



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:19 PM UTC

PDB ID : 8CDB / pdb_00008cdb
Title : Proulilysin E229A structure
Authors : Rodriguez-Banqueri, A.; Eckhard, U.; Gomis-Ruth, F.X.
Deposited on : 2023-01-30
Resolution : 4.50 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

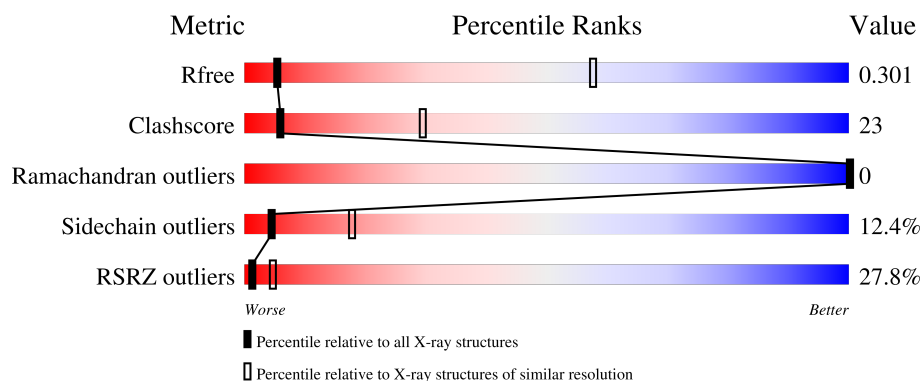
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	360	23% 41% 40% 15%
1	B	360	21% 42% 39% 15%
1	C	360	22% 42% 39% 15%
1	D	360	23% 43% 38% 15%
1	E	360	26% 44% 37% 15%

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Mol	Chain	Length	Quality of chain
1	F	360	
1	G	360	
1	H	360	
1	I	360	
1	J	360	
1	K	360	
1	L	360	
1	M	360	
1	N	360	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33614 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 Ulilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	B	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	C	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	D	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	E	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	F	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	G	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	H	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	I	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	J	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	K	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	L	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	M	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			
1	N	306	Total	C	N	O	S	0	0	0
			2399	1502	419	464	14			

There are 266 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	SER	-	expression tag	UNP Q8TL28
A	-15	SER	-	expression tag	UNP Q8TL28
A	-14	HIS	-	expression tag	UNP Q8TL28
A	-13	HIS	-	expression tag	UNP Q8TL28
A	-12	HIS	-	expression tag	UNP Q8TL28
A	-11	HIS	-	expression tag	UNP Q8TL28
A	-10	HIS	-	expression tag	UNP Q8TL28
A	-9	HIS	-	expression tag	UNP Q8TL28
A	-8	SER	-	expression tag	UNP Q8TL28
A	-7	SER	-	expression tag	UNP Q8TL28
A	-6	GLY	-	expression tag	UNP Q8TL28
A	-5	LEU	-	expression tag	UNP Q8TL28
A	-4	VAL	-	expression tag	UNP Q8TL28
A	-3	PRO	-	expression tag	UNP Q8TL28
A	-2	ARG	-	expression tag	UNP Q8TL28
A	-1	GLY	-	expression tag	UNP Q8TL28
A	0	SER	-	expression tag	UNP Q8TL28
A	229	ALA	GLU	variant	UNP Q8TL28
B	-17	GLY	-	expression tag	UNP Q8TL28
B	-16	SER	-	expression tag	UNP Q8TL28
B	-15	SER	-	expression tag	UNP Q8TL28
B	-14	HIS	-	expression tag	UNP Q8TL28
B	-13	HIS	-	expression tag	UNP Q8TL28
B	-12	HIS	-	expression tag	UNP Q8TL28
B	-11	HIS	-	expression tag	UNP Q8TL28
B	-10	HIS	-	expression tag	UNP Q8TL28
B	-9	HIS	-	expression tag	UNP Q8TL28
B	-8	SER	-	expression tag	UNP Q8TL28
B	-7	SER	-	expression tag	UNP Q8TL28
B	-6	GLY	-	expression tag	UNP Q8TL28
B	-5	LEU	-	expression tag	UNP Q8TL28
B	-4	VAL	-	expression tag	UNP Q8TL28
B	-3	PRO	-	expression tag	UNP Q8TL28
B	-2	ARG	-	expression tag	UNP Q8TL28
B	-1	GLY	-	expression tag	UNP Q8TL28
B	0	SER	-	expression tag	UNP Q8TL28
B	229	ALA	GLU	variant	UNP Q8TL28
C	-17	GLY	-	expression tag	UNP Q8TL28
C	-16	SER	-	expression tag	UNP Q8TL28
C	-15	SER	-	expression tag	UNP Q8TL28
C	-14	HIS	-	expression tag	UNP Q8TL28
C	-13	HIS	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q8TL28
C	-11	HIS	-	expression tag	UNP Q8TL28
C	-10	HIS	-	expression tag	UNP Q8TL28
C	-9	HIS	-	expression tag	UNP Q8TL28
C	-8	SER	-	expression tag	UNP Q8TL28
C	-7	SER	-	expression tag	UNP Q8TL28
C	-6	GLY	-	expression tag	UNP Q8TL28
C	-5	LEU	-	expression tag	UNP Q8TL28
C	-4	VAL	-	expression tag	UNP Q8TL28
C	-3	PRO	-	expression tag	UNP Q8TL28
C	-2	ARG	-	expression tag	UNP Q8TL28
C	-1	GLY	-	expression tag	UNP Q8TL28
C	0	SER	-	expression tag	UNP Q8TL28
C	229	ALA	GLU	variant	UNP Q8TL28
D	-17	GLY	-	expression tag	UNP Q8TL28
D	-16	SER	-	expression tag	UNP Q8TL28
D	-15	SER	-	expression tag	UNP Q8TL28
D	-14	HIS	-	expression tag	UNP Q8TL28
D	-13	HIS	-	expression tag	UNP Q8TL28
D	-12	HIS	-	expression tag	UNP Q8TL28
D	-11	HIS	-	expression tag	UNP Q8TL28
D	-10	HIS	-	expression tag	UNP Q8TL28
D	-9	HIS	-	expression tag	UNP Q8TL28
D	-8	SER	-	expression tag	UNP Q8TL28
D	-7	SER	-	expression tag	UNP Q8TL28
D	-6	GLY	-	expression tag	UNP Q8TL28
D	-5	LEU	-	expression tag	UNP Q8TL28
D	-4	VAL	-	expression tag	UNP Q8TL28
D	-3	PRO	-	expression tag	UNP Q8TL28
D	-2	ARG	-	expression tag	UNP Q8TL28
D	-1	GLY	-	expression tag	UNP Q8TL28
D	0	SER	-	expression tag	UNP Q8TL28
D	229	ALA	GLU	variant	UNP Q8TL28
E	-17	GLY	-	expression tag	UNP Q8TL28
E	-16	SER	-	expression tag	UNP Q8TL28
E	-15	SER	-	expression tag	UNP Q8TL28
E	-14	HIS	-	expression tag	UNP Q8TL28
E	-13	HIS	-	expression tag	UNP Q8TL28
E	-12	HIS	-	expression tag	UNP Q8TL28
E	-11	HIS	-	expression tag	UNP Q8TL28
E	-10	HIS	-	expression tag	UNP Q8TL28
E	-9	HIS	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	SER	-	expression tag	UNP Q8TL28
E	-7	SER	-	expression tag	UNP Q8TL28
E	-6	GLY	-	expression tag	UNP Q8TL28
E	-5	LEU	-	expression tag	UNP Q8TL28
E	-4	VAL	-	expression tag	UNP Q8TL28
E	-3	PRO	-	expression tag	UNP Q8TL28
E	-2	ARG	-	expression tag	UNP Q8TL28
E	-1	GLY	-	expression tag	UNP Q8TL28
E	0	SER	-	expression tag	UNP Q8TL28
E	229	ALA	GLU	variant	UNP Q8TL28
F	-17	GLY	-	expression tag	UNP Q8TL28
F	-16	SER	-	expression tag	UNP Q8TL28
F	-15	SER	-	expression tag	UNP Q8TL28
F	-14	HIS	-	expression tag	UNP Q8TL28
F	-13	HIS	-	expression tag	UNP Q8TL28
F	-12	HIS	-	expression tag	UNP Q8TL28
F	-11	HIS	-	expression tag	UNP Q8TL28
F	-10	HIS	-	expression tag	UNP Q8TL28
F	-9	HIS	-	expression tag	UNP Q8TL28
F	-8	SER	-	expression tag	UNP Q8TL28
F	-7	SER	-	expression tag	UNP Q8TL28
F	-6	GLY	-	expression tag	UNP Q8TL28
F	-5	LEU	-	expression tag	UNP Q8TL28
F	-4	VAL	-	expression tag	UNP Q8TL28
F	-3	PRO	-	expression tag	UNP Q8TL28
F	-2	ARG	-	expression tag	UNP Q8TL28
F	-1	GLY	-	expression tag	UNP Q8TL28
F	0	SER	-	expression tag	UNP Q8TL28
F	229	ALA	GLU	variant	UNP Q8TL28
G	-17	GLY	-	expression tag	UNP Q8TL28
G	-16	SER	-	expression tag	UNP Q8TL28
G	-15	SER	-	expression tag	UNP Q8TL28
G	-14	HIS	-	expression tag	UNP Q8TL28
G	-13	HIS	-	expression tag	UNP Q8TL28
G	-12	HIS	-	expression tag	UNP Q8TL28
G	-11	HIS	-	expression tag	UNP Q8TL28
G	-10	HIS	-	expression tag	UNP Q8TL28
G	-9	HIS	-	expression tag	UNP Q8TL28
G	-8	SER	-	expression tag	UNP Q8TL28
G	-7	SER	-	expression tag	UNP Q8TL28
G	-6	GLY	-	expression tag	UNP Q8TL28
G	-5	LEU	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	VAL	-	expression tag	UNP Q8TL28
G	-3	PRO	-	expression tag	UNP Q8TL28
G	-2	ARG	-	expression tag	UNP Q8TL28
G	-1	GLY	-	expression tag	UNP Q8TL28
G	0	SER	-	expression tag	UNP Q8TL28
G	229	ALA	GLU	variant	UNP Q8TL28
H	-17	GLY	-	expression tag	UNP Q8TL28
H	-16	SER	-	expression tag	UNP Q8TL28
H	-15	SER	-	expression tag	UNP Q8TL28
H	-14	HIS	-	expression tag	UNP Q8TL28
H	-13	HIS	-	expression tag	UNP Q8TL28
H	-12	HIS	-	expression tag	UNP Q8TL28
H	-11	HIS	-	expression tag	UNP Q8TL28
H	-10	HIS	-	expression tag	UNP Q8TL28
H	-9	HIS	-	expression tag	UNP Q8TL28
H	-8	SER	-	expression tag	UNP Q8TL28
H	-7	SER	-	expression tag	UNP Q8TL28
H	-6	GLY	-	expression tag	UNP Q8TL28
H	-5	LEU	-	expression tag	UNP Q8TL28
H	-4	VAL	-	expression tag	UNP Q8TL28
H	-3	PRO	-	expression tag	UNP Q8TL28
H	-2	ARG	-	expression tag	UNP Q8TL28
H	-1	GLY	-	expression tag	UNP Q8TL28
H	0	SER	-	expression tag	UNP Q8TL28
H	229	ALA	GLU	variant	UNP Q8TL28
I	-17	GLY	-	expression tag	UNP Q8TL28
I	-16	SER	-	expression tag	UNP Q8TL28
I	-15	SER	-	expression tag	UNP Q8TL28
I	-14	HIS	-	expression tag	UNP Q8TL28
I	-13	HIS	-	expression tag	UNP Q8TL28
I	-12	HIS	-	expression tag	UNP Q8TL28
I	-11	HIS	-	expression tag	UNP Q8TL28
I	-10	HIS	-	expression tag	UNP Q8TL28
I	-9	HIS	-	expression tag	UNP Q8TL28
I	-8	SER	-	expression tag	UNP Q8TL28
I	-7	SER	-	expression tag	UNP Q8TL28
I	-6	GLY	-	expression tag	UNP Q8TL28
I	-5	LEU	-	expression tag	UNP Q8TL28
I	-4	VAL	-	expression tag	UNP Q8TL28
I	-3	PRO	-	expression tag	UNP Q8TL28
I	-2	ARG	-	expression tag	UNP Q8TL28
I	-1	GLY	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	expression tag	UNP Q8TL28
I	229	ALA	GLU	variant	UNP Q8TL28
J	-17	GLY	-	expression tag	UNP Q8TL28
J	-16	SER	-	expression tag	UNP Q8TL28
J	-15	SER	-	expression tag	UNP Q8TL28
J	-14	HIS	-	expression tag	UNP Q8TL28
J	-13	HIS	-	expression tag	UNP Q8TL28
J	-12	HIS	-	expression tag	UNP Q8TL28
J	-11	HIS	-	expression tag	UNP Q8TL28
J	-10	HIS	-	expression tag	UNP Q8TL28
J	-9	HIS	-	expression tag	UNP Q8TL28
J	-8	SER	-	expression tag	UNP Q8TL28
J	-7	SER	-	expression tag	UNP Q8TL28
J	-6	GLY	-	expression tag	UNP Q8TL28
J	-5	LEU	-	expression tag	UNP Q8TL28
J	-4	VAL	-	expression tag	UNP Q8TL28
J	-3	PRO	-	expression tag	UNP Q8TL28
J	-2	ARG	-	expression tag	UNP Q8TL28
J	-1	GLY	-	expression tag	UNP Q8TL28
J	0	SER	-	expression tag	UNP Q8TL28
J	229	ALA	GLU	variant	UNP Q8TL28
K	-17	GLY	-	expression tag	UNP Q8TL28
K	-16	SER	-	expression tag	UNP Q8TL28
K	-15	SER	-	expression tag	UNP Q8TL28
K	-14	HIS	-	expression tag	UNP Q8TL28
K	-13	HIS	-	expression tag	UNP Q8TL28
K	-12	HIS	-	expression tag	UNP Q8TL28
K	-11	HIS	-	expression tag	UNP Q8TL28
K	-10	HIS	-	expression tag	UNP Q8TL28
K	-9	HIS	-	expression tag	UNP Q8TL28
K	-8	SER	-	expression tag	UNP Q8TL28
K	-7	SER	-	expression tag	UNP Q8TL28
K	-6	GLY	-	expression tag	UNP Q8TL28
K	-5	LEU	-	expression tag	UNP Q8TL28
K	-4	VAL	-	expression tag	UNP Q8TL28
K	-3	PRO	-	expression tag	UNP Q8TL28
K	-2	ARG	-	expression tag	UNP Q8TL28
K	-1	GLY	-	expression tag	UNP Q8TL28
K	0	SER	-	expression tag	UNP Q8TL28
K	229	ALA	GLU	variant	UNP Q8TL28
L	-17	GLY	-	expression tag	UNP Q8TL28
L	-16	SER	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-15	SER	-	expression tag	UNP Q8TL28
L	-14	HIS	-	expression tag	UNP Q8TL28
L	-13	HIS	-	expression tag	UNP Q8TL28
L	-12	HIS	-	expression tag	UNP Q8TL28
L	-11	HIS	-	expression tag	UNP Q8TL28
L	-10	HIS	-	expression tag	UNP Q8TL28
L	-9	HIS	-	expression tag	UNP Q8TL28
L	-8	SER	-	expression tag	UNP Q8TL28
L	-7	SER	-	expression tag	UNP Q8TL28
L	-6	GLY	-	expression tag	UNP Q8TL28
L	-5	LEU	-	expression tag	UNP Q8TL28
L	-4	VAL	-	expression tag	UNP Q8TL28
L	-3	PRO	-	expression tag	UNP Q8TL28
L	-2	ARG	-	expression tag	UNP Q8TL28
L	-1	GLY	-	expression tag	UNP Q8TL28
L	0	SER	-	expression tag	UNP Q8TL28
L	229	ALA	GLU	variant	UNP Q8TL28
M	-17	GLY	-	expression tag	UNP Q8TL28
M	-16	SER	-	expression tag	UNP Q8TL28
M	-15	SER	-	expression tag	UNP Q8TL28
M	-14	HIS	-	expression tag	UNP Q8TL28
M	-13	HIS	-	expression tag	UNP Q8TL28
M	-12	HIS	-	expression tag	UNP Q8TL28
M	-11	HIS	-	expression tag	UNP Q8TL28
M	-10	HIS	-	expression tag	UNP Q8TL28
M	-9	HIS	-	expression tag	UNP Q8TL28
M	-8	SER	-	expression tag	UNP Q8TL28
M	-7	SER	-	expression tag	UNP Q8TL28
M	-6	GLY	-	expression tag	UNP Q8TL28
M	-5	LEU	-	expression tag	UNP Q8TL28
M	-4	VAL	-	expression tag	UNP Q8TL28
M	-3	PRO	-	expression tag	UNP Q8TL28
M	-2	ARG	-	expression tag	UNP Q8TL28
M	-1	GLY	-	expression tag	UNP Q8TL28
M	0	SER	-	expression tag	UNP Q8TL28
M	229	ALA	GLU	variant	UNP Q8TL28
N	-17	GLY	-	expression tag	UNP Q8TL28
N	-16	SER	-	expression tag	UNP Q8TL28
N	-15	SER	-	expression tag	UNP Q8TL28
N	-14	HIS	-	expression tag	UNP Q8TL28
N	-13	HIS	-	expression tag	UNP Q8TL28
N	-12	HIS	-	expression tag	UNP Q8TL28

