



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:48 PM UTC

PDB ID : 3WST / pdb_00003wst
Title : Crystal structure of C.elegans PRMT7 in complex with SAH(P31)
Authors : Hasegawa, M.; Toma-fukai, S.; Shimizu, T.
Deposited on : 2014-03-21
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

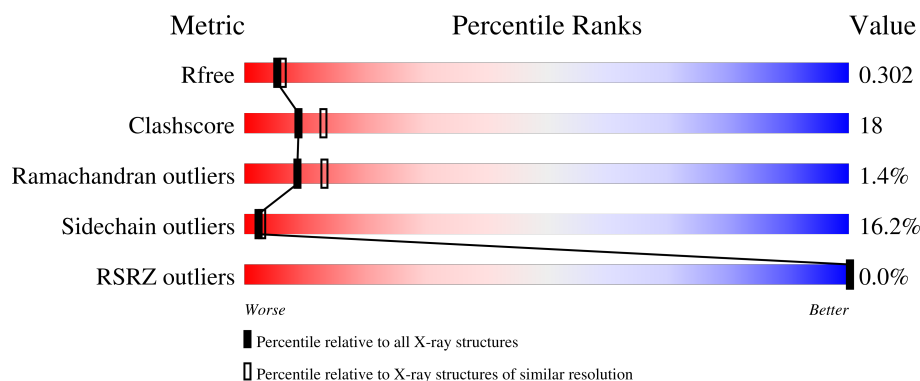
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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.



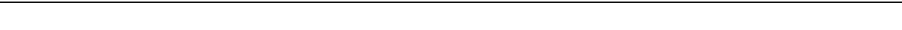
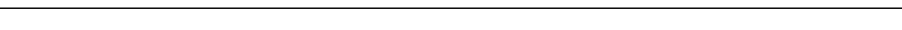
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	655	
1	B	655	
1	C	655	
1	D	655	
1	E	655	

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Mol	Chain	Length	Quality of chain
1	F	655	 59% 31% 7% . .
1	G	655	 60% 31% 7% .
1	H	655	 62% 30% 5% .
1	I	655	 59% 31% 8% . .
1	J	655	 56% 33% 8% . .
1	K	655	 50% 38% 9% . .
1	L	655	 64% 28% 6% .
1	M	655	 49% 37% 9% . .
1	N	655	 51% 37% 8% . .
1	O	655	 52% 38% 8% . .
1	P	655	 59% 31% 6% . .
1	Q	655	 49% 38% 8% . .
1	R	655	 52% 37% 8% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 92645 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 Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	D	637	Total	C	N	O	S	0	0	0
			5078	3231	852	968	27			
1	B	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	C	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	F	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	E	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	G	636	Total	C	N	O	S	0	0	0
			5070	3227	850	966	27			
1	H	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	I	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			
1	M	633	Total	C	N	O	S	0	0	0
			5049	3216	844	962	27			
1	N	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	O	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	P	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	Q	632	Total	C	N	O	S	0	0	0
			5039	3209	845	958	27			
1	R	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	J	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	L	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9XW42
A	-6	PRO	-	expression tag	UNP Q9XW42
A	-5	LEU	-	expression tag	UNP Q9XW42
A	-4	GLY	-	expression tag	UNP Q9XW42
A	-3	SER	-	expression tag	UNP Q9XW42
A	-2	GLY	-	expression tag	UNP Q9XW42
A	-1	ILE	-	expression tag	UNP Q9XW42
A	0	PRO	-	expression tag	UNP Q9XW42
D	-7	GLY	-	expression tag	UNP Q9XW42
D	-6	PRO	-	expression tag	UNP Q9XW42
D	-5	LEU	-	expression tag	UNP Q9XW42
D	-4	GLY	-	expression tag	UNP Q9XW42
D	-3	SER	-	expression tag	UNP Q9XW42
D	-2	GLY	-	expression tag	UNP Q9XW42
D	-1	ILE	-	expression tag	UNP Q9XW42
D	0	PRO	-	expression tag	UNP Q9XW42
B	-7	GLY	-	expression tag	UNP Q9XW42
B	-6	PRO	-	expression tag	UNP Q9XW42
B	-5	LEU	-	expression tag	UNP Q9XW42
B	-4	GLY	-	expression tag	UNP Q9XW42
B	-3	SER	-	expression tag	UNP Q9XW42
B	-2	GLY	-	expression tag	UNP Q9XW42
B	-1	ILE	-	expression tag	UNP Q9XW42
B	0	PRO	-	expression tag	UNP Q9XW42
C	-7	GLY	-	expression tag	UNP Q9XW42
C	-6	PRO	-	expression tag	UNP Q9XW42
C	-5	LEU	-	expression tag	UNP Q9XW42
C	-4	GLY	-	expression tag	UNP Q9XW42
C	-3	SER	-	expression tag	UNP Q9XW42
C	-2	GLY	-	expression tag	UNP Q9XW42
C	-1	ILE	-	expression tag	UNP Q9XW42
C	0	PRO	-	expression tag	UNP Q9XW42
F	-7	GLY	-	expression tag	UNP Q9XW42
F	-6	PRO	-	expression tag	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LEU	-	expression tag	UNP Q9XW42
F	-4	GLY	-	expression tag	UNP Q9XW42
F	-3	SER	-	expression tag	UNP Q9XW42
F	-2	GLY	-	expression tag	UNP Q9XW42
F	-1	ILE	-	expression tag	UNP Q9XW42
F	0	PRO	-	expression tag	UNP Q9XW42
E	-7	GLY	-	expression tag	UNP Q9XW42
E	-6	PRO	-	expression tag	UNP Q9XW42
E	-5	LEU	-	expression tag	UNP Q9XW42
E	-4	GLY	-	expression tag	UNP Q9XW42
E	-3	SER	-	expression tag	UNP Q9XW42
E	-2	GLY	-	expression tag	UNP Q9XW42
E	-1	ILE	-	expression tag	UNP Q9XW42
E	0	PRO	-	expression tag	UNP Q9XW42
G	-7	GLY	-	expression tag	UNP Q9XW42
G	-6	PRO	-	expression tag	UNP Q9XW42
G	-5	LEU	-	expression tag	UNP Q9XW42
G	-4	GLY	-	expression tag	UNP Q9XW42
G	-3	SER	-	expression tag	UNP Q9XW42
G	-2	GLY	-	expression tag	UNP Q9XW42
G	-1	ILE	-	expression tag	UNP Q9XW42
G	0	PRO	-	expression tag	UNP Q9XW42
H	-7	GLY	-	expression tag	UNP Q9XW42
H	-6	PRO	-	expression tag	UNP Q9XW42
H	-5	LEU	-	expression tag	UNP Q9XW42
H	-4	GLY	-	expression tag	UNP Q9XW42
H	-3	SER	-	expression tag	UNP Q9XW42
H	-2	GLY	-	expression tag	UNP Q9XW42
H	-1	ILE	-	expression tag	UNP Q9XW42
H	0	PRO	-	expression tag	UNP Q9XW42
I	-7	GLY	-	expression tag	UNP Q9XW42
I	-6	PRO	-	expression tag	UNP Q9XW42
I	-5	LEU	-	expression tag	UNP Q9XW42
I	-4	GLY	-	expression tag	UNP Q9XW42
I	-3	SER	-	expression tag	UNP Q9XW42
I	-2	GLY	-	expression tag	UNP Q9XW42
I	-1	ILE	-	expression tag	UNP Q9XW42
I	0	PRO	-	expression tag	UNP Q9XW42
M	-7	GLY	-	expression tag	UNP Q9XW42
M	-6	PRO	-	expression tag	UNP Q9XW42
M	-5	LEU	-	expression tag	UNP Q9XW42
M	-4	GLY	-	expression tag	UNP Q9XW42

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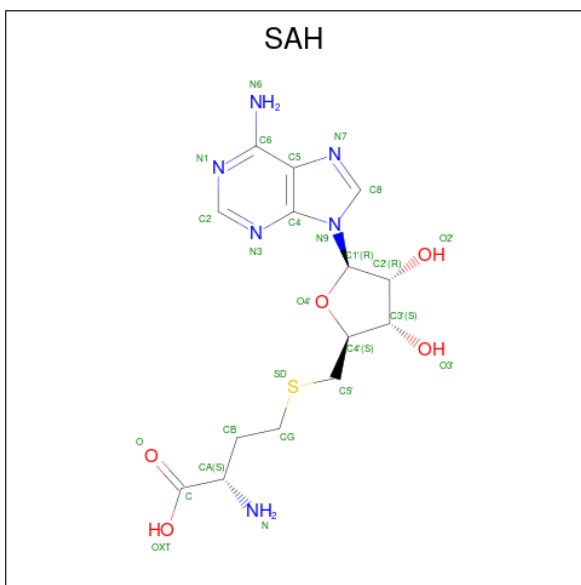
Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	SER	-	expression tag	UNP Q9XW42
M	-2	GLY	-	expression tag	UNP Q9XW42
M	-1	ILE	-	expression tag	UNP Q9XW42
M	0	PRO	-	expression tag	UNP Q9XW42
N	-7	GLY	-	expression tag	UNP Q9XW42
N	-6	PRO	-	expression tag	UNP Q9XW42
N	-5	LEU	-	expression tag	UNP Q9XW42
N	-4	GLY	-	expression tag	UNP Q9XW42
N	-3	SER	-	expression tag	UNP Q9XW42
N	-2	GLY	-	expression tag	UNP Q9XW42
N	-1	ILE	-	expression tag	UNP Q9XW42
N	0	PRO	-	expression tag	UNP Q9XW42
O	-7	GLY	-	expression tag	UNP Q9XW42
O	-6	PRO	-	expression tag	UNP Q9XW42
O	-5	LEU	-	expression tag	UNP Q9XW42
O	-4	GLY	-	expression tag	UNP Q9XW42
O	-3	SER	-	expression tag	UNP Q9XW42
O	-2	GLY	-	expression tag	UNP Q9XW42
O	-1	ILE	-	expression tag	UNP Q9XW42
O	0	PRO	-	expression tag	UNP Q9XW42
P	-7	GLY	-	expression tag	UNP Q9XW42
P	-6	PRO	-	expression tag	UNP Q9XW42
P	-5	LEU	-	expression tag	UNP Q9XW42
P	-4	GLY	-	expression tag	UNP Q9XW42
P	-3	SER	-	expression tag	UNP Q9XW42
P	-2	GLY	-	expression tag	UNP Q9XW42
P	-1	ILE	-	expression tag	UNP Q9XW42
P	0	PRO	-	expression tag	UNP Q9XW42
Q	-7	GLY	-	expression tag	UNP Q9XW42
Q	-6	PRO	-	expression tag	UNP Q9XW42
Q	-5	LEU	-	expression tag	UNP Q9XW42
Q	-4	GLY	-	expression tag	UNP Q9XW42
Q	-3	SER	-	expression tag	UNP Q9XW42
Q	-2	GLY	-	expression tag	UNP Q9XW42
Q	-1	ILE	-	expression tag	UNP Q9XW42
Q	0	PRO	-	expression tag	UNP Q9XW42
R	-7	GLY	-	expression tag	UNP Q9XW42
R	-6	PRO	-	expression tag	UNP Q9XW42
R	-5	LEU	-	expression tag	UNP Q9XW42
R	-4	GLY	-	expression tag	UNP Q9XW42
R	-3	SER	-	expression tag	UNP Q9XW42
R	-2	GLY	-	expression tag	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ILE	-	expression tag	UNP Q9XW42
R	0	PRO	-	expression tag	UNP Q9XW42
J	-7	GLY	-	expression tag	UNP Q9XW42
J	-6	PRO	-	expression tag	UNP Q9XW42
J	-5	LEU	-	expression tag	UNP Q9XW42
J	-4	GLY	-	expression tag	UNP Q9XW42
J	-3	SER	-	expression tag	UNP Q9XW42
J	-2	GLY	-	expression tag	UNP Q9XW42
J	-1	ILE	-	expression tag	UNP Q9XW42
J	0	PRO	-	expression tag	UNP Q9XW42
K	-7	GLY	-	expression tag	UNP Q9XW42
K	-6	PRO	-	expression tag	UNP Q9XW42
K	-5	LEU	-	expression tag	UNP Q9XW42
K	-4	GLY	-	expression tag	UNP Q9XW42
K	-3	SER	-	expression tag	UNP Q9XW42
K	-2	GLY	-	expression tag	UNP Q9XW42
K	-1	ILE	-	expression tag	UNP Q9XW42
K	0	PRO	-	expression tag	UNP Q9XW42
L	-7	GLY	-	expression tag	UNP Q9XW42
L	-6	PRO	-	expression tag	UNP Q9XW42
L	-5	LEU	-	expression tag	UNP Q9XW42
L	-4	GLY	-	expression tag	UNP Q9XW42
L	-3	SER	-	expression tag	UNP Q9XW42
L	-2	GLY	-	expression tag	UNP Q9XW42
L	-1	ILE	-	expression tag	UNP Q9XW42
L	0	PRO	-	expression tag	UNP Q9XW42

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



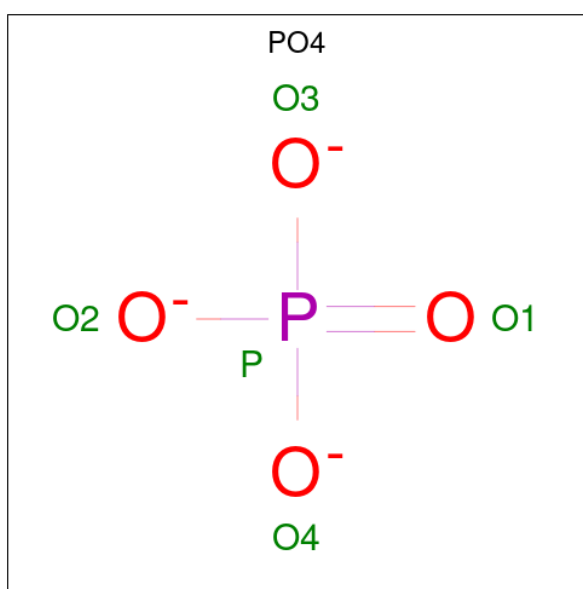
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	D	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	B	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	C	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	F	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	E	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	G	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	H	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	I	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	M	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	N	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	O	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	P	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	Q	1	Total 26	C 14	N 6	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	R	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	D	93	Total	O	0	0
			93	93		
4	B	26	Total	O	0	0
			26	26		
4	C	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		
4	E	41	Total	O	0	0
			41	41		
4	G	19	Total	O	0	0
			19	19		
4	H	59	Total	O	0	0
			59	59		

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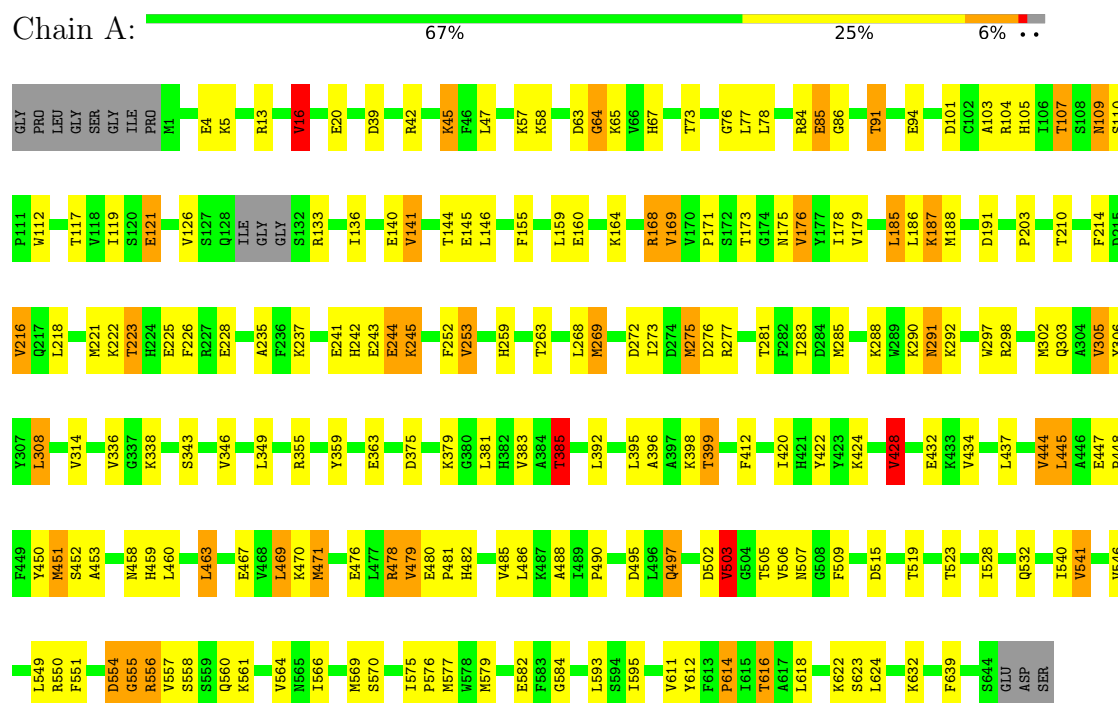
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	21	Total 21	O 21	0	0
4	M	2	Total 2	O 2	0	0
4	P	10	Total 10	O 10	0	0
4	Q	2	Total 2	O 2	0	0
4	R	2	Total 2	O 2	0	0
4	J	12	Total 12	O 12	0	0
4	K	6	Total 6	O 6	0	0
4	L	85	Total 85	O 85	0	0

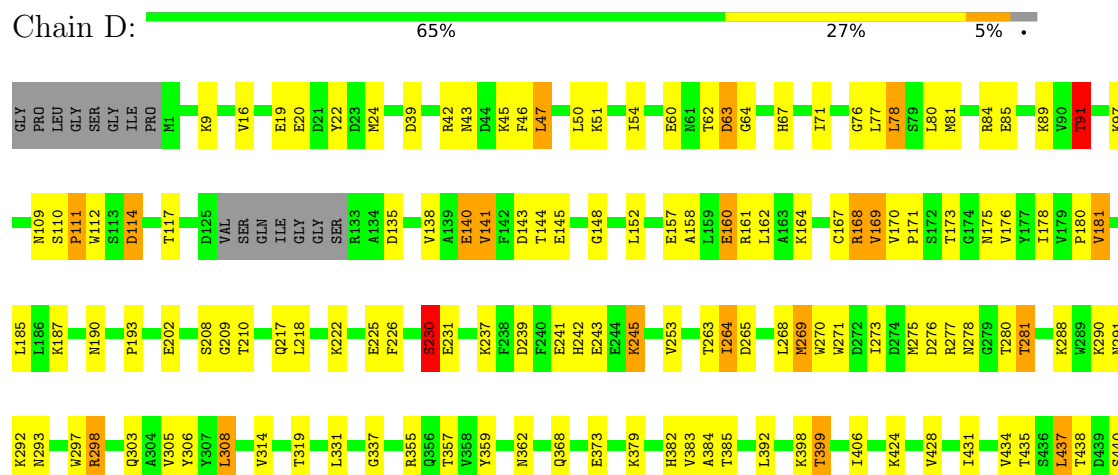
3 Residue-property plots [i](#)

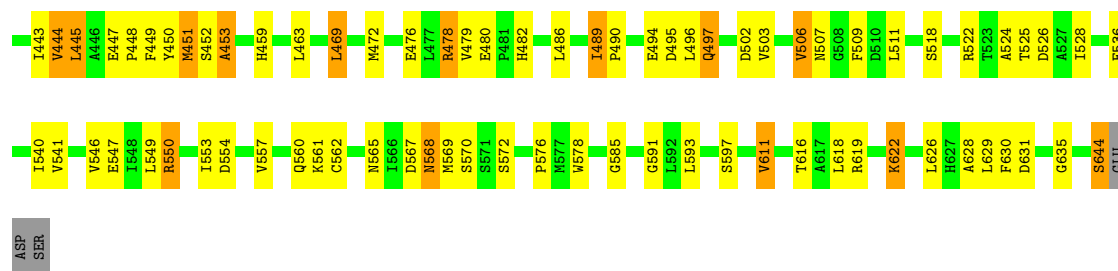
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein arginine N-methyltransferase 7



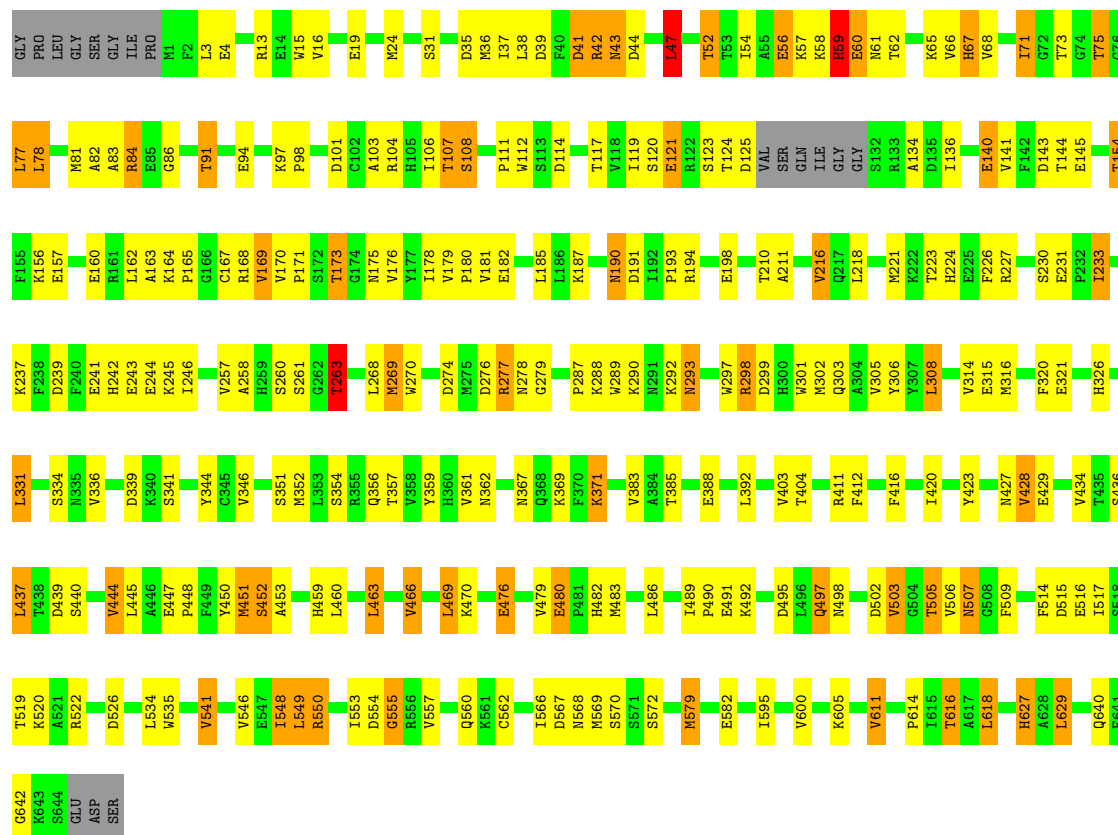
• Molecule 1: Protein arginine N-methyltransferase 7





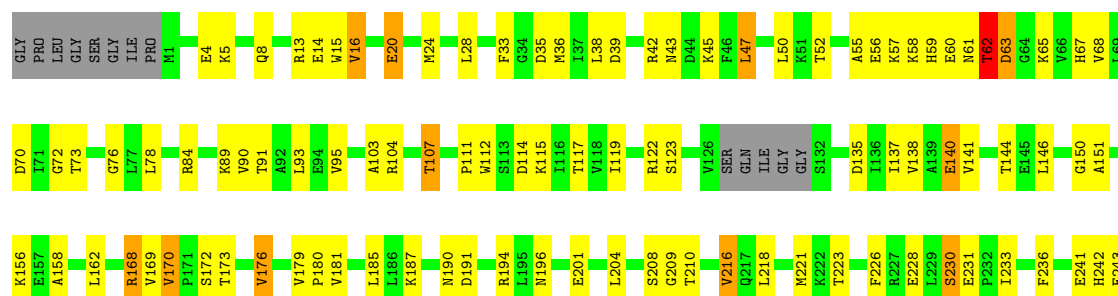
• Molecule 1: Protein arginine N-methyltransferase 7

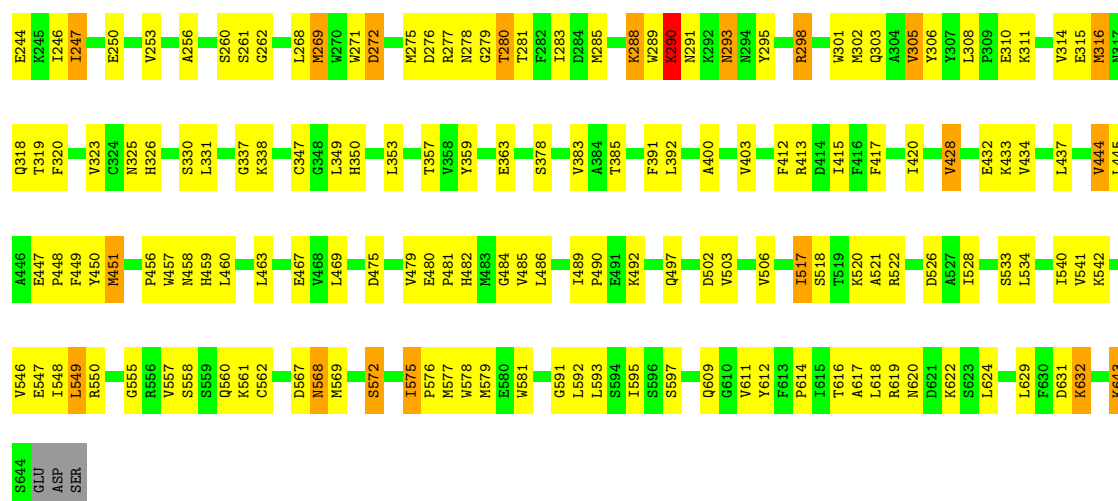
Chain B: 58% 31% 8% .



• Molecule 1: Protein arginine N-methyltransferase 7

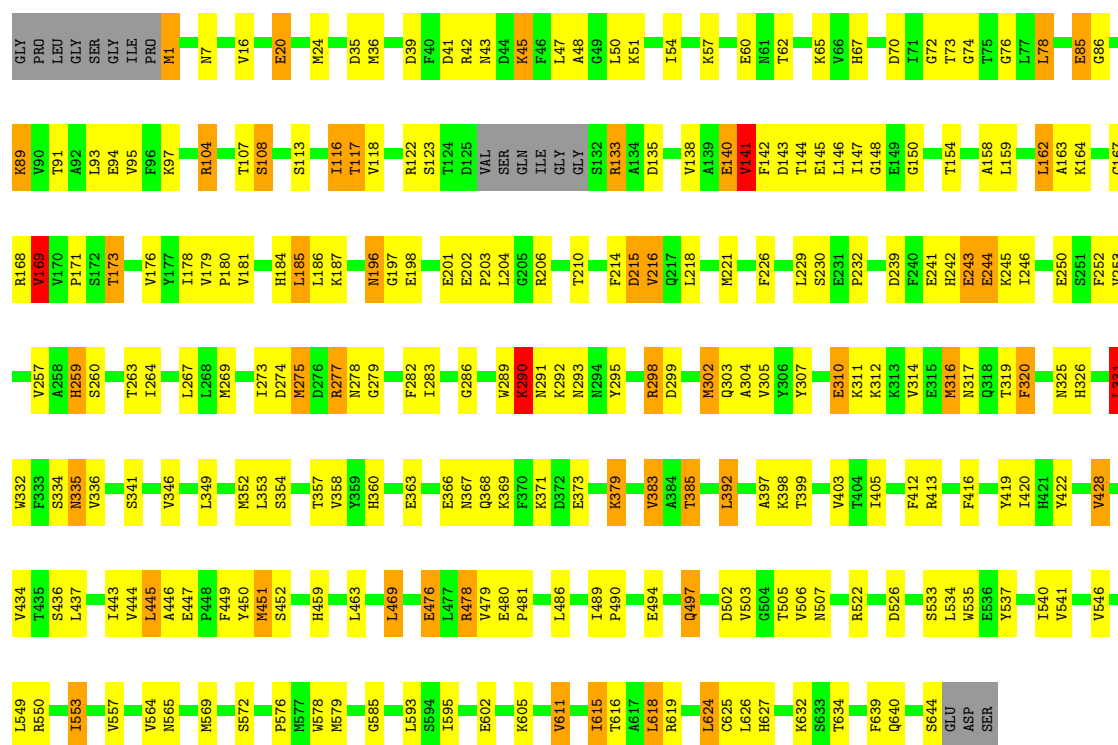
Chain C: 58% 34% 5% .





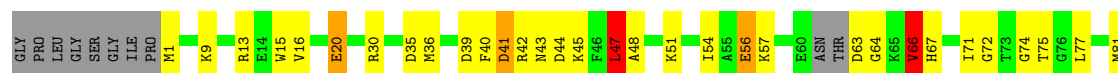
• Molecule 1: Protein arginine N-methyltransferase 7

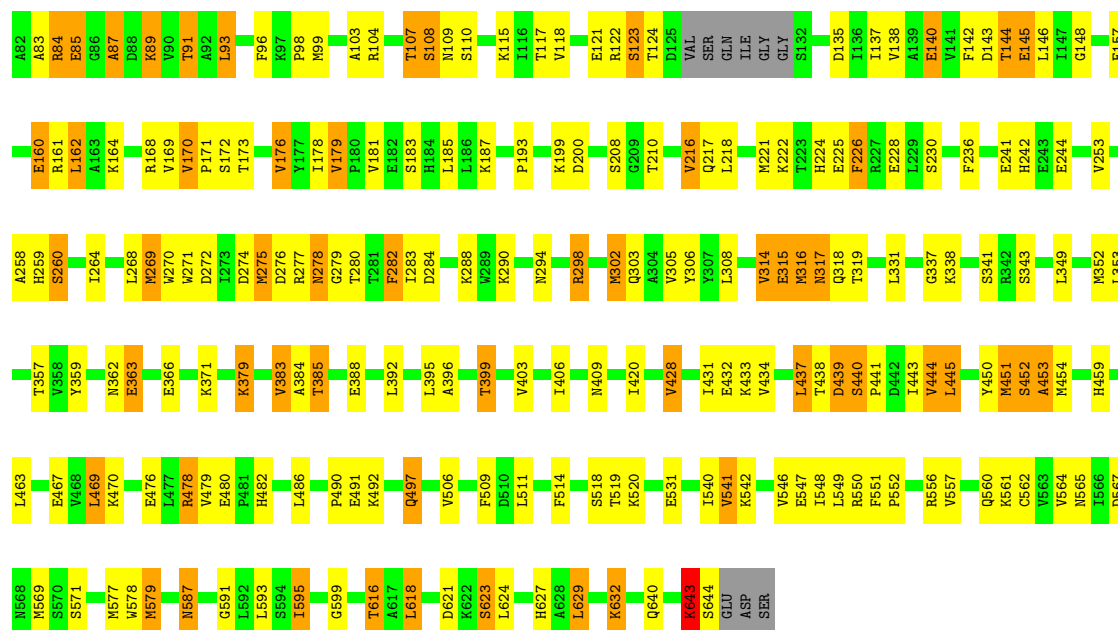
Chain F: 59% 31% 7% ..



• Molecule 1: Protein arginine N-methyltransferase 7

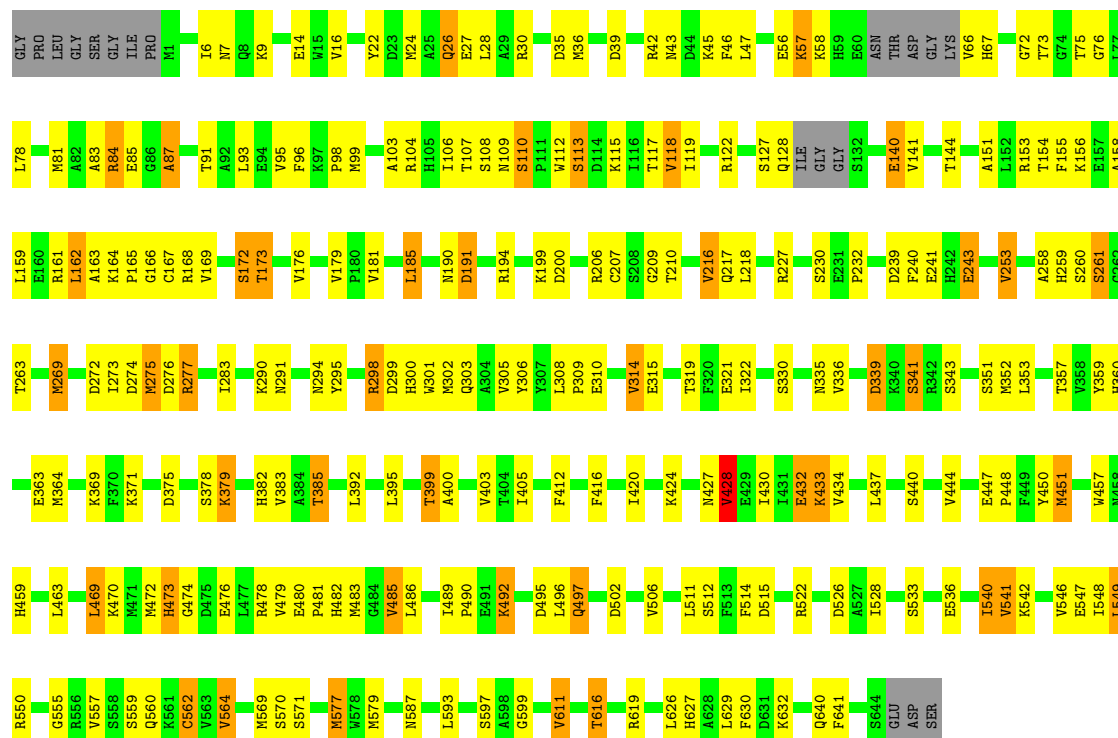
Chain E: 60% 28% 9% .





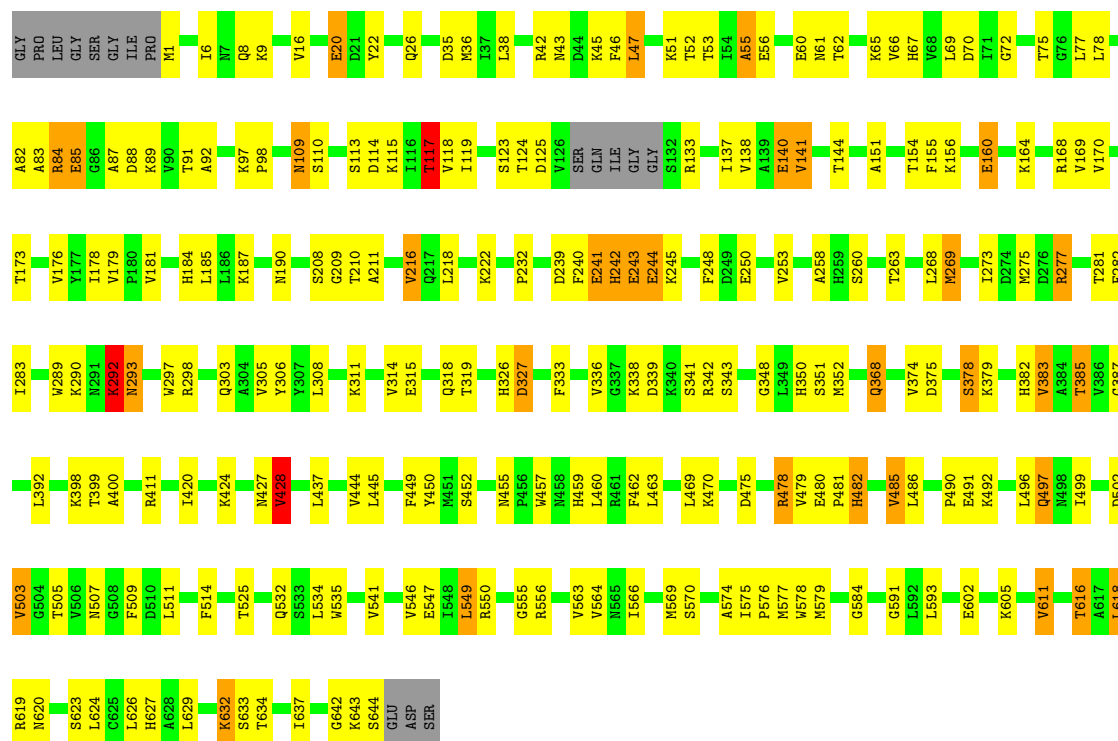
• Molecule 1: Protein arginine N-methyltransferase 7

Chain G: 60% 31% 7% .



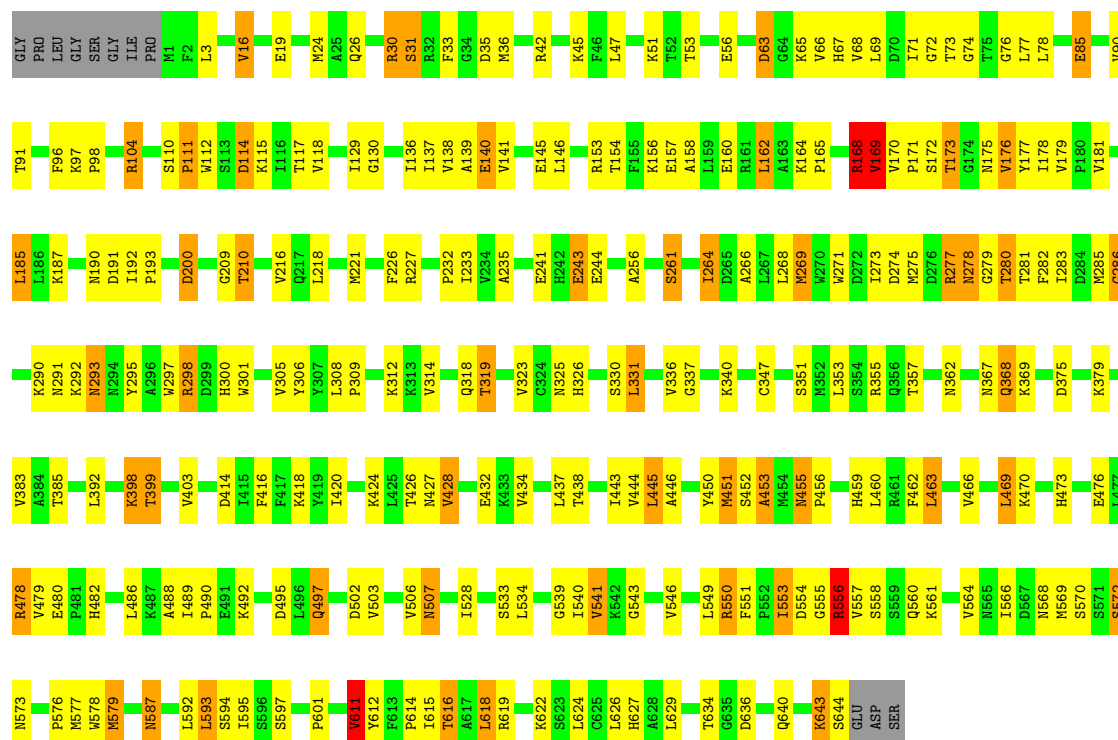
• Molecule 1: Protein arginine N-methyltransferase 7

Chain H: 62% 30% 5% .



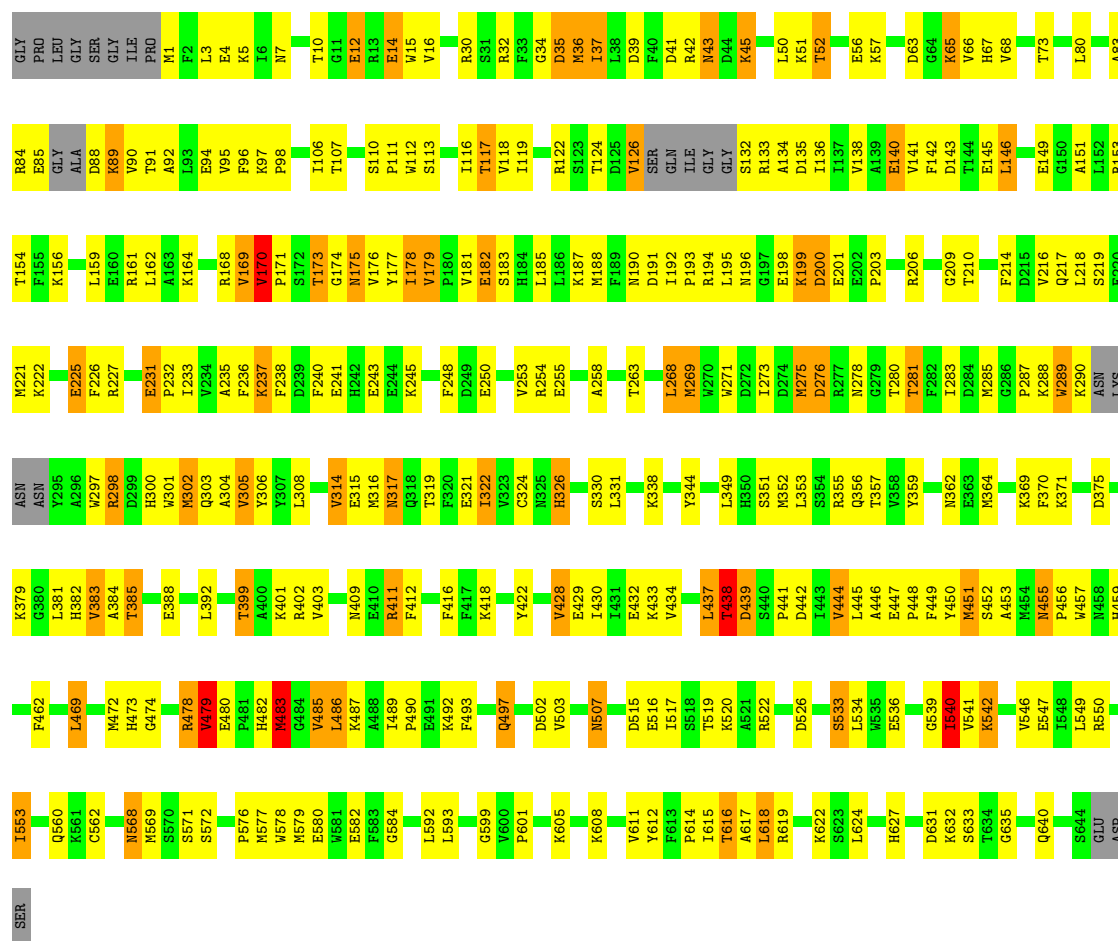
• Molecule 1: Protein arginine N-methyltransferase 7

Chain I: 59% 31% 8% ..



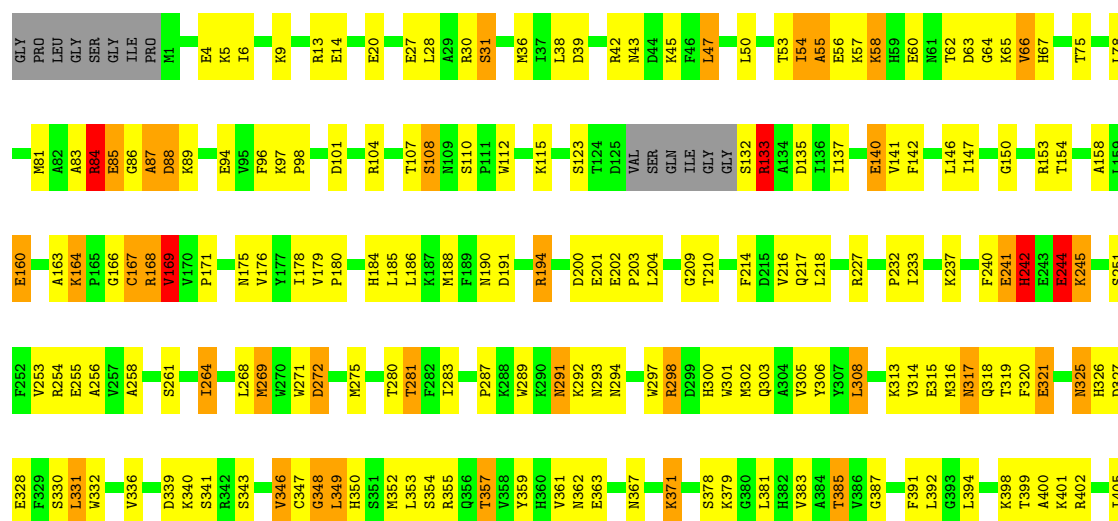
• Molecule 1: Protein arginine N-methyltransferase 7

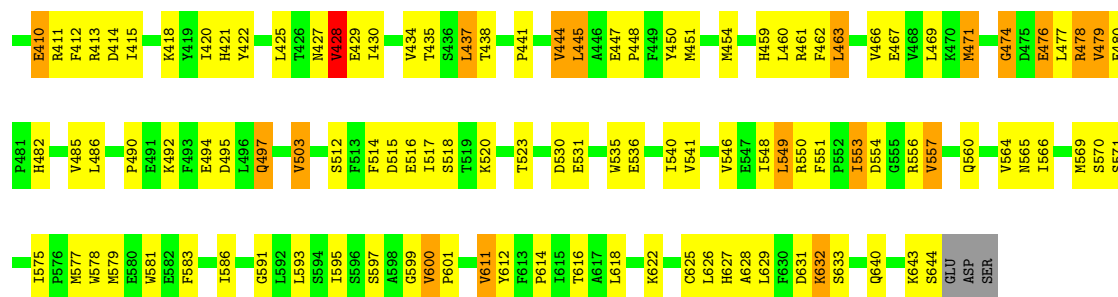
Chain M:  49% 37% 9% ..



• Molecule 1: Protein arginine N-methyltransferase 7

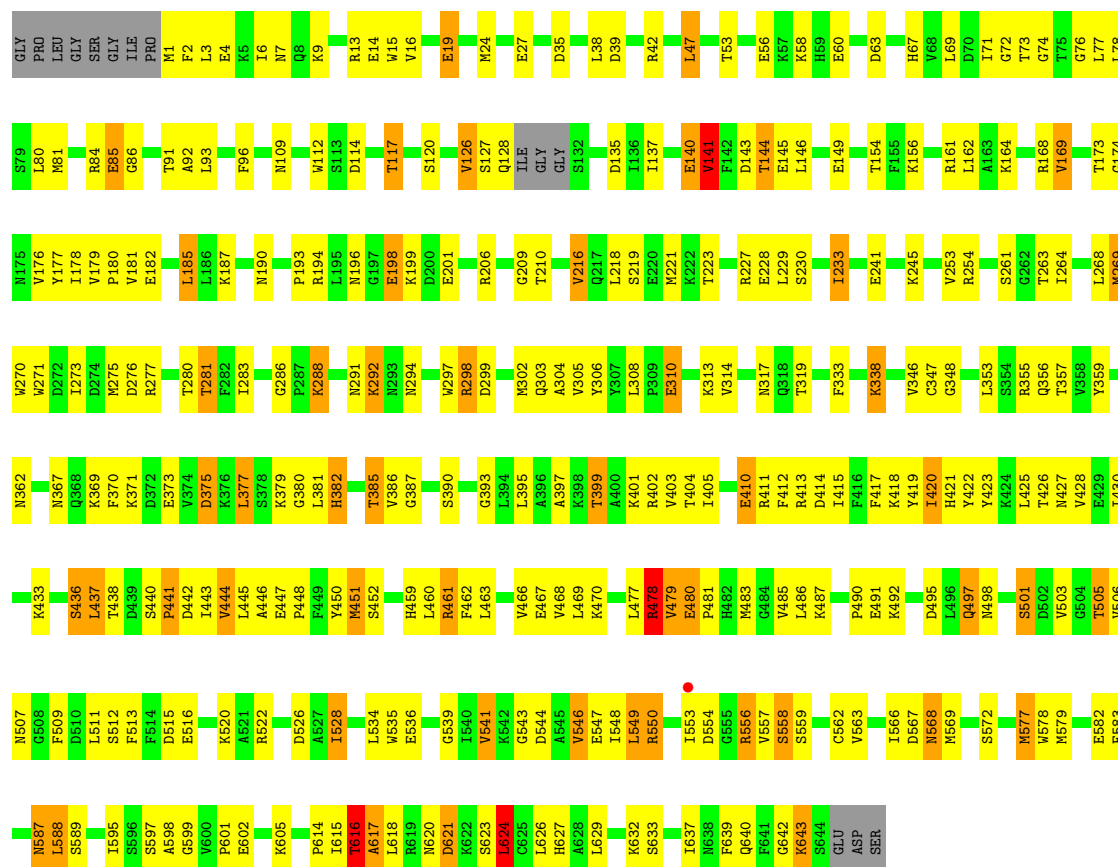
Chain N:  51% 37% 8% ..





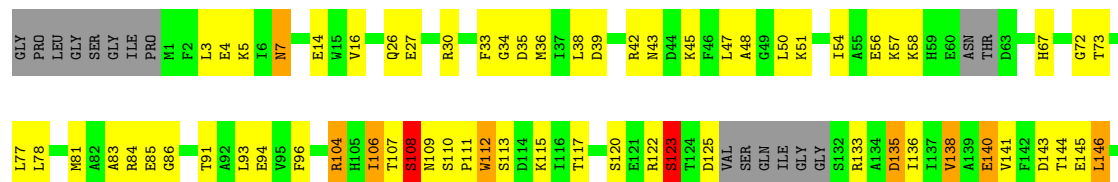
• Molecule 1: Protein arginine N-methyltransferase 7

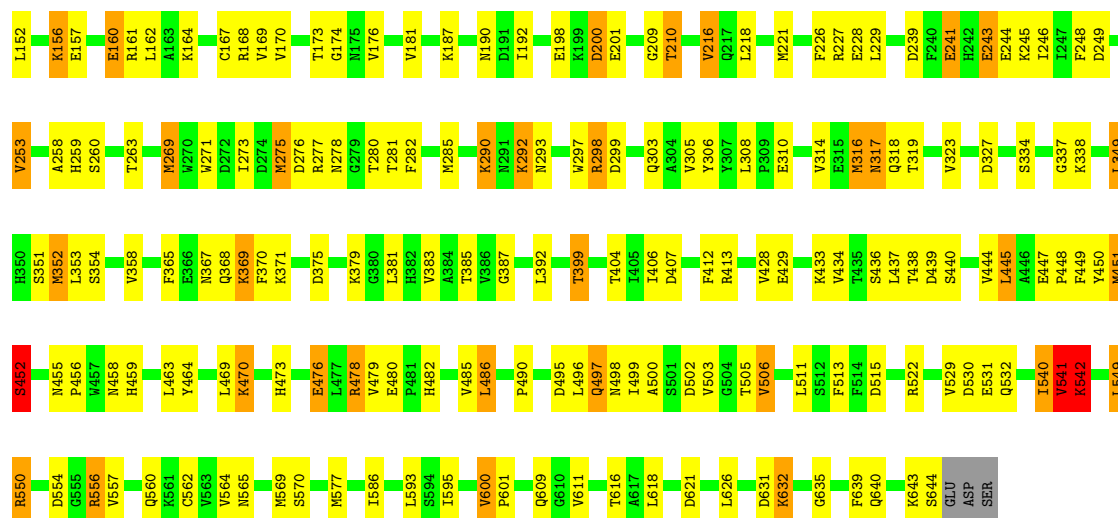
Chain O: 52% 38% 8% ..



• Molecule 1: Protein arginine N-methyltransferase 7

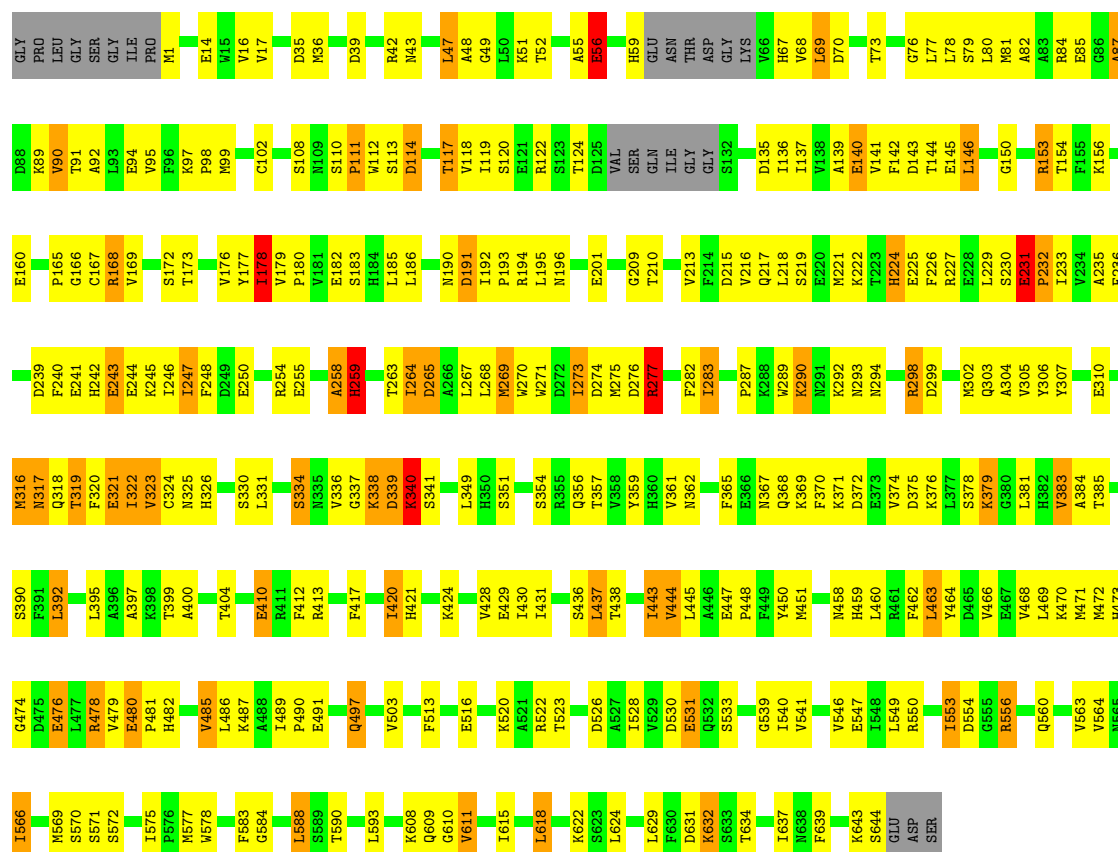
Chain P: 59% 31% 6% ..





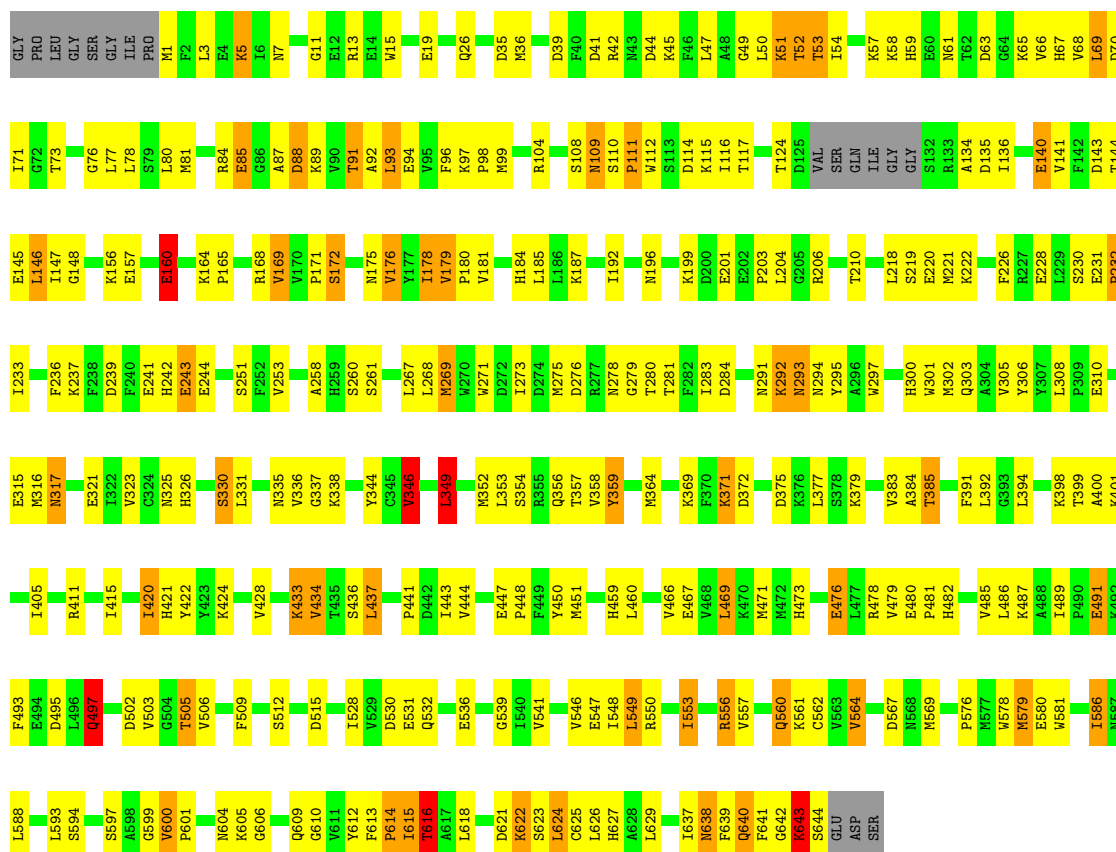
• Molecule 1: Protein arginine N-methyltransferase 7

Chain Q: 49% 38% 8% . .



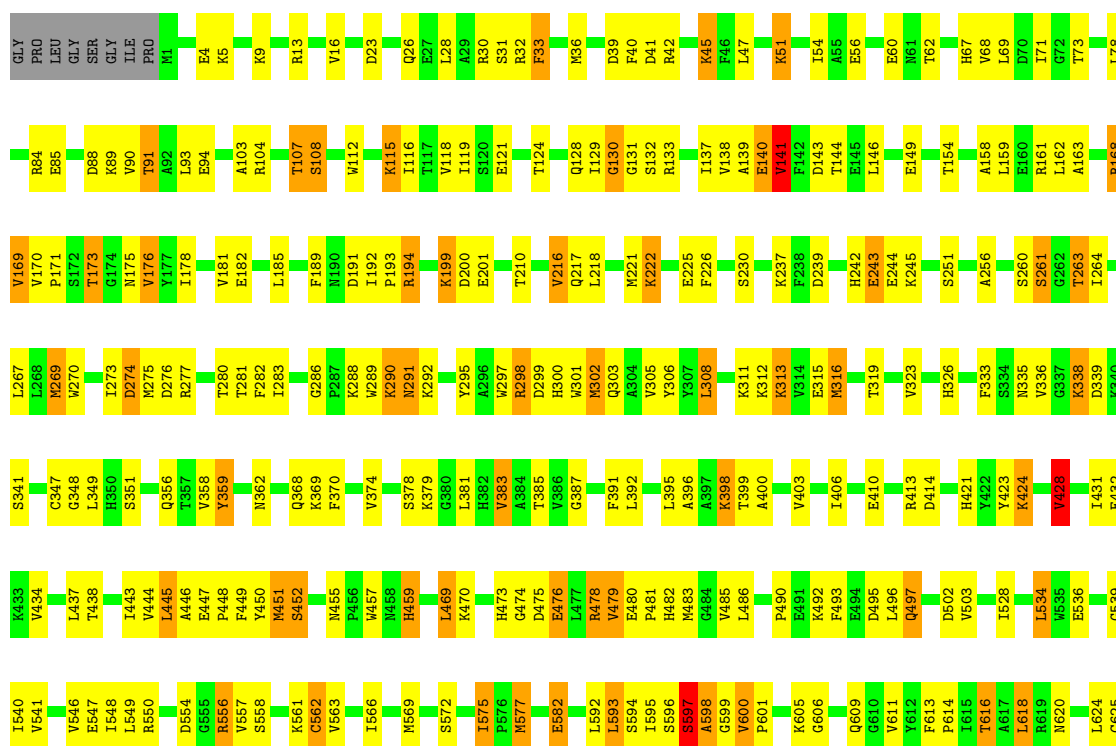
• Molecule 1: Protein arginine N-methyltransferase 7

Chain R: 52% 37% 8% . .



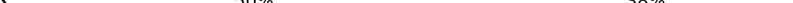
• Molecule 1: Protein arginine N-methyltransferase 7

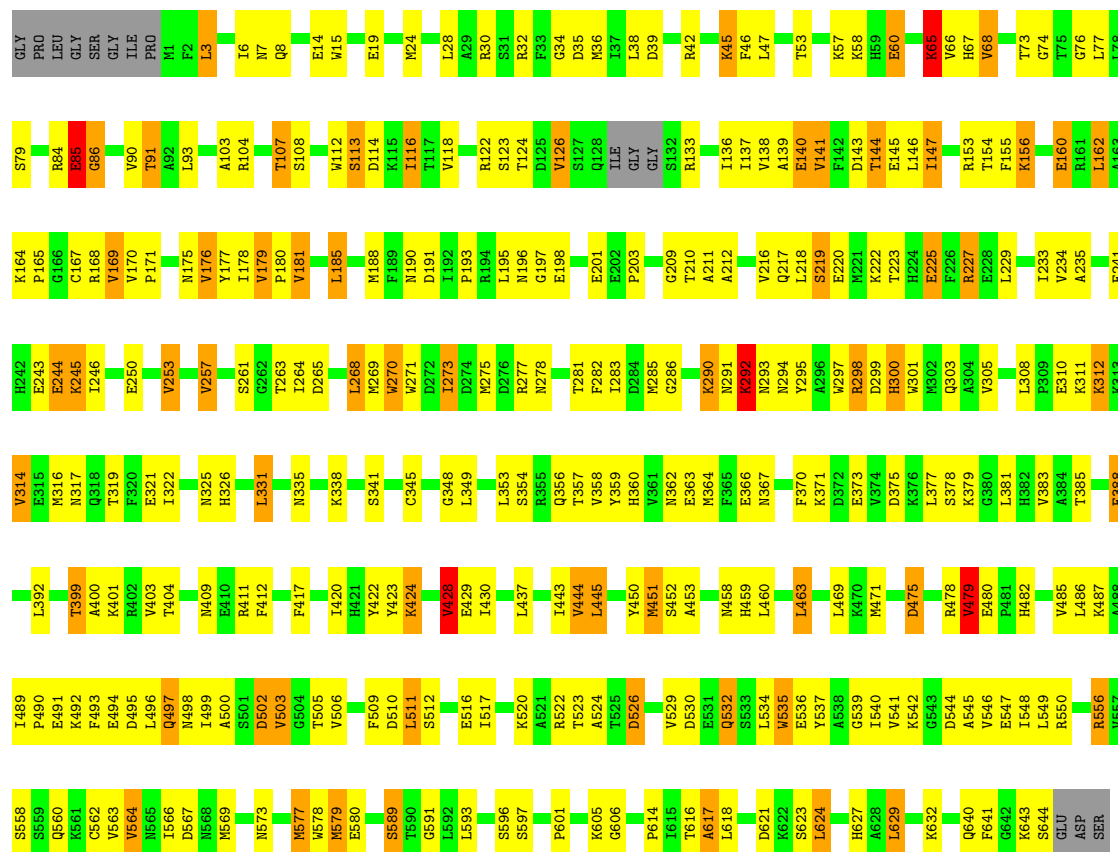
Chain J: 56% 33% 8% ..



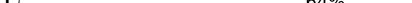


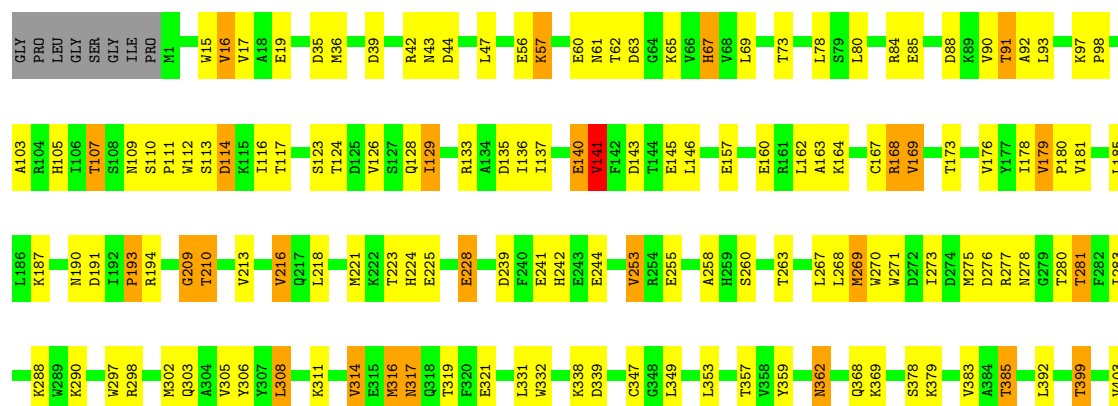
- Molecule 1: Protein arginine N-methyltransferase 7

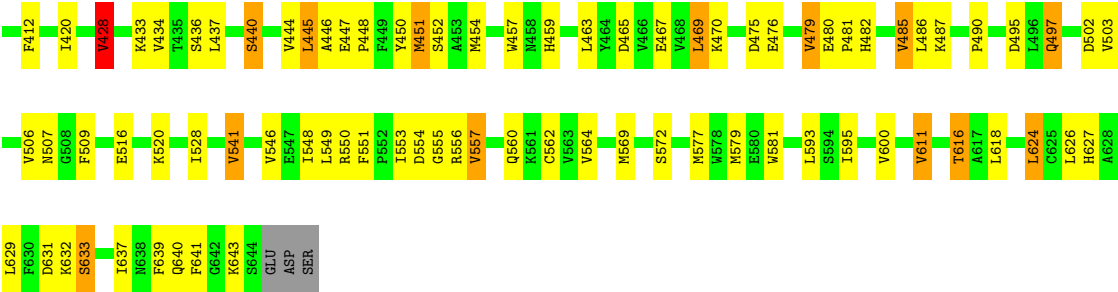
Chain K:  50% 38% 9% . .



