



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 06:24 AM EDT

PDB ID : 1KEE  
Title : Inactivation of the Amidotransferase Activity of Carbamoyl Phosphate Synthetase by the Antibiotic Acivicin  
Authors : Miles, B.W.; Thoden, J.B.; Holden, H.M.; Raushel, F.M.  
Deposited on : 2001-11-15  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

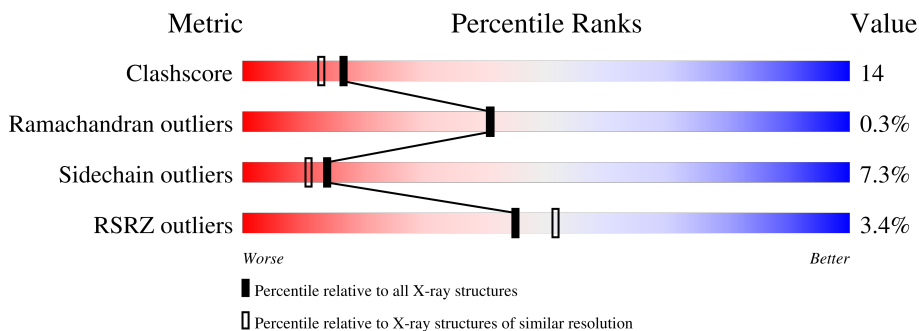
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	1073	 3% 63% 29% 6% ..
1	C	1073	 4% 63% 29% 7% ..
1	E	1073	 4% 64% 29% 5% ..
1	G	1073	 5% 60% 30% 7% ..
2	B	382	 % 62% 31% 5% .
2	D	382	 % 61% 34% ..

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Mol	Chain	Length	Quality of chain
2	F	382	
2	H	382	

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
2	143	B	269	X	-	-	-
2	143	D	269	X	-	-	-
2	143	F	269	X	-	-	-
2	143	H	269	X	-	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 48896 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
			Total	C	N	O	S			
1	A	1058	8181	5136	1425	1575	45	0	5	0
1	C	1058	8172	5130	1425	1572	45	0	2	0
1	E	1058	8204	5150	1430	1579	45	0	8	0
1	G	1058	8160	5123	1422	1570	45	0	0	0

- Molecule 2 is a protein called Carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	379	2912	1834	513	555	10	0	1	0
2	D	379	2907	1831	510	556	10	0	1	0
2	F	379	2905	1830	510	555	10	0	0	0
2	H	379	2905	1830	510	555	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	143	CYS	modified residue	UNP P00907
D	269	143	CYS	modified residue	UNP P00907
F	269	143	CYS	modified residue	UNP P00907
H	269	143	CYS	modified residue	UNP P00907

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

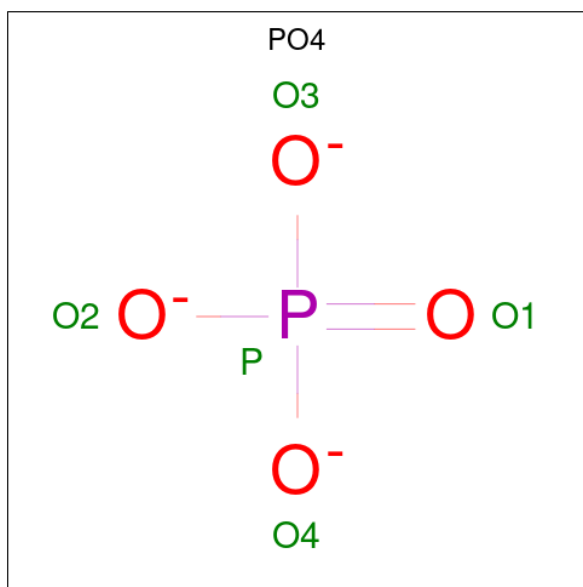
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Cl 5 5	0	0
5	B	1	Total Cl 1 1	0	0
5	C	5	Total Cl 5 5	0	0
5	D	1	Total Cl 1 1	0	0
5	E	4	Total Cl 4 4	0	0
5	F	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	4	Total	Cl	0	0
			4	4		
5	H	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



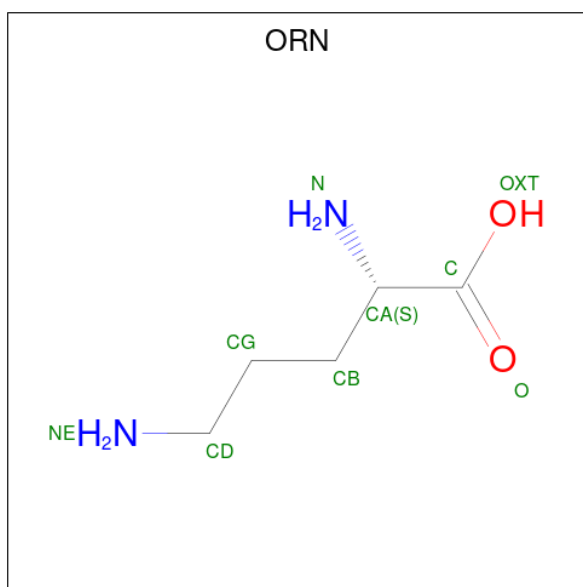
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



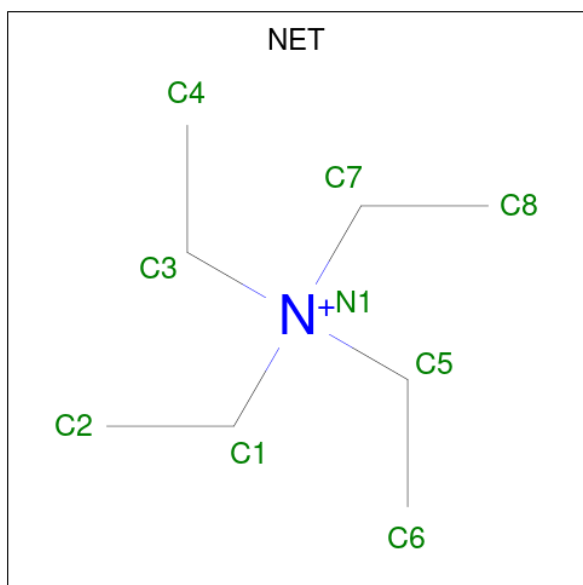
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			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<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



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

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





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

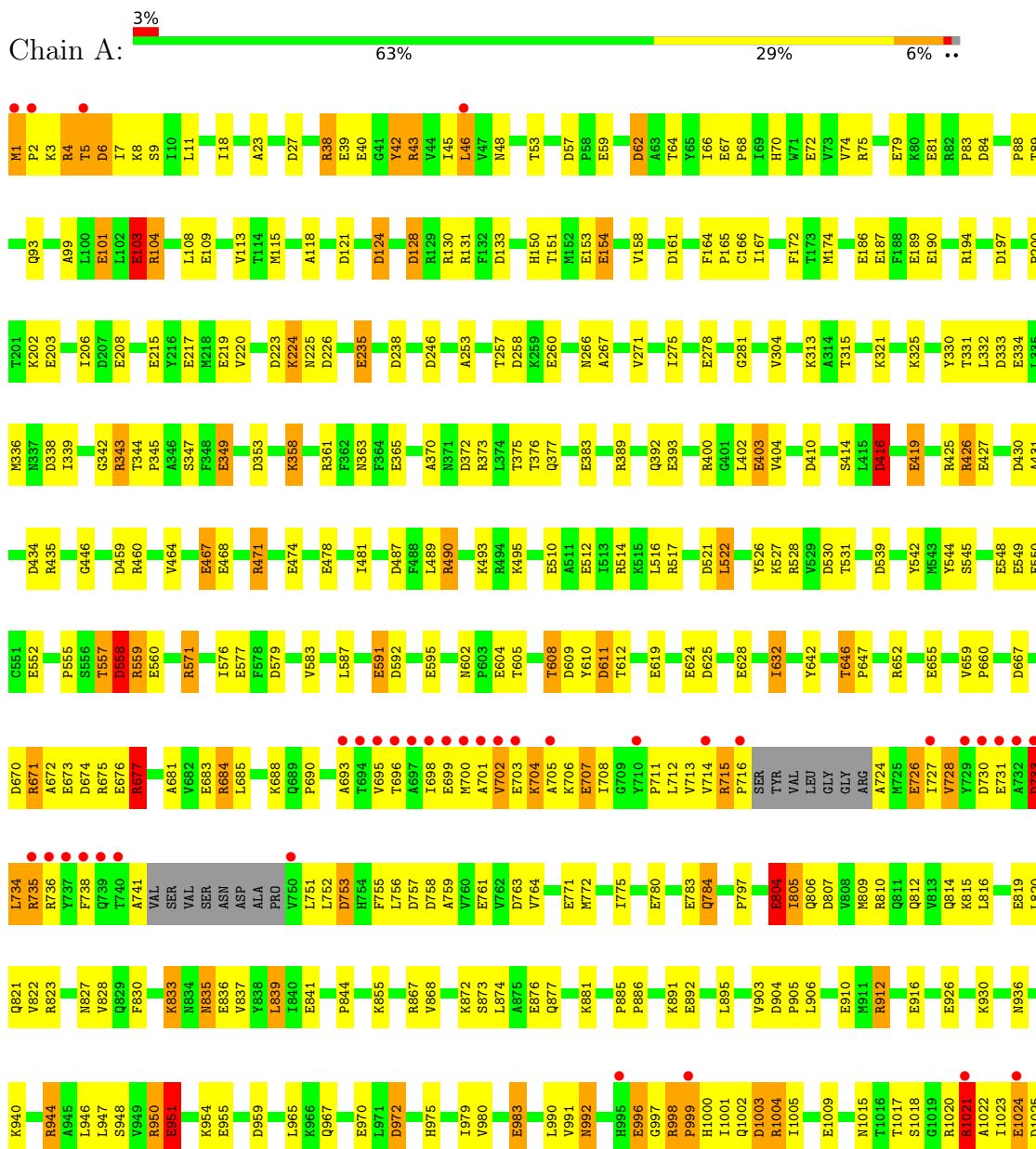
- Molecule 10 is water.

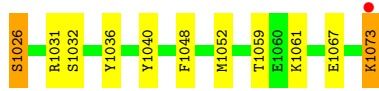
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	841	Total	O	0	0
			841	841		
10	B	230	Total	O	0	0
			230	230		
10	C	783	Total	O	0	0
			783	783		
10	D	304	Total	O	0	0
			304	304		
10	E	886	Total	O	0	0
			886	886		
10	F	263	Total	O	0	0
			263	263		
10	G	678	Total	O	0	0
			678	678		
10	H	191	Total	O	0	0
			191	191		

### 3 Residue-property plots i

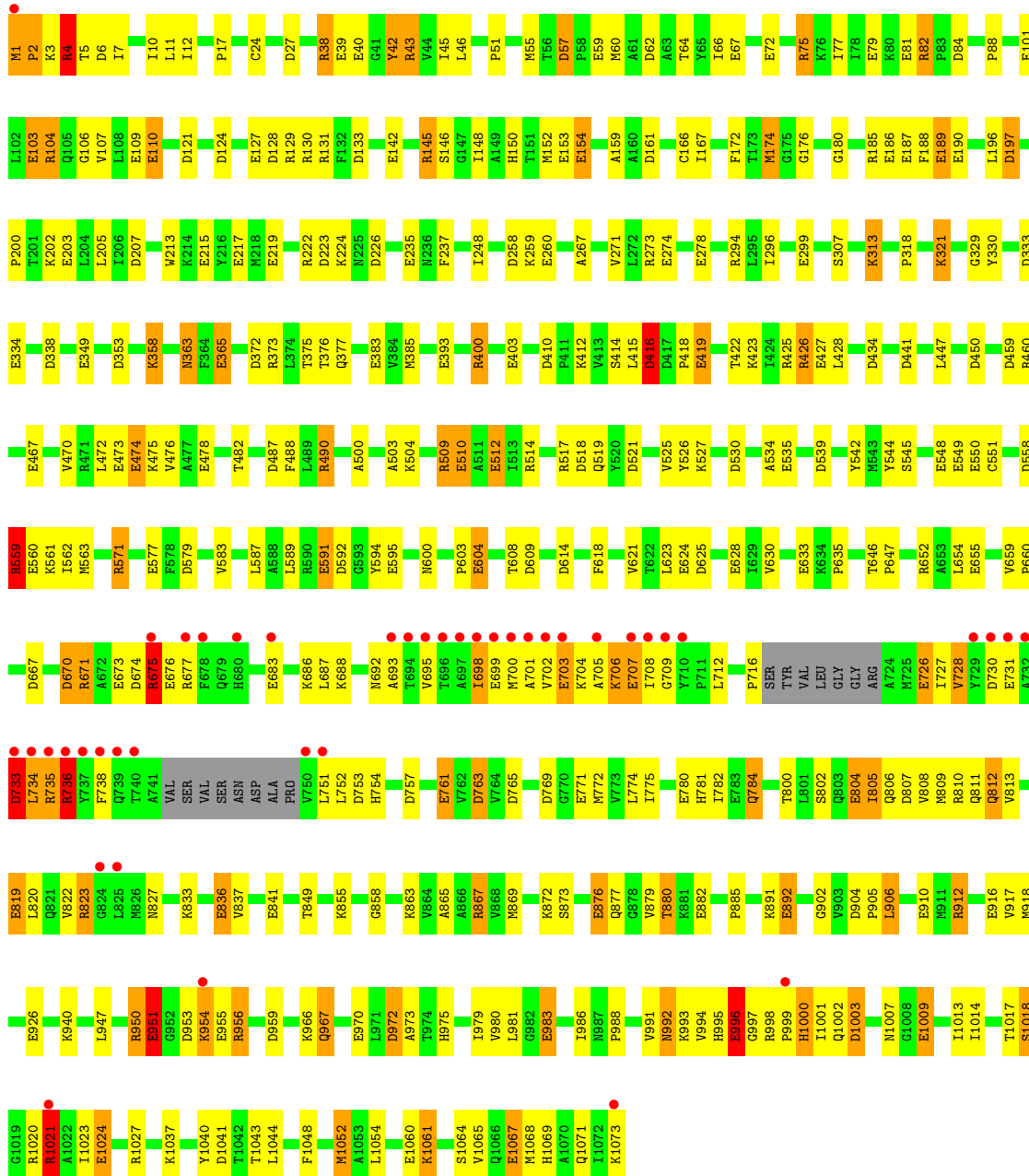
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Carbamoyl-phosphate synthetase large chain



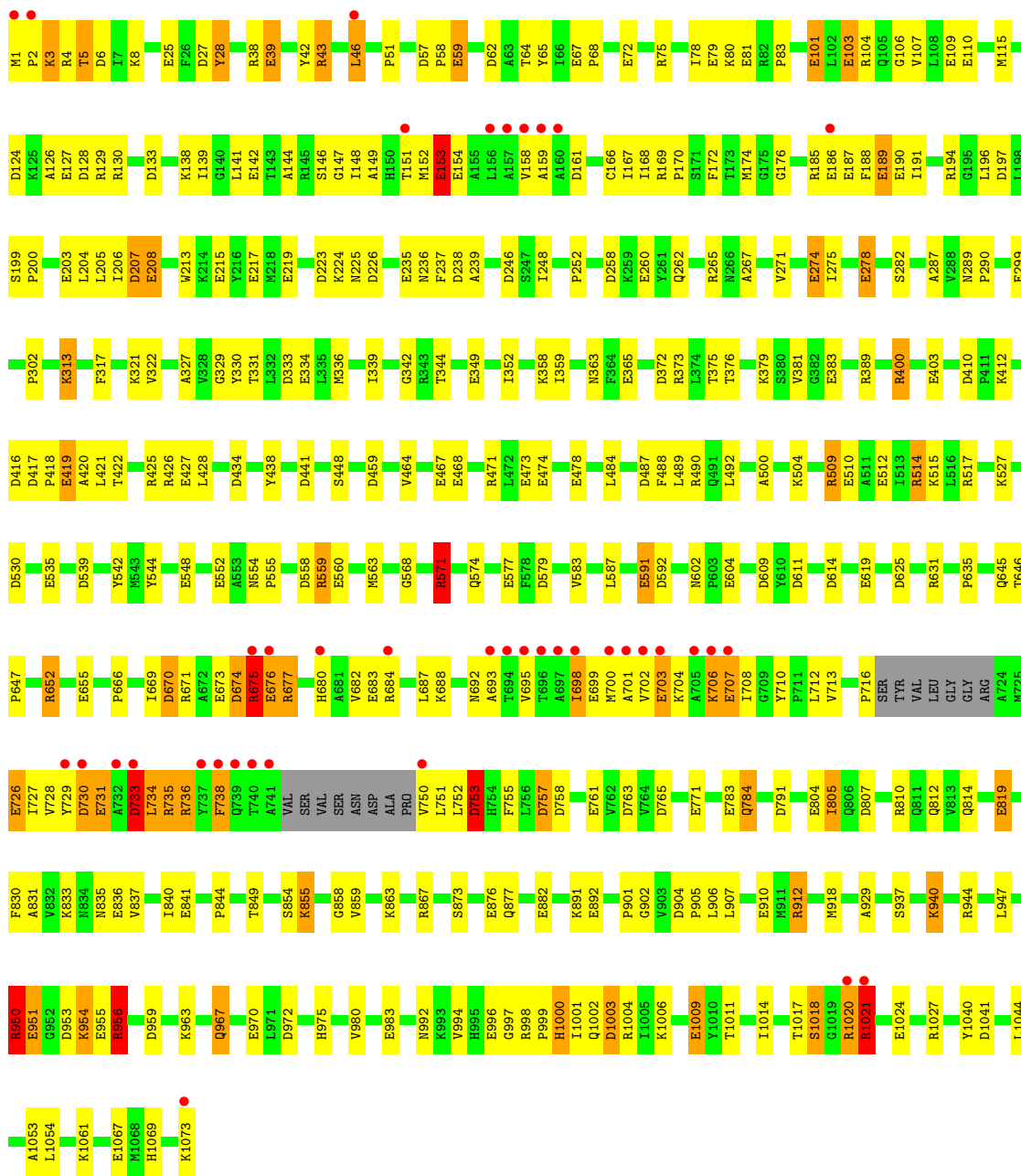


● Molecule 1: Carbamoyl-phosphate synthetase large chain

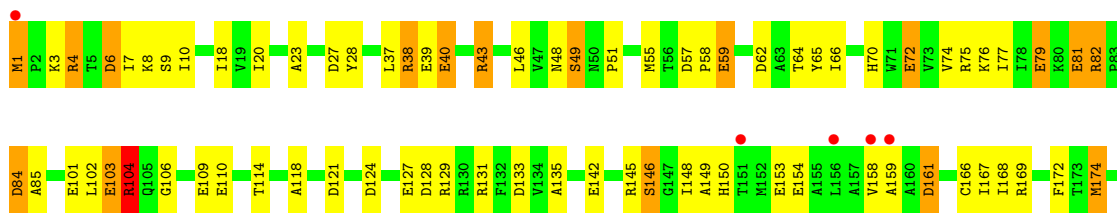


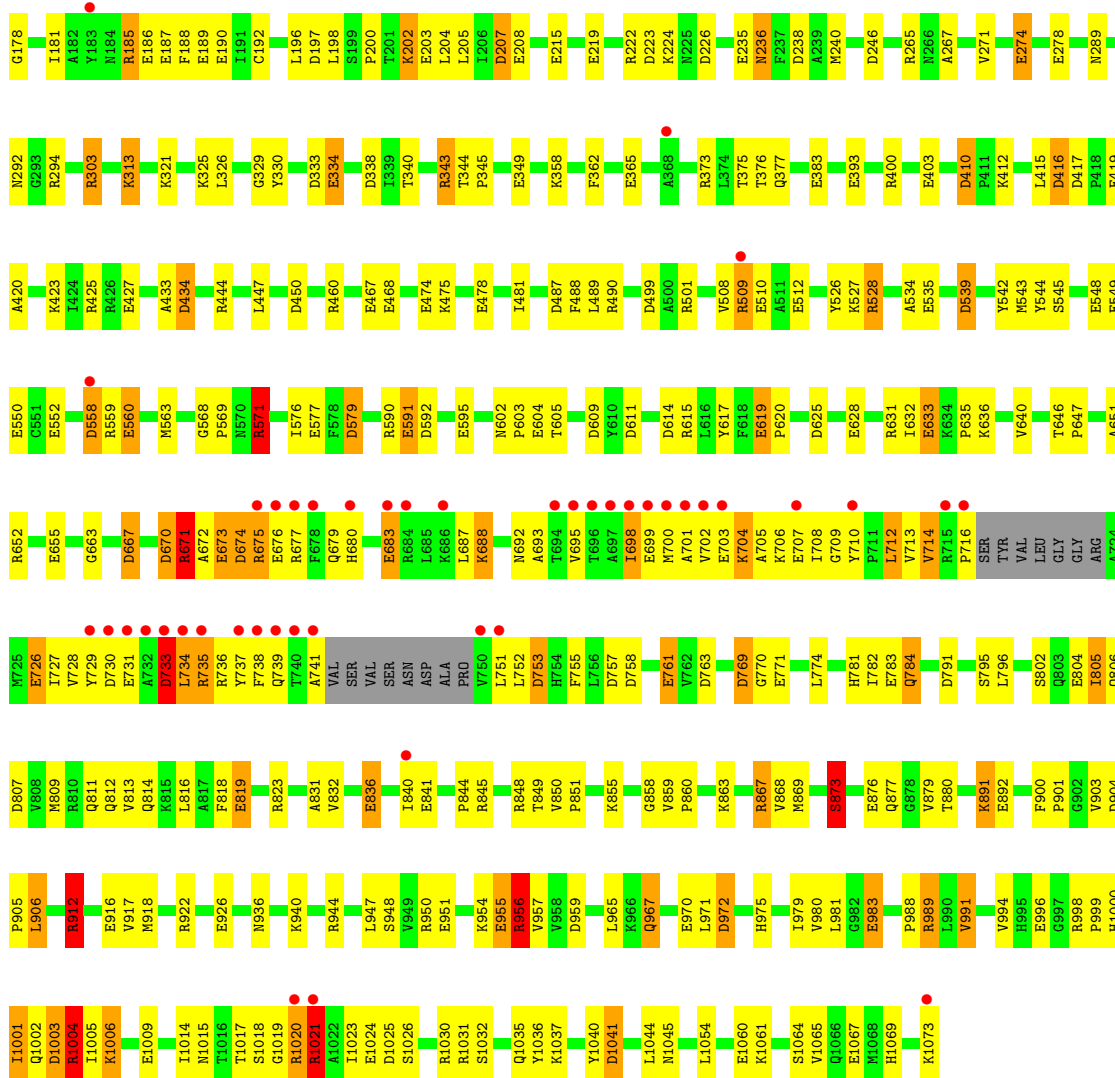
● Molecule 1: Carbamoyl-phosphate synthetase large chain



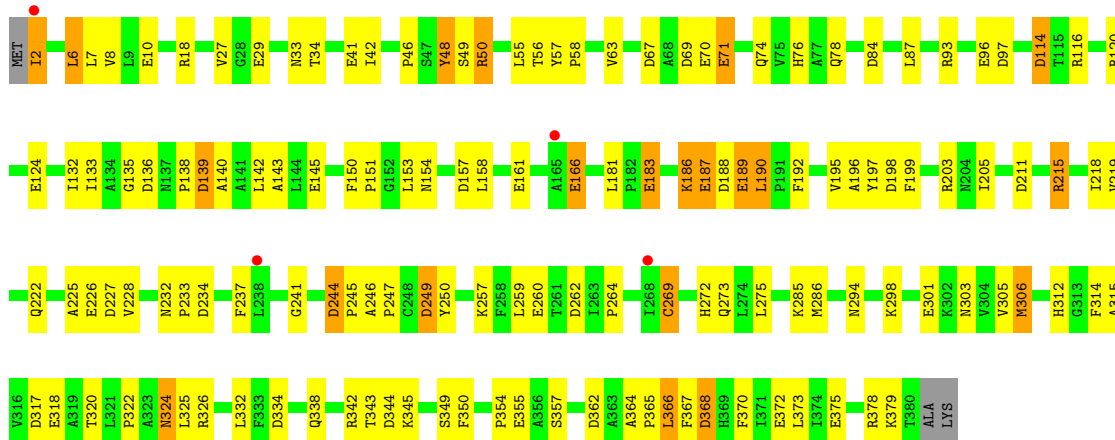


● Molecule 1: Carbamoyl-phosphate synthetase large chain



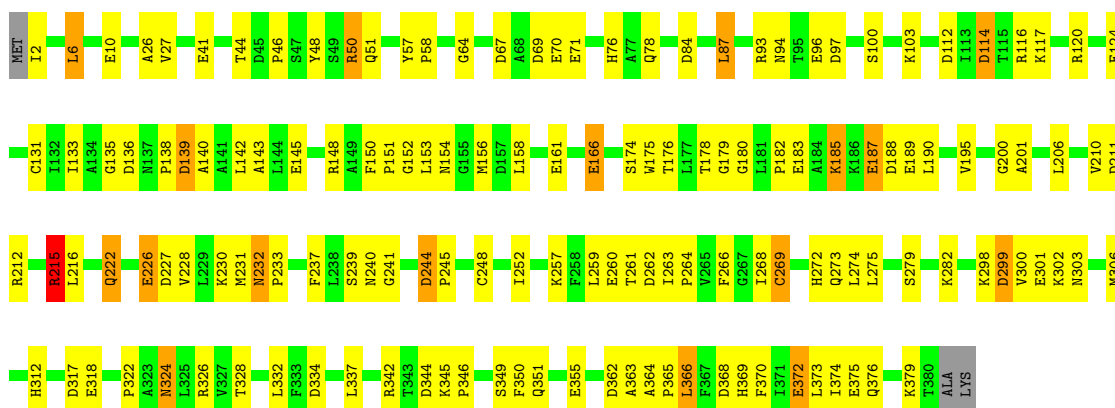


• Molecule 2: Carbamoyl-phosphate synthetase small chain



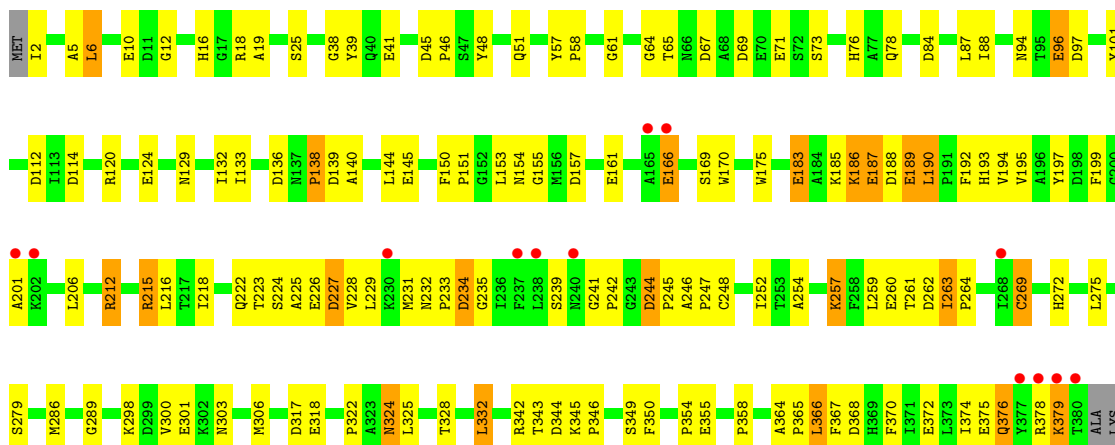
• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain D:  61% 34%



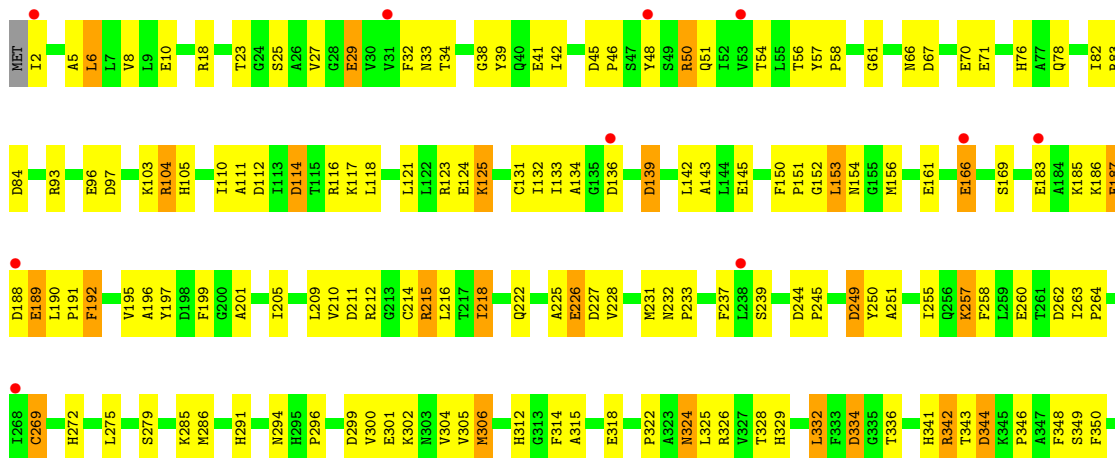
• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain F:  61% 33% 3% 6%



• Molecule 2: Carbamoyl-phosphate synthetase small chain

Chain H:  55% 36% 3% 7%



P354	E355	A356	S357	P358	D362	A363	A364	P365	L366	F367	D368	H369	F370	I371	E372	E375	T380	ALA	LYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.40Å 164.40Å 333.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.00-2.10) 88.9 (29.99-2.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.10Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.186 , 0.211 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 108.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	48896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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: NET, ADP, 143, MN, ORN, CL, K, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.99	76/8327 (0.9%)	1.38	120/11257 (1.1%)
1	C	0.99	79/8306 (1.0%)	1.34	111/11228 (1.0%)
1	E	1.00	77/8362 (0.9%)	1.34	118/11302 (1.0%)
1	G	0.97	74/8286 (0.9%)	1.38	120/11202 (1.1%)
2	B	0.88	20/2961 (0.7%)	1.28	38/4019 (0.9%)
2	D	0.90	19/2956 (0.6%)	1.29	33/4013 (0.8%)
2	F	0.90	18/2950 (0.6%)	1.31	39/4005 (1.0%)
2	H	0.88	20/2950 (0.7%)	1.28	36/4005 (0.9%)
All	All	0.96	383/45098 (0.8%)	1.34	615/61031 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0
2	D	1	0
2	F	1	0
2	H	1	0
All	All	4	0