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-11	HIS	-	expression tag	UNP Q8TL28
N	-10	HIS	-	expression tag	UNP Q8TL28
N	-9	HIS	-	expression tag	UNP Q8TL28
N	-8	SER	-	expression tag	UNP Q8TL28
N	-7	SER	-	expression tag	UNP Q8TL28
N	-6	GLY	-	expression tag	UNP Q8TL28
N	-5	LEU	-	expression tag	UNP Q8TL28
N	-4	VAL	-	expression tag	UNP Q8TL28
N	-3	PRO	-	expression tag	UNP Q8TL28
N	-2	ARG	-	expression tag	UNP Q8TL28
N	-1	GLY	-	expression tag	UNP Q8TL28
N	0	SER	-	expression tag	UNP Q8TL28
N	229	ALA	GLU	variant	UNP Q8TL28

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

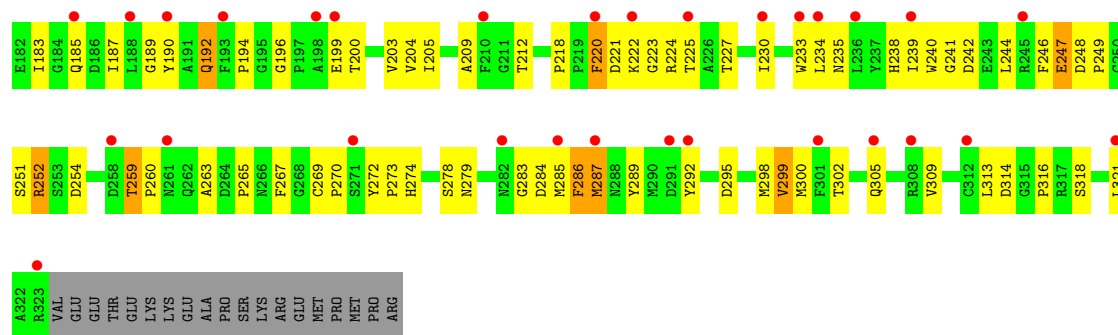
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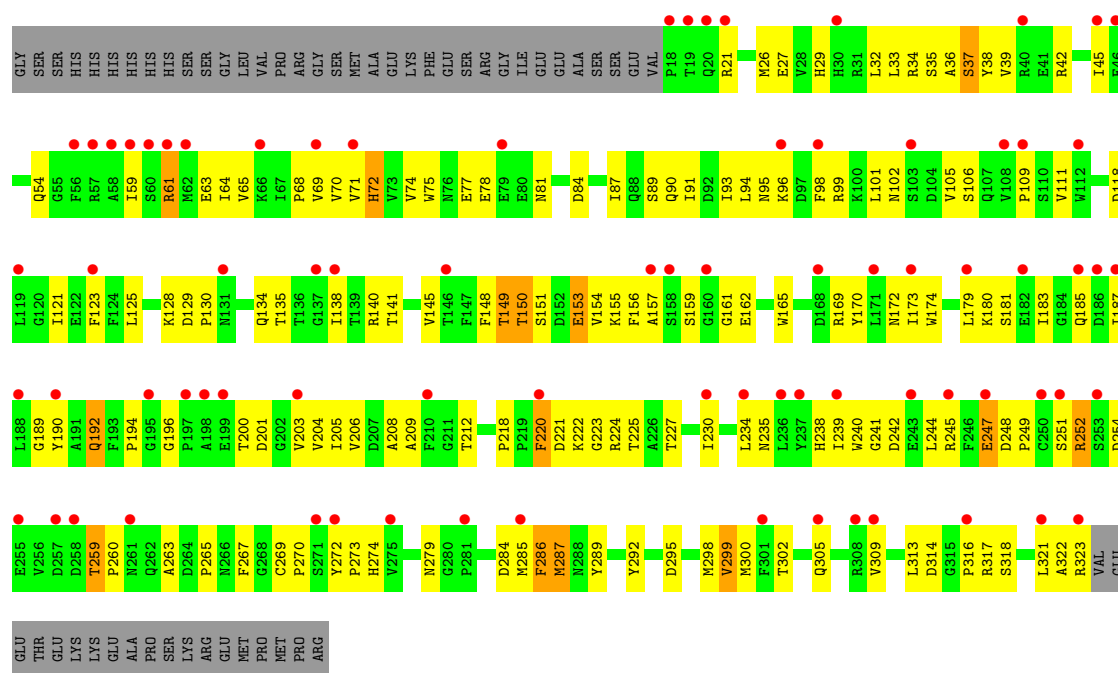
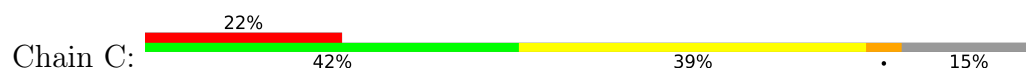
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	1	Total 1	Zn 1	0	0
2	N	1	Total 1	Zn 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

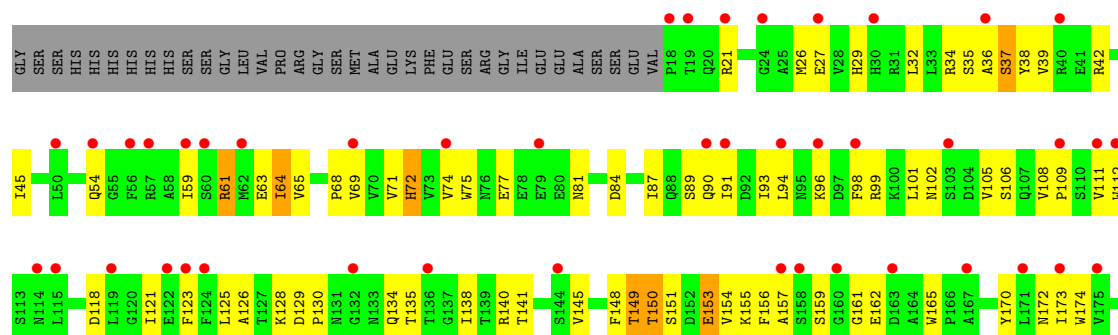
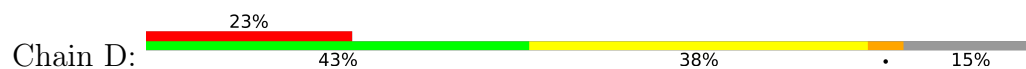
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	J	1	Total 1	Ca 1	0	0
3	K	1	Total 1	Ca 1	0	0
3	L	1	Total 1	Ca 1	0	0
3	M	1	Total 1	Ca 1	0	0
3	N	1	Total 1	Ca 1	0	0

