



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 02:46 PM EST

PDB ID : 1C3O
Title : CRYSTAL STRUCTURE OF THE CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT MUTANT C269S WITH BOUND GLUTAMINE
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-07-28
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

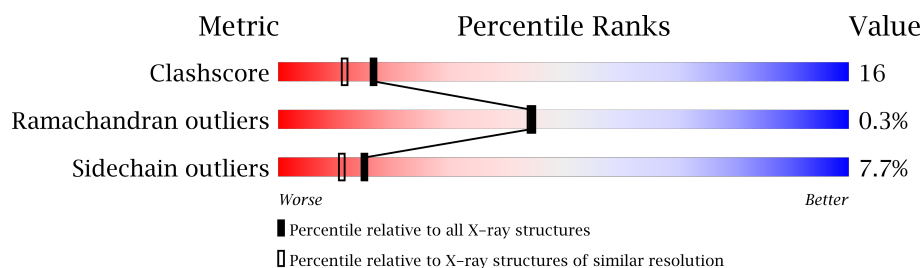
1 Overall quality at a glance

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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	 61% 30% 7% ..
1	C	1073	 60% 31% 6% ..
1	E	1073	 64% 28% 6% ..
1	G	1073	 56% 34% 7% ..
2	B	382	 58% 34% 7% .
2	D	382	 57% 36% 6% .
2	F	382	 55% 36% 7% .

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Mol	Chain	Length	Quality of chain
2	H	382	 <div>49% 42% 8%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	G	4083	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48477 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	6	0
			8195	5146	1433	1570	46			
1	C	1058	Total	C	N	O	S	0	7	0
			8192	5144	1428	1575	45			
1	E	1058	Total	C	N	O	S	0	10	0
			8211	5155	1431	1580	45			
1	G	1058	Total	C	N	O	S	0	4	0
			8180	5135	1425	1574	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	SER	CYS	ENGINEERED MUTATION	UNP P00907
D	269	SER	CYS	ENGINEERED MUTATION	UNP P00907
F	269	SER	CYS	ENGINEERED MUTATION	UNP P00907
H	269	SER	CYS	ENGINEERED MUTATION	UNP P00907

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	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	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	7	Total K 7 7	0	0
4	A	7	Total K 7 7	0	0
4	F	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	G	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	3	Total Cl 3 3	0	0
5	H	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0

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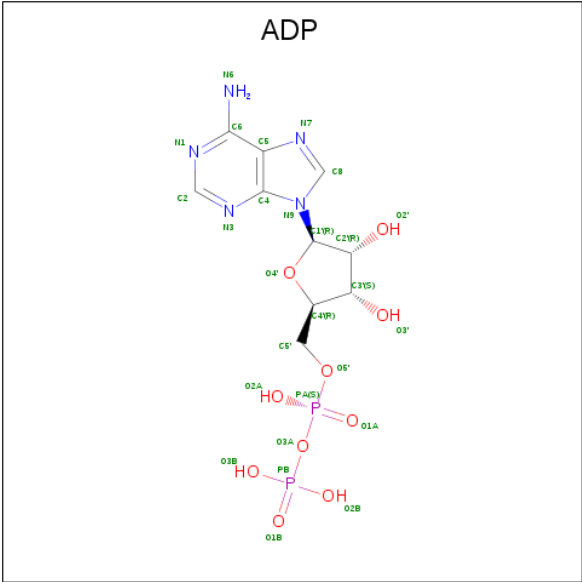
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



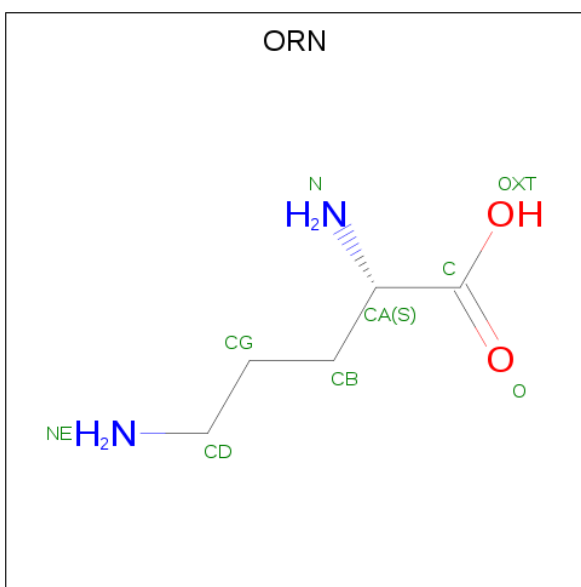
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



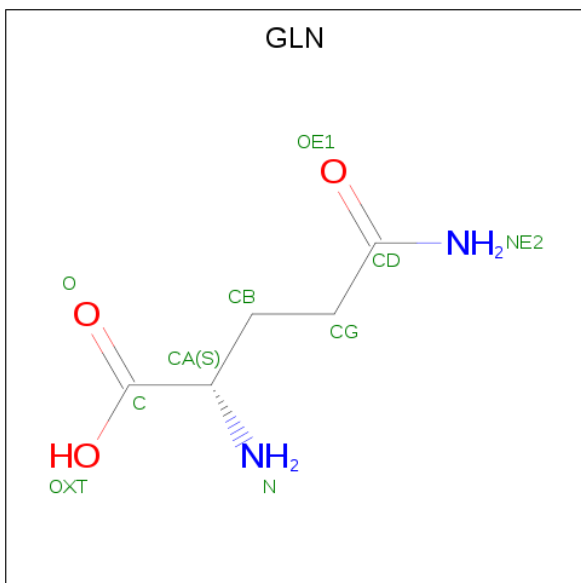
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



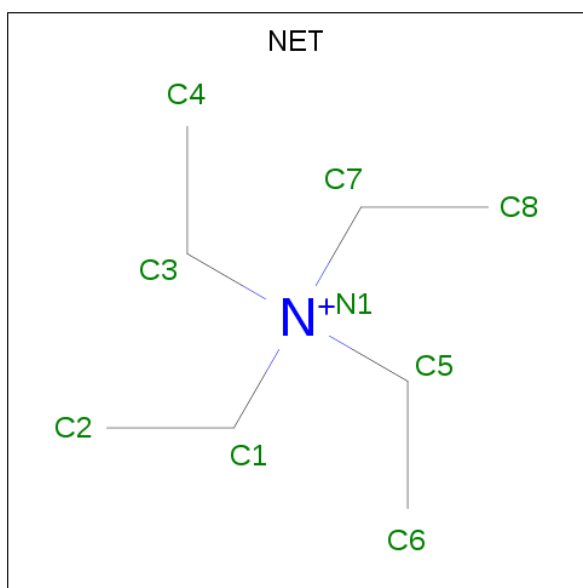
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			10	5	2	3		
9	B	1	Total	C	N	O	0	0
			10	5	2	3		
9	C	1	Total	C	N	O	0	0
			10	5	2	3		
9	D	1	Total	C	N	O	0	0
			10	5	2	3		
9	E	1	Total	C	N	O	0	0
			10	5	2	3		
9	F	1	Total	C	N	O	0	0
			10	5	2	3		
9	G	1	Total	C	N	O	0	0
			10	5	2	3		
9	H	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 10 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C₈H₂₀N).



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

- Molecule 11 is water.

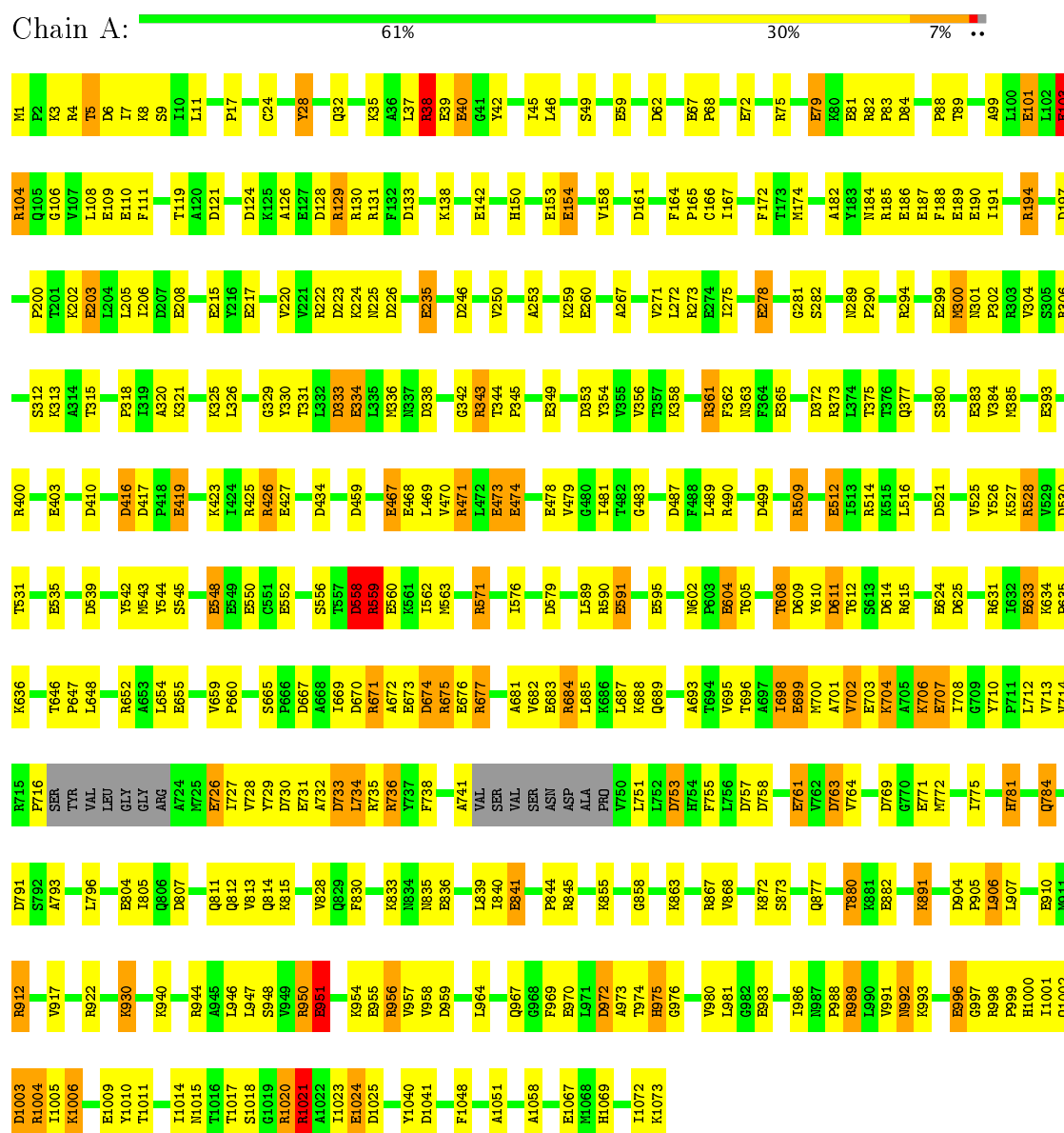
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	699	Total O 699 699	0	0
11	B	231	Total O 231 231	0	0
11	C	706	Total O 706 706	0	0
11	D	250	Total O 250 250	0	0
11	E	754	Total O 754 754	0	0
11	F	231	Total O 231 231	0	0
11	G	622	Total O 622 622	0	0
11	H	173	Total O 173 173	0	0

3 Residue-property plots

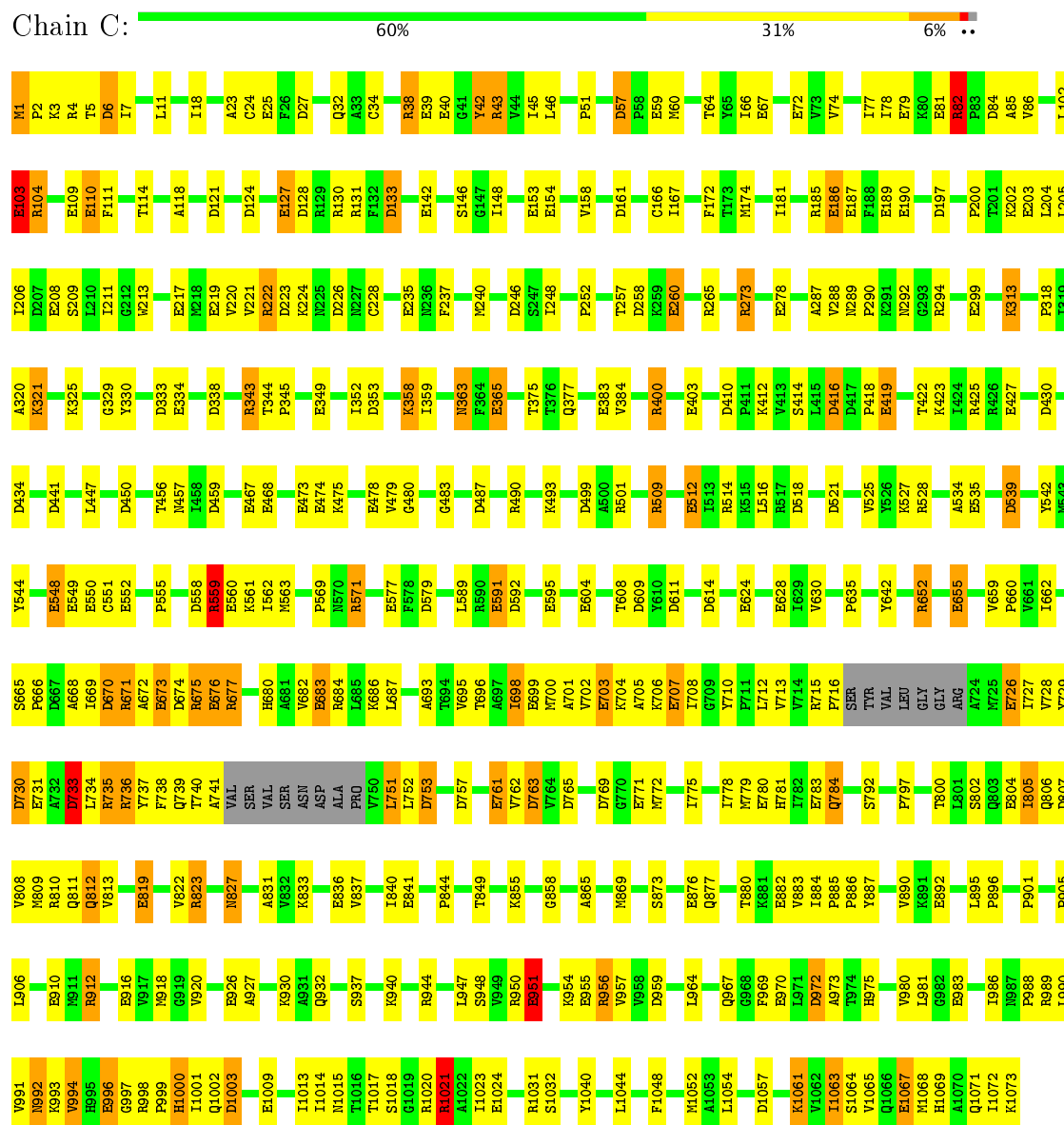
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

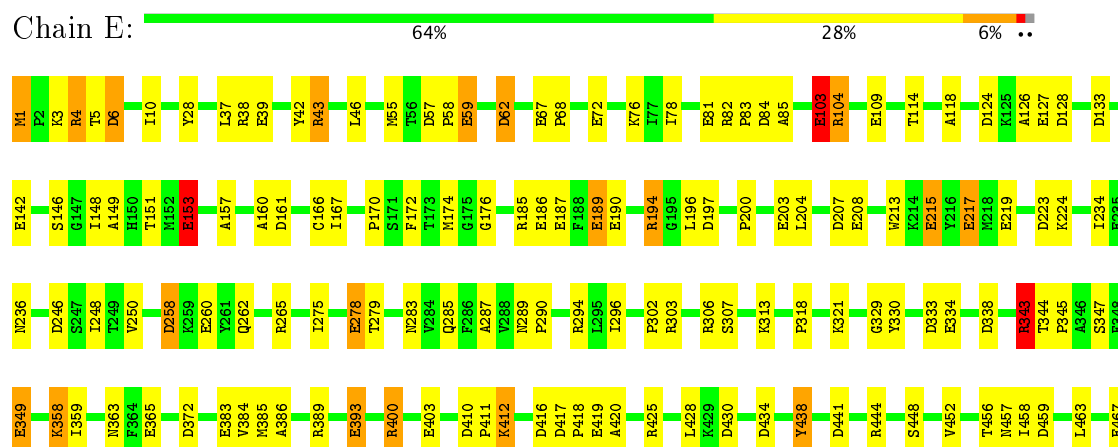
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

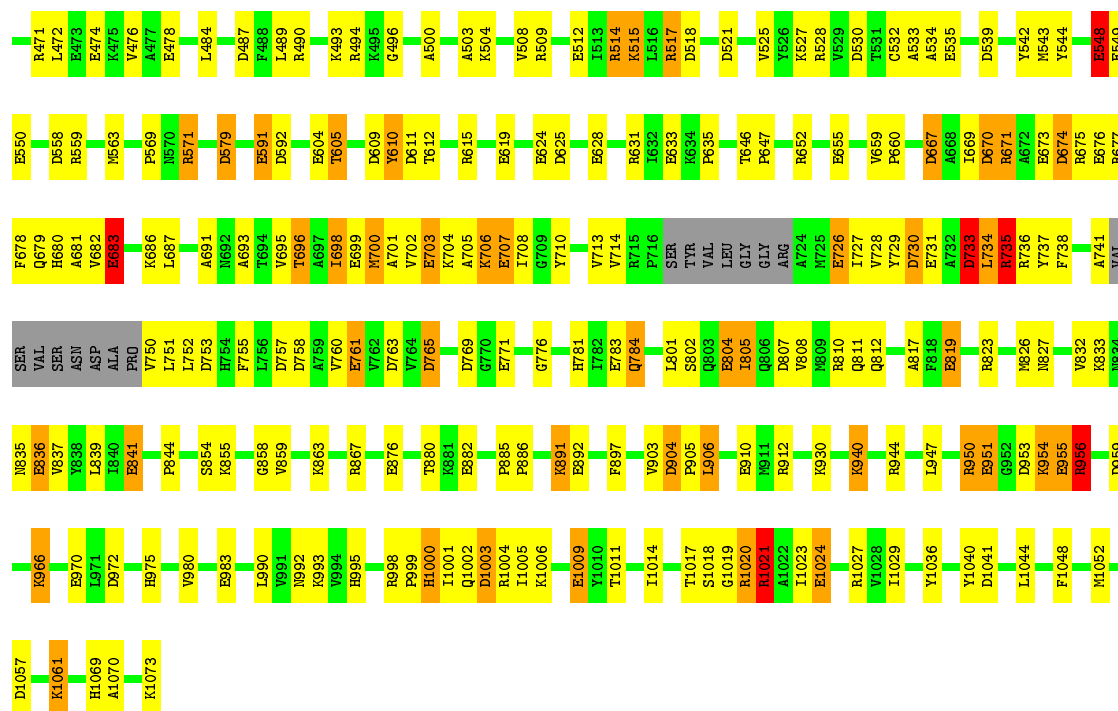


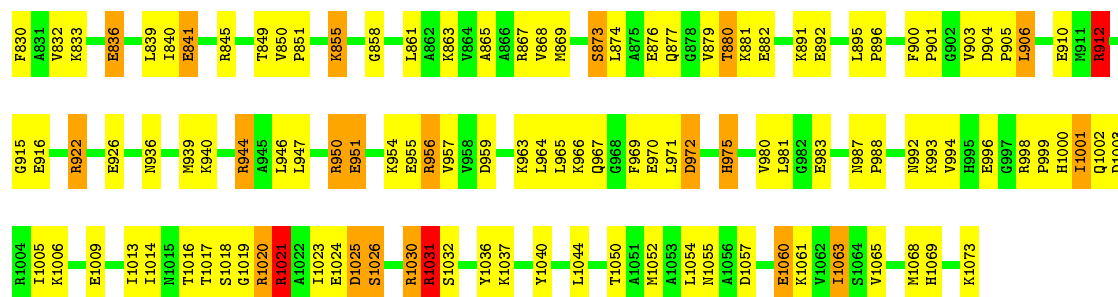
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

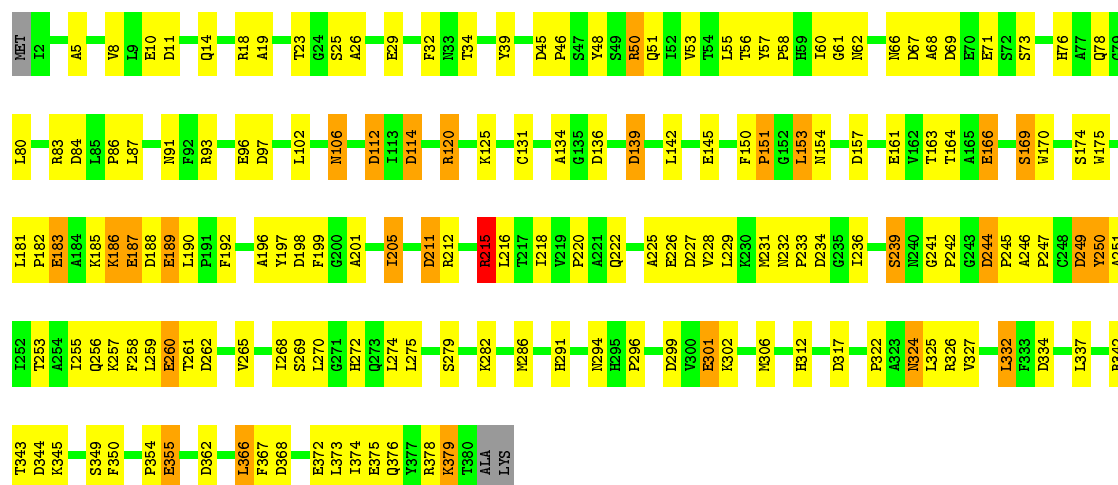


- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



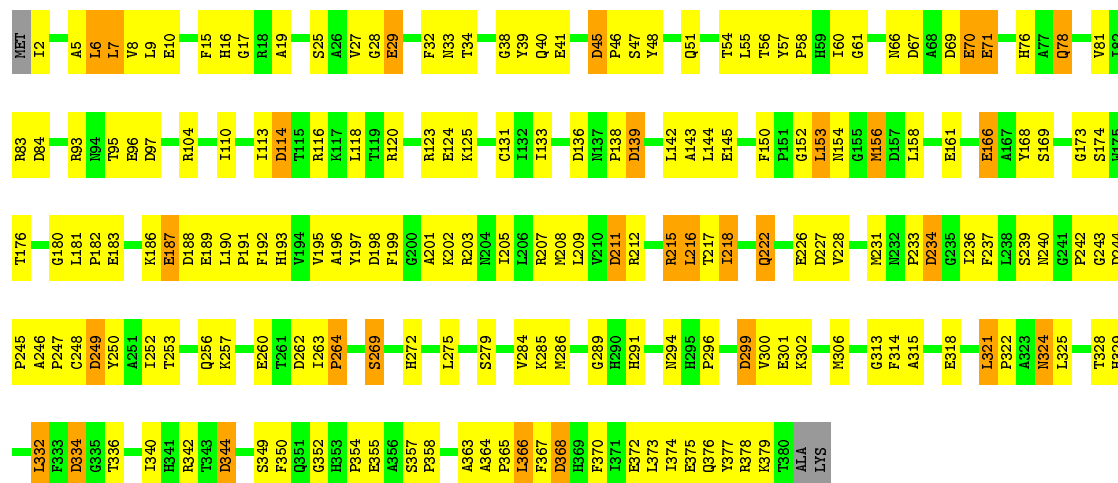






• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 49% 42% 8% •



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 164.40Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.4 (30.00-2.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.188 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48477	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	72/8345 (0.9%)	1.41	128/11276 (1.1%)
1	C	1.04	77/8346 (0.9%)	1.38	112/11281 (1.0%)
1	E	1.05	68/8377 (0.8%)	1.40	124/11320 (1.1%)
1	G	1.01	79/8322 (0.9%)	1.39	118/11249 (1.0%)
2	B	0.90	18/2957 (0.6%)	1.32	40/4016 (1.0%)
2	D	0.94	15/2957 (0.5%)	1.38	44/4016 (1.1%)
2	F	0.92	15/2957 (0.5%)	1.37	43/4016 (1.1%)
2	H	0.91	18/2957 (0.6%)	1.33	35/4016 (0.9%)
All	All	1.01	362/45218 (0.8%)	1.39	644/61190 (1.1%)