All (383) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	183	GLU	CD-OE2	8.23	1.34	1.25
1	C	110	GLU	CD-OE2	8.18	1.34	1.25
2	D	183	GLU	CD-OE2	8.05	1.34	1.25
1	E	467	GLU	CD-OE2	8.02	1.34	1.25
2	F	355	GLU	CD-OE2	8.01	1.34	1.25
2	B	183	GLU	CD-OE2	7.87	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	GLU	CD-OE2	7.79	1.34	1.25
1	C	1024	GLU	CD-OE2	7.72	1.34	1.25
2	F	183	GLU	CD-OE2	7.69	1.34	1.25
1	A	72	GLU	CD-OE2	7.54	1.33	1.25
1	E	771	GLU	CD-OE2	7.46	1.33	1.25
2	B	372	GLU	CD-OE2	7.43	1.33	1.25
2	F	189	GLU	CD-OE2	7.37	1.33	1.25
2	F	372	GLU	CD-OE2	7.23	1.33	1.25
1	E	215	GLU	CD-OE2	7.21	1.33	1.25
1	E	655[A]	GLU	CD-OE2	7.13	1.33	1.25
1	E	655[B]	GLU	CD-OE2	7.13	1.33	1.25
2	D	226	GLU	CD-OE2	7.11	1.33	1.25
1	A	683	GLU	CD-OE2	7.10	1.33	1.25
1	G	512	GLU	CD-OE2	7.10	1.33	1.25
1	E	474	GLU	CD-OE2	7.09	1.33	1.25
1	G	1024	GLU	CD-OE2	7.07	1.33	1.25
1	G	676	GLU	CD-OE2	7.06	1.33	1.25
2	H	226	GLU	CD-OE2	7.04	1.33	1.25
2	D	301	GLU	CD-OE2	7.04	1.33	1.25
1	A	512	GLU	CD-OE2	6.98	1.33	1.25
1	A	217	GLU	CD-OE2	6.97	1.33	1.25
1	G	186	GLU	CD-OE2	6.96	1.33	1.25
1	A	951	GLU	CD-OE2	6.94	1.33	1.25
2	F	226	GLU	CD-OE2	6.94	1.33	1.25
1	C	951	GLU	CD-OE2	6.92	1.33	1.25
2	F	166	GLU	CD-OE2	6.90	1.33	1.25
1	G	365	GLU	CD-OE2	6.89	1.33	1.25
1	A	703	GLU	CD-OE2	6.84	1.33	1.25
2	D	189	GLU	CD-OE2	6.84	1.33	1.25
1	A	836	GLU	CD-OE2	6.83	1.33	1.25
1	A	153	GLU	CD-OE2	6.83	1.33	1.25
1	A	577	GLU	CD-OE2	6.83	1.33	1.25
2	H	166	GLU	CD-OE2	6.81	1.33	1.25
1	A	955	GLU	CD-OE2	6.81	1.33	1.25
2	F	10	GLU	CD-OE2	6.80	1.33	1.25
1	C	703	GLU	CD-OE2	6.80	1.33	1.25
1	A	780	GLU	CD-OE2	6.80	1.33	1.25
2	F	71	GLU	CD-OE2	6.79	1.33	1.25
2	B	124	GLU	CD-OE2	6.79	1.33	1.25
1	C	836	GLU	CD-OE2	6.79	1.33	1.25
1	C	1009[A]	GLU	CD-OE2	6.79	1.33	1.25
1	C	1009[B]	GLU	CD-OE2	6.79	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	703	GLU	CD-OE2	6.78	1.33	1.25
1	E	478	GLU	CD-OE2	6.78	1.33	1.25
1	E	804	GLU	CD-OE2	6.75	1.33	1.25
1	A	1024	GLU	CD-OE2	6.74	1.33	1.25
2	D	166	GLU	CD-OE2	6.74	1.33	1.25
1	C	780	GLU	CD-OE2	6.72	1.33	1.25
1	E	699	GLU	CD-OE2	6.69	1.33	1.25
1	A	478	GLU	CD-OE2	6.69	1.33	1.25
1	E	260	GLU	CD-OE2	6.69	1.33	1.25
1	G	726	GLU	CD-OE2	6.68	1.32	1.25
1	C	186	GLU	CD-OE2	6.65	1.32	1.25
1	C	203	GLU	CD-OE2	6.64	1.32	1.25
1	E	365	GLU	CD-OE2	6.64	1.32	1.25
1	A	109	GLU	CD-OE2	6.62	1.32	1.25
1	C	153	GLU	CD-OE2	6.61	1.32	1.25
1	G	731	GLU	CD-OE2	6.60	1.32	1.25
1	G	215	GLU	CD-OE2	6.58	1.32	1.25
1	A	771	GLU	CD-OE2	6.58	1.32	1.25
1	C	187	GLU	CD-OE2	6.57	1.32	1.25
1	A	731	GLU	CD-OE2	6.57	1.32	1.25
1	E	560	GLU	CD-OE2	6.56	1.32	1.25
1	E	683	GLU	CD-OE2	6.56	1.32	1.25
1	G	110	GLU	CD-OE2	6.55	1.32	1.25
1	G	190	GLU	CD-OE2	6.55	1.32	1.25
1	G	783	GLU	CD-OE2	6.55	1.32	1.25
2	F	187	GLU	CD-OE2	6.51	1.32	1.25
1	A	655	GLU	CD-OE2	6.51	1.32	1.25
1	E	707	GLU	CD-OE2	6.49	1.32	1.25
1	G	655	GLU	CD-OE2	6.49	1.32	1.25
2	B	71	GLU	CD-OE2	6.48	1.32	1.25
1	E	676	GLU	CD-OE2	6.47	1.32	1.25
1	C	731	GLU	CD-OE2	6.45	1.32	1.25
1	A	550	GLU	CD-OE2	6.45	1.32	1.25
1	G	703	GLU	CD-OE2	6.44	1.32	1.25
2	D	355	GLU	CD-OE2	6.44	1.32	1.25
1	E	190	GLU	CD-OE2	6.43	1.32	1.25
2	F	96	GLU	CD-OE2	6.42	1.32	1.25
1	E	427	GLU	CD-OE2	6.42	1.32	1.25
1	G	699	GLU	CD-OE2	6.42	1.32	1.25
1	A	186	GLU	CD-OE2	6.42	1.32	1.25
1	G	478	GLU	CD-OE2	6.42	1.32	1.25
1	G	153	GLU	CD-OE2	6.41	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	187	GLU	CD-OE2	6.41	1.32	1.25
1	G	619	GLU	CD-OE2	6.40	1.32	1.25
1	G	876	GLU	CD-OE2	6.39	1.32	1.25
1	C	726	GLU	CD-OE2	6.38	1.32	1.25
1	A	549	GLU	CD-OE2	6.36	1.32	1.25
1	G	683	GLU	CD-OE2	6.35	1.32	1.25
2	B	41	GLU	CD-OE2	6.34	1.32	1.25
1	C	804	GLU	CD-OE2	6.34	1.32	1.25
1	E	673	GLU	CD-OE2	6.33	1.32	1.25
1	A	673	GLU	CD-OE2	6.32	1.32	1.25
1	E	1009[A]	GLU	CD-OE2	6.32	1.32	1.25
1	E	1009[B]	GLU	CD-OE2	6.32	1.32	1.25
1	A	365	GLU	CD-OE2	6.32	1.32	1.25
1	G	59	GLU	CD-OE2	6.31	1.32	1.25
1	A	699	GLU	CD-OE2	6.31	1.32	1.25
1	C	892	GLU	CD-OE2	6.31	1.32	1.25
2	B	166	GLU	CD-OE2	6.31	1.32	1.25
1	E	39	GLU	CD-OE2	6.30	1.32	1.25
1	C	595	GLU	CD-OE2	6.30	1.32	1.25
1	E	79	GLU	CD-OE2	6.30	1.32	1.25
1	A	474	GLU	CD-OE2	6.29	1.32	1.25
2	D	145	GLU	CD-OE2	6.29	1.32	1.25
1	C	419	GLU	CD-OE2	6.29	1.32	1.25
1	C	624	GLU	CD-OE2	6.29	1.32	1.25
2	D	375	GLU	CD-OE2	6.28	1.32	1.25
1	G	474	GLU	CD-OE2	6.28	1.32	1.25
2	B	70	GLU	CD-OE2	6.28	1.32	1.25
1	E	983	GLU	CD-OE2	6.28	1.32	1.25
1	G	510	GLU	CD-OE2	6.28	1.32	1.25
2	H	355	GLU	CD-OE2	6.26	1.32	1.25
1	C	349	GLU	CD-OE2	6.26	1.32	1.25
1	C	577	GLU	CD-OE2	6.25	1.32	1.25
2	B	226	GLU	CD-OE2	6.25	1.32	1.25
2	H	145	GLU	CD-OE2	6.24	1.32	1.25
1	E	819	GLU	CD-OE2	6.24	1.32	1.25
1	G	419	GLU	CD-OE2	6.24	1.32	1.25
1	A	804	GLU	CD-OE2	6.23	1.32	1.25
1	C	707	GLU	CD-OE2	6.23	1.32	1.25
1	E	841	GLU	CD-OE2	6.23	1.32	1.25
1	G	926	GLU	CD-OE2	6.22	1.32	1.25
1	G	836	GLU	CD-OE2	6.21	1.32	1.25
1	G	819	GLU	CD-OE2	6.20	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1009	GLU	CD-OE2	6.19	1.32	1.25
1	E	731	GLU	CD-OE2	6.19	1.32	1.25
1	A	604	GLU	CD-OE2	6.19	1.32	1.25
1	C	676	GLU	CD-OE2	6.19	1.32	1.25
1	C	473	GLU	CD-OE2	6.19	1.32	1.25
1	A	219	GLU	CD-OE2	6.17	1.32	1.25
1	A	595	GLU	CD-OE2	6.17	1.32	1.25
1	C	761	GLU	CD-OE2	6.17	1.32	1.25
1	E	591	GLU	CD-OE2	6.17	1.32	1.25
1	G	707	GLU	CD-OE2	6.16	1.32	1.25
1	C	109	GLU	CD-OE2	6.16	1.32	1.25
1	C	983	GLU	CD-OE2	6.15	1.32	1.25
1	C	365	GLU	CD-OE2	6.15	1.32	1.25
1	G	955	GLU	CD-OE2	6.15	1.32	1.25
2	D	71	GLU	CD-OE2	6.14	1.32	1.25
1	C	910	GLU	CD-OE2	6.14	1.32	1.25
1	E	72	GLU	CD-OE2	6.13	1.32	1.25
2	F	301	GLU	CD-OE2	6.13	1.32	1.25
1	E	59	GLU	CD-OE2	6.12	1.32	1.25
1	C	591	GLU	CD-OE2	6.09	1.32	1.25
1	G	951	GLU	CD-OE2	6.08	1.32	1.25
1	C	699	GLU	CD-OE2	6.08	1.32	1.25
1	A	468	GLU	CD-OE2	6.08	1.32	1.25
1	C	219	GLU	CD-OE2	6.08	1.32	1.25
1	C	955	GLU	CD-OE2	6.07	1.32	1.25
1	E	217	GLU	CD-OE2	6.07	1.32	1.25
1	A	707	GLU	CD-OE2	6.06	1.32	1.25
2	H	318	GLU	CD-OE2	6.06	1.32	1.25
1	A	187	GLU	CD-OE2	6.06	1.32	1.25
1	E	1024	GLU	CD-OE2	6.05	1.32	1.25
1	A	427	GLU	CD-OE2	6.04	1.32	1.25
2	D	318	GLU	CD-OE2	6.01	1.32	1.25
1	C	478	GLU	CD-OE2	6.01	1.32	1.25
1	A	676	GLU	CD-OE2	6.00	1.32	1.25
1	C	467	GLU	CD-OE2	6.00	1.32	1.25
1	C	549	GLU	CD-OE2	5.99	1.32	1.25
1	G	591	GLU	CD-OE2	5.99	1.32	1.25
1	G	577	GLU	CD-OE2	5.98	1.32	1.25
1	A	510	GLU	CD-OE2	5.97	1.32	1.25
2	B	301	GLU	CD-OE2	5.97	1.32	1.25
1	A	996	GLU	CD-OE2	5.97	1.32	1.25
1	E	535	GLU	CD-OE2	5.97	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	591	GLU	CD-OE2	5.96	1.32	1.25
1	G	804	GLU	CD-OE2	5.96	1.32	1.25
1	E	836	GLU	CD-OE2	5.96	1.32	1.25
1	E	219	GLU	CD-OE2	5.95	1.32	1.25
2	H	70	GLU	CD-OE2	5.95	1.32	1.25
2	H	301	GLU	CD-OE2	5.94	1.32	1.25
1	A	154	GLU	CD-OE2	5.94	1.32	1.25
1	E	186	GLU	CD-OE2	5.93	1.32	1.25
1	E	419	GLU	CD-OE2	5.93	1.32	1.25
1	C	655	GLU	CD-OE2	5.93	1.32	1.25
1	A	203	GLU	CD-OE2	5.92	1.32	1.25
1	E	109	GLU	CD-OE2	5.92	1.32	1.25
1	C	274	GLU	CD-OE2	5.92	1.32	1.25
1	E	910	GLU	CD-OE2	5.92	1.32	1.25
1	C	217	GLU	CD-OE2	5.92	1.32	1.25
1	A	190	GLU	CD-OE2	5.91	1.32	1.25
2	D	260	GLU	CD-OE2	5.91	1.32	1.25
2	B	187	GLU	CD-OE2	5.90	1.32	1.25
2	B	318	GLU	CD-OE2	5.90	1.32	1.25
1	C	474	GLU	CD-OE2	5.89	1.32	1.25
1	E	783	GLU	CD-OE2	5.89	1.32	1.25
1	G	274	GLU	CD-OE2	5.88	1.32	1.25
1	C	876	GLU	CD-OE2	5.88	1.32	1.25
1	G	628	GLU	CD-OE2	5.88	1.32	1.25
1	A	926	GLU	CD-OE2	5.87	1.32	1.25
1	E	203	GLU	CD-OE2	5.87	1.32	1.25
2	B	145	GLU	CD-OE2	5.86	1.32	1.25
2	B	355	GLU	CD-OE2	5.85	1.32	1.25
2	D	161	GLU	CD-OE2	5.84	1.32	1.25
1	A	726	GLU	CD-OE2	5.84	1.32	1.25
1	E	951	GLU	CD-OE2	5.84	1.32	1.25
1	E	876	GLU	CD-OE2	5.83	1.32	1.25
1	G	604	GLU	CD-OE2	5.83	1.32	1.25
1	E	189	GLU	CD-OE2	5.82	1.32	1.25
1	G	550	GLU	CD-OE2	5.82	1.32	1.25
1	C	771	GLU	CD-OE2	5.82	1.32	1.25
1	C	278	GLU	CD-OE2	5.81	1.32	1.25
1	A	970	GLU	CD-OE2	5.81	1.32	1.25
1	E	67	GLU	CD-OE2	5.81	1.32	1.25
1	E	154	GLU	CD-OE2	5.81	1.32	1.25
1	G	278	GLU	CD-OE2	5.81	1.32	1.25
1	E	278	GLU	CD-OE2	5.81	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	761	GLU	CD-OE2	5.80	1.32	1.25
2	H	71	GLU	CD-OE2	5.80	1.32	1.25
1	C	673	GLU	CD-OE2	5.79	1.32	1.25
1	A	628	GLU	CD-OE2	5.79	1.32	1.25
2	B	29	GLU	CD-OE2	5.79	1.32	1.25
1	E	403	GLU	CD-OE2	5.78	1.32	1.25
1	A	560	GLU	CD-OE2	5.78	1.32	1.25
1	C	628	GLU	CD-OE2	5.77	1.31	1.25
1	G	427	GLU	CD-OE2	5.77	1.31	1.25
1	G	552	GLU	CD-OE2	5.76	1.31	1.25
1	G	79	GLU	CD-OE2	5.76	1.31	1.25
2	F	145	GLU	CD-OE2	5.76	1.31	1.25
1	C	970	GLU	CD-OE2	5.75	1.31	1.25
1	C	560	GLU	CD-OE2	5.74	1.31	1.25
1	E	25	GLU	CD-OE2	5.74	1.31	1.25
1	G	109	GLU	CD-OE2	5.74	1.31	1.25
2	H	161	GLU	CD-OE2	5.74	1.31	1.25
1	A	1067	GLU	CD-OE2	5.72	1.31	1.25
1	C	403	GLU	CD-OE2	5.71	1.31	1.25
1	A	619	GLU	CD-OE2	5.71	1.31	1.25
1	C	189	GLU	CD-OE2	5.71	1.31	1.25
1	E	153[A]	GLU	CD-OE2	5.71	1.31	1.25
1	E	153[B]	GLU	CD-OE2	5.71	1.31	1.25
2	F	375	GLU	CD-OE2	5.71	1.31	1.25
1	G	208	GLU	CD-OE2	5.71	1.31	1.25
2	F	318	GLU	CD-OE2	5.70	1.31	1.25
1	G	103	GLU	CD-OE2	5.70	1.31	1.25
1	E	512	GLU	CD-OE2	5.70	1.31	1.25
1	G	127	GLU	CD-OE2	5.70	1.31	1.25
1	C	40	GLU	CD-OE2	5.68	1.31	1.25
1	C	127	GLU	CD-OE2	5.68	1.31	1.25
1	G	468	GLU	CD-OE2	5.68	1.31	1.25
1	E	577	GLU	CD-OE2	5.68	1.31	1.25
1	G	595	GLU	CD-OE2	5.68	1.31	1.25
1	G	535	GLU	CD-OE2	5.67	1.31	1.25
1	G	219	GLU	CD-OE2	5.66	1.31	1.25
1	E	970	GLU	CD-OE2	5.64	1.31	1.25
1	A	189	GLU	CD-OE2	5.64	1.31	1.25
1	E	334	GLU	CD-OE2	5.63	1.31	1.25
1	A	624	GLU	CD-OE2	5.63	1.31	1.25
2	D	70	GLU	CD-OE2	5.62	1.31	1.25
1	G	154	GLU	CD-OE2	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	349	GLU	CD-OE2	5.62	1.31	1.25
1	A	910	GLU	CD-OE2	5.62	1.31	1.25
1	A	208	GLU	CD-OE2	5.62	1.31	1.25
1	C	67	GLU	CD-OE2	5.62	1.31	1.25
1	C	996	GLU	CD-OE2	5.62	1.31	1.25
1	G	549	GLU	CD-OE2	5.61	1.31	1.25
2	H	260	GLU	CD-OE2	5.61	1.31	1.25
2	H	372	GLU	CD-OE2	5.61	1.31	1.25
1	A	983	GLU	CD-OE2	5.60	1.31	1.25
1	A	59[A]	GLU	CD-OE2	5.59	1.31	1.25
1	A	59[B]	GLU	CD-OE2	5.59	1.31	1.25
1	C	550	GLU	CD-OE2	5.59	1.31	1.25
1	E	103	GLU	CD-OE2	5.58	1.31	1.25
1	E	552	GLU	CD-OE2	5.58	1.31	1.25
2	B	189	GLU	CD-OE2	5.57	1.31	1.25
1	A	761	GLU	CD-OE2	5.57	1.31	1.25
1	A	349	GLU	CD-OE2	5.55	1.31	1.25
1	G	393	GLU	CD-OE2	5.55	1.31	1.25
2	H	189	GLU	CD-OE2	5.55	1.31	1.25
2	B	375	GLU	CD-OE2	5.55	1.31	1.25
1	A	79	GLU	CD-OE2	5.54	1.31	1.25
2	F	161	GLU	CD-OE2	5.54	1.31	1.25
1	C	819	GLU	CD-OE2	5.54	1.31	1.25
1	A	235	GLU	CD-OE2	5.54	1.31	1.25
1	G	970	GLU	CD-OE2	5.54	1.31	1.25
1	G	673	GLU	CD-OE2	5.53	1.31	1.25
1	C	535	GLU	CD-OE2	5.51	1.31	1.25
1	E	726	GLU	CD-OE2	5.51	1.31	1.25
1	G	1060	GLU	CD-OE2	5.51	1.31	1.25
1	E	187	GLU	CD-OE2	5.50	1.31	1.25
2	H	96	GLU	CD-OE2	5.50	1.31	1.25
1	G	983	GLU	CD-OE2	5.48	1.31	1.25
2	D	372	GLU	CD-OE2	5.47	1.31	1.25
1	E	882	GLU	CD-OE2	5.47	1.31	1.25
1	G	334	GLU	CD-OE2	5.47	1.31	1.25
1	E	510	GLU	CD-OE2	5.46	1.31	1.25
1	C	1067	GLU	CD-OE2	5.46	1.31	1.25
2	F	124	GLU	CD-OE2	5.46	1.31	1.25
1	C	190	GLU	CD-OE2	5.45	1.31	1.25
1	G	187	GLU	CD-OE2	5.45	1.31	1.25
1	E	299	GLU	CD-OE2	5.44	1.31	1.25
2	H	10	GLU	CD-OE2	5.43	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	GLU	CD-OE2	5.42	1.31	1.25
1	G	39	GLU	CD-OE2	5.41	1.31	1.25
2	D	41	GLU	CD-OE2	5.41	1.31	1.25
2	F	260	GLU	CD-OE2	5.41	1.31	1.25
1	C	39	GLU	CD-OE2	5.40	1.31	1.25
1	C	841	GLU	CD-OE2	5.40	1.31	1.25
1	E	127	GLU	CD-OE2	5.40	1.31	1.25
1	E	996	GLU	CD-OE2	5.40	1.31	1.25
1	C	926	GLU	CD-OE2	5.39	1.31	1.25
2	B	161	GLU	CD-OE2	5.39	1.31	1.25
1	C	510	GLU	CD-OE2	5.39	1.31	1.25
1	A	278	GLU	CD-OE2	5.38	1.31	1.25
2	H	124	GLU	CD-OE2	5.38	1.31	1.25
2	D	187	GLU	CD-OE2	5.38	1.31	1.25
1	G	771	GLU	CD-OE2	5.37	1.31	1.25
2	B	10	GLU	CD-OE2	5.37	1.31	1.25
1	G	40	GLU	CD-OE2	5.37	1.31	1.25
1	A	819	GLU	CD-OE2	5.36	1.31	1.25
1	C	1060	GLU	CD-OE2	5.35	1.31	1.25
1	A	876	GLU	CD-OE2	5.35	1.31	1.25
1	C	72	GLU	CD-OE2	5.35	1.31	1.25
1	C	235	GLU	CD-OE2	5.35	1.31	1.25
1	C	427	GLU	CD-OE2	5.34	1.31	1.25
1	E	1067	GLU	CD-OE2	5.34	1.31	1.25
2	F	41	GLU	CD-OE2	5.33	1.31	1.25
2	D	10	GLU	CD-OE2	5.33	1.31	1.25
1	C	393	GLU	CD-OE2	5.33	1.31	1.25
1	A	552	GLU	CD-OE2	5.32	1.31	1.25
1	A	916	GLU	CD-OE2	5.32	1.31	1.25
1	A	101	GLU	CD-OE2	5.32	1.31	1.25
1	C	383	GLU	CD-OE2	5.31	1.31	1.25
1	A	419	GLU	CD-OE2	5.31	1.31	1.25
1	C	512	GLU	CD-OE2	5.31	1.31	1.25
1	A	39	GLU	CD-OE2	5.30	1.31	1.25
1	E	142	GLU	CD-OE2	5.30	1.31	1.25
1	G	235	GLU	CD-OE2	5.30	1.31	1.25
1	A	841	GLU	CD-OE1	-5.29	1.19	1.25
1	C	142	GLU	CD-OE2	5.29	1.31	1.25
1	G	383	GLU	CD-OE2	5.28	1.31	1.25
1	A	103	GLU	CD-OE2	5.27	1.31	1.25
1	E	208	GLU	CD-OE2	5.27	1.31	1.25
1	E	619	GLU	CD-OE2	5.27	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	260	GLU	CD-OE2	5.26	1.31	1.25
1	A	215	GLU	CD-OE2	5.26	1.31	1.25
1	G	841	GLU	CD-OE2	5.25	1.31	1.25
1	C	79	GLU	CD-OE2	5.25	1.31	1.25
1	C	683	GLU	CD-OE2	5.24	1.31	1.25
1	E	235	GLU	CD-OE2	5.24	1.31	1.25
2	H	41	GLU	CD-OE2	5.23	1.31	1.25
1	G	761	GLU	CD-OE2	5.23	1.31	1.25
1	E	473	GLU	CD-OE2	5.22	1.31	1.25
1	G	403	GLU	CD-OE2	5.22	1.31	1.25
1	C	604	GLU	CD-OE2	5.21	1.31	1.25
1	C	916	GLU	CD-OE2	5.21	1.31	1.25
2	H	375	GLU	CD-OE2	5.21	1.31	1.25
1	A	260	GLU	CD-OE2	5.20	1.31	1.25
1	C	633	GLU	CD-OE2	5.19	1.31	1.25
1	A	393	GLU	CD-OE2	5.18	1.31	1.25
2	B	96	GLU	CD-OE2	5.18	1.31	1.25
1	A	467	GLU	CD-OE2	5.17	1.31	1.25
1	A	334	GLU	CD-OE2	5.16	1.31	1.25
1	E	110	GLU	CD-OE2	5.16	1.31	1.25
1	G	142	GLU	CD-OE2	5.14	1.31	1.25
1	G	633	GLU	CD-OE2	5.14	1.31	1.25
1	G	916	GLU	CD-OE2	5.14	1.31	1.25
1	A	783	GLU	CD-OE2	5.12	1.31	1.25
1	A	403	GLU	CD-OE2	5.12	1.31	1.25
1	G	1067	GLU	CD-OE2	5.11	1.31	1.25
1	E	274	GLU	CD-OE2	5.11	1.31	1.25
2	D	124	GLU	CD-OE2	5.09	1.31	1.25
1	G	72	GLU	CD-OE2	5.09	1.31	1.25
2	H	29	GLU	CD-OE2	5.08	1.31	1.25
1	C	103	GLU	CD-OE2	5.07	1.31	1.25
2	D	96	GLU	CD-OE2	5.07	1.31	1.25
1	G	189	GLU	CD-OE2	5.07	1.31	1.25
1	G	996	GLU	CD-OE2	5.05	1.31	1.25
1	A	892	GLU	CD-OE2	5.05	1.31	1.25
1	G	560	GLU	CD-OE2	5.04	1.31	1.25
1	E	101	GLU	CD-OE2	5.02	1.31	1.25
1	C	215	GLU	CD-OE2	5.01	1.31	1.25
1	E	955[A]	GLU	CD-OE2	5.01	1.31	1.25
1	E	955[B]	GLU	CD-OE2	5.01	1.31	1.25
1	G	467	GLU	CD-OE2	5.01	1.31	1.25