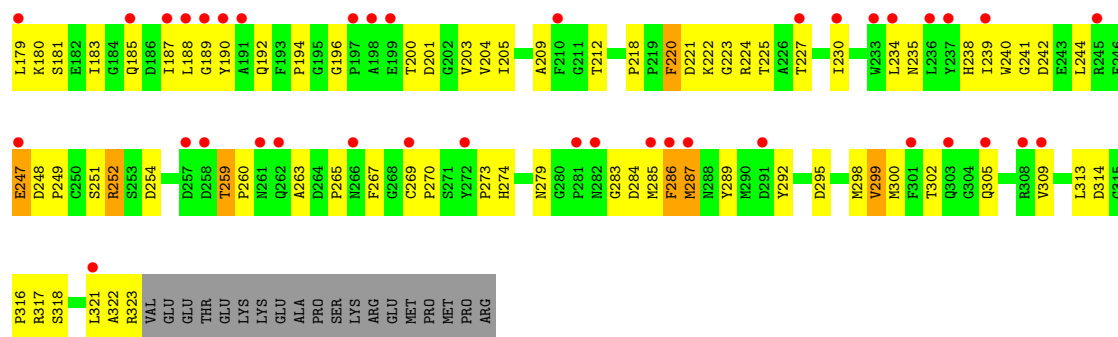


• Molecule 1: Ulilysin

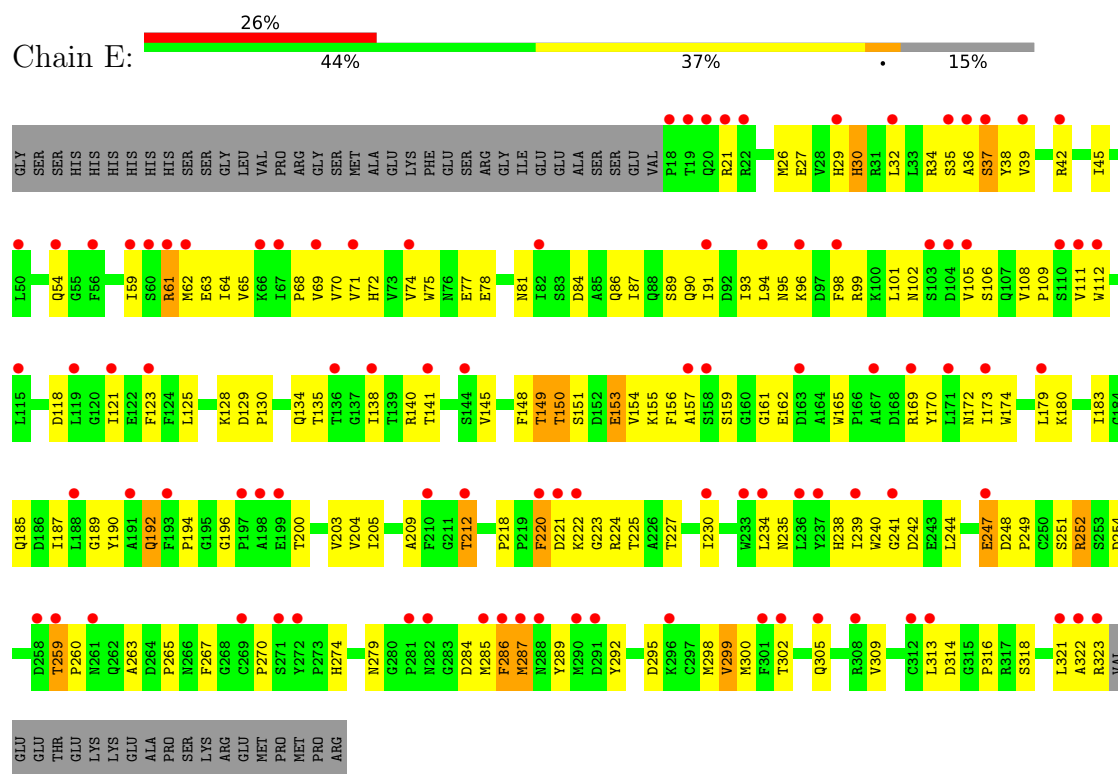


• Molecule 1: Ulilysin

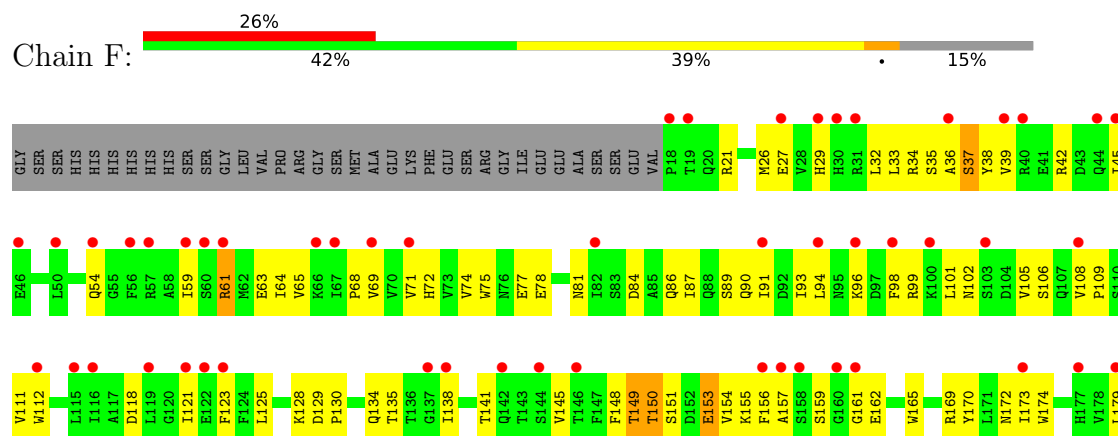


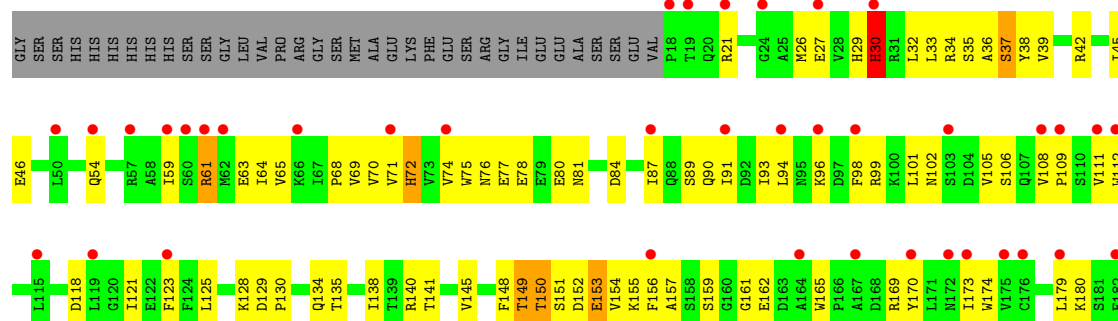


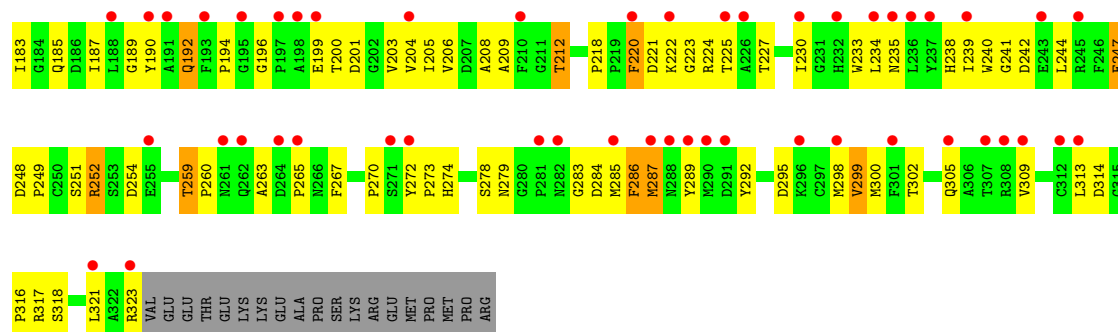
• Molecule 1: Ulilysin



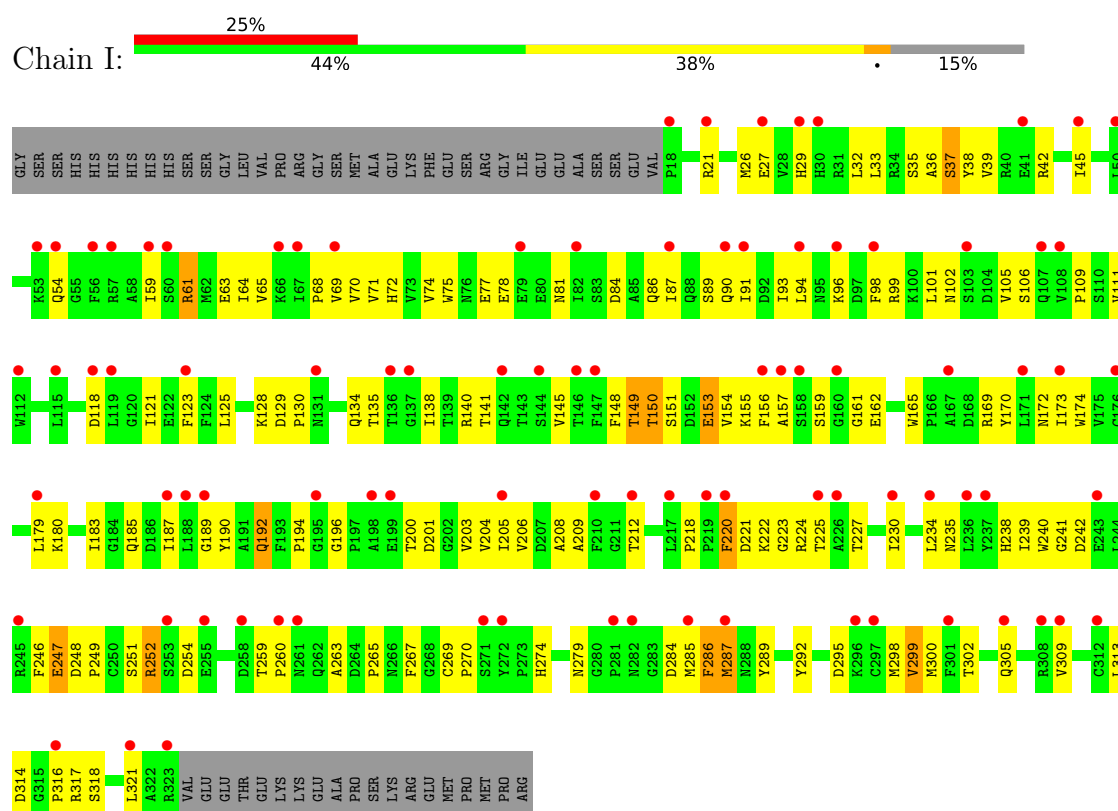
• Molecule 1: Ulilysin



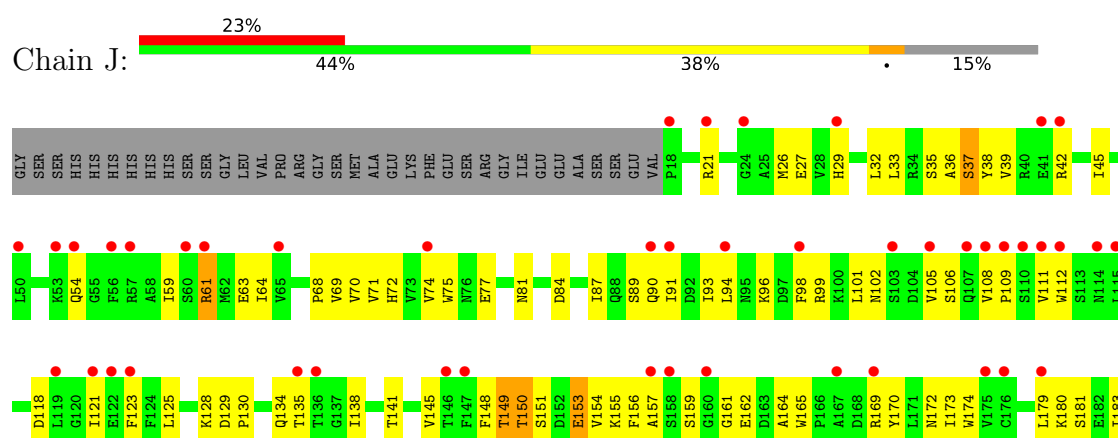


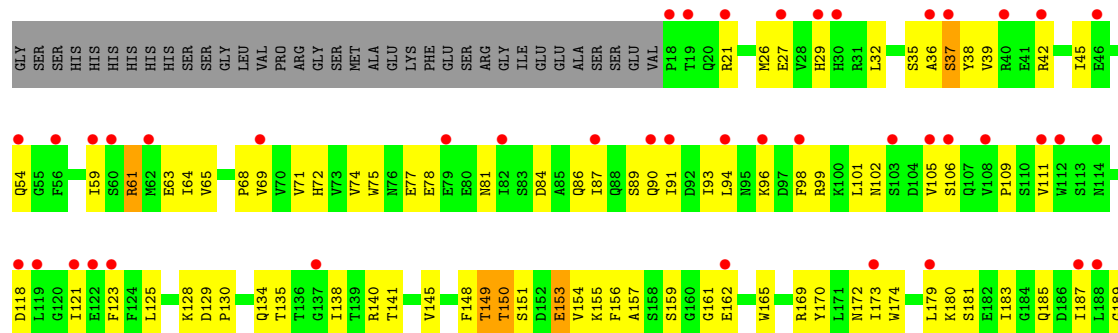


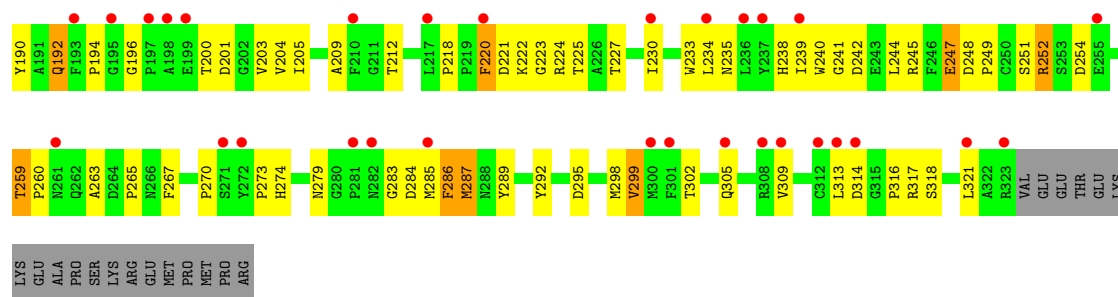
● Molecule 1: Ulilysin



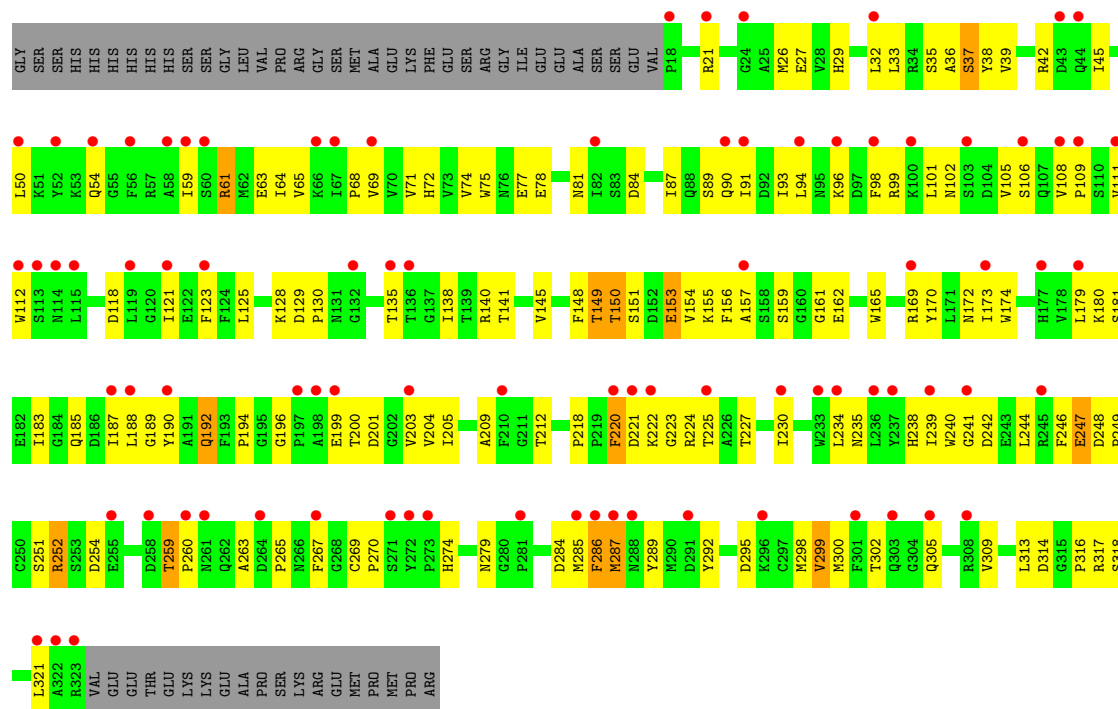
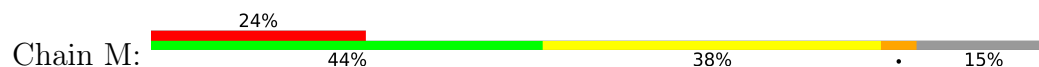
● Molecule 1: Ulilysin



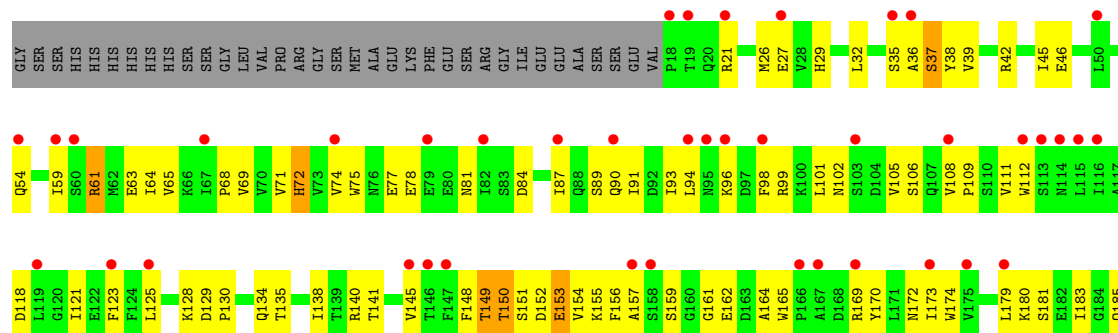


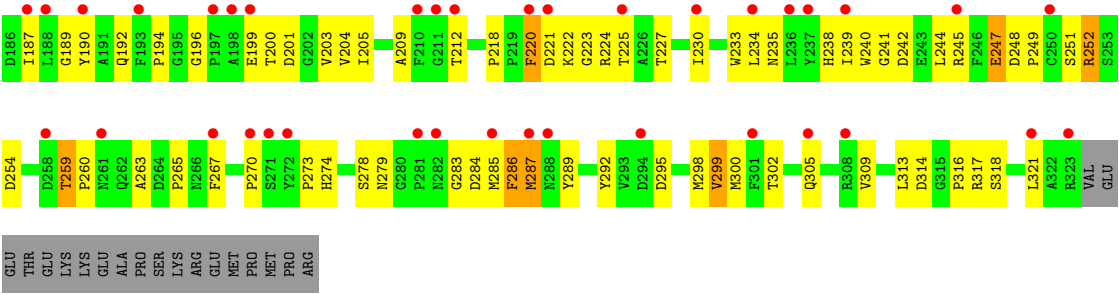


• Molecule 1: Ulilysin



• Molecule 1: Ulilysin





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	192.10Å 544.40Å 185.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.72 – 4.50 94.72 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (94.72-4.50) 99.5 (94.72-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 4.47Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.289 , 0.302 0.290 , 0.301	Depositor DCC
R_{free} test set	845 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	131.9	Xtrriage
Anisotropy	1.029	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 219.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33614	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3091e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, CA

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	0.32	0/2457	0.49	0/3340
1	B	0.36	0/2457	0.50	0/3340
1	C	0.32	0/2457	0.49	0/3340
1	D	0.34	0/2457	0.50	0/3340
1	E	0.35	0/2457	0.51	0/3340
1	F	0.35	0/2457	0.51	0/3340
1	G	0.37	0/2457	0.53	0/3340
1	H	0.47	4/2457 (0.2%)	0.55	0/3340
1	I	0.35	0/2457	0.51	0/3340
1	J	0.36	0/2457	0.51	0/3340
1	K	0.33	0/2457	0.50	0/3340
1	L	0.34	0/2457	0.50	0/3340
1	M	0.32	0/2457	0.49	0/3340
1	N	0.35	0/2457	0.51	0/3340
All	All	0.35	4/34398 (0.0%)	0.51	0/46760

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	30	HIS	CB-CG	6.79	1.59	1.50
1	H	30	HIS	CG-ND1	6.79	1.45	1.38
1	H	30	HIS	CE1-NE2	6.29	1.38	1.32
1	H	30	HIS	CG-CD2	5.40	1.41	1.35