- Molecule 1: Protein arginine N-methyltransferase 7

Chain L:  64% 28% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	190.70Å 190.70Å 373.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.41 – 2.39 47.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.41-2.39) 98.9 (47.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.303 0.233 , 0.302	Depositor DCC
R_{free} test set	29764 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.069 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	92645	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, 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	1.11	4/5217 (0.1%)	1.22	19/7044 (0.3%)
1	B	1.03	2/5195 (0.0%)	1.16	13/7014 (0.2%)
1	C	1.00	1/5202 (0.0%)	1.15	16/7024 (0.2%)
1	D	1.07	3/5189 (0.1%)	1.23	18/7006 (0.3%)
1	E	1.04	4/5179 (0.1%)	1.21	26/6990 (0.4%)
1	F	0.95	0/5195	1.15	20/7014 (0.3%)
1	G	1.00	2/5180 (0.0%)	1.13	14/6993 (0.2%)
1	H	1.07	5/5202 (0.1%)	1.21	17/7024 (0.2%)
1	I	1.00	0/5234	1.15	15/7068 (0.2%)
1	J	0.96	0/5234	1.16	23/7068 (0.3%)
1	K	0.95	1/5217 (0.0%)	1.13	20/7044 (0.3%)
1	L	1.11	7/5234 (0.1%)	1.23	22/7068 (0.3%)
1	M	0.89	0/5158	1.10	17/6962 (0.2%)
1	N	0.89	1/5195 (0.0%)	1.13	21/7014 (0.3%)
1	O	0.83	0/5217	1.05	9/7044 (0.1%)
1	P	0.94	0/5179	1.11	14/6990 (0.2%)
1	Q	0.86	0/5149	1.09	16/6951 (0.2%)
1	R	0.83	0/5195	1.06	17/7014 (0.2%)
All	All	0.98	30/93571 (0.0%)	1.15	317/126332 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	H	0	1
1	J	0	2
All	All	0	6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	HIS	CG-CD2	6.26	1.42	1.35
1	D	270	TRP	CA-C	-6.21	1.45	1.52
1	H	184	HIS	CG-CD2	6.18	1.42	1.35
1	A	242	HIS	CA-C	-5.79	1.46	1.53
1	A	179	VAL	CA-C	-5.62	1.48	1.52
1	G	259	HIS	CG-CD2	5.55	1.42	1.35
1	L	551	PHE	CA-C	-5.50	1.46	1.52
1	A	259	HIS	CE1-NE2	5.49	1.38	1.32
1	E	363	GLU	C-O	-5.46	1.17	1.24
1	L	362	ASN	C-O	-5.46	1.17	1.24
1	C	179	VAL	CA-C	-5.43	1.47	1.52
1	K	270	TRP	CA-C	-5.38	1.46	1.52
1	L	224	HIS	CE1-NE2	5.33	1.37	1.32
1	B	224	HIS	CG-CD2	5.33	1.41	1.35
1	D	152	LEU	N-CA	5.31	1.52	1.46
1	N	241	GLU	CA-C	5.31	1.58	1.52
1	G	382	HIS	CG-CD2	5.30	1.41	1.35
1	E	270	TRP	CA-C	-5.28	1.46	1.52
1	H	216	VAL	C-O	-5.27	1.18	1.24
1	L	67	HIS	CG-CD2	5.25	1.41	1.35
1	L	242	HIS	CA-C	-5.17	1.47	1.53
1	H	382	HIS	CG-CD2	5.17	1.41	1.35
1	H	151	ALA	N-CA	5.16	1.52	1.46
1	E	224	HIS	CG-CD2	5.15	1.41	1.35
1	E	632	LYS	CA-C	5.15	1.59	1.52
1	H	482	HIS	ND1-CE1	5.11	1.37	1.32
1	D	489	ILE	CA-C	-5.10	1.47	1.52
1	L	179	VAL	C-O	-5.06	1.18	1.23
1	L	332	TRP	CD2-CE2	5.05	1.50	1.41
1	B	270	TRP	CA-C	-5.03	1.46	1.52

All (317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	241	GLU	N-CA-C	13.44	130.36	113.43
1	F	346	VAL	N-CA-C	-12.93	100.86	113.53
1	N	346	VAL	N-CA-C	-12.16	101.52	113.20
1	C	62	THR	N-CA-C	9.77	121.92	111.28
1	L	643	LYS	N-CA-C	9.70	121.54	110.97
1	A	575	ILE	CA-C-N	9.39	129.45	119.78
1	A	575	ILE	C-N-CA	9.39	129.45	119.78
1	N	348	GLY	N-CA-C	-9.26	104.06	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	241	GLU	CA-C-N	9.14	138.16	121.70
1	H	241	GLU	C-N-CA	9.14	138.16	121.70
1	F	369	LYS	N-CA-C	-9.08	99.95	111.02
1	Q	611	VAL	CB-CA-C	-8.84	97.45	110.62
1	D	611	VAL	CB-CA-C	-8.83	96.34	110.28
1	L	611	VAL	CB-CA-C	-8.55	95.60	110.65
1	A	346	VAL	N-CA-C	-8.34	105.04	113.47
1	D	60	GLU	N-CA-C	8.11	120.83	111.11
1	L	428	VAL	N-CA-C	8.07	120.40	108.45
1	F	202	GLU	CA-C-N	7.98	127.62	119.56
1	F	202	GLU	C-N-CA	7.98	127.62	119.56
1	P	145	GLU	N-CA-C	7.97	123.18	113.38
1	F	86	GLY	N-CA-C	7.90	124.32	114.37
1	H	241	GLU	N-CA-C	7.89	123.09	111.96
1	O	63	ASP	N-CA-C	-7.73	100.91	110.41
1	I	169	VAL	N-CA-C	7.66	119.87	108.46
1	E	145	GLU	CA-C-N	7.59	135.37	121.70
1	E	145	GLU	C-N-CA	7.59	135.37	121.70
1	E	66	VAL	N-CA-C	7.48	118.45	107.37
1	O	126	VAL	N-CA-C	7.30	117.73	108.82
1	F	230	SER	N-CA-C	-7.28	98.12	108.96
1	J	387	GLY	N-CA-C	-7.17	100.28	110.88
1	F	169	VAL	N-CA-C	7.02	118.24	107.78
1	O	348	GLY	N-CA-C	-7.02	105.12	114.25
1	K	524	ALA	N-CA-C	7.00	119.80	111.33
1	P	145	GLU	CA-C-N	6.97	134.25	121.70
1	P	145	GLU	C-N-CA	6.97	134.25	121.70
1	D	308	LEU	CA-C-N	-6.96	111.81	119.19
1	D	308	LEU	C-N-CA	-6.96	111.81	119.19
1	C	643	LYS	N-CA-C	6.94	118.73	111.03
1	G	207	CYS	N-CA-C	-6.93	96.90	108.75
1	K	564	VAL	N-CA-C	6.93	118.70	108.45
1	J	31	SER	N-CA-C	6.92	121.33	112.34
1	K	526	ASP	N-CA-C	6.89	119.72	110.35
1	H	611	VAL	CB-CA-C	-6.88	98.55	110.65
1	N	241	GLU	CA-C-N	6.82	133.97	121.70
1	N	241	GLU	C-N-CA	6.82	133.97	121.70
1	E	643	LYS	N-CA-C	6.80	118.58	111.03
1	Q	195	LEU	N-CA-C	6.77	118.66	111.28
1	I	643	LYS	N-CA-C	6.74	120.72	112.23
1	E	264	ILE	CB-CA-C	-6.72	103.97	111.23
1	P	542	LYS	N-CA-C	6.71	120.15	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	44	ASP	N-CA-C	-6.67	104.09	111.36
1	Q	265	ASP	N-CA-C	6.67	121.01	112.34
1	H	619	ARG	N-CA-C	6.67	120.52	112.38
1	M	483	MET	N-CA-C	6.63	119.24	108.76
1	B	86	GLY	N-CA-C	6.63	123.92	114.64
1	Q	292	LYS	N-CA-C	-6.63	105.82	114.04
1	K	179	VAL	N-CA-C	6.62	114.68	107.60
1	L	308	LEU	CA-C-N	-6.61	111.71	119.05
1	L	308	LEU	C-N-CA	-6.61	111.71	119.05
1	L	440	SER	CA-C-N	-6.60	113.50	120.03
1	L	440	SER	C-N-CA	-6.60	113.50	120.03
1	R	349	LEU	N-CA-C	6.58	118.24	111.14
1	C	575	ILE	CA-C-N	6.57	126.49	119.85
1	C	575	ILE	C-N-CA	6.57	126.49	119.85
1	Q	443	ILE	N-CA-C	6.55	116.92	107.88
1	B	47	LEU	N-CA-C	-6.49	103.90	110.97
1	R	134	ALA	N-CA-C	6.47	119.11	109.59
1	K	147	ILE	N-CA-C	6.47	119.24	112.83
1	K	498	ASN	N-CA-C	6.44	118.38	111.36
1	A	252	PHE	CA-C-N	-6.44	114.06	122.37
1	A	252	PHE	C-N-CA	-6.44	114.06	122.37
1	I	611	VAL	CB-CA-C	-6.42	100.76	111.29
1	J	597	SER	CA-C-N	6.40	133.23	121.70
1	J	597	SER	C-N-CA	6.40	133.23	121.70
1	B	263	THR	N-CA-C	6.38	119.50	110.50
1	H	428	VAL	N-CA-C	6.38	117.48	108.17
1	N	85	GLU	N-CA-C	6.38	120.47	111.92
1	J	302	MET	N-CA-C	-6.38	99.82	108.24
1	J	192	ILE	CA-C-N	6.36	126.74	119.93
1	J	192	ILE	C-N-CA	6.36	126.74	119.93
1	G	473	HIS	N-CA-C	-6.35	100.80	110.14
1	M	479	VAL	N-CA-C	6.30	117.85	108.46
1	F	624	LEU	N-CA-C	6.26	119.74	109.85
1	I	168	ARG	N-CA-C	6.25	119.82	110.14
1	E	552	PRO	CA-C-N	-6.24	114.62	123.11
1	E	552	PRO	C-N-CA	-6.24	114.62	123.11
1	H	243	GLU	N-CA-C	6.23	118.88	111.71
1	L	347	CYS	N-CA-C	-6.23	105.50	113.23
1	N	87	ALA	CA-C-N	6.20	132.86	121.70
1	N	87	ALA	C-N-CA	6.20	132.86	121.70
1	R	586	ILE	N-CA-C	6.19	118.30	108.89
1	A	308	LEU	CA-C-N	-6.18	112.11	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	LEU	C-N-CA	-6.18	112.11	118.85
1	F	65	LYS	N-CA-C	6.15	119.73	109.95
1	Q	178	ILE	N-CA-C	-6.15	103.34	110.05
1	L	209	GLY	CA-C-N	-6.13	113.01	122.09
1	L	209	GLY	C-N-CA	-6.13	113.01	122.09
1	L	554	ASP	CB-CA-C	-6.13	98.30	111.78
1	N	164	LYS	CA-C-N	-6.10	113.67	120.14
1	N	164	LYS	C-N-CA	-6.10	113.67	120.14
1	O	428	VAL	N-CA-C	6.10	116.62	108.27
1	O	624	LEU	N-CA-C	6.05	116.41	107.88
1	O	546	VAL	N-CA-C	6.04	117.46	108.46
1	G	611	VAL	CB-CA-C	-6.02	100.77	110.28
1	E	118	VAL	N-CA-C	6.00	116.50	107.80
1	E	595	ILE	CB-CA-C	-6.00	102.25	110.77
1	P	586	ILE	N-CA-C	6.00	118.08	108.85
1	N	84	ARG	N-CA-C	-5.99	102.20	110.35
1	B	548	ILE	CB-CA-C	-5.98	105.05	110.91
1	B	226	PHE	N-CA-C	5.96	119.11	109.40
1	G	432	GLU	N-CA-C	5.96	117.85	111.36
1	J	459	HIS	N-CA-C	-5.95	104.67	112.41
1	N	47	LEU	N-CA-C	-5.95	104.79	111.28
1	R	600	VAL	N-CA-C	5.95	114.78	108.95
1	H	117	THR	CB-CA-C	5.94	121.03	109.33
1	I	455	ASN	CA-C-N	5.94	127.26	119.84
1	I	455	ASN	C-N-CA	5.94	127.26	119.84
1	L	479	VAL	N-CA-C	5.94	117.03	108.48
1	R	616	THR	N-CA-C	5.93	118.51	111.33
1	J	359	TYR	N-CA-C	-5.91	103.81	111.02
1	K	496	LEU	N-CA-C	5.91	118.48	111.33
1	E	145	GLU	N-CA-C	5.90	121.21	113.30
1	R	179	VAL	CA-C-N	5.90	126.20	119.83
1	R	179	VAL	C-N-CA	5.90	126.20	119.83
1	R	642	GLY	N-CA-C	5.89	119.74	111.14
1	K	86	GLY	N-CA-C	5.89	121.70	114.69
1	E	629	LEU	N-CA-C	5.88	118.30	108.02
1	A	428	VAL	N-CA-C	5.86	116.56	108.12
1	B	308	LEU	N-CA-C	-5.86	102.77	110.39
1	H	110	SER	CA-C-N	5.86	125.56	119.82
1	H	110	SER	C-N-CA	5.86	125.56	119.82
1	M	540	ILE	N-CA-C	5.86	116.30	108.27
1	N	461	ARG	N-CA-C	-5.86	105.23	112.38
1	Q	120	SER	N-CA-C	5.86	118.82	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	600	VAL	N-CA-C	5.85	112.88	107.56
1	F	331	LEU	CA-CB-CG	5.84	136.75	116.30
1	F	367	ASN	N-CA-C	5.84	117.72	108.67
1	M	12	GLU	N-CA-C	5.83	118.28	110.35
1	D	208	SER	CB-CA-C	-5.83	99.84	110.63
1	R	279	GLY	N-CA-C	-5.82	106.95	115.63
1	M	428	VAL	N-CA-C	5.82	116.75	108.42
1	A	86	GLY	N-CA-C	5.82	126.97	113.18
1	G	555	GLY	N-CA-C	5.82	121.07	114.67
1	L	141	VAL	N-CA-CB	-5.79	101.68	111.23
1	A	253	VAL	N-CA-CB	5.78	117.02	110.72
1	D	158	ALA	N-CA-C	-5.78	104.90	111.14
1	I	139	ALA	N-CA-C	5.78	117.54	107.49
1	R	372	ASP	N-CA-C	5.77	117.25	111.07
1	K	278	ASN	N-CA-C	5.77	120.32	113.28
1	K	428	VAL	N-CA-C	5.76	116.42	108.12
1	E	552	PRO	N-CA-C	-5.75	102.17	111.14
1	K	621	ASP	N-CA-C	5.74	117.70	110.24
1	I	192	ILE	CA-C-N	5.73	125.75	119.90
1	I	192	ILE	C-N-CA	5.73	125.75	119.90
1	R	330	SER	N-CA-C	5.72	118.79	109.06
1	P	192	ILE	CA-C-N	5.71	126.04	119.93
1	P	192	ILE	C-N-CA	5.71	126.04	119.93
1	J	597	SER	N-CA-C	5.71	122.95	110.80
1	J	348	GLY	N-CA-C	-5.70	107.87	115.40
1	I	187	LYS	N-CA-C	-5.69	105.22	111.82
1	E	179	VAL	CA-C-N	-5.69	114.73	120.31
1	E	179	VAL	C-N-CA	-5.69	114.73	120.31
1	C	347	CYS	N-CA-C	-5.69	106.69	113.97
1	N	330	SER	N-CA-C	5.69	118.95	110.14
1	E	440	SER	CA-C-N	5.68	125.87	120.31
1	E	440	SER	C-N-CA	5.68	125.87	120.31
1	Q	339	ASP	N-CA-C	5.68	118.31	107.75
1	L	368	GLN	N-CA-C	5.67	117.92	111.11
1	Q	166	GLY	N-CA-C	-5.67	107.92	115.40
1	E	145	GLU	O-C-N	-5.67	115.39	122.24
1	J	336	VAL	N-CA-C	5.66	116.71	109.30
1	M	164	LYS	CA-C-N	-5.65	114.43	120.03
1	M	164	LYS	C-N-CA	-5.65	114.43	120.03
1	N	175	ASN	CA-C-N	-5.65	115.78	123.12
1	N	175	ASN	C-N-CA	-5.65	115.78	123.12
1	I	179	VAL	CA-C-N	-5.63	114.18	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	179	VAL	C-N-CA	-5.63	114.18	120.14
1	Q	245	LYS	N-CA-C	-5.62	106.58	113.50
1	C	620	ASN	N-CA-C	5.62	120.29	113.38
1	F	286	GLY	CA-C-N	-5.60	113.84	120.11
1	F	286	GLY	C-N-CA	-5.60	113.84	120.11
1	E	579	MET	CG-SD-CE	-5.59	88.59	100.90
1	R	321	GLU	N-CA-C	5.59	118.69	109.85
1	O	199	LYS	N-CA-C	-5.59	102.00	110.28
1	E	226	PHE	N-CA-C	5.59	117.90	109.23
1	O	6	ILE	N-CA-C	5.58	115.98	108.17
1	B	423	TYR	N-CA-C	-5.58	106.14	113.17
1	H	485	VAL	N-CA-C	5.58	115.92	108.11
1	M	179	VAL	CA-C-N	5.57	126.00	119.99
1	M	179	VAL	C-N-CA	5.57	126.00	119.99
1	D	494	GLU	N-CA-C	-5.56	105.12	111.07
1	C	62	THR	CA-C-N	5.56	131.70	121.70
1	C	62	THR	C-N-CA	5.56	131.70	121.70
1	A	519	THR	N-CA-C	5.54	117.31	111.28
1	J	292	LYS	N-CA-C	-5.53	100.69	109.59
1	G	118	VAL	N-CA-C	5.53	117.29	108.89
1	Q	320	PHE	N-CA-C	5.52	117.49	108.76
1	C	449	PHE	N-CA-C	5.52	117.39	108.34
1	Q	412	PHE	N-CA-C	5.51	117.28	111.28
1	M	170	VAL	CB-CA-C	-5.50	104.55	111.04
1	G	110	SER	CA-C-N	5.49	126.71	119.84
1	G	110	SER	C-N-CA	5.49	126.71	119.84
1	D	110	SER	CA-C-N	-5.49	114.04	119.92
1	D	110	SER	C-N-CA	-5.49	114.04	119.92
1	E	47	LEU	N-CA-C	-5.49	104.98	110.97
1	R	600	VAL	CA-C-N	5.49	125.46	120.03
1	R	600	VAL	C-N-CA	5.49	125.46	120.03
1	G	440	SER	CA-C-N	-5.48	114.94	120.31
1	G	440	SER	C-N-CA	-5.48	114.94	120.31
1	G	428	VAL	N-CA-C	5.47	116.55	108.45
1	N	410	GLU	N-CA-C	5.46	117.67	111.11
1	N	428	VAL	N-CA-C	5.46	116.14	108.17
1	D	62	THR	N-CA-C	-5.46	105.41	111.36
1	K	116	ILE	N-CA-C	5.45	115.44	107.37
1	B	321	GLU	N-CA-C	5.45	118.28	109.40
1	K	388	GLU	N-CA-C	-5.44	99.23	108.26
1	C	305	VAL	N-CA-C	5.43	115.71	108.11
1	H	620	ASN	CB-CA-C	-5.43	102.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	231	GLU	CA-C-N	-5.43	113.05	119.84
1	Q	231	GLU	C-N-CA	-5.43	113.05	119.84
1	K	479	VAL	N-CA-C	5.41	115.68	108.11
1	D	619	ARG	N-CA-C	5.40	118.08	111.82
1	J	600	VAL	CA-C-N	5.39	125.81	119.99
1	J	600	VAL	C-N-CA	5.39	125.81	119.99
1	P	600	VAL	CA-C-N	5.39	125.56	119.90
1	P	600	VAL	C-N-CA	5.39	125.56	119.90
1	P	135	ASP	N-CA-C	-5.38	107.08	113.97
1	I	347	CYS	N-CA-C	-5.38	105.08	111.69
1	K	65	LYS	N-CA-C	5.37	118.59	110.64
1	A	385	THR	N-CA-C	-5.36	100.66	109.40
1	B	600	VAL	N-CA-C	5.36	112.44	107.56
1	D	97	LYS	CA-C-N	-5.36	113.51	119.19
1	D	97	LYS	C-N-CA	-5.36	113.51	119.19
1	P	541	VAL	N-CA-CB	-5.36	104.88	110.82
1	D	109	ASN	N-CA-C	-5.35	105.45	112.41
1	J	605	LYS	N-CA-C	-5.35	106.80	113.38
1	A	444	VAL	CB-CA-C	5.35	118.11	110.84
1	N	611	VAL	CB-CA-C	-5.33	102.54	111.29
1	F	428	VAL	N-CA-C	5.33	115.79	108.12
1	D	91	THR	CB-CA-C	5.32	118.92	110.19
1	K	502	ASP	N-CA-C	5.32	117.16	110.24
1	F	611	VAL	CB-CA-C	-5.32	101.29	110.65
1	E	541	VAL	N-CA-CB	-5.31	104.93	110.72
1	Q	226	PHE	N-CA-C	5.30	118.46	108.65
1	C	444	VAL	N-CA-CB	5.28	117.33	110.99
1	M	330	SER	N-CA-C	5.28	117.41	109.23
1	K	292	LYS	N-CA-C	5.27	117.72	107.71
1	E	302	MET	N-CA-CB	-5.26	102.77	110.97
1	D	524	ALA	N-CA-C	5.25	117.92	111.82
1	A	16	VAL	N-CA-C	-5.25	100.30	108.44
1	H	248	PHE	N-CA-C	5.25	117.08	111.36
1	L	116	ILE	CB-CA-C	-5.24	103.02	110.83
1	B	121	GLU	N-CA-C	-5.23	101.34	109.24
1	G	495	ASP	N-CA-C	5.23	120.03	113.43
1	M	134	ALA	N-CA-C	5.23	117.42	108.90
1	I	264	ILE	CB-CA-C	-5.23	106.26	111.80
1	A	503	VAL	CB-CA-C	5.22	117.96	111.80
1	J	256	ALA	N-CA-C	5.22	116.22	108.60
1	K	219	SER	N-CA-C	-5.22	106.96	113.38
1	M	226	PHE	N-CA-C	5.21	117.91	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	VAL	N-CA-C	5.20	117.34	108.86
1	F	578	TRP	N-CA-C	-5.19	101.37	108.38
1	J	428	VAL	N-CA-C	5.18	117.20	108.81
1	E	315	GLU	N-CA-C	5.18	117.61	108.75
1	H	327	ASP	N-CA-C	-5.17	99.78	110.80
1	J	23	ASP	N-CA-C	5.17	116.61	111.07
1	R	640	GLN	N-CA-C	-5.16	101.46	109.72
1	L	278	ASN	N-CA-C	5.15	119.43	113.20
1	L	90	VAL	CB-CA-C	-5.15	103.47	110.42
1	G	253	VAL	N-CA-CB	5.14	116.14	110.53
1	K	494	GLU	N-CA-C	-5.14	105.32	111.03
1	H	208	SER	N-CA-C	5.14	118.65	112.38
1	K	500	ALA	N-CA-C	5.14	120.20	113.88
1	M	455	ASN	CA-C-N	5.13	124.93	119.28
1	M	455	ASN	C-N-CA	5.13	124.93	119.28
1	E	200	ASP	CB-CA-C	-5.13	102.22	110.74
1	C	204	LEU	N-CA-C	-5.13	105.74	112.41
1	O	198	GLU	N-CA-C	5.13	117.43	108.76
1	D	111	PRO	N-CA-C	-5.12	103.41	111.34
1	B	211	ALA	N-CA-C	5.12	117.59	111.71
1	F	173	THR	CB-CA-C	-5.11	101.15	111.17
1	J	562	CYS	N-CA-C	5.11	115.91	108.14
1	L	624	LEU	N-CA-C	5.11	116.57	108.96
1	A	432	GLU	N-CA-C	5.10	117.96	111.69
1	A	458	ASN	N-CA-C	5.10	117.93	107.37
1	P	532	GLN	N-CA-CB	-5.10	103.13	111.24
1	N	523	THR	N-CA-C	-5.10	105.80	111.36
1	L	15	TRP	N-CA-C	5.09	116.93	109.24
1	M	474	GLY	N-CA-C	5.09	119.05	112.54
1	E	546	VAL	N-CA-C	5.08	115.23	108.11
1	D	230	SER	N-CA-C	-5.08	101.03	108.79
1	Q	283	ILE	N-CA-C	-5.08	101.10	108.36
1	L	141	VAL	CB-CA-C	5.07	119.60	111.29
1	B	97	LYS	CA-C-N	-5.07	113.82	119.19
1	B	97	LYS	C-N-CA	-5.07	113.82	119.19
1	C	158	ALA	N-CA-C	-5.06	105.67	111.14
1	G	330	SER	N-CA-C	5.05	117.35	109.52
1	R	491	GLU	N-CA-C	5.05	117.63	108.69
1	H	292	LYS	N-CA-C	-5.05	100.22	108.76
1	J	473	HIS	N-CA-C	-5.03	102.44	109.69
1	I	432	GLU	N-CA-C	5.03	117.88	111.69
1	A	285	MET	N-CA-C	-5.03	106.73	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	458	ASN	N-CA-C	5.03	116.80	107.60
1	H	241	GLU	O-C-N	-5.03	116.26	122.19
1	P	174	GLY	N-CA-C	5.03	118.40	110.91
1	F	302	MET	N-CA-CB	-5.02	103.38	110.51
1	F	215	ASP	N-CA-C	5.02	117.74	109.76
1	F	118	VAL	N-CA-C	5.02	115.54	108.36
1	M	182	GLU	N-CA-C	-5.02	101.78	109.76
1	P	243	GLU	N-CA-C	5.02	117.40	111.33
1	C	517	ILE	N-CA-C	5.01	115.73	110.62
1	C	609	GLN	N-CA-C	-5.01	102.77	110.14
1	E	13	ARG	N-CA-C	-5.01	102.86	110.28
1	J	475	ASP	N-CA-C	-5.01	107.14	113.20
1	J	452	SER	N-CA-C	5.00	117.47	111.71
1	N	169	VAL	N-CA-C	5.00	115.06	107.75
1	R	352	MET	N-CA-C	5.00	118.64	112.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLU	Peptide
1	E	282	PHE	Peptide
1	E	316	MET	Peptide
1	H	282	PHE	Peptide
1	J	291	ASN	Peptide
1	J	597	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5106	0	4989	137	0
1	B	5084	0	4967	192	0
1	C	5091	0	4976	169	1
1	D	5078	0	4962	146	1
1	E	5069	0	4953	174	0
1	F	5084	0	4967	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	5070	0	4955	161	0
1	H	5091	0	4976	148	0
1	I	5122	0	5007	187	0
1	J	5122	0	5007	197	0
1	K	5106	0	4989	223	0
1	L	5122	0	5007	149	0
1	M	5049	0	4935	274	0
1	N	5084	0	4967	241	1
1	O	5106	0	4989	226	0
1	P	5069	0	4953	168	1
1	Q	5039	0	4927	242	0
1	R	5084	0	4967	212	0
2	A	26	0	19	0	0
2	B	26	0	19	2	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
2	E	26	0	19	3	0
2	F	26	0	19	2	0
2	G	26	0	19	2	0
2	H	26	0	19	1	0
2	I	26	0	19	1	0
2	J	26	0	19	0	0
2	K	26	0	19	3	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
2	N	26	0	19	2	0
2	O	26	0	19	0	0
2	P	26	0	19	3	0
2	Q	26	0	19	2	0
2	R	26	0	19	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	1	0
3	R	5	0	0	0	0
4	A	105	0	0	0	0
4	B	26	0	0	0	0
4	C	16	0	0	1	0
4	D	93	0	0	3	0
4	E	41	0	0	0	0
4	F	12	0	0	1	0
4	G	19	0	0	1	0
4	H	59	0	0	1	0
4	I	21	0	0	3	0
4	J	12	0	0	1	0
4	K	6	0	0	0	0
4	L	85	0	0	4	0
4	M	2	0	0	2	0
4	P	10	0	0	2	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
All	All	92645	0	89835	3367	2

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 18.