All (615) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	38	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	E	956	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	642	TYR	CB-CG-CD2	-11.19	114.28	121.00
1	E	43	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	1004	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	G	43	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	G	43	ARG	NE-CZ-NH2	-10.05	115.28	120.30
1	G	104	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	A	642	TYR	CB-CG-CD1	9.86	126.92	121.00
1	C	400	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	A	416	ASP	CB-CG-OD2	-9.64	109.62	118.30
1	E	631	ARG	NE-CZ-NH1	9.44	125.02	120.30
2	F	139	ASP	CB-CG-OD2	-9.32	109.91	118.30
1	C	670	ASP	CB-CG-OD2	-9.29	109.94	118.30
1	E	670	ASP	CB-CG-OD2	-9.27	109.96	118.30
1	C	131	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	C	736	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	G	333	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	A	1004	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	E	579	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	G	956	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	G	944	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	223	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	A	610	TYR	CB-CG-CD2	-8.49	115.90	121.00
2	D	334	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	E	609	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	E	810	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	611	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	G	425	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	416	ASP	CB-CG-OD1	8.27	125.74	118.30
1	G	674	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	C	128	ASP	CB-CG-OD1	8.22	125.69	118.30
1	E	333	ASP	CB-CG-OD2	-8.21	110.91	118.30
2	B	362	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	E	1021	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	G	670	ASP	CB-CG-OD2	-8.13	110.99	118.30
1	G	410	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	E	333	ASP	CB-CG-OD1	8.09	125.58	118.30
1	C	579	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	C	84	ASP	CB-CG-OD1	8.04	125.53	118.30
2	D	211	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	A	373	ARG	NE-CZ-NH2	-8.00	116.30	120.30
2	H	262	ASP	CB-CG-OD2	-8.00	111.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	434	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	579	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	E	1041	ASP	CB-CG-OD1	7.99	125.49	118.30
2	H	97	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	E	912	ARG	NE-CZ-NH1	7.93	124.27	120.30
2	F	120	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	G	667	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	736	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	G	223	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	C	810	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	372	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	G	416	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	C	514	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	625	ASP	CB-CG-OD2	-7.79	111.29	118.30
2	D	368	ASP	CB-CG-OD2	-7.78	111.30	118.30
2	D	211	ASP	CB-CG-OD1	7.74	125.26	118.30
1	A	57	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	G	444	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	128	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	E	765	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	670	ASP	CB-CG-OD2	-7.68	111.39	118.30
2	H	84	ASP	CB-CG-OD1	7.62	125.16	118.30
1	G	169	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	610	TYR	CB-CG-CD1	7.61	125.56	121.00
2	B	50	ARG	NE-CZ-NH1	7.61	124.10	120.30
2	F	317	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	G	333	ASP	CB-CG-OD1	7.54	125.09	118.30
2	F	84	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	C	84	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	A	609	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	128	ASP	CB-CG-OD1	7.52	125.07	118.30
1	C	121	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C	459	ASP	CB-CG-OD2	-7.48	111.57	118.30
2	B	244	ASP	CB-CG-OD1	7.47	125.02	118.30
1	E	416	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	A	609	ASP	CB-CG-OD1	7.46	125.01	118.30
2	B	227	ASP	CB-CG-OD2	-7.45	111.59	118.30
2	B	211	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	G	1021	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	E	223	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	333	ASP	CB-CG-OD1	7.43	124.98	118.30
2	B	249	ASP	CB-CG-OD2	-7.42	111.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	TYR	CB-CG-CD1	-7.41	116.55	121.00
1	A	338	ASP	CB-CG-OD2	-7.41	111.64	118.30
1	G	75	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	B	244	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	G	6	ASP	CB-CG-OD2	-7.39	111.65	118.30
2	B	368	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	C	154	GLU	OE1-CD-OE2	-7.37	114.46	123.30
2	F	45	ASP	CB-CG-OD2	-7.36	111.68	118.30
2	H	136	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	C	400	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	959	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	A	677	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	G	75	ARG	NE-CZ-NH2	-7.28	116.66	120.30
2	D	262	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	G	757	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	E	1003	ASP	CB-CG-OD2	-7.22	111.80	118.30
2	F	188	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	223	ASP	CB-CG-OD1	7.22	124.80	118.30
1	E	128	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	G	238	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	E	614	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	223	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	671	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	G	223	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	246	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	675	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	G	265	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	H	211	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	C	530	ASP	CB-CG-OD1	7.07	124.67	118.30
2	F	212	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	514	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	G	416	ASP	CB-CG-OD1	7.04	124.64	118.30
1	E	972	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	E	246	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	972	ASP	CB-CG-OD2	-7.03	111.97	118.30
2	H	45	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	490	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	E	128	ASP	CB-CG-OD1	6.98	124.58	118.30
1	G	753	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	E	487	ASP	CB-CG-OD2	-6.98	112.02	118.30
2	F	120	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	425	ARG	NE-CZ-NH1	6.93	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	674	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	459	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	C	811	GLN	CB-CA-C	6.92	124.24	110.40
1	G	579	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	753	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	G	238	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	521	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	667	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	E	609	ASP	CB-CG-OD1	6.87	124.48	118.30
1	C	670	ASP	CB-CG-OD1	6.87	124.48	118.30
1	C	769	ASP	CB-CG-OD1	6.87	124.48	118.30
1	E	765	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	A	246	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	G	128	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	C	1003	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	G	185	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	867	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	C	27	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	104	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	G	592	ASP	CB-CG-OD2	-6.83	112.16	118.30
2	B	114	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	E	197	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	G	671	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	G	867	ARG	NE-CZ-NH1	6.81	123.71	120.30
2	H	227	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	E	753	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	611	ASP	CB-CG-OD1	6.81	124.42	118.30
2	D	112	ASP	CB-CG-OD1	6.80	124.42	118.30
1	G	757	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	441	ASP	CB-CG-OD1	6.78	124.41	118.30
2	B	136	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	E	579	ASP	CB-CG-OD1	6.76	124.39	118.30
1	E	611	ASP	CB-CG-OD1	6.76	124.38	118.30
1	G	848	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	B	326	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	75	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	459	ASP	CB-CG-OD1	6.73	124.35	118.30
1	G	434	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	514	ARG	NE-CZ-NH2	-6.71	116.95	120.30
2	D	139	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	G	128	ASP	CB-CG-OD1	6.67	124.30	118.30
2	F	157	ASP	CB-CG-OD1	6.67	124.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	670	ASP	CB-CG-OD1	6.67	124.30	118.30
1	G	499	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	E	631	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	539	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	1003	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	671	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	G	959	ASP	CB-CG-OD1	6.64	124.28	118.30
2	D	188	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	G	222	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	E	959	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	104	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	E	625	ASP	CB-CG-OD2	-6.63	112.34	118.30
2	D	93	ARG	NE-CZ-NH2	-6.61	116.99	120.30
2	H	249	ASP	CB-CG-OD1	6.61	124.25	118.30
1	E	959	ASP	CB-CG-OD2	-6.59	112.36	118.30
2	F	97	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	558	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	57	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	763	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	C	207	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	G	758	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	1021	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	F	101	TYR	CB-CG-CD2	6.54	124.92	121.00
2	H	116	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	G	614	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	121	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	410	ASP	CB-CG-OD2	-6.52	112.43	118.30
2	D	334	ASP	CB-CG-OD1	6.52	124.17	118.30
2	H	93	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	197	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	609	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	H	139	ASP	CB-CG-OD1	6.51	124.16	118.30
1	E	487	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	757	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	807	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	E	161	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	G	675	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	124	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	487	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	E	62	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	E	372	ASP	CB-CG-OD2	-6.45	112.49	118.30
2	H	368	ASP	CB-CG-OD2	-6.45	112.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	G	226	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	1031	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	G	27	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	124	ASP	CB-CG-OD1	6.43	124.09	118.30
1	G	769	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	G	246	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	518	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	410	ASP	CB-CG-OD1	6.42	124.07	118.30
1	G	667	ASP	CB-CG-OD1	6.41	124.06	118.30
1	G	121	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	G	27	ASP	CB-CG-OD1	6.40	124.06	118.30
1	G	487	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	B	262	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	G	675	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	E	677	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	F	317	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	521	ASP	CB-CG-OD1	6.38	124.04	118.30
1	G	558	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	6	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	530	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	514	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	G	62	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	F	227	ASP	CB-CG-OD1	6.36	124.03	118.30
1	E	43	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	62	ASP	CB-CG-OD1	6.35	124.02	118.30
2	H	188	ASP	CB-CG-OD1	6.35	124.01	118.30
1	E	611	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	G	674	ASP	CB-CG-OD1	6.34	124.00	118.30
1	C	161	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	G	338	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	C	716	PRO	N-CA-CB	6.32	110.89	103.30
1	G	609	ASP	CB-CG-OD1	6.32	123.99	118.30
1	C	258	ASP	CB-CG-OD1	6.32	123.99	118.30
2	D	139	ASP	CB-CG-OD1	6.32	123.98	118.30
1	E	265	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	B	93	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	C	614	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	959	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	G	609	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	E	207	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	E	197	ASP	CB-CG-OD1	6.30	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	161	ASP	CB-CG-OD2	-6.29	112.63	118.30
1	C	223	ASP	CB-CG-OD1	6.28	123.95	118.30
1	G	460	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	C	273	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	E	592	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	G	246	ASP	CB-CG-OD1	6.26	123.93	118.30
2	H	139	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	999	PRO	N-CA-CB	6.26	110.81	103.30
1	G	614	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	B	317	ASP	CB-CG-OD1	6.23	123.90	118.30
1	G	539	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	E	246	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	E	539	ASP	CB-CG-OD2	-6.21	112.71	118.30
2	F	84	ASP	CB-CG-OD1	6.21	123.89	118.30
2	B	157	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	57	ASP	CB-CG-OD1	6.20	123.88	118.30
2	F	67	ASP	CB-CG-OD2	-6.19	112.72	118.30
1	A	867	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	226	ASP	CB-CG-OD1	6.18	123.86	118.30
2	B	48	TYR	CB-CG-CD1	6.18	124.71	121.00
2	H	342	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	B	188	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	487	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	G	373	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	G	133	ASP	CB-CG-OD1	6.16	123.84	118.30
1	C	579	ASP	CB-CG-OD1	6.15	123.84	118.30
2	H	215	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	B	188	ASP	CB-CG-OD1	6.15	123.83	118.30
1	G	625	ASP	CB-CG-OD1	6.15	123.83	118.30
1	E	559	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	C	823	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	F	227	ASP	CB-CG-OD2	-6.13	112.78	118.30
2	B	97	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	G	410	ASP	CB-CG-OD1	6.13	123.82	118.30
2	D	97	ASP	CB-CG-OD1	6.13	123.82	118.30
1	G	6	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	904	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	E	28	TYR	CB-CG-CD1	6.13	124.68	121.00
1	G	956	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	82	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	G	571	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	E	372	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	PRO	N-CA-CB	6.11	110.63	103.30
1	C	6	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	416	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	G	716	PRO	N-CA-CB	6.10	110.62	103.30
2	H	84	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	E	194	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	733	ASP	CB-CG-OD2	-6.08	112.83	118.30
2	D	112	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	G	133	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	6	ASP	CB-CG-OD1	6.06	123.75	118.30
2	B	211	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	42	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	C	6	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	592	ASP	CB-CG-OD2	-6.04	112.86	118.30
2	D	344	ASP	CB-CG-OD2	-6.04	112.86	118.30
2	H	262	ASP	CB-CG-OD1	6.04	123.74	118.30
2	F	45	ASP	CB-CG-OD1	6.04	123.73	118.30
1	C	769	ASP	CB-CG-OD2	-6.04	112.87	118.30
2	F	244	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	E	716	PRO	N-CA-CB	6.03	110.53	103.30
2	H	334	ASP	CB-CG-OD2	-6.03	112.88	118.30
2	F	344	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	579	ASP	CB-CG-OD1	6.02	123.72	118.30
2	H	116	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	558	ASP	N-CA-CB	-6.02	99.77	110.60
2	F	101	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	84	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	944	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	950	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	226	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	75	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	389	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	H	112	ASP	CB-CG-OD1	5.98	123.68	118.30
1	E	226	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	121	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	E	674	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	E	410	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	E	675	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	38	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	E	517	ARG	NE-CZ-NH2	-5.95	117.32	120.30
2	D	84	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	G	733	ASP	CB-CG-OD2	-5.94	112.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	625	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	133	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	509	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	G	972	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	A	133	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	E	807	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	518	ASP	CB-CG-OD1	5.90	123.61	118.30
2	H	344	ASP	CB-CG-OD1	5.90	123.61	118.30
1	E	133	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	G	84	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	490	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	592	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	E	810	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	528	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	G	989	ARG	NE-CZ-NH1	-5.88	117.36	120.30
2	H	97	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	194	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	670	ASP	CB-CG-OD1	5.87	123.58	118.30
2	D	368	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	667	ASP	CB-CG-OD1	5.86	123.57	118.30
1	G	791	ASP	CB-CG-OD1	5.86	123.57	118.30
1	E	490	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	H	249	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	E	730	ASP	CB-CG-OD2	-5.85	113.03	118.30
2	D	317	ASP	CB-CG-OD1	5.85	123.56	118.30
1	E	38	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	D	362	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	C	441	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	C	154	GLU	CG-CD-OE1	5.82	129.95	118.30
1	C	972	ASP	CB-CG-OD2	-5.81	113.07	118.30
2	D	148	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	F	136	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	E	956	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	197	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	H	67	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	42	TYR	CB-CG-CD2	5.79	124.48	121.00
1	E	614	ASP	CB-CG-OD1	5.78	123.50	118.30
1	G	82	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	223	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	F	97	ASP	CB-CG-OD1	5.78	123.50	118.30
1	G	487	ASP	CB-CG-OD1	5.77	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	139	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	124	ASP	CB-CG-OD1	5.77	123.49	118.30
2	D	344	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	471	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	670	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C	410	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	C	530	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	C	450	ASP	CB-CG-OD2	-5.74	113.13	118.30
2	B	97	ASP	CB-CG-OD1	5.74	123.46	118.30
1	C	434	ASP	CB-CG-OD1	5.74	123.46	118.30
2	H	136	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	124	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	425	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	G	57	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	E	677	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	G	758	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	B	136	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	1003	ASP	CB-CG-OD1	5.69	123.42	118.30
1	E	530	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	G	791	ASP	CB-CG-OD2	-5.68	113.18	118.30
2	H	114	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	H	227	ASP	CB-CG-OD1	5.68	123.41	118.30
1	E	416	ASP	CB-CG-OD1	5.68	123.41	118.30
1	E	733	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	G	944	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	H	334	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	410	ASP	CB-CG-OD1	5.66	123.40	118.30
1	G	1041	ASP	CB-CG-OD2	-5.66	113.21	118.30
2	F	188	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	238	ASP	CB-CG-OD1	5.66	123.39	118.30
1	E	625	ASP	CB-CG-OD1	5.65	123.38	118.30
1	E	830	PHE	CB-CG-CD1	-5.64	116.85	120.80
2	B	249	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	753	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	B	344	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	194	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	E	459	ASP	CB-CG-OD1	5.62	123.36	118.30
2	D	136	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	757	ASP	CB-CG-OD1	5.62	123.36	118.30
1	G	671	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	684	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	G	121	ASP	CB-CG-OD1	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	373	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	E	27	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	715	ARG	CG-CD-NE	5.58	123.52	111.80
1	E	459	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	F	139	ASP	CB-CG-OD1	5.58	123.32	118.30
2	B	84	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	559	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	G	303	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	317	ASP	CB-CG-OD2	-5.57	113.28	118.30
2	F	262	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	43	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	197	ASP	CB-CG-OD1	5.56	123.31	118.30
1	E	27	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	400	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	G	1004	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	757	ASP	CB-CG-OD1	5.55	123.30	118.30
1	C	1021	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	372	ASP	CB-CG-OD2	-5.54	113.31	118.30
2	D	227	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	E	517	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	736	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	G	4	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	E	373	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	E	791	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	434	ASP	CB-CG-OD1	5.52	123.27	118.30
2	B	227	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	197	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	H	67	ASP	CB-CG-OD1	5.51	123.26	118.30
2	H	45	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	C	128	ASP	CB-CG-OD2	-5.50	113.34	118.30
1	C	736	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	131	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	130	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	124	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	E	558	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	G	590	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	558	ASP	CB-CG-OD1	5.47	123.22	118.30
1	G	39	GLU	CB-CA-C	-5.47	99.47	110.40
1	G	57	ASP	CB-CG-OD1	5.47	123.22	118.30
1	G	611	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	434	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	B	344	ASP	CB-CG-OD1	5.46	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	69	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	161	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	C	226	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	571	ARG	N-CA-CB	5.44	120.39	110.60
1	C	4	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	F	157	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	258	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	C	674	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	608	THR	CA-CB-CG2	-5.43	104.80	112.40
1	C	625	ASP	CB-CG-OD2	-5.42	113.42	118.30
2	B	334	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	E	530	ASP	CB-CG-OD1	5.42	123.18	118.30
1	E	730	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	867	ARG	NE-CZ-NH2	-5.41	117.60	120.30
2	D	262	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	609	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	207	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	287	ALA	N-CA-CB	5.38	117.63	110.10
2	F	234	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	344	THR	CA-CB-CG2	-5.38	104.88	112.40
1	G	460	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	E	1041	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	807	ASP	CB-CG-OD1	5.36	123.13	118.30
1	C	338	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	C	338	ASP	CB-CG-OD1	5.36	123.12	118.30
1	G	343	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	G	82	ARG	CG-CD-NE	-5.35	100.56	111.80
1	G	807	ASP	CB-CG-OD1	5.35	123.12	118.30
1	E	133	ASP	CB-CG-OD1	5.35	123.11	118.30
1	E	904	ASP	CB-CG-OD2	-5.35	113.48	118.30
2	F	136	ASP	CB-CG-OD1	5.35	123.11	118.30
1	E	161	ASP	CB-CG-OD1	5.34	123.11	118.30
1	E	471	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	B	114	ASP	CB-CG-OD1	5.34	123.10	118.30
1	G	972	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	333	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	E	434	ASP	CB-CG-OD1	5.33	123.10	118.30
2	F	378	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	D	326	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	E	757	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	726	GLU	N-CA-CB	5.33	120.19	110.60
1	E	1003	ASP	CB-CG-OD1	5.33	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	953	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	G	131	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	320	THR	CA-CB-CG2	-5.32	104.95	112.40
1	E	674	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	1025	ASP	CB-CG-OD1	5.32	123.09	118.30
1	E	807	ASP	CB-CG-OD1	5.32	123.08	118.30
1	G	592	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	104	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	416	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	389	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	E	62	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	758	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	H	368	ASP	CB-CG-OD1	5.31	123.08	118.30
2	F	372	GLU	CB-CA-C	-5.31	99.79	110.40
1	G	1020	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	F	368	ASP	CB-CG-OD2	-5.29	113.53	118.30
2	B	139	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	592	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	258	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	G	959	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	F	262	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	258	ASP	CB-CG-OD1	5.28	123.06	118.30
1	C	373	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	238	ASP	CB-CG-OD1	5.27	123.04	118.30
2	F	67	ASP	CB-CG-OD1	5.27	123.04	118.30
2	F	114	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	G	922	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	B	368	ASP	CB-CG-OD1	5.26	123.04	118.30
2	F	344	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	G	131	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	617	TYR	CB-CG-CD1	5.26	124.16	121.00
1	G	450	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	1031	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	753	ASP	CB-CG-OD1	5.25	123.02	118.30
1	G	338	ASP	CB-CG-OD1	5.25	123.02	118.30
2	B	50	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	C	222	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	D	114	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	998	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	62	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	539	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	E	238	ASP	CB-CG-OD2	-5.24	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	197	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	E	944	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	521	ASP	CB-CG-OD1	5.23	123.00	118.30
2	F	234	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	E	129	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	1025	ASP	CB-CG-OD1	5.22	123.00	118.30
2	B	67	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	522	LEU	CB-CA-C	5.22	120.11	110.20
1	E	438	TYR	CB-CG-CD1	5.21	124.13	121.00
1	C	425	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	557	THR	C-N-CA	5.21	134.72	121.70
1	C	110	GLU	OE1-CD-OE2	5.20	129.54	123.30
2	D	244	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	944	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	434	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	343	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	121	ASP	CB-CG-OD1	5.19	122.97	118.30
2	D	244	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	F	10	GLU	CB-CA-C	-5.18	100.03	110.40
1	A	610	TYR	N-CA-CB	5.18	119.92	110.60
1	C	1041	ASP	CB-CG-OD1	5.17	122.96	118.30
2	D	136	ASP	CB-CG-OD1	5.17	122.96	118.30
1	E	514	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	E	441	ASP	CB-CG-OD1	5.16	122.95	118.30
1	G	1041	ASP	CB-CG-OD1	5.16	122.94	118.30
2	H	112	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	H	362	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	1036	TYR	CB-CG-CD1	5.14	124.08	121.00