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2399	0	2279	116	0
1	B	2399	0	2279	117	1
1	C	2399	0	2279	111	0
1	D	2399	0	2279	112	0
1	E	2399	0	2279	108	0
1	F	2399	0	2279	117	0
1	G	2399	0	2279	112	0
1	H	2399	0	2279	115	0
1	I	2399	0	2279	108	0
1	J	2399	0	2279	110	0
1	K	2399	0	2279	109	0
1	L	2399	0	2279	103	0
1	M	2399	0	2279	105	0
1	N	2399	0	2279	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
All	All	33614	0	31906	1497	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1497) 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:N:174:TRP:HB2	1:N:204:VAL:HG22	1.61	0.82
1:H:174:TRP:HB2	1:H:204:VAL:HG22	1.62	0.82
1:I:174:TRP:HB2	1:I:204:VAL:HG22	1.62	0.81
1:B:174:TRP:HB2	1:B:204:VAL:HG22	1.62	0.80
1:G:174:TRP:HB2	1:G:204:VAL:HG22	1.64	0.79
1:K:174:TRP:HB2	1:K:204:VAL:HG22	1.65	0.79
1:D:174:TRP:HB2	1:D:204:VAL:HG22	1.64	0.79
1:L:174:TRP:HB2	1:L:204:VAL:HG22	1.64	0.79
1:M:174:TRP:HB2	1:M:204:VAL:HG22	1.66	0.78
1:F:174:TRP:HB2	1:F:204:VAL:HG22	1.64	0.78
1:N:29:HIS:HA	1:N:32:LEU:HD12	1.66	0.78
1:H:29:HIS:HA	1:H:32:LEU:HD12	1.65	0.77
1:J:174:TRP:HB2	1:J:204:VAL:HG22	1.66	0.77
1:E:29:HIS:HA	1:E:32:LEU:HD12	1.66	0.77
1:A:29:HIS:HA	1:A:32:LEU:HD12	1.66	0.76
1:K:224:ARG:HD2	1:K:289:TYR:HE1	1.50	0.76
1:A:174:TRP:HB2	1:A:204:VAL:HG22	1.67	0.76
1:J:29:HIS:HA	1:J:32:LEU:HD12	1.65	0.76
1:D:29:HIS:HA	1:D:32:LEU:HD12	1.68	0.76
1:E:174:TRP:HB2	1:E:204:VAL:HG22	1.66	0.76
1:K:29:HIS:HA	1:K:32:LEU:HD12	1.67	0.75
1:L:29:HIS:HA	1:L:32:LEU:HD12	1.68	0.75
1:A:279:ASN:HA	1:B:279:ASN:H	1.52	0.75
1:B:224:ARG:HD2	1:B:289:TYR:HE1	1.52	0.75
1:C:224:ARG:HD2	1:C:289:TYR:HE1	1.53	0.74
1:B:29:HIS:HA	1:B:32:LEU:HD12	1.69	0.74
1:C:174:TRP:HB2	1:C:204:VAL:HG22	1.68	0.74
1:I:29:HIS:HA	1:I:32:LEU:HD12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:HIS:HA	1:C:32:LEU:HD12	1.70	0.74
1:E:224:ARG:HD2	1:E:289:TYR:HE1	1.52	0.74
1:M:29:HIS:HA	1:M:32:LEU:HD12	1.67	0.74
1:G:224:ARG:HD2	1:G:289:TYR:HE1	1.52	0.74
1:J:224:ARG:HD2	1:J:289:TYR:HE1	1.52	0.74
1:M:224:ARG:HD2	1:M:289:TYR:HE1	1.52	0.74
1:M:151:SER:HB2	1:M:153:GLU:HG3	1.70	0.74
1:F:249:PRO:HB2	1:F:263:ALA:HB1	1.71	0.73
1:H:224:ARG:HD2	1:H:289:TYR:HE1	1.53	0.73
1:L:234:LEU:HB3	1:L:309:VAL:HG13	1.70	0.73
1:F:224:ARG:HD2	1:F:289:TYR:HE1	1.53	0.73
1:J:45:ILE:HG12	1:J:316:PRO:HG3	1.69	0.73
1:M:45:ILE:HG12	1:M:316:PRO:HG3	1.70	0.73
1:A:224:ARG:HD2	1:A:289:TYR:HE1	1.53	0.72
1:A:279:ASN:H	1:B:279:ASN:HA	1.54	0.72
1:G:45:ILE:HG12	1:G:316:PRO:HG3	1.69	0.72
1:D:224:ARG:HD2	1:D:289:TYR:HE1	1.53	0.72
1:I:151:SER:HB2	1:I:153:GLU:HG3	1.70	0.72
1:G:249:PRO:HB2	1:G:263:ALA:HB1	1.72	0.72
1:I:249:PRO:HB2	1:I:263:ALA:HB1	1.70	0.72
1:G:29:HIS:HA	1:G:32:LEU:HD12	1.71	0.72
1:E:45:ILE:HG12	1:E:316:PRO:HG3	1.72	0.72
1:B:45:ILE:HG12	1:B:316:PRO:HG3	1.72	0.71
1:K:151:SER:HB2	1:K:153:GLU:HG3	1.71	0.71
1:K:249:PRO:HB2	1:K:263:ALA:HB1	1.72	0.71
1:I:224:ARG:HD2	1:I:289:TYR:HE1	1.55	0.71
1:J:151:SER:HB2	1:J:153:GLU:HG3	1.72	0.71
1:N:224:ARG:HD2	1:N:289:TYR:HE1	1.53	0.71
1:A:249:PRO:HB2	1:A:263:ALA:HB1	1.72	0.71
1:F:29:HIS:HA	1:F:32:LEU:HD12	1.72	0.71
1:E:151:SER:HB2	1:E:153:GLU:HG3	1.72	0.71
1:B:249:PRO:HB2	1:B:263:ALA:HB1	1.72	0.71
1:J:249:PRO:HB2	1:J:263:ALA:HB1	1.72	0.71
1:F:151:SER:HB2	1:F:153:GLU:HG3	1.73	0.71
1:F:222:LYS:HB2	1:F:295:ASP:HB3	1.71	0.71
1:C:151:SER:HB2	1:C:153:GLU:HG3	1.72	0.71
1:C:247:GLU:HG2	1:C:251:SER:HB2	1.72	0.71
1:H:249:PRO:HB2	1:H:263:ALA:HB1	1.72	0.71
1:K:45:ILE:HG12	1:K:316:PRO:HG3	1.73	0.71
1:L:224:ARG:HD2	1:L:289:TYR:HE1	1.55	0.71
1:N:249:PRO:HB2	1:N:263:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:SER:HB2	1:D:153:GLU:HG3	1.73	0.70
1:M:247:GLU:HG2	1:M:251:SER:HB2	1.73	0.70
1:A:151:SER:HB2	1:A:153:GLU:HG3	1.71	0.70
1:I:259:THR:HG22	1:I:302:THR:HG21	1.74	0.70
1:L:249:PRO:HB2	1:L:263:ALA:HB1	1.71	0.70
1:K:234:LEU:HB3	1:K:309:VAL:HG13	1.73	0.70
1:H:151:SER:HB2	1:H:153:GLU:HG3	1.73	0.70
1:J:247:GLU:HG2	1:J:251:SER:HB2	1.72	0.70
1:L:151:SER:HB2	1:L:153:GLU:HG3	1.72	0.70
1:G:151:SER:HB2	1:G:153:GLU:HG3	1.74	0.70
1:B:151:SER:HB2	1:B:153:GLU:HG3	1.74	0.70
1:C:222:LYS:HB2	1:C:295:ASP:HB3	1.74	0.70
1:C:249:PRO:HB2	1:C:263:ALA:HB1	1.73	0.69
1:L:259:THR:HG22	1:L:302:THR:HG21	1.74	0.69
1:G:247:GLU:HG2	1:G:251:SER:HB2	1.74	0.69
1:K:222:LYS:HB2	1:K:295:ASP:HB3	1.74	0.69
1:A:45:ILE:HG12	1:A:316:PRO:HG3	1.74	0.69
1:C:45:ILE:HG12	1:C:316:PRO:HG3	1.73	0.69
1:D:45:ILE:HG12	1:D:316:PRO:HG3	1.73	0.69
1:E:249:PRO:HB2	1:E:263:ALA:HB1	1.73	0.69
1:I:45:ILE:HG12	1:I:316:PRO:HG3	1.73	0.69
1:L:45:ILE:HG12	1:L:316:PRO:HG3	1.73	0.69
1:F:45:ILE:HG12	1:F:316:PRO:HG3	1.75	0.69
1:M:249:PRO:HB2	1:M:263:ALA:HB1	1.73	0.69
1:N:45:ILE:HG12	1:N:316:PRO:HG3	1.75	0.69
1:N:151:SER:HB2	1:N:153:GLU:HG3	1.75	0.69
1:D:249:PRO:HB2	1:D:263:ALA:HB1	1.74	0.69
1:B:234:LEU:HB3	1:B:309:VAL:HG13	1.73	0.69
1:E:247:GLU:HG2	1:E:251:SER:HB2	1.74	0.69
1:H:222:LYS:HB2	1:H:295:ASP:HB3	1.75	0.69
1:J:234:LEU:HB3	1:J:309:VAL:HG13	1.74	0.69
1:M:259:THR:HG22	1:M:302:THR:HG21	1.75	0.69
1:C:234:LEU:HB3	1:C:309:VAL:HG13	1.76	0.68
1:D:247:GLU:HG2	1:D:251:SER:HB2	1.75	0.68
1:H:45:ILE:HG12	1:H:316:PRO:HG3	1.74	0.68
1:J:222:LYS:HB2	1:J:295:ASP:HB3	1.75	0.68
1:A:234:LEU:HB3	1:A:309:VAL:HG13	1.76	0.68
1:G:259:THR:HG22	1:G:302:THR:HG21	1.76	0.68
1:I:222:LYS:HB2	1:I:295:ASP:HB3	1.76	0.68
1:K:247:GLU:HG2	1:K:251:SER:HB2	1.75	0.68
1:D:259:THR:HG22	1:D:302:THR:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:LYS:NZ	1:L:134:GLN:OE1	2.27	0.68
1:N:259:THR:HG22	1:N:302:THR:HG21	1.76	0.68
1:D:222:LYS:HB2	1:D:295:ASP:HB3	1.75	0.68
1:E:222:LYS:HB2	1:E:295:ASP:HB3	1.76	0.68
1:F:247:GLU:HG2	1:F:251:SER:HB2	1.75	0.68
1:N:222:LYS:HB2	1:N:295:ASP:HB3	1.76	0.68
1:A:222:LYS:HB2	1:A:295:ASP:HB3	1.76	0.67
1:E:260:PRO:HD3	1:E:285:MET:HE3	1.76	0.67
1:H:247:GLU:HG2	1:H:251:SER:HB2	1.77	0.67
1:A:247:GLU:HG2	1:A:251:SER:HB2	1.77	0.67
1:F:259:THR:HG22	1:F:302:THR:HG21	1.77	0.67
1:G:222:LYS:HB2	1:G:295:ASP:HB3	1.77	0.67
1:G:234:LEU:HB3	1:G:309:VAL:HG13	1.75	0.67
1:C:260:PRO:HD3	1:C:285:MET:HE3	1.77	0.67
1:I:87:ILE:HD13	1:I:138:ILE:HD13	1.77	0.67
1:L:222:LYS:HB2	1:L:295:ASP:HB3	1.75	0.67
1:I:234:LEU:HB3	1:I:309:VAL:HG13	1.77	0.66
1:J:259:THR:HG22	1:J:302:THR:HG21	1.77	0.66
1:K:259:THR:HG22	1:K:302:THR:HG21	1.77	0.66
1:M:222:LYS:HB2	1:M:295:ASP:HB3	1.77	0.66
1:A:260:PRO:HD3	1:A:285:MET:HE3	1.77	0.66
1:B:259:THR:HG22	1:B:302:THR:HG21	1.77	0.66
1:H:234:LEU:HB3	1:H:309:VAL:HG13	1.76	0.66
1:B:222:LYS:HB2	1:B:295:ASP:HB3	1.78	0.66
1:H:260:PRO:HD3	1:H:285:MET:HE3	1.77	0.66
1:N:247:GLU:HG2	1:N:251:SER:HB2	1.77	0.66
1:B:241:GLY:HA3	1:B:252:ARG:HB2	1.78	0.66
1:J:260:PRO:HD3	1:J:285:MET:HE3	1.78	0.66
1:N:234:LEU:HB3	1:N:309:VAL:HG13	1.76	0.66
1:C:259:THR:HG22	1:C:302:THR:HG21	1.77	0.66
1:F:234:LEU:HB3	1:F:309:VAL:HG13	1.77	0.66
1:L:247:GLU:HG2	1:L:251:SER:HB2	1.77	0.66
1:D:87:ILE:HD13	1:D:138:ILE:HD13	1.78	0.65
1:B:247:GLU:HG2	1:B:251:SER:HB2	1.77	0.65
1:C:241:GLY:HA3	1:C:252:ARG:HB2	1.77	0.65
1:E:234:LEU:HB3	1:E:309:VAL:HG13	1.77	0.65
1:E:259:THR:HG22	1:E:302:THR:HG21	1.76	0.65
1:I:134:GLN:OE1	1:K:180:LYS:NZ	2.29	0.65
1:I:247:GLU:HG2	1:I:251:SER:HB2	1.79	0.65
1:G:241:GLY:HA3	1:G:252:ARG:HB2	1.79	0.65
1:D:234:LEU:HB3	1:D:309:VAL:HG13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:260:PRO:HD3	1:K:285:MET:HE3	1.79	0.65
1:M:260:PRO:HD3	1:M:285:MET:HE3	1.78	0.65
1:I:74:VAL:HG11	1:I:161:GLY:HA2	1.78	0.65
1:F:87:ILE:HD13	1:F:138:ILE:HD13	1.78	0.65
1:M:234:LEU:HB3	1:M:309:VAL:HG13	1.79	0.65
1:J:74:VAL:HG11	1:J:161:GLY:HA2	1.79	0.64
1:B:180:LYS:NZ	1:D:134:GLN:OE1	2.31	0.64
1:C:74:VAL:HG11	1:C:161:GLY:HA2	1.80	0.64
1:D:241:GLY:HA3	1:D:252:ARG:HB2	1.78	0.64
1:H:259:THR:HG22	1:H:302:THR:HG21	1.80	0.64
1:G:260:PRO:HD3	1:G:285:MET:HE3	1.79	0.64
1:H:21:ARG:HD2	1:H:292:TYR:HA	1.80	0.64
1:H:180:LYS:NZ	1:J:134:GLN:OE1	2.31	0.63
1:K:21:ARG:HD2	1:K:292:TYR:HA	1.79	0.63
1:E:89:SER:HB2	1:E:212:THR:HG23	1.81	0.63
1:G:21:ARG:HD2	1:G:292:TYR:HA	1.81	0.63
1:H:87:ILE:HD13	1:H:138:ILE:HD13	1.80	0.63
1:H:89:SER:HB2	1:H:212:THR:HG23	1.81	0.63
1:A:259:THR:HG22	1:A:302:THR:HG21	1.79	0.63
1:E:241:GLY:HA3	1:E:252:ARG:HB2	1.81	0.63
1:G:279:ASN:HA	1:H:279:ASN:H	1.64	0.63
1:H:190:TYR:O	1:H:203:VAL:HG13	1.99	0.63
1:A:72:HIS:HD2	1:A:162:GLU:HB3	1.64	0.63
1:G:218:PRO:HA	1:G:220:PHE:H	1.64	0.63
1:G:279:ASN:H	1:H:279:ASN:HA	1.63	0.63
1:I:148:PHE:CD1	1:I:154:VAL:HB	2.34	0.63
1:A:74:VAL:HG11	1:A:161:GLY:HA2	1.81	0.63
1:M:87:ILE:HD13	1:M:138:ILE:HD13	1.80	0.63
1:L:72:HIS:HD2	1:L:162:GLU:HB3	1.63	0.63
1:L:241:GLY:HA3	1:L:252:ARG:HB2	1.81	0.63
1:L:74:VAL:HG11	1:L:161:GLY:HA2	1.80	0.63