All (362) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419[A]	GLU	CD-OE2	-10.50	1.14	1.25
1	C	419[B]	GLU	CD-OE2	-10.50	1.14	1.25
1	C	110	GLU	CD-OE1	-10.46	1.14	1.25
1	C	1009	GLU	CD-OE2	9.29	1.35	1.25
1	A	109	GLU	CD-OE2	8.80	1.35	1.25
1	A	1009	GLU	CD-OE2	8.74	1.35	1.25
1	A	186	GLU	CD-OE2	8.57	1.35	1.25
1	C	1024	GLU	CD-OE2	8.50	1.34	1.25
1	E	726	GLU	CD-OE2	8.30	1.34	1.25
1	G	951	GLU	CD-OE2	8.19	1.34	1.25
2	H	166	GLU	CD-OE2	8.01	1.34	1.25
1	E	910	GLU	CD-OE2	7.80	1.34	1.25
2	B	166	GLU	CD-OE2	7.78	1.34	1.25
1	E	804	GLU	CD-OE2	7.78	1.34	1.25
1	A	110	GLU	CD-OE2	7.72	1.34	1.25
1	E	72	GLU	CD-OE2	7.70	1.34	1.25
2	F	372	GLU	CD-OE2	7.68	1.34	1.25
2	B	372	GLU	CD-OE2	7.67	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	226	GLU	CD-OE2	7.60	1.34	1.25
1	C	655	GLU	CD-OE2	7.51	1.33	1.25
1	G	1009	GLU	CD-OE2	7.47	1.33	1.25
2	D	183	GLU	CD-OE2	7.41	1.33	1.25
1	G	512	GLU	CD-OE2	7.33	1.33	1.25
1	G	1024	GLU	CD-OE2	7.31	1.33	1.25
1	E	819	GLU	CD-OE2	7.30	1.33	1.25
1	G	215	GLU	CD-OE2	7.29	1.33	1.25
1	C	676	GLU	CD-OE2	7.29	1.33	1.25
2	F	166	GLU	CD-OE2	7.29	1.33	1.25
1	C	683	GLU	CD-OE2	7.27	1.33	1.25
1	A	217	GLU	CD-OE2	7.26	1.33	1.25
1	E	59	GLU	CD-OE2	7.25	1.33	1.25
1	G	110	GLU	CD-OE2	7.24	1.33	1.25
1	A	604	GLU	CD-OE2	7.22	1.33	1.25
1	C	535	GLU	CD-OE2	7.21	1.33	1.25
2	H	70	GLU	CD-OE2	7.17	1.33	1.25
2	H	372	GLU	CD-OE2	7.16	1.33	1.25
1	C	703	GLU	CD-OE2	7.15	1.33	1.25
2	D	166	GLU	CD-OE2	7.14	1.33	1.25
1	G	699	GLU	CD-OE2	7.14	1.33	1.25
1	G	892	GLU	CD-OE2	7.13	1.33	1.25
1	G	707	GLU	CD-OE2	7.11	1.33	1.25
1	C	187	GLU	CD-OE2	7.08	1.33	1.25
1	G	676	GLU	CD-OE2	7.07	1.33	1.25
1	G	731	GLU	CD-OE2	7.07	1.33	1.25
1	C	876	GLU	CD-OE2	7.06	1.33	1.25
1	C	804	GLU	CD-OE2	7.02	1.33	1.25
1	A	703	GLU	CD-OE2	7.01	1.33	1.25
1	E	673	GLU	CD-OE2	7.00	1.33	1.25
1	A	512	GLU	CD-OE2	7.00	1.33	1.25
1	G	365	GLU	CD-OE2	6.99	1.33	1.25
1	E	1024	GLU	CD-OE2	6.98	1.33	1.25
1	A	591	GLU	CD-OE2	6.98	1.33	1.25
1	A	699	GLU	CD-OE2	6.97	1.33	1.25
1	A	683	GLU	CD-OE2	6.97	1.33	1.25
1	E	771	GLU	CD-OE2	6.96	1.33	1.25
1	A	955	GLU	CD-OE2	6.95	1.33	1.25
1	E	190	GLU	CD-OE2	6.93	1.33	1.25
1	E	761	GLU	CD-OE2	6.92	1.33	1.25
1	G	876	GLU	CD-OE2	6.90	1.33	1.25
1	C	103	GLU	CD-OE2	6.90	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	726	GLU	CD-OE2	6.88	1.33	1.25
1	A	655	GLU	CD-OE2	6.88	1.33	1.25
1	G	109	GLU	CD-OE2	6.87	1.33	1.25
1	E	403	GLU	CD-OE2	6.86	1.33	1.25
1	C	983	GLU	CD-OE2	6.85	1.33	1.25
2	D	301	GLU	CD-OE2	6.85	1.33	1.25
1	C	467	GLU	CD-OE2	6.85	1.33	1.25
1	A	836	GLU	CD-OE2	6.83	1.33	1.25
1	C	217	GLU	CD-OE2	6.83	1.33	1.25
1	E	349	GLU	CD-OE2	6.83	1.33	1.25
2	F	301	GLU	CD-OE2	6.80	1.33	1.25
1	C	699	GLU	CD-OE2	6.80	1.33	1.25
1	A	1067	GLU	CD-OE2	6.79	1.33	1.25
1	G	819	GLU	CD-OE2	6.76	1.33	1.25
1	A	153	GLU	CD-OE2	6.76	1.33	1.25
2	H	145	GLU	CD-OE2	6.74	1.33	1.25
1	G	510	GLU	CD-OE2	6.72	1.33	1.25
2	D	189	GLU	CD-OE2	6.70	1.33	1.25
1	E	676	GLU	CD-OE2	6.68	1.33	1.25
1	G	655	GLU	CD-OE2	6.66	1.32	1.25
1	G	334	GLU	CD-OE2	6.66	1.32	1.25
1	E	187	GLU	CD-OE2	6.62	1.32	1.25
1	A	535	GLU	CD-OE2	6.62	1.32	1.25
1	E	619	GLU	CD-OE2	6.62	1.32	1.25
1	C	951	GLU	CD-OE2	6.62	1.32	1.25
1	E	478[A]	GLU	CD-OE2	6.62	1.32	1.25
1	E	478[B]	GLU	CD-OE2	6.62	1.32	1.25
1	E	703	GLU	CD-OE2	6.62	1.32	1.25
1	E	707	GLU	CD-OE2	6.62	1.32	1.25
1	E	217	GLU	CD-OE2	6.60	1.32	1.25
1	C	731	GLU	CD-OE2	6.58	1.32	1.25
1	E	208	GLU	CD-OE2	6.58	1.32	1.25
1	E	683	GLU	CD-OE2	6.56	1.32	1.25
2	B	145	GLU	CD-OE2	6.56	1.32	1.25
1	C	59	GLU	CD-OE2	6.55	1.32	1.25
2	F	96	GLU	CD-OE2	6.55	1.32	1.25
2	B	187	GLU	CD-OE2	6.55	1.32	1.25
1	C	955	GLU	CD-OE2	6.54	1.32	1.25
1	A	1024	GLU	CD-OE2	6.54	1.32	1.25
1	G	804	GLU	CD-OE2	6.48	1.32	1.25
1	G	726	GLU	CD-OE2	6.48	1.32	1.25
1	G	79	GLU	CD-OE2	6.48	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	560	GLU	CD-OE2	6.47	1.32	1.25
1	A	676	GLU	CD-OE2	6.46	1.32	1.25
2	D	372	GLU	CD-OE2	6.45	1.32	1.25
2	H	29	GLU	CD-OE2	6.45	1.32	1.25
1	C	25	GLU	CD-OE2	6.45	1.32	1.25
1	A	633	GLU	CD-OE2	6.44	1.32	1.25
1	A	707	GLU	CD-OE2	6.42	1.32	1.25
2	H	183	GLU	CD-OE2	6.42	1.32	1.25
1	E	278	GLU	CD-OE2	6.40	1.32	1.25
1	G	591	GLU	CD-OE2	6.39	1.32	1.25
2	B	183	GLU	CD-OE2	6.38	1.32	1.25
2	H	187	GLU	CD-OE2	6.38	1.32	1.25
1	G	619	GLU	CD-OE2	6.36	1.32	1.25
1	G	190	GLU	CD-OE2	6.36	1.32	1.25
1	C	836	GLU	CD-OE2	6.35	1.32	1.25
1	G	683	GLU	CD-OE2	6.35	1.32	1.25
1	E	731	GLU	CD-OE2	6.35	1.32	1.25
1	G	478	GLU	CD-OE2	6.35	1.32	1.25
1	E	1009[A]	GLU	CD-OE2	6.34	1.32	1.25
1	E	1009[B]	GLU	CD-OE2	6.34	1.32	1.25
2	B	260	GLU	CD-OE2	6.33	1.32	1.25
1	C	153	GLU	CD-OE2	6.32	1.32	1.25
1	C	761	GLU	CD-OE2	6.32	1.32	1.25
1	G	186	GLU	CD-OE2	6.32	1.32	1.25
1	C	219	GLU	CD-OE2	6.32	1.32	1.25
1	E	951	GLU	CD-OE2	6.32	1.32	1.25
2	D	41	GLU	CD-OE2	6.31	1.32	1.25
1	G	419	GLU	CD-OE2	6.30	1.32	1.25
2	D	145	GLU	CD-OE2	6.30	1.32	1.25
1	A	81	GLU	CD-OE2	6.29	1.32	1.25
1	A	365	GLU	CD-OE2	6.27	1.32	1.25
2	D	355	GLU	CD-OE2	6.27	1.32	1.25
1	A	478	GLU	CD-OE2	6.26	1.32	1.25
1	E	955	GLU	CD-OE2	6.26	1.32	1.25
2	F	189	GLU	CD-OE2	6.26	1.32	1.25
1	C	771	GLU	CD-OE2	6.26	1.32	1.25
1	A	882	GLU	CD-OE2	6.25	1.32	1.25
1	G	703	GLU	CD-OE2	6.24	1.32	1.25
2	B	161	GLU	CD-OE2	6.24	1.32	1.25
1	G	154	GLU	CD-OE2	6.24	1.32	1.25
1	A	624	GLU	CD-OE1	-6.22	1.18	1.25
1	E	260	GLU	CD-OE2	6.22	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	226	GLU	CD-OE2	6.22	1.32	1.25
1	A	910	GLU	CD-OE2	6.21	1.32	1.25
1	G	474	GLU	CD-OE2	6.21	1.32	1.25
1	A	726	GLU	CD-OE2	6.18	1.32	1.25
1	E	699	GLU	CD-OE2	6.18	1.32	1.25
1	C	1067	GLU	CD-OE2	6.17	1.32	1.25
1	G	549	GLU	CD-OE2	6.17	1.32	1.25
2	F	226	GLU	CD-OE2	6.17	1.32	1.25
1	C	474	GLU	CD-OE2	6.17	1.32	1.25
1	C	970	GLU	CD-OE2	6.17	1.32	1.25
1	E	983	GLU	CD-OE2	6.16	1.32	1.25
2	H	301	GLU	CD-OE2	6.16	1.32	1.25
1	A	624	GLU	CD-OE2	6.15	1.32	1.25
1	A	39	GLU	CD-OE2	6.15	1.32	1.25
1	E	365	GLU	CD-OE2	6.14	1.32	1.25
1	E	836	GLU	CD-OE2	6.13	1.32	1.25
1	G	783	GLU	CD-OE2	6.13	1.32	1.25
1	A	208	GLU	CD-OE2	6.13	1.32	1.25
1	E	655[A]	GLU	CD-OE2	6.12	1.32	1.25
1	E	655[B]	GLU	CD-OE2	6.12	1.32	1.25
2	F	145	GLU	CD-OE2	6.12	1.32	1.25
2	B	70	GLU	CD-OE2	6.12	1.32	1.25
2	H	71	GLU	CD-OE2	6.12	1.32	1.25
1	C	512	GLU	CD-OE2	6.12	1.32	1.25
1	G	624	GLU	CD-OE2	6.12	1.32	1.25
1	C	996	GLU	CD-OE2	6.11	1.32	1.25
1	E	467	GLU	CD-OE2	6.11	1.32	1.25
2	B	226	GLU	CD-OE2	6.10	1.32	1.25
1	C	628	GLU	CD-OE2	6.09	1.32	1.25
2	H	10	GLU	CD-OE2	6.08	1.32	1.25
1	A	72	GLU	CD-OE2	6.08	1.32	1.25
1	C	190	GLU	CD-OE2	6.07	1.32	1.25
1	G	349	GLU	CD-OE2	6.07	1.32	1.25
1	C	349	GLU	CD-OE2	6.06	1.32	1.25
1	A	299	GLU	CD-OE2	6.05	1.32	1.25
2	B	318	GLU	CD-OE2	6.04	1.32	1.25
1	A	190	GLU	CD-OE2	6.04	1.32	1.25
1	C	473	GLU	CD-OE2	6.03	1.32	1.25
2	B	301	GLU	CD-OE2	6.03	1.32	1.25
1	G	633	GLU	CD-OE2	6.03	1.32	1.25
1	G	278	GLU	CD-OE2	6.02	1.32	1.25
1	E	189	GLU	CD-OE2	6.02	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	467	GLU	CD-OE2	6.01	1.32	1.25
1	E	334	GLU	CD-OE2	6.00	1.32	1.25
1	C	203	GLU	CD-OE2	5.99	1.32	1.25
1	C	819	GLU	CD-OE2	5.99	1.32	1.25
1	C	550	GLU	CD-OE2	5.99	1.32	1.25
1	C	882	GLU	CD-OE2	5.98	1.32	1.25
1	C	624	GLU	CD-OE2	5.98	1.32	1.25
1	G	103	GLU	CD-OE2	5.98	1.32	1.25
1	E	76	LYS	CE-NZ	-5.98	1.34	1.49
1	E	876	GLU	CD-OE2	5.98	1.32	1.25
1	C	926	GLU	CD-OE2	5.97	1.32	1.25
2	F	187	GLU	CD-OE2	5.97	1.32	1.25
1	E	970	GLU	CD-OE2	5.96	1.32	1.25
1	E	103	GLU	CD-OE2	5.96	1.32	1.25
1	C	109	GLU	CD-OE2	5.95	1.32	1.25
1	A	299	GLU	CD-OE1	-5.94	1.19	1.25
1	G	153	GLU	CD-OE2	5.94	1.32	1.25
1	A	59	GLU	CD-OE2	5.93	1.32	1.25
1	A	673	GLU	CD-OE2	5.92	1.32	1.25
1	G	983	GLU	CD-OE2	5.92	1.32	1.25
1	G	595	GLU	CD-OE2	5.91	1.32	1.25
1	A	951	GLU	CD-OE2	5.91	1.32	1.25
2	D	70	GLU	CD-OE2	5.91	1.32	1.25
1	G	761	GLU	CD-OE2	5.91	1.32	1.25
1	A	187	GLU	CD-OE2	5.90	1.32	1.25
1	E	127	GLU	CD-OE2	5.90	1.32	1.25
1	A	154	GLU	CD-OE2	5.89	1.32	1.25
1	C	478	GLU	CD-OE2	5.89	1.32	1.25
1	E	186	GLU	CD-OE2	5.88	1.32	1.25
1	A	334	GLU	CD-OE2	5.88	1.32	1.25
1	E	783	GLU	CD-OE2	5.88	1.32	1.25
1	G	836	GLU	CD-OE2	5.87	1.32	1.25
1	G	427	GLU	CD-OE2	5.87	1.32	1.25
1	E	512	GLU	CD-OE2	5.87	1.32	1.25
2	F	71	GLU	CD-OE2	5.87	1.32	1.25
1	C	673	GLU	CD-OE2	5.86	1.32	1.25
1	C	427	GLU	CD-OE2	5.84	1.32	1.25
1	A	731	GLU	CD-OE2	5.83	1.32	1.25
1	C	39	GLU	CD-OE2	5.83	1.32	1.25
1	A	970	GLU	CD-OE2	5.82	1.32	1.25
1	E	549	GLU	CD-OE2	5.82	1.32	1.25
1	C	72	GLU	CD-OE2	5.81	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	GLU	CD-OE2	5.81	1.32	1.25
1	G	916	GLU	CD-OE2	5.81	1.32	1.25
2	H	260	GLU	CD-OE2	5.80	1.32	1.25
1	G	473[A]	GLU	CD-OE2	5.79	1.32	1.25
1	G	473[B]	GLU	CD-OE2	5.79	1.32	1.25
1	C	560	GLU	CD-OE2	5.78	1.32	1.25
1	G	189	GLU	CD-OE2	5.78	1.32	1.25
1	G	560	GLU	CD-OE2	5.78	1.32	1.25
1	A	550	GLU	CD-OE2	5.78	1.32	1.25
1	C	910	GLU	CD-OE2	5.77	1.31	1.25
1	G	604	GLU	CD-OE2	5.77	1.31	1.25
2	F	375	GLU	CD-OE2	5.76	1.31	1.25
1	E	419	GLU	CD-OE2	5.76	1.31	1.25
1	G	970	GLU	CD-OE2	5.74	1.31	1.25
1	G	841	GLU	CD-OE2	5.74	1.31	1.25
1	C	79	GLU	CD-OE2	5.74	1.31	1.25
1	C	591	GLU	CD-OE2	5.73	1.31	1.25
2	H	161	GLU	CD-OE2	5.73	1.31	1.25
1	A	761	GLU	CD-OE2	5.72	1.31	1.25
1	C	916	GLU	CD-OE2	5.71	1.31	1.25
1	E	628	GLU	CD-OE2	5.71	1.31	1.25
1	A	474	GLU	CD-OE2	5.70	1.31	1.25
1	G	208	GLU	CD-OE2	5.70	1.31	1.25
1	E	393	GLU	CD-OE2	5.69	1.31	1.25
1	G	910	GLU	CD-OE2	5.68	1.31	1.25
1	C	278	GLU	CD-OE2	5.68	1.31	1.25
1	E	215	GLU	CD-OE2	5.68	1.31	1.25
1	G	468	GLU	CD-OE2	5.68	1.31	1.25
2	B	189	GLU	CD-OE2	5.67	1.31	1.25
1	A	419	GLU	CD-OE2	5.66	1.31	1.25
2	F	355	GLU	CD-OE1	-5.65	1.19	1.25
1	E	841	GLU	CD-OE2	5.64	1.31	1.25
1	A	79	GLU	CD-OE2	5.63	1.31	1.25
1	A	771	GLU	CD-OE2	5.63	1.31	1.25
1	A	40	GLU	CD-OE2	5.63	1.31	1.25
1	E	624	GLU	CD-OE2	5.63	1.31	1.25
1	A	142	GLU	CD-OE2	5.62	1.31	1.25
1	G	996	GLU	CD-OE2	5.62	1.31	1.25
1	A	403	GLU	CD-OE1	-5.62	1.19	1.25
1	G	403	GLU	CD-OE2	5.61	1.31	1.25
1	E	591	GLU	CD-OE2	5.60	1.31	1.25
2	D	375	GLU	CD-OE2	5.59	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	40	GLU	CD-OE2	5.58	1.31	1.25
2	H	375	GLU	CD-OE2	5.58	1.31	1.25
2	B	29	GLU	CD-OE2	5.57	1.31	1.25
1	A	393	GLU	CD-OE2	5.56	1.31	1.25
1	C	468	GLU	CD-OE2	5.56	1.31	1.25
2	D	187	GLU	CD-OE2	5.56	1.31	1.25
2	B	124	GLU	CD-OE2	5.55	1.31	1.25
1	G	219	GLU	CD-OE2	5.55	1.31	1.25
1	C	189	GLU	CD-OE2	5.54	1.31	1.25
1	G	926	GLU	CD-OE2	5.54	1.31	1.25
1	E	550	GLU	CD-OE1	-5.53	1.19	1.25
1	C	403	GLU	CD-OE2	5.52	1.31	1.25
1	E	548	GLU	CD-OE1	-5.51	1.19	1.25
2	B	96	GLU	CD-OE2	5.51	1.31	1.25
2	H	96	GLU	CD-OE2	5.51	1.31	1.25
1	A	278	GLU	CD-OE2	5.47	1.31	1.25
1	C	67	GLU	CD-OE2	5.46	1.31	1.25
1	C	235	GLU	CD-OE2	5.46	1.31	1.25
1	A	804	GLU	CD-OE2	5.44	1.31	1.25
1	E	189	GLU	CD-OE1	-5.44	1.19	1.25
1	C	549	GLU	CD-OE2	5.43	1.31	1.25
1	E	203	GLU	CD-OE2	5.42	1.31	1.25
2	F	10	GLU	CD-OE2	5.42	1.31	1.25
1	G	59	GLU	CD-OE2	5.42	1.31	1.25
1	E	474	GLU	CD-OE2	5.42	1.31	1.25
2	B	375	GLU	CD-OE2	5.41	1.31	1.25
1	E	219	GLU	CD-OE2	5.40	1.31	1.25
1	G	535	GLU	CD-OE2	5.40	1.31	1.25
1	E	39	GLU	CD-OE2	5.39	1.31	1.25
1	A	552	GLU	CD-OE2	5.39	1.31	1.25
1	E	109	GLU	CD-OE2	5.38	1.31	1.25
1	G	260	GLU	CD-OE2	5.38	1.31	1.25
1	G	955	GLU	CD-OE2	5.38	1.31	1.25
2	D	29	GLU	CD-OE2	5.36	1.31	1.25
2	H	318	GLU	CD-OE2	5.35	1.31	1.25
1	E	535	GLU	CD-OE2	5.35	1.31	1.25
1	G	673	GLU	CD-OE2	5.34	1.31	1.25
1	C	383	GLU	CD-OE2	5.34	1.31	1.25
1	A	996	GLU	CD-OE2	5.31	1.31	1.25
1	C	142	GLU	CD-OE2	5.30	1.31	1.25
2	B	10	GLU	CD-OE2	5.30	1.31	1.25
1	G	550	GLU	CD-OE2	5.29	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	41	GLU	CD-OE2	5.29	1.31	1.25
1	A	427	GLU	CD-OE2	5.29	1.31	1.25
1	C	577	GLU	CD-OE2	5.28	1.31	1.25
1	C	208	GLU	CD-OE2	5.28	1.31	1.25
1	G	577	GLU	CD-OE2	5.28	1.31	1.25
1	E	142	GLU	CD-OE2	5.27	1.31	1.25
1	C	783	GLU	CD-OE2	5.27	1.31	1.25
2	H	124	GLU	CD-OE2	5.27	1.31	1.25
1	G	72	GLU	CD-OE2	5.26	1.31	1.25
1	G	1060	GLU	CD-OE2	5.26	1.31	1.25
1	A	189	GLU	CD-OE2	5.25	1.31	1.25
1	A	473	GLU	CD-OE2	5.25	1.31	1.25
1	G	187	GLU	CD-OE2	5.25	1.31	1.25
1	C	127	GLU	CD-OE2	5.25	1.31	1.25
1	E	403	GLU	CD-OE1	-5.24	1.19	1.25
1	C	595	GLU	CD-OE2	5.24	1.31	1.25
1	G	235	GLU	CD-OE2	5.24	1.31	1.25
1	G	771	GLU	CD-OE2	5.24	1.31	1.25
2	D	96	GLU	CD-OE2	5.23	1.31	1.25
1	A	841	GLU	CD-OE2	5.23	1.31	1.25
1	G	39	GLU	CD-OE2	5.22	1.31	1.25
2	F	260	GLU	CD-OE2	5.22	1.31	1.25
1	A	595	GLU	CD-OE2	5.20	1.31	1.25
1	C	260	GLU	CD-OE2	5.20	1.31	1.25
1	A	468	GLU	CD-OE2	5.19	1.31	1.25
1	A	103	GLU	CD-OE2	5.18	1.31	1.25
1	A	215	GLU	CD-OE2	5.17	1.31	1.25
1	G	552	GLU	CD-OE2	5.16	1.31	1.25
1	E	153[A]	GLU	CD-OE2	5.14	1.31	1.25
1	E	153[B]	GLU	CD-OE2	5.14	1.31	1.25
1	A	203	GLU	CD-OE2	5.12	1.31	1.25
1	A	101	GLU	CD-OE2	5.12	1.31	1.25
1	C	334	GLU	CD-OE2	5.11	1.31	1.25
2	F	183	GLU	CD-OE2	5.11	1.31	1.25
1	A	235	GLU	CD-OE2	5.11	1.31	1.25
1	G	383	GLU	CD-OE1	-5.09	1.20	1.25
1	G	25	GLU	CD-OE2	5.08	1.31	1.25
1	C	707	GLU	CD-OE2	5.07	1.31	1.25
1	C	548	GLU	CD-OE2	5.07	1.31	1.25
2	D	10	GLU	CD-OE2	5.07	1.31	1.25
1	A	260	GLU	CD-OE2	5.05	1.31	1.25
1	C	780	GLU	CD-OE2	5.05	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	274	GLU	CD-OE2	5.05	1.31	1.25
2	B	41	GLU	CD-OE2	5.02	1.31	1.25
1	A	983	GLU	CD-OE2	5.02	1.31	1.25
1	A	467	GLU	CD-OE2	5.02	1.31	1.25
1	C	235	GLU	CD-OE1	-5.01	1.20	1.25
1	C	552	GLU	CD-OE1	-5.01	1.20	1.25
1	G	101	GLU	CD-OE2	5.00	1.31	1.25
2	F	161	GLU	CD-OE2	5.00	1.31	1.25