1	C	460	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	517	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	207	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	471	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	400	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	H	50	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	430	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	333	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	807	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	G	1003	ASP	CB-CG-OD1	5.11	122.89	118.30
1	G	904	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	D	326	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	758	ASP	CB-CG-OD2	-5.09	113.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	912	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	E	6	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	D	215	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	G	769	ASP	CB-CG-OD1	5.09	122.88	118.30
2	H	326	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	728	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	G	528	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	338	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	830	PHE	CB-CA-C	-5.08	100.25	110.40
2	D	67	ASP	CB-CG-OD1	5.07	122.87	118.30
1	C	129	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	D	188	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	912	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	G	81	GLU	CG-CD-OE2	-5.05	108.21	118.30
1	A	733	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	558	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	C	145	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	614	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	956	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	D	299	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	226	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	972	ASP	CB-CG-OD1	5.01	122.81	118.30
2	F	368	ASP	CB-CG-OD1	5.01	122.81	118.30
2	B	48	TYR	CB-CG-CD2	-5.00	118.00	121.00
1	C	953	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	E	124	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8181	0	8215	216	0
1	C	8172	0	8206	231	0
1	E	8204	0	8235	208	0
1	G	8160	0	8196	256	0
2	B	2912	0	2874	84	0
2	D	2907	0	2866	90	0
2	F	2905	0	2864	84	0
2	H	2905	0	2864	109	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	7	0	0	1	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	1	0
5	B	1	0	0	0	0
5	C	5	0	0	1	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
5	F	1	0	0	0	0
5	G	4	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	1	0
6	E	5	0	0	0	0
6	G	5	0	0	1	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	4	0
7	G	54	0	24	4	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	1	0
10	A	841	0	0	23	0
10	B	230	0	0	5	0
10	C	783	0	0	20	0
10	D	304	0	0	8	0
10	E	886	0	0	20	0
10	F	263	0	0	1	0
10	G	678	0	0	13	0
10	H	191	0	0	4	0
All	All	48896	0	44540	1267	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1267) 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:E:46:LEU:HD22	1:E:46:LEU:O	1.37	1.20
1:A:46:LEU:O	1:A:46:LEU:HD22	1.42	1.18
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.27	1.14
2:D:228:VAL:HA	2:D:231:MET:HE2	1.26	1.10
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.32	1.09
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.27	1.07
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.36	1.07
1:G:46:LEU:HD11	1:G:64:THR:HG23	1.36	1.06
1:E:46:LEU:HD21	1:E:64:THR:HG23	1.37	1.06
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.45	0.98
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.29	0.97
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.48	0.95
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.49	0.94
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.49	0.94
1:C:38[A]:ARG:HG3	1:C:38[A]:ARG:HH11	1.29	0.94
1:A:784:GLN:HE21	1:A:784:GLN:H	1.16	0.94
1:A:46:LEU:O	1:A:46:LEU:CD2	2.17	0.93
2:D:50:ARG:HH11	2:D:158:LEU:HD22	1.35	0.92
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.16	0.91
1:E:46:LEU:O	1:E:46:LEU:CD2	2.18	0.90
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.54	0.90
1:E:1:MET:H2	1:E:224:LYS:NZ	1.68	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.54	0.89
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.07	0.89
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.53	0.89
1:G:901:PRO:HD2	5:G:5084:CL:CL	2.08	0.89
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.02	0.89
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.51	0.89
1:E:1:MET:N	1:E:224:LYS:HZ1	1.72	0.87
1:E:728:VAL:CG1	1:E:733:ASP:HB3	2.04	0.87
1:E:1:MET:H2	1:E:224:LYS:HZ1	0.91	0.86
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.89	0.86
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.10	0.86
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.06	0.86
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.56	0.85
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.05	0.85
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.58	0.85
1:E:146:SER:HB2	1:E:205:LEU:HD11	1.58	0.85
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.55	0.85
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.56	0.84
2:F:259:LEU:HD13	2:F:342:ARG:NH1	1.91	0.84
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.59	0.84
1:A:46:LEU:CD2	1:A:46:LEU:C	2.44	0.84
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.57	0.84
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.56	0.84
1:G:698:ILE:HD12	1:G:698:ILE:H	1.43	0.83
1:A:46:LEU:HD21	1:A:64:THR:HG23	1.59	0.82
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.95	0.82
1:E:46:LEU:HD22	1:E:46:LEU:C	2.00	0.82
2:B:187:GLU:HG2	2:B:215[A]:ARG:HD2	1.61	0.82
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.61	0.81
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.63	0.81
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.46	0.81
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.15	0.81
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.43	0.81
2:B:324:ASN:HD22	2:B:324:ASN:N	1.76	0.80
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.45	0.80
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.10	0.80
1:E:994:VAL:HG13	1:E:1000:HIS:ND1	1.97	0.80
2:F:228:VAL:HA	2:F:231:MET:CE	2.12	0.79
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.63	0.79
1:C:46:LEU:HD12	1:C:46:LEU:C	2.03	0.79
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:GLU:O	2:B:203:ARG:HG3	1.83	0.78
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.66	0.78
1:E:1:MET:N	1:E:224:LYS:NZ	2.30	0.78
1:A:726:GLU:HG3	1:A:727:ILE:H	1.47	0.78
1:E:994:VAL:HG13	1:E:1000:HIS:CE1	2.19	0.78
1:G:784:GLN:H	1:G:784:GLN:HE21	1.29	0.77
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.66	0.77
1:G:873:SER:O	1:G:877:GLN:HG3	1.85	0.77
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.84	0.77
4:E:5053:K:K	10:E:5816:HOH:O	1.94	0.77
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.20	0.77
1:E:46:LEU:CD2	1:E:46:LEU:C	2.50	0.77
1:E:1001:ILE:HD12	1:E:1002:GLN:N	1.99	0.76
1:C:951:GLU:O	1:C:954:LYS:HB3	1.86	0.76
1:A:46:LEU:HD22	1:A:46:LEU:C	2.02	0.76
1:A:873:SER:O	1:A:877:GLN:HG3	1.85	0.76
2:D:185:LYS:HD3	2:D:190:LEU:HD21	1.66	0.76
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.68	0.76
2:D:322:PRO:HB2	2:D:324:ASN:ND2	2.01	0.76
1:C:882:GLU:HB2	10:C:5495:HOH:O	1.84	0.76
1:E:967[A]:GLN:HG3	1:E:1054:LEU:HD13	1.68	0.75
1:A:784:GLN:H	1:A:784:GLN:NE2	1.83	0.75
1:G:936:ASN:HB2	10:G:3407:HOH:O	1.86	0.75
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.68	0.75
2:F:322:PRO:HB2	2:F:324:ASN:ND2	2.01	0.75
2:H:322:PRO:HB2	2:H:324:ASN:ND2	2.02	0.75
1:E:734:LEU:HD12	1:E:734:LEU:O	1.87	0.74
2:F:228:VAL:HA	2:F:231:MET:HE3	1.70	0.74
1:G:784:GLN:H	1:G:784:GLN:NE2	1.85	0.74
1:C:734:LEU:O	1:C:734:LEU:HD12	1.88	0.74
1:G:967:GLN:HG3	1:G:1054:LEU:HD13	1.67	0.73
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.04	0.73
2:B:286:MET:HE1	2:B:315:ALA:HB2	1.69	0.73
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.18	0.73
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.24	0.72
2:H:187:GLU:HG2	2:H:215:ARG:CD	2.18	0.72
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.03	0.72
2:B:325:LEU:O	10:B:5179:HOH:O	2.06	0.72
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.71	0.72
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.04	0.72
1:A:646:THR:HB	1:A:647:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:784:GLN:H	1:E:784:GLN:HE21	1.35	0.72
1:E:736:ARG:NH2	10:E:5947:HOH:O	2.22	0.72
1:A:375:THR:HG23	1:A:377:GLN:H	1.54	0.72
1:C:772:MET:SD	1:C:880:THR:HG22	2.30	0.72
1:E:151:THR:OG1	1:E:153[B]:GLU:HG2	1.90	0.71
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.04	0.71
1:A:313:LYS:HE2	1:A:608:THR:O	1.88	0.71
1:G:1001:ILE:HD12	1:G:1002:GLN:N	2.06	0.71
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.72	0.71
2:D:228:VAL:CA	2:D:231:MET:HE2	2.15	0.71
2:H:300:VAL:HG22	2:H:328:THR:O	1.90	0.71
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.73	0.70
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.73	0.70
1:C:784:GLN:H	1:C:784:GLN:HE21	1.37	0.70
1:A:734:LEU:HD12	1:A:734:LEU:O	1.92	0.69
1:A:751:LEU:HD23	10:A:5738:HOH:O	1.92	0.69
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.73	0.69
2:H:269:143:HE	2:H:312:HIS:HB3	1.74	0.69
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.73	0.69
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.22	0.69
1:G:687:LEU:HD13	1:G:812:GLN:HG2	1.73	0.69
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.28	0.69
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.28	0.69
1:C:954:LYS:HB2	10:C:5808:HOH:O	1.92	0.69
1:C:46:LEU:HD12	1:C:46:LEU:O	1.92	0.69
1:G:734:LEU:HD12	1:G:734:LEU:O	1.92	0.69
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.28	0.68
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.56	0.68
2:F:186:LYS:O	2:F:189:GLU:HB2	1.93	0.68
1:A:950:ARG:HD3	10:A:5560:HOH:O	1.94	0.68
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.08	0.68
2:F:187:GLU:CG	2:F:215:ARG:HD2	2.20	0.68
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.94	0.68
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.23	0.68
1:C:548:GLU:OE1	2:D:114:ASP:HA	1.92	0.68
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.58	0.68
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.29	0.67
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.77	0.67
1:A:1021:ARG:HG3	1:A:1021:ARG:HH11	1.60	0.67
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.29	0.67
1:C:802:SER:O	1:C:806:GLN:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.10	0.67
1:G:726:GLU:HG3	1:G:727:ILE:N	2.09	0.67
1:E:784:GLN:H	1:E:784:GLN:NE2	1.92	0.67
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.95	0.67
1:C:416:ASP:O	1:C:418:PRO:HD3	1.94	0.67
2:B:324:ASN:ND2	2:B:324:ASN:N	2.44	0.67
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.76	0.66
1:A:681:ALA:O	1:A:685:LEU:HG	1.95	0.66
2:F:324:ASN:N	2:F:324:ASN:HD22	1.94	0.66
1:E:468:GLU:HG3	10:E:5429:HOH:O	1.95	0.66
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.78	0.66
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.77	0.66
1:A:715:ARG:HB3	10:A:5668:HOH:O	1.96	0.66
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.60	0.66
1:A:997:GLY:O	1:A:998:ARG:HG3	1.96	0.66
1:C:82:ARG:NH1	10:C:5109:HOH:O	2.26	0.66
1:E:703:GLU:O	1:E:706:LYS:HB2	1.96	0.66
1:G:64:THR:O	1:G:1065:VAL:HG23	1.96	0.65
2:B:324:ASN:HD22	2:B:324:ASN:H	1.44	0.65
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.31	0.65
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.29	0.65
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.28	0.65
1:E:645:GLN:HG3	10:E:5756:HOH:O	1.96	0.65
1:C:559:ARG:NH1	10:C:5704:HOH:O	2.29	0.65
2:H:186:LYS:O	2:H:189:GLU:HB2	1.96	0.65
2:B:259:LEU:HD13	2:B:342:ARG:NH1	2.11	0.65
2:F:248:CYS:O	2:F:252:ILE:HD12	1.96	0.65
1:C:509:ARG:NH1	1:C:512:GLU:OE1	2.29	0.65
1:E:278:GLU:HG2	10:E:5679:HOH:O	1.96	0.65
1:C:698:ILE:HD12	1:C:698:ILE:H	1.60	0.65
1:C:865:ALA:O	1:C:869:MET:HG3	1.97	0.65
1:G:712:LEU:HD23	1:G:752:LEU:HG	1.79	0.65
1:G:539:ASP:HB2	10:G:3694:HOH:O	1.96	0.64
1:C:130:ARG:HB2	1:C:148:ILE:CD1	2.27	0.64
1:G:166:CYS:C	1:G:167:ILE:HD12	2.18	0.64
2:B:298:LYS:HE2	2:B:303:ASN:OD1	1.96	0.64
1:C:313:LYS:HE2	1:C:608:THR:O	1.96	0.64
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.78	0.64
1:G:698:ILE:HD12	1:G:698:ILE:N	2.12	0.64
1:C:902:GLY:O	1:C:1027:ARG:NH2	2.30	0.64
1:A:358:LYS:HD2	1:A:383:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:5012:NET:H22	9:A:5012:NET:H42	1.80	0.64
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.96	0.64
1:C:110:GLU:OE2	10:C:5132:HOH:O	2.14	0.64
1:G:667:ASP:OD2	1:G:677:ARG:NH2	2.30	0.64
1:A:954:LYS:O	1:A:980:VAL:HG11	1.98	0.64
1:C:675:ARG:H	1:C:675:ARG:CD	2.08	0.64
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.79	0.64
1:G:701:ALA:O	1:G:705:ALA:N	2.30	0.64
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.78	0.64
1:C:809:MET:O	1:C:813:VAL:HG23	1.98	0.64
1:C:998:ARG:CB	1:C:999:PRO:HA	2.27	0.64
1:A:804:GLU:HB3	10:A:5750:HOH:O	1.98	0.63
1:C:873:SER:O	1:C:877:GLN:HG3	1.98	0.63
1:A:471:ARG:HB2	10:A:5388:HOH:O	1.98	0.63
2:F:324:ASN:HD22	2:F:324:ASN:H	1.45	0.63
2:B:272:HIS:ND1	2:B:349:SER:OG	2.30	0.63
2:B:338:GLN:NE2	10:B:5234:HOH:O	2.24	0.63
1:C:973:ALA:O	1:C:991:VAL:HG12	1.98	0.63
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.34	0.63
2:H:299:ASP:OD1	2:H:302:LYS:HD2	1.98	0.63
2:D:78:GLN:NE2	10:D:1782:HOH:O	2.29	0.63
1:G:710:TYR:HB3	1:G:729:TYR:O	1.99	0.63
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.81	0.63
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.98	0.63
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.81	0.63
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.80	0.63
2:F:223:THR:CG2	2:F:228:VAL:HG23	2.29	0.62
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.33	0.62
1:G:1004:ARG:O	1:G:1009:GLU:HG3	1.99	0.62
2:H:275:LEU:HD23	2:H:349:SER:OG	1.98	0.62
2:F:324:ASN:O	2:F:342:ARG:HD2	2.00	0.62
1:G:46:LEU:C	1:G:46:LEU:HD12	2.20	0.62
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.34	0.62
2:D:228:VAL:HA	2:D:231:MET:CE	2.18	0.62
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.00	0.62
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.27	0.62
2:H:324:ASN:HD22	2:H:324:ASN:H	1.48	0.62
2:F:46:PRO:O	2:F:242:PRO:HG3	2.00	0.62
1:C:726:GLU:HG3	1:C:727:ILE:H	1.65	0.62
2:D:228:VAL:O	2:D:231:MET:N	2.29	0.62
1:G:646:THR:HB	1:G:647:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1030:ARG:HH11	1:G:1030:ARG:HG3	1.64	0.62
1:A:816:LEU:HD11	1:A:839:LEU:HD21	1.82	0.62
1:E:954:LYS:O	1:E:980:VAL:HG11	2.00	0.62
2:H:34:THR:HA	2:H:56:THR:OG1	1.99	0.62
1:E:734:LEU:HD11	1:E:738:PHE:CE2	2.34	0.62
2:H:344:ASP:OD2	2:H:344:ASP:N	2.30	0.62
1:E:736:ARG:HH21	1:E:1020:ARG:HG2	1.65	0.61
1:C:267:ALA:O	1:C:271:VAL:HG23	2.00	0.61
1:E:4:ARG:HA	10:E:5629:HOH:O	2.00	0.61
1:A:89:THR:O	1:A:304:VAL:HG22	2.00	0.61
2:B:135:GLY:O	2:B:138:PRO:HD3	2.00	0.61
2:B:324:ASN:ND2	2:B:324:ASN:H	1.95	0.61
1:C:562:ILE:HG21	1:C:589:LEU:HD13	1.81	0.61
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.65	0.61
2:F:228:VAL:HA	2:F:231:MET:HE2	1.81	0.61
1:G:267:ALA:O	1:G:271:VAL:HG23	1.99	0.61
1:A:481:ILE:HG22	10:A:5397:HOH:O	2.00	0.61
2:B:190:LEU:HB2	2:B:215[B]:ARG:HB3	1.81	0.61
1:C:703:GLU:O	1:C:706:LYS:HB2	2.00	0.61
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.80	0.61
1:A:948:SER:O	1:A:1015:ASN:HA	2.00	0.61
2:B:186:LYS:O	2:B:189:GLU:HB2	2.01	0.61
1:E:950:ARG:HD3	10:E:5603:HOH:O	2.00	0.61
1:G:202:LYS:HG3	10:G:3585:HOH:O	2.00	0.61
1:A:726:GLU:HG3	1:A:727:ILE:N	2.13	0.61
1:A:738:PHE:O	1:A:741:ALA:HB3	2.01	0.61
2:B:275:LEU:HD23	2:B:349:SER:HB3	1.81	0.61
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.30	0.61
1:C:1017:THR:HG22	1:C:1023:ILE:HG13	1.83	0.61
1:G:101:GLU:OE2	1:G:104:ARG:NH2	2.29	0.61
1:G:698:ILE:H	1:G:698:ILE:CD1	2.11	0.61
1:G:1030:ARG:HG3	1:G:1030:ARG:NH1	2.14	0.61
2:H:249:ASP:OD2	2:H:250:TYR:N	2.31	0.61
1:A:1:MET:H1	1:A:224:LYS:HE3	1.66	0.61
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.31	0.61
1:G:809:MET:O	1:G:813:VAL:HG23	1.99	0.61
1:A:471:ARG:HD2	10:A:5687:HOH:O	2.00	0.61
1:A:1000:HIS:CD2	1:A:1002[B]:GLN:HB3	2.36	0.61
1:E:1000:HIS:O	1:E:1004[B]:ARG:HG3	2.01	0.61
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.31	0.61
1:A:991:VAL:HG23	1:A:1004:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:757:ASP:O	1:E:833:LYS:NZ	2.29	0.60
1:A:1073:LYS:NZ	10:A:5860:HOH:O	2.33	0.60
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.48	0.60
1:E:103:GLU:HG3	1:E:104:ARG:N	2.15	0.60
1:E:1021:ARG:HH11	1:E:1021:ARG:CG	2.14	0.60
2:H:78:GLN:NE2	10:H:4012:HOH:O	2.34	0.60
1:A:1021:ARG:HH11	1:A:1021:ARG:CG	2.14	0.60
2:H:324:ASN:HD22	2:H:324:ASN:N	1.99	0.60
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.82	0.60
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.49	0.60
1:G:1:MET:HA	1:G:224:LYS:HE3	1.83	0.60
1:A:822:VAL:O	1:A:823:ARG:HD3	2.02	0.60
1:E:997:GLY:C	1:E:998[B]:ARG:HG3	2.22	0.60
2:H:269:143:HE	2:H:312:HIS:CB	2.30	0.60
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.82	0.60
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.84	0.60
1:A:944:ARG:HD3	1:A:972:ASP:OD1	2.02	0.60
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.17	0.60
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.83	0.60
1:C:64:THR:O	1:C:1065:VAL:HG23	2.01	0.59
1:C:447:LEU:HD23	1:G:447:LEU:HD23	1.84	0.59
1:A:115:MET:HG2	1:A:118:ALA:O	2.03	0.59
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.84	0.59
2:B:249:ASP:OD2	2:B:250:TYR:N	2.33	0.59
1:E:698:ILE:O	1:E:702:VAL:HG23	2.03	0.59
2:B:225:ALA:O	2:B:228:VAL:HB	2.02	0.59
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.84	0.59
1:E:65:TYR:OH	1:E:80:LYS:HE2	2.03	0.59
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.02	0.59
1:C:695:VAL:CG1	1:C:701:ALA:HB2	2.17	0.59
1:E:710:TYR:HB3	1:E:729:TYR:O	2.03	0.59
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.17	0.59
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.85	0.59
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.84	0.59
2:D:226:GLU:O	2:D:230:LYS:HG3	2.02	0.59
2:H:286:MET:HE3	2:H:312:HIS:ND1	2.18	0.59
1:A:419:GLU:HB2	10:A:5681:HOH:O	2.02	0.59
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.33	0.59
2:F:195:VAL:CG2	2:F:233:PRO:HB3	2.29	0.59
1:G:1019:GLY:O	1:G:1023:ILE:HG13	2.03	0.59
1:G:1021:ARG:HG3	1:G:1021:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:THR:OG1	1:A:376:THR:N	2.35	0.58
1:G:343:ARG:HB3	10:G:4159:HOH:O	2.02	0.58
1:C:38[A]:ARG:HG3	1:C:38[A]:ARG:NH1	2.03	0.58
1:A:150:HIS:N	1:A:154:GLU:OE2	2.37	0.58
1:C:563:MET:CE	1:C:635:PRO:HG3	2.32	0.58
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.68	0.58
1:G:1021:ARG:HH11	1:G:1021:ARG:CG	2.16	0.58
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.85	0.58
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.33	0.58
2:D:233:PRO:HG2	2:D:263:ILE:HD13	1.85	0.58
1:E:130:ARG:HG3	1:E:148:ILE:HG13	1.85	0.58
2:F:218:ILE:HD13	2:F:218:ILE:N	2.18	0.58
1:G:687:LEU:CD1	1:G:812:GLN:HG2	2.34	0.58
1:A:1000:HIS:CD2	1:A:1002[A]:GLN:HB3	2.39	0.58
2:D:222:GLN:NE2	10:D:2212:HOH:O	2.26	0.58
1:E:967[B]:GLN:HG2	1:E:1054:LEU:HD13	1.84	0.58
1:C:950:ARG:HD3	10:C:5578:HOH:O	2.02	0.58
1:A:730:ASP:H	1:A:733:ASP:HB2	1.67	0.57
2:B:259:LEU:HD13	2:B:342:ARG:HH12	1.69	0.57
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.33	0.57
1:C:702:VAL:O	1:C:705:ALA:HB3	2.04	0.57
1:C:1061:LYS:HG2	10:C:5552:HOH:O	2.04	0.57
2:D:27:VAL:O	2:D:78:GLN:HG2	2.05	0.57
1:G:738:PHE:O	1:G:741:ALA:HB3	2.04	0.57
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.39	0.57
2:B:78:GLN:NE2	2:B:78:GLN:HA	2.19	0.57
1:E:1:MET:HB3	1:E:2:PRO:HD3	1.87	0.57
1:A:695:VAL:CG2	1:A:752:LEU:HD22	2.34	0.57
1:C:671:ARG:HG2	1:C:677:ARG:NH1	2.20	0.57
2:H:152:GLY:O	2:H:156:MET:HE3	2.05	0.57
1:C:43:ARG:NH2	1:C:81:GLU:OE2	2.36	0.57
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.40	0.57
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.29	0.57
1:A:489:LEU:HD22	1:A:516:LEU:HD23	1.87	0.57
1:C:130:ARG:HB2	1:C:148:ILE:HD12	1.86	0.57
2:F:232:ASN:N	2:F:233:PRO:HD3	2.18	0.57
1:G:954:LYS:O	1:G:957:VAL:HG12	2.05	0.57
2:H:103:LYS:NZ	10:H:3999:HOH:O	2.37	0.57
2:H:334:ASP:OD2	2:H:336:THR:HG23	2.05	0.57
1:C:75:ARG:HG3	1:C:107:VAL:CG1	2.35	0.57
1:C:998:ARG:CG	1:C:999:PRO:HA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1068:MET:O	1:C:1071:GLN:HB2	2.05	0.57
1:G:663:GLY:CA	1:G:869:MET:HG2	2.35	0.57
1:C:1:MET:HA	1:C:224:LYS:HE3	1.86	0.56
1:G:814:GLN:HG3	1:G:818:PHE:CE2	2.40	0.56
2:D:206:LEU:O	2:D:210:VAL:HG23	2.05	0.56
1:A:70:HIS:O	1:A:74:VAL:HG23	2.05	0.56
1:E:559:ARG:HB3	10:E:5812:HOH:O	2.04	0.56
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.86	0.56
1:G:46:LEU:CD1	1:G:64:THR:HG23	2.25	0.56
1:G:560:GLU:OE1	1:G:636:LYS:HE3	2.05	0.56
2:H:302:LYS:HB2	2:H:304:VAL:HG22	1.86	0.56
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.20	0.56
2:D:259:LEU:HD13	2:D:342:ARG:NH1	2.20	0.56
1:C:353:ASP:OD1	2:D:116:ARG:HD2	2.06	0.56
1:C:358:LYS:HE3	10:C:5075:HOH:O	2.05	0.56
2:H:46:PRO:HA	2:H:76:HIS:CG	2.41	0.56
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.87	0.56
2:B:286:MET:CE	2:B:315:ALA:HB2	2.35	0.56
1:G:735:ARG:O	1:G:738:PHE:N	2.38	0.56
2:D:324:ASN:N	2:D:324:ASN:HD22	2.01	0.56
1:E:1017:THR:HG22	1:E:1018:SER:N	2.21	0.56
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.36	0.56
1:A:646:THR:CB	1:A:647:PRO:HD3	2.36	0.56
2:D:200:GLY:HA2	10:D:2059:HOH:O	2.06	0.56
1:E:646:THR:HB	1:E:647:PRO:HD3	1.88	0.56
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.88	0.56
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.05	0.56
1:C:772:MET:HE2	1:C:880:THR:HA	1.87	0.55
2:H:251:ALA:O	2:H:255:ILE:HG13	2.06	0.55
1:A:353:ASP:OD1	2:B:116:ARG:HD2	2.06	0.55
1:E:702:VAL:CG1	1:E:731:GLU:HG3	2.35	0.55
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.70	0.55
1:G:1:MET:H1	1:G:224:LYS:HZ2	1.54	0.55
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.87	0.55
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.25	0.55
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.42	0.55
1:E:735:ARG:O	1:E:738:PHE:N	2.39	0.55
1:C:784:GLN:H	1:C:784:GLN:NE2	2.04	0.55
1:E:671:ARG:NH2	1:E:819:GLU:O	2.40	0.55
1:G:956:ARG:HB3	1:G:1044:LEU:HD21	1.87	0.55
2:D:300:VAL:HG22	2:D:328:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:LEU:HG	1:E:204:LEU:HD11	1.86	0.55
2:H:368:ASP:HB2	10:H:4261:HOH:O	2.06	0.55
1:C:975:HIS:HE2	1:E:992:ASN:ND2	2.05	0.55
1:E:805:ILE:HD13	1:E:837:VAL:CG2	2.37	0.55
1:G:998:ARG:HA	1:G:999:PRO:C	2.26	0.55
1:C:12:ILE:N	1:C:45:ILE:O	2.33	0.55
1:C:426:ARG:HD3	1:C:426:ARG:C	2.27	0.55
2:D:46:PRO:HA	2:D:76:HIS:CG	2.41	0.55
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.07	0.55
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.06	0.55
1:E:677:ARG:O	1:E:680:HIS:HB2	2.05	0.55
1:C:698:ILE:HD12	1:C:698:ILE:N	2.22	0.55
2:D:279:SER:O	2:D:322:PRO:HG3	2.07	0.55
1:E:814:GLN:NE2	10:E:5516:HOH:O	2.40	0.55
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.37	0.54
2:H:218:ILE:N	2:H:218:ILE:HD13	2.22	0.54
1:A:695:VAL:CG1	1:A:701:ALA:HB2	2.19	0.54
1:A:814:GLN:NE2	10:A:5474:HOH:O	2.40	0.54
1:E:358:LYS:HG2	1:E:359:ILE:N	2.21	0.54
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.88	0.54
1:G:814:GLN:HG3	1:G:818:PHE:HE2	1.73	0.54
1:A:46:LEU:C	1:A:46:LEU:HD23	2.26	0.54
1:A:704:LYS:O	1:A:707:GLU:HB2	2.06	0.54
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.09	0.54
1:C:101:GLU:OE2	1:C:104:ARG:NH2	2.33	0.54
2:D:156:MET:SD	2:D:158:LEU:HD21	2.48	0.54
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.07	0.54
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.37	0.54
1:G:340:THR:O	1:G:343:ARG:HB2	2.08	0.54
1:A:675:ARG:NH2	10:A:5504:HOH:O	2.29	0.54
1:C:224:LYS:HE2	1:C:329:GLY:O	2.07	0.54
2:D:178:THR:HG22	2:D:179:GLY:N	2.22	0.54
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.22	0.54
1:C:1021:ARG:HH11	1:C:1021:ARG:HG3	1.71	0.54
1:G:28:TYR:CE1	1:G:313:LYS:HE3	2.43	0.54
1:A:267:ALA:O	1:A:271:VAL:HG23	2.08	0.54
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.43	0.54
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.42	0.54
1:G:1:MET:N	1:G:224:LYS:NZ	2.55	0.54
1:A:224:LYS:NZ	10:A:5023:HOH:O	2.40	0.54
1:A:315:THR:O	1:A:531:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:VAL:O	2:B:78:GLN:HG2	2.08	0.54
2:B:232:ASN:N	2:B:233:PRO:HD3	2.22	0.54
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.43	0.54
2:D:231:MET:HA	10:D:2215:HOH:O	2.08	0.54
1:E:28:TYR:CE1	1:E:313:LYS:HE3	2.42	0.54
1:G:991:VAL:HG21	1:G:1001:ILE:HG22	1.90	0.54
2:F:298:LYS:HE2	2:F:303:ASN:OD1	2.08	0.54
1:G:167:ILE:HD12	1:G:167:ILE:N	2.22	0.54
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.39	0.53
1:A:698:ILE:O	1:A:702:VAL:HG23	2.07	0.53
1:C:1:MET:HB3	1:C:334:GLU:OE2	2.08	0.53
1:C:992:ASN:O	1:C:1000:HIS:HA	2.08	0.53
1:C:998:ARG:HG2	1:C:999:PRO:HA	1.90	0.53
2:D:275:LEU:HD23	2:D:349:SER:HB3	1.89	0.53
2:F:376:GLN:HA	2:F:379:LYS:NZ	2.23	0.53
1:G:733:ASP:HA	1:G:736:ARG:HH11	1.72	0.53
1:E:736:ARG:NH2	1:E:1020:ARG:HG2	2.23	0.53
1:A:1000:HIS:HD2	1:A:1003:ASP:N	1.97	0.53
1:C:994:VAL:HA	1:C:1000:HIS:CB	2.38	0.53
9:E:5056:NET:H42	9:E:5056:NET:H22	1.90	0.53
1:G:181:ILE:HD11	1:G:376:THR:HG23	1.91	0.53
2:H:232:ASN:N	2:H:233:PRO:HD3	2.23	0.53
2:B:46:PRO:HA	2:B:76:HIS:CG	2.43	0.53
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.08	0.53
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.08	0.53
2:D:350:PHE:HB2	2:D:366:LEU:HD22	1.91	0.53
2:F:279:SER:O	2:F:322:PRO:HG3	2.08	0.53
1:A:659:VAL:HG13	1:A:660:PRO:HD2	1.91	0.53
2:D:100:SER:O	10:D:1835:HOH:O	2.18	0.53
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.39	0.53
1:G:74:VAL:HG11	1:G:102:LEU:HD11	1.89	0.53
2:H:54:THR:HG21	2:H:118:LEU:HD23	1.89	0.53
1:C:46:LEU:C	1:C:46:LEU:CD1	2.75	0.53
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.38	0.53
1:G:663:GLY:HA3	1:G:869:MET:HG2	1.91	0.53
2:F:185:LYS:HD2	2:F:190:LEU:HD21	1.90	0.53
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.90	0.53
1:C:75:ARG:HG3	1:C:107:VAL:HG11	1.91	0.53
1:C:772:MET:CE	1:C:880:THR:HG22	2.39	0.53
2:D:26:ALA:O	2:D:131:CYS:HA	2.09	0.53
1:G:106:GLY:HA2	10:G:3478:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.24	0.52
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.24	0.52
1:C:872:LYS:HG3	1:C:876:GLU:HB3	1.91	0.52
1:C:885:PRO:HG2	10:C:5510:HOH:O	2.07	0.52
1:E:997:GLY:O	1:E:998[B]:ARG:HG3	2.09	0.52
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.90	0.52
1:G:236:ASN:HD22	1:G:236:ASN:N	2.07	0.52
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.39	0.52
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.40	0.52
1:A:734:LEU:HD12	1:A:734:LEU:C	2.28	0.52
2:F:201:ALA:HB2	2:F:239:SER:CB	2.40	0.52
2:D:50:ARG:NH1	2:D:158:LEU:HD22	2.13	0.52
1:E:735:ARG:O	1:E:738:PHE:HB2	2.10	0.52
2:F:194:VAL:HG13	2:F:235:GLY:O	2.09	0.52
1:G:150:HIS:CD2	1:G:203:GLU:HB2	2.44	0.52
1:A:344:THR:HB	1:A:345:PRO:HD2	1.92	0.52
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.39	0.52
2:D:152:GLY:O	2:D:156:MET:HE3	2.09	0.52
1:C:46:LEU:HD11	1:C:64:THR:HG23	1.92	0.52
2:F:376:GLN:HA	2:F:379:LYS:HZ2	1.74	0.52
1:G:375:THR:HG23	1:G:377:GLN:H	1.74	0.52
1:A:548:GLU:OE1	2:B:114:ASP:HA	2.09	0.52
1:C:623:LEU:HD12	1:C:654:LEU:HD23	1.92	0.52
2:D:298:LYS:HE2	2:D:303:ASN:OD1	2.09	0.52
1:E:78:ILE:HG23	1:E:83:PRO:HD2	1.92	0.52
1:E:146:SER:HB3	1:E:207:ASP:OD1	2.09	0.52
1:G:680:HIS:O	1:G:683:GLU:HB2	2.09	0.52
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.22	0.52
1:A:9:SER:OG	1:A:83:PRO:HA	2.10	0.52
2:D:324:ASN:HD22	2:D:324:ASN:H	1.57	0.52
1:G:146:SER:HB2	1:G:205:LEU:HD11	1.92	0.52
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.30	0.52
1:A:220:VAL:O	1:A:281:GLY:HA2	2.09	0.52
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.43	0.52
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.45	0.52
1:A:103:GLU:HG2	10:A:5598:HOH:O	2.08	0.51
1:A:426:ARG:HD3	1:A:426:ARG:C	2.31	0.51
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.10	0.51
1:C:363:ASN:ND2	1:C:365:GLU:OE1	2.39	0.51
1:E:652:ARG:HD2	1:E:666:PRO:HB2	1.92	0.51
1:A:999:PRO:HD2	1:G:983:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:ILE:HG21	1:C:589:LEU:CD1	2.39	0.51
1:G:713:VAL:HG12	1:G:713:VAL:O	2.08	0.51
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.92	0.51
1:A:339:ILE:HD11	1:A:531:THR:HG23	1.93	0.51
1:A:1000:HIS:CD2	1:A:1003:ASP:N	2.76	0.51
1:C:709:GLY:O	1:C:754:HIS:ND1	2.43	0.51
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.92	0.51
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.71	0.51
1:E:750:VAL:HG12	1:E:750:VAL:O	2.10	0.51
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.29	0.51
2:H:32:PHE:O	2:H:291:HIS:HB2	2.09	0.51
2:H:142:LEU:HD12	2:H:142:LEU:O	2.10	0.51
1:A:124:ASP:O	1:A:128:ASP:HB3	2.11	0.51
1:A:724:ALA:N	10:A:5721:HOH:O	2.44	0.51
1:C:630:VAL:HG11	1:C:659:VAL:HG22	1.93	0.51
1:E:1061:LYS:NZ	10:E:5578:HOH:O	2.42	0.51
1:G:3:LYS:HB3	1:G:330:TYR:CE1	2.45	0.51
1:G:129:ARG:HB3	1:G:205:LEU:HD22	1.93	0.51
1:G:734:LEU:HD12	1:G:734:LEU:C	2.27	0.51
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.92	0.51
2:D:201:ALA:HB2	2:D:239:SER:CB	2.41	0.51
1:E:375:THR:OG1	1:E:376:THR:N	2.43	0.51
1:A:1001:ILE:HD12	1:A:1002[B]:GLN:HB2	1.91	0.51
1:C:994:VAL:HA	1:C:1000:HIS:CG	2.46	0.51
1:E:1:MET:O	1:E:329:GLY:O	2.29	0.51
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.36	0.51
2:D:174:SER:O	2:D:182:PRO:HD3	2.10	0.51
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.76	0.51
2:B:199:PHE:O	2:B:241:GLY:HA3	2.10	0.51
1:C:38[B]:ARG:NH2	10:C:5086:HOH:O	2.27	0.51
2:B:120:ARG:HD2	10:B:5054:HOH:O	2.11	0.51
2:D:369:HIS:O	2:D:372:GLU:HB2	2.11	0.51
1:G:954:LYS:O	1:G:980:VAL:HG11	2.11	0.51
1:A:979:ILE:O	1:A:983:GLU:HG3	2.11	0.50
2:B:50:ARG:HD2	2:B:158:LEU:HD21	1.94	0.50
2:B:324:ASN:HA	2:B:343:THR:OG1	2.11	0.50
1:C:782:ILE:N	1:C:782:ILE:HD12	2.26	0.50
2:F:241:GLY:O	2:F:269:143:OF	2.28	0.50
1:C:197:ASP:OD2	1:C:1037:LYS:NZ	2.34	0.50
1:C:704:LYS:O	1:C:707:GLU:HB2	2.11	0.50
1:G:415:LEU:HB2	10:G:3828:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1017:THR:CG2	1:G:1023:ILE:HG12	2.42	0.50
1:C:1052:MET:HG2	10:C:5817:HOH:O	2.11	0.50
2:D:195:VAL:HG11	2:D:231:MET:HE1	1.93	0.50
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.93	0.50
1:G:814:GLN:CG	1:G:818:PHE:HE2	2.23	0.50
1:C:804:GLU:O	1:C:808:VAL:HG23	2.11	0.50
1:E:713:VAL:HB	1:E:753:ASP:HB2	1.93	0.50
1:A:344:THR:HA	10:A:5644:HOH:O	2.11	0.50
1:A:602:ASN:CG	1:A:605:THR:HG23	2.32	0.50
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.12	0.50
1:A:1001:ILE:O	1:A:1005:ILE:HG13	2.11	0.50
2:B:245:PRO:HG3	2:B:273:GLN:OE1	2.11	0.50
1:C:774:LEU:HD22	1:C:879:VAL:HG12	1.93	0.50
1:E:907:LEU:HD11	8:E:5055:ORN:HD3	1.93	0.50
1:G:181:ILE:HG13	1:G:376:THR:HG23	1.94	0.50
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.10	0.50
1:A:690:PRO:HG3	1:A:756:LEU:HD11	1.94	0.50
1:E:267:ALA:O	1:E:271:VAL:HG23	2.11	0.50
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.94	0.50
1:G:135:ALA:HB1	1:G:274:GLU:CG	2.42	0.50
2:H:324:ASN:O	2:H:342:ARG:HD2	2.12	0.50
2:D:248:CYS:O	2:D:252:ILE:HG13	2.11	0.50
1:G:51:PRO:HG3	1:G:918:MET:HB2	1.94	0.50
1:A:695:VAL:HG21	1:A:752:LEU:HD22	1.93	0.50
1:C:46:LEU:HD21	1:C:55:MET:O	2.11	0.50
1:C:986:ILE:O	1:C:988:PRO:HD3	2.12	0.50