1:A:241:GLY:HA3	1:A:252:ARG:HB2	1.82	0.62
1:E:190:TYR:O	1:E:203:VAL:HG13	1.99	0.62
1:B:87:ILE:HD13	1:B:138:ILE:HD13	1.80	0.62
1:L:87:ILE:HD13	1:L:138:ILE:HD13	1.79	0.62
1:N:260:PRO:HD3	1:N:285:MET:HE3	1.80	0.62
1:E:21:ARG:HD2	1:E:292:TYR:HA	1.82	0.62
1:I:260:PRO:HD3	1:I:285:MET:HE3	1.81	0.62
1:N:241:GLY:HA3	1:N:252:ARG:HB2	1.79	0.62
1:G:87:ILE:HD13	1:G:138:ILE:HD13	1.82	0.62
1:I:72:HIS:HD2	1:I:162:GLU:HB3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:ARG:HD2	1:J:292:TYR:HA	1.82	0.62
1:A:102:ASN:ND2	1:A:299:VAL:O	2.32	0.62
1:F:72:HIS:HD2	1:F:162:GLU:HB3	1.65	0.62
1:F:190:TYR:O	1:F:203:VAL:HG13	2.00	0.62
1:L:21:ARG:HD2	1:L:292:TYR:HA	1.82	0.62
1:E:148:PHE:CD1	1:E:154:VAL:HB	2.34	0.62
1:G:74:VAL:HG11	1:G:161:GLY:HA2	1.80	0.62
1:L:190:TYR:O	1:L:203:VAL:HG13	2.00	0.62
1:M:74:VAL:HG11	1:M:161:GLY:HA2	1.82	0.62
1:B:102:ASN:ND2	1:B:299:VAL:O	2.32	0.61
1:D:74:VAL:HG11	1:D:161:GLY:HA2	1.81	0.61
1:K:74:VAL:HG11	1:K:161:GLY:HA2	1.82	0.61
1:E:134:GLN:OE1	1:G:180:LYS:NZ	2.33	0.61
1:B:218:PRO:HA	1:B:220:PHE:H	1.65	0.61
1:J:190:TYR:O	1:J:203:VAL:HG13	2.00	0.61
1:E:87:ILE:HD13	1:E:138:ILE:HD13	1.82	0.61
1:H:241:GLY:HA3	1:H:252:ARG:HB2	1.82	0.61
1:B:154:VAL:O	1:B:161:GLY:HA3	2.00	0.61
1:B:260:PRO:HD3	1:B:285:MET:HE3	1.82	0.61
1:D:102:ASN:ND2	1:D:299:VAL:O	2.31	0.61
1:B:21:ARG:HD2	1:B:292:TYR:HA	1.81	0.61
1:J:72:HIS:HD2	1:J:162:GLU:HB3	1.65	0.61
1:K:241:GLY:HA3	1:K:252:ARG:HB2	1.81	0.61
1:D:21:ARG:HD2	1:D:292:TYR:HA	1.82	0.61
1:E:74:VAL:HG11	1:E:161:GLY:HA2	1.81	0.61
1:K:72:HIS:HD2	1:K:162:GLU:HB3	1.66	0.61
1:N:87:ILE:HD13	1:N:138:ILE:HD13	1.82	0.61
1:A:87:ILE:HD13	1:A:138:ILE:HD13	1.83	0.61
1:I:241:GLY:HA3	1:I:252:ARG:HB2	1.83	0.61
1:J:179:LEU:HB3	1:J:187:ILE:HG13	1.83	0.61
1:N:74:VAL:HG11	1:N:161:GLY:HA2	1.83	0.61
1:N:179:LEU:HB3	1:N:187:ILE:HG13	1.83	0.61
1:A:179:LEU:HB3	1:A:187:ILE:HG13	1.83	0.61
1:A:21:ARG:HD2	1:A:292:TYR:HA	1.83	0.60
1:L:260:PRO:HD3	1:L:285:MET:HE3	1.83	0.60
1:C:102:ASN:ND2	1:C:299:VAL:O	2.33	0.60
1:D:218:PRO:HA	1:D:220:PHE:H	1.66	0.60
1:F:260:PRO:HD3	1:F:285:MET:HE3	1.82	0.60
1:K:87:ILE:HD13	1:K:138:ILE:HD13	1.82	0.60
1:K:148:PHE:CD1	1:K:154:VAL:HB	2.36	0.60
1:L:180:LYS:NZ	1:N:134:GLN:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:218:PRO:HA	1:L:220:PHE:H	1.66	0.60
1:A:90:GLN:O	1:A:94:LEU:HG	2.01	0.60
1:A:154:VAL:O	1:A:161:GLY:HA3	2.02	0.60
1:C:87:ILE:HD13	1:C:138:ILE:HD13	1.83	0.60
1:K:179:LEU:HB3	1:K:187:ILE:HG13	1.83	0.60
1:A:218:PRO:HA	1:A:220:PHE:H	1.67	0.60
1:D:180:LYS:NZ	1:F:134:GLN:OE1	2.34	0.60
1:H:74:VAL:HG11	1:H:161:GLY:HA2	1.82	0.60
1:I:190:TYR:O	1:I:203:VAL:HG13	2.00	0.60
1:J:241:GLY:HA3	1:J:252:ARG:HB2	1.82	0.60
1:C:21:ARG:HD2	1:C:292:TYR:HA	1.84	0.60
1:C:148:PHE:CD1	1:C:154:VAL:HB	2.36	0.60
1:C:218:PRO:HA	1:C:220:PHE:H	1.67	0.60
1:D:148:PHE:CD1	1:D:154:VAL:HB	2.37	0.60
1:E:102:ASN:ND2	1:E:299:VAL:O	2.34	0.60
1:F:74:VAL:HG11	1:F:161:GLY:HA2	1.82	0.60
1:E:72:HIS:HD2	1:E:162:GLU:HB3	1.66	0.60
1:F:179:LEU:HB3	1:F:187:ILE:HG13	1.83	0.60
1:F:218:PRO:HA	1:F:220:PHE:H	1.66	0.60
1:M:21:ARG:HD2	1:M:292:TYR:HA	1.82	0.60
1:A:190:TYR:O	1:A:203:VAL:HG13	2.02	0.60
1:G:72:HIS:CD2	1:G:162:GLU:HB3	2.37	0.60
1:I:72:HIS:CD2	1:I:162:GLU:HB3	2.37	0.60
1:N:90:GLN:O	1:N:94:LEU:HG	2.02	0.60
1:F:89:SER:HB2	1:F:212:THR:HG23	1.84	0.59
1:K:218:PRO:HA	1:K:220:PHE:H	1.67	0.59
1:K:279:ASN:H	1:L:279:ASN:HA	1.67	0.59
1:M:218:PRO:HA	1:M:220:PHE:H	1.67	0.59
1:M:241:GLY:HA3	1:M:252:ARG:HB2	1.82	0.59
1:B:227:THR:HA	1:B:230:ILE:HD12	1.84	0.59
1:C:190:TYR:O	1:C:203:VAL:HG13	2.02	0.59
1:F:241:GLY:HA3	1:F:252:ARG:HB2	1.83	0.59
1:G:102:ASN:ND2	1:G:299:VAL:O	2.34	0.59
1:J:89:SER:HB2	1:J:212:THR:HG23	1.84	0.59
1:L:102:ASN:ND2	1:L:299:VAL:O	2.34	0.59
1:G:190:TYR:O	1:G:203:VAL:HG13	2.02	0.59
1:J:218:PRO:HA	1:J:220:PHE:H	1.66	0.59
1:L:72:HIS:CD2	1:L:162:GLU:HB3	2.37	0.59
1:L:89:SER:HB2	1:L:212:THR:HG23	1.84	0.59
1:N:190:TYR:O	1:N:203:VAL:HG13	2.02	0.59
1:C:90:GLN:O	1:C:94:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:148:PHE:CD1	1:J:154:VAL:HB	2.37	0.59
1:L:179:LEU:HB3	1:L:187:ILE:HG13	1.84	0.59
1:M:179:LEU:HB3	1:M:187:ILE:HG13	1.85	0.59
1:N:102:ASN:ND2	1:N:299:VAL:O	2.33	0.59
1:A:72:HIS:CD2	1:A:162:GLU:HB3	2.37	0.59
1:I:240:TRP:CZ3	1:I:265:PRO:HB3	2.36	0.59
1:A:96:LYS:HA	1:A:101:LEU:HB2	1.83	0.59
1:B:74:VAL:HG11	1:B:161:GLY:HA2	1.84	0.59
1:F:180:LYS:NZ	1:H:134:GLN:OE1	2.36	0.59
1:M:89:SER:HB2	1:M:212:THR:HG23	1.85	0.59
1:C:179:LEU:HB3	1:C:187:ILE:HG13	1.84	0.59
1:H:218:PRO:HA	1:H:220:PHE:H	1.66	0.59
1:M:190:TYR:O	1:M:203:VAL:HG13	2.02	0.59
1:B:96:LYS:HA	1:B:101:LEU:HB2	1.84	0.59
1:D:190:TYR:O	1:D:203:VAL:HG13	2.03	0.59
1:D:260:PRO:HD3	1:D:285:MET:HE3	1.83	0.59
1:G:134:GLN:OE1	1:I:180:LYS:NZ	2.36	0.59
1:G:148:PHE:CD1	1:G:154:VAL:HB	2.38	0.59
1:I:21:ARG:HD2	1:I:292:TYR:HA	1.84	0.59
1:K:190:TYR:O	1:K:203:VAL:HG13	2.03	0.59
1:G:89:SER:HB2	1:G:212:THR:HG23	1.85	0.59
1:J:87:ILE:HD13	1:J:138:ILE:HD13	1.84	0.59
1:F:21:ARG:HD2	1:F:292:TYR:HA	1.85	0.58
1:I:96:LYS:HA	1:I:101:LEU:HB2	1.85	0.58
1:I:102:ASN:ND2	1:I:299:VAL:O	2.35	0.58
1:M:72:HIS:HD2	1:M:162:GLU:HB3	1.66	0.58
1:N:148:PHE:CD1	1:N:154:VAL:HB	2.38	0.58
1:F:72:HIS:CD2	1:F:162:GLU:HB3	2.38	0.58
1:J:72:HIS:CD2	1:J:162:GLU:HB3	2.38	0.58
1:B:148:PHE:CD1	1:B:154:VAL:HB	2.38	0.58
1:H:148:PHE:CD1	1:H:154:VAL:HB	2.39	0.58
1:N:89:SER:HB2	1:N:212:THR:HG23	1.83	0.58
1:N:227:THR:HA	1:N:230:ILE:HD12	1.84	0.58
1:C:89:SER:HB2	1:C:212:THR:HG23	1.85	0.58
1:C:96:LYS:HA	1:C:101:LEU:HB2	1.86	0.58
1:E:90:GLN:O	1:E:94:LEU:HG	2.04	0.58
1:K:102:ASN:ND2	1:K:299:VAL:O	2.33	0.58
1:N:218:PRO:HA	1:N:220:PHE:H	1.67	0.58
1:B:190:TYR:O	1:B:203:VAL:HG13	2.03	0.58
1:F:154:VAL:O	1:F:161:GLY:HA3	2.04	0.58
1:B:34:ARG:HH22	1:D:323:ARG:C	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:HB3	1:D:187:ILE:HG13	1.85	0.58
1:I:179:LEU:HB3	1:I:187:ILE:HG13	1.84	0.58
1:L:148:PHE:CD1	1:L:154:VAL:HB	2.38	0.58
1:M:279:ASN:HA	1:N:279:ASN:H	1.69	0.58
1:D:240:TRP:CZ3	1:D:265:PRO:HB3	2.39	0.58
1:H:192:GLN:OE1	1:H:200:THR:OG1	2.17	0.58
1:I:153:GLU:O	1:I:159:SER:HB2	2.04	0.58
1:I:218:PRO:HA	1:I:220:PHE:H	1.67	0.58
1:N:154:VAL:O	1:N:161:GLY:HA3	2.03	0.58
1:D:227:THR:HA	1:D:230:ILE:HD12	1.86	0.58
1:H:154:VAL:O	1:H:161:GLY:HA3	2.04	0.58
1:K:96:LYS:HA	1:K:101:LEU:HB2	1.84	0.58
1:M:148:PHE:CD1	1:M:154:VAL:HB	2.39	0.58
1:K:183:ILE:HG13	1:K:185:GLN:H	1.69	0.57
1:M:154:VAL:O	1:M:161:GLY:HA3	2.03	0.57
1:N:21:ARG:HD2	1:N:292:TYR:HA	1.86	0.57
1:D:89:SER:HB2	1:D:212:THR:HG23	1.85	0.57
1:A:71:VAL:HA	1:A:173:ILE:HB	1.86	0.57
1:A:148:PHE:CD1	1:A:154:VAL:HB	2.39	0.57
1:E:96:LYS:HA	1:E:101:LEU:HB2	1.85	0.57
1:K:72:HIS:CD2	1:K:162:GLU:HB3	2.39	0.57
1:L:96:LYS:HA	1:L:101:LEU:HB2	1.86	0.57
1:M:90:GLN:O	1:M:94:LEU:HG	2.03	0.57
1:F:227:THR:HA	1:F:230:ILE:HD12	1.86	0.57
1:I:89:SER:HB2	1:I:212:THR:HG23	1.85	0.57
1:B:179:LEU:HB3	1:B:187:ILE:HG13	1.85	0.57
1:C:279:ASN:H	1:D:279:ASN:HA	1.69	0.57
1:D:154:VAL:O	1:D:161:GLY:HA3	2.05	0.57
1:M:153:GLU:O	1:M:159:SER:HB2	2.05	0.57
1:M:279:ASN:H	1:N:279:ASN:HA	1.70	0.57
1:D:72:HIS:CD2	1:D:162:GLU:HB3	2.39	0.57
1:F:148:PHE:CD1	1:F:154:VAL:HB	2.39	0.57
1:G:72:HIS:HD2	1:G:162:GLU:HB3	1.69	0.57
1:A:89:SER:HB2	1:A:212:THR:HG23	1.87	0.57
1:I:154:VAL:O	1:I:161:GLY:HA3	2.04	0.57
1:K:279:ASN:HA	1:L:279:ASN:H	1.69	0.57
1:N:96:LYS:HA	1:N:101:LEU:HB2	1.87	0.57
1:J:96:LYS:HA	1:J:101:LEU:HB2	1.85	0.57
1:K:89:SER:HB2	1:K:212:THR:HG23	1.86	0.57
1:D:34:ARG:HH22	1:F:323:ARG:C	2.13	0.57
1:E:179:LEU:HB3	1:E:187:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:GLN:O	1:G:94:LEU:HG	2.04	0.57
1:I:183:ILE:HG13	1:I:185:GLN:H	1.69	0.57
1:M:72:HIS:CD2	1:M:162:GLU:HB3	2.40	0.57
1:M:227:THR:HA	1:M:230:ILE:HD12	1.86	0.57
1:B:90:GLN:O	1:B:94:LEU:HG	2.05	0.56
1:H:227:THR:HA	1:H:230:ILE:HD12	1.87	0.56
1:K:90:GLN:O	1:K:94:LEU:HG	2.04	0.56
1:L:71:VAL:HA	1:L:173:ILE:HB	1.87	0.56
1:A:227:THR:HA	1:A:230:ILE:HD12	1.86	0.56
1:H:102:ASN:ND2	1:H:299:VAL:O	2.37	0.56
1:J:240:TRP:CZ3	1:J:265:PRO:HB3	2.40	0.56
1:E:72:HIS:CD2	1:E:162:GLU:HB3	2.39	0.56
1:E:218:PRO:HA	1:E:220:PHE:H	1.69	0.56
1:G:240:TRP:CZ3	1:G:265:PRO:HB3	2.40	0.56
1:K:240:TRP:CZ3	1:K:265:PRO:HB3	2.41	0.56
1:L:90:GLN:O	1:L:94:LEU:HG	2.06	0.56
1:L:227:THR:HA	1:L:230:ILE:HD12	1.86	0.56
1:N:72:HIS:CD2	1:N:162:GLU:HB3	2.39	0.56
1:B:89:SER:HB2	1:B:212:THR:HG23	1.86	0.56
1:I:227:THR:HA	1:I:230:ILE:HD12	1.86	0.56
1:C:154:VAL:O	1:C:161:GLY:HA3	2.05	0.56
1:D:96:LYS:HA	1:D:101:LEU:HB2	1.88	0.56
1:J:71:VAL:HA	1:J:173:ILE:HB	1.87	0.56
1:J:90:GLN:O	1:J:94:LEU:HG	2.06	0.56
1:L:154:VAL:O	1:L:161:GLY:HA3	2.05	0.56
1:N:71:VAL:HA	1:N:173:ILE:HB	1.88	0.56
1:C:153:GLU:O	1:C:159:SER:HB2	2.06	0.56