All (3367) 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:L:490:PRO:HB3	1:L:569:MET:CE	1.55	1.36
1:G:490:PRO:HB3	1:G:569:MET:CE	1.58	1.32
1:F:490:PRO:HB3	1:F:569:MET:CE	1.60	1.28
1:M:569:MET:HG3	1:M:624:LEU:CD1	1.67	1.23
1:B:490:PRO:HB3	1:B:569:MET:CE	1.71	1.20
1:D:497:GLN:NE2	1:D:497:GLN:H	1.42	1.18
1:N:379:LYS:HA	1:N:399:THR:HG22	1.28	1.16
1:A:490:PRO:HB3	1:A:569:MET:CE	1.76	1.16
1:E:478:ARG:HH21	1:E:478:ARG:HG2	0.99	1.15
1:L:273:ILE:HG13	1:L:275:MET:HE1	1.28	1.15
1:Q:375:ASP:HA	1:Q:399:THR:HG21	1.28	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:PRO:HB3	1:F:569:MET:HE1	1.22	1.14
1:O:393:GLY:HA3	1:O:405:ILE:CD1	1.77	1.13
1:Q:153:ARG:HG3	1:Q:153:ARG:HH11	1.04	1.12
1:Q:218:LEU:H	1:Q:303:GLN:NE2	1.44	1.12
1:J:597:SER:HB2	1:J:598:ALA:HB2	1.32	1.12
1:O:627:HIS:HB2	1:O:640:GLN:HB2	1.13	1.11
1:H:273:ILE:HG13	1:H:275:MET:HE1	1.21	1.11
1:H:490:PRO:HB3	1:H:569:MET:CE	1.81	1.11
1:L:67:HIS:CE1	1:L:91:THR:HG23	1.86	1.11
1:F:218:LEU:H	1:F:303:GLN:NE2	1.49	1.10
1:Q:68:VAL:HG13	1:Q:90:VAL:HG13	1.30	1.10
1:C:490:PRO:HB3	1:C:569:MET:CE	1.82	1.10
1:L:490:PRO:HB3	1:L:569:MET:HE1	1.26	1.09
1:B:490:PRO:HB3	1:B:569:MET:HE1	1.34	1.09
1:F:50:LEU:O	1:F:54:ILE:HD12	1.52	1.09
1:K:67:HIS:CE1	1:K:91:THR:HG22	1.85	1.09
1:L:67:HIS:HE1	1:L:91:THR:HG23	0.96	1.08
1:C:169:VAL:HG22	1:C:241:GLU:HG2	1.14	1.08
1:I:26:GLN:HG2	1:I:30:ARG:HH12	1.12	1.08
1:M:280:THR:HG23	1:M:281:THR:HG22	1.35	1.08
1:J:490:PRO:HB3	1:J:569:MET:CE	1.84	1.08
1:G:169:VAL:HG12	1:G:241:GLU:HG3	1.25	1.08
1:Q:264:ILE:O	1:Q:264:ILE:HG12	1.44	1.07
1:R:433:LYS:H	1:R:433:LYS:HE2	1.20	1.06
1:M:569:MET:HG3	1:M:624:LEU:HD12	1.32	1.06
1:N:54:ILE:CA	1:N:58:LYS:HZ3	1.69	1.06
1:O:227:ARG:NH2	1:O:261:SER:O	1.88	1.06
1:M:91:THR:HG22	1:M:117:THR:HG23	1.32	1.05
1:K:67:HIS:HE1	1:K:91:THR:HG22	0.94	1.05
1:Q:39:ASP:OD2	1:Q:298:ARG:HD3	1.56	1.05
1:C:168:ARG:HG2	1:C:168:ARG:HH11	0.90	1.05
1:A:490:PRO:HB3	1:A:569:MET:HE1	1.40	1.04
1:A:168:ARG:HG2	1:A:168:ARG:HH11	0.89	1.03
1:H:273:ILE:CG1	1:H:275:MET:HE1	1.88	1.03
1:N:55:ALA:N	1:N:58:LYS:HZ2	1.54	1.03
1:J:490:PRO:HB3	1:J:569:MET:HE3	1.07	1.03
1:I:51:LYS:HE2	1:I:85:GLU:OE2	1.56	1.03
1:N:269:MET:HG2	1:N:306:TYR:HE1	1.24	1.03
1:Q:168:ARG:HH11	1:Q:168:ARG:HG2	1.24	1.03
1:K:67:HIS:HE1	1:K:91:THR:CG2	1.69	1.03
1:M:478:ARG:HH21	1:M:478:ARG:HG2	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:444:VAL:HG13	1:N:479:VAL:HB	1.40	1.03
1:A:103:ALA:O	1:A:107:THR:HB	1.57	1.02
1:N:54:ILE:HA	1:N:58:LYS:NZ	1.75	1.02
1:C:450:TYR:H	1:C:459:HIS:HD2	1.08	1.02
1:N:54:ILE:HA	1:N:58:LYS:HZ3	0.87	1.02
1:I:210:THR:HG21	4:I:809:HOH:O	1.60	1.02
1:N:63:ASP:HB2	1:N:65:LYS:H	1.23	1.02
1:J:490:PRO:CB	1:J:569:MET:HE3	1.90	1.02
1:G:490:PRO:CB	1:G:569:MET:CE	2.38	1.01
1:H:547:GLU:OE2	1:H:550:ARG:NH1	1.92	1.01
1:I:497:GLN:HE21	1:I:497:GLN:N	1.56	1.01
1:A:420:ILE:HD11	1:A:428:VAL:HG22	1.43	1.01
1:H:490:PRO:HB3	1:H:569:MET:HE2	1.38	1.01
1:A:577:MET:HE1	1:A:639:PHE:CE1	1.97	1.00
1:C:168:ARG:HG2	1:C:168:ARG:NH1	1.72	1.00
1:I:67:HIS:HE1	1:I:91:THR:HG23	1.26	1.00
1:P:241:GLU:HG3	1:P:277:ARG:HH21	1.26	1.00
1:J:490:PRO:CB	1:J:569:MET:CE	2.39	1.00
1:Q:137:ILE:HG13	1:Q:169:VAL:HG12	1.44	1.00
1:K:68:VAL:HG22	1:K:136:ILE:HB	1.43	0.99
1:O:393:GLY:HA3	1:O:405:ILE:HD11	1.03	0.99
1:A:478:ARG:HG2	1:A:478:ARG:HH21	1.26	0.99
1:J:39:ASP:OD2	1:J:298:ARG:HD3	1.61	0.98
1:G:490:PRO:HB3	1:G:569:MET:HE1	1.44	0.98
1:H:497:GLN:NE2	1:H:497:GLN:H	1.60	0.98
1:H:478:ARG:HH21	1:H:478:ARG:HG2	1.29	0.98
1:H:497:GLN:H	1:H:497:GLN:HE21	1.09	0.98
1:Q:68:VAL:HG13	1:Q:90:VAL:CG1	1.94	0.98
1:I:26:GLN:HG2	1:I:30:ARG:NH1	1.76	0.98
1:K:273:ILE:HD12	1:K:275:MET:HE1	1.46	0.98
1:R:450:TYR:H	1:R:459:HIS:CD2	1.82	0.97
1:K:67:HIS:CE1	1:K:91:THR:CG2	2.47	0.97
1:G:490:PRO:CB	1:G:569:MET:HE1	1.95	0.97
1:H:480:GLU:OE2	1:H:482:HIS:HD2	1.44	0.97
1:D:490:PRO:HB3	1:D:569:MET:HE3	1.47	0.97
1:R:556:ARG:HH11	1:R:556:ARG:HG3	1.29	0.97
1:G:490:PRO:HB3	1:G:569:MET:HE3	1.47	0.96
1:A:67:HIS:HE1	1:A:91:THR:CG2	1.77	0.96
1:C:169:VAL:CG2	1:C:241:GLU:HG2	1.95	0.96
1:A:168:ARG:HG2	1:A:168:ARG:NH1	1.69	0.96
1:I:497:GLN:H	1:I:497:GLN:NE2	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:450:TYR:H	1:R:459:HIS:HD2	1.04	0.96
1:J:273:ILE:HG13	1:J:275:MET:HE1	1.45	0.96
1:E:317:ASN:HD22	1:E:317:ASN:H	0.99	0.96
1:M:478:ARG:HH21	1:M:478:ARG:CG	1.79	0.96
1:Q:42:ARG:NH1	1:Q:140:GLU:HG2	1.80	0.96
1:E:67:HIS:HE1	1:E:91:THR:HG23	1.30	0.96
1:J:597:SER:HB2	1:J:598:ALA:CB	1.94	0.96
1:A:497:GLN:NE2	1:A:497:GLN:H	1.63	0.95
1:N:438:THR:HG21	1:O:629:LEU:HD21	1.48	0.95
1:Q:218:LEU:N	1:Q:303:GLN:HE21	1.63	0.95
1:D:280:THR:HG23	1:D:281:THR:HG22	1.46	0.95
1:N:169:VAL:HG11	1:N:240:PHE:O	1.68	0.94
1:D:168:ARG:HG2	1:D:168:ARG:HH11	1.32	0.94
1:O:73:THR:HB	1:O:92:ALA:HB1	1.49	0.94
1:A:497:GLN:H	1:A:497:GLN:HE21	1.08	0.94
1:B:39:ASP:OD2	1:B:298:ARG:HD3	1.66	0.94
1:A:502:ASP:OD2	1:A:616:THR:HG21	1.66	0.94
1:H:480:GLU:OE2	1:H:482:HIS:CD2	2.21	0.94
1:F:42:ARG:NH1	1:F:140:GLU:HG2	1.83	0.94
1:M:450:TYR:H	1:M:459:HIS:HD2	1.01	0.94
1:E:67:HIS:CE1	1:E:91:THR:HG23	2.03	0.93
1:P:450:TYR:H	1:P:459:HIS:HD2	1.07	0.93
1:D:497:GLN:HE21	1:D:497:GLN:N	1.64	0.93
1:D:490:PRO:HB3	1:D:569:MET:CE	1.97	0.93
1:J:158:ALA:HA	1:J:162:LEU:HD23	1.50	0.93
1:N:168:ARG:HG2	1:N:168:ARG:HH11	1.34	0.93
1:N:255:GLU:HG2	1:N:321:GLU:HG2	1.51	0.92
1:A:228:GLU:OE2	1:A:290:LYS:NZ	2.02	0.92
1:J:168:ARG:HG2	1:J:168:ARG:HH11	1.33	0.92
1:B:450:TYR:H	1:B:459:HIS:HD2	0.99	0.92
1:E:259:HIS:HD2	1:E:260:SER:OG	1.51	0.92
1:P:157:GLU:HA	1:P:160:GLU:HG3	1.51	0.92
1:H:87:ALA:O	1:H:115:LYS:HE3	1.67	0.92
1:A:133:ARG:HB2	1:A:164:LYS:HG3	1.51	0.92
1:E:490:PRO:HB3	1:E:569:MET:CE	1.99	0.92
1:O:218:LEU:H	1:O:303:GLN:NE2	1.68	0.92
1:E:169:VAL:HG12	1:E:241:GLU:HG2	1.52	0.92
1:J:497:GLN:H	1:J:497:GLN:HE21	1.16	0.92
1:L:490:PRO:CB	1:L:569:MET:HE1	2.00	0.92
1:D:478:ARG:HG2	1:D:478:ARG:HH21	1.35	0.91
1:E:478:ARG:HG2	1:E:478:ARG:NH2	1.79	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:ARG:NH1	1:L:140:GLU:HG2	1.85	0.91
1:P:490:PRO:HB3	1:P:569:MET:CE	2.00	0.91
1:D:168:ARG:NH2	1:D:276:ASP:O	2.03	0.91
1:F:218:LEU:H	1:F:303:GLN:HE21	1.13	0.91
1:E:42:ARG:NH1	1:E:140:GLU:HG2	1.84	0.91
1:H:117:THR:OG1	1:J:131:GLY:HA3	1.70	0.91
1:H:273:ILE:HG13	1:H:275:MET:CE	2.00	0.91
1:P:478:ARG:HH21	1:P:478:ARG:HG2	1.36	0.91
1:Q:180:PRO:HG2	1:Q:230:SER:HB3	1.52	0.91
1:D:497:GLN:H	1:D:497:GLN:HE21	0.97	0.91
1:C:137:ILE:HB	1:C:169:VAL:HG12	1.50	0.91
1:D:480:GLU:OE2	1:D:482:HIS:HD2	1.54	0.91
1:O:39:ASP:OD2	1:O:298:ARG:HD3	1.71	0.90
1:P:42:ARG:NH1	1:P:140:GLU:HG2	1.86	0.90
1:L:168:ARG:HG2	1:L:168:ARG:HH11	1.35	0.90
1:C:168:ARG:HH11	1:C:168:ARG:CG	1.81	0.90
1:M:91:THR:HG22	1:M:117:THR:CG2	2.02	0.90
1:O:497:GLN:HE21	1:O:497:GLN:H	1.14	0.90
1:L:169:VAL:HG13	1:L:241:GLU:HG2	1.52	0.90
1:R:196:ASN:HB2	1:R:201:GLU:OE2	1.71	0.90
1:M:497:GLN:NE2	1:M:497:GLN:H	1.68	0.90
1:D:434:VAL:CG1	1:D:469:LEU:HD13	2.02	0.90
1:C:490:PRO:HB3	1:C:569:MET:HE3	1.52	0.90
1:M:42:ARG:HH11	1:M:140:GLU:HG3	1.36	0.90
1:L:67:HIS:HE1	1:L:91:THR:CG2	1.81	0.90
1:D:42:ARG:HH11	1:D:140:GLU:HG2	1.34	0.90
1:L:379:LYS:HA	1:L:399:THR:HG23	1.53	0.90
1:I:450:TYR:H	1:I:459:HIS:HD2	1.12	0.89
1:K:123:SER:HB3	2:K:701:SAH:HN62	1.34	0.89
1:M:178:ILE:O	1:M:233:ILE:HG22	1.72	0.89
1:G:379:LYS:HA	1:G:399:THR:HG23	1.55	0.89
1:C:314:VAL:HG21	1:C:320:PHE:CD2	2.06	0.89
1:E:379:LYS:HA	1:E:399:THR:CG2	2.03	0.89
1:A:67:HIS:HE1	1:A:91:THR:HG22	1.37	0.89
1:A:168:ARG:HH11	1:A:168:ARG:CG	1.81	0.89
1:M:483:MET:HE1	1:M:550:ARG:HG2	1.51	0.89
1:P:42:ARG:HH11	1:P:140:GLU:HG2	1.36	0.89
1:I:379:LYS:HA	1:I:399:THR:HG23	1.53	0.89
1:J:370:PHE:O	1:J:374:VAL:HG23	1.72	0.89
1:A:434:VAL:CG1	1:A:469:LEU:HD13	2.03	0.88
1:N:55:ALA:N	1:N:58:LYS:NZ	2.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:196:ASN:HB2	1:Q:201:GLU:OE2	1.72	0.88
1:O:490:PRO:HB3	1:O:569:MET:CE	2.03	0.88
1:M:450:TYR:H	1:M:459:HIS:CD2	1.89	0.88
1:F:490:PRO:CB	1:F:569:MET:HE1	2.04	0.88
1:G:379:LYS:HA	1:G:399:THR:CG2	2.04	0.88
1:I:67:HIS:CE1	1:I:91:THR:HG23	2.08	0.88
1:F:497:GLN:HE21	1:F:497:GLN:H	1.19	0.88
1:O:643:LYS:H	1:O:643:LYS:HD2	1.37	0.88
1:R:291:ASN:HB3	1:R:295:TYR:HB2	1.56	0.88
1:L:490:PRO:CB	1:L:569:MET:CE	2.50	0.88
1:Q:153:ARG:HG3	1:Q:153:ARG:NH1	1.74	0.88
1:J:194:ARG:HG2	1:J:201:GLU:HB2	1.54	0.87
1:R:547:GLU:OE2	1:R:550:ARG:NH2	2.07	0.87
1:Q:68:VAL:CG1	1:Q:90:VAL:HG13	2.03	0.87
1:D:379:LYS:HA	1:D:399:THR:HG23	1.56	0.87
1:M:497:GLN:H	1:M:497:GLN:HE21	1.19	0.87
1:O:373:GLU:O	1:O:377:LEU:HD12	1.75	0.87
1:B:490:PRO:CB	1:B:569:MET:HE1	2.05	0.87
1:H:450:TYR:H	1:H:459:HIS:HD2	1.22	0.87
1:M:68:VAL:HG22	1:M:136:ILE:HB	1.55	0.87
1:Q:450:TYR:H	1:Q:459:HIS:HD2	1.18	0.87
1:N:147:ILE:HD11	1:N:331:LEU:HD13	1.57	0.86
1:I:570:SER:HB3	1:I:622:LYS:HG2	1.54	0.86
1:B:550:ARG:H	1:B:560:GLN:HE22	1.23	0.86
1:N:478:ARG:HG2	1:N:478:ARG:HH21	1.39	0.86
1:D:379:LYS:HA	1:D:399:THR:CG2	2.06	0.86
1:E:57:LYS:O	1:E:66:VAL:HG21	1.75	0.86
1:D:145:GLU:HA	1:D:269:MET:HE1	1.58	0.86
1:F:379:LYS:HA	1:F:399:THR:HG22	1.57	0.86
1:P:146:LEU:HD23	1:P:146:LEU:H	1.40	0.86
1:K:42:ARG:NH1	1:K:140:GLU:HG2	1.89	0.86
1:M:379:LYS:HA	1:M:399:THR:CG2	2.06	0.86
1:J:483:MET:HB3	1:J:582:GLU:HG3	1.55	0.86
1:M:181:VAL:HG21	1:M:268:LEU:HD11	1.57	0.86
1:F:39:ASP:OD2	1:F:298:ARG:HD3	1.76	0.85
1:O:393:GLY:CA	1:O:405:ILE:HD11	1.99	0.85
1:P:104:ARG:HB2	1:P:104:ARG:CZ	2.04	0.85
1:F:450:TYR:H	1:F:459:HIS:HD2	1.25	0.85
1:I:323:VAL:HG11	1:I:340:LYS:HD3	1.57	0.85
1:D:42:ARG:NH1	1:D:140:GLU:HG2	1.90	0.85
1:N:50:LEU:O	1:N:54:ILE:HG23	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:153:ARG:HH11	1:Q:153:ARG:CG	1.89	0.85
1:L:168:ARG:NH1	1:L:241:GLU:OE2	2.08	0.85
1:F:218:LEU:HD12	1:F:303:GLN:CB	2.06	0.85
1:M:478:ARG:HG2	1:M:478:ARG:NH2	1.89	0.85
1:C:450:TYR:H	1:C:459:HIS:CD2	1.94	0.85
1:L:490:PRO:HB3	1:L:569:MET:HE2	1.58	0.85
1:M:379:LYS:HA	1:M:399:THR:HG23	1.57	0.85
1:N:58:LYS:HE2	1:N:66:VAL:HG21	1.57	0.85
1:K:569:MET:HG3	1:K:624:LEU:HD11	1.58	0.85
1:R:622:LYS:H	1:R:622:LYS:HD2	1.41	0.85
1:N:566:ILE:CG2	1:N:569:MET:HE3	2.07	0.84
1:B:104:ARG:O	1:B:108:SER:HB3	1.77	0.84
1:K:169:VAL:HG13	1:K:241:GLU:HG2	1.57	0.84
1:F:565:ASN:HD21	1:F:644:SER:HB2	1.42	0.84
1:B:163:ALA:HB1	1:B:167:CYS:SG	2.17	0.84
1:O:528:ILE:H	1:O:528:ILE:HD12	1.41	0.84
1:J:438:THR:HG21	1:K:629:LEU:HD21	1.59	0.84
1:A:490:PRO:CB	1:A:569:MET:HE1	2.08	0.84
1:D:434:VAL:HG12	1:D:469:LEU:HD13	1.60	0.84
1:G:497:GLN:HE21	1:G:497:GLN:H	1.25	0.84
1:O:373:GLU:HG3	1:O:377:LEU:HD11	1.59	0.83
1:F:553:ILE:HG22	1:F:553:ILE:O	1.77	0.83
1:P:450:TYR:H	1:P:459:HIS:CD2	1.94	0.83
1:E:87:ALA:O	1:E:115:LYS:HE2	1.78	0.83
1:R:51:LYS:HZ2	1:R:51:LYS:HB2	1.43	0.83
1:A:273:ILE:HG13	1:A:275:MET:HE1	1.60	0.83
1:D:490:PRO:CB	1:D:569:MET:CE	2.56	0.83
1:A:67:HIS:CE1	1:A:91:THR:CG2	2.62	0.83
1:O:233:ILE:HD11	1:O:254:ARG:CB	2.08	0.83
1:R:66:VAL:HA	1:R:135:ASP:OD2	1.76	0.83
1:F:150:GLY:O	1:F:154:THR:OG1	1.96	0.83
1:N:379:LYS:HA	1:N:399:THR:CG2	2.08	0.83
1:N:480:GLU:OE2	1:N:482:HIS:HD2	1.60	0.83
1:R:379:LYS:HA	1:R:399:THR:CG2	2.08	0.83
1:Q:378:SER:HB2	1:Q:399:THR:HG23	1.60	0.82
1:K:550:ARG:H	1:K:560:GLN:HE22	1.24	0.82
1:L:577:MET:HE2	1:L:626:LEU:HD11	1.61	0.82
1:N:27:GLU:OE2	1:N:96:PHE:CE1	2.32	0.82
1:N:254:ARG:O	1:N:321:GLU:HA	1.79	0.82
1:B:450:TYR:H	1:B:459:HIS:CD2	1.91	0.82
1:M:110:SER:HB2	1:M:111:PRO:HD2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:254:ARG:O	1:Q:321:GLU:HA	1.79	0.82
1:G:66:VAL:HG12	1:G:87:ALA:HA	1.62	0.82
1:O:450:TYR:H	1:O:459:HIS:HD2	1.27	0.82
1:K:379:LYS:HA	1:K:399:THR:HG23	1.60	0.82
1:K:388:GLU:OE1	1:K:452:SER:HB2	1.79	0.82
1:L:631:ASP:OD1	1:L:633:SER:HB2	1.80	0.82
1:A:506:VAL:HG12	1:A:507:ASN:HD22	1.45	0.82
1:L:577:MET:CE	1:L:641:PHE:HZ	1.92	0.82
1:P:104:ARG:O	1:P:108:SER:HB2	1.80	0.81
1:J:189:PHE:CD1	1:J:359:TYR:HB2	2.14	0.81
1:F:553:ILE:O	1:F:553:ILE:CG2	2.29	0.81
1:N:63:ASP:CB	1:N:65:LYS:H	1.93	0.81
1:K:42:ARG:HH12	1:K:140:GLU:HG2	1.45	0.81
1:C:314:VAL:CG2	1:C:320:PHE:CD2	2.63	0.81
1:Q:183:SER:H	1:Q:265:ASP:HB2	1.46	0.81
1:Q:478:ARG:HG2	1:Q:478:ARG:HH21	1.45	0.81
1:H:42:ARG:HH11	1:H:140:GLU:HG2	1.46	0.81
1:J:243:GLU:OE1	1:J:243:GLU:N	2.12	0.81
1:D:291:ASN:H	1:D:292:LYS:HZ3	1.28	0.81
1:P:259:HIS:HD2	1:P:260:SER:OG	1.62	0.81
1:C:480:GLU:OE2	1:C:482:HIS:HD2	1.64	0.81
1:G:169:VAL:CG1	1:G:241:GLU:HG3	2.09	0.81
1:M:50:LEU:HD23	1:M:170:VAL:HG21	1.62	0.81
1:N:269:MET:HG2	1:N:306:TYR:CE1	2.13	0.81
1:J:497:GLN:H	1:J:497:GLN:NE2	1.78	0.81
1:R:556:ARG:HH11	1:R:556:ARG:CG	1.93	0.81
1:B:216:VAL:O	1:B:302:MET:HG2	1.81	0.80
1:E:379:LYS:HA	1:E:399:THR:HG23	1.63	0.80
1:I:275:MET:HA	1:I:275:MET:HE2	1.61	0.80
1:M:444:VAL:HG13	1:M:479:VAL:HB	1.61	0.80
1:D:450:TYR:H	1:D:459:HIS:HD2	1.27	0.80
1:Q:216:VAL:O	1:Q:302:MET:HG2	1.81	0.80
1:Q:264:ILE:HD11	1:Q:267:LEU:HD21	1.63	0.80
1:M:95:VAL:CG2	1:M:122:ARG:HG3	2.11	0.80
1:P:379:LYS:HA	1:P:399:THR:HG23	1.63	0.80
1:F:275:MET:HE3	1:F:283:ILE:HG13	1.61	0.80
1:E:478:ARG:HH21	1:E:478:ARG:CG	1.90	0.80
1:Q:264:ILE:O	1:Q:264:ILE:CG1	2.29	0.80
1:L:451:MET:HE2	1:L:451:MET:O	1.82	0.80
1:E:258:ALA:HB3	1:E:315:GLU:O	1.82	0.79
1:E:317:ASN:H	1:E:317:ASN:ND2	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:379:LYS:HA	1:R:399:THR:HG21	1.64	0.79
1:R:567:ASP:HA	1:R:623:SER:HB2	1.64	0.79
1:B:140:GLU:HG3	1:B:140:GLU:O	1.82	0.79
1:M:39:ASP:OD2	1:M:298:ARG:HD2	1.81	0.79
1:J:450:TYR:H	1:J:459:HIS:HD2	1.31	0.79
1:J:596:SER:O	1:J:599:GLY:N	2.11	0.79
1:I:169:VAL:HG13	1:I:241:GLU:HG2	1.65	0.79
1:P:5:LYS:HA	1:R:420:ILE:HD11	1.65	0.79
1:D:169:VAL:HG13	1:D:241:GLU:HG2	1.63	0.79
1:F:50:LEU:O	1:F:54:ILE:CD1	2.31	0.79
1:B:39:ASP:O	1:B:43:ASN:ND2	2.16	0.79
1:N:242:HIS:HB3	1:N:245:LYS:HD3	1.64	0.79
1:K:141:VAL:HG13	1:K:141:VAL:O	1.81	0.79
1:L:210:THR:HB	4:L:815:HOH:O	1.83	0.79
1:B:218:LEU:HD22	1:B:221:MET:HE2	1.64	0.79
1:G:158:ALA:HA	1:G:162:LEU:HD23	1.64	0.79
1:M:132:SER:N	1:P:104:ARG:NH2	2.31	0.79
1:M:569:MET:CG	1:M:624:LEU:CD1	2.58	0.78
1:Q:168:ARG:HH11	1:Q:168:ARG:CG	1.96	0.78
1:B:566:ILE:HG22	1:B:569:MET:HE3	1.64	0.78
1:J:239:ASP:OD2	1:J:242:HIS:HD2	1.66	0.78
1:A:169:VAL:HG13	1:A:241:GLU:HG2	1.63	0.78
1:M:41:ASP:O	1:M:45:LYS:HB2	1.83	0.78
1:O:233:ILE:HD11	1:O:254:ARG:HB3	1.65	0.78
1:Q:218:LEU:N	1:Q:303:GLN:NE2	2.25	0.78
1:A:490:PRO:HB3	1:A:569:MET:HE2	1.65	0.78
1:M:480:GLU:OE2	1:M:482:HIS:HD2	1.67	0.78
1:G:497:GLN:H	1:G:497:GLN:NE2	1.82	0.78
1:R:73:THR:OG1	1:R:76:GLY:HA2	1.83	0.78
1:O:42:ARG:NH1	1:O:140:GLU:HG2	1.98	0.78
1:K:76:GLY:O	1:K:79:SER:N	2.17	0.78
1:G:450:TYR:H	1:G:459:HIS:HD2	1.31	0.78
1:K:450:TYR:H	1:K:459:HIS:HD2	1.30	0.78
1:E:317:ASN:HD22	1:E:317:ASN:N	1.75	0.78
1:L:42:ARG:HH11	1:L:140:GLU:HG2	1.48	0.78
1:N:142:PHE:CD1	1:N:146:LEU:HD12	2.20	0.77
1:N:133:ARG:HB3	1:N:133:ARG:HH21	1.48	0.77
1:Q:178:ILE:HD13	1:Q:235:ALA:HB2	1.65	0.77
1:K:541:VAL:HG23	1:K:601:PRO:HG3	1.66	0.77
1:F:450:TYR:H	1:F:459:HIS:CD2	2.02	0.77
1:N:67:HIS:H	1:N:135:ASP:HB2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:232:PRO:HG2	1:Q:290:LYS:HE2	1.65	0.77
1:J:480:GLU:OE2	1:J:482:HIS:HD2	1.66	0.77
1:D:67:HIS:HE1	1:D:91:THR:CG2	1.96	0.77
1:B:490:PRO:CB	1:B:569:MET:CE	2.60	0.77
1:C:490:PRO:CB	1:C:569:MET:CE	2.63	0.77
1:M:280:THR:HG23	1:M:281:THR:CG2	2.14	0.77
1:Q:247:ILE:HG12	1:Q:250:GLU:OE2	1.84	0.77
1:B:243:GLU:OE1	1:B:243:GLU:N	2.13	0.77
1:J:383:VAL:HG21	1:J:445:LEU:HD22	1.67	0.77
1:E:434:VAL:CG1	1:E:469:LEU:HD13	2.15	0.77
1:G:103:ALA:O	1:G:107:THR:HG23	1.84	0.77
1:Q:218:LEU:H	1:Q:303:GLN:HE21	0.78	0.77
1:B:179:VAL:HG12	1:B:180:PRO:O	1.85	0.77
1:F:104:ARG:O	1:F:108:SER:HB3	1.84	0.77
1:A:450:TYR:H	1:A:459:HIS:HD2	1.33	0.77
1:G:95:VAL:HG22	1:G:95:VAL:O	1.85	0.77
1:N:530:ASP:OD1	1:N:531:GLU:N	2.17	0.77
1:E:41:ASP:C	1:E:41:ASP:OD1	2.27	0.76
1:B:42:ARG:NH1	1:B:140:GLU:HG2	2.00	0.76
1:F:206:ARG:HH12	1:F:310:GLU:HG3	1.50	0.76
1:N:566:ILE:HG22	1:N:569:MET:CE	2.15	0.76
1:B:269:MET:HG2	1:B:306:TYR:HE2	1.50	0.76
1:C:489:ILE:O	1:C:576:PRO:HD2	1.86	0.76
1:H:450:TYR:H	1:H:459:HIS:CD2	2.04	0.76
1:O:411:ARG:O	1:O:415:ILE:HD12	1.84	0.76
1:R:450:TYR:N	1:R:459:HIS:HD2	1.80	0.76
1:A:67:HIS:CE1	1:A:91:THR:HG22	2.20	0.76
1:I:273:ILE:HD12	1:I:275:MET:HE1	1.68	0.76
1:D:80:LEU:HB3	1:D:509:PHE:CE1	2.19	0.76
1:R:478:ARG:HH21	1:R:478:ARG:HG2	1.50	0.76
1:L:467:GLU:HG3	1:L:555:GLY:O	1.86	0.76
1:M:278:ASN:O	1:M:280:THR:HG22	1.85	0.76
1:D:291:ASN:H	1:D:292:LYS:NZ	1.84	0.75
1:H:497:GLN:HE21	1:H:497:GLN:N	1.83	0.75
1:I:227:ARG:NH2	1:I:261:SER:O	2.19	0.75
1:M:222:LYS:O	1:M:225:GLU:HG2	1.86	0.75
1:K:480:GLU:OE2	1:K:482:HIS:HD2	1.67	0.75
1:F:218:LEU:HD12	1:F:303:GLN:HB3	1.67	0.75
1:C:4:GLU:OE2	1:C:13:ARG:HD3	1.86	0.75
1:Q:232:PRO:CG	1:Q:290:LYS:HE2	2.17	0.75
1:Q:276:ASP:O	1:Q:277:ARG:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:568:ASN:O	1:I:572:SER:OG	2.03	0.75
1:M:412:PHE:HE2	1:M:451:MET:HG2	1.51	0.75
1:Q:480:GLU:HG3	1:Q:584:GLY:H	1.52	0.75
1:I:434:VAL:HG12	1:I:469:LEU:HD13	1.69	0.75
1:C:42:ARG:NH1	1:C:140:GLU:HG2	2.02	0.75
1:C:616:THR:O	1:C:619:ARG:HG2	1.85	0.75
1:H:478:ARG:HH21	1:H:478:ARG:CG	2.00	0.75
1:O:442:ASP:O	1:O:478:ARG:HB2	1.87	0.75
1:R:291:ASN:C	1:R:292:LYS:HD2	2.12	0.75
1:N:450:TYR:H	1:N:459:HIS:HD2	1.34	0.75
1:J:168:ARG:HG2	1:J:168:ARG:NH1	2.02	0.75
1:I:141:VAL:O	1:I:141:VAL:HG12	1.85	0.74
1:M:553:ILE:HG13	1:M:553:ILE:O	1.84	0.74
1:B:169:VAL:HG13	1:B:241:GLU:HG2	1.70	0.74
1:E:42:ARG:HH12	1:E:140:GLU:HG2	1.49	0.74
1:E:450:TYR:H	1:E:459:HIS:HD2	1.32	0.74
1:M:5:LYS:HA	1:O:420:ILE:HD11	1.69	0.74
1:M:615:ILE:O	1:M:617:ALA:N	2.20	0.74
1:C:4:GLU:OE2	1:C:13:ARG:CD	2.36	0.74
1:F:275:MET:CE	1:F:283:ILE:HG13	2.16	0.74
1:E:497:GLN:NE2	1:E:497:GLN:H	1.84	0.74
1:F:497:GLN:H	1:F:497:GLN:NE2	1.86	0.74
1:M:95:VAL:HG21	1:M:122:ARG:HG3	1.69	0.74
1:O:169:VAL:HG13	1:O:241:GLU:HG2	1.68	0.74
1:O:566:ILE:O	1:O:623:SER:HA	1.85	0.74
1:N:150:GLY:O	1:N:154:THR:OG1	2.06	0.74
1:P:490:PRO:HB3	1:P:569:MET:HE1	1.70	0.74
1:L:577:MET:HE3	1:L:641:PHE:HZ	1.51	0.74
1:R:371:LYS:O	1:R:375:ASP:OD1	2.06	0.74
1:D:67:HIS:HE1	1:D:91:THR:HG23	1.49	0.74
1:M:480:GLU:OE2	1:M:482:HIS:CD2	2.41	0.74
1:C:67:HIS:HE1	1:C:91:THR:HG22	1.53	0.74
1:O:4:GLU:OE2	1:O:13:ARG:HD3	1.88	0.74
1:R:51:LYS:HB2	1:R:51:LYS:NZ	2.02	0.73
1:H:66:VAL:N	1:H:88:ASP:OD2	2.21	0.73
1:Q:590:THR:O	1:Q:609:GLN:NE2	2.20	0.73
1:R:384:ALA:HB3	1:R:444:VAL:HG12	1.70	0.73
1:B:314:VAL:HG22	1:B:315:GLU:H	1.53	0.73
1:M:450:TYR:N	1:M:459:HIS:HD2	1.81	0.73
1:O:382:HIS:CD2	1:O:441:PRO:HA	2.23	0.73
1:K:271:TRP:O	1:K:285:MET:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:MET:HA	1:J:300:HIS:CD2	2.22	0.73
1:O:643:LYS:H	1:O:643:LYS:CD	1.99	0.73
1:N:104:ARG:O	1:N:108:SER:OG	2.04	0.73
1:J:273:ILE:CG1	1:J:275:MET:HE1	2.19	0.73
1:O:627:HIS:CB	1:O:640:GLN:HB2	2.08	0.73
1:K:550:ARG:N	1:K:560:GLN:HE22	1.87	0.73
1:L:103:ALA:O	1:L:107:THR:HB	1.89	0.73
1:Q:222:LYS:HB2	1:Q:225:GLU:HG2	1.71	0.73
1:L:378:SER:HB2	1:L:399:THR:HG22	1.71	0.73
1:I:278:ASN:O	1:I:280:THR:HG23	1.89	0.72
1:K:73:THR:OG1	1:K:76:GLY:HA2	1.89	0.72
1:H:42:ARG:NH1	1:H:140:GLU:HG2	2.04	0.72
1:H:490:PRO:CB	1:H:569:MET:CE	2.64	0.72
1:N:81:MET:O	1:N:84:ARG:O	2.07	0.72
1:B:218:LEU:H	1:B:303:GLN:NE2	1.87	0.72
1:B:392:LEU:HD23	1:B:392:LEU:O	1.89	0.72
1:M:42:ARG:NH1	1:M:140:GLU:HG3	2.04	0.72
1:M:245:LYS:HE3	1:R:337:GLY:HA2	1.70	0.72
1:B:43:ASN:H	1:B:43:ASN:HD22	1.38	0.72
1:M:412:PHE:CE2	1:M:451:MET:HG2	2.24	0.72
1:N:87:ALA:HA	1:N:88:ASP:HB2	1.69	0.72
1:D:39:ASP:OD2	1:D:298:ARG:HD3	1.88	0.72
1:H:549:LEU:HD23	1:H:637:ILE:HD13	1.70	0.72
1:M:126:VAL:H	1:M:161:ARG:NH2	1.86	0.72
1:O:190:ASN:HD21	1:O:209:GLY:HA3	1.53	0.72
1:O:497:GLN:H	1:O:497:GLN:NE2	1.87	0.72
1:P:365:PHE:O	1:P:371:LYS:CE	2.37	0.72
1:E:146:LEU:HB3	1:E:271:TRP:CD1	2.25	0.72
1:H:244:GLU:CD	1:H:244:GLU:H	1.97	0.72
1:A:478:ARG:HH21	1:A:478:ARG:CG	2.03	0.72
1:Q:570:SER:HB2	1:Q:622:LYS:HD3	1.72	0.72
1:I:434:VAL:CG1	1:I:469:LEU:HD13	2.20	0.72
1:N:39:ASP:OD2	1:N:298:ARG:CD	2.38	0.72
1:L:497:GLN:HE21	1:L:497:GLN:H	1.35	0.72
1:F:203:PRO:HA	1:F:422:TYR:CD2	2.25	0.71
1:F:244:GLU:OE1	1:F:245:LYS:HG3	1.90	0.71
1:H:169:VAL:HG12	1:H:241:GLU:HG2	1.70	0.71
1:Q:450:TYR:H	1:Q:459:HIS:CD2	2.07	0.71
1:F:616:THR:O	1:F:619:ARG:NH1	2.21	0.71
1:P:57:LYS:HE2	1:P:135:ASP:HB3	1.71	0.71
1:R:176:VAL:CG1	1:R:236:PHE:HB2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:GLU:OE1	2:F:701:SAH:O2'	2.08	0.71
1:E:259:HIS:CD2	1:E:260:SER:OG	2.41	0.71
1:P:317:ASN:ND2	1:P:317:ASN:O	2.22	0.71
1:P:478:ARG:HH21	1:P:478:ARG:CG	2.03	0.71
1:Q:367:ASN:OD1	1:Q:370:PHE:HB2	1.90	0.71
1:M:91:THR:CG2	1:M:117:THR:HG23	2.14	0.71
1:N:133:ARG:HG3	1:N:164:LYS:HG3	1.73	0.71
1:E:550:ARG:H	1:E:560:GLN:HE22	1.37	0.71
1:I:450:TYR:H	1:I:459:HIS:CD2	2.03	0.71
1:M:45:LYS:O	1:M:275:MET:HG2	1.89	0.71
1:B:145:GLU:HG2	1:B:331:LEU:HD22	1.73	0.71
1:C:244:GLU:HA	1:C:244:GLU:OE2	1.91	0.71
1:M:145:GLU:HG3	1:M:331:LEU:HD13	1.72	0.71
1:I:443:ILE:HG12	1:I:445:LEU:HD13	1.73	0.71
1:Q:217:GLN:NE2	1:Q:298:ARG:O	2.14	0.71
1:B:460:LEU:HD21	1:B:579:MET:HE1	1.73	0.71
1:N:55:ALA:HA	1:N:58:LYS:HD2	1.73	0.71
1:O:490:PRO:HB3	1:O:569:MET:HE3	1.72	0.71
1:Q:169:VAL:HG21	1:Q:240:PHE:HB2	1.73	0.71
1:J:173:THR:HG22	1:J:274:ASP:HB3	1.71	0.70
1:K:412:PHE:HE2	1:K:451:MET:HG2	1.56	0.70
1:E:595:ILE:CG2	1:E:599:GLY:HA2	2.21	0.70
1:K:420:ILE:HD11	1:K:428:VAL:HG22	1.72	0.70
1:K:547:GLU:OE2	1:K:550:ARG:NH1	2.20	0.70
1:B:497:GLN:H	1:B:497:GLN:HE21	1.39	0.70
1:M:489:ILE:O	1:M:576:PRO:HD2	1.91	0.70
1:B:241:GLU:HB2	1:B:277:ARG:HH21	1.56	0.70
1:K:138:VAL:HG23	1:K:170:VAL:HB	1.71	0.70
1:M:321:GLU:O	1:M:322:ILE:HD12	1.90	0.70
1:B:450:TYR:N	1:B:459:HIS:HD2	1.82	0.70
1:I:490:PRO:HB3	1:I:569:MET:CE	2.21	0.70
1:R:489:ILE:O	1:R:576:PRO:HD2	1.91	0.70
1:N:566:ILE:HG22	1:N:569:MET:HE3	1.73	0.70
1:P:269:MET:HG2	1:P:306:TYR:HE1	1.55	0.70
1:K:460:LEU:HB3	1:K:463:LEU:HD23	1.72	0.70
1:B:168:ARG:NH1	1:B:241:GLU:OE2	2.24	0.70
1:H:275:MET:HE3	1:H:283:ILE:H	1.56	0.70
1:N:88:ASP:O	1:N:89:LYS:HG3	1.92	0.70
1:B:66:VAL:HG12	1:B:67:HIS:N	2.07	0.70
1:B:227:ARG:NH2	1:B:261:SER:O	2.25	0.70
1:C:95:VAL:HG21	1:C:122:ARG:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ASP:OD2	1:G:298:ARG:HD3	1.91	0.70
1:R:269:MET:HG2	1:R:306:TYR:HE1	1.57	0.70
1:E:84:ARG:NH1	1:E:509:PHE:CZ	2.60	0.69
1:G:22:TYR:CE2	1:G:26:GLN:OE1	2.45	0.69
1:D:480:GLU:OE2	1:D:482:HIS:CD2	2.41	0.69
1:I:73:THR:OG1	1:I:76:GLY:HA2	1.92	0.69
1:N:566:ILE:HG21	1:N:569:MET:HE3	1.73	0.69
1:R:349:LEU:HD12	1:R:415:ILE:HD13	1.74	0.69
1:G:547:GLU:OE2	1:G:550:ARG:NH2	2.24	0.69
1:H:169:VAL:CG1	1:H:241:GLU:HG2	2.22	0.69
1:I:550:ARG:H	1:I:560:GLN:HE22	1.38	0.69
1:O:233:ILE:HD11	1:O:254:ARG:HB2	1.74	0.69
1:K:169:VAL:HG13	1:K:241:GLU:CG	2.21	0.69
1:A:420:ILE:CD1	1:A:428:VAL:HG22	2.21	0.69
1:B:497:GLN:H	1:B:497:GLN:NE2	1.90	0.69
1:F:206:ARG:HH12	1:F:310:GLU:CG	2.06	0.69
1:J:193:PRO:HA	1:J:362:ASN:HD21	1.57	0.69
1:B:73:THR:HG22	1:B:94:GLU:HB2	1.72	0.69
1:P:278:ASN:HB2	1:P:280:THR:HG22	1.74	0.69
1:K:516:GLU:O	1:K:520:LYS:HG3	1.91	0.69
1:D:490:PRO:CB	1:D:569:MET:HE1	2.21	0.69
1:B:392:LEU:HD23	1:B:392:LEU:C	2.17	0.69
1:B:447:GLU:N	1:B:448:PRO:HA	2.08	0.69
1:G:27:GLU:HG2	1:G:96:PHE:CE1	2.26	0.69
1:H:269:MET:HG2	1:H:306:TYR:CE1	2.28	0.69
1:N:169:VAL:CG1	1:N:241:GLU:HG2	2.22	0.69
1:P:210:THR:HG21	4:P:810:HOH:O	1.93	0.69
1:J:67:HIS:HE1	1:J:91:THR:HG22	1.57	0.69
1:K:497:GLN:NE2	1:K:573:ASN:ND2	2.40	0.69
1:E:450:TYR:H	1:E:459:HIS:CD2	2.09	0.69
1:Q:42:ARG:HH12	1:Q:140:GLU:HG2	1.58	0.69
1:A:269:MET:HG2	1:A:306:TYR:HE1	1.58	0.69
1:I:210:THR:HB	4:I:807:HOH:O	1.92	0.69
1:M:51:LYS:HG2	1:M:85:GLU:HG2	1.73	0.69
1:M:483:MET:HE1	1:M:550:ARG:CG	2.23	0.69
1:N:87:ALA:CA	1:N:88:ASP:HB2	2.22	0.69
1:P:227:ARG:NH1	1:P:229:LEU:HD21	2.08	0.69
1:D:67:HIS:CE1	1:D:91:THR:HG23	2.28	0.69
1:H:51:LYS:CG	1:H:85:GLU:HG3	2.23	0.69
1:M:37:ILE:HG21	1:M:503:VAL:CG1	2.23	0.69
1:N:27:GLU:OE2	1:N:96:PHE:CD1	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:HIS:CE1	1:L:91:THR:CG2	2.66	0.69
1:A:434:VAL:HG12	1:A:469:LEU:HD13	1.74	0.69
1:C:39:ASP:OD2	1:C:298:ARG:HD3	1.93	0.69
1:N:566:ILE:CG2	1:N:569:MET:CE	2.70	0.69
1:C:140:GLU:HG3	1:C:140:GLU:O	1.92	0.68
1:Q:643:LYS:O	1:Q:644:SER:HB3	1.93	0.68
1:A:291:ASN:H	1:A:292:LYS:HZ3	1.41	0.68
1:B:412:PHE:HE2	1:B:451:MET:HG2	1.58	0.68
1:G:412:PHE:HE2	1:G:451:MET:HG2	1.58	0.68
1:O:567:ASP:O	1:O:568:ASN:HB2	1.93	0.68
1:A:141:VAL:O	1:A:141:VAL:HG13	1.92	0.68
1:B:42:ARG:HH11	1:B:140:GLU:HG2	1.58	0.68
1:B:169:VAL:CG1	1:B:241:GLU:HG2	2.24	0.68
1:F:490:PRO:HB3	1:F:569:MET:HE3	1.67	0.68
1:H:269:MET:HG2	1:H:306:TYR:HE1	1.58	0.68
2:M:701:SAH:HB1	2:M:701:SAH:H4'	1.76	0.68
1:M:145:GLU:CG	1:M:331:LEU:HD13	2.24	0.68
1:P:190:ASN:HD21	1:P:209:GLY:HA3	1.59	0.68
1:R:433:LYS:H	1:R:433:LYS:CE	2.03	0.68
1:K:84:ARG:O	1:K:85:GLU:HB2	1.93	0.68
1:K:580:GLU:HG2	1:K:589:SER:HB2	1.76	0.68
1:D:222:LYS:O	1:D:225:GLU:HB2	1.93	0.68
1:R:433:LYS:HE2	1:R:433:LYS:N	2.02	0.68
1:N:315:GLU:HB2	1:N:318:GLN:HG2	1.75	0.68
1:J:597:SER:CB	1:J:598:ALA:HB2	2.19	0.68
1:A:39:ASP:OD2	1:A:298:ARG:HD3	1.93	0.68
1:B:490:PRO:HB3	1:B:569:MET:HE2	1.71	0.68
1:H:490:PRO:HB3	1:H:569:MET:HE3	1.75	0.68
1:M:569:MET:HG3	1:M:624:LEU:HD11	1.74	0.68
1:Q:480:GLU:OE2	1:Q:482:HIS:HD2	1.77	0.68
1:J:42:ARG:NH1	1:J:140:GLU:HG2	2.09	0.68
1:J:480:GLU:OE2	1:J:482:HIS:CD2	2.46	0.68
1:L:280:THR:HG23	1:L:281:THR:HG22	1.74	0.68
1:D:502:ASP:OD2	1:D:616:THR:HG21	1.94	0.68
1:C:490:PRO:HB3	1:C:569:MET:HE1	1.74	0.68
1:P:42:ARG:HH21	1:P:43:ASN:HD21	1.41	0.68
1:I:210:THR:CG2	4:I:809:HOH:O	2.29	0.67
1:M:522:ARG:O	1:M:526:ASP:HB2	1.94	0.67
1:N:147:ILE:HD11	1:N:331:LEU:CD1	2.24	0.67
1:Q:264:ILE:HD11	1:Q:267:LEU:CD2	2.23	0.67
1:K:65:LYS:HA	1:K:65:LYS:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:177:TYR:O	1:I:269:MET:HA	1.93	0.67
1:A:497:GLN:HE21	1:A:497:GLN:N	1.87	0.67
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.59	0.67
1:Q:137:ILE:CG1	1:Q:169:VAL:HG12	2.22	0.67
1:B:175:ASN:HD22	1:B:237:LYS:HG2	1.58	0.67
1:I:173:THR:HG22	1:I:274:ASP:HB3	1.76	0.67
1:Q:190:ASN:HD21	1:Q:209:GLY:HA3	1.59	0.67
1:A:480:GLU:CG	1:A:584:GLY:H	2.08	0.67
1:C:95:VAL:CG2	1:C:122:ARG:HG3	2.25	0.67
1:M:258:ALA:HB2	1:M:314:VAL:HG13	1.77	0.67
1:D:522:ARG:O	1:D:526:ASP:HB2	1.95	0.67
1:D:497:GLN:NE2	1:D:497:GLN:N	2.25	0.67
1:D:550:ARG:H	1:D:560:GLN:HE22	1.43	0.67
1:B:43:ASN:O	1:B:81:MET:HE1	1.95	0.67
1:C:618:LEU:HD23	1:C:624:LEU:HD22	1.75	0.67
1:H:478:ARG:HG2	1:H:478:ARG:NH2	2.04	0.67
1:M:214:PHE:CD2	1:M:305:VAL:HG22	2.30	0.67
1:N:63:ASP:HB2	1:N:65:LYS:N	2.05	0.67
1:O:506:VAL:O	1:O:509:PHE:HB2	1.95	0.67
1:P:152:LEU:HD22	1:P:246:ILE:HG23	1.76	0.67
1:P:275:MET:HE2	1:P:275:MET:N	2.10	0.67
1:E:565:ASN:HA	1:E:624:LEU:O	1.93	0.67
1:G:169:VAL:HG12	1:G:241:GLU:CG	2.16	0.67
1:D:42:ARG:NH1	1:D:140:GLU:CG	2.58	0.67
1:F:42:ARG:HH11	1:F:140:GLU:HG2	1.57	0.67
1:I:104:ARG:HG3	1:I:118:VAL:HB	1.76	0.67
1:M:490:PRO:HB3	1:M:569:MET:CE	2.25	0.67
1:N:497:GLN:HE21	1:N:497:GLN:H	1.41	0.67
1:F:141:VAL:O	1:F:141:VAL:HG12	1.94	0.66
1:O:444:VAL:HG13	1:O:479:VAL:HA	1.76	0.66
1:Q:480:GLU:OE2	1:Q:482:HIS:CD2	2.48	0.66
1:R:218:LEU:H	1:R:303:GLN:HE21	1.43	0.66
1:R:384:ALA:HB2	1:R:437:LEU:HD11	1.76	0.66
1:J:218:LEU:H	1:J:303:GLN:HE21	1.43	0.66
1:A:434:VAL:CG1	1:A:469:LEU:CD1	2.73	0.66
1:E:169:VAL:CG1	1:E:241:GLU:HG2	2.24	0.66
1:G:42:ARG:HH21	1:G:43:ASN:ND2	1.93	0.66
1:N:137:ILE:HD11	1:N:163:ALA:HB2	1.77	0.66
1:N:163:ALA:HB1	1:N:167:CYS:SG	2.35	0.66
1:R:50:LEU:O	1:R:54:ILE:HB	1.94	0.66
1:C:141:VAL:O	1:C:141:VAL:HG12	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:497:GLN:H	1:N:497:GLN:NE2	1.93	0.66
1:J:490:PRO:HB2	1:J:569:MET:CE	2.26	0.66
1:D:489:ILE:HG13	1:D:490:PRO:HD2	1.78	0.66
1:G:478:ARG:HH21	1:G:478:ARG:HG3	1.60	0.66
1:N:478:ARG:HH21	1:N:478:ARG:CG	2.09	0.66
1:P:506:VAL:HG23	1:P:511:LEU:HD12	1.78	0.66
1:Q:191:ASP:OD2	1:Q:194:ARG:NH1	2.29	0.66
1:R:460:LEU:HD11	1:R:637:ILE:HD11	1.78	0.66
1:J:239:ASP:OD2	1:J:242:HIS:CD2	2.49	0.66
1:E:318:GLN:OE1	1:H:368:GLN:HG2	1.96	0.66
1:I:414:ASP:O	1:I:418:LYS:HG3	1.96	0.66
1:Q:91:THR:HG22	1:Q:117:THR:HG23	1.77	0.66
1:D:193:PRO:HA	1:D:362:ASN:HD21	1.61	0.66
1:P:490:PRO:HB3	1:P:569:MET:HE2	1.78	0.66
1:I:541:VAL:HG23	1:I:601:PRO:HG3	1.78	0.66
1:M:83:ALA:HB1	1:M:112:TRP:CG	2.30	0.66
1:N:480:GLU:OE2	1:N:482:HIS:CD2	2.45	0.66
1:O:528:ILE:HD12	1:O:528:ILE:N	2.10	0.66
1:Q:69:LEU:HB3	1:Q:137:ILE:HG22	1.78	0.66
1:M:84:ARG:HD3	1:M:112:TRP:CH2	2.31	0.66
1:N:39:ASP:OD2	1:N:298:ARG:HD3	1.95	0.66
1:J:67:HIS:CE1	1:J:89:LYS:HD3	2.31	0.66
1:A:218:LEU:H	1:A:303:GLN:NE2	1.94	0.66
1:P:146:LEU:HB3	1:P:271:TRP:CD1	2.31	0.66
1:J:601:PRO:HD2	4:J:812:HOH:O	1.95	0.66
1:F:171:PRO:HB3	1:F:273:ILE:HD12	1.76	0.66
1:M:218:LEU:HD22	1:M:221:MET:HE2	1.78	0.66
1:K:349:LEU:HD11	1:K:353:LEU:HD12	1.78	0.66
1:G:559:SER:OG	1:G:632:LYS:HB2	1.95	0.65
1:N:242:HIS:O	1:N:245:LYS:HG2	1.94	0.65
1:A:141:VAL:O	1:A:141:VAL:CG1	2.44	0.65
1:A:269:MET:HG2	1:A:306:TYR:CE1	2.31	0.65
1:G:173:THR:HB	1:G:274:ASP:HB3	1.78	0.65
1:I:275:MET:HE2	1:I:275:MET:CA	2.25	0.65
1:N:583:PHE:O	1:N:586:ILE:HG12	1.95	0.65
1:O:218:LEU:HD13	1:O:268:LEU:HD13	1.78	0.65
1:Q:85:GLU:O	1:Q:85:GLU:HG3	1.96	0.65
1:K:297:TRP:CD2	1:K:495:ASP:HB3	2.31	0.65
1:N:381:LEU:O	1:N:400:ALA:HB1	1.95	0.65
1:O:126:VAL:O	1:O:161:ARG:NH2	2.27	0.65
1:J:73:THR:HG22	1:J:94:GLU:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PRO:CB	1:A:569:MET:CE	2.64	0.65
1:D:67:HIS:CE1	1:D:91:THR:CG2	2.79	0.65
1:C:314:VAL:HG21	1:C:320:PHE:CE2	2.31	0.65
1:O:382:HIS:ND1	1:O:402:ARG:HD3	2.12	0.65
1:C:489:ILE:HD13	1:C:541:VAL:HG21	1.78	0.65
1:O:7:ASN:HD21	1:O:640:GLN:HE22	1.42	0.65
1:O:42:ARG:HH11	1:O:140:GLU:HG2	1.59	0.65
1:O:433:LYS:O	1:O:436:SER:HB2	1.97	0.65
1:Q:421:HIS:O	1:Q:424:LYS:HD3	1.97	0.65
1:R:597:SER:HA	1:R:599:GLY:H	1.62	0.65
1:D:42:ARG:HH11	1:D:140:GLU:CG	2.07	0.65
1:D:193:PRO:HA	1:D:362:ASN:ND2	2.11	0.65
1:Q:84:ARG:O	1:Q:85:GLU:HB3	1.95	0.65
1:L:168:ARG:NH2	1:L:276:ASP:O	2.28	0.65
1:A:480:GLU:OE2	1:A:482:HIS:CD2	2.49	0.65
1:C:262:GLY:O	1:C:314:VAL:HG12	1.96	0.65
1:H:623:SER:O	1:H:624:LEU:HD23	1.97	0.65
1:K:250:GLU:HB2	1:K:326:HIS:NE2	2.12	0.65
1:G:42:ARG:HH21	1:G:43:ASN:HD21	1.44	0.65
1:K:283:ILE:HG23	1:K:298:ARG:HH21	1.62	0.65
1:L:273:ILE:CG1	1:L:275:MET:HE1	2.17	0.65
1:D:616:THR:HG23	4:D:822:HOH:O	1.95	0.65
1:E:145:GLU:O	1:E:145:GLU:HG2	1.95	0.65
1:H:273:ILE:CD1	1:H:275:MET:HE1	2.26	0.65
1:N:54:ILE:C	1:N:58:LYS:NZ	2.55	0.65
1:J:159:LEU:HA	1:J:163:ALA:HB3	1.79	0.65
1:K:217:GLN:HB2	1:K:536:GLU:HB3	1.78	0.65
1:D:169:VAL:HG22	1:D:171:PRO:O	1.97	0.64
1:C:314:VAL:CG2	1:C:320:PHE:HD2	2.10	0.64
1:F:368:GLN:NE2	1:F:371:LYS:HE3	2.12	0.64
1:M:359:TYR:CE2	1:M:605:LYS:HB2	2.32	0.64
1:Q:143:ASP:O	1:Q:145:GLU:N	2.30	0.64
1:R:168:ARG:NH1	1:R:241:GLU:OE2	2.29	0.64
1:D:629:LEU:HD21	1:E:438:THR:HG21	1.79	0.64
1:H:378:SER:HB3	1:H:383:VAL:HG11	1.79	0.64
1:H:502:ASP:OD2	1:H:616:THR:HG21	1.98	0.64
1:Q:323:VAL:HG11	1:Q:340:LYS:HE2	1.78	0.64
1:D:111:PRO:O	1:D:112:TRP:HB2	1.97	0.64
1:I:277:ARG:HG2	1:I:277:ARG:O	1.96	0.64
1:N:87:ALA:O	1:N:115:LYS:HE3	1.97	0.64
1:P:352:MET:HG2	1:P:412:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:478:ARG:HG2	1:P:478:ARG:NH2	2.11	0.64
1:J:243:GLU:H	1:J:243:GLU:CD	2.00	0.64
1:N:39:ASP:OD2	1:N:298:ARG:HD2	1.98	0.64
1:P:84:ARG:C	1:P:86:GLY:H	2.05	0.64
1:Q:168:ARG:HG2	1:Q:168:ARG:NH1	2.02	0.64
1:L:317:ASN:H	1:L:317:ASN:HD22	1.44	0.64
1:A:63:ASP:OD1	1:A:63:ASP:O	2.16	0.64
1:F:565:ASN:ND2	1:F:644:SER:HB2	2.12	0.64
1:N:55:ALA:H	1:N:58:LYS:HZ2	1.45	0.64
1:N:550:ARG:H	1:N:560:GLN:HE22	1.45	0.64
1:R:280:THR:HG23	1:R:281:THR:H	1.63	0.64
1:H:61:ASN:ND2	1:H:65:LYS:O	2.28	0.64
1:N:50:LEU:O	1:N:54:ILE:CG2	2.46	0.64
1:P:4:GLU:O	1:R:420:ILE:HD11	1.98	0.64
1:K:218:LEU:HB2	1:K:303:GLN:HE21	1.62	0.64
1:G:45:LYS:O	1:G:275:MET:HG2	1.98	0.64
1:B:476:GLU:CD	1:B:476:GLU:H	2.05	0.64
1:G:24:MET:HE3	1:G:98:PRO:HG3	1.78	0.64
1:O:3:LEU:O	1:O:15:TRP:HA	1.98	0.64
1:Q:231:GLU:O	1:Q:232:PRO:C	2.39	0.64
1:N:462:PHE:O	1:N:466:VAL:HG23	1.98	0.64
1:B:4:GLU:OE2	1:B:13:ARG:HD3	1.98	0.64
1:B:41:ASP:O	1:B:42:ARG:C	2.41	0.64
1:C:42:ARG:HH21	1:C:43:ASN:HD21	1.46	0.64
1:G:218:LEU:H	1:G:303:GLN:NE2	1.96	0.64
1:G:474:GLY:HA3	1:G:476:GLU:OE2	1.98	0.64
1:H:490:PRO:CB	1:H:569:MET:HE2	2.23	0.64
1:R:176:VAL:HG13	1:R:236:PHE:HB2	1.80	0.64
1:J:218:LEU:H	1:J:303:GLN:NE2	1.96	0.64
1:A:218:LEU:HD12	1:A:303:GLN:HB2	1.80	0.63
1:P:38:LEU:HD13	1:P:498:ASN:HD22	1.63	0.63
1:P:375:ASP:O	1:P:399:THR:HG21	1.97	0.63
1:K:122:ARG:HD3	1:K:124:THR:OG1	1.98	0.63
1:C:269:MET:HG2	1:C:306:TYR:CE1	2.33	0.63
1:K:516:GLU:HG3	1:K:520:LYS:HE3	1.79	0.63
1:I:218:LEU:HD13	1:I:268:LEU:HD13	1.80	0.63
1:I:497:GLN:HE21	1:I:497:GLN:H	0.77	0.63
1:M:83:ALA:HB1	1:M:112:TRP:CB	2.28	0.63
1:P:141:VAL:O	1:P:141:VAL:HG12	1.96	0.63
1:L:450:TYR:H	1:L:459:HIS:HD2	1.45	0.63
1:L:168:ARG:HH11	1:L:168:ARG:CG	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLU:OE2	1:A:482:HIS:HD2	1.80	0.63
1:M:43:ASN:HD22	1:M:43:ASN:N	1.96	0.63
1:K:46:PHE:CE2	1:K:140:GLU:HB2	2.33	0.63
1:K:68:VAL:CG2	1:K:136:ILE:HB	2.26	0.63
1:E:103:ALA:O	1:E:107:THR:HB	1.97	0.63
1:H:84:ARG:O	1:H:85:GLU:HB2	1.99	0.63
1:A:109:ASN:HD22	1:A:109:ASN:N	1.96	0.63
1:I:543:GLY:HA3	1:I:568:ASN:ND2	2.14	0.63
1:O:218:LEU:H	1:O:303:GLN:HE21	1.43	0.63
1:R:497:GLN:HE21	1:R:497:GLN:H	1.44	0.63
1:K:624:LEU:H	1:K:624:LEU:HD12	1.64	0.63
1:B:41:ASP:O	1:B:44:ASP:N	2.30	0.63
1:H:83:ALA:C	1:H:84:ARG:O	2.39	0.63
1:H:156:LYS:O	1:H:160:GLU:HG2	1.98	0.63
1:M:434:VAL:CG1	1:M:469:LEU:HD13	2.28	0.63
1:Q:169:VAL:HG23	1:Q:172:SER:HA	1.79	0.63
1:Q:528:ILE:HD13	1:Q:639:PHE:O	1.99	0.63
1:C:103:ALA:O	1:C:107:THR:HB	1.99	0.63
1:E:176:VAL:HG13	1:E:236:PHE:HB2	1.81	0.63
1:Q:73:THR:OG1	1:Q:76:GLY:HA2	1.98	0.63
1:K:169:VAL:HG22	1:K:171:PRO:O	1.99	0.63
1:E:490:PRO:HB3	1:E:569:MET:HE3	1.81	0.62
1:I:193:PRO:HA	1:I:362:ASN:HD21	1.63	0.62
1:I:171:PRO:HB3	1:I:275:MET:CE	2.29	0.62
1:K:141:VAL:O	1:K:141:VAL:CG1	2.47	0.62
1:C:353:LEU:HD22	1:C:357:THR:HG21	1.81	0.62
1:E:135:ASP:OD1	1:E:164:LYS:HD2	2.00	0.62
1:H:42:ARG:HH21	1:H:43:ASN:HD21	1.47	0.62
1:I:63:ASP:OD2	1:I:65:LYS:HB2	2.00	0.62
1:I:534:LEU:HD11	1:I:576:PRO:HB3	1.80	0.62
1:G:161:ARG:HB2	1:G:162:LEU:HD22	1.82	0.62
1:I:157:GLU:HA	1:I:160:GLU:HG2	1.81	0.62
1:K:510:ASP:OD2	1:K:512:SER:HB3	1.99	0.62
1:I:420:ILE:CD1	1:I:428:VAL:HG22	2.29	0.62
1:O:112:TRP:CZ3	1:O:509:PHE:HE1	2.18	0.62
1:C:191:ASP:OD2	1:C:194:ARG:NH1	2.32	0.62
1:G:72:GLY:O	2:G:701:SAH:N	2.31	0.62
1:I:178:ILE:HA	1:I:268:LEU:O	1.98	0.62
1:M:382:HIS:CD2	1:M:402:ARG:HG3	2.34	0.62
1:R:467:GLU:HG3	1:R:556:ARG:HD2	1.81	0.62
1:F:42:ARG:HH21	1:F:43:ASN:HD21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:356:GLN:O	1:M:359:TYR:HB3	1.99	0.62
1:N:54:ILE:HD11	1:N:87:ALA:N	2.14	0.62
1:K:108:SER:O	1:K:113:SER:HB2	1.99	0.62
1:L:506:VAL:HG12	1:L:507:ASN:HD22	1.64	0.62
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.07	0.62
1:C:194:ARG:HB3	1:C:201:GLU:OE1	2.00	0.62
1:E:274:ASP:HA	1:E:282:PHE:HD1	1.64	0.62
1:H:51:LYS:HG3	1:H:85:GLU:HG3	1.81	0.62
1:I:490:PRO:HB3	1:I:569:MET:HE2	1.81	0.62
1:R:356:GLN:O	1:R:606:GLY:HA2	2.00	0.62
1:I:26:GLN:CG	1:I:30:ARG:HH12	1.99	0.62
1:N:218:LEU:H	1:N:303:GLN:NE2	1.98	0.62
1:O:419:TYR:O	1:O:420:ILE:C	2.42	0.62
1:Q:97:LYS:HB2	1:Q:98:PRO:HD3	1.80	0.62
1:Q:379:LYS:HA	1:Q:399:THR:OG1	2.00	0.62
1:J:39:ASP:OD2	1:J:298:ARG:CD	2.43	0.62
1:D:622:LYS:HD3	1:D:622:LYS:H	1.64	0.62
1:I:176:VAL:HG22	1:I:235:ALA:HB3	1.82	0.62
1:I:292:LYS:HG2	1:I:293:ASN:HA	1.79	0.62
1:N:379:LYS:CA	1:N:399:THR:HG22	2.18	0.62
1:P:227:ARG:HH12	1:P:229:LEU:HD21	1.64	0.62
1:K:167:CYS:SG	1:K:168:ARG:N	2.73	0.62
1:O:7:ASN:HB2	1:O:14:GLU:CD	2.24	0.61
1:J:129:ILE:O	1:J:130:GLY:C	2.43	0.61
1:N:133:ARG:CG	1:N:164:LYS:HG3	2.29	0.61
1:L:379:LYS:CA	1:L:399:THR:HG23	2.28	0.61
1:A:144:THR:O	1:A:269:MET:HE1	1.99	0.61
1:C:337:GLY:O	1:C:338:LYS:HD2	2.00	0.61
1:F:259:HIS:HD2	1:F:260:SER:OG	1.83	0.61
1:E:497:GLN:H	1:E:497:GLN:HE21	1.46	0.61
1:I:480:GLU:OE2	1:I:482:HIS:HD2	1.83	0.61
1:N:565:ASN:ND2	1:N:644:SER:OG	2.32	0.61
1:Q:43:ASN:HB3	1:Q:81:MET:HE1	1.82	0.61
1:K:250:GLU:HB2	1:K:326:HIS:CD2	2.33	0.61
1:D:622:LYS:HD3	1:D:622:LYS:N	2.15	0.61
1:F:243:GLU:HA	1:F:246:ILE:HD12	1.82	0.61
1:G:95:VAL:O	1:G:95:VAL:CG2	2.47	0.61
1:P:352:MET:HG2	1:P:412:PHE:CZ	2.35	0.61
1:J:563:VAL:HG13	1:J:625:CYS:SG	2.40	0.61
1:K:445:LEU:HD12	1:K:480:GLU:HB2	1.81	0.61
1:O:548:ILE:O	1:O:549:LEU:HD13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:417:PHE:CZ	1:Q:430:ILE:HB	2.36	0.61
1:J:470:LYS:HD2	1:J:554:ASP:O	2.00	0.61
1:B:39:ASP:OD2	1:B:298:ARG:CD	2.45	0.61
1:M:3:LEU:HD22	1:O:418:LYS:HA	1.83	0.61
1:N:218:LEU:HD12	1:N:303:GLN:HB2	1.81	0.61
1:P:550:ARG:H	1:P:560:GLN:HE22	1.47	0.61
1:K:77:LEU:HD22	1:K:511:LEU:HD11	1.83	0.61
1:K:573:ASN:O	1:K:614:PRO:HD2	1.99	0.61
1:C:5:LYS:NZ	1:C:14:GLU:OE1	2.34	0.61
1:G:108:SER:O	1:G:109:ASN:HB2	2.01	0.61
1:G:218:LEU:H	1:G:303:GLN:HE21	1.48	0.61
1:C:216:VAL:O	1:C:302:MET:HG2	2.00	0.61
1:M:42:ARG:HA	1:M:283:ILE:HD11	1.82	0.61
1:N:444:VAL:CG1	1:N:479:VAL:HB	2.24	0.61
1:K:475:ASP:OD1	1:K:475:ASP:N	2.33	0.61
1:O:587:ASN:HD22	1:O:588:LEU:N	1.98	0.61
1:Q:92:ALA:HB3	1:Q:118:VAL:HG23	1.83	0.61
1:Q:460:LEU:HB3	1:Q:463:LEU:HD23	1.81	0.61
1:J:189:PHE:CE1	1:J:359:TYR:HB2	2.36	0.61
1:J:577:MET:HE1	1:J:626:LEU:HD11	1.81	0.61
1:K:39:ASP:O	1:K:42:ARG:HB3	2.01	0.61
1:L:133:ARG:HB2	1:L:164:LYS:HG3	1.81	0.61
1:L:168:ARG:HH12	1:L:241:GLU:CD	2.08	0.61
1:B:447:GLU:H	1:B:448:PRO:HA	1.64	0.61
1:C:288:LYS:C	1:C:290:LYS:H	2.08	0.61
1:E:241:GLU:HG3	1:E:277:ARG:HH21	1.65	0.61
1:M:196:ASN:HB2	1:M:201:GLU:OE2	2.01	0.61
1:Q:35:ASP:OD1	1:Q:299:ASP:HB3	2.01	0.61
1:J:67:HIS:HE1	1:J:91:THR:CG2	2.14	0.61
1:B:269:MET:HG2	1:B:306:TYR:CE2	2.35	0.60
1:F:218:LEU:N	1:F:303:GLN:NE2	2.34	0.60
1:H:190:ASN:HD21	1:H:209:GLY:HA3	1.66	0.60
1:P:490:PRO:CB	1:P:569:MET:HE1	2.30	0.60
1:Q:69:LEU:HD12	1:Q:91:THR:OG1	2.02	0.60
1:J:182:GLU:HG3	1:J:263:THR:O	2.01	0.60
1:A:480:GLU:HG3	1:A:481:PRO:HA	1.84	0.60
1:C:490:PRO:CB	1:C:569:MET:HE1	2.30	0.60
1:E:511:LEU:O	1:E:514:PHE:N	2.30	0.60
1:H:420:ILE:HD11	1:H:428:VAL:HG22	1.83	0.60
1:P:5:LYS:NZ	1:P:14:GLU:OE1	2.34	0.60
1:R:146:LEU:HB2	1:R:271:TRP:CD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:502:ASP:CG	1:K:616:THR:HG21	2.25	0.60
1:M:182:GLU:OE2	1:M:227:ARG:NH1	2.34	0.60
1:M:478:ARG:CG	1:M:478:ARG:NH2	2.50	0.60
1:K:241:GLU:HB2	1:K:277:ARG:HH21	1.65	0.60
1:A:291:ASN:H	1:A:292:LYS:NZ	1.99	0.60
1:C:460:LEU:HB3	1:C:463:LEU:HD23	1.83	0.60
1:E:72:GLY:HA3	2:E:701:SAH:O4'	2.01	0.60
1:E:258:ALA:O	1:E:317:ASN:HA	2.01	0.60
1:I:502:ASP:OD2	1:I:616:THR:HG21	2.01	0.60
1:P:365:PHE:O	1:P:371:LYS:HE3	2.01	0.60
1:R:562:CYS:SG	1:R:564:VAL:HG13	2.42	0.60
1:A:45:LYS:O	1:A:275:MET:HG2	2.02	0.60
1:F:196:ASN:O	1:F:198:GLU:N	2.33	0.60
1:M:143:ASP:HB3	1:M:149:GLU:OE1	2.01	0.60
1:D:114:ASP:HB3	1:B:65:LYS:NZ	2.16	0.60
1:F:35:ASP:O	1:F:36:MET:C	2.45	0.60
1:A:185:LEU:O	1:A:188:MET:HB2	2.01	0.60
1:R:203:PRO:HA	1:R:422:TYR:CG	2.37	0.60
1:L:577:MET:CE	1:L:626:LEU:HD11	2.31	0.60
1:C:168:ARG:NH2	1:C:276:ASP:O	2.34	0.60
1:O:135:ASP:OD1	1:O:164:LYS:HD2	2.02	0.60
1:O:615:ILE:O	1:O:616:THR:C	2.45	0.60
1:J:91:THR:HG21	1:J:129:ILE:CG2	2.32	0.60
1:J:597:SER:CB	1:J:598:ALA:CB	2.77	0.60
1:L:446:ALA:O	1:L:481:PRO:HD3	2.01	0.60
1:C:489:ILE:CD1	1:C:541:VAL:HG21	2.31	0.60
1:G:169:VAL:HG13	1:G:172:SER:HA	1.82	0.60
1:Q:95:VAL:HB	1:Q:122:ARG:HG3	1.84	0.60
1:Q:583:PHE:HB3	1:Q:588:LEU:HD12	1.82	0.60
1:J:141:VAL:HG13	1:J:141:VAL:O	2.00	0.60
1:D:622:LYS:H	1:D:622:LYS:CD	2.15	0.60
1:C:547:GLU:OE1	1:C:550:ARG:NH1	2.35	0.60
1:I:470:LYS:O	1:I:473:HIS:O	2.20	0.60
1:M:218:LEU:H	1:M:303:GLN:NE2	2.00	0.60
1:N:36:MET:HA	1:N:300:HIS:CD2	2.36	0.60
1:Q:480:GLU:CG	1:Q:584:GLY:H	2.14	0.60
1:B:66:VAL:HG12	1:B:67:HIS:H	1.66	0.59
1:B:480:GLU:OE2	1:B:482:HIS:HD2	1.86	0.59
1:B:506:VAL:O	1:B:507:ASN:C	2.44	0.59
1:P:33:PHE:HB2	1:P:36:MET:HE2	1.84	0.59
1:Q:569:MET:HE1	1:Q:575:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:373:GLU:OE1	1:K:373:GLU:HA	2.02	0.59
1:D:434:VAL:CG1	1:D:469:LEU:CD1	2.80	0.59
1:F:142:PHE:CD1	1:F:146:LEU:HD12	2.37	0.59
1:E:359:TYR:C	1:E:359:TYR:CD1	2.81	0.59
1:G:22:TYR:HE2	1:G:26:GLN:OE1	1.83	0.59
1:N:168:ARG:HG2	1:N:168:ARG:NH1	2.13	0.59
1:Q:77:LEU:HA	1:Q:80:LEU:HD12	1.83	0.59
1:Q:550:ARG:H	1:Q:560:GLN:HE21	1.50	0.59
1:B:54:ILE:O	1:B:58:LYS:HG2	2.03	0.59
1:G:434:VAL:CG1	1:G:469:LEU:HD13	2.32	0.59
1:M:492:LYS:HB2	1:M:572:SER:HA	1.84	0.59
1:P:310:GLU:OE2	1:P:338:LYS:HD2	2.02	0.59
1:Q:480:GLU:HG3	1:Q:584:GLY:N	2.18	0.59
1:R:175:ASN:HD21	1:R:237:LYS:HG2	1.66	0.59
1:D:143:ASP:OD2	1:D:148:GLY:HA3	2.02	0.59
1:D:379:LYS:CA	1:D:399:THR:CG2	2.80	0.59
1:C:291:ASN:HB3	1:C:295:TYR:HB2	1.83	0.59
1:F:451:MET:HG3	1:F:452:SER:N	2.18	0.59
1:M:84:ARG:HD3	1:M:112:TRP:HH2	1.66	0.59
1:P:190:ASN:ND2	1:P:209:GLY:HA3	2.17	0.59
1:Q:73:THR:O	2:Q:701:SAH:HA	2.02	0.59
1:L:126:VAL:HG11	1:L:129:ILE:HD13	1.85	0.59
1:A:67:HIS:HE1	1:A:91:THR:HG23	1.66	0.59
1:A:497:GLN:NE2	1:A:497:GLN:N	2.46	0.59
1:I:269:MET:HG2	1:I:306:TYR:HE1	1.68	0.59
1:R:556:ARG:CG	1:R:556:ARG:NH1	2.62	0.59
1:H:52:THR:O	1:H:55:ALA:HB3	2.02	0.59
1:N:142:PHE:CD1	1:N:146:LEU:CD1	2.85	0.59
1:K:190:ASN:HD21	1:K:209:GLY:HA3	1.67	0.59
1:C:84:ARG:NH1	1:O:280:THR:HG23	2.18	0.59
1:F:42:ARG:HH12	1:F:140:GLU:HG2	1.62	0.59
1:P:138:VAL:HG23	1:P:170:VAL:HB	1.83	0.59
1:P:156:LYS:O	1:P:160:GLU:HG2	2.02	0.59
1:I:35:ASP:OD1	1:I:300:HIS:HD2	1.86	0.59
1:M:84:ARG:HG2	1:M:85:GLU:OE1	2.01	0.59
1:M:141:VAL:O	1:M:141:VAL:HG12	2.02	0.59
1:N:54:ILE:HD11	1:N:87:ALA:H	1.67	0.59
1:Q:102:CYS:HA	1:Q:513:PHE:HE2	1.68	0.59
1:L:577:MET:HE1	1:L:641:PHE:HZ	1.68	0.59
1:M:32:ARG:HG3	1:M:34:GLY:H	1.68	0.59
1:M:379:LYS:CA	1:M:399:THR:CG2	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:254:ARG:O	1:N:321:GLU:CA	2.49	0.59
1:O:67:HIS:HE1	1:O:91:THR:OG1	1.86	0.59
1:P:5:LYS:CA	1:R:420:ILE:HD11	2.33	0.59
1:Q:577:MET:HE1	1:Q:639:PHE:CE1	2.38	0.59
1:Q:583:PHE:CB	1:Q:588:LEU:HD12	2.33	0.59
1:B:47:LEU:HG	1:B:81:MET:HE2	1.85	0.58
1:B:245:LYS:HE3	1:E:337:GLY:HA2	1.85	0.58
1:I:497:GLN:CD	1:I:573:ASN:ND2	2.59	0.58
1:M:280:THR:HG23	1:M:281:THR:N	2.18	0.58
1:O:373:GLU:HG3	1:O:377:LEU:CD1	2.32	0.58
1:Q:258:ALA:O	1:Q:259:HIS:HB3	2.03	0.58
1:Q:365:PHE:O	1:Q:371:LYS:HE3	2.03	0.58
1:Q:375:ASP:HA	1:Q:399:THR:CG2	2.18	0.58
1:R:181:VAL:HG22	1:R:228:GLU:HA	1.85	0.58
1:K:53:THR:HG22	1:K:168:ARG:HE	1.68	0.58
1:C:486:LEU:HD12	1:C:548:ILE:HB	1.85	0.58
1:P:241:GLU:CG	1:P:277:ARG:HH21	2.10	0.58
1:P:367:ASN:OD1	1:P:369:LYS:HG2	2.02	0.58
1:R:491:GLU:HG2	1:R:493:PHE:CD2	2.38	0.58
1:J:4:GLU:OE2	1:J:13:ARG:HD3	2.02	0.58
1:L:497:GLN:H	1:L:497:GLN:NE2	2.01	0.58
1:A:434:VAL:HG12	1:A:469:LEU:CD1	2.34	0.58
1:M:37:ILE:HG21	1:M:503:VAL:HG11	1.85	0.58
1:M:176:VAL:HG21	1:M:236:PHE:HD2	1.68	0.58
1:B:140:GLU:OE1	1:B:301:TRP:HZ2	1.86	0.58
1:M:110:SER:HB2	1:M:111:PRO:CD	2.31	0.58
1:K:39:ASP:OD1	1:K:298:ARG:NH1	2.36	0.58
1:E:142:PHE:CD1	1:E:146:LEU:HD12	2.39	0.58
1:E:218:LEU:H	1:E:303:GLN:NE2	2.00	0.58
1:O:168:ARG:NH2	1:O:276:ASP:O	2.33	0.58
1:O:245:LYS:HD3	1:P:337:GLY:HA2	1.86	0.58
1:P:497:GLN:NE2	1:P:497:GLN:H	2.01	0.58
1:Q:497:GLN:NE2	1:Q:497:GLN:H	2.02	0.58
1:J:451:MET:HG3	1:J:452:SER:N	2.18	0.58
1:L:577:MET:CE	1:L:641:PHE:CZ	2.80	0.58
1:F:522:ARG:O	1:F:526:ASP:HB2	2.04	0.58
1:H:385:THR:HG22	4:H:820:HOH:O	2.04	0.58
1:N:184:HIS:O	1:N:188:MET:HG3	2.03	0.58
1:O:370:PHE:HE1	1:O:588:LEU:CD2	2.17	0.58
1:P:146:LEU:H	1:P:146:LEU:CD2	2.12	0.58
1:R:180:PRO:HD2	1:R:230:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:VAL:HG21	1:E:445:LEU:HD22	1.84	0.58
1:E:551:PHE:CE2	1:E:579:MET:HE1	2.38	0.58
1:M:169:VAL:HG11	1:M:241:GLU:HA	1.86	0.58
1:N:58:LYS:CE	1:N:66:VAL:HG21	2.31	0.58
1:Q:222:LYS:CB	1:Q:224:HIS:HB3	2.33	0.58
1:J:403:VAL:HB	1:J:428:VAL:HB	1.85	0.58
1:G:385:THR:HG21	1:G:405:ILE:HG23	1.86	0.58
1:H:141:VAL:HG13	1:H:141:VAL:O	2.04	0.58
1:N:53:THR:O	1:N:58:LYS:NZ	2.37	0.58
1:P:541:VAL:HG23	1:P:601:PRO:HG3	1.84	0.58
1:Q:39:ASP:OD2	1:Q:298:ARG:HB3	2.04	0.58
1:F:168:ARG:HA	1:F:241:GLU:OE2	2.04	0.58
1:F:206:ARG:NH1	1:F:310:GLU:HG3	2.17	0.58
1:F:277:ARG:C	1:F:279:GLY:H	2.12	0.58
1:M:36:MET:HB3	1:M:300:HIS:CG	2.39	0.58
1:N:354:SER:OG	1:N:357:THR:OG1	2.21	0.58
1:O:497:GLN:HE21	1:O:497:GLN:N	1.95	0.58
1:P:7:ASN:HD21	1:P:640:GLN:HE22	1.51	0.58
1:R:530:ASP:O	1:R:610:GLY:HA2	2.04	0.58
1:C:68:VAL:HB	1:C:90:VAL:HG22	1.85	0.58
1:F:373:GLU:OE2	1:F:585:GLY:N	2.26	0.58
1:E:317:ASN:ND2	1:E:317:ASN:N	2.41	0.58
1:G:66:VAL:CG1	1:G:87:ALA:HA	2.34	0.58
1:I:478:ARG:HH21	1:I:478:ARG:CG	2.16	0.58
1:O:112:TRP:HZ3	1:O:509:PHE:HE1	1.52	0.58
1:Q:110:SER:HB2	1:Q:111:PRO:CD	2.34	0.58
1:R:80:LEU:HB3	1:R:509:PHE:CD1	2.39	0.58
1:L:480:GLU:OE2	1:L:482:HIS:HD2	1.87	0.58
1:B:94:GLU:OE2	2:B:701:SAH:O3'	2.22	0.57
1:I:157:GLU:HA	1:I:160:GLU:CG	2.34	0.57
1:I:278:ASN:O	1:I:280:THR:N	2.37	0.57
1:M:37:ILE:HG21	1:M:503:VAL:HG13	1.85	0.57
1:N:242:HIS:HB3	1:N:245:LYS:CD	2.34	0.57
1:O:80:LEU:HB3	1:O:509:PHE:CZ	2.38	0.57
1:Q:122:ARG:HH21	1:Q:124:THR:HG21	1.69	0.57
1:K:122:ARG:O	1:K:123:SER:C	2.45	0.57
1:B:480:GLU:OE2	1:B:482:HIS:CD2	2.57	0.57
1:M:67:HIS:CD2	1:M:133:ARG:O	2.56	0.57
1:O:194:ARG:HG2	1:O:201:GLU:CB	2.34	0.57
1:K:84:ARG:HB2	1:K:112:TRP:CE2	2.39	0.57
1:L:403:VAL:HB	1:L:428:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:CG	1:A:306:TYR:HE1	2.17	0.57
1:D:45:LYS:HB3	1:D:275:MET:HE3	1.84	0.57
1:E:383:VAL:HB	1:E:443:ILE:HG23	1.84	0.57
1:G:99:MET:HE1	1:G:514:PHE:CE1	2.38	0.57
1:P:45:LYS:HG2	1:P:282:PHE:O	2.04	0.57
1:Q:150:GLY:O	1:Q:154:THR:OG1	2.22	0.57
1:Q:259:HIS:C	1:Q:259:HIS:CD2	2.82	0.57
1:J:144:THR:O	1:J:269:MET:CE	2.53	0.57
1:J:618:LEU:HG	1:J:624:LEU:HD22	1.86	0.57
1:K:179:VAL:HG21	1:K:270:TRP:CH2	2.39	0.57
1:D:50:LEU:O	1:D:54:ILE:HG13	2.05	0.57
1:D:373:GLU:OE2	1:D:585:GLY:N	2.26	0.57
1:C:288:LYS:O	1:C:290:LYS:N	2.37	0.57
1:G:81:MET:O	1:G:84:ARG:HB3	2.04	0.57
1:M:95:VAL:HG13	1:M:96:PHE:N	2.19	0.57
1:O:193:PRO:HA	1:O:362:ASN:HD21	1.69	0.57
1:P:253:VAL:CG2	1:P:253:VAL:O	2.52	0.57
1:L:434:VAL:CG1	1:L:469:LEU:HD13	2.35	0.57
1:L:541:VAL:HG11	1:L:595:ILE:HD13	1.86	0.57
1:A:155:PHE:O	1:A:159:LEU:HG	2.04	0.57
1:D:43:ASN:HB3	1:D:507:ASN:HD21	1.68	0.57
1:F:141:VAL:O	1:F:141:VAL:CG1	2.51	0.57
1:E:35:ASP:O	1:E:36:MET:C	2.46	0.57
1:E:439:ASP:N	1:E:439:ASP:OD1	2.36	0.57
1:H:77:LEU:HD13	1:H:511:LEU:HD11	1.86	0.57
1:M:32:ARG:HG3	1:M:34:GLY:N	2.19	0.57
1:O:557:VAL:HG22	1:O:632:LYS:HB2	1.85	0.57
1:Q:239:ASP:OD1	1:Q:241:GLU:HB2	2.03	0.57
1:J:158:ALA:HA	1:J:162:LEU:CD2	2.30	0.57
1:J:274:ASP:OD2	1:J:277:ARG:HA	2.04	0.57
1:K:548:ILE:HG22	1:K:549:LEU:HD22	1.87	0.57
1:L:577:MET:HE1	1:L:641:PHE:CZ	2.40	0.57
1:A:168:ARG:NH2	1:A:276:ASP:O	2.37	0.57
1:A:379:LYS:HA	1:A:399:THR:HG23	1.86	0.57
1:I:169:VAL:HG22	1:I:171:PRO:O	2.04	0.57
1:Q:236:PHE:CZ	1:Q:324:CYS:HB3	2.40	0.57
1:J:497:GLN:NE2	1:J:497:GLN:N	2.51	0.57
1:L:187:LYS:O	1:L:191:ASP:HB2	2.03	0.57
1:L:239:ASP:OD1	1:L:277:ARG:NH2	2.36	0.57
1:C:269:MET:HG2	1:C:306:TYR:HE1	1.69	0.57
1:M:353:LEU:HD22	1:M:357:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:493:PHE:HA	1:M:539:GLY:HA3	1.86	0.57
1:O:173:THR:CG2	1:O:174:GLY:N	2.68	0.57
1:P:123:SER:HB3	2:P:701:SAH:HN62	1.69	0.57
1:K:140:GLU:HG3	1:K:140:GLU:O	2.04	0.57
1:F:506:VAL:HG12	1:F:507:ASN:HD22	1.70	0.57
1:N:39:ASP:C	1:N:39:ASP:OD1	2.47	0.57
1:O:420:ILE:HG13	1:O:421:HIS:N	2.19	0.57
1:P:221:MET:HG2	1:P:226:PHE:CD1	2.39	0.57
1:R:622:LYS:HD2	1:R:622:LYS:N	2.17	0.57
1:J:67:HIS:CE1	1:J:91:THR:CG2	2.87	0.57
1:L:56:GLU:OE1	1:L:168:ARG:HD2	2.04	0.57
1:M:188:MET:HE2	1:M:359:TYR:CE1	2.39	0.57
1:M:192:ILE:O	1:M:194:ARG:HD3	2.05	0.57
1:M:541:VAL:CG2	1:M:601:PRO:HG3	2.35	0.57
1:O:56:GLU:O	1:O:60:GLU:HG2	2.05	0.57
1:O:77:LEU:HD13	1:O:511:LEU:HD11	1.86	0.57
1:O:485:VAL:HG21	1:O:547:GLU:HG2	1.87	0.57
1:Q:356:GLN:NE2	1:Q:608:LYS:HE3	2.20	0.57
1:J:67:HIS:HD2	1:J:133:ARG:O	1.86	0.57
1:D:111:PRO:O	1:D:112:TRP:CB	2.52	0.57
1:G:480:GLU:OE2	1:G:482:HIS:HD2	1.88	0.57
1:P:77:LEU:HD11	1:P:81:MET:HE3	1.87	0.57
1:Q:447:GLU:N	1:Q:448:PRO:HA	2.20	0.57
1:L:193:PRO:HA	1:L:362:ASN:HD21	1.70	0.57
1:B:68:VAL:HG22	1:B:136:ILE:HD12	1.86	0.56
1:F:335:ASN:N	1:F:335:ASN:OD1	2.37	0.56
1:E:67:HIS:HE1	1:E:91:THR:CG2	2.11	0.56
1:N:140:GLU:OE1	1:N:301:TRP:HZ2	1.87	0.56
1:P:490:PRO:HA	1:P:569:MET:HE1	1.86	0.56
1:P:549:LEU:HD12	1:P:560:GLN:NE2	2.18	0.56
1:R:353:LEU:HD22	1:R:357:THR:HG21	1.87	0.56
1:K:283:ILE:HG23	1:K:298:ARG:NH2	2.20	0.56
1:K:356:GLN:O	1:K:359:TYR:HB3	2.04	0.56
1:E:490:PRO:CB	1:E:569:MET:CE	2.79	0.56
1:R:622:LYS:H	1:R:622:LYS:CD	2.16	0.56
1:K:451:MET:HE3	1:K:452:SER:HA	1.87	0.56
1:B:314:VAL:HG21	1:B:320:PHE:CD1	2.40	0.56
1:B:534:LEU:HD21	1:B:611:VAL:HG11	1.88	0.56
1:F:218:LEU:N	1:F:303:GLN:HE21	1.94	0.56
1:F:259:HIS:C	1:F:259:HIS:CD2	2.83	0.56
1:F:383:VAL:HG13	1:F:403:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:460:LEU:HB3	1:I:463:LEU:HD22	1.88	0.56
1:I:490:PRO:HB3	1:I:569:MET:HE1	1.87	0.56
1:M:300:HIS:CE1	1:M:301:TRP:CD2	2.93	0.56
1:N:168:ARG:HH11	1:N:168:ARG:CG	2.13	0.56
1:N:280:THR:OG1	1:N:281:THR:HG22	2.04	0.56
1:Q:216:VAL:C	1:Q:302:MET:HG2	2.29	0.56
1:Q:255:GLU:OE1	1:Q:319:THR:HG22	2.05	0.56
1:Q:289:TRP:O	1:Q:289:TRP:HE3	1.88	0.56
1:Q:491:GLU:OE1	1:Q:539:GLY:HA3	2.05	0.56
1:R:45:LYS:O	1:R:275:MET:HG2	2.05	0.56
1:R:52:THR:HG21	1:R:276:ASP:HB2	1.87	0.56
1:R:181:VAL:HG11	1:R:226:PHE:HB2	1.88	0.56
1:R:297:TRP:CE3	1:R:495:ASP:HB3	2.40	0.56
1:K:145:GLU:HG3	1:K:331:LEU:HD22	1.87	0.56
1:L:317:ASN:H	1:L:317:ASN:ND2	2.03	0.56
1:E:379:LYS:CA	1:E:399:THR:CG2	2.81	0.56
1:O:616:THR:OG1	1:O:617:ALA:N	2.39	0.56
1:Q:516:GLU:O	1:Q:520:LYS:HG3	2.05	0.56
1:R:80:LEU:HD13	1:R:509:PHE:HB3	1.88	0.56
1:L:480:GLU:OE2	1:L:482:HIS:CD2	2.58	0.56
1:I:566:ILE:CG2	1:I:569:MET:HE3	2.35	0.56
1:M:3:LEU:O	1:M:15:TRP:HA	2.05	0.56
1:M:37:ILE:CG2	1:M:503:VAL:HG13	2.36	0.56
1:M:169:VAL:CG1	1:M:241:GLU:HA	2.35	0.56
1:O:444:VAL:CG1	1:O:479:VAL:HA	2.35	0.56
1:O:624:LEU:HB2	1:O:643:LYS:HA	1.86	0.56
1:Q:356:GLN:HE22	1:Q:608:LYS:HE3	1.71	0.56
1:J:556:ARG:O	1:J:556:ARG:HG2	2.04	0.56
1:K:133:ARG:HB2	1:K:164:LYS:HG3	1.87	0.56
1:K:218:LEU:CD1	1:K:268:LEU:HD22	2.36	0.56
1:L:114:ASP:OD1	1:L:114:ASP:N	2.35	0.56
1:F:145:GLU:HG2	1:F:331:LEU:HD22	1.87	0.56
1:I:141:VAL:O	1:I:141:VAL:CG1	2.52	0.56
1:N:179:VAL:HG22	1:N:232:PRO:HA	1.87	0.56
1:K:354:SER:O	1:K:358:VAL:HG23	2.05	0.56
1:A:73:THR:HG22	1:A:94:GLU:HB2	1.87	0.56
1:B:216:VAL:C	1:B:302:MET:HG2	2.30	0.56
1:C:522:ARG:O	1:C:526:ASP:HB2	2.05	0.56
1:M:7:ASN:HB2	1:M:14:GLU:OE1	2.05	0.56
1:R:310:GLU:OE1	1:R:338:LYS:HG3	2.06	0.56
1:R:437:LEU:O	1:R:473:HIS:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ARG:NH1	1:K:526:ASP:OD1	2.39	0.56
1:A:218:LEU:H	1:A:303:GLN:HE21	1.52	0.56
1:C:517:ILE:HG13	1:C:518:SER:N	2.19	0.56
1:I:643:LYS:O	1:I:644:SER:CB	2.54	0.56
1:N:57:LYS:NZ	1:N:166:GLY:O	2.39	0.56
1:O:505:THR:HA	1:O:509:PHE:O	2.05	0.56
1:L:191:ASP:OD2	1:L:194:ARG:NH1	2.38	0.56
1:C:42:ARG:HH11	1:C:140:GLU:HG2	1.71	0.56
1:F:291:ASN:HB3	1:F:295:TYR:HB2	1.88	0.56
1:F:443:ILE:HG12	1:F:445:LEU:HD13	1.87	0.56
1:G:489:ILE:HD13	1:G:541:VAL:HG21	1.87	0.56
1:M:138:VAL:HG23	1:M:170:VAL:HB	1.88	0.56
1:K:241:GLU:HB2	1:K:277:ARG:NH2	2.21	0.56
1:A:39:ASP:OD2	1:A:298:ARG:CD	2.54	0.56
1:C:567:ASP:C	1:C:568:ASN:HD22	2.14	0.56
1:N:378:SER:HB3	1:N:400:ALA:HB2	1.87	0.56
1:R:69:LEU:HD12	1:R:70:ASP:N	2.20	0.56
1:F:163:ALA:HB1	1:F:167:CYS:SG	2.46	0.55
1:F:478:ARG:HG2	1:F:478:ARG:HH21	1.71	0.55
1:E:480:GLU:OE2	1:E:482:HIS:HD2	1.89	0.55
1:I:488:ALA:HB2	1:I:577:MET:HE3	1.88	0.55
1:M:198:GLU:HB2	1:M:201:GLU:OE2	2.06	0.55
1:Q:370:PHE:HE2	1:Q:588:LEU:HD21	1.71	0.55
1:R:369:LYS:HE3	1:R:586:ILE:HG21	1.89	0.55
1:E:140:GLU:O	1:E:140:GLU:HG3	2.04	0.55
1:G:434:VAL:HG12	1:G:469:LEU:HD13	1.89	0.55
1:Q:222:LYS:HB2	1:Q:224:HIS:HB3	1.87	0.55
1:Q:231:GLU:C	1:Q:232:PRO:O	2.49	0.55
1:R:481:PRO:HG2	1:R:581:TRP:CE3	2.41	0.55
1:K:156:LYS:O	1:K:160:GLU:HG2	2.06	0.55
1:A:221:MET:HE3	1:A:226:PHE:CD1	2.41	0.55
1:B:344:TYR:O	1:B:346:VAL:HG13	2.07	0.55
1:E:352:MET:HE1	1:E:409:ASN:HD21	1.70	0.55
1:M:66:VAL:O	1:M:88:ASP:HB2	2.06	0.55
1:M:126:VAL:H	1:M:161:ARG:HH22	1.51	0.55
1:M:490:PRO:HB3	1:M:569:MET:HE2	1.88	0.55
1:N:58:LYS:N	1:N:58:LYS:HE3	2.21	0.55
1:N:348:GLY:O	1:N:415:ILE:HD11	2.07	0.55
1:Q:180:PRO:CG	1:Q:230:SER:HB3	2.31	0.55
1:L:502:ASP:OD2	1:L:616:THR:HG21	2.07	0.55
1:D:180:PRO:HB3	1:D:264:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD21	1:B:503:VAL:HA	1.87	0.55
1:B:483:MET:HB3	1:B:582:GLU:HG3	1.87	0.55
1:E:72:GLY:CA	2:E:701:SAH:O4'	2.54	0.55
1:R:434:VAL:HG12	1:R:469:LEU:HD13	1.88	0.55
1:C:460:LEU:HD22	1:C:463:LEU:HD21	1.88	0.55
1:F:385:THR:HB	1:F:405:ILE:HA	1.88	0.55
1:G:36:MET:HA	1:G:300:HIS:CD2	2.41	0.55
1:I:478:ARG:HH21	1:I:478:ARG:HG2	1.70	0.55
1:N:123:SER:OG	2:N:701:SAH:N6	2.38	0.55
1:J:137:ILE:HD11	1:J:163:ALA:HB2	1.89	0.55
1:K:145:GLU:CG	1:K:331:LEU:HD22	2.37	0.55
1:A:379:LYS:HA	1:A:399:THR:CG2	2.36	0.55
1:F:218:LEU:H	1:F:303:GLN:HE22	1.48	0.55
1:N:275:MET:HE1	1:N:283:ILE:N	2.22	0.55
1:O:141:VAL:O	1:O:141:VAL:HG13	2.05	0.55
1:O:643:LYS:HD2	1:O:643:LYS:N	2.14	0.55
1:P:210:THR:HB	4:P:804:HOH:O	2.05	0.55
1:Q:354:SER:HB2	3:Q:702:PO4:O3	2.07	0.55
1:K:38:LEU:HD21	1:K:503:VAL:HA	1.89	0.55
1:L:136:ILE:HA	1:L:168:ARG:O	2.07	0.55
1:L:627:HIS:HB2	1:L:640:GLN:HB2	1.88	0.55
1:B:239:ASP:OD2	1:B:242:HIS:HD2	1.89	0.55
1:G:412:PHE:CE2	1:G:451:MET:HG2	2.40	0.55
1:H:577:MET:HE1	1:H:626:LEU:HD11	1.88	0.55
1:M:145:GLU:HG2	1:M:331:LEU:CD1	2.36	0.55
1:R:80:LEU:HB3	1:R:509:PHE:CE1	2.41	0.55
1:R:379:LYS:HA	1:R:399:THR:HG22	1.89	0.55
1:J:222:LYS:HB2	1:J:225:GLU:HG2	1.89	0.55
1:K:143:ASP:O	1:K:144:THR:C	2.50	0.55
1:B:392:LEU:C	1:B:392:LEU:CD2	2.79	0.55
1:C:522:ARG:HG2	1:C:526:ASP:OD2	2.07	0.55
1:F:218:LEU:HD22	1:F:221:MET:HE2	1.88	0.55
1:H:218:LEU:H	1:H:303:GLN:HE21	1.55	0.55
1:N:367:ASN:O	1:N:371:LYS:HD3	2.07	0.55
1:J:497:GLN:HE21	1:J:497:GLN:N	1.96	0.55
1:K:616:THR:C	1:K:618:LEU:H	2.15	0.55
1:C:550:ARG:H	1:C:560:GLN:HE22	1.54	0.55
1:F:143:ASP:OD1	1:F:143:ASP:N	2.37	0.55
1:M:434:VAL:CG1	1:M:469:LEU:CD1	2.85	0.55
1:N:315:GLU:HB2	1:N:318:GLN:CG	2.35	0.55
1:Q:42:ARG:HH11	1:Q:140:GLU:HG2	1.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:THR:O	1:J:269:MET:HE1	2.07	0.55
1:J:383:VAL:CG2	1:J:445:LEU:HD22	2.37	0.55
1:D:42:ARG:HH21	1:D:43:ASN:HD21	1.54	0.54
1:D:157:GLU:HA	1:D:160:GLU:HG3	1.90	0.54
1:C:502:ASP:OD2	1:C:616:THR:CG2	2.55	0.54
1:M:568:ASN:HD22	1:M:568:ASN:N	2.05	0.54
1:N:132:SER:HB2	1:R:104:ARG:CZ	2.36	0.54
1:N:142:PHE:HD1	1:N:146:LEU:HD12	1.69	0.54
1:N:359:TYR:CD1	1:N:359:TYR:C	2.85	0.54
1:P:503:VAL:H	1:P:515:ASP:CG	2.15	0.54
1:R:460:LEU:HD21	1:R:579:MET:CE	2.37	0.54
1:L:297:TRP:CD2	1:L:495:ASP:HB3	2.42	0.54
1:D:565:ASN:HD21	1:D:644:SER:HB3	1.71	0.54
1:B:241:GLU:HB2	1:B:277:ARG:NH2	2.21	0.54
1:B:550:ARG:H	1:B:560:GLN:NE2	1.99	0.54
1:B:554:ASP:O	1:B:555:GLY:O	2.26	0.54
1:C:84:ARG:NH1	1:O:280:THR:CG2	2.70	0.54
1:E:89:LYS:HZ3	1:E:91:THR:HG22	1.72	0.54
1:E:420:ILE:HD11	1:E:428:VAL:HG22	1.90	0.54
1:I:353:LEU:HD22	1:I:357:THR:HG21	1.88	0.54
1:M:402:ARG:NH2	1:M:429:GLU:OE1	2.28	0.54
1:B:67:HIS:C	1:B:67:HIS:ND1	2.64	0.54
1:B:218:LEU:H	1:B:303:GLN:HE21	1.52	0.54
1:B:452:SER:O	1:B:453:ALA:C	2.51	0.54
1:B:534:LEU:HD11	1:B:611:VAL:HG13	1.90	0.54
1:C:480:GLU:HA	1:C:481:PRO:C	2.33	0.54
1:E:39:ASP:OD2	1:E:298:ARG:HD3	2.07	0.54
1:M:486:LEU:HD22	1:M:578:TRP:O	2.07	0.54
1:J:71:ILE:HG21	1:J:154:THR:CG2	2.37	0.54
1:J:339:ASP:OD1	1:J:341:SER:HB2	2.06	0.54
1:I:534:LEU:CD1	1:I:576:PRO:HB3	2.37	0.54
1:M:485:VAL:HG13	1:M:487:LYS:HG3	1.88	0.54
1:O:180:PRO:HB2	1:O:264:ILE:HG12	1.89	0.54
1:O:182:GLU:OE1	1:O:263:THR:HG22	2.07	0.54
1:P:50:LEU:O	1:P:54:ILE:HB	2.06	0.54
1:P:470:LYS:O	1:P:473:HIS:O	2.26	0.54
1:K:578:TRP:CG	1:K:591:GLY:HA3	2.43	0.54
1:B:43:ASN:ND2	1:B:43:ASN:N	2.55	0.54
1:B:505:THR:HA	1:B:509:PHE:O	2.06	0.54
1:C:55:ALA:HB1	1:O:292:LYS:HE3	1.90	0.54
1:C:467:GLU:HG3	1:C:555:GLY:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:ILE:CD1	1:H:428:VAL:HG22	2.37	0.54
1:I:129:ILE:HG22	1:I:130:GLY:O	2.06	0.54
1:I:269:MET:HG2	1:I:306:TYR:CE1	2.42	0.54
1:N:169:VAL:CG1	1:N:240:PHE:O	2.51	0.54
1:P:5:LYS:HA	1:R:420:ILE:CD1	2.36	0.54
1:R:179:VAL:HG22	1:R:232:PRO:HA	1.88	0.54
1:K:485:VAL:HG13	1:K:487:LYS:HG3	1.90	0.54
1:K:556:ARG:H	1:K:556:ARG:CZ	2.20	0.54
1:E:168:ARG:HH22	1:E:276:ASP:C	2.15	0.54
1:E:216:VAL:HG23	1:E:217:GLN:N	2.21	0.54
1:E:490:PRO:HB3	1:E:569:MET:HE1	1.87	0.54
1:G:432:GLU:HG2	1:G:433:LYS:HG3	1.89	0.54
1:I:539:GLY:O	1:I:540:ILE:HD13	2.07	0.54
1:N:275:MET:H	1:N:275:MET:HE2	1.73	0.54
1:K:84:ARG:O	1:K:85:GLU:CB	2.56	0.54
1:B:123:SER:O	1:B:125:ASP:N	2.41	0.54
1:B:194:ARG:HD2	1:B:198:GLU:O	2.08	0.54
1:N:84:ARG:HB3	1:N:112:TRP:CZ2	2.43	0.54
1:P:379:LYS:HA	1:P:399:THR:CG2	2.37	0.54
1:F:626:LEU:HD23	1:F:626:LEU:C	2.32	0.54
1:M:169:VAL:HG11	1:M:240:PHE:O	2.08	0.54
1:P:110:SER:HB2	1:P:112:TRP:CE3	2.43	0.54
1:A:245:LYS:HD3	1:D:337:GLY:HA2	1.90	0.54
1:D:46:PHE:CZ	1:D:140:GLU:HB2	2.42	0.54
1:D:291:ASN:O	1:D:292:LYS:HD3	2.08	0.54
1:M:190:ASN:HD21	1:M:209:GLY:HA3	1.73	0.54
1:M:533:SER:O	1:M:536:GLU:HB2	2.08	0.54
1:N:137:ILE:O	1:N:169:VAL:HA	2.08	0.54
1:O:417:PHE:CZ	1:O:430:ILE:HB	2.43	0.54
1:R:447:GLU:N	1:R:448:PRO:HA	2.23	0.54
1:L:168:ARG:HG2	1:L:168:ARG:NH1	2.15	0.54
1:C:45:LYS:O	1:C:275:MET:HG2	2.08	0.54
1:M:434:VAL:HG13	1:M:469:LEU:HD13	1.90	0.54
1:N:490:PRO:HB3	1:N:569:MET:CE	2.38	0.54
1:O:460:LEU:C	1:O:462:PHE:N	2.65	0.54
1:Q:178:ILE:CD1	1:Q:235:ALA:HB2	2.35	0.54
1:Q:276:ASP:O	1:Q:277:ARG:CB	2.56	0.54
1:R:87:ALA:O	1:R:88:ASP:C	2.51	0.54
1:K:179:VAL:HG21	1:K:270:TRP:HH2	1.72	0.54
1:I:489:ILE:O	1:I:576:PRO:HD2	2.08	0.53
1:Q:530:ASP:O	1:Q:610:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:592:LEU:HD21	1:J:595:ILE:HD11	1.90	0.53
1:A:467:GLU:CD	1:A:557:VAL:HG12	2.34	0.53
1:B:297:TRP:CZ2	1:B:299:ASP:HB2	2.43	0.53
1:E:138:VAL:HG23	1:E:170:VAL:HB	1.89	0.53
1:G:56:GLU:C	1:G:58:LYS:H	2.16	0.53
1:I:42:ARG:HH11	1:I:140:GLU:HG3	1.72	0.53
1:I:171:PRO:HB3	1:I:275:MET:HE1	1.90	0.53
1:O:4:GLU:OE2	1:O:13:ARG:NH1	2.42	0.53
1:O:73:THR:OG1	1:O:76:GLY:HA2	2.08	0.53
1:P:168:ARG:HH22	1:P:276:ASP:C	2.16	0.53
1:P:297:TRP:CE3	1:P:495:ASP:HB3	2.44	0.53
1:D:243:GLU:OE1	1:D:243:GLU:N	2.30	0.53
1:B:627:HIS:CD2	1:B:627:HIS:N	2.76	0.53
1:G:141:VAL:O	1:G:141:VAL:HG12	2.08	0.53
1:I:193:PRO:HA	1:I:362:ASN:ND2	2.23	0.53
1:M:111:PRO:C	1:M:113:SER:H	2.17	0.53
1:O:229:LEU:HD13	1:O:314:VAL:HG12	1.89	0.53
1:J:88:ASP:O	1:J:115:LYS:HG2	2.08	0.53
1:A:176:VAL:HG22	1:A:235:ALA:HB3	1.90	0.53
1:A:566:ILE:HG22	1:A:569:MET:HE3	1.90	0.53
1:D:242:HIS:HB2	1:D:245:LYS:HG3	1.90	0.53
1:F:91:THR:HG22	1:F:117:THR:HG22	1.89	0.53
1:G:490:PRO:HB3	1:G:569:MET:HE2	1.76	0.53
1:M:132:SER:N	1:P:104:ARG:HH21	2.06	0.53
1:M:375:ASP:O	1:M:399:THR:HG21	2.09	0.53
1:Q:179:VAL:HG22	1:Q:232:PRO:HA	1.89	0.53
1:K:505:THR:HA	1:K:509:PHE:O	2.08	0.53
1:A:214:PHE:CD2	1:A:305:VAL:HG22	2.44	0.53
1:E:41:ASP:O	1:E:42:ARG:C	2.51	0.53
1:E:241:GLU:CG	1:E:277:ARG:HH21	2.20	0.53
1:E:274:ASP:HA	1:E:282:PHE:CD1	2.43	0.53
1:G:6:ILE:HG13	1:I:426:THR:HB	1.91	0.53
1:I:68:VAL:O	1:I:90:VAL:HA	2.08	0.53
1:M:92:ALA:HB3	1:M:118:VAL:HG22	1.90	0.53
1:M:258:ALA:CB	1:M:314:VAL:HG13	2.38	0.53
1:N:55:ALA:CA	1:N:58:LYS:HZ2	2.22	0.53
1:P:490:PRO:CA	1:P:569:MET:HE1	2.39	0.53
1:R:489:ILE:HD11	1:R:541:VAL:HG11	1.91	0.53
1:K:36:MET:HA	1:K:300:HIS:CD2	2.43	0.53
1:L:528:ILE:HD13	1:L:639:PHE:O	2.08	0.53
1:A:502:ASP:CG	1:A:616:THR:HG21	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLU:HB2	1:H:326:HIS:NE2	2.23	0.53
1:P:198:GLU:HB2	1:P:201:GLU:HG3	1.90	0.53
1:Q:447:GLU:H	1:Q:448:PRO:HA	1.73	0.53
1:R:218:LEU:C	1:R:220:GLU:H	2.16	0.53
1:R:300:HIS:CE1	1:R:301:TRP:CD2	2.97	0.53
1:K:534:LEU:O	1:K:536:GLU:N	2.42	0.53
1:D:78:LEU:O	1:D:81:MET:HB2	2.09	0.53
1:D:178:ILE:HA	1:D:268:LEU:O	2.09	0.53
1:B:75:THR:HG22	1:B:77:LEU:H	1.73	0.53
1:E:434:VAL:HG13	1:E:469:LEU:HD13	1.91	0.53
1:I:379:LYS:HA	1:I:399:THR:CG2	2.33	0.53
1:N:450:TYR:H	1:N:459:HIS:CD2	2.22	0.53
1:R:144:THR:HG23	1:R:302:MET:O	2.09	0.53
1:K:123:SER:HB3	2:K:701:SAH:N6	2.13	0.53
1:E:627:HIS:HB2	1:E:640:GLN:HB2	1.90	0.53
1:Q:51:LYS:HA	1:Q:85:GLU:CD	2.33	0.53
1:R:156:LYS:HG3	1:R:157:GLU:N	2.22	0.53
1:J:264:ILE:HD12	1:J:312:LYS:HG3	1.90	0.53
1:L:258:ALA:CB	1:L:314:VAL:HG13	2.39	0.53
1:L:280:THR:HG23	1:L:281:THR:CG2	2.38	0.53
1:A:109:ASN:N	1:A:109:ASN:ND2	2.57	0.53
1:F:216:VAL:O	1:F:302:MET:HG2	2.09	0.53
1:G:190:ASN:HD21	1:G:209:GLY:HA3	1.73	0.53
1:I:168:ARG:HG2	1:I:168:ARG:HH11	1.72	0.53
1:I:587:ASN:ND2	1:I:587:ASN:C	2.67	0.53
1:M:84:ARG:O	1:M:85:GLU:HB2	2.09	0.53
1:O:387:GLY:HA2	1:O:450:TYR:CE1	2.43	0.53
1:P:496:LEU:O	1:P:499:ILE:HG12	2.09	0.53
1:Q:392:LEU:CD1	1:Q:445:LEU:HB3	2.38	0.53
1:L:553:ILE:HD11	1:L:581:TRP:HZ3	1.73	0.53
1:B:84:ARG:HB3	1:B:112:TRP:CH2	2.44	0.53
1:E:278:ASN:O	1:E:280:THR:N	2.40	0.53
1:M:409:ASN:OD1	1:M:411:ARG:HG2	2.09	0.53
1:M:615:ILE:HG13	1:M:618:LEU:HD22	1.90	0.53
1:N:87:ALA:CB	1:N:88:ASP:HB2	2.38	0.53
1:Q:410:GLU:HG3	1:Q:413:ARG:NH2	2.23	0.53
1:R:49:GLY:O	1:R:53:THR:OG1	2.27	0.53
1:R:178:ILE:HG13	1:R:267:LEU:HD22	1.90	0.53
1:R:184:HIS:HA	1:R:187:LYS:HD3	1.90	0.53
1:J:128:GLN:OE1	1:J:129:ILE:O	2.27	0.53
1:J:378:SER:HB3	1:J:400:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:VAL:HG12	1:K:162:LEU:HD11	1.90	0.53
1:K:143:ASP:O	1:K:146:LEU:N	2.32	0.53
1:M:516:GLU:HG2	1:M:520:LYS:HE3	1.90	0.52
1:Q:143:ASP:C	1:Q:145:GLU:H	2.17	0.52
1:R:157:GLU:O	1:R:160:GLU:HG2	2.09	0.52
1:J:410:GLU:OE2	1:K:19:GLU:HB3	2.09	0.52
1:K:485:VAL:O	1:K:579:MET:HG3	2.09	0.52
1:D:269:MET:HG2	1:D:306:TYR:HE1	1.73	0.52
1:D:445:LEU:HD12	1:D:480:GLU:HB2	1.91	0.52
1:B:567:ASP:O	1:B:568:ASN:HB2	2.09	0.52
1:F:239:ASP:OD2	1:F:242:HIS:HD2	1.92	0.52
1:I:570:SER:HB3	1:I:622:LYS:HA	1.92	0.52
1:I:577:MET:HE1	1:I:626:LEU:HD11	1.90	0.52
1:O:280:THR:HG22	1:O:281:THR:HG22	1.90	0.52
1:R:597:SER:HA	1:R:599:GLY:N	2.23	0.52
1:J:561:LYS:O	1:J:562:CYS:HB3	2.09	0.52
1:K:45:LYS:NZ	1:K:294:ASN:HD22	2.07	0.52
1:L:275:MET:HE3	1:L:283:ILE:H	1.74	0.52
1:E:595:ILE:HG22	1:E:599:GLY:HA2	1.90	0.52
1:I:615:ILE:O	1:I:616:THR:C	2.52	0.52
1:M:457:TRP:CD1	1:M:457:TRP:O	2.62	0.52
1:O:145:GLU:HA	1:O:269:MET:HE2	1.91	0.52
1:O:291:ASN:OD1	1:O:294:ASN:HB2	2.10	0.52
1:R:502:ASP:OD2	1:R:616:THR:HG21	2.08	0.52
1:K:285:MET:O	1:K:285:MET:HE3	2.10	0.52
1:B:163:ALA:CB	1:B:167:CYS:SG	2.95	0.52
1:G:540:ILE:HD11	1:G:542:LYS:HE2	1.91	0.52
1:N:566:ILE:HG22	1:N:569:MET:HE2	1.88	0.52
1:R:145:GLU:HA	1:R:269:MET:HE2	1.92	0.52
1:J:548:ILE:HD12	1:J:626:LEU:HD13	1.92	0.52
1:K:185:LEU:O	1:K:188:MET:HB2	2.10	0.52
1:K:379:LYS:CA	1:K:399:THR:HG23	2.38	0.52
1:L:57:LYS:HG2	1:L:135:ASP:HB3	1.91	0.52
1:A:76:GLY:O	1:A:77:LEU:C	2.53	0.52
1:D:626:LEU:HD21	1:D:628:ALA:HB2	1.90	0.52
1:C:489:ILE:HG12	1:C:541:VAL:CG2	2.39	0.52
1:F:147:ILE:HD11	1:F:331:LEU:HD13	1.91	0.52
1:F:478:ARG:HH21	1:F:478:ARG:CG	2.22	0.52
1:E:218:LEU:H	1:E:303:GLN:HE21	1.55	0.52
1:E:506:VAL:N	1:E:509:PHE:O	2.37	0.52
1:N:169:VAL:HG13	1:N:241:GLU:HG2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:506:VAL:HG12	1:O:507:ASN:HD22	1.74	0.52
1:J:478:ARG:HH21	1:J:478:ARG:HG2	1.74	0.52
1:L:297:TRP:CE3	1:L:495:ASP:HB3	2.45	0.52
1:A:541:VAL:HG11	1:A:595:ILE:HD13	1.91	0.52
1:D:630:PHE:CE1	1:D:635:GLY:HA2	2.44	0.52
1:G:73:THR:OG1	1:G:76:GLY:HA2	2.09	0.52
1:G:379:LYS:CA	1:G:399:THR:CG2	2.83	0.52
1:M:5:LYS:HD3	1:O:417:PHE:HE1	1.75	0.52
1:N:141:VAL:O	1:N:141:VAL:HG12	2.09	0.52
1:R:478:ARG:HG2	1:R:478:ARG:NH2	2.21	0.52
1:K:497:GLN:NE2	1:K:497:GLN:H	2.08	0.52
1:D:114:ASP:HB3	1:B:65:LYS:HZ1	1.73	0.52
1:E:490:PRO:CB	1:E:569:MET:HE1	2.40	0.52
1:G:104:ARG:HB3	1:G:118:VAL:HB	1.91	0.52
1:G:490:PRO:CA	1:G:569:MET:HE1	2.39	0.52
1:I:643:LYS:O	1:I:644:SER:HB2	2.10	0.52
1:P:7:ASN:HD21	1:P:640:GLN:NE2	2.08	0.52
1:J:91:THR:HG21	1:J:129:ILE:HG21	1.92	0.52
1:J:169:VAL:HG23	1:J:171:PRO:O	2.10	0.52
1:I:616:THR:O	1:I:619:ARG:HG2	2.10	0.52
1:R:35:ASP:OD2	1:R:300:HIS:HD2	1.93	0.52
1:R:243:GLU:H	1:R:243:GLU:CD	2.16	0.52
1:R:291:ASN:CB	1:R:295:TYR:HB2	2.32	0.52
1:R:433:LYS:HE3	1:R:436:SER:OG	2.10	0.52
1:J:71:ILE:HG12	1:J:93:LEU:HD12	1.91	0.52
1:J:406:ILE:HG12	1:J:431:ILE:HD11	1.91	0.52
1:K:177:TYR:HA	1:K:233:ILE:O	2.09	0.52
1:K:529:VAL:HG12	1:K:530:ASP:O	2.10	0.52
1:A:452:SER:O	1:A:453:ALA:C	2.53	0.52
1:D:547:GLU:OE2	1:D:550:ARG:NH1	2.37	0.52
1:B:24:MET:HE2	1:B:98:PRO:HG3	1.91	0.52
1:B:218:LEU:HD12	1:B:303:GLN:HB3	1.92	0.52
1:C:35:ASP:O	1:C:36:MET:C	2.53	0.52
1:C:73:THR:OG1	1:C:76:GLY:HA2	2.10	0.52
1:C:221:MET:HE3	1:C:226:PHE:CE1	2.44	0.52
1:C:432:GLU:HG2	1:C:433:LYS:HG3	1.92	0.52
1:M:39:ASP:OD2	1:M:298:ARG:CD	2.57	0.52
1:P:577:MET:HE1	1:P:639:PHE:CE1	2.45	0.52
1:Q:275:MET:HE1	1:Q:283:ILE:H	1.74	0.52
1:R:280:THR:HG23	1:R:281:THR:N	2.24	0.52
1:R:292:LYS:HA	1:R:293:ASN:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MET:N	1:A:275:MET:HE2	2.25	0.52
1:A:577:MET:CE	1:A:639:PHE:CE1	2.84	0.52
1:D:135:ASP:OD1	1:D:164:LYS:HD2	2.09	0.52
1:B:460:LEU:HB3	1:B:463:LEU:HD22	1.91	0.52
1:G:27:GLU:HG2	1:G:96:PHE:CZ	2.45	0.52
1:M:542:LYS:HG3	1:M:571:SER:HB2	1.91	0.52
1:N:154:THR:O	1:N:158:ALA:HB2	2.09	0.52
1:P:94:GLU:O	1:P:120:SER:HA	2.10	0.52
1:J:483:MET:HG2	1:J:550:ARG:HH21	1.75	0.52
1:A:471:MET:HA	1:A:471:MET:HE3	1.92	0.51
1:I:145:GLU:OE2	1:I:331:LEU:HB2	2.10	0.51
1:I:398:LYS:NZ	1:I:398:LYS:HB3	2.25	0.51
1:M:73:THR:HB	1:M:92:ALA:HB1	1.92	0.51
1:M:269:MET:HG2	1:M:306:TYR:HE2	1.75	0.51
1:O:587:ASN:HD22	1:O:587:ASN:C	2.18	0.51
1:J:217:GLN:HB2	1:J:536:GLU:HB3	1.93	0.51
1:B:43:ASN:O	1:B:81:MET:CE	2.58	0.51
1:C:67:HIS:HE1	1:C:91:THR:CG2	2.23	0.51
1:I:3:LEU:HB2	1:I:16:VAL:HG12	1.93	0.51
1:I:138:VAL:HG23	1:I:170:VAL:HB	1.92	0.51
1:I:275:MET:HE2	1:I:275:MET:N	2.25	0.51
1:I:337:GLY:HA2	1:K:245:LYS:HD3	1.92	0.51
1:M:178:ILE:HG13	1:M:233:ILE:HG23	1.93	0.51
1:M:550:ARG:H	1:M:560:GLN:HE22	1.58	0.51
1:N:171:PRO:O	1:N:240:PHE:HD2	1.93	0.51
1:N:471:MET:HE1	1:N:556:ARG:HH12	1.75	0.51
1:P:450:TYR:N	1:P:459:HIS:HD2	1.92	0.51
1:K:139:ALA:HB3	1:K:155:PHE:CZ	2.45	0.51
1:B:41:ASP:O	1:B:43:ASN:N	2.43	0.51
1:C:111:PRO:HA	1:O:47:LEU:HD13	1.92	0.51
1:F:164:LYS:O	1:F:167:CYS:HB2	2.11	0.51
1:G:619:ARG:HG2	1:G:619:ARG:HH11	1.75	0.51
1:M:447:GLU:N	1:M:448:PRO:HA	2.26	0.51
1:M:492:LYS:O	1:M:540:ILE:N	2.38	0.51
1:N:595:ILE:CG2	1:N:599:GLY:HA2	2.40	0.51
1:O:229:LEU:HD13	1:O:314:VAL:CG1	2.40	0.51
1:O:535:TRP:CD2	1:O:605:LYS:HG2	2.45	0.51
1:O:632:LYS:HG3	1:O:633:SER:N	2.25	0.51
1:K:57:LYS:HA	1:K:60:GLU:HB2	1.93	0.51
1:K:522:ARG:O	1:K:526:ASP:HB2	2.10	0.51
1:B:59:HIS:O	1:B:60:GLU:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:VAL:HG11	1:F:226:PHE:HB2	1.92	0.51
1:F:449:PHE:CD1	1:F:449:PHE:C	2.89	0.51
1:E:567:ASP:OD1	1:E:623:SER:OG	2.29	0.51
1:G:626:LEU:HG	1:G:641:PHE:CE2	2.45	0.51
1:M:190:ASN:ND2	1:M:209:GLY:HA3	2.26	0.51
1:M:449:PHE:HA	1:M:459:HIS:CD2	2.46	0.51
1:N:217:GLN:NE2	1:N:298:ARG:O	2.31	0.51
1:N:517:ILE:HG13	1:N:518:SER:N	2.25	0.51
1:L:129:ILE:HG23	1:L:129:ILE:O	2.09	0.51
1:A:556:ARG:HG2	1:A:556:ARG:HH11	1.75	0.51
1:H:51:LYS:HG2	1:H:85:GLU:HG3	1.92	0.51
1:M:238:PHE:HB3	1:M:240:PHE:CE1	2.45	0.51
1:M:258:ALA:HB3	1:M:315:GLU:O	2.10	0.51
1:M:482:HIS:HA	1:M:553:ILE:HG12	1.92	0.51
1:N:63:ASP:N	1:N:64:GLY:HA2	2.25	0.51
1:O:450:TYR:H	1:O:459:HIS:CD2	2.18	0.51
1:Q:232:PRO:HG3	1:Q:290:LYS:HE2	1.89	0.51
1:J:483:MET:HG2	1:J:550:ARG:NH2	2.26	0.51
1:K:68:VAL:O	1:K:90:VAL:HA	2.10	0.51
1:L:550:ARG:H	1:L:560:GLN:HE22	1.57	0.51
1:D:271:TRP:CZ3	1:D:273:ILE:HG12	2.46	0.51
1:G:95:VAL:HB	1:G:122:ARG:HG3	1.92	0.51
1:M:83:ALA:HB2	1:M:116:ILE:HD11	1.92	0.51
1:M:203:PRO:HA	1:M:422:TYR:CG	2.45	0.51
1:M:356:GLN:NE2	1:M:608:LYS:HE3	2.25	0.51
1:M:379:LYS:HA	1:M:399:THR:HG22	1.90	0.51
1:O:2:PHE:CD2	1:O:520:LYS:HB3	2.46	0.51
1:Q:302:MET:HG2	1:Q:303:GLN:H	1.75	0.51
1:R:638:ASN:HD22	1:R:638:ASN:N	2.09	0.51
1:A:379:LYS:O	1:A:381:LEU:HG	2.11	0.51
1:D:269:MET:HG2	1:D:306:TYR:CE1	2.45	0.51
1:B:3:LEU:O	1:B:15:TRP:HA	2.11	0.51
1:H:626:LEU:HD23	1:H:627:HIS:N	2.25	0.51
1:M:385:THR:CG2	4:M:802:HOH:O	2.59	0.51
1:M:616:THR:O	1:M:619:ARG:HB2	2.11	0.51
1:N:569:MET:HE1	1:N:575:ILE:HG12	1.93	0.51
1:O:194:ARG:HG2	1:O:201:GLU:HB3	1.93	0.51
1:O:441:PRO:O	1:O:477:LEU:HD11	2.11	0.51
1:Q:464:TYR:O	1:Q:468:VAL:HG23	2.11	0.51
1:A:244:GLU:CD	1:A:244:GLU:H	2.18	0.51
1:A:480:GLU:HA	1:A:481:PRO:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:ARG:HG2	1:D:478:ARG:NH2	2.13	0.51
1:B:94:GLU:O	1:B:120:SER:HA	2.10	0.51
1:F:1:MET:N	4:F:801:HOH:O	2.43	0.51
1:F:73:THR:O	1:F:74:GLY:C	2.54	0.51
1:E:547:GLU:OE1	1:E:550:ARG:NH1	2.44	0.51
1:N:326:HIS:HB2	1:N:331:LEU:HD12	1.92	0.51
1:P:379:LYS:CA	1:P:399:THR:HG23	2.37	0.51
1:R:146:LEU:HD23	1:R:147:ILE:HG23	1.93	0.51
1:R:258:ALA:C	1:R:260:SER:H	2.19	0.51
1:J:51:LYS:HG3	1:J:85:GLU:CD	2.34	0.51
1:K:34:GLY:C	1:K:499:ILE:HA	2.36	0.51
1:C:196:ASN:HB2	1:C:201:GLU:OE2	2.11	0.51
1:F:497:GLN:HE21	1:F:497:GLN:N	1.98	0.51
1:H:490:PRO:HA	1:H:569:MET:HE1	1.93	0.51
1:Q:243:GLU:HA	1:Q:246:ILE:HD12	1.92	0.51
1:Q:339:ASP:C	1:Q:341:SER:H	2.19	0.51
1:Q:553:ILE:O	1:Q:553:ILE:CG2	2.59	0.51
1:J:103:ALA:O	1:J:107:THR:HB	2.11	0.51
1:J:275:MET:HE3	1:J:283:ILE:H	1.76	0.51
1:L:412:PHE:HE2	1:L:451:MET:HG2	1.74	0.51
1:A:58:LYS:HD3	1:A:64:GLY:O	2.10	0.51
1:D:506:VAL:O	1:D:507:ASN:C	2.53	0.51
1:C:502:ASP:OD2	1:C:616:THR:HG21	2.11	0.51
1:C:631:ASP:C	1:C:631:ASP:OD1	2.54	0.51
1:E:157:GLU:O	1:E:160:GLU:HG3	2.11	0.51
1:I:114:ASP:OD1	1:I:114:ASP:N	2.38	0.51
1:M:447:GLU:H	1:M:448:PRO:HA	1.75	0.51
1:O:173:THR:HG22	1:O:174:GLY:N	2.25	0.51
1:R:220:GLU:HG3	1:R:536:GLU:O	2.11	0.51
1:R:593:LEU:O	1:R:594:SER:HB3	2.10	0.51
1:L:73:THR:HB	1:L:92:ALA:HB1	1.91	0.51
1:A:272:ASP:C	1:A:272:ASP:OD1	2.54	0.50
1:B:173:THR:HG22	1:B:274:ASP:HB3	1.93	0.50
1:C:233:ILE:HG12	1:C:256:ALA:HB2	1.94	0.50
1:C:569:MET:HA	1:C:572:SER:HB2	1.93	0.50
1:F:446:ALA:O	1:F:481:PRO:HD3	2.12	0.50
1:F:480:GLU:HA	1:F:481:PRO:C	2.35	0.50
1:M:142:PHE:HD2	1:M:146:LEU:HD12	1.76	0.50
1:R:35:ASP:O	1:R:36:MET:C	2.53	0.50
1:L:39:ASP:OD2	1:L:298:ARG:CD	2.60	0.50
1:A:447:GLU:N	1:A:448:PRO:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:THR:O	1:E:110:SER:OG	2.28	0.50
1:G:522:ARG:O	1:G:526:ASP:HB2	2.10	0.50
1:O:73:THR:HG23	1:O:74:GLY:N	2.26	0.50
1:O:91:THR:HG22	1:O:117:THR:HG23	1.93	0.50
1:O:194:ARG:HG2	1:O:201:GLU:HB2	1.93	0.50
1:P:26:GLN:O	1:P:30:ARG:CD	2.59	0.50
1:Q:82:ALA:O	1:Q:87:ALA:HB3	2.11	0.50
1:Q:550:ARG:H	1:Q:560:GLN:NE2	2.08	0.50
1:J:269:MET:HG2	1:J:306:TYR:HE1	1.76	0.50
1:A:101:ASP:O	1:A:105:HIS:HB2	2.11	0.50
1:B:123:SER:C	1:B:125:ASP:H	2.18	0.50
1:C:35:ASP:O	1:C:38:LEU:N	2.44	0.50
1:C:42:ARG:NH2	1:C:43:ASN:HD21	2.09	0.50
1:F:289:TRP:O	1:F:290:LYS:HG2	2.11	0.50
1:I:627:HIS:HB2	1:I:640:GLN:HB2	1.94	0.50
1:M:541:VAL:HG22	1:M:601:PRO:HG3	1.92	0.50
1:N:203:PRO:HA	1:N:422:TYR:CD2	2.46	0.50
1:N:578:TRP:CB	1:N:591:GLY:HA3	2.41	0.50
1:J:300:HIS:CE1	1:J:301:TRP:CD2	2.99	0.50
1:K:65:LYS:HA	1:K:65:LYS:CE	2.41	0.50
1:K:556:ARG:H	1:K:556:ARG:NH1	2.09	0.50
1:L:84:ARG:HG3	1:L:112:TRP:CZ2	2.46	0.50
1:D:434:VAL:HG12	1:D:469:LEU:CD1	2.36	0.50
1:N:153:ARG:HB2	1:N:328:GLU:OE2	2.12	0.50
1:N:579:MET:HE2	1:N:581:TRP:CZ2	2.46	0.50
1:O:27:GLU:HB3	1:O:96:PHE:CZ	2.47	0.50
1:P:269:MET:HG2	1:P:306:TYR:CE1	2.40	0.50
1:Q:395:LEU:C	1:Q:397:ALA:H	2.18	0.50
1:R:218:LEU:HD13	1:R:268:LEU:HD13	1.93	0.50
1:K:217:GLN:HG3	1:K:537:TYR:CE1	2.46	0.50
1:K:356:GLN:HG2	1:K:357:THR:H	1.75	0.50
1:B:78:LEU:O	1:B:81:MET:HB2	2.12	0.50
1:E:42:ARG:HH11	1:E:140:GLU:HG2	1.72	0.50
1:G:457:TRP:HA	4:G:811:HOH:O	2.09	0.50
1:M:269:MET:O	1:M:269:MET:HG3	2.11	0.50
1:O:39:ASP:OD2	1:O:298:ARG:CD	2.54	0.50
1:O:397:ALA:HA	1:O:403:VAL:HG21	1.93	0.50
1:K:103:ALA:O	1:K:107:THR:HB	2.11	0.50
1:L:490:PRO:HB3	1:L:569:MET:HE3	1.75	0.50
1:D:528:ILE:H	1:D:528:ILE:HD12	1.76	0.50
1:E:161:ARG:HB3	1:E:162:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:142:PHE:CD2	1:M:146:LEU:HD12	2.46	0.50
1:O:73:THR:CB	1:O:92:ALA:HB1	2.32	0.50
1:O:353:LEU:HB3	1:O:357:THR:HB	1.94	0.50
1:Q:14:GLU:HG2	1:Q:523:THR:HG21	1.93	0.50
1:Q:629:LEU:O	1:Q:637:ILE:HA	2.12	0.50
1:R:359:TYR:CZ	1:R:605:LYS:HB2	2.46	0.50
1:R:421:HIS:O	1:R:424:LYS:HE3	2.12	0.50
1:D:379:LYS:CA	1:D:399:THR:HG23	2.37	0.50
1:B:486:LEU:HD12	1:B:548:ILE:HB	1.94	0.50
1:F:489:ILE:O	1:F:576:PRO:HD2	2.12	0.50
1:E:222:LYS:O	1:E:225:GLU:HG2	2.12	0.50
1:I:168:ARG:HG2	1:I:168:ARG:NH1	2.24	0.50
1:I:375:ASP:O	1:I:399:THR:HG21	2.12	0.50
1:O:275:MET:HE1	1:O:283:ILE:H	1.76	0.50
1:O:477:LEU:O	1:O:479:VAL:HG12	2.12	0.50
1:P:143:ASP:O	1:P:146:LEU:HA	2.12	0.50
1:Q:480:GLU:HA	1:Q:481:PRO:C	2.36	0.50
1:L:65:LYS:HA	1:L:88:ASP:OD2	2.12	0.50
1:D:230:SER:OG	1:D:231:GLU:O	2.28	0.50
1:B:339:ASP:OD1	1:B:341:SER:HB2	2.12	0.50
1:E:83:ALA:O	1:E:84:ARG:C	2.55	0.50
1:G:273:ILE:HG13	1:G:273:ILE:O	2.10	0.50
1:R:460:LEU:HD21	1:R:579:MET:HE1	1.93	0.50
1:J:168:ARG:NH2	1:J:276:ASP:O	2.43	0.50
1:J:625:CYS:SG	1:J:627:HIS:CD2	3.05	0.50
1:K:84:ARG:HB2	1:K:112:TRP:NE1	2.27	0.50
1:K:487:LYS:HE3	1:K:547:GLU:HG2	1.94	0.50
1:C:244:GLU:OE2	1:C:244:GLU:CA	2.60	0.50
1:E:56:GLU:HG3	1:E:57:LYS:N	2.25	0.50
1:E:452:SER:O	1:E:453:ALA:C	2.54	0.50
1:N:4:GLU:OE2	1:N:13:ARG:HD3	2.11	0.50
1:O:77:LEU:O	1:O:81:MET:HG3	2.11	0.50
1:Q:35:ASP:O	1:Q:36:MET:C	2.53	0.50
1:Q:367:ASN:HD21	1:Q:369:LYS:HG2	1.77	0.50
1:R:41:ASP:O	1:R:45:LYS:HB2	2.12	0.50
1:R:556:ARG:HG3	1:R:556:ARG:NH1	2.09	0.50