1:E:138:LYS:HD3	1:E:274:GLU:OE1	2.12	0.50
1:E:225:ASN:ND2	1:E:331:THR:HG21	2.26	0.50
1:G:700:MET:O	1:G:704:LYS:HB2	2.10	0.50
2:H:367:PHE:O	2:H:370:PHE:HB3	2.11	0.50
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.44	0.49
1:C:698:ILE:H	1:C:698:ILE:CD1	2.22	0.49
1:E:39:GLU:HG3	10:E:5114:HOH:O	2.12	0.49
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.93	0.49
1:C:152:MET:SD	1:C:189:GLU:HG2	2.52	0.49
2:F:354:PRO:HB2	2:F:367:PHE:CE2	2.47	0.49
1:G:224:LYS:HE2	1:G:329:GLY:O	2.12	0.49
1:G:400:ARG:HB3	10:G:3730:HOH:O	2.12	0.49
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.94	0.49
1:C:11:LEU:HA	1:C:45:ILE:O	2.12	0.49
1:C:167:ILE:HD12	1:C:167:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:755:PHE:CD1	7:G:2072:ADP:C2	3.00	0.49
1:C:519:GLN:NE2	10:C:5775:HOH:O	2.45	0.49
1:C:993:LYS:O	1:C:1000:HIS:HB3	2.13	0.49
1:C:997:GLY:O	1:C:998:ARG:HG3	2.13	0.49
1:E:734:LEU:HD12	1:E:734:LEU:C	2.29	0.49
1:G:1017:THR:HG22	1:G:1023:ILE:HG12	1.94	0.49
1:C:482:THR:HB	10:C:5689:HOH:O	2.11	0.49
2:D:345:LYS:HB3	2:D:346:PRO:CD	2.40	0.49
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.47	0.49
1:G:948:SER:O	1:G:1015:ASN:HA	2.13	0.49
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.60	0.49
1:C:701:ALA:O	1:C:705:ALA:N	2.37	0.49
1:C:980:VAL:HG13	10:C:5728:HOH:O	2.13	0.49
1:E:500:ALA:O	1:E:504:LYS:HG3	2.12	0.49
1:E:854:SER:HA	1:E:859:VAL:O	2.12	0.49
1:G:1:MET:H1	1:G:224:LYS:NZ	2.10	0.49
1:G:796:LEU:C	1:G:796:LEU:HD23	2.33	0.49
2:B:259:LEU:O	2:B:345:LYS:HE3	2.13	0.49
1:E:568:GLY:O	1:E:602:ASN:HB2	2.12	0.49
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.95	0.49
1:E:929:ALA:HB2	1:E:1053:ALA:HB1	1.93	0.49
1:G:1030:ARG:HH11	1:G:1030:ARG:CG	2.25	0.49
2:D:269:143:HE	2:D:312:HIS:CB	2.43	0.49
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.93	0.49
2:F:223:THR:HG21	2:F:228:VAL:HG23	1.93	0.49
2:F:225:ALA:O	2:F:229:LEU:HG	2.12	0.49
1:G:129:ARG:NH2	7:G:2066:ADP:O3B	2.39	0.49
2:H:38:GLY:HA3	2:H:358:PRO:HB3	1.95	0.49
1:A:998:ARG:CB	1:A:999:PRO:HA	2.43	0.49
1:C:1017:THR:CG2	1:C:1023:ILE:HG13	2.42	0.49
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.47	0.49
2:D:241:GLY:O	2:D:269:143:OF	2.30	0.49
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.48	0.49
2:H:324:ASN:ND2	2:H:324:ASN:H	2.10	0.49
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.78	0.49
1:A:402:LEU:O	1:A:403:GLU:HB2	2.13	0.48
1:A:775:ILE:HG13	1:A:810:ARG:HG2	1.94	0.48
1:A:951:GLU:OE1	1:A:951:GLU:HA	2.10	0.48
2:B:364:ALA:N	2:B:365:PRO:HD2	2.28	0.48
1:E:224:LYS:HE2	1:E:329:GLY:O	2.13	0.48
2:H:322:PRO:HG2	2:H:324:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:OE1	1:A:495:LYS:HD3	2.13	0.48
2:B:367:PHE:O	2:B:370:PHE:HB3	2.13	0.48
1:C:490:ARG:HD3	10:C:5655:HOH:O	2.13	0.48
1:C:500:ALA:O	1:C:504:LYS:HG3	2.13	0.48
2:B:34:THR:HA	2:B:56:THR:OG1	2.13	0.48
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.95	0.48
1:C:695:VAL:HG11	1:C:701:ALA:CA	2.43	0.48
1:E:998[A]:ARG:HB3	1:E:999:PRO:HA	1.95	0.48
1:G:362:PHE:CD2	1:G:433:ALA:HB1	2.48	0.48
1:G:410:ASP:OD1	1:G:501:ARG:NH1	2.47	0.48
1:A:772:MET:HG3	1:A:874:LEU:HD12	1.95	0.48
1:C:509:ARG:HD3	10:C:5680:HOH:O	2.14	0.48
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.96	0.48
1:C:1064:SER:OG	1:C:1067:GLU:HG3	2.12	0.48
2:F:169:SER:HA	2:F:216:LEU:O	2.13	0.48
1:C:561:LYS:HE2	10:C:5448:HOH:O	2.12	0.48
1:C:734:LEU:HD12	1:C:734:LEU:C	2.29	0.48
1:E:213:TRP:O	1:E:239:ALA:HB1	2.12	0.48
1:G:774:LEU:HD22	1:G:879:VAL:HG12	1.96	0.48
1:C:1:MET:CB	1:C:2:PRO:HD3	2.43	0.48
2:D:135:GLY:O	2:D:138:PRO:HD3	2.13	0.48
1:E:172:PHE:CB	1:E:200:PRO:HG2	2.31	0.48
1:E:676:GLU:O	1:E:680:HIS:ND1	2.46	0.48
1:G:65:TYR:CE2	1:G:77:ILE:HG23	2.49	0.48
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.78	0.48
1:E:464:VAL:HG11	2:F:88:ILE:HD13	1.96	0.48
1:E:571:ARG:HD3	1:E:574:GLN:HB2	1.95	0.48
1:G:181:ILE:CG1	1:G:376:THR:HG23	2.42	0.48
1:G:702:VAL:HG11	1:G:735:ARG:HH22	1.76	0.48
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.95	0.48
1:A:460:ARG:O	1:A:464:VAL:HG13	2.12	0.48
1:A:954:LYS:HB3	1:A:980:VAL:HG21	1.96	0.48
1:C:24:CYS:HB2	1:C:604:GLU:HB3	1.94	0.48
1:C:600:ASN:O	1:C:618:PHE:HA	2.13	0.48
2:D:363:ALA:C	2:D:365:PRO:HD2	2.34	0.48
1:G:733:ASP:O	1:G:736:ARG:NH1	2.46	0.48
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.77	0.48
1:A:88:PRO:HB3	1:A:99:ALA:HB2	1.95	0.48
1:C:375:THR:HG23	1:C:377:GLN:H	1.79	0.48
2:D:142:LEU:HD12	2:D:142:LEU:O	2.14	0.48
1:G:947:LEU:HD12	1:G:947:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:341:HIS:CD2	2:H:348:PHE:HB3	2.48	0.48
1:A:759:ALA:HB2	1:A:833:LYS:HG3	1.95	0.48
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.49	0.48
2:D:228:VAL:O	2:D:231:MET:HB2	2.14	0.48
1:E:805:ILE:HD13	1:E:837:VAL:HG23	1.96	0.48
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.43	0.48
1:G:965:LEU:HA	1:G:965:LEU:HD23	1.75	0.48
1:G:972:ASP:HA	1:G:989:ARG:O	2.14	0.48
1:C:166:CYS:C	1:C:167:ILE:HD12	2.34	0.47
1:G:18:ILE:HG23	1:G:23:ALA:HA	1.96	0.47
1:G:150:HIS:HD2	1:G:203:GLU:HB2	1.77	0.47
1:G:344:THR:HB	1:G:345:PRO:HD2	1.95	0.47
1:G:730:ASP:H	1:G:733:ASP:HB2	1.79	0.47
1:G:735:ARG:O	1:G:738:PHE:HB2	2.14	0.47
1:A:5:THR:C	1:A:7:ILE:H	2.17	0.47
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.29	0.47
2:B:286:MET:CE	2:B:312:HIS:ND1	2.78	0.47
2:F:332:LEU:HD12	2:F:332:LEU:HA	1.62	0.47
2:B:6:LEU:HD12	2:B:7:LEU:N	2.29	0.47
1:G:174:MET:HB2	6:G:2071:PO4:O1	2.14	0.47
2:H:264:PRO:HA	2:H:346:PRO:HB2	1.97	0.47
1:C:872:LYS:HG2	1:C:877:GLN:HG2	1.97	0.47
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.96	0.47
1:G:38:ARG:HG3	1:G:38:ARG:HH11	1.79	0.47
1:A:713:VAL:HG12	1:A:713:VAL:O	2.15	0.47
1:C:822:VAL:O	1:C:823:ARG:HD3	2.14	0.47
1:E:167:ILE:N	1:E:167:ILE:HD12	2.29	0.47
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.27	0.47
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.44	0.47
1:C:213:TRP:CZ3	1:C:296:ILE:HD12	2.49	0.47
2:F:275:LEU:HD23	2:F:349:SER:OG	2.14	0.47
1:G:135:ALA:HB1	1:G:274:GLU:HG3	1.96	0.47
1:G:196:LEU:HG	1:G:204:LEU:HD11	1.96	0.47
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.45	0.47
1:A:27:ASP:OD2	1:A:53:THR:HB	2.15	0.47
1:A:266:ASN:ND2	10:A:5275:HOH:O	2.45	0.47
1:A:583:VAL:HG13	1:A:612:THR:CG2	2.45	0.47
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.49	0.47
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.44	0.47
1:E:166:CYS:C	1:E:167:ILE:HD12	2.34	0.47
1:E:902:GLY:O	1:E:1027:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1000:HIS:CD2	1:E:1000:HIS:H	2.28	0.47
1:E:1021:ARG:HH11	1:E:1021:ARG:HG2	1.80	0.47
2:F:269:143:O	2:F:272:HIS:HB3	2.15	0.47
1:G:569:PRO:O	1:G:571:ARG:HD2	2.14	0.47
1:G:1005:ILE:HG21	1:G:1032:SER:HB3	1.96	0.47
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	1.96	0.47
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.50	0.47
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.79	0.47
1:C:671:ARG:NH2	1:C:819:GLU:O	2.48	0.47
1:C:998:ARG:HA	1:C:999:PRO:C	2.34	0.47
1:G:48:ASN:O	1:G:66:ILE:HA	2.14	0.47
1:G:181:ILE:CD1	1:G:376:THR:HG23	2.45	0.47
2:H:38:GLY:HA3	2:H:358:PRO:CB	2.45	0.47
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.33	0.47
1:E:692:ASN:HA	1:E:752:LEU:O	2.15	0.47
1:G:9:SER:O	1:G:84:ASP:HB2	2.15	0.47
1:G:632:ILE:HG13	1:G:633:GLU:N	2.30	0.47
1:G:1001:ILE:CD1	1:G:1002:GLN:N	2.75	0.47
1:A:675:ARG:NH2	10:A:5768:HOH:O	2.49	0.46
1:C:735:ARG:O	1:C:738:PHE:N	2.47	0.46
2:D:264:PRO:HB3	2:D:373:LEU:HB3	1.98	0.46
1:E:46:LEU:HD13	1:E:46:LEU:N	2.30	0.46
1:E:891:LYS:HG2	1:E:892:GLU:N	2.29	0.46
1:G:1:MET:O	1:G:334:GLU:OE1	2.33	0.46
1:A:735:ARG:O	1:A:738:PHE:N	2.47	0.46
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.98	0.46
1:C:726:GLU:CG	1:C:727:ILE:N	2.78	0.46
1:C:995:HIS:O	1:C:997:GLY:N	2.48	0.46
2:D:139:ASP:OD2	2:D:142:LEU:HB2	2.15	0.46
1:E:169:ARG:NH1	7:E:2045:ADP:O2A	2.47	0.46
1:E:863:LYS:O	1:E:867:ARG:HG3	2.15	0.46
2:F:194:VAL:HG13	2:F:235:GLY:C	2.35	0.46
1:G:434:ASP:HB2	10:G:3716:HOH:O	2.15	0.46
1:G:734:LEU:O	1:G:737:TYR:HB3	2.15	0.46
2:H:29:GLU:HB2	2:H:153:LEU:HD22	1.97	0.46
2:H:210:VAL:HG22	2:H:214:CYS:O	2.15	0.46
1:A:930:LYS:HE3	10:A:5080:HOH:O	2.15	0.46
1:E:702:VAL:O	1:E:706:LYS:HD3	2.15	0.46
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.50	0.46
2:D:116:ARG:O	2:D:120:ARG:HG3	2.15	0.46
2:D:222:GLN:H	2:D:222:GLN:HE21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:679:GLN:HG2	1:G:683:GLU:OE2	2.15	0.46
1:A:990:LEU:HG	1:G:979:ILE:CD1	2.46	0.46
2:B:196:ALA:O	2:B:219:VAL:HG22	2.14	0.46
1:C:695:VAL:HG21	1:C:701:ALA:CA	2.36	0.46
1:E:151:THR:CB	1:E:153[B]:GLU:HG2	2.45	0.46
1:E:317:PHE:CE1	1:E:322:VAL:HG21	2.51	0.46
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.46
2:F:272:HIS:HA	2:F:349:SER:HB2	1.97	0.46
1:G:563:MET:CE	1:G:635:PRO:HG3	2.45	0.46
1:G:568:GLY:O	1:G:602:ASN:HB2	2.15	0.46
1:G:906:LEU:O	1:G:912:ARG:NH2	2.39	0.46
2:H:286:MET:CE	2:H:312:HIS:ND1	2.78	0.46
1:A:414:SER:OG	1:A:416:ASP:OD2	2.30	0.46
2:B:365:PRO:O	2:B:368:ASP:HB2	2.16	0.46
1:C:991:VAL:O	10:C:5809:HOH:O	2.21	0.46
1:C:1023:ILE:HG22	1:C:1024:GLU:N	2.31	0.46
1:G:1004:ARG:HA	1:G:1009:GLU:HG3	1.98	0.46
2:H:350:PHE:HB2	2:H:366:LEU:HD23	1.98	0.46
1:A:370:ALA:HB2	1:A:903:VAL:CG2	2.45	0.46
1:A:726:GLU:CG	1:A:727:ILE:N	2.78	0.46
1:C:802:SER:OG	1:C:805:ILE:HB	2.16	0.46
2:F:367:PHE:O	2:F:370:PHE:HB3	2.16	0.46
1:G:40:GLU:HG2	1:G:325:LYS:HE2	1.98	0.46
1:G:289:ASN:HB3	1:G:292:ASN:OD1	2.14	0.46
1:A:446:GLY:O	1:E:448:SER:N	2.45	0.46
1:E:51:PRO:HG3	1:E:918:MET:HB2	1.97	0.46
1:E:998[B]:ARG:HB3	1:E:999:PRO:HA	1.96	0.46
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.46	0.46
1:G:712:LEU:CD2	1:G:752:LEU:HG	2.44	0.46
1:A:835:ASN:HD22	1:A:835:ASN:HA	1.64	0.46
1:C:589:LEU:O	1:C:594:TYR:HB2	2.15	0.46
2:D:269:143:HE	2:D:312:HIS:HB2	1.98	0.46
1:G:695:VAL:CG1	1:G:700:MET:HB3	2.40	0.46
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.81	0.46
1:A:805:ILE:HD13	1:A:837:VAL:CG2	2.46	0.46
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.84	0.46
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.81	0.46
1:E:57:ASP:HB3	1:E:59:GLU:OE2	2.16	0.46
1:E:152:MET:SD	1:E:189:GLU:HG2	2.56	0.46
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.98	0.46
1:G:118:ALA:HA	10:G:3483:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.46	0.46
1:A:820:LEU:O	1:A:821:GLN:HB2	2.16	0.45
1:C:979:ILE:O	1:C:983:GLU:HG3	2.15	0.45
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.32	0.45
1:E:5:THR:O	1:E:8:LYS:NZ	2.49	0.45
1:E:147:GLY:HA3	1:E:158:VAL:HG13	1.98	0.45
1:G:158:VAL:O	1:G:161:ASP:HB3	2.15	0.45
1:G:548:GLU:OE1	2:H:114:ASP:HA	2.16	0.45
1:G:859:VAL:HA	1:G:860:PRO:HD2	1.82	0.45
2:H:212:ARG:HG3	2:H:212:ARG:HH11	1.80	0.45
1:A:6:ASP:OD2	1:A:6:ASP:N	2.45	0.45
1:A:701:ALA:O	1:A:705:ALA:N	2.40	0.45
2:B:2:ILE:HD12	10:B:5202:HOH:O	2.15	0.45
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.17	0.45
1:C:892:GLU:OE1	8:C:5033:ORN:NE	2.50	0.45
1:E:46:LEU:HD21	1:E:64:THR:CG2	2.26	0.45
1:E:258:ASP:O	1:E:262:GLN:HG2	2.16	0.45
1:E:675:ARG:CD	1:E:675:ARG:H	2.29	0.45
1:E:873:SER:O	1:E:877:GLN:HG3	2.17	0.45
1:E:998[B]:ARG:HG3	1:E:998[B]:ARG:HH11	1.81	0.45
2:F:324:ASN:HA	2:F:343:THR:OG1	2.16	0.45
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.59	0.45
2:H:218:ILE:N	2:H:218:ILE:CD1	2.79	0.45
2:H:355:GLU:OE2	2:H:355:GLU:N	2.40	0.45
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.50	0.45
1:C:1:MET:N	1:C:2:PRO:CD	2.79	0.45
1:G:784:GLN:HE21	1:G:784:GLN:N	2.04	0.45
2:H:192:PHE:O	2:H:215:ARG:HB3	2.16	0.45
1:A:583:VAL:O	1:A:587:LEU:HG	2.15	0.45
1:C:571:ARG:HD3	1:C:571:ARG:N	2.30	0.45
2:D:44:THR:O	2:D:46:PRO:HD3	2.17	0.45
1:G:1017:THR:HG22	1:G:1018:SER:N	2.32	0.45
1:A:166:CYS:C	1:A:167:ILE:HD12	2.37	0.45
1:A:583:VAL:HG13	1:A:612:THR:HG21	1.99	0.45
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.46	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:106:GLY:HA2	10:C:5129:HOH:O	2.17	0.45
1:C:237:PHE:HB3	1:C:248:ILE:O	2.16	0.45
1:C:385:MET:HB2	1:C:603:PRO:HG3	1.98	0.45
1:C:583:VAL:O	1:C:587:LEU:HG	2.15	0.45
2:F:78:GLN:NE2	10:F:2863:HOH:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:272:HIS:HA	2:F:349:SER:CB	2.47	0.45
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.98	0.45
1:A:734:LEU:CD1	1:A:738:PHE:CE2	3.00	0.45
2:B:232:ASN:N	2:B:233:PRO:CD	2.80	0.45
2:D:364:ALA:N	2:D:365:PRO:CD	2.80	0.45
1:E:176:GLY:N	7:E:2045:ADP:O2B	2.42	0.45
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.51	0.45
2:D:175:TRP:HA	2:D:180:GLY:O	2.17	0.45
2:D:370:PHE:O	2:D:374:ILE:HG13	2.17	0.45
1:E:282:SER:OG	1:E:302:PRO:HA	2.17	0.45
1:E:698:ILE:CD1	1:E:698:ILE:N	2.79	0.45
1:G:240:MET:HE3	7:G:2066:ADP:C4	2.52	0.45
1:G:292:ASN:OD1	1:G:294:ARG:HB2	2.16	0.45
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.52	0.45
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.52	0.45
1:G:1017:THR:CG2	1:G:1018:SER:N	2.79	0.45
1:A:1:MET:N	1:A:224:LYS:HE3	2.29	0.45
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.32	0.45
1:C:534:ALA:HB1	2:D:120:ARG:HG2	1.98	0.45
1:C:761:GLU:CG	1:C:781:HIS:CE1	3.00	0.45
1:G:10:ILE:HD13	1:G:37:LEU:HD13	1.98	0.45
1:G:640:VAL:HG21	1:G:651:ALA:HB2	1.99	0.45
1:G:671:ARG:NH2	1:G:819:GLU:O	2.50	0.45
1:A:555:PRO:HG3	1:A:632:ILE:HD12	1.99	0.45
1:A:1061:LYS:HD3	10:A:5534:HOH:O	2.16	0.45
1:C:525:VAL:HB	1:C:551:CYS:HA	1.98	0.45
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.46	0.45
1:E:75:ARG:HG3	1:E:107:VAL:HG13	1.98	0.45
1:E:147:GLY:HA3	1:E:158:VAL:CG1	2.47	0.45
2:B:33:ASN:HB3	2:B:55:LEU:HD23	1.98	0.45
2:B:74:GLN:HG3	2:B:76:HIS:NE2	2.32	0.45
1:C:735:ARG:O	1:C:738:PHE:HB2	2.17	0.45
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.99	0.45
1:G:167:ILE:N	1:G:167:ILE:CD1	2.80	0.45
1:A:1001:ILE:HD12	1:A:1002[A]:GLN:HB2	1.97	0.44
1:A:1022:ALA:O	1:A:1026:SER:OG	2.30	0.44
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.52	0.44
1:G:527:LYS:O	1:G:543:MET:HB3	2.17	0.44
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.99	0.44
2:H:6:LEU:CD1	2:H:8:VAL:HG23	2.39	0.44
1:A:672:ALA:HB3	1:A:844:PRO:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.52	0.44
1:C:176:GLY:HA3	1:C:377:GLN:HA	1.97	0.44
1:C:400:ARG:HD3	10:C:5346:HOH:O	2.18	0.44
1:C:726:GLU:HG3	1:C:727:ILE:N	2.30	0.44
2:F:46:PRO:HA	2:F:76:HIS:CG	2.51	0.44
1:G:782:ILE:O	1:G:1045:ASN:HB3	2.16	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:167:ILE:HD12	1:A:167:ILE:N	2.32	0.44
1:A:257:THR:HG22	2:B:63:VAL:HG21	2.00	0.44
1:C:736:ARG:CZ	1:C:736:ARG:HB3	2.48	0.44
1:E:168:ILE:HD13	1:E:191:ILE:CG2	2.47	0.44
1:E:687:LEU:HD22	1:E:812:GLN:HG2	2.00	0.44
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.99	0.44
1:G:148:ILE:HG22	1:G:149:ALA:N	2.33	0.44
2:H:150:PHE:CD2	2:H:151:PRO:HD2	2.52	0.44
2:H:324:ASN:HA	2:H:343:THR:OG1	2.17	0.44
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.59	0.44
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.49	0.44
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.99	0.44
1:A:698:ILE:HD12	1:A:698:ILE:H	1.82	0.44
2:B:197:TYR:HB3	2:B:199:PHE:CZ	2.52	0.44
1:C:259:LYS:HD2	2:D:69:ASP:OD2	2.18	0.44
2:D:324:ASN:ND2	2:D:324:ASN:H	2.16	0.44
1:E:755:PHE:CD1	7:E:2051:ADP:C2	3.06	0.44
1:E:1004[B]:ARG:NH2	10:E:5070:HOH:O	2.50	0.44
1:A:1073:LYS:HD2	1:A:1073:LYS:N	2.32	0.44
2:D:212:ARG:HH11	2:D:212:ARG:CG	2.30	0.44
1:E:901:PRO:HD2	5:E:5063:CL:CL	2.54	0.44
2:F:193:HIS:N	2:F:234:ASP:OD2	2.42	0.44
2:F:212:ARG:HG3	2:F:212:ARG:HH11	1.82	0.44
2:F:246:ALA:N	2:F:247:PRO:HD2	2.31	0.44
2:F:254:ALA:O	2:F:257:LYS:HB2	2.17	0.44
1:G:726:GLU:CG	1:G:727:ILE:N	2.79	0.44
1:G:812:GLN:O	1:G:816:LEU:HD12	2.17	0.44
2:H:38:GLY:O	2:H:358:PRO:HG3	2.17	0.44
2:H:286:MET:CE	2:H:315:ALA:HB2	2.48	0.44
1:A:11:LEU:HA	1:A:45:ILE:O	2.18	0.44
1:C:687:LEU:HD11	1:C:812:GLN:HG2	1.95	0.44
2:D:232:ASN:N	2:D:233:PRO:HD3	2.31	0.44
1:E:1:MET:N	1:E:224:LYS:CE	2.80	0.44
2:F:246:ALA:N	2:F:247:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:GLU:O	2:H:294:ASN:HB2	2.17	0.44
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.99	0.44
1:A:1:MET:CB	1:A:2:PRO:HD3	2.48	0.44
1:A:571:ARG:HD3	1:A:571:ARG:N	2.32	0.44
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.75	0.44
1:E:583:VAL:O	1:E:587:LEU:HG	2.17	0.44
1:E:687:LEU:HD22	1:E:812:GLN:CG	2.48	0.44
1:G:159:ALA:HB2	1:G:188:PHE:CZ	2.52	0.44
1:G:534:ALA:O	2:H:123:ARG:HD3	2.17	0.44
1:G:802:SER:O	1:G:806:GLN:HG3	2.18	0.44
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.53	0.44
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.48	0.44
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.80	0.44
2:B:285:LYS:HG3	2:B:314:PHE:CZ	2.52	0.44
1:A:659:VAL:CG1	1:A:660:PRO:HD2	2.47	0.44
1:A:991:VAL:CG2	1:A:1004:ARG:NH1	2.80	0.44
1:C:51:PRO:HG3	1:C:918:MET:HB2	2.00	0.44
1:E:554:ASN:N	1:E:555:PRO:HD3	2.33	0.44
1:E:704:LYS:O	1:E:707:GLU:HB2	2.17	0.44
1:E:994:VAL:HG13	1:E:1000:HIS:CG	2.51	0.44
1:G:46:LEU:HD12	1:G:46:LEU:O	2.17	0.44
2:H:350:PHE:CG	2:H:366:LEU:CD2	3.00	0.44
1:A:700:MET:O	1:A:704:LYS:HB2	2.18	0.43
2:D:6:LEU:HD21	2:D:140:ALA:HA	2.00	0.43
1:G:148:ILE:CG2	1:G:149:ALA:N	2.81	0.43
1:G:489:LEU:HD12	1:G:489:LEU:HA	1.83	0.43
2:H:305:VAL:HG12	2:H:306:MET:N	2.32	0.43
1:C:734:LEU:CD1	1:C:738:PHE:CE2	3.00	0.43
2:D:299:ASP:OD1	2:D:302:LYS:HD2	2.19	0.43
1:G:602:ASN:HA	1:G:603:PRO:HD2	1.93	0.43
2:H:364:ALA:N	2:H:365:PRO:HD2	2.33	0.43
1:A:93:GLN:HG2	5:A:5017:CL:CL	2.56	0.43
1:A:344:THR:HB	1:A:345:PRO:CD	2.48	0.43
1:A:735:ARG:O	1:A:738:PHE:HB2	2.17	0.43
2:D:231:MET:HB2	2:D:231:MET:HE3	1.84	0.43
1:E:426:ARG:C	1:E:426:ARG:HD3	2.37	0.43
1:E:488:PHE:O	1:E:492:LEU:HG	2.18	0.43
1:E:753:ASP:HB2	10:E:5830:HOH:O	2.17	0.43
2:F:324:ASN:ND2	2:F:324:ASN:H	2.14	0.43
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.99	0.43
1:G:879:VAL:HA	10:G:3925:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:ARG:HG3	2:H:212:ARG:NH1	2.33	0.43
1:A:99:ALA:HB1	1:A:115:MET:CE	2.48	0.43
1:C:695:VAL:CG2	1:C:752:LEU:HD22	2.48	0.43
1:E:726:GLU:OE1	1:E:1020:ARG:HD3	2.18	0.43
2:F:6:LEU:HD13	2:F:16:HIS:CE1	2.53	0.43
2:F:155:GLY:N	2:F:244:ASP:OD1	2.46	0.43
2:F:364:ALA:N	2:F:365:PRO:HD2	2.33	0.43
1:G:805:ILE:HD12	1:G:832:VAL:HG11	2.00	0.43
1:G:891:LYS:HG2	1:G:892:GLU:N	2.31	0.43
1:G:955:GLU:HB3	10:G:3973:HOH:O	2.17	0.43
1:G:1002:GLN:O	1:G:1006:LYS:HB3	2.18	0.43
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.61	0.43
1:A:602:ASN:ND2	1:A:605:THR:HG23	2.33	0.43
1:C:174:MET:HB2	6:C:2028:PO4:O1	2.18	0.43
1:C:975:HIS:O	1:C:979:ILE:HG12	2.18	0.43
1:E:106:GLY:HA2	10:E:5155:HOH:O	2.17	0.43
1:E:159:ALA:HB2	1:E:188:PHE:CZ	2.53	0.43
1:E:363:ASN:OD1	1:E:381:VAL:HG21	2.18	0.43
1:E:484:LEU:HD23	1:E:484:LEU:HA	1.76	0.43
1:G:188:PHE:O	1:G:192:CYS:HB2	2.18	0.43
1:G:646:THR:HB	1:G:647:PRO:CD	2.49	0.43
2:H:25:SER:HA	2:H:132:ILE:O	2.19	0.43
2:H:169:SER:HA	2:H:216:LEU:O	2.18	0.43
2:B:259:LEU:O	2:B:345:LYS:HD2	2.19	0.43
1:C:775:ILE:HD13	1:C:775:ILE:HA	1.89	0.43
1:C:967:GLN:HG3	1:C:1054:LEU:CD1	2.35	0.43
1:E:239:ALA:HB2	10:E:5283:HOH:O	2.17	0.43
2:F:245:PRO:C	2:F:247:PRO:HD2	2.39	0.43
1:G:674:ASP:HB3	1:G:677:ARG:HG3	2.00	0.43
1:C:621:VAL:HG12	1:C:621:VAL:O	2.18	0.43
1:C:646:THR:HB	1:C:647:PRO:HD3	2.00	0.43
1:C:947:LEU:N	1:C:947:LEU:HD12	2.33	0.43
2:D:364:ALA:N	2:D:365:PRO:HD2	2.34	0.43
1:E:139:ILE:HG13	1:E:141:LEU:HG	2.00	0.43
2:H:6:LEU:HD11	2:H:8:VAL:HG22	1.98	0.43
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.79	0.43
2:F:65:THR:OG1	2:F:96:GLU:O	2.30	0.43
1:G:18:ILE:HD12	1:G:23:ALA:HA	2.01	0.43
1:G:196:LEU:HG	1:G:204:LEU:CD1	2.49	0.43
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.48	0.43
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1021:ARG:CG	1:G:1021:ARG:NH1	2.80	0.43
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.54	0.43
1:A:806:GLN:HA	1:A:809:MET:HE2	2.00	0.43
1:A:885:PRO:HA	1:A:886:PRO:HD3	1.87	0.43
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.49	0.43
1:C:906:LEU:O	1:C:912:ARG:NH2	2.47	0.43
1:G:49:SER:O	1:G:51:PRO:HD3	2.18	0.43
1:G:713:VAL:HG23	1:G:755:PHE:HB2	2.01	0.43
1:G:755:PHE:CE1	7:G:2072:ADP:C2	3.07	0.43
1:G:900:PHE:O	1:G:903:VAL:HG23	2.19	0.43
1:G:1035:GLN:NE2	10:G:3567:HOH:O	2.51	0.43
9:G:5077:NET:H63	9:G:5077:NET:H31	1.84	0.43
2:H:5:ALA:HB3	2:H:110:ILE:HG13	2.01	0.43
1:A:576:ILE:HD13	1:A:576:ILE:HG21	1.71	0.43
1:A:764:VAL:O	1:A:827:ASN:HA	2.19	0.43
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.00	0.43
2:F:25:SER:HA	2:F:132:ILE:O	2.19	0.43
1:A:151:THR:HB	10:A:5633:HOH:O	2.19	0.42
1:A:868:VAL:HA	1:A:872:LYS:O	2.19	0.42
9:A:5012:NET:H23	9:A:5012:NET:H71	1.72	0.42
1:C:698:ILE:O	1:C:702:VAL:HG23	2.19	0.42
1:E:101:GLU:OE2	1:E:104:ARG:NH2	2.37	0.42
1:G:178:GLY:HA3	1:G:198:LEU:HD23	2.00	0.42
1:G:769:ASP:N	1:G:769:ASP:OD2	2.52	0.42
2:H:114:ASP:O	2:H:117:LYS:HB3	2.19	0.42
1:E:146:SER:HB2	1:E:205:LEU:CD1	2.39	0.42
2:F:286:MET:HE3	2:F:289:GLY:HA2	2.01	0.42
1:G:1000:HIS:O	1:G:1004:ARG:HG3	2.19	0.42
2:H:249:ASP:OD2	2:H:250:TYR:HD2	2.01	0.42
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.50	0.42
1:C:294:ARG:HD2	5:C:5040:CL:CL	2.57	0.42
2:D:324:ASN:O	2:D:342:ARG:HA	2.19	0.42
1:E:1021:ARG:CG	1:E:1021:ARG:NH1	2.80	0.42
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.75	0.42
1:G:688:LYS:HE3	1:G:836:GLU:CD	2.39	0.42
1:G:850:VAL:HB	1:G:851:PRO:HD3	2.00	0.42
1:A:936:ASN:HB2	10:A:5036:HOH:O	2.19	0.42
2:B:6:LEU:O	2:B:132:ILE:HA	2.20	0.42
1:C:470:VAL:O	1:C:474:GLU:HG3	2.20	0.42
1:C:472:LEU:O	1:C:476:VAL:HG23	2.19	0.42
1:C:475:LYS:HD3	1:C:488:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:ASP:H	1:C:733:ASP:HB2	1.85	0.42
1:C:863:LYS:O	1:C:867:ARG:HG3	2.18	0.42
2:D:117:LYS:NZ	10:D:1605:HOH:O	2.52	0.42
2:F:5:ALA:HB2	2:F:19:ALA:HB2	2.00	0.42
1:A:40:GLU:OE1	1:A:325:LYS:NZ	2.30	0.42
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.85	0.42
1:A:558:ASP:HB3	1:A:559:ARG:H	1.59	0.42
1:C:10:ILE:HD12	1:C:42:TYR:HB3	2.02	0.42
1:E:670:ASP:CB	1:E:677:ARG:HH21	2.22	0.42
1:E:734:LEU:CD1	1:E:738:PHE:CE2	3.02	0.42
1:G:831:ALA:HB2	1:G:840:ILE:HD11	2.01	0.42
2:H:121:LEU:CD1	2:H:125:LYS:HD3	2.49	0.42
1:A:349:GLU:O	2:B:294:ASN:HB2	2.18	0.42
2:B:305:VAL:HG12	2:B:306:MET:N	2.35	0.42
2:B:378:ARG:NH1	2:B:378:ARG:HG2	2.33	0.42
1:C:563:MET:HE2	1:C:563:MET:HB2	1.78	0.42
1:C:904:ASP:HA	1:C:905:PRO:HD3	1.81	0.42
1:G:49:SER:HB2	1:G:917:VAL:HG12	2.02	0.42
1:G:168:ILE:HG23	1:G:204:LEU:HD22	2.00	0.42
1:G:663:GLY:HA2	1:G:869:MET:HG2	2.01	0.42
1:G:863:LYS:O	1:G:867:ARG:HG3	2.20	0.42
2:H:226:GLU:OE1	2:H:257:LYS:HE3	2.20	0.42
2:H:228:VAL:HA	2:H:231:MET:HE3	2.01	0.42
9:A:5012:NET:H31	9:A:5012:NET:H63	1.67	0.42
2:B:49:SER:HA	2:B:76:HIS:O	2.19	0.42
2:B:264:PRO:HB3	2:B:373:LEU:HB3	2.01	0.42
2:D:275:LEU:HD12	2:D:275:LEU:O	2.18	0.42
1:E:237:PHE:HB3	1:E:248:ILE:O	2.20	0.42
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.20	0.42
2:F:261:THR:OG1	2:F:263:ILE:HG13	2.20	0.42
1:A:1017:THR:CG2	1:A:1018:SER:N	2.82	0.42
1:E:327:ALA:HB2	10:E:5322:HOH:O	2.19	0.42
2:F:300:VAL:HG22	2:F:328:THR:O	2.19	0.42
1:G:619:GLU:HB3	1:G:620:PRO:HD2	2.02	0.42
1:E:379:LYS:HE2	10:E:5358:HOH:O	2.19	0.42
1:E:733:ASP:HA	1:E:736:ARG:HH11	1.84	0.42
1:G:159:ALA:HB2	1:G:188:PHE:CE2	2.55	0.42
2:H:209:LEU:HD23	2:H:209:LEU:HA	1.95	0.42
1:A:325:LYS:O	1:A:330:TYR:HB2	2.20	0.42
2:B:244:ASP:O	2:B:247:PRO:HD2	2.19	0.42
2:B:246:ALA:N	2:B:247:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLY:HA2	1:C:376:THR:OG1	2.20	0.42
1:C:196:LEU:HD23	1:C:196:LEU:HA	1.95	0.42
1:C:695:VAL:HG11	1:C:701:ALA:N	2.35	0.42
2:D:103:LYS:NZ	10:D:1769:HOH:O	2.48	0.42
1:E:252:PRO:HD3	1:E:352:ILE:HD11	2.01	0.42
1:E:728:VAL:HG12	1:E:733:ASP:HB3	1.95	0.42
1:G:375:THR:OG1	1:G:376:THR:N	2.52	0.42
2:H:296:PRO:HB2	2:H:332:LEU:HB2	2.01	0.42
2:H:324:ASN:O	2:H:342:ARG:HA	2.20	0.42
1:A:46:LEU:CD2	1:A:64:THR:HA	2.50	0.41
1:A:48:ASN:O	1:A:66:ILE:HA	2.20	0.41
1:A:321:LYS:NZ	1:A:611:ASP:OD1	2.49	0.41
1:A:602:ASN:ND2	1:A:605:THR:CG2	2.83	0.41
1:C:1:MET:O	1:C:329:GLY:O	2.38	0.41
1:C:820:LEU:HD23	1:C:820:LEU:HA	1.91	0.41
1:E:421:LEU:HD23	1:E:421:LEU:HA	1.90	0.41
2:H:42:ILE:HG23	2:H:48:TYR:CE2	2.55	0.41
2:H:324:ASN:ND2	2:H:324:ASN:N	2.67	0.41
1:A:704:LYS:HD2	1:A:704:LYS:HA	1.69	0.41
1:A:728:VAL:H	1:A:728:VAL:HG23	1.64	0.41
9:A:5012:NET:H42	9:A:5012:NET:C2	2.44	0.41
2:B:232:ASN:O	10:B:5245:HOH:O	2.22	0.41
1:C:11:LEU:HA	1:C:45:ILE:HB	2.02	0.41
1:C:670:ASP:HB3	1:C:677:ARG:NH2	2.34	0.41
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.20	0.41
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.19	0.41
1:C:1071:GLN:HE21	1:C:1071:GLN:HB3	1.70	0.41
1:A:702:VAL:HG11	1:A:735:ARG:NH2	2.35	0.41
2:B:46:PRO:HA	2:B:76:HIS:CB	2.50	0.41
2:B:190:LEU:HB2	2:B:215[A]:ARG:HB3	2.03	0.41
1:C:415:LEU:HA	1:C:415:LEU:HD23	1.87	0.41
2:D:212:ARG:CG	2:D:212:ARG:NH1	2.81	0.41
1:E:400:ARG:HD3	10:E:5372:HOH:O	2.19	0.41
1:E:1021:ARG:HH11	1:E:1021:ARG:HG3	1.84	0.41
2:F:6:LEU:HD21	2:F:140:ALA:HA	2.02	0.41
1:G:1:MET:H2	1:G:224:LYS:HZ1	1.69	0.41
1:G:79:GLU:O	1:G:82:ARG:HD2	2.19	0.41
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.85	0.41
1:G:1041:ASP:HA	8:G:5076:ORN:O	2.20	0.41
2:H:33:ASN:HA	2:H:291:HIS:O	2.20	0.41
1:A:431:ALA:HB2	1:A:435:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:ASP:OD2	1:C:827:ASN:HB2	2.20	0.41
1:E:336:MET:HB3	1:E:342:GLY:HA2	2.02	0.41
1:E:855:LYS:HA	1:E:855:LYS:HD2	1.82	0.41
2:F:112:ASP:N	2:F:112:ASP:OD2	2.53	0.41
2:F:248:CYS:C	2:F:252:ILE:HD12	2.41	0.41
1:G:423:LYS:H	1:G:423:LYS:HG3	1.62	0.41
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.36	0.41
1:A:108:LEU:HD22	1:A:113:VAL:HB	2.02	0.41
1:A:332:LEU:HB3	1:A:347:SER:HB3	2.02	0.41
1:A:419:GLU:HG3	10:E:5067:HOH:O	2.19	0.41
1:A:517:ARG:HD2	1:A:522:LEU:O	2.21	0.41
2:B:269:143:HE	2:B:312:HIS:CB	2.51	0.41
2:B:269:143:HE	2:B:312:HIS:HB3	2.02	0.41
1:C:66:ILE:CG2	1:C:918:MET:HB3	2.50	0.41
2:D:372:GLU:HG3	10:D:2246:HOH:O	2.20	0.41
1:E:940:LYS:HG3	1:E:1011:THR:HB	2.01	0.41
2:H:82:ILE:O	2:H:111:ALA:HA	2.20	0.41
2:H:350:PHE:CD1	2:H:366:LEU:HD21	2.56	0.41
1:A:18:ILE:HG23	1:A:23:ALA:HA	2.02	0.41
1:A:828:VAL:CG1	1:A:839:LEU:HD11	2.51	0.41
2:B:6:LEU:HD21	2:B:140:ALA:HA	2.02	0.41
1:C:891:LYS:HG2	1:C:892:GLU:N	2.36	0.41
1:C:994:VAL:HA	1:C:1000:HIS:ND1	2.35	0.41
1:C:1017:THR:CG2	1:C:1018:SER:N	2.83	0.41
2:D:176:THR:O	2:D:180:GLY:N	2.52	0.41
1:E:237:PHE:HB3	1:E:248:ILE:HB	2.03	0.41
1:E:419:GLU:O	1:E:422:THR:HB	2.21	0.41
1:E:514:ARG:HD3	10:E:5436:HOH:O	2.20	0.41
1:E:669:ILE:HA	1:E:844:PRO:HG2	2.03	0.41
2:F:223:THR:HG22	2:F:228:VAL:HG23	2.03	0.41
1:G:688:LYS:HD3	10:G:4241:HOH:O	2.19	0.41
2:H:66:ASN:ND2	10:H:3649:HOH:O	2.35	0.41
2:B:259:LEU:HA	2:B:259:LEU:HD23	1.80	0.41
2:B:298:LYS:HB2	2:B:332:LEU:HD11	2.02	0.41
1:C:1021:ARG:HH11	1:C:1021:ARG:CG	2.34	0.41
2:D:228:VAL:HG22	2:D:231:MET:CE	2.50	0.41
1:E:1:MET:CB	1:E:2:PRO:HD3	2.50	0.41
1:E:489:LEU:HD12	1:E:489:LEU:HA	1.88	0.41
1:E:755:PHE:CE1	7:E:2051:ADP:C2	3.08	0.41
2:F:374:ILE:O	2:F:374:ILE:HG22	2.21	0.41
1:G:994:VAL:HG13	1:G:1000:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD21	1:A:64:THR:CG2	2.42	0.41
1:A:467:GLU:O	1:A:471:ARG:HG2	2.21	0.41
1:A:695:VAL:HG23	1:A:752:LEU:HD22	2.01	0.41
1:C:318:PRO:HB2	1:C:321:LYS:HB2	2.03	0.41
1:C:992:ASN:ND2	1:E:975:HIS:NE2	2.68	0.41
2:D:272:HIS:HA	2:D:349:SER:HB2	2.02	0.41
1:G:892:GLU:OE1	8:G:5076:ORN:NE	2.51	0.41
2:H:23:THR:HG23	2:H:134:ALA:O	2.21	0.41
2:H:201:ALA:HB2	2:H:239:SER:CB	2.50	0.41
2:H:205:ILE:HG13	2:H:355:GLU:HG3	2.03	0.41
1:A:728:VAL:HG12	1:A:733:ASP:HB3	2.02	0.41
1:A:797:PRO:HB3	10:A:5497:HOH:O	2.20	0.41
2:B:378:ARG:HG2	2:B:378:ARG:HH11	1.85	0.41
1:C:150:HIS:N	1:C:154:GLU:OE2	2.54	0.41
1:C:385:MET:HB3	1:C:618:PHE:CE1	2.56	0.41
1:C:419:GLU:O	1:C:423:LYS:HG3	2.21	0.41
1:C:526:TYR:CE1	1:C:545:SER:HB3	2.56	0.41
1:C:805:ILE:HD13	1:C:837:VAL:CG2	2.51	0.41
1:C:833:LYS:O	1:C:836:GLU:HB2	2.21	0.41
1:E:170:PRO:HB3	1:E:199:SER:HB2	2.03	0.41
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.78	0.41
1:G:58:PRO:HD2	1:G:59:GLU:OE2	2.21	0.41
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.56	0.41
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.73	0.41
1:A:164:PHE:HA	1:A:165:PRO:C	2.39	0.41
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.56	0.41
1:A:672:ALA:HB2	1:A:844:PRO:HG3	2.01	0.41
1:A:946:LEU:C	1:A:947:LEU:HD12	2.42	0.41
1:C:1:MET:N	1:C:2:PRO:HD2	2.36	0.41
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.56	0.41
2:F:129:ASN:CG	2:F:150:PHE:HD1	2.25	0.41
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.03	0.41
1:G:85:ALA:HB1	1:G:114:THR:O	2.21	0.41
1:G:726:GLU:HG3	1:G:727:ILE:H	1.82	0.41
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.33	0.41
2:H:279:SER:O	2:H:322:PRO:HG3	2.21	0.41
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.85	0.40
2:B:187:GLU:CG	2:B:215[A]:ARG:HD2	2.42	0.40
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.56	0.40
1:C:46:LEU:CD2	1:C:55:MET:O	2.69	0.40
1:C:423:LYS:HG3	1:C:423:LYS:H	1.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:CD1	1:C:837:VAL:CG2	2.99	0.40
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.71	0.40
1:E:1017:THR:CG2	1:E:1018:SER:N	2.84	0.40
2:H:286:MET:HE2	2:H:314:PHE:C	2.42	0.40
1:A:4:ARG:HD3	1:A:7:ILE:HD12	2.03	0.40
1:A:167:ILE:N	1:A:167:ILE:CD1	2.84	0.40
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.56	0.40
1:A:998:ARG:HA	1:A:999:PRO:C	2.39	0.40
2:D:324:ASN:ND2	2:D:324:ASN:N	2.68	0.40
2:D:337:LEU:HD12	2:D:337:LEU:HA	1.83	0.40
1:G:6:ASP:OD2	1:G:6:ASP:N	2.49	0.40
1:G:579:ASP:OD1	1:G:605:THR:HB	2.21	0.40
1:G:738:PHE:HA	1:G:741:ALA:HB3	2.03	0.40
1:G:770:GLY:CA	1:G:823:ARG:CZ	3.00	0.40
1:G:770:GLY:HA3	1:G:823:ARG:CZ	2.52	0.40
2:D:201:ALA:HA	2:D:240:ASN:OD1	2.22	0.40
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.69	0.40
1:E:3:LYS:HB2	1:E:42:TYR:HH	1.82	0.40
1:E:148:ILE:CG2	1:E:149:ALA:N	2.85	0.40
1:E:1001:ILE:HD12	1:E:1002:GLN:CA	2.52	0.40
2:F:38:GLY:HA3	2:F:358:PRO:HB3	2.02	0.40
1:G:1065:VAL:HG23	1:G:1065:VAL:H	1.59	0.40
2:H:196:ALA:HA	2:H:237:PHE:O	2.22	0.40
1:A:944:ARG:HD3	1:A:972:ASP:CG	2.42	0.40
1:C:77:ILE:O	1:C:81:GLU:N	2.51	0.40
1:C:992:ASN:ND2	1:C:996:GLU:HB3	2.36	0.40
1:E:728:VAL:HG11	1:E:734:LEU:HA	2.03	0.40
1:E:730:ASP:H	1:E:733:ASP:HB2	1.86	0.40
1:E:730:ASP:O	1:E:733:ASP:HB2	2.21	0.40
1:G:7:ILE:HG21	1:G:7:ILE:HD13	1.80	0.40
1:G:671:ARG:CG	1:G:677:ARG:NH1	2.82	0.40
2:H:121:LEU:HD11	2:H:125:LYS:HD3	2.03	0.40
2:H:363:ALA:C	2:H:365:PRO:HD2	2.42	0.40
1:A:681:ALA:HA	1:A:684:ARG:HB3	2.02	0.40
1:A:812:GLN:NE2	10:A:5766:HOH:O	2.29	0.40
1:A:1048:PHE:O	1:A:1052:MET:HG3	2.21	0.40
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.84	0.40
1:C:693:ALA:HB2	1:C:708:ILE:HD11	2.02	0.40
1:C:947:LEU:HG	1:C:1014:ILE:HG21	2.03	0.40
1:E:146:SER:HA	1:E:206:ILE:O	2.22	0.40
1:E:693:ALA:CB	1:E:708:ILE:HD11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:LEU:HD22	2:F:216:LEU:HD13	2.04	0.40
1:G:1:MET:N	1:G:224:LYS:HZ1	2.19	0.40
1:G:709:GLY:O	1:G:712:LEU:HD12	2.20	0.40
1:G:981:LEU:HA	1:G:981:LEU:HD23	1.91	0.40
2:H:185:LYS:HD2	2:H:190:LEU:HD21	2.04	0.40
2:H:190:LEU:HD23	2:H:190:LEU:HA	1.78	0.40
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.57	0.40
2:H:350:PHE:CG	2:H:366:LEU:HD21	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1057/1073 (98%)	998 (94%)	56 (5%)	3 (0%)	41	41
1	C	1054/1073 (98%)	1002 (95%)	48 (5%)	4 (0%)	34	32
1	E	1060/1073 (99%)	1012 (96%)	45 (4%)	3 (0%)	41	41
1	G	1052/1073 (98%)	998 (95%)	49 (5%)	5 (0%)	29	26
2	B	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	376/382 (98%)	364 (97%)	12 (3%)	0	100	100
2	H	376/382 (98%)	362 (96%)	14 (4%)	0	100	100
All	All	5729/5820 (98%)	5462 (95%)	252 (4%)	15 (0%)	41	41

