



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:55 PM UTC

PDB ID : 3RYO / pdb_00003ryo
Title : Crystal Structure of Enhanced Intracellular Survival (Eis) Protein from Mycobacterium tuberculosis with Acetyl CoA
Authors : Kim, K.H.; An, D.R.; Yoon, J.Y.; Kim, H.S.; Yoon, H.J.; Song, J.; Im, H.N.; Kim, J.; Kim, D.J.; Lee, S.J.; Kim, H.J.; Lee, J.Y.; Suh, S.W.
Deposited on : 2011-05-11
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

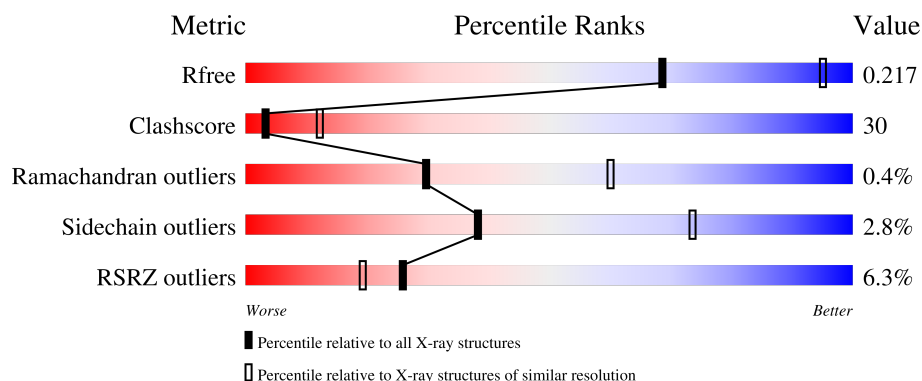
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



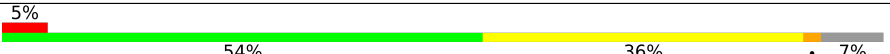
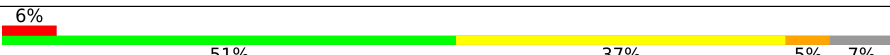
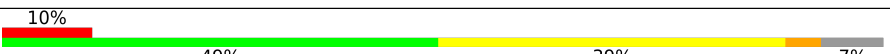
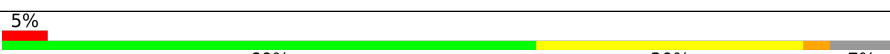
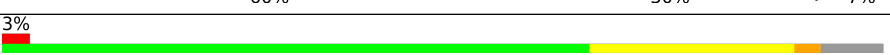
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	428	 6% 57% 33% 7%
1	B	428	 5% 59% 31% 7%
1	C	428	 5% 58% 32% 7%
1	D	428	 6% 56% 34% 7%

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Mol	Chain	Length	Quality of chain
1	E	428	
1	F	428	
1	G	428	
1	H	428	
1	I	428	
1	J	428	
1	K	428	
1	L	428	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37731 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 Enhanced intracellular survival protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	B	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	C	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	D	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	E	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	F	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	G	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	H	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	I	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	J	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	K	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0
1	L	396	Total 3053	C 1921	N 560	O 560	S 5	Se 7	0	0	0

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP P71727
A	-18	GLY	-	expression tag	UNP P71727
A	-17	SER	-	expression tag	UNP P71727
A	-16	SER	-	expression tag	UNP P71727
A	-15	HIS	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P71727
A	-13	HIS	-	expression tag	UNP P71727
A	-12	HIS	-	expression tag	UNP P71727
A	-11	HIS	-	expression tag	UNP P71727
A	-10	HIS	-	expression tag	UNP P71727
A	-9	SER	-	expression tag	UNP P71727
A	-8	SER	-	expression tag	UNP P71727
A	-7	GLY	-	expression tag	UNP P71727
A	-6	LEU	-	expression tag	UNP P71727
A	-5	VAL	-	expression tag	UNP P71727
A	-4	PRO	-	expression tag	UNP P71727
A	-3	ARG	-	expression tag	UNP P71727
A	-2	GLY	-	expression tag	UNP P71727
A	-1	SER	-	expression tag	UNP P71727
A	0	HIS	-	expression tag	UNP P71727
B	-19	MSE	-	expression tag	UNP P71727
B	-18	GLY	-	expression tag	UNP P71727
B	-17	SER	-	expression tag	UNP P71727
B	-16	SER	-	expression tag	UNP P71727
B	-15	HIS	-	expression tag	UNP P71727
B	-14	HIS	-	expression tag	UNP P71727
B	-13	HIS	-	expression tag	UNP P71727
B	-12	HIS	-	expression tag	UNP P71727
B	-11	HIS	-	expression tag	UNP P71727
B	-10	HIS	-	expression tag	UNP P71727
B	-9	SER	-	expression tag	UNP P71727
B	-8	SER	-	expression tag	UNP P71727
B	-7	GLY	-	expression tag	UNP P71727
B	-6	LEU	-	expression tag	UNP P71727
B	-5	VAL	-	expression tag	UNP P71727
B	-4	PRO	-	expression tag	UNP P71727
B	-3	ARG	-	expression tag	UNP P71727
B	-2	GLY	-	expression tag	UNP P71727
B	-1	SER	-	expression tag	UNP P71727
B	0	HIS	-	expression tag	UNP P71727
C	-19	MSE	-	expression tag	UNP P71727
C	-18	GLY	-	expression tag	UNP P71727
C	-17	SER	-	expression tag	UNP P71727
C	-16	SER	-	expression tag	UNP P71727
C	-15	HIS	-	expression tag	UNP P71727
C	-14	HIS	-	expression tag	UNP P71727
C	-13	HIS	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP P71727
C	-11	HIS	-	expression tag	UNP P71727
C	-10	HIS	-	expression tag	UNP P71727
C	-9	SER	-	expression tag	UNP P71727
C	-8	SER	-	expression tag	UNP P71727
C	-7	GLY	-	expression tag	UNP P71727
C	-6	LEU	-	expression tag	UNP P71727
C	-5	VAL	-	expression tag	UNP P71727
C	-4	PRO	-	expression tag	UNP P71727
C	-3	ARG	-	expression tag	UNP P71727
C	-2	GLY	-	expression tag	UNP P71727
C	-1	SER	-	expression tag	UNP P71727
C	0	HIS	-	expression tag	UNP P71727
D	-19	MSE	-	expression tag	UNP P71727
D	-18	GLY	-	expression tag	UNP P71727
D	-17	SER	-	expression tag	UNP P71727
D	-16	SER	-	expression tag	UNP P71727
D	-15	HIS	-	expression tag	UNP P71727
D	-14	HIS	-	expression tag	UNP P71727
D	-13	HIS	-	expression tag	UNP P71727
D	-12	HIS	-	expression tag	UNP P71727
D	-11	HIS	-	expression tag	UNP P71727
D	-10	HIS	-	expression tag	UNP P71727
D	-9	SER	-	expression tag	UNP P71727
D	-8	SER	-	expression tag	UNP P71727
D	-7	GLY	-	expression tag	UNP P71727
D	-6	LEU	-	expression tag	UNP P71727
D	-5	VAL	-	expression tag	UNP P71727
D	-4	PRO	-	expression tag	UNP P71727
D	-3	ARG	-	expression tag	UNP P71727
D	-2	GLY	-	expression tag	UNP P71727
D	-1	SER	-	expression tag	UNP P71727
D	0	HIS	-	expression tag	UNP P71727
E	-19	MSE	-	expression tag	UNP P71727
E	-18	GLY	-	expression tag	UNP P71727
E	-17	SER	-	expression tag	UNP P71727
E	-16	SER	-	expression tag	UNP P71727
E	-15	HIS	-	expression tag	UNP P71727
E	-14	HIS	-	expression tag	UNP P71727
E	-13	HIS	-	expression tag	UNP P71727
E	-12	HIS	-	expression tag	UNP P71727
E	-11	HIS	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P71727
E	-9	SER	-	expression tag	UNP P71727
E	-8	SER	-	expression tag	UNP P71727
E	-7	GLY	-	expression tag	UNP P71727
E	-6	LEU	-	expression tag	UNP P71727
E	-5	VAL	-	expression tag	UNP P71727
E	-4	PRO	-	expression tag	UNP P71727
E	-3	ARG	-	expression tag	UNP P71727
E	-2	GLY	-	expression tag	UNP P71727
E	-1	SER	-	expression tag	UNP P71727
E	0	HIS	-	expression tag	UNP P71727
F	-19	MSE	-	expression tag	UNP P71727
F	-18	GLY	-	expression tag	UNP P71727
F	-17	SER	-	expression tag	UNP P71727
F	-16	SER	-	expression tag	UNP P71727
F	-15	HIS	-	expression tag	UNP P71727
F	-14	HIS	-	expression tag	UNP P71727
F	-13	HIS	-	expression tag	UNP P71727
F	-12	HIS	-	expression tag	UNP P71727
F	-11	HIS	-	expression tag	UNP P71727
F	-10	HIS	-	expression tag	UNP P71727
F	-9	SER	-	expression tag	UNP P71727
F	-8	SER	-	expression tag	UNP P71727
F	-7	GLY	-	expression tag	UNP P71727
F	-6	LEU	-	expression tag	UNP P71727
F	-5	VAL	-	expression tag	UNP P71727
F	-4	PRO	-	expression tag	UNP P71727
F	-3	ARG	-	expression tag	UNP P71727
F	-2	GLY	-	expression tag	UNP P71727
F	-1	SER	-	expression tag	UNP P71727
F	0	HIS	-	expression tag	UNP P71727
G	-19	MSE	-	expression tag	UNP P71727
G	-18	GLY	-	expression tag	UNP P71727
G	-17	SER	-	expression tag	UNP P71727
G	-16	SER	-	expression tag	UNP P71727
G	-15	HIS	-	expression tag	UNP P71727
G	-14	HIS	-	expression tag	UNP P71727
G	-13	HIS	-	expression tag	UNP P71727
G	-12	HIS	-	expression tag	UNP P71727
G	-11	HIS	-	expression tag	UNP P71727
G	-10	HIS	-	expression tag	UNP P71727
G	-9	SER	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP P71727
G	-7	GLY	-	expression tag	UNP P71727
G	-6	LEU	-	expression tag	UNP P71727
G	-5	VAL	-	expression tag	UNP P71727
G	-4	PRO	-	expression tag	UNP P71727
G	-3	ARG	-	expression tag	UNP P71727
G	-2	GLY	-	expression tag	UNP P71727
G	-1	SER	-	expression tag	UNP P71727
G	0	HIS	-	expression tag	UNP P71727
H	-19	MSE	-	expression tag	UNP P71727
H	-18	GLY	-	expression tag	UNP P71727
H	-17	SER	-	expression tag	UNP P71727
H	-16	SER	-	expression tag	UNP P71727
H	-15	HIS	-	expression tag	UNP P71727
H	-14	HIS	-	expression tag	UNP P71727
H	-13	HIS	-	expression tag	UNP P71727
H	-12	HIS	-	expression tag	UNP P71727
H	-11	HIS	-	expression tag	UNP P71727
H	-10	HIS	-	expression tag	UNP P71727
H	-9	SER	-	expression tag	UNP P71727
H	-8	SER	-	expression tag	UNP P71727
H	-7	GLY	-	expression tag	UNP P71727
H	-6	LEU	-	expression tag	UNP P71727
H	-5	VAL	-	expression tag	UNP P71727
H	-4	PRO	-	expression tag	UNP P71727
H	-3	ARG	-	expression tag	UNP P71727
H	-2	GLY	-	expression tag	UNP P71727
H	-1	SER	-	expression tag	UNP P71727
H	0	HIS	-	expression tag	UNP P71727
I	-19	MSE	-	expression tag	UNP P71727
I	-18	GLY	-	expression tag	UNP P71727
I	-17	SER	-	expression tag	UNP P71727
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I	-11	HIS	-	expression tag	UNP P71727
I	-10	HIS	-	expression tag	UNP P71727
I	-9	SER	-	expression tag	UNP P71727
I	-8	SER	-	expression tag	UNP P71727
I	-7	GLY	-	expression tag	UNP P71727

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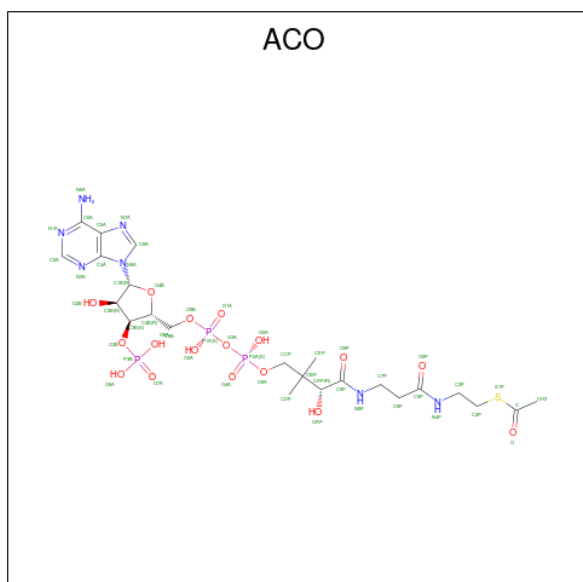
Chain	Residue	Modelled	Actual	Comment	Reference
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I	-4	PRO	-	expression tag	UNP P71727
I	-3	ARG	-	expression tag	UNP P71727
I	-2	GLY	-	expression tag	UNP P71727
I	-1	SER	-	expression tag	UNP P71727
I	0	HIS	-	expression tag	UNP P71727
J	-19	MSE	-	expression tag	UNP P71727
J	-18	GLY	-	expression tag	UNP P71727
J	-17	SER	-	expression tag	UNP P71727
J	-16	SER	-	expression tag	UNP P71727
J	-15	HIS	-	expression tag	UNP P71727
J	-14	HIS	-	expression tag	UNP P71727
J	-13	HIS	-	expression tag	UNP P71727
J	-12	HIS	-	expression tag	UNP P71727
J	-11	HIS	-	expression tag	UNP P71727
J	-10	HIS	-	expression tag	UNP P71727
J	-9	SER	-	expression tag	UNP P71727
J	-8	SER	-	expression tag	UNP P71727
J	-7	GLY	-	expression tag	UNP P71727
J	-6	LEU	-	expression tag	UNP P71727
J	-5	VAL	-	expression tag	UNP P71727
J	-4	PRO	-	expression tag	UNP P71727
J	-3	ARG	-	expression tag	UNP P71727
J	-2	GLY	-	expression tag	UNP P71727
J	-1	SER	-	expression tag	UNP P71727
J	0	HIS	-	expression tag	UNP P71727
K	-19	MSE	-	expression tag	UNP P71727
K	-18	GLY	-	expression tag	UNP P71727
K	-17	SER	-	expression tag	UNP P71727
K	-16	SER	-	expression tag	UNP P71727
K	-15	HIS	-	expression tag	UNP P71727
K	-14	HIS	-	expression tag	UNP P71727
K	-13	HIS	-	expression tag	UNP P71727
K	-12	HIS	-	expression tag	UNP P71727
K	-11	HIS	-	expression tag	UNP P71727
K	-10	HIS	-	expression tag	UNP P71727
K	-9	SER	-	expression tag	UNP P71727
K	-8	SER	-	expression tag	UNP P71727
K	-7	GLY	-	expression tag	UNP P71727
K	-6	LEU	-	expression tag	UNP P71727
K	-5	VAL	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P71727
K	-3	ARG	-	expression tag	UNP P71727
K	-2	GLY	-	expression tag	UNP P71727
K	-1	SER	-	expression tag	UNP P71727
K	0	HIS	-	expression tag	UNP P71727
L	-19	MSE	-	expression tag	UNP P71727
L	-18	GLY	-	expression tag	UNP P71727
L	-17	SER	-	expression tag	UNP P71727
L	-16	SER	-	expression tag	UNP P71727
L	-15	HIS	-	expression tag	UNP P71727
L	-14	HIS	-	expression tag	UNP P71727
L	-13	HIS	-	expression tag	UNP P71727
L	-12	HIS	-	expression tag	UNP P71727
L	-11	HIS	-	expression tag	UNP P71727
L	-10	HIS	-	expression tag	UNP P71727
L	-9	SER	-	expression tag	UNP P71727
L	-8	SER	-	expression tag	UNP P71727
L	-7	GLY	-	expression tag	UNP P71727
L	-6	LEU	-	expression tag	UNP P71727
L	-5	VAL	-	expression tag	UNP P71727
L	-4	PRO	-	expression tag	UNP P71727
L	-3	ARG	-	expression tag	UNP P71727
L	-2	GLY	-	expression tag	UNP P71727
L	-1	SER	-	expression tag	UNP P71727
L	0	HIS	-	expression tag	UNP P71727

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	74	Total	O	0	0
			74	74		
3	C	54	Total	O	0	0
			54	54		
3	D	51	Total	O	0	0
			51	51		
3	E	47	Total	O	0	0
			47	47		
3	F	48	Total	O	0	0
			48	48		
3	G	31	Total	O	0	0
			31	31		
3	H	39	Total	O	0	0
			39	39		

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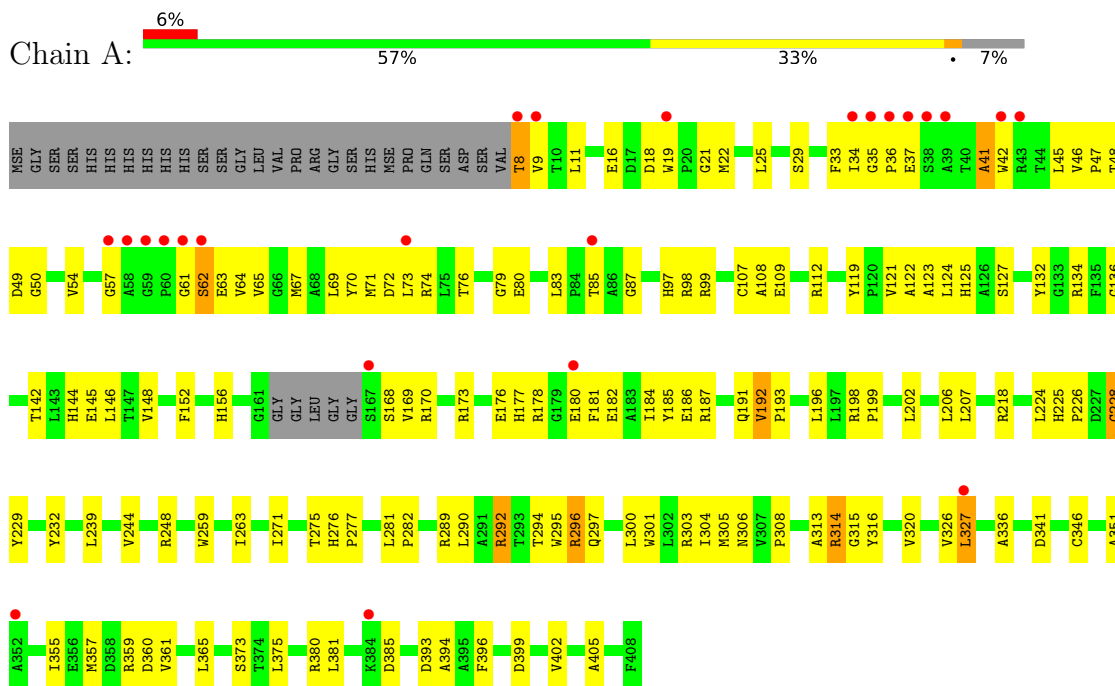
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	17	Total 17	O 17	0	0
3	J	9	Total 9	O 9	0	0
3	K	29	Total 29	O 29	0	0
3	L	38	Total 38	O 38	0	0

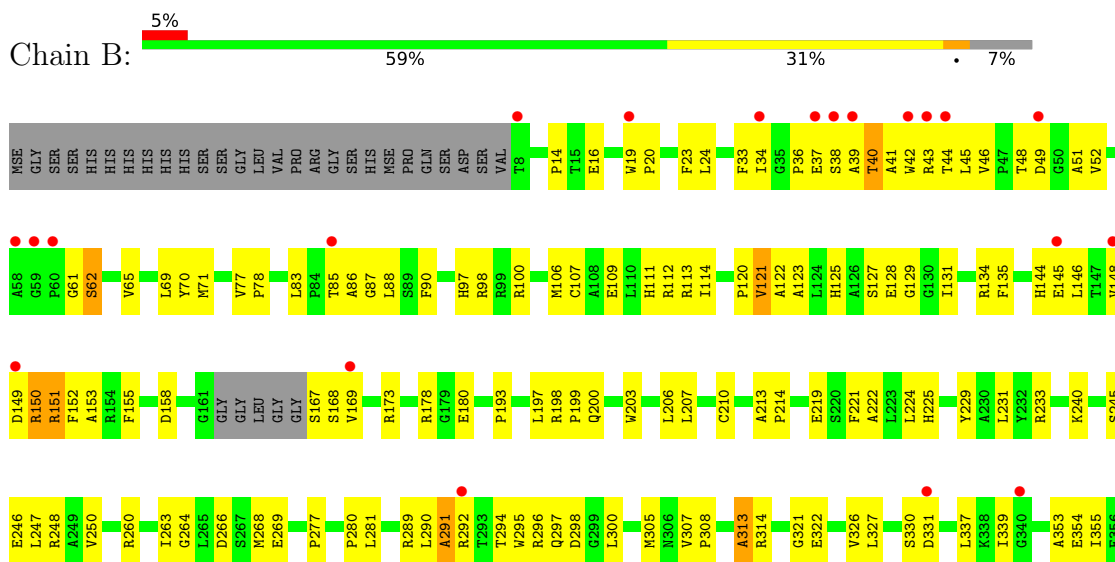
3 Residue-property plots

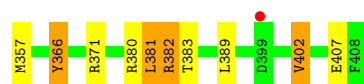
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

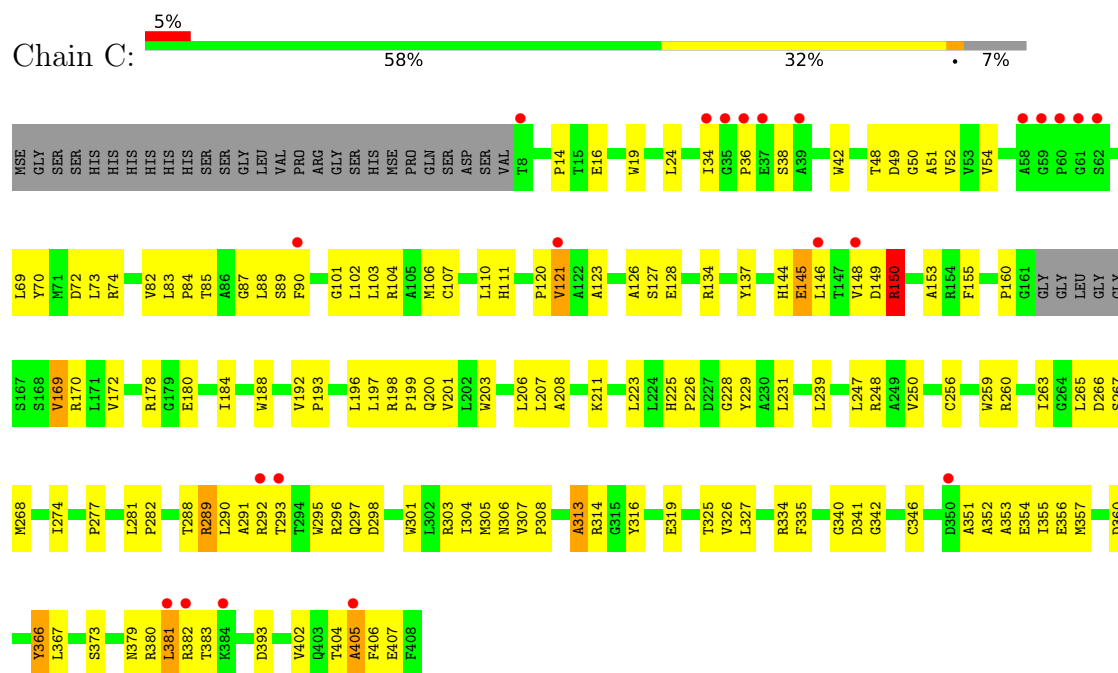


• Molecule 1: Enhanced intracellular survival protein

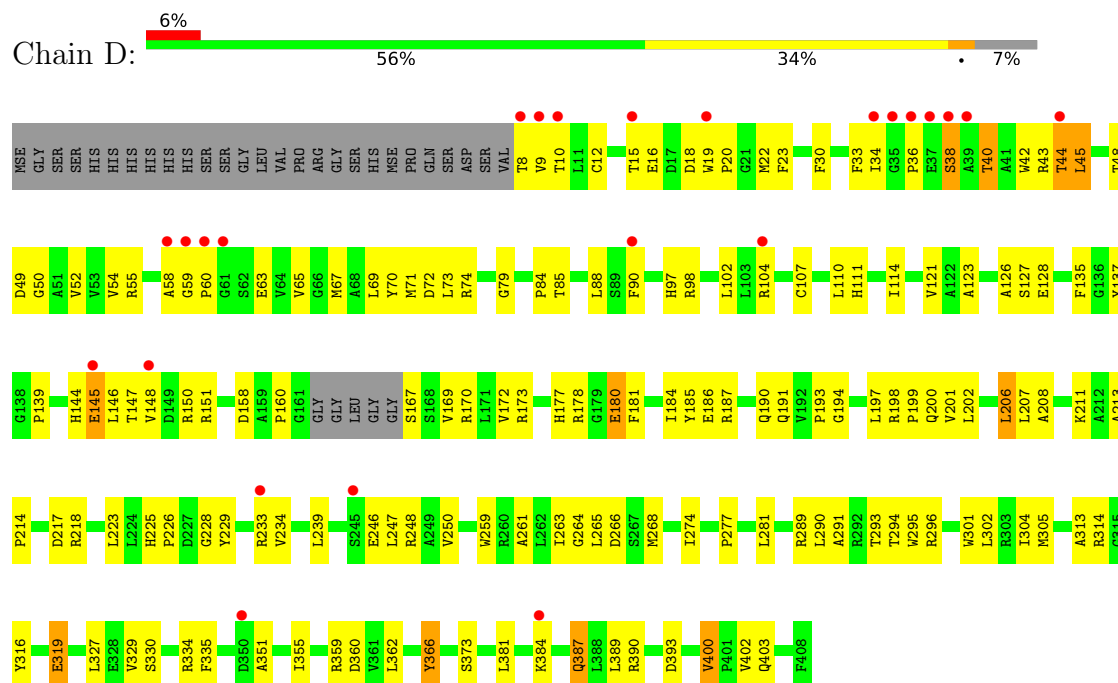




- Molecule 1: Enhanced intracellular survival protein

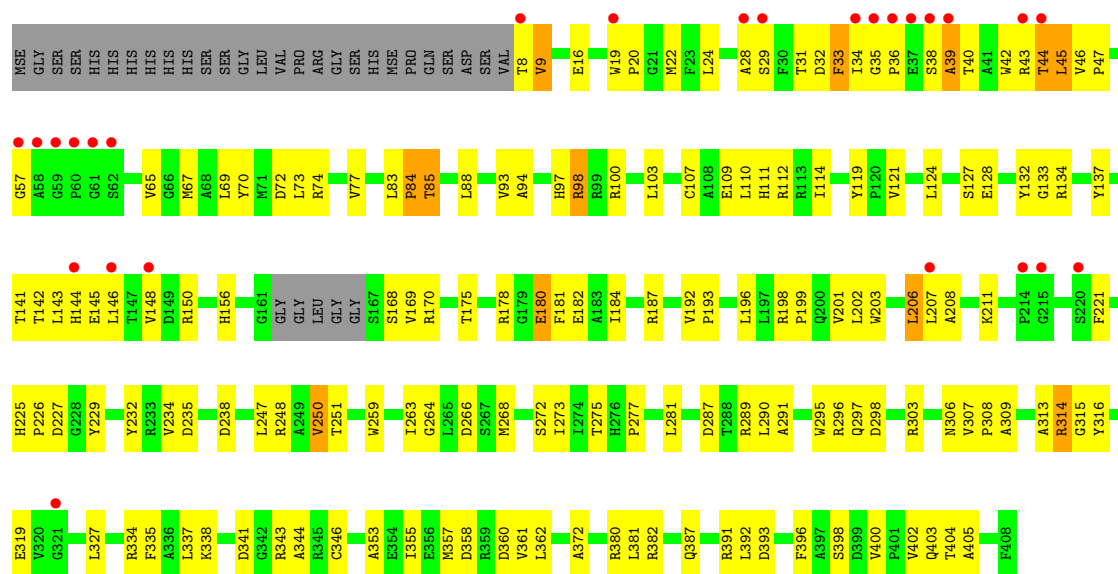


- Molecule 1: Enhanced intracellular survival protein

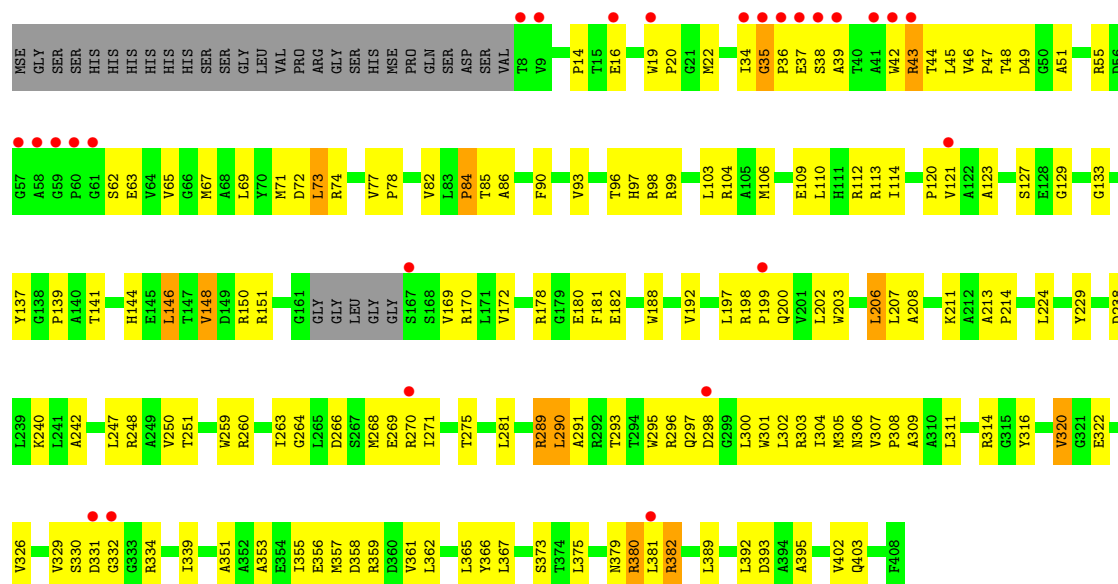


- Molecule 1: Enhanced intracellular survival protein

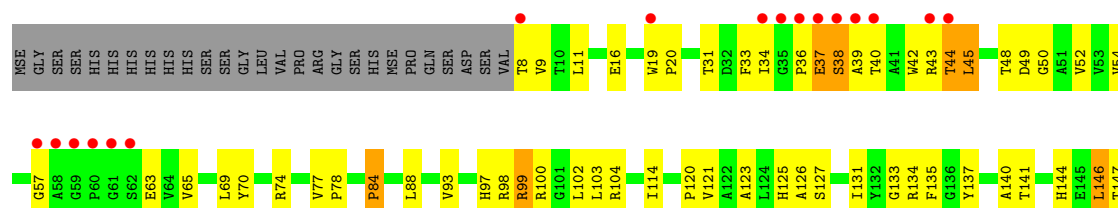


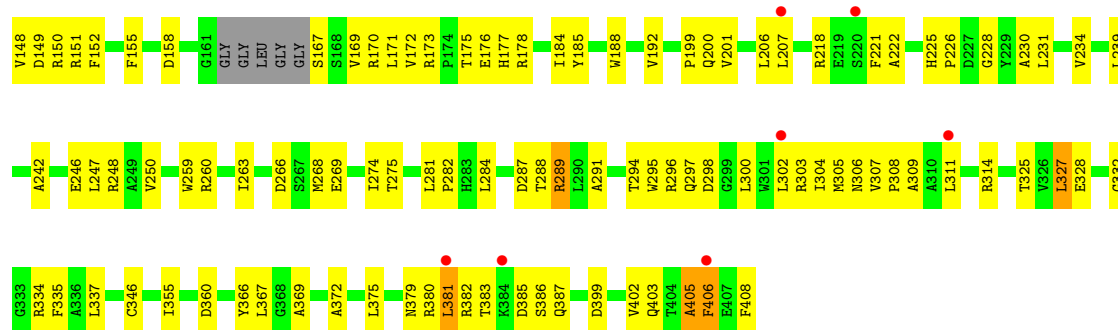


• Molecule 1: Enhanced intracellular survival protein

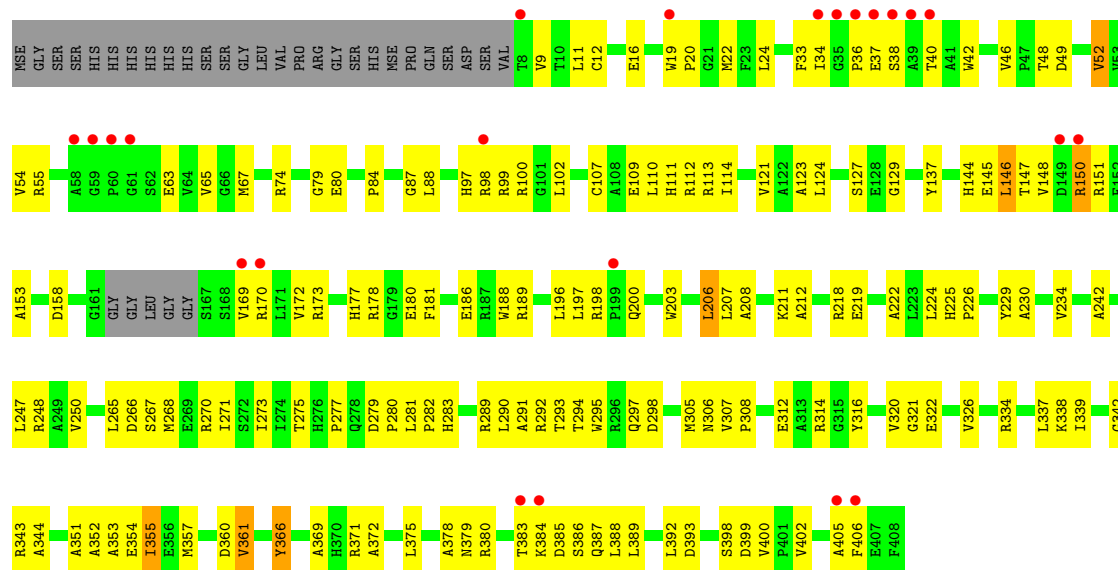


• Molecule 1: Enhanced intracellular survival protein

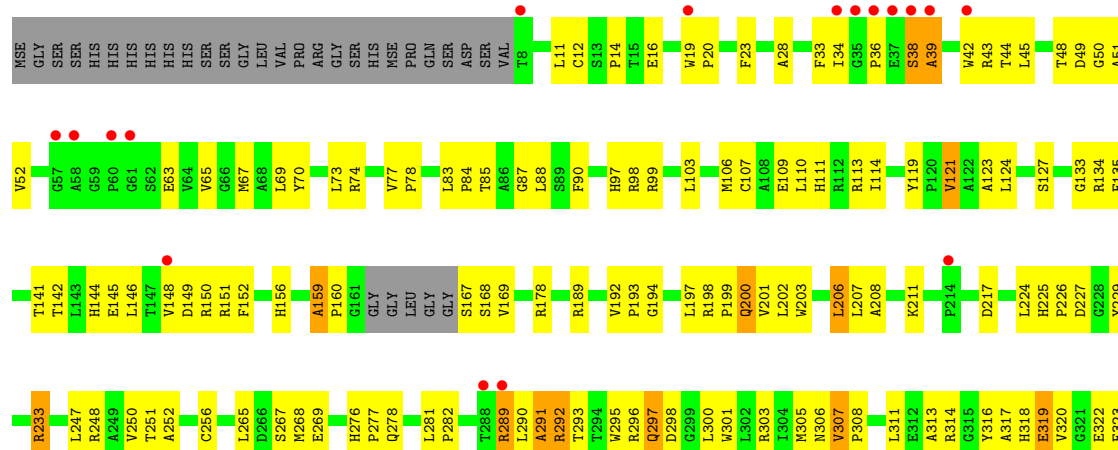


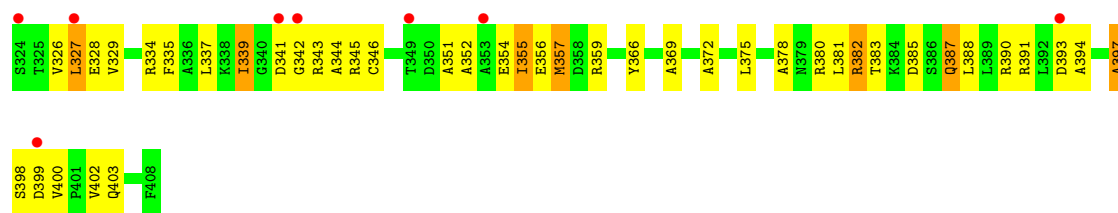


• Molecule 1: Enhanced intracellular survival protein

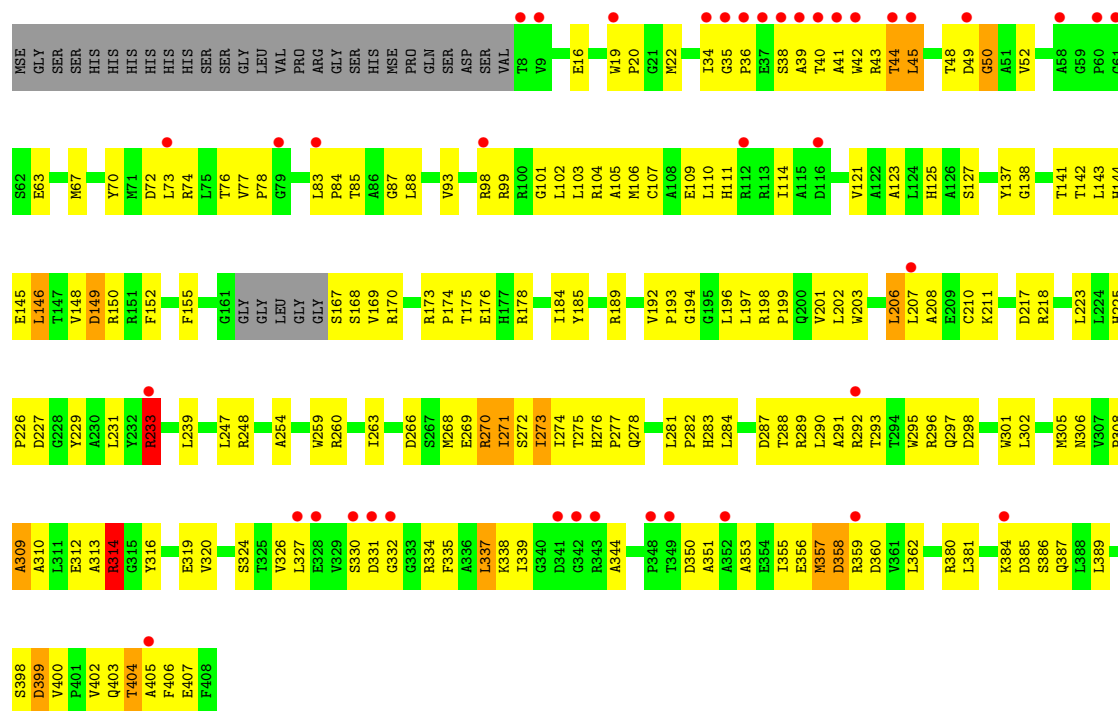


• Molecule 1: Enhanced intracellular survival protein

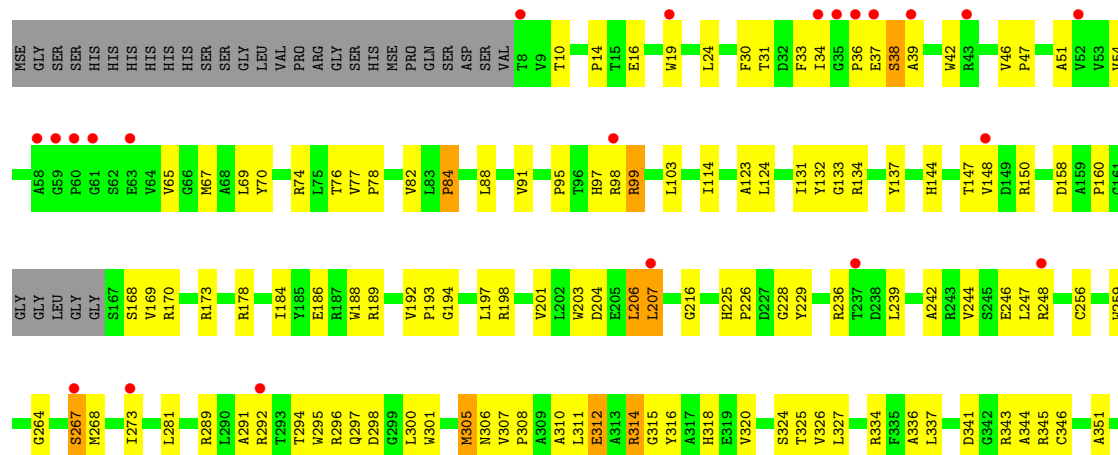


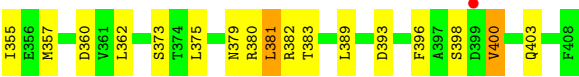


● Molecule 1: Enhanced intracellular survival protein

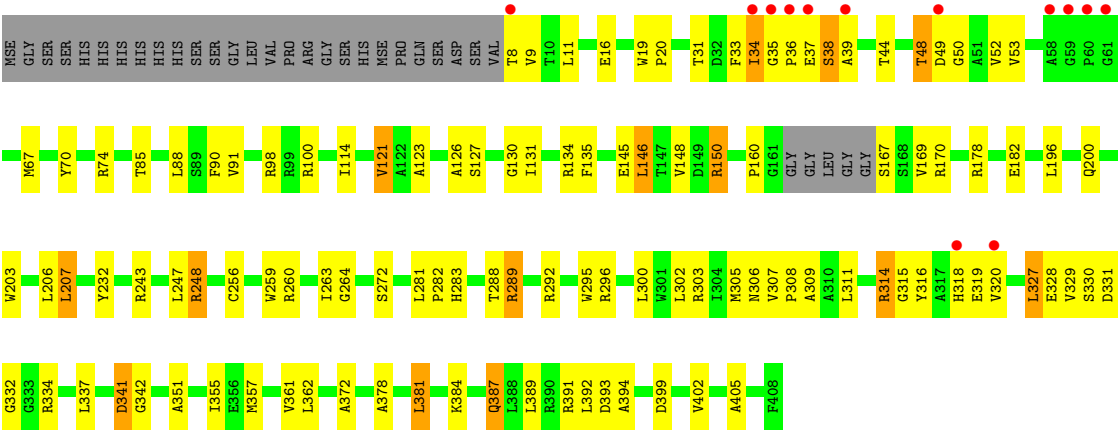


● Molecule 1: Enhanced intracellular survival protein





● Molecule 1: Enhanced intracellular survival protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.13Å 150.19Å 184.38Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	29.94 – 2.80 29.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.4 (29.94-2.80) 95.3 (29.94-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.87 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.192 , 0.248 0.219 , 0.217	Depositor DCC
R_{free} test set	13782 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	37731	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: ACO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/3115	0.97	10/4226 (0.2%)
1	B	0.53	0/3115	0.95	11/4226 (0.3%)
1	C	0.54	0/3115	0.94	13/4226 (0.3%)
1	D	0.55	0/3115	0.97	12/4226 (0.3%)
1	E	0.53	0/3115	0.95	9/4226 (0.2%)
1	F	0.55	0/3115	0.97	8/4226 (0.2%)
1	G	0.52	0/3115	0.94	8/4226 (0.2%)
1	H	0.51	0/3115	0.88	5/4226 (0.1%)
1	I	0.46	0/3115	0.94	13/4226 (0.3%)
1	J	0.49	0/3115	0.93	8/4226 (0.2%)
1	K	0.49	0/3115	0.90	7/4226 (0.2%)
1	L	0.54	0/3115	0.92	4/4226 (0.1%)
All	All	0.53	0/37380	0.94	108/50712 (0.2%)