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	G	75	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	G	265	ARG	NE-CZ-NH1	12.54	126.57	120.30
2	D	120	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	E	343	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	G	261	TYR	CB-CG-CD2	-10.78	114.53	121.00
1	C	223	ASP	CB-CG-OD2	-10.65	108.72	118.30
2	B	211	ASP	CB-CG-OD2	-10.18	109.14	118.30
1	A	223	ASP	CB-CG-OD2	-10.15	109.16	118.30
1	A	944	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	E	753	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	C	736	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	E	514	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	C	490[A]	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	C	490[B]	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	G	75	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	194	ARG	NE-CZ-NH2	-9.15	115.72	120.30
2	F	97	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	G	223	ASP	CB-CG-OD2	-9.11	110.10	118.30
2	F	67	ASP	CB-CG-OD2	-9.10	110.11	118.30
2	H	334	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	A	1003	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	E	494	ARG	NE-CZ-NH1	8.95	124.78	120.30
2	D	334	ASP	CB-CG-OD2	-8.93	110.27	118.30
2	D	207	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	129	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	E	38	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	C	521	ASP	CB-CG-OD1	8.75	126.18	118.30
1	E	904	ASP	CB-CG-OD2	-8.69	110.48	118.30
2	H	45	ASP	CB-CG-OD1	8.65	126.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	368	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	514	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	C	131	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	C	956	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	G	261	TYR	CB-CG-CD1	8.57	126.14	121.00
1	A	867	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	E	197	ASP	CB-CG-OD2	-8.56	110.60	118.30
1	C	501	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	E	38	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	H	368	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	G	333	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	E	609	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	G	161	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	E	333	ASP	CB-CG-OD1	8.41	125.87	118.30
1	C	972	ASP	CB-CG-OD1	8.39	125.85	118.30
1	C	121	ASP	CB-CG-OD1	8.35	125.82	118.30
1	G	614	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	E	670	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	124	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	C	670	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	A	904	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	C	972	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	G	667	ASP	CB-CG-OD2	-8.20	110.92	118.30
2	F	139	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	G	609	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	D	215	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	C	959	ASP	CB-CG-OD2	-8.17	110.95	118.30
2	F	139	ASP	CB-CG-OD1	8.16	125.65	118.30
1	C	441	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	C	501	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	E	43	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	G	460	ARG	NE-CZ-NH1	8.09	124.35	120.30
2	D	18	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	C	6	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	E	372	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	E	104	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	867	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	G	57	ASP	CB-CG-OD1	7.93	125.44	118.30
2	F	317	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	G	434	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	G	609	ASP	CB-CG-OD1	7.88	125.39	118.30
1	E	625	ASP	CB-CG-OD1	7.84	125.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	823	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	F	368	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	E	410	ASP	CB-CG-OD1	7.80	125.32	118.30
1	E	625	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	A	128	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	G	1030	ARG	NE-CZ-NH2	-7.71	116.44	120.30
2	B	249	ASP	CB-CG-OD2	-7.71	111.37	118.30
1	E	444	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	670	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	A	197	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	C	27	ASP	CB-CG-OD1	7.67	125.21	118.30
1	A	246	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	G	944	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	G	124	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	539	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	G	410	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	C	528	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	H	97	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	G	333	ASP	CB-CG-OD1	7.56	125.11	118.30
1	A	1021	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	959	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	611	ASP	CB-CG-OD1	7.55	125.10	118.30
2	B	362	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	E	333	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	129	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	G	1057	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	G	670	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	G	6	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	E	6	ASP	CB-CG-OD1	7.47	125.03	118.30
1	A	372	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	C	614	ASP	CB-CG-OD2	-7.46	111.59	118.30
2	D	262	ASP	CB-CG-OD2	-7.46	111.59	118.30
2	H	264	PRO	N-CA-CB	7.44	112.22	103.30
1	E	509	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	677	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	H	299	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	E	959	ASP	CB-CG-OD1	7.39	124.95	118.30
2	F	334	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	C	197	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	E	944	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	C	133	ASP	CB-CG-OD1	7.35	124.91	118.30
1	A	338	ASP	CB-CG-OD2	-7.33	111.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1003	ASP	CB-CG-OD2	-7.31	111.72	118.30
2	F	120	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	D	67	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	G	145	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	343	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	E	810	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	128	ASP	CB-CG-OD1	7.28	124.85	118.30
1	E	487	ASP	CB-CG-OD1	7.28	124.85	118.30
1	E	223	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	716	PRO	N-CA-CB	7.27	112.02	103.30
1	E	416	ASP	CB-CG-OD2	-7.27	111.76	118.30
2	F	368	ASP	CB-CG-OD1	7.26	124.83	118.30
2	H	211	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	131	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	490	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	G	128	ASP	CB-CG-OD1	7.23	124.81	118.30
2	D	368	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	G	410	ASP	CB-CG-OD1	7.23	124.81	118.30
2	H	139	ASP	CB-CG-OD1	7.21	124.79	118.30
1	E	487	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	C	558	ASP	N-CA-CB	-7.19	97.66	110.60
1	E	124	ASP	CB-CG-OD1	7.19	124.77	118.30
1	C	131	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	E	400	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	611	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	E	410	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	615	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	E	1003	ASP	CB-CG-OD2	-7.12	111.89	118.30
2	D	203	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	539	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	E	265	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	E	1027	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	226	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	C	128	ASP	CB-CG-OD1	7.08	124.67	118.30
2	F	45	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	E	161	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	C	223	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	733	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	E	128	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	C	226	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	E	82	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	B	326	ARG	NE-CZ-NH2	-7.00	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	763	ASP	CB-CG-OD2	-7.00	112.00	118.30
2	D	114	ASP	CB-CG-OD1	6.99	124.59	118.30
1	G	223	ASP	CB-CG-OD1	6.99	124.59	118.30
1	E	904	ASP	CB-CG-OD1	6.98	124.58	118.30
1	E	769	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	E	223	ASP	CB-CG-OD2	-6.95	112.04	118.30
2	B	368	ASP	CB-CG-OD1	6.94	124.55	118.30
1	E	763	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	736	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	D	112	ASP	CB-CG-OD1	6.91	124.52	118.30
2	D	188	ASP	CB-CG-OD2	-6.91	112.08	118.30
2	D	188	ASP	CB-CG-OD1	6.89	124.50	118.30
1	E	6	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	559	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	539	ASP	CB-CG-OD1	6.88	124.49	118.30
2	H	215	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	6	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	558	ASP	CB-CG-OD2	-6.84	112.14	118.30
2	B	97	ASP	CB-CG-OD1	6.83	124.45	118.30
1	G	226	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	161	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	F	249	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	G	197	ASP	CB-CG-OD2	-6.80	112.17	118.30
1	E	736	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	G	674	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	F	67	ASP	CB-CG-OD1	6.78	124.40	118.30
1	G	499	ASP	CB-CG-OD2	-6.76	112.21	118.30
2	H	84	ASP	CB-CG-OD1	6.76	124.39	118.30
1	E	128	ASP	CB-CG-OD1	6.75	124.38	118.30
2	H	136	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	G	959	ASP	CB-CG-OD1	6.74	124.36	118.30
1	G	425	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	G	959	ASP	CB-CG-OD2	-6.73	112.24	118.30
2	F	97	ASP	CB-CG-OD1	6.73	124.36	118.30
1	E	610	TYR	CB-CG-CD2	6.71	125.03	121.00
1	E	765	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	223	ASP	CB-CG-OD1	6.70	124.33	118.30
2	D	362	ASP	CB-CG-OD2	-6.70	112.27	118.30
2	F	120	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	674	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	E	611	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	222	ARG	NE-CZ-NH1	6.67	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	517	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	972	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	G	258	ASP	CB-CG-OD1	6.66	124.30	118.30
2	F	344	ASP	CB-CG-OD1	6.66	124.29	118.30
1	E	611	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	C	430	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	C	518	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	416	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	D	299	ASP	CB-CG-OD1	6.63	124.27	118.30
1	E	416	ASP	CB-CG-OD1	6.63	124.27	118.30
1	G	972	ASP	CB-CG-OD1	6.62	124.26	118.30
2	D	97	ASP	CB-CG-OD1	6.61	124.25	118.30
1	E	197	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	677	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	E	592	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	C	450	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	G	614	ASP	CB-CG-OD1	6.57	124.22	118.30
2	D	139	ASP	CB-CG-OD1	6.57	124.21	118.30
2	B	262	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	G	769	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	C	197	ASP	CB-CG-OD1	6.55	124.19	118.30
1	G	670	ASP	CB-CG-OD1	6.54	124.18	118.30
1	C	558	ASP	CB-CG-OD2	-6.52	112.43	118.30
2	F	227	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	E	133	ASP	CB-CG-OD1	6.52	124.17	118.30
2	D	299	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	G	625	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	499	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	F	211	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	G	226	ASP	CB-CG-OD2	-6.50	112.45	118.30
2	D	227	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	G	306	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	G	372	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	104	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	G	972	ASP	CB-CG-OD2	-6.49	112.46	118.30
2	H	67	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	E	558	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	528	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	1041	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	226	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	124	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	C	416	ASP	CB-CG-OD2	-6.45	112.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	944	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	E	459	ASP	CB-CG-OD1	6.44	124.09	118.30
2	B	211	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	625	ASP	CB-CG-OD2	-6.43	112.52	118.30
2	B	139	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	G	592	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	E	84	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	E	674	ASP	CB-CG-OD2	-6.42	112.53	118.30
2	F	188	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	487	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	G	128	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	G	579	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	H	116	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	H	188	ASP	CB-CG-OD1	6.39	124.05	118.30
2	B	344	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	E	758	ASP	CB-CG-OD1	6.38	124.05	118.30
2	D	368	ASP	CB-CG-OD1	6.38	124.05	118.30
1	C	539	ASP	CB-CG-OD1	6.38	124.04	118.30
2	F	45	ASP	CB-CG-OD1	6.37	124.04	118.30
1	G	133	ASP	CB-CG-OD2	-6.37	112.56	118.30
2	H	97	ASP	CB-CG-OD1	6.37	124.04	118.30
2	D	114	ASP	CB-CG-OD2	-6.37	112.56	118.30
2	D	139	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	F	227	ASP	CB-CG-OD1	6.37	124.03	118.30
1	E	194	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	807	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	459	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	6	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	614	ASP	CB-CG-OD1	6.34	124.01	118.30
1	G	736	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	D	211	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	956	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	D	192	PHE	CB-CG-CD2	6.32	125.22	120.80
1	E	1041	ASP	CB-CG-OD1	6.31	123.98	118.30
1	G	389	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	128	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	E	769	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	185	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	333	ASP	CB-CG-OD2	-6.28	112.65	118.30
2	F	244	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	G	757[A]	ASP	CB-CG-OD2	-6.28	112.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	757[B]	ASP	CB-CG-OD2	-6.28	112.65	118.30
2	D	262	ASP	CB-CG-OD1	6.27	123.95	118.30
1	C	441	ASP	CB-CG-OD1	6.27	123.94	118.30
2	F	211	ASP	CB-CG-OD1	6.27	123.94	118.30
1	G	57	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	H	299	ASP	CB-CG-OD1	6.26	123.93	118.30
2	F	198	ASP	CB-CG-OD1	6.25	123.93	118.30
1	E	438	TYR	CB-CG-CD1	6.25	124.75	121.00
1	E	343	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	959	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	C	1003	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	333	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	84	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	H	212	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	609	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	410	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	G	667	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	194	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	E	539	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	956[A]	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	956[B]	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	539	ASP	CB-CG-OD1	6.20	123.88	118.30
2	D	112	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	F	262	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	C	82	ARG	CA-CB-CG	-6.17	99.82	113.40
1	C	684	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	124	ASP	CB-CG-OD1	6.17	123.85	118.30
1	E	670	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	763	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	133	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	769	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	G	43	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	E	521	ASP	CB-CG-OD1	6.14	123.82	118.30
2	B	136	ASP	CB-CG-OD1	6.13	123.82	118.30
1	E	438	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	C	487	ASP	CB-CG-OD1	6.11	123.80	118.30
1	G	730	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	C	670	ASP	CB-CG-OD1	6.11	123.80	118.30
2	B	227	ASP	CB-CG-OD1	6.10	123.79	118.30
1	E	441	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	509	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	D	192	PHE	CB-CG-CD1	-6.10	116.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	C	763	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	1041	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	G	625	ASP	CB-CG-OD2	-6.08	112.83	118.30
2	H	378	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	H	227	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	G	42	TYR	CB-CG-CD1	-6.07	117.36	121.00
2	B	203	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	H	234	ASP	CB-CG-OD2	-6.05	112.85	118.30
2	B	69	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	C	343	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	G	757[A]	ASP	CB-CG-OD1	6.05	123.75	118.30
1	G	757[B]	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	300	MET	CG-SD-CE	6.05	109.88	100.20
1	A	416	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	410	ASP	CB-CG-OD1	6.05	123.74	118.30
1	E	1021	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	763	ASP	CB-CG-OD1	6.04	123.73	118.30
2	H	114	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	E	430	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	E	579	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	1021	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	912	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	E	807	ASP	CB-CG-OD2	-6.00	112.90	118.30
2	B	317	ASP	CB-CG-OD1	6.00	123.70	118.30
2	H	344	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	38[A]	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	38[B]	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	487	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	D	136	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	684	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	B	227	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	C	514	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	G	514	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	609	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	1021	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	H	211	ASP	CB-CG-OD1	5.94	123.64	118.30
1	E	592	ASP	CB-CG-OD1	5.93	123.64	118.30
1	E	674	ASP	CB-CG-OD1	5.93	123.64	118.30
1	G	716	PRO	N-CA-CB	5.93	110.41	103.30
1	E	133	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	614	ASP	CB-CG-OD1	5.92	123.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	989	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	F	157	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	514	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	H	249	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	A	372	ASP	CB-CG-OD1	5.88	123.59	118.30
1	E	124	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	425	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	758	ASP	CB-CG-OD2	-5.88	113.01	118.30
2	H	136	ASP	CB-CG-OD1	5.87	123.59	118.30
1	G	674	ASP	CB-CG-OD1	5.86	123.57	118.30
2	F	362	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	G	124	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	G	416	ASP	CB-CG-OD2	-5.83	113.05	118.30
2	D	104	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	E	1027	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	G	161	ASP	CB-CG-OD1	5.83	123.55	118.30
2	B	262	ASP	CB-CG-OD1	5.83	123.54	118.30
1	C	459	ASP	CB-CG-OD1	5.83	123.54	118.30
1	E	459	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	E	956[A]	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	956[B]	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	G	753	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	E	294	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	F	188	ASP	CB-CG-OD2	-5.82	113.07	118.30
2	B	299	ASP	CB-CG-OD2	-5.81	113.07	118.30
2	F	262	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	579	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	F	234	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	69	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	425	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	G	521	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	H	198	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	E	765	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	G	246	ASP	CB-CG-OD1	5.76	123.49	118.30
2	H	139	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	670	ASP	CB-CG-OD1	5.76	123.49	118.30
2	D	136	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	G	922	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	667	ASP	CB-CG-OD1	5.75	123.48	118.30
2	F	114	ASP	CB-CG-OD1	5.75	123.47	118.30
1	G	426[A]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	G	426[B]	ARG	NE-CZ-NH2	-5.75	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	C	333	ASP	CB-CG-OD2	-5.74	113.13	118.30
2	D	67	ASP	CB-CG-OD1	5.74	123.47	118.30
1	E	1036	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	434	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	490	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	265	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	G	904	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	G	1031	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	791	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	922	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	G	487	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	B	50	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	G	246	ASP	CB-CG-OD2	-5.72	113.16	118.30
2	D	45	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	609	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	G	121	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	609	ASP	CB-CG-OD1	5.70	123.43	118.30
2	F	84	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	H	262	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	E	735	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	D	234	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	471	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	F	84	ASP	CB-CG-OD1	5.68	123.42	118.30
1	E	631	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	716	PRO	N-CA-CB	5.68	110.11	103.30
2	F	11	ASP	CB-CG-OD1	5.68	123.41	118.30
1	G	237	PHE	CB-CG-CD2	5.67	124.77	120.80
1	C	246	ASP	CB-CG-OD1	5.67	123.40	118.30
2	H	198	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	972	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	333	ASP	CB-CG-OD1	5.65	123.39	118.30
1	E	1041	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	631	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	B	84	ASP	CB-CG-OD1	5.65	123.39	118.30
2	D	69	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	426	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	G	539	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	D	227	ASP	CB-CG-OD1	5.63	123.37	118.30
2	H	249	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	400	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	G	27	ASP	CB-CG-OD2	-5.63	113.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	675	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	G	791	ASP	CB-CG-OD1	5.63	123.37	118.30
1	G	453	PHE	CB-CG-CD2	-5.62	116.86	120.80
1	G	1025	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	E	303	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	265	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	753	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	104	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	530	ASP	CB-CG-OD1	5.60	123.34	118.30
1	G	956	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	590	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	75	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	119	THR	CA-CB-CG2	-5.59	104.58	112.40
2	B	45	ASP	CB-CG-OD1	5.59	123.33	118.30
1	G	730	ASP	CB-CG-OD1	5.58	123.32	118.30
1	G	416	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	197	ASP	CB-CG-OD1	5.57	123.31	118.30
1	G	528	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	1003	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	769	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	959	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	471	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	G	611	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	84	ASP	CB-CG-OD1	5.55	123.29	118.30
1	E	258	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	C	246	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	G	499	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	28	TYR	CB-CG-CD1	-5.53	117.69	121.00
1	C	450	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	42	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	361	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	354	TYR	CB-CG-CD2	5.52	124.31	121.00
1	E	605	THR	CA-CB-CG2	-5.52	104.67	112.40
2	D	148	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	E	730	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	C	609	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	642	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	A	807	ASP	CB-CG-OD1	5.50	123.25	118.30
1	E	733	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	G	590	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	559	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	D	317	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	317	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	361	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	1025	ASP	CB-CG-OD1	5.49	123.24	118.30
1	E	730	ASP	CB-CG-OD1	5.48	123.24	118.30
1	C	769	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	530	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	434	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	G	237	PHE	CB-CG-CD1	-5.47	116.97	120.80
2	B	157	ASP	CB-CG-OD1	5.46	123.22	118.30
1	E	62	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	G	430	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	G	1057	ASP	CB-CG-OD1	5.46	123.21	118.30
2	H	215	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	B	93	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	675	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	G	27	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	807	ASP	CB-CG-OD1	5.43	123.19	118.30
1	G	912	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	E	530	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	C	807	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	499	ASP	CB-CG-OD2	-5.42	113.42	118.30
2	B	136	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	161	ASP	CB-CG-OD1	5.41	123.17	118.30
2	H	69	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	C	82	ARG	CG-CD-NE	-5.40	100.45	111.80
1	C	959	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	807	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	E	434	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	B	244	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	E	279	THR	CA-CB-CG2	-5.40	104.84	112.40
1	C	82	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	84	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	441	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	A	769	ASP	CB-CG-OD1	5.39	123.15	118.30
2	D	344	ASP	CB-CG-OD1	5.39	123.15	118.30
2	B	11	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	B	188	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	444	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	F	378	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	E	1021	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	G	121	ASP	CB-CG-OD1	5.37	123.14	118.30
1	E	189	GLU	CA-CB-CG	-5.37	101.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1057	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	758	ASP	CB-CG-OD1	5.36	123.13	118.30
1	C	57	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	C	434	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	226	ASP	CB-CG-OD1	5.35	123.12	118.30
1	G	84	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	E	558	ASP	N-CA-CB	-5.35	100.97	110.60
1	E	579	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	204	LEU	CB-CA-C	-5.34	100.05	110.20
2	F	250	TYR	CB-CG-CD2	-5.34	117.80	121.00
2	B	344	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	904	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	509	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	E	763	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	434	ASP	CB-CG-OD1	5.31	123.08	118.30
1	G	133	ASP	CB-CG-OD1	5.31	123.08	118.30
2	B	249	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	677	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	425	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	F	198	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	G	81	GLU	CG-CD-OE2	-5.29	107.72	118.30
1	A	625	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	459	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	674	ASP	CB-CG-OD1	5.28	123.05	118.30
2	F	69	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	161	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	521	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	753	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	258	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	373	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	G	558	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	133	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	C	273	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	E	246	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	E	1057	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	G	769	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	306	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	989	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	667	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	830	PHE	CB-CG-CD1	-5.23	117.14	120.80
2	B	198	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	E	287	ALA	N-CA-CB	5.22	117.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	GLU	CG-CD-OE2	-5.22	107.87	118.30
1	A	121	ASP	CB-CG-OD1	5.21	122.99	118.30
2	F	50	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	F	234	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	D	211	ASP	CB-CG-OD1	5.20	122.98	118.30
2	B	95	THR	CA-CB-CG2	-5.20	105.13	112.40
1	E	338	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	G	238	ASP	CB-CG-OD1	5.19	122.97	118.30
1	G	400	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	6	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	D	249	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	5	THR	CA-CB-CG2	-5.18	105.15	112.40
1	C	677	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	124	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	338	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	487	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	807	ASP	CB-CG-OD1	5.17	122.95	118.30
2	F	215	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	G	518	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	D	120	ARG	CD-NE-CZ	5.17	130.83	123.60
1	G	530	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	674	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	133	ASP	CB-CG-OD1	5.16	122.94	118.30
2	D	334	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	62	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	684	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	667	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	B	316	VAL	CA-CB-CG1	-5.14	103.19	110.90
1	A	39	GLU	CB-CA-C	-5.14	100.12	110.40
2	B	203	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	G	1016	THR	CA-CB-CG2	-5.13	105.21	112.40
1	C	84	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	608	THR	CA-CB-CG2	-5.13	105.22	112.40
2	F	136	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	592	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	C	730	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	E	118	ALA	N-CA-CB	5.12	117.26	110.10
1	C	579	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	G	1025	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	338	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	97	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	B	45	ASP	CB-CG-OD2	-5.09	113.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	781	HIS	CB-CA-C	-5.09	100.22	110.40
1	A	1004	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	E	880	THR	CA-CB-CG2	-5.09	105.28	112.40
2	H	114	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	130	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	306	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	H	262	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	791	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	G	338	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	E	389	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	D	326	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	994	VAL	CG1-CB-CG2	-5.06	102.80	110.90
2	B	207	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	G	438	TYR	CB-CG-CD2	-5.05	117.97	121.00
2	B	320	THR	CA-CB-CG2	-5.03	105.35	112.40
1	C	912	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	F	112	ASP	CB-CG-OD1	5.03	122.83	118.30
1	E	518	ASP	CB-CG-OD1	5.03	122.82	118.30
1	C	400	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	E	823	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	G	353	ASP	CB-CG-OD1	5.01	122.81	118.30
2	H	344	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	372	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	471	ARG	NE-CZ-NH2	-5.00	117.80	120.30
2	D	344	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	A	521	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

