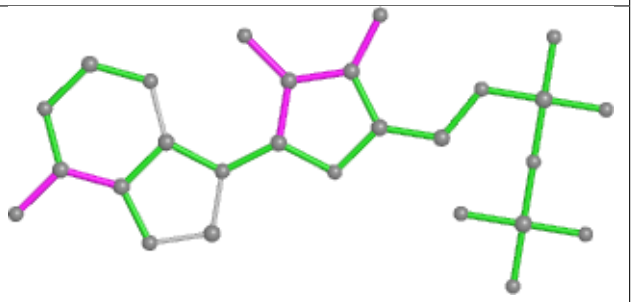


Rings

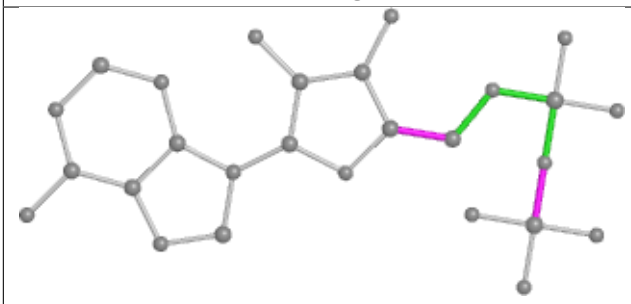
Ligand ADP C 3910



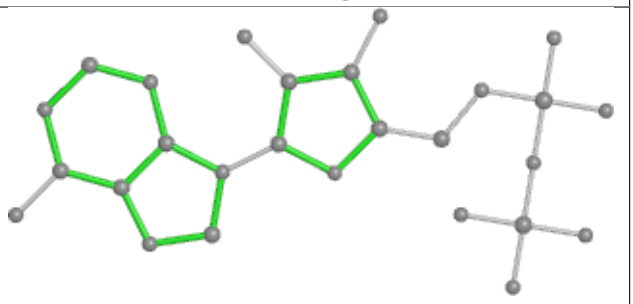
Bond lengths



Bond angles

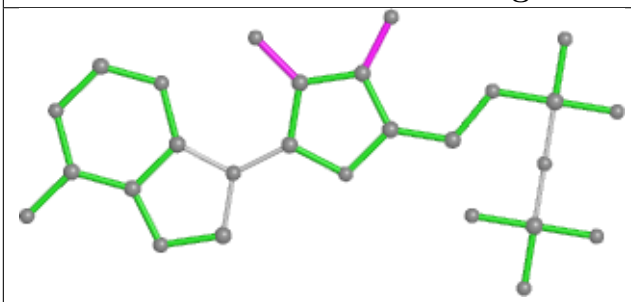


Torsions

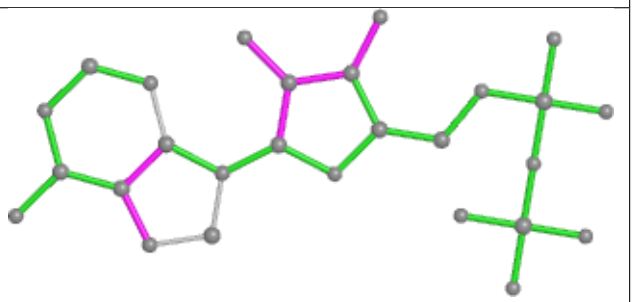


Rings

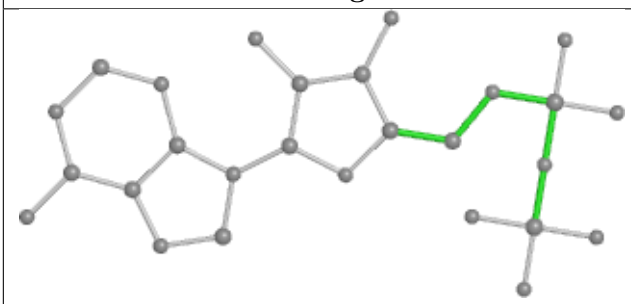
Ligand ADP G 7910



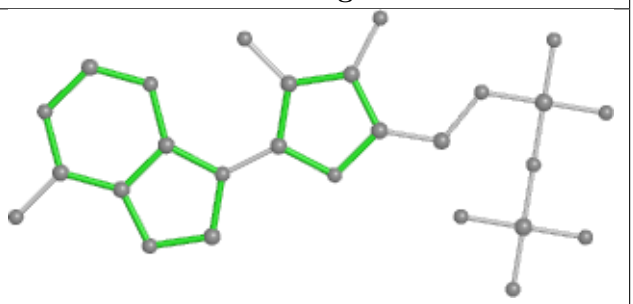