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	C	0	1
1	F	0	1
1	J	0	2
All	All	0	5

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	THR	N-CA-C	10.08	122.34	111.36
1	A	168	SER	N-CA-C	-9.81	100.23	112.88
1	E	168	SER	N-CA-C	-9.57	101.29	113.16
1	L	35	GLY	N-CA-C	9.42	127.18	115.22
1	E	44	THR	N-CA-C	8.54	120.67	111.36
1	I	289	ARG	N-CA-C	8.11	120.12	111.28
1	L	37	GLU	N-CA-C	7.99	119.77	111.14
1	B	40	THR	N-CA-C	7.91	119.90	111.28
1	B	121	VAL	N-CA-C	7.91	118.78	108.35
1	D	12	CYS	N-CA-C	7.70	119.36	108.74
1	A	33	PHE	N-CA-C	7.69	121.55	110.10
1	F	366	TYR	N-CA-C	7.68	119.65	111.28
1	B	33	PHE	N-CA-C	7.65	121.32	110.23
1	G	44	THR	N-CA-C	7.51	119.55	111.36
1	J	44	THR	N-CA-C	7.41	119.35	111.28
1	I	399	ASP	N-CA-C	-7.38	103.23	111.28
1	L	38	SER	N-CA-C	7.25	119.26	111.36
1	D	40	THR	CA-C-N	7.21	129.81	120.44
1	D	40	THR	C-N-CA	7.21	129.81	120.44
1	F	38	SER	N-CA-C	7.07	119.07	111.36
1	G	405	ALA	N-CA-C	7.00	118.56	111.07
1	F	43	ARG	N-CA-C	6.93	118.91	111.36
1	A	292	ARG	N-CA-C	6.91	120.32	109.96
1	C	406	PHE	N-CA-C	6.87	120.19	110.23
1	G	38	SER	N-CA-C	6.81	118.79	111.36
1	J	404	THR	N-CA-C	6.78	120.06	110.23
1	E	45	LEU	N-CA-C	6.77	121.70	113.17
1	J	168	SER	N-CA-C	-6.72	105.23	113.50
1	K	400	VAL	N-CA-C	-6.64	100.66	107.89
1	B	168	SER	N-CA-C	-6.57	104.50	113.30
1	D	40	THR	N-CA-C	6.51	118.46	111.36
1	L	48	THR	N-CA-C	-6.49	101.09	110.24
1	C	382	ARG	N-CA-C	6.36	119.52	108.76
1	B	382	ARG	N-CA-C	6.29	119.38	108.76
1	K	310	ALA	N-CA-C	6.28	118.12	111.28
1	J	399	ASP	N-CA-C	-6.21	104.52	111.28
1	A	327	LEU	N-CA-C	6.20	118.63	108.52
1	D	400	VAL	N-CA-C	-6.18	100.76	108.05
1	E	29	SER	N-CA-C	6.17	118.08	111.36
1	H	40	THR	CA-C-N	6.15	128.99	120.63
1	H	40	THR	C-N-CA	6.15	128.99	120.63
1	A	314	ARG	N-CA-C	6.10	119.31	110.28
1	I	200	GLN	N-CA-C	-6.09	104.64	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	84	PRO	N-CA-C	-6.09	101.65	111.03
1	G	84	PRO	N-CA-C	-6.04	101.72	111.03
1	G	45	LEU	N-CA-C	6.04	121.45	112.94
1	H	40	THR	N-CA-C	6.00	117.82	111.28
1	E	85	THR	N-CA-C	5.98	118.87	108.76
1	I	39	ALA	N-CA-C	5.97	117.79	111.28
1	I	354	GLU	N-CA-C	-5.91	105.90	113.23
1	I	307	VAL	CB-CA-C	-5.89	108.11	113.70
1	I	168	SER	N-CA-C	-5.88	106.06	113.18
1	H	366	TYR	N-CA-C	5.87	118.43	111.33
1	A	41	ALA	N-CA-C	5.83	117.30	111.07
1	C	192	VAL	CA-C-N	-5.77	113.59	119.83
1	C	192	VAL	C-N-CA	-5.77	113.59	119.83
1	J	50	GLY	N-CA-C	-5.68	105.72	115.61
1	A	399	ASP	N-CA-C	-5.63	104.83	110.97
1	F	382	ARG	N-CA-C	5.63	118.64	109.24
1	F	84	PRO	N-CA-C	-5.63	102.36	111.03
1	C	289	ARG	N-CA-C	5.62	119.24	112.38
1	B	402	VAL	N-CA-C	5.62	116.83	109.58
1	F	289	ARG	N-CA-C	5.62	117.41	111.28
1	D	45	LEU	N-CA-C	5.62	120.83	113.30
1	D	313	ALA	N-CA-C	5.59	117.38	111.28
1	C	313	ALA	N-CA-C	5.59	117.45	111.36
1	F	358	ASP	N-CA-C	-5.58	103.02	110.55
1	K	168	SER	N-CA-C	-5.55	106.28	113.16
1	E	38	SER	N-CA-C	5.53	117.31	111.28
1	J	149	ASP	N-CA-C	-5.53	100.11	108.67
1	D	145	GLU	N-CA-C	-5.51	101.00	109.76
1	B	291	ALA	N-CA-C	-5.48	103.06	110.68
1	G	406	PHE	N-CA-C	5.46	116.44	108.14
1	C	172	VAL	N-CA-C	5.46	117.95	108.95
1	I	382	ARG	N-CA-C	5.45	117.78	108.90
1	K	312	GLU	N-CA-C	5.36	117.20	111.36
1	C	405	ALA	N-CA-C	-5.35	101.51	109.96
1	E	39	ALA	N-CA-C	5.35	117.80	111.33
1	E	84	PRO	N-CA-C	-5.35	102.79	111.03
1	D	384	LYS	N-CA-C	-5.33	106.55	113.16
1	D	79	GLY	N-CA-C	-5.32	107.45	115.32
1	K	38	SER	N-CA-C	5.32	117.08	111.28
1	E	132	TYR	N-CA-C	5.30	119.59	113.18
1	I	159	ALA	CA-C-N	5.28	125.28	119.90
1	I	159	ALA	C-N-CA	5.28	125.28	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ARG	N-CA-C	5.24	117.00	111.28
1	I	291	ALA	N-CA-C	-5.22	101.79	109.62
1	A	192	VAL	CA-C-N	-5.21	114.40	119.76
1	A	192	VAL	C-N-CA	-5.21	114.40	119.76
1	C	38	SER	N-CA-C	5.21	116.95	111.28
1	B	366	TYR	N-CA-C	5.19	117.61	111.33
1	H	361	VAL	N-CA-C	-5.15	105.52	110.72
1	I	329	VAL	N-CA-C	-5.13	100.99	108.17
1	C	149	ASP	N-CA-C	-5.13	102.46	110.10
1	C	381	LEU	N-CA-C	-5.13	100.54	108.90
1	A	228	GLY	N-CA-C	5.12	118.06	110.63
1	J	270	ARG	N-CA-C	5.12	117.60	109.50
1	B	150	ARG	N-CA-C	5.09	116.83	111.28
1	D	366	TYR	N-CA-C	5.08	117.48	111.33
1	G	99	ARG	N-CA-C	5.06	118.57	111.74
1	I	292	ARG	N-CA-C	5.06	117.64	110.50
1	C	121	VAL	N-CA-C	5.05	115.45	108.23
1	G	37	GLU	N-CA-C	5.04	116.85	111.36
1	K	99	ARG	N-CA-C	5.03	118.53	111.74
1	C	366	TYR	N-CA-C	5.01	116.74	111.28
1	F	35	GLY	O-C-N	5.01	122.87	121.07
1	B	313	ALA	N-CA-C	5.00	116.81	111.36
1	J	45	LEU	N-CA-C	5.00	120.76	114.31

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ARG	Sidechain
1	C	150	ARG	Sidechain
1	F	380	ARG	Sidechain
1	J	233	ARG	Sidechain
1	J	314	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3053	0	3020	164	0
1	B	3053	0	3020	177	0
1	C	3053	0	3020	201	0
1	D	3053	0	3020	220	0
1	E	3053	0	3020	208	2
1	F	3053	0	3020	240	0
1	G	3053	0	3020	190	0
1	H	3053	0	3020	246	0
1	I	3053	0	3020	255	0
1	J	3053	0	3020	227	1
1	K	3053	0	3020	170	1
1	L	3053	0	3018	88	2
2	A	51	0	34	6	0
2	B	51	0	33	4	0
2	C	51	0	34	12	0
2	D	51	0	33	2	0
2	E	51	0	34	8	0
2	F	51	0	33	5	0
2	G	51	0	33	6	0
2	H	51	0	33	2	0
2	I	51	0	34	7	0
2	J	51	0	34	3	0
2	K	51	0	34	10	0
2	L	51	0	33	5	0
3	A	46	0	0	2	0
3	B	74	0	0	6	0
3	C	54	0	0	6	0
3	D	51	0	0	5	0
3	E	47	0	0	2	0
3	F	48	0	0	2	0
3	G	31	0	0	3	0
3	H	39	0	0	4	0
3	I	17	0	0	1	0
3	J	9	0	0	6	0
3	K	29	0	0	4	0
3	L	38	0	0	3	0
All	All	37731	0	36640	2250	3

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 30.