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	8195	0	8247	239	0
1	C	8192	0	8230	247	0
1	E	8211	0	8245	225	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	8180	0	8214	291	0
2	B	2895	0	2861	91	0
2	D	2895	0	2861	98	0
2	F	2895	0	2861	107	0
2	H	2895	0	2861	134	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	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	1	0
5	B	1	0	0	0	0
5	C	3	0	0	2	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
5	G	3	0	0	3	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	0	0
7	C	54	0	24	1	0
7	E	54	0	24	4	0
7	G	54	0	24	2	0
8	A	9	0	11	1	0
8	C	9	0	11	1	0
8	E	9	0	11	0	0
8	G	9	0	11	0	0
9	A	10	0	7	0	0
9	B	10	0	7	3	0
9	C	10	0	7	0	0
9	D	10	0	7	2	0
9	E	10	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	10	0	7	3	0
9	G	10	0	7	0	0
9	H	10	0	7	2	0
10	A	9	0	20	0	0
10	C	9	0	20	1	0
10	E	9	0	20	2	0
10	G	9	0	20	0	0
11	A	699	0	0	14	0
11	B	231	0	0	4	0
11	C	706	0	0	19	0
11	D	250	0	0	5	0
11	E	754	0	0	23	0
11	F	231	0	0	4	0
11	G	622	0	0	20	0
11	H	173	0	0	4	0
All	All	48477	0	44656	1411	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1411) 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:808:VAL:HA	1:E:811[B]:GLN:HE21	1.12	1.11
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.10
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.36	1.08
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.38	1.04
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.35	1.03
1:G:784:GLN:NE2	1:G:784:GLN:H	1.57	1.00
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.44	0.99
1:C:1063:ILE:HD13	1:C:1068:MET:HG3	1.41	0.99
1:E:1002:GLN:HE22	1:E:1006[B]:LYS:NZ	1.60	0.97
1:A:784:GLN:HE21	1:A:784:GLN:H	0.98	0.96
1:A:784:GLN:NE2	1:A:784:GLN:H	1.64	0.95
1:A:956[B]:ARG:HH11	1:A:956[B]:ARG:HG2	1.31	0.94
1:G:784:GLN:N	1:G:784:GLN:HE21	1.64	0.94
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.47	0.93
1:A:38[A]:ARG:HH11	1:A:38[A]:ARG:HG3	1.34	0.93
1:E:696:THR:H	1:E:700:MET:HE3	1.31	0.93
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.51	0.92
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:VAL:HA	2:D:231:MET:HE2	1.51	0.91
1:E:1002:GLN:HE22	1:E:1006[B]:LYS:HZ3	1.11	0.91
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.84	0.91
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.53	0.90
1:G:1021:ARG:HH11	1:G:1021:ARG:HG2	1.38	0.89
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.88	0.88
2:B:324:ASN:N	2:B:324:ASN:HD22	1.70	0.88
1:E:808:VAL:HA	1:E:811[B]:GLN:NE2	1.89	0.88
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.56	0.87
2:B:324:ASN:H	2:B:324:ASN:HD22	1.18	0.87
1:C:994:VAL:HG13	1:C:1000:HIS:ND1	1.89	0.87
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.04	0.87
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.03	0.87
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.57	0.86
1:E:698:ILE:HG13	1:E:738:PHE:CD1	2.11	0.86
1:E:784:GLN:H	1:E:784:GLN:NE2	1.73	0.86
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.05	0.85
1:G:563:MET:CE	1:G:635:PRO:HG3	2.08	0.84
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.92	0.84
1:A:1001:ILE:HD12	1:A:1002:GLN:N	1.90	0.84
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.12	0.84
1:E:784:GLN:H	1:E:784:GLN:HE21	1.23	0.84
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.93	0.83
1:G:1063:ILE:HD13	1:G:1068:MET:HG3	1.59	0.83
1:C:670:ASP:HB3	1:C:677:ARG:HH21	1.43	0.83
2:F:228:VAL:HA	2:F:231:MET:CE	2.09	0.83
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.14	0.82
1:C:563:MET:CE	1:C:635:PRO:HG3	2.09	0.82
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.59	0.82
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.94	0.82
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.62	0.82
2:D:241:GLY:O	9:D:4034:GLN:HG3	1.80	0.81
2:H:187:GLU:HG2	2:H:215:ARG:CD	2.10	0.81
1:G:663:GLY:HA3	1:G:869:MET:HE3	1.63	0.81
2:F:201:ALA:HB2	2:F:239:SER:CB	2.10	0.81
1:C:670:ASP:HB3	1:C:677:ARG:NH2	1.97	0.80
1:A:734:LEU:O	1:A:734:LEU:HD12	1.82	0.80
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.44	0.80
1:A:38[B]:ARG:HH11	1:A:38[B]:ARG:HG2	1.43	0.80
1:A:313:LYS:HE2	1:A:608:THR:O	1.82	0.80
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:ASN:H	2:B:324:ASN:ND2	1.80	0.79
1:E:1002:GLN:NE2	1:E:1006[B]:LYS:NZ	2.31	0.79
1:C:74:VAL:HG11	1:C:102:LEU:HD11	1.64	0.79
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.64	0.79
2:F:241:GLY:O	9:F:4056:GLN:HG3	1.82	0.79
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.65	0.79
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.65	0.79
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.62	0.79
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.11	0.78
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.18	0.78
1:E:1:MET:HB2	1:E:224:LYS:NZ	1.97	0.78
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.46	0.78
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.14	0.77
1:E:151:THR:HB	1:E:153[B]:GLU:OE2	1.85	0.77
1:C:1:MET:HB2	1:C:224:LYS:NZ	1.99	0.77
1:G:181:ILE:HD11	1:G:376:THR:HG23	1.65	0.77
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.66	0.77
1:E:1:MET:HB2	1:E:224:LYS:HZ2	1.47	0.77
1:G:64:THR:O	1:G:1065:VAL:HG23	1.85	0.77
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.66	0.77
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.20	0.77
1:G:704:LYS:O	1:G:708:ILE:HD12	1.85	0.77
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.65	0.76
1:E:808:VAL:CA	1:E:811[B]:GLN:HE21	1.94	0.76
1:G:903:VAL:HG13	11:G:3404:HOH:O	1.86	0.76
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.67	0.76
2:D:228:VAL:HA	2:D:231:MET:CE	2.14	0.76
2:H:299:ASP:OD1	2:H:302:LYS:HD3	1.85	0.76
2:B:226:GLU:O	2:B:230:LYS:HG3	1.86	0.76
2:D:324:ASN:HD22	2:D:324:ASN:H	1.31	0.76
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.50	0.76
1:C:363:ASN:HA	1:C:365:GLU:OE2	1.86	0.76
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.20	0.76
1:A:784:GLN:HE21	1:A:784:GLN:N	1.80	0.76
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.68	0.75
1:C:973:ALA:O	1:C:991[A]:VAL:HG12	1.85	0.75
1:G:385:MET:HG2	1:G:618:PHE:CE1	2.21	0.75
2:H:324:ASN:HD22	2:H:324:ASN:H	1.35	0.75
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.69	0.75
1:E:153[A]:GLU:HG2	11:E:4283:HOH:O	1.85	0.75
1:E:698:ILE:O	1:E:702:VAL:HG23	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:ARG:HD3	11:C:4652:HOH:O	1.87	0.74
1:G:865:ALA:O	1:G:869:MET:HG3	1.86	0.74
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.17	0.74
1:C:1:MET:HB2	1:C:224:LYS:HZ2	1.51	0.74
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.68	0.74
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.70	0.74
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.67	0.74
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.18	0.74
2:H:54:THR:HG21	2:H:118:LEU:HD23	1.70	0.74
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.23	0.73
2:H:71:GLU:O	2:H:203:ARG:HG3	1.87	0.73
1:A:681:ALA:O	1:A:685:LEU:HG	1.88	0.73
2:B:71:GLU:O	2:B:203:ARG:HG3	1.87	0.73
1:C:38:ARG:NH1	1:C:38:ARG:HG3	2.02	0.73
1:G:954:LYS:O	1:G:957:VAL:HG12	1.88	0.73
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.70	0.73
1:A:772:MET:SD	1:A:880:THR:HG22	2.29	0.73
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.89	0.73
1:C:802:SER:O	1:C:806:GLN:HG3	1.89	0.73
2:H:324:ASN:HD22	2:H:324:ASN:N	1.87	0.73
1:A:973:ALA:O	1:A:991:VAL:HG12	1.88	0.73
1:A:930:LYS:HE3	11:A:4162:HOH:O	1.89	0.73
1:C:358:LYS:HE3	11:C:4153:HOH:O	1.89	0.72
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.71	0.72
1:C:400:ARG:HD3	11:C:4391:HOH:O	1.88	0.72
1:G:873:SER:O	1:G:877:GLN:HG3	1.89	0.72
2:H:228:VAL:HA	2:H:231:MET:CE	2.18	0.72
1:A:772:MET:HE2	1:A:880:THR:HA	1.72	0.72
1:A:698:ILE:H	1:A:698:ILE:HD12	1.54	0.72
1:E:863:LYS:O	1:E:867:ARG:HG3	1.89	0.72
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.54	0.72
1:G:181:ILE:CD1	1:G:376:THR:HG23	2.20	0.72
2:F:251:ALA:O	2:F:255:ILE:HD12	1.88	0.72
1:G:57:ASP:HB3	1:G:59:GLU:OE2	1.89	0.72
2:F:228:VAL:HA	2:F:231:MET:HE2	1.72	0.72
1:A:318:PRO:HG3	1:A:610:TYR:OH	1.88	0.72
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.72	0.72
1:E:1004:ARG:HD3	1:E:1009[B]:GLU:OE2	1.90	0.71
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.72	0.71
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.20	0.71
1:A:997:GLY:O	1:A:998:ARG:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.73	0.71
1:G:734:LEU:HD12	1:G:734:LEU:O	1.89	0.71
1:G:663:GLY:HA3	1:G:869:MET:CE	2.21	0.71
2:B:117:LYS:HE3	11:B:4071:HOH:O	1.89	0.71
1:G:58:PRO:HD2	1:G:59:GLU:OE2	1.90	0.71
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.54	0.71
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.73	0.71
2:F:324:ASN:O	2:F:342:ARG:HD2	1.91	0.70
2:D:246:ALA:HB3	2:D:247:PRO:HD3	1.73	0.70
2:D:259:LEU:HD13	2:D:342:ARG:NH1	2.06	0.70
1:G:998:ARG:HA	1:G:999:PRO:C	2.12	0.70
1:A:873:SER:O	1:A:877:GLN:HG3	1.92	0.70
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.27	0.70
1:A:38[A]:ARG:NH1	1:A:38[A]:ARG:HG3	2.02	0.70
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.16	0.70
1:C:726:GLU:HG3	1:C:727:ILE:H	1.55	0.70
2:H:218:ILE:N	2:H:218:ILE:HD13	2.07	0.69
1:G:548:GLU:HG2	2:H:114:ASP:CG	2.12	0.69
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.73	0.69
1:C:998:ARG:HG2	1:C:999:PRO:HA	1.73	0.69
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.27	0.69
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.27	0.69
2:F:324:ASN:H	2:F:324:ASN:HD22	1.40	0.69
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.57	0.69
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.75	0.69
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.74	0.69
1:E:1001:ILE:HD12	1:E:1002:GLN:N	2.07	0.69
1:G:648:LEU:HD22	1:G:845:ARG:HD3	1.75	0.69
1:A:974:THR:HG21	1:A:993[B]:LYS:HD3	1.74	0.69
1:E:166:CYS:C	1:E:167:ILE:HD12	2.13	0.69
1:E:1:MET:N	1:E:224:LYS:HE3	2.07	0.69
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.73	0.69
2:H:6:LEU:HD12	2:H:7:LEU:N	2.08	0.69
2:H:34:THR:HA	2:H:56:THR:OG1	1.92	0.68
1:G:784:GLN:HE21	1:G:784:GLN:H	0.79	0.68
2:H:286:MET:CE	2:H:289:GLY:HA2	2.23	0.68
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.29	0.68
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.23	0.68
1:E:103:GLU:HG3	1:E:104:ARG:N	2.06	0.68
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.74	0.68
1:C:726:GLU:HG3	1:C:727:ILE:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.29	0.68
1:C:883:VAL:O	1:C:884:ILE:HD13	1.94	0.68
1:E:224:LYS:HE2	1:E:329:GLY:O	1.94	0.68
1:G:563:MET:HE1	1:G:635:PRO:HG3	1.73	0.68
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.08	0.68
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.27	0.68
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.74	0.68
2:B:324:ASN:O	2:B:342:ARG:HD2	1.94	0.67
1:C:1063:ILE:CD1	1:C:1068:MET:HG3	2.22	0.67
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.60	0.67
1:E:1021:ARG:HG2	1:E:1021:ARG:HH11	1.57	0.67
1:E:1:MET:N	11:E:4680:HOH:O	2.25	0.67
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.29	0.67
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.22	0.67
1:E:696:THR:N	1:E:700:MET:HE3	2.07	0.67
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.74	0.67
1:G:273:ARG:HD2	11:G:3191:HOH:O	1.95	0.67
2:F:139:ASP:OD2	2:F:142:LEU:HB2	1.94	0.67
2:H:228:VAL:HA	2:H:231:MET:HE2	1.76	0.67
2:H:6:LEU:HD11	2:H:8:VAL:HG22	1.77	0.67
1:G:4:ARG:HD3	1:G:7:ILE:HD12	1.76	0.67
1:G:475:LYS:O	1:G:479:VAL:HG13	1.95	0.67
1:A:698:ILE:O	1:A:701:ALA:HB3	1.95	0.66
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.77	0.66
1:A:563:MET:CE	1:A:635:PRO:HG3	2.24	0.66
1:C:698:ILE:H	1:C:698:ILE:HD12	1.61	0.66
1:G:166:CYS:C	1:G:167:ILE:HD12	2.15	0.66
1:C:224:LYS:HE2	1:C:329:GLY:O	1.95	0.66
1:A:772:MET:CE	1:A:880:THR:HG22	2.26	0.66
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.76	0.66
1:G:1:MET:HB2	1:G:224:LYS:NZ	2.11	0.66
1:C:32:GLN:OE1	1:C:320:ALA:HB3	1.95	0.65
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.77	0.65
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.77	0.65
1:G:1030:ARG:NH1	1:G:1030:ARG:HG3	2.10	0.65
1:G:936:ASN:HB2	11:G:2917:HOH:O	1.97	0.65
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.27	0.65
2:B:218:ILE:N	2:B:218:ILE:HD13	2.12	0.65
2:D:64:GLY:HA3	2:D:94:ASN:OD1	1.97	0.65
1:G:695:VAL:CG1	1:G:700:MET:HB3	2.21	0.65
2:B:279:SER:O	2:B:322:PRO:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:954:LYS:O	1:E:980:VAL:HG11	1.96	0.65
2:H:205:ILE:HG13	2:H:355:GLU:HG3	1.79	0.65
1:A:726:GLU:HG3	1:A:727:ILE:H	1.62	0.65
1:C:708:ILE:HG21	1:C:712:LEU:HD11	1.79	0.65
2:F:232:ASN:N	2:F:233:PRO:HD3	2.11	0.65
2:F:8:VAL:HG22	2:F:14:GLN:HG2	1.78	0.65
2:H:324:ASN:O	2:H:342:ARG:HD2	1.97	0.65
1:C:652:ARG:NH1	1:C:670:ASP:OD2	2.30	0.64
2:D:205:ILE:HG13	2:D:355:GLU:HG3	1.79	0.64
1:G:772:MET:SD	1:G:880:THR:HG22	2.37	0.64
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.43	0.64
1:C:154:GLU:OE1	11:C:4246:HOH:O	2.15	0.64
1:E:515:LYS:HD3	1:E:515:LYS:O	1.98	0.64
1:E:343:ARG:NH2	11:E:4720:HOH:O	2.30	0.64
2:F:218:ILE:HD13	2:F:218:ILE:N	2.12	0.64
1:A:358:LYS:HE3	11:A:4129:HOH:O	1.97	0.64
1:C:734:LEU:O	1:C:734:LEU:HD12	1.97	0.64
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.79	0.64
2:B:249:ASP:OD2	2:B:250:TYR:N	2.31	0.64
1:C:994:VAL:HG13	1:C:1000:HIS:CE1	2.31	0.64
2:H:286:MET:HE2	2:H:289:GLY:HA2	1.79	0.64
2:B:272:HIS:ND1	2:B:349:SER:OG	2.30	0.64
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.28	0.64
1:A:698:ILE:CD1	1:A:698:ILE:H	2.11	0.64
2:F:186:LYS:O	2:F:189:GLU:HB2	1.97	0.64
1:E:646:THR:HB	1:E:647:PRO:HD3	1.80	0.64
1:G:1030:ARG:HH11	1:G:1030:ARG:HG3	1.63	0.64
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.44	0.63
1:E:998:ARG:HG2	1:E:999:PRO:HA	1.80	0.63
1:G:901:PRO:HD2	5:G:4084:CL:CL	2.36	0.63
1:E:6:ASP:N	1:E:6:ASP:OD2	2.29	0.63
1:A:648:LEU:HD22	1:A:845:ARG:HD3	1.79	0.63
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.34	0.63
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.79	0.63
1:A:38[B]:ARG:HG2	1:A:38[B]:ARG:NH1	2.04	0.63
1:C:695:VAL:CG1	1:C:701:ALA:HB2	2.24	0.63
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.80	0.63
1:A:956[B]:ARG:NH1	1:A:956[B]:ARG:HG2	2.03	0.63
1:A:976:GLY:O	1:A:980:VAL:HG23	1.99	0.63
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.98	0.63
1:G:698:ILE:HD12	1:G:698:ILE:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:LYS:NZ	11:A:4560:HOH:O	2.30	0.63
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.63	0.63
1:E:151:THR:OG1	1:E:153[B]:GLU:HG2	1.99	0.63
1:G:817:ALA:HB2	1:G:826:MET:SD	2.39	0.63
2:H:269:SER:HB3	9:H:4079:GLN:OE1	1.99	0.63
1:A:150:HIS:N	1:A:154:GLU:OE2	2.32	0.62
1:C:890:VAL:HG23	1:C:927:ALA:HB1	1.79	0.62
2:F:225:ALA:O	2:F:229:LEU:HG	1.99	0.62
1:A:905:PRO:HB2	1:A:1040:TYR:OH	2.00	0.62
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.18	0.62
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.34	0.62
1:A:659:VAL:HG13	1:A:660:PRO:HD2	1.81	0.62
1:A:698:ILE:N	1:A:698:ILE:HD12	2.13	0.62
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.64	0.62
1:C:947:LEU:N	1:C:947:LEU:HD12	2.13	0.62
1:G:167:ILE:HD12	1:G:167:ILE:N	2.15	0.62
1:A:726:GLU:HG3	1:A:727:ILE:N	2.15	0.62
1:A:4:ARG:HD3	1:A:7:ILE:HD12	1.82	0.62
1:A:992:ASN:ND2	1:G:975:HIS:NE2	2.48	0.62
1:C:687:LEU:HD11	1:C:812:GLN:HG2	1.80	0.61
1:E:4:ARG:HA	11:E:4160:HOH:O	1.99	0.61
1:E:734:LEU:O	1:E:734:LEU:HD12	2.00	0.61
1:G:757[B]:ASP:OD1	1:G:833:LYS:NZ	2.33	0.61
2:H:328:THR:HG21	11:H:3665:HOH:O	1.99	0.61
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.81	0.61
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.21	0.61
1:A:907:LEU:HD11	8:A:4011:ORN:HD3	1.82	0.61
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.35	0.61
1:C:784:GLN:H	1:C:784:GLN:HE21	1.49	0.61
1:E:167:ILE:N	1:E:167:ILE:HD12	2.15	0.61
1:C:698:ILE:N	1:C:698:ILE:HD12	2.16	0.61
1:E:1021:ARG:CG	1:E:1021:ARG:HH11	2.14	0.61
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.00	0.61
1:A:1021:ARG:CG	1:A:1021:ARG:HH11	2.13	0.61
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.83	0.61
1:C:416:ASP:O	1:C:418:PRO:HD3	2.01	0.61
2:D:195:VAL:HG11	2:D:231:MET:HE1	1.81	0.61
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.83	0.61
2:H:284:VAL:O	2:H:315:ALA:N	2.33	0.61
1:C:812:GLN:NE2	11:C:4684:HOH:O	2.06	0.60
1:A:375:THR:HG23	1:A:377:GLN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ARG:CD	1:C:675:ARG:H	2.11	0.60
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.82	0.60
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.30	0.60
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.01	0.60
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.84	0.60
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.83	0.60
1:G:10:ILE:HD12	1:G:42:TYR:HB3	1.83	0.60
1:A:956[A]:ARG:HD3	11:A:4668:HOH:O	2.01	0.60
1:C:698:ILE:H	1:C:698:ILE:CD1	2.15	0.60
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.82	0.60
1:G:1001:ILE:CD1	1:G:1002:GLN:N	2.65	0.60
1:A:757:ASP:O	1:A:833:LYS:NZ	2.32	0.60
1:E:956[A]:ARG:HB3	1:E:1044:LEU:CD2	2.31	0.60
1:E:702:VAL:HG11	1:E:735:ARG:NH2	2.15	0.60
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.66	0.60
1:C:1021:ARG:HH11	1:C:1021:ARG:HG3	1.65	0.60
1:C:822:VAL:O	1:C:823:ARG:HD3	2.01	0.60
2:F:228:VAL:HA	2:F:231:MET:HE3	1.80	0.60
2:F:324:ASN:HD22	2:F:324:ASN:N	1.99	0.60
2:H:158:LEU:CB	2:H:242:PRO:HB2	2.31	0.60
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.17	0.60
1:C:890:VAL:HG23	1:C:927:ALA:CB	2.31	0.60
1:E:812:GLN:NE2	11:E:4800:HOH:O	2.35	0.60
2:H:33:ASN:HA	2:H:291:HIS:O	2.02	0.60
2:H:344:ASP:OD2	2:H:344:ASP:N	2.34	0.60
2:B:186:LYS:O	2:B:189:GLU:HB2	2.02	0.59
2:B:370:PHE:O	2:B:374:ILE:HG13	2.02	0.59
1:G:676:GLU:O	1:G:680:HIS:ND1	2.35	0.59
1:C:784:GLN:H	1:C:784:GLN:NE2	1.99	0.59
1:E:563:MET:CE	1:E:635:PRO:HG3	2.32	0.59
1:C:708:ILE:CG2	1:C:712:LEU:HD11	2.31	0.59
1:G:282:SER:N	11:G:3572:HOH:O	2.35	0.59
1:G:343:ARG:NH1	11:G:3545:HOH:O	2.34	0.59
1:A:646:THR:HB	1:A:647:PRO:HD3	1.83	0.59
1:A:954:LYS:O	1:A:957:VAL:HG12	2.02	0.59
1:C:313:LYS:HE2	1:C:608:THR:O	2.02	0.59
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.50	0.59
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.85	0.59
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.50	0.59
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.83	0.59
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:509:ARG:HB2	1:G:509:ARG:HH11	1.66	0.59
2:H:55:LEU:CD1	2:H:60:ILE:HD12	2.32	0.59
2:D:174:SER:O	2:D:182:PRO:HD3	2.03	0.59
1:A:675:ARG:CD	1:A:675:ARG:H	2.15	0.59
1:A:906:LEU:O	1:A:912:ARG:NH2	2.30	0.59
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.17	0.59
2:D:26:ALA:O	2:D:131:CYS:HA	2.03	0.59
1:C:509:ARG:NH1	1:C:512:GLU:OE1	2.35	0.59
1:C:954:LYS:O	1:C:957:VAL:HG12	2.02	0.59
2:F:379:LYS:HZ3	2:F:379:LYS:HB2	1.67	0.59
1:E:1020:ARG:O	1:E:1024:GLU:HG3	2.03	0.59
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.84	0.59
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.26	0.58
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.85	0.58
1:A:315:THR:O	1:A:531:THR:HG22	2.03	0.58
1:C:975:HIS:HE2	1:E:992:ASN:ND2	2.01	0.58
2:H:46:PRO:O	2:H:242:PRO:HG3	2.03	0.58
1:C:133:ASP:OD2	11:C:4117:HOH:O	2.17	0.58
2:H:324:ASN:H	2:H:324:ASN:ND2	2.00	0.58
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.03	0.58
1:G:698:ILE:N	1:G:698:ILE:HD12	2.18	0.58
2:B:46:PRO:HA	2:B:76:HIS:CG	2.37	0.58
1:C:447:LEU:HD23	1:G:446:GLY:O	2.02	0.58
1:C:998:ARG:CG	1:C:999:PRO:HA	2.33	0.58
2:D:118:LEU:O	2:D:118:LEU:HD12	2.04	0.58
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.33	0.58
2:H:363:ALA:C	2:H:365:PRO:HD2	2.23	0.58
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.39	0.58
1:G:165:PRO:HA	1:G:182:ALA:O	2.04	0.58
1:C:1052:MET:HG2	11:C:4681:HOH:O	2.04	0.58
1:C:980:VAL:HG13	11:C:4704:HOH:O	2.03	0.58
2:F:269:SER:HB3	9:F:4056:GLN:OE1	2.04	0.58
1:G:1021:ARG:CG	1:G:1021:ARG:HH11	2.12	0.58
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.33	0.58
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.07	0.58
1:A:272:LEU:HD11	1:A:282:SER:HB2	1.85	0.58
2:B:350:PHE:HB2	2:B:366:LEU:HD22	1.86	0.58
1:C:1063:ILE:HD13	1:C:1068:MET:CG	2.26	0.58
1:A:863:LYS:HE2	11:A:4575:HOH:O	2.03	0.57
2:D:350:PHE:HB2	2:D:366:LEU:HD22	1.86	0.57
1:G:809:MET:O	1:G:813:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:CYS:C	1:A:167:ILE:HD12	2.25	0.57
1:A:964:LEU:O	1:A:969:PHE:HB2	2.03	0.57
2:B:313:GLY:HA3	11:B:4020:HOH:O	2.04	0.57
1:C:103:GLU:HG3	1:C:104:ARG:N	2.15	0.57
1:C:695:VAL:CG1	1:C:700:MET:HB3	2.34	0.57
2:D:6:LEU:HD13	2:D:16:HIS:CE1	2.39	0.57
1:C:479:VAL:CG2	1:C:483:GLY:HA3	2.34	0.57
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.52	0.57
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.69	0.57
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.85	0.57
1:E:194:ARG:HD3	11:E:4114:HOH:O	2.04	0.57
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.40	0.57
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.85	0.57
1:A:1011:THR:HG23	11:A:4539:HOH:O	2.04	0.57
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.35	0.57
1:E:213:TRP:CE2	1:E:289:ASN:HB2	2.39	0.57
1:G:729:TYR:CE1	1:G:1019:GLY:HA2	2.39	0.57
1:G:560:GLU:OE1	1:G:636:LYS:HE3	2.05	0.57
2:H:78:GLN:NE2	2:H:78:GLN:HA	2.19	0.57
1:E:1017:THR:HG22	1:E:1023:ILE:HG13	1.87	0.57
1:A:194:ARG:NH2	11:A:4602:HOH:O	2.28	0.57
2:D:286:MET:CE	2:D:312:HIS:ND1	2.67	0.57
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.86	0.57
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.86	0.57
1:C:419[B]:GLU:OE1	1:G:422:THR:HG21	2.05	0.57
1:C:559:ARG:HH11	1:C:559:ARG:HG3	1.69	0.57
1:E:344:THR:HB	1:E:345:PRO:HD2	1.87	0.57
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.86	0.57
2:B:139:ASP:OD2	2:B:142:LEU:HB2	2.05	0.56
1:C:901:PRO:HD2	5:C:4039:CL:CL	2.42	0.56
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.87	0.56
1:A:562:ILE:HG21	1:A:589:LEU:CD1	2.35	0.56
1:A:321:LYS:NZ	1:A:611:ASP:OD1	2.36	0.56
2:F:253:THR:O	2:F:256:GLN:HB2	2.05	0.56
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.40	0.56
1:C:375:THR:HG23	1:C:377:GLN:H	1.69	0.56
1:C:693:ALA:HB1	1:C:704:LYS:HG2	1.86	0.56
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.86	0.56
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.87	0.56
1:A:344:THR:HB	1:A:345:PRO:HD2	1.86	0.56
1:C:40:GLU:OE1	1:C:325:LYS:HE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:534:ALA:O	2:H:123:ARG:HD3	2.05	0.56
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.87	0.56
1:A:973:ALA:C	1:A:991:VAL:HG12	2.26	0.56
1:A:998:ARG:CB	1:A:999:PRO:HA	2.34	0.56
1:E:196:LEU:HG	1:E:204:LEU:HD11	1.86	0.56