Bond lengths



Bond angles

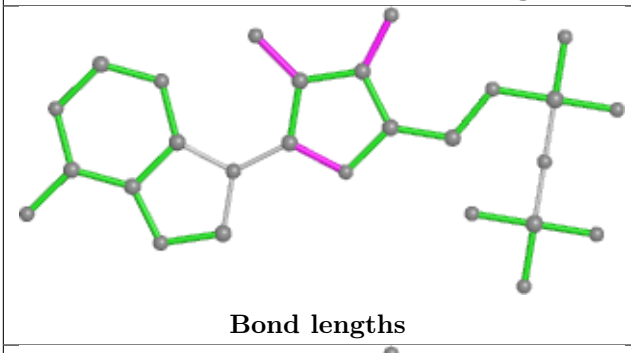


Torsions

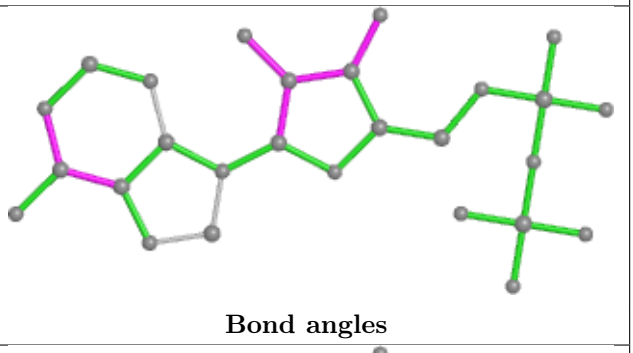


Rings

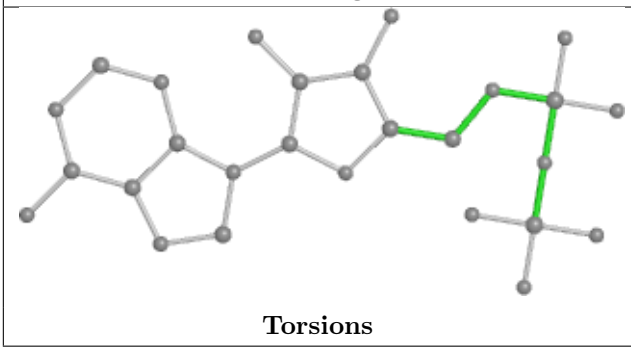
Ligand ADP E 5910



Bond lengths



Bond angles



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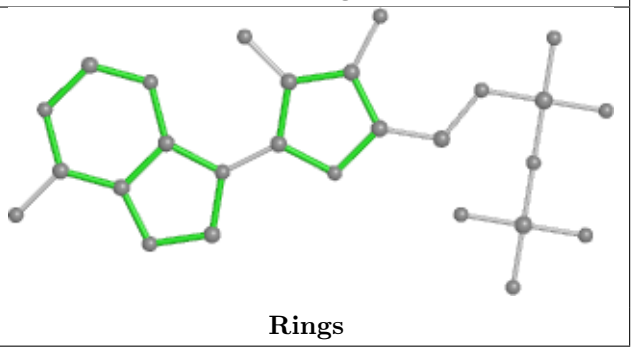
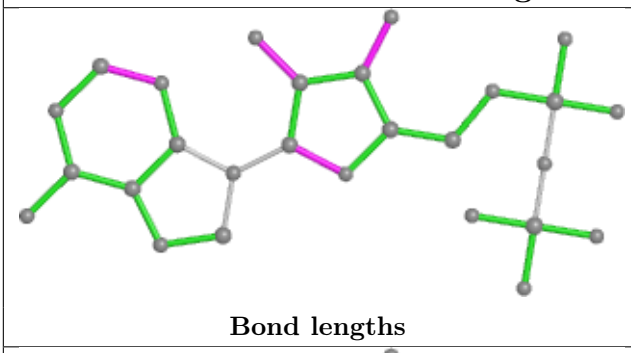