1:H:179:LEU:HB3	1:H:187:ILE:HG13	1.87	0.56
1:A:153:GLU:O	1:A:159:SER:HB2	2.04	0.56
1:C:72:HIS:CD2	1:C:162:GLU:HB3	2.40	0.56
1:C:183:ILE:HG13	1:C:185:GLN:H	1.71	0.56
1:C:279:ASN:HA	1:D:279:ASN:H	1.70	0.56
1:M:26:MET:HG3	1:M:242:ASP:CG	2.31	0.56
1:B:72:HIS:CD2	1:B:162:GLU:HB3	2.40	0.56
1:D:153:GLU:O	1:D:159:SER:HB2	2.05	0.56
1:F:96:LYS:HA	1:F:101:LEU:HB2	1.88	0.56
1:H:90:GLN:O	1:H:94:LEU:HG	2.05	0.56
1:I:279:ASN:H	1:J:279:ASN:HA	1.71	0.56
1:M:96:LYS:HA	1:M:101:LEU:HB2	1.87	0.56
1:F:201:ASP:OD1	1:F:317:ARG:NH2	2.30	0.56
1:H:72:HIS:CD2	1:H:162:GLU:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:HB2	1:A:111:VAL:HG12	1.88	0.55
1:G:154:VAL:O	1:G:161:GLY:HA3	2.06	0.55
1:G:179:LEU:HB3	1:G:187:ILE:HG13	1.87	0.55
1:H:183:ILE:HG13	1:H:185:GLN:H	1.70	0.55
1:H:240:TRP:CZ3	1:H:265:PRO:HB3	2.41	0.55
1:L:153:GLU:O	1:L:159:SER:HB2	2.06	0.55
1:M:183:ILE:HG13	1:M:185:GLN:H	1.71	0.55
1:E:154:VAL:O	1:E:161:GLY:HA3	2.06	0.55
1:F:153:GLU:O	1:F:159:SER:HB2	2.07	0.55
1:K:154:VAL:O	1:K:161:GLY:HA3	2.05	0.55
1:M:240:TRP:CZ3	1:M:265:PRO:HB3	2.42	0.55
1:E:240:TRP:CZ3	1:E:265:PRO:HB3	2.41	0.55
1:F:183:ILE:HG13	1:F:185:GLN:H	1.70	0.55
1:I:279:ASN:HA	1:J:279:ASN:H	1.71	0.55
1:J:149:THR:HB	1:J:151:SER:H	1.71	0.55
1:K:153:GLU:O	1:K:159:SER:HB2	2.06	0.55
1:J:227:THR:HA	1:J:230:ILE:HD12	1.88	0.55
1:A:26:MET:HG3	1:A:242:ASP:CG	2.31	0.55
1:D:90:GLN:O	1:D:94:LEU:HG	2.07	0.55
1:E:227:THR:HA	1:E:230:ILE:HD12	1.88	0.55
1:F:102:ASN:ND2	1:F:299:VAL:O	2.34	0.55
1:C:309:VAL:O	1:C:313:LEU:HG	2.06	0.55
1:F:26:MET:HG3	1:F:242:ASP:CG	2.32	0.55
1:K:149:THR:HB	1:K:151:SER:H	1.72	0.55
1:M:102:ASN:ND2	1:M:299:VAL:O	2.34	0.55
1:D:26:MET:HG3	1:D:242:ASP:CG	2.30	0.55
1:G:35:SER:C	1:G:37:SER:H	2.15	0.55
1:N:61:ARG:HH12	1:N:121:ILE:HD11	1.72	0.55
1:B:26:MET:HG3	1:B:242:ASP:CG	2.31	0.55
1:C:71:VAL:HA	1:C:173:ILE:HB	1.88	0.55
1:K:26:MET:HG3	1:K:242:ASP:CG	2.32	0.55
1:D:309:VAL:O	1:D:313:LEU:HG	2.07	0.55
1:E:26:MET:HG3	1:E:242:ASP:CG	2.32	0.55
1:K:71:VAL:HA	1:K:173:ILE:HB	1.89	0.55
1:B:209:ALA:HA	1:B:220:PHE:HB2	1.88	0.54
1:C:72:HIS:HD2	1:C:162:GLU:HB3	1.73	0.54
1:D:149:THR:HB	1:D:151:SER:H	1.72	0.54
1:K:227:THR:HA	1:K:230:ILE:HD12	1.88	0.54
1:L:240:TRP:CZ3	1:L:265:PRO:HB3	2.41	0.54
1:N:26:MET:HG3	1:N:242:ASP:CG	2.32	0.54
1:D:183:ILE:HG13	1:D:185:GLN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:PRO:HB2	1:H:111:VAL:HG12	1.88	0.54
1:I:90:GLN:O	1:I:94:LEU:HG	2.06	0.54
1:M:270:PRO:HG2	1:M:286:PHE:CG	2.43	0.54
1:C:87:ILE:O	1:C:91:ILE:HG12	2.07	0.54
1:J:109:PRO:HB2	1:J:111:VAL:HG12	1.87	0.54
1:M:68:PRO:HB2	1:M:170:TYR:HD1	1.72	0.54
1:I:192:GLN:OE1	1:I:200:THR:OG1	2.20	0.54
1:I:289:TYR:HA	1:I:298:MET:HB2	1.88	0.54
1:B:153:GLU:O	1:B:159:SER:HB2	2.07	0.54
1:B:240:TRP:CZ3	1:B:265:PRO:HB3	2.42	0.54
1:B:309:VAL:O	1:B:313:LEU:HG	2.08	0.54
1:E:109:PRO:HB2	1:E:111:VAL:HG12	1.89	0.54
1:H:26:MET:HG3	1:H:242:ASP:CG	2.32	0.54
1:I:26:MET:HG3	1:I:242:ASP:CG	2.33	0.54
1:H:270:PRO:HG2	1:H:286:PHE:CG	2.43	0.54
1:B:68:PRO:HB2	1:B:170:TYR:HD1	1.73	0.54
1:C:227:THR:HA	1:C:230:ILE:HD12	1.88	0.54
1:F:149:THR:HB	1:F:151:SER:H	1.72	0.54
1:H:96:LYS:HA	1:H:101:LEU:HB2	1.89	0.54
1:K:35:SER:C	1:K:37:SER:H	2.16	0.54
1:A:240:TRP:CZ3	1:A:265:PRO:HB3	2.42	0.54
1:B:109:PRO:HB2	1:B:111:VAL:HG12	1.90	0.54
1:C:109:PRO:HB2	1:C:111:VAL:HG12	1.90	0.54
1:F:240:TRP:CZ3	1:F:265:PRO:HB3	2.43	0.54
1:G:227:THR:HA	1:G:230:ILE:HD12	1.88	0.54
1:N:72:HIS:HD2	1:N:162:GLU:HB3	1.72	0.54
1:N:109:PRO:HB2	1:N:111:VAL:HG12	1.89	0.54
1:D:209:ALA:HA	1:D:220:PHE:HB2	1.89	0.54
1:E:183:ILE:HG13	1:E:185:GLN:H	1.72	0.54
1:E:309:VAL:O	1:E:313:LEU:HG	2.07	0.54
1:G:26:MET:HG3	1:G:242:ASP:CG	2.33	0.54
1:G:71:VAL:HA	1:G:173:ILE:HB	1.90	0.54
1:G:84:ASP:OD1	1:G:140:ARG:NH2	2.35	0.54
1:G:183:ILE:HG13	1:G:185:GLN:H	1.71	0.54
1:J:309:VAL:O	1:J:313:LEU:HG	2.08	0.54
1:L:183:ILE:HG13	1:L:185:GLN:H	1.73	0.54
1:M:309:VAL:O	1:M:313:LEU:HG	2.07	0.54
1:A:149:THR:HB	1:A:151:SER:H	1.73	0.54
1:B:183:ILE:HG13	1:B:185:GLN:H	1.73	0.54
1:E:279:ASN:HA	1:F:279:ASN:H	1.72	0.54
1:J:183:ILE:HG13	1:J:185:GLN:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:THR:HB	1:L:151:SER:H	1.73	0.54
1:M:149:THR:HB	1:M:151:SER:H	1.73	0.54
1:I:270:PRO:HG2	1:I:286:PHE:CG	2.43	0.53
1:J:153:GLU:O	1:J:159:SER:HB2	2.07	0.53
1:L:289:TYR:HA	1:L:298:MET:HB2	1.90	0.53
1:N:87:ILE:O	1:N:91:ILE:HG12	2.08	0.53
1:E:68:PRO:HB2	1:E:170:TYR:HD1	1.74	0.53
1:E:270:PRO:HG2	1:E:286:PHE:CG	2.44	0.53
1:M:35:SER:C	1:M:37:SER:H	2.16	0.53
1:N:183:ILE:HG13	1:N:185:GLN:H	1.71	0.53
1:N:240:TRP:CZ3	1:N:265:PRO:HB3	2.43	0.53
1:D:155:LYS:HD3	1:D:200:THR:HA	1.91	0.53
1:G:109:PRO:HB2	1:G:111:VAL:HG12	1.89	0.53
1:G:270:PRO:HG2	1:G:286:PHE:CG	2.44	0.53
1:K:289:TYR:HA	1:K:298:MET:HB2	1.89	0.53
1:D:27:GLU:HB2	1:D:150:THR:HG21	1.91	0.53
1:G:149:THR:HB	1:G:151:SER:H	1.73	0.53
1:C:270:PRO:HG2	1:C:286:PHE:CG	2.43	0.53
1:G:209:ALA:HA	1:G:220:PHE:HB2	1.90	0.53
1:H:72:HIS:HD2	1:H:162:GLU:HB3	1.72	0.53
1:H:129:ASP:HB2	1:H:130:PRO:HD2	1.90	0.53
1:N:35:SER:C	1:N:37:SER:H	2.17	0.53
1:B:71:VAL:HA	1:B:173:ILE:HB	1.89	0.53
1:D:71:VAL:HA	1:D:173:ILE:HB	1.89	0.53
1:M:155:LYS:HD3	1:M:200:THR:HA	1.91	0.53
1:N:149:THR:HB	1:N:151:SER:H	1.72	0.53
1:M:87:ILE:O	1:M:91:ILE:HG12	2.09	0.53
1:A:209:ALA:HA	1:A:220:PHE:HB2	1.91	0.53
1:E:35:SER:C	1:E:37:SER:H	2.16	0.53
1:F:109:PRO:HB2	1:F:111:VAL:HG12	1.90	0.53
1:F:309:VAL:O	1:F:313:LEU:HG	2.08	0.53
1:I:149:THR:HB	1:I:151:SER:H	1.73	0.53
1:I:209:ALA:HA	1:I:220:PHE:HB2	1.91	0.53
1:J:87:ILE:O	1:J:91:ILE:HG12	2.09	0.53
1:K:155:LYS:HD3	1:K:200:THR:HA	1.91	0.53
1:M:201:ASP:OD1	1:M:317:ARG:NH2	2.32	0.53
1:A:183:ILE:HG13	1:A:185:GLN:H	1.73	0.53
1:B:35:SER:C	1:B:37:SER:H	2.17	0.53
1:I:35:SER:C	1:I:37:SER:H	2.17	0.53
1:I:84:ASP:HA	1:I:87:ILE:HD12	1.91	0.53
1:J:35:SER:C	1:J:37:SER:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:155:LYS:HD3	1:N:200:THR:HA	1.91	0.53
1:D:72:HIS:HD2	1:D:162:GLU:HB3	1.72	0.53
1:E:129:ASP:HB2	1:E:130:PRO:HD2	1.91	0.53
1:E:149:THR:HB	1:E:151:SER:H	1.74	0.53
1:H:289:TYR:HA	1:H:298:MET:HB2	1.90	0.53
1:I:68:PRO:HB2	1:I:170:TYR:HD1	1.74	0.53
1:J:153:GLU:CD	1:J:153:GLU:H	2.17	0.53
1:J:154:VAL:O	1:J:161:GLY:HA3	2.09	0.53
1:B:149:THR:HB	1:B:151:SER:H	1.73	0.52
1:C:35:SER:C	1:C:37:SER:H	2.17	0.52
1:D:84:ASP:HA	1:D:87:ILE:HD12	1.91	0.52
1:D:87:ILE:O	1:D:91:ILE:HG12	2.09	0.52
1:F:90:GLN:O	1:F:94:LEU:HG	2.09	0.52
1:G:130:PRO:HD3	1:G:165:TRP:CE3	2.44	0.52
1:I:71:VAL:HA	1:I:173:ILE:HB	1.90	0.52
1:J:289:TYR:HA	1:J:298:MET:HB2	1.90	0.52
1:N:309:VAL:O	1:N:313:LEU:HG	2.07	0.52
1:C:26:MET:HG3	1:C:242:ASP:CG	2.35	0.52
1:E:130:PRO:HD3	1:E:165:TRP:CE3	2.43	0.52
1:F:90:GLN:NE2	1:F:223:GLY:O	2.42	0.52
1:I:109:PRO:HB2	1:I:111:VAL:HG12	1.89	0.52
1:K:87:ILE:O	1:K:91:ILE:HG12	2.09	0.52
1:M:130:PRO:HD3	1:M:165:TRP:CE3	2.44	0.52
1:N:209:ALA:HA	1:N:220:PHE:HB2	1.91	0.52
1:A:289:TYR:HA	1:A:298:MET:HB2	1.91	0.52
1:B:129:ASP:HB2	1:B:130:PRO:HD2	1.91	0.52
1:D:35:SER:C	1:D:37:SER:H	2.15	0.52
1:G:42:ARG:NH1	1:G:235:ASN:HD21	2.07	0.52
1:K:27:GLU:HB2	1:K:150:THR:HG21	1.91	0.52
1:K:134:GLN:OE1	1:M:180:LYS:NZ	2.43	0.52
1:M:71:VAL:HA	1:M:173:ILE:HB	1.91	0.52
1:M:109:PRO:HB2	1:M:111:VAL:HG12	1.90	0.52
1:N:153:GLU:O	1:N:159:SER:HB2	2.09	0.52
1:F:129:ASP:HB2	1:F:130:PRO:HD2	1.91	0.52
1:H:155:LYS:HD3	1:H:200:THR:HA	1.92	0.52
1:K:42:ARG:NH1	1:K:235:ASN:HD21	2.07	0.52
1:L:155:LYS:HD3	1:L:200:THR:HA	1.92	0.52
1:A:278:SER:HB2	1:B:279:ASN:C	2.35	0.52
1:D:270:PRO:HG2	1:D:286:PHE:CG	2.44	0.52
1:F:61:ARG:HH12	1:F:121:ILE:HD11	1.74	0.52
1:L:35:SER:C	1:L:37:SER:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:HIS:HD2	1:B:162:GLU:HB3	1.73	0.52
1:B:130:PRO:HD3	1:B:165:TRP:CE3	2.44	0.52
1:C:155:LYS:HD3	1:C:200:THR:HA	1.91	0.52
1:E:279:ASN:H	1:F:279:ASN:HA	1.75	0.52
1:F:71:VAL:HA	1:F:173:ILE:HB	1.91	0.52
1:F:289:TYR:HA	1:F:298:MET:HB2	1.91	0.52
1:J:270:PRO:HG2	1:J:286:PHE:CG	2.45	0.52
1:A:27:GLU:HB2	1:A:150:THR:HG21	1.91	0.52
1:C:149:THR:HB	1:C:151:SER:H	1.75	0.52
1:H:35:SER:C	1:H:37:SER:H	2.18	0.52
1:K:109:PRO:HB2	1:K:111:VAL:HG12	1.90	0.52
1:L:61:ARG:HH12	1:L:121:ILE:HD11	1.75	0.52
1:L:270:PRO:HG2	1:L:286:PHE:CG	2.44	0.52
1:M:84:ASP:HA	1:M:87:ILE:HD12	1.92	0.52
1:N:27:GLU:HB2	1:N:150:THR:HG21	1.91	0.52
1:F:130:PRO:HD3	1:F:165:TRP:CE3	2.45	0.52
1:G:192:GLN:OE1	1:G:200:THR:OG1	2.21	0.52
1:G:289:TYR:HA	1:G:298:MET:HB2	1.91	0.52
1:K:130:PRO:HD3	1:K:165:TRP:CE3	2.45	0.52
1:L:109:PRO:HB2	1:L:111:VAL:HG12	1.90	0.52
1:L:209:ALA:HA	1:L:220:PHE:HB2	1.91	0.52
1:M:27:GLU:HB2	1:M:150:THR:HG21	1.92	0.52
1:D:26:MET:HG3	1:D:242:ASP:OD1	2.10	0.52
1:H:84:ASP:HA	1:H:87:ILE:HD12	1.92	0.52