1:E:698:ILE:HG13	1:E:738:PHE:CG	2.39	0.56
1:G:349:GLU:O	2:H:294:ASN:HB2	2.04	0.56
1:G:954:LYS:O	1:G:980:VAL:HG11	2.06	0.56
1:E:1019:GLY:O	1:E:1023:ILE:HD12	2.05	0.56
1:E:726:GLU:HG3	1:E:1020:ARG:NH2	2.21	0.56
1:A:489:LEU:HD22	1:A:516:LEU:HD23	1.86	0.56
1:C:695:VAL:HG21	1:C:752:LEU:HD22	1.88	0.56
1:G:569:PRO:O	1:G:571:ARG:HD2	2.06	0.56
1:C:3:LYS:HG2	11:C:4580:HOH:O	2.04	0.56
2:D:286:MET:HE3	2:D:312:HIS:ND1	2.21	0.56
2:F:272:HIS:HA	2:F:349:SER:HB2	1.88	0.56
2:H:248:CYS:O	2:H:252:ILE:HG13	2.06	0.56
2:D:44:THR:O	2:D:46:PRO:HD3	2.06	0.56
1:G:1001:ILE:HD12	1:G:1002:GLN:N	2.20	0.56
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.06	0.56
1:A:682:VAL:HG11	1:A:689:GLN:HE21	1.71	0.56
1:E:757:ASP:O	1:E:833:LYS:NZ	2.27	0.56
1:G:964:LEU:O	1:G:969:PHE:HB2	2.06	0.56
1:G:679:GLN:HG2	1:G:689:GLN:HE22	1.71	0.55
2:H:169:SER:HA	2:H:216:LEU:O	2.07	0.55
2:H:228:VAL:HA	2:H:231:MET:HE3	1.86	0.55
1:A:700:MET:O	1:A:704:LYS:HB2	2.06	0.55
1:A:1020:ARG:HH21	1:A:1023:ILE:HG21	1.70	0.55
2:B:172:GLN:O	2:B:207:ARG:HA	2.06	0.55
2:B:259:LEU:O	2:B:345:LYS:HE3	2.07	0.55
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.07	0.55
1:G:548:GLU:HG2	2:H:114:ASP:OD1	2.05	0.55
1:C:1068:MET:O	1:C:1071:GLN:HB2	2.07	0.55
1:C:858:GLY:HA2	1:C:1069:HIS:NE2	2.21	0.55
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.36	0.55
1:A:103:GLU:HG2	1:A:108:LEU:HD12	1.89	0.55
1:A:948:SER:O	1:A:1015:ASN:HA	2.06	0.55
2:B:46:PRO:HA	2:B:76:HIS:CB	2.37	0.55
1:C:735:ARG:O	1:C:738:PHE:HB2	2.07	0.55
2:D:178:THR:HB	11:D:1596:HOH:O	2.06	0.55
1:E:998:ARG:HA	1:E:999:PRO:C	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:668:ALA:O	1:G:671:ARG:HB2	2.07	0.55
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.41	0.55
1:E:950:ARG:HD3	11:E:4812:HOH:O	2.06	0.55
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.37	0.55
1:A:88:PRO:HB3	1:A:99:ALA:HB2	1.88	0.55
1:A:947:LEU:N	1:A:947:LEU:HD12	2.21	0.55
1:C:222:ARG:NH1	1:C:273:ARG:HA	2.21	0.55
1:C:735:ARG:O	1:C:738:PHE:N	2.39	0.55
2:D:206:LEU:O	2:D:210:VAL:HG23	2.07	0.55
1:E:1:MET:H2	1:E:224:LYS:HE3	1.70	0.55
1:G:556:SER:HB2	1:G:558:ASP:HB2	1.88	0.55
2:B:364:ALA:N	2:B:365:PRO:HD2	2.22	0.55
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.37	0.55
2:D:240:ASN:HB2	9:D:4034:GLN:OE1	2.06	0.55
1:A:167:ILE:N	1:A:167:ILE:HD12	2.22	0.54
2:D:46:PRO:HA	2:D:76:HIS:CG	2.41	0.54
1:E:652:ARG:NH2	1:E:667:ASP:OD2	2.40	0.54
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.88	0.54
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.22	0.54
2:B:46:PRO:O	2:B:242:PRO:HG3	2.06	0.54
2:D:285:LYS:HG3	2:D:314:PHE:CE1	2.42	0.54
1:A:28:TYR:O	1:A:32:GLN:HG3	2.07	0.54
1:C:992:ASN:ND2	1:C:996:GLU:HB3	2.23	0.54
1:E:897:PHE:HB3	11:E:4620:HOH:O	2.08	0.54
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.88	0.54
2:H:173:GLY:O	2:H:207:ARG:HG2	2.08	0.54
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.21	0.54
1:G:701:ALA:O	1:G:705:ALA:N	2.30	0.54
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.87	0.54
1:E:185:ARG:HG2	1:E:189:GLU:OE2	2.07	0.54
2:F:78:GLN:NE2	11:F:2502:HOH:O	2.33	0.54
1:G:540:THR:HG22	1:G:541:ALA:N	2.23	0.54
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.90	0.54
1:A:79:GLU:HB2	1:A:111:PHE:CZ	2.42	0.54
1:C:353:ASP:OD1	2:D:116:ARG:HD2	2.08	0.54
1:E:726:GLU:HG3	1:E:1020:ARG:HH21	1.72	0.54
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.37	0.54
1:E:703:GLU:O	1:E:706:LYS:HB2	2.07	0.54
1:G:181:ILE:HD11	1:G:376:THR:CG2	2.35	0.54
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.89	0.54
1:E:956[B]:ARG:HB3	1:E:1044:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:730:ASP:O	1:E:733:ASP:HB2	2.07	0.54
1:G:671:ARG:NH2	1:G:819:GLU:O	2.40	0.54
1:C:257:THR:HG23	2:D:91:ASN:ND2	2.23	0.54
1:C:670:ASP:CB	1:C:677:ARG:HH21	2.18	0.54
2:H:186:LYS:O	2:H:189:GLU:HB2	2.08	0.54
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.38	0.54
1:A:998:ARG:HG2	1:A:999:PRO:HA	1.90	0.54
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.08	0.54
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.08	0.54
1:E:710:TYR:HB3	1:E:729:TYR:O	2.08	0.54
1:E:802:SER:OG	1:E:805:ILE:HB	2.08	0.54
1:E:808:VAL:HA	1:E:811[B]:GLN:HG3	1.90	0.54
1:G:148:ILE:HG22	1:G:149:ALA:N	2.22	0.54
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.23	0.53
1:G:922:ARG:NH2	1:G:1060:GLU:OE2	2.41	0.53
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.42	0.53
1:C:237:PHE:HB3	1:C:248:ILE:O	2.07	0.53
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.43	0.53
2:D:355:GLU:N	2:D:355:GLU:OE2	2.37	0.53
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.90	0.53
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.07	0.53
1:A:362:PHE:CE1	1:A:380:SER:HB3	2.43	0.53
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.09	0.53
1:E:682:VAL:CG1	1:E:687:LEU:HB2	2.38	0.53
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.89	0.53
2:H:193:HIS:O	2:H:234:ASP:HB2	2.08	0.53
2:H:352:GLY:O	2:H:354:PRO:HD3	2.08	0.53
2:H:365:PRO:HA	2:H:368:ASP:OD1	2.08	0.53
1:E:1002:GLN:NE2	1:E:1006[B]:LYS:HZ2	2.05	0.53
2:F:272:HIS:HA	2:F:349:SER:CB	2.39	0.53
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.25	0.53
1:A:481:ILE:HG22	11:A:4626:HOH:O	2.08	0.53
1:A:695:VAL:HG11	1:A:701:ALA:N	2.23	0.53
2:B:105:HIS:ND1	11:B:4218:HOH:O	2.34	0.53
1:C:252:PRO:HD3	1:C:352:ILE:HD11	1.90	0.53
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.38	0.53
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.89	0.53
1:E:930:LYS:HE3	11:E:4218:HOH:O	2.09	0.53
1:G:475:LYS:NZ	11:G:3293:HOH:O	2.33	0.53
1:A:713:VAL:HG12	1:A:713:VAL:O	2.08	0.53
1:A:4:ARG:CD	1:A:7:ILE:HD12	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LEU:HD22	1:A:812:GLN:HG2	1.91	0.53
1:E:947:LEU:N	1:E:947:LEU:HD12	2.24	0.53
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.23	0.53
1:E:1:MET:H3	1:E:224:LYS:HE3	1.73	0.53
1:G:340:THR:O	1:G:343:ARG:HB2	2.09	0.53
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.31	0.53
2:H:46:PRO:HA	2:H:76:HIS:CG	2.43	0.53
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.24	0.53
1:C:695:VAL:HG11	1:C:701:ALA:CA	2.38	0.53
1:C:695:VAL:HG11	1:C:701:ALA:N	2.23	0.53
1:A:331:THR:O	1:A:334:GLU:HB2	2.09	0.53
1:A:734:LEU:C	1:A:734:LEU:HD12	2.25	0.53
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.44	0.53
1:C:676:GLU:O	1:C:680:HIS:ND1	2.42	0.53
2:H:156:MET:HG2	2:H:158:LEU:HG	1.91	0.53
1:G:1001:ILE:O	1:G:1005:ILE:HG13	2.08	0.52
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.19	0.52
2:B:41:GLU:N	2:B:41:GLU:OE2	2.36	0.52
1:C:762:VAL:HG13	1:C:779:MET:O	2.08	0.52
2:D:286:MET:HE2	2:D:314:PHE:C	2.30	0.52
1:E:103:GLU:HG2	11:E:4778:HOH:O	2.09	0.52
1:E:701:ALA:O	1:E:705:ALA:N	2.28	0.52
1:E:734:LEU:C	1:E:734:LEU:HD12	2.27	0.52
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.44	0.52
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.39	0.52
1:G:761:GLU:HG2	1:G:781:HIS:CE1	2.44	0.52
1:E:213:TRP:HZ3	1:E:296:ILE:HD12	1.74	0.52
1:G:151:THR:HG21	11:G:3075:HOH:O	2.09	0.52
1:A:659:VAL:CG1	1:A:660:PRO:HD2	2.39	0.52
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.90	0.52
1:C:805:ILE:HD13	1:C:837:VAL:CG2	2.40	0.52
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.44	0.52
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.75	0.52
2:F:324:ASN:HA	2:F:343:THR:OG1	2.10	0.52
1:G:993:LYS:NZ	11:G:3612:HOH:O	2.29	0.52
1:A:419:GLU:HG3	11:E:4704:HOH:O	2.10	0.52
1:C:110:GLU:HG2	1:C:111:PHE:CE1	2.44	0.52
2:D:156:MET:HA	11:D:1820:HOH:O	2.10	0.52
2:F:197:TYR:O	2:F:239:SER:HB3	2.10	0.52
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.28	0.52
1:G:158:VAL:O	1:G:161:ASP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:361:ARG:CZ	1:G:571:ARG:HG2	2.40	0.52
2:H:193:HIS:NE2	2:H:217:THR:OG1	2.27	0.52
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.22	0.52
2:F:205:ILE:HG12	2:F:355:GLU:CG	2.40	0.52
1:G:489:LEU:HD13	1:G:522:LEU:HD23	1.92	0.52
1:A:556:SER:HB2	1:A:558:ASP:HB2	1.92	0.52
1:A:986:ILE:O	1:A:988:PRO:HD3	2.10	0.52
2:D:272:HIS:HA	2:D:349:SER:HB2	1.90	0.52
2:H:168:TYR:CE2	2:H:218:ILE:HG12	2.44	0.52
2:H:264:PRO:HB3	2:H:373:LEU:HB3	1.91	0.52
2:D:246:ALA:HB3	2:D:247:PRO:CD	2.39	0.52
1:E:956[A]:ARG:HB3	1:E:1044:LEU:HD21	1.91	0.52
1:E:784:GLN:HE21	1:E:784:GLN:N	2.00	0.52
1:A:975:HIS:HE2	1:G:992:ASN:HD21	1.58	0.52
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.39	0.52
2:D:272:HIS:HA	2:D:349:SER:CB	2.40	0.52
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.45	0.52
1:G:79:GLU:HG2	1:G:111:PHE:CZ	2.45	0.52
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.25	0.52
1:A:975:HIS:HE2	1:G:992:ASN:ND2	2.08	0.52
1:A:349:GLU:O	2:B:294:ASN:HB2	2.10	0.51
1:C:695:VAL:CG2	1:C:752:LEU:HD22	2.40	0.51
2:B:27:VAL:O	2:B:78:GLN:HG2	2.10	0.51
1:E:1061:LYS:HE2	11:E:4658:HOH:O	2.09	0.51
1:G:950:ARG:HD3	11:G:3654:HOH:O	2.10	0.51
1:A:101:GLU:HA	1:A:101:GLU:OE2	2.11	0.51
1:C:997:GLY:O	1:C:998:ARG:HG3	2.10	0.51
1:G:1030:ARG:CG	1:G:1030:ARG:HH11	2.23	0.51
2:D:279:SER:O	2:D:322:PRO:HG3	2.09	0.51
2:F:279:SER:O	2:F:322:PRO:HG3	2.10	0.51
1:G:1:MET:N	1:G:224:LYS:HE3	2.25	0.51
1:G:18:ILE:HG23	1:G:23:ALA:HA	1.91	0.51
1:G:47:VAL:O	1:G:47:VAL:HG13	2.10	0.51
1:G:796:LEU:HD23	1:G:796:LEU:C	2.31	0.51
2:H:174:SER:HB2	2:H:211:ASP:OD2	2.10	0.51
1:C:673:GLU:O	1:C:675:ARG:NH1	2.43	0.51
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.75	0.51
1:E:966:LYS:O	1:E:966:LYS:HG3	2.10	0.51
2:B:249:ASP:HB3	11:B:4178:HOH:O	2.10	0.51
2:B:364:ALA:N	2:B:365:PRO:CD	2.73	0.51
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ASP:O	1:E:262:GLN:HG2	2.10	0.51
1:G:292:ASN:OD1	1:G:294:ARG:HB2	2.10	0.51
1:A:222:ARG:CZ	1:A:273:ARG:HG2	2.41	0.51
1:C:740:THR:O	1:C:741:ALA:O	2.29	0.51
1:E:1001:ILE:O	1:E:1005:ILE:HG13	2.11	0.51
1:E:3:LYS:HB2	1:E:42:TYR:OH	2.10	0.51
2:F:257:LYS:O	2:F:260:GLU:HB2	2.11	0.51
1:C:539:ASP:HB2	11:C:4614:HOH:O	2.09	0.51
1:E:1048:PHE:O	1:E:1052:MET:HG3	2.11	0.51
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.93	0.51
1:G:713:VAL:HG23	1:G:755:PHE:HB2	1.91	0.51
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.94	0.51
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.46	0.51
1:C:127:GLU:HB2	1:C:172:PHE:CZ	2.45	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.51
1:E:998:ARG:CG	1:E:999:PRO:HA	2.40	0.51
1:E:817:ALA:HB2	1:E:826:MET:SD	2.50	0.51
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.45	0.51
1:G:692:ASN:HA	1:G:752:LEU:O	2.11	0.51
2:H:158:LEU:HB3	2:H:242:PRO:HB2	1.92	0.51
2:B:66:ASN:HB3	2:B:93:ARG:O	2.12	0.50
1:C:669:ILE:HA	1:C:844:PRO:HG2	1.92	0.50
2:D:353:HIS:CE1	11:D:1634:HOH:O	2.64	0.50
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.29	0.50
1:E:62:ASP:OD2	11:E:4634:HOH:O	2.18	0.50
1:G:150:HIS:CD2	1:G:203:GLU:HB2	2.46	0.50
1:G:730:ASP:H	1:G:733:ASP:HB2	1.76	0.50
2:H:158:LEU:HB2	2:H:242:PRO:HB2	1.92	0.50
2:D:218:ILE:HD13	2:D:218:ILE:N	2.27	0.50
2:D:286:MET:CE	2:D:315:ALA:HB2	2.40	0.50
2:D:327:VAL:HG13	2:D:337:LEU:CD1	2.41	0.50
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.27	0.50
2:H:81:VAL:CG1	2:H:113:ILE:HD11	2.42	0.50
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.75	0.50
1:A:333:ASP:N	1:A:333:ASP:OD1	2.44	0.50
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.46	0.50
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.46	0.50
1:E:126:ALA:CB	1:E:302:PRO:HG3	2.39	0.50
1:G:361:ARG:NH2	1:G:571:ARG:HG2	2.27	0.50
2:H:250:TYR:CD2	2:H:250:TYR:N	2.79	0.50
2:H:6:LEU:HD12	2:H:7:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:O	1:A:474:GLU:HG3	2.11	0.50
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.41	0.50
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.11	0.50
1:C:726:GLU:CG	1:C:727:ILE:N	2.74	0.50
1:A:728:VAL:HG12	1:A:733:ASP:HB3	1.92	0.50
1:G:729:TYR:HE1	1:G:1019:GLY:HA2	1.76	0.50
1:G:698:ILE:O	1:G:701:ALA:HB3	2.12	0.50
1:A:11:LEU:HA	1:A:45:ILE:O	2.11	0.50
1:A:950:ARG:HD3	11:A:4711:HOH:O	2.11	0.50
1:C:11:LEU:HA	1:C:45:ILE:O	2.12	0.50
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.46	0.50
1:E:234:ILE:HG23	1:E:250:VAL:O	2.11	0.50
1:E:693:ALA:CB	1:E:708:ILE:HD11	2.42	0.50
1:C:562:ILE:HG21	1:C:589:LEU:CD1	2.42	0.50
1:E:393:GLU:HA	1:E:496:GLY:HA3	1.94	0.50
1:G:947:LEU:HG	1:G:1014:ILE:CG2	2.41	0.50
2:D:232:ASN:N	2:D:233:PRO:HD3	2.27	0.50
1:A:710:TYR:HB3	1:A:729:TYR:O	2.11	0.50
2:B:290:HIS:HB2	2:B:312:HIS:NE2	2.27	0.50
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.47	0.50
2:D:174:SER:HB2	2:D:211:ASP:OD2	2.12	0.50
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.47	0.50
1:E:808:VAL:O	1:E:811[B]:GLN:HG3	2.11	0.50
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.93	0.50
1:G:294:ARG:HD2	5:G:4083:CL:CL	2.49	0.50
2:H:324:ASN:N	2:H:324:ASN:ND2	2.58	0.50
1:A:1001:ILE:O	1:A:1005:ILE:HG13	2.12	0.49
1:A:417:ASP:OD1	1:A:423:LYS:NZ	2.35	0.49
1:A:704:LYS:O	1:A:707:GLU:HB2	2.11	0.49
2:D:370:PHE:O	2:D:374:ILE:HG13	2.12	0.49
1:E:358:LYS:HG2	1:E:359:ILE:N	2.26	0.49
2:F:32:PHE:O	2:F:291:HIS:HB2	2.11	0.49
2:H:16:HIS:O	2:H:113:ILE:HG22	2.12	0.49
2:B:290:HIS:HB2	2:B:312:HIS:CD2	2.47	0.49
1:C:288:VAL:O	1:C:290:PRO:HD3	2.12	0.49
1:C:713:VAL:O	1:C:713:VAL:HG12	2.12	0.49
2:D:324:ASN:ND2	2:D:324:ASN:H	2.06	0.49
1:E:67:GLU:HB3	1:E:68:PRO:HD2	1.94	0.49
1:G:103:GLU:HG3	1:G:104:ARG:N	2.19	0.49
1:G:636:LYS:HD3	11:G:3354:HOH:O	2.11	0.49
1:A:947:LEU:N	1:A:947:LEU:CD1	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:SER:HB2	2:F:211:ASP:OD2	2.12	0.49
2:F:322:PRO:HD2	2:F:325:LEU:HD12	1.93	0.49
1:G:167:ILE:CD1	1:G:167:ILE:N	2.75	0.49
2:F:376:GLN:O	2:F:376:GLN:HG2	2.08	0.49
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.47	0.49
1:C:972:ASP:OD2	1:C:991[B]:VAL:HG21	2.12	0.49
2:B:270:LEU:HA	2:B:273:GLN:OE1	2.13	0.49
2:F:249:ASP:OD2	2:F:250:TYR:N	2.45	0.49
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.47	0.49
1:G:1021:ARG:NH1	1:G:1021:ARG:HG2	2.16	0.49
1:G:1005:ILE:HG21	1:G:1032:SER:HB3	1.93	0.49
1:G:434:ASP:HB2	11:G:3231:HOH:O	2.12	0.49
1:A:278:GLU:HG2	11:A:4597:HOH:O	2.13	0.49
2:B:245:PRO:HG3	2:B:273:GLN:OE1	2.13	0.49
1:C:802:SER:OG	1:C:805:ILE:HB	2.13	0.49
1:E:738:PHE:O	1:E:741:ALA:HB3	2.12	0.49
2:F:269:SER:O	2:F:272:HIS:HB3	2.13	0.49
1:G:56:THR:OG1	1:G:855:LYS:NZ	2.34	0.49
1:C:130:ARG:HG3	1:C:148:ILE:HG13	1.95	0.49
1:E:1020:ARG:HD3	1:E:1020:ARG:HA	1.46	0.49
1:G:441:ASP:OD2	1:G:444:ARG:NH1	2.44	0.49
1:A:106:GLY:HA2	11:A:4176:HOH:O	2.13	0.49
1:A:981:LEU:CD1	1:A:988:PRO:HG3	2.43	0.49
1:C:110:GLU:HG2	1:C:111:PHE:CD1	2.48	0.49
1:C:534:ALA:HB2	2:D:116:ARG:NH1	2.27	0.49
2:H:153:LEU:HA	2:H:156:MET:HE3	1.95	0.49
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.47	0.49
1:C:805:ILE:CD1	1:C:837:VAL:HG23	2.43	0.49
1:E:760:VAL:HG11	1:E:801:LEU:HD11	1.94	0.49
1:G:1017:THR:HG22	1:G:1018:SER:N	2.28	0.49
1:G:298:ILE:HG13	11:G:3128:HOH:O	2.11	0.49
1:G:738:PHE:O	1:G:741:ALA:HB3	2.13	0.49
1:G:951:GLU:HA	1:G:954:LYS:HD2	1.94	0.49
1:G:967:GLN:HG3	1:G:1054:LEU:HD13	1.95	0.49
2:D:212:ARG:CG	2:D:212:ARG:HH11	2.25	0.48
2:H:48:TYR:O	2:H:51:GLN:HB2	2.12	0.48
1:A:665:SER:O	1:A:669:ILE:HG13	2.12	0.48
1:G:710:TYR:HB3	1:G:729:TYR:O	2.12	0.48
1:E:493:LYS:HE2	1:E:517:ARG:HD3	1.95	0.48
1:A:562:ILE:HG21	1:A:589:LEU:HD12	1.94	0.48
1:A:726:GLU:CG	1:A:727:ILE:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:ALA:HB3	2:B:218:ILE:HD12	1.94	0.48
1:C:18:ILE:HG23	1:C:23:ALA:HA	1.95	0.48
1:E:349:GLU:O	2:F:294:ASN:HB2	2.13	0.48
2:F:275:LEU:HD23	2:F:349:SER:OG	2.13	0.48
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.94	0.48
2:H:176:THR:O	2:H:180:GLY:N	2.40	0.48
1:A:558:ASP:HB3	1:A:559:ARG:H	1.38	0.48
1:C:240:MET:HE2	1:C:287:ALA:HB2	1.96	0.48
2:F:48:TYR:HA	2:F:51:GLN:NE2	2.28	0.48
1:G:67:GLU:HB3	1:G:68:PRO:HD2	1.94	0.48
1:G:734:LEU:HD12	1:G:734:LEU:C	2.30	0.48
1:G:830:PHE:CE1	1:G:839:LEU:HD13	2.48	0.48
1:C:209:SER:OG	1:C:211:ILE:HG13	2.14	0.48
2:F:125:LYS:NZ	11:F:2862:HOH:O	2.46	0.48
2:F:201:ALA:CB	2:F:239:SER:HB2	2.38	0.48
1:E:347:SER:O	2:F:296:PRO:HB3	2.14	0.48
1:A:954:LYS:O	1:A:980:VAL:HG11	2.14	0.48
1:A:972:ASP:OD1	1:A:989:ARG:HB3	2.14	0.48
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.48	0.48
1:E:671:ARG:NH2	1:E:819:GLU:O	2.47	0.48
2:F:34:THR:HA	2:F:56:THR:OG1	2.13	0.48
1:G:726:GLU:CG	1:G:727:ILE:N	2.77	0.48
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.49	0.48
1:A:167:ILE:CD1	1:A:167:ILE:N	2.77	0.48
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.29	0.48
1:C:993:LYS:O	1:C:1000:HIS:HB3	2.14	0.48
1:G:240:MET:HE3	7:G:4068:ADP:C4	2.49	0.48
1:G:579:ASP:OD1	1:G:605:THR:HB	2.14	0.48
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.43	0.48
1:A:891:LYS:NZ	11:A:4492:HOH:O	2.47	0.48
1:C:698:ILE:O	1:C:702:VAL:HG23	2.14	0.48
2:D:269:SER:O	2:D:272:HIS:HB3	2.14	0.48
1:E:170:PRO:HA	1:E:204:LEU:HD23	1.95	0.48
1:E:448:SER:O	1:E:452:VAL:HG23	2.14	0.48
2:F:286:MET:HE1	2:F:312:HIS:O	2.13	0.48
1:G:1:MET:H1	1:G:224:LYS:HE3	1.79	0.48
1:G:679:GLN:HG2	1:G:689:GLN:NE2	2.28	0.48
2:H:218:ILE:N	2:H:218:ILE:CD1	2.75	0.48
1:A:467:GLU:O	1:A:471:ARG:HG2	2.14	0.48
1:A:525:VAL:HG22	1:A:548:GLU:H	1.79	0.48
1:C:4:ARG:CD	1:C:7:ILE:HD12	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:LEU:HD23	2:D:15:PHE:CD2	2.49	0.48
2:D:85:LEU:HD12	2:D:86:PRO:HD2	1.95	0.48
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.50	0.48
1:E:804:GLU:O	1:E:808:VAL:HG23	2.14	0.48
1:G:956:ARG:HB3	1:G:1044:LEU:HD21	1.96	0.48
1:A:89:THR:O	1:A:304:VAL:HG22	2.14	0.47
2:B:173:GLY:O	2:B:207:ARG:HG2	2.14	0.47
2:B:232:ASN:N	2:B:233:PRO:HD3	2.30	0.47
1:E:726:GLU:CG	1:E:727:ILE:N	2.77	0.47
2:F:322:PRO:HB2	2:F:324:ASN:HD22	1.77	0.47
1:G:805:ILE:HD12	1:G:832:VAL:CG1	2.43	0.47
2:H:322:PRO:CB	2:H:324:ASN:HD21	2.24	0.47
1:A:17:PRO:HG3	1:A:917:VAL:HG13	1.95	0.47
1:C:668:ALA:O	1:C:671:ARG:HB2	2.15	0.47
1:C:703:GLU:HA	1:C:703:GLU:OE2	2.14	0.47
1:C:973:ALA:C	1:C:991[A]:VAL:HG12	2.33	0.47
1:G:738:PHE:HA	1:G:741:ALA:HB3	1.96	0.47
1:A:1:MET:HB2	1:A:224:LYS:NZ	2.29	0.47
1:A:730:ASP:H	1:A:733:ASP:HB2	1.77	0.47
1:E:278:GLU:HG2	11:E:4235:HOH:O	2.14	0.47
1:E:525:VAL:HG22	1:E:548:GLU:H	1.78	0.47
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.50	0.47
1:A:224:LYS:HE2	1:A:329:GLY:O	2.14	0.47
1:A:82:ARG:NH1	1:A:82:ARG:HG3	2.30	0.47
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.32	0.47
2:F:106:ASN:ND2	11:F:2545:HOH:O	2.47	0.47
2:F:164:THR:O	2:F:220:PRO:HB3	2.15	0.47
1:G:423:LYS:HB3	11:G:3274:HOH:O	2.14	0.47
1:A:951:GLU:HA	1:A:954:LYS:HD2	1.96	0.47
1:A:998:ARG:HA	1:A:999:PRO:C	2.32	0.47
2:B:205:ILE:O	2:B:209:LEU:HG	2.15	0.47
2:B:222:GLN:HA	2:B:250:TYR:CD1	2.50	0.47
1:C:992:ASN:O	1:C:1000:HIS:HA	2.14	0.47
1:C:865:ALA:O	1:C:869:MET:HG3	2.13	0.47
1:G:906:LEU:O	1:G:912:ARG:NH2	2.31	0.47
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.97	0.47
1:C:1000:HIS:H	1:C:1000:HIS:CD2	2.33	0.47
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.50	0.47
1:C:704:LYS:HD2	1:C:707:GLU:OE1	2.14	0.47
1:C:737:TYR:O	1:C:741:ALA:HB2	2.15	0.47
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8:VAL:HG12	2:H:9:LEU:N	2.29	0.47
1:A:693:ALA:HB2	1:A:708:ILE:HD11	1.96	0.47
1:A:734:LEU:CD1	1:A:738:PHE:CE2	2.98	0.47
2:F:259:LEU:O	2:F:345:LYS:HE2	2.15	0.47
1:G:1017:THR:CG2	1:G:1018:SER:N	2.77	0.47
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.22	0.47
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.95	0.47
1:C:167:ILE:HG13	1:C:181:ILE:HG12	1.96	0.47
1:E:1017:THR:CG2	1:E:1023:ILE:HG13	2.43	0.47
1:E:698:ILE:CD1	1:E:698:ILE:N	2.77	0.47
1:E:841:GLU:HB2	11:E:4625:HOH:O	2.15	0.47
2:F:236:ILE:O	2:F:265:VAL:HA	2.15	0.47
1:G:224:LYS:HE2	1:G:329:GLY:O	2.14	0.47
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.45	0.47
1:G:863:LYS:O	1:G:867:ARG:HG3	2.14	0.47
2:H:322:PRO:HD2	2:H:325:LEU:HD12	1.97	0.47
1:A:184:ASN:O	1:A:188:PHE:HB2	2.15	0.47
1:A:772:MET:CE	1:A:880:THR:HA	2.44	0.47
1:C:294:ARG:HD2	5:C:4038:CL:CL	2.51	0.47
1:C:64:THR:O	1:C:1065:VAL:HG23	2.14	0.47
1:C:986:ILE:O	1:C:988:PRO:HD3	2.14	0.47
2:F:244:ASP:OD2	2:F:245:PRO:HD2	2.14	0.47
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.45	0.47
1:A:698:ILE:O	1:A:702:VAL:HG23	2.15	0.47
1:C:130:ARG:HB2	1:C:148:ILE:HD12	1.95	0.47
1:E:500:ALA:O	1:E:504:LYS:HG3	2.15	0.47
2:F:26:ALA:O	2:F:131:CYS:HA	2.15	0.47
1:A:1021:ARG:HG2	1:A:1021:ARG:HH11	1.80	0.47
1:C:74:VAL:CG1	1:C:102:LEU:HD11	2.42	0.47
1:C:808:VAL:HA	1:C:811[B]:GLN:OE1	2.14	0.47
2:D:118:LEU:C	2:D:118:LEU:HD12	2.36	0.47
1:E:904:ASP:O	1:E:906:LEU:N	2.45	0.47
2:F:83:ARG:O	2:F:112:ASP:HA	2.15	0.47
1:G:11:LEU:HA	1:G:45:ILE:O	2.14	0.47
1:A:24:CYS:SG	1:A:576:ILE:HB	2.55	0.46
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.39	0.46
1:E:1017:THR:HG21	1:E:1023:ILE:HA	1.97	0.46
1:E:458:ILE:O	1:E:463:LEU:HD11	2.15	0.46
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.28	0.46
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.53	0.46
2:H:40:GLN:HE21	2:H:70:GLU:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:OE2	1:A:604:GLU:OE1	2.34	0.46
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.51	0.46
1:C:318:PRO:HB2	1:C:321:LYS:HB2	1.97	0.46
1:E:1017:THR:HG22	1:E:1018:SER:N	2.30	0.46
2:F:55:LEU:HD13	2:F:60:ILE:HD12	1.97	0.46
1:G:277:VAL:HG12	1:G:277:VAL:O	2.15	0.46
2:H:45:ASP:HB3	2:H:48:TYR:HD2	1.80	0.46
1:A:469:LEU:O	1:A:473:GLU:HG3	2.15	0.46
1:A:9:SER:OG	1:A:83:PRO:HA	2.16	0.46
2:D:173:GLY:O	2:D:207:ARG:HG2	2.15	0.46
2:D:286:MET:HE1	2:D:315:ALA:HB2	1.97	0.46
1:E:678:PHE:O	1:E:681:ALA:N	2.48	0.46
1:G:148:ILE:CG2	1:G:149:ALA:N	2.78	0.46
2:H:325:LEU:HA	2:H:325:LEU:HD23	1.68	0.46
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.40	0.46
1:C:733:ASP:OD1	1:C:736:ARG:NH1	2.48	0.46
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.69	0.46
1:E:734:LEU:O	1:E:737:TYR:HB3	2.14	0.46
2:H:144:LEU:O	2:H:144:LEU:HD12	2.16	0.46
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.97	0.46
2:B:121:LEU:O	2:B:121:LEU:HD12	2.15	0.46
1:C:166:CYS:C	1:C:167:ILE:HD12	2.35	0.46
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.16	0.46
1:C:66:ILE:CG2	1:C:918:MET:HB3	2.45	0.46
1:C:51:PRO:HG3	1:C:918:MET:HB2	1.97	0.46
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.49	0.46
1:G:939:MET:HE1	1:G:1050:THR:HG21	1.97	0.46
1:G:702:VAL:O	1:G:706:LYS:HD3	2.15	0.46
10:C:4036:NET:H71	10:C:4036:NET:H23	1.62	0.46
1:C:885:PRO:HG2	11:C:4735:HOH:O	2.16	0.46
1:C:990:LEU:HD13	1:E:990:LEU:HD22	1.98	0.46
2:D:201:ALA:HB2	2:D:239:SER:CB	2.46	0.46
2:D:45:ASP:HB3	2:D:48:TYR:HD2	1.80	0.46
1:E:735:ARG:O	1:E:738:PHE:HB2	2.16	0.46
1:G:598:MET:HG3	1:G:599:VAL:N	2.31	0.46
1:G:874:LEU:HB3	1:G:879:VAL:O	2.16	0.46
2:H:286:MET:HB3	2:H:286:MET:HE2	1.83	0.46
1:C:365:GLU:HG3	1:C:365:GLU:H	1.04	0.46
1:C:77:ILE:O	1:C:81:GLU:N	2.43	0.46
1:E:1017:THR:CG2	1:E:1018:SER:N	2.78	0.46
1:E:412:LYS:HG2	1:E:438:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:PRO:HA	2:F:76:HIS:CG	2.50	0.46