All (2250) 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:F:22:MSE:HE2	1:F:42:TRP:CH2	1.32	1.64
1:C:357:MSE:HE2	1:C:381:LEU:CD1	1.21	1.57
1:F:357:MSE:HE2	1:F:381:LEU:CD1	1.27	1.57
1:D:148:VAL:CG2	1:D:291:ALA:HA	1.31	1.55
1:H:354:GLU:HA	1:H:384:LYS:NZ	1.18	1.51
1:F:22:MSE:CE	1:F:42:TRP:CH2	1.88	1.49
1:I:357:MSE:CE	1:I:381:LEU:HD13	1.39	1.48
1:C:148:VAL:CG2	1:C:291:ALA:HA	1.44	1.48
1:F:144:HIS:NE2	1:F:296:ARG:NH1	1.66	1.44
1:F:42:TRP:CE2	1:F:69:LEU:CD2	2.02	1.41
1:C:148:VAL:HG22	1:C:291:ALA:CA	1.51	1.40
1:D:148:VAL:HG22	1:D:291:ALA:CA	1.50	1.39
1:F:42:TRP:NE1	1:F:69:LEU:HD22	1.38	1.38
1:E:148:VAL:CG2	1:E:291:ALA:HA	1.56	1.35
1:K:244:VAL:CG2	1:K:273:ILE:HD11	1.58	1.34
1:F:42:TRP:CZ2	1:F:69:LEU:HD23	1.61	1.33
1:C:357:MSE:CE	1:C:381:LEU:CD1	2.06	1.33
1:I:357:MSE:HE2	1:I:381:LEU:CD1	1.58	1.31
1:H:180:GLU:OE2	1:H:224:LEU:HD21	1.20	1.29
1:G:40:THR:O	1:G:44:THR:HG22	1.30	1.28
1:B:85:THR:HG23	1:B:121:VAL:O	1.18	1.28
1:I:44:THR:O	1:I:45:LEU:HD23	1.31	1.28
1:K:244:VAL:HG21	1:K:273:ILE:CD1	1.63	1.28
1:K:244:VAL:HB	1:K:273:ILE:CG1	1.63	1.27
1:I:357:MSE:CE	1:I:381:LEU:CD1	2.10	1.26
1:A:180:GLU:OE2	1:A:224:LEU:HD21	1.21	1.26
1:C:52:VAL:CG2	1:C:110:LEU:HD11	1.67	1.24
1:E:148:VAL:HG22	1:E:291:ALA:CA	1.67	1.23
1:H:34:ILE:HB	1:H:37:GLU:CG	1.66	1.23
1:H:354:GLU:CA	1:H:384:LYS:NZ	2.03	1.22
1:H:169:VAL:HG13	1:H:224:LEU:O	1.12	1.22
1:K:244:VAL:CB	1:K:273:ILE:HG12	1.69	1.21
1:G:150:ARG:HD3	1:G:268:MSE:O	1.34	1.21
1:H:169:VAL:HG13	1:H:224:LEU:C	1.62	1.21
1:G:11:LEU:HD11	1:G:52:VAL:CG2	1.69	1.21
1:C:106:MSE:O	1:C:110:LEU:HD13	1.37	1.20
1:I:34:ILE:HG22	1:I:36:PRO:HD2	1.18	1.18
1:C:52:VAL:HG21	1:C:110:LEU:CD1	1.72	1.18
1:D:150:ARG:NH2	1:D:266:ASP:HA	1.59	1.18
1:B:180:GLU:OE2	1:B:224:LEU:HD21	1.44	1.16
1:F:22:MSE:CE	1:F:42:TRP:CZ2	2.28	1.16
1:F:357:MSE:CE	1:F:381:LEU:CD1	2.24	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LEU:HD12	1:E:275:THR:CG2	1.76	1.15
1:E:327:LEU:HD11	1:E:357:MSE:HE3	1.18	1.15
1:K:244:VAL:HG11	1:K:273:ILE:HD13	1.24	1.15
1:D:34:ILE:HG22	1:D:36:PRO:HD2	1.26	1.14
1:D:40:THR:O	1:D:44:THR:HG22	1.44	1.14
1:L:34:ILE:HG22	1:L:36:PRO:HD2	1.28	1.14
1:B:150:ARG:HD3	1:B:268:MSE:O	1.47	1.14
1:H:34:ILE:HB	1:H:37:GLU:HG2	1.14	1.14
1:G:11:LEU:HD11	1:G:52:VAL:HG21	1.27	1.13
1:H:385:ASP:OD2	1:H:387:GLN:HG2	1.45	1.13
1:I:148:VAL:HG22	1:I:291:ALA:HA	1.25	1.13
1:G:222:ALA:HB2	1:G:231:LEU:HD23	1.27	1.13
1:C:357:MSE:CE	1:C:381:LEU:HD13	1.73	1.13
1:I:323:PHE:HB2	1:I:391:ARG:NH1	1.64	1.12
1:F:121:VAL:HG12	1:F:304:ILE:HA	1.30	1.12
1:F:22:MSE:HE1	1:F:42:TRP:CZ2	1.84	1.12
1:C:106:MSE:O	1:C:110:LEU:CD1	1.98	1.12
1:E:146:LEU:CD1	1:E:275:THR:HG21	1.80	1.12
1:D:148:VAL:HG13	1:D:290:LEU:C	1.75	1.11
1:C:145:GLU:CB	1:C:295:TRP:HB3	1.81	1.11
1:I:149:ASP:OD2	1:I:152:PHE:HE1	1.30	1.11
1:C:357:MSE:HE2	1:C:381:LEU:HD11	1.29	1.11
1:D:146:LEU:HD21	1:D:148:VAL:CG2	1.80	1.10
1:F:121:VAL:HA	1:F:305:MSE:HG2	1.32	1.10
1:I:148:VAL:CG2	1:I:291:ALA:HA	1.79	1.10
1:J:203:TRP:O	1:J:207:LEU:HD13	1.51	1.10
1:C:357:MSE:HE2	1:C:381:LEU:CG	1.82	1.10
1:D:146:LEU:HD21	1:D:148:VAL:HG23	1.13	1.10
1:H:178:ARG:NH1	1:H:207:LEU:CD1	2.15	1.10
1:I:148:VAL:HG13	1:I:290:LEU:O	1.51	1.10
1:K:327:LEU:HD11	1:K:357:MSE:HE3	1.35	1.09
1:C:145:GLU:HB2	1:C:295:TRP:HB3	1.22	1.09
1:D:33:PHE:HE1	1:D:38:SER:OG	1.36	1.09
1:D:146:LEU:CD2	1:D:148:VAL:HG23	1.81	1.08
1:E:44:THR:HG21	1:E:201:VAL:HG11	1.35	1.08
1:C:178:ARG:HD2	1:C:207:LEU:HD11	1.33	1.08
1:H:169:VAL:CG1	1:H:224:LEU:O	2.01	1.08
1:D:10:THR:HG21	1:H:384:LYS:HD2	1.36	1.08
1:F:72:ASP:C	1:F:73:LEU:HD12	1.79	1.07
1:F:150:ARG:HD3	1:F:268:MSE:O	1.52	1.07
1:J:357:MSE:HE1	1:J:362:LEU:HB2	1.25	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:TRP:CZ2	1:F:69:LEU:CD2	2.32	1.06
1:I:149:ASP:OD2	1:I:152:PHE:CE1	2.06	1.06
1:C:357:MSE:HE2	1:C:381:LEU:HD13	1.09	1.06
1:F:42:TRP:NE1	1:F:69:LEU:CD2	2.12	1.06
1:G:222:ALA:HB2	1:G:231:LEU:CD2	1.85	1.06
1:H:34:ILE:HB	1:H:37:GLU:CD	1.80	1.05
1:F:357:MSE:CE	1:F:381:LEU:HD13	1.84	1.05
1:G:150:ARG:CD	1:G:268:MSE:O	2.04	1.05
1:J:74:ARG:HD3	1:J:84:PRO:HA	1.39	1.05
1:E:327:LEU:CD1	1:E:357:MSE:HE3	1.86	1.04
1:H:178:ARG:NH1	1:H:207:LEU:HD12	1.73	1.04
1:K:327:LEU:CD1	1:K:357:MSE:HE3	1.87	1.04
1:G:44:THR:HG21	1:G:201:VAL:HG11	1.39	1.04
1:D:193:PRO:HD3	1:D:400:VAL:HG21	1.38	1.04
1:F:357:MSE:HE2	1:F:381:LEU:HD11	1.07	1.04
1:H:109:GLU:O	1:H:112:ARG:HG2	1.57	1.04
1:H:354:GLU:CA	1:H:384:LYS:HZ1	1.64	1.04
1:G:104:ARG:NH2	2:G:501:ACO:O8A	1.91	1.03
1:H:34:ILE:CB	1:H:37:GLU:HG2	1.87	1.03
1:C:121:VAL:HA	1:C:305:MSE:HG2	1.37	1.03
1:H:33:PHE:CE1	1:H:38:SER:OG	2.10	1.03
1:C:107:CYS:O	1:C:111:HIS:ND1	1.91	1.03
1:C:178:ARG:HD2	1:C:207:LEU:CD1	1.88	1.03
1:E:295:TRP:HZ2	1:E:297:GLN:NE2	1.54	1.02
1:J:34:ILE:HG22	1:J:36:PRO:HD2	1.09	1.02
1:E:148:VAL:HG13	1:E:290:LEU:C	1.84	1.02
1:G:175:THR:HA	1:G:207:LEU:HD11	1.34	1.02
1:I:169:VAL:HG22	1:I:225:HIS:HB2	1.38	1.01
1:C:357:MSE:HB3	1:C:381:LEU:HD13	1.41	1.01
1:J:34:ILE:HG22	1:J:36:PRO:CD	1.90	1.01
1:J:43:ARG:HH11	1:J:43:ARG:HA	1.23	1.01
1:B:42:TRP:NE1	1:B:90:PHE:CE2	2.29	1.01
1:A:355:ILE:HD11	1:A:381:LEU:HD13	1.41	1.01
1:E:146:LEU:HD12	1:E:275:THR:HG21	1.06	1.01
1:G:11:LEU:CD1	1:G:52:VAL:CG2	2.38	1.01
1:F:34:ILE:HG22	1:F:36:PRO:HD2	1.37	1.00
1:K:314:ARG:NH1	1:K:315:GLY:O	1.93	1.00
1:F:357:MSE:HE2	1:F:381:LEU:HD13	1.06	1.00
1:E:295:TRP:CZ2	1:E:297:GLN:NE2	2.30	1.00
1:C:34:ILE:HG22	1:C:36:PRO:HD2	1.43	1.00
1:C:357:MSE:CE	1:C:381:LEU:HD11	1.81	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:GLU:O	1:F:381:LEU:HD12	1.62	1.00
1:K:244:VAL:CB	1:K:273:ILE:CD1	2.39	1.00
1:A:73:LEU:CD1	1:A:87:GLY:HA3	1.91	1.00
1:L:34:ILE:CG2	1:L:36:PRO:HD2	1.92	1.00
1:I:323:PHE:HB2	1:I:391:ARG:HH11	1.18	0.99
1:F:22:MSE:CE	1:F:42:TRP:HH2	1.48	0.99
1:D:178:ARG:HG3	1:D:207:LEU:HD11	1.42	0.99
1:C:357:MSE:HE2	1:C:381:LEU:CD2	1.93	0.99
1:H:150:ARG:HD3	1:H:151:ARG:N	1.78	0.99
1:H:295:TRP:CZ2	1:H:297:GLN:NE2	2.30	0.99
1:E:358:ASP:O	1:E:361:VAL:HG12	1.60	0.98
1:F:357:MSE:CE	1:F:381:LEU:HD11	1.88	0.98
1:I:357:MSE:HE3	1:I:381:LEU:CD1	1.91	0.98
1:C:104:ARG:NH2	3:C:635:HOH:O	1.95	0.98
1:D:148:VAL:CG2	1:D:291:ALA:CA	2.24	0.98
1:H:385:ASP:CG	1:H:387:GLN:HG2	1.87	0.97
1:B:85:THR:CG2	1:B:121:VAL:O	2.12	0.97
1:H:180:GLU:OE2	1:H:224:LEU:CD2	2.11	0.97
1:C:150:ARG:HH21	1:C:266:ASP:HA	1.29	0.97
1:E:156:HIS:CE1	1:F:380:ARG:NH1	2.33	0.97
1:B:45:LEU:HD11	1:B:199:PRO:HG2	1.43	0.97
1:I:45:LEU:HD11	1:I:199:PRO:HG2	1.46	0.97
1:J:189:ARG:HH11	1:J:197:LEU:HD13	1.28	0.97
1:F:42:TRP:CE2	1:F:69:LEU:HD21	1.98	0.96
1:H:295:TRP:HZ2	1:H:297:GLN:NE2	1.63	0.96
1:J:405:ALA:HB3	3:J:602:HOH:O	1.64	0.96
1:K:144:HIS:NE2	1:K:296:ARG:NH1	2.13	0.96
1:J:227:ASP:OD2	3:J:603:HOH:O	1.84	0.96
1:K:244:VAL:HG11	1:K:273:ILE:CD1	1.95	0.96
1:C:144:HIS:CD2	1:C:277:PRO:HG3	2.01	0.95
1:G:303:ARG:NH1	1:G:305:MSE:SE	2.49	0.95
1:E:34:ILE:HG22	1:E:36:PRO:HD2	1.48	0.95
1:E:297:GLN:HG3	1:F:289:ARG:HD3	1.47	0.95
1:A:85:THR:HG23	1:A:121:VAL:O	1.66	0.95
1:A:178:ARG:HG3	1:A:207:LEU:HD11	1.46	0.95
1:B:148:VAL:HG22	1:B:291:ALA:HA	1.47	0.94
1:E:93:VAL:O	1:E:98:ARG:NH2	2.00	0.94
1:I:34:ILE:CG2	1:I:36:PRO:HD2	1.96	0.94
1:A:320:VAL:CG2	1:A:394:ALA:HB1	1.97	0.94
1:D:8:THR:N	1:H:353:ALA:H	1.64	0.94
1:H:98:ARG:HH21	1:H:99:ARG:NH2	1.64	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:VAL:CG1	1:F:304:ILE:HA	1.97	0.94
1:G:9:VAL:CG1	1:G:54:VAL:CG1	2.46	0.94
1:H:354:GLU:HA	1:H:384:LYS:HZ2	1.32	0.94
1:J:295:TRP:HZ2	1:J:297:GLN:NE2	1.67	0.93
1:C:178:ARG:CD	1:C:207:LEU:HD11	1.98	0.93
1:C:357:MSE:CE	1:C:381:LEU:CD2	2.46	0.93
1:I:356:GLU:O	1:I:381:LEU:HD12	1.67	0.93
1:K:193:PRO:HD3	1:K:400:VAL:HG11	1.51	0.93
1:J:34:ILE:CG2	1:J:36:PRO:HD2	1.98	0.92
1:K:193:PRO:CD	1:K:400:VAL:CG1	2.48	0.92
1:C:355:ILE:HD11	1:C:381:LEU:HD21	1.48	0.92
1:G:355:ILE:HD11	1:G:381:LEU:HD21	1.52	0.92
1:I:193:PRO:HD3	1:I:400:VAL:HG21	1.49	0.92
1:K:244:VAL:CG1	1:K:273:ILE:HD13	1.98	0.92
1:H:146:LEU:HD23	1:H:275:THR:HG22	1.50	0.92
1:E:193:PRO:HD3	1:E:400:VAL:HG21	1.50	0.92
1:D:145:GLU:HB3	1:D:295:TRP:HB3	1.49	0.91
1:I:357:MSE:HE3	1:I:381:LEU:HD11	1.51	0.91
1:H:178:ARG:HH11	1:H:207:LEU:CD1	1.81	0.91
1:F:42:TRP:HE1	1:F:69:LEU:HD22	1.35	0.91
1:H:385:ASP:OD2	1:H:387:GLN:CG	2.17	0.91
1:I:327:LEU:C	1:I:327:LEU:HD23	1.94	0.91
1:I:327:LEU:HD23	1:I:328:GLU:N	1.85	0.91
1:G:44:THR:CG2	1:G:201:VAL:HG11	2.00	0.91
1:D:193:PRO:CD	1:D:400:VAL:CG2	2.48	0.91
1:J:40:THR:O	1:J:44:THR:HG22	1.71	0.91
1:C:357:MSE:HB3	1:C:381:LEU:CD1	2.00	0.91
1:H:144:HIS:CD2	1:H:277:PRO:HG3	2.05	0.91
1:I:193:PRO:CD	1:I:400:VAL:HG23	2.00	0.90
1:A:73:LEU:O	1:A:85:THR:N	2.04	0.90
1:B:145:GLU:HB3	1:B:295:TRP:HB3	1.51	0.90
1:C:121:VAL:HG12	1:C:304:ILE:HA	1.50	0.90
1:E:206:LEU:HD23	1:E:206:LEU:C	1.96	0.90
1:E:193:PRO:CD	1:E:400:VAL:HG23	2.01	0.90
1:H:178:ARG:HH12	1:H:207:LEU:HD12	1.33	0.90
1:J:203:TRP:O	1:J:207:LEU:CD1	2.20	0.90
1:H:150:ARG:HH11	1:H:150:ARG:C	1.80	0.90
1:K:244:VAL:CB	1:K:273:ILE:CG1	2.36	0.90
1:I:323:PHE:CB	1:I:391:ARG:NH1	2.34	0.90
1:I:289:ARG:HD3	1:J:297:GLN:HG3	1.53	0.89
1:J:206:LEU:O	1:J:206:LEU:HD23	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:206:LEU:HD23	1:J:206:LEU:C	1.97	0.89
1:I:206:LEU:C	1:I:206:LEU:HD23	1.97	0.89
1:D:10:THR:OG1	1:H:384:LYS:HD3	1.72	0.89
1:F:199:PRO:HD2	1:F:202:LEU:HD12	1.55	0.89
1:D:42:TRP:NE1	1:D:90:PHE:CZ	2.41	0.89
1:J:144:HIS:NE2	1:J:296:ARG:NH1	2.21	0.89
1:I:52:VAL:HG13	1:I:110:LEU:HD21	1.53	0.89
1:K:148:VAL:HG22	1:K:291:ALA:HA	1.54	0.89
1:F:98:ARG:HG2	1:F:99:ARG:HG2	1.54	0.89
1:D:65:VAL:HG11	1:D:97:HIS:CE1	2.06	0.89
1:G:65:VAL:HG11	1:G:97:HIS:CE1	2.08	0.88
1:K:314:ARG:NH2	1:K:396:PHE:O	2.06	0.88
1:F:357:MSE:HB3	1:F:381:LEU:HD13	1.53	0.88
1:I:193:PRO:HD3	1:I:400:VAL:CG2	2.03	0.88
1:J:405:ALA:CB	3:J:602:HOH:O	2.20	0.88
1:B:144:HIS:NE2	1:B:296:ARG:NH1	2.22	0.88
1:E:144:HIS:HE1	1:E:296:ARG:HE	1.22	0.88
1:J:295:TRP:CZ2	1:J:297:GLN:NE2	2.41	0.88
1:A:73:LEU:HD11	1:A:87:GLY:HA3	1.53	0.88
1:A:144:HIS:NE2	1:A:296:ARG:NH1	2.22	0.88
1:G:144:HIS:NE2	1:G:296:ARG:NH1	2.22	0.88
1:B:144:HIS:CE1	1:B:296:ARG:HH11	1.91	0.87
1:K:193:PRO:CD	1:K:400:VAL:HG11	2.04	0.87
1:E:146:LEU:CD1	1:E:275:THR:CG2	2.46	0.87
1:E:206:LEU:HD23	1:E:206:LEU:O	1.74	0.87
1:I:289:ARG:HD3	1:J:297:GLN:CG	2.05	0.87
1:B:233:ARG:NH1	3:B:627:HOH:O	2.01	0.87
1:A:180:GLU:OE2	1:A:224:LEU:CD2	2.17	0.87
1:I:52:VAL:HG13	1:I:110:LEU:CD2	2.05	0.87
1:K:206:LEU:HD23	1:K:206:LEU:O	1.73	0.87
1:E:109:GLU:OE1	1:E:112:ARG:NH2	2.07	0.86
1:A:314:ARG:NH2	1:A:396:PHE:O	2.08	0.86
1:A:34:ILE:HG22	1:A:36:PRO:HD2	1.55	0.86
1:F:22:MSE:HE3	1:F:42:TRP:CH2	2.05	0.86
1:F:22:MSE:HE3	1:F:42:TRP:HH2	1.36	0.86
1:F:98:ARG:HG3	1:F:99:ARG:NH1	1.90	0.86
1:J:357:MSE:HE1	1:J:362:LEU:CB	2.05	0.86
1:H:196:LEU:HB2	1:H:406:PHE:CE2	2.11	0.86
1:F:206:LEU:O	1:F:206:LEU:HD23	1.73	0.86
1:J:193:PRO:HD3	1:J:400:VAL:HG21	1.58	0.86
1:G:148:VAL:HG22	1:G:291:ALA:HA	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:PRO:CD	1:E:400:VAL:CG2	2.54	0.86
1:F:208:ALA:O	1:F:211:LYS:HG2	1.74	0.86
1:G:222:ALA:CB	1:G:231:LEU:HD23	2.06	0.86
1:I:148:VAL:HG22	1:I:291:ALA:CA	2.05	0.86
1:K:244:VAL:CG1	1:K:273:ILE:CD1	2.54	0.85
1:B:40:THR:O	1:B:44:THR:HG23	1.76	0.85
1:D:43:ARG:HA	1:D:43:ARG:HH11	1.40	0.85
1:F:206:LEU:HD23	1:F:206:LEU:C	2.01	0.85
1:H:178:ARG:NH1	1:H:207:LEU:HD11	1.90	0.85
1:K:244:VAL:CG2	1:K:273:ILE:CG1	2.53	0.85
1:E:357:MSE:HB2	1:E:361:VAL:HG11	1.58	0.85
1:A:34:ILE:HD12	1:A:37:GLU:OE1	1.77	0.85
1:C:356:GLU:O	1:C:381:LEU:HD12	1.77	0.85
1:H:206:LEU:HD23	1:H:206:LEU:O	1.76	0.85
1:I:193:PRO:CD	1:I:400:VAL:CG2	2.54	0.85
1:E:297:GLN:CG	1:F:289:ARG:HD3	2.06	0.85
1:F:71:MSE:HB2	1:F:73:LEU:HD11	1.55	0.85
1:G:327:LEU:HD23	1:G:327:LEU:C	2.01	0.85
1:C:193:PRO:HB2	1:C:402:VAL:HG22	1.59	0.84
1:D:150:ARG:NH2	1:D:266:ASP:CA	2.39	0.84
1:A:72:ASP:OD1	1:A:119:TYR:OH	1.92	0.84
1:D:10:THR:HG21	1:H:384:LYS:CD	2.06	0.84
1:G:248:ARG:NH2	1:G:405:ALA:O	2.09	0.84
1:G:381:LEU:HD23	1:G:381:LEU:C	2.01	0.84
1:D:193:PRO:HD3	1:D:400:VAL:CG2	2.06	0.84
1:J:357:MSE:HE3	1:J:358:ASP:O	1.77	0.84
1:H:196:LEU:HB2	1:H:406:PHE:HE2	1.43	0.84
1:I:44:THR:O	1:I:45:LEU:CD2	2.23	0.84
1:B:123:ALA:HB1	1:B:300:LEU:HD11	1.58	0.84
1:C:148:VAL:CG2	1:C:291:ALA:CA	2.29	0.84
1:H:206:LEU:HD23	1:H:206:LEU:C	2.02	0.84
1:F:188:TRP:CH2	1:F:248:ARG:NH1	2.46	0.84
1:J:208:ALA:O	1:J:211:LYS:HG2	1.77	0.84
1:A:145:GLU:HB3	1:A:295:TRP:HB3	1.59	0.84
1:H:109:GLU:OE1	1:H:112:ARG:HD3	1.77	0.84
1:I:206:LEU:HD23	1:I:206:LEU:O	1.77	0.84
1:E:193:PRO:HD3	1:E:400:VAL:CG2	2.07	0.84
1:I:267:SER:O	1:I:268:MSE:HE2	1.78	0.84
1:F:357:MSE:HB3	1:F:381:LEU:CD1	2.08	0.83
1:I:323:PHE:CB	1:I:391:ARG:HH11	1.90	0.83
1:F:34:ILE:HG22	1:F:36:PRO:CD	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:LEU:HD23	1:G:328:GLU:N	1.92	0.83
1:I:23:PHE:HE1	1:I:38:SER:HG	1.24	0.83
1:D:40:THR:O	1:D:44:THR:CG2	2.25	0.83
1:G:303:ARG:HH11	1:G:305:MSE:SE	2.08	0.83
1:K:244:VAL:CG2	1:K:273:ILE:CD1	2.31	0.83
1:K:337:LEU:HD12	1:K:345:ARG:O	1.78	0.83
1:E:145:GLU:CB	1:E:295:TRP:HB3	2.08	0.83
1:G:188:TRP:CH2	1:G:248:ARG:NH1	2.47	0.82
1:C:146:LEU:HD11	1:C:291:ALA:C	2.04	0.82
1:F:303:ARG:NH1	1:F:359:ARG:HH11	1.76	0.82
1:G:11:LEU:CD1	1:G:52:VAL:HG22	2.07	0.82
1:I:200:GLN:HA	1:I:200:GLN:HE21	1.44	0.82
1:D:193:PRO:CD	1:D:400:VAL:HG23	2.10	0.82
1:H:34:ILE:N	1:H:37:GLU:OE1	2.12	0.82
1:D:144:HIS:CD2	1:D:277:PRO:HG3	2.15	0.82
1:K:193:PRO:HD2	1:K:400:VAL:HG13	1.61	0.82
1:K:206:LEU:HD23	1:K:206:LEU:C	2.04	0.81
1:K:289:ARG:NH2	1:L:126:ALA:O	2.13	0.81
1:A:178:ARG:CG	1:A:207:LEU:HD11	2.11	0.80
1:F:192:VAL:HG11	1:F:403:GLN:HB2	1.63	0.80
1:B:42:TRP:HZ2	1:B:90:PHE:CE1	1.99	0.80
1:F:150:ARG:CD	1:F:268:MSE:O	2.30	0.80
1:C:206:LEU:HD23	1:C:206:LEU:O	1.80	0.80
1:I:98:ARG:HG2	1:I:99:ARG:HG2	1.63	0.80
1:B:169:VAL:HG13	1:B:224:LEU:C	2.06	0.80
1:D:145:GLU:CB	1:D:295:TRP:HB3	2.10	0.80
1:K:244:VAL:HB	1:K:273:ILE:HG12	0.84	0.80
1:J:78:PRO:HG2	1:J:314:ARG:HH21	1.47	0.80
1:E:145:GLU:HB3	1:E:295:TRP:HB3	1.62	0.80
1:G:9:VAL:HG13	1:G:54:VAL:HG12	1.63	0.80
1:B:169:VAL:CG2	1:B:225:HIS:HD2	1.93	0.80
1:E:44:THR:CG2	1:E:201:VAL:HG11	2.10	0.80
1:D:145:GLU:OE2	1:D:295:TRP:CB	2.30	0.79
1:G:34:ILE:HG22	1:G:36:PRO:HD2	1.62	0.79
1:G:43:ARG:HH11	1:G:43:ARG:HA	1.47	0.79
1:J:271:ILE:N	1:J:271:ILE:HD12	1.96	0.79
1:B:169:VAL:CG2	1:B:225:HIS:CD2	2.65	0.79
1:C:150:ARG:NH2	1:C:266:ASP:HA	1.96	0.79
1:E:144:HIS:CE1	1:E:296:ARG:HE	2.00	0.79
1:F:14:PRO:HD2	1:F:51:ALA:O	1.82	0.79
1:K:193:PRO:HD2	1:K:400:VAL:CG1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HD23	1:B:206:LEU:C	2.07	0.79
1:I:34:ILE:HG22	1:I:36:PRO:CD	2.09	0.79
1:E:144:HIS:HE1	1:E:296:ARG:NE	1.80	0.79
1:J:270:ARG:C	1:J:271:ILE:HD12	2.07	0.79
1:A:327:LEU:HD13	1:A:355:ILE:HG23	1.64	0.79
1:E:144:HIS:CE1	1:E:296:ARG:HG3	2.18	0.79
1:I:107:CYS:O	1:I:111:HIS:ND1	2.15	0.79
1:H:169:VAL:CG2	1:H:225:HIS:HB2	2.12	0.79
1:E:148:VAL:HG13	1:E:290:LEU:O	1.82	0.78
1:F:71:MSE:CB	1:F:73:LEU:HD11	2.13	0.78
1:I:45:LEU:CD1	1:I:199:PRO:HG2	2.12	0.78
1:E:314:ARG:NH2	1:E:396:PHE:O	2.17	0.78
1:F:303:ARG:CZ	1:F:359:ARG:HH11	1.96	0.78
1:H:169:VAL:HG22	1:H:225:HIS:HB2	1.65	0.78
1:I:144:HIS:NE2	1:I:296:ARG:NH1	2.31	0.78
1:K:381:LEU:HD23	1:K:382:ARG:N	1.98	0.78
1:F:98:ARG:HE	1:F:99:ARG:NH2	1.82	0.78
1:C:206:LEU:HD23	1:C:206:LEU:C	2.08	0.78
1:F:65:VAL:HG11	1:F:97:HIS:CE1	2.18	0.78
1:G:218:ARG:NH2	1:G:239:LEU:HD21	1.97	0.78
1:C:178:ARG:HH11	1:C:207:LEU:HD12	1.50	0.78
1:D:148:VAL:HG21	1:D:291:ALA:HA	1.59	0.78
1:F:42:TRP:CD1	1:F:46:VAL:HG21	2.19	0.78
1:H:98:ARG:NH2	1:H:99:ARG:NH2	2.31	0.78
1:E:33:PHE:CD1	1:E:33:PHE:C	2.62	0.77
1:H:121:VAL:HA	1:H:305:MSE:HG2	1.66	0.77
1:L:318:HIS:CE1	1:L:342:GLY:HA3	2.19	0.77
1:I:148:VAL:HG13	1:I:290:LEU:C	2.09	0.77
1:J:78:PRO:HG2	1:J:314:ARG:NH2	2.00	0.77
1:K:65:VAL:HG11	1:K:97:HIS:CE1	2.20	0.77
1:D:146:LEU:HD23	1:D:147:THR:N	1.98	0.77
1:H:146:LEU:HD23	1:H:275:THR:CG2	2.14	0.77
1:B:206:LEU:HD23	1:B:206:LEU:O	1.85	0.77
1:E:192:VAL:HG11	1:E:403:GLN:HB2	1.65	0.77
1:F:34:ILE:HB	1:F:37:GLU:HG2	1.66	0.77
1:H:383:THR:HG21	1:H:389:LEU:HB2	1.66	0.77
1:D:148:VAL:HG13	1:D:290:LEU:O	1.83	0.77
1:E:334:ARG:HD3	1:E:353:ALA:HB2	1.67	0.77
1:B:144:HIS:CD2	1:B:277:PRO:HG3	2.20	0.77
1:E:307:VAL:HB	1:E:308:PRO:HD3	1.66	0.77
1:F:34:ILE:CG2	1:F:36:PRO:HD2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:ARG:HG2	1:K:99:ARG:HG2	1.66	0.76
1:B:14:PRO:HD2	1:B:51:ALA:O	1.84	0.76
1:H:169:VAL:HG22	1:H:225:HIS:CB	2.16	0.76
1:G:9:VAL:HG13	1:G:54:VAL:CG1	2.16	0.76
1:I:38:SER:HB2	1:I:42:TRP:CZ2	2.19	0.76
1:D:34:ILE:CG2	1:D:36:PRO:HD2	2.11	0.76
1:D:44:THR:HG21	1:D:201:VAL:HG21	1.67	0.76
1:D:206:LEU:C	1:D:206:LEU:HD23	2.11	0.76
1:C:52:VAL:HG21	1:C:110:LEU:HD11	0.83	0.76
1:D:169:VAL:HG22	1:D:225:HIS:HB2	1.67	0.76
1:D:206:LEU:HD23	1:D:206:LEU:O	1.84	0.76
1:A:73:LEU:HB2	1:A:85:THR:O	1.86	0.76
1:F:22:MSE:HE2	1:F:42:TRP:CZ3	2.14	0.76
1:F:330:SER:O	3:F:629:HOH:O	2.02	0.76
1:C:145:GLU:HG2	1:C:274:ILE:CD1	2.15	0.76
1:J:150:ARG:HD3	1:J:268:MSE:O	1.86	0.76
1:A:320:VAL:HG21	1:A:394:ALA:CB	2.16	0.76
1:D:146:LEU:HD23	1:D:146:LEU:C	2.10	0.76
1:I:43:ARG:HA	1:I:43:ARG:HH11	1.49	0.76
1:B:24:LEU:HD13	1:D:173:ARG:HG2	1.68	0.75
1:E:144:HIS:CE1	1:E:296:ARG:NE	2.54	0.75
1:G:40:THR:O	1:G:44:THR:CG2	2.24	0.75
1:A:178:ARG:HH11	1:A:207:LEU:HD12	1.51	0.75
1:A:320:VAL:HG22	1:A:394:ALA:HB1	1.68	0.75
1:B:169:VAL:HG22	1:B:225:HIS:CB	2.17	0.75
1:C:121:VAL:CA	1:C:305:MSE:HG2	2.16	0.75
1:C:355:ILE:HD11	1:C:381:LEU:CD2	2.15	0.75
1:H:109:GLU:O	1:H:112:ARG:CG	2.33	0.75
1:C:326:VAL:CG1	1:C:353:ALA:HA	2.16	0.75
1:A:42:TRP:CD1	1:A:69:LEU:HD21	2.21	0.75
1:A:65:VAL:HG11	1:A:97:HIS:CE1	2.21	0.75
1:A:73:LEU:HD12	1:A:87:GLY:CA	2.17	0.75
1:C:134:ARG:NH1	2:C:501:ACO:H1B	2.00	0.75
1:J:44:THR:HG21	1:J:201:VAL:HG21	1.68	0.75
1:B:169:VAL:HG23	1:B:225:HIS:HD2	1.52	0.75
1:I:169:VAL:HG22	1:I:225:HIS:CB	2.17	0.75
1:J:193:PRO:CD	1:J:400:VAL:HG23	2.16	0.75
1:B:150:ARG:CD	1:B:268:MSE:O	2.31	0.75
1:D:355:ILE:HD11	1:D:381:LEU:HD13	1.68	0.75
1:J:74:ARG:CD	1:J:84:PRO:HA	2.17	0.75
1:D:10:THR:CG2	1:H:384:LYS:HD2	2.14	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:193:PRO:HD3	1:J:400:VAL:CG2	2.16	0.75
1:C:357:MSE:CB	1:C:381:LEU:HD13	2.17	0.75
1:I:148:VAL:CG1	1:I:290:LEU:O	2.31	0.75
1:I:355:ILE:HD11	1:I:381:LEU:CG	2.17	0.75
1:C:144:HIS:NE2	1:C:277:PRO:HG3	2.02	0.75
1:B:48:THR:O	1:B:49:ASP:CG	2.30	0.74
1:G:126:ALA:O	1:H:289:ARG:NH2	2.21	0.74
1:E:360:ASP:OD2	1:E:380:ARG:NH2	2.20	0.74
1:F:98:ARG:NE	1:F:99:ARG:CZ	2.50	0.74
1:B:169:VAL:HG13	1:B:224:LEU:O	1.86	0.74
1:D:74:ARG:HD3	1:D:84:PRO:HA	1.69	0.74
1:B:144:HIS:HB3	1:B:146:LEU:HD11	1.69	0.74
1:B:380:ARG:O	3:B:604:HOH:O	2.06	0.74
1:E:83:LEU:HD21	1:E:313:ALA:HB1	1.68	0.74
1:I:320:VAL:HG23	1:J:319:GLU:HB3	1.69	0.74
1:C:127:SER:HB3	2:C:501:ACO:H22	1.68	0.74
1:I:289:ARG:CD	1:J:297:GLN:HG3	2.17	0.74
1:A:365:LEU:HD21	1:A:375:LEU:HD12	1.70	0.74
1:C:357:MSE:HE3	1:C:381:LEU:HD11	1.68	0.74
1:D:48:THR:O	1:D:49:ASP:CG	2.30	0.74
1:J:355:ILE:HD11	1:J:381:LEU:HD13	1.70	0.74
1:K:355:ILE:HD11	1:K:381:LEU:HD21	1.70	0.74
1:I:169:VAL:HG13	1:I:224:LEU:O	1.87	0.74
1:J:339:ILE:HG12	1:J:344:ALA:HB2	1.70	0.74
1:I:327:LEU:C	1:I:327:LEU:CD2	2.61	0.73
1:C:70:TYR:HA	1:C:87:GLY:O	1.87	0.73
1:J:193:PRO:CG	1:J:400:VAL:HG23	2.18	0.73
1:A:145:GLU:CB	1:A:295:TRP:HB3	2.17	0.73
1:B:145:GLU:CB	1:B:295:TRP:HB3	2.17	0.73
1:D:150:ARG:HH21	1:D:266:ASP:C	1.96	0.73
1:A:121:VAL:HG13	1:A:303:ARG:O	1.88	0.73
1:D:145:GLU:OE2	1:D:295:TRP:HB2	1.86	0.73
1:G:175:THR:CA	1:G:207:LEU:HD11	2.16	0.73
1:J:43:ARG:HA	1:J:43:ARG:NH1	2.02	0.73
1:D:193:PRO:CD	1:D:400:VAL:HG21	2.12	0.73
1:G:44:THR:HG21	1:G:201:VAL:CG1	2.18	0.73
1:E:156:HIS:CE1	1:F:380:ARG:HH12	2.07	0.73
1:J:178:ARG:HD2	1:J:207:LEU:CD2	2.19	0.73
1:G:169:VAL:HG22	1:G:225:HIS:HB2	1.71	0.72
1:H:354:GLU:CA	1:H:384:LYS:HZ3	2.01	0.72
1:I:38:SER:O	1:I:42:TRP:CD1	2.41	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:THR:HG23	1:J:121:VAL:HG23	1.71	0.72
1:L:31:THR:HG23	3:L:621:HOH:O	1.88	0.72
1:C:314:ARG:NH1	1:C:366:TYR:O	2.22	0.72
1:H:48:THR:O	1:H:49:ASP:OD1	2.08	0.72
1:I:307:VAL:HB	1:I:308:PRO:HD3	1.70	0.72
1:C:120:PRO:O	1:C:305:MSE:HB2	1.88	0.72
1:F:303:ARG:HH12	1:F:359:ARG:NH1	1.86	0.72
1:H:107:CYS:O	1:H:111:HIS:ND1	2.21	0.72
1:K:98:ARG:HG3	1:K:99:ARG:NH1	2.04	0.72
1:C:357:MSE:CE	1:C:381:LEU:HD22	2.20	0.72
1:I:200:GLN:HA	1:I:200:GLN:NE2	2.04	0.72
1:J:178:ARG:HD2	1:J:207:LEU:HD21	1.69	0.72
1:I:327:LEU:O	1:I:335:PHE:N	2.22	0.72
1:E:156:HIS:NE2	1:F:380:ARG:NH1	2.38	0.72
1:H:98:ARG:HG2	1:H:99:ARG:HG2	1.72	0.72
1:I:107:CYS:C	1:I:111:HIS:HD1	1.98	0.72
1:D:247:LEU:HD23	1:D:247:LEU:C	2.15	0.72
1:E:150:ARG:HD3	1:E:268:MSE:O	1.90	0.72
1:B:42:TRP:O	1:B:46:VAL:HB	1.89	0.71
1:F:326:VAL:HG12	1:F:353:ALA:HA	1.72	0.71
1:H:322:GLU:OE1	1:H:338:LYS:HE2	1.90	0.71
1:I:337:LEU:HD12	1:I:345:ARG:O	1.89	0.71
1:I:357:MSE:HE2	1:I:381:LEU:HD13	0.72	0.71
1:F:98:ARG:HE	1:F:99:ARG:CZ	2.03	0.71
1:I:276:HIS:HD2	1:I:278:GLN:H	1.37	0.71
1:I:289:ARG:HD3	1:J:297:GLN:CD	2.15	0.71
1:F:303:ARG:NH1	1:F:359:ARG:NH1	2.37	0.71
1:I:355:ILE:CD1	1:I:381:LEU:HD11	2.20	0.71
1:D:146:LEU:HD11	1:D:291:ALA:HB1	1.71	0.71
1:E:297:GLN:HG3	1:F:289:ARG:CD	2.19	0.71
1:I:83:LEU:HD21	1:I:313:ALA:HB1	1.71	0.71
1:K:201:VAL:O	1:K:204:ASP:HB2	1.89	0.71
1:H:178:ARG:HH11	1:H:207:LEU:HD11	1.50	0.71
1:B:178:ARG:NH1	1:B:207:LEU:HD12	2.06	0.71
1:J:110:LEU:O	1:J:114:ILE:HG13	1.91	0.71
1:A:320:VAL:HG21	1:A:394:ALA:HB1	1.69	0.71
1:C:319:GLU:O	1:D:319:GLU:O	2.08	0.71
1:E:358:ASP:O	1:E:361:VAL:CG1	2.38	0.71
1:F:16:GLU:HA	1:F:19:TRP:CD1	2.26	0.71
1:G:289:ARG:NH1	1:H:298:ASP:OD2	2.23	0.71
1:D:150:ARG:CZ	1:D:266:ASP:HA	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:SER:HB3	2:E:501:ACO:H22	1.71	0.71
1:I:169:VAL:CG2	1:I:225:HIS:HB2	2.19	0.71
1:C:148:VAL:HG21	1:C:291:ALA:CB	2.21	0.71
1:D:18:ASP:OD2	1:D:55:ARG:NH2	2.24	0.71
1:D:49:ASP:C	1:D:49:ASP:OD1	2.34	0.71
1:E:297:GLN:OE1	1:F:289:ARG:CD	2.38	0.71
1:I:289:ARG:CG	1:J:298:ASP:OD1	2.39	0.71
1:J:193:PRO:CD	1:J:400:VAL:CG2	2.69	0.71
1:K:244:VAL:HG21	1:K:273:ILE:HD11	0.77	0.71
1:A:320:VAL:CG2	1:A:394:ALA:CB	2.68	0.70
1:C:110:LEU:HD12	1:C:110:LEU:H	1.56	0.70
1:C:407:GLU:HB2	3:C:636:HOH:O	1.91	0.70
1:D:33:PHE:CE1	1:D:38:SER:CB	2.73	0.70
1:I:65:VAL:HG11	1:I:97:HIS:CE1	2.26	0.70
1:A:73:LEU:CD1	1:A:87:GLY:CA	2.67	0.70
1:B:314:ARG:NH1	1:B:366:TYR:O	2.24	0.70
1:C:334:ARG:HD3	1:C:351:ALA:O	1.91	0.70
1:D:33:PHE:CE1	1:D:38:SER:OG	2.22	0.70
1:E:206:LEU:C	1:E:206:LEU:CD2	2.64	0.70
1:J:337:LEU:HD11	1:J:339:ILE:HD11	1.72	0.70
1:K:381:LEU:HD23	1:K:381:LEU:C	2.16	0.70
1:C:357:MSE:SE	1:C:381:LEU:HD13	2.41	0.70
1:G:33:PHE:O	1:G:34:ILE:HG13	1.92	0.70
1:D:52:VAL:HG13	1:D:110:LEU:HD21	1.74	0.70
1:F:121:VAL:HG12	1:F:304:ILE:CA	2.16	0.70
1:E:65:VAL:HG11	1:E:97:HIS:CE1	2.26	0.70
1:I:148:VAL:HG21	1:I:291:ALA:HA	1.71	0.70
1:J:44:THR:HG21	1:J:201:VAL:HG11	1.72	0.70
1:J:197:LEU:O	1:J:199:PRO:HD3	1.90	0.70
1:A:73:LEU:HD12	1:A:87:GLY:HA3	1.74	0.70
1:B:127:SER:HB3	2:B:501:ACO:H22	1.71	0.70
1:C:85:THR:HG23	1:C:121:VAL:O	1.91	0.70
1:I:217:ASP:OD1	1:I:233:ARG:NH1	2.24	0.70
1:C:107:CYS:C	1:C:111:HIS:HD1	1.98	0.70
1:D:217:ASP:HB3	1:D:233:ARG:HD2	1.72	0.70
1:I:355:ILE:HG12	1:I:356:GLU:N	2.07	0.70
1:G:50:GLY:HA2	1:G:70:TYR:CE1	2.27	0.69
1:G:69:LEU:C	1:G:69:LEU:HD12	2.17	0.69
1:H:169:VAL:CG1	1:H:224:LEU:C	2.55	0.69
1:I:206:LEU:C	1:I:206:LEU:CD2	2.65	0.69
1:K:123:ALA:HB1	1:K:300:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:GLU:O	1:G:19:TRP:HD1	1.75	0.69
1:J:149:ASP:OD2	1:J:152:PHE:CE1	2.44	0.69
1:C:357:MSE:HE1	1:C:381:LEU:CD2	2.20	0.69
1:D:8:THR:HG23	1:D:9:VAL:N	2.05	0.69
1:G:281:LEU:HB3	1:G:282:PRO:HD3	1.73	0.69
1:J:206:LEU:C	1:J:206:LEU:CD2	2.64	0.69
1:L:256:CYS:O	1:L:260:ARG:HG3	1.91	0.69
1:C:148:VAL:CG2	1:C:291:ALA:CB	2.69	0.69
1:G:98:ARG:HD2	1:L:264:GLY:CA	2.23	0.69
1:G:327:LEU:C	1:G:327:LEU:CD2	2.65	0.69
1:I:355:ILE:HD11	1:I:381:LEU:HD11	1.73	0.69
1:K:178:ARG:NH1	1:K:207:LEU:HD23	2.06	0.69
1:A:248:ARG:NH2	1:A:405:ALA:O	2.22	0.69
1:I:217:ASP:CG	1:I:233:ARG:NH1	2.50	0.69
1:B:85:THR:HG23	1:B:121:VAL:C	2.14	0.69
1:B:221:PHE:CE2	1:E:28:ALA:HA	2.28	0.69
1:C:148:VAL:HG13	1:C:290:LEU:C	2.17	0.69
1:G:149:ASP:OD2	1:G:152:PHE:CE2	2.45	0.69
1:K:314:ARG:HD3	1:K:316:TYR:CE2	2.27	0.69
1:B:178:ARG:HG3	1:B:207:LEU:HD11	1.73	0.69
1:C:34:ILE:CG2	1:C:36:PRO:HD2	2.21	0.69
1:D:178:ARG:CG	1:D:207:LEU:HD11	2.19	0.69
1:C:146:LEU:HD11	1:C:291:ALA:O	1.92	0.69
1:D:150:ARG:NH2	1:D:266:ASP:O	2.26	0.69
1:G:149:ASP:OD2	1:G:152:PHE:HE2	1.74	0.69
1:I:44:THR:O	1:I:44:THR:HG22	1.91	0.69
1:C:178:ARG:HH21	1:C:200:GLN:NE2	1.90	0.69
1:D:8:THR:HG23	1:D:9:VAL:H	1.57	0.69
1:E:127:SER:H	2:E:501:ACO:H21	1.58	0.69
1:L:372:ALA:HB1	1:L:381:LEU:HD21	1.75	0.69
1:E:42:TRP:CH2	1:E:67:MSE:HE1	2.27	0.69
1:K:34:ILE:HG22	1:K:36:PRO:HD2	1.73	0.69
1:B:381:LEU:HD23	1:B:381:LEU:C	2.18	0.68
1:G:266:ASP:OD1	1:I:98:ARG:HD2	1.92	0.68
1:H:34:ILE:CB	1:H:37:GLU:CD	2.63	0.68
1:K:14:PRO:HD2	1:K:51:ALA:O	1.93	0.68
1:I:355:ILE:HG12	1:I:356:GLU:H	1.58	0.68
1:B:327:LEU:HD11	1:B:357:MSE:HE3	1.73	0.68
1:J:357:MSE:CE	1:J:362:LEU:HB2	2.14	0.68
1:K:216:GLY:HA2	1:K:236:ARG:HE	1.57	0.68
1:A:121:VAL:HG12	1:A:122:ALA:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:NE	3:B:633:HOH:O	2.26	0.68
1:I:114:ILE:CG2	1:I:305:MSE:HE2	2.24	0.68
1:J:149:ASP:OD2	1:J:152:PHE:HE1	1.76	0.68
1:K:188:TRP:CZ2	1:K:248:ARG:NH1	2.61	0.68
1:B:169:VAL:HG22	1:B:225:HIS:HB2	1.76	0.68
1:G:44:THR:HG21	1:G:201:VAL:HG21	1.76	0.68
1:D:10:THR:OG1	1:H:384:LYS:CD	2.41	0.68
1:H:203:TRP:O	1:H:207:LEU:HG	1.93	0.68
1:I:98:ARG:HG3	1:I:99:ARG:NH1	2.09	0.68
1:A:373:SER:HB3	1:A:393:ASP:OD2	1.94	0.68
1:I:198:ARG:HG2	1:I:203:TRP:CD1	2.29	0.68
1:L:34:ILE:HG22	1:L:36:PRO:CD	2.17	0.68
1:E:193:PRO:HD2	1:E:400:VAL:HG23	1.74	0.67
1:K:311:LEU:HD21	1:K:362:LEU:HD11	1.75	0.67
1:F:188:TRP:CZ2	1:F:248:ARG:NH1	2.62	0.67
1:G:295:TRP:HZ2	1:G:297:GLN:NE2	1.91	0.67
1:G:300:LEU:HD21	1:G:302:LEU:HD21	1.76	0.67
1:H:197:LEU:HD12	1:H:198:ARG:N	2.09	0.67
1:H:385:ASP:OD1	1:H:387:GLN:N	2.26	0.67
1:D:73:LEU:O	1:D:85:THR:N	2.15	0.67
1:G:355:ILE:CD1	1:G:381:LEU:HD21	2.23	0.67
1:I:339:ILE:HD13	1:I:344:ALA:HB2	1.74	0.67
1:C:144:HIS:CD2	1:C:277:PRO:CG	2.76	0.67
1:G:120:PRO:O	1:G:305:MSE:HB2	1.94	0.67
1:H:399:ASP:OD2	3:H:619:HOH:O	2.11	0.67
1:I:337:LEU:HD13	1:I:346:CYS:HB2	1.76	0.67
1:C:357:MSE:CE	1:C:381:LEU:HD21	2.24	0.67
1:F:22:MSE:HE2	1:F:42:TRP:HH2	1.09	0.67
1:G:146:LEU:HD22	1:G:275:THR:HG21	1.75	0.67
1:K:189:ARG:NH1	1:K:197:LEU:HD13	2.10	0.67
1:K:327:LEU:HD13	1:K:357:MSE:HE3	1.73	0.67
1:D:193:PRO:HD2	1:D:400:VAL:HG23	1.75	0.67
1:E:148:VAL:HA	1:E:290:LEU:O	1.94	0.67
1:F:121:VAL:HB	1:F:303:ARG:O	1.95	0.67
1:D:217:ASP:HB3	1:D:233:ARG:CD	2.24	0.67
1:G:381:LEU:C	1:G:381:LEU:CD2	2.68	0.67
1:J:41:ALA:HA	1:J:44:THR:CG2	2.25	0.67
1:B:14:PRO:HD3	1:B:52:VAL:HA	1.75	0.66
1:E:40:THR:O	1:E:44:THR:HG22	1.95	0.66
1:F:73:LEU:HD12	1:F:73:LEU:N	2.09	0.66
1:B:149:ASP:OD2	1:B:152:PHE:CE2	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:HG3	1:D:135:PHE:HE1	1.59	0.66
1:E:297:GLN:OE1	1:F:289:ARG:HD3	1.96	0.66
1:H:385:ASP:OD1	1:H:387:GLN:HG2	1.96	0.66
1:B:40:THR:O	1:B:44:THR:CG2	2.42	0.66
1:B:109:GLU:OE1	1:B:112:ARG:HD3	1.95	0.66
1:G:295:TRP:CZ2	1:G:297:GLN:NE2	2.64	0.66
1:H:196:LEU:HD13	1:H:406:PHE:CZ	2.31	0.66
1:K:312:GLU:OE1	1:K:346:CYS:N	2.27	0.66
1:G:307:VAL:HG13	1:G:311:LEU:HD11	1.76	0.66
1:K:267:SER:O	1:K:268:MSE:HE2	1.96	0.66
1:A:48:THR:O	1:A:49:ASP:OD1	2.13	0.66
1:A:177:HIS:O	1:A:181:PHE:CD2	2.49	0.66
1:F:206:LEU:C	1:F:206:LEU:CD2	2.68	0.66
1:F:295:TRP:CZ2	1:F:297:GLN:HB3	2.31	0.66
1:H:354:GLU:HA	1:H:384:LYS:HZ1	0.81	0.66
1:K:188:TRP:CE2	1:K:248:ARG:NH1	2.64	0.66
1:A:8:THR:HA	1:A:57:GLY:HA2	1.78	0.66
1:E:156:HIS:NE2	1:F:380:ARG:CZ	2.58	0.66
1:I:289:ARG:CD	1:J:297:GLN:CD	2.69	0.66
1:J:381:LEU:HD11	1:J:389:LEU:HD21	1.76	0.66
1:K:247:LEU:C	1:K:247:LEU:HD23	2.20	0.66
1:H:146:LEU:HD13	1:H:293:THR:HA	1.77	0.66
1:A:73:LEU:N	1:A:85:THR:O	2.29	0.65
1:B:49:ASP:C	1:B:49:ASP:OD1	2.38	0.65
1:B:247:LEU:HD23	1:B:248:ARG:N	2.11	0.65
1:C:306:ASN:OD1	1:C:308:PRO:HD2	1.95	0.65
1:F:365:LEU:HD21	1:F:375:LEU:HD12	1.77	0.65
1:I:169:VAL:HG13	1:I:224:LEU:C	2.21	0.65
1:I:178:ARG:HD2	1:I:207:LEU:CD1	2.26	0.65
1:J:203:TRP:C	1:J:207:LEU:HD13	2.19	0.65
1:I:124:LEU:HD12	1:I:301:TRP:HB2	1.77	0.65
1:C:106:MSE:O	1:C:110:LEU:HD12	1.93	0.65
1:B:169:VAL:HG22	1:B:225:HIS:CD2	2.30	0.65
1:I:45:LEU:HD11	1:I:199:PRO:CG	2.24	0.65
1:B:42:TRP:CZ2	1:B:90:PHE:CE1	2.85	0.65
1:B:292:ARG:NH1	1:B:294:THR:HG22	2.12	0.65
1:C:178:ARG:CG	1:C:207:LEU:HD11	2.26	0.65
1:D:148:VAL:HA	1:D:290:LEU:O	1.96	0.65
1:E:314:ARG:HD3	1:E:316:TYR:CZ	2.32	0.65
1:G:98:ARG:CD	1:L:264:GLY:HA2	2.27	0.65
1:I:193:PRO:HD2	1:I:400:VAL:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ARG:NH2	1:F:266:ASP:OD1	2.29	0.65
1:G:170:ARG:HD2	1:I:63:GLU:OE1	1.97	0.65
1:G:289:ARG:HH11	1:H:298:ASP:CG	2.03	0.65
1:H:198:ARG:HD2	1:H:203:TRP:CE2	2.31	0.65
1:I:247:LEU:HD23	1:I:247:LEU:C	2.21	0.65
1:J:189:ARG:NH1	1:J:197:LEU:HD13	2.08	0.65
1:C:106:MSE:C	1:C:110:LEU:HD13	2.19	0.65
1:C:146:LEU:HD21	1:C:291:ALA:HB1	1.78	0.65
1:C:357:MSE:HE1	1:C:381:LEU:HD21	1.79	0.65
1:D:67:MSE:HE2	1:D:90:PHE:HB3	1.78	0.65
1:I:198:ARG:HD2	1:I:203:TRP:CE2	2.32	0.65
1:I:337:LEU:HD11	1:I:344:ALA:HB1	1.79	0.65
1:I:355:ILE:HD11	1:I:381:LEU:CD1	2.26	0.65
1:C:326:VAL:HG11	1:C:353:ALA:HA	1.77	0.65
1:G:178:ARG:HH21	1:G:200:GLN:NE2	1.94	0.65
1:H:178:ARG:HG3	1:H:207:LEU:HD11	1.77	0.65
1:H:267:SER:C	1:H:268:MSE:HE2	2.22	0.65
1:H:342:GLY:O	1:H:343:ARG:HD2	1.97	0.65
1:L:34:ILE:CG2	1:L:36:PRO:CD	2.73	0.65
1:B:246:GLU:CD	1:B:248:ARG:HE	2.03	0.65
1:C:48:THR:O	1:C:49:ASP:OD1	2.14	0.65
1:F:16:GLU:HA	1:F:19:TRP:NE1	2.11	0.65
1:H:107:CYS:C	1:H:111:HIS:HD1	2.04	0.65
1:J:74:ARG:CZ	1:J:84:PRO:HB3	2.26	0.65
1:B:292:ARG:HH11	1:B:294:THR:HG22	1.61	0.65
1:F:103:LEU:HD22	2:F:501:ACO:H121	1.79	0.65
1:L:178:ARG:HH21	1:L:200:GLN:NE2	1.95	0.65
1:A:121:VAL:HG22	1:A:304:ILE:HA	1.78	0.64
1:E:44:THR:HG21	1:E:201:VAL:CG1	2.20	0.64
1:G:9:VAL:CG1	1:G:54:VAL:HG13	2.25	0.64
1:I:23:PHE:HE1	1:I:38:SER:OG	1.80	0.64
1:K:192:VAL:HG11	1:K:403:GLN:HB2	1.79	0.64
1:B:246:GLU:OE1	1:B:248:ARG:NE	2.22	0.64
1:D:246:GLU:OE1	1:D:248:ARG:NE	2.19	0.64
1:H:146:LEU:HD22	1:H:146:LEU:N	2.11	0.64
1:A:123:ALA:HB1	1:A:300:LEU:HD11	1.79	0.64
1:G:250:VAL:O	1:G:250:VAL:HG12	1.95	0.64
1:L:319:GLU:OE1	1:L:319:GLU:N	2.30	0.64
1:L:381:LEU:C	1:L:381:LEU:HD12	2.21	0.64
1:E:148:VAL:HG22	1:E:291:ALA:HA	0.72	0.64
1:I:320:VAL:HA	1:J:319:GLU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:HD12	3:D:608:HOH:O	1.98	0.64
1:E:227:ASP:HB3	1:E:250:VAL:HG22	1.78	0.64
1:F:35:GLY:N	1:F:36:PRO:HD2	2.11	0.64
1:J:72:ASP:OD1	1:J:74:ARG:NH1	2.30	0.64
1:K:206:LEU:C	1:K:206:LEU:CD2	2.70	0.64
1:I:103:LEU:HD22	2:I:501:ACO:H121	1.79	0.64
1:J:43:ARG:HH11	1:J:43:ARG:CA	2.04	0.64
1:J:44:THR:CG2	1:J:201:VAL:HG11	2.27	0.64
1:J:247:LEU:HD23	1:J:247:LEU:C	2.23	0.64
1:H:150:ARG:HD3	1:H:150:ARG:C	2.22	0.64
1:J:227:ASP:HB2	1:J:254:ALA:HB2	1.80	0.64
1:C:148:VAL:HG21	1:C:291:ALA:HB2	1.80	0.64
1:D:259:TRP:O	1:D:263:ILE:HG12	1.97	0.64
1:E:145:GLU:HB2	1:E:295:TRP:HB3	1.78	0.64
1:I:127:SER:HB3	2:I:501:ACO:H22	1.80	0.64
1:A:34:ILE:HB	1:A:37:GLU:HG2	1.78	0.64
1:C:355:ILE:CD1	1:C:381:LEU:HD21	2.24	0.64
1:J:143:LEU:HD21	1:J:404:THR:HG21	1.77	0.64
1:A:42:TRP:CD1	1:A:69:LEU:CD2	2.81	0.64
1:C:54:VAL:HG11	1:C:102:LEU:HD22	1.79	0.64
1:D:72:ASP:O	1:D:73:LEU:HD23	1.98	0.64
1:F:98:ARG:HG3	1:F:99:ARG:HH11	1.63	0.64
1:H:34:ILE:HG22	1:H:36:PRO:HD2	1.79	0.64
1:K:247:LEU:HD23	1:K:248:ARG:N	2.11	0.64
1:B:107:CYS:O	1:B:111:HIS:ND1	2.26	0.63
1:K:193:PRO:CD	1:K:400:VAL:HG13	2.18	0.63
1:D:139:PRO:HB2	3:D:627:HOH:O	1.97	0.63
1:H:148:VAL:HG22	1:H:291:ALA:HA	1.80	0.63
1:D:98:ARG:HD2	1:E:264:GLY:CA	2.28	0.63
1:E:247:LEU:HD23	1:E:247:LEU:C	2.24	0.63
1:H:206:LEU:C	1:H:206:LEU:CD2	2.70	0.63
1:I:303:ARG:HH11	1:I:305:MSE:SE	2.31	0.63
1:B:85:THR:HG22	1:B:86:ALA:N	2.14	0.63
1:D:72:ASP:OD1	1:D:74:ARG:NH1	2.30	0.63
1:D:150:ARG:NH2	1:D:266:ASP:C	2.55	0.63
1:F:74:ARG:HB3	1:F:82:VAL:CG1	2.29	0.63
1:H:312:GLU:HG2	1:H:344:ALA:O	1.99	0.63
1:J:194:GLY:O	1:J:405:ALA:HB2	1.99	0.63
1:A:121:VAL:CG1	1:A:122:ALA:N	2.62	0.63
1:D:144:HIS:NE2	1:D:296:ARG:NH1	2.47	0.63
1:E:146:LEU:O	1:E:272:SER:HA	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:TRP:NE1	1:K:403:GLN:OE1	2.30	0.63
1:C:110:LEU:HD12	1:C:110:LEU:N	2.13	0.63
1:F:34:ILE:HB	1:F:37:GLU:CG	2.28	0.63
1:I:375:LEU:HD21	1:J:283:HIS:CE1	2.34	0.63
1:J:196:LEU:HG	1:J:405:ALA:CB	2.29	0.63
1:A:98:ARG:HH11	1:A:99:ARG:NH2	1.97	0.63
1:D:42:TRP:NE1	1:D:90:PHE:CE2	2.65	0.63
1:I:73:LEU:HB2	1:I:85:THR:O	1.98	0.63
1:C:404:THR:HG22	1:C:405:ALA:O	1.99	0.63
1:H:306:ASN:OD1	1:H:308:PRO:HD2	1.98	0.63
1:J:45:LEU:HD11	1:J:199:PRO:HG2	1.80	0.63
1:C:121:VAL:CG1	1:C:304:ILE:HA	2.28	0.62
1:C:178:ARG:NH1	1:C:207:LEU:HD12	2.12	0.62
1:C:247:LEU:HD13	3:C:650:HOH:O	1.98	0.62
1:J:312:GLU:HG2	1:J:344:ALA:O	1.98	0.62
1:B:145:GLU:OE2	1:B:295:TRP:CB	2.47	0.62
1:I:150:ARG:HG2	1:I:269:GLU:O	1.99	0.62
1:D:373:SER:HB3	1:D:393:ASP:OD2	2.00	0.62
1:E:127:SER:HB3	2:E:501:ACO:C2P	2.29	0.62
1:F:355:ILE:HD11	1:F:381:LEU:HD21	1.81	0.62
1:I:148:VAL:HG22	1:I:290:LEU:O	2.00	0.62
1:I:199:PRO:HB2	1:I:201:VAL:HG12	1.80	0.62
1:B:45:LEU:CD1	1:B:199:PRO:HG2	2.26	0.62
1:E:355:ILE:HD11	1:E:381:LEU:HD13	1.80	0.62
1:F:98:ARG:CG	1:F:99:ARG:NH1	2.62	0.62
1:I:38:SER:HB2	1:I:42:TRP:CE2	2.35	0.62
1:A:74:ARG:O	1:A:196:LEU:HD23	1.98	0.62
1:C:127:SER:CB	2:C:501:ACO:H22	2.29	0.62
1:D:114:ILE:HG22	1:D:305:MSE:HE2	1.80	0.62
1:I:247:LEU:HD23	1:I:248:ARG:N	2.13	0.62
1:J:98:ARG:HD2	1:K:264:GLY:CA	2.29	0.62
1:D:54:VAL:HG11	1:D:102:LEU:HD13	1.81	0.62
1:F:334:ARG:HD3	1:F:351:ALA:O	1.99	0.62
1:I:52:VAL:CG1	1:I:110:LEU:HD21	2.29	0.62
1:J:102:LEU:O	1:J:103:LEU:C	2.42	0.62
1:K:314:ARG:HD3	1:K:316:TYR:CZ	2.35	0.62
1:B:240:LYS:HB3	1:B:269:GLU:HB2	1.81	0.62
2:C:501:ACO:O5P	2:C:501:ACO:H141	1.98	0.62
1:K:244:VAL:CG2	1:K:273:ILE:HG12	2.25	0.62
1:E:314:ARG:NH1	1:E:315:GLY:O	2.31	0.62
1:K:314:ARG:HH11	1:K:314:ARG:CG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:HIS:HD2	1:D:277:PRO:HG3	1.64	0.62
1:I:306:ASN:OD1	1:I:308:PRO:HD2	2.00	0.62
1:L:387:GLN:HE22	1:L:391:ARG:NH2	1.97	0.62
1:F:71:MSE:C	1:F:73:LEU:CD1	2.72	0.62
1:G:167:SER:N	3:G:603:HOH:O	2.33	0.62
1:G:325:THR:O	1:G:337:LEU:N	2.26	0.61
1:I:107:CYS:HB3	1:I:111:HIS:CE1	2.34	0.61
1:J:247:LEU:HD23	1:J:248:ARG:N	2.15	0.61
1:B:98:ARG:HD2	1:D:264:GLY:CA	2.30	0.61
1:B:247:LEU:HD23	1:B:247:LEU:C	2.25	0.61
1:B:381:LEU:HD23	1:B:382:ARG:N	2.15	0.61
1:F:110:LEU:O	1:F:114:ILE:HG13	1.99	0.61
1:E:247:LEU:HD23	1:E:248:ARG:N	2.14	0.61
1:A:144:HIS:CE1	1:A:296:ARG:NH1	2.68	0.61
1:A:173:ARG:HG3	1:C:24:LEU:HD13	1.82	0.61
1:B:23:PHE:HE1	1:B:42:TRP:HZ3	1.47	0.61
1:G:100:ARG:NH1	1:L:167:SER:OG	2.34	0.61
1:G:121:VAL:HG12	1:G:304:ILE:HA	1.82	0.61
1:G:218:ARG:HH21	1:G:239:LEU:HD21	1.65	0.61
1:H:145:GLU:HB3	1:H:295:TRP:HB3	1.81	0.61
1:I:52:VAL:CG1	1:I:110:LEU:CD2	2.76	0.61
1:E:144:HIS:CD2	1:E:277:PRO:HG3	2.35	0.61
1:B:383:THR:CG2	1:B:389:LEU:HD21	2.30	0.61
1:E:144:HIS:CE1	1:E:296:ARG:CD	2.83	0.61
1:F:34:ILE:HB	1:F:37:GLU:CD	2.24	0.61
1:F:242:ALA:HB2	1:F:268:MSE:HG3	1.82	0.61
1:F:303:ARG:NH2	1:F:359:ARG:NH1	2.49	0.61
1:H:354:GLU:CB	1:H:384:LYS:NZ	2.63	0.61
1:F:14:PRO:CD	1:F:51:ALA:O	2.48	0.61
1:K:76:THR:O	1:K:193:PRO:HA	1.99	0.61
1:B:149:ASP:OD2	1:B:152:PHE:HE2	1.83	0.61
1:E:19:TRP:N	1:E:20:PRO:HD2	2.16	0.61
1:G:123:ALA:HB2	1:G:302:LEU:CD2	2.30	0.61
1:H:109:GLU:CD	1:H:112:ARG:HD3	2.26	0.61
1:J:289:ARG:O	1:J:292:ARG:HG3	1.99	0.61
1:C:101:GLY:HA2	2:C:501:ACO:O2A	2.01	0.61
1:E:107:CYS:O	1:E:111:HIS:ND1	2.34	0.61
1:H:19:TRP:N	1:H:20:PRO:HD2	2.16	0.61
1:A:45:LEU:HD13	1:A:71:MSE:HE2	1.83	0.61
1:A:381:LEU:C	1:A:381:LEU:HD12	2.26	0.61
1:B:109:GLU:O	1:B:112:ARG:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:TRP:CZ2	1:C:297:GLN:NE2	2.69	0.61
1:D:16:GLU:HA	1:D:19:TRP:CD1	2.36	0.61
1:D:177:HIS:HB3	1:D:180:GLU:HG3	1.81	0.61
1:G:302:LEU:HD11	1:G:367:LEU:HD11	1.83	0.61
1:G:311:LEU:HD22	1:G:346:CYS:SG	2.40	0.61
1:I:293:THR:O	3:I:608:HOH:O	2.17	0.61
1:I:289:ARG:CD	1:J:297:GLN:OE1	2.48	0.60
1:B:198:ARG:HD2	1:B:203:TRP:CE2	2.36	0.60
1:G:77:VAL:HB	1:G:78:PRO:HD2	1.82	0.60
1:J:41:ALA:C	1:J:44:THR:HG22	2.26	0.60
1:A:85:THR:HG23	1:A:121:VAL:C	2.25	0.60
1:B:42:TRP:HZ2	1:B:90:PHE:CD1	2.20	0.60
1:E:103:LEU:HD22	2:E:501:ACO:H142	1.83	0.60
1:D:177:HIS:ND1	1:D:180:GLU:OE1	2.20	0.60
1:G:34:ILE:CG2	1:G:36:PRO:HD2	2.31	0.60
1:H:146:LEU:CD2	1:H:275:THR:HG22	2.26	0.60
1:H:150:ARG:NH1	1:H:150:ARG:O	2.33	0.60
1:I:167:SER:OG	1:L:100:ARG:NH1	2.33	0.60
1:B:38:SER:O	1:B:39:ALA:C	2.45	0.60
1:D:148:VAL:CG1	1:D:290:LEU:HB3	2.32	0.60
1:G:303:ARG:HH12	1:G:305:MSE:SE	2.32	0.60
1:F:170:ARG:O	1:F:172:VAL:HG13	2.02	0.60
1:F:357:MSE:SE	1:F:381:LEU:HD13	2.51	0.60
1:B:34:ILE:HB	1:B:37:GLU:HG2	1.82	0.60
1:C:356:GLU:C	1:C:381:LEU:HD12	2.26	0.60
1:I:289:ARG:NH1	1:J:298:ASP:OD2	2.35	0.60
1:K:184:ILE:HG21	1:K:228:GLY:HA2	1.82	0.60
1:B:34:ILE:HG22	1:B:36:PRO:HD2	1.82	0.60
1:C:247:LEU:C	1:C:247:LEU:HD23	2.26	0.60
1:D:33:PHE:CE1	1:D:38:SER:HB2	2.36	0.60
1:H:34:ILE:CB	1:H:37:GLU:OE1	2.50	0.60
1:H:314:ARG:NH1	1:H:366:TYR:O	2.35	0.60
1:D:206:LEU:C	1:D:206:LEU:CD2	2.75	0.60
1:F:98:ARG:HH11	1:F:99:ARG:NH2	2.00	0.60
1:K:337:LEU:HD13	1:K:346:CYS:HB2	1.84	0.60
1:F:121:VAL:HA	1:F:305:MSE:CG	2.20	0.59
1:J:35:GLY:N	1:J:36:PRO:HD2	2.17	0.59
1:J:193:PRO:HG2	1:J:400:VAL:HG23	1.82	0.59
1:A:178:ARG:NH1	1:A:207:LEU:HD12	2.16	0.59
1:E:296:ARG:HB3	1:F:293:THR:HB	1.84	0.59
1:E:319:GLU:O	1:F:320:VAL:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:ARG:HH22	1:F:359:ARG:NH1	2.00	0.59
1:H:65:VAL:HG11	1:H:97:HIS:CE1	2.37	0.59
1:B:383:THR:HG22	1:B:389:LEU:HD21	1.83	0.59
1:C:297:GLN:OE1	1:D:289:ARG:CZ	2.50	0.59
1:D:10:THR:CG2	1:H:384:LYS:CD	2.77	0.59
1:K:19:TRP:HZ3	1:K:42:TRP:HE3	1.50	0.59
1:B:131:ILE:HG12	2:B:501:ACO:C6A	2.32	0.59
1:E:33:PHE:CD1	1:E:34:ILE:N	2.70	0.59
1:J:270:ARG:NH1	1:J:270:ARG:HB2	2.17	0.59
1:J:271:ILE:N	1:J:271:ILE:CD1	2.65	0.59
1:A:132:TYR:OH	2:A:501:ACO:H31	2.03	0.59
1:C:206:LEU:C	1:C:206:LEU:CD2	2.75	0.59
1:E:114:ILE:CG2	1:E:119:TYR:HB2	2.33	0.59
1:F:303:ARG:NH2	1:F:359:ARG:HH11	2.01	0.59
1:A:314:ARG:NH1	1:A:316:TYR:CD2	2.71	0.59
1:B:16:GLU:HA	1:B:19:TRP:CD1	2.37	0.59
1:D:234:VAL:HG23	3:D:626:HOH:O	2.03	0.59
1:I:99:ARG:NH1	2:I:501:ACO:O5A	2.35	0.59
1:D:247:LEU:HD23	1:D:248:ARG:N	2.18	0.59
1:I:250:VAL:HG23	1:I:251:THR:HG23	1.85	0.59
1:B:169:VAL:CG2	1:B:225:HIS:HB2	2.32	0.59
1:C:16:GLU:HA	1:C:19:TRP:CD1	2.38	0.59
1:H:385:ASP:OD1	1:H:386:SER:N	2.36	0.59
1:I:225:HIS:CE1	1:I:226:PRO:HD2	2.38	0.59
1:B:206:LEU:C	1:B:206:LEU:CD2	2.75	0.59
1:D:10:THR:HG21	1:H:384:LYS:CE	2.33	0.59
1:D:52:VAL:HG13	1:D:110:LEU:CD2	2.32	0.59
1:D:98:ARG:HD2	1:E:264:GLY:HA2	1.85	0.59
1:I:289:ARG:HD3	1:J:297:GLN:OE1	2.02	0.59
1:A:42:TRP:NE1	1:A:69:LEU:HD21	2.18	0.58
1:G:385:ASP:C	1:G:385:ASP:OD1	2.46	0.58
1:H:34:ILE:HG13	1:H:37:GLU:OE1	2.03	0.58
1:B:167:SER:N	3:B:621:HOH:O	2.35	0.58
1:B:169:VAL:HG22	1:B:225:HIS:CG	2.38	0.58
1:E:142:THR:HG22	1:E:144:HIS:CD2	2.38	0.58
1:F:71:MSE:O	1:F:73:LEU:HD13	2.03	0.58
1:G:69:LEU:HD12	1:G:69:LEU:O	2.02	0.58
1:H:127:SER:HB3	2:H:501:ACO:H22	1.84	0.58
1:L:329:VAL:O	1:L:332:GLY:N	2.30	0.58
1:L:330:SER:O	1:L:331:ASP:HB2	2.03	0.58
1:A:173:ARG:HB2	1:A:176:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:CYS:C	1:B:111:HIS:HD1	2.11	0.58
1:A:16:GLU:HA	1:A:19:TRP:CD1	2.38	0.58
1:C:355:ILE:HG12	1:C:381:LEU:HD11	1.85	0.58
1:F:326:VAL:CG1	1:F:353:ALA:HA	2.32	0.58
1:G:9:VAL:HG11	1:G:54:VAL:CG1	2.32	0.58
1:A:34:ILE:HG22	1:A:36:PRO:CD	2.32	0.58
1:A:306:ASN:OD1	1:A:308:PRO:HD2	2.02	0.58
1:E:148:VAL:CG2	1:E:291:ALA:CA	2.48	0.58
1:G:33:PHE:O	1:G:34:ILE:CG1	2.51	0.58
1:E:44:THR:HG23	1:E:45:LEU:HG	1.86	0.58
1:I:19:TRP:N	1:I:20:PRO:HD2	2.18	0.58
1:J:52:VAL:CG1	1:J:110:LEU:HD21	2.34	0.58
1:A:187:ARG:O	1:A:191:GLN:HG3	2.04	0.58
1:C:150:ARG:NH1	1:C:150:ARG:O	2.36	0.58
1:D:146:LEU:CD2	1:D:146:LEU:C	2.76	0.58
1:H:34:ILE:CG2	1:H:36:PRO:HD2	2.33	0.58
1:K:188:TRP:CH2	1:K:248:ARG:NH1	2.71	0.58
1:F:320:VAL:HG11	1:F:395:ALA:HA	1.86	0.58
1:H:79:GLY:O	1:H:80:GLU:HB2	2.02	0.58
1:J:98:ARG:CD	1:K:264:GLY:HA2	2.34	0.58
1:A:327:LEU:CD1	1:A:355:ILE:HG23	2.33	0.58
1:E:297:GLN:CD	1:F:289:ARG:HD3	2.28	0.58
1:H:150:ARG:NH2	1:H:266:ASP:OD1	2.37	0.58
1:I:355:ILE:HD11	1:I:381:LEU:HG	1.84	0.58
1:D:218:ARG:HH21	1:D:239:LEU:HD21	1.69	0.58
1:G:40:THR:C	1:G:44:THR:HG22	2.21	0.58
1:I:193:PRO:CG	1:I:400:VAL:HG23	2.33	0.58
2:I:501:ACO:H4B	2:I:501:ACO:O8A	2.04	0.58
1:J:273:ILE:HG12	1:J:274:ILE:N	2.18	0.57
1:E:8:THR:O	1:E:57:GLY:N	2.37	0.57
1:E:199:PRO:HD2	1:E:202:LEU:HD12	1.85	0.57
1:F:242:ALA:HB3	1:F:271:ILE:CD1	2.35	0.57
1:H:107:CYS:HB3	1:H:111:HIS:CE1	2.39	0.57
1:A:146:LEU:HD13	1:A:275:THR:HG22	1.85	0.57
1:D:145:GLU:OE2	1:D:295:TRP:HB3	2.02	0.57
1:G:225:HIS:CG	1:G:226:PRO:HD2	2.38	0.57
1:K:69:LEU:HD12	1:K:69:LEU:O	2.03	0.57
1:C:198:ARG:HD2	1:C:203:TRP:CE2	2.39	0.57
1:D:33:PHE:O	1:D:34:ILE:HD13	2.04	0.57
1:J:16:GLU:HA	1:J:19:TRP:CD1	2.39	0.57
1:A:361:VAL:HG13	1:A:375:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:CD1	1:C:110:LEU:H	2.17	0.57
1:E:156:HIS:NE2	1:F:380:ARG:NH2	2.52	0.57
1:H:326:VAL:HG21	1:H:352:ALA:O	2.04	0.57
1:J:400:VAL:HG23	1:J:400:VAL:O	2.04	0.57
1:E:144:HIS:CE1	1:E:296:ARG:CG	2.88	0.57
1:I:225:HIS:ND1	1:I:226:PRO:HD2	2.18	0.57
1:K:131:ILE:HG12	2:K:501:ACO:C6A	2.34	0.57
1:E:69:LEU:HD12	1:E:69:LEU:O	2.04	0.57
1:I:149:ASP:OD2	1:I:152:PHE:CD1	2.55	0.57
1:B:77:VAL:HB	1:B:78:PRO:HD2	1.86	0.57
1:C:52:VAL:CG2	1:C:110:LEU:CD1	2.55	0.57
1:F:250:VAL:HG23	1:F:251:THR:HG23	1.86	0.57
1:G:16:GLU:HA	1:G:19:TRP:CD1	2.39	0.57
1:H:225:HIS:CG	1:H:226:PRO:HD2	2.40	0.57
1:C:134:ARG:NH1	2:C:501:ACO:C1B	2.67	0.57
1:D:18:ASP:O	1:D:22:MSE:HG3	2.05	0.57
1:G:65:VAL:CG1	1:G:97:HIS:CE1	2.86	0.57
1:I:357:MSE:HE2	1:I:381:LEU:CG	2.31	0.57
1:I:375:LEU:O	1:I:380:ARG:HB2	2.05	0.57
1:K:198:ARG:HG2	1:K:203:TRP:CD1	2.40	0.57
1:B:69:LEU:C	1:B:69:LEU:HD12	2.30	0.57
1:B:193:PRO:O	1:B:402:VAL:HG23	2.05	0.57
1:C:170:ARG:HD2	1:F:63:GLU:CD	2.29	0.57
1:D:127:SER:H	2:D:501:ACO:H21	1.69	0.57
1:E:387:GLN:HE22	1:E:391:ARG:NH2	2.03	0.57
1:H:148:VAL:HG21	1:H:281:LEU:HD21	1.86	0.57
1:G:242:ALA:HB2	1:G:268:MSE:HG3	1.86	0.56
1:I:267:SER:C	1:I:268:MSE:HE2	2.29	0.56
1:H:169:VAL:HG21	1:H:225:HIS:HB2	1.86	0.56
1:A:34:ILE:HB	1:A:37:GLU:OE1	2.05	0.56
1:A:50:GLY:HA2	1:A:70:TYR:CE2	2.40	0.56
1:B:43:ARG:HH11	1:B:43:ARG:HA	1.69	0.56
1:D:16:GLU:O	1:D:19:TRP:HD1	1.88	0.56
1:G:289:ARG:NH1	1:H:298:ASP:CG	2.62	0.56
1:G:311:LEU:N	1:G:311:LEU:HD12	2.20	0.56
1:H:197:LEU:HD12	1:H:198:ARG:H	1.69	0.56
1:H:385:ASP:OD1	1:H:385:ASP:C	2.48	0.56
1:K:158:ASP:OD2	3:K:604:HOH:O	2.17	0.56
1:K:355:ILE:CD1	1:K:381:LEU:HD21	2.34	0.56
1:A:83:LEU:HD21	1:A:313:ALA:HB1	1.86	0.56
1:F:242:ALA:HB3	1:F:271:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:ALA:HA	1:G:230:ALA:O	2.04	0.56
1:K:292:ARG:CG	3:K:605:HOH:O	2.54	0.56
1:K:242:ALA:HB2	1:K:268:MSE:SE	2.55	0.56
1:G:34:ILE:HB	1:G:37:GLU:HG2	1.87	0.56
1:J:217:ASP:HB3	1:J:233:ARG:HD2	1.87	0.56
1:I:323:PHE:CG	1:I:391:ARG:HD3	2.39	0.56
1:D:193:PRO:CG	1:D:400:VAL:CG2	2.84	0.56
1:E:193:PRO:CG	1:E:400:VAL:HG23	2.35	0.56
1:J:142:THR:O	1:J:277:PRO:HD3	2.05	0.56
1:B:144:HIS:CE1	1:B:296:ARG:NH1	2.63	0.56
1:I:225:HIS:CG	1:I:226:PRO:HD2	2.40	0.56
1:I:342:GLY:O	1:I:343:ARG:CG	2.54	0.56
1:I:342:GLY:O	1:I:343:ARG:HG3	2.05	0.56
1:J:41:ALA:CA	1:J:44:THR:HG22	2.36	0.56
1:J:107:CYS:O	1:J:111:HIS:ND1	2.38	0.56
1:K:324:SER:O	1:K:325:THR:HB	2.04	0.56
1:C:267:SER:O	1:C:268:MSE:HE2	2.06	0.56
1:H:196:LEU:HD12	1:H:406:PHE:CE2	2.41	0.56
1:I:150:ARG:HD3	1:I:268:MSE:O	2.06	0.56
1:B:83:LEU:HD21	1:B:313:ALA:HB1	1.87	0.55
1:D:193:PRO:O	1:D:402:VAL:HG23	2.06	0.55
1:I:48:THR:O	1:I:49:ASP:OD1	2.24	0.55
1:J:127:SER:HB3	2:J:501:ACO:H22	1.89	0.55
1:B:52:VAL:CG1	1:B:113:ARG:NH1	2.70	0.55
1:C:83:LEU:HD21	1:C:313:ALA:HB1	1.89	0.55
1:I:296:ARG:HD3	1:J:293:THR:OG1	2.05	0.55
1:A:355:ILE:HD11	1:A:381:LEU:CD1	2.28	0.55
1:D:43:ARG:HA	1:D:43:ARG:NH1	2.16	0.55
1:D:58:ALA:CB	1:H:384:LYS:HG3	2.37	0.55
1:E:43:ARG:HH11	1:E:43:ARG:HA	1.69	0.55
1:E:178:ARG:O	1:E:182:GLU:HG3	2.07	0.55
1:E:208:ALA:O	1:E:211:LYS:HG2	2.06	0.55
1:E:221:PHE:O	1:E:232:TYR:CD1	2.59	0.55
1:J:314:ARG:HD3	1:J:316:TYR:CZ	2.41	0.55
1:K:134:ARG:NH1	2:K:501:ACO:H1B	2.22	0.55
1:A:109:GLU:OE2	1:A:112:ARG:NH2	2.39	0.55
1:A:134:ARG:NH1	2:A:501:ACO:H1B	2.21	0.55
1:H:208:ALA:O	1:H:211:LYS:HG2	2.06	0.55
1:I:356:GLU:OE2	1:I:382:ARG:NE	2.32	0.55
1:K:400:VAL:HG13	1:K:400:VAL:O	2.07	0.55
1:L:33:PHE:O	1:L:34:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:259:TRP:O	1:L:263:ILE:HG12	2.05	0.55
1:B:23:PHE:CE1	1:B:42:TRP:HZ3	2.24	0.55
1:C:153:ALA:HA	1:C:290:LEU:CD1	2.36	0.55
1:F:42:TRP:CD2	1:F:69:LEU:HD21	2.40	0.55
1:F:43:ARG:HA	1:F:43:ARG:HH11	1.71	0.55
1:F:259:TRP:CE2	1:F:281:LEU:HD22	2.42	0.55
1:K:34:ILE:HB	1:K:37:GLU:HG2	1.88	0.55
1:G:355:ILE:HD11	1:G:381:LEU:CD2	2.33	0.55
1:K:192:VAL:CG1	1:K:403:GLN:HB2	2.36	0.55
1:B:150:ARG:CZ	1:B:266:ASP:HA	2.37	0.55
1:C:144:HIS:NE2	1:C:296:ARG:NH1	2.54	0.55
1:C:160:PRO:HG2	1:C:256:CYS:SG	2.46	0.55
1:D:327:LEU:O	1:D:335:PHE:N	2.39	0.55
1:A:35:GLY:N	1:A:36:PRO:HD2	2.22	0.55
1:C:178:ARG:HG3	1:C:207:LEU:HD11	1.89	0.55
1:F:123:ALA:HB1	1:F:300:LEU:HD11	1.89	0.55
1:K:297:GLN:CG	1:L:289:ARG:HD3	2.36	0.55
1:H:146:LEU:CD2	1:H:275:THR:CG2	2.84	0.55
1:J:196:LEU:HG	1:J:405:ALA:HB1	1.88	0.55
1:K:192:VAL:HG11	1:K:403:GLN:CG	2.36	0.55
1:D:148:VAL:HG21	1:D:291:ALA:CB	2.36	0.55
1:I:217:ASP:CG	1:I:233:ARG:HH11	2.14	0.55
1:J:50:GLY:HA2	1:J:70:TYR:CE1	2.41	0.55
1:D:247:LEU:C	1:D:247:LEU:CD2	2.80	0.54
1:H:22:MSE:HE2	1:H:42:TRP:CZ3	2.42	0.54
1:K:160:PRO:HG2	1:K:256:CYS:CB	2.37	0.54
1:L:327:LEU:C	1:L:327:LEU:CD2	2.79	0.54
1:A:123:ALA:HA	1:A:301:TRP:O	2.07	0.54
1:C:88:LEU:HD12	1:C:88:LEU:N	2.22	0.54
1:C:199:PRO:HB2	1:C:201:VAL:HG12	1.89	0.54
1:E:175:THR:HA	1:E:207:LEU:HD11	1.90	0.54
1:J:334:ARG:NH1	1:J:350:ASP:O	2.40	0.54
1:D:400:VAL:HG23	1:D:400:VAL:O	2.07	0.54
1:E:107:CYS:C	1:E:111:HIS:HD1	2.15	0.54
1:H:145:GLU:C	1:H:146:LEU:HD22	2.32	0.54
1:H:188:TRP:CH2	1:H:248:ARG:NH1	2.75	0.54
1:H:196:LEU:CD1	1:H:406:PHE:CE2	2.90	0.54
1:H:212:ALA:HB2	1:H:219:GLU:N	2.21	0.54
1:I:39:ALA:O	1:I:43:ARG:HG2	2.07	0.54
1:J:326:VAL:O	1:J:355:ILE:HG22	2.06	0.54
1:L:381:LEU:HD12	1:L:381:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:CG2	1:A:36:PRO:HD2	2.33	0.54
1:C:367:LEU:O	1:C:402:VAL:HG21	2.08	0.54
1:H:19:TRP:HZ3	1:H:42:TRP:HE3	1.55	0.54
1:H:198:ARG:HG2	1:H:203:TRP:CD1	2.43	0.54
1:I:52:VAL:HG13	1:I:110:LEU:HD23	1.86	0.54
1:J:101:GLY:O	1:J:104:ARG:HB3	2.08	0.54
1:K:381:LEU:C	1:K:381:LEU:CD2	2.79	0.54
1:D:186:GLU:O	1:D:190:GLN:HG3	2.06	0.54
1:F:77:VAL:HB	1:F:78:PRO:HD2	1.90	0.54
1:F:330:SER:O	1:F:331:ASP:HB2	2.07	0.54
1:G:9:VAL:HG11	1:G:102:LEU:HD21	1.90	0.54
1:H:34:ILE:HB	1:H:37:GLU:OE1	2.05	0.54
1:D:148:VAL:HG13	1:D:290:LEU:HB3	1.90	0.54
1:J:98:ARG:NH2	1:J:99:ARG:NH2	2.56	0.54
1:A:34:ILE:HB	1:A:37:GLU:CG	2.37	0.54
1:D:10:THR:CB	1:H:384:LYS:CD	2.86	0.54
1:D:314:ARG:O	1:D:316:TYR:CE1	2.61	0.54
1:K:77:VAL:HB	1:K:78:PRO:HD2	1.90	0.54
1:K:373:SER:HB3	1:K:393:ASP:OD2	2.08	0.54
1:A:98:ARG:HD3	1:F:264:GLY:HA2	1.89	0.54
1:B:41:ALA:O	1:B:45:LEU:N	2.35	0.54
1:C:148:VAL:HG13	1:C:290:LEU:HB3	1.90	0.54
1:D:44:THR:HG21	1:D:201:VAL:HG11	1.90	0.54
1:E:248:ARG:NH2	1:E:405:ALA:O	2.41	0.54
1:F:144:HIS:CE1	1:F:296:ARG:HH12	2.23	0.54
1:G:74:ARG:HD3	1:G:84:PRO:HA	1.89	0.54
1:G:103:LEU:HD22	2:G:501:ACO:H133	1.90	0.54
1:I:44:THR:C	1:I:45:LEU:HD23	2.24	0.54
1:A:297:GLN:HG3	1:B:289:ARG:HD3	1.88	0.54
1:C:247:LEU:HD23	1:C:248:ARG:N	2.23	0.54
1:D:304:ILE:O	1:D:359:ARG:NH1	2.40	0.54
1:B:19:TRP:N	1:B:20:PRO:HD2	2.23	0.54
1:C:145:GLU:HB3	1:C:295:TRP:HB3	1.82	0.54
1:E:192:VAL:HG11	1:E:403:GLN:CB	2.35	0.54
1:H:247:LEU:HD23	1:H:248:ARG:N	2.23	0.54
1:I:42:TRP:CD1	1:I:42:TRP:N	2.74	0.54
1:K:203:TRP:O	1:K:207:LEU:HD22	2.07	0.54
1:L:123:ALA:HB1	1:L:300:LEU:HD11	1.88	0.54
1:A:314:ARG:HH22	1:A:396:PHE:C	2.15	0.53
1:E:22:MSE:HE2	1:E:67:MSE:HE3	1.88	0.53
1:H:34:ILE:O	1:H:37:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:LEU:HD12	1:H:273:ILE:CD1	2.38	0.53
1:A:45:LEU:CD1	1:A:71:MSE:CE	2.85	0.53
1:B:98:ARG:HD2	1:D:264:GLY:HA3	1.90	0.53
1:G:311:LEU:HD12	1:G:311:LEU:H	1.73	0.53
1:J:72:ASP:O	1:J:73:LEU:HD23	2.07	0.53
1:J:77:VAL:HB	1:J:78:PRO:HD2	1.89	0.53
1:D:225:HIS:CE1	1:D:226:PRO:HD2	2.44	0.53
1:E:387:GLN:NE2	1:E:391:ARG:NH2	2.57	0.53
1:F:192:VAL:CG1	1:F:403:GLN:HB2	2.36	0.53
1:I:192:VAL:HG11	1:I:403:GLN:HB2	1.90	0.53