1:R:612:TYR:OH	1:R:615:ILE:HD12	2.11	0.50
1:J:26:GLN:O	1:J:30:ARG:HD2	2.12	0.50
1:A:273:ILE:HD11	1:A:283:ILE:HD12	1.93	0.49
1:A:490:PRO:CA	1:A:569:MET:HE1	2.41	0.49
1:D:489:ILE:CG1	1:D:490:PRO:HD2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:VAL:CG2	1:C:547:GLU:HG3	2.42	0.49
1:F:299:ASP:OD1	1:F:537:TYR:OH	2.15	0.49
1:H:222:LYS:NZ	1:H:602:GLU:OE2	2.44	0.49
1:I:278:ASN:O	1:I:280:THR:CG2	2.58	0.49
1:N:87:ALA:HB1	1:N:88:ASP:HB2	1.94	0.49
1:O:356:GLN:O	1:O:359:TYR:HB3	2.12	0.49
1:P:368:GLN:O	1:P:369:LYS:C	2.55	0.49
1:Q:141:VAL:O	1:Q:141:VAL:HG12	2.12	0.49
1:R:7:ASN:O	1:R:11:GLY:N	2.40	0.49
1:R:218:LEU:O	1:R:220:GLU:N	2.44	0.49
1:J:406:ILE:HG21	1:J:434:VAL:HG22	1.94	0.49
1:L:253:VAL:HG22	1:L:253:VAL:O	2.10	0.49
1:A:550:ARG:H	1:A:560:GLN:NE2	2.10	0.49
1:B:141:VAL:HG12	1:B:141:VAL:O	2.12	0.49
1:E:403:VAL:HB	1:E:428:VAL:HB	1.94	0.49
1:H:61:ASN:O	1:H:62:THR:C	2.55	0.49
1:R:626:LEU:HD21	1:R:639:PHE:HD2	1.77	0.49
1:J:69:LEU:HD12	1:J:91:THR:O	2.12	0.49
1:J:563:VAL:CG1	1:J:625:CYS:SG	3.00	0.49
1:L:557:VAL:HG23	1:L:632:LYS:HB2	1.95	0.49
1:B:37:ILE:O	1:B:37:ILE:HG22	2.13	0.49
1:B:629:LEU:O	1:B:629:LEU:HG	2.12	0.49
1:C:67:HIS:CE1	1:C:91:THR:HG22	2.42	0.49
1:C:612:TYR:CE2	1:C:614:PRO:HA	2.47	0.49
1:F:144:THR:HG21	1:F:215:ASP:HB3	1.93	0.49
1:F:218:LEU:HD12	1:F:303:GLN:HB2	1.90	0.49
1:E:315:GLU:HB3	1:E:318:GLN:HG3	1.93	0.49
1:H:618:LEU:HD21	1:H:642:GLY:HA2	1.95	0.49
1:I:256:ALA:O	1:I:319:THR:HA	2.10	0.49
1:M:136:ILE:HA	1:M:168:ARG:O	2.11	0.49
1:O:196:ASN:HB2	1:O:201:GLU:OE2	2.12	0.49
1:P:146:LEU:HB3	1:P:271:TRP:NE1	2.26	0.49
1:P:317:ASN:C	1:P:317:ASN:HD22	2.16	0.49
1:P:354:SER:O	1:P:358:VAL:HG23	2.12	0.49
1:Q:114:ASP:OD1	1:Q:114:ASP:N	2.44	0.49
1:Q:186:LEU:O	1:Q:307:TYR:OH	2.17	0.49
1:Q:269:MET:SD	1:Q:270:TRP:N	2.85	0.49
1:R:51:LYS:NZ	1:R:51:LYS:CB	2.74	0.49
1:R:261:SER:OG	1:R:316:MET:N	2.43	0.49
1:J:67:HIS:CE1	1:J:91:THR:HG22	2.43	0.49
1:K:137:ILE:O	1:K:169:VAL:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:218:LEU:H	1:L:303:GLN:HE21	1.60	0.49
1:E:39:ASP:OD2	1:E:298:ARG:CD	2.60	0.49
1:H:138:VAL:HG23	1:H:170:VAL:HB	1.94	0.49
1:H:379:LYS:HA	1:H:399:THR:HG23	1.94	0.49
1:O:194:ARG:HD2	1:O:198:GLU:O	2.13	0.49
1:Q:153:ARG:NH1	1:Q:248:PHE:CZ	2.80	0.49
1:R:143:ASP:OD2	1:R:148:GLY:HA3	2.13	0.49
1:R:297:TRP:CD2	1:R:495:ASP:HB3	2.48	0.49
1:J:42:ARG:HH11	1:J:140:GLU:HG2	1.76	0.49
1:G:239:ASP:OD2	1:G:277:ARG:NH2	2.45	0.49
1:M:434:VAL:HG12	1:M:469:LEU:CD1	2.42	0.49
1:K:326:HIS:HB3	1:K:331:LEU:HD12	1.93	0.49
1:L:218:LEU:H	1:L:303:GLN:NE2	2.09	0.49
1:A:375:ASP:O	1:A:399:THR:HG21	2.13	0.49
1:D:452:SER:O	1:D:453:ALA:C	2.54	0.49
1:F:67:HIS:ND1	1:F:89:LYS:HB3	2.27	0.49
1:G:405:ILE:HB	1:G:430:ILE:HG12	1.93	0.49
1:I:634:THR:OG1	1:I:636:ASP:HB2	2.12	0.49
1:O:190:ASN:ND2	1:O:209:GLY:HA3	2.26	0.49
1:P:451:MET:HG3	1:P:452:SER:N	2.28	0.49
1:R:476:GLU:H	1:R:476:GLU:CD	2.20	0.49
1:D:406:ILE:HG12	1:D:431:ILE:HD11	1.95	0.49
1:G:272:ASP:HA	1:G:283:ILE:O	2.12	0.49
1:H:42:ARG:NH2	1:H:43:ASN:HD21	2.09	0.49
1:I:35:ASP:OD1	1:I:300:HIS:CD2	2.65	0.49
1:I:452:SER:O	1:I:453:ALA:C	2.56	0.49
1:M:287:PRO:O	1:M:288:LYS:C	2.56	0.49
1:O:624:LEU:HB2	1:O:642:GLY:O	2.11	0.49
1:P:292:LYS:HB3	1:P:293:ASN:OD1	2.12	0.49
1:P:349:LEU:HD11	1:P:353:LEU:HD12	1.94	0.49
1:R:553:ILE:HD12	1:R:553:ILE:H	1.77	0.49
1:R:567:ASP:HA	1:R:623:SER:CB	2.37	0.49
1:K:58:LYS:NZ	1:K:86:GLY:O	2.45	0.49
1:K:493:PHE:HA	1:K:539:GLY:HA2	1.94	0.49
1:L:241:GLU:HB2	1:L:277:ARG:NH2	2.27	0.49
1:F:45:LYS:HE2	1:F:282:PHE:O	2.12	0.49
1:I:69:LEU:HD23	1:I:137:ILE:HG12	1.95	0.49
1:I:190:ASN:O	1:I:190:ASN:CG	2.56	0.49
1:M:569:MET:HG3	1:M:624:LEU:HD13	1.83	0.49
1:N:255:GLU:HA	1:N:320:PHE:O	2.13	0.49
1:Q:139:ALA:O	1:Q:142:PHE:CE1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:109:ASN:HD22	1:R:109:ASN:N	2.10	0.49
1:R:172:SER:HB3	1:R:241:GLU:OE2	2.12	0.49
1:L:39:ASP:OD2	1:L:298:ARG:HD3	2.13	0.49
1:F:171:PRO:CB	1:F:273:ILE:HD12	2.43	0.49
1:F:353:LEU:HD22	1:F:357:THR:HG21	1.95	0.49
1:I:497:GLN:N	1:I:497:GLN:NE2	2.38	0.49
1:M:35:ASP:O	1:M:37:ILE:N	2.45	0.49
1:N:28:LEU:O	1:N:31:SER:HB2	2.13	0.49
1:Q:443:ILE:HG13	1:Q:478:ARG:O	2.13	0.49
1:R:42:ARG:HH11	1:R:140:GLU:HG2	1.78	0.49
1:D:355:ARG:HD3	4:D:806:HOH:O	2.11	0.49
1:B:447:GLU:N	1:B:448:PRO:CA	2.76	0.49
1:C:15:TRP:CD2	1:C:520:LYS:HG2	2.48	0.49
1:C:168:ARG:NH1	1:C:241:GLU:OE2	2.46	0.49
1:C:378:SER:HB3	1:C:400:ALA:HB2	1.95	0.49
1:G:470:LYS:O	1:G:473:HIS:O	2.30	0.49
1:H:42:ARG:HH11	1:H:140:GLU:CG	2.22	0.49
1:M:214:PHE:HD2	1:M:305:VAL:HG22	1.75	0.49
1:M:569:MET:CG	1:M:624:LEU:HD12	2.22	0.49
1:Q:643:LYS:O	1:Q:644:SER:CB	2.61	0.49
1:J:443:ILE:HG12	1:J:445:LEU:HD13	1.95	0.49
1:J:449:PHE:C	1:J:449:PHE:CD1	2.91	0.49
1:L:490:PRO:CA	1:L:569:MET:HE1	2.42	0.49
1:D:140:GLU:C	1:D:140:GLU:OE1	2.56	0.48
1:F:145:GLU:CG	1:F:331:LEU:HD22	2.42	0.48
1:G:353:LEU:HD22	1:G:357:THR:HG21	1.94	0.48
1:I:175:ASN:O	1:I:271:TRP:HA	2.13	0.48
1:M:278:ASN:O	1:M:280:THR:N	2.44	0.48
1:O:467:GLU:OE1	1:O:467:GLU:HA	2.13	0.48
1:O:535:TRP:CD1	1:O:605:LYS:HA	2.48	0.48
1:P:273:ILE:HG13	1:P:275:MET:HE1	1.95	0.48
1:R:169:VAL:HG23	1:R:171:PRO:O	2.13	0.48
1:R:284:ASP:HB3	1:R:291:ASN:HD21	1.78	0.48
1:K:90:VAL:HB	1:K:116:ILE:HG12	1.94	0.48
1:K:244:GLU:H	1:K:244:GLU:CD	2.19	0.48
1:K:299:ASP:O	1:K:301:TRP:N	2.46	0.48
1:L:359:TYR:CD1	1:L:359:TYR:C	2.90	0.48
1:A:218:LEU:HD12	1:A:303:GLN:CB	2.42	0.48
1:D:80:LEU:HD13	1:D:509:PHE:CD1	2.48	0.48
1:C:218:LEU:HD13	1:C:268:LEU:HD13	1.95	0.48
1:E:144:THR:O	1:E:269:MET:HE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:175:ASN:ND2	1:R:237:LYS:HG2	2.28	0.48
1:R:201:GLU:C	1:R:203:PRO:HD3	2.37	0.48
1:K:316:MET:HG2	1:K:317:ASN:N	2.27	0.48
1:L:193:PRO:HA	1:L:362:ASN:ND2	2.28	0.48
1:B:66:VAL:CG1	1:B:67:HIS:N	2.76	0.48
1:C:218:LEU:H	1:C:303:GLN:HE21	1.61	0.48
1:N:188:MET:O	1:N:362:ASN:OD1	2.31	0.48
1:P:106:ILE:HD11	1:P:513:PHE:HB3	1.96	0.48
1:P:141:VAL:O	1:P:141:VAL:CG1	2.61	0.48
1:P:500:ALA:HB1	1:P:522:ARG:HH22	1.78	0.48
1:R:539:GLY:O	1:R:601:PRO:HD2	2.13	0.48
1:K:444:VAL:HG13	1:K:479:VAL:HB	1.95	0.48
1:B:218:LEU:HD12	1:B:303:GLN:CB	2.43	0.48
1:C:57:LYS:HE2	1:C:135:ASP:HB3	1.95	0.48
1:C:62:THR:N	1:C:63:ASP:HB3	2.29	0.48
1:E:63:ASP:CG	1:E:64:GLY:H	2.21	0.48
1:E:74:GLY:C	1:E:99:MET:HE3	2.38	0.48
1:I:45:LYS:NZ	1:I:282:PHE:O	2.45	0.48
1:I:291:ASN:ND2	1:I:295:TYR:HA	2.29	0.48
1:I:490:PRO:CB	1:I:569:MET:HE1	2.44	0.48
1:N:56:GLU:OE1	1:N:168:ARG:HD2	2.14	0.48
1:O:599:GLY:O	1:O:601:PRO:HD3	2.13	0.48
1:Q:269:MET:HG2	1:Q:306:TYR:HE1	1.79	0.48
1:J:242:HIS:O	1:J:245:LYS:HB2	2.12	0.48
1:K:510:ASP:C	1:K:512:SER:H	2.22	0.48
1:B:519:THR:O	1:B:520:LYS:C	2.54	0.48
1:C:280:THR:HG23	1:C:281:THR:HG23	1.95	0.48
1:E:36:MET:SD	2:E:701:SAH:HG1	2.54	0.48
1:E:168:ARG:HA	1:E:241:GLU:OE2	2.13	0.48
1:M:550:ARG:O	1:M:560:GLN:OE1	2.31	0.48
1:O:297:TRP:CD2	1:O:495:ASP:HB3	2.48	0.48
1:O:467:GLU:OE2	1:O:556:ARG:HA	2.13	0.48
1:O:569:MET:HA	1:O:572:SER:HB2	1.95	0.48
1:P:280:THR:HG23	1:P:281:THR:HG23	1.94	0.48
1:P:631:ASP:O	1:P:635:GLY:N	2.41	0.48
1:Q:570:SER:CB	1:Q:622:LYS:HD3	2.40	0.48
1:H:51:LYS:HG3	1:H:85:GLU:CG	2.43	0.48
1:I:136:ILE:HA	1:I:168:ARG:O	2.13	0.48
1:O:548:ILE:O	1:O:562:CYS:SG	2.67	0.48
1:R:36:MET:HA	1:R:300:HIS:CD2	2.48	0.48
1:L:420:ILE:HD11	1:L:428:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:PRO:CA	1:D:569:MET:HE1	2.44	0.48
1:D:528:ILE:HD12	1:D:528:ILE:N	2.28	0.48
1:B:178:ILE:HA	1:B:268:LEU:O	2.14	0.48
1:C:484:GLY:HA3	1:C:581:TRP:CZ3	2.49	0.48
1:E:226:PHE:N	1:E:226:PHE:CD1	2.81	0.48
1:I:543:GLY:HA3	1:I:568:ASN:HD22	1.77	0.48
1:N:84:ARG:HD2	1:N:85:GLU:HG2	1.95	0.48
1:O:535:TRP:O	1:O:535:TRP:CE3	2.67	0.48
1:R:69:LEU:HD12	1:R:69:LEU:C	2.39	0.48
1:J:169:VAL:CG2	1:J:171:PRO:O	2.62	0.48
1:J:308:LEU:HD13	1:J:333:PHE:O	2.13	0.48
1:L:290:LYS:O	1:L:290:LYS:HG2	2.13	0.48
1:A:359:TYR:CD1	1:A:359:TYR:C	2.92	0.48
1:D:489:ILE:O	1:D:576:PRO:HD2	2.13	0.48
1:E:75:THR:O	1:E:103:ALA:HA	2.13	0.48
1:N:42:ARG:NH1	1:N:140:GLU:HG2	2.28	0.48
1:N:84:ARG:O	1:N:85:GLU:HB2	2.14	0.48
1:N:387:GLY:HA2	1:N:450:TYR:CE2	2.48	0.48
1:O:553:ILE:HG13	1:O:554:ASP:H	1.79	0.48
1:P:228:GLU:OE2	1:P:290:LYS:NZ	2.47	0.48
1:P:455:ASN:HB2	1:P:458:ASN:HB2	1.96	0.48
1:R:338:LYS:HA	1:R:338:LYS:HD3	1.52	0.48
1:J:193:PRO:HA	1:J:362:ASN:ND2	2.26	0.48
1:J:490:PRO:HB2	1:J:569:MET:HE2	1.96	0.48
1:K:534:LEU:C	1:K:536:GLU:H	2.22	0.48
1:B:218:LEU:HD13	1:B:268:LEU:HD13	1.96	0.48
1:E:388:GLU:OE1	1:E:452:SER:HB2	2.13	0.48
1:H:38:LEU:HD21	1:H:503:VAL:HA	1.96	0.48
1:I:273:ILE:HG13	1:I:283:ILE:HB	1.96	0.48
1:M:159:LEU:HD13	1:M:243:GLU:N	2.29	0.48
1:M:300:HIS:CE1	1:M:301:TRP:CE2	3.02	0.48
1:N:405:ILE:HB	1:N:430:ILE:HG12	1.95	0.48
1:Q:143:ASP:C	1:Q:145:GLU:N	2.71	0.48
1:Q:356:GLN:O	1:Q:359:TYR:HB3	2.13	0.48
1:R:548:ILE:HG22	1:R:549:LEU:HD22	1.95	0.48
1:K:145:GLU:HG3	1:K:331:LEU:CD2	2.44	0.48
1:K:218:LEU:HD13	1:K:268:LEU:HD22	1.95	0.48
1:K:220:GLU:HG3	1:K:536:GLU:O	2.13	0.48
1:D:443:ILE:HG13	1:D:478:ARG:HB3	1.95	0.48
1:C:293:ASN:OD1	1:C:293:ASN:N	2.46	0.48
1:O:382:HIS:HD2	1:O:441:PRO:HA	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:522:ARG:O	1:O:526:ASP:HB2	2.14	0.48
1:O:534:LEU:C	1:O:536:GLU:H	2.22	0.48
1:K:297:TRP:CE3	1:K:495:ASP:HB3	2.48	0.48
1:A:612:TYR:CE2	1:A:614:PRO:HA	2.49	0.47
1:D:578:TRP:CG	1:D:591:GLY:HA3	2.49	0.47
1:C:323:VAL:HG12	1:C:325:ASN:HD21	1.79	0.47
1:F:497:GLN:NE2	1:F:497:GLN:N	2.59	0.47
1:H:20:GLU:H	1:H:20:GLU:HG3	1.52	0.47
1:I:398:LYS:HB3	1:I:398:LYS:HZ3	1.79	0.47
1:M:271:TRP:O	1:M:285:MET:HB2	2.14	0.47
1:N:67:HIS:HB3	1:N:135:ASP:H	1.79	0.47
1:N:339:ASP:HA	1:Q:244:GLU:HG3	1.96	0.47
1:O:375:ASP:HB3	1:O:399:THR:OG1	2.14	0.47
1:P:72:GLY:O	2:P:701:SAH:N	2.42	0.47
1:P:531:GLU:HA	1:P:609:GLN:O	2.14	0.47
1:Q:489:ILE:HG22	1:Q:578:TRP:HZ3	1.79	0.47
1:J:423:TYR:O	1:J:424:LYS:C	2.57	0.47
1:K:291:ASN:HB3	1:K:295:TYR:HB2	1.96	0.47
1:K:490:PRO:HG3	1:K:569:MET:HE2	1.95	0.47
1:D:22:TYR:CE2	1:D:525:THR:HG22	2.50	0.47
1:D:67:HIS:HE1	1:D:91:THR:HG22	1.77	0.47
1:D:202:GLU:HA	4:D:852:HOH:O	2.14	0.47
1:D:239:ASP:OD2	1:D:242:HIS:HD2	1.96	0.47
1:D:435:THR:HA	1:D:472:MET:SD	2.54	0.47
1:M:89:LYS:HZ2	1:M:89:LYS:HB3	1.79	0.47
1:M:497:GLN:HE21	1:M:497:GLN:N	1.99	0.47
1:N:84:ARG:CB	1:N:112:TRP:CZ2	2.97	0.47
1:N:180:PRO:HB2	1:N:264:ILE:HG12	1.96	0.47
1:N:327:ASP:C	1:N:327:ASP:OD1	2.58	0.47
1:O:35:ASP:CG	1:O:299:ASP:H	2.22	0.47
1:O:85:GLU:OE1	1:O:85:GLU:HA	2.14	0.47
1:Q:236:PHE:CE2	1:Q:326:HIS:HD2	2.32	0.47
1:R:45:LYS:HB3	1:R:275:MET:HE3	1.96	0.47
1:R:359:TYR:C	1:R:359:TYR:CD1	2.91	0.47
1:L:385:THR:HG22	4:L:825:HOH:O	2.13	0.47
1:B:491:GLU:HG3	1:B:492:LYS:N	2.29	0.47
1:C:28:LEU:HD23	1:C:521:ALA:HB2	1.95	0.47
1:C:480:GLU:OE2	1:C:482:HIS:CD2	2.55	0.47
1:F:140:GLU:HG3	1:F:140:GLU:O	2.14	0.47
1:G:35:ASP:O	1:G:36:MET:C	2.56	0.47
1:G:118:VAL:C	1:G:119:ILE:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:489:ILE:HG13	1:G:490:PRO:HD2	1.95	0.47
1:H:51:LYS:NZ	1:H:51:LYS:CB	2.78	0.47
1:H:218:LEU:HD13	1:H:268:LEU:HD13	1.96	0.47
1:M:111:PRO:HG2	1:M:112:TRP:CE3	2.48	0.47
1:M:250:GLU:HB2	1:M:326:HIS:CD2	2.49	0.47
1:M:507:ASN:HD22	1:M:507:ASN:N	2.11	0.47
1:O:218:LEU:H	1:O:303:GLN:HE22	1.57	0.47
1:Q:357:THR:O	1:Q:361:VAL:HG23	2.15	0.47
1:Q:547:GLU:CD	1:Q:550:ARG:HH11	2.23	0.47
1:R:291:ASN:O	1:R:292:LYS:HD2	2.12	0.47
1:J:270:TRP:CE2	1:J:286:GLY:HA2	2.49	0.47
1:J:356:GLN:O	1:J:606:GLY:HA2	2.14	0.47
1:J:569:MET:HE2	1:J:572:SER:HB2	1.96	0.47
1:K:353:LEU:HD22	1:K:357:THR:HG21	1.95	0.47
1:K:532:GLN:HE21	1:K:532:GLN:HB2	1.45	0.47
1:L:317:ASN:ND2	1:L:317:ASN:N	2.63	0.47
1:A:243:GLU:HG2	1:A:244:GLU:OE1	2.14	0.47
1:B:535:TRP:CE3	1:B:605:LYS:HE3	2.49	0.47
1:F:42:ARG:HH21	1:F:43:ASN:ND2	2.11	0.47
1:E:157:GLU:HA	1:E:160:GLU:CG	2.45	0.47
1:E:218:LEU:HD22	1:E:221:MET:HE2	1.96	0.47
1:E:284:ASP:HB3	1:E:294:ASN:HB2	1.96	0.47
1:G:478:ARG:NH2	1:G:480:GLU:OE1	2.47	0.47
1:O:146:LEU:HB2	1:O:271:TRP:CD1	2.49	0.47
1:O:168:ARG:HG2	1:O:241:GLU:OE2	2.14	0.47
1:O:490:PRO:HB3	1:O:569:MET:HE1	1.94	0.47
1:R:643:LYS:O	1:R:644:SER:HB3	2.15	0.47
1:J:450:TYR:H	1:J:459:HIS:CD2	2.20	0.47
1:K:193:PRO:HA	1:K:362:ASN:ND2	2.28	0.47
1:K:196:ASN:HB2	1:K:201:GLU:OE2	2.15	0.47
1:K:412:PHE:CE2	1:K:451:MET:HG2	2.44	0.47
1:K:489:ILE:HD12	1:K:545:ALA:HB2	1.95	0.47
1:B:507:ASN:HD22	1:B:507:ASN:N	2.13	0.47
1:F:250:GLU:OE2	1:F:252:PHE:CE2	2.68	0.47
1:H:277:ARG:O	1:H:277:ARG:HG2	2.13	0.47
1:I:218:LEU:HD22	1:I:221:MET:HE2	1.96	0.47
1:M:10:THR:C	1:M:12:GLU:H	2.22	0.47
1:R:218:LEU:N	1:R:303:GLN:HE21	2.11	0.47
1:J:490:PRO:HB2	1:J:572:SER:OG	2.14	0.47
1:L:253:VAL:O	1:L:253:VAL:CG2	2.61	0.47
1:A:623:SER:O	1:A:624:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LYS:NZ	1:B:553:ILE:O	2.47	0.47
1:G:112:TRP:HD1	1:G:115:LYS:HD2	1.78	0.47
1:G:490:PRO:CB	1:G:569:MET:HE2	2.39	0.47
1:I:420:ILE:HD11	1:I:428:VAL:HG22	1.95	0.47
1:N:625:CYS:HB2	1:N:643:LYS:O	2.13	0.47
1:O:556:ARG:O	1:O:558:SER:OG	2.30	0.47
1:R:437:LEU:HD13	1:R:441:PRO:HD3	1.95	0.47
1:R:548:ILE:HD12	1:R:564:VAL:HG21	1.96	0.47
1:J:143:ASP:HB3	1:J:149:GLU:HG3	1.95	0.47
1:J:480:GLU:HA	1:J:481:PRO:C	2.39	0.47
1:L:61:ASN:O	1:L:63:ASP:O	2.33	0.47
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.29	0.47
1:D:218:LEU:H	1:D:303:GLN:HE21	1.62	0.47
1:D:379:LYS:HA	1:D:399:THR:HG22	1.92	0.47
1:B:258:ALA:O	1:B:316:MET:HA	2.14	0.47
1:C:261:SER:OG	1:C:316:MET:N	2.47	0.47
1:F:316:MET:HA	1:F:317:ASN:HA	1.63	0.47
1:E:71:ILE:HG23	1:E:93:LEU:HD12	1.96	0.47
1:E:108:SER:O	1:E:110:SER:N	2.47	0.47
1:E:451:MET:HG3	1:E:452:SER:N	2.28	0.47
1:G:352:MET:O	1:G:451:MET:HE3	2.15	0.47
1:G:514:PHE:O	1:G:515:ASP:C	2.57	0.47
1:H:123:SER:C	1:H:125:ASP:H	2.22	0.47
1:H:450:TYR:N	1:H:459:HIS:HD2	2.02	0.47
1:H:497:GLN:NE2	1:H:497:GLN:N	2.43	0.47
1:I:137:ILE:O	1:I:169:VAL:HA	2.15	0.47
1:I:297:TRP:CD2	1:I:495:ASP:HB3	2.50	0.47
1:M:179:VAL:HG22	1:M:232:PRO:HA	1.96	0.47
1:M:181:VAL:HG21	1:M:268:LEU:CD1	2.37	0.47
1:M:540:ILE:HD12	1:M:542:LYS:HE2	1.97	0.47
1:M:568:ASN:N	1:M:568:ASN:ND2	2.62	0.47
1:N:325:ASN:HB2	1:N:332:TRP:CE2	2.50	0.47
1:O:177:TYR:O	1:O:269:MET:HA	2.14	0.47
1:O:539:GLY:O	1:O:601:PRO:HD2	2.14	0.47
1:P:84:ARG:C	1:P:86:GLY:N	2.73	0.47
1:P:387:GLY:HA2	1:P:450:TYR:CE1	2.50	0.47
1:Q:438:THR:HG21	1:R:629:LEU:HD21	1.97	0.47
1:R:13:ARG:NH1	1:R:13:ARG:HB2	2.30	0.47
1:R:69:LEU:HD11	1:R:71:ILE:HG12	1.97	0.47
1:R:110:SER:C	1:R:112:TRP:H	2.23	0.47
1:J:444:VAL:HG13	1:J:479:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:569:MET:HE2	1:J:572:SER:CB	2.44	0.47
1:K:534:LEU:C	1:K:536:GLU:N	2.72	0.47
1:D:278:ASN:HB2	1:D:280:THR:HG22	1.95	0.47
1:B:78:LEU:HD22	2:B:701:SAH:HN2	1.80	0.47
1:B:460:LEU:HD21	1:B:579:MET:CE	2.44	0.47
1:C:272:ASP:OD1	1:C:272:ASP:C	2.58	0.47
1:E:45:LYS:O	1:E:275:MET:HG2	2.15	0.47
1:G:112:TRP:O	1:G:113:SER:C	2.58	0.47
1:M:95:VAL:CB	1:M:122:ARG:HG3	2.44	0.47
1:M:194:ARG:O	1:M:195:LEU:C	2.58	0.47
1:N:43:ASN:N	1:N:43:ASN:HD22	2.12	0.47
1:P:367:ASN:HD21	1:P:369:LYS:HD3	1.80	0.47
1:Q:478:ARG:HH21	1:Q:478:ARG:CG	2.20	0.47
1:R:604:ASN:OD1	1:R:606:GLY:N	2.33	0.47
1:K:423:TYR:O	1:K:424:LYS:C	2.58	0.47
1:C:221:MET:HE3	1:C:226:PHE:CD1	2.50	0.47
1:F:416:PHE:O	1:F:420:ILE:HG13	2.15	0.47
1:G:375:ASP:O	1:G:399:THR:HG21	2.14	0.47
1:H:35:ASP:O	1:H:36:MET:C	2.57	0.47
1:I:177:TYR:HA	1:I:233:ILE:O	2.14	0.47
1:N:57:LYS:HB3	1:N:66:VAL:HG11	1.97	0.47
1:R:84:ARG:O	1:R:85:GLU:HB2	2.15	0.47
1:R:354:SER:O	1:R:358:VAL:HG23	2.14	0.47
1:R:578:TRP:HE1	1:R:580:GLU:HG3	1.80	0.47
1:K:168:ARG:HG2	1:K:168:ARG:HH11	1.80	0.47
1:A:241:GLU:HG3	1:A:277:ARG:HH21	1.79	0.47
1:D:292:LYS:HA	1:D:293:ASN:HA	1.53	0.47
1:B:416:PHE:O	1:B:420:ILE:HG13	2.15	0.47
1:C:349:LEU:O	1:C:350:HIS:C	2.58	0.47
1:F:57:LYS:HG2	1:F:135:ASP:HB3	1.97	0.47
1:F:184:HIS:O	1:F:185:LEU:C	2.58	0.47
1:E:275:MET:HE1	1:E:283:ILE:H	1.79	0.47
1:G:179:VAL:HG22	1:G:232:PRO:HA	1.96	0.47
1:I:298:ARG:HD2	1:I:301:TRP:HE3	1.80	0.47
1:M:111:PRO:HG2	1:M:112:TRP:CZ3	2.50	0.47
1:M:615:ILE:O	1:M:615:ILE:HG13	2.14	0.47
1:N:514:PHE:O	1:N:518:SER:CB	2.63	0.47
1:P:529:VAL:HG12	1:P:530:ASP:O	2.15	0.47
1:Q:55:ALA:O	1:Q:56:GLU:C	2.58	0.47
1:Q:222:LYS:HB3	1:Q:224:HIS:HB3	1.96	0.47
1:Q:395:LEU:C	1:Q:397:ALA:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:97:LYS:HB2	1:R:98:PRO:HD3	1.96	0.47
1:J:129:ILE:O	1:J:131:GLY:N	2.47	0.47
1:K:181:VAL:HG21	1:K:268:LEU:HD11	1.97	0.47
1:B:516:GLU:HG2	1:B:517:ILE:N	2.30	0.46
1:C:73:THR:O	2:C:701:SAH:HA	2.15	0.46
1:C:288:LYS:C	1:C:290:LYS:N	2.72	0.46
1:F:41:ASP:OD1	1:F:45:LYS:NZ	2.47	0.46
1:F:259:HIS:CD2	1:F:259:HIS:O	2.68	0.46
1:E:84:ARG:HG3	1:E:85:GLU:N	2.31	0.46
1:E:216:VAL:O	1:E:302:MET:HG2	2.16	0.46
1:G:57:LYS:NZ	1:G:166:GLY:O	2.48	0.46
1:G:483:MET:SD	1:G:550:ARG:HG3	2.55	0.46
1:G:492:LYS:HB2	1:G:571:SER:O	2.14	0.46
1:H:137:ILE:O	1:H:169:VAL:HA	2.15	0.46
1:H:574:ALA:C	1:H:575:ILE:HG13	2.40	0.46
1:I:146:LEU:HB2	1:I:271:TRP:CD1	2.50	0.46
1:I:616:THR:C	1:I:618:LEU:H	2.22	0.46
1:N:460:LEU:C	1:N:462:PHE:N	2.70	0.46
1:N:512:SER:O	1:N:515:ASP:HB2	2.15	0.46
1:N:595:ILE:HG22	1:N:599:GLY:HA2	1.97	0.46
1:O:269:MET:HG3	1:O:304:ALA:HB3	1.97	0.46
1:P:285:MET:O	1:P:303:GLN:OE1	2.33	0.46
1:P:407:ASP:O	1:P:413:ARG:HD3	2.15	0.46
1:Q:179:VAL:HG21	1:Q:270:TRP:CH2	2.51	0.46
1:Q:460:LEU:HD22	1:Q:463:LEU:HD21	1.97	0.46
1:R:580:GLU:HA	1:R:588:LEU:O	2.15	0.46
1:K:180:PRO:O	1:K:181:VAL:HG23	2.16	0.46
1:L:412:PHE:CE2	1:L:451:MET:HG2	2.49	0.46
1:L:631:ASP:CG	1:L:633:SER:HB2	2.40	0.46
1:B:297:TRP:CE3	1:B:298:ARG:HA	2.50	0.46
1:B:434:VAL:HG12	1:B:469:LEU:HD13	1.97	0.46
1:F:198:GLU:O	1:F:201:GLU:HG3	2.16	0.46
1:E:179:VAL:HG11	1:E:228:GLU:HG2	1.97	0.46
1:E:258:ALA:HB2	1:E:314:VAL:HG13	1.98	0.46
1:E:406:ILE:HG12	1:E:431:ILE:HD11	1.97	0.46
1:N:27:GLU:HB3	1:N:96:PHE:CE1	2.50	0.46
1:N:56:GLU:O	1:N:60:GLU:HG3	2.14	0.46
1:O:419:TYR:O	1:O:422:TYR:N	2.44	0.46
1:R:53:THR:HB	1:R:136:ILE:HD13	1.96	0.46
1:J:381:LEU:HD23	1:J:381:LEU:HA	1.73	0.46
1:K:104:ARG:HA	1:K:107:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASP:HA	1:C:138:VAL:O	2.14	0.46
1:C:168:ARG:NH1	1:C:168:ARG:CG	2.52	0.46
1:C:295:TYR:CD2	1:C:295:TYR:C	2.93	0.46
1:F:107:THR:HG21	1:F:116:ILE:HG21	1.97	0.46
1:F:273:ILE:HG13	1:F:275:MET:HE1	1.96	0.46
1:F:360:HIS:NE2	1:F:447:GLU:OE2	2.40	0.46
1:E:242:HIS:HB3	1:E:244:GLU:OE2	2.15	0.46
1:G:75:THR:O	1:G:106:ILE:HD12	2.15	0.46
1:G:472:MET:HE2	1:G:472:MET:HB3	1.81	0.46
1:G:550:ARG:H	1:G:560:GLN:HE22	1.64	0.46
1:H:178:ILE:HA	1:H:268:LEU:O	2.15	0.46
1:I:271:TRP:HZ3	1:I:283:ILE:HG22	1.79	0.46
1:M:94:GLU:OE2	2:M:701:SAH:H1'	2.15	0.46
1:M:381:LEU:HB3	1:M:442:ASP:HB2	1.97	0.46
1:N:160:GLU:H	1:N:160:GLU:HG2	1.55	0.46
1:N:549:LEU:HD12	1:N:560:GLN:NE2	2.30	0.46
1:N:553:ILE:HD12	1:N:553:ILE:HA	1.72	0.46
1:O:84:ARG:HG3	1:O:112:TRP:CZ2	2.50	0.46
1:O:216:VAL:C	1:O:302:MET:HG2	2.40	0.46
1:Q:169:VAL:HG21	1:Q:240:PHE:C	2.41	0.46
1:Q:191:ASP:O	1:Q:192:ILE:C	2.58	0.46
1:R:181:VAL:CG1	1:R:226:PHE:HB2	2.45	0.46
1:R:267:LEU:C	1:R:268:LEU:HD23	2.41	0.46
1:R:480:GLU:OE2	1:R:482:HIS:HD2	1.97	0.46
1:K:218:LEU:HD11	1:K:268:LEU:HD22	1.98	0.46
1:C:144:THR:O	1:C:271:TRP:CD1	2.68	0.46
1:G:169:VAL:HG11	1:G:240:PHE:C	2.41	0.46
1:H:250:GLU:HB2	1:H:326:HIS:CD2	2.51	0.46
1:H:449:PHE:CD1	1:H:449:PHE:C	2.94	0.46
1:I:495:ASP:C	1:I:497:GLN:NE2	2.74	0.46
1:I:555:GLY:HA3	1:I:556:ARG:O	2.14	0.46
1:M:175:ASN:HD21	1:M:237:LYS:NZ	2.13	0.46
1:M:193:PRO:HA	1:M:362:ASN:HD21	1.81	0.46
1:O:38:LEU:HD21	1:O:503:VAL:HA	1.96	0.46
1:O:410:GLU:O	1:O:410:GLU:HG3	2.14	0.46
1:O:498:ASN:HA	1:O:501:SER:OG	2.15	0.46
1:Q:254:ARG:O	1:Q:321:GLU:CA	2.59	0.46
1:Q:392:LEU:HD12	1:Q:445:LEU:HB3	1.97	0.46
1:Q:522:ARG:O	1:Q:526:ASP:HB2	2.14	0.46
1:R:553:ILE:HD12	1:R:553:ILE:N	2.29	0.46
1:J:175:ASN:ND2	1:J:237:LYS:HG2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:391:PHE:O	1:J:392:LEU:C	2.58	0.46
1:K:28:LEU:HD11	1:K:517:ILE:HD12	1.98	0.46
1:C:320:PHE:CD1	1:C:320:PHE:C	2.93	0.46
1:C:490:PRO:HA	1:C:569:MET:HE1	1.96	0.46
1:F:169:VAL:HG22	1:F:241:GLU:HG2	1.97	0.46
1:G:144:THR:HG23	1:G:302:MET:O	2.16	0.46
1:G:258:ALA:HB3	1:G:315:GLU:O	2.15	0.46
1:H:218:LEU:H	1:H:303:GLN:NE2	2.12	0.46
1:N:349:LEU:HD23	1:N:350:HIS:N	2.30	0.46
1:P:107:THR:C	1:P:109:ASN:N	2.74	0.46
1:P:157:GLU:O	1:P:161:ARG:HB2	2.15	0.46
1:P:447:GLU:N	1:P:448:PRO:HA	2.30	0.46
1:Q:420:ILE:HD11	1:R:5:LYS:HA	1.98	0.46
1:R:140:GLU:HG3	1:R:140:GLU:O	2.16	0.46
1:B:71:ILE:HG21	1:B:154:THR:HG23	1.98	0.46
1:C:56:GLU:OE1	1:C:168:ARG:HD2	2.16	0.46
1:E:67:HIS:CE1	1:E:91:THR:CG2	2.88	0.46
1:G:559:SER:HA	1:G:630:PHE:O	2.16	0.46
1:H:258:ALA:HB2	1:H:314:VAL:CG2	2.46	0.46
1:M:217:GLN:C	1:M:219:SER:H	2.22	0.46
1:M:218:LEU:H	1:M:303:GLN:HE21	1.62	0.46
1:N:379:LYS:CA	1:N:399:THR:CG2	2.86	0.46
1:N:627:HIS:HB2	1:N:640:GLN:HB2	1.98	0.46
1:O:621:ASP:OD1	1:O:621:ASP:N	2.46	0.46
1:J:323:VAL:HG23	1:J:335:ASN:HA	1.96	0.46
1:J:421:HIS:HB2	1:K:3:LEU:HB3	1.97	0.46
1:K:335:ASN:O	1:K:338:LYS:HB2	2.16	0.46
1:L:145:GLU:HG3	1:L:213:VAL:HG21	1.96	0.46
1:L:146:LEU:HB2	1:L:271:TRP:CD1	2.49	0.46
1:L:179:VAL:HG21	1:L:270:TRP:CH2	2.50	0.46
1:L:190:ASN:HD21	1:L:209:GLY:HA3	1.81	0.46
1:A:168:ARG:NH1	1:A:241:GLU:OE2	2.49	0.46
1:A:169:VAL:HG22	1:A:171:PRO:O	2.15	0.46
1:A:175:ASN:ND2	1:A:237:LYS:HG2	2.30	0.46
1:B:156:LYS:HE2	1:B:246:ILE:O	2.16	0.46
1:C:190:ASN:ND2	1:C:209:GLY:HA3	2.31	0.46
1:C:490:PRO:CA	1:C:569:MET:HE1	2.46	0.46
1:E:143:ASP:O	1:E:146:LEU:HA	2.16	0.46
1:G:502:ASP:OD2	1:G:616:THR:HG21	2.16	0.46
1:H:478:ARG:CG	1:H:478:ARG:NH2	2.70	0.46
1:I:478:ARG:HG2	1:I:478:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:111:PRO:C	1:M:113:SER:N	2.72	0.46
1:N:385:THR:HA	1:N:445:LEU:O	2.15	0.46
1:P:216:VAL:HG22	1:P:218:LEU:HD23	1.98	0.46
1:P:253:VAL:O	1:P:253:VAL:HG23	2.15	0.46
1:Q:139:ALA:O	1:Q:142:PHE:HE1	1.99	0.46
1:J:502:ASP:OD2	1:J:616:THR:HG21	2.16	0.46
1:K:123:SER:CB	2:K:701:SAH:HN62	2.17	0.46
1:A:145:GLU:O	1:A:146:LEU:HB3	2.16	0.46
1:C:16:VAL:HG22	4:C:811:HOH:O	2.16	0.46
1:C:314:VAL:HG23	1:C:320:PHE:CD2	2.50	0.46
1:F:7:ASN:ND2	1:F:640:GLN:OE1	2.45	0.46
1:G:93:LEU:CD2	1:G:119:ILE:HB	2.46	0.46
1:G:151:ALA:O	1:G:155:PHE:HD2	1.99	0.46
1:I:379:LYS:CA	1:I:399:THR:HG23	2.36	0.46
1:M:67:HIS:HD2	1:M:133:ARG:O	1.98	0.46
1:M:218:LEU:N	1:M:303:GLN:NE2	2.64	0.46
1:M:280:THR:CG2	1:M:281:THR:N	2.79	0.46
1:N:327:ASP:OD1	1:N:328:GLU:N	2.49	0.46
1:P:73:THR:O	2:P:701:SAH:HA	2.15	0.46
1:Q:42:ARG:HE	1:Q:43:ASN:ND2	2.14	0.46
1:R:218:LEU:HD22	1:R:221:MET:HE2	1.97	0.46
1:J:274:ASP:OD2	1:J:277:ARG:CA	2.63	0.46
1:K:32:ARG:O	1:K:36:MET:HE2	2.14	0.46
1:K:143:ASP:C	1:K:145:GLU:N	2.73	0.46
1:A:275:MET:HE2	1:A:275:MET:CA	2.45	0.46
1:A:554:ASP:O	1:A:555:GLY:O	2.34	0.46
1:D:626:LEU:CD2	1:D:628:ALA:HB2	2.45	0.46
1:F:203:PRO:HA	1:F:422:TYR:CG	2.51	0.46
1:E:42:ARG:HE	1:E:43:ASN:HD21	1.64	0.46
1:E:385:THR:HA	1:E:445:LEU:O	2.16	0.46
1:G:156:LYS:HA	1:G:243:GLU:HB3	1.97	0.46
1:G:190:ASN:ND2	1:G:209:GLY:HA3	2.31	0.46
1:H:67:HIS:CE1	1:H:89:LYS:HE3	2.51	0.46
1:H:242:HIS:O	1:H:245:LYS:HB2	2.16	0.46
1:I:298:ARG:O	1:I:301:TRP:O	2.34	0.46
1:I:492:LYS:HA	1:I:573:ASN:OD1	2.16	0.46
1:I:616:THR:C	1:I:618:LEU:N	2.74	0.46
1:M:364:MET:HG3	1:M:370:PHE:CE2	2.51	0.46
1:P:406:ILE:HD13	1:P:434:VAL:HA	1.97	0.46
1:R:231:GLU:O	1:R:232:PRO:C	2.57	0.46
1:K:257:VAL:HG12	1:K:257:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:HG23	1:D:170:VAL:HB	1.97	0.46
1:C:140:GLU:O	1:C:140:GLU:CG	2.61	0.46
1:C:150:GLY:O	1:C:151:ALA:C	2.59	0.46
1:F:48:ALA:O	1:F:51:LYS:N	2.48	0.46
1:F:73:THR:O	1:F:76:GLY:N	2.49	0.46
1:G:35:ASP:OD1	1:G:35:ASP:N	2.48	0.46
1:H:133:ARG:HG3	1:H:164:LYS:HG2	1.98	0.46
1:H:239:ASP:OD1	1:H:242:HIS:HB2	2.16	0.46
1:H:460:LEU:HD21	1:H:579:MET:CE	2.46	0.46
1:M:289:TRP:O	1:M:290:LYS:HG2	2.16	0.46
1:M:418:LYS:HE3	1:M:418:LYS:HB2	1.79	0.46
1:M:534:LEU:C	1:M:536:GLU:N	2.72	0.46
1:N:214:PHE:CD1	1:N:214:PHE:C	2.91	0.46
1:O:144:THR:O	1:O:269:MET:HE1	2.16	0.46
1:P:502:ASP:OD2	1:P:616:THR:HB	2.15	0.46
1:P:554:ASP:C	1:P:556:ARG:H	2.24	0.46
1:J:216:VAL:O	1:J:302:MET:HG2	2.16	0.46
1:K:164:LYS:O	1:K:165:PRO:C	2.59	0.46
1:K:367:ASN:OD1	1:K:370:PHE:N	2.48	0.46
1:D:45:LYS:O	1:D:275:MET:HG2	2.15	0.45
1:C:61:ASN:HD22	1:C:61:ASN:N	2.14	0.45
1:C:247:ILE:HB	1:C:250:GLU:OE2	2.16	0.45
1:C:616:THR:C	1:C:618:LEU:H	2.24	0.45
1:G:217:GLN:HB2	1:G:536:GLU:HB3	1.98	0.45
1:O:412:PHE:HE2	1:O:451:MET:HG2	1.81	0.45
1:P:164:LYS:O	1:P:167:CYS:HB2	2.16	0.45
1:Q:99:MET:O	1:Q:102:CYS:HB3	2.16	0.45
1:R:243:GLU:OE1	1:R:243:GLU:N	2.43	0.45
1:R:316:MET:HA	1:R:317:ASN:HA	1.69	0.45
1:R:353:LEU:HD22	1:R:357:THR:CG2	2.46	0.45
1:R:375:ASP:OD1	1:R:375:ASP:N	2.48	0.45
1:J:291:ASN:HB3	1:J:295:TYR:HB2	1.98	0.45
1:K:360:HIS:HB2	1:K:606:GLY:HA3	1.98	0.45
1:K:404:THR:HG23	1:K:429:GLU:HG3	1.99	0.45
1:L:353:LEU:HD22	1:L:357:THR:HG21	1.97	0.45
1:A:84:ARG:HG3	1:A:112:TRP:CZ2	2.50	0.45
1:A:186:LEU:O	1:A:187:LYS:C	2.59	0.45
1:A:385:THR:HA	1:A:445:LEU:O	2.16	0.45
1:D:437:LEU:HD22	1:D:437:LEU:C	2.41	0.45
1:B:466:VAL:HG11	1:B:553:ILE:CG2	2.46	0.45
1:B:569:MET:HA	1:B:572:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:502:ASP:OD2	1:F:616:THR:HG21	2.17	0.45
1:E:48:ALA:HA	1:E:51:LYS:HB2	1.98	0.45
1:G:478:ARG:HH21	1:G:478:ARG:CG	2.29	0.45
1:G:489:ILE:HG12	1:G:541:VAL:HG22	1.99	0.45
1:H:327:ASP:C	1:H:327:ASP:OD1	2.60	0.45
1:N:566:ILE:HG21	1:N:569:MET:CE	2.42	0.45
1:O:143:ASP:HB3	1:O:149:GLU:HG3	1.98	0.45
1:O:427:ASN:OD1	1:O:427:ASN:N	2.49	0.45
1:P:39:ASP:OD2	1:P:298:ARG:HD3	2.16	0.45
1:Q:218:LEU:HA	1:Q:218:LEU:HD23	1.42	0.45
1:Q:287:PRO:HG2	1:Q:289:TRP:CZ2	2.50	0.45
1:Q:468:VAL:O	1:Q:472:MET:HG3	2.16	0.45
1:J:144:THR:O	1:J:144:THR:CG2	2.64	0.45
1:J:218:LEU:N	1:J:303:GLN:NE2	2.62	0.45
1:J:358:VAL:O	1:J:359:TYR:C	2.59	0.45
1:K:179:VAL:CG2	1:K:270:TRP:CH2	2.99	0.45
1:K:193:PRO:HA	1:K:362:ASN:HD21	1.82	0.45
1:L:447:GLU:N	1:L:448:PRO:HA	2.32	0.45
1:A:447:GLU:H	1:A:448:PRO:HA	1.82	0.45
1:B:119:ILE:HG22	1:B:121:GLU:HG2	1.99	0.45
1:B:164:LYS:O	1:B:165:PRO:C	2.58	0.45
1:B:190:ASN:O	1:B:190:ASN:ND2	2.50	0.45
1:B:297:TRP:CE3	1:B:495:ASP:HB3	2.51	0.45
1:B:357:THR:O	1:B:361:VAL:HG23	2.16	0.45
1:C:456:PRO:HD2	1:C:457:TRP:CE3	2.51	0.45
1:C:592:LEU:HD21	1:C:595:ILE:HD11	1.97	0.45
1:F:72:GLY:CA	2:F:701:SAH:O4'	2.65	0.45
1:F:144:THR:O	1:F:269:MET:HE1	2.17	0.45
1:G:540:ILE:HB	1:G:599:GLY:O	2.15	0.45
1:H:47:LEU:HD22	1:H:51:LYS:CD	2.46	0.45
1:H:269:MET:CG	1:H:306:TYR:HE1	2.27	0.45
1:M:35:ASP:HB3	1:M:300:HIS:H	1.80	0.45
1:M:174:GLY:HA2	1:M:273:ILE:HA	1.98	0.45
1:N:315:GLU:CB	1:N:318:GLN:HG2	2.44	0.45
1:O:185:LEU:C	1:O:185:LEU:HD23	2.41	0.45
1:O:460:LEU:HD11	1:O:637:ILE:HD11	1.98	0.45
1:P:110:SER:HB2	1:P:112:TRP:CZ3	2.51	0.45
1:R:36:MET:HE1	2:R:701:SAH:SD	2.55	0.45
1:K:292:LYS:HA	1:K:293:ASN:HB3	1.98	0.45
1:L:157:GLU:HA	1:L:160:GLU:HG2	1.97	0.45
1:L:316:MET:HE2	1:L:316:MET:HB3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:579:MET:HE2	1:L:581:TRP:CZ2	2.51	0.45
1:A:4:GLU:OE2	1:A:13:ARG:NH1	2.50	0.45
1:A:480:GLU:HG2	1:A:584:GLY:H	1.79	0.45
1:B:287:PRO:O	1:B:289:TRP:N	2.50	0.45
1:B:534:LEU:HD11	1:B:611:VAL:CG1	2.46	0.45
1:B:535:TRP:CG	1:B:605:LYS:HG2	2.51	0.45
1:C:285:MET:HE2	1:C:301:TRP:HB3	1.99	0.45
1:F:179:VAL:HG22	1:F:232:PRO:HA	1.98	0.45
1:F:214:PHE:O	1:F:304:ALA:HA	2.17	0.45
1:G:258:ALA:CB	1:G:314:VAL:HG13	2.47	0.45
1:I:72:GLY:O	2:I:701:SAH:N	2.50	0.45
1:I:420:ILE:HD11	1:I:428:VAL:CG2	2.46	0.45
1:M:385:THR:HG22	4:M:802:HOH:O	2.15	0.45
1:N:287:PRO:O	1:N:291:ASN:HB3	2.16	0.45
1:K:181:VAL:O	1:K:265:ASP:N	2.49	0.45
1:K:616:THR:C	1:K:618:LEU:N	2.73	0.45
1:L:137:ILE:HB	1:L:169:VAL:HB	1.97	0.45
1:A:488:ALA:HA	1:A:576:PRO:O	2.16	0.45
1:D:359:TYR:CD1	1:D:359:TYR:C	2.94	0.45
1:B:56:GLU:O	1:B:59:HIS:HB2	2.17	0.45
1:B:193:PRO:HA	1:B:362:ASN:ND2	2.32	0.45
1:C:349:LEU:HD11	1:C:391:PHE:HZ	1.82	0.45
1:I:111:PRO:HB2	1:I:112:TRP:CE3	2.52	0.45
1:I:612:TYR:CZ	1:I:614:PRO:HA	2.51	0.45
1:M:42:ARG:HH11	1:M:140:GLU:CG	2.20	0.45
1:M:67:HIS:N	1:M:135:ASP:OD2	2.36	0.45
1:N:577:MET:CE	1:N:626:LEU:HD11	2.47	0.45
1:O:567:ASP:O	1:O:568:ASN:CB	2.62	0.45
1:P:258:ALA:O	1:P:317:ASN:HA	2.17	0.45
1:J:45:LYS:O	1:J:275:MET:HG3	2.17	0.45
1:K:299:ASP:C	1:K:301:TRP:N	2.75	0.45
1:L:631:ASP:OD1	1:L:631:ASP:C	2.59	0.45
1:D:550:ARG:H	1:D:560:GLN:NE2	2.11	0.45
1:D:631:ASP:C	1:D:631:ASP:OD1	2.59	0.45
1:B:567:ASP:O	1:B:568:ASN:CB	2.64	0.45
1:C:349:LEU:HD12	1:C:415:ILE:HD13	1.99	0.45
1:F:95:VAL:HG23	1:F:122:ARG:HB2	1.98	0.45
1:E:161:ARG:HB3	1:E:162:LEU:CD1	2.46	0.45
1:E:241:GLU:HG3	1:E:277:ARG:NH2	2.31	0.45
1:E:275:MET:CE	1:E:283:ILE:HG13	2.46	0.45
1:E:443:ILE:HG12	1:E:445:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:ASP:OD2	1:M:65:LYS:HB2	2.16	0.45
1:M:432:GLU:HG2	1:M:433:LYS:HG3	1.98	0.45
1:N:346:VAL:O	1:N:347:CYS:C	2.60	0.45
1:O:470:LYS:HE3	1:O:554:ASP:HA	1.98	0.45
1:J:597:SER:HB2	1:J:598:ALA:HB3	1.91	0.45
1:K:188:MET:O	1:K:359:TYR:HA	2.16	0.45
1:K:203:PRO:HA	1:K:422:TYR:CG	2.52	0.45
1:L:216:VAL:O	1:L:302:MET:HG2	2.17	0.45
1:B:292:LYS:HA	1:B:293:ASN:HA	1.75	0.45
1:C:323:VAL:HG12	1:C:325:ASN:ND2	2.31	0.45
1:E:258:ALA:CB	1:E:314:VAL:HG13	2.47	0.45
1:H:56:GLU:O	1:H:60:GLU:HG2	2.17	0.45
1:H:258:ALA:HB2	1:H:314:VAL:HG22	1.97	0.45
1:M:169:VAL:HG22	1:M:171:PRO:O	2.16	0.45
1:M:485:VAL:HG12	1:M:580:GLU:HB2	1.98	0.45
1:N:146:LEU:HB2	1:N:271:TRP:CD1	2.52	0.45
1:N:268:LEU:HD12	1:N:289:TRP:HH2	1.82	0.45
1:N:471:MET:HE1	1:N:556:ARG:NH1	2.31	0.45
1:O:277:ARG:HG2	1:O:277:ARG:O	2.17	0.45
1:P:168:ARG:HE	1:P:168:ARG:HB3	1.67	0.45
1:Q:68:VAL:HG13	1:Q:90:VAL:HG12	1.90	0.45
1:Q:68:VAL:HG23	1:Q:136:ILE:HB	1.99	0.45
1:Q:437:LEU:HD23	1:Q:437:LEU:HA	1.87	0.45
1:J:199:LYS:HA	1:J:200:ASP:HA	1.71	0.45
1:K:491:GLU:OE1	1:K:539:GLY:HA3	2.16	0.45
1:K:497:GLN:H	1:K:497:GLN:CD	2.25	0.45
1:A:104:ARG:HA	1:A:107:THR:HG22	1.99	0.45
1:A:178:ILE:HA	1:A:268:LEU:O	2.17	0.45
1:B:412:PHE:CE2	1:B:451:MET:HG2	2.44	0.45
1:F:158:ALA:HA	1:F:162:LEU:HB2	1.98	0.45
1:M:379:LYS:CA	1:M:399:THR:HG23	2.38	0.45
1:M:447:GLU:HB2	1:M:449:PHE:N	2.32	0.45
1:N:297:TRP:CD2	1:N:495:ASP:HB3	2.52	0.45
1:N:549:LEU:HD21	1:N:628:ALA:HB1	1.98	0.45
1:P:241:GLU:HG3	1:P:277:ARG:NH2	2.10	0.45
1:Q:95:VAL:CB	1:Q:122:ARG:HG3	2.46	0.45
1:Q:316:MET:HA	1:Q:317:ASN:HA	1.70	0.45
1:Q:321:GLU:O	1:Q:322:ILE:HD12	2.17	0.45
1:Q:381:LEU:O	1:Q:400:ALA:HB1	2.17	0.45
1:Q:466:VAL:CG1	1:Q:470:LYS:HE2	2.46	0.45
1:R:344:TYR:O	1:R:346:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:373:GLU:O	1:K:377:LEU:HD12	2.17	0.45
1:L:16:VAL:CG1	1:L:17:VAL:N	2.79	0.45
1:L:275:MET:HE3	1:L:283:ILE:N	2.31	0.45
1:L:629:LEU:O	1:L:637:ILE:HA	2.17	0.45
1:F:20:GLU:H	1:F:20:GLU:HG3	1.62	0.45
1:E:84:ARG:NH1	1:E:509:PHE:CE2	2.85	0.45
1:I:164:LYS:O	1:I:165:PRO:C	2.59	0.45
1:I:200:ASP:OD1	1:I:200:ASP:N	2.39	0.45
1:M:141:VAL:O	1:M:141:VAL:CG1	2.65	0.45
1:M:382:HIS:HD2	1:M:402:ARG:HG3	1.80	0.45
1:M:450:TYR:HE1	1:M:462:PHE:HB2	1.82	0.45
1:M:542:LYS:CG	1:M:571:SER:HB2	2.46	0.45
1:N:178:ILE:HG13	1:N:233:ILE:HB	1.99	0.45
1:N:400:ALA:C	1:N:402:ARG:N	2.75	0.45
1:N:414:ASP:O	1:N:418:LYS:HG3	2.17	0.45
1:N:490:PRO:HB3	1:N:569:MET:HE2	1.99	0.45
1:O:19:GLU:O	1:O:19:GLU:HG2	2.14	0.45
1:O:292:LYS:HD2	1:O:292:LYS:HA	1.54	0.45
1:J:534:LEU:HG	1:J:609:GLN:HB2	1.98	0.45
1:K:168:ARG:HG2	1:K:168:ARG:NH1	2.32	0.45
1:K:176:VAL:HG22	1:K:235:ALA:HB3	1.99	0.45
1:K:617:ALA:C	1:K:618:LEU:HD12	2.42	0.45
1:L:275:MET:HE2	1:L:275:MET:N	2.32	0.45
1:A:84:ARG:O	1:A:85:GLU:HB2	2.17	0.45
1:A:225:GLU:HA	1:A:225:GLU:OE1	2.17	0.45
1:B:157:GLU:HA	1:B:160:GLU:HG2	1.98	0.45
1:F:325:ASN:HB3	1:F:332:TRP:CE2	2.52	0.45
1:E:587:ASN:ND2	1:E:587:ASN:C	2.75	0.45
1:M:95:VAL:HG13	1:M:96:PHE:H	1.80	0.45
1:M:493:PHE:HA	1:M:539:GLY:CA	2.47	0.45
1:O:72:GLY:N	1:O:93:LEU:O	2.48	0.45
1:Q:431:ILE:HD12	1:Q:436:SER:HB2	1.99	0.45
1:Q:631:ASP:HB3	1:Q:634:THR:OG1	2.16	0.45
1:R:92:ALA:C	1:R:93:LEU:HD23	2.42	0.45
1:J:414:ASP:OD2	1:K:19:GLU:HG2	2.17	0.45
1:K:143:ASP:O	1:K:145:GLU:N	2.50	0.45
1:B:427:ASN:HA	1:C:8:GLN:HE22	1.81	0.44
1:E:432:GLU:HG2	1:E:433:LYS:HG2	1.99	0.44
1:G:420:ILE:HD11	1:G:428:VAL:HG22	1.99	0.44
1:I:181:VAL:HG21	1:I:226:PHE:HB2	1.98	0.44
1:M:569:MET:CG	1:M:624:LEU:HD11	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:54:ILE:HG13	1:N:58:LYS:HD3	1.99	0.44
1:O:480:GLU:HG3	1:O:481:PRO:HA	1.99	0.44
1:O:512:SER:O	1:O:515:ASP:HB2	2.17	0.44
1:P:26:GLN:O	1:P:30:ARG:HD2	2.17	0.44
1:P:136:ILE:HA	1:P:168:ARG:O	2.16	0.44
1:P:365:PHE:O	1:P:371:LYS:NZ	2.50	0.44
1:Q:480:GLU:CG	1:Q:584:GLY:N	2.78	0.44
1:R:505:THR:HA	1:R:509:PHE:O	2.17	0.44
1:J:600:VAL:HA	1:J:601:PRO:HD3	1.86	0.44
1:D:218:LEU:H	1:D:303:GLN:NE2	2.15	0.44
1:F:319:THR:O	1:F:320:PHE:HB3	2.17	0.44
1:G:56:GLU:C	1:G:58:LYS:N	2.75	0.44
1:H:632:LYS:HG2	1:H:633:SER:N	2.31	0.44
1:M:231:GLU:H	1:M:231:GLU:HG2	1.58	0.44
1:M:276:ASP:OD1	1:M:278:ASN:HB2	2.16	0.44
1:M:316:MET:HA	1:M:317:ASN:HA	1.78	0.44
1:N:352:MET:HE2	1:N:411:ARG:HB2	1.99	0.44
1:O:353:LEU:HD22	1:O:357:THR:HG21	1.98	0.44
1:O:483:MET:CG	1:O:550:ARG:HH21	2.30	0.44
1:O:541:VAL:N	1:O:599:GLY:O	2.41	0.44
1:O:577:MET:HE2	1:O:639:PHE:CZ	2.53	0.44
1:O:623:SER:O	1:O:624:LEU:HB3	2.17	0.44
1:J:368:GLN:O	1:J:369:LYS:C	2.59	0.44
1:L:228:GLU:OE2	1:L:290:LYS:HE2	2.17	0.44
1:L:631:ASP:OD1	1:L:633:SER:N	2.47	0.44
1:A:67:HIS:CE1	1:A:91:THR:HG23	2.47	0.44
1:C:447:GLU:N	1:C:448:PRO:HA	2.33	0.44
1:C:547:GLU:CD	1:C:550:ARG:NH1	2.74	0.44
1:E:492:LYS:HB2	1:E:542:LYS:HE2	1.99	0.44
1:G:450:TYR:H	1:G:459:HIS:CD2	2.22	0.44
1:I:551:PHE:CE2	1:I:579:MET:HE1	2.52	0.44
1:N:378:SER:O	1:N:379:LYS:C	2.59	0.44
1:N:460:LEU:HB3	1:N:463:LEU:HD22	1.99	0.44
1:P:48:ALA:HA	1:P:51:LYS:HD2	1.99	0.44
1:Q:569:MET:CE	1:Q:575:ILE:HG12	2.47	0.44
1:J:300:HIS:HE1	1:J:301:TRP:CE3	2.35	0.44
1:K:378:SER:HB2	1:K:399:THR:HG22	1.99	0.44
1:B:35:ASP:O	1:B:36:MET:C	2.60	0.44
1:F:159:LEU:HB3	1:F:243:GLU:HG2	1.98	0.44
1:E:20:GLU:H	1:E:20:GLU:HG3	1.21	0.44
1:G:67:HIS:HE1	1:G:91:THR:HG23	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:THR:CG2	1:G:405:ILE:HG23	2.47	0.44
1:H:190:ASN:ND2	1:H:209:GLY:HA3	2.31	0.44
1:I:507:ASN:N	1:I:507:ASN:ND2	2.65	0.44
1:M:68:VAL:HA	1:M:136:ILE:O	2.17	0.44
1:N:353:LEU:HB3	1:N:357:THR:HB	1.99	0.44
1:O:395:LEU:HD23	1:O:395:LEU:HA	1.75	0.44
1:P:26:GLN:O	1:P:30:ARG:HD3	2.16	0.44
1:P:42:ARG:NH2	1:P:43:ASN:HD21	2.09	0.44
1:Q:583:PHE:CB	1:Q:588:LEU:CD1	2.96	0.44
1:R:192:ILE:HG23	1:R:204:LEU:HD12	1.99	0.44
1:R:379:LYS:CA	1:R:399:THR:HG21	2.42	0.44
1:J:178:ILE:HB	1:J:267:LEU:HD22	1.99	0.44
1:J:300:HIS:CE1	1:J:301:TRP:CE3	3.05	0.44
1:K:169:VAL:CG1	1:K:241:GLU:HG2	2.39	0.44
1:K:375:ASP:O	1:K:399:THR:HG21	2.17	0.44
1:L:516:GLU:O	1:L:520:LYS:HG3	2.18	0.44
1:A:566:ILE:CG2	1:A:569:MET:HE3	2.47	0.44
1:B:41:ASP:C	1:B:41:ASP:OD1	2.59	0.44
1:F:51:LYS:HG3	1:F:85:GLU:HG3	1.98	0.44
1:G:28:LEU:O	1:G:28:LEU:HG	2.17	0.44
1:I:31:SER:O	1:I:33:PHE:CD2	2.71	0.44
1:I:156:LYS:NZ	1:I:243:GLU:O	2.51	0.44
1:M:80:LEU:HD21	1:M:107:THR:HG22	2.00	0.44
1:M:269:MET:HG2	1:M:306:TYR:CE2	2.51	0.44
1:M:502:ASP:OD1	1:M:616:THR:HG21	2.17	0.44
1:N:218:LEU:HD12	1:N:303:GLN:CB	2.47	0.44
1:N:272:ASP:C	1:N:272:ASP:OD1	2.60	0.44
1:N:387:GLY:HA2	1:N:450:TYR:CZ	2.53	0.44
1:O:550:ARG:HD2	1:O:550:ARG:HA	1.80	0.44
1:Q:216:VAL:HG13	1:Q:218:LEU:HG	2.00	0.44
1:L:143:ASP:O	1:L:146:LEU:N	2.43	0.44
1:D:50:LEU:O	1:D:54:ILE:CG1	2.65	0.44
1:B:43:ASN:HD22	1:B:43:ASN:N	2.07	0.44
1:F:392:LEU:O	1:F:392:LEU:HD22	2.17	0.44
1:E:362:ASN:O	1:E:366:GLU:HG2	2.18	0.44
1:G:239:ASP:CG	1:G:277:ARG:NH2	2.76	0.44
1:G:403:VAL:HB	1:G:428:VAL:HB	1.99	0.44
1:I:367:ASN:C	1:I:367:ASN:OD1	2.60	0.44
1:M:269:MET:HG3	1:M:304:ALA:HB3	2.00	0.44
1:M:316:MET:HG3	1:M:316:MET:O	2.17	0.44
1:M:472:MET:HE2	1:M:473:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:ARG:NH1	1:N:241:GLU:OE2	2.51	0.44
1:Q:108:SER:HA	1:Q:113:SER:HB2	1.99	0.44
1:Q:375:ASP:CA	1:Q:399:THR:HG21	2.21	0.44
1:Q:404:THR:HG23	1:Q:429:GLU:HG3	2.00	0.44
1:Q:490:PRO:HB2	1:Q:572:SER:OG	2.18	0.44
1:A:412:PHE:HE2	1:A:451:MET:HG2	1.82	0.44
1:D:495:ASP:O	1:D:496:LEU:C	2.61	0.44
1:B:489:ILE:HD13	1:B:541:VAL:HG22	1.99	0.44
1:F:277:ARG:O	1:F:279:GLY:N	2.51	0.44
1:H:211:ALA:HB2	1:H:343:SER:O	2.17	0.44
1:I:51:LYS:HG3	1:I:85:GLU:HG2	2.00	0.44
1:I:185:LEU:O	1:I:185:LEU:HD22	2.18	0.44
1:N:94:GLU:OE1	2:N:701:SAH:O2'	2.27	0.44
1:N:201:GLU:HA	1:N:422:TYR:OH	2.17	0.44
1:P:497:GLN:H	1:P:497:GLN:HE21	1.65	0.44
1:Q:52:THR:O	1:Q:55:ALA:HB3	2.17	0.44
1:Q:235:ALA:HB1	1:Q:324:CYS:SG	2.58	0.44
1:Q:383:VAL:HG23	1:Q:384:ALA:N	2.33	0.44
1:R:94:GLU:OE2	2:R:701:SAH:H1'	2.18	0.44
1:J:56:GLU:OE1	1:J:168:ARG:HD2	2.18	0.44
1:J:273:ILE:CD1	1:J:275:MET:HE1	2.48	0.44
1:J:395:LEU:O	1:J:398:LYS:HB2	2.18	0.44
1:A:434:VAL:HG13	1:A:469:LEU:CD1	2.47	0.44
1:B:503:VAL:H	1:B:515:ASP:CG	2.26	0.44
1:C:57:LYS:HG2	1:C:135:ASP:HB3	1.99	0.44
1:F:186:LEU:O	1:F:307:TYR:OH	2.21	0.44
1:F:264:ILE:HB	1:F:312:LYS:HB3	2.00	0.44
1:G:35:ASP:CG	1:G:299:ASP:H	2.23	0.44
1:I:145:GLU:HG3	1:I:331:LEU:HD22	2.00	0.44
1:M:383:VAL:HG13	1:M:403:VAL:HG22	2.00	0.44
1:O:145:GLU:HA	1:O:269:MET:CE	2.48	0.44
1:O:233:ILE:CD1	1:O:254:ARG:HB3	2.42	0.44
1:P:84:ARG:O	1:P:85:GLU:HB2	2.18	0.44
1:P:110:SER:O	1:P:113:SER:HB3	2.18	0.44
1:Q:146:LEU:HD13	1:Q:271:TRP:CD2	2.53	0.44
1:Q:168:ARG:CG	1:Q:168:ARG:NH1	2.65	0.44
1:R:69:LEU:HD13	1:R:91:THR:HG23	1.99	0.44
1:J:359:TYR:C	1:J:359:TYR:CD1	2.96	0.44
1:J:593:LEU:HD12	1:J:593:LEU:HA	1.91	0.44
1:A:103:ALA:O	1:A:107:THR:CB	2.47	0.44
1:D:297:TRP:CE3	1:D:495:ASP:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLU:CD	1:B:301:TRP:HZ2	2.26	0.44
1:B:231:GLU:O	1:B:233:ILE:HG22	2.18	0.44
1:F:292:LYS:HD2	1:F:292:LYS:HA	1.74	0.44
1:G:42:ARG:HG3	1:G:301:TRP:CH2	2.53	0.44
1:G:107:THR:O	1:G:110:SER:OG	2.35	0.44
1:I:36:MET:HE2	1:I:36:MET:HB3	1.86	0.44
1:M:68:VAL:HB	1:M:90:VAL:HG22	2.00	0.44
1:M:235:ALA:HA	1:M:254:ARG:HG3	2.00	0.44
1:M:269:MET:CG	1:M:304:ALA:HB3	2.48	0.44
1:O:297:TRP:CE3	1:O:495:ASP:HB3	2.52	0.44
1:Q:169:VAL:HG22	1:Q:241:GLU:HG2	2.00	0.44
1:Q:460:LEU:C	1:Q:462:PHE:N	2.71	0.44
1:R:67:HIS:CE1	1:R:89:LYS:HG2	2.53	0.44
1:R:168:ARG:HG2	1:R:241:GLU:OE1	2.18	0.44
1:R:275:MET:HE1	1:R:283:ILE:HG13	1.99	0.44
1:R:550:ARG:CZ	1:R:550:ARG:HB2	2.47	0.44
1:K:147:ILE:HD11	1:K:331:LEU:HD13	2.00	0.44
1:K:217:GLN:C	1:K:219:SER:H	2.26	0.44
1:L:80:LEU:HB3	1:L:509:PHE:CE1	2.53	0.44
1:B:169:VAL:HG22	1:B:171:PRO:O	2.17	0.43
1:C:338:LYS:N	1:F:244:GLU:HG3	2.32	0.43
1:F:218:LEU:CD2	1:F:221:MET:HE2	2.47	0.43
1:F:625:CYS:HB2	1:F:644:SER:HA	2.00	0.43
1:E:480:GLU:OE2	1:E:482:HIS:CD2	2.69	0.43
1:G:497:GLN:NE2	1:G:497:GLN:N	2.60	0.43
1:I:63:ASP:OD1	1:I:63:ASP:N	2.48	0.43
1:O:219:SER:HB3	1:O:288:LYS:HB2	2.00	0.43
1:O:404:THR:HG21	1:O:437:LEU:HD23	2.00	0.43
1:O:442:ASP:O	1:O:478:ARG:CB	2.62	0.43
1:O:451:MET:HG3	1:O:452:SER:N	2.32	0.43
1:P:464:TYR:OH	1:P:632:LYS:O	2.28	0.43
1:Q:274:ASP:OD2	1:Q:277:ARG:N	2.50	0.43
1:Q:513:PHE:O	1:Q:516:GLU:HB3	2.18	0.43
1:R:35:ASP:OD1	1:R:300:HIS:N	2.47	0.43
1:R:239:ASP:CG	1:R:242:HIS:HD2	2.26	0.43
1:J:191:ASP:OD2	1:J:194:ARG:NH1	2.51	0.43
1:D:490:PRO:HA	1:D:569:MET:HE1	2.00	0.43
1:D:518:SER:O	1:D:522:ARG:HG3	2.18	0.43
1:B:168:ARG:NH1	1:B:168:ARG:HG2	2.31	0.43
1:C:146:LEU:HD13	1:C:271:TRP:CG	2.53	0.43
1:C:230:SER:OG	1:C:231:GLU:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:LYS:HG3	1:C:295:TYR:CE2	2.53	0.43
1:C:403:VAL:HB	1:C:428:VAL:HB	2.00	0.43
1:C:578:TRP:CB	1:C:591:GLY:HA3	2.48	0.43
1:F:39:ASP:C	1:F:39:ASP:OD1	2.60	0.43
1:M:632:LYS:HG3	1:M:633:SER:N	2.32	0.43
1:N:251:SER:OG	1:N:340:LYS:HD3	2.18	0.43
1:N:258:ALA:HB3	1:N:315:GLU:O	2.18	0.43
1:N:400:ALA:O	1:N:401:LYS:C	2.61	0.43
1:O:414:ASP:O	1:O:418:LYS:HG3	2.17	0.43
1:P:486:LEU:HD11	1:P:577:MET:HE2	1.99	0.43
1:Q:67:HIS:O	1:Q:135:ASP:N	2.47	0.43
1:R:39:ASP:C	1:R:39:ASP:OD1	2.59	0.43
1:R:178:ILE:HA	1:R:268:LEU:O	2.18	0.43
1:J:54:ILE:HD13	1:J:85:GLU:HB3	1.99	0.43
1:K:348:GLY:CA	1:K:411:ARG:HH22	2.31	0.43
1:L:190:ASN:ND2	1:L:209:GLY:HA3	2.33	0.43
1:B:514:PHE:HA	1:B:517:ILE:HG12	1.99	0.43
1:F:178:ILE:HB	1:F:267:LEU:HD22	1.99	0.43
1:E:623:SER:O	1:E:624:LEU:HD23	2.18	0.43
1:H:70:ASP:HA	1:H:138:VAL:O	2.18	0.43
1:H:455:ASN:HB3	1:H:457:TRP:CE2	2.53	0.43
1:I:451:MET:HE3	1:I:451:MET:O	2.18	0.43
1:I:593:LEU:HD12	1:I:593:LEU:HA	1.73	0.43
1:M:349:LEU:HD11	1:M:353:LEU:HD12	1.99	0.43
1:N:339:ASP:OD1	1:N:340:LYS:N	2.51	0.43
1:N:410:GLU:CD	1:O:19:GLU:HB2	2.42	0.43
1:N:447:GLU:N	1:N:448:PRO:HA	2.32	0.43
1:N:474:GLY:HA3	1:N:476:GLU:OE2	2.18	0.43
1:O:198:GLU:O	1:O:201:GLU:HB2	2.17	0.43
1:O:548:ILE:HD12	1:O:626:LEU:HD13	2.01	0.43
1:P:83:ALA:HB1	1:P:112:TRP:CG	2.53	0.43
1:P:156:LYS:O	1:P:160:GLU:CG	2.65	0.43
1:Q:67:HIS:HA	1:Q:89:LYS:O	2.17	0.43
1:R:218:LEU:HD23	1:R:218:LEU:HA	1.72	0.43
1:R:485:VAL:HA	1:R:549:LEU:O	2.19	0.43
1:R:512:SER:O	1:R:515:ASP:HB2	2.18	0.43
1:J:124:THR:O	1:J:161:ARG:NH2	2.51	0.43
1:J:194:ARG:HG2	1:J:201:GLU:CB	2.37	0.43
1:K:229:LEU:CD1	1:K:314:VAL:HG12	2.48	0.43
1:K:641:PHE:N	1:K:641:PHE:CD1	2.85	0.43
1:L:84:ARG:HG3	1:L:112:TRP:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TRP:CE3	1:A:495:ASP:HB3	2.53	0.43
1:D:622:LYS:N	1:D:622:LYS:CD	2.79	0.43
1:B:111:PRO:HG2	1:B:112:TRP:CH2	2.53	0.43
1:E:643:LYS:O	1:E:644:SER:OG	2.27	0.43
1:H:244:GLU:CD	1:H:244:GLU:N	2.73	0.43
1:N:190:ASN:HD21	1:N:209:GLY:HA3	1.83	0.43
1:O:24:MET:HE3	1:O:24:MET:HB2	1.96	0.43
1:O:178:ILE:HG21	1:O:333:PHE:CZ	2.53	0.43
1:O:367:ASN:O	1:O:371:LYS:HD3	2.18	0.43
1:O:466:VAL:HA	1:O:469:LEU:HB2	1.99	0.43
1:O:483:MET:HB3	1:O:582:GLU:HG2	1.99	0.43
1:O:578:TRP:CD1	1:O:589:SER:HG	2.36	0.43
1:Q:140:GLU:HG3	1:Q:140:GLU:O	2.17	0.43
1:R:52:THR:HG21	1:R:276:ASP:CB	2.46	0.43
1:R:466:VAL:HG11	1:R:553:ILE:HG21	2.00	0.43
1:J:68:VAL:O	1:J:90:VAL:HA	2.18	0.43
1:J:93:LEU:HD23	1:J:119:ILE:HB	2.01	0.43
1:J:226:PHE:CZ	1:J:289:TRP:CZ2	3.06	0.43
1:J:261:SER:OG	1:J:316:MET:N	2.52	0.43
1:B:388:GLU:OE1	1:B:452:SER:HB2	2.19	0.43
1:F:143:ASP:O	1:F:146:LEU:N	2.34	0.43
1:F:368:GLN:NE2	1:F:371:LYS:CE	2.80	0.43
1:F:476:GLU:H	1:F:476:GLU:CD	2.27	0.43
1:G:42:ARG:HG3	1:G:301:TRP:CZ3	2.53	0.43
1:G:378:SER:O	1:G:400:ALA:HA	2.18	0.43
1:H:375:ASP:O	1:H:399:THR:HG21	2.19	0.43
1:M:480:GLU:CG	1:M:584:GLY:H	2.32	0.43
1:N:55:ALA:CA	1:N:58:LYS:HD2	2.47	0.43
1:N:612:TYR:CE2	1:N:614:PRO:HA	2.53	0.43
1:P:600:VAL:HA	1:P:601:PRO:HD3	1.86	0.43
1:Q:1:MET:O	1:Q:17:VAL:HG12	2.19	0.43
1:R:136:ILE:HG23	1:R:168:ARG:O	2.18	0.43
1:R:487:LYS:HE3	1:R:547:GLU:HG2	2.00	0.43
1:J:290:LYS:HD3	1:J:290:LYS:HA	1.92	0.43
1:K:492:LYS:HD3	1:K:542:LYS:NZ	2.33	0.43
1:A:216:VAL:O	1:A:302:MET:HG2	2.18	0.43
1:B:490:PRO:CA	1:B:569:MET:HE1	2.47	0.43
1:C:176:VAL:HG13	1:C:236:PHE:HB2	1.99	0.43
1:C:275:MET:HE1	1:C:283:ILE:H	1.84	0.43
1:E:269:MET:HG2	1:E:306:TYR:CE1	2.54	0.43
1:E:384:ALA:O	1:E:444:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ARG:O	1:G:154:THR:C	2.61	0.43
1:H:449:PHE:HA	1:H:459:HIS:CD2	2.54	0.43
1:I:264:ILE:HD12	1:I:312:LYS:HG2	2.00	0.43
1:I:550:ARG:HH11	1:I:550:ARG:CG	2.30	0.43
1:M:4:GLU:O	1:O:420:ILE:HD11	2.19	0.43
1:M:515:ASP:O	1:M:519:THR:HB	2.18	0.43
1:N:437:LEU:HD11	1:N:441:PRO:HD3	2.00	0.43
1:O:303:GLN:N	1:O:303:GLN:CD	2.76	0.43
1:P:144:THR:O	1:P:269:MET:HE1	2.18	0.43
1:P:480:GLU:OE2	1:P:482:HIS:HD2	2.01	0.43
1:R:218:LEU:C	1:R:220:GLU:N	2.77	0.43
1:R:297:TRP:CZ3	1:R:495:ASP:HB3	2.54	0.43
1:J:326:HIS:ND1	1:J:326:HIS:C	2.76	0.43
1:K:253:VAL:O	1:K:253:VAL:CG2	2.66	0.43
1:K:264:ILE:HD12	1:K:312:LYS:HG3	2.01	0.43
1:K:550:ARG:O	1:K:560:GLN:OE1	2.36	0.43
1:K:616:THR:O	1:K:618:LEU:N	2.52	0.43
1:L:569:MET:HA	1:L:572:SER:HB2	2.00	0.43
1:A:460:LEU:HD22	1:A:463:LEU:HD22	2.00	0.43
1:A:480:GLU:HG2	1:A:584:GLY:N	2.34	0.43
1:D:47:LEU:HD22	1:D:51:LYS:HE2	2.01	0.43
1:D:84:ARG:HG3	1:D:112:TRP:CZ2	2.54	0.43
1:D:190:ASN:ND2	1:D:209:GLY:HA3	2.33	0.43
1:B:566:ILE:CG2	1:B:569:MET:HE3	2.40	0.43
1:C:489:ILE:HG12	1:C:541:VAL:HG22	1.99	0.43
1:G:427:ASN:HA	1:H:8:GLN:OE1	2.18	0.43
1:G:489:ILE:CD1	1:G:541:VAL:HG21	2.48	0.43
1:H:480:GLU:HG3	1:H:584:GLY:H	1.84	0.43
1:I:24:MET:HE3	1:I:24:MET:HB2	1.57	0.43
1:I:570:SER:CB	1:I:622:LYS:HG2	2.38	0.43
1:M:151:ALA:O	1:M:154:THR:HG22	2.18	0.43
1:M:615:ILE:CG1	1:M:618:LEU:HD22	2.48	0.43
1:N:169:VAL:HG12	1:N:241:GLU:HG2	2.00	0.43
1:N:631:ASP:O	1:N:632:LYS:C	2.61	0.43
1:O:7:ASN:HD21	1:O:640:GLN:NE2	2.14	0.43
1:O:269:MET:HG2	1:O:306:TYR:CE1	2.54	0.43
1:P:161:ARG:HB3	1:P:162:LEU:HD13	2.01	0.43
1:P:218:LEU:H	1:P:303:GLN:HE21	1.66	0.43
1:L:338:LYS:O	1:L:339:ASP:C	2.61	0.43
1:A:203:PRO:HA	1:A:422:TYR:CG	2.54	0.43
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:HG2	1:B:112:TRP:CZ3	2.54	0.43
1:C:315:GLU:HB3	1:C:318:GLN:HG3	1.99	0.43
1:C:403:VAL:O	1:C:428:VAL:HA	2.19	0.43
1:F:534:LEU:HD23	1:F:534:LEU:HA	1.88	0.43
1:E:54:ILE:HD13	1:E:87:ALA:H	1.83	0.43
1:E:176:VAL:CG1	1:E:236:PHE:HB2	2.49	0.43
1:G:269:MET:HG2	1:G:306:TYR:CE1	2.53	0.43
1:I:291:ASN:HD21	1:I:295:TYR:HA	1.84	0.43
1:R:385:THR:HG21	1:R:405:ILE:HG23	2.01	0.43
1:R:569:MET:HG3	1:R:624:LEU:HG	2.00	0.43
1:J:138:VAL:HG23	1:J:170:VAL:HB	2.00	0.43
1:L:69:LEU:HD12	1:L:91:THR:O	2.18	0.43
1:L:163:ALA:HB1	1:L:167:CYS:SG	2.58	0.43
1:L:258:ALA:O	1:L:317:ASN:HA	2.18	0.43
1:A:63:ASP:C	1:A:65:LYS:H	2.27	0.43
1:D:567:ASP:C	1:D:568:ASN:ND2	2.77	0.43
1:D:569:MET:HA	1:D:572:SER:HB2	2.01	0.43
1:B:103:ALA:O	1:B:107:THR:HB	2.19	0.43
1:B:170:VAL:HA	1:B:171:PRO:HA	1.85	0.43
1:B:367:ASN:O	1:B:371:LYS:HD3	2.18	0.43
1:E:170:VAL:HA	1:E:171:PRO:HA	1.92	0.43
1:G:485:VAL:N	1:G:579:MET:HE3	2.34	0.43
1:H:67:HIS:CE1	1:H:91:THR:HG22	2.53	0.43
1:H:92:ALA:HB3	1:H:118:VAL:HG22	2.00	0.43
1:I:502:ASP:OD2	1:I:616:THR:CG2	2.65	0.43
1:M:43:ASN:N	1:M:43:ASN:ND2	2.64	0.43
1:M:96:PHE:CD2	1:M:98:PRO:HD2	2.54	0.43
1:M:176:VAL:CG2	1:M:236:PHE:HD2	2.31	0.43
1:N:63:ASP:CB	1:N:65:LYS:N	2.72	0.43
1:P:476:GLU:C	1:P:476:GLU:CD	2.87	0.43
1:Q:215:ASP:HA	1:Q:304:ALA:HA	2.00	0.43
1:L:141:VAL:O	1:L:141:VAL:CG1	2.66	0.43
1:C:20:GLU:H	1:C:20:GLU:HG3	1.40	0.43
1:F:277:ARG:C	1:F:279:GLY:N	2.76	0.43
1:G:339:ASP:OD1	1:G:341:SER:HB2	2.18	0.43
1:G:357:THR:O	1:G:360:HIS:HB3	2.19	0.43
1:H:97:LYS:N	1:H:98:PRO:CD	2.82	0.43
1:H:178:ILE:HG21	1:H:333:PHE:CZ	2.54	0.43
1:N:254:ARG:O	1:N:321:GLU:HB3	2.19	0.43
1:N:535:TRP:CE2	1:N:536:GLU:HG3	2.54	0.43
1:O:71:ILE:HG21	1:O:154:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:566:ILE:CG2	1:Q:569:MET:CE	2.97	0.43
1:R:164:LYS:O	1:R:165:PRO:C	2.62	0.43
1:J:274:ASP:HB2	1:J:282:PHE:CE1	2.54	0.43
1:J:547:GLU:OE2	1:J:550:ARG:CG	2.66	0.43
1:K:7:ASN:HB2	1:K:14:GLU:CD	2.44	0.43
1:L:378:SER:O	1:L:379:LYS:C	2.62	0.43
1:A:550:ARG:NH1	1:A:550:ARG:HB2	2.33	0.42
1:D:490:PRO:HB2	1:D:569:MET:CE	2.45	0.42
1:D:506:VAL:HG21	1:D:511:LEU:HD12	2.00	0.42
1:B:143:ASP:O	1:B:144:THR:C	2.60	0.42
1:B:502:ASP:OD2	1:B:616:THR:HG21	2.19	0.42
1:E:108:SER:C	1:E:110:SER:H	2.27	0.42
1:E:122:ARG:O	1:E:123:SER:C	2.60	0.42
1:E:169:VAL:HG13	1:E:172:SER:HA	2.01	0.42
1:E:621:ASP:OD1	1:E:621:ASP:N	2.52	0.42
1:G:159:LEU:HB2	1:G:243:GLU:HG3	2.01	0.42
1:G:291:ASN:HB3	1:G:295:TYR:HB2	2.01	0.42
1:H:303:GLN:CD	1:H:303:GLN:N	2.77	0.42
1:H:563:VAL:HG22	1:H:627:HIS:CG	2.54	0.42
1:H:578:TRP:CG	1:H:591:GLY:HA3	2.54	0.42
1:I:77:LEU:HD11	1:I:506:VAL:HG12	2.00	0.42
1:I:162:LEU:HD13	1:I:162:LEU:N	2.34	0.42
1:M:627:HIS:HB2	1:M:640:GLN:HB2	2.01	0.42
1:N:65:LYS:HA	1:N:88:ASP:OD2	2.19	0.42
1:O:275:MET:CE	1:O:283:ILE:H	2.31	0.42
1:O:379:LYS:O	1:O:381:LEU:N	2.52	0.42
1:Q:80:LEU:C	1:Q:82:ALA:N	2.77	0.42
1:Q:566:ILE:HG22	1:Q:569:MET:HE2	2.01	0.42
1:J:51:LYS:HG3	1:J:85:GLU:OE2	2.19	0.42
1:J:146:LEU:HD22	1:J:176:VAL:HG12	2.01	0.42
1:L:239:ASP:CG	1:L:277:ARG:HH22	2.27	0.42
1:D:180:PRO:CB	1:D:264:ILE:HD13	2.50	0.42
1:C:138:VAL:HG23	1:C:170:VAL:HB	2.01	0.42
1:F:142:PHE:HD1	1:F:146:LEU:HD12	1.80	0.42
1:F:615:ILE:CG1	1:F:618:LEU:HD22	2.49	0.42
1:E:548:ILE:HD12	1:E:564:VAL:HG21	2.00	0.42
1:H:496:LEU:O	1:H:499:ILE:HG12	2.19	0.42
1:I:416:PHE:O	1:I:420:ILE:HG13	2.18	0.42
1:I:615:ILE:HG12	1:I:618:LEU:HD22	2.01	0.42
1:M:95:VAL:HB	1:M:122:ARG:HG3	2.02	0.42
1:M:599:GLY:O	1:M:601:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:LYS:HE3	1:Q:337:GLY:O	2.18	0.42
1:N:308:LEU:HD12	1:N:308:LEU:HA	1.91	0.42
1:O:490:PRO:HG2	1:O:543:GLY:HA3	2.01	0.42
1:P:239:ASP:OD1	1:P:277:ARG:NH2	2.52	0.42
1:K:253:VAL:O	1:K:253:VAL:HG23	2.19	0.42
1:K:490:PRO:HG3	1:K:566:ILE:HG22	2.01	0.42
1:L:42:ARG:HH12	1:L:140:GLU:HG2	1.75	0.42
1:L:470:LYS:HG2	1:L:475:ASP:HA	1.99	0.42
1:A:470:LYS:NZ	1:A:554:ASP:HA	2.34	0.42
1:A:503:VAL:HB	1:A:515:ASP:OD1	2.19	0.42
1:B:39:ASP:C	1:B:39:ASP:OD1	2.61	0.42
1:C:277:ARG:C	1:C:279:GLY:H	2.26	0.42
1:F:310:GLU:CD	1:F:310:GLU:H	2.28	0.42
1:G:46:PHE:CZ	1:G:140:GLU:HB3	2.54	0.42
1:H:69:LEU:CD1	1:H:91:THR:HG23	2.49	0.42
1:H:72:GLY:O	2:H:701:SAH:N	2.53	0.42
1:H:144:THR:O	1:H:269:MET:HE1	2.19	0.42
1:H:563:VAL:HA	1:H:626:LEU:O	2.19	0.42
1:M:51:LYS:HD3	1:M:85:GLU:OE2	2.19	0.42
1:N:38:LEU:HD21	1:N:503:VAL:HA	2.00	0.42
1:N:391:PHE:O	1:N:394:LEU:HB2	2.19	0.42
1:N:550:ARG:O	1:N:560:GLN:OE1	2.37	0.42
1:O:423:TYR:HB2	1:O:425:LEU:HG	2.01	0.42
1:O:440:SER:HA	1:O:441:PRO:HD3	1.86	0.42
1:O:483:MET:HB3	1:O:582:GLU:CG	2.49	0.42
1:P:323:VAL:HB	1:P:334:SER:OG	2.19	0.42
1:Q:273:ILE:O	1:Q:282:PHE:HA	2.19	0.42
1:R:578:TRP:NE1	1:R:580:GLU:HG3	2.34	0.42
1:K:53:THR:HG22	1:K:168:ARG:NE	2.34	0.42
1:L:210:THR:HG21	4:L:809:HOH:O	2.18	0.42
1:D:190:ASN:HD21	1:D:209:GLY:HA3	1.84	0.42
1:D:217:GLN:HB2	1:D:536:GLU:HB3	2.00	0.42
1:D:550:ARG:O	1:D:560:GLN:OE1	2.37	0.42
1:C:463:LEU:H	1:C:463:LEU:HD22	1.83	0.42
1:G:627:HIS:HB2	1:G:640:GLN:HB2	2.01	0.42
1:H:82:ALA:O	1:H:84:ARG:O	2.37	0.42
1:H:491:GLU:HG3	1:H:492:LYS:N	2.34	0.42
1:I:145:GLU:CG	1:I:331:LEU:HD22	2.49	0.42
1:N:516:GLU:O	1:N:520:LYS:HG3	2.20	0.42
1:O:144:THR:C	1:O:146:LEU:H	2.27	0.42
1:O:480:GLU:HA	1:O:481:PRO:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:491:GLU:HG3	1:O:492:LYS:N	2.34	0.42
1:P:56:GLU:O	1:P:56:GLU:HG2	2.19	0.42
1:R:613:PHE:HA	1:R:614:PRO:HD2	1.93	0.42
1:J:107:THR:HG22	1:J:108:SER:N	2.35	0.42
1:L:178:ILE:HA	1:L:268:LEU:O	2.18	0.42
1:L:241:GLU:HB2	1:L:277:ARG:HH21	1.85	0.42
1:C:288:LYS:HG3	1:C:295:TYR:CZ	2.54	0.42
1:F:299:ASP:O	1:F:302:MET:HE3	2.20	0.42
1:G:67:HIS:CE1	1:G:91:THR:HG23	2.54	0.42
1:H:75:THR:HG22	1:H:514:PHE:CD1	2.55	0.42
1:N:55:ALA:H	1:N:58:LYS:NZ	2.05	0.42
1:N:420:ILE:CD1	1:N:428:VAL:HG22	2.50	0.42
1:N:477:LEU:O	1:N:479:VAL:HG12	2.20	0.42
1:O:369:LYS:O	1:O:370:PHE:C	2.62	0.42
1:O:618:LEU:HB3	1:O:624:LEU:HD11	2.01	0.42
1:P:292:LYS:HA	1:P:292:LYS:NZ	2.34	0.42
1:Q:182:GLU:HG3	1:Q:263:THR:O	2.20	0.42
1:Q:182:GLU:HB2	1:Q:229:LEU:HD11	2.02	0.42
1:R:326:HIS:HA	1:R:330:SER:O	2.20	0.42
1:R:627:HIS:HB2	1:R:640:GLN:HB2	2.00	0.42
1:J:275:MET:HE2	1:J:275:MET:N	2.35	0.42
1:K:325:ASN:O	1:K:331:LEU:HA	2.19	0.42
1:L:485:VAL:HG22	1:L:487:LYS:HG3	2.01	0.42
1:A:551:PHE:CE1	1:A:579:MET:HE1	2.54	0.42
1:B:541:VAL:HG11	1:B:595:ILE:HD13	2.02	0.42
1:C:169:VAL:HG23	1:C:172:SER:HA	2.01	0.42
1:C:412:PHE:O	1:C:413:ARG:C	2.63	0.42
1:C:542:LYS:HD3	1:C:542:LYS:HA	1.78	0.42
1:F:133:ARG:HB2	1:F:164:LYS:HG3	2.02	0.42
1:F:399:THR:HG22	1:F:399:THR:O	2.19	0.42
1:E:77:LEU:O	1:E:81:MET:HG3	2.20	0.42
1:E:434:VAL:HG13	1:E:469:LEU:CD1	2.49	0.42
1:E:616:THR:C	1:E:618:LEU:N	2.77	0.42
1:G:416:PHE:O	1:G:420:ILE:HG13	2.19	0.42
1:H:22:TYR:CE1	1:H:525:THR:HG22	2.54	0.42
1:I:158:ALA:HA	1:I:162:LEU:HD22	2.00	0.42
1:I:273:ILE:CD1	1:I:275:MET:HE1	2.41	0.42
1:I:368:GLN:O	1:I:369:LYS:C	2.63	0.42
1:I:379:LYS:N	1:I:399:THR:CG2	2.83	0.42
1:M:91:THR:CG2	1:M:117:THR:CG2	2.86	0.42
1:Q:177:TYR:N	1:Q:177:TYR:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:497:GLN:H	1:R:497:GLN:NE2	2.11	0.42
1:J:474:GLY:C	1:J:476:GLU:H	2.27	0.42
1:K:195:LEU:HB3	1:K:423:TYR:CZ	2.54	0.42
1:L:97:LYS:O	1:L:98:PRO:C	2.62	0.42
1:L:269:MET:HG3	1:L:306:TYR:HE1	1.85	0.42
1:A:395:LEU:O	1:A:396:ALA:C	2.60	0.42
1:D:76:GLY:O	1:D:77:LEU:C	2.62	0.42
1:D:218:LEU:HD13	1:D:268:LEU:HD13	2.02	0.42
1:B:182:GLU:OE2	1:B:227:ARG:NH1	2.52	0.42
1:B:302:MET:HE3	1:B:302:MET:HB2	1.93	0.42
1:C:534:LEU:HD21	1:C:611:VAL:HG11	2.02	0.42
1:F:93:LEU:HD13	1:F:123:SER:HA	2.02	0.42
1:F:158:ALA:O	1:F:162:LEU:N	2.52	0.42
1:F:397:ALA:O	1:F:399:THR:N	2.52	0.42
1:E:44:ASP:O	1:E:47:LEU:HB3	2.20	0.42
1:E:445:LEU:HD12	1:E:480:GLU:HB2	2.01	0.42
1:G:96:PHE:HD2	1:G:99:MET:HG2	1.84	0.42
1:G:619:ARG:HG2	1:G:619:ARG:NH1	2.34	0.42
1:I:592:LEU:HD21	1:I:595:ILE:HD11	2.02	0.42
1:M:181:VAL:HG12	1:M:183:SER:HB3	2.02	0.42
1:N:27:GLU:HB3	1:N:96:PHE:CZ	2.55	0.42
1:N:96:PHE:CD2	1:N:98:PRO:HD2	2.54	0.42
1:N:316:MET:HA	1:N:317:ASN:HA	1.65	0.42
1:Q:323:VAL:HG23	1:Q:334:SER:O	2.20	0.42
1:R:391:PHE:O	1:R:394:LEU:HB2	2.20	0.42
1:K:45:LYS:HE2	1:K:282:PHE:O	2.19	0.42
1:L:269:MET:CG	1:L:306:TYR:HE1	2.32	0.42
1:A:57:LYS:HD2	1:A:57:LYS:HA	1.82	0.42
1:A:612:TYR:CZ	1:A:614:PRO:HA	2.55	0.42
1:C:190:ASN:HD21	1:C:209:GLY:HA3	1.85	0.42
1:F:73:THR:HG22	1:F:94:GLU:HB2	2.01	0.42
1:F:229:LEU:HD23	1:F:229:LEU:HA	1.63	0.42
1:F:354:SER:O	1:F:358:VAL:HG23	2.19	0.42
1:E:269:MET:HG2	1:E:306:TYR:HE1	1.84	0.42
1:E:491:GLU:HG3	1:E:540:ILE:O	2.19	0.42
1:G:119:ILE:HD12	1:G:119:ILE:N	2.35	0.42
1:G:447:GLU:N	1:G:448:PRO:HA	2.35	0.42
1:H:119:ILE:HG23	1:J:128:GLN:HG2	2.02	0.42
1:H:169:VAL:HG11	1:H:240:PHE:O	2.20	0.42
1:N:551:PHE:CD1	1:N:579:MET:HE1	2.54	0.42
1:O:58:LYS:NZ	1:O:86:GLY:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:481:PRO:HB3	1:O:583:PHE:HD1	1.85	0.42
1:P:379:LYS:O	1:P:381:LEU:HG	2.20	0.42
1:Q:474:GLY:C	1:Q:476:GLU:N	2.74	0.42
1:J:141:VAL:O	1:J:141:VAL:CG1	2.68	0.42
1:J:168:ARG:HH22	1:J:277:ARG:HB2	1.84	0.42
1:K:532:GLN:HG2	1:K:537:TYR:HE2	1.85	0.42
1:L:577:MET:HE3	1:L:641:PHE:CZ	2.42	0.42
1:A:566:ILE:O	1:A:623:SER:HA	2.20	0.42
1:F:91:THR:HG22	1:F:117:THR:CG2	2.50	0.42
1:G:269:MET:HG2	1:G:306:TYR:HE1	1.84	0.42
1:G:480:GLU:HA	1:G:481:PRO:C	2.45	0.42
1:H:6:ILE:O	1:H:8:GLN:NE2	2.50	0.42
1:H:51:LYS:NZ	1:H:51:LYS:HB3	2.35	0.42
1:H:53:THR:HG22	1:H:168:ARG:HE	1.85	0.42
1:I:403:VAL:HB	1:I:428:VAL:HB	2.00	0.42
1:I:577:MET:HA	1:I:578:TRP:CE3	2.55	0.42
1:M:301:TRP:O	1:M:302:MET:HB3	2.20	0.42
1:M:384:ALA:O	1:M:444:VAL:HA	2.19	0.42
1:N:467:GLU:OE1	1:N:557:VAL:HG13	2.20	0.42
1:Q:190:ASN:ND2	1:Q:209:GLY:HA3	2.29	0.42
1:R:3:LEU:O	1:R:15:TRP:HA	2.20	0.42
1:J:51:LYS:HA	1:J:85:GLU:HG2	2.02	0.42
1:B:339:ASP:OD1	1:B:341:SER:N	2.45	0.42
1:C:190:ASN:O	1:C:190:ASN:CG	2.63	0.42
1:C:359:TYR:CD1	1:C:359:TYR:C	2.98	0.42
1:C:412:PHE:HE2	1:C:451:MET:HG2	1.85	0.42
1:C:569:MET:SD	1:C:575:ILE:HD11	2.60	0.42
1:E:146:LEU:HD23	1:E:146:LEU:H	1.85	0.42
1:E:569:MET:HE2	1:E:569:MET:HA	2.01	0.42
1:G:309:PRO:HB2	1:G:310:GLU:CD	2.45	0.42
1:I:550:ARG:HH11	1:I:550:ARG:HB2	1.85	0.42
1:M:66:VAL:HA	1:M:135:ASP:OD2	2.20	0.42
1:M:455:ASN:HA	1:M:456:PRO:HD3	1.87	0.42
1:N:227:ARG:NH2	1:N:261:SER:O	2.53	0.42
1:Q:186:LEU:HD11	1:Q:268:LEU:HD21	2.02	0.42
1:Q:193:PRO:HA	1:Q:362:ASN:HD21	1.84	0.42
1:Q:390:SER:OG	1:Q:447:GLU:OE1	2.31	0.42
1:Q:553:ILE:O	1:Q:553:ILE:HG23	2.19	0.42
1:Q:618:LEU:HG	1:Q:624:LEU:HD22	2.01	0.42
1:R:57:LYS:O	1:R:61:ASN:ND2	2.52	0.42
1:R:323:VAL:HG12	1:R:325:ASN:HD21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:550:ARG:O	1:R:560:GLN:NE2	2.48	0.42
1:R:616:THR:C	1:R:618:LEU:H	2.28	0.42
1:J:434:VAL:HG12	1:J:469:LEU:HD13	2.01	0.42
1:J:563:VAL:HG22	1:J:627:HIS:CD2	2.55	0.42
1:K:310:GLU:OE2	1:K:338:LYS:HG2	2.20	0.42
1:K:403:VAL:HB	1:K:428:VAL:HB	2.02	0.42
1:A:505:THR:HA	1:A:509:PHE:O	2.20	0.41
1:B:59:HIS:O	1:B:61:ASN:N	2.52	0.41
1:B:134:ALA:HB3	1:B:163:ALA:HA	2.01	0.41
1:B:522:ARG:O	1:B:526:ASP:HB2	2.19	0.41
1:F:502:ASP:CG	1:F:616:THR:HG21	2.45	0.41
1:F:535:TRP:CG	1:F:605:LYS:HG2	2.54	0.41
1:G:191:ASP:OD2	1:G:194:ARG:NH1	2.42	0.41
1:G:369:LYS:HE3	1:G:369:LYS:HB3	1.93	0.41
1:G:577:MET:HE3	1:G:577:MET:HB3	1.83	0.41
1:H:84:ARG:O	1:H:85:GLU:CB	2.62	0.41
1:H:97:LYS:HB2	1:H:98:PRO:HD3	2.02	0.41
1:H:374:VAL:O	1:H:378:SER:OG	2.37	0.41
1:M:217:GLN:C	1:M:219:SER:N	2.77	0.41
1:M:416:PHE:HB2	1:M:430:ILE:HD13	2.00	0.41
1:M:534:LEU:C	1:M:536:GLU:H	2.26	0.41
1:M:612:TYR:CE2	1:M:614:PRO:HA	2.55	0.41
1:O:179:VAL:HG11	1:O:228:GLU:HG2	2.00	0.41
1:Q:218:LEU:HD22	1:Q:221:MET:HE2	2.02	0.41
1:J:447:GLU:N	1:J:448:PRO:HA	2.35	0.41
1:K:153:ARG:O	1:K:154:THR:C	2.62	0.41
1:K:178:ILE:HA	1:K:268:LEU:O	2.20	0.41
1:K:359:TYR:CZ	1:K:605:LYS:HB2	2.55	0.41
1:L:39:ASP:OD2	1:L:298:ARG:HD2	2.20	0.41
1:A:222:LYS:O	1:A:223:THR:C	2.63	0.41
1:A:570:SER:HB3	1:A:622:LYS:HG3	2.02	0.41
1:B:66:VAL:CG1	1:B:67:HIS:H	2.32	0.41
1:B:403:VAL:HB	1:B:428:VAL:HB	2.01	0.41
1:B:437:LEU:HD22	1:B:439:ASP:O	2.19	0.41
1:E:96:PHE:CZ	1:E:98:PRO:HG2	2.55	0.41
1:E:550:ARG:H	1:E:560:GLN:NE2	2.13	0.41
1:H:178:ILE:HG21	1:H:333:PHE:CE2	2.55	0.41
1:H:179:VAL:HG22	1:H:232:PRO:HA	2.02	0.41
1:H:387:GLY:HA2	1:H:450:TYR:CE2	2.55	0.41
1:I:110:SER:C	1:I:112:TRP:H	2.28	0.41
1:I:478:ARG:CG	1:I:478:ARG:NH2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:THR:HG21	1:M:278:ASN:HD21	1.85	0.41
1:M:392:LEU:HD12	1:M:446:ALA:C	2.45	0.41
1:Q:231:GLU:H	1:Q:231:GLU:HG2	1.68	0.41
1:Q:269:MET:HG2	1:Q:306:TYR:CE1	2.54	0.41
1:Q:458:ASN:C	1:Q:458:ASN:OD1	2.63	0.41
1:R:54:ILE:HD13	1:R:54:ILE:HA	1.90	0.41
1:R:385:THR:CG2	1:R:405:ILE:HG23	2.49	0.41
1:J:478:ARG:HH21	1:J:478:ARG:CG	2.33	0.41
1:K:198:GLU:O	1:K:201:GLU:HG3	2.19	0.41
1:L:280:THR:HG23	1:L:281:THR:N	2.35	0.41
1:D:24:MET:HE3	1:D:24:MET:HB2	1.95	0.41
1:D:357:THR:HG21	1:D:449:PHE:CZ	2.54	0.41
1:B:182:GLU:HG3	1:B:263:THR:O	2.19	0.41
1:C:47:LEU:HD23	1:C:47:LEU:HA	1.83	0.41
1:C:228:GLU:OE2	1:C:290:LYS:NZ	2.51	0.41
1:H:348:GLY:O	1:H:352:MET:HG2	2.20	0.41
1:I:576:PRO:HA	1:I:611:VAL:HA	2.02	0.41
1:M:631:ASP:O	1:M:635:GLY:N	2.50	0.41
1:N:27:GLU:OE2	1:N:96:PHE:HE1	1.96	0.41
1:N:133:ARG:HH21	1:N:133:ARG:CB	2.25	0.41
1:N:514:PHE:O	1:N:518:SER:HB3	2.20	0.41
1:N:548:ILE:O	1:N:549:LEU:HD13	2.21	0.41
1:O:185:LEU:C	1:O:185:LEU:CD2	2.93	0.41
1:O:385:THR:HB	1:O:405:ILE:HD13	2.01	0.41
1:O:597:SER:HB3	1:O:598:ALA:H	1.73	0.41
1:Q:70:ASP:HB3	1:Q:79:SER:OG	2.20	0.41
1:Q:190:ASN:ND2	1:Q:190:ASN:O	2.54	0.41
1:Q:216:VAL:N	1:Q:302:MET:SD	2.93	0.41
1:K:6:ILE:O	1:K:8:GLN:NE2	2.53	0.41
1:K:136:ILE:HA	1:K:168:ARG:O	2.20	0.41
1:D:382:HIS:C	1:D:382:HIS:CD2	2.95	0.41
1:D:437:LEU:C	1:D:437:LEU:CD2	2.93	0.41
1:D:451:MET:HE2	1:D:451:MET:O	2.20	0.41
1:B:427:ASN:HA	1:C:8:GLN:NE2	2.35	0.41
1:F:42:ARG:HH11	1:F:140:GLU:CG	2.30	0.41
1:F:264:ILE:N	1:F:312:LYS:O	2.54	0.41
1:F:569:MET:HA	1:F:572:SER:HB2	2.01	0.41
1:E:143:ASP:OD2	1:E:148:GLY:HA3	2.19	0.41
1:E:379:LYS:HA	1:E:399:THR:HG22	1.93	0.41
1:E:395:LEU:O	1:E:396:ALA:C	2.60	0.41
1:E:467:GLU:OE1	1:E:556:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:LYS:HD2	1:G:9:LYS:HA	1.72	0.41
1:G:83:ALA:HA	1:G:87:ALA:HB3	2.01	0.41
1:G:364:MET:HE3	1:G:395:LEU:HD12	2.02	0.41
1:G:562:CYS:SG	1:G:564:VAL:HG22	2.60	0.41
1:H:155:PHE:O	1:H:156:LYS:C	2.62	0.41
1:H:400:ALA:O	1:H:427:ASN:ND2	2.50	0.41
1:H:460:LEU:HD21	1:H:579:MET:HE3	2.02	0.41
1:H:535:TRP:CE3	1:H:605:LYS:HE3	2.55	0.41
1:M:153:ARG:HB2	1:M:248:PHE:CZ	2.54	0.41
1:M:173:THR:HG23	1:M:174:GLY:N	2.35	0.41
1:M:173:THR:CG2	1:M:174:GLY:N	2.83	0.41
1:M:199:LYS:HA	1:M:200:ASP:HA	1.34	0.41
1:M:235:ALA:HB1	1:M:324:CYS:HB3	2.03	0.41
1:M:382:HIS:ND1	1:M:441:PRO:HA	2.35	0.41
1:N:54:ILE:CA	1:N:58:LYS:NZ	2.51	0.41
1:N:451:MET:SD	1:N:451:MET:C	3.03	0.41
1:O:53:THR:HG22	1:O:168:ARG:HE	1.84	0.41
1:O:346:VAL:O	1:O:347:CYS:C	2.63	0.41
1:O:513:PHE:O	1:O:516:GLU:HB3	2.21	0.41
1:P:39:ASP:OD2	1:P:298:ARG:CD	2.68	0.41
1:P:540:ILE:HG22	1:P:542:LYS:HE3	2.03	0.41
1:J:104:ARG:HA	1:J:118:VAL:HG21	2.02	0.41
1:J:594:SER:C	1:J:595:ILE:HG13	2.44	0.41
1:J:613:PHE:HA	1:J:614:PRO:HD2	1.89	0.41
1:K:35:ASP:O	1:K:36:MET:C	2.61	0.41
1:K:417:PHE:CZ	1:K:430:ILE:HB	2.55	0.41
1:K:443:ILE:HG13	1:K:478:ARG:HB3	2.03	0.41
1:B:164:LYS:O	1:B:167:CYS:HB2	2.20	0.41
1:B:326:HIS:ND1	1:B:326:HIS:C	2.77	0.41
1:B:476:GLU:CD	1:B:476:GLU:N	2.72	0.41
1:B:549:LEU:HD12	1:B:549:LEU:HA	1.93	0.41
1:F:180:PRO:HB2	1:F:229:LEU:HB2	2.03	0.41
1:E:84:ARG:HD3	1:O:620:ASN:HD21	1.84	0.41
1:G:7:ASN:HB2	1:G:14:GLU:CD	2.46	0.41
1:G:164:LYS:O	1:G:165:PRO:C	2.62	0.41
1:H:109:ASN:HD22	1:H:109:ASN:N	2.18	0.41
1:H:141:VAL:O	1:H:141:VAL:CG1	2.69	0.41
1:I:129:ILE:HG22	1:I:130:GLY:N	2.36	0.41
1:M:68:VAL:HG22	1:M:136:ILE:CB	2.40	0.41
1:M:176:VAL:HG22	1:M:236:PHE:HB2	2.01	0.41
1:M:297:TRP:CE3	1:M:298:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:42:ARG:HH11	1:N:140:GLU:HG2	1.85	0.41
1:N:216:VAL:HG13	1:N:218:LEU:HG	2.03	0.41
1:N:412:PHE:O	1:N:413:ARG:C	2.63	0.41
1:P:111:PRO:HD2	1:P:112:TRP:CZ3	2.54	0.41
1:Q:374:VAL:O	1:Q:375:ASP:C	2.63	0.41
1:R:639:PHE:HB3	1:R:641:PHE:CE1	2.55	0.41
1:J:495:ASP:O	1:J:496:LEU:C	2.63	0.41
1:J:643:LYS:HG3	1:J:644:SER:H	1.86	0.41
1:K:104:ARG:NH1	1:K:118:VAL:HG12	2.34	0.41
1:K:218:LEU:HB2	1:K:303:GLN:NE2	2.31	0.41
1:A:16:VAL:HG11	1:C:417:PHE:CG	2.55	0.41
1:B:444:VAL:O	1:B:445:LEU:HD12	2.21	0.41
1:C:84:ARG:HG3	1:C:112:TRP:CZ2	2.55	0.41
1:F:169:VAL:O	1:F:171:PRO:C	2.63	0.41
1:E:518:SER:O	1:E:519:THR:C	2.63	0.41
1:E:616:THR:C	1:E:618:LEU:H	2.27	0.41
1:H:480:GLU:HA	1:H:481:PRO:C	2.45	0.41
1:N:36:MET:HA	1:N:300:HIS:NE2	2.35	0.41
1:N:85:GLU:N	1:N:86:GLY:HA2	2.36	0.41
1:N:110:SER:C	1:N:112:TRP:H	2.28	0.41
1:O:386:VAL:HG23	1:O:446:ALA:HB2	2.02	0.41
1:O:390:SER:OG	1:O:447:GLU:OE1	2.33	0.41
1:O:632:LYS:HG3	1:O:633:SER:H	1.86	0.41
1:P:259:HIS:CD2	1:P:260:SER:OG	2.54	0.41
1:P:316:MET:HA	1:P:317:ASN:HA	1.71	0.41
1:Q:110:SER:HB2	1:Q:111:PRO:HD2	2.01	0.41
1:J:618:LEU:O	1:J:620:ASN:N	2.53	0.41
1:K:312:LYS:HA	1:K:312:LYS:HD3	1.87	0.41
1:K:458:ASN:C	1:K:458:ASN:OD1	2.63	0.41
1:L:35:ASP:O	1:L:36:MET:C	2.64	0.41
1:L:93:LEU:CD1	1:L:123:SER:HA	2.50	0.41
1:B:314:VAL:HG22	1:B:315:GLU:N	2.30	0.41
1:E:437:LEU:HD11	1:E:441:PRO:HG3	2.01	0.41
1:G:108:SER:O	1:G:109:ASN:CB	2.67	0.41
1:G:163:ALA:HB1	1:G:167:CYS:SG	2.61	0.41
1:G:239:ASP:OD1	1:G:277:ARG:NH2	2.54	0.41
1:I:153:ARG:O	1:I:154:THR:C	2.62	0.41
1:I:355:ARG:NE	3:I:702:PO4:O1	2.45	0.41
1:I:553:ILE:H	1:I:553:ILE:HD12	1.86	0.41
1:M:218:LEU:HB2	1:M:303:GLN:HE21	1.86	0.41
1:M:222:LYS:O	1:M:225:GLU:CG	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:460:LEU:O	1:O:461:ARG:C	2.63	0.41
1:P:27:GLU:HB3	1:P:96:PHE:CZ	2.56	0.41
1:P:45:LYS:O	1:P:275:MET:HG2	2.21	0.41
1:P:67:HIS:HE1	1:P:91:THR:HG23	1.85	0.41
1:P:297:TRP:CD2	1:P:495:ASP:HB3	2.55	0.41
1:P:369:LYS:CG	1:P:370:PHE:N	2.82	0.41
1:Q:137:ILE:O	1:Q:169:VAL:HA	2.21	0.41
1:Q:378:SER:HB2	1:Q:399:THR:CG2	2.41	0.41
1:Q:473:HIS:O	1:Q:474:GLY:C	2.62	0.41
1:Q:556:ARG:HE	1:Q:556:ARG:HB2	1.67	0.41
1:J:84:ARG:HG3	1:J:112:TRP:CZ2	2.56	0.41
1:J:263:THR:HA	1:J:313:LYS:HA	2.02	0.41
1:K:156:LYS:HG3	1:K:246:ILE:HB	2.02	0.41
1:K:381:LEU:O	1:K:400:ALA:HB1	2.20	0.41
1:K:535:TRP:O	1:K:535:TRP:CE3	2.74	0.41
1:L:180:PRO:HA	1:L:267:LEU:HD23	2.01	0.41
1:D:629:LEU:CD2	1:E:438:THR:HG21	2.48	0.41
1:B:82:ALA:O	1:B:83:ALA:C	2.63	0.41
1:B:354:SER:OG	1:B:356:GLN:CD	2.64	0.41
1:B:359:TYR:CD1	1:B:359:TYR:C	2.98	0.41
1:F:412:PHE:O	1:F:413:ARG:C	2.64	0.41
1:E:57:LYS:O	1:E:66:VAL:CG2	2.58	0.41
1:E:74:GLY:O	1:E:75:THR:C	2.64	0.41
1:E:595:ILE:HG23	1:E:599:GLY:HA2	2.02	0.41
1:G:168:ARG:NH2	1:G:276:ASP:O	2.54	0.41
1:I:71:ILE:HG21	1:I:154:THR:HG23	2.02	0.41
1:I:445:LEU:HD12	1:I:480:GLU:HB2	2.02	0.41
1:I:446:ALA:HB3	1:I:462:PHE:CE1	2.56	0.41
1:M:177:TYR:HA	1:M:233:ILE:O	2.21	0.41
1:N:58:LYS:CE	1:N:58:LYS:N	2.84	0.41
1:N:186:LEU:HD23	1:N:186:LEU:HA	1.95	0.41
1:N:467:GLU:CD	1:N:557:VAL:HG13	2.46	0.41
1:O:7:ASN:HB2	1:O:14:GLU:OE1	2.21	0.41
1:O:182:GLU:HB2	1:O:229:LEU:HD21	2.03	0.41
1:O:410:GLU:HB2	1:O:413:ARG:NH2	2.35	0.41
1:O:443:ILE:HA	1:O:478:ARG:O	2.20	0.41
1:O:447:GLU:H	1:O:448:PRO:HA	1.85	0.41
1:P:35:ASP:CG	1:P:299:ASP:H	2.29	0.41
1:Q:485:VAL:HG12	1:Q:487:LYS:HG3	2.02	0.41
1:R:471:MET:HG3	1:R:556:ARG:NH2	2.35	0.41
1:J:493:PHE:HA	1:J:539:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:TRP:O	1:K:114:ASP:N	2.54	0.41
1:L:255:GLU:HG2	1:L:321:GLU:HG2	2.03	0.41
1:L:288:LYS:HB3	1:L:288:LYS:HE2	1.63	0.41
1:A:478:ARG:CG	1:A:478:ARG:NH2	2.70	0.41
1:D:167:CYS:SG	1:D:168:ARG:O	2.79	0.41
1:B:38:LEU:HD13	1:B:498:ASN:HD22	1.86	0.41
1:C:141:VAL:O	1:C:141:VAL:CG1	2.65	0.41
1:C:180:PRO:C	1:C:181:VAL:HG23	2.46	0.41
1:F:60:GLU:O	1:F:60:GLU:HG3	2.21	0.41
1:F:70:ASP:HA	1:F:138:VAL:O	2.20	0.41
1:F:627:HIS:O	1:F:639:PHE:HA	2.21	0.41
1:E:15:TRP:NE1	1:E:520:LYS:HE2	2.36	0.41
1:E:42:ARG:HE	1:E:43:ASN:ND2	2.18	0.41
1:E:316:MET:HA	1:E:317:ASN:HA	1.86	0.41
1:E:353:LEU:HD22	1:E:357:THR:HG21	2.02	0.41
1:G:169:VAL:HG11	1:G:240:PHE:O	2.21	0.41
1:G:185:LEU:HD23	1:G:359:TYR:HE2	1.86	0.41
1:G:448:PRO:O	1:G:448:PRO:HG2	2.21	0.41
1:H:46:PHE:CZ	1:H:140:GLU:HB2	2.56	0.41
1:H:123:SER:C	1:H:125:ASP:N	2.77	0.41
1:H:268:LEU:HD12	1:H:289:TRP:HH2	1.85	0.41
1:I:96:PHE:CZ	1:I:98:PRO:HG2	2.56	0.41
1:I:190:ASN:HD21	1:I:209:GLY:HA3	1.86	0.41
1:I:243:GLU:HG2	1:I:244:GLU:N	2.34	0.41
1:I:326:HIS:HA	1:I:330:SER:O	2.21	0.41
1:I:455:ASN:HA	1:I:456:PRO:HD2	1.65	0.41
1:M:52:THR:HG21	1:M:278:ASN:ND2	2.36	0.41
1:M:57:LYS:HD3	1:M:57:LYS:HA	1.96	0.41
1:M:437:LEU:HD23	1:M:437:LEU:HA	1.88	0.41
1:M:482:HIS:CE1	1:M:582:GLU:HB3	2.56	0.41
1:M:487:LYS:O	1:M:577:MET:HA	2.21	0.41
1:N:302:MET:HG2	1:N:303:GLN:H	1.86	0.41
1:N:427:ASN:N	1:N:427:ASN:OD1	2.53	0.41
1:P:449:PHE:HA	1:P:459:HIS:CD2	2.56	0.41
1:Q:48:ALA:O	1:Q:49:GLY:C	2.64	0.41
1:R:84:ARG:O	1:R:85:GLU:CB	2.68	0.41
1:R:96:PHE:HD2	1:R:99:MET:HG2	1.85	0.41
1:R:550:ARG:H	1:R:560:GLN:NE2	2.18	0.41
1:J:32:ARG:O	1:J:33:PHE:C	2.64	0.41
1:J:119:ILE:HG22	1:J:121:GLU:HG3	2.02	0.41
1:J:413:ARG:NH1	1:J:432:GLU:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:446:ALA:O	1:J:481:PRO:HD3	2.21	0.41
1:J:547:GLU:OE2	1:J:550:ARG:HD2	2.21	0.41
1:K:478:ARG:NH2	1:K:480:GLU:OE1	2.54	0.41
1:K:516:GLU:CG	1:K:520:LYS:HE3	2.50	0.41
1:K:623:SER:O	1:K:644:SER:OG	2.30	0.41
1:L:42:ARG:HH21	1:L:43:ASN:HD21	1.68	0.41
1:L:105:HIS:O	1:L:109:ASN:ND2	2.46	0.41
1:A:119:ILE:HG22	1:A:121:GLU:HG2	2.02	0.41
1:D:226:PHE:CD1	1:D:226:PHE:N	2.89	0.41
1:D:447:GLU:N	1:D:448:PRO:HA	2.35	0.41
1:C:242:HIS:C	1:C:244:GLU:H	2.29	0.41
1:C:420:ILE:HD11	1:C:428:VAL:HG22	2.02	0.41
1:C:549:LEU:HD12	1:C:549:LEU:HA	1.68	0.41
1:F:434:VAL:CG1	1:F:469:LEU:HD13	2.52	0.41
1:E:216:VAL:C	1:E:302:MET:HG2	2.46	0.41
1:E:383:VAL:HB	1:E:443:ILE:CG2	2.51	0.41
1:G:216:VAL:CG2	1:G:217:GLN:N	2.83	0.41
1:H:292:LYS:HA	1:H:293:ASN:HA	1.93	0.41
1:H:460:LEU:C	1:H:462:PHE:N	2.76	0.41
1:H:505:THR:HA	1:H:509:PHE:O	2.20	0.41
1:N:292:LYS:HD2	1:N:293:ASN:ND2	2.37	0.41
1:N:600:VAL:HA	1:N:601:PRO:HD3	1.85	0.41
1:P:445:LEU:HD12	1:P:480:GLU:HB2	2.03	0.41
1:Q:323:VAL:HB	1:Q:334:SER:OG	2.21	0.41
1:Q:531:GLU:O	1:Q:531:GLU:HG2	2.21	0.41
1:R:77:LEU:HD11	1:R:81:MET:HE3	2.02	0.41
1:J:455:ASN:HB3	1:J:457:TRP:CE2	2.56	0.41
1:K:227:ARG:NH2	1:K:261:SER:O	2.53	0.41
1:L:168:ARG:NH1	1:L:168:ARG:CG	2.75	0.41
1:D:157:GLU:HB3	1:D:161:ARG:NH1	2.36	0.40
1:B:37:ILE:O	1:B:37:ILE:CG2	2.68	0.40
1:B:57:LYS:HG3	1:B:57:LYS:O	2.21	0.40
1:B:489:ILE:HD13	1:B:541:VAL:CG2	2.51	0.40
1:B:553:ILE:O	1:B:553:ILE:HG22	2.21	0.40
1:C:72:GLY:N	1:C:93:LEU:O	2.53	0.40
1:F:78:LEU:HD12	1:F:78:LEU:HA	1.83	0.40
1:F:274:ASP:OD1	1:F:277:ARG:N	2.45	0.40
1:E:178:ILE:HA	1:E:268:LEU:O	2.21	0.40
1:H:342:ARG:HH11	1:H:342:ARG:HD3	1.69	0.40
1:H:534:LEU:CD1	1:H:576:PRO:HB3	2.51	0.40
1:I:427:ASN:OD1	1:I:427:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:LEU:HD23	1:O:137:ILE:HG12	2.03	0.40
1:O:270:TRP:CE2	1:O:286:GLY:HA2	2.57	0.40
1:P:404:THR:HG23	1:P:429:GLU:HG3	2.03	0.40
1:P:447:GLU:H	1:P:448:PRO:HA	1.87	0.40
1:R:108:SER:C	1:R:110:SER:H	2.30	0.40
1:J:71:ILE:HB	1:J:139:ALA:HB2	2.02	0.40
1:J:566:ILE:HG21	1:J:575:ILE:HD13	2.04	0.40
1:K:222:LYS:HB2	1:K:225:GLU:CG	2.51	0.40
1:D:175:ASN:ND2	1:D:237:LYS:HG2	2.37	0.40
1:C:59:HIS:HD2	1:C:60:GLU:HG3	1.85	0.40
1:C:547:GLU:OE2	1:C:550:ARG:NH1	2.52	0.40
1:F:204:LEU:HD21	1:F:419:TYR:CE1	2.56	0.40
1:G:321:GLU:O	1:G:322:ILE:HD13	2.21	0.40
1:I:73:THR:O	1:I:74:GLY:C	2.62	0.40
1:M:194:ARG:HB3	1:M:201:GLU:OE1	2.21	0.40
1:M:344:TYR:CD1	1:M:344:TYR:N	2.89	0.40
1:M:438:THR:HB	1:M:439:ASP:OD1	2.22	0.40
1:P:198:GLU:HB3	1:P:200:ASP:HB2	2.04	0.40
1:P:275:MET:HE2	1:P:275:MET:CA	2.52	0.40
1:P:541:VAL:HG11	1:P:595:ILE:HD13	2.03	0.40
1:Q:94:GLU:OE1	2:Q:701:SAH:O2'	2.36	0.40
1:Q:216:VAL:C	1:Q:302:MET:CG	2.94	0.40
1:Q:216:VAL:CA	1:Q:302:MET:SD	3.10	0.40
1:Q:242:HIS:O	1:Q:243:GLU:C	2.64	0.40
1:Q:287:PRO:HG2	1:Q:289:TRP:CH2	2.56	0.40
1:Q:460:LEU:HD22	1:Q:463:LEU:CD2	2.51	0.40
1:J:40:PHE:CD1	1:J:41:ASP:N	2.90	0.40
1:J:144:THR:O	1:J:144:THR:HG22	2.20	0.40
1:J:297:TRP:CZ2	1:J:299:ASP:HB2	2.56	0.40
1:J:338:LYS:HD2	1:J:338:LYS:HA	1.90	0.40
1:K:277:ARG:O	1:K:277:ARG:HG2	2.21	0.40
1:L:63:ASP:OD1	1:L:63:ASP:N	2.36	0.40
1:L:110:SER:C	1:L:112:TRP:H	2.29	0.40
1:L:445:LEU:HD12	1:L:480:GLU:HB2	2.03	0.40
1:L:457:TRP:HA	4:L:831:HOH:O	2.20	0.40
1:L:465:ASP:O	1:L:469:LEU:HD22	2.21	0.40
1:A:136:ILE:HA	1:A:168:ARG:O	2.21	0.40
1:B:618:LEU:HD21	1:B:642:GLY:HA2	2.03	0.40
1:F:216:VAL:C	1:F:302:MET:HG2	2.46	0.40
1:E:578:TRP:CG	1:E:591:GLY:HA3	2.57	0.40
1:G:548:ILE:HG22	1:G:549:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:TRP:CE3	1:H:298:ARG:HA	2.56	0.40
1:M:434:VAL:HG12	1:M:469:LEU:HD12	2.03	0.40
1:N:140:GLU:OE1	1:N:301:TRP:CZ2	2.71	0.40
1:N:194:ARG:HB3	1:N:201:GLU:HG3	2.04	0.40
1:O:185:LEU:HD23	1:O:185:LEU:O	2.21	0.40
1:O:549:LEU:HD12	1:O:549:LEU:HA	1.81	0.40
1:P:122:ARG:O	1:P:125:ASP:HB2	2.22	0.40
1:Q:47:LEU:O	1:Q:51:LYS:HB2	2.21	0.40
1:Q:179:VAL:HA	1:Q:180:PRO:HD2	1.88	0.40
1:Q:372:ASP:O	1:Q:376:LYS:HB2	2.21	0.40
1:R:612:TYR:OH	1:R:615:ILE:CD1	2.70	0.40
1:J:261:SER:OG	1:J:315:GLU:HA	2.21	0.40
1:J:392:LEU:HD23	1:J:392:LEU:HA	1.90	0.40
1:K:175:ASN:O	1:K:271:TRP:HA	2.22	0.40
1:K:549:LEU:HD12	1:K:560:GLN:HB3	2.02	0.40
1:L:269:MET:HG2	1:L:306:TYR:CE1	2.56	0.40
1:D:63:ASP:CG	1:D:64:GLY:H	2.30	0.40
1:D:181:VAL:O	1:D:265:ASP:N	2.54	0.40
1:B:91:THR:HG23	1:B:119:ILE:CD1	2.52	0.40
1:B:277:ARG:C	1:B:279:GLY:H	2.29	0.40
1:C:275:MET:CE	1:C:283:ILE:H	2.34	0.40
1:E:122:ARG:O	1:E:124:THR:N	2.55	0.40
1:G:35:ASP:OD2	1:G:299:ASP:N	2.40	0.40
1:G:227:ARG:NH2	1:G:261:SER:O	2.55	0.40
1:G:310:GLU:OE1	1:G:335:ASN:OD1	2.40	0.40
1:G:448:PRO:O	1:G:448:PRO:CG	2.69	0.40
1:H:315:GLU:HB3	1:H:318:GLN:HB2	2.03	0.40
1:H:470:LYS:HD2	1:H:555:GLY:HA3	2.04	0.40
1:I:181:VAL:HG12	1:I:266:ALA:O	2.22	0.40
1:I:285:MET:O	1:I:286:GLY:C	2.64	0.40
1:I:566:ILE:HG22	1:I:569:MET:HE3	2.03	0.40
1:M:280:THR:CG2	1:M:281:THR:HG22	2.26	0.40
1:M:388:GLU:HB3	1:M:450:TYR:HA	2.03	0.40
1:N:233:ILE:HG12	1:N:256:ALA:HB2	2.04	0.40
1:N:244:GLU:CD	1:N:244:GLU:H	2.30	0.40
1:N:420:ILE:HA	1:N:425:LEU:HD12	2.03	0.40
1:O:375:ASP:HA	1:O:399:THR:OG1	2.21	0.40
1:P:248:PHE:O	1:P:327:ASP:C	2.65	0.40
1:P:455:ASN:HA	1:P:456:PRO:HD3	1.89	0.40
1:R:111:PRO:HD2	1:R:112:TRP:CZ3	2.57	0.40
1:R:531:GLU:HA	1:R:609:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:409:ASN:OD1	1:K:409:ASN:C	2.64	0.40
1:A:490:PRO:HA	1:A:569:MET:HE1	2.04	0.40
1:D:384:ALA:O	1:D:444:VAL:HA	2.21	0.40
1:D:565:ASN:ND2	1:D:644:SER:HB3	2.37	0.40
1:B:168:ARG:NH2	1:B:276:ASP:O	2.55	0.40
1:B:352:MET:HE2	1:B:411:ARG:HB2	2.03	0.40
1:B:404:THR:HG23	1:B:429:GLU:HG3	2.03	0.40
1:C:156:LYS:NZ	1:C:246:ILE:O	2.46	0.40
1:F:259:HIS:CD2	1:F:260:SER:OG	2.70	0.40
1:E:193:PRO:HA	1:E:362:ASN:ND2	2.36	0.40
1:G:73:THR:HA	2:G:701:SAH:N	2.36	0.40
1:H:239:ASP:CG	1:H:277:ARG:HH22	2.30	0.40
1:I:162:LEU:N	1:I:162:LEU:CD1	2.85	0.40
1:I:619:ARG:HG2	1:I:619:ARG:HH11	1.86	0.40
1:M:96:PHE:CE2	1:M:98:PRO:HD2	2.56	0.40
1:M:145:GLU:O	1:M:146:LEU:HB3	2.21	0.40
1:M:174:GLY:HA3	1:M:273:ILE:HG22	2.03	0.40
1:M:388:GLU:HG2	1:M:451:MET:HG3	2.04	0.40
1:N:141:VAL:O	1:N:141:VAL:CG1	2.69	0.40
1:N:242:HIS:HB3	1:N:245:LYS:CG	2.50	0.40
1:N:357:THR:O	1:N:361:VAL:HG23	2.22	0.40
1:O:310:GLU:OE2	1:O:338:LYS:HG2	2.22	0.40
1:O:557:VAL:CG2	1:O:632:LYS:HB2	2.49	0.40
1:Q:410:GLU:HG3	1:Q:413:ARG:HH22	1.87	0.40
1:Q:443:ILE:CG1	1:Q:444:VAL:N	2.85	0.40
1:Q:468:VAL:O	1:Q:471:MET:HB3	2.21	0.40
1:R:278:ASN:HB2	1:R:280:THR:HG22	2.01	0.40
1:R:377:LEU:HB3	1:R:443:ILE:HD13	2.03	0.40
1:R:600:VAL:HA	1:R:601:PRO:HD2	1.82	0.40
1:J:264:ILE:HD12	1:J:312:LYS:CG	2.52	0.40
1:J:315:GLU:O	1:J:316:MET:C	2.64	0.40
1:J:347:CYS:C	1:J:349:LEU:H	2.30	0.40
1:K:211:ALA:O	1:K:212:ALA:C	2.64	0.40
1:K:577:MET:HE3	1:K:577:MET:HB3	1.88	0.40
1:K:627:HIS:HB2	1:K:640:GLN:HB2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ASP:OD1	1:C:550:ARG:NH2[3_554]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:554:ASP:OD1	1:P:550:ARG:NH2[3_654]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/655 (97%)	600 (94%)	34 (5%)	3 (0%)	24	37
1	B	634/655 (97%)	561 (88%)	62 (10%)	11 (2%)	7	10
1	C	635/655 (97%)	578 (91%)	47 (7%)	10 (2%)	7	11
1	D	633/655 (97%)	595 (94%)	34 (5%)	4 (1%)	21	32
1	E	630/655 (96%)	569 (90%)	53 (8%)	8 (1%)	9	14
1	F	634/655 (97%)	563 (89%)	62 (10%)	9 (1%)	9	13
1	G	630/655 (96%)	575 (91%)	50 (8%)	5 (1%)	16	25
1	H	635/655 (97%)	590 (93%)	39 (6%)	6 (1%)	14	22
1	I	642/655 (98%)	572 (89%)	58 (9%)	12 (2%)	6	8
1	J	642/655 (98%)	578 (90%)	54 (8%)	10 (2%)	7	11
1	K	637/655 (97%)	570 (90%)	53 (8%)	14 (2%)	5	6
1	L	642/655 (98%)	607 (94%)	34 (5%)	1 (0%)	43	58
1	M	625/655 (95%)	551 (88%)	65 (10%)	9 (1%)	9	13
1	N	634/655 (97%)	558 (88%)	67 (11%)	9 (1%)	9	13
1	O	637/655 (97%)	567 (89%)	61 (10%)	9 (1%)	9	13
1	P	630/655 (96%)	576 (91%)	48 (8%)	6 (1%)	12	20
1	Q	626/655 (96%)	526 (84%)	81 (13%)	19 (3%)	3	3
1	R	634/655 (97%)	567 (89%)	52 (8%)	15 (2%)	4	5
All	All	11417/11790 (97%)	10303 (90%)	954 (8%)	160 (1%)	9	13