2:H:249:ASP:HB3	11:H:3526:HOH:O	2.14	0.46
2:H:300:VAL:HG22	2:H:328:THR:O	2.16	0.46
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.60	0.46
1:G:53:THR:OG1	1:G:56:THR:HG23	2.16	0.46
1:G:648:LEU:CD2	1:G:845:ARG:HD3	2.45	0.46
1:A:840:ILE:O	1:A:841:GLU:HB3	2.14	0.46
2:B:185:LYS:CD	2:B:190:LEU:HD21	2.46	0.46
1:C:130:ARG:HB2	1:C:148:ILE:CD1	2.45	0.46
1:G:1052:MET:O	1:G:1055:ASN:HB2	2.16	0.46
1:G:315:THR:O	1:G:531:THR:HG22	2.15	0.46
1:A:38[B]:ARG:CG	1:A:38[B]:ARG:HH11	2.20	0.46
1:A:764:VAL:HG11	1:A:813:VAL:HG21	1.97	0.46
1:A:814:GLN:NE2	11:A:4511:HOH:O	2.48	0.46
2:B:241:GLY:N	9:B:4012:GLN:OE1	2.39	0.46
1:C:710:TYR:HB3	1:C:729:TYR:O	2.15	0.46
2:D:286:MET:HE1	2:D:312:HIS:CE1	2.51	0.46
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.45	0.46
2:H:222:GLN:HA	2:H:250:TYR:CD1	2.51	0.46
1:C:1021:ARG:HH11	1:C:1021:ARG:CG	2.28	0.45
1:C:118:ALA:HA	11:C:4198:HOH:O	2.16	0.45
1:C:186:GLU:N	11:C:4608:HOH:O	2.43	0.45
1:C:655:GLU:CD	1:C:666:PRO:HG2	2.36	0.45
1:E:146:SER:HB3	1:E:207:ASP:OD1	2.15	0.45
1:A:336[A]:MET:HB3	1:A:342:GLY:HA2	1.98	0.45
2:B:266:PHE:HB2	2:B:370:PHE:CD1	2.50	0.45
2:B:6:LEU:HD23	2:B:138:PRO:HB2	1.97	0.45
1:C:479:VAL:HG23	1:C:480:GLY:O	2.16	0.45
2:F:379:LYS:NZ	2:F:379:LYS:HB2	2.31	0.45
1:G:250:VAL:HA	1:G:356:VAL:O	2.16	0.45
1:G:475:LYS:CE	11:G:3293:HOH:O	2.64	0.45
1:G:726:GLU:HG3	1:G:727:ILE:N	2.30	0.45
2:H:208:MET:SD	2:H:355:GLU:HA	2.56	0.45
2:H:313:GLY:HA3	11:H:2933:HOH:O	2.15	0.45
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.45
1:A:32:GLN:OE1	1:A:320:ALA:HB3	2.16	0.45
1:E:400:ARG:HD3	11:E:4438:HOH:O	2.17	0.45
1:E:679:GLN:O	1:E:683:GLU:HB2	2.16	0.45
1:G:294:ARG:NH1	5:G:4083:CL:CL	2.86	0.45
1:G:550:GLU:CD	2:H:120:ARG:HH21	2.19	0.45
1:C:715:ARG:HB2	1:C:751:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:CD1	1:C:837:VAL:CG2	2.94	0.45
1:C:975:HIS:HE2	1:E:992:ASN:HD21	1.63	0.45
2:D:298:LYS:O	2:D:329:HIS:HA	2.17	0.45
2:F:169:SER:HA	2:F:216:LEU:O	2.16	0.45
1:G:540:THR:CG2	1:G:541:ALA:N	2.78	0.45
1:G:559:ARG:HG3	1:G:559:ARG:HH11	1.81	0.45
1:G:833:LYS:O	1:G:836:GLU:HB2	2.15	0.45
1:A:1:MET:HB2	1:A:224:LYS:HZ2	1.81	0.45
1:A:384:VAL:HG22	1:A:385:MET:N	2.32	0.45
1:E:953:ASP:O	1:E:955:GLU:N	2.50	0.45
1:E:956[B]:ARG:HB3	1:E:1044:LEU:HD21	1.96	0.45
2:F:46:PRO:O	2:F:242:PRO:HG3	2.16	0.45
1:A:671:ARG:HG2	1:A:677:ARG:NH1	2.32	0.45
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.82	0.45
2:B:142:LEU:O	2:B:145:GLU:HB3	2.17	0.45
1:C:186:GLU:HB2	11:C:4608:HOH:O	2.16	0.45
1:C:698:ILE:N	1:C:698:ILE:CD1	2.79	0.45
1:C:86:VAL:HG13	1:C:86:VAL:O	2.15	0.45
2:D:298:LYS:HE2	2:D:303:ASN:OD1	2.16	0.45
2:D:39:TYR:CZ	2:D:61:GLY:HA2	2.51	0.45
1:E:669:ILE:HA	1:E:844:PRO:HG2	1.98	0.45
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.81	0.45
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.82	0.45
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.69	0.45
1:A:633:GLU:O	1:A:634:LYS:HB2	2.17	0.45
2:F:23:THR:HG23	2:F:134:ALA:O	2.16	0.45
1:G:40:GLU:HG2	1:G:325:LYS:HE2	1.98	0.45
1:G:475:LYS:HE3	11:G:3293:HOH:O	2.15	0.45
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.52	0.45
2:B:324:ASN:N	2:B:324:ASN:ND2	2.39	0.45
1:E:157:ALA:HA	11:E:4288:HOH:O	2.16	0.45
1:E:612:THR:O	1:E:612:THR:HG22	2.16	0.45
2:F:270:LEU:HB2	9:F:4056:GLN:HG2	1.98	0.45
2:F:53:VAL:O	2:F:80:LEU:HD12	2.16	0.45
1:A:250:VAL:HA	1:A:356:VAL:O	2.17	0.45
2:B:232:ASN:N	2:B:233:PRO:CD	2.80	0.45
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.52	0.45
2:D:165:ALA:HB3	11:D:1800:HOH:O	2.17	0.45
1:E:167:ILE:CD1	1:E:167:ILE:N	2.80	0.45
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.98	0.45
1:A:38[A]:ARG:HH11	1:A:38[A]:ARG:CG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:ARG:CG	1:A:999:PRO:HA	2.46	0.45
2:B:321:LEU:HD21	2:B:337:LEU:HD21	1.99	0.45
2:B:367:PHE:O	2:B:370:PHE:HB3	2.17	0.45
1:C:456:THR:O	1:C:457:ASN:HB2	2.16	0.45
2:D:2:ILE:HD12	2:D:3:LYS:H	1.81	0.45
2:D:2:ILE:HD12	2:D:3:LYS:N	2.32	0.45
1:E:704:LYS:O	1:E:707:GLU:HB2	2.17	0.45
1:E:995:HIS:CD2	1:E:995:HIS:H	2.33	0.45
1:G:301:ASN:HA	1:G:302:PRO:HD3	1.87	0.45
1:G:820:LEU:O	1:G:821:GLN:HB2	2.17	0.45
2:H:275:LEU:O	2:H:275:LEU:HD12	2.17	0.45
2:H:202:LYS:NZ	2:H:355:GLU:OE1	2.30	0.45
1:A:509:ARG:O	1:A:512:GLU:HB2	2.16	0.44
1:C:213:TRP:HH2	1:C:294:ARG:HD3	1.82	0.44
1:C:325:LYS:O	1:C:330:TYR:HB2	2.16	0.44
1:E:1:MET:HB2	1:E:224:LYS:HZ1	1.81	0.44
1:E:215:GLU:OE1	7:E:4045:ADP:O3'	2.31	0.44
2:F:185:LYS:HD2	2:F:190:LEU:HD21	1.99	0.44
1:G:473[B]:GLU:OE1	1:G:501:ARG:NH2	2.43	0.44
1:G:698:ILE:CD1	1:G:698:ILE:H	2.29	0.44
2:H:240:ASN:HB2	9:H:4079:GLN:OE1	2.16	0.44
2:D:286:MET:HE1	2:D:312:HIS:ND1	2.31	0.44
1:E:176:GLY:N	7:E:4045:ADP:O2B	2.43	0.44
1:E:503:ALA:HB1	1:E:508:VAL:O	2.18	0.44
2:F:218:ILE:N	2:F:218:ILE:CD1	2.79	0.44
2:F:5:ALA:HB2	2:F:19:ALA:HB2	2.00	0.44
2:H:253:THR:O	2:H:256:GLN:HB2	2.17	0.44
2:B:344:ASP:OD2	2:B:344:ASP:N	2.39	0.44
7:C:4029:ADP:H5'2	11:C:4571:HOH:O	2.17	0.44
2:D:327:VAL:HG23	11:D:1624:HOH:O	2.16	0.44
1:E:805:ILE:CD1	1:E:837:VAL:CG2	2.95	0.44
1:G:79:GLU:CG	1:G:111:PHE:CZ	3.00	0.44
1:G:632:ILE:HG13	1:G:633:GLU:N	2.32	0.44
1:G:693:ALA:HB3	1:G:708:ILE:HD11	1.98	0.44
1:G:87:LEU:HD12	1:G:87:LEU:HA	1.66	0.44
1:G:882:GLU:HB3	11:G:3372:HOH:O	2.16	0.44
2:H:196:ALA:HA	2:H:237:PHE:O	2.17	0.44
2:H:71:GLU:C	2:H:203:ARG:HG3	2.37	0.44
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.50	0.44
1:A:1021:ARG:HG3	1:A:1021:ARG:HH11	1.82	0.44
1:A:730:ASP:O	1:A:733:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:948:SER:O	1:C:1015:ASN:HA	2.17	0.44
1:C:994:VAL:HG23	11:C:4748:HOH:O	2.17	0.44
1:E:157:ALA:O	1:E:160:ALA:HB3	2.18	0.44
1:E:384:VAL:HG22	1:E:385:MET:N	2.32	0.44
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.16	0.44
1:E:750:VAL:O	1:E:750:VAL:HG12	2.17	0.44
1:G:150:HIS:HD2	1:G:203:GLU:HB2	1.82	0.44
1:G:683:GLU:HA	1:G:683:GLU:OE2	2.15	0.44
1:G:76:LYS:HA	1:G:76:LYS:HD2	1.71	0.44
1:C:559:ARG:NH1	1:C:559:ARG:HG3	2.31	0.44
1:C:998:ARG:CB	1:C:999:PRO:HA	2.46	0.44
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.53	0.44
2:D:226:GLU:O	2:D:230:LYS:HG3	2.17	0.44
1:G:675:ARG:CD	1:G:675:ARG:H	2.28	0.44
1:A:220:VAL:O	1:A:281:GLY:HA2	2.17	0.44
1:E:283:ASN:HB2	11:E:4666:HOH:O	2.17	0.44
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.43	0.44
1:G:784:GLN:N	1:G:784:GLN:NE2	2.40	0.44
1:A:129:ARG:HB3	1:A:205:LEU:HD22	1.99	0.44
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.98	0.44
1:A:602:ASN:CG	1:A:605:THR:HG23	2.38	0.44
2:B:102:LEU:HD23	2:B:102:LEU:HA	1.74	0.44
2:B:334:ASP:CG	2:B:336:THR:HG23	2.38	0.44
1:C:675:ARG:HD3	1:C:675:ARG:H	1.83	0.44
1:C:831:ALA:HB2	1:C:840:ILE:HD11	1.99	0.44
1:G:654:LEU:HD22	1:G:659:VAL:HG21	1.98	0.44
1:G:726:GLU:HG3	1:G:727:ILE:H	1.83	0.44
2:H:374:ILE:O	2:H:377:TYR:HB3	2.18	0.44
1:A:675:ARG:HG3	1:A:751:LEU:HD21	1.98	0.44
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.82	0.44
1:C:358:LYS:HG2	1:C:359:ILE:N	2.32	0.44
2:F:199:PHE:O	2:F:241:GLY:HA3	2.18	0.44
2:B:13:THR:HG22	2:B:15:PHE:CE2	2.52	0.44
2:B:218:ILE:N	2:B:218:ILE:CD1	2.80	0.44
1:C:158:VAL:HG11	1:C:206:ILE:HB	1.99	0.44
1:C:666:PRO:O	1:C:669:ILE:HB	2.18	0.44
1:C:671:ARG:NH2	1:C:819:GLU:O	2.51	0.44
1:C:686:LYS:O	1:C:687:LEU:HD23	2.18	0.44
1:E:903:VAL:O	1:E:905:PRO:HD3	2.18	0.44
1:G:563:MET:HB3	1:G:638:VAL:HG22	1.99	0.44
1:G:946:LEU:HB3	1:G:1013:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:994:VAL:HG13	1:G:1000:HIS:CE1	2.53	0.44
2:B:199:PHE:O	2:B:241:GLY:HA3	2.18	0.43
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.48	0.43
2:B:265:VAL:O	2:B:347:ALA:HA	2.18	0.43
1:C:772:MET:SD	1:C:880:THR:HG22	2.57	0.43
1:C:775:ILE:HG13	1:C:810:ARG:HG2	2.00	0.43
1:E:148:ILE:CG2	1:E:149:ALA:N	2.81	0.43
1:E:57:ASP:HA	1:E:58:PRO:HD3	1.79	0.43
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.81	0.43
2:F:373:LEU:HD23	2:F:373:LEU:HA	1.78	0.43
1:G:947:LEU:N	1:G:947:LEU:HD12	2.33	0.43
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.45	0.43
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.99	0.43
1:A:612:THR:HG22	1:A:612:THR:O	2.18	0.43
1:C:384:VAL:HB	1:C:569:PRO:HG3	1.99	0.43
10:E:4058:NET:H63	10:E:4058:NET:H31	1.53	0.43
1:E:515:LYS:HD3	1:E:515:LYS:C	2.38	0.43
1:E:686:LYS:C	1:E:687:LEU:HD23	2.38	0.43
1:E:713:VAL:HG12	1:E:713:VAL:O	2.17	0.43
1:E:808:VAL:HG13	1:E:811[B]:GLN:NE2	2.32	0.43
1:G:1021:ARG:NH1	1:G:1021:ARG:CG	2.78	0.43
1:G:104:ARG:HB2	11:G:2906:HOH:O	2.18	0.43
1:G:308:SER:HB3	11:G:3571:HOH:O	2.17	0.43
2:H:279:SER:O	2:H:322:PRO:HG3	2.18	0.43
2:H:321:LEU:HD12	2:H:321:LEU:HA	1.78	0.43
1:C:920:VAL:O	1:C:930:LYS:HD3	2.18	0.43
1:E:385:MET:HG2	1:E:386:ALA:N	2.32	0.43
1:G:1001:ILE:HD13	1:G:1002:GLN:N	2.32	0.43
1:G:734:LEU:CD1	1:G:738:PHE:CD2	3.02	0.43
2:H:5:ALA:HB2	2:H:19:ALA:HB2	1.99	0.43
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.51	0.43
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.19	0.43
1:C:765:ASP:OD2	1:C:827:ASN:HB2	2.18	0.43
1:E:659:VAL:HG13	1:E:660:PRO:HD2	2.00	0.43
1:A:479:VAL:CG2	1:A:483:GLY:HA3	2.49	0.43
1:A:828:VAL:CG1	1:A:839:LEU:HD11	2.49	0.43
1:E:1:MET:CB	1:E:224:LYS:NZ	2.76	0.43
2:F:205:ILE:HG12	2:F:355:GLU:HG3	2.00	0.43
1:G:358:LYS:HG2	1:G:359:ILE:N	2.31	0.43
1:G:456:THR:O	1:G:457:ASN:HB2	2.18	0.43
1:G:965:LEU:HA	1:G:965:LEU:HD23	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ILE:HA	2:B:258:PHE:HD2	1.84	0.43
1:C:1063:ILE:CD1	1:C:1068:MET:CG	2.93	0.43
1:C:895:LEU:HA	1:C:896:PRO:HD3	1.83	0.43
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.99	0.43
1:E:472:LEU:O	1:E:476:VAL:HG23	2.19	0.43
2:F:163:THR:OG1	2:F:164:THR:N	2.50	0.43
1:G:385:MET:HG3	1:G:386:ALA:N	2.34	0.43
1:G:24:CYS:HB2	1:G:604:GLU:HB3	2.00	0.43
2:H:17:GLY:HA3	2:H:110:ILE:HD11	2.01	0.43
1:A:671:ARG:CG	1:A:677:ARG:NH1	2.81	0.43
1:A:793:ALA:HA	1:A:891:LYS:O	2.19	0.43
2:B:324:ASN:HA	2:B:343:THR:OG1	2.18	0.43
2:B:350:PHE:CB	2:B:366:LEU:HD22	2.47	0.43
1:C:1061:LYS:HD3	11:C:4585:HOH:O	2.18	0.43
2:D:376:GLN:HA	2:D:379:LYS:NZ	2.33	0.43
1:E:735:ARG:O	1:E:738:PHE:N	2.51	0.43
1:G:509:ARG:HB2	1:G:509:ARG:NH1	2.32	0.43
1:A:38[B]:ARG:CG	1:A:38[B]:ARG:NH1	2.80	0.43
1:A:682:VAL:HG11	1:A:689:GLN:NE2	2.32	0.43
1:A:954:LYS:HB3	1:A:980:VAL:HG11	2.01	0.43
2:B:249:ASP:HA	2:B:252:ILE:HD12	2.00	0.43
2:B:269:SER:OG	9:B:4012:GLN:HG2	2.18	0.43
1:E:579:ASP:OD1	1:E:605:THR:HB	2.19	0.43
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.01	0.43
1:G:1021:ARG:O	1:G:1025:ASP:OD2	2.36	0.43
1:G:1017:THR:HG22	1:G:1023:ILE:HG13	1.99	0.43
1:G:339:ILE:HD11	1:G:531:THR:HG23	2.00	0.43
1:G:588:ALA:O	1:G:591:GLU:HB3	2.19	0.43
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.48	0.43
1:C:167:ILE:N	1:C:167:ILE:HD12	2.33	0.43
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	1.99	0.43
7:E:4051:ADP:H5'2	11:E:4614:HOH:O	2.18	0.43
1:E:765:ASP:O	1:E:776:GLY:N	2.51	0.43
1:G:246:ASP:C	1:G:360:PRO:HG3	2.40	0.43
1:G:339:ILE:HD12	1:G:529:VAL:O	2.19	0.43
1:G:905:PRO:HG2	1:G:1030:ARG:HB3	2.00	0.43
1:G:944:ARG:NH1	1:G:972:ASP:OD1	2.52	0.43
2:H:28:GLY:HA2	2:H:150:PHE:CE2	2.54	0.43
2:D:259:LEU:HD13	2:D:342:ARG:HH12	1.82	0.43
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.54	0.43
2:F:102:LEU:HD23	2:F:102:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:370:ALA:HB2	1:G:900:PHE:HB3	2.00	0.43
1:G:695:VAL:HG11	1:G:701:ALA:N	2.34	0.43
1:G:733:ASP:HA	1:G:736:ARG:HH11	1.83	0.43
2:H:334:ASP:OD2	2:H:336:THR:HG23	2.19	0.43
2:H:66:ASN:HB3	2:H:93:ARG:O	2.18	0.43
1:A:267:ALA:O	1:A:271:VAL:HG23	2.19	0.42
1:A:426:ARG:C	1:A:426:ARG:HD3	2.40	0.42
1:A:738:PHE:O	1:A:741:ALA:HB3	2.19	0.42
2:D:178:THR:HG22	2:D:179:GLY:N	2.32	0.42
2:D:33:ASN:HA	2:D:291:HIS:O	2.18	0.42
1:E:456:THR:O	1:E:457:ASN:HB2	2.19	0.42
2:H:209:LEU:HD23	2:H:209:LEU:HA	1.79	0.42
2:D:186:LYS:H	2:D:189:GLU:CD	2.22	0.42
1:E:569:PRO:O	1:E:571:ARG:HD2	2.19	0.42
1:E:854:SER:HA	1:E:859:VAL:O	2.19	0.42
2:F:86:PRO:HA	11:F:2685:HOH:O	2.19	0.42
2:B:208:MET:O	2:B:211:ASP:HB2	2.19	0.42
1:C:677:ARG:O	1:C:680:HIS:HB2	2.19	0.42
1:C:778:ILE:HD11	1:C:810:ARG:HG3	2.02	0.42
1:E:1070:ALA:HB3	11:E:4646:HOH:O	2.19	0.42
1:E:548:GLU:HG2	2:F:114:ASP:HB2	2.01	0.42
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.93	0.42
2:H:373:LEU:HA	2:H:373:LEU:HD23	1.74	0.42
1:A:259:LYS:HD3	2:B:175:TRP:CZ3	2.55	0.42
1:C:1:MET:N	1:C:224:LYS:HE3	2.34	0.42
1:C:221:VAL:O	1:C:228:CYS:HA	2.19	0.42
1:C:493:LYS:HD2	1:C:493:LYS:HA	1.86	0.42
1:C:905:PRO:HB2	1:C:1040:TYR:HH	1.84	0.42
2:D:333:PHE:HA	2:D:333:PHE:HD1	1.77	0.42
1:E:808:VAL:CA	1:E:811[B]:GLN:HG3	2.49	0.42
1:E:534:ALA:HB1	2:F:120:ARG:HG2	2.01	0.42
2:F:196:ALA:HB3	2:F:218:ILE:HD12	2.01	0.42
1:G:267:ALA:O	1:G:271:VAL:HG23	2.19	0.42
1:G:915:GLY:HA2	11:G:2979:HOH:O	2.18	0.42
2:H:367:PHE:O	2:H:370:PHE:HB3	2.19	0.42
1:A:35:LYS:HD2	11:A:4141:HOH:O	2.19	0.42
1:A:868:VAL:HA	1:A:872:LYS:O	2.19	0.42
2:B:87:LEU:HA	2:B:87:LEU:HD12	1.72	0.42
2:D:208:MET:O	2:D:211:ASP:HB2	2.20	0.42
1:E:714:VAL:HG13	1:E:752:LEU:HD12	2.00	0.42
1:E:891:LYS:HG2	1:E:892:GLU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:940:LYS:HG3	1:E:1011:THR:HB	2.01	0.42
2:F:342:ARG:HD2	2:F:342:ARG:HA	1.92	0.42
1:G:1032:SER:O	1:G:1036:TYR:HD1	2.02	0.42
1:G:361:ARG:O	1:G:380:SER:HB2	2.19	0.42
1:G:402:LEU:O	1:G:403:GLU:HB2	2.19	0.42
1:G:482:THR:HG22	1:G:483:GLY:N	2.34	0.42
1:G:735:ARG:O	1:G:738:PHE:HB2	2.19	0.42
1:G:946:LEU:C	1:G:947:LEU:HD12	2.39	0.42
1:A:775:ILE:HA	1:A:775:ILE:HD13	1.86	0.42
1:C:730:ASP:H	1:C:733:ASP:HB2	1.84	0.42
2:D:325:LEU:HA	2:D:325:LEU:HD23	1.82	0.42
1:E:755:PHE:CE1	7:E:4051:ADP:C2	3.08	0.42
1:E:493:LYS:HD2	1:E:493:LYS:HA	1.78	0.42
2:F:66:ASN:OD1	2:F:68:ALA:HB3	2.19	0.42
1:G:170:PRO:HA	1:G:204:LEU:HD23	2.01	0.42
1:G:185:ARG:O	1:G:188:PHE:HB3	2.19	0.42
1:G:329:GLY:CA	11:G:2959:HOH:O	2.68	0.42
1:G:828:VAL:CG1	1:G:839:LEU:HD11	2.50	0.42
1:G:965:LEU:HG	1:G:971:LEU:HD11	2.02	0.42
1:A:548:GLU:OE1	2:B:83:ARG:HD3	2.19	0.42
1:A:981:LEU:HD12	1:A:988:PRO:HG3	2.02	0.42
1:E:217:GLU:HG2	1:E:285:GLN:HG2	2.01	0.42
2:F:91:ASN:OD1	2:F:93:ARG:HB2	2.19	0.42
1:A:336[B]:MET:HB3	1:A:342:GLY:HA2	2.02	0.42
1:C:257:THR:HG23	1:C:260:GLU:OE2	2.19	0.42
1:C:840:ILE:O	1:C:841:GLU:HB3	2.20	0.42
1:C:892:GLU:OE1	8:C:4033:ORN:NE	2.52	0.42
2:D:212:ARG:NH1	2:D:212:ARG:CG	2.78	0.42
1:E:85:ALA:HA	1:E:114:THR:O	2.20	0.42
2:F:46:PRO:HA	2:F:76:HIS:CB	2.50	0.42
1:G:987:ASN:HA	1:G:988:PRO:HD2	1.91	0.42
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.68	0.42
2:H:376:GLN:HG3	2:H:376:GLN:O	2.20	0.42
1:A:1021:ARG:NH1	1:A:1021:ARG:CG	2.80	0.42
1:E:248:ILE:HA	1:E:358:LYS:O	2.20	0.42
1:E:10:ILE:HD13	1:E:37:LEU:HD13	2.02	0.42
1:E:528:ARG:HG2	1:E:543:MET:HG2	2.01	0.42
1:G:453:PHE:C	1:G:453:PHE:CD1	2.92	0.42
1:A:313:LYS:HE2	1:A:608:THR:C	2.39	0.42
1:A:528:ARG:HG2	1:A:543:MET:HG2	2.02	0.42
1:C:1064:SER:OG	1:C:1067:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLU:CG	1:C:325:LYS:HE2	2.49	0.42
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.79	0.42
1:E:514:ARG:HD3	11:E:4483:HOH:O	2.20	0.42
1:G:48:ASN:O	1:G:66:ILE:HA	2.20	0.42
2:H:7:LEU:HD23	2:H:15:PHE:CD2	2.54	0.42
1:A:191:ILE:HG21	1:A:191:ILE:HD13	1.91	0.41
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.20	0.41
1:A:702:VAL:O	1:A:706:LYS:HD3	2.20	0.41
1:C:1064:SER:O	1:C:1068:MET:HG3	2.20	0.41
1:C:24:CYS:HB2	1:C:604:GLU:HB3	2.02	0.41
1:E:882:GLU:HB3	11:E:4757:HOH:O	2.19	0.41
2:F:228:VAL:HG11	2:F:258:PHE:CE1	2.55	0.41
2:F:286:MET:CE	2:F:312:HIS:ND1	2.83	0.41
1:G:752:LEU:HA	1:G:752:LEU:HD12	1.72	0.41
2:H:150:PHE:CE1	2:H:152:GLY:HA2	2.55	0.41
1:A:659:VAL:HG12	1:A:660:PRO:N	2.34	0.41
2:D:364:ALA:N	2:D:365:PRO:CD	2.83	0.41
1:E:765:ASP:OD2	1:E:827:ASN:HB2	2.20	0.41
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.83	0.41
1:G:145:ARG:HB2	1:G:208:GLU:CD	2.40	0.41
1:G:755:PHE:CD1	7:G:4074:ADP:C2	3.08	0.41
1:A:734:LEU:CD1	1:A:738:PHE:CD2	3.03	0.41
2:B:75:VAL:HG11	2:B:107:ILE:HG13	2.02	0.41
1:C:662:ILE:HG21	1:C:662:ILE:HD13	1.84	0.41
1:C:967:GLN:HG3	1:C:1054:LEU:CD1	2.45	0.41
2:D:163:THR:OG1	2:D:164:THR:N	2.54	0.41
1:E:489:LEU:HD12	1:E:489:LEU:HA	1.89	0.41
1:G:734:LEU:O	1:G:737:TYR:HB3	2.20	0.41
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.36	0.41
1:G:981:LEU:HD23	1:G:981:LEU:HA	1.87	0.41
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.55	0.41
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.36	0.41
1:A:654:LEU:HD22	1:A:659:VAL:HG21	2.02	0.41
1:A:796:LEU:C	1:A:796:LEU:HD23	2.40	0.41
1:A:946:LEU:C	1:A:947:LEU:HD12	2.41	0.41
2:B:240:ASN:HB2	9:B:4012:GLN:OE1	2.21	0.41
1:C:994:VAL:HG23	1:C:1001:ILE:HD11	2.01	0.41
2:D:172:GLN:O	2:D:207:ARG:HA	2.21	0.41
2:D:190:LEU:HB2	2:D:215:ARG:HB3	2.02	0.41
2:D:229:LEU:HA	2:D:229:LEU:HD23	1.82	0.41
1:E:726:GLU:HG3	1:E:727:ILE:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:726:GLU:OE1	1:G:1020:ARG:HD3	2.20	0.41
2:H:201:ALA:HB2	2:H:239:SER:CB	2.51	0.41
1:A:654:LEU:O	1:A:659:VAL:HG23	2.20	0.41
1:A:698:ILE:HG22	1:A:699:GLU:N	2.36	0.41
1:A:957:VAL:HG13	1:A:958:VAL:N	2.36	0.41
1:C:34:CYS:SG	1:C:46:LEU:HD22	2.60	0.41
1:C:4:ARG:NH1	11:C:4132:HOH:O	2.54	0.41
1:C:525:VAL:HG12	1:C:551:CYS:HB2	2.03	0.41
1:C:571:ARG:HD3	1:C:571:ARG:N	2.35	0.41
1:C:682:VAL:HG13	1:C:687:LEU:HB2	2.02	0.41
2:D:171:THR:O	2:D:185:LYS:N	2.47	0.41
1:G:516:LEU:HA	1:G:516:LEU:HD12	1.77	0.41
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.35	0.41
2:H:181:LEU:HA	2:H:182:PRO:HD3	1.91	0.41
1:A:353:ASP:N	1:A:353:ASP:OD2	2.51	0.41
1:C:964:LEU:O	1:C:969:PHE:HB2	2.20	0.41
2:D:369:HIS:O	2:D:372:GLU:HB2	2.20	0.41
1:E:1021:ARG:CG	1:E:1021:ARG:NH1	2.80	0.41
1:E:532:CYS:O	1:E:533:ALA:HB3	2.21	0.41
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.20	0.41
1:E:78:ILE:HG23	1:E:83:PRO:HD2	2.02	0.41
2:F:374:ILE:O	2:F:374:ILE:HG22	2.19	0.41
1:G:479:VAL:HG23	1:G:480:GLY:O	2.20	0.41
1:G:622:THR:OG1	1:G:625:ASP:OD1	2.27	0.41
2:H:376:GLN:HG2	2:H:377:TYR:N	2.35	0.41
2:H:95:THR:HG21	11:H:3459:HOH:O	2.21	0.41
1:C:85:ALA:HA	1:C:114:THR:O	2.20	0.41
2:D:188:ASP:N	2:D:188:ASP:OD2	2.51	0.41
10:E:4058:NET:H42	10:E:4058:NET:H22	2.03	0.41
1:E:615:ARG:NE	1:E:633:GLU:OE1	2.44	0.41
1:E:670:ASP:CB	1:E:677:ARG:HH21	2.24	0.41
2:F:212:ARG:HH11	2:F:212:ARG:HG3	1.86	0.41
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.20	0.41
1:G:469:LEU:O	1:G:473[B]:GLU:HB2	2.20	0.41
2:H:354:PRO:HB2	2:H:367:PHE:CE2	2.56	0.41
1:C:57:ASP:HB2	1:C:60:MET:HG2	2.03	0.41
1:C:886:PRO:HD2	1:C:887:TYR:CD1	2.56	0.41
1:C:932:GLN:HG2	1:C:937:SER:HB3	2.02	0.41
2:D:259:LEU:HD23	2:D:259:LEU:HA	1.87	0.41
2:D:43:LEU:HB3	2:D:75:VAL:HG13	2.03	0.41
1:E:696:THR:N	1:E:700:MET:CE	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:VAL:HG11	2:F:258:PHE:CZ	2.55	0.41
1:G:895:LEU:HA	1:G:896:PRO:HD3	1.98	0.41
2:H:350:PHE:HB2	2:H:366:LEU:HD22	2.03	0.41
1:A:947:LEU:HA	1:A:1014:ILE:HG23	2.03	0.41
1:C:43:ARG:NH2	1:C:81:GLU:OE2	2.50	0.41
2:F:354:PRO:HB2	2:F:367:PHE:CE2	2.55	0.41
1:A:1048:PHE:O	1:A:1051:ALA:HB3	2.21	0.41
1:A:164:PHE:HA	1:A:165:PRO:C	2.40	0.41
1:A:4:ARG:NE	1:A:7:ILE:HD12	2.36	0.41
2:B:285:LYS:HG3	2:B:314:PHE:CZ	2.54	0.41
1:C:563:MET:HE1	1:C:635:PRO:HG3	1.96	0.41
2:D:371:ILE:O	2:D:374:ILE:HB	2.20	0.41
1:E:411:PRO:HD2	11:E:4697:HOH:O	2.20	0.41
1:E:832:VAL:HA	1:E:836:GLU:O	2.21	0.41
2:F:142:LEU:HA	2:F:142:LEU:HD12	1.78	0.41
2:F:205:ILE:HD13	2:F:268:ILE:HD12	2.03	0.41
2:F:29:GLU:HB2	2:F:153:LEU:HD22	2.01	0.41
1:G:840:ILE:O	1:G:841:GLU:HB3	2.21	0.41
1:G:861:LEU:HA	1:G:861:LEU:HD23	1.75	0.41
1:A:930:LYS:HG3	1:A:1058:ALA:HB1	2.03	0.41
1:A:294:ARG:HD2	5:A:4016:CL:CL	2.58	0.41
1:A:930:LYS:HG3	1:A:1058:ALA:CB	2.51	0.41
2:F:322:PRO:CB	2:F:324:ASN:HD21	2.31	0.41
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.51	0.41
1:G:734:LEU:HD12	1:G:738:PHE:CD2	2.55	0.41
1:G:780:GLU:OE2	1:G:798:ALA:HB1	2.20	0.41
2:H:38:GLY:HA3	2:H:358:PRO:CB	2.51	0.41
1:A:713:VAL:HG23	1:A:755:PHE:HB2	2.03	0.40
1:C:220:VAL:C	1:C:221:VAL:HG23	2.42	0.40
1:C:516:LEU:HA	1:C:516:LEU:HD12	1.59	0.40
1:C:78:ILE:O	1:C:82:ARG:N	2.34	0.40
1:E:1001:ILE:HD13	1:E:1029:ILE:HG13	2.03	0.40
1:E:148:ILE:HG22	1:E:149:ALA:N	2.36	0.40
1:E:1:MET:CB	1:E:224:LYS:HZ1	2.32	0.40
2:F:62:ASN:OD1	2:F:86:PRO:HG3	2.22	0.40
1:G:250:VAL:HG12	1:G:357:THR:HG23	2.03	0.40
1:G:620:PRO:HB2	1:G:622:THR:HG23	2.02	0.40
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.37	0.40
1:A:126:ALA:HB3	1:A:302:PRO:HG3	2.02	0.40
1:C:475:LYS:O	1:C:479:VAL:HG13	2.20	0.40
1:C:805:ILE:HD11	1:C:837:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:286:MET:CE	2:F:312:HIS:O	2.69	0.40
1:G:362:PHE:CD2	1:G:433:ALA:HB1	2.56	0.40
1:G:472:LEU:O	1:G:476:VAL:HG23	2.21	0.40
1:G:788:HIS:ND1	1:G:790:GLY:N	2.60	0.40
2:H:250:TYR:H	2:H:250:TYR:HD2	1.63	0.40
1:A:1006:LYS:HB3	1:A:1006:LYS:HE3	2.00	0.40
2:B:34:THR:HA	2:B:56:THR:OG1	2.22	0.40
1:C:6:ASP:OD2	1:C:6:ASP:N	2.49	0.40
1:C:873:SER:O	1:C:877:GLN:HG3	2.21	0.40
2:D:294:ASN:OD1	2:D:294:ASN:N	2.54	0.40
1:G:1031:ARG:HB3	1:G:1031:ARG:HE	1.56	0.40
2:H:236:ILE:HD12	2:H:263:ILE:CG2	2.51	0.40
2:H:296:PRO:HB2	2:H:332:LEU:HB2	2.02	0.40
1:A:732:ALA:O	1:A:736:ARG:HB2	2.21	0.40
1:C:561:LYS:HE2	11:C:4472:HOH:O	2.21	0.40
1:C:701:ALA:O	1:C:705:ALA:N	2.49	0.40
1:E:484:LEU:HD23	1:E:484:LEU:HA	1.96	0.40
1:E:713:VAL:HG23	1:E:755:PHE:HB2	2.04	0.40
1:E:950:ARG:HH11	1:E:950:ARG:HD2	1.68	0.40
2:F:246:ALA:N	2:F:247:PRO:HD2	2.36	0.40
2:F:274:LEU:HA	2:F:274:LEU:HD23	1.92	0.40
1:G:939:MET:CE	1:G:1050:THR:CG2	2.99	0.40
2:H:32:PHE:O	2:H:291:HIS:HB2	2.20	0.40
1:A:1004:ARG:HD2	1:A:1010:TYR:OH	2.20	0.40
1:A:165:PRO:HA	1:A:182:ALA:O	2.21	0.40
1:A:345:PRO:HG3	2:B:332:LEU:HB3	2.03	0.40
1:C:630:VAL:HG11	1:C:659:VAL:HG22	2.04	0.40
1:C:809:MET:O	1:C:813:VAL:HG23	2.21	0.40
2:D:139:ASP:OD2	2:D:142:LEU:HB2	2.21	0.40
2:D:345:LYS:HB3	2:D:346:PRO:HD2	2.04	0.40
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.36	0.40
2:F:181:LEU:HA	2:F:182:PRO:HD3	1.98	0.40
2:F:286:MET:HE1	2:F:312:HIS:ND1	2.36	0.40
2:F:299:ASP:OD1	2:F:302:LYS:HD2	2.22	0.40
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.56	0.40
1:G:712:LEU:O	1:G:727:ILE:HA	2.20	0.40
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1058/1073 (99%)	1004 (95%)	51 (5%)	3 (0%)	44	44
1	C	1059/1073 (99%)	1005 (95%)	50 (5%)	4 (0%)	38	35
1	E	1062/1073 (99%)	1004 (94%)	56 (5%)	2 (0%)	51	52
1	G	1056/1073 (98%)	991 (94%)	59 (6%)	6 (1%)	28	24
2	B	377/382 (99%)	362 (96%)	15 (4%)	0	100	100
2	D	377/382 (99%)	357 (95%)	18 (5%)	2 (0%)	32	28
2	F	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
2	H	377/382 (99%)	353 (94%)	22 (6%)	2 (0%)	32	28
All	All	5743/5820 (99%)	5434 (95%)	290 (5%)	19 (0%)	44	44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	E	954	LYS
1	G	558	ASP
1	G	873	SER
1	A	975	HIS
1	C	739	GLN
1	E	975	HIS
1	G	739	GLN
1	G	975	HIS
2	D	229	LEU
2	H	269	SER
2	D	127	ALA
1	C	951	GLU
1	G	2	PRO
1	G	788	HIS
1	A	698	ILE
1	C	2	PRO