1:H:149:THR:HB	1:H:151:SER:H	1.74	0.52
1:K:153:GLU:H	1:K:153:GLU:CD	2.18	0.52
1:K:192:GLN:OE1	1:K:200:THR:OG1	2.21	0.52
1:L:26:MET:HG3	1:L:242:ASP:CG	2.34	0.52
1:A:84:ASP:HA	1:A:87:ILE:HD12	1.92	0.51
1:B:34:ARG:NH1	1:D:322:ALA:O	2.42	0.51
1:C:289:TYR:HA	1:C:298:MET:HB2	1.91	0.51
1:G:96:LYS:HA	1:G:101:LEU:HB2	1.90	0.51
1:G:155:LYS:HD3	1:G:200:THR:HA	1.92	0.51
1:H:201:ASP:OD1	1:H:317:ARG:NH2	2.33	0.51
1:H:309:VAL:O	1:H:313:LEU:HG	2.10	0.51
1:L:99:ARG:NH1	1:L:118:ASP:HB2	2.25	0.51
1:L:153:GLU:CD	1:L:153:GLU:H	2.18	0.51
1:M:26:MET:HG3	1:M:242:ASP:OD1	2.10	0.51
1:N:129:ASP:HB2	1:N:130:PRO:HD2	1.91	0.51
1:A:270:PRO:HG2	1:A:286:PHE:CG	2.45	0.51
1:B:87:ILE:O	1:B:91:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ASP:HB2	1:G:130:PRO:HD2	1.91	0.51
1:A:314:ASP:O	1:A:318:SER:HB3	2.10	0.51
1:B:61:ARG:HH12	1:B:121:ILE:HD11	1.76	0.51
1:E:87:ILE:O	1:E:91:ILE:HG12	2.09	0.51
1:I:61:ARG:HH12	1:I:121:ILE:HD11	1.75	0.51
1:I:129:ASP:HB2	1:I:130:PRO:HD2	1.93	0.51
1:E:155:LYS:HD3	1:E:200:THR:HA	1.92	0.51
1:J:27:GLU:HB2	1:J:150:THR:HG21	1.92	0.51
1:N:270:PRO:HG2	1:N:286:PHE:CG	2.45	0.51
1:K:84:ASP:HA	1:K:87:ILE:HD12	1.93	0.51
1:D:289:TYR:HA	1:D:298:MET:HB2	1.92	0.51
1:E:289:TYR:HA	1:E:298:MET:HB2	1.90	0.51
1:F:42:ARG:NH1	1:F:235:ASN:HD21	2.08	0.51
1:G:61:ARG:HH12	1:G:121:ILE:HD11	1.76	0.51
1:G:68:PRO:HB2	1:G:170:TYR:HD1	1.75	0.51
1:K:68:PRO:HB2	1:K:170:TYR:HD1	1.75	0.51
1:K:270:PRO:HG2	1:K:286:PHE:CG	2.46	0.51
1:N:84:ASP:HA	1:N:87:ILE:HD12	1.92	0.51
1:B:155:LYS:HD3	1:B:200:THR:HA	1.93	0.51
1:B:270:PRO:HG2	1:B:286:PHE:CG	2.45	0.51
1:C:240:TRP:CZ3	1:C:265:PRO:HB3	2.46	0.51
1:D:34:ARG:NH1	1:F:322:ALA:O	2.44	0.51
1:D:38:TYR:CE2	1:D:42:ARG:HG3	2.46	0.51
1:D:129:ASP:HB2	1:D:130:PRO:HD2	1.92	0.51
1:J:68:PRO:HB2	1:J:170:TYR:HD1	1.74	0.51
1:J:155:LYS:HD3	1:J:200:THR:HA	1.93	0.51
1:L:90:GLN:NE2	1:L:223:GLY:O	2.44	0.51
1:B:84:ASP:OD1	1:B:140:ARG:NH2	2.39	0.51
1:E:32:LEU:HB3	1:E:38:TYR:CE2	2.46	0.51
1:E:209:ALA:HA	1:E:220:PHE:HB2	1.92	0.51
1:G:153:GLU:O	1:G:159:SER:HB2	2.11	0.51
1:J:26:MET:HG3	1:J:242:ASP:CG	2.35	0.51
1:L:87:ILE:O	1:L:91:ILE:HG12	2.11	0.51
1:A:68:PRO:HB2	1:A:170:TYR:HD1	1.76	0.51
1:A:129:ASP:HB2	1:A:130:PRO:HD2	1.93	0.51
1:B:212:THR:HA	1:B:221:ASP:O	2.11	0.51
1:B:289:TYR:HA	1:B:298:MET:HB2	1.91	0.51
1:I:98:PHE:CE1	1:I:227:THR:HG23	2.45	0.51
1:L:129:ASP:HB2	1:L:130:PRO:HD2	1.93	0.51
1:N:289:TYR:HA	1:N:298:MET:HB2	1.91	0.51
1:D:109:PRO:HB2	1:D:111:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ARG:NH1	1:F:118:ASP:HB2	2.26	0.51
1:H:305:GLN:O	1:H:309:VAL:HG23	2.11	0.51
1:I:27:GLU:HB2	1:I:150:THR:HG21	1.93	0.51
1:J:32:LEU:HD13	1:J:38:TYR:CZ	2.46	0.51
1:J:102:ASN:ND2	1:J:299:VAL:O	2.36	0.51
1:J:209:ALA:HA	1:J:220:PHE:HB2	1.93	0.51
1:L:27:GLU:HB2	1:L:150:THR:HG21	1.93	0.51
1:M:289:TYR:HA	1:M:298:MET:HB2	1.92	0.51
1:B:38:TYR:CE2	1:B:42:ARG:HG3	2.46	0.50
1:B:84:ASP:HA	1:B:87:ILE:HD12	1.93	0.50
1:D:130:PRO:HD3	1:D:165:TRP:CE3	2.46	0.50
1:H:287:MET:H	1:H:287:MET:CE	2.25	0.50
1:I:87:ILE:O	1:I:91:ILE:HG12	2.11	0.50
1:M:42:ARG:NH1	1:M:235:ASN:HD21	2.09	0.50
1:N:38:TYR:CE2	1:N:42:ARG:HG3	2.46	0.50
1:A:26:MET:HG3	1:A:242:ASP:OD1	2.12	0.50
1:B:27:GLU:HB2	1:B:150:THR:HG21	1.92	0.50
1:E:84:ASP:HA	1:E:87:ILE:HD12	1.93	0.50
1:F:35:SER:C	1:F:37:SER:H	2.18	0.50
1:H:209:ALA:HA	1:H:220:PHE:HB2	1.93	0.50
1:J:287:MET:H	1:J:287:MET:CE	2.24	0.50
1:K:201:ASP:OD1	1:K:317:ARG:NH2	2.32	0.50
1:K:209:ALA:HA	1:K:220:PHE:HB2	1.91	0.50
1:L:84:ASP:HA	1:L:87:ILE:HD12	1.93	0.50
1:A:130:PRO:HD3	1:A:165:TRP:CE3	2.46	0.50
1:A:153:GLU:CD	1:A:153:GLU:H	2.19	0.50
1:A:155:LYS:HD3	1:A:200:THR:HA	1.94	0.50
1:E:27:GLU:HB2	1:E:150:THR:HG21	1.92	0.50
1:G:218:PRO:HA	1:G:220:PHE:N	2.26	0.50
1:H:153:GLU:O	1:H:159:SER:HB2	2.12	0.50
1:A:35:SER:C	1:A:37:SER:H	2.19	0.50
1:A:38:TYR:CE2	1:A:42:ARG:HG3	2.47	0.50
1:D:153:GLU:CD	1:D:153:GLU:H	2.19	0.50
1:F:68:PRO:HB2	1:F:170:TYR:HD1	1.76	0.50
1:F:209:ALA:HA	1:F:220:PHE:HB2	1.93	0.50
1:L:38:TYR:CE2	1:L:42:ARG:HG3	2.46	0.50
1:M:209:ALA:HA	1:M:220:PHE:HB2	1.92	0.50
1:M:270:PRO:HG2	1:M:286:PHE:CD2	2.47	0.50
1:B:192:GLN:OE1	1:B:200:THR:OG1	2.21	0.50
1:C:84:ASP:HA	1:C:87:ILE:HD12	1.94	0.50
1:F:84:ASP:HA	1:F:87:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:PRO:HG2	1:F:286:PHE:CG	2.47	0.50
1:H:61:ARG:HH12	1:H:121:ILE:HD11	1.75	0.50
1:I:155:LYS:HD3	1:I:200:THR:HA	1.94	0.50
1:I:189:GLY:HA3	1:I:205:ILE:HD13	1.94	0.50
1:J:32:LEU:HB3	1:J:38:TYR:CE2	2.46	0.50
1:J:61:ARG:HH12	1:J:121:ILE:HD11	1.77	0.50
1:K:309:VAL:O	1:K:313:LEU:HG	2.11	0.50
1:C:61:ARG:HH12	1:C:121:ILE:HD11	1.77	0.50
1:D:270:PRO:HG2	1:D:286:PHE:CD2	2.46	0.50
1:F:32:LEU:HD13	1:F:38:TYR:CZ	2.47	0.50
1:G:274:HIS:O	1:G:284:ASP:N	2.43	0.50
1:H:130:PRO:HD3	1:H:165:TRP:CE3	2.47	0.50
1:M:84:ASP:OD1	1:M:140:ARG:NH2	2.38	0.50
1:C:27:GLU:HB2	1:C:150:THR:HG21	1.92	0.50
1:E:32:LEU:HD13	1:E:38:TYR:CZ	2.47	0.50
1:G:75:TRP:CG	1:G:81:ASN:HB2	2.47	0.50
1:I:309:VAL:O	1:I:313:LEU:HG	2.12	0.50
1:J:99:ARG:HB2	1:J:101:LEU:HG	1.94	0.50
1:N:130:PRO:HD3	1:N:165:TRP:CE3	2.46	0.50
1:C:68:PRO:HB2	1:C:170:TYR:HD1	1.76	0.50
1:G:84:ASP:HA	1:G:87:ILE:HD12	1.94	0.50
1:H:34:ARG:HH22	1:J:323:ARG:C	2.20	0.50
1:N:68:PRO:HB2	1:N:170:TYR:HD1	1.77	0.50
1:A:87:ILE:O	1:A:91:ILE:HG12	2.12	0.50
1:C:32:LEU:HB3	1:C:38:TYR:CE2	2.47	0.50
1:E:153:GLU:O	1:E:159:SER:HB2	2.12	0.50
1:N:99:ARG:NH1	1:N:118:ASP:HB2	2.27	0.50
1:A:61:ARG:HH12	1:A:121:ILE:HD11	1.76	0.49
1:A:279:ASN:C	1:B:278:SER:HB2	2.37	0.49
1:E:71:VAL:HA	1:E:173:ILE:HB	1.93	0.49
1:F:155:LYS:HD3	1:F:200:THR:HA	1.94	0.49
1:H:270:PRO:HG2	1:H:286:PHE:CD2	2.47	0.49
1:J:99:ARG:NH1	1:J:118:ASP:HB2	2.27	0.49
1:J:130:PRO:HD3	1:J:165:TRP:CE3	2.47	0.49
1:N:109:PRO:HD2	1:N:287:MET:SD	2.52	0.49
1:C:209:ALA:HA	1:C:220:PHE:HB2	1.93	0.49
1:E:153:GLU:CD	1:E:153:GLU:H	2.19	0.49
1:E:287:MET:CE	1:E:287:MET:H	2.24	0.49
1:G:87:ILE:O	1:G:91:ILE:HG12	2.12	0.49
1:J:270:PRO:HG2	1:J:286:PHE:CD2	2.47	0.49
1:F:192:GLN:OE1	1:F:200:THR:OG1	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:VAL:HG12	1:F:313:LEU:HD21	1.95	0.49
1:G:26:MET:HG3	1:G:242:ASP:OD1	2.11	0.49
1:I:270:PRO:HG2	1:I:286:PHE:CD2	2.47	0.49
1:L:98:PHE:CE1	1:L:227:THR:HG23	2.47	0.49
1:M:32:LEU:HD13	1:M:38:TYR:CZ	2.47	0.49
1:A:99:ARG:NH1	1:A:118:ASP:HB2	2.27	0.49
1:C:129:ASP:HB2	1:C:130:PRO:HD2	1.94	0.49
1:C:153:GLU:CD	1:C:153:GLU:H	2.19	0.49
1:E:323:ARG:C	1:G:34:ARG:HH22	2.19	0.49
1:L:42:ARG:NH1	1:L:235:ASN:HD21	2.09	0.49
1:L:218:PRO:HA	1:L:220:PHE:N	2.27	0.49
1:E:274:HIS:O	1:E:284:ASP:N	2.41	0.49
1:H:38:TYR:CE2	1:H:42:ARG:HG3	2.47	0.49
1:K:26:MET:HG3	1:K:242:ASP:OD1	2.12	0.49
1:K:129:ASP:HB2	1:K:130:PRO:HD2	1.93	0.49
1:L:270:PRO:HG2	1:L:286:PHE:CD2	2.48	0.49
1:I:42:ARG:NH1	1:I:235:ASN:HD21	2.10	0.49
1:L:32:LEU:HD13	1:L:38:TYR:CZ	2.48	0.49
1:M:129:ASP:HB2	1:M:130:PRO:HD2	1.94	0.49
1:M:165:TRP:N	1:M:172:ASN:OD1	2.45	0.49
1:N:26:MET:HG3	1:N:242:ASP:OD1	2.13	0.49
1:I:153:GLU:CD	1:I:153:GLU:H	2.20	0.49
1:N:305:GLN:O	1:N:309:VAL:HG23	2.13	0.49
1:E:94:LEU:O	1:E:98:PHE:HD1	1.96	0.49
1:E:314:ASP:O	1:E:318:SER:HB3	2.12	0.49
1:G:287:MET:CE	1:G:287:MET:H	2.25	0.49
1:H:27:GLU:HB2	1:H:150:THR:HG21	1.95	0.49
1:H:68:PRO:HB2	1:H:170:TYR:HD1	1.78	0.49
1:H:71:VAL:HA	1:H:173:ILE:HB	1.95	0.49
1:H:274:HIS:O	1:H:284:ASP:N	2.42	0.49
1:A:42:ARG:NH1	1:A:235:ASN:HD21	2.11	0.49
1:F:287:MET:H	1:F:287:MET:CE	2.25	0.49
1:G:38:TYR:CE2	1:G:42:ARG:HG3	2.48	0.49
1:H:94:LEU:O	1:H:98:PHE:HD1	1.96	0.49
1:K:99:ARG:HB2	1:K:101:LEU:HG	1.95	0.49
1:K:99:ARG:NH1	1:K:118:ASP:HB2	2.26	0.49
1:M:32:LEU:HB3	1:M:38:TYR:CE2	2.48	0.49
1:C:130:PRO:HD3	1:C:165:TRP:CE3	2.47	0.49
1:C:323:ARG:C	1:E:34:ARG:HH22	2.21	0.49
1:E:99:ARG:NH1	1:E:118:ASP:HB2	2.28	0.49
1:E:270:PRO:HG2	1:E:286:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:ASP:OD1	1:G:317:ARG:NH2	2.36	0.49
1:H:157:ALA:HA	1:H:161:GLY:O	2.12	0.49
1:I:32:LEU:HB3	1:I:38:TYR:CE2	2.48	0.49
1:L:130:PRO:HD3	1:L:165:TRP:CE3	2.47	0.49
1:L:309:VAL:O	1:L:313:LEU:HG	2.13	0.49
1:M:153:GLU:CD	1:M:153:GLU:H	2.19	0.49
1:B:26:MET:HG3	1:B:242:ASP:OD1	2.13	0.48
1:B:32:LEU:HD13	1:B:38:TYR:CZ	2.48	0.48
1:B:157:ALA:HA	1:B:161:GLY:O	2.13	0.48
1:D:287:MET:H	1:D:287:MET:CE	2.26	0.48
1:F:218:PRO:HA	1:F:220:PHE:N	2.26	0.48
1:I:130:PRO:HD3	1:I:165:TRP:CE3	2.48	0.48
1:I:218:PRO:HA	1:I:220:PHE:N	2.27	0.48
1:K:314:ASP:O	1:K:318:SER:HB3	2.13	0.48
1:L:84:ASP:OD1	1:L:140:ARG:NH2	2.41	0.48
1:M:61:ARG:HH12	1:M:121:ILE:HD11	1.77	0.48
1:M:287:MET:H	1:M:287:MET:CE	2.25	0.48
1:A:309:VAL:O	1:A:313:LEU:HG	2.13	0.48
1:B:218:PRO:HA	1:B:220:PHE:N	2.27	0.48
1:C:26:MET:HG3	1:C:242:ASP:OD1	2.13	0.48
1:C:99:ARG:NH1	1:C:118:ASP:HB2	2.28	0.48