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	ASP
1	B	59	HIS
1	B	60	GLU
1	B	278	ASN
1	F	290	LYS
1	G	87	ALA
1	I	279	GLY
1	M	35	ASP
1	M	36	MET
1	M	438	THR
1	M	616	THR
1	N	88	ASP
1	O	568	ASN
1	P	438	THR
1	Q	144	THR
1	Q	259	HIS
1	Q	336	VAL
1	R	88	ASP
1	R	219	SER
1	R	400	ALA
1	J	141	VAL
1	K	300	HIS
1	A	555	GLY
1	D	277	ARG
1	D	453	ALA
1	B	77	LEU
1	B	288	LYS
1	B	555	GLY
1	C	63	ASP
1	C	289	TRP
1	C	290	LYS
1	C	617	ALA
1	F	197	GLY
1	F	278	ASN
1	F	398	LYS
1	E	87	ALA
1	E	109	ASN
1	E	123	SER
1	E	183	SER
1	H	113	SER
1	I	286	GLY
1	I	453	ALA
1	M	146	LEU

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Mol	Chain	Res	Type
1	N	264	ILE
1	N	291	ASN
1	N	474	GLY
1	O	141	VAL
1	O	380	GLY
1	O	461	ARG
1	O	478	ARG
1	O	617	ALA
1	P	108	SER
1	P	123	SER
1	P	452	SER
1	Q	56	GLU
1	Q	219	SER
1	Q	258	ALA
1	Q	277	ARG
1	R	346	VAL
1	J	130	GLY
1	J	396	ALA
1	J	598	ALA
1	K	85	GLU
1	K	113	SER
1	K	286	GLY
1	K	535	TRP
1	B	41	ASP
1	B	42	ARG
1	B	124	THR
1	C	243	GLU
1	F	148	GLY
1	G	113	SER
1	G	496	LEU
1	H	242	HIS
1	I	111	PRO
1	I	533	SER
1	M	276	ASP
1	M	289	TRP
1	Q	224	HIS
1	Q	227	ARG
1	Q	232	PRO
1	Q	340	LYS
1	R	614	PRO
1	J	597	SER
1	J	632	LYS