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Mol	Chain	Res	Type
2	H	243	GLY
1	C	698	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	871/878 (99%)	810 (93%)	61 (7%)	18	14
1	C	872/878 (99%)	805 (92%)	67 (8%)	15	11
1	E	875/878 (100%)	817 (93%)	58 (7%)	19	16
1	G	869/878 (99%)	796 (92%)	73 (8%)	13	8
2	B	308/310 (99%)	277 (90%)	31 (10%)	9	5
2	D	308/310 (99%)	289 (94%)	19 (6%)	21	18
2	F	308/310 (99%)	280 (91%)	28 (9%)	11	7
2	H	308/310 (99%)	283 (92%)	25 (8%)	14	9
All	All	4719/4752 (99%)	4357 (92%)	362 (8%)	15	11

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	8	LYS
1	A	38[A]	ARG
1	A	38[B]	ARG
1	A	46	LEU
1	A	49	SER
1	A	103	GLU
1	A	138	LYS
1	A	174	MET
1	A	202	LYS
1	A	275	ILE
1	A	300	MET
1	A	312	SER

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	343	ARG
1	A	363	ASN
1	A	416	ASP
1	A	542	TYR
1	A	548	GLU
1	A	559	ARG
1	A	571	ARG
1	A	591	GLU
1	A	652[A]	ARG
1	A	652[B]	ARG
1	A	671	ARG
1	A	675	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	805	ILE
1	A	811	GLN
1	A	815	LYS
1	A	835	ASN
1	A	855	LYS
1	A	880	THR
1	A	891	LYS
1	A	906	LEU
1	A	912	ARG
1	A	930	LYS
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	967	GLN
1	A	992	ASN