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	996	GLU
1	G	873	SER

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Mol	Chain	Res	Type
1	A	558	ASP
1	A	975	HIS
1	E	675	ARG
1	E	954	LYS
1	G	975	HIS
1	G	558	ASP
1	G	739	GLN
1	A	646	THR
1	C	88	PRO
1	E	738	PHE
1	G	698	ILE
1	C	2	PRO
1	C	698	ILE

### 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	870/878 (99%)	808 (93%)	62 (7%)	14	11
1	C	867/878 (99%)	797 (92%)	70 (8%)	11	8
1	E	873/878 (99%)	818 (94%)	55 (6%)	18	15
1	G	865/878 (98%)	793 (92%)	72 (8%)	11	7
2	B	308/309 (100%)	288 (94%)	20 (6%)	17	14
2	D	308/309 (100%)	288 (94%)	20 (6%)	17	14
2	F	307/309 (99%)	281 (92%)	26 (8%)	10	7
2	H	307/309 (99%)	286 (93%)	21 (7%)	16	13
All	All	4705/4748 (99%)	4359 (93%)	346 (7%)	14	10

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	5	THR
1	A	8	LYS
1	A	38	ARG
1	A	46	LEU
1	A	62	ASP
1	A	103	GLU
1	A	174	MET
1	A	202	LYS
1	A	224	LYS
1	A	275	ILE
1	A	343	ARG
1	A	358	LYS
1	A	363	ASN
1	A	416	ASP
1	A	426	ARG
1	A	490	ARG
1	A	542	TYR
1	A	557	THR
1	A	571	ARG
1	A	591	GLU
1	A	632	ILE
1	A	652	ARG
1	A	671	ARG
1	A	677	ARG
1	A	684	ARG
1	A	688	LYS
1	A	696	THR
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	712	LEU
1	A	714	VAL
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	804	GLU
1	A	805	ILE
1	A	815	LYS
1	A	833	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	835	ASN
1	A	839	LEU
1	A	855	LYS
1	A	881	LYS
1	A	891	LYS
1	A	895	LEU
1	A	906	LEU
1	A	912	ARG
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	967	GLN
1	A	992	ASN
1	A	1021	ARG
1	A	1026	SER
1	A	1032	SER
1	A	1059	THR
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	18	ARG
2	B	87	LEU
2	B	153	LEU
2	B	154	ASN
2	B	166	GLU
2	B	183	GLU
2	B	186	LYS
2	B	190	LEU
2	B	192	PHE
2	B	215[A]	ARG
2	B	215[B]	ARG
2	B	222	GLN
2	B	257	LYS
2	B	306	MET
2	B	324	ASN
2	B	357	SER
2	B	366	LEU
2	B	379	LYS
1	C	1	MET
1	C	4	ARG
1	C	5	THR
1	C	38[A]	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	38[B]	ARG
1	C	43	ARG
1	C	103	GLU
1	C	145	ARG
1	C	174	MET
1	C	185	ARG
1	C	202	LYS
1	C	299	GLU
1	C	307	SER
1	C	313	LYS
1	C	321	LYS
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	414	SER
1	C	416	ASP
1	C	422	THR
1	C	426	ARG
1	C	428	LEU
1	C	509	ARG
1	C	542	TYR
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	652	ARG
1	C	671	ARG
1	C	675	ARG
1	C	686	LYS
1	C	688	LYS
1	C	692	ASN
1	C	706	LYS
1	C	712	LEU
1	C	728	VAL
1	C	733	ASP
1	C	734	LEU
1	C	735	ARG
1	C	736	ARG
1	C	751	LEU
1	C	763	ASP
1	C	784	GLN
1	C	800	THR
1	C	805	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	812	GLN
1	C	849	THR
1	C	855	LYS
1	C	880	THR
1	C	906	LEU
1	C	912	ARG
1	C	940	LYS
1	C	950	ARG
1	C	951	GLU
1	C	954	LYS
1	C	966	LYS
1	C	967	GLN
1	C	972	ASP
1	C	992	ASN
1	C	1000	HIS
1	C	1007	ASN
1	C	1009[A]	GLU
1	C	1009[B]	GLU
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1052	MET
1	C	1061	LYS
1	C	1073	LYS
2	D	2	ILE
2	D	6	LEU
2	D	50	ARG
2	D	87	LEU
2	D	153	LEU
2	D	154	ASN
2	D	166	GLU
2	D	185	LYS
2	D	215	ARG
2	D	222	GLN
2	D	232	ASN
2	D	257	LYS
2	D	261	THR
2	D	282	LYS
2	D	306	MET
2	D	324	ASN
2	D	332	LEU
2	D	366	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	376	GLN
2	D	379	LYS
1	E	3	LYS
1	E	5	THR
1	E	46	LEU
1	E	68	PRO
1	E	115	MET
1	E	153[A]	GLU
1	E	153[B]	GLU
1	E	174	MET
1	E	185	ARG
1	E	236	ASN
1	E	275	ILE
1	E	313	LYS
1	E	321	LYS
1	E	339	ILE
1	E	412	LYS
1	E	428	LEU
1	E	509	ARG
1	E	515	LYS
1	E	542	TYR
1	E	548	GLU
1	E	571	ARG
1	E	591	GLU
1	E	652	ARG
1	E	675	ARG
1	E	688	LYS
1	E	698	ILE
1	E	706	LYS
1	E	712	LEU
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	751	LEU
1	E	753	ASP
1	E	763	ASP
1	E	784	GLN
1	E	805	ILE
1	E	835	ASN
1	E	849	THR
1	E	855	LYS
1	E	906	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	912	ARG
1	E	937	SER
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG
1	E	963	LYS
1	E	967[A]	GLN
1	E	967[B]	GLN
1	E	1000	HIS
1	E	1006	LYS
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1073	LYS
2	F	2	ILE
2	F	6	LEU
2	F	18	ARG
2	F	73	SER
2	F	87	LEU
2	F	138	PRO
2	F	153	LEU
2	F	154	ASN
2	F	166	GLU
2	F	175	TRP
2	F	183	GLU
2	F	186	LYS
2	F	190	LEU
2	F	192	PHE
2	F	215	ARG
2	F	222	GLN
2	F	224	SER
2	F	227	ASP
2	F	257	LYS
2	F	263	ILE
2	F	306	MET
2	F	324	ASN
2	F	332	LEU
2	F	366	LEU
2	F	376	GLN
2	F	379	LYS
1	G	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	4	ARG
1	G	8	LYS
1	G	20	ILE
1	G	49	SER
1	G	55	MET
1	G	76	LYS
1	G	103	GLU
1	G	104	ARG
1	G	145	ARG
1	G	146	SER
1	G	174	MET
1	G	185	ARG
1	G	202	LYS
1	G	207	ASP
1	G	236	ASN
1	G	303	ARG
1	G	313	LYS
1	G	321	LYS
1	G	326	LEU
1	G	358	LYS
1	G	412	LYS
1	G	416	ASP
1	G	490	ARG
1	G	509	ARG
1	G	542	TYR
1	G	559	ARG
1	G	571	ARG
1	G	576	ILE
1	G	591	GLU
1	G	631	ARG
1	G	652	ARG
1	G	671	ARG
1	G	673	GLU
1	G	675	ARG
1	G	688	LYS
1	G	692	ASN
1	G	704	LYS
1	G	706	LYS
1	G	712	LEU
1	G	714	VAL
1	G	733	ASP
1	G	734	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	735	ARG
1	G	751	LEU
1	G	753	ASP
1	G	763	ASP
1	G	784	GLN
1	G	795	SER
1	G	805	ILE
1	G	811	GLN
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	873	SER
1	G	880	THR
1	G	891	LYS
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	950	ARG
1	G	956	ARG
1	G	967	GLN
1	G	991	VAL
1	G	1001	ILE
1	G	1004	ARG
1	G	1006	LYS
1	G	1020	ARG
1	G	1021	ARG
1	G	1061	LYS
1	G	1064	SER
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	18	ARG
2	H	50	ARG
2	H	104	ARG
2	H	125	LYS
2	H	153	LEU
2	H	154	ASN
2	H	166	GLU
2	H	191	PRO
2	H	192	PHE
2	H	218	ILE
2	H	222	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	257	LYS
2	H	263	ILE
2	H	306	MET
2	H	324	ASN
2	H	332	LEU
2	H	357	SER
2	H	365	PRO
2	H	372	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
1	A	679	GLN
1	A	689	GLN
1	A	784	GLN
1	A	803	GLN
1	A	814	GLN
1	A	834	ASN
1	A	835	ASN
1	A	967	GLN
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	645	GLN
1	C	679	GLN
1	C	689	GLN
1	C	784	GLN
1	C	803	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	812	GLN
1	C	936	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1007	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	14	GLN
2	D	51	GLN
2	D	154	ASN
2	D	222	GLN
2	D	324	ASN
2	D	351	GLN
1	E	105	GLN
1	E	266	ASN
1	E	457	ASN
1	E	679	GLN
1	E	689	GLN
1	E	784	GLN
1	E	814	GLN
1	E	835	ASN
1	E	987	ASN
1	E	992	ASN
1	E	1000	HIS
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	16	HIS
2	F	51	GLN
2	F	154	ASN
2	F	324	ASN
1	G	105	GLN
1	G	150	HIS
1	G	457	ASN
1	G	523	HIS
1	G	679	GLN
1	G	689	GLN
1	G	692	ASN
1	G	784	GLN

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Mol	Chain	Res	Type
1	G	803	GLN
1	G	814	GLN
1	G	936	ASN
1	G	942	HIS
1	G	987	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	154	ASN
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	143	F	269	2	9,16,17	7.68	4 (44%)	3,21,23	1.86	1 (33%)
2	143	D	269	2	9,16,17	6.57	5 (55%)	3,21,23	1.34	0
2	143	B	269	2	9,16,17	5.18	4 (44%)	3,21,23	1.81	1 (33%)
2	143	H	269	2	9,16,17	8.70	5 (55%)	3,21,23	1.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	143	F	269	2	1/1/5/8	4/9/24/26	0/1/1/1
2	143	D	269	2	1/1/5/8	3/9/24/26	0/1/1/1
2	143	B	269	2	1/1/5/8	3/9/24/26	0/1/1/1
2	143	H	269	2	1/1/5/8	4/9/24/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	143	CD-NX	-20.68	1.17	1.45
2	F	269	143	CD-NX	-19.40	1.19	1.45
2	D	269	143	CD-NX	-16.99	1.22	1.45
2	B	269	143	CD-NX	-13.21	1.27	1.45
2	H	269	143	CD-CE	-12.18	1.33	1.49
2	F	269	143	CB-SG	-7.69	1.73	1.82
2	F	269	143	CD-CE	-7.10	1.40	1.49
2	H	269	143	OJ2-CJ	7.05	1.43	1.22
2	H	269	143	CB-SG	-6.76	1.74	1.82
2	D	269	143	CB-SG	-6.36	1.75	1.82
2	F	269	143	OJ2-CJ	6.22	1.41	1.22
2	B	269	143	CB-SG	-5.96	1.75	1.82
2	D	269	143	OJ2-CJ	5.52	1.39	1.22
2	B	269	143	OJ2-CJ	4.77	1.36	1.22
2	D	269	143	CD-CE	-4.47	1.43	1.49
2	B	269	143	OJ1-CJ	2.37	1.38	1.30
2	H	269	143	OJ1-CJ	2.07	1.37	1.30
2	D	269	143	OJ1-CJ	2.05	1.37	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	143	OJ1-CJ-OJ2	-2.82	117.68	124.09
2	F	269	143	OJ1-CJ-OJ2	-2.43	118.57	124.09

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD

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Mol	Chain	Res	Type	Atom
2	H	269	143	CD

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	143	N-CA-CB-SG
2	B	269	143	OF-CF-CI-CJ
2	D	269	143	N-CA-CB-SG
2	D	269	143	OF-CF-CI-CJ
2	F	269	143	N-CA-CB-SG
2	F	269	143	C-CA-CB-SG
2	F	269	143	OF-CF-CI-CJ
2	H	269	143	N-CA-CB-SG
2	H	269	143	C-CA-CB-SG
2	H	269	143	OF-CF-CI-CJ
2	B	269	143	NI-CI-CJ-OJ1
2	D	269	143	NI-CI-CJ-OJ1
2	F	269	143	NI-CI-CJ-OJ1
2	H	269	143	NI-CI-CJ-OJ1

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	269	143	2	0
2	D	269	143	3	0
2	B	269	143	2	0
2	H	269	143	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 66 are monoatomic - leaving 20 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
7	ADP	E	2045	3	24,29,29	1.01	2 (8%)	29,45,45	1.25	2 (6%)
6	PO4	E	2050	3	4,4,4	1.99	3 (75%)	6,6,6	1.07	0
7	ADP	C	2029	4,3	24,29,29	1.10	2 (8%)	29,45,45	1.29	4 (13%)
7	ADP	A	2001	3	24,29,29	1.21	2 (8%)	29,45,45	1.26	4 (13%)
7	ADP	G	2066	3	24,29,29	1.16	3 (12%)	29,45,45	1.28	4 (13%)
8	ORN	G	5076	-	7,8,8	0.97	1 (14%)	8,9,9	1.11	1 (12%)
6	PO4	A	2006	3	4,4,4	1.85	2 (50%)	6,6,6	1.28	1 (16%)
7	ADP	A	2007	4,3	24,29,29	1.01	1 (4%)	29,45,45	1.27	3 (10%)
7	ADP	G	2072	4,3	24,29,29	1.20	4 (16%)	29,45,45	1.37	4 (13%)
8	ORN	C	5033	-	7,8,8	0.87	0	8,9,9	1.11	1 (12%)
9	NET	G	5077	-	8,8,8	0.83	0	10,10,10	0.35	0
7	ADP	C	2023	3	24,29,29	1.26	4 (16%)	29,45,45	1.22	5 (17%)
6	PO4	C	2028	3	4,4,4	2.28	2 (50%)	6,6,6	0.98	0
9	NET	E	5056	-	8,8,8	0.79	0	10,10,10	0.35	0
7	ADP	E	2051	4,3	24,29,29	1.15	4 (16%)	29,45,45	1.06	3 (10%)
9	NET	C	5034	-	8,8,8	0.60	0	10,10,10	0.45	0
9	NET	A	5012	-	8,8,8	0.64	0	10,10,10	0.52	0
8	ORN	A	5011	-	7,8,8	0.79	0	8,9,9	1.54	2 (25%)
6	PO4	G	2071	3	4,4,4	2.07	1 (25%)	6,6,6	1.05	0
8	ORN	E	5055	-	7,8,8	0.95	0	8,9,9	1.25	1 (12%)