1:B:42:TRP:NE1	1:B:90:PHE:CD2	2.70	0.53
1:E:74:ARG:HD3	1:E:84:PRO:HA	1.90	0.53
1:E:381:LEU:C	1:E:381:LEU:HD12	2.34	0.53
1:I:293:THR:HB	1:J:296:ARG:HB3	1.89	0.53
1:K:169:VAL:HG22	1:K:225:HIS:HB2	1.91	0.53
1:B:178:ARG:HH11	1:B:207:LEU:HD12	1.71	0.53
1:D:121:VAL:HG12	1:D:304:ILE:HA	1.91	0.53
1:D:381:LEU:HD11	1:D:389:LEU:HD21	1.90	0.53
1:E:146:LEU:HB2	1:E:273:ILE:HG23	1.90	0.53
1:F:197:LEU:O	1:F:199:PRO:HD3	2.09	0.53
1:G:188:TRP:CZ2	1:G:248:ARG:NH1	2.77	0.53
1:D:16:GLU:HA	1:D:19:TRP:NE1	2.24	0.53
1:E:355:ILE:HG13	1:E:382:ARG:O	2.09	0.53
1:G:259:TRP:O	1:G:263:ILE:HG12	2.09	0.53
2:G:501:ACO:O8A	2:G:501:ACO:H4B	2.08	0.53
1:H:144:HIS:HD2	1:H:277:PRO:HG3	1.66	0.53
1:B:100:ARG:NH2	1:D:167:SER:OG	2.42	0.53
1:C:259:TRP:CE2	1:C:281:LEU:HD22	2.44	0.53
1:D:181:PHE:HD1	1:D:229:TYR:CG	2.26	0.53
1:D:259:TRP:CE2	1:D:281:LEU:HD22	2.44	0.53
1:E:144:HIS:HE1	1:E:296:ARG:CD	2.20	0.53
1:K:244:VAL:HB	1:K:273:ILE:CD1	2.15	0.53
1:L:48:THR:O	1:L:49:ASP:OD1	2.26	0.53
1:E:107:CYS:HB3	1:E:111:HIS:CE1	2.44	0.53
1:E:297:GLN:HG2	1:E:298:ASP:N	2.24	0.53
1:H:98:ARG:NE	1:H:99:ARG:CZ	2.71	0.53
1:B:23:PHE:HE1	1:B:42:TRP:CZ3	2.26	0.53
1:C:89:SER:O	1:C:90:PHE:HB2	2.09	0.53
1:D:63:GLU:CD	1:E:170:ARG:HD2	2.34	0.53
1:E:143:LEU:HD21	1:E:404:THR:CB	2.39	0.53
1:I:114:ILE:HG22	1:I:305:MSE:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:ARG:CD	1:J:297:GLN:CG	2.80	0.53
1:L:145:GLU:HB3	1:L:295:TRP:HB3	1.89	0.53
1:F:43:ARG:HH11	1:F:43:ARG:CA	2.22	0.53
1:F:314:ARG:O	1:F:316:TYR:CE1	2.62	0.53
1:G:192:VAL:HG11	1:G:403:GLN:HB2	1.90	0.53
1:I:44:THR:O	1:I:44:THR:CG2	2.56	0.53
1:J:34:ILE:HG22	1:J:36:PRO:CG	2.38	0.53
1:F:77:VAL:HB	1:F:78:PRO:CD	2.39	0.52
1:F:198:ARG:HD2	1:F:203:TRP:CE2	2.44	0.52
1:G:372:ALA:HB1	1:G:381:LEU:HD13	1.91	0.52
1:J:330:SER:O	1:J:331:ASP:HB2	2.09	0.52
1:L:34:ILE:HG23	1:L:36:PRO:HD2	1.89	0.52
1:A:45:LEU:HD12	1:A:71:MSE:CE	2.39	0.52
1:A:199:PRO:HD2	1:A:202:LEU:HD12	1.90	0.52
1:B:98:ARG:HD2	1:D:264:GLY:HA2	1.92	0.52
1:B:355:ILE:HD11	1:B:381:LEU:HD21	1.90	0.52
1:D:98:ARG:CD	1:E:264:GLY:HA2	2.39	0.52
1:F:22:MSE:HE1	1:F:42:TRP:HZ2	1.65	0.52
1:F:39:ALA:O	1:F:43:ARG:HG2	2.08	0.52
1:G:150:ARG:HG2	1:G:269:GLU:O	2.09	0.52
1:I:289:ARG:HG3	1:J:298:ASP:OD1	2.09	0.52
1:I:372:ALA:HB3	1:I:393:ASP:OD1	2.09	0.52
1:I:390:ARG:HD3	1:J:399:ASP:OD2	2.08	0.52
1:I:400:VAL:HG23	1:I:400:VAL:O	2.08	0.52
1:J:19:TRP:N	1:J:20:PRO:HD2	2.24	0.52
1:A:127:SER:HB3	2:A:501:ACO:H22	1.89	0.52
1:B:145:GLU:C	1:B:146:LEU:HD12	2.34	0.52
1:D:8:THR:N	1:H:353:ALA:HB3	2.24	0.52
1:E:381:LEU:HD12	1:E:381:LEU:O	2.10	0.52
1:I:289:ARG:CZ	1:J:297:GLN:OE1	2.57	0.52
1:J:193:PRO:CG	1:J:400:VAL:CG2	2.86	0.52
1:A:42:TRP:HA	1:A:46:VAL:HG23	1.92	0.52
1:A:156:HIS:CE1	1:B:380:ARG:NH1	2.78	0.52
1:B:85:THR:CG2	1:B:86:ALA:N	2.72	0.52
1:B:145:GLU:OE2	1:B:295:TRP:HB3	2.08	0.52
1:B:326:VAL:HB	1:B:354:GLU:H	1.75	0.52
1:C:146:LEU:HD12	1:C:292:ARG:O	2.10	0.52
1:K:307:VAL:HB	1:K:308:PRO:HD3	1.92	0.52
1:B:381:LEU:C	1:B:381:LEU:CD2	2.83	0.52
1:D:63:GLU:OE1	1:E:170:ARG:HD2	2.10	0.52
1:E:110:LEU:O	1:E:114:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:MSE:O	1:F:73:LEU:CD1	2.58	0.52
1:F:192:VAL:HG11	1:F:403:GLN:CB	2.39	0.52
1:G:123:ALA:CB	1:G:302:LEU:HD23	2.39	0.52
1:G:406:PHE:O	3:G:629:HOH:O	2.18	0.52
1:H:247:LEU:HD23	1:H:247:LEU:C	2.34	0.52
1:H:339:ILE:HG12	1:H:344:ALA:HB2	1.90	0.52
1:J:207:LEU:HD12	1:J:207:LEU:N	2.24	0.52
1:K:98:ARG:HE	1:K:99:ARG:NH2	2.08	0.52
1:C:180:GLU:O	1:C:184:ILE:HG13	2.09	0.52
2:E:501:ACO:H4B	2:E:501:ACO:O8A	2.08	0.52
1:F:361:VAL:HG13	1:F:375:LEU:HD13	1.90	0.52
1:H:145:GLU:OE2	1:H:295:TRP:CB	2.58	0.52
1:I:198:ARG:NH1	1:I:206:LEU:CD1	2.73	0.52
1:I:293:THR:OG1	1:J:296:ARG:HD3	2.10	0.52
1:K:311:LEU:O	1:K:316:TYR:OH	2.13	0.52
1:A:121:VAL:HA	1:A:305:MSE:HG2	1.90	0.52
2:B:501:ACO:H4B	2:B:501:ACO:O8A	2.10	0.52
1:D:107:CYS:O	1:D:111:HIS:ND1	2.39	0.52
1:E:196:LEU:HD12	1:E:405:ALA:HB3	1.91	0.52
1:E:360:ASP:CG	1:E:380:ARG:HH22	2.17	0.52
1:F:98:ARG:HH11	1:F:99:ARG:HH21	1.57	0.52
1:J:52:VAL:HG12	1:J:110:LEU:HD21	1.90	0.52
1:C:316:TYR:O	1:C:342:GLY:HA2	2.10	0.52
1:F:73:LEU:N	1:F:73:LEU:CD1	2.73	0.52
1:I:318:HIS:C	1:I:320:VAL:H	2.18	0.52
1:B:197:LEU:O	1:B:199:PRO:HD3	2.09	0.52
1:D:402:VAL:HG12	3:D:621:HOH:O	2.09	0.52
1:E:141:THR:HG22	1:E:402:VAL:HG11	1.93	0.52
1:F:120:PRO:O	1:F:305:MSE:HB2	2.10	0.52
1:F:133:GLY:HA2	1:F:137:TYR:O	2.10	0.52
1:G:98:ARG:HD2	1:L:264:GLY:HA2	1.88	0.52
1:I:52:VAL:CG1	1:I:110:LEU:HD23	2.39	0.52
1:B:155:PHE:CZ	1:B:260:ARG:HA	2.44	0.51
1:I:178:ARG:HD2	1:I:207:LEU:HD11	1.92	0.51
1:I:200:GLN:HE21	1:I:200:GLN:CA	2.15	0.51
1:A:276:HIS:HB2	1:A:277:PRO:HD2	1.92	0.51
1:A:314:ARG:NH2	1:A:396:PHE:C	2.68	0.51
1:B:24:LEU:HD13	1:D:173:ARG:CG	2.37	0.51
1:B:330:SER:O	1:B:331:ASP:HB2	2.09	0.51
1:D:250:VAL:HG12	1:D:250:VAL:O	2.09	0.51
1:G:98:ARG:HD2	1:L:264:GLY:HA3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:HIS:CD2	1:H:277:PRO:CG	2.88	0.51
1:H:281:LEU:O	1:H:282:PRO:C	2.54	0.51
1:B:178:ARG:CG	1:B:207:LEU:HD11	2.40	0.51
1:B:219:GLU:HG3	3:B:623:HOH:O	2.09	0.51
1:C:357:MSE:CG	1:C:381:LEU:HD13	2.40	0.51
1:G:43:ARG:HA	1:G:43:ARG:NH1	2.21	0.51
1:I:23:PHE:CE1	1:I:38:SER:OG	2.56	0.51
1:K:225:HIS:CG	1:K:226:PRO:HD2	2.46	0.51
1:A:314:ARG:HG2	1:A:315:GLY:O	2.10	0.51
1:A:381:LEU:HD12	1:A:381:LEU:O	2.11	0.51
1:C:74:ARG:HD3	1:C:84:PRO:HA	1.93	0.51
1:E:156:HIS:HE2	1:F:380:ARG:NH2	2.08	0.51
1:E:181:PHE:HD1	1:E:229:TYR:CG	2.29	0.51
1:F:392:LEU:O	1:F:393:ASP:C	2.53	0.51
1:H:98:ARG:NE	1:H:99:ARG:NH1	2.57	0.51
1:I:208:ALA:O	1:I:211:LYS:HG2	2.10	0.51
1:I:323:PHE:CD2	1:I:391:ARG:HD3	2.45	0.51
1:K:314:ARG:HH11	1:K:314:ARG:HG2	1.74	0.51
1:A:145:GLU:C	1:A:146:LEU:HD12	2.36	0.51
1:B:200:GLN:HA	1:B:200:GLN:NE2	2.25	0.51
1:F:247:LEU:HD23	1:F:248:ARG:N	2.25	0.51
1:I:323:PHE:CE2	1:I:391:ARG:HB3	2.45	0.51
1:I:355:ILE:HD11	1:I:381:LEU:HD21	1.93	0.51
1:L:314:ARG:HD3	1:L:315:GLY:O	2.11	0.51
1:C:120:PRO:C	1:C:305:MSE:HB2	2.35	0.51
1:D:150:ARG:NE	1:D:265:LEU:O	2.44	0.51
1:D:208:ALA:O	1:D:211:LYS:HG2	2.10	0.51
1:H:109:GLU:C	1:H:112:ARG:HG2	2.33	0.51
1:B:42:TRP:CZ2	1:B:90:PHE:CD1	2.99	0.51
1:C:150:ARG:HH21	1:C:266:ASP:CA	2.13	0.51
1:C:340:GLY:O	1:C:341:ASP:HB2	2.11	0.51
1:D:148:VAL:HG22	1:D:291:ALA:HA	0.56	0.51
1:H:107:CYS:HB3	1:H:111:HIS:HE1	1.76	0.51
1:I:247:LEU:C	1:I:247:LEU:CD2	2.83	0.51
1:A:45:LEU:CD1	1:A:71:MSE:HE2	2.40	0.51
1:A:98:ARG:CD	1:F:264:GLY:HA2	2.41	0.51
1:B:34:ILE:HB	1:B:37:GLU:OE1	2.11	0.51
1:C:327:LEU:O	1:C:335:PHE:N	2.44	0.51
1:G:284:LEU:HD23	1:H:378:ALA:HB1	1.92	0.51
1:G:289:ARG:NE	1:H:297:GLN:OE1	2.43	0.51
1:I:251:THR:O	1:I:252:ALA:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:ARG:CD	1:J:207:LEU:HD21	2.38	0.51
1:F:39:ALA:O	1:F:43:ARG:CG	2.59	0.51
1:F:144:HIS:CD2	1:F:296:ARG:NH1	2.68	0.51
1:F:260:ARG:HG2	1:F:260:ARG:HH11	1.76	0.51
1:G:184:ILE:HG21	1:G:228:GLY:HA2	1.91	0.51
1:H:354:GLU:CB	1:H:384:LYS:HZ3	2.24	0.51
1:I:317:ALA:HB3	1:I:394:ALA:O	2.11	0.51
1:I:342:GLY:C	1:I:343:ARG:HG3	2.36	0.51
1:E:128:GLU:HA	1:F:289:ARG:NH2	2.26	0.51
1:G:33:PHE:C	1:G:34:ILE:HG13	2.35	0.51
1:I:178:ARG:CG	1:I:207:LEU:HD11	2.41	0.51
1:I:355:ILE:HG13	1:I:383:THR:HB	1.92	0.51
1:J:41:ALA:CA	1:J:44:THR:CG2	2.89	0.51
1:B:144:HIS:HB3	1:B:146:LEU:CD1	2.39	0.50
1:B:247:LEU:O	1:B:248:ARG:HD3	2.11	0.50
1:C:357:MSE:HB3	1:C:381:LEU:HD12	1.90	0.50
1:D:199:PRO:O	1:D:200:GLN:C	2.54	0.50
1:E:341:ASP:OD2	1:E:343:ARG:NH2	2.44	0.50
1:G:93:VAL:HG23	2:G:501:ACO:H132	1.93	0.50
1:I:114:ILE:HG23	1:I:119:TYR:HB2	1.92	0.50
1:I:197:LEU:HD12	1:I:198:ARG:H	1.77	0.50
1:I:311:LEU:HD13	1:I:337:LEU:HD22	1.93	0.50
2:K:501:ACO:H52A	3:K:622:HOH:O	2.10	0.50
1:A:18:ASP:O	1:A:19:TRP:C	2.54	0.50
1:G:375:LEU:HD21	1:H:283:HIS:CE1	2.46	0.50
1:I:369:ALA:HB2	1:I:402:VAL:HG11	1.93	0.50
1:J:263:ILE:O	1:J:263:ILE:HG22	2.11	0.50
1:B:34:ILE:HB	1:B:37:GLU:CG	2.41	0.50
1:F:16:GLU:O	1:F:19:TRP:CD1	2.64	0.50
1:F:34:ILE:HG22	1:F:36:PRO:CG	2.40	0.50
1:F:127:SER:HB3	2:F:501:ACO:H22	1.94	0.50
1:F:247:LEU:HD23	1:F:247:LEU:C	2.35	0.50
1:F:379:ASN:ND2	1:F:382:ARG:HD3	2.26	0.50
1:G:104:ARG:HG3	1:G:135:PHE:HE1	1.77	0.50
1:G:250:VAL:O	1:G:250:VAL:CG1	2.59	0.50
1:G:289:ARG:HG3	1:H:129:GLY:HA3	1.91	0.50
1:J:247:LEU:C	1:J:247:LEU:CD2	2.84	0.50
1:K:38:SER:O	1:K:39:ALA:C	2.55	0.50
1:K:198:ARG:HD2	1:K:203:TRP:CE2	2.47	0.50
1:K:247:LEU:C	1:K:247:LEU:CD2	2.85	0.50
1:D:148:VAL:CG2	1:D:291:ALA:CB	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ASP:C	1:F:49:ASP:OD1	2.54	0.50
1:J:98:ARG:HD2	1:K:264:GLY:HA3	1.93	0.50
1:C:198:ARG:NH1	1:C:206:LEU:CD1	2.75	0.50
1:E:156:HIS:HE2	1:F:380:ARG:HH22	1.59	0.50
1:G:385:ASP:OD1	1:G:387:GLN:N	2.45	0.50
1:K:16:GLU:HA	1:K:19:TRP:CD1	2.46	0.50
1:C:373:SER:HB3	1:C:393:ASP:OD2	2.11	0.50
1:J:405:ALA:N	3:J:602:HOH:O	2.09	0.50
1:L:334:ARG:HD2	1:L:351:ALA:O	2.11	0.50
1:A:69:LEU:C	1:A:69:LEU:HD12	2.37	0.50
1:A:385:ASP:C	1:A:385:ASP:OD1	2.54	0.50
1:C:178:ARG:HH21	1:C:200:GLN:HE21	1.57	0.50
1:C:293:THR:N	3:C:604:HOH:O	2.03	0.50
1:C:295:TRP:HZ2	1:C:297:GLN:NE2	2.08	0.50
1:D:181:PHE:HD1	1:D:229:TYR:CD2	2.30	0.50
1:E:187:ARG:NH2	1:E:250:VAL:HG21	2.27	0.50
1:E:192:VAL:HG11	1:E:403:GLN:CG	2.42	0.50
1:E:341:ASP:OD1	1:E:341:ASP:O	2.30	0.50
1:F:16:GLU:O	1:F:19:TRP:HD1	1.95	0.50
1:G:185:TYR:CD1	1:G:185:TYR:C	2.89	0.50
1:H:247:LEU:O	1:H:248:ARG:HD3	2.11	0.50
1:J:225:HIS:CG	1:J:226:PRO:HD2	2.46	0.50
1:J:297:GLN:HG2	1:J:298:ASP:N	2.26	0.50
1:K:192:VAL:HG11	1:K:403:GLN:CB	2.42	0.50
1:G:9:VAL:HG12	1:G:54:VAL:HG13	1.92	0.50
1:G:172:VAL:HB	1:G:177:HIS:CD2	2.47	0.50
1:I:107:CYS:HB3	1:I:111:HIS:HE1	1.75	0.50
1:I:141:THR:HG22	1:I:402:VAL:HG21	1.92	0.50
1:J:339:ILE:HG12	1:J:344:ALA:CB	2.40	0.50
1:L:178:ARG:HG3	1:L:207:LEU:HD21	1.94	0.50
1:B:34:ILE:HB	1:B:37:GLU:CD	2.37	0.50
1:C:326:VAL:HG21	1:C:352:ALA:O	2.11	0.50
1:E:85:THR:HG23	1:E:121:VAL:HG23	1.93	0.50
1:F:148:VAL:HG13	1:F:271:ILE:HB	1.94	0.50
1:G:9:VAL:HG11	1:G:54:VAL:HG11	1.93	0.50
1:H:34:ILE:O	1:H:37:GLU:CG	2.60	0.50
1:H:98:ARG:HD2	1:J:266:ASP:OD2	2.12	0.50
1:C:325:THR:OG1	1:C:326:VAL:N	2.45	0.49
1:D:48:THR:O	1:D:49:ASP:OD1	2.30	0.49
1:E:400:VAL:HG23	1:E:400:VAL:O	2.11	0.49
1:G:16:GLU:HA	1:G:19:TRP:NE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:381:LEU:CD2	1:G:381:LEU:O	2.59	0.49
1:H:42:TRP:CH2	1:H:67:MSE:HE1	2.47	0.49
1:K:334:ARG:HD2	1:K:351:ALA:O	2.12	0.49
1:A:336:ALA:O	1:A:346:CYS:HA	2.12	0.49
1:B:266:ASP:H	1:E:98:ARG:HH11	1.59	0.49
1:D:178:ARG:NH1	1:D:207:LEU:HD12	2.27	0.49
1:E:88:LEU:N	1:E:88:LEU:HD12	2.27	0.49
1:F:98:ARG:NE	1:F:99:ARG:NH2	2.55	0.49
1:G:48:THR:O	1:G:49:ASP:OD1	2.30	0.49
1:I:77:VAL:HB	1:I:78:PRO:CD	2.42	0.49
1:L:182:GLU:HA	1:L:203:TRP:CZ2	2.47	0.49
1:A:73:LEU:CB	1:A:85:THR:O	2.59	0.49
1:A:173:ARG:CG	1:C:24:LEU:HD13	2.42	0.49
1:B:150:ARG:HG2	1:B:269:GLU:C	2.37	0.49
1:B:307:VAL:HB	1:B:308:PRO:HD3	1.94	0.49
1:C:266:ASP:OD2	1:F:98:ARG:HD2	2.12	0.49
1:F:259:TRP:CZ2	1:F:281:LEU:HD22	2.48	0.49
1:H:188:TRP:CZ2	1:H:248:ARG:NH1	2.80	0.49
1:H:292:ARG:HA	3:H:605:HOH:O	2.13	0.49
1:C:145:GLU:HG2	1:C:274:ILE:HD13	1.95	0.49
1:C:326:VAL:HB	1:C:354:GLU:H	1.76	0.49
1:F:19:TRP:N	1:F:20:PRO:HD2	2.26	0.49
1:H:145:GLU:CB	1:H:295:TRP:HB3	2.41	0.49
1:J:76:THR:O	1:J:193:PRO:HA	2.12	0.49
1:A:79:GLY:O	1:A:80:GLU:HB2	2.12	0.49
1:F:121:VAL:HG12	1:F:305:MSE:H	1.76	0.49
1:G:150:ARG:HG2	1:G:269:GLU:C	2.38	0.49
1:I:276:HIS:HD2	1:I:278:GLN:N	2.08	0.49
1:I:323:PHE:HB3	1:I:391:ARG:NH1	2.25	0.49
1:I:355:ILE:HD11	1:I:381:LEU:CD2	2.42	0.49
1:J:83:LEU:HD11	1:J:313:ALA:CB	2.42	0.49
1:D:172:VAL:HB	1:D:177:HIS:CD2	2.48	0.49
1:D:223:LEU:HD13	1:D:261:ALA:HB1	1.95	0.49
1:F:42:TRP:CD1	1:F:69:LEU:HD22	2.34	0.49
1:F:141:THR:HG22	1:F:402:VAL:HG11	1.93	0.49
1:H:34:ILE:CB	1:H:37:GLU:CG	2.58	0.49
1:K:10:THR:O	1:K:54:VAL:HA	2.12	0.49
1:L:150:ARG:NH1	1:L:263:ILE:O	2.43	0.49
1:L:381:LEU:HD11	1:L:389:LEU:HD21	1.95	0.49
1:B:231:LEU:HB2	1:B:245:SER:OG	2.11	0.49
1:C:155:PHE:CE2	1:C:260:ARG:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:ALA:HB2	1:G:302:LEU:HD23	1.95	0.49
1:H:147:THR:OG1	1:H:294:THR:HG21	2.12	0.49
1:K:51:ALA:HA	1:K:69:LEU:HB3	1.94	0.49
1:D:148:VAL:HG13	1:D:290:LEU:CB	2.42	0.49
1:E:16:GLU:HA	1:E:19:TRP:CD1	2.46	0.49
1:E:72:ASP:O	1:E:73:LEU:HD23	2.12	0.49
1:F:35:GLY:N	1:F:36:PRO:CD	2.75	0.49
1:F:303:ARG:HD3	1:F:305:MSE:SE	2.62	0.49
1:G:98:ARG:CD	1:L:264:GLY:CA	2.86	0.49
1:H:295:TRP:CH2	1:H:297:GLN:NE2	2.66	0.49
1:J:98:ARG:HD2	1:K:264:GLY:HA2	1.93	0.49
1:A:320:VAL:HG21	1:A:394:ALA:HB3	1.94	0.49
1:D:150:ARG:NE	1:D:268:MSE:O	2.46	0.49
1:E:198:ARG:CZ	1:E:206:LEU:HD12	2.43	0.49
1:F:150:ARG:CZ	1:F:266:ASP:HA	2.43	0.49
1:H:33:PHE:CZ	1:H:38:SER:OG	2.55	0.49
1:B:145:GLU:OE2	1:B:295:TRP:HB2	2.12	0.49
1:C:50:GLY:HA2	1:C:70:TYR:CE1	2.48	0.49
1:E:114:ILE:HG22	1:E:119:TYR:HB2	1.94	0.49
1:E:247:LEU:C	1:E:247:LEU:CD2	2.86	0.49
1:F:295:TRP:HZ2	1:F:297:GLN:NE2	2.11	0.49
1:F:311:LEU:HD21	1:F:362:LEU:HD11	1.95	0.49
1:G:54:VAL:HG11	1:G:102:LEU:HD22	1.95	0.49
1:I:178:ARG:HG3	1:I:207:LEU:HD11	1.95	0.49
1:J:169:VAL:HG11	1:J:223:LEU:HB3	1.95	0.49
1:A:125:HIS:HE1	3:A:618:HOH:O	1.94	0.48
1:B:42:TRP:HD1	1:B:71:MSE:HE3	1.78	0.48
1:C:134:ARG:CZ	2:C:501:ACO:H1B	2.43	0.48
1:D:144:HIS:CD2	1:D:277:PRO:CG	2.92	0.48
1:E:314:ARG:HD3	1:E:316:TYR:CE2	2.48	0.48
1:H:144:HIS:NE2	1:H:277:PRO:HG3	2.27	0.48
1:H:170:ARG:O	1:H:172:VAL:HG13	2.11	0.48
1:H:297:GLN:HG2	1:H:298:ASP:N	2.28	0.48
1:J:43:ARG:NH1	1:J:43:ARG:CA	2.69	0.48
1:J:357:MSE:HE1	1:J:362:LEU:CA	2.42	0.48
1:K:360:ASP:OD2	1:K:380:ARG:NH2	2.45	0.48
1:L:311:LEU:HD21	1:L:362:LEU:HD11	1.95	0.48
2:B:501:ACO:O5P	2:B:501:ACO:H141	2.13	0.48
1:C:200:GLN:NE2	1:C:200:GLN:HA	2.28	0.48
1:G:11:LEU:HD12	1:G:52:VAL:CG2	2.37	0.48
1:G:114:ILE:HG22	1:G:305:MSE:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:VAL:HB	1:G:308:PRO:HD3	1.95	0.48
1:I:178:ARG:CD	1:I:207:LEU:HD11	2.42	0.48
1:K:229:TYR:N	1:K:248:ARG:O	2.45	0.48
1:K:297:GLN:HG3	1:L:289:ARG:HD3	1.94	0.48
1:B:48:THR:O	1:B:49:ASP:OD1	2.30	0.48
1:B:65:VAL:HG11	1:B:97:HIS:CE1	2.48	0.48
1:B:148:VAL:HG13	1:B:290:LEU:O	2.14	0.48
1:D:148:VAL:HG21	1:D:291:ALA:CA	2.26	0.48
1:E:148:VAL:HG21	1:E:281:LEU:HD21	1.95	0.48
1:F:46:VAL:CG2	1:F:69:LEU:HD13	2.44	0.48
1:G:48:THR:O	1:G:49:ASP:CG	2.56	0.48
1:I:70:TYR:HB3	1:I:88:LEU:HD23	1.94	0.48
1:I:227:ASP:HB3	1:I:250:VAL:HG22	1.95	0.48
1:J:146:LEU:O	1:J:272:SER:HA	2.13	0.48
1:J:184:ILE:HG21	1:J:229:TYR:HD1	1.78	0.48
1:K:103:LEU:HB2	2:K:501:ACO:O6A	2.14	0.48
1:K:383:THR:HG21	1:K:389:LEU:HG	1.94	0.48
1:A:145:GLU:HB3	1:A:295:TRP:CB	2.38	0.48
1:A:360:ASP:CG	1:A:380:ARG:HH22	2.21	0.48
1:C:239:LEU:O	1:C:268:MSE:HE1	2.13	0.48
1:G:140:ALA:O	1:G:369:ALA:HB2	2.13	0.48
1:H:34:ILE:CG1	1:H:37:GLU:OE1	2.61	0.48
1:J:77:VAL:HB	1:J:78:PRO:CD	2.43	0.48
1:K:316:TYR:CE1	1:K:344:ALA:HB2	2.48	0.48
1:C:155:PHE:CZ	1:C:260:ARG:HA	2.48	0.48
1:D:137:TYR:O	1:D:360:ASP:HB2	2.13	0.48
1:E:69:LEU:HD12	1:E:69:LEU:C	2.39	0.48
1:G:222:ALA:CB	1:G:231:LEU:CD2	2.75	0.48
1:I:398:SER:OG	1:I:400:VAL:O	2.30	0.48
1:B:326:VAL:CG1	1:B:353:ALA:HA	2.44	0.48
1:C:150:ARG:HD3	1:C:265:LEU:O	2.13	0.48
1:C:307:VAL:HB	1:C:308:PRO:HD3	1.96	0.48
1:D:33:PHE:O	1:D:34:ILE:CD1	2.62	0.48
1:D:59:GLY:O	1:D:60:PRO:C	2.57	0.48
1:F:144:HIS:CE1	1:F:296:ARG:NH1	2.67	0.48
1:H:34:ILE:C	1:H:37:GLU:HG2	2.38	0.48
1:H:145:GLU:OE2	1:H:295:TRP:HB3	2.14	0.48
1:I:69:LEU:C	1:I:69:LEU:HD12	2.38	0.48
1:J:281:LEU:O	1:J:282:PRO:C	2.54	0.48
1:J:295:TRP:CZ2	1:J:297:GLN:HB3	2.49	0.48
1:B:42:TRP:NE1	1:B:90:PHE:CZ	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:CD	1:D:264:GLY:HA2	2.43	0.48
1:D:9:VAL:O	1:H:352:ALA:HB1	2.14	0.48
1:E:144:HIS:NE2	1:E:277:PRO:HG3	2.29	0.48
1:F:74:ARG:HB3	1:F:82:VAL:HG11	1.95	0.48
1:F:139:PRO:HD3	1:F:301:TRP:CZ3	2.49	0.48
1:G:133:GLY:HA2	1:G:137:TYR:O	2.13	0.48
1:I:70:TYR:HA	1:I:87:GLY:O	2.14	0.48
1:J:404:THR:HG22	1:J:405:ALA:O	2.14	0.48
1:A:144:HIS:HB3	1:A:146:LEU:HD11	1.95	0.48
1:A:263:ILE:HG22	1:A:263:ILE:O	2.13	0.48
1:B:34:ILE:CG2	1:B:36:PRO:HD2	2.44	0.48
1:B:371:ARG:NH2	3:B:652:HOH:O	2.46	0.48
1:D:19:TRP:N	1:D:20:PRO:HD2	2.28	0.48
1:D:88:LEU:HD11	1:D:137:TYR:OH	2.13	0.48
1:F:306:ASN:HB3	1:F:309:ALA:HB3	1.95	0.48
1:G:360:ASP:OD2	1:G:380:ARG:NH2	2.46	0.48
1:K:169:VAL:HG12	1:K:170:ARG:N	2.27	0.48
1:F:71:MSE:HB2	1:F:73:LEU:CD1	2.37	0.48
1:I:133:GLY:C	1:I:135:PHE:H	2.22	0.48
1:J:338:LYS:O	1:J:344:ALA:HA	2.13	0.48
1:K:69:LEU:HD12	1:K:69:LEU:C	2.38	0.48
1:D:400:VAL:CG2	1:D:400:VAL:O	2.62	0.48
1:I:134:ARG:CZ	2:I:501:ACO:H1B	2.44	0.48
1:J:141:THR:HG22	1:J:402:VAL:HG21	1.95	0.48
1:L:307:VAL:HB	1:L:308:PRO:HD3	1.95	0.48
1:C:303:ARG:HH11	1:C:305:MSE:SE	2.47	0.47
1:D:334:ARG:HD3	1:D:351:ALA:O	2.14	0.47
1:F:74:ARG:HD3	1:F:84:PRO:HA	1.95	0.47
1:F:367:LEU:O	1:F:402:VAL:CG2	2.62	0.47
1:G:225:HIS:O	1:G:226:PRO:C	2.56	0.47
1:G:379:ASN:OD1	1:G:382:ARG:HG2	2.14	0.47
1:H:34:ILE:CA	1:H:37:GLU:HG2	2.43	0.47
1:I:148:VAL:CB	1:I:290:LEU:O	2.62	0.47
1:I:296:ARG:HB3	1:J:293:THR:HB	1.95	0.47
1:A:184:ILE:HG21	1:A:228:GLY:HA2	1.96	0.47
1:C:266:ASP:C	1:C:268:MSE:H	2.22	0.47
1:G:8:THR:O	1:G:57:GLY:N	2.46	0.47
1:I:44:THR:HG21	1:I:201:VAL:HB	1.96	0.47
1:J:155:PHE:CZ	1:J:260:ARG:HA	2.49	0.47
1:K:103:LEU:HD22	2:K:501:ACO:H121	1.95	0.47
1:A:21:GLY:HA3	1:A:64:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:LEU:HB3	1:C:282:PRO:HD3	1.96	0.47
1:D:8:THR:N	1:H:353:ALA:N	2.47	0.47
1:D:225:HIS:ND1	1:D:226:PRO:HD2	2.29	0.47
1:F:289:ARG:O	1:F:290:LEU:C	2.57	0.47
1:I:14:PRO:HD2	1:I:51:ALA:O	2.14	0.47
1:J:145:GLU:HB3	1:J:295:TRP:HB3	1.96	0.47
1:K:314:ARG:NH1	1:K:314:ARG:CG	2.72	0.47
1:L:33:PHE:CD1	1:L:34:ILE:N	2.82	0.47
1:B:247:LEU:C	1:B:247:LEU:CD2	2.87	0.47
1:D:8:THR:N	1:H:353:ALA:CB	2.78	0.47
1:D:10:THR:CG2	1:H:384:LYS:HE3	2.44	0.47
1:E:192:VAL:CG1	1:E:403:GLN:HB2	2.39	0.47
1:G:248:ARG:HH22	1:G:405:ALA:C	2.22	0.47
1:H:98:ARG:HH21	1:H:99:ARG:HH21	1.52	0.47
1:I:289:ARG:HG2	1:J:298:ASP:OD1	2.13	0.47
1:J:218:ARG:HH21	1:J:239:LEU:HD21	1.79	0.47
1:K:297:GLN:CD	1:L:289:ARG:HD3	2.39	0.47
1:A:326:VAL:HG21	1:A:351:ALA:HB3	1.95	0.47
1:B:40:THR:O	1:B:44:THR:OG1	2.30	0.47
1:B:150:ARG:NH2	1:B:266:ASP:OD1	2.48	0.47
1:D:42:TRP:NE1	1:D:90:PHE:CE1	2.77	0.47
1:F:109:GLU:O	1:F:113:ARG:HG3	2.14	0.47
1:F:357:MSE:HB3	1:F:381:LEU:HD12	1.90	0.47
1:G:171:LEU:HD21	1:I:28:ALA:CB	2.45	0.47
1:H:137:TYR:O	1:H:360:ASP:HB2	2.14	0.47
1:H:247:LEU:C	1:H:247:LEU:CD2	2.87	0.47
1:K:98:ARG:NE	1:K:99:ARG:CZ	2.78	0.47
1:K:225:HIS:O	1:K:226:PRO:C	2.56	0.47
1:A:185:TYR:C	1:A:185:TYR:CD1	2.92	0.47
1:C:148:VAL:HG13	1:C:290:LEU:O	2.15	0.47
1:C:225:HIS:CG	1:C:226:PRO:HD2	2.50	0.47
1:D:16:GLU:O	1:D:19:TRP:CD1	2.67	0.47
1:D:65:VAL:CG1	1:D:97:HIS:CE1	2.88	0.47
1:E:314:ARG:O	1:E:316:TYR:CE1	2.67	0.47
1:G:218:ARG:HD2	1:G:234:VAL:HB	1.96	0.47
1:J:146:LEU:HD22	1:J:275:THR:HG21	1.97	0.47
1:J:169:VAL:CG1	1:J:223:LEU:HB3	2.44	0.47
1:A:124:LEU:C	1:A:124:LEU:HD12	2.39	0.47
1:C:198:ARG:NH1	1:C:206:LEU:HD12	2.30	0.47
1:C:355:ILE:HD11	1:C:381:LEU:CG	2.44	0.47
1:D:193:PRO:CG	1:D:400:VAL:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ARG:HG3	1:D:316:TYR:CZ	2.49	0.47
1:E:111:HIS:CD2	1:E:303:ARG:HD3	2.49	0.47
1:E:128:GLU:C	1:F:289:ARG:NH2	2.73	0.47
1:G:131:ILE:O	1:G:134:ARG:HG2	2.14	0.47
1:G:158:ASP:HB3	1:H:379:ASN:O	2.14	0.47
1:H:109:GLU:OE1	1:H:112:ARG:CD	2.56	0.47
1:I:193:PRO:CG	1:I:400:VAL:CG2	2.92	0.47
1:J:381:LEU:HD12	1:J:381:LEU:C	2.40	0.47
1:B:264:GLY:O	1:E:98:ARG:NE	2.43	0.47
1:B:321:GLY:O	1:B:322:GLU:C	2.58	0.47
1:D:15:THR:HG23	1:D:55:ARG:HH22	1.80	0.47
1:D:114:ILE:CG2	1:D:305:MSE:HE2	2.45	0.47
1:D:225:HIS:CG	1:D:226:PRO:HD2	2.49	0.47
1:F:43:ARG:HB3	1:F:43:ARG:NH1	2.29	0.47
1:F:93:VAL:HG23	2:F:501:ACO:H132	1.97	0.47
1:J:35:GLY:N	1:J:36:PRO:CD	2.78	0.47
1:J:45:LEU:CD1	1:J:199:PRO:HG2	2.43	0.47
1:J:109:GLU:HA	1:J:109:GLU:OE2	2.15	0.47
1:K:336:ALA:O	1:K:346:CYS:HA	2.15	0.47
1:B:51:ALA:CB	1:B:69:LEU:HB3	2.45	0.47
1:D:98:ARG:HD2	1:E:264:GLY:HA3	1.95	0.47
1:D:294:THR:O	1:D:295:TRP:HB2	2.14	0.47
1:E:250:VAL:HG23	1:E:251:THR:HG23	1.96	0.47
1:H:150:ARG:HH21	1:H:266:ASP:HA	1.80	0.47
1:A:276:HIS:HB2	1:A:277:PRO:CD	2.44	0.47
1:D:387:GLN:HG3	1:D:390:ARG:HH21	1.80	0.47
1:G:307:VAL:CG1	1:G:311:LEU:HD11	2.45	0.47
1:G:314:ARG:NH1	1:G:366:TYR:O	2.47	0.47
1:H:11:LEU:HD11	1:H:52:VAL:HG22	1.96	0.47
1:H:360:ASP:OD2	1:H:380:ARG:NH2	2.47	0.47
1:I:74:ARG:HD3	1:I:84:PRO:HA	1.97	0.47
1:I:318:HIS:O	1:I:320:VAL:N	2.44	0.47
1:J:150:ARG:HB3	1:J:271:ILE:HD13	1.97	0.47
1:J:155:PHE:CE1	1:J:260:ARG:HA	2.50	0.47
1:J:218:ARG:NH2	1:J:239:LEU:HD21	2.30	0.47
1:K:239:LEU:O	1:K:268:MSE:HE1	2.15	0.47
1:K:259:TRP:CZ2	1:K:281:LEU:HD22	2.49	0.47
1:E:114:ILE:HG23	1:E:119:TYR:HB2	1.98	0.46
1:E:314:ARG:HH11	1:E:314:ARG:CG	2.29	0.46
1:F:289:ARG:O	1:F:291:ALA:N	2.47	0.46
1:G:44:THR:HG21	1:G:201:VAL:CG2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:355:ILE:HG13	1:G:383:THR:HB	1.98	0.46
1:J:332:GLY:O	1:J:335:PHE:CE1	2.68	0.46
1:F:229:TYR:C	1:F:229:TYR:CD1	2.93	0.46
1:H:100:ARG:N	3:H:601:HOH:O	2.09	0.46
1:H:361:VAL:HG13	1:H:375:LEU:HD13	1.95	0.46
1:I:320:VAL:O	1:I:320:VAL:HG13	2.15	0.46
1:A:121:VAL:CG1	1:A:122:ALA:H	2.27	0.46
1:B:198:ARG:NH1	1:B:206:LEU:HD12	2.30	0.46
1:B:327:LEU:CD1	1:B:357:MSE:HE3	2.44	0.46
1:C:379:ASN:HB2	1:D:160:PRO:HD3	1.97	0.46
1:D:314:ARG:NH1	1:D:366:TYR:O	2.48	0.46
1:E:77:VAL:HG11	1:E:83:LEU:HD12	1.97	0.46
1:E:221:PHE:O	1:E:232:TYR:CE1	2.68	0.46
1:G:385:ASP:OD1	1:G:386:SER:N	2.48	0.46
1:H:369:ALA:HB2	1:H:402:VAL:HG11	1.97	0.46
1:J:42:TRP:O	1:J:43:ARG:C	2.58	0.46
1:J:72:ASP:CG	1:J:74:ARG:HH12	2.24	0.46
1:B:109:GLU:O	1:B:112:ARG:CG	2.63	0.46
1:E:259:TRP:O	1:E:263:ILE:HG12	2.14	0.46
1:G:372:ALA:HB1	1:G:381:LEU:CD1	2.45	0.46
1:I:198:ARG:CD	1:I:203:TRP:CE2	2.99	0.46
1:A:47:PRO:O	1:A:48:THR:C	2.59	0.46
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.15	0.46
1:A:192:VAL:HG12	1:A:193:PRO:O	2.15	0.46
1:B:146:LEU:HD12	1:B:146:LEU:N	2.30	0.46
1:C:126:ALA:HB1	1:C:128:GLU:O	2.16	0.46
1:C:314:ARG:HD2	1:C:366:TYR:CE1	2.51	0.46
1:F:121:VAL:CA	1:F:305:MSE:HG2	2.22	0.46
1:G:247:LEU:HD23	1:G:247:LEU:C	2.40	0.46
1:H:98:ARG:CZ	1:H:99:ARG:CZ	2.93	0.46
1:H:169:VAL:HG22	1:H:225:HIS:CA	2.45	0.46
1:J:385:ASP:OD1	1:J:386:SER:N	2.48	0.46
1:K:379:ASN:HB2	1:L:160:PRO:HD3	1.98	0.46
1:E:47:PRO:HG2	1:E:70:TYR:CE1	2.51	0.46
1:E:128:GLU:CA	1:F:289:ARG:NH2	2.79	0.46
1:H:42:TRP:HA	1:H:46:VAL:HG23	1.98	0.46
1:I:38:SER:O	1:I:42:TRP:CG	2.68	0.46
1:I:318:HIS:CE1	1:I:342:GLY:HA3	2.50	0.46
1:K:292:ARG:HG3	3:K:605:HOH:O	2.16	0.46
1:A:127:SER:H	2:A:501:ACO:H21	1.80	0.46
1:B:109:GLU:O	1:B:113:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:THR:CB	1:H:384:LYS:HD2	2.45	0.46
1:G:297:GLN:CG	1:G:298:ASP:N	2.79	0.46
1:G:379:ASN:O	1:H:158:ASP:HB3	2.16	0.46
1:G:381:LEU:HD23	1:G:381:LEU:O	2.16	0.46
1:H:218:ARG:HD2	1:H:234:VAL:HB	1.98	0.46
1:I:281:LEU:HB3	1:I:282:PRO:HD3	1.98	0.46
1:J:63:GLU:OE1	1:K:170:ARG:HD2	2.16	0.46
1:K:19:TRP:HZ3	1:K:42:TRP:CE3	2.33	0.46
1:K:77:VAL:HB	1:K:78:PRO:CD	2.46	0.46
2:L:501:ACO:O5P	2:L:501:ACO:H141	2.16	0.46
1:D:145:GLU:HB2	1:D:295:TRP:HE3	1.80	0.46
1:L:131:ILE:HG12	2:L:501:ACO:C6A	2.46	0.46
1:L:146:LEU:O	1:L:272:SER:HA	2.16	0.46
1:L:327:LEU:HD23	1:L:328:GLU:N	2.31	0.46
1:B:144:HIS:NE2	1:B:277:PRO:HG3	2.29	0.46
1:C:42:TRP:NE1	1:C:90:PHE:CE2	2.80	0.46
1:D:233:ARG:HD2	3:D:612:HOH:O	2.14	0.46
1:D:304:ILE:HG13	1:D:362:LEU:HD23	1.97	0.46
1:E:128:GLU:HA	1:F:289:ARG:HH21	1.80	0.46
1:F:289:ARG:C	1:F:291:ALA:N	2.74	0.46
1:H:19:TRP:N	1:H:20:PRO:CD	2.79	0.46
1:H:339:ILE:HG12	1:H:344:ALA:CB	2.46	0.46
1:K:375:LEU:HD21	1:L:283:HIS:CE1	2.51	0.46
1:L:70:TYR:HB3	1:L:88:LEU:HD23	1.97	0.46
1:A:34:ILE:CD1	1:A:37:GLU:OE1	2.56	0.46
1:C:188:TRP:CH2	1:C:248:ARG:NH1	2.84	0.46
1:D:33:PHE:CZ	1:D:38:SER:CB	2.99	0.46
1:J:185:TYR:CE2	1:J:198:ARG:HB2	2.51	0.46
1:I:146:LEU:HA	1:I:292:ARG:O	2.16	0.45
1:I:378:ALA:HB1	1:J:284:LEU:HD23	1.98	0.45
1:J:287:ASP:HB3	1:J:290:LEU:HD12	1.97	0.45
1:J:288:THR:HG23	3:J:606:HOH:O	2.16	0.45
1:K:312:GLU:HG2	1:K:344:ALA:O	2.16	0.45
1:A:98:ARG:O	1:A:99:ARG:HB2	2.16	0.45
1:H:11:LEU:HD12	1:H:12:CYS:N	2.30	0.45
1:H:281:LEU:HB3	1:H:282:PRO:HD3	1.98	0.45
1:H:380:ARG:HD2	1:H:380:ARG:HA	1.81	0.45
1:J:149:ASP:OD2	1:J:152:PHE:CD1	2.70	0.45
1:J:381:LEU:HD12	1:J:381:LEU:O	2.16	0.45
1:L:49:ASP:OD1	1:L:49:ASP:C	2.59	0.45
1:D:194:GLY:HA3	1:D:403:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:THR:O	1:E:57:GLY:HA2	2.16	0.45
1:E:289:ARG:HD3	1:F:297:GLN:HG3	1.99	0.45
1:F:120:PRO:C	1:F:121:VAL:HG13	2.41	0.45
1:H:196:LEU:CD1	1:H:406:PHE:CZ	2.98	0.45
1:I:16:GLU:HA	1:I:19:TRP:CD1	2.51	0.45
1:J:314:ARG:HD3	1:J:316:TYR:CE2	2.52	0.45
1:D:274:ILE:HD13	1:D:274:ILE:N	2.31	0.45
1:F:67:MSE:HE2	1:F:90:PHE:HB3	1.98	0.45
1:G:248:ARG:HH22	1:G:405:ALA:HA	1.82	0.45
1:I:67:MSE:N	1:I:106:MSE:SE	3.00	0.45
1:I:134:ARG:NH1	2:I:501:ACO:H1B	2.31	0.45
1:I:150:ARG:HG3	1:I:151:ARG:N	2.32	0.45
1:I:308:PRO:HA	1:I:346:CYS:SG	2.57	0.45
1:J:206:LEU:HD21	1:J:231:LEU:HD11	1.98	0.45
1:L:33:PHE:CD1	1:L:33:PHE:C	2.95	0.45
1:L:123:ALA:HB2	1:L:302:LEU:HD23	1.98	0.45
1:L:306:ASN:ND2	1:L:309:ALA:HB2	2.30	0.45
1:B:120:PRO:C	1:B:121:VAL:HG13	2.41	0.45
1:B:322:GLU:HA	1:B:339:ILE:O	2.17	0.45
1:D:202:LEU:HA	1:D:202:LEU:HD23	1.69	0.45
1:F:104:ARG:NH2	2:F:501:ACO:O8A	2.49	0.45
1:F:182:GLU:HG2	1:F:203:TRP:CE2	2.51	0.45
1:G:150:ARG:HG3	1:G:151:ARG:N	2.31	0.45
1:I:356:GLU:C	1:I:357:MSE:HG2	2.42	0.45
1:J:40:THR:C	1:J:44:THR:HG22	2.40	0.45
1:J:125:HIS:CE1	1:J:407:GLU:HA	2.50	0.45
1:K:173:ARG:HG2	1:K:173:ARG:HH11	1.82	0.45
1:K:281:LEU:HD12	1:K:281:LEU:O	2.16	0.45
1:K:398:SER:OG	1:K:400:VAL:O	2.30	0.45
1:A:16:GLU:HA	1:A:19:TRP:NE1	2.32	0.45
1:A:98:ARG:NH1	1:A:99:ARG:NH2	2.65	0.45
1:C:144:HIS:HD2	1:C:277:PRO:HG3	1.70	0.45
1:C:178:ARG:HH11	1:C:207:LEU:CD1	2.25	0.45
1:C:247:LEU:C	1:C:247:LEU:CD2	2.89	0.45
2:C:501:ACO:O5P	2:C:501:ACO:N8P	2.49	0.45
1:E:39:ALA:O	1:E:43:ARG:HG2	2.17	0.45
1:E:142:THR:HG21	1:E:144:HIS:NE2	2.32	0.45
1:H:173:ARG:HG2	1:K:24:LEU:HD13	1.99	0.45
1:K:67:MSE:HE3	1:K:67:MSE:HB2	1.94	0.45
1:A:259:TRP:CZ2	1:A:281:LEU:HD22	2.52	0.45
1:D:85:THR:HG23	1:D:121:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ALA:HB2	1:D:302:LEU:HD23	1.99	0.45
1:E:33:PHE:C	1:E:33:PHE:HD1	2.19	0.45
1:F:34:ILE:HG22	1:F:36:PRO:HG2	1.98	0.45
1:F:55:ARG:HB3	1:F:62:SER:HB2	1.98	0.45
1:G:69:LEU:C	1:G:69:LEU:CD1	2.87	0.45
1:H:153:ALA:HA	1:H:290:LEU:CD1	2.47	0.45
1:H:222:ALA:HA	1:H:230:ALA:O	2.17	0.45
1:H:265:LEU:HD23	1:K:95:PRO:HB3	1.98	0.45
1:J:259:TRP:CE2	1:J:281:LEU:HD22	2.52	0.45
1:K:389:LEU:HD23	1:K:389:LEU:HA	1.78	0.45
1:A:145:GLU:HB2	1:A:295:TRP:HB3	1.98	0.45
1:C:153:ALA:HA	1:C:290:LEU:HD13	1.98	0.45
1:H:98:ARG:NH2	1:H:99:ARG:CZ	2.79	0.45
1:H:98:ARG:HG3	1:H:99:ARG:NH1	2.31	0.45
1:J:83:LEU:HD21	1:J:313:ALA:HB1	1.98	0.45
1:J:106:MSE:O	1:J:110:LEU:HG	2.17	0.45
1:K:192:VAL:O	1:K:193:PRO:C	2.60	0.45
2:L:501:ACO:O5P	2:L:501:ACO:N8P	2.48	0.45
1:B:125:HIS:CE1	1:B:407:GLU:HA	2.51	0.45
1:C:69:LEU:C	1:C:69:LEU:HD12	2.42	0.45
1:E:107:CYS:HB3	1:E:111:HIS:HE1	1.82	0.45
1:E:297:GLN:OE1	1:F:289:ARG:NE	2.49	0.45
1:H:188:TRP:HH2	1:H:405:ALA:HB2	1.81	0.45
1:H:270:ARG:NH1	3:H:620:HOH:O	2.34	0.45
1:I:148:VAL:CG2	1:I:290:LEU:O	2.65	0.45
1:I:318:HIS:HA	1:I:341:ASP:OD1	2.16	0.45
1:J:50:GLY:CA	1:J:70:TYR:CE1	3.00	0.45
1:K:74:ARG:HD3	1:K:84:PRO:HA	1.98	0.45
1:K:98:ARG:CG	1:K:99:ARG:NH1	2.77	0.45
1:L:281:LEU:HB3	1:L:282:PRO:HD3	1.99	0.45
1:A:169:VAL:HG22	1:A:170:ARG:N	2.30	0.45
1:D:52:VAL:CG1	1:D:110:LEU:CD2	2.95	0.45
1:D:246:GLU:CD	1:D:248:ARG:HE	2.17	0.45
1:F:307:VAL:HB	1:F:308:PRO:HD3	1.99	0.45
1:H:124:LEU:C	1:H:124:LEU:HD12	2.41	0.45
1:I:43:ARG:HH11	1:I:43:ARG:CA	2.25	0.45
1:I:276:HIS:CD2	1:I:278:GLN:H	2.27	0.45
1:K:192:VAL:HG11	1:K:403:GLN:CD	2.42	0.45
1:L:318:HIS:CE1	1:L:341:ASP:O	2.70	0.45
1:A:142:THR:HG21	1:A:296:ARG:NH2	2.32	0.44
1:B:145:GLU:HB2	1:B:295:TRP:HE3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ARG:NH1	1:D:158:ASP:OD2	2.45	0.44
1:G:380:ARG:NH1	1:H:158:ASP:OD2	2.48	0.44
1:G:408:PHE:CD1	1:G:408:PHE:C	2.95	0.44
1:H:87:GLY:HA2	1:H:123:ALA:O	2.16	0.44
2:I:501:ACO:O5P	2:I:501:ACO:H141	2.17	0.44
1:J:297:GLN:CG	1:J:298:ASP:N	2.80	0.44
1:J:327:LEU:HD12	1:J:355:ILE:HG23	1.98	0.44
1:K:70:TYR:HB3	1:K:88:LEU:HD23	1.98	0.44
1:L:392:LEU:O	1:L:393:ASP:C	2.60	0.44
1:A:225:HIS:O	1:A:226:PRO:C	2.61	0.44
1:A:289:ARG:HG3	1:B:129:GLY:HA3	1.99	0.44
1:B:114:ILE:HG22	1:B:305:MSE:HE2	1.98	0.44
1:E:124:LEU:C	1:E:124:LEU:HD12	2.42	0.44
1:F:42:TRP:CD1	1:F:46:VAL:CG2	2.96	0.44
1:F:198:ARG:HD2	1:F:203:TRP:CZ2	2.51	0.44
1:G:206:LEU:HD23	1:G:206:LEU:C	2.43	0.44
1:H:16:GLU:HA	1:H:19:TRP:CD1	2.51	0.44
1:H:146:LEU:N	1:H:146:LEU:CD2	2.78	0.44
1:I:145:GLU:HB3	1:I:295:TRP:HB3	1.99	0.44
1:I:194:GLY:HA3	1:I:403:GLN:O	2.16	0.44
1:A:70:TYR:O	1:A:70:TYR:CD1	2.70	0.44
1:D:16:GLU:C	1:D:18:ASP:H	2.26	0.44
1:D:50:GLY:HA2	1:D:70:TYR:CE2	2.53	0.44
1:D:218:ARG:HD2	1:D:234:VAL:HB	1.99	0.44
1:F:72:ASP:O	1:F:73:LEU:HD12	2.11	0.44
1:I:67:MSE:HE2	1:I:90:PHE:HB3	1.99	0.44
1:I:334:ARG:HD3	1:I:351:ALA:O	2.17	0.44
1:J:38:SER:O	1:J:39:ALA:C	2.60	0.44
1:K:103:LEU:N	2:K:501:ACO:O2A	2.47	0.44
1:K:400:VAL:CG1	1:K:400:VAL:O	2.65	0.44
1:C:266:ASP:C	1:C:268:MSE:N	2.76	0.44
2:C:501:ACO:O8A	2:C:501:ACO:H4B	2.17	0.44
1:F:123:ALA:HB2	1:F:302:LEU:HD23	1.99	0.44
1:F:178:ARG:O	1:F:182:GLU:HG3	2.17	0.44
1:G:16:GLU:HA	1:G:19:TRP:HE1	1.82	0.44
1:H:242:ALA:HB2	1:H:268:MSE:HG3	1.99	0.44
1:I:65:VAL:CG1	1:I:97:HIS:CE1	2.99	0.44
1:A:134:ARG:CZ	2:A:501:ACO:H1B	2.48	0.44
1:E:9:VAL:O	1:E:9:VAL:HG12	2.16	0.44
1:J:74:ARG:CD	1:J:84:PRO:CA	2.93	0.44
1:J:184:ILE:HG21	1:J:229:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:327:LEU:CD1	1:J:355:ILE:HG23	2.48	0.44
1:J:400:VAL:CG2	1:J:400:VAL:O	2.66	0.44
1:K:194:GLY:HA3	1:K:403:GLN:O	2.17	0.44
1:L:134:ARG:CZ	2:L:501:ACO:H1B	2.48	0.44
1:E:44:THR:HG21	1:E:201:VAL:HG21	1.98	0.44
1:G:121:VAL:HA	1:G:305:MSE:HG2	1.99	0.44
1:L:130:GLY:N	3:L:628:HOH:O	2.47	0.44
1:L:320:VAL:HG21	1:L:394:ALA:CB	2.47	0.44
1:C:121:VAL:HB	1:C:303:ARG:O	2.17	0.44
1:C:170:ARG:HD2	1:F:63:GLU:OE2	2.18	0.44
1:C:206:LEU:HD21	1:C:231:LEU:CD1	2.47	0.44
1:C:292:ARG:HG2	1:C:293:THR:O	2.18	0.44
1:F:146:LEU:HD22	1:F:275:THR:HG21	2.00	0.44
1:F:181:PHE:HE1	1:F:224:LEU:HD13	1.83	0.44
1:H:9:VAL:HB	1:H:55:ARG:O	2.17	0.44
1:H:198:ARG:NH1	1:H:206:LEU:HD12	2.33	0.44
1:I:198:ARG:NH1	1:I:206:LEU:HD12	2.33	0.44
1:G:63:GLU:OE1	1:L:170:ARG:HD2	2.17	0.44
1:H:354:GLU:C	1:H:384:LYS:NZ	2.73	0.44
1:I:289:ARG:NH1	1:J:297:GLN:OE1	2.50	0.44
1:J:305:MSE:HA	1:J:359:ARG:HH21	1.83	0.44
1:K:188:TRP:CG	1:K:248:ARG:HD2	2.52	0.44
1:L:320:VAL:CG2	1:L:394:ALA:HB1	2.48	0.44
2:A:501:ACO:H62	2:A:501:ACO:O9P	2.18	0.44
1:C:296:ARG:HD3	1:D:293:THR:OG1	2.18	0.44
1:D:23:PHE:CE1	1:D:42:TRP:CZ3	3.06	0.44
1:D:381:LEU:C	1:D:381:LEU:HD12	2.42	0.44
1:G:147:THR:OG1	1:G:294:THR:HG21	2.17	0.44
1:H:88:LEU:HB2	1:H:124:LEU:HB3	2.00	0.44
1:H:337:LEU:HD11	1:H:344:ALA:HB1	2.00	0.44
1:J:41:ALA:HA	1:J:44:THR:HG21	2.00	0.44
1:J:326:VAL:CG1	1:J:353:ALA:HA	2.48	0.44
1:A:45:LEU:HD21	1:A:199:PRO:HG2	1.99	0.43
1:B:61:GLY:O	1:B:62:SER:C	2.60	0.43
1:B:222:ALA:HB2	1:B:231:LEU:HD23	1.99	0.43
1:E:225:HIS:CG	1:E:226:PRO:HD2	2.53	0.43
1:F:42:TRP:O	1:F:46:VAL:HB	2.18	0.43
1:F:295:TRP:CZ2	1:F:297:GLN:CB	3.01	0.43
1:F:329:VAL:HB	1:F:332:GLY:HA3	2.00	0.43
1:I:160:PRO:HG2	1:I:256:CYS:CB	2.47	0.43
1:A:41:ALA:O	1:A:45:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:VAL:HA	1:E:47:PRO:HD3	1.88	0.43
1:H:200:GLN:HA	1:H:200:GLN:OE1	2.18	0.43
1:I:317:ALA:CB	1:I:394:ALA:O	2.66	0.43
1:J:85:THR:CG2	1:J:121:VAL:HG23	2.44	0.43
1:K:34:ILE:CG2	1:K:36:PRO:HD2	2.44	0.43
1:A:144:HIS:CD2	1:A:296:ARG:HG3	2.53	0.43
1:A:281:LEU:N	1:A:282:PRO:CD	2.82	0.43
1:B:198:ARG:HD2	1:B:203:TRP:CZ2	2.53	0.43
1:C:72:ASP:O	1:C:73:LEU:HD23	2.18	0.43
1:E:308:PRO:HD3	1:E:335:PHE:CE2	2.53	0.43
1:E:337:LEU:HD13	1:E:346:CYS:HB2	2.01	0.43
1:F:150:ARG:HG3	1:F:151:ARG:N	2.33	0.43
1:L:247:LEU:HD23	1:L:248:ARG:N	2.33	0.43
1:D:169:VAL:HG12	1:D:170:ARG:N	2.33	0.43
1:F:19:TRP:HB2	1:F:20:PRO:CD	2.48	0.43
1:F:71:MSE:C	1:F:73:LEU:HD12	2.43	0.43
1:G:19:TRP:N	1:G:20:PRO:HD2	2.33	0.43
1:J:202:LEU:CD1	1:J:406:PHE:CE2	3.01	0.43
1:K:193:PRO:CG	1:K:400:VAL:CG1	2.96	0.43
1:K:326:VAL:CG1	1:K:334:ARG:HG2	2.49	0.43
1:L:19:TRP:HB2	1:L:20:PRO:CD	2.47	0.43
1:B:150:ARG:HG2	1:B:269:GLU:O	2.18	0.43
1:B:153:ALA:CB	1:B:263:ILE:HD12	2.47	0.43
1:B:280:PRO:O	1:B:281:LEU:C	2.60	0.43
1:C:137:TYR:O	1:C:360:ASP:HB2	2.18	0.43
1:C:259:TRP:O	1:C:263:ILE:HG12	2.18	0.43
1:D:334:ARG:CD	1:D:351:ALA:O	2.67	0.43
1:E:198:ARG:HD2	1:E:203:TRP:CE2	2.53	0.43
1:F:247:LEU:C	1:F:247:LEU:CD2	2.91	0.43
1:F:298:ASP:OD2	1:F:301:TRP:CZ2	2.72	0.43
1:G:125:HIS:HE1	3:G:629:HOH:O	2.00	0.43
1:H:295:TRP:CH2	1:H:297:GLN:HB3	2.53	0.43
1:K:98:ARG:HH21	1:K:99:ARG:NH2	2.17	0.43
1:K:188:TRP:CD2	1:K:248:ARG:NH1	2.82	0.43
1:D:30:PHE:HB2	1:D:33:PHE:HB2	1.99	0.43
1:D:52:VAL:CG1	1:D:110:LEU:HD21	2.47	0.43
1:D:123:ALA:HA	1:D:301:TRP:O	2.19	0.43
1:E:307:VAL:HB	1:E:308:PRO:CD	2.44	0.43
1:F:44:THR:O	1:F:45:LEU:HD23	2.19	0.43
1:G:282:PRO:O	1:G:288:THR:HG22	2.19	0.43
1:I:393:ASP:O	1:I:397:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:VAL:HG23	2:J:501:ACO:H132	1.99	0.43
1:J:137:TYR:O	1:J:360:ASP:HB2	2.19	0.43
1:K:327:LEU:HD13	1:K:355:ILE:HG23	2.00	0.43
1:L:127:SER:HB3	2:L:501:ACO:H22	2.01	0.43
1:L:316:TYR:O	1:L:342:GLY:HA2	2.19	0.43
1:A:148:VAL:HA	1:A:290:LEU:O	2.18	0.43
1:B:213:ALA:HA	1:B:214:PRO:HD2	1.86	0.43
1:D:58:ALA:HB2	1:H:384:LYS:HG3	2.01	0.43
1:E:287:ASP:OD1	1:F:129:GLY:HA3	2.18	0.43
1:E:372:ALA:HB1	1:E:381:LEU:HD21	2.01	0.43
1:G:146:LEU:HA	1:G:146:LEU:HD12	1.79	0.43
1:H:24:LEU:HD13	1:J:173:ARG:CG	2.49	0.43
1:J:45:LEU:HD13	1:J:73:LEU:HD21	2.01	0.43
1:J:324:SER:OG	1:J:338:LYS:HD2	2.19	0.43
1:L:121:VAL:HA	1:L:305:MSE:HG2	2.01	0.43
1:L:247:LEU:HD23	1:L:247:LEU:C	2.43	0.43
1:L:355:ILE:HD11	1:L:381:LEU:HD13	2.00	0.43
1:A:63:GLU:OE1	1:F:170:ARG:HD2	2.18	0.43
1:D:10:THR:CG2	1:H:384:LYS:CE	2.96	0.43
1:E:42:TRP:N	1:E:42:TRP:CD1	2.87	0.43
1:E:142:THR:CG2	1:E:144:HIS:NE2	2.82	0.43
1:G:247:LEU:HD23	1:G:248:ARG:N	2.34	0.43
1:G:289:ARG:HD3	1:H:298:ASP:OD1	2.19	0.43
1:G:297:GLN:HG2	1:G:298:ASP:N	2.33	0.43
1:H:145:GLU:OE2	1:H:295:TRP:HB2	2.19	0.43
1:J:123:ALA:HB2	1:J:302:LEU:HD23	1.99	0.43
1:E:193:PRO:CG	1:E:400:VAL:CG2	2.94	0.43
1:E:193:PRO:HG2	1:E:400:VAL:HG23	2.00	0.43
1:F:238:ASP:C	1:F:240:LYS:H	2.26	0.43
1:H:121:VAL:CA	1:H:305:MSE:HG2	2.41	0.43
1:H:150:ARG:HD3	1:H:151:ARG:CA	2.47	0.43
1:H:371:ARG:HE	1:H:371:ARG:HB3	1.56	0.43
1:I:297:GLN:CG	1:I:298:ASP:N	2.81	0.43
1:I:385:ASP:OD2	1:I:388:LEU:HB2	2.19	0.43
1:L:49:ASP:OD1	1:L:49:ASP:O	2.37	0.43
1:A:152:PHE:HE1	1:D:151:ARG:HB3	1.83	0.43
1:A:178:ARG:O	1:A:182:GLU:HG3	2.19	0.43
1:A:292:ARG:O	1:A:294:THR:HG23	2.19	0.43
1:D:45:LEU:HB2	1:D:71:MSE:HE2	2.01	0.43
1:D:185:TYR:CD2	1:D:185:TYR:C	2.96	0.43
1:E:73:LEU:O	1:E:85:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:ASN:OD1	1:F:308:PRO:HD2	2.19	0.43
1:F:322:GLU:HA	1:F:339:ILE:O	2.18	0.43
1:G:306:ASN:HB3	1:G:309:ALA:HB3	2.00	0.43
1:H:169:VAL:CG2	1:H:225:HIS:CD2	3.02	0.43
1:H:196:LEU:CB	1:H:406:PHE:CE2	2.95	0.43
2:H:501:ACO:O5P	2:H:501:ACO:N8P	2.52	0.43
1:I:50:GLY:HA2	1:I:70:TYR:CE1	2.54	0.43
1:J:192:VAL:HG11	1:J:403:GLN:HB2	2.01	0.43
1:J:217:ASP:OD2	1:J:233:ARG:NH1	2.51	0.43
1:J:334:ARG:HD2	1:J:351:ALA:O	2.19	0.43
1:K:306:ASN:OD1	1:K:308:PRO:HD2	2.19	0.43
1:K:341:ASP:O	1:K:343:ARG:HG3	2.18	0.43
1:L:378:ALA:O	3:L:611:HOH:O	2.21	0.43
1:A:76:THR:O	1:A:193:PRO:HA	2.20	0.42
1:A:98:ARG:HD3	1:F:264:GLY:CA	2.49	0.42
1:B:24:LEU:CD1	1:D:173:ARG:HG2	2.45	0.42
1:D:187:ARG:O	1:D:191:GLN:HG3	2.18	0.42
1:E:297:GLN:OE1	1:F:289:ARG:CZ	2.67	0.42
1:G:99:ARG:NH1	2:G:501:ACO:O5A	2.52	0.42
1:H:11:LEU:CD1	1:H:52:VAL:HG22	2.49	0.42
1:H:334:ARG:HD2	1:H:351:ALA:O	2.19	0.42
1:J:138:GLY:O	1:J:301:TRP:HA	2.18	0.42
1:L:11:LEU:HD12	1:L:53:VAL:O	2.19	0.42
1:C:208:ALA:O	1:C:211:LYS:HG2	2.19	0.42
1:E:145:GLU:HB3	1:E:295:TRP:CB	2.42	0.42
1:E:392:LEU:O	1:E:393:ASP:C	2.62	0.42
1:F:137:TYR:CD2	1:F:303:ARG:HB2	2.54	0.42
1:J:150:ARG:HG2	1:J:269:GLU:O	2.17	0.42
2:K:501:ACO:O5P	2:K:501:ACO:H141	2.19	0.42
1:L:281:LEU:N	1:L:282:PRO:HD2	2.35	0.42
1:A:69:LEU:HD12	1:A:69:LEU:O	2.19	0.42
1:A:303:ARG:HH11	1:A:305:MSE:SE	2.53	0.42
1:A:359:ARG:NH1	3:A:610:HOH:O	2.53	0.42
1:C:144:HIS:HD2	1:C:277:PRO:CD	2.32	0.42
1:C:200:GLN:HE21	1:C:200:GLN:HA	1.84	0.42
1:D:184:ILE:HG21	1:D:228:GLY:HA2	2.01	0.42
1:H:54:VAL:HG11	1:H:102:LEU:HD22	2.01	0.42
1:I:109:GLU:O	1:I:113:ARG:HG3	2.19	0.42
1:I:123:ALA:HB1	1:I:300:LEU:HD11	2.01	0.42
1:K:30:PHE:O	1:K:31:THR:C	2.62	0.42
1:K:147:THR:HB	1:K:294:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD13	1:A:54:VAL:HG22	2.02	0.42
1:A:259:TRP:CE2	1:A:281:LEU:HD22	2.55	0.42
1:B:14:PRO:CD	1:B:51:ALA:O	2.63	0.42
1:C:314:ARG:O	1:C:316:TYR:CE1	2.72	0.42
1:F:169:VAL:HG23	1:F:224:LEU:C	2.44	0.42
1:H:229:TYR:CD1	1:H:229:TYR:C	2.98	0.42
1:H:280:PRO:O	1:H:281:LEU:C	2.62	0.42
1:I:33:PHE:CG	1:I:34:ILE:N	2.88	0.42
1:I:289:ARG:NE	1:J:297:GLN:OE1	2.53	0.42
1:I:327:LEU:HD23	1:I:328:GLU:CA	2.49	0.42
1:L:88:LEU:HD23	1:L:88:LEU:HA	1.78	0.42
1:L:330:SER:O	1:L:331:ASP:CB	2.67	0.42
1:A:61:GLY:O	1:A:62:SER:C	2.61	0.42
1:A:181:PHE:HD1	1:A:229:TYR:CG	2.38	0.42
1:C:367:LEU:O	1:C:402:VAL:CG2	2.66	0.42
1:E:133:GLY:HA2	1:E:137:TYR:O	2.19	0.42
1:E:134:ARG:N	3:E:629:HOH:O	2.45	0.42
1:E:146:LEU:HD12	1:E:275:THR:HG22	1.85	0.42
1:E:148:VAL:HG13	1:E:291:ALA:N	2.32	0.42
1:H:112:ARG:HG3	1:H:113:ARG:N	2.34	0.42
1:I:83:LEU:HD21	1:I:313:ALA:CB	2.46	0.42
1:I:133:GLY:C	1:I:135:PHE:N	2.76	0.42
1:I:357:MSE:CE	1:I:381:LEU:CD2	2.98	0.42
1:A:42:TRP:HA	1:A:46:VAL:CG2	2.50	0.42
1:A:136:GLY:O	1:A:303:ARG:HG3	2.20	0.42
1:C:110:LEU:CD1	1:C:110:LEU:N	2.80	0.42
1:E:327:LEU:HD13	1:E:357:MSE:HE3	1.89	0.42
1:G:311:LEU:H	1:G:311:LEU:CD1	2.32	0.42
1:H:279:ASP:O	1:H:282:PRO:HD2	2.18	0.42
1:I:11:LEU:HD12	1:I:12:CYS:N	2.34	0.42
1:I:110:LEU:O	1:I:114:ILE:HG13	2.20	0.42
1:K:281:LEU:HD12	1:K:281:LEU:C	2.45	0.42
1:K:297:GLN:HG2	1:K:298:ASP:N	2.35	0.42
1:L:206:LEU:HD23	1:L:207:LEU:HD13	2.01	0.42
1:A:25:LEU:O	1:A:29:SER:HB2	2.20	0.42
1:A:63:GLU:OE1	1:F:170:ARG:HB3	2.19	0.42
1:A:314:ARG:NH1	1:A:315:GLY:O	2.52	0.42
1:B:87:GLY:HA2	1:B:123:ALA:O	2.20	0.42
1:C:308:PRO:HA	1:C:346:CYS:SG	2.60	0.42
1:C:357:MSE:HE1	1:C:381:LEU:HD22	1.92	0.42
1:D:44:THR:CG2	1:D:201:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:ACO:OAP	1:E:266:ASP:OD2	2.38	0.42
1:E:281:LEU:HD23	1:E:291:ALA:HB1	2.00	0.42
1:F:269:GLU:C	1:F:270:ARG:HG3	2.44	0.42
1:G:155:PHE:CZ	1:G:260:ARG:HA	2.54	0.42
1:G:171:LEU:HD11	1:G:221:PHE:HB3	2.01	0.42
1:H:11:LEU:HD11	1:H:52:VAL:CG2	2.49	0.42
1:H:188:TRP:CH2	1:H:405:ALA:HB2	2.54	0.42
1:I:156:HIS:CE1	1:J:380:ARG:NH1	2.88	0.42
1:J:40:THR:O	1:J:41:ALA:C	2.62	0.42
1:J:102:LEU:O	1:J:105:ALA:N	2.53	0.42
1:J:174:PRO:C	1:J:176:GLU:H	2.27	0.42
1:L:114:ILE:HG22	1:L:305:MSE:HE2	2.02	0.42
1:L:361:VAL:O	1:L:362:LEU:C	2.62	0.42
1:A:357:MSE:HE2	1:A:381:LEU:HB2	2.01	0.42
1:A:380:ARG:HD2	1:B:158:ASP:OD2	2.19	0.42
1:E:127:SER:CB	2:E:501:ACO:C2P	2.96	0.42
1:E:235:ASP:HB3	1:E:238:ASP:O	2.19	0.42
1:F:200:GLN:NE2	1:F:200:GLN:HA	2.35	0.42
1:F:303:ARG:HH11	1:F:305:MSE:SE	2.53	0.42
1:H:326:VAL:CG1	1:H:353:ALA:HA	2.50	0.42
1:H:387:GLN:HG3	1:H:388:LEU:N	2.34	0.42
2:J:501:ACO:O8A	2:J:501:ACO:H4B	2.20	0.42
1:K:124:LEU:HD23	1:K:137:TYR:CE2	2.54	0.42
1:K:134:ARG:CZ	2:K:501:ACO:H1B	2.50	0.42
1:K:379:ASN:CB	1:L:160:PRO:HD3	2.49	0.42
1:L:259:TRP:O	1:L:263:ILE:CG1	2.68	0.42
1:C:103:LEU:HD22	2:C:501:ACO:H133	2.01	0.42
1:C:268:MSE:HE2	1:C:268:MSE:HA	2.02	0.42
1:C:288:THR:HG23	1:C:289:ARG:N	2.35	0.42
1:F:98:ARG:NH1	1:F:99:ARG:NH2	2.67	0.42
1:F:298:ASP:OD2	1:F:301:TRP:HZ2	2.02	0.42
1:G:173:ARG:HD2	1:G:176:GLU:OE2	2.19	0.42
1:H:63:GLU:OE1	1:J:170:ARG:HD2	2.20	0.42
1:H:307:VAL:HB	1:H:308:PRO:HD3	2.02	0.42
1:I:148:VAL:HA	1:I:290:LEU:O	2.19	0.42
1:I:387:GLN:O	1:I:391:ARG:HG3	2.20	0.42
1:J:40:THR:OG1	1:J:41:ALA:N	2.53	0.42
1:K:173:ARG:HG2	1:K:173:ARG:NH1	2.35	0.42
1:K:186:GLU:OE1	1:K:186:GLU:HA	2.18	0.42
1:K:327:LEU:HD12	1:K:355:ILE:O	2.20	0.42
1:A:218:ARG:NH2	1:A:239:LEU:HD21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG22	1:F:96:THR:CG2	2.50	0.42
1:E:45:LEU:HD21	1:E:199:PRO:HG2	2.02	0.42
1:F:151:ARG:CZ	1:F:269:GLU:HG3	2.50	0.42
1:G:45:LEU:HD21	1:G:199:PRO:HG2	2.02	0.42
1:H:314:ARG:O	1:H:316:TYR:CE1	2.73	0.42
1:J:384:LYS:HG2	1:J:384:LYS:O	2.20	0.42
1:K:298:ASP:OD2	1:K:301:TRP:NE1	2.47	0.42
2:K:501:ACO:O5P	2:K:501:ACO:N8P	2.53	0.42
1:L:38:SER:O	1:L:39:ALA:C	2.63	0.42
1:L:327:LEU:HG	1:L:357:MSE:HE3	2.02	0.42
1:A:70:TYR:CD1	1:A:70:TYR:C	2.98	0.41
1:A:206:LEU:C	1:A:206:LEU:HD23	2.45	0.41
1:C:74:ARG:HB3	1:C:82:VAL:CG1	2.49	0.41
1:E:110:LEU:HD23	1:E:110:LEU:HA	1.84	0.41
1:F:213:ALA:HA	1:F:214:PRO:HD2	1.92	0.41
1:H:110:LEU:O	1:H:114:ILE:HG13	2.20	0.41
1:I:142:THR:O	1:I:277:PRO:HD3	2.20	0.41
1:J:281:LEU:C	1:J:283:HIS:N	2.77	0.41
1:K:327:LEU:HD11	1:K:357:MSE:CE	2.26	0.41
1:L:16:GLU:HA	1:L:19:TRP:CD1	2.55	0.41
1:A:232:TYR:HB3	1:A:244:VAL:HG22	2.02	0.41
1:B:246:GLU:CD	1:B:248:ARG:NE	2.76	0.41
1:B:297:GLN:HG2	1:B:298:ASP:N	2.35	0.41
1:C:123:ALA:HA	1:C:301:TRP:O	2.20	0.41
1:C:169:VAL:HG22	1:F:96:THR:HG22	2.01	0.41
2:E:501:ACO:O9P	2:E:501:ACO:H131	2.20	0.41
1:H:354:GLU:HB3	1:H:384:LYS:HZ3	1.84	0.41
1:I:297:GLN:HG3	1:I:298:ASP:N	2.35	0.41
1:J:148:VAL:HG22	1:J:291:ALA:HA	2.01	0.41
1:J:309:ALA:O	1:J:310:ALA:C	2.63	0.41
1:J:360:ASP:OD2	1:J:380:ARG:NH2	2.53	0.41
1:K:259:TRP:CE2	1:K:281:LEU:HD22	2.55	0.41
1:A:61:GLY:C	1:A:62:SER:O	2.62	0.41
1:B:297:GLN:CG	1:B:298:ASP:N	2.82	0.41
1:C:197:LEU:HB3	3:C:627:HOH:O	2.19	0.41
1:D:44:THR:HG21	1:D:201:VAL:CG2	2.44	0.41
1:D:58:ALA:HB1	1:H:384:LYS:HG3	2.01	0.41
1:D:281:LEU:HD12	1:D:281:LEU:O	2.20	0.41
1:F:181:PHE:CE1	1:F:224:LEU:HD13	2.55	0.41
1:F:314:ARG:HG3	1:F:316:TYR:CE1	2.55	0.41
1:G:49:ASP:OD1	1:G:49:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:ILE:HG21	1:I:305:MSE:HE2	2.00	0.41
1:J:83:LEU:HD11	1:J:313:ALA:HB1	2.02	0.41
1:J:360:ASP:CG	1:J:380:ARG:HH22	2.28	0.41
1:J:405:ALA:CA	3:J:602:HOH:O	2.53	0.41
1:L:67:MSE:HE2	1:L:90:PHE:HB3	2.02	0.41
1:B:86:ALA:O	1:B:122:ALA:HA	2.19	0.41
1:B:229:TYR:CD1	1:B:229:TYR:C	2.98	0.41
1:C:14:PRO:HD2	1:C:51:ALA:O	2.20	0.41
1:C:297:GLN:HG2	1:C:298:ASP:N	2.35	0.41
1:E:93:VAL:HG12	1:E:94:ALA:O	2.20	0.41
1:G:287:ASP:C	1:G:287:ASP:OD1	2.63	0.41
1:I:276:HIS:ND1	1:I:403:GLN:HG2	2.35	0.41
1:I:319:GLU:HB3	1:J:320:VAL:HG23	2.01	0.41
1:I:375:LEU:CD2	1:J:283:HIS:CE1	3.02	0.41
1:K:91:VAL:O	2:K:501:ACO:N4P	2.53	0.41
1:K:188:TRP:CZ3	1:K:248:ARG:NH1	2.88	0.41
1:K:305:MSE:HE3	1:K:305:MSE:HB3	1.75	0.41
1:A:22:MSE:HE3	1:A:67:MSE:HE3	2.02	0.41
1:B:149:ASP:OD2	1:B:152:PHE:CD2	2.73	0.41
1:C:134:ARG:HH12	2:C:501:ACO:H1B	1.82	0.41
1:C:380:ARG:O	3:C:614:HOH:O	2.22	0.41
1:F:85:THR:HG22	1:F:86:ALA:N	2.34	0.41
1:G:127:SER:H	2:G:501:ACO:H21	1.84	0.41
1:G:307:VAL:CG1	1:G:311:LEU:CD1	2.98	0.41
1:H:177:HIS:O	1:H:181:PHE:CD2	2.74	0.41
1:I:229:TYR:CD1	1:I:229:TYR:C	2.99	0.41
1:J:169:VAL:HG22	1:J:225:HIS:HB2	2.02	0.41
1:K:318:HIS:C	1:K:320:VAL:H	2.29	0.41
1:L:232:TYR:HA	1:L:243:ARG:O	2.21	0.41
1:B:134:ARG:HG3	1:B:135:PHE:CD1	2.56	0.41
1:C:144:HIS:CE1	1:C:296:ARG:NH1	2.88	0.41
1:E:148:VAL:CG2	1:E:291:ALA:CB	2.97	0.41
1:E:387:GLN:O	1:E:391:ARG:HG3	2.20	0.41
1:F:314:ARG:HG3	1:F:316:TYR:CZ	2.56	0.41
1:G:206:LEU:HD21	1:G:231:LEU:CD1	2.50	0.41
1:H:169:VAL:HG22	1:H:225:HIS:HA	2.01	0.41
1:H:320:VAL:HG22	1:H:321:GLY:N	2.36	0.41
1:I:334:ARG:CD	1:I:351:ALA:O	2.68	0.41
1:L:67:MSE:O	1:L:91:VAL:HA	2.21	0.41
1:A:35:GLY:N	1:A:36:PRO:CD	2.83	0.41
1:B:150:ARG:HG3	1:B:151:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HA	1:C:290:LEU:O	2.20	0.41
1:D:104:ARG:HG3	1:D:135:PHE:CE1	2.48	0.41
1:E:32:ASP:OD1	1:E:33:PHE:N	2.54	0.41
1:E:169:VAL:HG22	1:E:170:ARG:N	2.34	0.41
1:E:362:LEU:HD12	1:E:362:LEU:HA	1.86	0.41
1:F:269:GLU:C	1:F:270:ARG:CG	2.94	0.41
1:F:373:SER:HA	1:F:389:LEU:HD22	2.02	0.41
1:G:54:VAL:HG11	1:G:102:LEU:CD2	2.49	0.41
1:J:22:MSE:HB3	1:J:67:MSE:CE	2.51	0.41
1:J:98:ARG:NH2	1:J:99:ARG:CZ	2.84	0.41
1:J:276:HIS:CD2	1:J:278:GLN:H	2.39	0.41
1:J:357:MSE:HB3	1:J:381:LEU:CB	2.50	0.41
1:K:33:PHE:CG	1:K:34:ILE:N	2.89	0.41
1:B:167:SER:OG	1:E:100:ARG:NH1	2.53	0.41
1:B:207:LEU:O	1:B:210:CYS:HB2	2.20	0.41
1:B:383:THR:HG21	1:B:389:LEU:CD2	2.51	0.41
1:D:213:ALA:HA	1:D:214:PRO:HD2	1.85	0.41
1:D:329:VAL:O	1:D:330:SER:C	2.63	0.41
1:F:98:ARG:NE	1:F:99:ARG:NH1	2.68	0.41
1:I:225:HIS:CG	1:I:226:PRO:CD	3.04	0.41
1:I:322:GLU:HA	1:I:339:ILE:O	2.20	0.41
1:J:207:LEU:O	1:J:210:CYS:HB2	2.21	0.41
1:A:34:ILE:HD12	1:A:37:GLU:CD	2.44	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.88	0.41
1:B:70:TYR:HA	1:B:87:GLY:O	2.21	0.41
1:B:167:SER:OG	1:E:100:ARG:CZ	2.69	0.41
1:B:198:ARG:HG2	1:B:203:TRP:CD1	2.56	0.41
1:C:70:TYR:CA	1:C:87:GLY:O	2.66	0.41
1:C:148:VAL:HG22	1:C:291:ALA:HA	0.56	0.41
1:C:188:TRP:CZ2	1:C:248:ARG:NH1	2.89	0.41
1:C:223:LEU:O	1:C:229:TYR:HA	2.21	0.41
1:D:8:THR:CG2	1:D:9:VAL:H	2.19	0.41
1:D:126:ALA:HB1	1:D:128:GLU:O	2.21	0.41
1:D:198:ARG:HA	1:D:199:PRO:HD3	1.80	0.41
1:E:34:ILE:HG22	1:E:35:GLY:N	2.34	0.41
1:E:306:ASN:HB3	1:E:309:ALA:HB3	2.03	0.41
1:F:34:ILE:CG2	1:F:36:PRO:HG2	2.51	0.41
1:F:103:LEU:HD22	2:F:501:ACO:CCP	2.50	0.41
1:F:150:ARG:NH2	1:F:263:ILE:O	2.51	0.41
1:F:169:VAL:HG23	1:F:224:LEU:O	2.21	0.41
1:G:33:PHE:CG	1:G:34:ILE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:THR:HG22	1:G:402:VAL:HG11	2.02	0.41
1:G:246:GLU:HG2	1:G:248:ARG:HG2	2.02	0.41
1:G:247:LEU:C	1:G:247:LEU:CD2	2.94	0.41
1:G:274:ILE:N	1:G:274:ILE:HD13	2.36	0.41
1:G:367:LEU:O	1:G:402:VAL:CG2	2.69	0.41
1:H:98:ARG:HD2	1:J:266:ASP:CG	2.46	0.41
1:H:100:ARG:NH1	1:J:167:SER:OG	2.54	0.41
1:H:186:GLU:OE2	1:H:189:ARG:NH1	2.52	0.41
1:H:342:GLY:C	1:H:343:ARG:HD2	2.45	0.41
1:H:372:ALA:N	1:H:393:ASP:OD1	2.54	0.41
1:I:98:ARG:HE	1:I:99:ARG:NH2	2.18	0.41
1:I:300:LEU:HG	1:I:301:TRP:N	2.35	0.41
1:I:326:VAL:HG11	1:I:352:ALA:O	2.21	0.41
1:J:385:ASP:OD1	1:J:387:GLN:N	2.45	0.41
1:C:184:ILE:HG21	1:C:228:GLY:HA2	2.02	0.41
1:C:355:ILE:HG13	1:C:383:THR:HB	2.02	0.41
1:G:328:GLU:HB2	1:G:334:ARG:HG3	2.03	0.41
1:H:355:ILE:CD1	1:H:392:LEU:HD11	2.50	0.41
1:I:314:ARG:O	1:I:316:TYR:CE1	2.74	0.41
1:J:202:LEU:HD23	1:J:202:LEU:HA	1.86	0.41
1:K:132:TYR:O	1:K:133:GLY:C	2.64	0.41
1:L:327:LEU:C	1:L:327:LEU:HD23	2.46	0.41
1:A:107:CYS:O	1:A:108:ALA:C	2.63	0.40
1:A:124:LEU:HD12	1:A:301:TRP:HB2	2.02	0.40
1:A:144:HIS:HB3	1:A:146:LEU:CD1	2.51	0.40
1:B:169:VAL:HG22	1:B:225:HIS:CA	2.51	0.40
1:E:93:VAL:HG23	2:E:501:ACO:H132	2.03	0.40
1:E:180:GLU:O	1:E:184:ILE:HG13	2.21	0.40
1:H:98:ARG:CG	1:H:99:ARG:NH1	2.84	0.40
1:I:189:ARG:HH11	1:I:197:LEU:HD13	1.87	0.40
1:I:314:ARG:NH1	1:I:366:TYR:O	2.54	0.40
1:I:357:MSE:HB3	1:I:381:LEU:HD12	2.03	0.40
1:K:70:TYR:HB3	1:K:88:LEU:CD2	2.52	0.40
1:A:98:ARG:NH1	1:A:99:ARG:CZ	2.85	0.40
1:B:173:ARG:HG2	1:E:24:LEU:HD13	2.02	0.40
1:C:101:GLY:CA	2:C:501:ACO:O2A	2.68	0.40
1:C:144:HIS:CD2	1:C:277:PRO:CD	3.04	0.40
1:D:144:HIS:CE1	1:D:296:ARG:NH1	2.89	0.40
1:D:250:VAL:O	1:D:250:VAL:CG1	2.69	0.40
1:E:234:VAL:HG23	3:E:614:HOH:O	2.21	0.40
1:E:338:LYS:O	1:E:344:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:VAL:HA	1:F:47:PRO:HD3	1.91	0.40
1:F:49:ASP:OD1	1:F:49:ASP:O	2.39	0.40
1:G:266:ASP:CG	1:I:98:ARG:HD2	2.46	0.40
1:I:202:LEU:HD23	1:I:202:LEU:HA	1.84	0.40
1:J:70:TYR:HA	1:J:87:GLY:O	2.21	0.40
1:B:42:TRP:HA	1:B:46:VAL:HG23	2.02	0.40
1:C:74:ARG:O	1:C:196:LEU:HA	2.21	0.40
1:D:145:GLU:HB2	1:D:295:TRP:HB3	1.99	0.40
1:D:148:VAL:CG1	1:D:290:LEU:C	2.69	0.40
1:F:48:THR:O	1:F:49:ASP:OD1	2.39	0.40
1:H:74:ARG:HD3	1:H:84:PRO:HA	2.03	0.40
1:H:150:ARG:HD2	1:H:268:MSE:O	2.21	0.40
1:H:385:ASP:CG	1:H:387:GLN:CG	2.75	0.40
1:H:398:SER:OG	1:H:400:VAL:O	2.33	0.40
1:I:85:THR:HG23	1:I:121:VAL:HG23	2.03	0.40
1:L:50:GLY:HA2	1:L:70:TYR:CE1	2.57	0.40
1:B:298:ASP:OD1	1:B:298:ASP:O	2.39	0.40
1:E:398:SER:OG	1:E:400:VAL:O	2.30	0.40
1:F:46:VAL:HG22	1:F:69:LEU:HD13	2.04	0.40
1:G:38:SER:O	1:G:39:ALA:C	2.64	0.40
1:G:42:TRP:O	1:G:43:ARG:C	2.62	0.40
1:J:45:LEU:HD13	1:J:73:LEU:CD2	2.52	0.40
1:J:398:SER:OG	1:J:400:VAL:O	2.30	0.40
1:A:198:ARG:HA	1:A:199:PRO:HD3	1.93	0.40
1:D:48:THR:O	1:D:49:ASP:CB	2.70	0.40
1:E:319:GLU:HG3	3:F:628:HOH:O	2.21	0.40
1:G:77:VAL:HB	1:G:78:PRO:CD	2.49	0.40
1:G:327:LEU:O	1:G:335:PHE:N	2.55	0.40
1:H:355:ILE:HD11	1:H:357:MSE:HE2	2.03	0.40
1:I:159:ALA:HA	1:I:160:PRO:HD2	1.83	0.40
1:J:306:ASN:OD1	1:J:308:PRO:HD2	2.21	0.40
1:K:46:VAL:HA	1:K:47:PRO:HD3	1.96	0.40
1:K:74:ARG:HB3	1:K:82:VAL:HG13	2.03	0.40
1:L:74:ARG:O	1:L:196:LEU:HA	2.21	0.40
1:L:135:PHE:O	1:L:303:ARG:NE	2.54	0.40