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Mol	Chain	Res	Type
1	A	1006	LYS
1	A	1018	SER
1	A	1020	ARG
1	A	1021	ARG
1	A	1072	ILE
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	18	ARG
2	B	25	SER
2	B	35	SER
2	B	50	ARG
2	B	87	LEU
2	B	154	ASN
2	B	174	SER
2	B	183	GLU
2	B	186	LYS
2	B	192	PHE
2	B	215	ARG
2	B	218	ILE
2	B	222	GLN
2	B	239	SER
2	B	257	LYS
2	B	269	SER
2	B	282	LYS
2	B	302	LYS
2	B	306	MET
2	B	321	LEU
2	B	324	ASN
2	B	326	ARG
2	B	332	LEU
2	B	333	PHE
2	B	357	SER
2	B	360	PRO
2	B	366	LEU
2	B	372	GLU
2	B	379	LYS
1	C	1	MET
1	C	5	THR
1	C	38	ARG
1	C	43	ARG
1	C	82	ARG

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Mol	Chain	Res	Type
1	C	103	GLU
1	C	174	MET
1	C	185	ARG
1	C	202	LYS
1	C	299	GLU
1	C	313	LYS
1	C	321	LYS
1	C	343	ARG
1	C	358	LYS
1	C	363	ASN
1	C	365	GLU
1	C	412	LYS
1	C	414	SER
1	C	422	THR
1	C	423	LYS
1	C	509	ARG
1	C	542	TYR
1	C	548	GLU
1	C	555	PRO
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	652	ARG
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	683	GLU
1	C	696	THR
1	C	706	LYS
1	C	733	ASP
1	C	735	ARG
1	C	751	LEU
1	C	753	ASP
1	C	757	ASP
1	C	763	ASP
1	C	784	GLN
1	C	792	SER
1	C	797	PRO
1	C	800	THR
1	C	805	ILE
1	C	812	GLN
1	C	827	ASN

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Mol	Chain	Res	Type
1	C	833	LYS
1	C	849	THR
1	C	855	LYS
1	C	906	LEU
1	C	912	ARG
1	C	940	LYS
1	C	950	ARG
1	C	951	GLU
1	C	992	ASN
1	C	1000	HIS
1	C	1014	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1031	ARG
1	C	1032	SER
1	C	1061	LYS
1	C	1063	ILE
1	C	1072	ILE
1	C	1073	LYS
2	D	6	LEU
2	D	18	ARG
2	D	47	SER
2	D	87	LEU
2	D	154	ASN
2	D	166	GLU
2	D	174	SER
2	D	183	GLU
2	D	222	GLN
2	D	257	LYS
2	D	261	THR
2	D	269	SER
2	D	282	LYS
2	D	324	ASN
2	D	326	ARG
2	D	332	LEU
2	D	333	PHE
2	D	366	LEU
2	D	379	LYS
1	E	1	MET
1	E	4	ARG
1	E	5	THR

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Mol	Chain	Res	Type
1	E	46	LEU
1	E	55	MET
1	E	103	GLU
1	E	153[A]	GLU
1	E	153[B]	GLU
1	E	174	MET
1	E	236	ASN
1	E	275	ILE
1	E	307	SER
1	E	321	LYS
1	E	343	ARG
1	E	358	LYS
1	E	363	ASN
1	E	412	LYS
1	E	428	LEU
1	E	490	ARG
1	E	515	LYS
1	E	542	TYR
1	E	548	GLU
1	E	559	ARG
1	E	571	ARG
1	E	591	GLU
1	E	671	ARG
1	E	675	ARG
1	E	680	HIS
1	E	683	GLU
1	E	696	THR
1	E	698	ILE
1	E	700	MET
1	E	706	LYS
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	751	LEU
1	E	784	GLN
1	E	805	ILE
1	E	835	ASN
1	E	839	LEU
1	E	855	LYS
1	E	891	LYS
1	E	906	LEU
1	E	912[A]	ARG

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Mol	Chain	Res	Type
1	E	912[B]	ARG
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956[A]	ARG
1	E	956[B]	ARG
1	E	966	LYS
1	E	993	LYS
1	E	1000	HIS
1	E	1020	ARG
1	E	1021	ARG
1	E	1061	LYS
1	E	1073	LYS
2	F	18	ARG
2	F	25	SER
2	F	50	ARG
2	F	73	SER
2	F	87	LEU
2	F	106	ASN
2	F	151	PRO
2	F	153	LEU
2	F	154	ASN
2	F	166	GLU
2	F	169	SER
2	F	175	TRP
2	F	183	GLU
2	F	186	LYS
2	F	192	PHE
2	F	205	ILE
2	F	215	ARG
2	F	222	GLN
2	F	239	SER
2	F	261	THR
2	F	282	LYS
2	F	301	GLU
2	F	306	MET
2	F	324	ASN
2	F	326	ARG
2	F	332	LEU
2	F	366	LEU
2	F	379	LYS
1	G	4	ARG

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Mol	Chain	Res	Type
1	G	8	LYS
1	G	43	ARG
1	G	46	LEU
1	G	49	SER
1	G	59	GLU
1	G	76	LYS
1	G	145	ARG
1	G	174	MET
1	G	207	ASP
1	G	236	ASN
1	G	275	ILE
1	G	307	SER
1	G	313	LYS
1	G	321	LYS
1	G	326	LEU
1	G	343	ARG
1	G	363	ASN
1	G	387	ILE
1	G	412	LYS
1	G	416	ASP
1	G	428	LEU
1	G	482	THR
1	G	489	LEU
1	G	509	ARG
1	G	519	GLN
1	G	542	TYR
1	G	543	MET
1	G	548	GLU
1	G	558	ASP
1	G	559	ARG
1	G	571	ARG
1	G	591	GLU
1	G	652	ARG
1	G	665	SER
1	G	671	ARG
1	G	675	ARG
1	G	683	GLU
1	G	688	LYS
1	G	704	LYS
1	G	706	LYS
1	G	714	VAL
1	G	733	ASP

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Mol	Chain	Res	Type
1	G	734	LEU
1	G	735	ARG
1	G	751	LEU
1	G	752	LEU
1	G	753	ASP
1	G	763	ASP
1	G	784	GLN
1	G	800	THR
1	G	805	ILE
1	G	815	LYS
1	G	849	THR
1	G	855	LYS
1	G	880	THR
1	G	881	LYS
1	G	891	LYS
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	950	ARG
1	G	963	LYS
1	G	966	LYS
1	G	1001	ILE
1	G	1006	LYS
1	G	1020	ARG
1	G	1021	ARG
1	G	1026	SER
1	G	1031	ARG
1	G	1061	LYS
1	G	1063	ILE
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	7	LEU
2	H	25	SER
2	H	47	SER
2	H	78	GLN
2	H	104	ARG
2	H	125	LYS
2	H	153	LEU
2	H	154	ASN
2	H	156	MET
2	H	166	GLU

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Mol	Chain	Res	Type
2	H	192	PHE
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	257	LYS
2	H	306	MET
2	H	321	LEU
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	357	SER
2	H	366	LEU
2	H	379	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
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	936	ASN
1	A	942	HIS
1	A	967	GLN
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1007	ASN
1	A	1035	GLN
1	A	1071	GLN
2	B	51	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN

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Mol	Chain	Res	Type
1	C	457	ASN
1	C	645	GLN
1	C	689	GLN
1	C	784	GLN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	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	803	GLN
1	E	814	GLN
1	E	835	ASN
1	E	942	HIS
1	E	987	ASN
1	E	992	ASN
1	E	1000	HIS
1	E	1002	GLN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN
2	F	106	ASN
2	F	154	ASN
2	F	222	GLN
2	F	324	ASN
1	G	105	GLN
1	G	457	ASN
1	G	523	HIS
1	G	689	GLN

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Mol	Chain	Res	Type
1	G	784	GLN
1	G	803	GLN
1	G	834	ASN
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	78	GLN
2	H	154	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 60 are monoatomic - leaving 29 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	A	4000	3	25,29,29	1.17	3 (12%)	24,45,45	1.05	0
6	PO4	A	4006	3,4	4,4,4	2.01	2 (50%)	6,6,6	0.87	0
7	ADP	A	4007	3,4	25,29,29	0.95	0	24,45,45	1.18	2 (8%)
8	ORN	A	4011	-	3,8,8	0.60	0	2,9,9	0.70	0
9	GLN	A	4013	-	4,9,9	0.58	0	5,11,11	0.91	0
10	NET	A	4014	-	8,8,8	0.67	0	10,10,10	0.54	0
9	GLN	B	4012	-	4,9,9	0.25	0	5,11,11	1.10	0
7	ADP	C	4023	3	25,29,29	1.14	2 (8%)	24,45,45	0.72	0
6	PO4	C	4028	3,4	4,4,4	2.43	2 (50%)	6,6,6	0.99	0
7	ADP	C	4029	3,4	25,29,29	1.59	4 (16%)	24,45,45	1.07	2 (8%)
8	ORN	C	4033	-	3,8,8	0.48	0	2,9,9	0.21	0
9	GLN	C	4035	-	4,9,9	0.40	0	5,11,11	0.81	0
10	NET	C	4036	-	8,8,8	0.53	0	10,10,10	0.45	0
9	GLN	D	4034	-	4,9,9	0.60	0	5,11,11	2.39	2 (40%)
7	ADP	E	4045	3	25,29,29	1.24	3 (12%)	24,45,45	1.04	1 (4%)
6	PO4	E	4050	3,4	4,4,4	1.99	3 (75%)	6,6,6	0.99	0
7	ADP	E	4051	3,4	25,29,29	1.28	5 (20%)	24,45,45	0.95	1 (4%)
8	ORN	E	4055	-	3,8,8	0.41	0	2,9,9	0.45	0
9	GLN	E	4057	-	4,9,9	0.56	0	5,11,11	1.18	0
10	NET	E	4058	-	8,8,8	0.53	0	10,10,10	0.71	0
6	PO4	E	4067	-	4,4,4	1.22	0	6,6,6	0.59	0
9	GLN	F	4056	-	4,9,9	0.60	0	5,11,11	1.63	1 (20%)
7	ADP	G	4068	3	25,29,29	1.15	3 (12%)	24,45,45	1.32	4 (16%)
6	PO4	G	4073	3,4	4,4,4	1.63	1 (25%)	6,6,6	0.89	0
7	ADP	G	4074	3,4	25,29,29	1.44	4 (16%)	24,45,45	1.23	2 (8%)
8	ORN	G	4078	-	3,8,8	0.28	0	2,9,9	0.51	0
9	GLN	G	4080	-	4,9,9	0.64	0	5,11,11	0.67	0
10	NET	G	4081	-	8,8,8	0.64	0	10,10,10	0.44	0
9	GLN	H	4079	-	4,9,9	0.32	0	5,11,11	1.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	A	4000	3	-	0/12/32/32	0/3/3/3
6	PO4	A	4006	3,4	-	0/0/0/0	0/0/0/0
7	ADP	A	4007	3,4	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	A	4011	-	-	0/4/8/8	0/0/0/0
9	GLN	A	4013	-	-	0/5/9/9	0/0/0/0
10	NET	A	4014	-	-	0/12/12/12	0/0/0/0
9	GLN	B	4012	-	-	0/5/9/9	0/0/0/0
7	ADP	C	4023	3	-	0/12/32/32	0/3/3/3
6	PO4	C	4028	3,4	-	0/0/0/0	0/0/0/0
7	ADP	C	4029	3,4	-	0/12/32/32	0/3/3/3
8	ORN	C	4033	-	-	0/4/8/8	0/0/0/0
9	GLN	C	4035	-	-	0/5/9/9	0/0/0/0
10	NET	C	4036	-	-	0/12/12/12	0/0/0/0
9	GLN	D	4034	-	-	0/5/9/9	0/0/0/0
7	ADP	E	4045	3	-	0/12/32/32	0/3/3/3
6	PO4	E	4050	3,4	-	0/0/0/0	0/0/0/0
7	ADP	E	4051	3,4	-	0/12/32/32	0/3/3/3
8	ORN	E	4055	-	-	0/4/8/8	0/0/0/0
9	GLN	E	4057	-	-	0/5/9/9	0/0/0/0
10	NET	E	4058	-	-	0/12/12/12	0/0/0/0
6	PO4	E	4067	-	-	0/0/0/0	0/0/0/0
9	GLN	F	4056	-	-	0/5/9/9	0/0/0/0
7	ADP	G	4068	3	-	0/12/32/32	0/3/3/3
6	PO4	G	4073	3,4	-	0/0/0/0	0/0/0/0
7	ADP	G	4074	3,4	-	0/12/32/32	0/3/3/3
8	ORN	G	4078	-	-	0/4/8/8	0/0/0/0
9	GLN	G	4080	-	-	0/5/9/9	0/0/0/0
10	NET	G	4081	-	-	0/12/12/12	0/0/0/0
9	GLN	H	4079	-	-	0/5/9/9	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	4028	PO4	P-O4	-3.15	1.43	1.54
6	C	4028	PO4	P-O2	-2.87	1.44	1.54
7	G	4074	ADP	O4'-C1'	-2.62	1.37	1.41
6	A	4006	PO4	P-O2	-2.59	1.45	1.54
7	A	4000	ADP	O4'-C1'	-2.51	1.37	1.41
6	G	4073	PO4	P-O2	-2.50	1.45	1.54
7	E	4045	ADP	O4'-C1'	-2.42	1.37	1.41
7	E	4051	ADP	O4'-C1'	-2.34	1.38	1.41
6	E	4050	PO4	P-O3	-2.32	1.46	1.54
6	A	4006	PO4	P-O4	-2.31	1.46	1.54
6	E	4050	PO4	P-O2	-2.25	1.46	1.54
6	E	4050	PO4	P-O4	-2.12	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	4023	ADP	O4'-C1'	-2.09	1.38	1.41
7	G	4068	ADP	O4'-C1'	-2.07	1.38	1.41
7	E	4051	ADP	O3'-C3'	2.03	1.47	1.43
7	A	4000	ADP	C2-N1	2.08	1.37	1.33
7	C	4029	ADP	C2-N1	2.25	1.38	1.33
7	E	4051	ADP	C2-N1	2.25	1.38	1.33
7	E	4051	ADP	O2'-C2'	2.28	1.48	1.43
7	G	4068	ADP	O2'-C2'	2.37	1.48	1.43
7	A	4000	ADP	O3'-C3'	2.52	1.48	1.43
7	G	4074	ADP	O2'-C2'	2.67	1.49	1.43
7	C	4029	ADP	O2'-C2'	2.67	1.49	1.43
7	C	4023	ADP	O2'-C2'	2.87	1.49	1.43
7	E	4045	ADP	O3'-C3'	2.94	1.49	1.43
7	G	4068	ADP	O3'-C3'	2.99	1.49	1.43
7	E	4045	ADP	PB-O3A	3.00	1.64	1.60
7	G	4074	ADP	PB-O3A	3.51	1.65	1.60
7	C	4029	ADP	O3'-C3'	3.70	1.51	1.43
7	G	4074	ADP	O3'-C3'	3.81	1.51	1.43
7	E	4051	ADP	PB-O3A	3.83	1.66	1.60
7	C	4029	ADP	PB-O3A	5.22	1.68	1.60

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	4034	GLN	CG-CB-CA	-3.88	104.78	113.84
9	F	4056	GLN	CG-CB-CA	-2.76	107.39	113.84
9	D	4034	GLN	OE1-CD-CG	-2.61	113.45	121.06
7	A	4007	ADP	C2'-C3'-C4'	-2.48	97.79	102.62
7	E	4045	ADP	C5-C6-N6	2.04	124.63	120.47
7	C	4029	ADP	O2'-C2'-C3'	2.11	118.59	111.83
7	C	4029	ADP	O3'-C3'-C2'	2.13	118.66	111.83
7	E	4051	ADP	C4-C5-N7	2.15	111.48	109.41
7	G	4068	ADP	N3-C2-N1	2.15	130.73	128.86
7	G	4068	ADP	O2'-C2'-C3'	2.48	119.78	111.83
7	G	4074	ADP	C5-C6-N6	2.55	125.66	120.47
7	G	4068	ADP	N6-C6-N1	2.58	123.88	118.77
7	G	4074	ADP	O3'-C3'-C2'	2.71	120.51	111.83
7	G	4068	ADP	O3'-C3'-C2'	2.73	120.57	111.83
7	A	4007	ADP	C5-C6-N6	3.12	126.83	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4011	ORN	1	0
9	B	4012	GLN	3	0
7	C	4029	ADP	1	0
8	C	4033	ORN	1	0
10	C	4036	NET	1	0
9	D	4034	GLN	2	0
7	E	4045	ADP	2	0
7	E	4051	ADP	2	0
10	E	4058	NET	2	0
9	F	4056	GLN	3	0
7	G	4068	ADP	1	0
7	G	4074	ADP	1	0
9	H	4079	GLN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.