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Mol	Chain	Res	Type
1	J	643	LYS
1	K	144	THR
1	K	345	CYS
1	K	453	ALA
1	K	511	LEU
1	A	291	ASN
1	B	277	ARG
1	C	33	PHE
1	C	278	ASN
1	C	316	MET
1	C	475	ASP
1	F	185	LEU
1	E	288	LYS
1	E	453	ALA
1	G	277	ARG
1	H	84	ARG
1	H	277	ARG
1	I	277	ARG
1	I	594	SER
1	I	616	THR
1	M	302	MET
1	M	453	ALA
1	N	55	ALA
1	N	83	ALA
1	N	133	ARG
1	O	616	THR
1	Q	87	ALA
1	Q	243	GLU
1	Q	293	ASN
1	Q	338	LYS
1	R	52	THR
1	R	85	GLU
1	R	160	GLU
1	R	497	GLN
1	R	643	LYS
1	J	316	MET
1	K	74	GLY
1	K	617	ALA
1	B	52	THR
1	C	632	LYS
1	F	379	LYS
1	E	108	SER

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Mol	Chain	Res	Type
1	G	57	LYS
1	H	55	ALA
1	I	556	ARG
1	P	7	ASN
1	Q	146	LEU
1	Q	632	LYS
1	R	26	GLN
1	R	243	GLU
1	J	424	LYS
1	K	290	LYS
1	K	523	THR
1	H	350	HIS
1	I	309	PRO
1	N	242	HIS
1	N	244	GLU
1	O	441	PRO
1	O	614	PRO
1	R	557	VAL
1	J	33	PHE
1	A	64	GLY
1	E	279	GLY
1	R	111	PRO
1	L	111	PRO
1	D	141	VAL
1	F	615	ILE
1	P	34	GLY
1	K	197	GLY
1	F	141	VAL
1	I	553	ILE
1	R	232	PRO
1	I	232	PRO
1	Q	111	PRO
1	Q	165	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	556/569 (98%)	472 (85%)	84 (15%)	3	3
1	B	553/569 (97%)	466 (84%)	87 (16%)	2	3
1	C	554/569 (97%)	470 (85%)	84 (15%)	3	3
1	D	552/569 (97%)	472 (86%)	80 (14%)	3	4
1	E	551/569 (97%)	458 (83%)	93 (17%)	2	3
1	F	553/569 (97%)	462 (84%)	91 (16%)	2	3
1	G	552/569 (97%)	469 (85%)	83 (15%)	3	3
1	H	554/569 (97%)	471 (85%)	83 (15%)	3	3
1	I	557/569 (98%)	468 (84%)	89 (16%)	2	3
1	J	557/569 (98%)	469 (84%)	88 (16%)	2	3
1	K	556/569 (98%)	459 (83%)	97 (17%)	2	2
1	L	557/569 (98%)	473 (85%)	84 (15%)	3	3
1	M	550/569 (97%)	456 (83%)	94 (17%)	2	2
1	N	553/569 (97%)	448 (81%)	105 (19%)	1	2
1	O	556/569 (98%)	466 (84%)	90 (16%)	2	3
1	P	551/569 (97%)	457 (83%)	94 (17%)	2	2
1	Q	548/569 (96%)	456 (83%)	92 (17%)	2	3
1	R	553/569 (97%)	459 (83%)	94 (17%)	2	2
All	All	9963/10242 (97%)	8351 (84%)	1612 (16%)	2	3

All (1612) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	VAL
1	A	20	GLU
1	A	42	ARG
1	A	45	LYS
1	A	47	LEU
1	A	78	LEU
1	A	91	THR
1	A	107	THR
1	A	109	ASN
1	A	110	SER
1	A	117	THR
1	A	121	GLU
1	A	126	VAL

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Mol	Chain	Res	Type
1	A	140	GLU
1	A	141	VAL
1	A	160	GLU
1	A	168	ARG
1	A	169	VAL
1	A	173	THR
1	A	176	VAL
1	A	185	LEU
1	A	187	LYS
1	A	191	ASP
1	A	210	THR
1	A	216	VAL
1	A	223	THR
1	A	244	GLU
1	A	245	LYS
1	A	253	VAL
1	A	263	THR
1	A	269	MET
1	A	275	MET
1	A	281	THR
1	A	288	LYS
1	A	305	VAL
1	A	308	LEU
1	A	314	VAL
1	A	336	VAL
1	A	338	LYS
1	A	343	SER
1	A	349	LEU
1	A	355	ARG
1	A	363	GLU
1	A	383	VAL
1	A	385	THR
1	A	392	LEU
1	A	398	LYS
1	A	399	THR
1	A	424	LYS
1	A	428	VAL
1	A	437	LEU
1	A	444	VAL
1	A	445	LEU
1	A	451	MET
1	A	463	LEU

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Mol	Chain	Res	Type
1	A	469	LEU
1	A	471	MET
1	A	476	GLU
1	A	478	ARG
1	A	479	VAL
1	A	485	VAL
1	A	486	LEU
1	A	497	GLN
1	A	503	VAL
1	A	523	THR
1	A	528	ILE
1	A	532	GLN
1	A	540	ILE
1	A	541	VAL
1	A	546	VAL
1	A	549	LEU
1	A	554	ASP
1	A	556	ARG
1	A	558	SER
1	A	561	LYS
1	A	564	VAL
1	A	582	GLU
1	A	593	LEU
1	A	611	VAL
1	A	614	PRO
1	A	616	THR
1	A	618	LEU
1	A	632	LYS
1	D	9	LYS
1	D	16	VAL
1	D	19	GLU
1	D	20	GLU
1	D	47	LEU
1	D	71	ILE
1	D	78	LEU
1	D	85	GLU
1	D	89	LYS
1	D	91	THR
1	D	114	ASP
1	D	117	THR
1	D	140	GLU
1	D	141	VAL

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Mol	Chain	Res	Type
1	D	144	THR
1	D	160	GLU
1	D	162	LEU
1	D	168	ARG
1	D	169	VAL
1	D	173	THR
1	D	176	VAL
1	D	181	VAL
1	D	185	LEU
1	D	187	LYS
1	D	210	THR
1	D	230	SER
1	D	245	LYS
1	D	253	VAL
1	D	263	THR
1	D	264	ILE
1	D	269	MET
1	D	281	THR
1	D	288	LYS
1	D	290	LYS
1	D	298	ARG
1	D	305	VAL
1	D	308	LEU
1	D	314	VAL
1	D	319	THR
1	D	331	LEU
1	D	368	GLN
1	D	383	VAL
1	D	385	THR
1	D	392	LEU
1	D	398	LYS
1	D	399	THR
1	D	424	LYS
1	D	428	VAL
1	D	437	LEU
1	D	438	THR
1	D	440	SER
1	D	444	VAL
1	D	445	LEU
1	D	451	MET
1	D	463	LEU
1	D	469	LEU

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Mol	Chain	Res	Type
1	D	476	GLU
1	D	478	ARG
1	D	479	VAL
1	D	486	LEU
1	D	497	GLN
1	D	503	VAL
1	D	506	VAL
1	D	540	ILE
1	D	541	VAL
1	D	546	VAL
1	D	549	LEU
1	D	550	ARG
1	D	553	ILE
1	D	557	VAL
1	D	561	LYS
1	D	562	CYS
1	D	568	ASN
1	D	570	SER
1	D	593	LEU
1	D	597	SER
1	D	611	VAL
1	D	618	LEU
1	D	622	LYS
1	D	644	SER
1	B	16	VAL
1	B	19	GLU
1	B	31	SER
1	B	43	ASN
1	B	47	LEU
1	B	52	THR
1	B	56	GLU
1	B	59	HIS
1	B	62	THR
1	B	67	HIS
1	B	71	ILE
1	B	75	THR
1	B	78	LEU
1	B	84	ARG
1	B	91	THR
1	B	101	ASP
1	B	106	ILE
1	B	107	THR

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Mol	Chain	Res	Type
1	B	108	SER
1	B	114	ASP
1	B	117	THR
1	B	140	GLU
1	B	154	THR
1	B	162	LEU
1	B	169	VAL
1	B	173	THR
1	B	176	VAL
1	B	181	VAL
1	B	185	LEU
1	B	187	LYS
1	B	190	ASN
1	B	191	ASP
1	B	210	THR
1	B	216	VAL
1	B	223	THR
1	B	230	SER
1	B	233	ILE
1	B	244	GLU
1	B	257	VAL
1	B	260	SER
1	B	263	THR
1	B	269	MET
1	B	290	LYS
1	B	293	ASN
1	B	298	ARG
1	B	305	VAL
1	B	308	LEU
1	B	331	LEU
1	B	334	SER
1	B	336	VAL
1	B	351	SER
1	B	369	LYS
1	B	371	LYS
1	B	383	VAL
1	B	385	THR
1	B	428	VAL
1	B	436	SER
1	B	437	LEU
1	B	440	SER
1	B	444	VAL

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Mol	Chain	Res	Type
1	B	451	MET
1	B	452	SER
1	B	463	LEU
1	B	466	VAL
1	B	469	LEU
1	B	476	GLU
1	B	479	VAL
1	B	480	GLU
1	B	497	GLN
1	B	503	VAL
1	B	505	THR
1	B	507	ASN
1	B	541	VAL
1	B	546	VAL
1	B	549	LEU
1	B	550	ARG
1	B	557	VAL
1	B	562	CYS
1	B	570	SER
1	B	579	MET
1	B	611	VAL
1	B	614	PRO
1	B	616	THR
1	B	618	LEU
1	B	627	HIS
1	B	629	LEU
1	B	640	GLN
1	C	16	VAL
1	C	20	GLU
1	C	24	MET
1	C	47	LEU
1	C	50	LEU
1	C	52	THR
1	C	58	LYS
1	C	62	THR
1	C	65	LYS
1	C	78	LEU
1	C	89	LYS
1	C	104	ARG
1	C	107	THR
1	C	114	ASP
1	C	115	LYS

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Mol	Chain	Res	Type
1	C	117	THR
1	C	119	ILE
1	C	123	SER
1	C	140	GLU
1	C	162	LEU
1	C	168	ARG
1	C	170	VAL
1	C	173	THR
1	C	176	VAL
1	C	185	LEU
1	C	187	LYS
1	C	208	SER
1	C	210	THR
1	C	216	VAL
1	C	223	THR
1	C	230	SER
1	C	247	ILE
1	C	253	VAL
1	C	260	SER
1	C	269	MET
1	C	272	ASP
1	C	280	THR
1	C	288	LYS
1	C	290	LYS
1	C	293	ASN
1	C	298	ARG
1	C	305	VAL
1	C	308	LEU
1	C	310	GLU
1	C	311	LYS
1	C	319	THR
1	C	326	HIS
1	C	330	SER
1	C	331	LEU
1	C	363	GLU
1	C	383	VAL
1	C	385	THR
1	C	392	LEU
1	C	428	VAL
1	C	434	VAL
1	C	437	LEU
1	C	444	VAL

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Mol	Chain	Res	Type
1	C	445	LEU
1	C	451	MET
1	C	469	LEU
1	C	479	VAL
1	C	492	LYS
1	C	497	GLN
1	C	503	VAL
1	C	506	VAL
1	C	528	ILE
1	C	533	SER
1	C	540	ILE
1	C	546	VAL
1	C	549	LEU
1	C	557	VAL
1	C	558	SER
1	C	561	LYS
1	C	562	CYS
1	C	568	ASN
1	C	572	SER
1	C	577	MET
1	C	579	MET
1	C	593	LEU
1	C	597	SER
1	C	622	LYS
1	C	629	LEU
1	C	632	LYS
1	C	643	LYS
1	F	1	MET
1	F	16	VAL
1	F	20	GLU
1	F	24	MET
1	F	45	LYS
1	F	47	LEU
1	F	62	THR
1	F	78	LEU
1	F	85	GLU
1	F	89	LYS
1	F	97	LYS
1	F	104	ARG
1	F	108	SER
1	F	113	SER
1	F	116	ILE

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Mol	Chain	Res	Type
1	F	117	THR
1	F	133	ARG
1	F	140	GLU
1	F	141	VAL
1	F	162	LEU
1	F	169	VAL
1	F	173	THR
1	F	176	VAL
1	F	187	LYS
1	F	196	ASN
1	F	210	THR
1	F	216	VAL
1	F	243	GLU
1	F	244	GLU
1	F	253	VAL
1	F	257	VAL
1	F	259	HIS
1	F	263	THR
1	F	275	MET
1	F	277	ARG
1	F	290	LYS
1	F	293	ASN
1	F	298	ARG
1	F	305	VAL
1	F	310	GLU
1	F	311	LYS
1	F	314	VAL
1	F	316	MET
1	F	320	PHE
1	F	326	HIS
1	F	331	LEU
1	F	334	SER
1	F	335	ASN
1	F	336	VAL
1	F	341	SER
1	F	349	LEU
1	F	352	MET
1	F	363	GLU
1	F	366	GLU
1	F	383	VAL
1	F	385	THR
1	F	392	LEU

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Mol	Chain	Res	Type
1	F	428	VAL
1	F	436	SER
1	F	437	LEU
1	F	444	VAL
1	F	445	LEU
1	F	451	MET
1	F	463	LEU
1	F	469	LEU
1	F	476	GLU
1	F	478	ARG
1	F	479	VAL
1	F	486	LEU
1	F	494	GLU
1	F	497	GLN
1	F	503	VAL
1	F	505	THR
1	F	533	SER
1	F	540	ILE
1	F	541	VAL
1	F	546	VAL
1	F	549	LEU
1	F	550	ARG
1	F	553	ILE
1	F	557	VAL
1	F	564	VAL
1	F	579	MET
1	F	593	LEU
1	F	595	ILE
1	F	602	GLU
1	F	611	VAL
1	F	618	LEU
1	F	624	LEU
1	F	632	LYS
1	F	634	THR
1	E	1	MET
1	E	9	LYS
1	E	16	VAL
1	E	20	GLU
1	E	30	ARG
1	E	40	PHE
1	E	41	ASP
1	E	47	LEU

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Mol	Chain	Res	Type
1	E	56	GLU
1	E	66	VAL
1	E	84	ARG
1	E	85	GLU
1	E	89	LYS
1	E	91	THR
1	E	93	LEU
1	E	104	ARG
1	E	107	THR
1	E	117	THR
1	E	121	GLU
1	E	137	ILE
1	E	140	GLU
1	E	144	THR
1	E	160	GLU
1	E	162	LEU
1	E	170	VAL
1	E	173	THR
1	E	176	VAL
1	E	181	VAL
1	E	185	LEU
1	E	187	LYS
1	E	199	LYS
1	E	208	SER
1	E	210	THR
1	E	216	VAL
1	E	230	SER
1	E	253	VAL
1	E	260	SER
1	E	269	MET
1	E	272	ASP
1	E	275	MET
1	E	278	ASN
1	E	290	LYS
1	E	298	ARG
1	E	305	VAL
1	E	308	LEU
1	E	314	VAL
1	E	317	ASN
1	E	319	THR
1	E	331	LEU
1	E	338	LYS

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Mol	Chain	Res	Type
1	E	341	SER
1	E	343	SER
1	E	349	LEU
1	E	363	GLU
1	E	371	LYS
1	E	379	LYS
1	E	383	VAL
1	E	385	THR
1	E	392	LEU
1	E	399	THR
1	E	428	VAL
1	E	437	LEU
1	E	439	ASP
1	E	440	SER
1	E	444	VAL
1	E	445	LEU
1	E	451	MET
1	E	452	SER
1	E	454	MET
1	E	463	LEU
1	E	469	LEU
1	E	470	LYS
1	E	476	GLU
1	E	478	ARG
1	E	479	VAL
1	E	486	LEU
1	E	497	GLN
1	E	531	GLU
1	E	541	VAL
1	E	549	LEU
1	E	557	VAL
1	E	561	LYS
1	E	562	CYS
1	E	571	SER
1	E	577	MET
1	E	587	ASN
1	E	593	LEU
1	E	616	THR
1	E	618	LEU
1	E	623	SER
1	E	629	LEU
1	E	632	LYS

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Mol	Chain	Res	Type
1	E	643	LYS
1	G	16	VAL
1	G	26	GLN
1	G	30	ARG
1	G	47	LEU
1	G	78	LEU
1	G	84	ARG
1	G	85	GLU
1	G	117	THR
1	G	127	SER
1	G	128	GLN
1	G	140	GLU
1	G	162	LEU
1	G	172	SER
1	G	173	THR
1	G	176	VAL
1	G	181	VAL
1	G	185	LEU
1	G	191	ASP
1	G	199	LYS
1	G	200	ASP
1	G	206	ARG
1	G	210	THR
1	G	216	VAL
1	G	230	SER
1	G	243	GLU
1	G	253	VAL
1	G	260	SER
1	G	261	SER
1	G	263	THR
1	G	269	MET
1	G	275	MET
1	G	290	LYS
1	G	294	ASN
1	G	298	ARG
1	G	305	VAL
1	G	308	LEU
1	G	314	VAL
1	G	319	THR
1	G	336	VAL
1	G	339	ASP
1	G	341	SER

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Mol	Chain	Res	Type
1	G	343	SER
1	G	351	SER
1	G	363	GLU
1	G	371	LYS
1	G	379	LYS
1	G	383	VAL
1	G	385	THR
1	G	392	LEU
1	G	399	THR
1	G	424	LYS
1	G	428	VAL
1	G	433	LYS
1	G	437	LEU
1	G	444	VAL
1	G	451	MET
1	G	463	LEU
1	G	469	LEU
1	G	479	VAL
1	G	485	VAL
1	G	486	LEU
1	G	492	LYS
1	G	497	GLN
1	G	506	VAL
1	G	511	LEU
1	G	512	SER
1	G	528	ILE
1	G	533	SER
1	G	540	ILE
1	G	541	VAL
1	G	546	VAL
1	G	549	LEU
1	G	557	VAL
1	G	562	CYS
1	G	564	VAL
1	G	570	SER
1	G	577	MET
1	G	587	ASN
1	G	593	LEU
1	G	597	SER
1	G	611	VAL
1	G	616	THR
1	G	629	LEU

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Mol	Chain	Res	Type
1	H	1	MET
1	H	9	LYS
1	H	16	VAL
1	H	20	GLU
1	H	26	GLN
1	H	45	LYS
1	H	47	LEU
1	H	78	LEU
1	H	85	GLU
1	H	109	ASN
1	H	114	ASP
1	H	117	THR
1	H	124	THR
1	H	140	GLU
1	H	141	VAL
1	H	154	THR
1	H	160	GLU
1	H	173	THR
1	H	176	VAL
1	H	181	VAL
1	H	185	LEU
1	H	187	LYS
1	H	210	THR
1	H	216	VAL
1	H	243	GLU
1	H	244	GLU
1	H	253	VAL
1	H	260	SER
1	H	263	THR
1	H	269	MET
1	H	281	THR
1	H	290	LYS
1	H	292	LYS
1	H	293	ASN
1	H	305	VAL
1	H	308	LEU
1	H	311	LYS
1	H	319	THR
1	H	336	VAL
1	H	338	LYS
1	H	339	ASP
1	H	341	SER

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Mol	Chain	Res	Type
1	H	351	SER
1	H	368	GLN
1	H	378	SER
1	H	383	VAL
1	H	385	THR
1	H	392	LEU
1	H	398	LYS
1	H	411	ARG
1	H	424	LYS
1	H	428	VAL
1	H	437	LEU
1	H	444	VAL
1	H	445	LEU
1	H	452	SER
1	H	463	LEU
1	H	469	LEU
1	H	475	ASP
1	H	478	ARG
1	H	479	VAL
1	H	485	VAL
1	H	486	LEU
1	H	497	GLN
1	H	503	VAL
1	H	507	ASN
1	H	532	GLN
1	H	541	VAL
1	H	546	VAL
1	H	549	LEU
1	H	556	ARG
1	H	564	VAL
1	H	566	ILE
1	H	570	SER
1	H	593	LEU
1	H	611	VAL
1	H	616	THR
1	H	618	LEU
1	H	629	LEU
1	H	632	LYS
1	H	634	THR
1	H	643	LYS
1	H	644	SER
1	I	16	VAL

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Mol	Chain	Res	Type
1	I	19	GLU
1	I	30	ARG
1	I	31	SER
1	I	47	LEU
1	I	53	THR
1	I	56	GLU
1	I	63	ASP
1	I	66	VAL
1	I	78	LEU
1	I	85	GLU
1	I	97	LYS
1	I	104	ARG
1	I	114	ASP
1	I	115	LYS
1	I	117	THR
1	I	140	GLU
1	I	162	LEU
1	I	168	ARG
1	I	169	VAL
1	I	172	SER
1	I	173	THR
1	I	176	VAL
1	I	185	LEU
1	I	191	ASP
1	I	200	ASP
1	I	210	THR
1	I	216	VAL
1	I	243	GLU
1	I	261	SER
1	I	269	MET
1	I	278	ASN
1	I	280	THR
1	I	281	THR
1	I	290	LYS
1	I	293	ASN
1	I	298	ARG
1	I	305	VAL
1	I	308	LEU
1	I	314	VAL
1	I	318	GLN
1	I	319	THR
1	I	325	ASN

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Mol	Chain	Res	Type
1	I	331	LEU
1	I	336	VAL
1	I	351	SER
1	I	368	GLN
1	I	383	VAL
1	I	385	THR
1	I	392	LEU
1	I	398	LYS
1	I	399	THR
1	I	424	LYS
1	I	428	VAL
1	I	437	LEU
1	I	438	THR
1	I	444	VAL
1	I	445	LEU
1	I	451	MET
1	I	463	LEU
1	I	466	VAL
1	I	469	LEU
1	I	476	GLU
1	I	478	ARG
1	I	479	VAL
1	I	486	LEU
1	I	497	GLN
1	I	503	VAL
1	I	507	ASN
1	I	528	ILE
1	I	541	VAL
1	I	546	VAL
1	I	549	LEU
1	I	550	ARG
1	I	554	ASP
1	I	556	ARG
1	I	557	VAL
1	I	558	SER
1	I	561	LYS
1	I	564	VAL
1	I	572	SER
1	I	579	MET
1	I	587	ASN
1	I	593	LEU
1	I	597	SER

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Mol	Chain	Res	Type
1	I	611	VAL
1	I	618	LEU
1	I	624	LEU
1	I	629	LEU
1	M	1	MET
1	M	14	GLU
1	M	16	VAL
1	M	30	ARG
1	M	37	ILE
1	M	43	ASN
1	M	45	LYS
1	M	52	THR
1	M	56	GLU
1	M	65	LYS
1	M	89	LYS
1	M	97	LYS
1	M	106	ILE
1	M	117	THR
1	M	119	ILE
1	M	124	THR
1	M	126	VAL
1	M	140	GLU
1	M	156	LYS
1	M	162	LEU
1	M	169	VAL
1	M	170	VAL
1	M	173	THR
1	M	175	ASN
1	M	178	ILE
1	M	185	LEU
1	M	187	LYS
1	M	191	ASP
1	M	199	LYS
1	M	200	ASP
1	M	206	ARG
1	M	210	THR
1	M	216	VAL
1	M	225	GLU
1	M	231	GLU
1	M	237	LYS
1	M	253	VAL
1	M	255	GLU

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Mol	Chain	Res	Type
1	M	263	THR
1	M	268	LEU
1	M	269	MET
1	M	275	MET
1	M	281	THR
1	M	298	ARG
1	M	305	VAL
1	M	308	LEU
1	M	314	VAL
1	M	317	ASN
1	M	319	THR
1	M	322	ILE
1	M	326	HIS
1	M	338	LYS
1	M	351	SER
1	M	352	MET
1	M	355	ARG
1	M	369	LYS
1	M	371	LYS
1	M	383	VAL
1	M	385	THR
1	M	399	THR
1	M	401	LYS
1	M	411	ARG
1	M	428	VAL
1	M	437	LEU
1	M	438	THR
1	M	439	ASP
1	M	444	VAL
1	M	445	LEU
1	M	451	MET
1	M	452	SER
1	M	469	LEU
1	M	478	ARG
1	M	479	VAL
1	M	483	MET
1	M	485	VAL
1	M	486	LEU
1	M	497	GLN
1	M	507	ASN
1	M	517	ILE
1	M	533	SER

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Mol	Chain	Res	Type
1	M	540	ILE
1	M	542	LYS
1	M	546	VAL
1	M	547	GLU
1	M	549	LEU
1	M	553	ILE
1	M	562	CYS
1	M	568	ASN
1	M	579	MET
1	M	592	LEU
1	M	593	LEU
1	M	611	VAL
1	M	618	LEU
1	M	622	LYS
1	N	5	LYS
1	N	6	ILE
1	N	9	LYS
1	N	14	GLU
1	N	20	GLU
1	N	30	ARG
1	N	31	SER
1	N	45	LYS
1	N	47	LEU
1	N	54	ILE
1	N	58	LYS
1	N	62	THR
1	N	66	VAL
1	N	75	THR
1	N	78	LEU
1	N	84	ARG
1	N	97	LYS
1	N	101	ASP
1	N	107	THR
1	N	108	SER
1	N	133	ARG
1	N	140	GLU
1	N	160	GLU
1	N	167	CYS
1	N	168	ARG
1	N	169	VAL
1	N	176	VAL
1	N	185	LEU

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Mol	Chain	Res	Type
1	N	191	ASP
1	N	194	ARG
1	N	200	ASP
1	N	202	GLU
1	N	204	LEU
1	N	210	THR
1	N	237	LYS
1	N	242	HIS
1	N	244	GLU
1	N	245	LYS
1	N	253	VAL
1	N	269	MET
1	N	272	ASP
1	N	281	THR
1	N	294	ASN
1	N	298	ARG
1	N	305	VAL
1	N	308	LEU
1	N	313	LYS
1	N	314	VAL
1	N	317	ASN
1	N	319	THR
1	N	321	GLU
1	N	325	ASN
1	N	331	LEU
1	N	336	VAL
1	N	341	SER
1	N	343	SER
1	N	349	LEU
1	N	355	ARG
1	N	357	THR
1	N	363	GLU
1	N	371	LYS
1	N	383	VAL
1	N	385	THR
1	N	392	LEU
1	N	398	LYS
1	N	421	HIS
1	N	428	VAL
1	N	429	GLU
1	N	434	VAL
1	N	435	THR

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Mol	Chain	Res	Type
1	N	437	LEU
1	N	444	VAL
1	N	445	LEU
1	N	454	MET
1	N	463	LEU
1	N	469	LEU
1	N	471	MET
1	N	476	GLU
1	N	478	ARG
1	N	479	VAL
1	N	485	VAL
1	N	486	LEU
1	N	492	LYS
1	N	494	GLU
1	N	497	GLN
1	N	503	VAL
1	N	540	ILE
1	N	541	VAL
1	N	546	VAL
1	N	549	LEU
1	N	553	ILE
1	N	557	VAL
1	N	564	VAL
1	N	570	SER
1	N	571	SER
1	N	593	LEU
1	N	597	SER
1	N	600	VAL
1	N	611	VAL
1	N	616	THR
1	N	618	LEU
1	N	622	LYS
1	N	629	LEU
1	N	632	LYS
1	N	633	SER
1	O	1	MET
1	O	9	LYS
1	O	16	VAL
1	O	19	GLU
1	O	47	LEU
1	O	78	LEU
1	O	85	GLU

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Mol	Chain	Res	Type
1	O	109	ASN
1	O	114	ASP
1	O	117	THR
1	O	120	SER
1	O	127	SER
1	O	128	GLN
1	O	140	GLU
1	O	141	VAL
1	O	144	THR
1	O	156	LYS
1	O	162	LEU
1	O	169	VAL
1	O	176	VAL
1	O	181	VAL
1	O	185	LEU
1	O	187	LYS
1	O	206	ARG
1	O	210	THR
1	O	216	VAL
1	O	221	MET
1	O	223	THR
1	O	230	SER
1	O	233	ILE
1	O	253	VAL
1	O	269	MET
1	O	273	ILE
1	O	281	THR
1	O	288	LYS
1	O	292	LYS
1	O	298	ARG
1	O	305	VAL
1	O	308	LEU
1	O	310	GLU
1	O	313	LYS
1	O	317	ASN
1	O	319	THR
1	O	338	LYS
1	O	355	ARG
1	O	375	ASP
1	O	377	LEU
1	O	382	HIS
1	O	385	THR

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Mol	Chain	Res	Type
1	O	399	THR
1	O	401	LYS
1	O	410	GLU
1	O	420	ILE
1	O	426	THR
1	O	436	SER
1	O	437	LEU
1	O	438	THR
1	O	444	VAL
1	O	445	LEU
1	O	451	MET
1	O	463	LEU
1	O	468	VAL
1	O	478	ARG
1	O	479	VAL
1	O	480	GLU
1	O	486	LEU
1	O	487	LYS
1	O	497	GLN
1	O	501	SER
1	O	505	THR
1	O	528	ILE
1	O	541	VAL
1	O	544	ASP
1	O	546	VAL
1	O	549	LEU
1	O	550	ARG
1	O	556	ARG
1	O	558	SER
1	O	559	SER
1	O	563	VAL
1	O	577	MET
1	O	579	MET
1	O	587	ASN
1	O	588	LEU
1	O	595	ILE
1	O	602	GLU
1	O	616	THR
1	O	621	ASP
1	O	624	LEU
1	O	643	LYS
1	P	3	LEU

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Mol	Chain	Res	Type
1	P	16	VAL
1	P	47	LEU
1	P	58	LYS
1	P	78	LEU
1	P	93	LEU
1	P	104	ARG
1	P	106	ILE
1	P	108	SER
1	P	112	TRP
1	P	115	LYS
1	P	117	THR
1	P	123	SER
1	P	133	ARG
1	P	138	VAL
1	P	140	GLU
1	P	146	LEU
1	P	156	LYS
1	P	160	GLU
1	P	169	VAL
1	P	173	THR
1	P	176	VAL
1	P	181	VAL
1	P	187	LYS
1	P	200	ASP
1	P	210	THR
1	P	216	VAL
1	P	241	GLU
1	P	243	GLU
1	P	244	GLU
1	P	245	LYS
1	P	249	ASP
1	P	253	VAL
1	P	263	THR
1	P	269	MET
1	P	275	MET
1	P	290	LYS
1	P	292	LYS
1	P	298	ARG
1	P	305	VAL
1	P	308	LEU
1	P	314	VAL
1	P	316	MET

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Mol	Chain	Res	Type
1	P	317	ASN
1	P	318	GLN
1	P	319	THR
1	P	349	LEU
1	P	351	SER
1	P	352	MET
1	P	369	LYS
1	P	383	VAL
1	P	385	THR
1	P	392	LEU
1	P	399	THR
1	P	428	VAL
1	P	433	LYS
1	P	436	SER
1	P	437	LEU
1	P	439	ASP
1	P	440	SER
1	P	444	VAL
1	P	445	LEU
1	P	451	MET
1	P	452	SER
1	P	463	LEU
1	P	469	LEU
1	P	470	LYS
1	P	476	GLU
1	P	478	ARG
1	P	479	VAL
1	P	485	VAL
1	P	486	LEU
1	P	497	GLN
1	P	505	THR
1	P	506	VAL
1	P	540	ILE
1	P	541	VAL
1	P	542	LYS
1	P	549	LEU
1	P	550	ARG
1	P	556	ARG
1	P	557	VAL
1	P	562	CYS
1	P	564	VAL
1	P	565	ASN

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Mol	Chain	Res	Type
1	P	570	SER
1	P	593	LEU
1	P	611	VAL
1	P	618	LEU
1	P	621	ASP
1	P	626	LEU
1	P	632	LYS
1	P	643	LYS
1	P	644	SER
1	Q	16	VAL
1	Q	47	LEU
1	Q	56	GLU
1	Q	59	HIS
1	Q	69	LEU
1	Q	78	LEU
1	Q	90	VAL
1	Q	112	TRP
1	Q	114	ASP
1	Q	117	THR
1	Q	119	ILE
1	Q	140	GLU
1	Q	153	ARG
1	Q	156	LYS
1	Q	160	GLU
1	Q	167	CYS
1	Q	168	ARG
1	Q	173	THR
1	Q	176	VAL
1	Q	178	ILE
1	Q	185	LEU
1	Q	191	ASP
1	Q	210	THR
1	Q	213	VAL
1	Q	231	GLU
1	Q	233	ILE
1	Q	247	ILE
1	Q	259	HIS
1	Q	264	ILE
1	Q	269	MET
1	Q	273	ILE
1	Q	277	ARG
1	Q	290	LYS

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Mol	Chain	Res	Type
1	Q	294	ASN
1	Q	298	ARG
1	Q	305	VAL
1	Q	310	GLU
1	Q	316	MET
1	Q	317	ASN
1	Q	318	GLN
1	Q	319	THR
1	Q	321	GLU
1	Q	322	ILE
1	Q	323	VAL
1	Q	325	ASN
1	Q	330	SER
1	Q	331	LEU
1	Q	334	SER
1	Q	338	LYS
1	Q	340	LYS
1	Q	349	LEU
1	Q	351	SER
1	Q	368	GLN
1	Q	379	LYS
1	Q	383	VAL
1	Q	385	THR
1	Q	392	LEU
1	Q	410	GLU
1	Q	420	ILE
1	Q	428	VAL
1	Q	437	LEU
1	Q	444	VAL
1	Q	451	MET
1	Q	463	LEU
1	Q	469	LEU
1	Q	476	GLU
1	Q	478	ARG
1	Q	479	VAL
1	Q	480	GLU
1	Q	485	VAL
1	Q	486	LEU
1	Q	497	GLN
1	Q	503	VAL
1	Q	531	GLU
1	Q	533	SER

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Mol	Chain	Res	Type
1	Q	540	ILE
1	Q	541	VAL
1	Q	546	VAL
1	Q	549	LEU
1	Q	553	ILE
1	Q	554	ASP
1	Q	556	ARG
1	Q	563	VAL
1	Q	564	VAL
1	Q	566	ILE
1	Q	571	SER
1	Q	588	LEU
1	Q	593	LEU
1	Q	611	VAL
1	Q	615	ILE
1	Q	618	LEU
1	Q	632	LYS
1	R	1	MET
1	R	5	LYS
1	R	19	GLU
1	R	44	ASP
1	R	47	LEU
1	R	51	LYS
1	R	53	THR
1	R	58	LYS
1	R	59	HIS
1	R	63	ASP
1	R	65	LYS
1	R	68	VAL
1	R	69	LEU
1	R	78	LEU
1	R	91	THR
1	R	93	LEU
1	R	109	ASN
1	R	114	ASP
1	R	115	LYS
1	R	116	ILE
1	R	117	THR
1	R	124	THR
1	R	140	GLU
1	R	141	VAL
1	R	146	LEU