All (3) 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:E:9:VAL:CG1	1:L:8:THR:OG1[2_545]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:ASP:OD1	1:K:345:ARG:NH1[2_645]	1.83	0.37
1:E:9:VAL:O	1:L:8:THR:OG1[2_545]	2.14	0.06

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	392/428 (92%)	375 (96%)	15 (4%)	2 (0%)	24	55
1	B	392/428 (92%)	373 (95%)	18 (5%)	1 (0%)	36	66
1	C	392/428 (92%)	374 (95%)	18 (5%)	0	100	100
1	D	392/428 (92%)	376 (96%)	15 (4%)	1 (0%)	36	66
1	E	392/428 (92%)	376 (96%)	16 (4%)	0	100	100
1	F	392/428 (92%)	369 (94%)	22 (6%)	1 (0%)	36	66
1	G	392/428 (92%)	379 (97%)	12 (3%)	1 (0%)	36	66
1	H	392/428 (92%)	377 (96%)	15 (4%)	0	100	100
1	I	392/428 (92%)	365 (93%)	23 (6%)	4 (1%)	12	38
1	J	392/428 (92%)	357 (91%)	31 (8%)	4 (1%)	12	38
1	K	392/428 (92%)	367 (94%)	23 (6%)	2 (0%)	24	55
1	L	392/428 (92%)	370 (94%)	21 (5%)	1 (0%)	36	66
All	All	4704/5136 (92%)	4458 (95%)	229 (5%)	17 (0%)	30	60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	I	319	GLU
1	I	357	MSE
1	I	397	ALA
1	J	175	THR