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
8	ORN	E	5055	-	-	6/8/8/8	-
9	NET	E	5056	-	-	3/12/12/12	-
7	ADP	A	2007	4,3	-	3/12/32/32	0/3/3/3
7	ADP	C	2029	4,3	-	3/12/32/32	0/3/3/3
7	ADP	A	2001	3	-	0/12/32/32	0/3/3/3
7	ADP	E	2051	4,3	-	3/12/32/32	0/3/3/3
7	ADP	G	2072	4,3	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	C	5033	-	-	7/8/8/8	-
9	NET	A	5012	-	-	10/12/12/12	-
8	ORN	A	5011	-	-	5/8/8/8	-
7	ADP	G	2066	3	-	0/12/32/32	0/3/3/3
7	ADP	C	2023	3	-	2/12/32/32	0/3/3/3
9	NET	C	5034	-	-	0/12/12/12	-
8	ORN	G	5076	-	-	6/8/8/8	-
7	ADP	E	2045	3	-	0/12/32/32	0/3/3/3
9	NET	G	5077	-	-	3/12/12/12	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2029	ADP	O3'-C3'	3.44	1.51	1.43
7	G	2066	ADP	O2'-C2'	2.99	1.50	1.43
7	A	2001	ADP	O3'-C3'	2.96	1.49	1.43
7	C	2023	ADP	O3'-C3'	2.95	1.49	1.43
7	C	2023	ADP	O4'-C1'	-2.94	1.37	1.41
6	C	2028	PO4	P-O4	-2.81	1.46	1.54
6	G	2071	PO4	P-O2	-2.76	1.46	1.54
7	A	2001	ADP	O2'-C2'	2.69	1.49	1.43
7	E	2051	ADP	O2'-C2'	2.61	1.49	1.43
7	G	2072	ADP	O4'-C1'	-2.60	1.37	1.41
6	C	2028	PO4	P-O2	-2.59	1.46	1.54
7	G	2066	ADP	O3'-C3'	2.53	1.48	1.43
7	E	2051	ADP	O4'-C1'	-2.51	1.37	1.41
7	C	2023	ADP	O2'-C2'	2.48	1.48	1.43
7	C	2029	ADP	O2'-C2'	2.45	1.48	1.43
7	E	2045	ADP	O3'-C3'	2.39	1.48	1.43
6	E	2050	PO4	P-O3	-2.32	1.47	1.54
8	G	5076	ORN	O-C	2.28	1.29	1.22
6	A	2006	PO4	P-O4	-2.27	1.47	1.54
7	E	2045	ADP	O2'-C2'	2.26	1.48	1.43
6	E	2050	PO4	P-O4	-2.23	1.47	1.54
7	G	2072	ADP	C2-N1	2.21	1.38	1.33
7	E	2051	ADP	C2-N1	2.19	1.38	1.33
7	E	2051	ADP	O3'-C3'	2.16	1.48	1.43
7	G	2072	ADP	O3'-C3'	2.13	1.48	1.43
7	C	2023	ADP	C2-N1	2.12	1.37	1.33
6	A	2006	PO4	P-O3	-2.10	1.48	1.54
7	G	2072	ADP	O2'-C2'	2.10	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	2050	PO4	P-O2	-2.06	1.48	1.54
7	A	2007	ADP	PB-O2B	-2.06	1.46	1.54
7	G	2066	ADP	C2-N1	2.03	1.37	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	2072	ADP	O3B-PB-O3A	3.94	117.86	104.64
7	E	2045	ADP	C5-C6-N6	3.71	125.99	120.35
7	C	2029	ADP	C5-C6-N6	3.35	125.44	120.35
7	G	2066	ADP	O2'-C2'-C3'	3.19	122.15	111.82
7	A	2007	ADP	C5-C6-N6	3.17	125.17	120.35
7	A	2001	ADP	C5-C6-N1	-2.98	113.59	120.35
7	G	2066	ADP	O3'-C3'-C2'	2.95	121.37	111.82
7	C	2029	ADP	O2'-C2'-C3'	2.86	121.06	111.82
7	A	2007	ADP	C3'-C2'-C1'	2.84	105.26	100.98
7	G	2072	ADP	O2'-C2'-C3'	2.75	120.70	111.82
7	E	2045	ADP	C3'-C2'-C1'	2.74	105.11	100.98
7	C	2029	ADP	O3'-C3'-C2'	2.74	120.67	111.82
7	A	2001	ADP	C3'-C2'-C1'	2.63	104.94	100.98
7	A	2007	ADP	O2B-PB-O3A	2.62	113.44	104.64
7	C	2023	ADP	O2'-C2'-C3'	2.54	120.04	111.82
6	A	2006	PO4	O4-P-O2	2.53	116.08	107.97
7	C	2023	ADP	C3'-C2'-C1'	2.51	104.76	100.98
7	C	2023	ADP	O3'-C3'-C2'	2.44	119.72	111.82
7	G	2072	ADP	C5-C6-N6	2.41	124.02	120.35
7	C	2029	ADP	C3'-C2'-C1'	2.40	104.60	100.98
7	A	2001	ADP	N6-C6-N1	2.40	123.55	118.57
8	A	5011	ORN	CB-CA-C	-2.38	104.64	110.30
8	E	5055	ORN	OXT-C-O	-2.38	118.69	124.09
7	G	2066	ADP	C5-C6-N1	-2.32	115.08	120.35
8	G	5076	ORN	OXT-C-CA	2.18	120.80	113.38
8	C	5033	ORN	OXT-C-CA	2.14	120.67	113.38
7	G	2066	ADP	C5-C6-N6	2.14	123.60	120.35
7	E	2051	ADP	C5-C6-N6	2.13	123.59	120.35
7	E	2051	ADP	O3'-C3'-C2'	2.11	118.63	111.82
8	A	5011	ORN	OXT-C-CA	2.09	120.50	113.38
7	C	2023	ADP	C2'-C3'-C4'	-2.08	98.61	102.64
7	C	2023	ADP	C5-C6-N1	-2.05	115.70	120.35
7	G	2072	ADP	O3'-C3'-C2'	2.05	118.45	111.82
7	A	2001	ADP	O2'-C2'-C3'	2.01	118.33	111.82
7	E	2051	ADP	C2'-C3'-C4'	-2.01	98.74	102.64

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2007	ADP	PA-O3A-PB-O3B
7	C	2029	ADP	PA-O3A-PB-O3B
7	E	2051	ADP	PA-O3A-PB-O3B
8	A	5011	ORN	N-CA-CB-CG
8	A	5011	ORN	C-CA-CB-CG
8	C	5033	ORN	N-CA-CB-CG
8	C	5033	ORN	C-CA-CB-CG
8	E	5055	ORN	N-CA-CB-CG
8	E	5055	ORN	C-CA-CB-CG
8	G	5076	ORN	N-CA-CB-CG
8	G	5076	ORN	C-CA-CB-CG
8	G	5076	ORN	O-C-CA-N
9	A	5012	NET	C4-C3-N1-C1
9	A	5012	NET	C4-C3-N1-C7
9	A	5012	NET	C4-C3-N1-C5
8	E	5055	ORN	CA-CB-CG-CD
9	A	5012	NET	C8-C7-N1-C3
8	C	5033	ORN	OXT-C-CA-N
9	A	5012	NET	C8-C7-N1-C1
9	A	5012	NET	C8-C7-N1-C5
8	G	5076	ORN	CA-CB-CG-CD
8	G	5076	ORN	OXT-C-CA-N
8	C	5033	ORN	CA-CB-CG-CD
7	E	2051	ADP	PA-O3A-PB-O1B
7	G	2072	ADP	PA-O3A-PB-O1B
9	G	5077	NET	C4-C3-N1-C1
9	E	5056	NET	C4-C3-N1-C7
8	A	5011	ORN	O-C-CA-N
8	C	5033	ORN	O-C-CA-N
8	E	5055	ORN	O-C-CA-N
9	G	5077	NET	C4-C3-N1-C7
9	A	5012	NET	C6-C5-N1-C3
8	A	5011	ORN	NE-CD-CG-CB
8	C	5033	ORN	NE-CD-CG-CB
8	G	5076	ORN	NE-CD-CG-CB
9	G	5077	NET	C4-C3-N1-C5
7	G	2072	ADP	C5'-O5'-PA-O3A
7	A	2007	ADP	PB-O3A-PA-O2A
7	C	2023	ADP	PB-O3A-PA-O1A
9	E	5056	NET	C4-C3-N1-C5

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Mol	Chain	Res	Type	Atoms
9	A	5012	NET	C6-C5-N1-C1
9	E	5056	NET	C4-C3-N1-C1
8	A	5011	ORN	CA-CB-CG-CD
8	E	5055	ORN	O-C-CA-CB
9	A	5012	NET	C6-C5-N1-C7
7	C	2029	ADP	PB-O3A-PA-O2A
7	E	2051	ADP	PB-O3A-PA-O2A
7	A	2007	ADP	PA-O3A-PB-O1B
7	G	2072	ADP	PB-O3A-PA-O2A
7	C	2029	ADP	PA-O3A-PB-O1B
8	E	5055	ORN	OXT-C-CA-N
7	C	2023	ADP	C5'-O5'-PA-O1A
8	C	5033	ORN	O-C-CA-CB
9	A	5012	NET	C2-C1-N1-C5

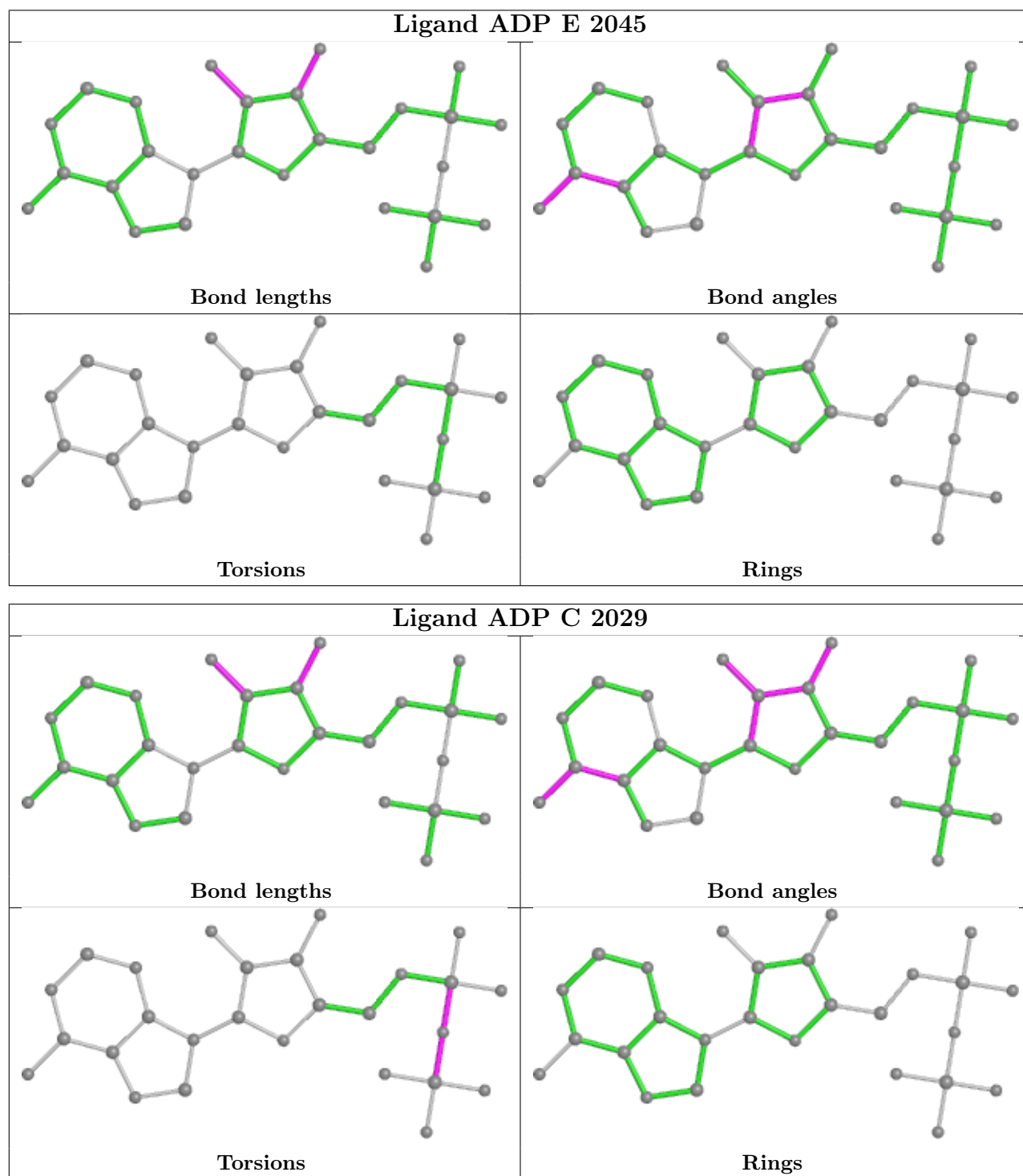
There are no ring outliers.

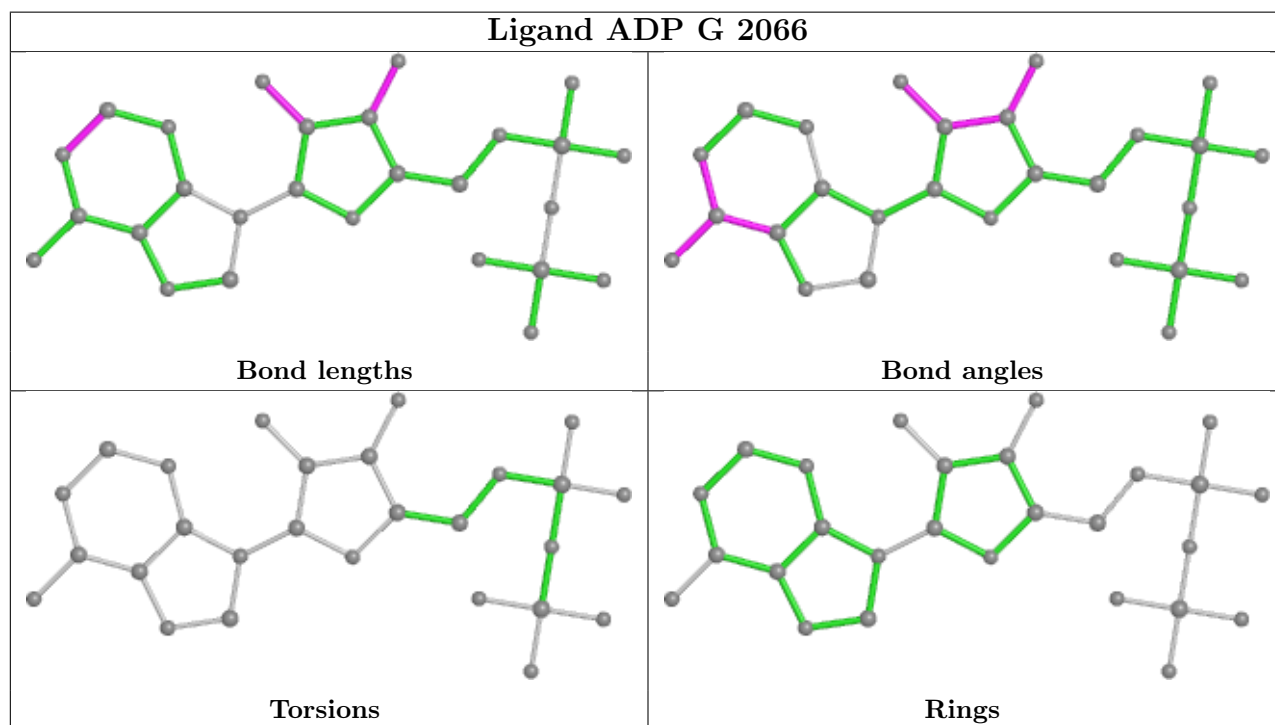
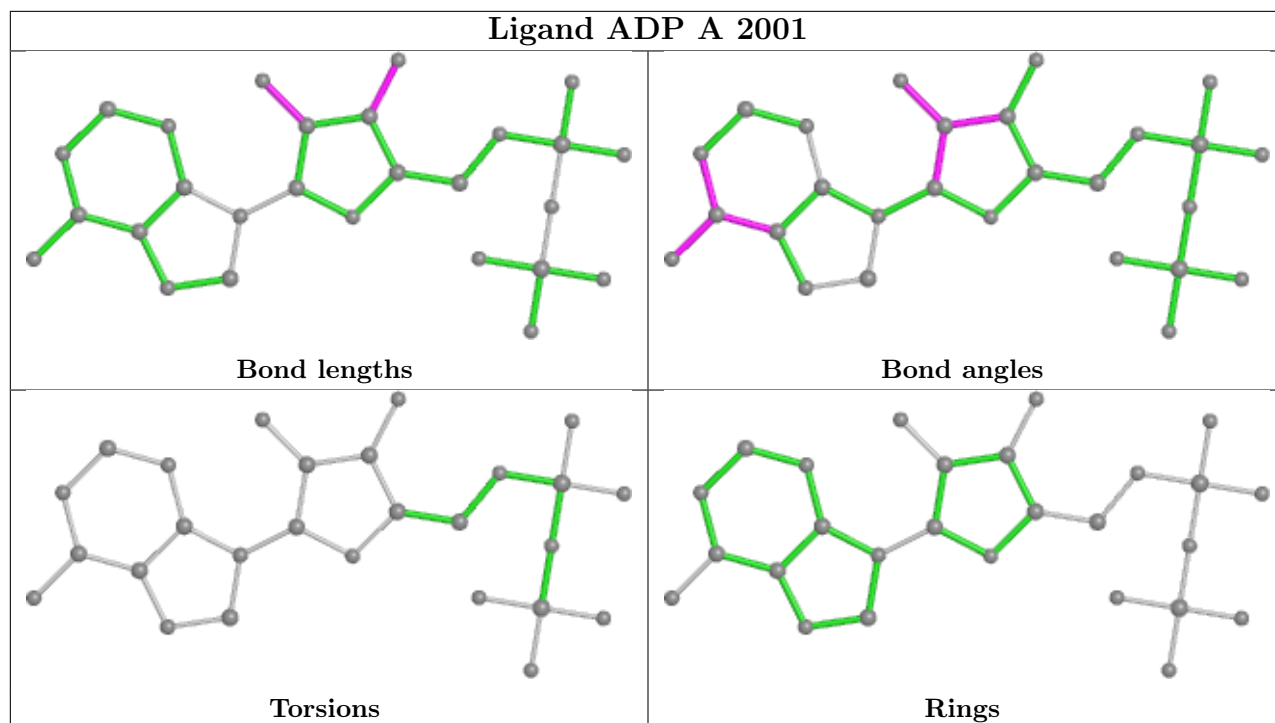
12 monomers are involved in 20 short contacts:

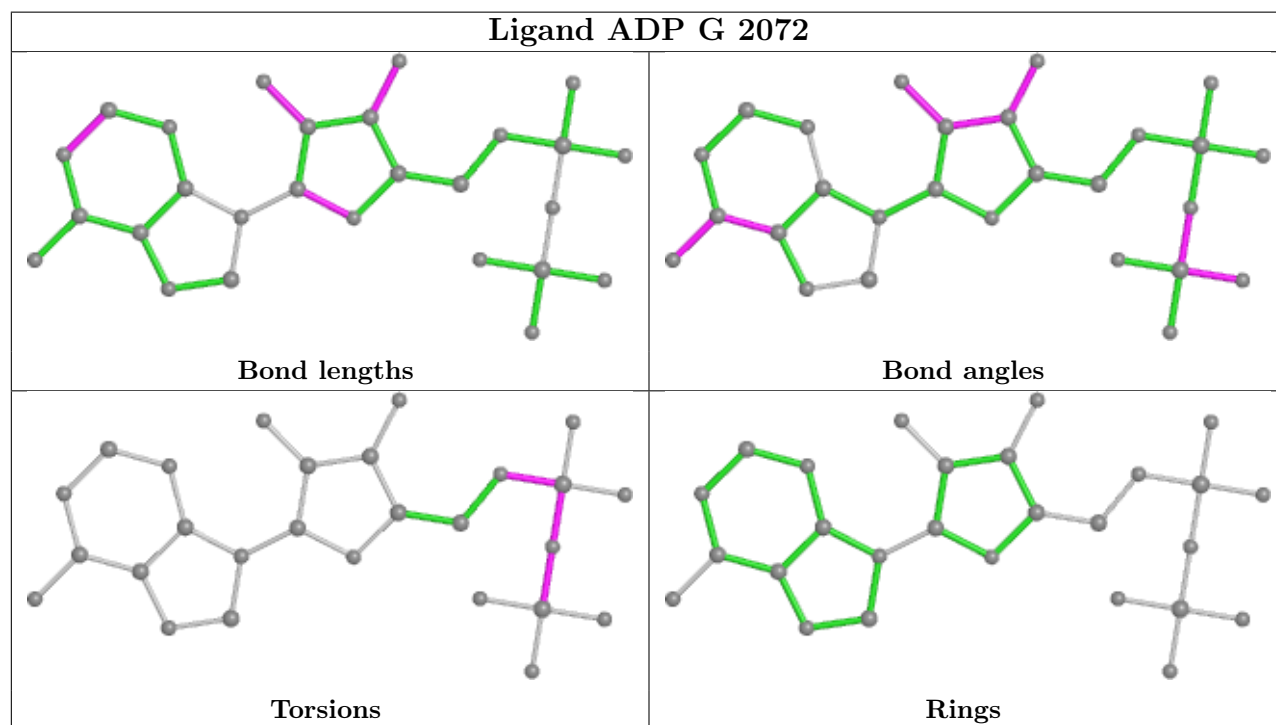
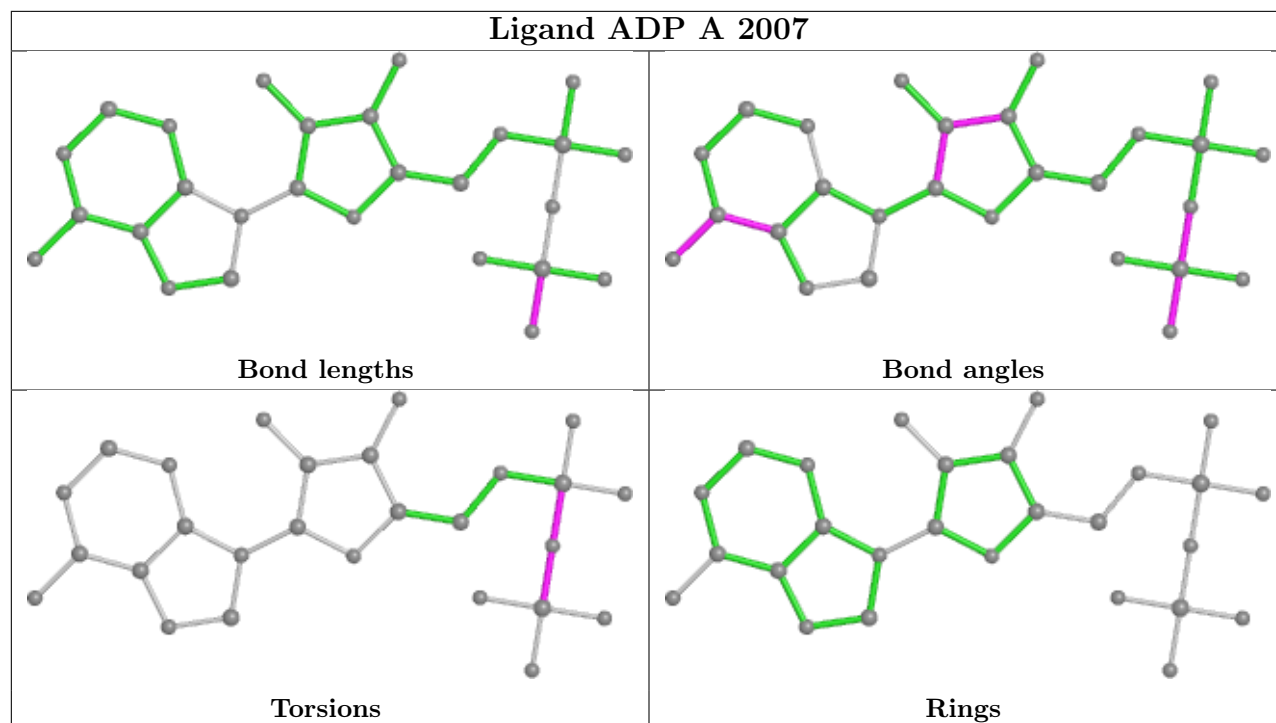
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	2045	ADP	2	0
7	G	2066	ADP	2	0
8	G	5076	ORN	2	0
7	G	2072	ADP	2	0
8	C	5033	ORN	1	0
9	G	5077	NET	1	0
6	C	2028	PO4	1	0
9	E	5056	NET	1	0
7	E	2051	ADP	2	0
9	A	5012	NET	4	0
6	G	2071	PO4	1	0
8	E	5055	ORN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