Rings

Ligand ADP E 5900



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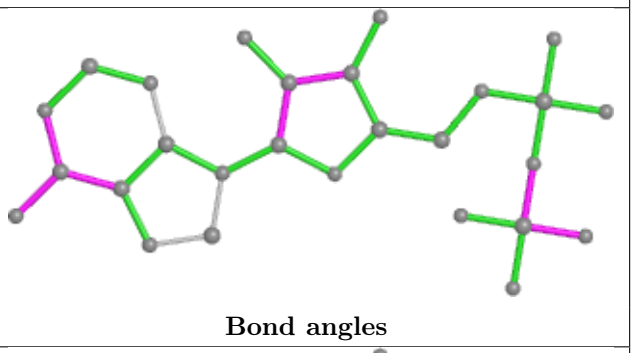
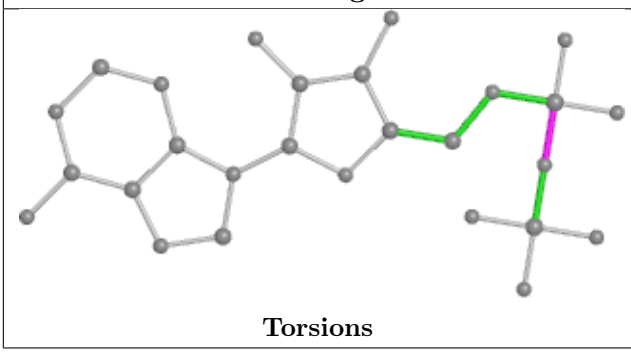


Bond angles



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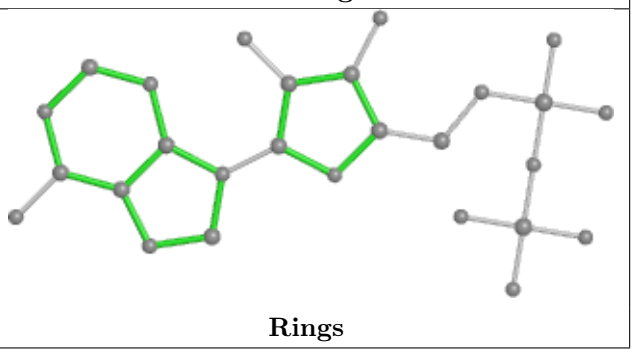
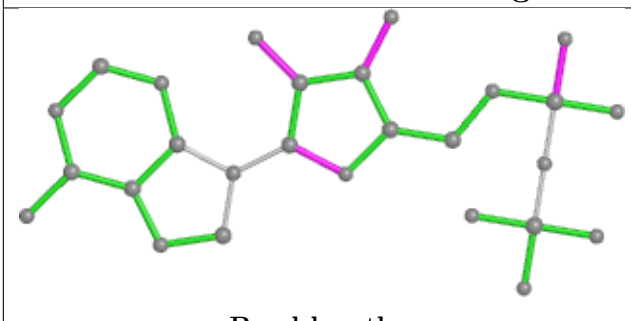


Rings

Ligand ADP A 1900



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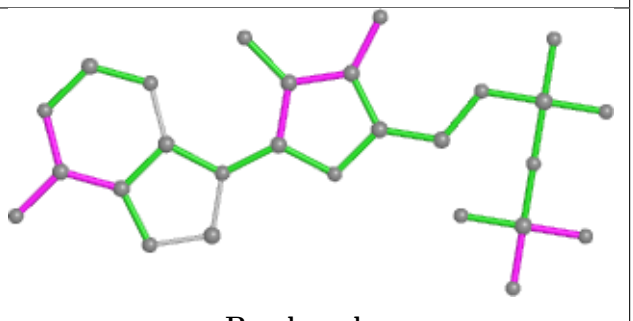
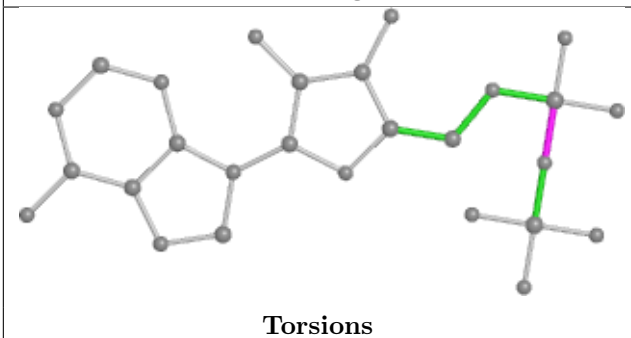