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Mol	Chain	Res	Type
1	J	309	ALA
1	J	357	MSE
1	J	358	ASP
1	B	62	SER
1	F	290	LEU
1	I	265	LEU
1	L	405	ALA
1	A	62	SER
1	D	319	GLU
1	K	295	TRP
1	G	332	GLY
1	K	114	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/327 (95%)	307 (99%)	4 (1%)	61	86
1	B	311/327 (95%)	305 (98%)	6 (2%)	50	81
1	C	311/327 (95%)	307 (99%)	4 (1%)	61	86
1	D	311/327 (95%)	306 (98%)	5 (2%)	55	83
1	E	311/327 (95%)	303 (97%)	8 (3%)	40	75
1	F	311/327 (95%)	302 (97%)	9 (3%)	37	73
1	G	311/327 (95%)	304 (98%)	7 (2%)	44	78
1	H	311/327 (95%)	304 (98%)	7 (2%)	44	78
1	I	311/327 (95%)	301 (97%)	10 (3%)	34	70
1	J	311/327 (95%)	301 (97%)	10 (3%)	34	70
1	K	311/327 (95%)	303 (97%)	8 (3%)	40	75
1	L	311/327 (95%)	285 (92%)	26 (8%)	10	32
All	All	3732/3924 (95%)	3628 (97%)	104 (3%)	38	73

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	271	ILE
1	A	341	ASP
1	A	402	VAL
1	B	88	LEU
1	B	106	MSE
1	B	128	GLU
1	B	250	VAL
1	B	337	LEU
1	B	381	LEU
1	C	145	GLU
1	C	150	ARG
1	C	169	VAL
1	C	250	VAL
1	D	38	SER
1	D	69	LEU
1	D	180	GLU
1	D	206	LEU
1	D	387	GLN
1	E	9	VAL
1	E	31	THR
1	E	33	PHE
1	E	98	ARG
1	E	180	GLU
1	E	206	LEU
1	E	250	VAL
1	E	314	ARG
1	F	73	LEU
1	F	106	MSE
1	F	112	ARG
1	F	146	LEU
1	F	148	VAL
1	F	180	GLU
1	F	206	LEU
1	F	207	LEU
1	F	320	VAL
1	G	31	THR
1	G	88	LEU
1	G	146	LEU
1	G	289	ARG
1	G	327	LEU
1	G	381	LEU
1	G	399	ASP

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Mol	Chain	Res	Type
1	H	52	VAL
1	H	146	LEU
1	H	150	ARG
1	H	206	LEU
1	H	250	VAL
1	H	271	ILE
1	H	355	ILE
1	I	38	SER
1	I	121	VAL
1	I	206	LEU
1	I	233	ARG
1	I	297	GLN
1	I	327	LEU
1	I	339	ILE
1	I	355	ILE
1	I	359	ARG
1	I	387	GLN
1	J	48	THR
1	J	88	LEU
1	J	146	LEU
1	J	206	LEU
1	J	233	ARG
1	J	271	ILE
1	J	273	ILE
1	J	314	ARG
1	J	337	LEU
1	J	356	GLU
1	K	150	ARG
1	K	206	LEU
1	K	207	LEU
1	K	246	GLU
1	K	267	SER
1	K	305	MSE
1	K	314	ARG
1	K	381	LEU
1	L	9	VAL
1	L	34	ILE
1	L	44	THR
1	L	52	VAL
1	L	85	THR
1	L	98	ARG
1	L	121	VAL

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Mol	Chain	Res	Type
1	L	146	LEU
1	L	148	VAL
1	L	150	ARG
1	L	169	VAL
1	L	207	LEU
1	L	248	ARG
1	L	288	THR
1	L	289	ARG
1	L	292	ARG
1	L	296	ARG
1	L	314	ARG
1	L	327	LEU
1	L	337	LEU
1	L	341	ASP
1	L	381	LEU
1	L	384	LYS
1	L	387	GLN
1	L	399	ASP
1	L	402	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	200	GLN
1	A	255	HIS
1	B	125	HIS
1	B	200	GLN
1	C	144	HIS
1	C	200	GLN
1	C	255	HIS
1	C	276	HIS
1	C	403	GLN
1	D	125	HIS
1	D	403	GLN
1	E	97	HIS
1	E	144	HIS
1	E	190	GLN
1	E	387	GLN
1	F	125	HIS
1	F	177	HIS
1	F	200	GLN

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Mol	Chain	Res	Type
1	F	255	HIS
1	F	297	GLN
1	G	125	HIS
1	G	200	GLN
1	G	297	GLN
1	G	387	GLN
1	H	144	HIS
1	H	177	HIS
1	H	255	HIS
1	H	283	HIS
1	H	387	GLN
1	I	200	GLN
1	I	276	HIS
1	I	283	HIS
1	J	97	HIS
1	J	125	HIS
1	J	177	HIS
1	J	255	HIS
1	J	283	HIS
1	J	318	HIS
1	K	125	HIS
1	K	200	GLN
1	K	255	HIS
1	L	190	GLN
1	L	200	GLN
1	L	318	HIS
1	L	387	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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
2	ACO	H	501	-	51,53,53	1.73	7 (13%)	73,79,79	2.04	20 (27%)
2	ACO	G	501	-	51,53,53	1.79	8 (15%)	73,79,79	1.94	16 (21%)
2	ACO	K	501	-	51,53,53	1.74	7 (13%)	73,79,79	2.18	22 (30%)
2	ACO	F	501	-	51,53,53	1.81	9 (17%)	73,79,79	2.06	18 (24%)
2	ACO	J	501	-	51,53,53	1.69	8 (15%)	73,79,79	2.06	21 (28%)
2	ACO	I	501	-	51,53,53	1.75	8 (15%)	73,79,79	1.92	15 (20%)
2	ACO	E	501	-	51,53,53	1.76	7 (13%)	73,79,79	2.06	21 (28%)
2	ACO	L	501	-	51,53,53	1.82	10 (19%)	73,79,79	2.13	20 (27%)
2	ACO	C	501	-	51,53,53	1.72	9 (17%)	73,79,79	1.92	21 (28%)
2	ACO	D	501	-	51,53,53	1.71	8 (15%)	73,79,79	2.22	19 (26%)
2	ACO	A	501	-	51,53,53	1.78	8 (15%)	73,79,79	2.11	21 (28%)
2	ACO	B	501	-	51,53,53	1.81	9 (17%)	73,79,79	2.09	22 (30%)

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	ACO	H	501	-	-	15/51/67/67	0/3/3/3
2	ACO	G	501	-	-	10/51/67/67	0/3/3/3
2	ACO	K	501	-	-	16/51/67/67	0/3/3/3
2	ACO	F	501	-	-	16/51/67/67	0/3/3/3
2	ACO	J	501	-	-	18/51/67/67	0/3/3/3
2	ACO	I	501	-	-	14/51/67/67	0/3/3/3
2	ACO	E	501	-	-	14/51/67/67	0/3/3/3
2	ACO	L	501	-	-	9/51/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	C	501	-	-	15/51/67/67	0/3/3/3
2	ACO	D	501	-	-	15/51/67/67	0/3/3/3
2	ACO	A	501	-	-	11/51/67/67	0/3/3/3
2	ACO	B	501	-	-	14/51/67/67	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	ACO	C9P-N8P	5.36	1.46	1.33
2	A	501	ACO	C5P-N4P	5.27	1.45	1.33
2	L	501	ACO	C5P-N4P	5.27	1.45	1.33
2	I	501	ACO	C9P-N8P	5.13	1.45	1.33
2	F	501	ACO	C5P-N4P	5.11	1.45	1.33
2	E	501	ACO	C9P-N8P	5.09	1.45	1.33
2	K	501	ACO	C5P-N4P	5.04	1.45	1.33
2	E	501	ACO	C6A-N6A	5.01	1.47	1.34
2	E	501	ACO	C5P-N4P	5.01	1.45	1.33
2	B	501	ACO	C9P-N8P	4.98	1.45	1.33
2	H	501	ACO	C5P-N4P	4.94	1.45	1.33
2	I	501	ACO	C5P-N4P	4.93	1.45	1.33
2	B	501	ACO	C5P-N4P	4.93	1.45	1.33
2	C	501	ACO	C9P-N8P	4.90	1.45	1.33
2	D	501	ACO	C5P-N4P	4.89	1.45	1.33
2	J	501	ACO	C9P-N8P	4.88	1.45	1.33
2	J	501	ACO	C5P-N4P	4.88	1.45	1.33
2	K	501	ACO	C9P-N8P	4.83	1.45	1.33
2	D	501	ACO	C9P-N8P	4.82	1.44	1.33
2	F	501	ACO	C9P-N8P	4.81	1.44	1.33
2	K	501	ACO	C6A-N6A	4.79	1.46	1.34
2	L	501	ACO	C9P-N8P	4.79	1.44	1.33
2	I	501	ACO	C6A-N6A	4.79	1.46	1.34
2	A	501	ACO	C9P-N8P	4.77	1.44	1.33
2	H	501	ACO	C9P-N8P	4.75	1.44	1.33
2	G	501	ACO	C5P-N4P	4.69	1.44	1.33
2	A	501	ACO	C6A-N6A	4.65	1.46	1.34
2	D	501	ACO	C6A-N6A	4.65	1.46	1.34
2	C	501	ACO	C6A-N6A	4.63	1.46	1.34
2	H	501	ACO	C6A-N6A	4.63	1.46	1.34
2	L	501	ACO	C6A-N6A	4.62	1.46	1.34
2	J	501	ACO	C6A-N6A	4.57	1.45	1.34
2	F	501	ACO	C6A-N6A	4.53	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	ACO	C6A-N6A	4.52	1.45	1.34
2	B	501	ACO	C6A-N6A	4.45	1.45	1.34
2	B	501	ACO	C2B-C3B	-4.45	1.43	1.53
2	C	501	ACO	C5P-N4P	4.45	1.43	1.33
2	G	501	ACO	C2B-C3B	-4.31	1.43	1.53
2	F	501	ACO	C2B-C3B	-4.15	1.43	1.53
2	A	501	ACO	C2B-C3B	-4.14	1.43	1.53
2	L	501	ACO	C2B-C3B	-4.13	1.44	1.53
2	H	501	ACO	C2B-C3B	-3.97	1.44	1.53
2	L	501	ACO	OAP-CAP	-3.74	1.35	1.42
2	C	501	ACO	C2B-C3B	-3.69	1.44	1.53
2	I	501	ACO	C2B-C3B	-3.57	1.45	1.53
2	K	501	ACO	C2B-C3B	-3.55	1.45	1.53
2	D	501	ACO	OAP-CAP	-3.52	1.36	1.42
2	E	501	ACO	C2B-C3B	-3.49	1.45	1.53
2	J	501	ACO	C2B-C3B	-3.41	1.45	1.53
2	D	501	ACO	C2B-C3B	-3.40	1.45	1.53
2	B	501	ACO	OAP-CAP	-3.39	1.36	1.42
2	H	501	ACO	OAP-CAP	-3.18	1.36	1.42
2	F	501	ACO	OAP-CAP	-3.16	1.36	1.42
2	G	501	ACO	OAP-CAP	-3.14	1.36	1.42
2	K	501	ACO	OAP-CAP	-3.10	1.36	1.42
2	I	501	ACO	OAP-CAP	-3.03	1.37	1.42
2	A	501	ACO	OAP-CAP	-2.98	1.37	1.42
2	E	501	ACO	OAP-CAP	-2.98	1.37	1.42
2	C	501	ACO	C3B-C4B	-2.88	1.45	1.52
2	F	501	ACO	C3B-C4B	-2.87	1.45	1.52
2	I	501	ACO	C3B-C4B	-2.79	1.45	1.52
2	J	501	ACO	OAP-CAP	-2.75	1.37	1.42
2	E	501	ACO	C3B-C4B	-2.74	1.45	1.52
2	H	501	ACO	C3B-C4B	-2.69	1.46	1.52
2	K	501	ACO	C3B-C4B	-2.69	1.46	1.52
2	G	501	ACO	C3B-C4B	-2.68	1.46	1.52
2	C	501	ACO	OAP-CAP	-2.64	1.37	1.42
2	J	501	ACO	C3B-C4B	-2.52	1.46	1.52
2	A	501	ACO	C3B-C4B	-2.49	1.46	1.52
2	B	501	ACO	C3B-C4B	-2.48	1.46	1.52
2	F	501	ACO	P3B-O3B	-2.47	1.55	1.59
2	L	501	ACO	P3B-O3B	-2.44	1.55	1.59
2	E	501	ACO	C5B-C4B	-2.41	1.44	1.51
2	L	501	ACO	C5A-N7A	-2.41	1.34	1.39
2	H	501	ACO	C5B-C4B	-2.30	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ACO	C3B-C4B	-2.30	1.47	1.52
2	L	501	ACO	C3B-C4B	-2.28	1.47	1.52
2	I	501	ACO	C1B-N9A	2.25	1.52	1.46
2	I	501	ACO	C5B-C4B	-2.24	1.44	1.51
2	D	501	ACO	C5B-C4B	-2.18	1.45	1.51
2	C	501	ACO	C5B-C4B	-2.16	1.45	1.51
2	F	501	ACO	C5B-C4B	-2.15	1.45	1.51
2	K	501	ACO	C5B-C4B	-2.13	1.45	1.51
2	C	501	ACO	C1B-N9A	2.13	1.52	1.46
2	J	501	ACO	C5B-C4B	-2.13	1.45	1.51
2	A	501	ACO	C1B-N9A	2.12	1.52	1.46
2	G	501	ACO	C5A-N7A	-2.12	1.35	1.39
2	J	501	ACO	C1B-N9A	2.11	1.52	1.46
2	B	501	ACO	P2A-O3A	2.10	1.61	1.59
2	B	501	ACO	P3B-O3B	-2.08	1.55	1.59
2	L	501	ACO	C8A-N9A	-2.08	1.34	1.37
2	B	501	ACO	C1B-N9A	2.05	1.52	1.46
2	D	501	ACO	C1B-N9A	2.05	1.52	1.46
2	L	501	ACO	CCP-CBP	2.04	1.55	1.52
2	A	501	ACO	C8A-N7A	2.03	1.35	1.31
2	G	501	ACO	O2B-C2B	-2.01	1.38	1.43
2	F	501	ACO	C1B-N9A	2.01	1.51	1.46
2	C	501	ACO	P3B-O3B	-2.01	1.56	1.59