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Mol	Chain	Res	Type
1	R	160	GLU
1	R	169	VAL
1	R	172	SER
1	R	176	VAL
1	R	178	ILE
1	R	185	LEU
1	R	199	LYS
1	R	206	ARG
1	R	210	THR
1	R	222	LYS
1	R	233	ILE
1	R	244	GLU
1	R	251	SER
1	R	253	VAL
1	R	269	MET
1	R	273	ILE
1	R	292	LYS
1	R	293	ASN
1	R	294	ASN
1	R	305	VAL
1	R	308	LEU
1	R	315	GLU
1	R	317	ASN
1	R	331	LEU
1	R	335	ASN
1	R	336	VAL
1	R	346	VAL
1	R	349	LEU
1	R	359	TYR
1	R	364	MET
1	R	371	LYS
1	R	383	VAL
1	R	385	THR
1	R	392	LEU
1	R	398	LYS
1	R	401	LYS
1	R	411	ARG
1	R	420	ILE
1	R	428	VAL
1	R	433	LYS
1	R	434	VAL
1	R	437	LEU

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Mol	Chain	Res	Type
1	R	451	MET
1	R	469	LEU
1	R	476	GLU
1	R	479	VAL
1	R	486	LEU
1	R	497	GLN
1	R	503	VAL
1	R	505	THR
1	R	506	VAL
1	R	528	ILE
1	R	532	GLN
1	R	546	VAL
1	R	549	LEU
1	R	553	ILE
1	R	556	ARG
1	R	560	GLN
1	R	561	LYS
1	R	564	VAL
1	R	579	MET
1	R	615	ILE
1	R	616	THR
1	R	621	ASP
1	R	622	LYS
1	R	624	LEU
1	R	625	CYS
1	R	638	ASN
1	R	643	LYS
1	J	5	LYS
1	J	9	LYS
1	J	16	VAL
1	J	28	LEU
1	J	45	LYS
1	J	47	LEU
1	J	51	LYS
1	J	60	GLU
1	J	62	THR
1	J	78	LEU
1	J	91	THR
1	J	107	THR
1	J	108	SER
1	J	115	LYS
1	J	116	ILE

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Mol	Chain	Res	Type
1	J	132	SER
1	J	140	GLU
1	J	141	VAL
1	J	168	ARG
1	J	169	VAL
1	J	173	THR
1	J	176	VAL
1	J	181	VAL
1	J	185	LEU
1	J	194	ARG
1	J	199	LYS
1	J	210	THR
1	J	216	VAL
1	J	221	MET
1	J	222	LYS
1	J	230	SER
1	J	243	GLU
1	J	244	GLU
1	J	251	SER
1	J	260	SER
1	J	261	SER
1	J	263	THR
1	J	269	MET
1	J	274	ASP
1	J	280	THR
1	J	281	THR
1	J	288	LYS
1	J	290	LYS
1	J	298	ARG
1	J	305	VAL
1	J	308	LEU
1	J	311	LYS
1	J	313	LYS
1	J	319	THR
1	J	338	LYS
1	J	351	SER
1	J	379	LYS
1	J	383	VAL
1	J	385	THR
1	J	398	LYS
1	J	399	THR
1	J	428	VAL

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Mol	Chain	Res	Type
1	J	437	LEU
1	J	445	LEU
1	J	451	MET
1	J	469	LEU
1	J	476	GLU
1	J	478	ARG
1	J	479	VAL
1	J	485	VAL
1	J	486	LEU
1	J	492	LYS
1	J	497	GLN
1	J	503	VAL
1	J	528	ILE
1	J	534	LEU
1	J	540	ILE
1	J	541	VAL
1	J	546	VAL
1	J	549	LEU
1	J	556	ARG
1	J	557	VAL
1	J	558	SER
1	J	575	ILE
1	J	577	MET
1	J	582	GLU
1	J	593	LEU
1	J	611	VAL
1	J	616	THR
1	J	618	LEU
1	J	629	LEU
1	J	632	LYS
1	J	643	LYS
1	K	3	LEU
1	K	15	TRP
1	K	24	MET
1	K	45	LYS
1	K	47	LEU
1	K	60	GLU
1	K	65	LYS
1	K	66	VAL
1	K	68	VAL
1	K	85	GLU
1	K	91	THR

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Mol	Chain	Res	Type
1	K	93	LEU
1	K	107	THR
1	K	126	VAL
1	K	140	GLU
1	K	141	VAL
1	K	156	LYS
1	K	160	GLU
1	K	162	LEU
1	K	169	VAL
1	K	176	VAL
1	K	181	VAL
1	K	185	LEU
1	K	191	ASP
1	K	210	THR
1	K	216	VAL
1	K	223	THR
1	K	225	GLU
1	K	227	ARG
1	K	234	VAL
1	K	243	GLU
1	K	244	GLU
1	K	245	LYS
1	K	253	VAL
1	K	257	VAL
1	K	263	THR
1	K	268	LEU
1	K	269	MET
1	K	273	ILE
1	K	281	THR
1	K	290	LYS
1	K	292	LYS
1	K	298	ARG
1	K	305	VAL
1	K	308	LEU
1	K	311	LYS
1	K	312	LYS
1	K	314	VAL
1	K	319	THR
1	K	321	GLU
1	K	322	ILE
1	K	331	LEU
1	K	341	SER

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Mol	Chain	Res	Type
1	K	363	GLU
1	K	364	MET
1	K	366	GLU
1	K	371	LYS
1	K	383	VAL
1	K	385	THR
1	K	392	LEU
1	K	399	THR
1	K	401	LYS
1	K	424	LYS
1	K	428	VAL
1	K	437	LEU
1	K	444	VAL
1	K	445	LEU
1	K	451	MET
1	K	463	LEU
1	K	469	LEU
1	K	471	MET
1	K	475	ASP
1	K	479	VAL
1	K	486	LEU
1	K	497	GLN
1	K	503	VAL
1	K	506	VAL
1	K	532	GLN
1	K	540	ILE
1	K	544	ASP
1	K	546	VAL
1	K	556	ARG
1	K	558	SER
1	K	562	CYS
1	K	563	VAL
1	K	564	VAL
1	K	567	ASP
1	K	577	MET
1	K	579	MET
1	K	589	SER
1	K	593	LEU
1	K	596	SER
1	K	597	SER
1	K	624	LEU
1	K	629	LEU

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Mol	Chain	Res	Type
1	K	632	LYS
1	K	643	LYS
1	L	16	VAL
1	L	19	GLU
1	L	47	LEU
1	L	57	LYS
1	L	60	GLU
1	L	62	THR
1	L	78	LEU
1	L	85	GLU
1	L	91	THR
1	L	107	THR
1	L	113	SER
1	L	114	ASP
1	L	117	THR
1	L	124	THR
1	L	128	GLN
1	L	129	ILE
1	L	140	GLU
1	L	141	VAL
1	L	162	LEU
1	L	168	ARG
1	L	169	VAL
1	L	173	THR
1	L	176	VAL
1	L	181	VAL
1	L	185	LEU
1	L	193	PRO
1	L	210	THR
1	L	216	VAL
1	L	221	MET
1	L	223	THR
1	L	225	GLU
1	L	228	GLU
1	L	244	GLU
1	L	253	VAL
1	L	260	SER
1	L	263	THR
1	L	269	MET
1	L	281	THR
1	L	305	VAL
1	L	308	LEU

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Mol	Chain	Res	Type
1	L	311	LYS
1	L	314	VAL
1	L	316	MET
1	L	317	ASN
1	L	319	THR
1	L	331	LEU
1	L	349	LEU
1	L	369	LYS
1	L	383	VAL
1	L	385	THR
1	L	392	LEU
1	L	399	THR
1	L	428	VAL
1	L	433	LYS
1	L	436	SER
1	L	437	LEU
1	L	440	SER
1	L	444	VAL
1	L	445	LEU
1	L	451	MET
1	L	452	SER
1	L	454	MET
1	L	463	LEU
1	L	469	LEU
1	L	476	GLU
1	L	479	VAL
1	L	485	VAL
1	L	486	LEU
1	L	497	GLN
1	L	503	VAL
1	L	541	VAL
1	L	546	VAL
1	L	548	ILE
1	L	549	LEU
1	L	556	ARG
1	L	557	VAL
1	L	562	CYS
1	L	564	VAL
1	L	593	LEU
1	L	611	VAL
1	L	616	THR
1	L	618	LEU

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Mol	Chain	Res	Type
1	L	624	LEU
1	L	633	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (326) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	43	ASN
1	A	67	HIS
1	A	109	ASN
1	A	175	ASN
1	A	242	HIS
1	A	259	HIS
1	A	303	GLN
1	A	362	ASN
1	A	368	GLN
1	A	459	HIS
1	A	482	HIS
1	A	497	GLN
1	A	498	ASN
1	A	507	ASN
1	A	560	GLN
1	D	43	ASN
1	D	67	HIS
1	D	105	HIS
1	D	109	ASN
1	D	175	ASN
1	D	190	ASN
1	D	242	HIS
1	D	259	HIS
1	D	293	ASN
1	D	303	GLN
1	D	335	ASN
1	D	362	ASN
1	D	368	GLN
1	D	459	HIS
1	D	482	HIS
1	D	497	GLN
1	D	507	ASN
1	D	560	GLN
1	D	565	ASN
1	B	109	ASN

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Mol	Chain	Res	Type
1	B	175	ASN
1	B	190	ASN
1	B	242	HIS
1	B	259	HIS
1	B	291	ASN
1	B	303	GLN
1	B	335	ASN
1	B	362	ASN
1	B	455	ASN
1	B	459	HIS
1	B	482	HIS
1	B	497	GLN
1	B	498	ASN
1	B	507	ASN
1	B	560	GLN
1	B	620	ASN
1	C	43	ASN
1	C	59	HIS
1	C	61	ASN
1	C	67	HIS
1	C	109	ASN
1	C	184	HIS
1	C	190	ASN
1	C	242	HIS
1	C	259	HIS
1	C	294	ASN
1	C	303	GLN
1	C	335	ASN
1	C	362	ASN
1	C	368	GLN
1	C	459	HIS
1	C	482	HIS
1	C	497	GLN
1	C	498	ASN
1	C	507	ASN
1	C	560	GLN
1	C	565	ASN
1	C	568	ASN
1	C	587	ASN
1	C	620	ASN
1	F	43	ASN
1	F	61	ASN

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Mol	Chain	Res	Type
1	F	105	HIS
1	F	242	HIS
1	F	259	HIS
1	F	278	ASN
1	F	294	ASN
1	F	303	GLN
1	F	362	ASN
1	F	368	GLN
1	F	455	ASN
1	F	459	HIS
1	F	497	GLN
1	F	507	ASN
1	F	565	ASN
1	F	587	ASN
1	F	620	ASN
1	E	26	GLN
1	E	43	ASN
1	E	67	HIS
1	E	109	ASN
1	E	175	ASN
1	E	259	HIS
1	E	303	GLN
1	E	317	ASN
1	E	362	ASN
1	E	459	HIS
1	E	482	HIS
1	E	497	GLN
1	E	560	GLN
1	E	587	ASN
1	E	638	ASN
1	G	43	ASN
1	G	59	HIS
1	G	67	HIS
1	G	109	ASN
1	G	190	ASN
1	G	259	HIS
1	G	300	HIS
1	G	303	GLN
1	G	335	ASN
1	G	362	ASN
1	G	459	HIS
1	G	482	HIS

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Mol	Chain	Res	Type
1	G	497	GLN
1	G	498	ASN
1	G	560	GLN
1	G	587	ASN
1	H	26	GLN
1	H	43	ASN
1	H	67	HIS
1	H	109	ASN
1	H	175	ASN
1	H	190	ASN
1	H	224	HIS
1	H	303	GLN
1	H	335	ASN
1	H	362	ASN
1	H	459	HIS
1	H	482	HIS
1	H	497	GLN
1	H	507	ASN
1	H	638	ASN
1	I	26	GLN
1	I	43	ASN
1	I	67	HIS
1	I	105	HIS
1	I	190	ASN
1	I	259	HIS
1	I	294	ASN
1	I	300	HIS
1	I	303	GLN
1	I	335	ASN
1	I	362	ASN
1	I	368	GLN
1	I	459	HIS
1	I	473	HIS
1	I	482	HIS
1	I	497	GLN
1	I	498	ASN
1	I	507	ASN
1	I	560	GLN
1	I	568	ASN
1	I	587	ASN
1	I	620	ASN
1	M	43	ASN

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Mol	Chain	Res	Type
1	M	67	HIS
1	M	109	ASN
1	M	175	ASN
1	M	190	ASN
1	M	278	ASN
1	M	303	GLN
1	M	325	ASN
1	M	335	ASN
1	M	362	ASN
1	M	459	HIS
1	M	482	HIS
1	M	497	GLN
1	M	498	ASN
1	M	560	GLN
1	M	568	ASN
1	N	26	GLN
1	N	43	ASN
1	N	105	HIS
1	N	109	ASN
1	N	175	ASN
1	N	190	ASN
1	N	259	HIS
1	N	291	ASN
1	N	293	ASN
1	N	294	ASN
1	N	303	GLN
1	N	317	ASN
1	N	335	ASN
1	N	362	ASN
1	N	459	HIS
1	N	482	HIS
1	N	497	GLN
1	N	507	ASN
1	N	560	GLN
1	N	565	ASN
1	O	43	ASN
1	O	67	HIS
1	O	105	HIS
1	O	175	ASN
1	O	190	ASN
1	O	303	GLN
1	O	335	ASN

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Mol	Chain	Res	Type
1	O	362	ASN
1	O	459	HIS
1	O	497	GLN
1	O	498	ASN
1	O	507	ASN
1	O	565	ASN
1	O	568	ASN
1	O	587	ASN
1	O	638	ASN
1	O	640	GLN
1	P	43	ASN
1	P	67	HIS
1	P	175	ASN
1	P	190	ASN
1	P	259	HIS
1	P	294	ASN
1	P	303	GLN
1	P	317	ASN
1	P	362	ASN
1	P	368	GLN
1	P	459	HIS
1	P	482	HIS
1	P	497	GLN
1	P	498	ASN
1	P	507	ASN
1	P	532	GLN
1	P	560	GLN
1	P	565	ASN
1	P	587	ASN
1	P	620	ASN
1	P	640	GLN
1	Q	8	GLN
1	Q	43	ASN
1	Q	67	HIS
1	Q	105	HIS
1	Q	190	ASN
1	Q	196	ASN
1	Q	242	HIS
1	Q	259	HIS
1	Q	303	GLN
1	Q	362	ASN
1	Q	409	ASN

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Mol	Chain	Res	Type
1	Q	455	ASN
1	Q	459	HIS
1	Q	482	HIS
1	Q	497	GLN
1	Q	498	ASN
1	Q	532	GLN
1	Q	560	GLN
1	Q	568	ASN
1	R	43	ASN
1	R	61	ASN
1	R	67	HIS
1	R	109	ASN
1	R	175	ASN
1	R	242	HIS
1	R	259	HIS
1	R	291	ASN
1	R	293	ASN
1	R	294	ASN
1	R	300	HIS
1	R	303	GLN
1	R	325	ASN
1	R	362	ASN
1	R	368	GLN
1	R	459	HIS
1	R	482	HIS
1	R	497	GLN
1	R	507	ASN
1	R	560	GLN
1	R	638	ASN
1	J	26	GLN
1	J	43	ASN
1	J	67	HIS
1	J	190	ASN
1	J	242	HIS
1	J	278	ASN
1	J	291	ASN
1	J	300	HIS
1	J	303	GLN
1	J	362	ASN
1	J	459	HIS
1	J	473	HIS
1	J	482	HIS

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Mol	Chain	Res	Type
1	J	497	GLN
1	J	498	ASN
1	J	627	HIS
1	K	67	HIS
1	K	105	HIS
1	K	109	ASN
1	K	190	ASN
1	K	259	HIS
1	K	294	ASN
1	K	303	GLN
1	K	317	ASN
1	K	335	ASN
1	K	362	ASN
1	K	459	HIS
1	K	482	HIS
1	K	497	GLN
1	K	498	ASN
1	K	532	GLN
1	K	560	GLN
1	K	640	GLN
1	L	26	GLN
1	L	43	ASN
1	L	61	ASN
1	L	67	HIS
1	L	190	ASN
1	L	242	HIS
1	L	259	HIS
1	L	294	ASN
1	L	303	GLN
1	L	317	ASN
1	L	362	ASN
1	L	368	GLN
1	L	459	HIS
1	L	482	HIS
1	L	497	GLN
1	L	507	ASN
1	L	560	GLN
1	L	620	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	I	702	-	4,4,4	1.18	0	6,6,6	1.51	2 (33%)
3	PO4	K	702	-	4,4,4	0.98	0	6,6,6	0.63	0
3	PO4	C	702	-	4,4,4	0.79	0	6,6,6	1.19	1 (16%)
3	PO4	O	702	-	4,4,4	0.86	0	6,6,6	0.42	0
3	PO4	D	702	-	4,4,4	1.10	0	6,6,6	1.75	2 (33%)
2	SAH	M	701	-	27,28,28	1.78	6 (22%)	36,40,40	2.35	12 (33%)
2	SAH	E	701	-	27,28,28	1.49	5 (18%)	36,40,40	2.16	14 (38%)
3	PO4	F	702	-	4,4,4	1.05	0	6,6,6	1.44	1 (16%)
3	PO4	P	702	-	4,4,4	0.90	0	6,6,6	1.02	0
2	SAH	B	701	-	27,28,28	1.41	5 (18%)	36,40,40	2.10	13 (36%)
3	PO4	M	702	-	4,4,4	0.80	0	6,6,6	0.83	0
3	PO4	J	702	-	4,4,4	1.07	0	6,6,6	0.79	0
3	PO4	G	702	-	4,4,4	1.10	0	6,6,6	1.00	0
2	SAH	F	701	-	27,28,28	1.36	4 (14%)	36,40,40	2.19	12 (33%)
3	PO4	L	702	-	4,4,4	1.11	0	6,6,6	0.93	0
3	PO4	E	702	-	4,4,4	0.71	0	6,6,6	0.95	0
3	PO4	B	702	-	4,4,4	0.87	0	6,6,6	1.12	0
2	SAH	A	701	-	27,28,28	1.61	5 (18%)	36,40,40	2.16	14 (38%)
2	SAH	K	701	-	27,28,28	1.40	5 (18%)	36,40,40	2.27	14 (38%)
2	SAH	C	701	-	27,28,28	1.35	4 (14%)	36,40,40	2.21	12 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	Q	702	-	4,4,4	1.00	0	6,6,6	0.58	0
3	PO4	R	702	-	4,4,4	0.72	0	6,6,6	0.82	0
3	PO4	H	702	-	4,4,4	0.74	0	6,6,6	1.52	1 (16%)
2	SAH	R	701	-	27,28,28	1.51	6 (22%)	36,40,40	2.05	10 (27%)
2	SAH	N	701	-	27,28,28	1.47	5 (18%)	36,40,40	2.27	15 (41%)
3	PO4	A	702	-	4,4,4	0.67	0	6,6,6	1.36	1 (16%)
2	SAH	O	701	-	27,28,28	1.46	5 (18%)	36,40,40	2.25	14 (38%)
2	SAH	I	701	-	27,28,28	1.50	6 (22%)	36,40,40	2.32	17 (47%)
2	SAH	Q	701	-	27,28,28	1.39	4 (14%)	36,40,40	2.04	12 (33%)
3	PO4	N	702	-	4,4,4	1.01	0	6,6,6	0.75	0
2	SAH	L	701	-	27,28,28	1.55	6 (22%)	36,40,40	2.39	15 (41%)
2	SAH	H	701	-	27,28,28	1.59	5 (18%)	36,40,40	2.53	11 (30%)
2	SAH	J	701	-	27,28,28	1.37	4 (14%)	36,40,40	2.11	12 (33%)
2	SAH	D	701	-	27,28,28	1.54	5 (18%)	36,40,40	2.25	14 (38%)
2	SAH	G	701	-	27,28,28	1.60	4 (14%)	36,40,40	2.20	14 (38%)
2	SAH	P	701	-	27,28,28	1.58	5 (18%)	36,40,40	2.07	14 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	701	-	-	0/15/31/31	0/3/3/3
2	SAH	I	701	-	-	1/15/31/31	0/3/3/3
2	SAH	C	701	-	-	1/15/31/31	0/3/3/3
2	SAH	O	701	-	-	0/15/31/31	0/3/3/3
2	SAH	M	701	-	-	3/15/31/31	0/3/3/3
2	SAH	K	701	-	-	0/15/31/31	0/3/3/3
2	SAH	D	701	-	-	0/15/31/31	0/3/3/3
2	SAH	G	701	-	-	4/15/31/31	0/3/3/3
2	SAH	Q	701	-	-	2/15/31/31	0/3/3/3
2	SAH	L	701	-	-	2/15/31/31	0/3/3/3
2	SAH	H	701	-	-	3/15/31/31	0/3/3/3
2	SAH	R	701	-	-	2/15/31/31	0/3/3/3
2	SAH	N	701	-	-	5/15/31/31	0/3/3/3
2	SAH	J	701	-	-	1/15/31/31	0/3/3/3
2	SAH	F	701	-	-	2/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	E	701	-	-	0/15/31/31	0/3/3/3
2	SAH	B	701	-	-	1/15/31/31	0/3/3/3
2	SAH	P	701	-	-	2/15/31/31	0/3/3/3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	701	SAH	C5-C4	5.42	1.48	1.39
2	P	701	SAH	C5-C4	5.27	1.48	1.39
2	G	701	SAH	C5-C4	5.06	1.48	1.39
2	L	701	SAH	C5-C4	4.98	1.48	1.39
2	A	701	SAH	C5-C4	4.96	1.47	1.39
2	R	701	SAH	C5-C4	4.82	1.47	1.39
2	D	701	SAH	C5-C4	4.65	1.47	1.39
2	E	701	SAH	C5-C4	4.56	1.47	1.39
2	H	701	SAH	C5-C4	4.50	1.47	1.39
2	B	701	SAH	C5-C4	4.42	1.47	1.39
2	J	701	SAH	C5-C4	4.39	1.46	1.39
2	N	701	SAH	C5-C4	4.36	1.46	1.39
2	O	701	SAH	C5-C4	4.30	1.46	1.39
2	I	701	SAH	C5-C4	4.25	1.46	1.39
2	Q	701	SAH	C5-C4	4.22	1.46	1.39
2	C	701	SAH	C5-C4	3.78	1.45	1.39
2	F	701	SAH	C5-C4	3.58	1.45	1.39
2	L	701	SAH	C5-C6	3.33	1.50	1.41
2	K	701	SAH	C5-C4	3.33	1.45	1.39
2	P	701	SAH	C5-C6	3.22	1.50	1.41
2	A	701	SAH	C5-N7	-3.18	1.33	1.39
2	G	701	SAH	C5-C6	3.11	1.49	1.41
2	H	701	SAH	C5-C6	3.00	1.49	1.41
2	M	701	SAH	C4-N3	3.00	1.40	1.34
2	D	701	SAH	C5-C6	2.93	1.49	1.41
2	B	701	SAH	C5-C6	2.88	1.49	1.41
2	D	701	SAH	C5-N7	-2.86	1.33	1.39
2	J	701	SAH	C5-N7	-2.85	1.33	1.39
2	I	701	SAH	C8-N7	2.83	1.37	1.31
2	E	701	SAH	C5-C6	2.82	1.48	1.41
2	M	701	SAH	C5-C6	2.80	1.48	1.41
2	M	701	SAH	C5-N7	-2.77	1.34	1.39
2	K	701	SAH	C8-N9	-2.77	1.32	1.37
2	Q	701	SAH	C5-C6	2.75	1.48	1.41
2	C	701	SAH	C5-C6	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	701	SAH	C5-C6	2.66	1.48	1.41
2	E	701	SAH	C8-N7	2.62	1.36	1.31
2	N	701	SAH	C4-N3	2.59	1.39	1.34
2	R	701	SAH	C5-N7	-2.59	1.34	1.39
2	Q	701	SAH	C5-N7	-2.58	1.34	1.39
2	N	701	SAH	C5-C6	2.58	1.48	1.41
2	F	701	SAH	C5-C6	2.54	1.48	1.41
2	J	701	SAH	C8-N7	2.53	1.36	1.31
2	R	701	SAH	C5-C6	2.52	1.48	1.41
2	C	701	SAH	C5-N7	-2.52	1.34	1.39
2	F	701	SAH	OXT-C	-2.51	1.22	1.30
2	D	701	SAH	C4-N9	-2.51	1.32	1.37
2	G	701	SAH	C8-N7	2.50	1.36	1.31
2	A	701	SAH	C4-N9	-2.49	1.32	1.37
2	R	701	SAH	C8-N7	2.47	1.36	1.31
2	O	701	SAH	C5-N7	-2.47	1.34	1.39
2	H	701	SAH	C2-N3	2.46	1.38	1.33
2	B	701	SAH	C5-N7	-2.45	1.34	1.39
2	N	701	SAH	C8-N7	2.45	1.36	1.31
2	K	701	SAH	C5-N7	-2.39	1.34	1.39
2	M	701	SAH	C8-N7	2.39	1.36	1.31
2	R	701	SAH	C4-N9	-2.33	1.32	1.37
2	P	701	SAH	C8-N7	2.32	1.36	1.31
2	K	701	SAH	C4-N9	-2.32	1.32	1.37
2	I	701	SAH	C4-N9	-2.31	1.32	1.37
2	A	701	SAH	C8-N7	2.31	1.36	1.31
2	O	701	SAH	C8-N7	2.29	1.36	1.31
2	I	701	SAH	C5-C6	2.27	1.47	1.41
2	G	701	SAH	OXT-C	-2.24	1.23	1.30
2	J	701	SAH	C4-N9	-2.24	1.33	1.37
2	B	701	SAH	C4-N9	-2.21	1.33	1.37
2	B	701	SAH	C8-N7	2.21	1.35	1.31
2	H	701	SAH	C8-N7	2.21	1.35	1.31
2	F	701	SAH	C8-N7	2.20	1.35	1.31
2	D	701	SAH	OXT-C	-2.19	1.23	1.30
2	L	701	SAH	C8-N7	2.18	1.35	1.31
2	E	701	SAH	C5-N7	-2.18	1.35	1.39
2	L	701	SAH	C4-N9	-2.17	1.33	1.37
2	R	701	SAH	OXT-C	-2.16	1.23	1.30
2	I	701	SAH	O4'-C4'	-2.16	1.40	1.45
2	A	701	SAH	C5-C6	2.15	1.47	1.41
2	C	701	SAH	OXT-C	-2.15	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	701	SAH	C5-N7	-2.15	1.35	1.39
2	N	701	SAH	OXT-C	-2.12	1.23	1.30
2	M	701	SAH	C2-N1	2.12	1.37	1.33
2	O	701	SAH	C4-N9	-2.11	1.33	1.37
2	P	701	SAH	OXT-C	-2.09	1.24	1.30
2	Q	701	SAH	C8-N7	2.08	1.35	1.31
2	L	701	SAH	OXT-C	-2.06	1.24	1.30
2	E	701	SAH	C4-N9	-2.05	1.33	1.37
2	K	701	SAH	C8-N7	2.05	1.35	1.31
2	H	701	SAH	O4'-C4'	-2.05	1.40	1.45
2	L	701	SAH	C5-N7	-2.05	1.35	1.39
2	P	701	SAH	C4-N9	-2.02	1.33	1.37

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	SAH	O4'-C1'-N9	-6.79	95.05	108.09
2	K	701	SAH	O4'-C1'-N9	-6.45	95.70	108.09
2	C	701	SAH	C5-C4-N3	-6.40	117.90	126.72
2	H	701	SAH	C5-C4-N3	-6.33	118.00	126.72
2	G	701	SAH	C5-C4-N3	-5.68	118.90	126.72
2	F	701	SAH	C5-C4-N3	-5.65	118.94	126.72
2	D	701	SAH	C5-C4-N3	-5.63	118.96	126.72
2	L	701	SAH	C5-C4-N3	-5.55	119.07	126.72
2	M	701	SAH	N3-C4-N9	5.50	136.53	127.17
2	M	701	SAH	C5-C4-N3	-5.43	119.23	126.72
2	Q	701	SAH	C5-C4-N3	-5.40	119.28	126.72
2	E	701	SAH	C5-C4-N3	-5.35	119.35	126.72
2	R	701	SAH	C5-C4-N3	-5.34	119.36	126.72
2	B	701	SAH	C5-C4-N3	-5.29	119.43	126.72
2	C	701	SAH	N3-C4-N9	5.19	136.00	127.17
2	M	701	SAH	C2'-C1'-N9	5.06	125.88	113.30
2	N	701	SAH	N3-C4-N9	5.02	135.70	127.17
2	J	701	SAH	O4'-C1'-N9	-4.97	98.54	108.09
2	A	701	SAH	O4'-C1'-N9	-4.94	98.60	108.09
2	H	701	SAH	N3-C4-N9	4.90	135.50	127.17
2	F	701	SAH	N3-C4-N9	4.89	135.49	127.17
2	N	701	SAH	C5-C4-N3	-4.89	119.99	126.72
2	A	701	SAH	C5-C4-N3	-4.87	120.01	126.72
2	Q	701	SAH	N3-C4-N9	4.83	135.38	127.17
2	J	701	SAH	C5-C4-N3	-4.82	120.08	126.72
2	H	701	SAH	C2'-C1'-N9	4.81	125.25	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	701	SAH	C5-C4-N3	-4.79	120.12	126.72
2	G	701	SAH	N3-C4-N9	4.72	135.19	127.17
2	D	701	SAH	N3-C4-N9	4.71	135.18	127.17
2	I	701	SAH	C5-C4-N3	-4.71	120.23	126.72
2	R	701	SAH	N3-C4-N9	4.57	134.93	127.17
2	P	701	SAH	C5-C4-N3	-4.52	120.49	126.72
2	K	701	SAH	C5-C4-N3	-4.51	120.50	126.72
2	O	701	SAH	O4'-C1'-N9	-4.51	99.43	108.09
2	L	701	SAH	N3-C4-N9	4.49	134.81	127.17
2	N	701	SAH	N3-C2-N1	-4.45	121.85	128.58
2	A	701	SAH	N3-C4-N9	4.44	134.72	127.17
2	I	701	SAH	N3-C2-N1	-4.42	121.90	128.58
2	O	701	SAH	N3-C4-N9	4.36	134.59	127.17
2	H	701	SAH	C2-N3-C4	4.30	122.34	111.83
2	N	701	SAH	C4-N9-C8	4.29	110.24	105.74
2	C	701	SAH	C2-N3-C4	4.24	122.20	111.83
2	L	701	SAH	C2-N3-C4	4.24	122.19	111.83
2	B	701	SAH	N3-C4-N9	4.21	134.32	127.17
2	K	701	SAH	N3-C4-N9	4.19	134.28	127.17
2	D	701	SAH	O4'-C1'-N9	-4.17	100.09	108.09
2	L	701	SAH	N3-C2-N1	-4.11	122.36	128.58
2	P	701	SAH	N3-C4-N9	4.09	134.12	127.17
2	O	701	SAH	N3-C2-N1	-4.07	122.42	128.58
2	E	701	SAH	N3-C4-N9	4.05	134.05	127.17
2	K	701	SAH	C4-N9-C8	3.96	109.89	105.74
2	E	701	SAH	C2-N3-C4	3.94	121.46	111.83
2	M	701	SAH	N3-C2-N1	-3.92	122.64	128.58
2	J	701	SAH	N3-C4-N9	3.92	133.83	127.17
2	Q	701	SAH	C2-N3-C4	3.90	121.36	111.83
2	F	701	SAH	C4-N9-C8	3.90	109.83	105.74
2	B	701	SAH	C2-N3-C4	3.88	121.31	111.83
2	Q	701	SAH	N3-C2-N1	-3.85	122.75	128.58
2	G	701	SAH	C4-C5-N7	-3.85	106.18	110.58
2	I	701	SAH	C2-N3-C4	3.82	121.16	111.83
2	F	701	SAH	C2-N3-C4	3.81	121.14	111.83
2	D	701	SAH	OXT-C-O	-3.79	115.48	124.08
2	H	701	SAH	N3-C2-N1	-3.77	122.88	128.58
2	R	701	SAH	N3-C2-N1	-3.76	122.88	128.58
2	L	701	SAH	C4-C5-N7	-3.76	106.28	110.58
2	P	701	SAH	C4-N9-C8	3.76	109.68	105.74
2	F	701	SAH	N3-C2-N1	-3.74	122.92	128.58
2	I	701	SAH	C4-C5-N7	-3.71	106.34	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	701	SAH	C2-N3-C4	3.71	120.89	111.83
2	L	701	SAH	O4'-C1'-N9	-3.70	100.98	108.09
2	E	701	SAH	N3-C2-N1	-3.69	123.00	128.58
2	O	701	SAH	C4-N9-C8	3.69	109.61	105.74
2	O	701	SAH	C2'-C1'-N9	3.66	122.41	113.30
2	P	701	SAH	N3-C2-N1	-3.65	123.06	128.58
2	N	701	SAH	C2-N3-C4	3.64	120.72	111.83
2	G	701	SAH	C2-N3-C4	3.63	120.71	111.83
2	R	701	SAH	OXT-C-O	-3.59	115.94	124.08
2	R	701	SAH	C2-N3-C4	3.56	120.53	111.83
2	M	701	SAH	N6-C6-N1	3.56	126.30	118.38
2	K	701	SAH	N3-C2-N1	-3.54	123.22	128.58
2	D	701	SAH	C2-N3-C4	3.54	120.47	111.83
2	G	701	SAH	N3-C2-N1	-3.53	123.24	128.58
2	E	701	SAH	O4'-C1'-N9	-3.52	101.34	108.09
2	M	701	SAH	C2-N3-C4	3.52	120.42	111.83
2	K	701	SAH	C2'-C1'-N9	3.51	122.03	113.30
2	G	701	SAH	C4-N9-C8	3.46	109.37	105.74
2	P	701	SAH	C2-N3-C4	3.45	120.27	111.83
2	I	701	SAH	N3-C4-N9	3.45	133.04	127.17
2	B	701	SAH	N3-C2-N1	-3.45	123.36	128.58
2	M	701	SAH	O4'-C1'-N9	-3.43	101.50	108.09
2	C	701	SAH	N3-C2-N1	-3.43	123.39	128.58
2	L	701	SAH	C4-N9-C8	3.42	109.33	105.74
2	I	701	SAH	OXT-C-O	-3.33	116.53	124.08
2	C	701	SAH	C4-C5-N7	-3.32	106.79	110.58
2	A	701	SAH	N3-C2-N1	-3.31	123.57	128.58
2	Q	701	SAH	C4-N9-C8	3.26	109.16	105.74
2	A	701	SAH	C4-N9-C8	3.24	109.14	105.74
2	H	701	SAH	C4-C5-N7	-3.24	106.88	110.58
2	P	701	SAH	C4-C5-N7	-3.22	106.90	110.58
2	I	701	SAH	C6-C5-N7	3.21	138.28	132.09
2	B	701	SAH	C4-C5-N7	-3.20	106.92	110.58
2	A	701	SAH	O3'-C3'-C4'	-3.18	101.96	111.08
2	R	701	SAH	C4-N9-C8	3.17	109.07	105.74
2	E	701	SAH	C4-C5-N7	-3.17	106.96	110.58
2	I	701	SAH	C4-N9-C1'	-3.17	119.23	126.63
2	I	701	SAH	C4-N9-C8	3.15	109.05	105.74
2	C	701	SAH	C2'-C1'-N9	3.12	121.05	113.30
2	J	701	SAH	C4-N9-C8	3.10	109.00	105.74
2	J	701	SAH	C2-N3-C4	3.08	119.36	111.83
2	I	701	SAH	CB-CG-SD	-3.05	106.64	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	702	PO4	O4-P-O2	3.05	117.39	107.91
2	J	701	SAH	C4-C5-N7	-3.02	107.12	110.58
2	L	701	SAH	C5-N7-C8	3.02	108.20	103.45
2	D	701	SAH	CB-CG-SD	-3.02	106.72	113.45
2	I	701	SAH	C2'-C3'-C4'	2.99	108.38	102.61
2	N	701	SAH	N9-C8-N7	-2.98	109.71	113.94
2	O	701	SAH	C2'-C3'-C4'	2.97	108.36	102.61
2	F	701	SAH	N9-C8-N7	-2.97	109.72	113.94
2	L	701	SAH	C6-C5-N7	2.96	137.80	132.09
2	L	701	SAH	O2'-C2'-C1'	-2.96	99.93	110.10
2	K	701	SAH	C2-N3-C4	2.94	119.02	111.83
2	J	701	SAH	N3-C2-N1	-2.94	124.13	128.58
2	A	701	SAH	C2-N3-C4	2.93	119.00	111.83
2	B	701	SAH	C4-N9-C8	2.93	108.81	105.74
2	D	701	SAH	C4-C5-N7	-2.91	107.25	110.58
2	G	701	SAH	CB-CG-SD	-2.90	106.99	113.45
2	D	701	SAH	O3'-C3'-C4'	-2.90	102.76	111.08
2	C	701	SAH	O4'-C1'-N9	-2.89	102.54	108.09
2	F	701	SAH	C4-C5-N7	-2.89	107.28	110.58
2	R	701	SAH	C4-C5-N7	-2.89	107.28	110.58
2	A	701	SAH	C2'-C1'-N9	2.87	120.42	113.30
2	N	701	SAH	C2'-C1'-N9	2.82	120.32	113.30
2	N	701	SAH	C2-N1-C6	2.80	123.33	118.73
2	J	701	SAH	N9-C8-N7	-2.78	109.99	113.94
2	P	701	SAH	C6-C5-N7	2.78	137.45	132.09
2	G	701	SAH	C5-N7-C8	2.78	107.81	103.45
2	O	701	SAH	N9-C8-N7	-2.77	110.00	113.94
2	D	701	SAH	C4-N9-C8	2.77	108.64	105.74
2	E	701	SAH	C4'-C5'-SD	-2.74	103.99	113.78
2	J	701	SAH	C5-N7-C8	2.73	107.74	103.45
2	L	701	SAH	N9-C8-N7	-2.73	110.06	113.94
2	N	701	SAH	CB-CA-N	2.72	117.21	110.12
2	B	701	SAH	C5-N7-C8	2.72	107.72	103.45
2	L	701	SAH	CB-CG-SD	-2.70	107.42	113.45
2	I	701	SAH	O3'-C3'-C4'	-2.70	103.33	111.08
2	E	701	SAH	C6-C5-N7	2.70	137.29	132.09
3	D	702	PO4	O4-P-O3	2.70	116.31	107.91
2	C	701	SAH	C5-N7-C8	2.67	107.65	103.45
2	D	701	SAH	N3-C2-N1	-2.67	124.54	128.58
2	L	701	SAH	C2'-C1'-N9	2.66	119.91	113.30
2	G	701	SAH	O4'-C1'-N9	2.66	113.19	108.09
2	J	701	SAH	O3'-C3'-C4'	-2.65	103.47	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	701	SAH	C5-N7-C8	2.64	107.60	103.45
2	F	701	SAH	C5-N7-C8	2.64	107.60	103.45
2	G	701	SAH	C2'-C1'-N9	-2.63	106.77	113.30
2	M	701	SAH	C5-C6-N6	-2.63	116.77	123.29
2	B	701	SAH	O3'-C3'-C2'	-2.63	103.38	111.82
2	K	701	SAH	C4-C5-N7	-2.61	107.60	110.58
2	M	701	SAH	C4-N9-C8	2.60	108.47	105.74
2	L	701	SAH	O3'-C3'-C4'	-2.60	103.60	111.08
2	F	701	SAH	C2'-C3'-C4'	2.60	107.63	102.61
2	H	701	SAH	CB-CG-SD	-2.60	107.66	113.45
2	A	701	SAH	C4-C5-N7	-2.59	107.62	110.58
2	E	701	SAH	O3'-C3'-C4'	-2.59	103.65	111.08
2	I	701	SAH	C2-N1-C6	2.58	122.97	118.73
2	B	701	SAH	C2'-C3'-C4'	2.57	107.58	102.61
3	A	702	PO4	O4-P-O3	2.57	115.91	107.91
2	Q	701	SAH	C4-C5-N7	-2.57	107.64	110.58
2	B	701	SAH	N9-C8-N7	-2.57	110.29	113.94
2	R	701	SAH	C2-N1-C6	2.57	122.95	118.73
2	G	701	SAH	C2-N1-C6	2.55	122.92	118.73
3	D	702	PO4	O3-P-O1	-2.54	101.97	110.95
2	P	701	SAH	C4-N9-C1'	-2.52	120.75	126.63
2	M	701	SAH	C2-N1-C6	2.51	122.85	118.73
2	H	701	SAH	C4'-O4'-C1'	2.50	115.00	109.47
2	C	701	SAH	O3'-C3'-C4'	-2.50	103.91	111.08
2	M	701	SAH	C4'-O4'-C1'	2.49	114.97	109.47
2	F	701	SAH	CB-CA-N	2.49	116.60	110.12
2	B	701	SAH	OXT-C-O	-2.49	118.44	124.08
2	B	701	SAH	O4'-C1'-N9	-2.48	103.32	108.09
2	E	701	SAH	C4-N9-C8	2.47	108.34	105.74
2	O	701	SAH	C5-N7-C8	2.46	107.32	103.45
2	I	701	SAH	C5-N7-C8	2.46	107.31	103.45
2	O	701	SAH	C4-C5-N7	-2.46	107.77	110.58
2	N	701	SAH	N6-C6-N1	2.45	123.84	118.38
2	P	701	SAH	C2'-C3'-C4'	2.45	107.34	102.61
2	K	701	SAH	C4-N9-C1'	-2.44	120.92	126.63
2	J	701	SAH	C2'-C3'-C4'	2.43	107.31	102.61
2	B	701	SAH	C6-C5-N7	2.42	136.75	132.09
2	D	701	SAH	C5-N7-C8	2.41	107.24	103.45
2	A	701	SAH	OXT-C-O	-2.38	118.68	124.08
2	I	701	SAH	N9-C8-N7	-2.38	110.56	113.94
2	K	701	SAH	N9-C8-N7	-2.37	110.57	113.94
2	C	701	SAH	C4-N9-C8	2.37	108.22	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	SAH	C2'-C3'-C4'	2.36	107.18	102.61
2	K	701	SAH	C2-N1-C6	2.35	122.60	118.73
2	P	701	SAH	C5-N7-C8	2.35	107.15	103.45
2	G	701	SAH	OXT-C-O	-2.35	118.75	124.08
2	R	701	SAH	CB-CG-SD	-2.33	108.24	113.45
2	Q	701	SAH	C5-N7-C8	2.32	107.09	103.45
2	E	701	SAH	C5-N7-C8	2.30	107.07	103.45
2	P	701	SAH	C2-N1-C6	2.30	122.51	118.73
2	I	701	SAH	C5'-SD-CG	-2.29	95.46	102.26
2	P	701	SAH	O3'-C3'-C4'	-2.27	104.57	111.08
2	G	701	SAH	N9-C8-N7	-2.27	110.72	113.94
2	D	701	SAH	C2'-C1'-N9	2.26	118.92	113.30
2	A	701	SAH	C2-N1-C6	2.26	122.44	118.73
3	I	702	PO4	O4-P-O1	2.25	118.92	110.95
2	G	701	SAH	C6-C5-N7	2.25	136.43	132.09
2	O	701	SAH	CB-CG-SD	-2.25	108.44	113.45
2	K	701	SAH	N6-C6-N1	2.24	123.37	118.38
2	K	701	SAH	C2'-C3'-C4'	2.24	106.93	102.61
3	F	702	PO4	O4-P-O2	2.22	114.83	107.91
2	Q	701	SAH	N9-C8-N7	-2.22	110.78	113.94
2	N	701	SAH	OXT-C-O	-2.21	119.07	124.08
2	Q	701	SAH	CB-CG-SD	-2.20	108.53	113.45
2	N	701	SAH	CB-CG-SD	-2.20	108.54	113.45
2	D	701	SAH	O4'-C1'-C2'	-2.19	101.93	106.62
2	P	701	SAH	N9-C8-N7	-2.18	110.84	113.94
2	E	701	SAH	C3'-C2'-C1'	2.18	105.59	101.46
2	E	701	SAH	OXT-C-O	-2.17	119.17	124.08
2	Q	701	SAH	N6-C6-N1	2.17	123.20	118.38
3	I	702	PO4	O2-P-O1	-2.16	103.32	110.95
2	L	701	SAH	C2-N1-C6	2.15	122.26	118.73
2	M	701	SAH	C5-N7-C8	2.14	106.82	103.45
2	N	701	SAH	C4-C5-N7	-2.14	108.14	110.58
2	O	701	SAH	N6-C6-N1	2.12	123.11	118.38
2	D	701	SAH	N9-C8-N7	-2.11	110.94	113.94
2	P	701	SAH	C2'-C1'-N9	2.10	118.53	113.30
2	J	701	SAH	C6-C5-N7	2.10	136.14	132.09
2	R	701	SAH	C5-N7-C8	2.10	106.75	103.45
2	A	701	SAH	C5-N7-C8	2.09	106.73	103.45
3	C	702	PO4	O4-P-O2	2.09	114.41	107.91
2	C	701	SAH	C2'-C3'-C4'	2.08	106.63	102.61
2	O	701	SAH	C2-N1-C6	2.08	122.15	118.73
2	H	701	SAH	C4-N9-C8	2.07	107.91	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	701	SAH	C1'-N9-C8	2.06	131.66	127.09
2	E	701	SAH	N9-C8-N7	-2.05	111.03	113.94
2	Q	701	SAH	CB-CA-N	2.04	115.44	110.12
2	N	701	SAH	C5-C6-N6	-2.03	118.25	123.29
2	A	701	SAH	CB-CG-SD	-2.03	108.91	113.45
2	F	701	SAH	C6-C5-N7	2.03	136.00	132.09
2	H	701	SAH	C2'-C3'-C4'	2.03	106.53	102.61
2	F	701	SAH	C2'-C1'-N9	2.03	118.34	113.30
2	Q	701	SAH	C2-N1-C6	2.01	122.03	118.73
2	K	701	SAH	C5-N7-C8	2.01	106.61	103.45
2	C	701	SAH	OXT-C-O	-2.01	119.53	124.08

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	701	SAH	O4'-C4'-C5'-SD
2	G	701	SAH	O4'-C4'-C5'-SD
2	G	701	SAH	C3'-C4'-C5'-SD
2	N	701	SAH	O-C-CA-N
2	N	701	SAH	O4'-C4'-C5'-SD
2	N	701	SAH	C3'-C4'-C5'-SD
2	P	701	SAH	O4'-C4'-C5'-SD
2	P	701	SAH	C3'-C4'-C5'-SD
2	Q	701	SAH	O4'-C4'-C5'-SD
2	Q	701	SAH	C3'-C4'-C5'-SD
2	R	701	SAH	O4'-C4'-C5'-SD
2	R	701	SAH	C3'-C4'-C5'-SD
2	N	701	SAH	OXT-C-CA-N
2	H	701	SAH	C-CA-CB-CG
2	M	701	SAH	C-CA-CB-CG
2	G	701	SAH	C2'-C1'-N9-C8
2	F	701	SAH	C3'-C4'-C5'-SD
2	H	701	SAH	N-CA-CB-CG
2	L	701	SAH	C3'-C4'-C5'-SD
2	M	701	SAH	O4'-C4'-C5'-SD
2	L	701	SAH	O4'-C4'-C5'-SD
2	H	701	SAH	CB-CG-SD-C5'
2	J	701	SAH	CB-CG-SD-C5'
2	I	701	SAH	C-CA-CB-CG
2	G	701	SAH	O4'-C1'-N9-C8
2	N	701	SAH	CB-CG-SD-C5'

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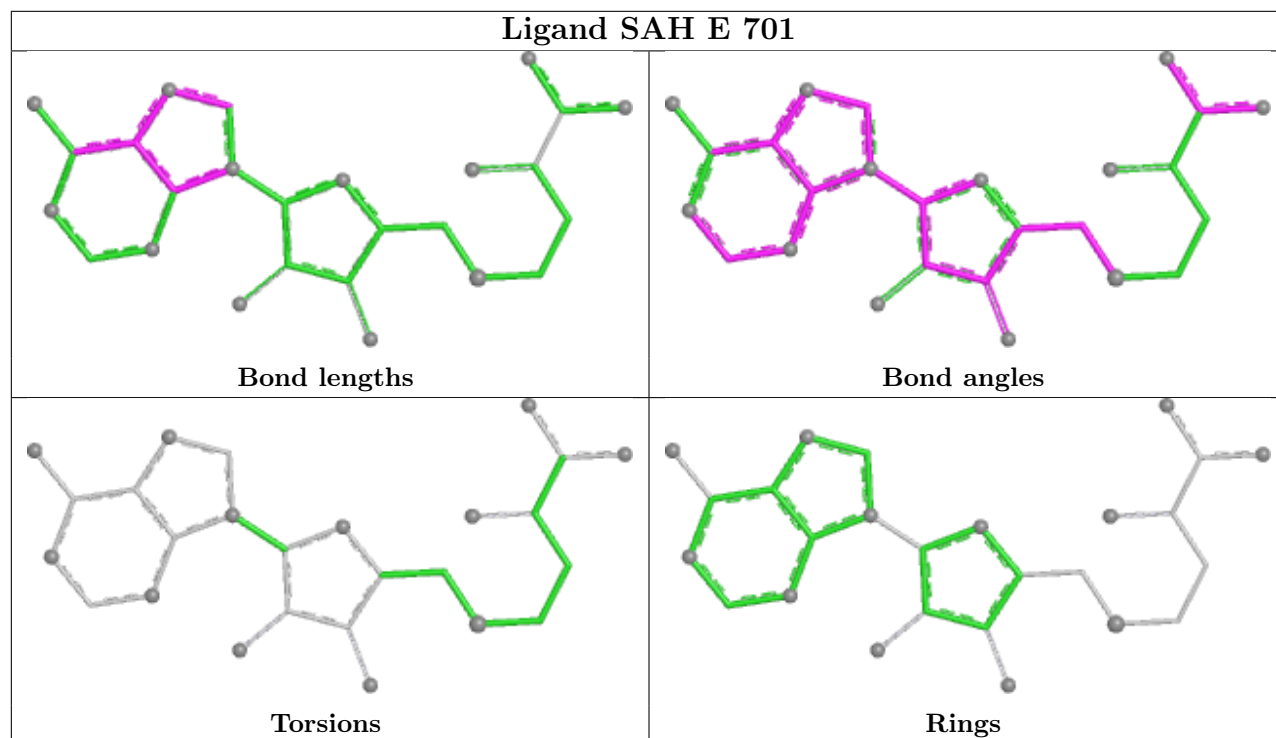
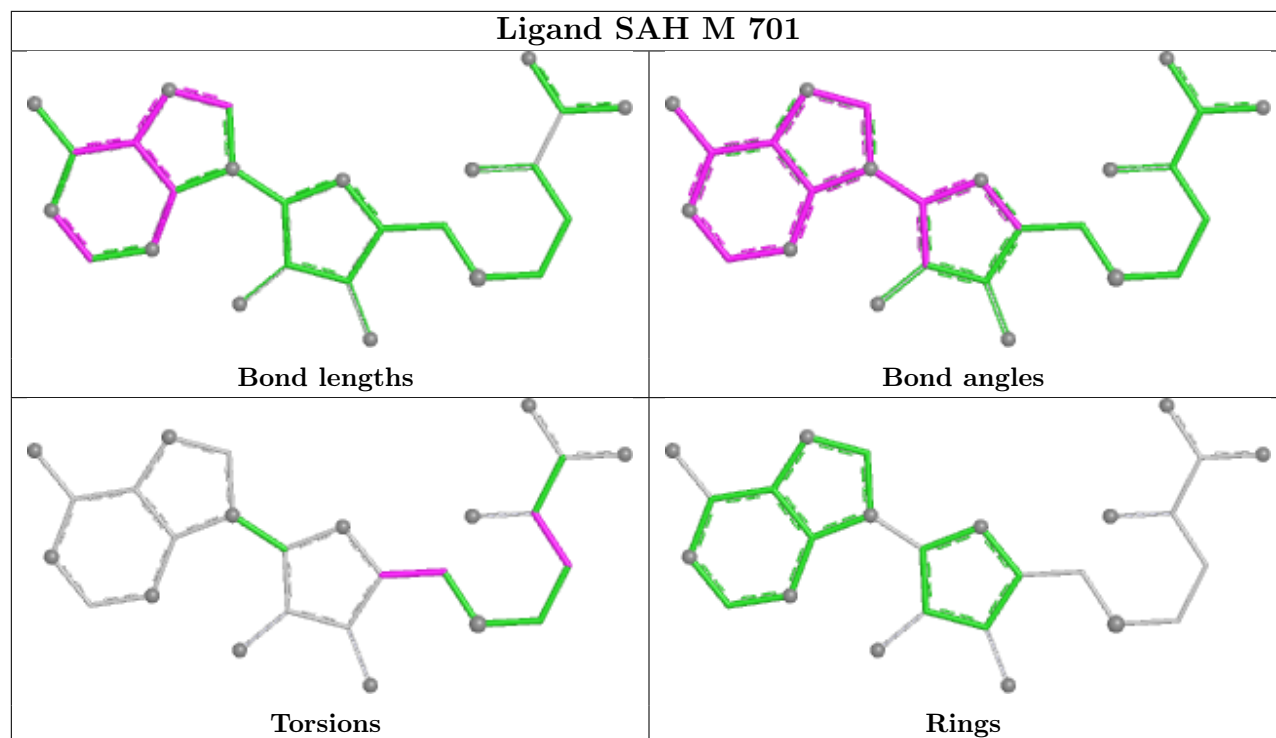
Mol	Chain	Res	Type	Atoms
2	B	701	SAH	C3'-C4'-C5'-SD
2	C	701	SAH	C3'-C4'-C5'-SD
2	M	701	SAH	C3'-C4'-C5'-SD

There are no ring outliers.

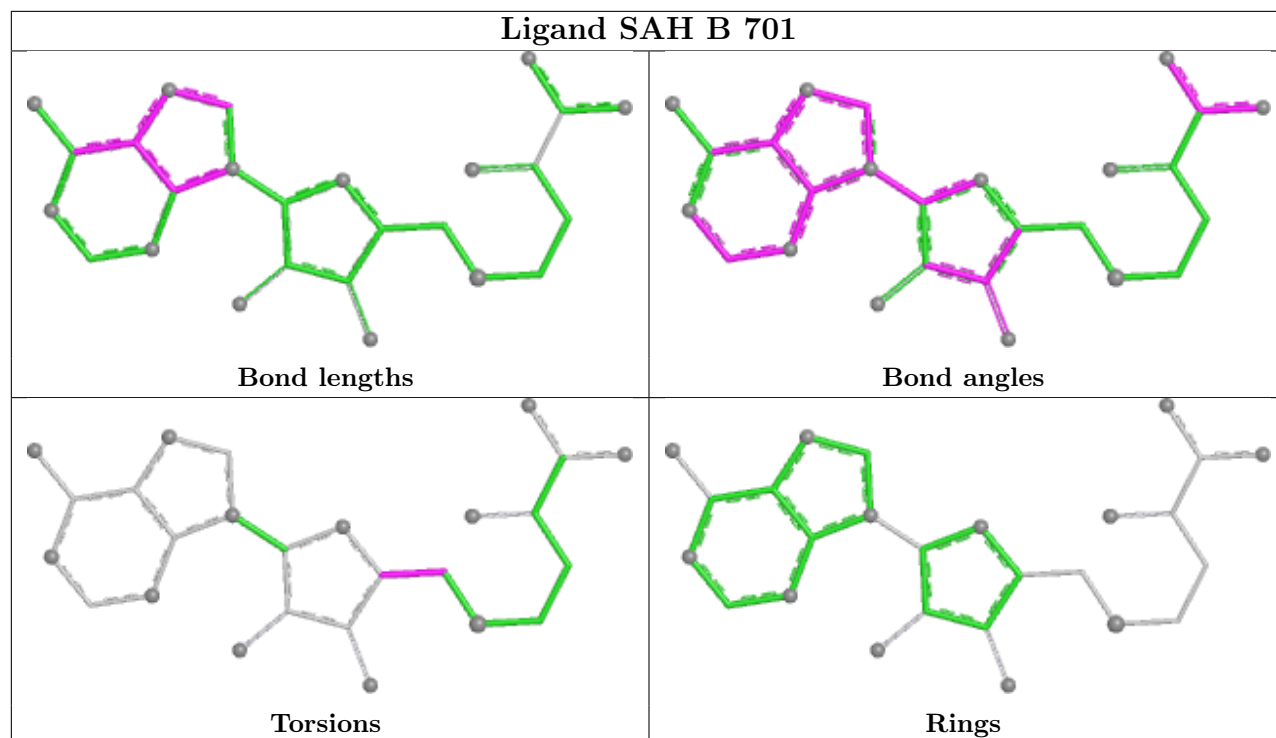
15 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	702	PO4	1	0
2	M	701	SAH	2	0
2	E	701	SAH	3	0
2	B	701	SAH	2	0
2	F	701	SAH	2	0
2	K	701	SAH	3	0
2	C	701	SAH	1	0
3	Q	702	PO4	1	0
2	R	701	SAH	2	0
2	N	701	SAH	2	0
2	I	701	SAH	1	0
2	Q	701	SAH	2	0
2	H	701	SAH	1	0
2	G	701	SAH	2	0
2	P	701	SAH	3	0

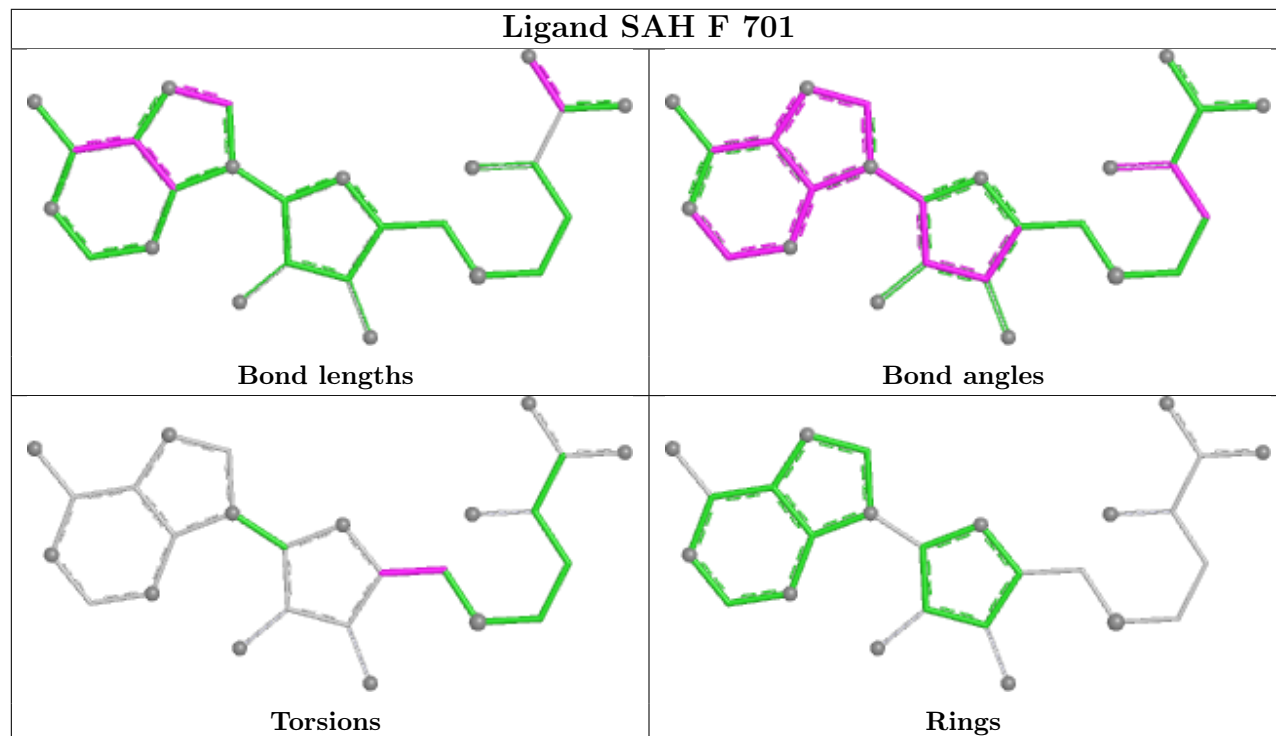
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