Bond angles



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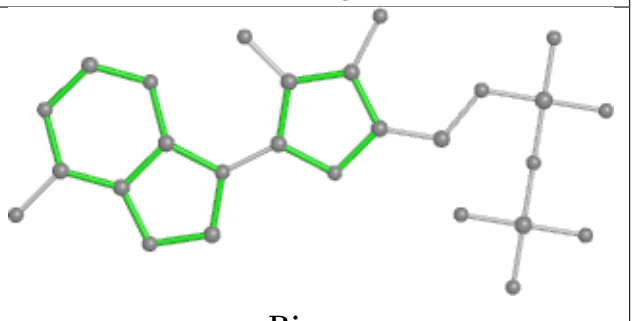
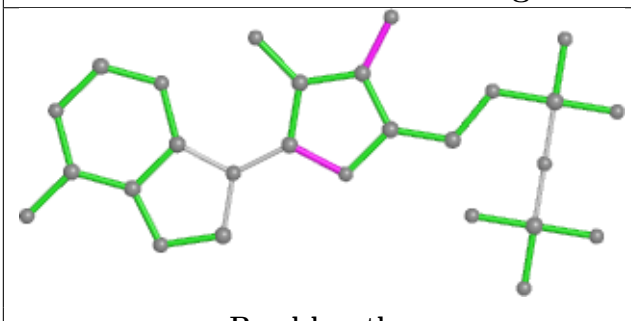


Rings

Ligand ADP A 1910



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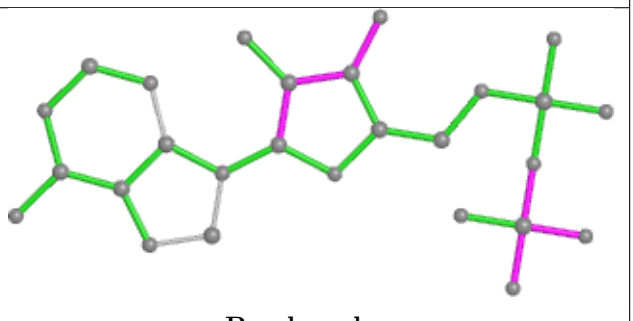
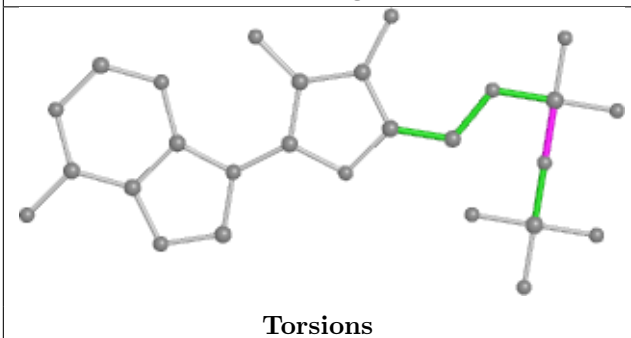
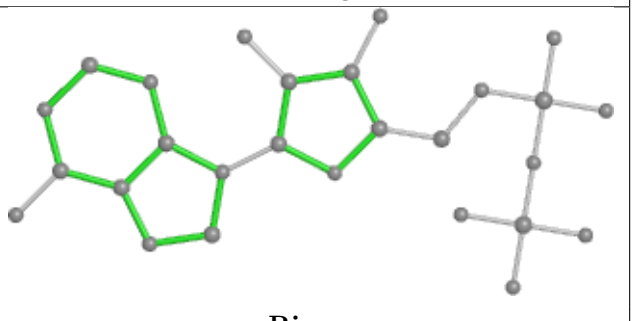


Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.