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	ACO	O6A-CCP-CBP	7.73	122.97	110.55
2	K	501	ACO	O6A-CCP-CBP	7.39	122.42	110.55
2	L	501	ACO	O6A-CCP-CBP	7.18	122.09	110.55
2	J	501	ACO	O6A-CCP-CBP	6.84	121.54	110.55
2	F	501	ACO	C2P-C3P-N4P	6.65	126.30	112.41
2	I	501	ACO	O6A-CCP-CBP	6.40	120.84	110.55
2	E	501	ACO	O6A-CCP-CBP	6.30	120.68	110.55
2	A	501	ACO	O4B-C1B-N9A	5.96	119.54	108.09
2	B	501	ACO	O6A-CCP-CBP	5.71	119.72	110.55
2	D	501	ACO	O4B-C1B-N9A	5.58	118.81	108.09
2	C	501	ACO	C5A-C4A-N3A	-5.36	119.34	126.72
2	J	501	ACO	O4B-C1B-N9A	5.30	118.26	108.09
2	L	501	ACO	C5A-C4A-N3A	-5.26	119.48	126.72
2	F	501	ACO	C5A-C4A-N3A	-5.15	119.62	126.72
2	K	501	ACO	O4B-C1B-N9A	5.14	117.96	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	ACO	C2P-C3P-N4P	5.14	123.14	112.41
2	I	501	ACO	N3A-C2A-N1A	-5.10	120.86	128.58
2	L	501	ACO	C2P-C3P-N4P	5.10	123.06	112.41
2	G	501	ACO	C5A-C4A-N3A	-5.08	119.72	126.72
2	B	501	ACO	O4B-C1B-N9A	5.02	117.73	108.09
2	C	501	ACO	O4B-C1B-N9A	4.97	117.64	108.09
2	F	501	ACO	O6A-CCP-CBP	4.86	118.35	110.55
2	K	501	ACO	C4A-N9A-C8A	4.85	110.83	105.74
2	A	501	ACO	N3A-C2A-N1A	-4.84	121.25	128.58
2	H	501	ACO	C5A-C4A-N3A	-4.81	120.09	126.72
2	B	501	ACO	N3A-C2A-N1A	-4.80	121.31	128.58
2	A	501	ACO	C5A-C4A-N3A	-4.78	120.13	126.72
2	H	501	ACO	N3A-C2A-N1A	-4.77	121.36	128.58
2	F	501	ACO	O4B-C1B-N9A	4.75	117.22	108.09
2	L	501	ACO	N3A-C4A-N9A	4.73	135.22	127.17
2	I	501	ACO	C5A-C4A-N3A	-4.69	120.25	126.72
2	B	501	ACO	C5A-C4A-N3A	-4.69	120.26	126.72
2	K	501	ACO	N3A-C2A-N1A	-4.69	121.48	128.58
2	H	501	ACO	O4B-C1B-N9A	4.67	117.05	108.09
2	J	501	ACO	C5A-C4A-N3A	-4.64	120.32	126.72
2	K	501	ACO	N9A-C8A-N7A	-4.63	107.36	113.94
2	A	501	ACO	O6A-CCP-CBP	4.63	117.98	110.55
2	E	501	ACO	N3A-C2A-N1A	-4.61	121.61	128.58
2	F	501	ACO	N3A-C4A-N9A	4.52	134.85	127.17
2	L	501	ACO	N9A-C8A-N7A	-4.50	107.56	113.94
2	E	501	ACO	C5A-C4A-N3A	-4.46	120.58	126.72
2	D	501	ACO	N3A-C2A-N1A	-4.40	121.92	128.58
2	H	501	ACO	C4A-N9A-C8A	4.40	110.35	105.74
2	H	501	ACO	N3A-C4A-N9A	4.39	134.63	127.17
2	L	501	ACO	C4A-N9A-C8A	4.36	110.32	105.74
2	H	501	ACO	O6A-CCP-CBP	4.36	117.56	110.55
2	G	501	ACO	O6A-CCP-CBP	4.35	117.55	110.55
2	C	501	ACO	N3A-C4A-N9A	4.35	134.56	127.17
2	K	501	ACO	C5A-C4A-N3A	-4.33	120.75	126.72
2	I	501	ACO	N3A-C4A-N9A	4.32	134.52	127.17
2	F	501	ACO	N3A-C2A-N1A	-4.32	122.05	128.58
2	D	501	ACO	N9A-C8A-N7A	-4.31	107.83	113.94
2	D	501	ACO	C4A-N9A-C8A	4.28	110.23	105.74
2	D	501	ACO	C5A-C4A-N3A	-4.24	120.88	126.72
2	H	501	ACO	N9A-C8A-N7A	-4.22	107.94	113.94
2	G	501	ACO	C2P-C3P-N4P	4.22	121.23	112.41
2	I	501	ACO	O4B-C1B-N9A	4.22	116.19	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	ACO	N3A-C4A-N9A	4.21	134.33	127.17
2	B	501	ACO	N9A-C8A-N7A	-4.17	108.02	113.94
2	G	501	ACO	N3A-C2A-N1A	-4.16	122.28	128.58
2	C	501	ACO	N3A-C2A-N1A	-4.12	122.34	128.58
2	F	501	ACO	N9A-C8A-N7A	-4.11	108.11	113.94
2	L	501	ACO	N3A-C2A-N1A	-4.10	122.38	128.58
2	E	501	ACO	O4B-C1B-N9A	4.09	115.95	108.09
2	J	501	ACO	N3A-C2A-N1A	-4.09	122.40	128.58
2	B	501	ACO	N3A-C4A-N9A	4.06	134.07	127.17
2	B	501	ACO	C4A-N9A-C8A	4.05	109.99	105.74
2	F	501	ACO	C4A-N9A-C8A	4.05	109.99	105.74
2	G	501	ACO	C6P-C5P-N4P	4.04	123.71	116.34
2	A	501	ACO	CAP-C9P-N8P	4.02	124.11	116.48
2	L	501	ACO	O4B-C1B-N9A	4.01	115.80	108.09
2	A	501	ACO	N3A-C4A-N9A	4.00	133.97	127.17
2	D	501	ACO	C6P-C5P-N4P	3.99	123.61	116.34
2	K	501	ACO	N3A-C4A-N9A	3.99	133.95	127.17
2	C	501	ACO	N9A-C8A-N7A	-3.97	108.30	113.94
2	J	501	ACO	N3A-C4A-N9A	3.97	133.92	127.17
2	E	501	ACO	C4A-N9A-C8A	3.94	109.88	105.74
2	A	501	ACO	N9A-C8A-N7A	-3.93	108.36	113.94
2	E	501	ACO	N3A-C4A-N9A	3.92	133.84	127.17
2	I	501	ACO	C4A-N9A-C8A	3.91	109.85	105.74
2	G	501	ACO	O4B-C1B-N9A	3.91	115.59	108.09
2	C	501	ACO	O6A-CCP-CBP	3.90	116.82	110.55
2	I	501	ACO	N9A-C8A-N7A	-3.82	108.52	113.94
2	E	501	ACO	CAP-C9P-N8P	3.81	123.72	116.48
2	G	501	ACO	N9A-C8A-N7A	-3.79	108.56	113.94
2	A	501	ACO	C4A-N9A-C8A	3.78	109.71	105.74
2	E	501	ACO	C2P-C3P-N4P	3.77	120.28	112.41
2	H	501	ACO	C2P-C3P-N4P	3.76	120.26	112.41
2	E	501	ACO	N9A-C8A-N7A	-3.74	108.62	113.94
2	J	501	ACO	N9A-C8A-N7A	-3.74	108.63	113.94
2	J	501	ACO	C2P-C3P-N4P	3.68	120.09	112.41
2	J	501	ACO	CAP-C9P-N8P	3.65	123.41	116.48
2	H	501	ACO	CAP-C9P-N8P	3.63	123.37	116.48
2	J	501	ACO	C4A-N9A-C8A	3.61	109.53	105.74
2	A	501	ACO	C7P-N8P-C9P	-3.61	116.06	122.55
2	B	501	ACO	C2P-C3P-N4P	3.61	119.94	112.41
2	L	501	ACO	CAP-C9P-N8P	3.58	123.27	116.48
2	I	501	ACO	C2A-N3A-C4A	3.57	120.54	111.83
2	D	501	ACO	N3A-C4A-N9A	3.55	133.21	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	ACO	C5A-N7A-C8A	3.54	109.01	103.45
2	A	501	ACO	C2A-N3A-C4A	3.52	120.42	111.83
2	H	501	ACO	C2A-N3A-C4A	3.51	120.41	111.83
2	F	501	ACO	C2A-N3A-C4A	3.50	120.39	111.83
2	C	501	ACO	C4A-N9A-C8A	3.50	109.42	105.74
2	G	501	ACO	CAP-C9P-N8P	3.48	123.09	116.48
2	D	501	ACO	C4A-N9A-C1B	-3.47	118.52	126.63
2	C	501	ACO	C2A-N3A-C4A	3.44	120.23	111.83
2	E	501	ACO	C2A-N3A-C4A	3.42	120.18	111.83
2	B	501	ACO	C2A-N3A-C4A	3.40	120.12	111.83
2	D	501	ACO	C3P-N4P-C5P	-3.37	116.56	122.82
2	A	501	ACO	C2P-C3P-N4P	3.36	119.43	112.41
2	K	501	ACO	C2P-C3P-N4P	3.33	119.37	112.41
2	B	501	ACO	O5P-C5P-N4P	-3.33	116.50	123.03
2	L	501	ACO	C2A-N3A-C4A	3.32	119.95	111.83
2	G	501	ACO	C2A-N3A-C4A	3.32	119.94	111.83
2	L	501	ACO	C6P-C5P-N4P	3.32	122.39	116.34
2	G	501	ACO	C4A-N9A-C8A	3.32	109.22	105.74
2	F	501	ACO	C5A-N7A-C8A	3.31	108.65	103.45
2	K	501	ACO	C5A-N7A-C8A	3.29	108.62	103.45
2	K	501	ACO	C2A-N3A-C4A	3.29	119.87	111.83
2	E	501	ACO	O5P-C5P-N4P	-3.28	116.59	123.03
2	E	501	ACO	C6P-C5P-N4P	3.28	122.31	116.34
2	B	501	ACO	C5A-N7A-C8A	3.27	108.59	103.45
2	D	501	ACO	C5A-N7A-C8A	3.26	108.57	103.45
2	H	501	ACO	C5A-N7A-C8A	3.24	108.55	103.45
2	C	501	ACO	C5A-N7A-C8A	3.24	108.54	103.45
2	D	501	ACO	C2A-N3A-C4A	3.19	119.63	111.83
2	K	501	ACO	CAP-C9P-N8P	3.19	122.53	116.48
2	K	501	ACO	C4A-N9A-C1B	-3.15	119.26	126.63
2	D	501	ACO	O5P-C5P-N4P	-3.14	116.87	123.03
2	A	501	ACO	C5A-N7A-C8A	3.14	108.38	103.45
2	J	501	ACO	C2A-N3A-C4A	3.11	119.43	111.83
2	J	501	ACO	C3P-N4P-C5P	-3.11	117.04	122.82
2	B	501	ACO	C6P-C5P-N4P	3.10	121.99	116.34
2	G	501	ACO	C5A-N7A-C8A	3.07	108.28	103.45
2	H	501	ACO	C6P-C7P-N8P	3.07	118.53	112.00
2	K	501	ACO	O5B-C5B-C4B	3.04	119.36	108.99
2	J	501	ACO	C6P-C5P-N4P	3.02	121.84	116.34
2	J	501	ACO	C3B-C2B-C1B	3.01	106.51	99.89
2	E	501	ACO	C7P-N8P-C9P	-2.98	117.19	122.55
2	J	501	ACO	C5A-N7A-C8A	2.98	108.14	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	ACO	C3B-C2B-C1B	2.98	106.43	99.89
2	I	501	ACO	C5A-N7A-C8A	2.95	108.08	103.45
2	B	501	ACO	CAP-C9P-N8P	2.94	122.07	116.48
2	A	501	ACO	C6P-C5P-N4P	2.92	121.67	116.34
2	H	501	ACO	C6P-C5P-N4P	2.90	121.63	116.34
2	C	501	ACO	C3P-N4P-C5P	-2.86	117.50	122.82
2	A	501	ACO	C4A-N9A-C1B	-2.85	119.97	126.63
2	K	501	ACO	C6P-C5P-N4P	2.84	121.51	116.34
2	G	501	ACO	O5P-C5P-N4P	-2.83	117.47	123.03
2	C	501	ACO	O5P-C5P-N4P	-2.82	117.50	123.03
2	E	501	ACO	C4A-N9A-C1B	-2.81	120.06	126.63
2	B	501	ACO	C3B-C2B-C1B	2.78	106.00	99.89
2	C	501	ACO	O5B-C5B-C4B	2.77	118.42	108.99
2	C	501	ACO	C2P-C3P-N4P	2.76	118.17	112.41
2	E	501	ACO	C5A-N7A-C8A	2.74	107.75	103.45
2	D	501	ACO	C4A-C5A-N7A	-2.73	107.46	110.58
2	E	501	ACO	C7P-C6P-C5P	2.73	116.94	112.39
2	I	501	ACO	O5B-C5B-C4B	2.73	118.27	108.99
2	K	501	ACO	O5P-C5P-N4P	-2.70	117.73	123.03
2	A	501	ACO	O5B-C5B-C4B	2.68	118.13	108.99
2	K	501	ACO	C3B-C2B-C1B	2.68	105.78	99.89
2	G	501	ACO	C3B-C2B-C1B	2.67	105.75	99.89
2	H	501	ACO	C3B-C2B-C1B	2.65	105.73	99.89
2	G	501	ACO	O5B-C5B-C4B	2.65	118.03	108.99
2	A	501	ACO	C3B-C2B-C1B	2.64	105.70	99.89
2	H	501	ACO	O9P-C9P-N8P	-2.64	117.40	122.98
2	B	501	ACO	O5B-C5B-C4B	2.63	117.93	108.99
2	B	501	ACO	C7P-C6P-C5P	2.60	116.73	112.39
2	C	501	ACO	C4A-C5A-N7A	-2.58	107.63	110.58
2	D	501	ACO	CAP-C9P-N8P	2.58	121.37	116.48
2	A	501	ACO	C4A-C5A-N7A	-2.57	107.65	110.58
2	H	501	ACO	C4A-N9A-C1B	-2.56	120.65	126.63
2	K	501	ACO	C5B-C4B-C3B	-2.53	105.95	114.38
2	F	501	ACO	O5B-C5B-C4B	2.53	117.61	108.99
2	J	501	ACO	O5B-C5B-C4B	2.51	117.56	108.99
2	B	501	ACO	C4A-C5A-N7A	-2.51	107.71	110.58
2	F	501	ACO	C4A-C5A-N7A	-2.50	107.72	110.58
2	E	501	ACO	O9P-C9P-N8P	-2.47	117.75	122.98
2	C	501	ACO	C3B-C2B-C1B	2.46	105.31	99.89
2	I	501	ACO	C6P-C5P-N4P	2.45	120.81	116.34
2	A	501	ACO	C2P-S1P-C	2.45	113.19	101.42
2	H	501	ACO	O5P-C5P-N4P	-2.44	118.23	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ACO	C4A-N9A-C1B	-2.44	120.92	126.63
2	I	501	ACO	C4A-N9A-C1B	-2.44	120.92	126.63
2	E	501	ACO	C3P-N4P-C5P	-2.43	118.29	122.82
2	D	501	ACO	CDP-CBP-CCP	2.43	112.24	108.22
2	L	501	ACO	C4A-C5A-N7A	-2.43	107.80	110.58
2	B	501	ACO	C2B-C1B-N9A	-2.41	107.31	113.30
2	F	501	ACO	C6P-C5P-N4P	2.41	120.74	116.34
2	D	501	ACO	C3B-C2B-C1B	2.37	105.10	99.89
2	K	501	ACO	C4A-C5A-N7A	-2.37	107.87	110.58
2	L	501	ACO	C2B-C1B-N9A	-2.37	107.42	113.30
2	H	501	ACO	C4A-C5A-N7A	-2.36	107.88	110.58
2	J	501	ACO	C4A-N9A-C1B	-2.36	121.12	126.63
2	J	501	ACO	O9P-C9P-N8P	-2.34	118.02	122.98
2	F	501	ACO	CAP-C9P-N8P	2.33	120.91	116.48
2	J	501	ACO	O5P-C5P-N4P	-2.33	118.45	123.03
2	K	501	ACO	C2B-C1B-N9A	-2.33	107.51	113.30
2	C	501	ACO	C6P-C5P-N4P	2.33	120.59	116.34
2	H	501	ACO	C7P-N8P-C9P	-2.32	118.38	122.55
2	J	501	ACO	C4A-C5A-N7A	-2.31	107.94	110.58
2	C	501	ACO	O2A-P1A-O3A	2.31	113.51	107.27
2	L	501	ACO	C2P-S1P-C	2.31	112.52	101.42
2	A	501	ACO	O3B-C3B-C2B	-2.31	103.41	111.68
2	J	501	ACO	C2B-C1B-N9A	-2.28	107.63	113.30
2	B	501	ACO	C2P-S1P-C	2.28	112.38	101.42
2	I	501	ACO	C2P-S1P-C	2.28	112.38	101.42
2	F	501	ACO	C4A-N9A-C1B	-2.28	121.31	126.63
2	G	501	ACO	C4A-C5A-N7A	-2.27	107.98	110.58
2	K	501	ACO	C7P-C6P-C5P	2.27	116.18	112.39
2	C	501	ACO	C4A-N9A-C1B	-2.27	121.33	126.63
2	E	501	ACO	O2A-P1A-O3A	2.26	113.39	107.27
2	L	501	ACO	O5P-C5P-N4P	-2.24	118.64	123.03
2	B	501	ACO	O3B-C3B-C2B	-2.24	103.66	111.68
2	F	501	ACO	P3B-O3B-C3B	-2.23	117.47	123.43
2	E	501	ACO	C6P-C7P-N8P	2.22	116.72	112.00
2	C	501	ACO	CAP-C9P-N8P	2.20	120.67	116.48
2	K	501	ACO	O4B-C4B-C3B	2.20	109.55	104.92
2	L	501	ACO	C3B-C2B-C1B	2.20	104.72	99.89
2	F	501	ACO	C2P-S1P-C	2.18	111.92	101.42
2	A	501	ACO	O9P-C9P-N8P	-2.18	118.37	122.98
2	L	501	ACO	O9P-C9P-N8P	-2.18	118.37	122.98
2	L	501	ACO	O5B-C5B-C4B	2.18	116.42	108.99
2	H	501	ACO	C3P-N4P-C5P	-2.16	118.81	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	ACO	C4A-C5A-N7A	-2.12	108.16	110.58
2	L	501	ACO	O3B-C3B-C2B	-2.10	104.13	111.68
2	F	501	ACO	CEP-CBP-CCP	2.10	111.70	108.22
2	D	501	ACO	C7P-C6P-C5P	2.10	115.89	112.39
2	B	501	ACO	O4B-C4B-C3B	2.09	109.32	104.92
2	J	501	ACO	C6P-C7P-N8P	2.06	116.39	112.00
2	K	501	ACO	C7P-N8P-C9P	-2.06	118.84	122.55
2	C	501	ACO	C5B-C4B-C3B	-2.02	107.66	114.38
2	I	501	ACO	CAP-C9P-N8P	2.01	120.30	116.48
2	C	501	ACO	C2P-S1P-C	2.01	111.09	101.42
2	A	501	ACO	O5P-C5P-N4P	-2.00	119.10	123.03

There are no chirality outliers.

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ACO	O4B-C4B-C5B-O5B
2	A	501	ACO	C5B-O5B-P1A-O2A
2	A	501	ACO	C5B-O5B-P1A-O3A
2	A	501	ACO	CDP-CBP-CCP-O6A
2	A	501	ACO	CEP-CBP-CCP-O6A
2	A	501	ACO	CAP-CBP-CCP-O6A
2	A	501	ACO	O-C-S1P-C2P
2	A	501	ACO	CH3-C-S1P-C2P
2	B	501	ACO	C4B-C3B-O3B-P3B
2	B	501	ACO	O4B-C4B-C5B-O5B
2	B	501	ACO	C5B-O5B-P1A-O1A
2	B	501	ACO	C5B-O5B-P1A-O2A
2	B	501	ACO	C5B-O5B-P1A-O3A
2	B	501	ACO	CDP-CBP-CCP-O6A
2	B	501	ACO	CEP-CBP-CCP-O6A
2	B	501	ACO	CAP-CBP-CCP-O6A
2	B	501	ACO	C5P-C6P-C7P-N8P
2	B	501	ACO	O-C-S1P-C2P
2	B	501	ACO	CH3-C-S1P-C2P
2	C	501	ACO	C4B-C3B-O3B-P3B
2	C	501	ACO	O4B-C4B-C5B-O5B
2	C	501	ACO	C5B-O5B-P1A-O1A
2	C	501	ACO	C5B-O5B-P1A-O2A
2	C	501	ACO	C5B-O5B-P1A-O3A
2	C	501	ACO	C5P-C6P-C7P-N8P
2	C	501	ACO	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
2	C	501	ACO	O-C-S1P-C2P
2	C	501	ACO	CH3-C-S1P-C2P
2	D	501	ACO	O4B-C4B-C5B-O5B
2	D	501	ACO	C5B-O5B-P1A-O1A
2	D	501	ACO	C5B-O5B-P1A-O2A
2	D	501	ACO	C5B-O5B-P1A-O3A
2	D	501	ACO	CDP-CBP-CCP-O6A
2	D	501	ACO	CEP-CBP-CCP-O6A
2	D	501	ACO	CAP-CBP-CCP-O6A
2	D	501	ACO	S1P-C2P-C3P-N4P
2	D	501	ACO	O-C-S1P-C2P
2	D	501	ACO	CH3-C-S1P-C2P
2	E	501	ACO	O4B-C4B-C5B-O5B
2	E	501	ACO	C5B-O5B-P1A-O2A
2	E	501	ACO	C5B-O5B-P1A-O3A
2	E	501	ACO	CDP-CBP-CCP-O6A
2	E	501	ACO	CEP-CBP-CCP-O6A
2	E	501	ACO	CAP-CBP-CCP-O6A
2	E	501	ACO	C5P-C6P-C7P-N8P
2	E	501	ACO	S1P-C2P-C3P-N4P
2	E	501	ACO	O-C-S1P-C2P
2	E	501	ACO	CH3-C-S1P-C2P
2	F	501	ACO	O4B-C4B-C5B-O5B
2	F	501	ACO	C5B-O5B-P1A-O1A
2	F	501	ACO	C5B-O5B-P1A-O2A
2	F	501	ACO	C5B-O5B-P1A-O3A
2	F	501	ACO	CDP-CBP-CCP-O6A
2	F	501	ACO	CEP-CBP-CCP-O6A
2	F	501	ACO	CAP-CBP-CCP-O6A
2	F	501	ACO	S1P-C2P-C3P-N4P
2	F	501	ACO	O-C-S1P-C2P
2	F	501	ACO	CH3-C-S1P-C2P
2	G	501	ACO	CEP-CBP-CCP-O6A
2	G	501	ACO	O-C-S1P-C2P
2	G	501	ACO	CH3-C-S1P-C2P
2	H	501	ACO	O4B-C4B-C5B-O5B
2	H	501	ACO	C5B-O5B-P1A-O1A
2	H	501	ACO	C5B-O5B-P1A-O2A
2	H	501	ACO	C5B-O5B-P1A-O3A
2	H	501	ACO	CDP-CBP-CCP-O6A
2	H	501	ACO	CEP-CBP-CCP-O6A
2	H	501	ACO	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	H	501	ACO	C5P-C6P-C7P-N8P
2	H	501	ACO	O-C-S1P-C2P
2	H	501	ACO	CH3-C-S1P-C2P
2	I	501	ACO	C4B-C3B-O3B-P3B
2	I	501	ACO	O4B-C4B-C5B-O5B
2	I	501	ACO	C5B-O5B-P1A-O1A
2	I	501	ACO	C5B-O5B-P1A-O2A
2	I	501	ACO	C5B-O5B-P1A-O3A
2	I	501	ACO	CDP-CBP-CCP-O6A
2	I	501	ACO	CEP-CBP-CCP-O6A
2	I	501	ACO	CAP-CBP-CCP-O6A
2	I	501	ACO	S1P-C2P-C3P-N4P
2	I	501	ACO	O-C-S1P-C2P
2	I	501	ACO	CH3-C-S1P-C2P
2	J	501	ACO	C4B-C3B-O3B-P3B
2	J	501	ACO	O4B-C4B-C5B-O5B
2	J	501	ACO	C5B-O5B-P1A-O1A
2	J	501	ACO	C5B-O5B-P1A-O2A
2	J	501	ACO	C5B-O5B-P1A-O3A
2	J	501	ACO	CDP-CBP-CCP-O6A
2	J	501	ACO	CEP-CBP-CCP-O6A
2	J	501	ACO	CAP-CBP-CCP-O6A
2	J	501	ACO	S1P-C2P-C3P-N4P
2	J	501	ACO	O-C-S1P-C2P
2	J	501	ACO	CH3-C-S1P-C2P
2	K	501	ACO	C4B-C3B-O3B-P3B
2	K	501	ACO	C3B-C4B-C5B-O5B
2	K	501	ACO	O4B-C4B-C5B-O5B
2	K	501	ACO	C5B-O5B-P1A-O1A
2	K	501	ACO	C5B-O5B-P1A-O3A
2	K	501	ACO	CDP-CBP-CCP-O6A
2	K	501	ACO	CEP-CBP-CCP-O6A
2	K	501	ACO	CAP-CBP-CCP-O6A
2	K	501	ACO	C5P-C6P-C7P-N8P
2	K	501	ACO	S1P-C2P-C3P-N4P
2	K	501	ACO	O-C-S1P-C2P
2	K	501	ACO	CH3-C-S1P-C2P
2	L	501	ACO	C5P-C6P-C7P-N8P
2	L	501	ACO	S1P-C2P-C3P-N4P
2	L	501	ACO	O-C-S1P-C2P
2	L	501	ACO	CH3-C-S1P-C2P
2	C	501	ACO	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	501	ACO	C3B-C4B-C5B-O5B
2	E	501	ACO	C3B-C4B-C5B-O5B
2	G	501	ACO	O4B-C4B-C5B-O5B
2	I	501	ACO	C3B-C4B-C5B-O5B
2	L	501	ACO	O4B-C4B-C5B-O5B
2	D	501	ACO	C4B-C3B-O3B-P3B
2	E	501	ACO	C4B-C3B-O3B-P3B
2	H	501	ACO	C4B-C3B-O3B-P3B
2	L	501	ACO	C4B-C3B-O3B-P3B
2	F	501	ACO	C6P-C7P-N8P-C9P
2	G	501	ACO	C6P-C7P-N8P-C9P
2	B	501	ACO	C3B-C4B-C5B-O5B
2	F	501	ACO	C3B-C4B-C5B-O5B
2	G	501	ACO	C2B-C3B-O3B-P3B
2	G	501	ACO	C4B-C3B-O3B-P3B
2	A	501	ACO	C3B-C4B-C5B-O5B
2	H	501	ACO	C3B-C4B-C5B-O5B
2	J	501	ACO	C3B-C4B-C5B-O5B
2	J	501	ACO	C5P-C6P-C7P-N8P
2	G	501	ACO	C3B-C4B-C5B-O5B
2	L	501	ACO	C3B-C4B-C5B-O5B
2	D	501	ACO	C6P-C7P-N8P-C9P
2	C	501	ACO	C2B-C3B-O3B-P3B
2	F	501	ACO	C2B-C3B-O3B-P3B
2	F	501	ACO	C4B-C3B-O3B-P3B
2	D	501	ACO	C9P-CAP-CBP-CDP
2	K	501	ACO	C9P-CAP-CBP-CDP
2	F	501	ACO	P1A-O3A-P2A-O4A
2	H	501	ACO	P1A-O3A-P2A-O4A
2	K	501	ACO	P1A-O3A-P2A-O4A
2	C	501	ACO	CDP-CBP-CCP-O6A
2	G	501	ACO	CDP-CBP-CCP-O6A
2	A	501	ACO	C6P-C7P-N8P-C9P
2	C	501	ACO	C3P-C2P-S1P-C
2	L	501	ACO	C6P-C7P-N8P-C9P
2	K	501	ACO	C5B-O5B-P1A-O2A
2	J	501	ACO	P2A-O3A-P1A-O2A
2	C	501	ACO	C3B-O3B-P3B-O8A
2	E	501	ACO	C3B-O3B-P3B-O8A
2	K	501	ACO	C3B-O3B-P3B-O8A
2	L	501	ACO	C3B-O3B-P3B-O8A
2	J	501	ACO	C6P-C7P-N8P-C9P

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Mol	Chain	Res	Type	Atoms
2	I	501	ACO	C6P-C7P-N8P-C9P
2	E	501	ACO	C2B-C3B-O3B-P3B
2	B	501	ACO	P1A-O3A-P2A-O4A
2	I	501	ACO	C5P-C6P-C7P-N8P
2	D	501	ACO	OAP-CAP-CBP-CEP
2	J	501	ACO	P2A-O3A-P1A-O1A
2	J	501	ACO	P1A-O3A-P2A-O5A
2	J	501	ACO	C3B-O3B-P3B-O8A
2	A	501	ACO	C4B-C3B-O3B-P3B
2	C	501	ACO	CEP-CBP-CCP-O6A
2	G	501	ACO	CAP-CBP-CCP-O6A
2	B	501	ACO	P1A-O3A-P2A-O5A
2	F	501	ACO	P1A-O3A-P2A-O5A
2	H	501	ACO	P2A-O3A-P1A-O2A
2	H	501	ACO	P1A-O3A-P2A-O5A

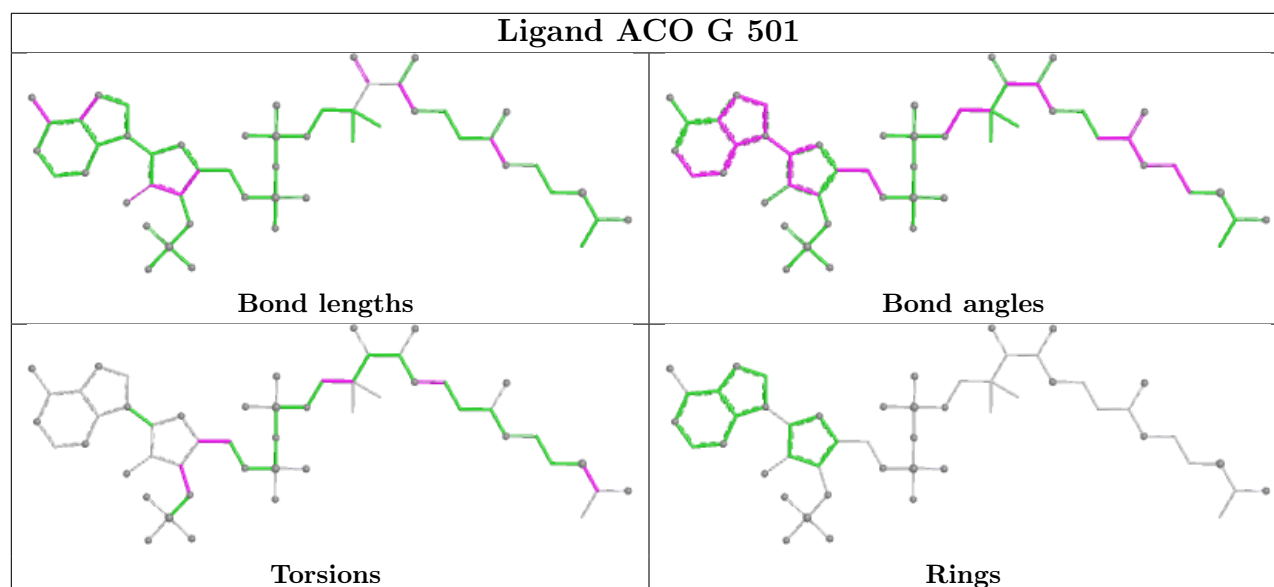
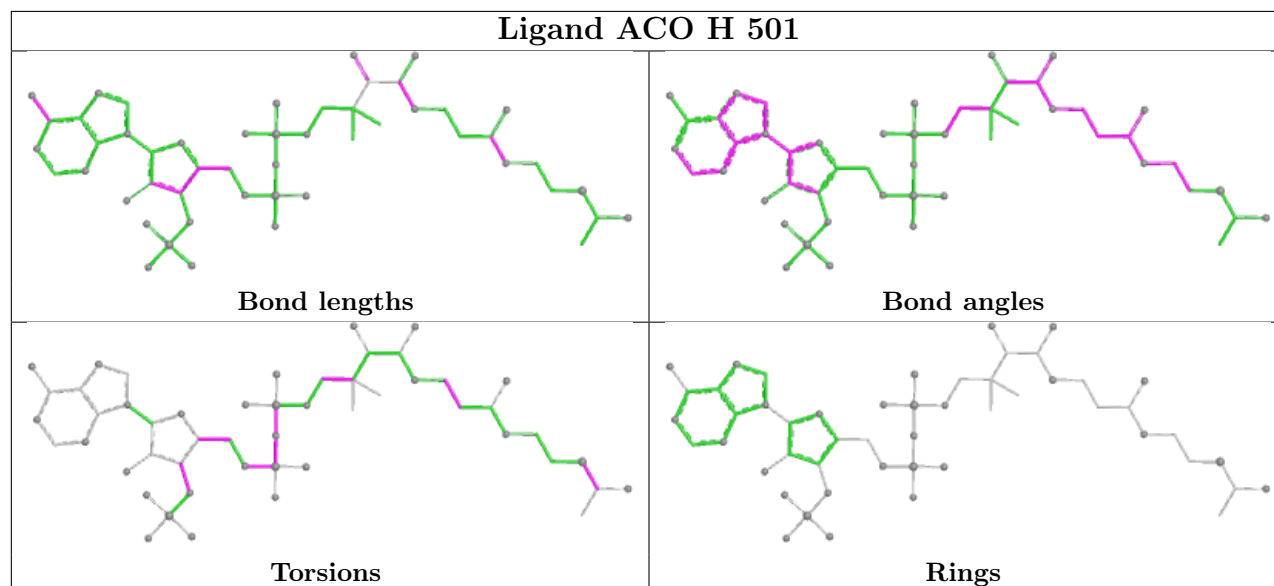
There are no ring outliers.

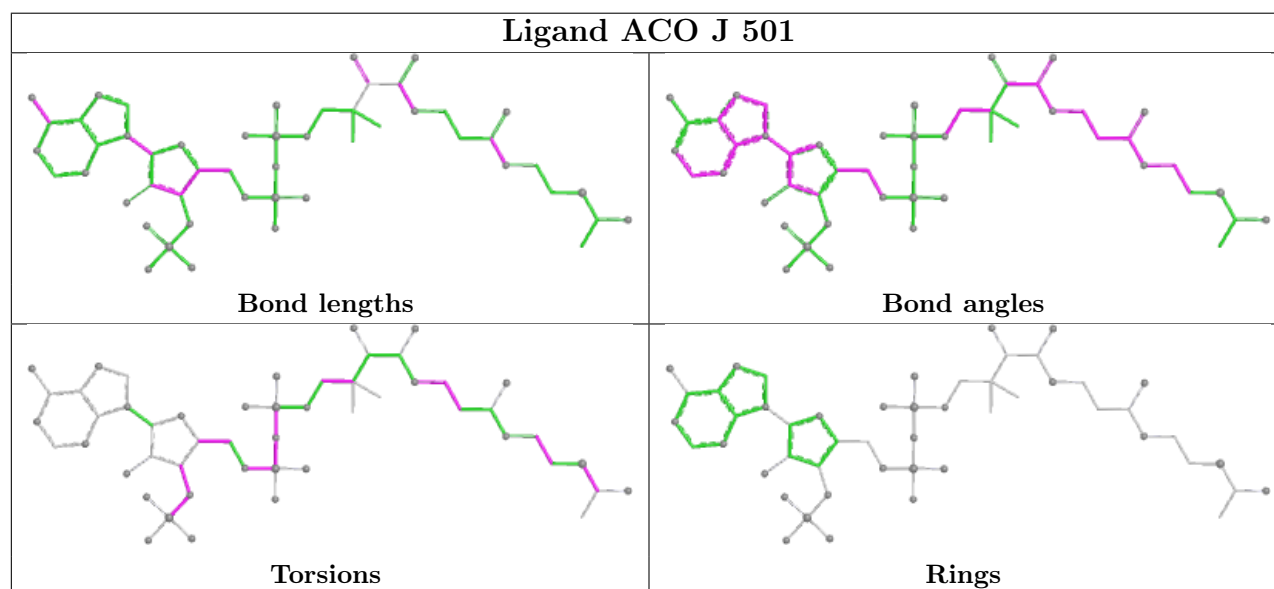
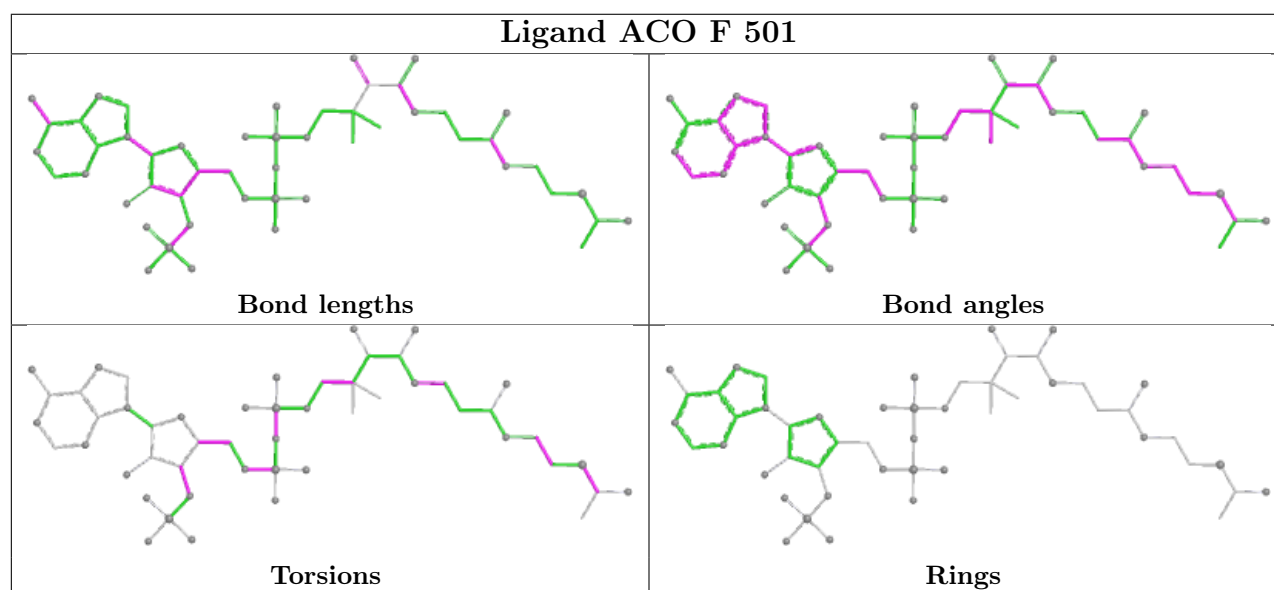
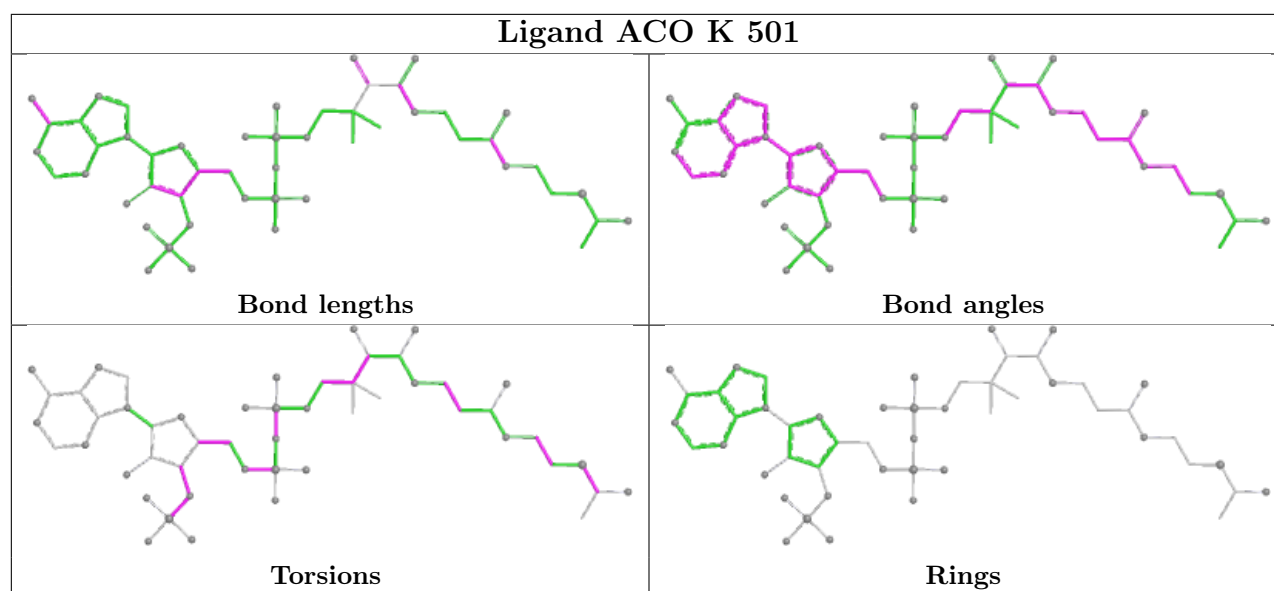
12 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	ACO	2	0
2	G	501	ACO	6	0
2	K	501	ACO	10	0
2	F	501	ACO	5	0
2	J	501	ACO	3	0
2	I	501	ACO	7	0
2	E	501	ACO	8	0
2	L	501	ACO	5	0
2	C	501	ACO	12	0
2	D	501	ACO	2	0
2	A	501	ACO	6	0
2	B	501	ACO	4	0

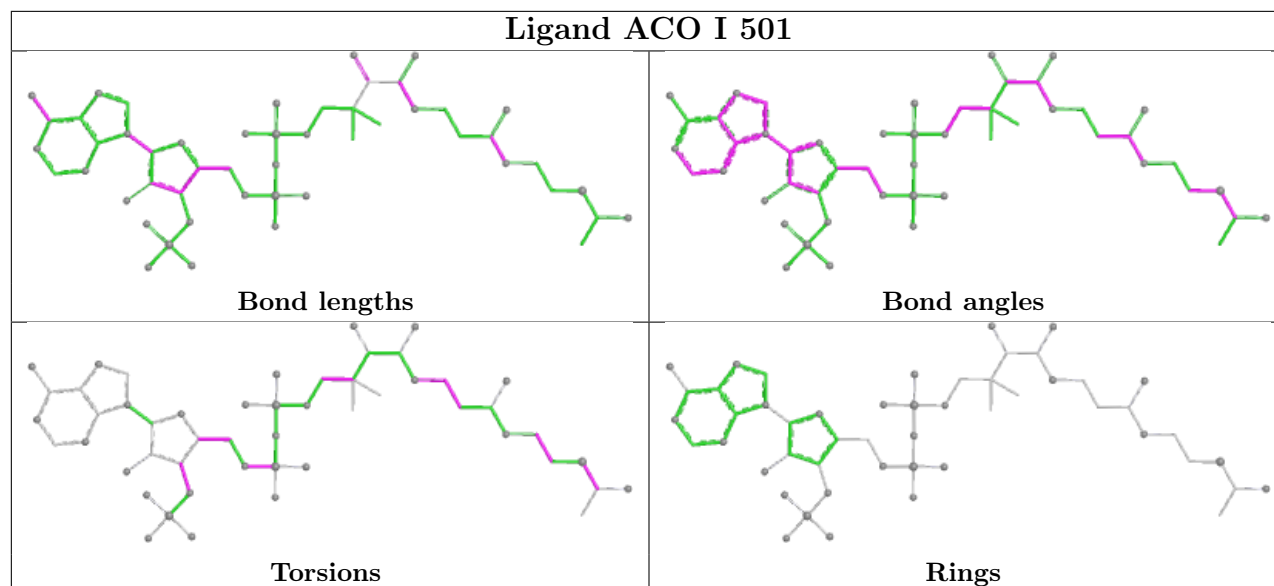
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