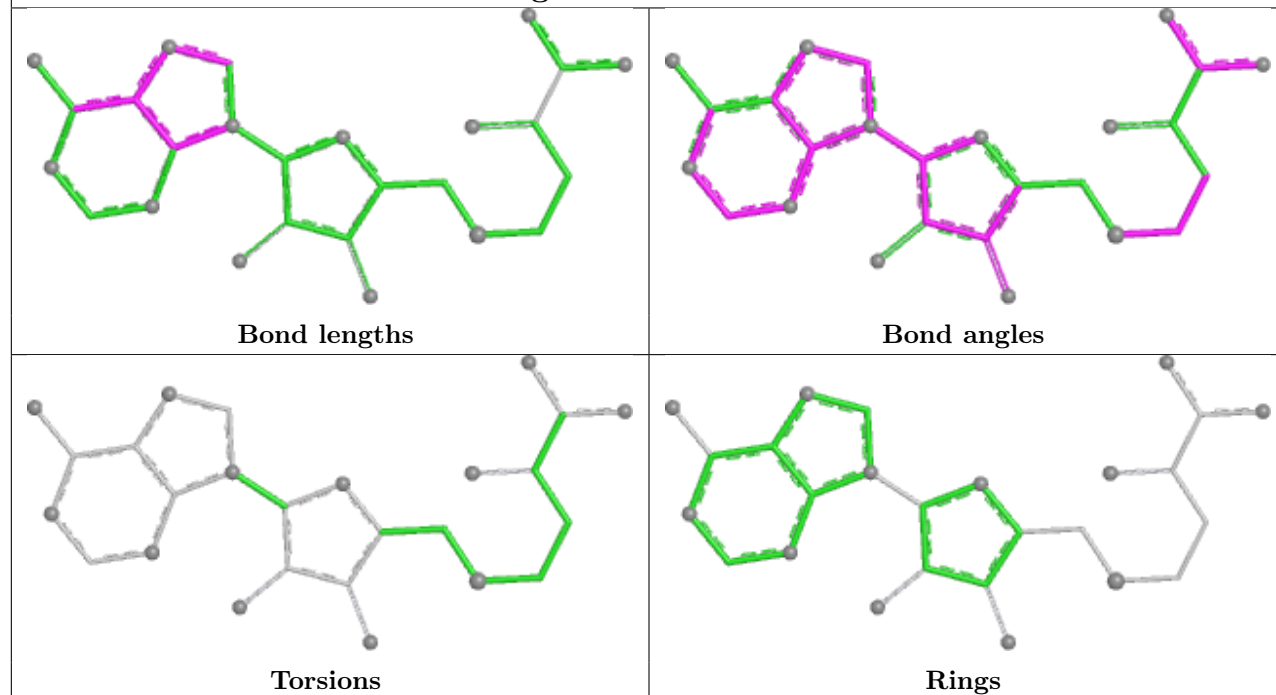
Ligand SAH B 701



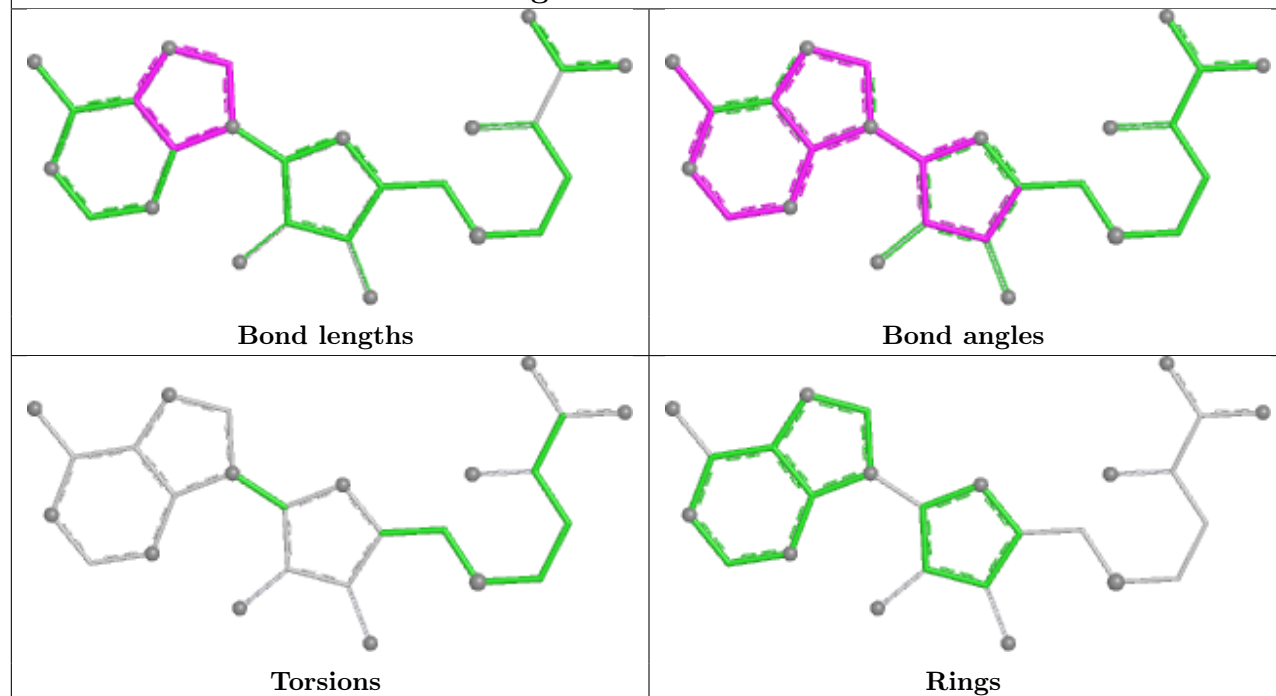
Ligand SAH F 701



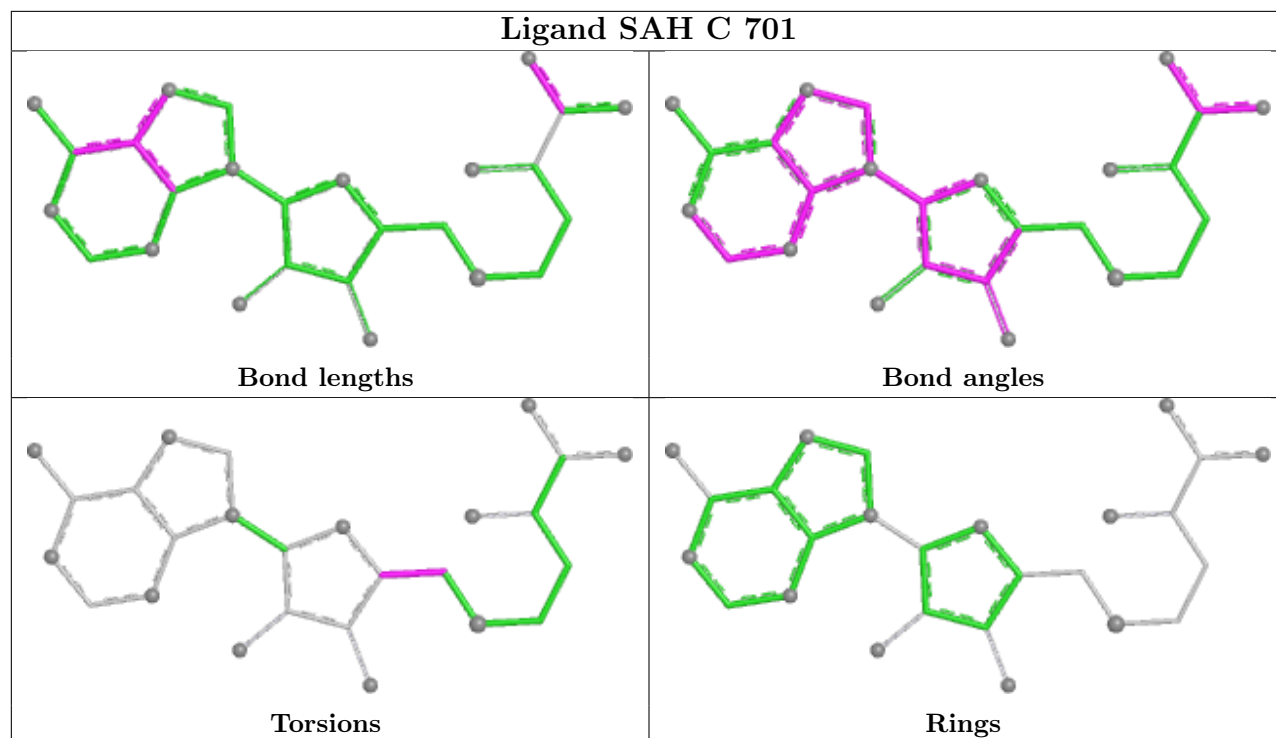
Ligand SAH A 701



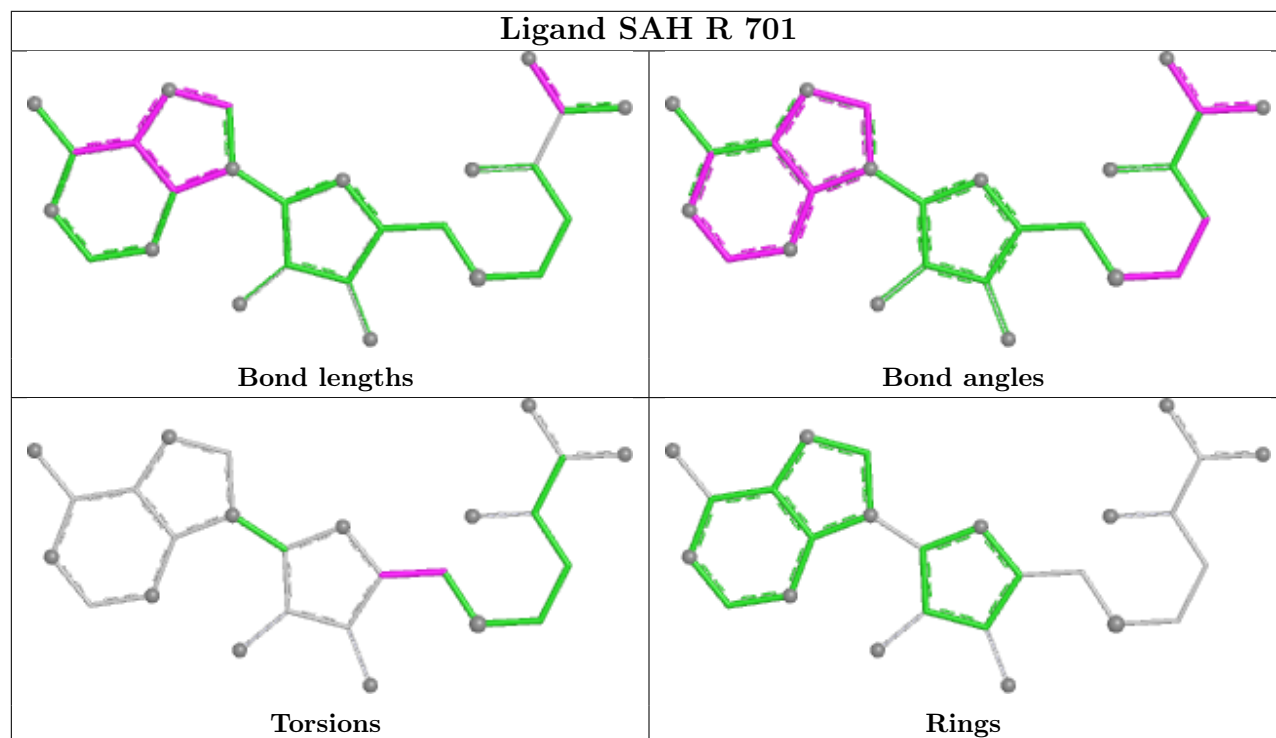
Ligand SAH K 701

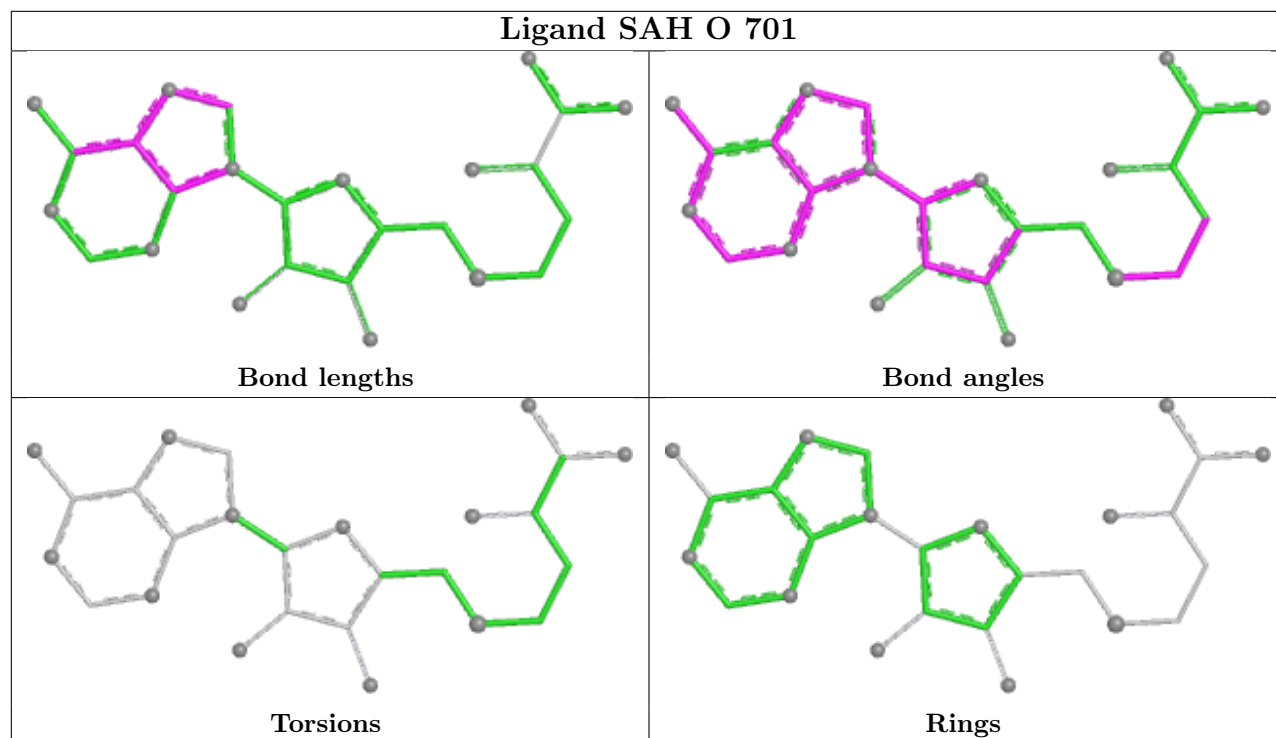
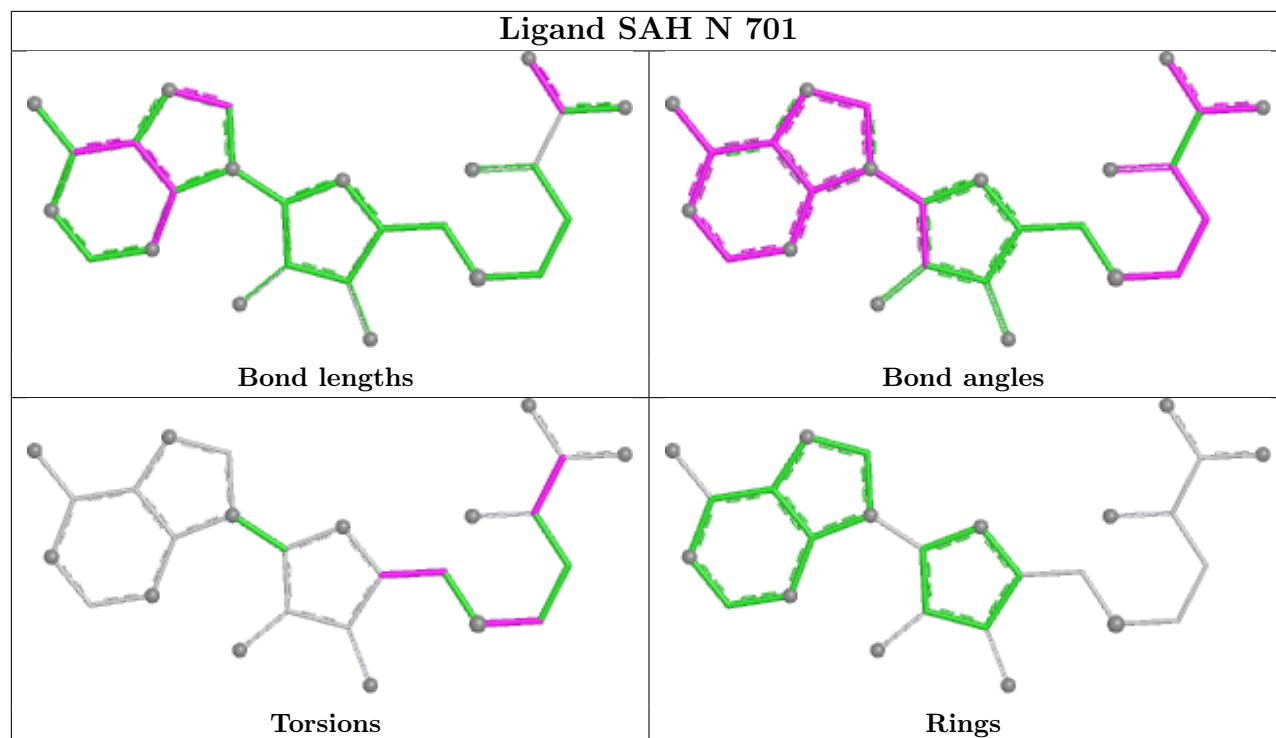


Ligand SAH C 701

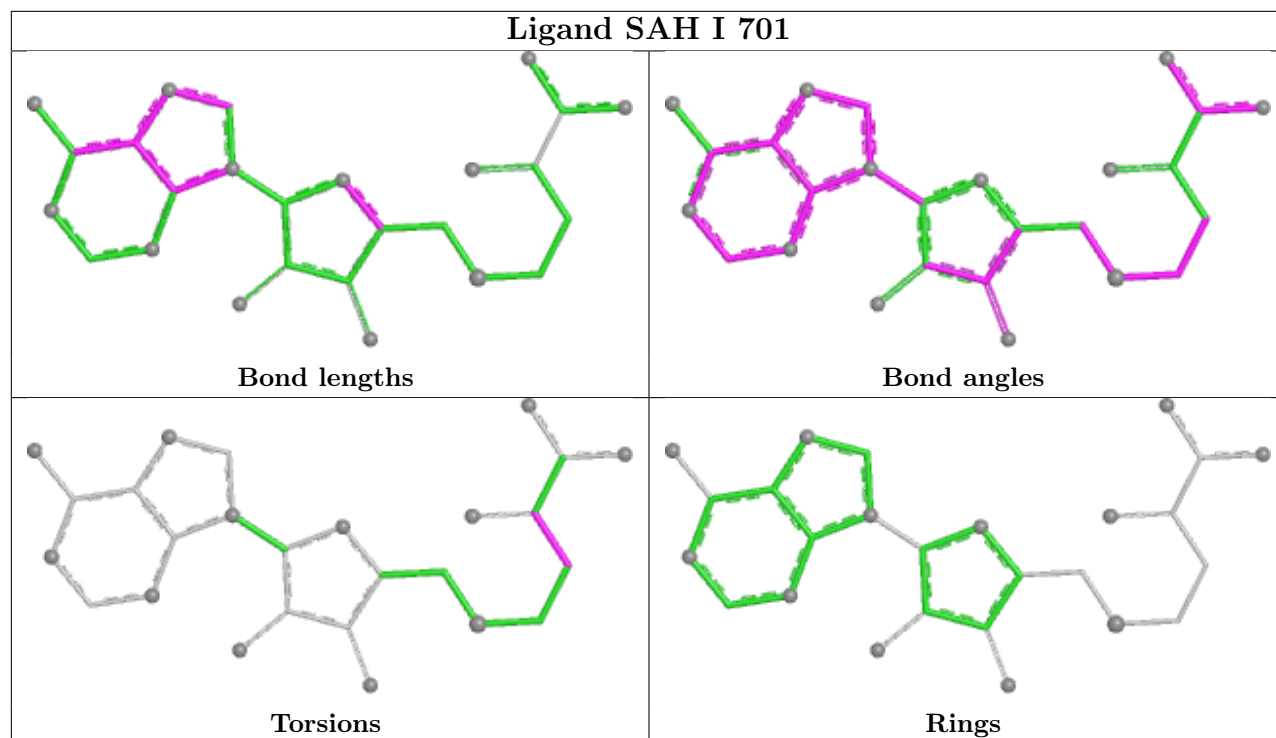


Ligand SAH R 701

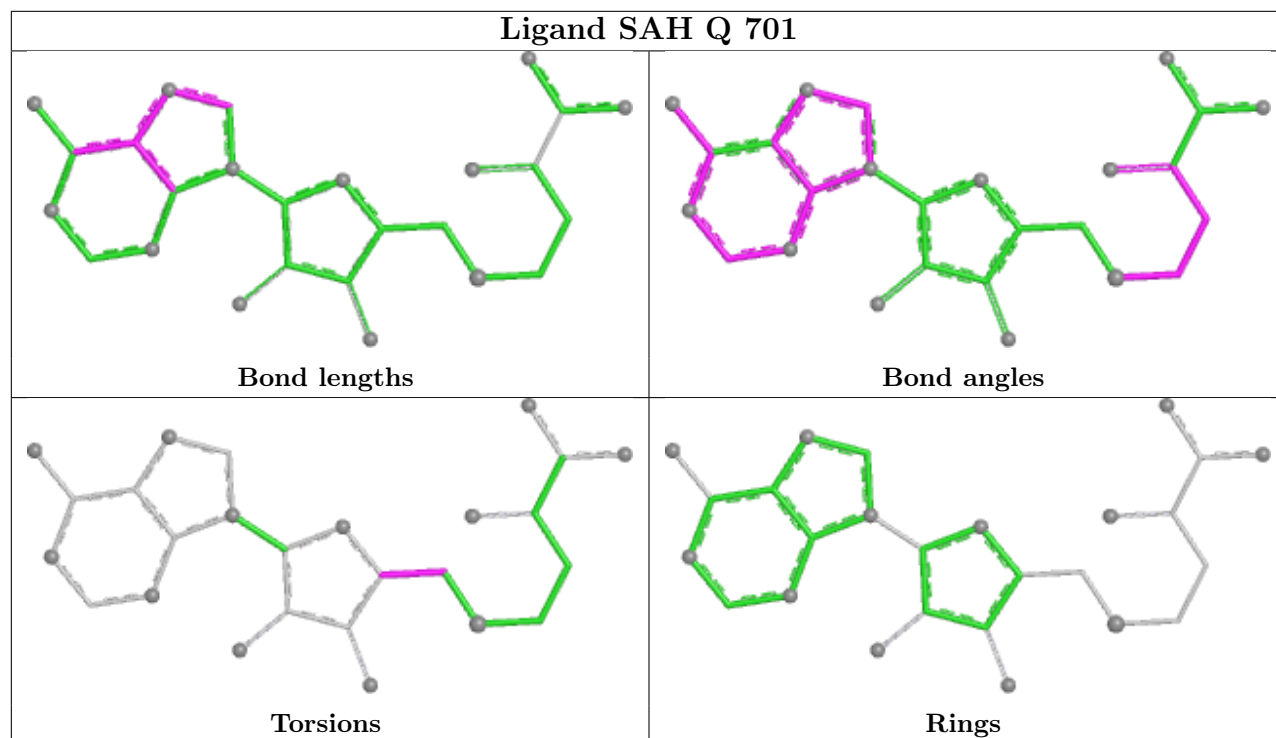




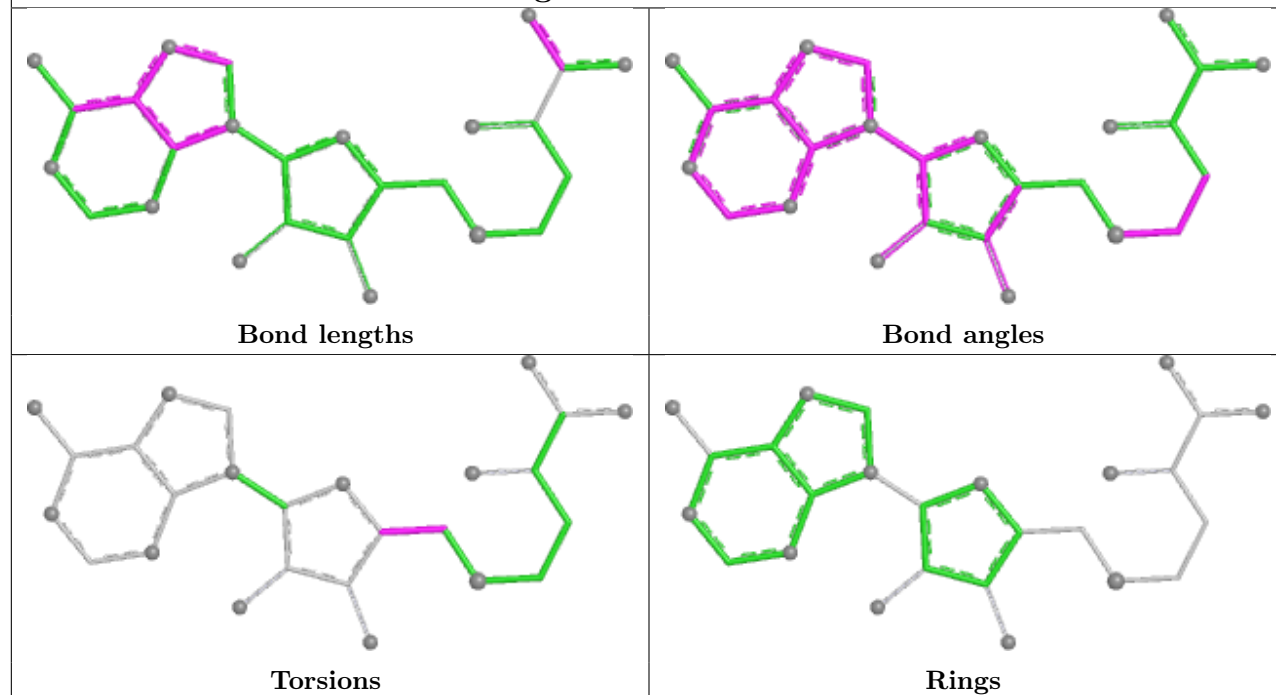
Ligand SAH I 701



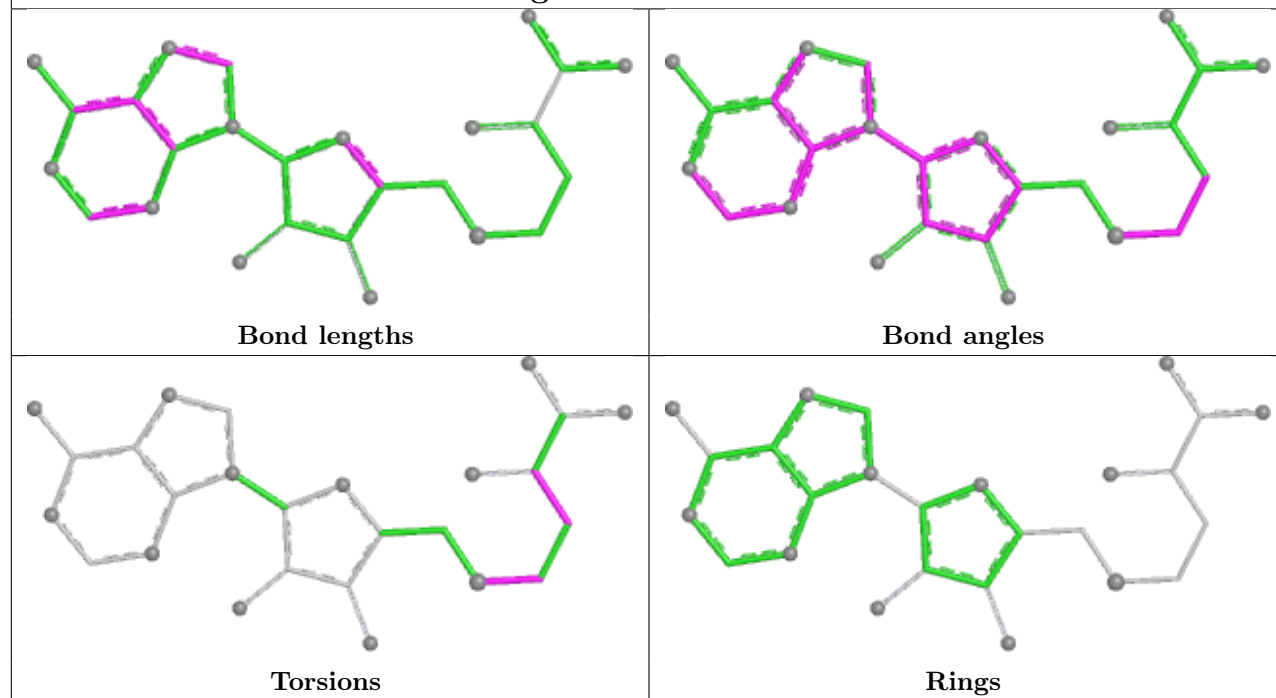
Ligand SAH Q 701



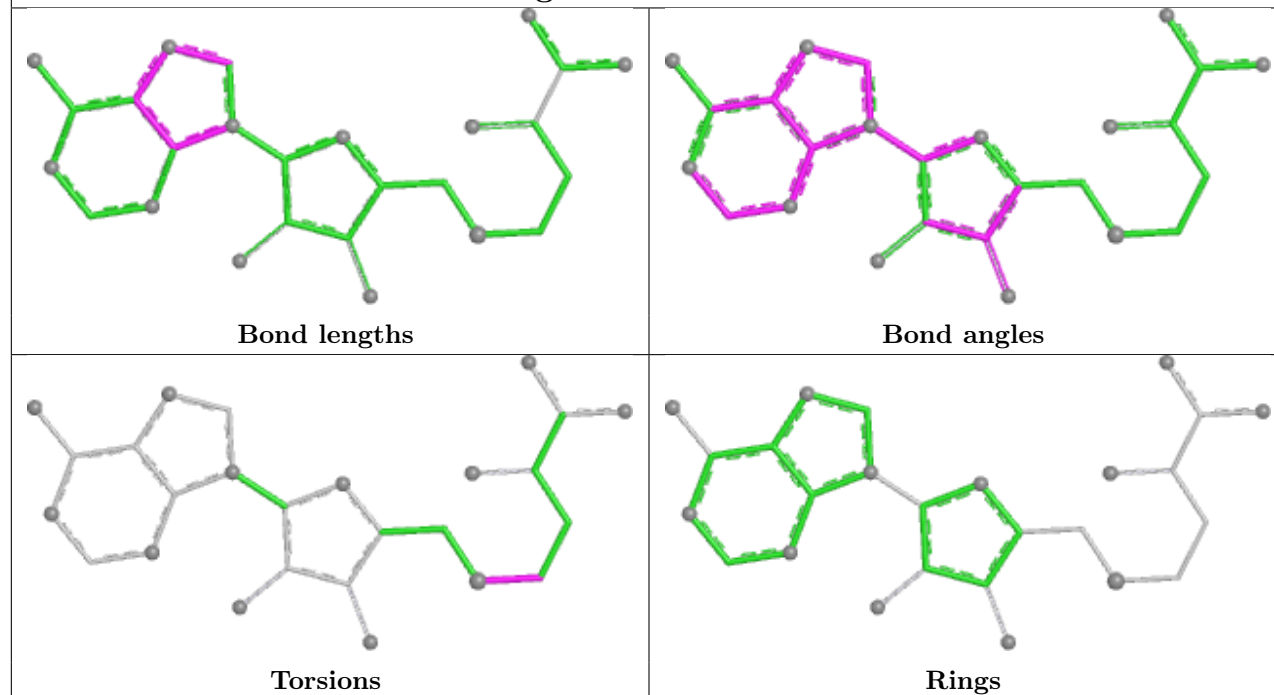
Ligand SAH L 701



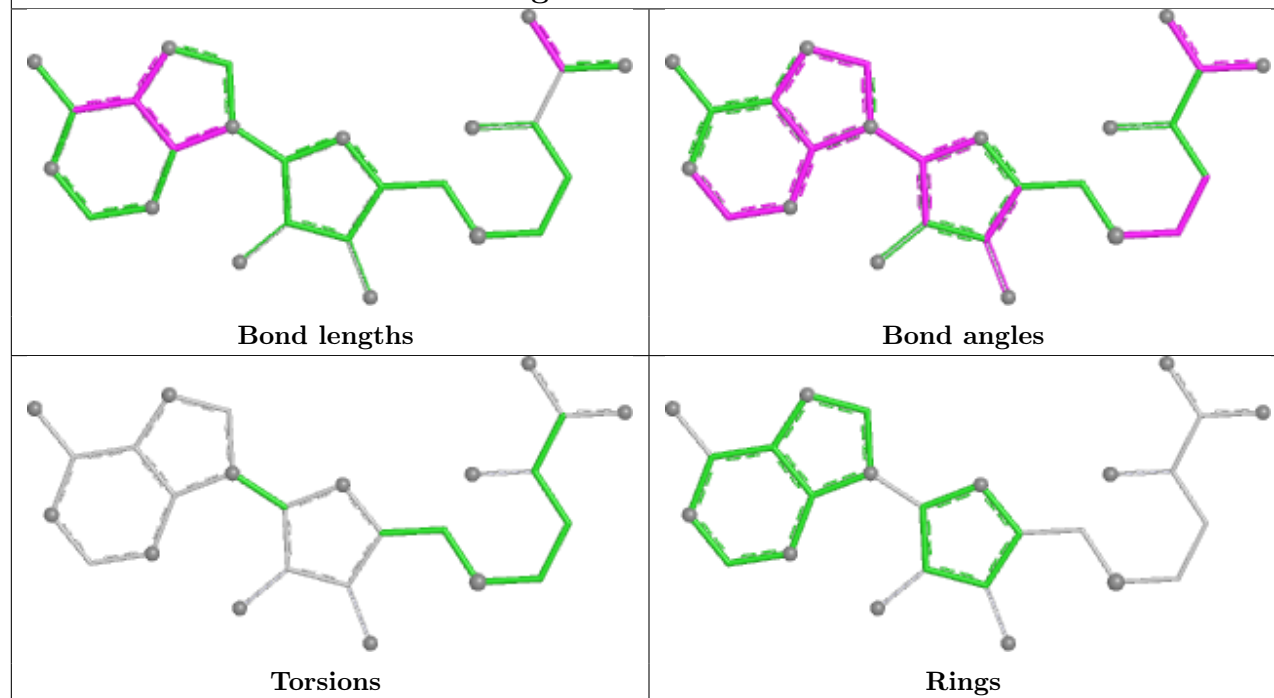
Ligand SAH H 701

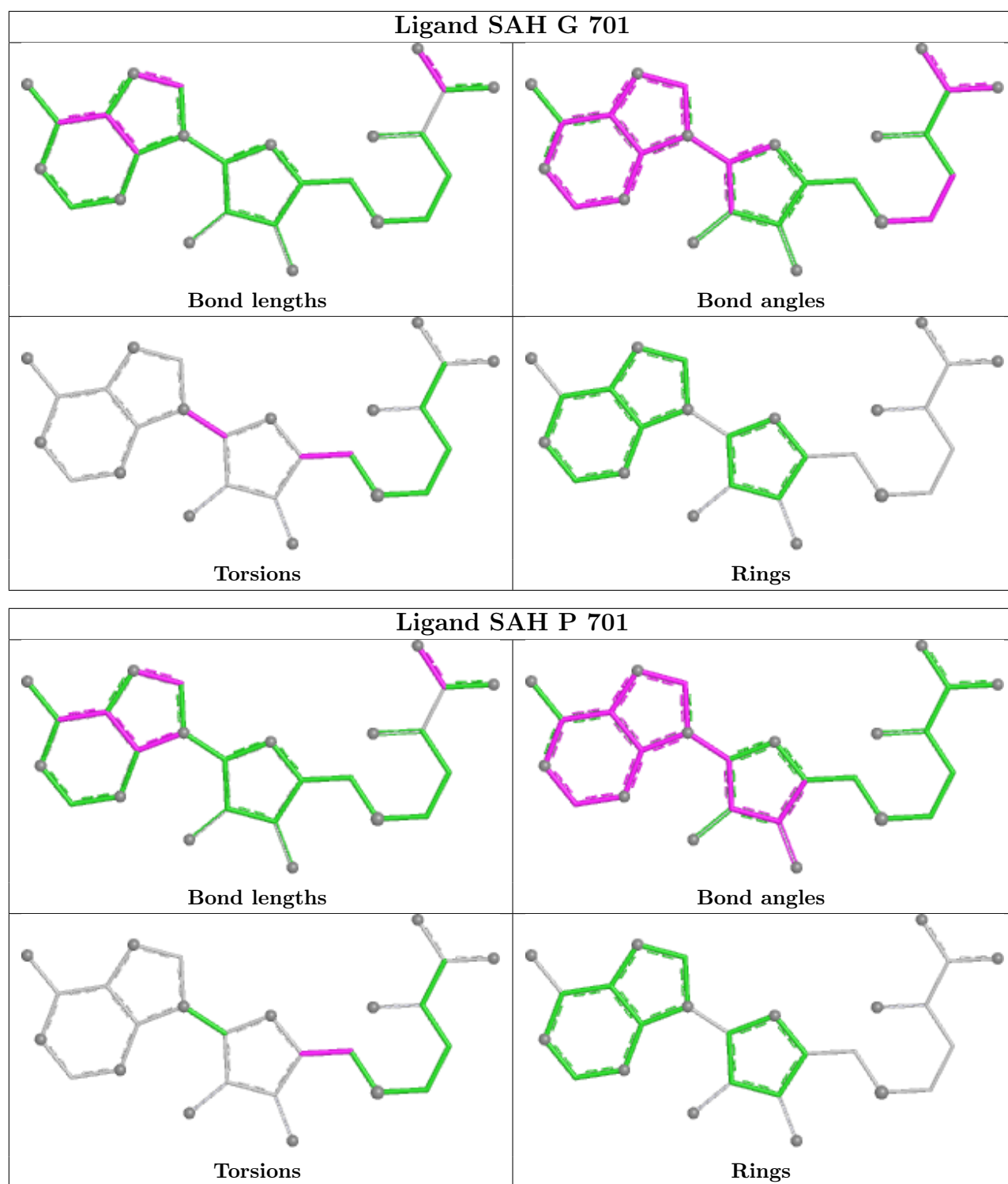


Ligand SAH J 701



Ligand SAH D 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	641/655 (97%)	-1.27	0 100 100	16, 33, 57, 83	0
1	B	638/655 (97%)	-1.14	0 100 100	24, 43, 74, 103	0
1	C	639/655 (97%)	-1.13	0 100 100	26, 44, 68, 100	0
1	D	637/655 (97%)	-1.26	0 100 100	19, 34, 56, 101	0
1	E	636/655 (97%)	-1.12	0 100 100	21, 41, 80, 124	0
1	F	638/655 (97%)	-1.06	0 100 100	27, 48, 75, 120	0
1	G	636/655 (97%)	-1.12	0 100 100	23, 43, 81, 129	0
1	H	639/655 (97%)	-1.22	0 100 100	18, 38, 60, 91	0
1	I	644/655 (98%)	-1.15	0 100 100	28, 44, 68, 94	0
1	J	644/655 (98%)	-1.08	0 100 100	29, 47, 69, 92	0
1	K	641/655 (97%)	-1.04	0 100 100	26, 52, 77, 99	0
1	L	644/655 (98%)	-1.29	0 100 100	19, 33, 55, 78	0
1	M	633/655 (96%)	-0.91	0 100 100	38, 61, 84, 110	0
1	N	638/655 (97%)	-1.01	0 100 100	36, 55, 75, 93	0
1	O	641/655 (97%)	-0.88	1 (0%) 91 89	39, 64, 96, 127	0
1	P	636/655 (97%)	-1.03	0 100 100	30, 51, 82, 105	0
1	Q	632/655 (96%)	-0.86	0 100 100	37, 62, 99, 124	0
1	R	638/655 (97%)	-0.80	0 100 100	44, 69, 99, 131	0
All	All	11495/11790 (97%)	-1.08	1 (0%) 100 100	16, 48, 82, 131	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	553	ILE	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

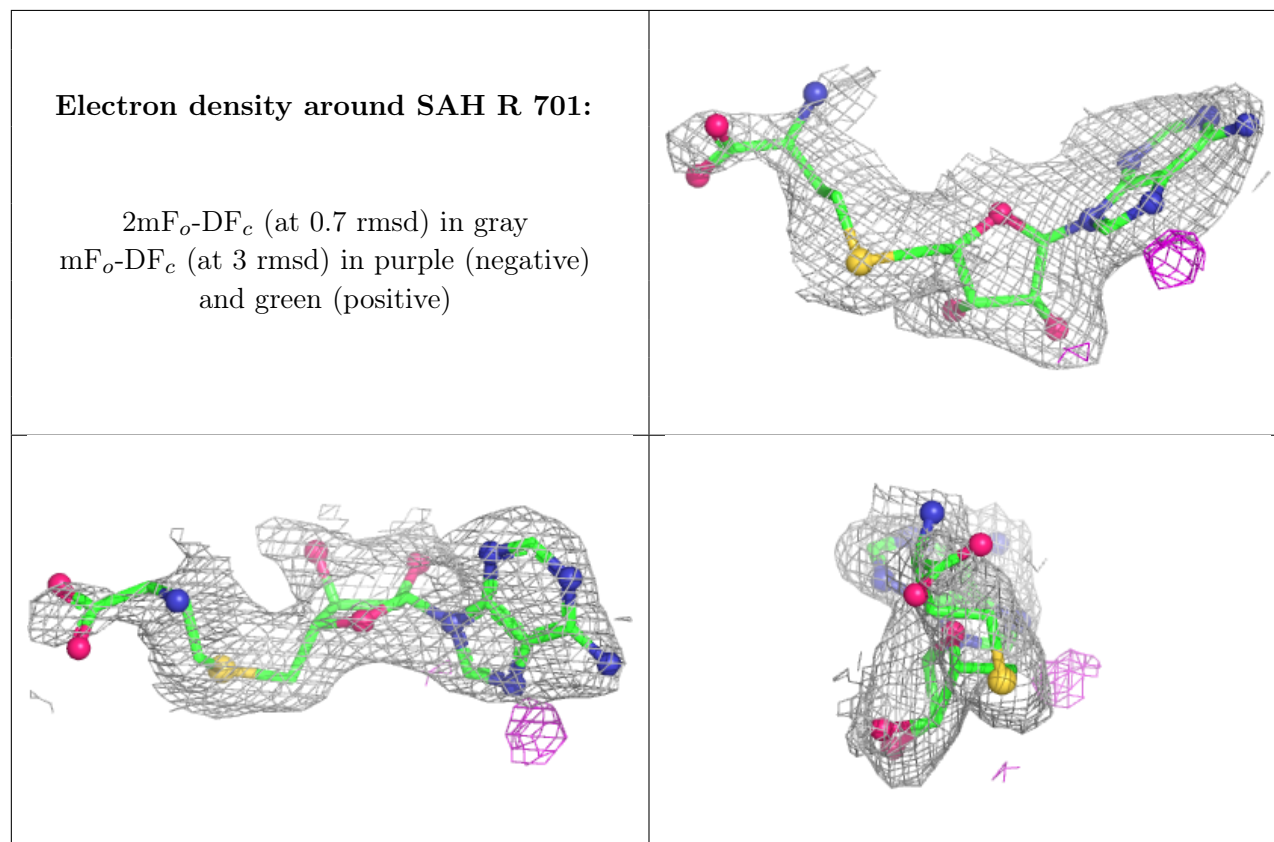
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	R	701	26/26	0.98	0.06	47,56,92,99	0
3	PO4	M	702	5/5	0.98	0.05	70,71,74,78	0
3	PO4	N	702	5/5	0.98	0.03	52,57,62,66	0
3	PO4	O	702	5/5	0.98	0.04	57,58,70,72	0
3	PO4	R	702	5/5	0.98	0.05	52,55,59,61	0
2	SAH	E	701	26/26	0.99	0.04	43,53,63,65	0
2	SAH	G	701	26/26	0.99	0.04	46,63,72,72	0
2	SAH	H	701	26/26	0.99	0.03	24,29,33,34	0
2	SAH	I	701	26/26	0.99	0.03	35,38,45,47	0
2	SAH	M	701	26/26	0.99	0.04	36,61,74,79	0
2	SAH	N	701	26/26	0.99	0.04	40,53,58,58	0
2	SAH	O	701	26/26	0.99	0.03	37,41,47,52	0
2	SAH	P	701	26/26	0.99	0.04	43,53,63,65	0
2	SAH	Q	701	26/26	0.99	0.05	48,64,75,76	0
2	SAH	A	701	26/26	0.99	0.04	27,33,38,38	0
2	SAH	J	701	26/26	0.99	0.04	34,38,44,46	0
2	SAH	K	701	26/26	0.99	0.04	37,41,47,51	0
2	SAH	L	701	26/26	0.99	0.03	27,33,36,39	0
3	PO4	A	702	5/5	0.99	0.03	31,32,37,39	0
3	PO4	B	702	5/5	0.99	0.04	36,39,45,48	0
3	PO4	C	702	5/5	0.99	0.04	37,41,44,44	0
3	PO4	F	702	5/5	0.99	0.04	38,42,49,56	0
3	PO4	E	702	5/5	0.99	0.03	36,40,43,47	0
3	PO4	G	702	5/5	0.99	0.03	42,42,49,50	0
3	PO4	H	702	5/5	0.99	0.02	28,34,36,37	0
3	PO4	I	702	5/5	0.99	0.04	36,37,44,49	0
2	SAH	D	701	26/26	0.99	0.05	32,37,45,46	0

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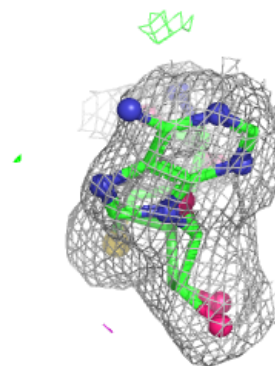
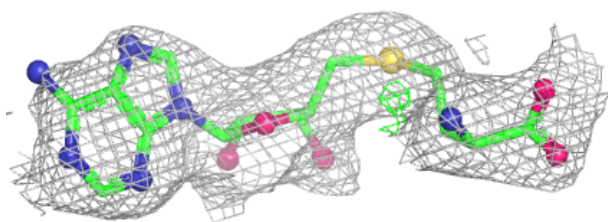
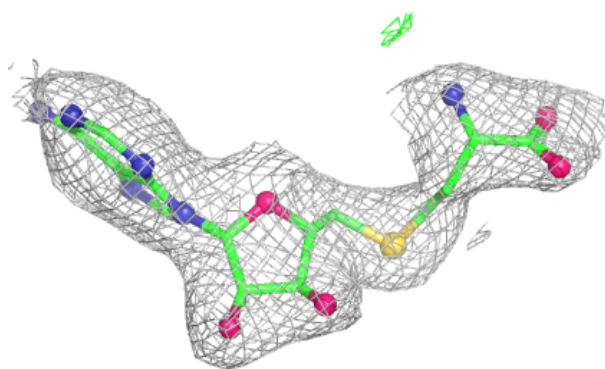
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	B	701	26/26	0.99	0.04	36,43,57,58	0
2	SAH	C	701	26/26	0.99	0.03	36,48,57,59	0
3	PO4	P	702	5/5	0.99	0.03	43,43,45,47	0
3	PO4	Q	702	5/5	0.99	0.04	59,63,72,72	0
2	SAH	F	701	26/26	0.99	0.04	35,46,61,64	0
3	PO4	J	702	5/5	0.99	0.03	45,46,49,51	0
3	PO4	K	702	5/5	0.99	0.03	43,45,46,51	0
3	PO4	D	702	5/5	1.00	0.03	31,35,36,37	0
3	PO4	L	702	5/5	1.00	0.03	32,32,35,37	0

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

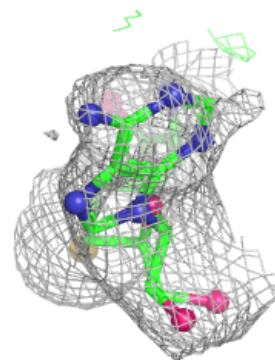
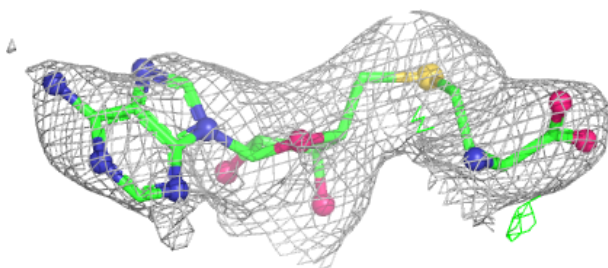
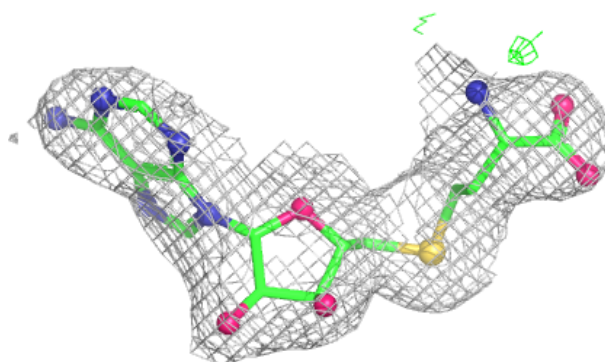


Electron density around SAH E 701:

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

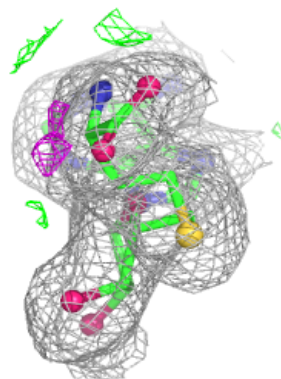
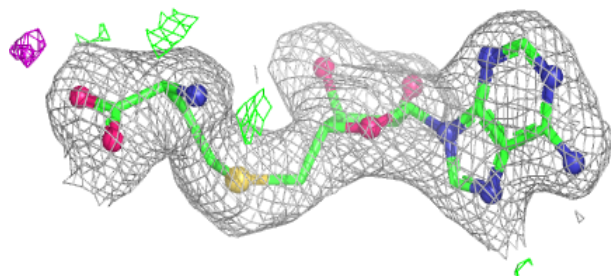
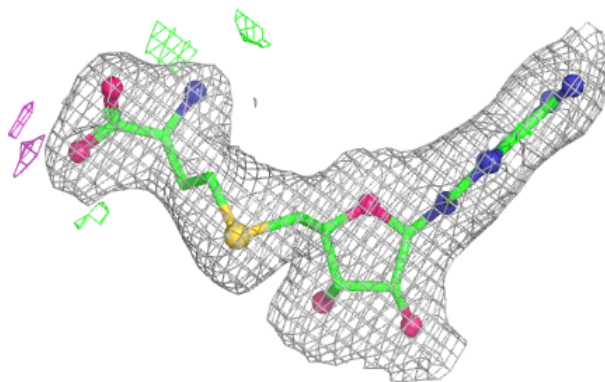
**Electron density around SAH G 701:**

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and green (positive)

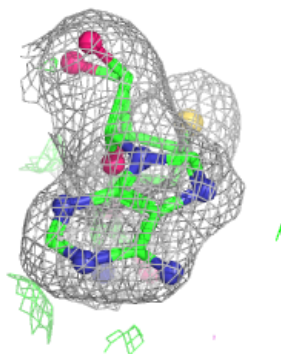
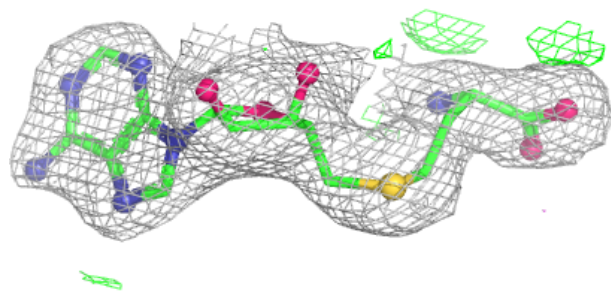
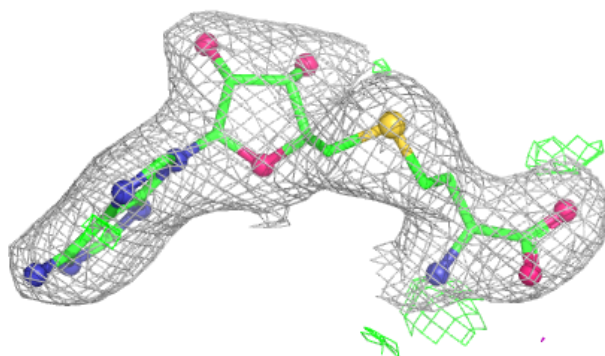


Electron density around SAH H 701:

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and green (positive)

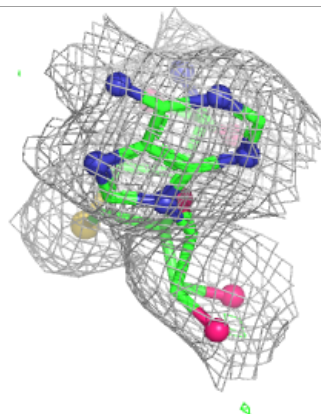
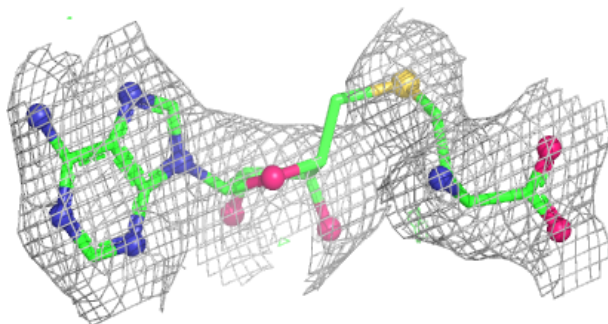
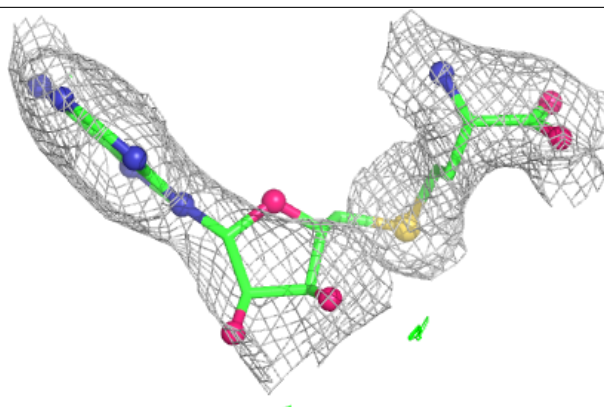
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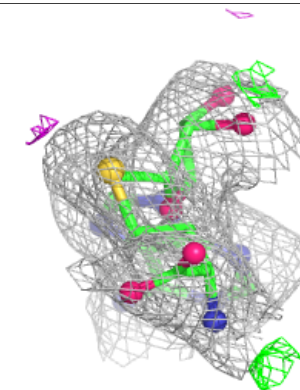
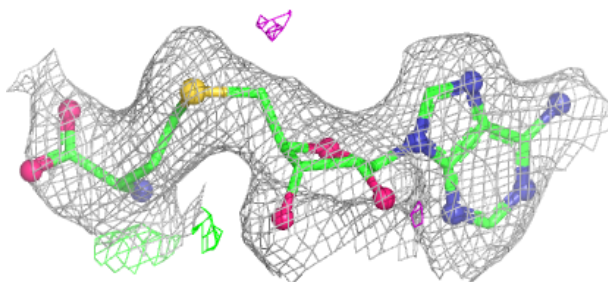
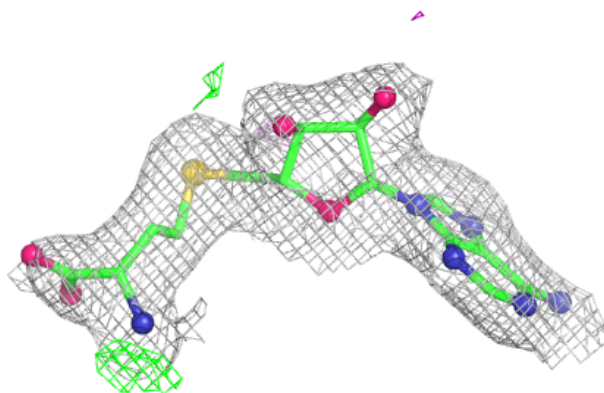


Electron density around SAH M 701:

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and green (positive)

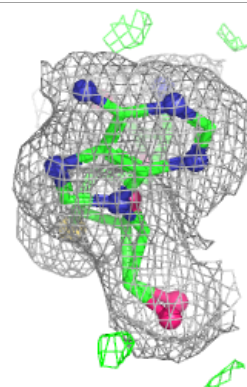
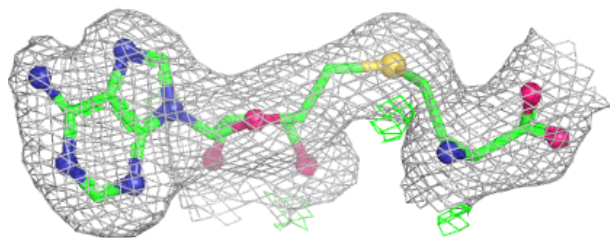
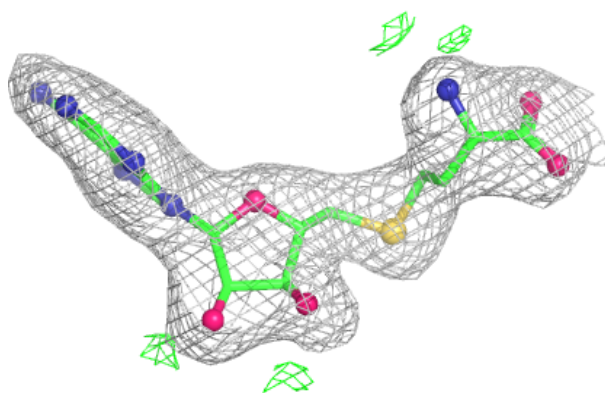
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and green (positive)

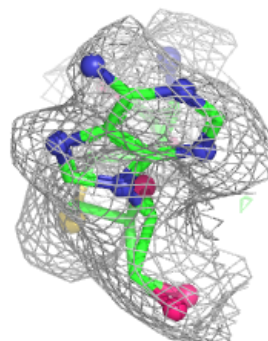
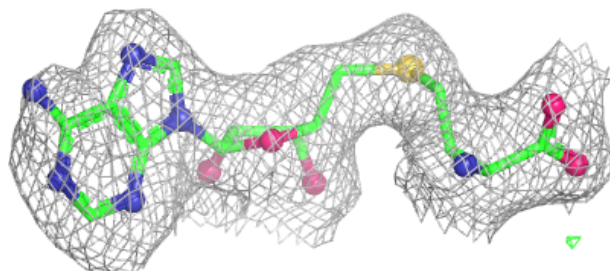
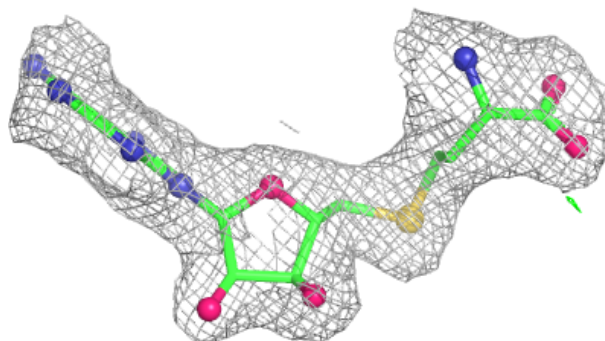


Electron density around SAH O 701:

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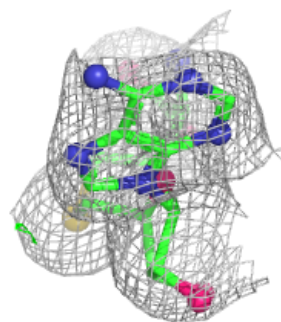
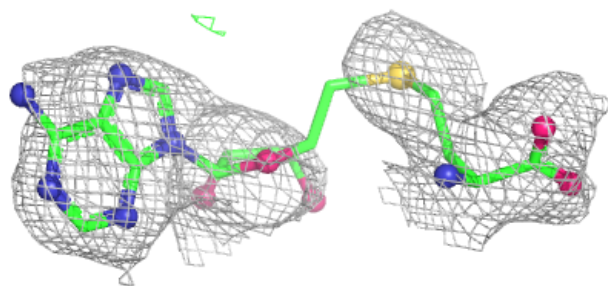
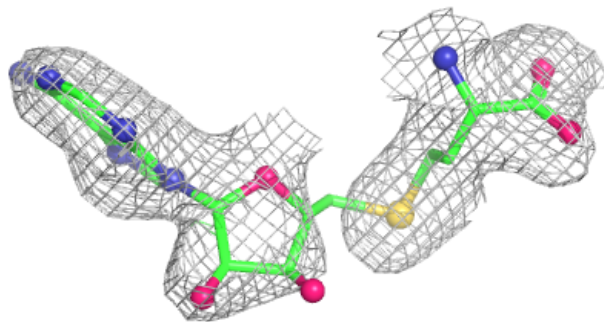
**Electron density around SAH P 701:**

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and green (positive)

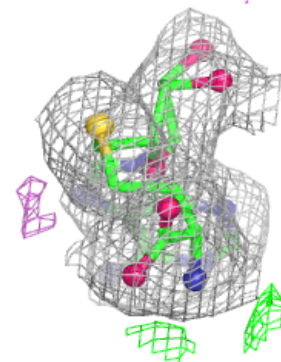
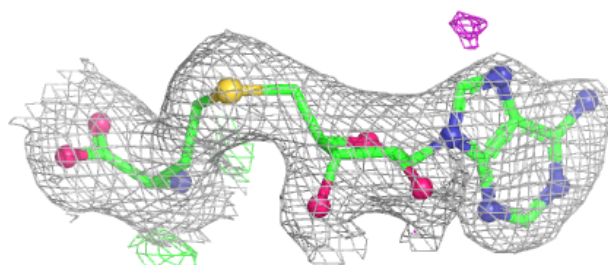
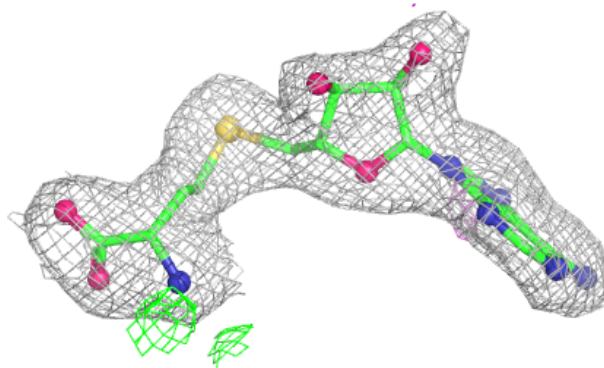


Electron density around SAH Q 701:

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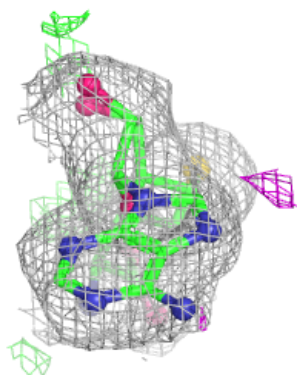
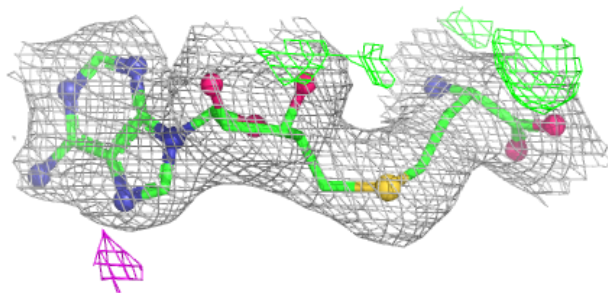
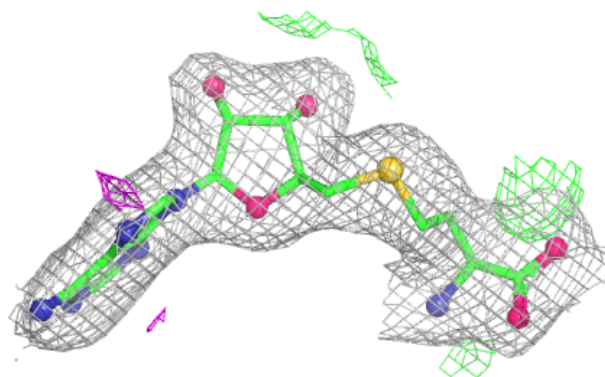
**Electron density around SAH A 701:**

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and green (positive)

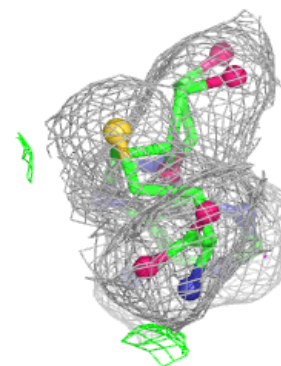
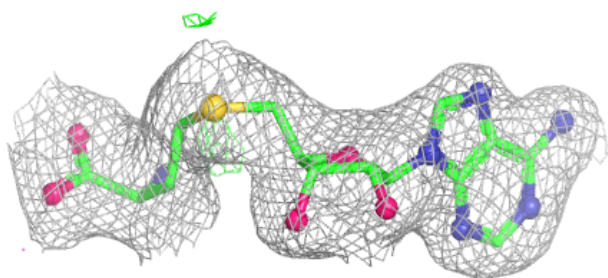
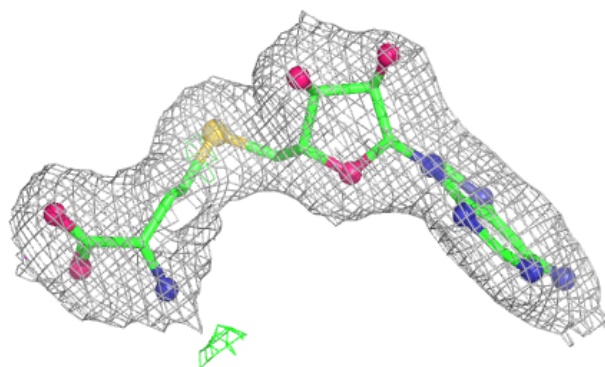


Electron density around SAH J 701:

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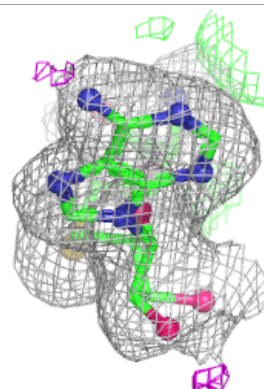
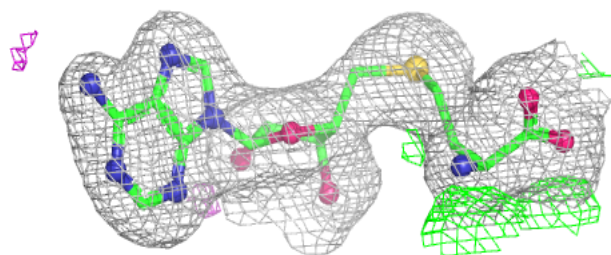
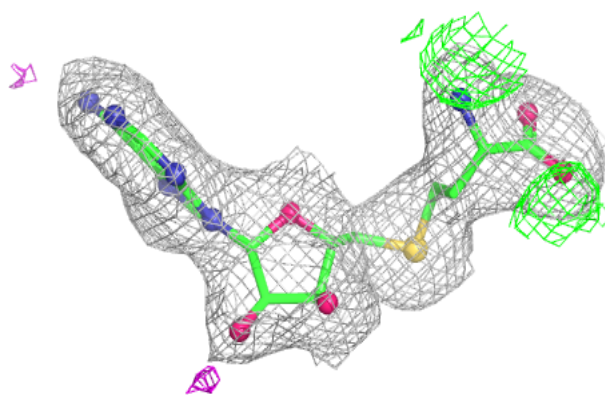
**Electron density around SAH K 701:**

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and green (positive)

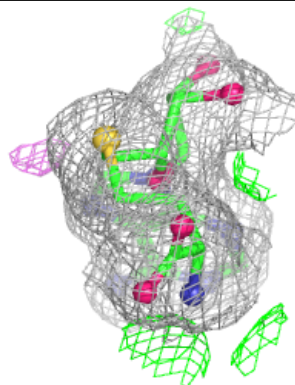
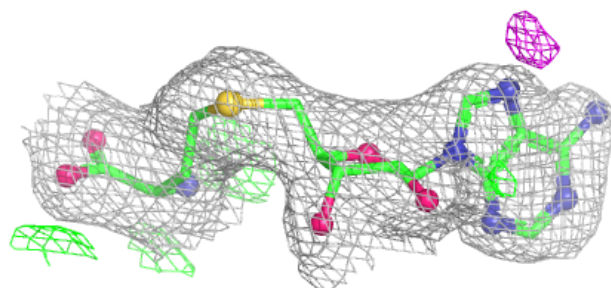
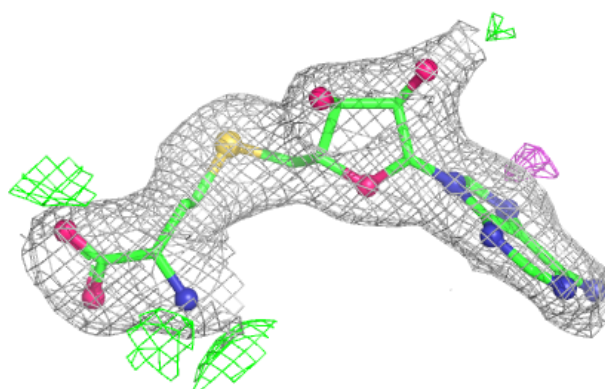


Electron density around SAH L 701:

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

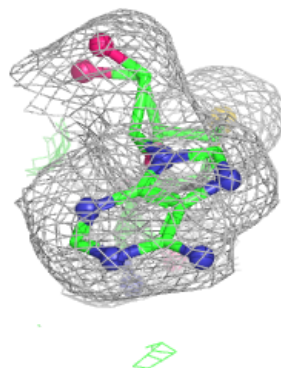
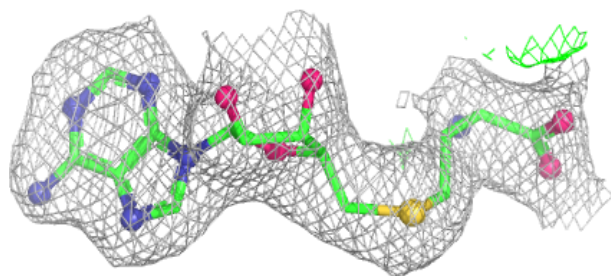
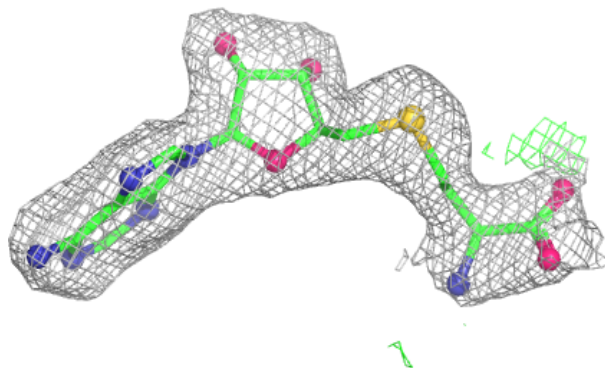
**Electron density around SAH D 701:**

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

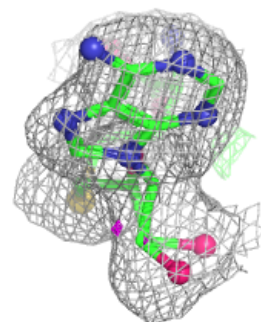
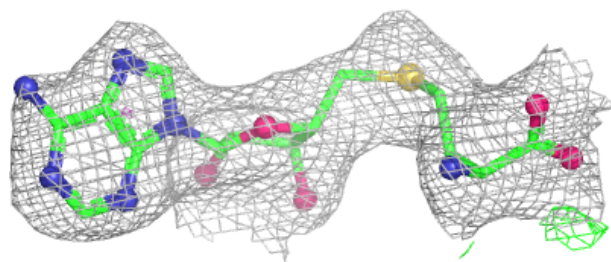
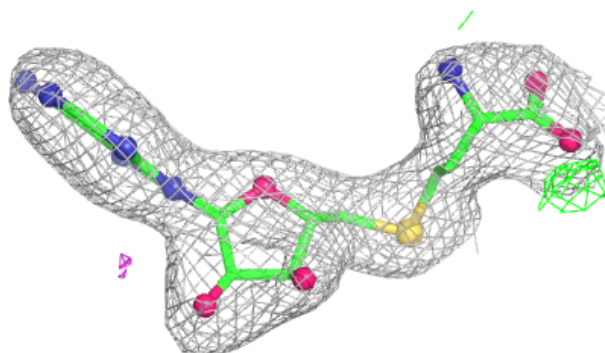


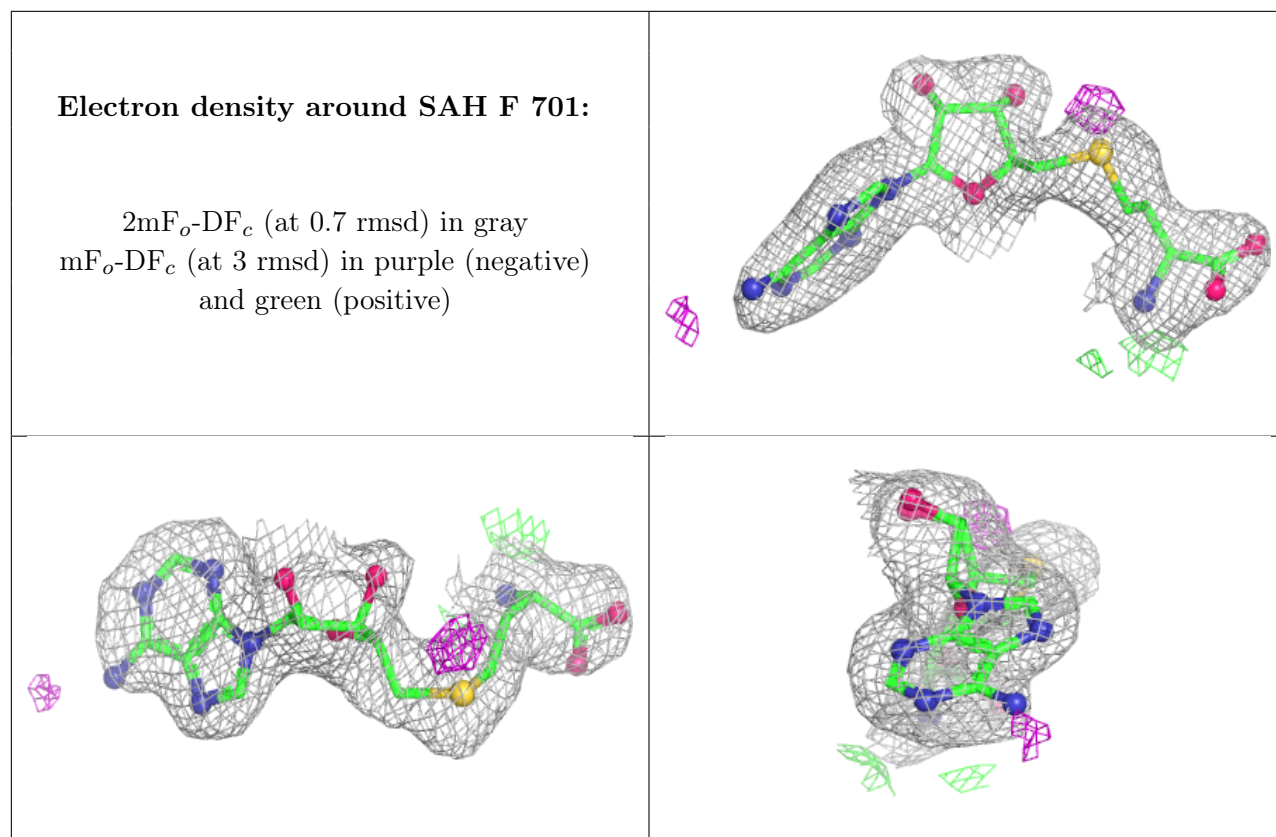
Electron density around SAH B 701:

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

**Electron density around SAH C 701:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.