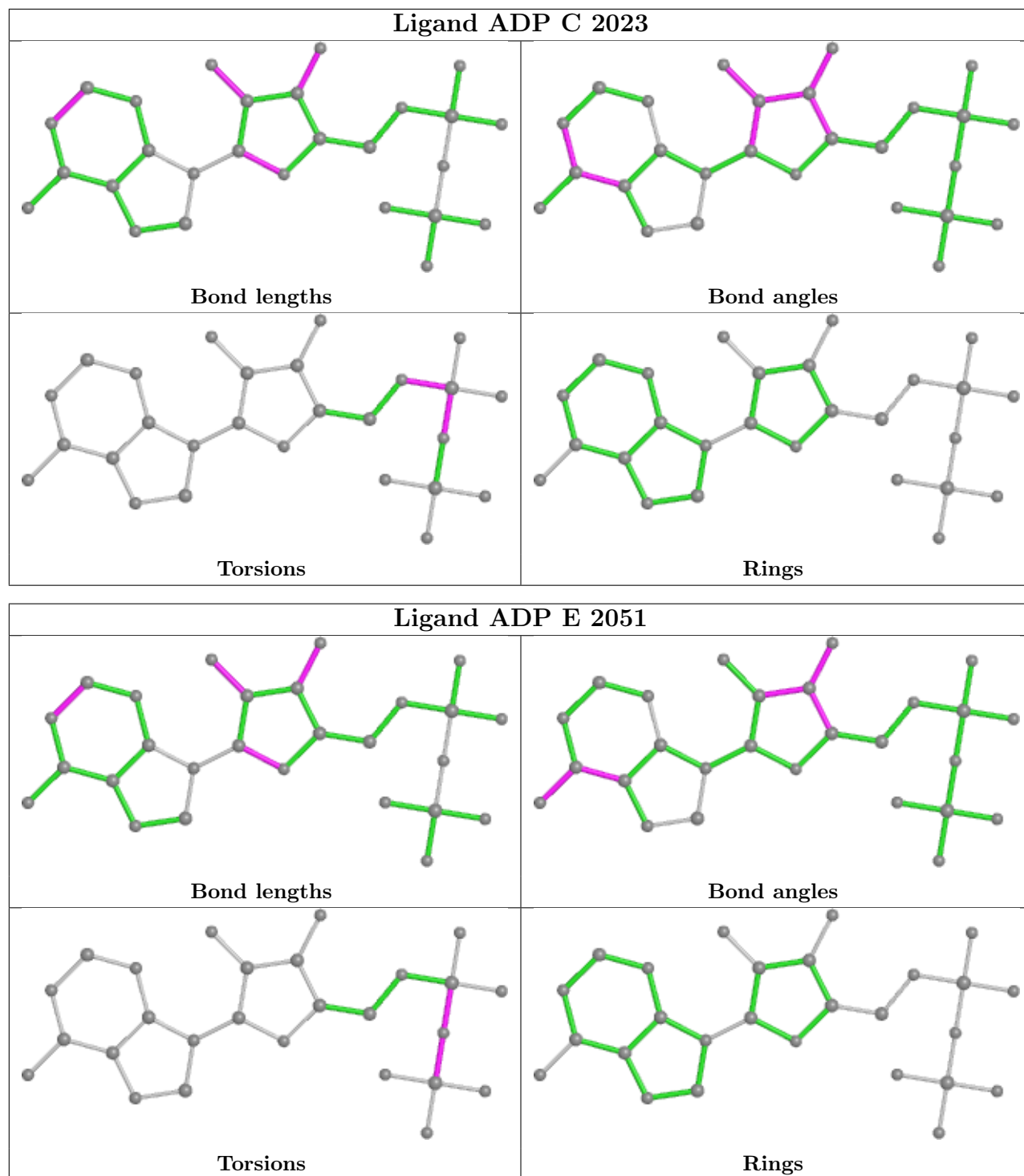
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1058/1073 (98%)	-0.33	37 (3%) 44 50	15, 32, 80, 100	0
1	C	1058/1073 (98%)	-0.31	42 (3%) 38 44	15, 33, 81, 100	0
1	E	1058/1073 (98%)	-0.32	40 (3%) 40 46	16, 29, 82, 100	0
1	G	1058/1073 (98%)	-0.20	49 (4%) 32 38	16, 37, 87, 100	0
2	B	378/382 (98%)	-0.29	4 (1%) 80 84	19, 41, 75, 100	0
2	D	378/382 (98%)	-0.39	0 100 100	18, 33, 63, 92	0
2	F	378/382 (98%)	-0.28	13 (3%) 45 51	18, 35, 74, 99	0
2	H	378/382 (98%)	-0.12	10 (2%) 56 61	25, 45, 78, 98	0
All	All	5744/5820 (98%)	-0.29	195 (3%) 45 51	15, 34, 80, 100	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.4
1	A	738	PHE	10.3
1	A	740	THR	9.9
1	A	739	GLN	8.8
1	C	695	VAL	8.3
1	G	1	MET	8.2
1	A	698	ILE	8.2
1	A	732	ALA	7.9
1	G	738	PHE	7.8
1	E	750	VAL	7.7
1	C	738	PHE	7.5
1	A	750	VAL	7.4
1	E	1	MET	7.3
1	E	738	PHE	7.3
1	G	740	THR	6.9
1	A	693	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	G	739	GLN	6.8
1	C	1	MET	6.7
1	A	736	ARG	6.6
1	C	740	THR	6.4
1	C	696	THR	6.2
1	C	739	GLN	6.0
1	E	739	GLN	6.0
1	G	729	TYR	5.9
1	C	698	ILE	5.9
1	A	737	TYR	5.7
1	E	694	THR	5.6
1	G	697	ALA	5.4
1	C	733	ASP	5.3
1	A	730	ASP	5.3
1	A	695	VAL	5.2
1	C	736	ARG	5.2
1	E	740	THR	5.1
1	A	696	THR	5.1
1	C	731	GLU	5.1
1	C	729	TYR	5.0
1	C	732	ALA	4.9
1	E	741	ALA	4.9
1	G	741	ALA	4.8
1	E	695	VAL	4.8
1	E	737	TYR	4.8
1	C	750	VAL	4.7
1	G	716	PRO	4.7
1	G	695	VAL	4.7
1	A	729	TYR	4.7
1	A	710	TYR	4.6
1	G	694	THR	4.6
1	C	702	VAL	4.5
1	G	733	ASP	4.5
1	G	732	ALA	4.3
1	C	710	TYR	4.3
1	C	734	LEU	4.3
1	A	697	ALA	4.2
1	E	697	ALA	4.2
1	A	735	ARG	4.2
1	C	697	ALA	4.1
1	C	694	THR	4.1
1	E	2	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	700	MET	4.1
1	G	750	VAL	4.1
1	C	701	ALA	4.1
1	G	680	HIS	4.1
1	E	729	TYR	4.1
1	A	699	GLU	4.1
1	G	703	GLU	4.0
1	C	737	TYR	4.0
1	A	733	ASP	4.0
1	G	710	TYR	4.0
2	F	380	THR	3.9
1	C	677	ARG	3.9
1	G	698	ILE	3.9
1	E	701	ALA	3.8
1	G	678	PHE	3.8
1	E	703	GLU	3.8
1	E	732	ALA	3.8
1	C	705	ALA	3.7
1	A	731	GLU	3.7
1	E	680	HIS	3.7
1	G	734	LEU	3.7
1	E	700	MET	3.6
1	G	737	TYR	3.6
1	C	700	MET	3.6
1	C	680	HIS	3.6
1	G	676	GLU	3.6
1	C	709	GLY	3.6
1	G	368	ALA	3.5
1	G	701	ALA	3.5
1	C	730	ASP	3.5
2	B	2	ILE	3.5
1	A	703	GLU	3.5
1	G	751	LEU	3.5
1	E	1021	ARG	3.4
1	E	675	ARG	3.4
1	E	156	LEU	3.4
1	A	716	PRO	3.4
1	G	675	ARG	3.4
1	C	703	GLU	3.4
1	E	696	THR	3.4
1	G	1021	ARG	3.3
1	G	731	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	705	ALA	3.3
1	E	706	LYS	3.2
2	F	201	ALA	3.2
1	G	677	ARG	3.2
2	H	136	ASP	3.1
1	A	714	VAL	3.1
1	E	733	ASP	3.1
1	A	1021	ARG	3.1
2	F	268	ILE	3.1
2	H	53	VAL	3.0
1	G	696	THR	3.0
1	E	730	ASP	3.0
1	G	151	THR	3.0
1	C	708	ILE	3.0
1	C	1073	LYS	3.0
1	E	1073	LYS	3.0
2	B	268	ILE	2.9
2	F	379	LYS	2.9
1	G	702	VAL	2.9
1	A	700	MET	2.9
1	G	840	ILE	2.9
2	H	188	ASP	2.9
1	G	686	LYS	2.9
1	E	159	ALA	2.8
1	C	825	LEU	2.8
1	G	156	LEU	2.8
1	C	675	ARG	2.8
2	F	237	PHE	2.8
1	A	702	VAL	2.8
1	G	159	ALA	2.8
2	H	268	ILE	2.8
1	A	705	ALA	2.7
1	E	698	ILE	2.7
1	A	1073	LYS	2.7
1	E	707	GLU	2.7
2	F	166	GLU	2.7
2	H	31	VAL	2.7
1	E	157	ALA	2.7
1	E	151	THR	2.7
1	E	158	VAL	2.6
1	G	684	ARG	2.6
1	C	693	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	694	THR	2.6
1	A	995	HIS	2.6
2	B	165	ALA	2.6
2	H	2	ILE	2.6
1	C	1021	ARG	2.5
1	G	715	ARG	2.5
1	E	684	ARG	2.5
1	E	702	VAL	2.5
1	G	699	GLU	2.5
1	G	735	ARG	2.5
2	F	165	ALA	2.5
1	C	683	GLU	2.5
1	A	701	ALA	2.4
1	A	999	PRO	2.4
2	F	240	ASN	2.4
1	C	699	GLU	2.4
1	E	693	ALA	2.4
1	G	730	ASP	2.4
2	H	166	GLU	2.3
1	G	509	ARG	2.3
1	C	824	GLY	2.3
2	H	238	LEU	2.3
1	E	160	ALA	2.3
2	B	238	LEU	2.2
2	F	238	LEU	2.2
1	G	683	GLU	2.2
2	F	378	ARG	2.2
1	G	1073	LYS	2.2
1	E	676	GLU	2.2
1	G	1020	ARG	2.2
2	F	230	LYS	2.2
1	C	999	PRO	2.2
2	F	377	TYR	2.2
2	H	48	TYR	2.2
1	A	5	THR	2.2
1	C	954	LYS	2.2
1	C	678	PHE	2.1
2	F	202	LYS	2.1
1	C	707	GLU	2.1
1	C	751	LEU	2.1
1	C	735	ARG	2.1
1	A	727	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	46	LEU	2.1
1	G	558	ASP	2.1
1	A	1024	GLU	2.1
2	H	183	GLU	2.1
1	G	707	GLU	2.0
1	A	2	PRO	2.0
1	G	183	TYR	2.0
1	E	46	LEU	2.0
1	E	186	GLU	2.0
1	E	1020	ARG	2.0
1	G	158	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	143	H	269	16/17	0.90	0.21	29,71,100,100	0
2	143	B	269	16/17	0.91	0.18	34,46,87,90	0
2	143	F	269	16/17	0.93	0.20	25,46,100,100	0
2	143	D	269	16/17	0.94	0.20	21,32,100,100	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	K	C	5031	1/1	0.89	0.11	52,52,52,52	0
4	K	A	5013	1/1	0.93	0.10	59,59,59,59	0
5	CL	A	5020	1/1	0.93	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	E	5062	1/1	0.94	0.07	59,59,59,59	0
4	K	C	5035	1/1	0.95	0.06	48,48,48,48	0
8	ORN	G	5076	9/9	0.95	0.16	18,27,35,49	0
9	NET	E	5056	9/9	0.95	0.15	19,29,41,43	0
6	PO4	A	2006	5/5	0.96	0.07	22,25,39,50	0
6	PO4	G	2071	5/5	0.96	0.08	20,28,40,56	0
8	ORN	A	5011	9/9	0.96	0.15	21,24,31,40	0
8	ORN	C	5033	9/9	0.96	0.16	12,21,37,46	0
4	K	E	5057	1/1	0.96	0.06	59,59,59,59	0
5	CL	G	5084	1/1	0.96	0.11	65,65,65,65	0
9	NET	G	5077	9/9	0.96	0.15	23,39,55,64	0
5	CL	C	5044	1/1	0.97	0.06	39,39,39,39	0
4	K	C	5036	1/1	0.97	0.07	56,56,56,56	0
5	CL	G	5083	1/1	0.97	0.05	40,40,40,40	0
4	K	C	5037	1/1	0.97	0.08	62,62,62,62	0
5	CL	G	5085	1/1	0.97	0.07	68,68,68,68	0
4	K	A	5009	1/1	0.97	0.13	38,38,38,38	0
4	K	E	5058	1/1	0.97	0.09	53,53,53,53	0
7	ADP	G	2072	27/27	0.97	0.07	24,38,60,83	0
4	K	G	5074	1/1	0.97	0.16	67,67,67,67	0
4	K	G	5079	1/1	0.97	0.09	71,71,71,71	0
4	K	A	5015	1/1	0.97	0.05	54,54,54,54	0
9	NET	A	5012	9/9	0.97	0.12	20,29,37,45	0
5	CL	C	5040	1/1	0.97	0.04	35,35,35,35	0
5	CL	C	5042	1/1	0.97	0.07	55,55,55,55	0
6	PO4	E	2050	5/5	0.98	0.07	22,25,48,48	0
4	K	E	5053	1/1	0.98	0.09	51,51,51,51	0
7	ADP	C	2029	27/27	0.98	0.07	16,35,60,82	0
7	ADP	E	2051	27/27	0.98	0.07	20,32,49,89	0
7	ADP	G	2066	27/27	0.98	0.10	15,21,36,38	0
4	K	G	5080	1/1	0.98	0.07	43,43,43,43	0
4	K	H	5081	1/1	0.98	0.12	57,57,57,57	0
5	CL	A	5019	1/1	0.98	0.06	40,40,40,40	0
8	ORN	E	5055	9/9	0.98	0.11	21,23,35,53	0
4	K	E	5059	1/1	0.98	0.04	43,43,43,43	0
5	CL	A	5022	1/1	0.98	0.17	74,74,74,74	0
5	CL	H	5086	1/1	0.98	0.11	47,47,47,47	0
4	K	C	5027	1/1	0.98	0.10	29,29,29,29	0
5	CL	F	5065	1/1	0.99	0.08	31,31,31,31	0
5	CL	G	5082	1/1	0.99	0.08	39,39,39,39	0
4	K	G	5070	1/1	0.99	0.12	36,36,36,36	0
4	K	A	5010	1/1	0.99	0.08	24,24,24,24	0

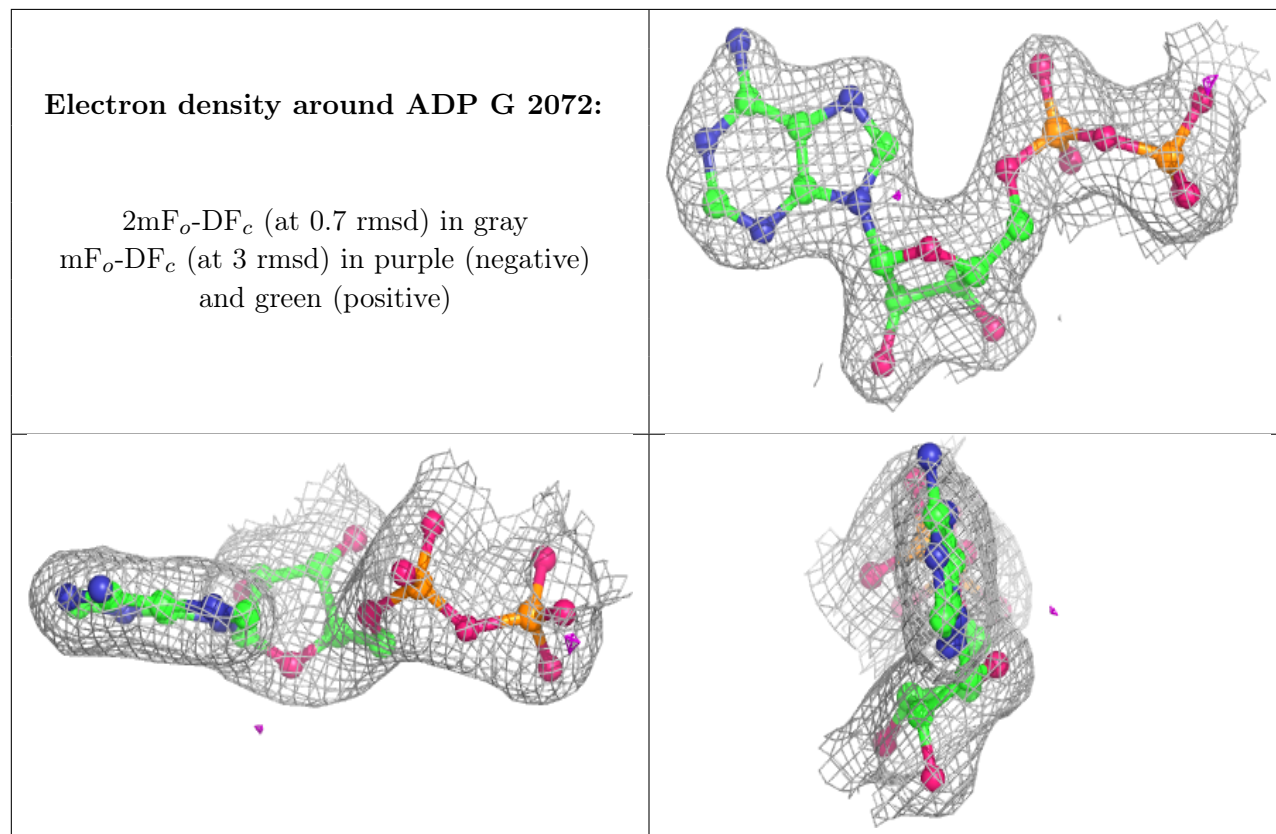
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	G	5078	1/1	0.99	0.06	54,54,54,54	0
3	MN	C	2024	1/1	0.99	0.09	28,28,28,28	0
4	K	A	5014	1/1	0.99	0.10	52,52,52,52	0
6	PO4	C	2028	5/5	0.99	0.08	13,16,31,35	0
4	K	D	5038	1/1	0.99	0.06	37,37,37,37	0
5	CL	A	5018	1/1	0.99	0.04	34,34,34,34	0
7	ADP	A	2001	27/27	0.99	0.10	16,25,33,41	0
7	ADP	A	2007	27/27	0.99	0.07	17,26,37,45	0
7	ADP	C	2023	27/27	0.99	0.12	13,21,23,26	0
4	K	E	2048	1/1	0.99	0.08	24,24,24,24	0
7	ADP	E	2045	27/27	0.99	0.12	16,27,43,64	0
4	K	E	5049	1/1	0.99	0.13	30,30,30,30	0
3	MN	G	2067	1/1	0.99	0.06	36,36,36,36	0
5	CL	B	5021	1/1	0.99	0.06	33,33,33,33	0
4	K	B	5016	1/1	0.99	0.08	45,45,45,45	0
3	MN	G	2073	1/1	0.99	0.06	42,42,42,42	0
3	MN	A	5008	1/1	0.99	0.06	28,28,28,28	0
5	CL	D	5043	1/1	0.99	0.06	30,30,30,30	0
4	K	F	5060	1/1	0.99	0.09	42,42,42,42	0
9	NET	C	5034	9/9	0.99	0.12	17,19,27,30	0
5	CL	E	5063	1/1	0.99	0.05	45,45,45,45	0
5	CL	E	5064	1/1	0.99	0.05	54,54,54,54	0
3	MN	A	2002	1/1	1.00	0.06	31,31,31,31	0
4	K	C	5026	1/1	1.00	0.12	18,18,18,18	0
5	CL	C	5039	1/1	1.00	0.11	27,27,27,27	0
3	MN	G	2068	1/1	1.00	0.07	25,25,25,25	0
5	CL	C	5041	1/1	1.00	0.05	36,36,36,36	0
3	MN	A	2003	1/1	1.00	0.08	25,25,25,25	0
4	K	G	2069	1/1	1.00	0.09	23,23,23,23	0
4	K	C	5032	1/1	1.00	0.07	31,31,31,31	0
5	CL	E	5061	1/1	1.00	0.12	30,30,30,30	0
4	K	A	5004	1/1	1.00	0.10	24,24,24,24	0
4	K	G	5075	1/1	1.00	0.08	29,29,29,29	0
4	K	A	5005	1/1	1.00	0.09	27,27,27,27	0
3	MN	C	2025	1/1	1.00	0.09	22,22,22,22	0
3	MN	C	2030	1/1	1.00	0.06	38,38,38,38	0
3	MN	E	2046	1/1	1.00	0.08	34,34,34,34	0
5	CL	A	5017	1/1	1.00	0.07	29,29,29,29	0
3	MN	E	2047	1/1	1.00	0.08	27,27,27,27	0
3	MN	E	2052	1/1	1.00	0.05	34,34,34,34	0
4	K	E	5054	1/1	1.00	0.07	24,24,24,24	0

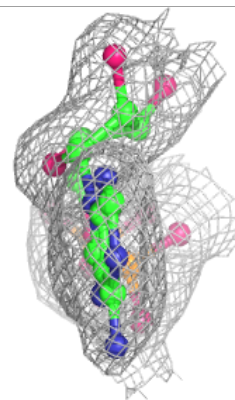
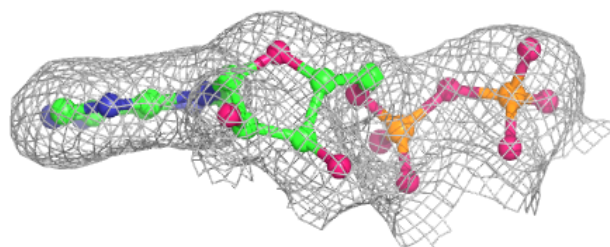
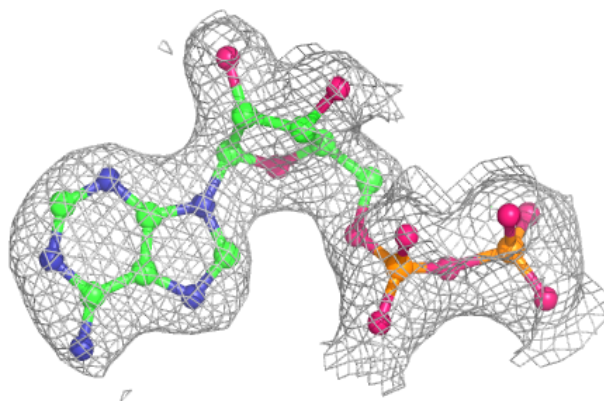
The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

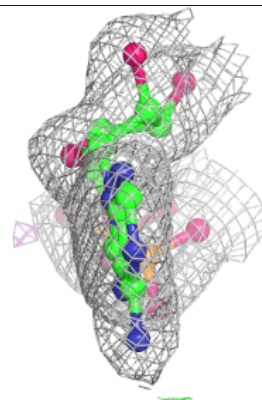
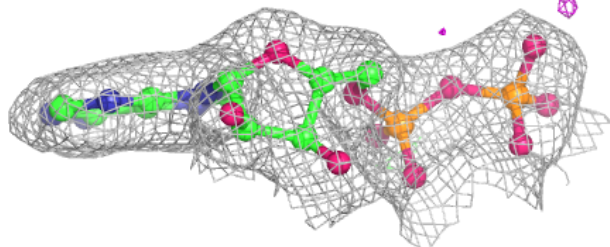
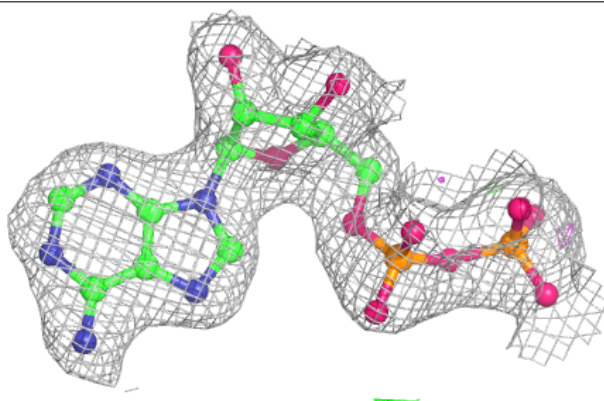


**Electron density around ADP C 2029:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

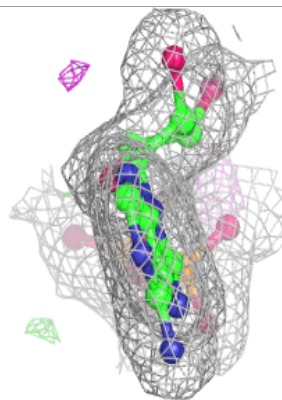
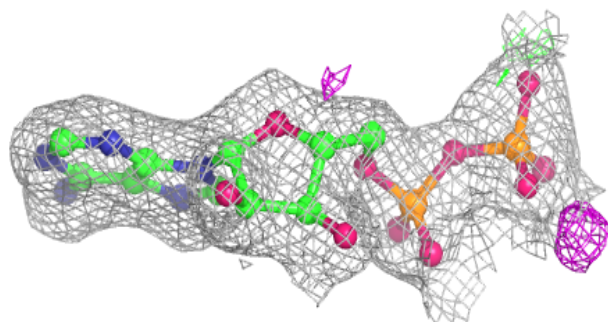
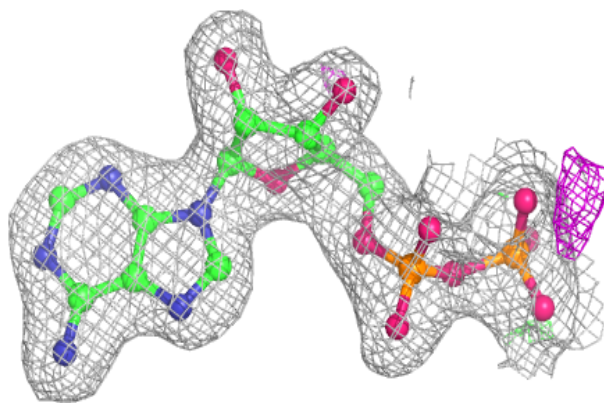
**Electron density around ADP E 2051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

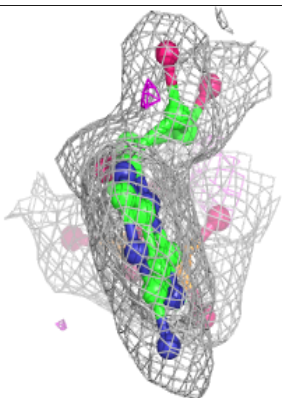
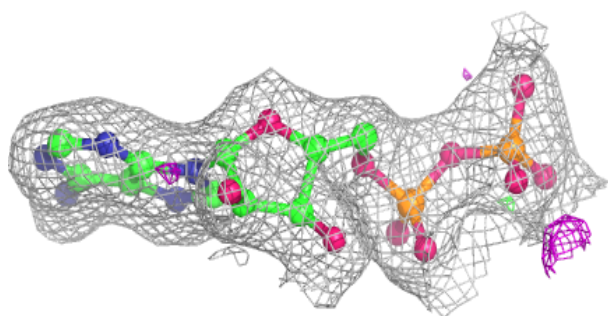
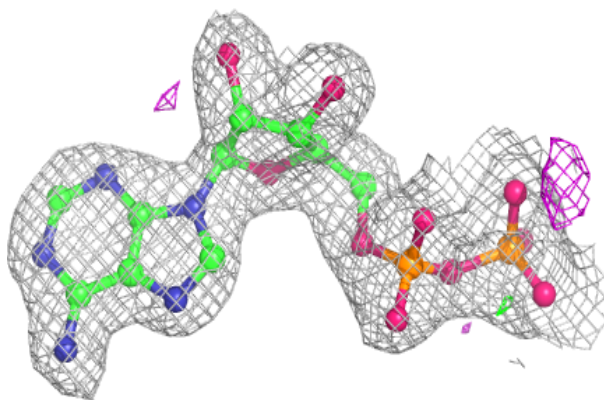


**Electron density around ADP G 2066:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

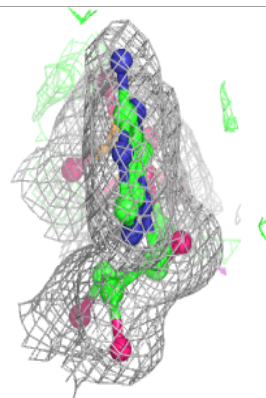
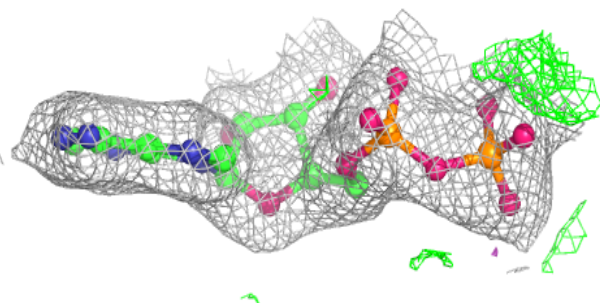
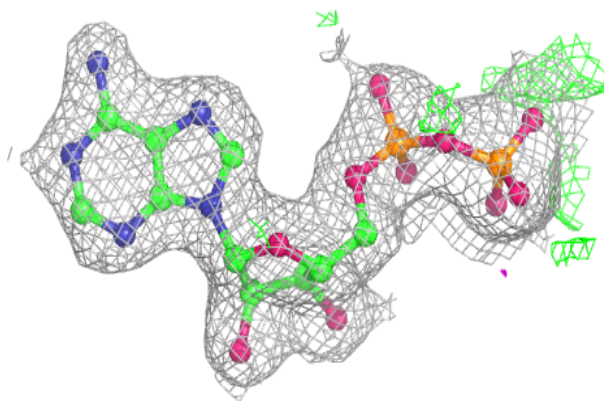
**Electron density around ADP A 2001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

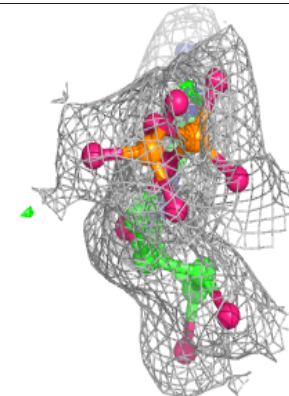
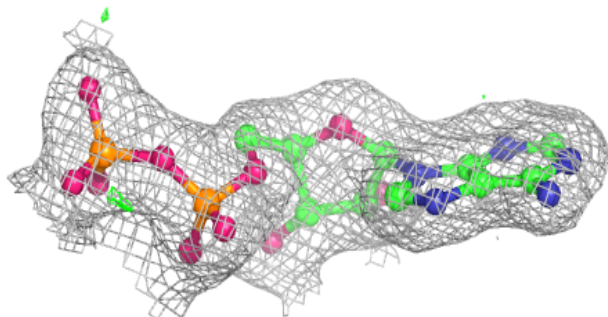
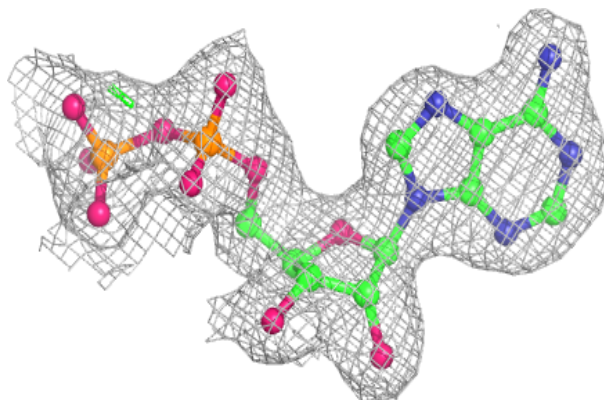


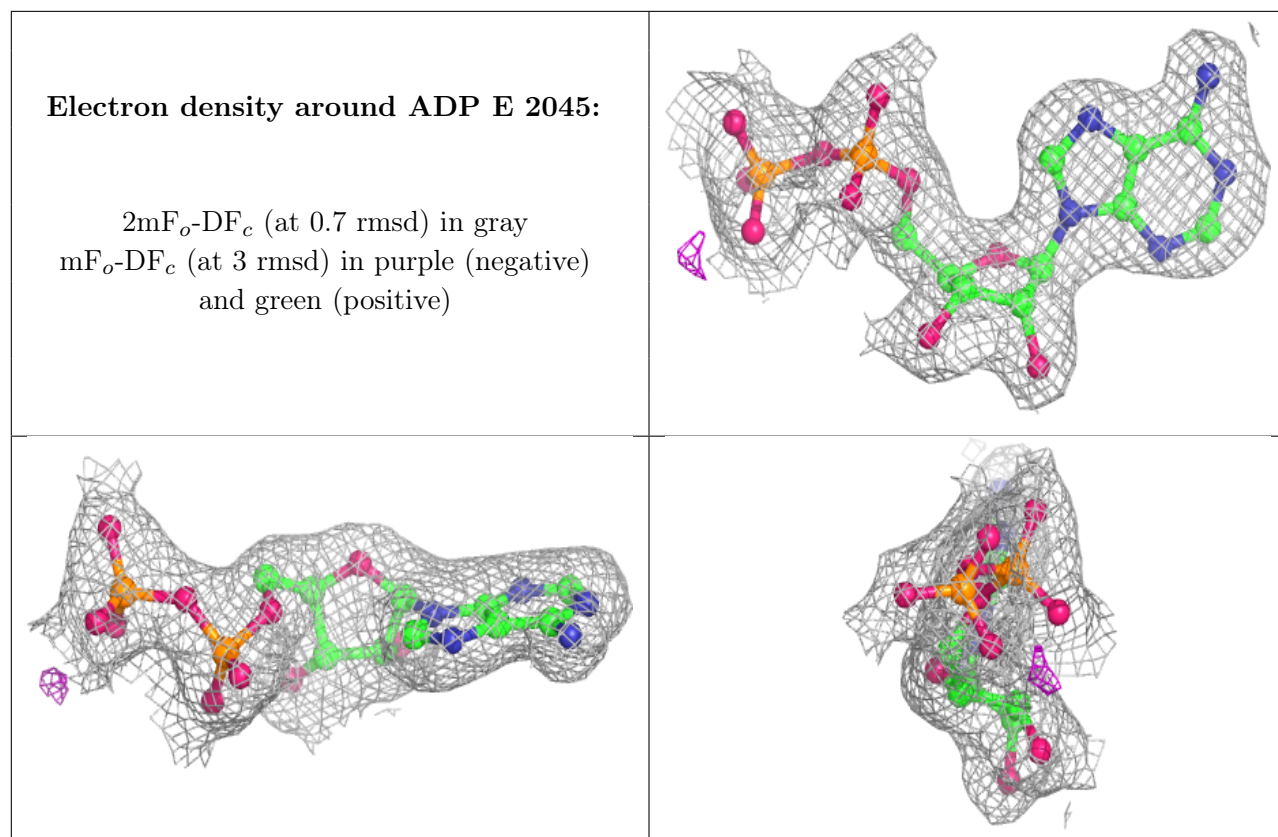
**Electron density around ADP A 2007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP C 2023:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.