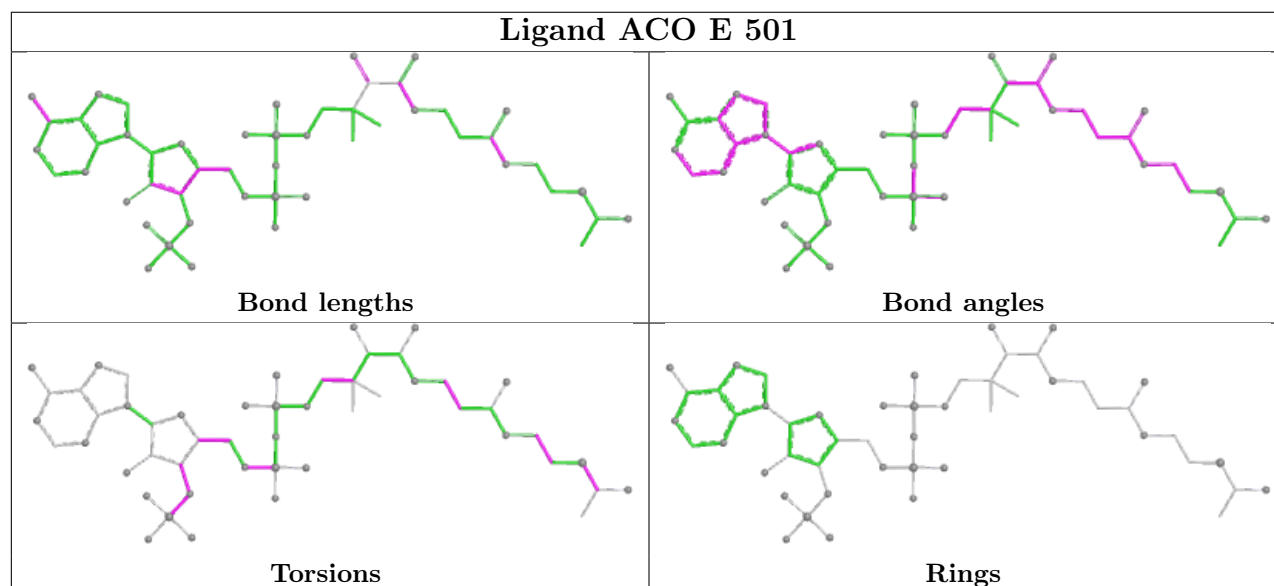




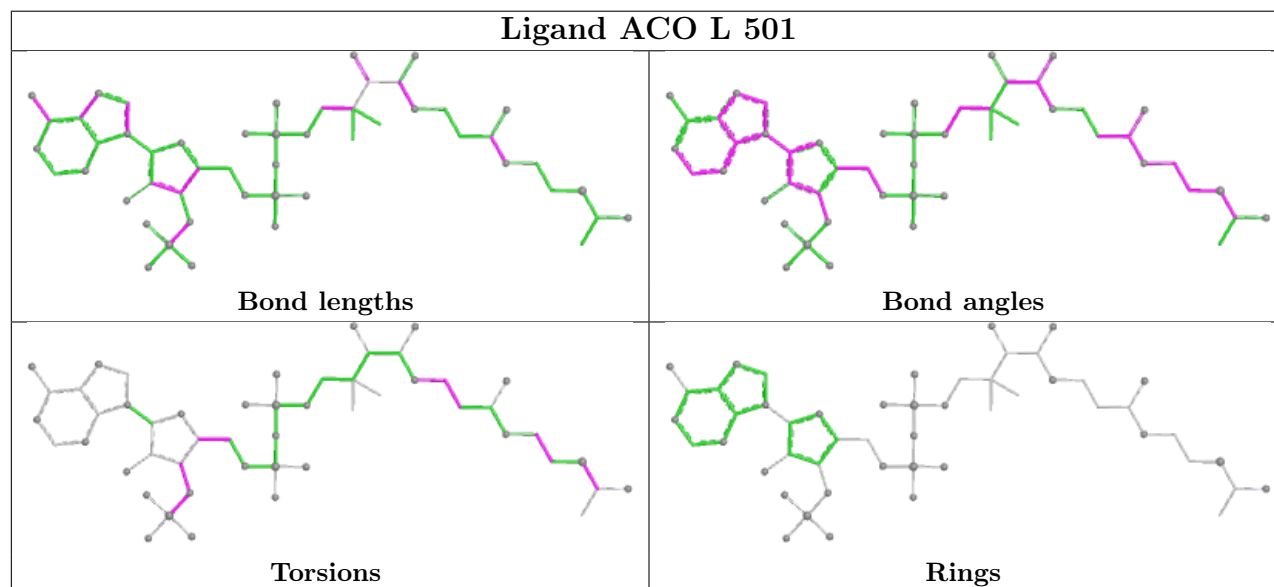
Ligand ACO I 501

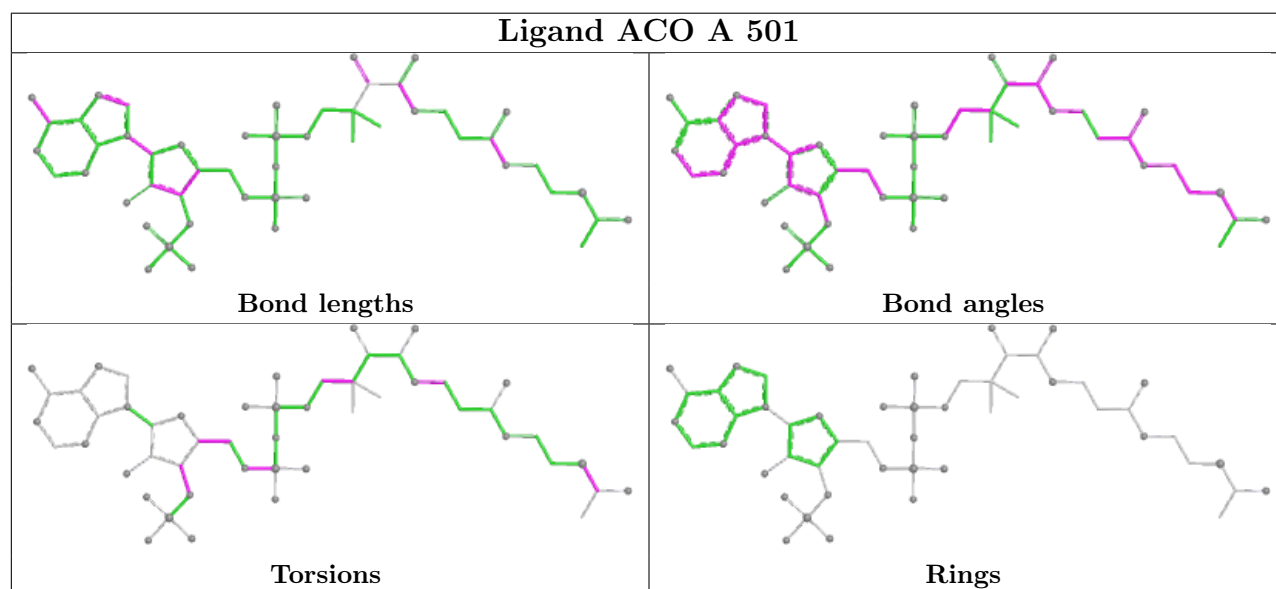
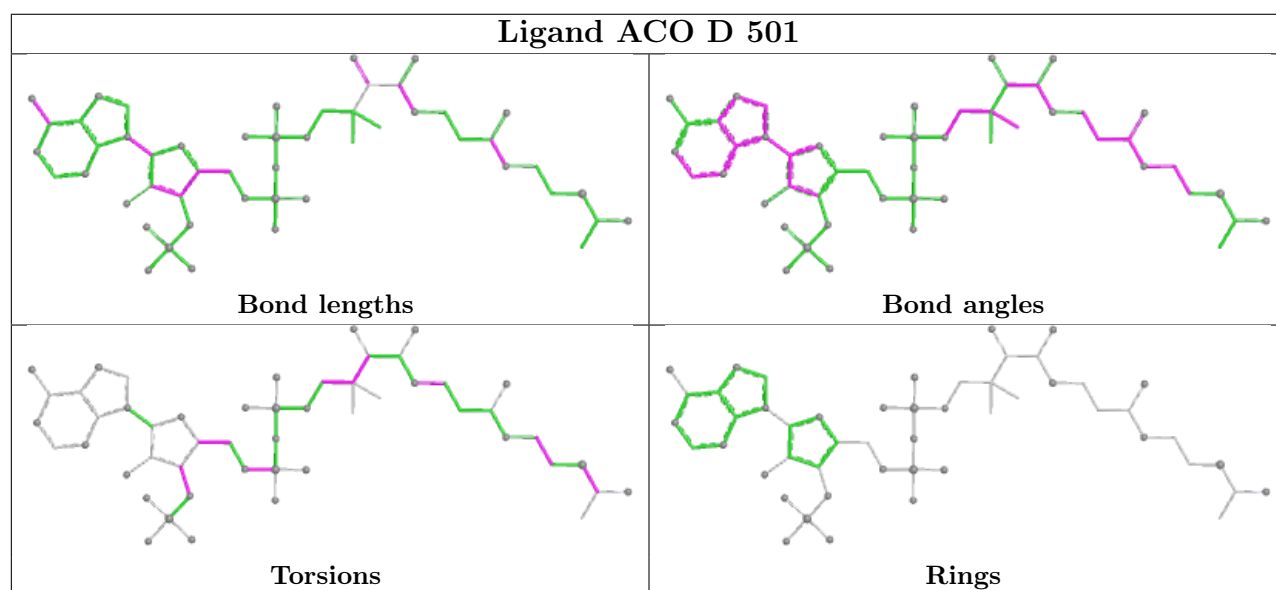
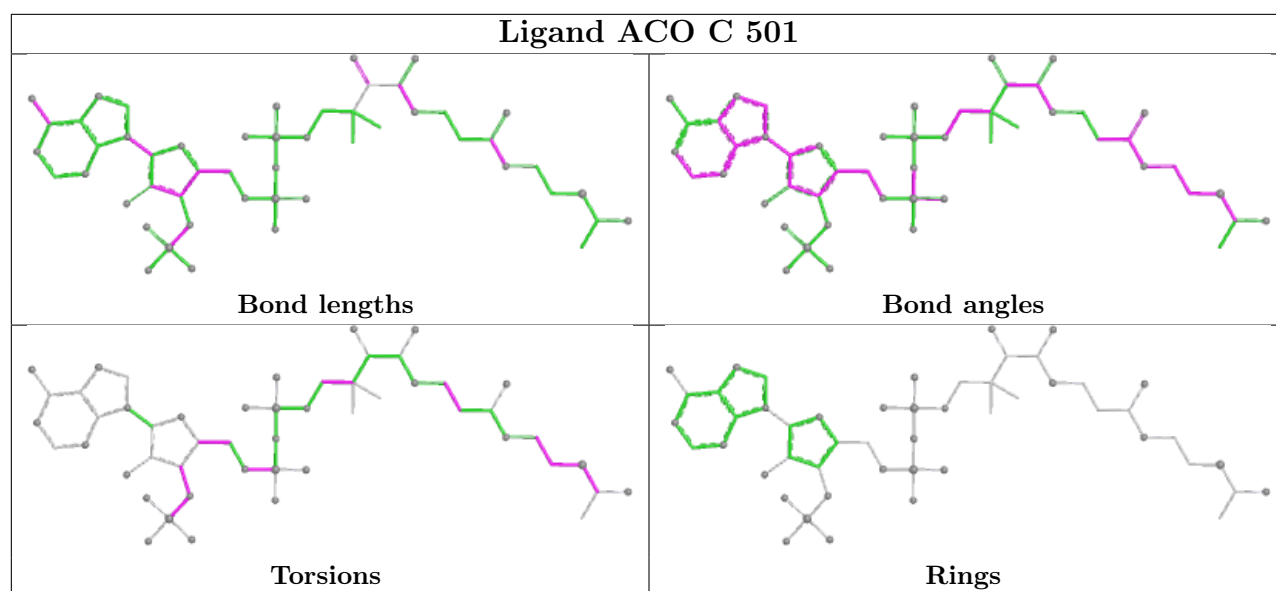


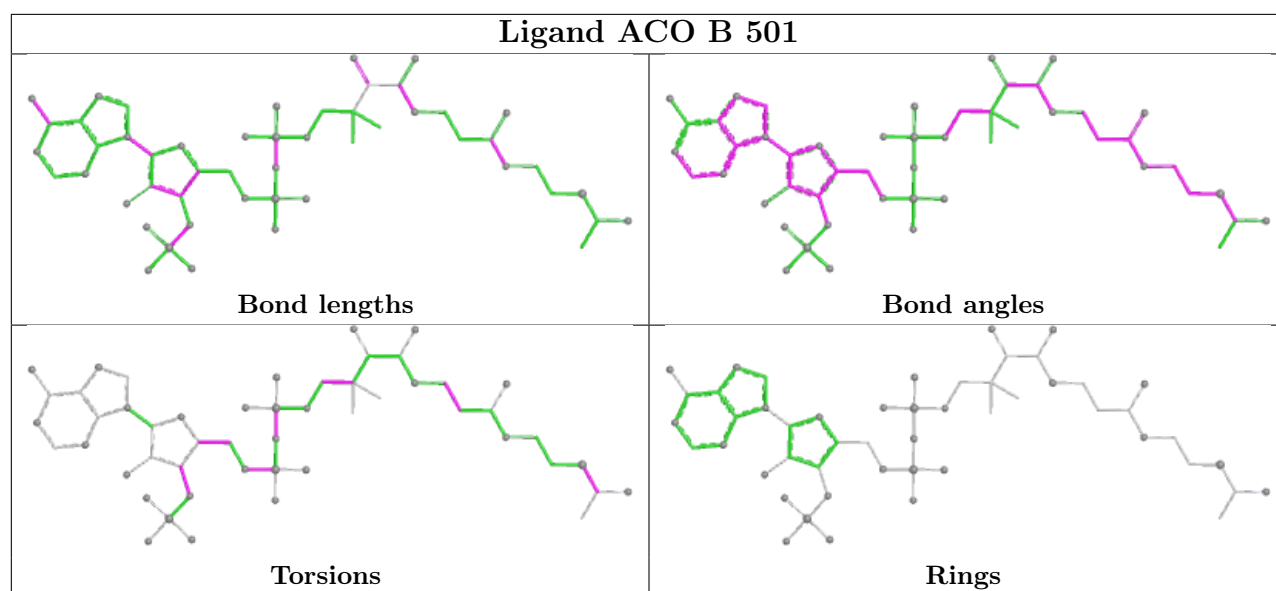
Ligand ACO E 501



Ligand ACO L 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	389/428 (90%)	-0.02	24 (6%)	26	20	16, 28, 63, 139	0
1	B	389/428 (90%)	-0.02	22 (5%)	29	22	18, 27, 65, 161	0
1	C	389/428 (90%)	0.08	22 (5%)	29	22	21, 30, 66, 152	0
1	D	389/428 (90%)	0.11	24 (6%)	26	20	18, 29, 65, 144	0
1	E	389/428 (90%)	0.16	26 (6%)	24	17	17, 30, 66, 158	0
1	F	389/428 (90%)	0.15	26 (6%)	24	17	20, 30, 72, 125	0
1	G	389/428 (90%)	0.21	24 (6%)	26	20	22, 35, 67, 162	0
1	H	389/428 (90%)	0.22	23 (5%)	28	21	23, 36, 72, 165	0
1	I	389/428 (90%)	0.52	25 (6%)	25	18	24, 47, 78, 163	0
1	J	389/428 (90%)	0.75	41 (10%)	11	8	24, 51, 81, 166	0
1	K	389/428 (90%)	0.31	23 (5%)	28	21	24, 43, 78, 157	0
1	L	389/428 (90%)	0.00	13 (3%)	49	39	23, 35, 69, 160	0
All	All	4668/5136 (90%)	0.21	293 (6%)	26	19	16, 35, 74, 166	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	TRP	14.2
1	E	60	PRO	8.5
1	A	60	PRO	7.6
1	A	8	THR	7.4
1	B	42	TRP	7.1
1	E	59	GLY	7.0
1	F	60	PRO	6.9
1	E	58	ALA	6.9
1	J	405	ALA	6.6
1	C	34	ILE	6.1
1	E	8	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	L	60	PRO	5.8
1	A	73	LEU	5.7
1	D	60	PRO	5.7
1	G	60	PRO	5.6
1	H	384	LYS	5.6
1	D	38	SER	5.6
1	I	60	PRO	5.2
1	F	61	GLY	5.2
1	D	8	THR	5.1
1	J	34	ILE	5.1
1	K	60	PRO	5.0
1	A	61	GLY	5.0
1	C	60	PRO	5.0
1	E	36	PRO	4.9
1	I	341	ASP	4.9
1	I	38	SER	4.9
1	A	59	GLY	4.8
1	E	37	GLU	4.8
1	I	34	ILE	4.8
1	I	61	GLY	4.8
1	B	60	PRO	4.8
1	D	148	VAL	4.8
1	K	34	ILE	4.7
1	G	8	THR	4.7
1	J	60	PRO	4.6
1	H	149	ASP	4.6
1	F	332	GLY	4.5
1	D	36	PRO	4.5
1	D	10	THR	4.5
1	C	148	VAL	4.5
1	C	58	ALA	4.4
1	F	19	TRP	4.4
1	D	61	GLY	4.4
1	E	61	GLY	4.3
1	A	34	ILE	4.3
1	H	58	ALA	4.3
1	E	34	ILE	4.2
1	F	9	VAL	4.1
1	H	39	ALA	4.1
1	D	35	GLY	4.1
1	H	34	ILE	4.0
1	E	144	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	61	GLY	4.0
1	G	34	ILE	4.0
1	H	60	PRO	4.0
1	J	331	ASP	3.9
1	I	148	VAL	3.9
1	B	340	GLY	3.9
1	D	59	GLY	3.8
1	G	58	ALA	3.8
1	I	8	THR	3.8
1	C	8	THR	3.8
1	C	36	PRO	3.7
1	G	39	ALA	3.7
1	K	35	GLY	3.7
1	L	61	GLY	3.7
1	G	59	GLY	3.7
1	E	38	SER	3.7
1	G	35	GLY	3.7
1	C	39	ALA	3.7
1	L	34	ILE	3.7
1	B	37	GLU	3.6
1	H	169	VAL	3.6
1	L	36	PRO	3.6
1	A	384	LYS	3.6
1	I	37	GLU	3.6
1	A	58	ALA	3.6
1	F	35	GLY	3.6
1	H	8	THR	3.6
1	C	292	ARG	3.5
1	E	35	GLY	3.5
1	L	59	GLY	3.5
1	J	42	TRP	3.5
1	J	36	PRO	3.5
1	G	43	ARG	3.5
1	D	9	VAL	3.5
1	G	220	SER	3.5
1	G	62	SER	3.5
1	J	19	TRP	3.5
1	B	34	ILE	3.4
1	F	121	VAL	3.4
1	G	207	LEU	3.4
1	I	58	ALA	3.4
1	E	44	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	8	THR	3.4
1	L	35	GLY	3.4
1	H	37	GLU	3.4
1	D	44	THR	3.4
1	E	215	GLY	3.3
1	G	57	GLY	3.3
1	E	220	SER	3.3
1	C	37	GLU	3.3
1	J	384	LYS	3.3
1	K	399	ASP	3.3
1	E	214	PRO	3.3
1	D	39	ALA	3.3
1	J	45	LEU	3.3
1	C	35	GLY	3.3
1	H	35	GLY	3.2
1	B	39	ALA	3.2
1	F	381	LEU	3.2
1	G	44	THR	3.2
1	E	19	TRP	3.2
1	B	49	ASP	3.2
1	B	43	ARG	3.2
1	H	19	TRP	3.2
1	B	331	ASP	3.2
1	E	39	ALA	3.2
1	J	292	ARG	3.2
1	J	343	ARG	3.2
1	J	35	GLY	3.2
1	D	58	ALA	3.1
1	I	35	GLY	3.1
1	J	58	ALA	3.1
1	K	39	ALA	3.1
1	J	330	SER	3.1
1	K	61	GLY	3.1
1	J	83	LEU	3.1
1	B	169	VAL	3.0
1	I	393	ASP	3.0
1	K	59	GLY	3.0
1	K	248	ARG	3.0
1	E	148	VAL	3.0
1	A	57	GLY	3.0
1	J	332	GLY	3.0
1	H	36	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	15	THR	3.0
1	H	383	THR	3.0
1	J	352	ALA	3.0
1	L	39	ALA	3.0
1	A	42	TRP	3.0
1	E	146	LEU	3.0
1	J	112	ARG	3.0
1	I	19	TRP	2.9
1	F	199	PRO	2.9
1	J	37	GLU	2.9
1	F	58	ALA	2.9
1	J	8	THR	2.9
1	A	36	PRO	2.9
1	G	37	GLU	2.9
1	F	34	ILE	2.9
1	K	37	GLU	2.8
1	A	39	ALA	2.8
1	F	331	ASP	2.8
1	D	37	GLU	2.8
1	I	39	ALA	2.8
1	J	40	THR	2.8
1	K	267	SER	2.8
1	L	320	VAL	2.8
1	C	121	VAL	2.7
1	K	148	VAL	2.7
1	K	8	THR	2.7
1	F	39	ALA	2.7
1	K	273	ILE	2.7
1	G	36	PRO	2.7
1	G	38	SER	2.7
1	J	61	GLY	2.7
1	J	349	THR	2.7
1	I	324	SER	2.7
1	F	41	ALA	2.7
1	D	233	ARG	2.7
1	H	170	ARG	2.7
1	H	61	GLY	2.7
1	A	62	SER	2.7
1	E	29	SER	2.7
1	J	327	LEU	2.7
1	J	41	ALA	2.6
1	J	98	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	58	ALA	2.6
1	K	98	ARG	2.6
1	F	8	THR	2.6
1	A	327	LEU	2.6
1	E	43	ARG	2.6
1	H	150	ARG	2.6
1	H	38	SER	2.6
1	A	43	ARG	2.6
1	A	19	TRP	2.6
1	F	57	GLY	2.6
1	J	79	GLY	2.6
1	I	36	PRO	2.5
1	J	44	THR	2.5
1	K	58	ALA	2.5
1	B	149	ASP	2.5
1	E	57	GLY	2.5
1	F	36	PRO	2.5
1	I	42	TRP	2.5
1	H	406	PHE	2.5
1	C	382	ARG	2.5
1	C	384	LYS	2.5
1	F	38	SER	2.4
1	F	167	SER	2.4
1	G	19	TRP	2.4
1	K	19	TRP	2.4
1	K	43	ARG	2.4
1	C	146	LEU	2.4
1	C	350	ASP	2.4
1	J	116	ASP	2.4
1	J	341	ASP	2.4
1	F	59	GLY	2.4
1	D	245	SER	2.4
1	B	19	TRP	2.4
1	G	406	PHE	2.4
1	B	44	THR	2.4
1	I	349	THR	2.4
1	C	381	LEU	2.4
1	K	207	LEU	2.4
1	D	34	ILE	2.4
1	B	59	GLY	2.4
1	F	43	ARG	2.4
1	G	384	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	348	PRO	2.4
1	E	321	GLY	2.3
1	J	342	GLY	2.3
1	J	359	ARG	2.3
1	J	39	ALA	2.3
1	L	37	GLU	2.3
1	A	38	SER	2.3
1	B	85	THR	2.3
1	F	270	ARG	2.3
1	A	35	GLY	2.3
1	C	90	PHE	2.3
1	A	37	GLU	2.3
1	H	405	ALA	2.3
1	E	207	LEU	2.3
1	G	40	THR	2.3
1	C	61	GLY	2.3
1	K	292	ARG	2.3
1	A	352	ALA	2.3
1	L	58	ALA	2.3
1	J	207	LEU	2.3
1	B	8	THR	2.3
1	D	19	TRP	2.3
1	J	38	SER	2.3
1	B	148	VAL	2.3
1	H	199	PRO	2.3
1	C	405	ALA	2.2
1	J	328	GLU	2.2
1	G	311	LEU	2.2
1	J	73	LEU	2.2
1	A	9	VAL	2.2
1	B	145	GLU	2.2
1	F	298	ASP	2.2
1	H	98	ARG	2.2
1	H	40	THR	2.2
1	K	36	PRO	2.2
1	C	62	SER	2.2
1	D	384	LYS	2.2
1	I	353	ALA	2.2
1	H	59	GLY	2.2
1	I	327	LEU	2.2
1	F	16	GLU	2.2
1	D	350	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	399	ASP	2.2
1	D	90	PHE	2.2
1	L	318	HIS	2.1
1	J	9	VAL	2.1
1	B	399	ASP	2.1
1	L	49	ASP	2.1
1	C	59	GLY	2.1
1	G	381	LEU	2.1
1	J	49	ASP	2.1
1	K	237	THR	2.1
1	A	167	SER	2.1
1	K	63	GLU	2.1
1	I	214	PRO	2.1
1	I	342	GLY	2.1
1	A	85	THR	2.1
1	I	288	THR	2.1
1	I	289	ARG	2.1
1	D	145	GLU	2.1
1	F	37	GLU	2.1
1	B	38	SER	2.1
1	D	104	ARG	2.1
1	G	302	LEU	2.0
1	J	233	ARG	2.0
1	E	28	ALA	2.0
1	E	62	SER	2.0
1	K	52	VAL	2.0
1	B	292	ARG	2.0
1	I	57	GLY	2.0
1	C	293	THR	2.0
1	A	180	GLU	2.0

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

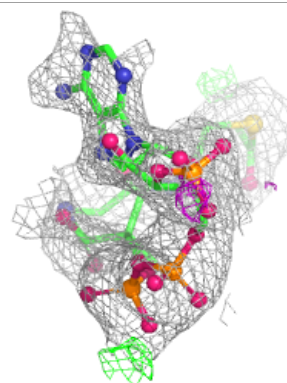
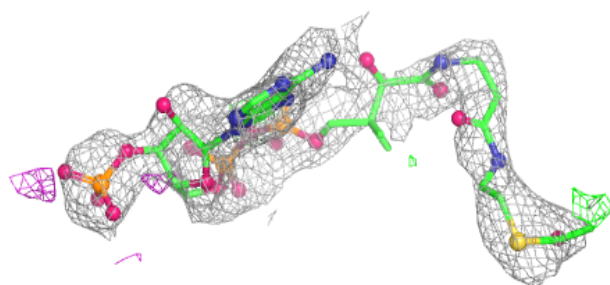
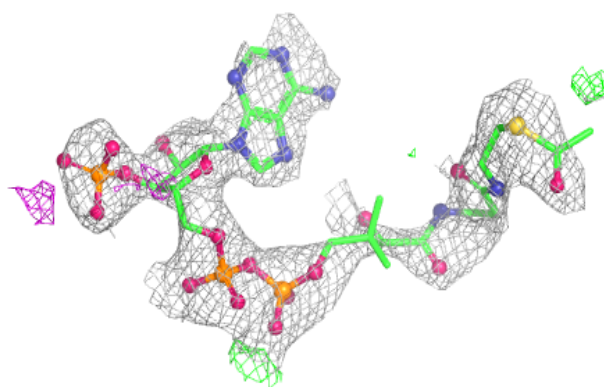
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACO	J	501	51/51	0.79	0.15	54,68,82,89	0
2	ACO	I	501	51/51	0.80	0.13	44,63,78,97	0
2	ACO	E	501	51/51	0.81	0.14	38,57,82,89	0
2	ACO	H	501	51/51	0.82	0.13	41,57,73,81	0
2	ACO	D	501	51/51	0.86	0.12	34,51,70,81	0
2	ACO	K	501	51/51	0.86	0.11	45,56,70,77	0
2	ACO	F	501	51/51	0.87	0.11	34,48,66,73	0
2	ACO	C	501	51/51	0.88	0.11	33,50,71,83	0
2	ACO	A	501	51/51	0.88	0.11	30,46,67,81	0
2	ACO	B	501	51/51	0.91	0.10	29,42,54,61	0
2	ACO	G	501	51/51	0.92	0.09	28,40,60,73	0
2	ACO	L	501	51/51	0.92	0.10	26,38,61,72	0

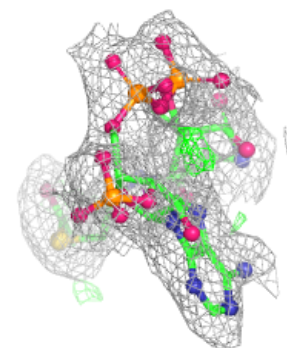
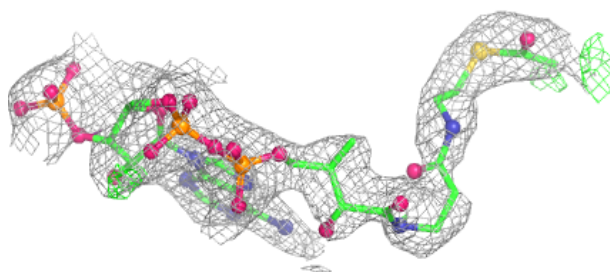
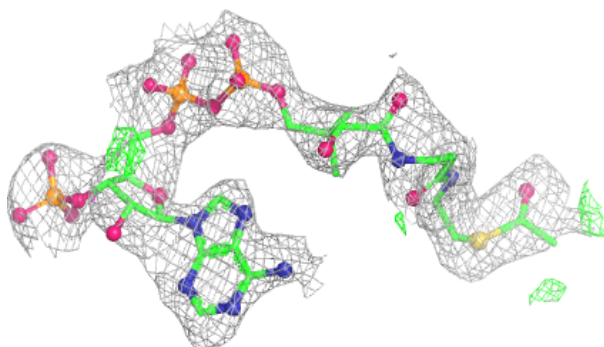
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO J 501:

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

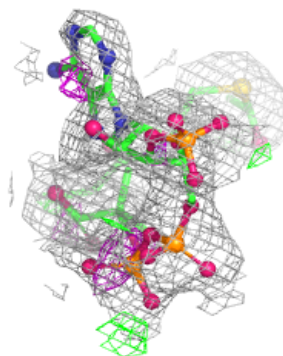
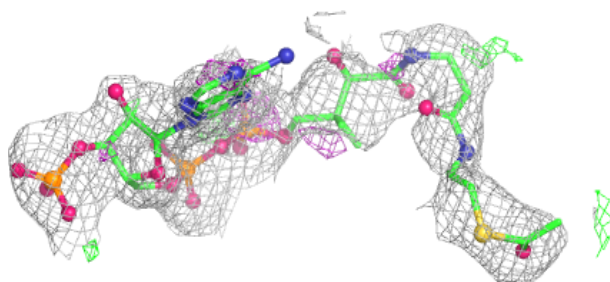
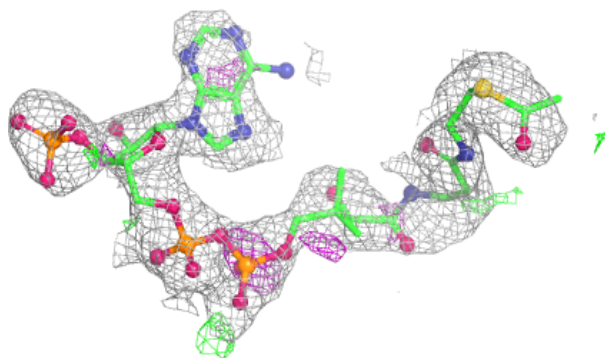
**Electron density around ACO I 501:**

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

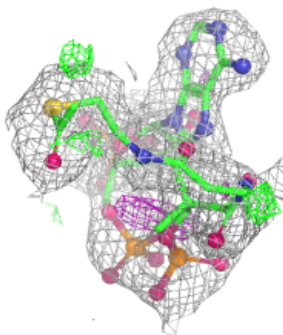
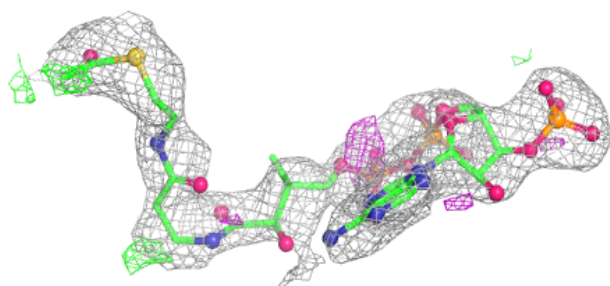
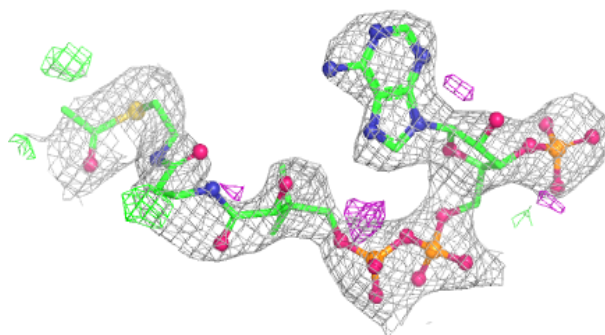


Electron density around ACO E 501:

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

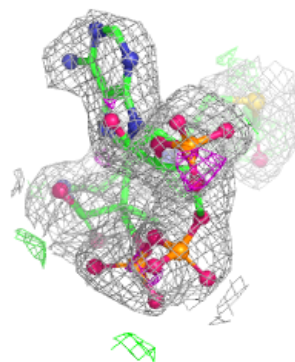
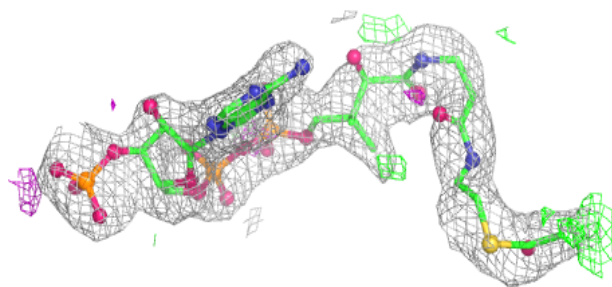
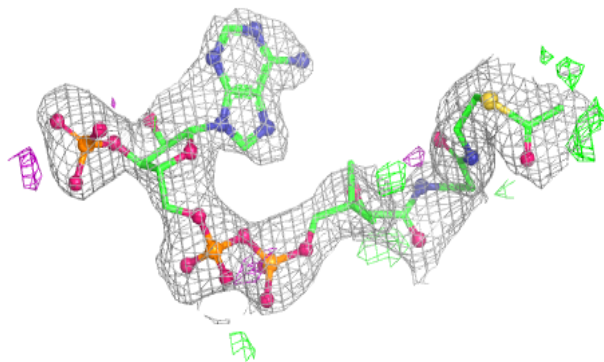
**Electron density around ACO H 501:**

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

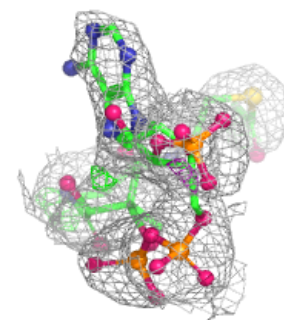
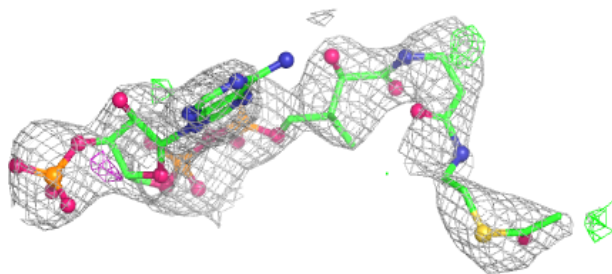
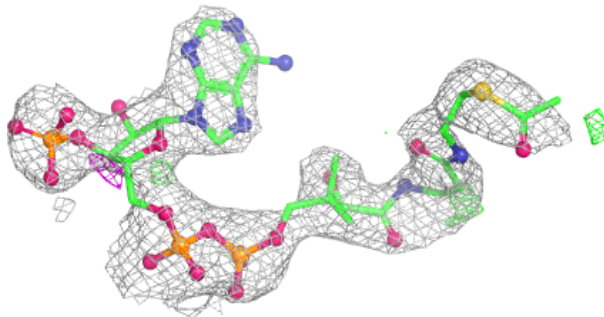


Electron density around ACO D 501:

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

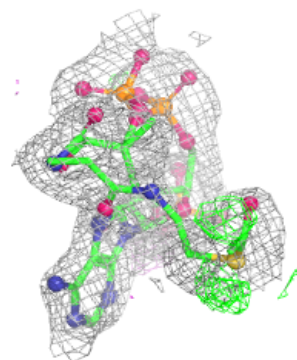
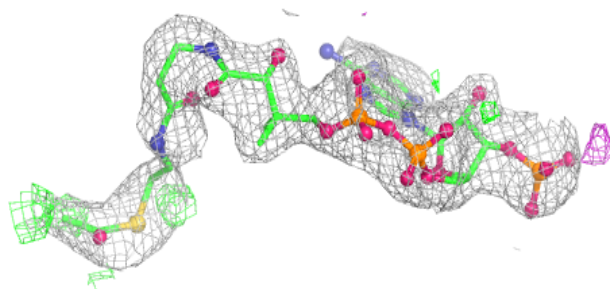
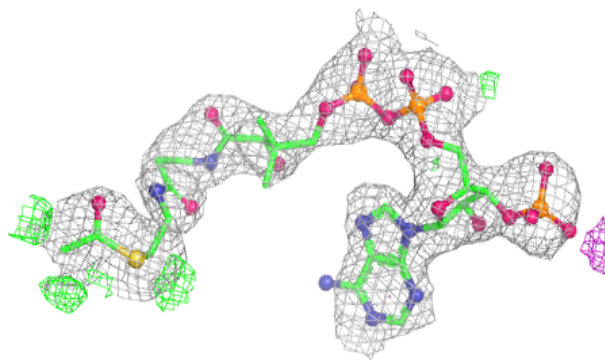
**Electron density around ACO K 501:**

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

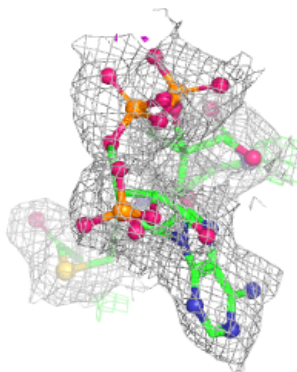
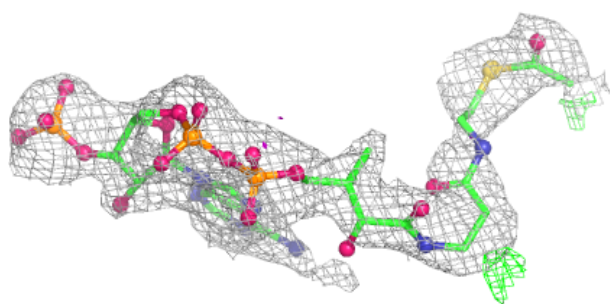
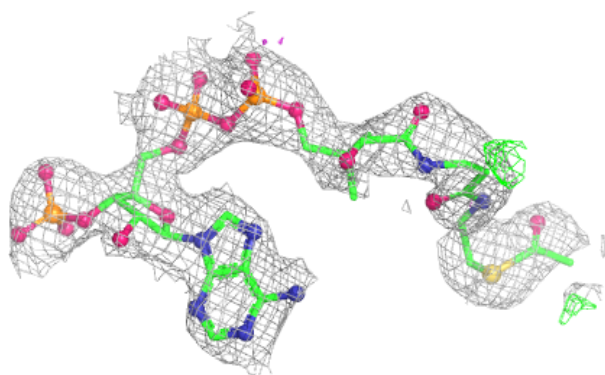


Electron density around ACO F 501:

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

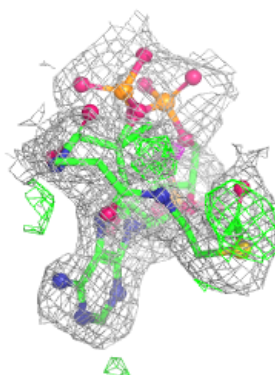
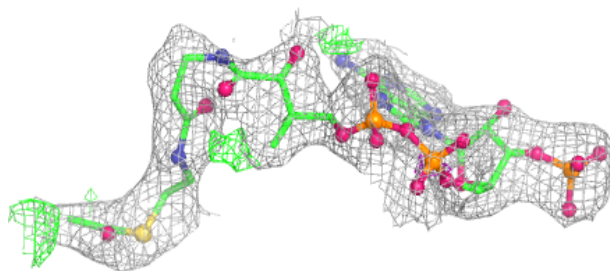
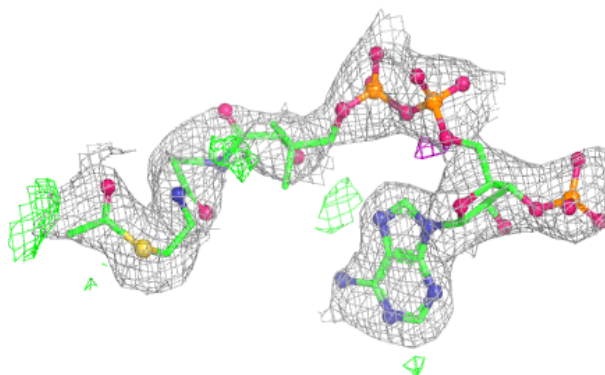
**Electron density around ACO C 501:**

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

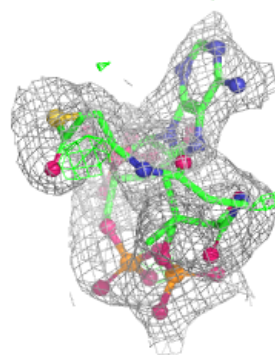
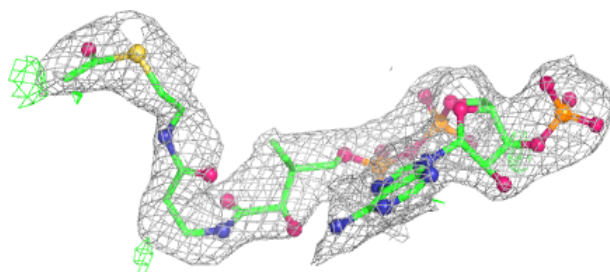
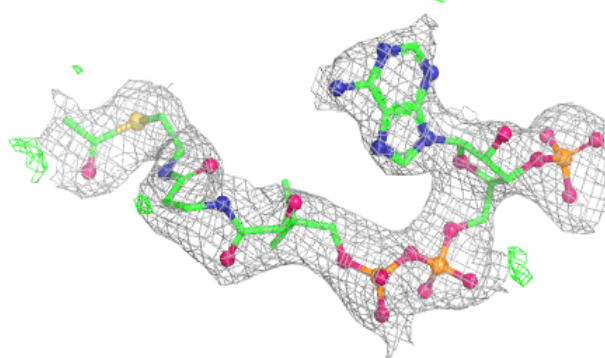


Electron density around ACO A 501:

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

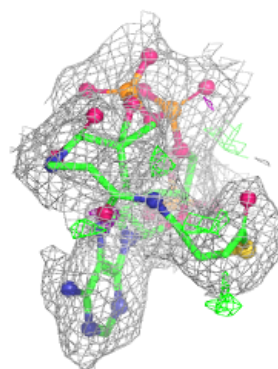
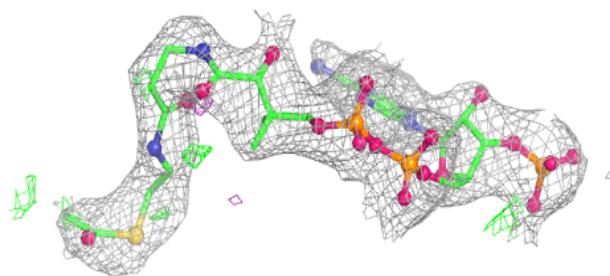
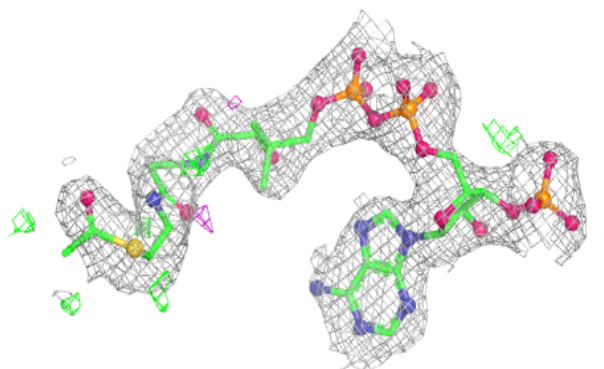
**Electron density around ACO B 501:**

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

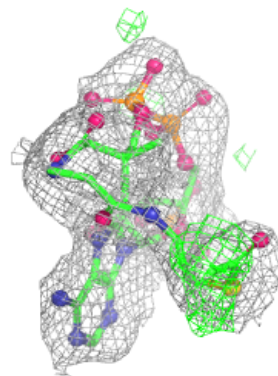
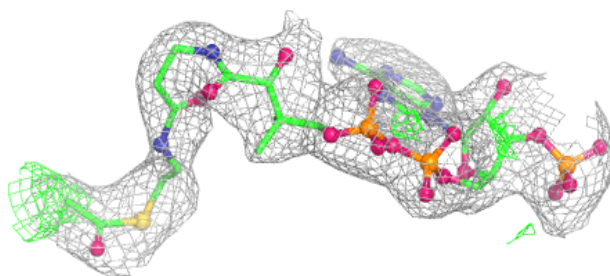
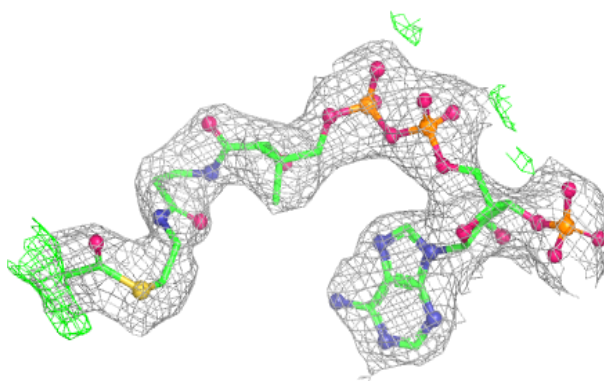


Electron density around ACO G 501:

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

**Electron density around ACO L 501:**

$2mF_o-DF_c$ (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.