1:C:270:PRO:HG2	1:C:286:PHE:CD2	2.48	0.48
1:D:42:ARG:NH1	1:D:235:ASN:HD21	2.11	0.48
1:D:68:PRO:HB2	1:D:170:TYR:HD1	1.78	0.48
1:D:218:PRO:HA	1:D:220:PHE:N	2.27	0.48
1:E:26:MET:HG3	1:E:242:ASP:OD1	2.13	0.48
1:E:99:ARG:HB2	1:E:101:LEU:HG	1.95	0.48
1:F:87:ILE:O	1:F:91:ILE:HG12	2.13	0.48
1:F:153:GLU:CD	1:F:153:GLU:H	2.21	0.48
1:G:305:GLN:O	1:G:309:VAL:HG23	2.12	0.48
1:I:314:ASP:O	1:I:318:SER:HB3	2.13	0.48
1:J:90:GLN:NE2	1:J:223:GLY:O	2.45	0.48
1:L:26:MET:HG3	1:L:242:ASP:OD1	2.13	0.48
1:F:27:GLU:HB2	1:F:150:THR:HG21	1.95	0.48
1:F:94:LEU:O	1:F:98:PHE:HD1	1.96	0.48
1:G:153:GLU:CD	1:G:153:GLU:H	2.21	0.48
1:H:87:ILE:O	1:H:91:ILE:HG12	2.13	0.48
1:H:99:ARG:HB2	1:H:101:LEU:HG	1.95	0.48
1:I:99:ARG:HB2	1:I:101:LEU:HG	1.96	0.48
1:C:94:LEU:O	1:C:98:PHE:HD1	1.97	0.48
1:E:109:PRO:HD2	1:E:287:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:287:MET:H	1:K:287:MET:CE	2.26	0.48
1:A:287:MET:H	1:A:287:MET:CE	2.26	0.48
1:H:314:ASP:O	1:H:318:SER:HB3	2.13	0.48
1:I:75:TRP:CG	1:I:81:ASN:HB2	2.48	0.48
1:J:218:PRO:HA	1:J:220:PHE:N	2.28	0.48
1:A:218:PRO:HA	1:A:220:PHE:N	2.28	0.48
1:B:42:ARG:NH1	1:B:235:ASN:HD21	2.10	0.48
1:B:314:ASP:O	1:B:318:SER:HB3	2.14	0.48
1:C:75:TRP:CG	1:C:81:ASN:HB2	2.48	0.48
1:D:99:ARG:HB2	1:D:101:LEU:HG	1.95	0.48
1:I:26:MET:HG3	1:I:242:ASP:OD1	2.13	0.48
1:I:75:TRP:HB2	1:I:77:GLU:O	2.13	0.48
1:I:99:ARG:NH1	1:I:118:ASP:HB2	2.28	0.48
1:N:32:LEU:HD13	1:N:38:TYR:CZ	2.49	0.48
1:B:75:TRP:CG	1:B:81:ASN:HB2	2.48	0.48
1:F:32:LEU:HB3	1:F:38:TYR:CE2	2.48	0.48
1:G:38:TYR:HD1	1:G:196:GLY:HA2	1.78	0.48
1:I:32:LEU:HD13	1:I:38:TYR:CZ	2.49	0.48
1:I:155:LYS:HA	1:I:174:TRP:NE1	2.29	0.48
1:A:32:LEU:HD13	1:A:38:TYR:CZ	2.48	0.48
1:H:32:LEU:HD13	1:H:38:TYR:CZ	2.49	0.48
1:K:32:LEU:HD13	1:K:38:TYR:CZ	2.49	0.48
1:K:38:TYR:CE2	1:K:42:ARG:HG3	2.48	0.48
1:B:99:ARG:HB2	1:B:101:LEU:HG	1.96	0.48
1:D:61:ARG:HH12	1:D:121:ILE:HD11	1.79	0.48
1:E:61:ARG:HH12	1:E:121:ILE:HD11	1.78	0.48
1:E:155:LYS:HA	1:E:174:TRP:NE1	2.28	0.48
1:H:75:TRP:CG	1:H:81:ASN:HB2	2.49	0.48
1:J:129:ASP:HB2	1:J:130:PRO:HD2	1.96	0.48
1:A:75:TRP:HB2	1:A:77:GLU:O	2.14	0.48
1:F:38:TYR:CE2	1:F:42:ARG:HG3	2.49	0.48
1:I:38:TYR:CE2	1:I:42:ARG:HG3	2.49	0.48
1:J:75:TRP:CG	1:J:81:ASN:HB2	2.49	0.48
1:N:270:PRO:HG2	1:N:286:PHE:CD2	2.48	0.48
1:C:32:LEU:HD13	1:C:38:TYR:CZ	2.48	0.47
1:D:32:LEU:HD13	1:D:38:TYR:CZ	2.49	0.47
1:E:42:ARG:NH1	1:E:235:ASN:HD21	2.12	0.47
1:H:189:GLY:HA3	1:H:205:ILE:HD13	1.95	0.47
1:N:90:GLN:NE2	1:N:223:GLY:O	2.45	0.47
1:G:270:PRO:HG2	1:G:286:PHE:CD2	2.49	0.47
1:H:90:GLN:NE2	1:H:223:GLY:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:192:GLN:OE1	1:J:200:THR:OG1	2.21	0.47
1:K:61:ARG:HH12	1:K:121:ILE:HD11	1.78	0.47
1:M:99:ARG:NH1	1:M:118:ASP:HB2	2.30	0.47
1:B:270:PRO:HG2	1:B:286:PHE:CD2	2.50	0.47
1:C:314:ASP:O	1:C:318:SER:HB3	2.15	0.47
1:D:90:GLN:NE2	1:D:223:GLY:O	2.46	0.47
1:G:27:GLU:HB2	1:G:150:THR:HG21	1.96	0.47
1:G:99:ARG:HB2	1:G:101:LEU:HG	1.97	0.47
1:G:99:ARG:NH1	1:G:118:ASP:HB2	2.28	0.47
1:H:218:PRO:HA	1:H:220:PHE:N	2.27	0.47
1:J:314:ASP:O	1:J:318:SER:HB3	2.14	0.47
1:K:112:TRP:CD2	1:K:285:MET:HE2	2.49	0.47
1:K:305:GLN:O	1:K:309:VAL:HG23	2.15	0.47
1:N:94:LEU:O	1:N:98:PHE:HD1	1.97	0.47
1:N:153:GLU:CD	1:N:153:GLU:H	2.21	0.47
1:N:218:PRO:HA	1:N:220:PHE:N	2.29	0.47
1:N:238:HIS:O	1:N:254:ASP:HB3	2.14	0.47
1:C:38:TYR:CE2	1:C:42:ARG:HG3	2.49	0.47
1:L:194:PRO:HD2	1:L:235:ASN:ND2	2.30	0.47
1:L:287:MET:CE	1:L:287:MET:H	2.26	0.47
1:M:38:TYR:CE2	1:M:42:ARG:HG3	2.49	0.47
1:N:42:ARG:NH1	1:N:235:ASN:HD21	2.11	0.47
1:N:157:ALA:HA	1:N:161:GLY:O	2.14	0.47
1:A:201:ASP:OD1	1:A:317:ARG:NH2	2.33	0.47
1:C:99:ARG:HB2	1:C:101:LEU:HG	1.96	0.47
1:H:26:MET:HG3	1:H:242:ASP:OD1	2.14	0.47
1:H:152:ASP:OD2	1:H:155:LYS:NZ	2.33	0.47
1:K:98:PHE:CE1	1:K:227:THR:HG23	2.50	0.47
1:B:189:GLY:HA3	1:B:205:ILE:HD13	1.96	0.47
1:C:98:PHE:CE1	1:C:227:THR:HG23	2.50	0.47
1:J:84:ASP:HA	1:J:87:ILE:HD12	1.96	0.47
1:M:94:LEU:O	1:M:98:PHE:HD1	1.97	0.47
1:A:189:GLY:HA3	1:A:205:ILE:HD13	1.97	0.47
1:A:270:PRO:HG2	1:A:286:PHE:CD2	2.50	0.47
1:B:99:ARG:NH1	1:B:118:ASP:HB2	2.30	0.47
1:B:287:MET:CE	1:B:287:MET:H	2.27	0.47
1:C:201:ASP:OD1	1:C:317:ARG:NH2	2.35	0.47
1:D:75:TRP:CG	1:D:81:ASN:HB2	2.50	0.47
1:F:26:MET:HG3	1:F:242:ASP:OD1	2.14	0.47
1:F:65:VAL:HG21	1:F:321:LEU:HD22	1.97	0.47
1:F:75:TRP:HB2	1:F:77:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:LEU:HB3	1:G:38:TYR:CE2	2.49	0.47
1:H:153:GLU:CD	1:H:153:GLU:H	2.21	0.47
1:L:75:TRP:HB2	1:L:77:GLU:O	2.15	0.47
1:M:189:GLY:HA3	1:M:205:ILE:HD13	1.97	0.47
1:N:194:PRO:HD2	1:N:235:ASN:ND2	2.30	0.47
1:A:32:LEU:HB3	1:A:38:TYR:CE2	2.50	0.47
1:A:212:THR:HA	1:A:221:ASP:O	2.14	0.47
1:C:218:PRO:HA	1:C:220:PHE:N	2.29	0.47
1:L:238:HIS:O	1:L:254:ASP:HB3	2.15	0.47
1:M:309:VAL:HG12	1:M:313:LEU:HD21	1.96	0.47
1:N:314:ASP:O	1:N:318:SER:HB3	2.14	0.47
1:B:194:PRO:HD2	1:B:235:ASN:ND2	2.29	0.47
1:B:249:PRO:O	1:B:252:ARG:HG3	2.15	0.47
1:B:274:HIS:O	1:B:284:ASP:N	2.46	0.47
1:E:75:TRP:CG	1:E:81:ASN:HB2	2.50	0.47
1:E:192:GLN:OE1	1:E:200:THR:OG1	2.24	0.47
1:I:84:ASP:OD1	1:I:140:ARG:NH2	2.38	0.47
1:I:305:GLN:O	1:I:309:VAL:HG23	2.15	0.47
1:L:274:HIS:O	1:L:284:ASP:N	2.46	0.47
1:C:84:ASP:OD1	1:C:140:ARG:NH2	2.42	0.47
1:D:94:LEU:O	1:D:98:PHE:HD1	1.98	0.47
1:E:84:ASP:OD1	1:E:140:ARG:NH2	2.38	0.47
1:G:94:LEU:O	1:G:98:PHE:HD1	1.98	0.47
1:G:314:ASP:O	1:G:318:SER:HB3	2.14	0.47
1:K:84:ASP:OD1	1:K:140:ARG:NH2	2.41	0.47
1:L:68:PRO:HB2	1:L:170:TYR:HD1	1.80	0.47
1:L:75:TRP:CG	1:L:81:ASN:HB2	2.50	0.47
1:L:94:LEU:O	1:L:98:PHE:HD1	1.97	0.47
1:A:134:GLN:OE1	1:C:180:LYS:NZ	2.49	0.46
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.78	0.46
1:C:42:ARG:NH1	1:C:235:ASN:HD21	2.12	0.46
1:D:309:VAL:HG12	1:D:313:LEU:HD21	1.98	0.46
1:D:314:ASP:O	1:D:318:SER:HB3	2.14	0.46
1:E:300:MET:HE2	1:E:300:MET:HB2	1.84	0.46
1:G:32:LEU:HD13	1:G:38:TYR:CZ	2.50	0.46
1:G:179:LEU:HD23	1:G:179:LEU:HA	1.80	0.46
1:I:220:PHE:HB3	1:I:225:THR:OG1	2.15	0.46
1:J:21:ARG:NH1	1:J:225:THR:HG23	2.30	0.46
1:J:98:PHE:CE1	1:J:227:THR:HG23	2.50	0.46
1:M:99:ARG:HB2	1:M:101:LEU:HG	1.97	0.46
1:N:155:LYS:HA	1:N:174:TRP:NE1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLU:CD	1:B:153:GLU:H	2.21	0.46
1:C:212:THR:HA	1:C:221:ASP:O	2.15	0.46
1:C:274:HIS:O	1:C:284:ASP:N	2.44	0.46
1:F:314:ASP:O	1:F:318:SER:HB3	2.15	0.46
1:I:212:THR:HA	1:I:221:ASP:O	2.15	0.46
1:K:32:LEU:HB3	1:K:38:TYR:CE2	2.50	0.46
1:K:94:LEU:O	1:K:98:PHE:HD1	1.99	0.46
1:M:98:PHE:CE1	1:M:227:THR:HG23	2.50	0.46
1:M:192:GLN:OE1	1:M:200:THR:OG1	2.24	0.46
1:C:26:MET:HE3	1:C:244:LEU:HD23	1.96	0.46
1:D:99:ARG:NH1	1:D:118:ASP:HB2	2.30	0.46
1:E:38:TYR:CE2	1:E:42:ARG:HG3	2.50	0.46
1:E:218:PRO:HA	1:E:220:PHE:N	2.30	0.46
1:E:305:GLN:O	1:E:309:VAL:HG23	2.14	0.46
1:G:194:PRO:HD2	1:G:235:ASN:ND2	2.30	0.46
1:L:32:LEU:HB3	1:L:38:TYR:CE2	2.51	0.46
1:N:75:TRP:CG	1:N:81:ASN:HB2	2.50	0.46
1:B:238:HIS:O	1:B:254:ASP:HB3	2.15	0.46
1:C:109:PRO:HD2	1:C:287:MET:SD	2.55	0.46
1:F:90:GLN:HE22	1:F:223:GLY:C	2.23	0.46
1:L:189:GLY:HA3	1:L:205:ILE:HD13	1.97	0.46
1:M:274:HIS:O	1:M:284:ASP:N	2.44	0.46
1:N:230:ILE:O	1:N:233:TRP:N	2.46	0.46
1:N:274:HIS:O	1:N:284:ASP:N	2.46	0.46
1:C:21:ARG:NH1	1:C:225:THR:HG23	2.31	0.46
1:D:38:TYR:HD1	1:D:196:GLY:HA2	1.81	0.46
1:F:98:PHE:CE1	1:F:227:THR:HG23	2.51	0.46
1:F:274:HIS:O	1:F:284:ASP:N	2.47	0.46
1:G:212:THR:HA	1:G:221:ASP:O	2.16	0.46
1:I:179:LEU:HD23	1:I:179:LEU:HA	1.76	0.46
1:J:94:LEU:O	1:J:98:PHE:HD1	1.99	0.46
1:J:212:THR:HA	1:J:221:ASP:O	2.15	0.46
1:K:218:PRO:HA	1:K:220:PHE:N	2.28	0.46
1:M:157:ALA:HA	1:M:161:GLY:O	2.16	0.46
1:M:220:PHE:HB3	1:M:225:THR:OG1	2.15	0.46
1:C:134:GLN:OE1	1:E:180:LYS:NZ	2.48	0.46
1:E:21:ARG:NH1	1:E:225:THR:HG23	2.31	0.46
1:E:90:GLN:NE2	1:E:223:GLY:O	2.48	0.46
1:H:42:ARG:NH1	1:H:235:ASN:HD21	2.13	0.46
1:I:157:ALA:HA	1:I:161:GLY:O	2.16	0.46
1:I:300:MET:HE2	1:I:300:MET:HB2	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:PRO:HD2	1:J:287:MET:SD	2.56	0.46
1:N:65:VAL:HG21	1:N:321:LEU:HD22	1.98	0.46
1:B:90:GLN:NE2	1:B:223:GLY:O	2.46	0.46
1:D:212:THR:HA	1:D:221:ASP:O	2.15	0.46
1:D:238:HIS:O	1:D:254:ASP:HB3	2.16	0.46
1:J:179:LEU:HD23	1:J:179:LEU:HA	1.82	0.46
1:M:155:LYS:HA	1:M:174:TRP:NE1	2.31	0.46
1:M:314:ASP:O	1:M:318:SER:HB3	2.16	0.46
1:B:68:PRO:HB2	1:B:170:TYR:CD1	2.51	0.46
1:E:36:ALA:HA	1:E:39:VAL:HB	1.98	0.46
1:J:26:MET:HG3	1:J:242:ASP:OD1	2.16	0.46
1:J:305:GLN:O	1:J:309:VAL:HG23	2.14	0.46
1:L:155:LYS:HA	1:L:174:TRP:NE1	2.31	0.46
1:M:212:THR:HA	1:M:221:ASP:O	2.15	0.46
1:M:305:GLN:O	1:M:309:VAL:HG23	2.16	0.46
1:N:287:MET:CE	1:N:287:MET:H	2.28	0.46
1:A:194:PRO:HD2	1:A:235:ASN:ND2	2.31	0.46
1:A:305:GLN:O	1:A:309:VAL:HG23	2.15	0.46
1:C:287:MET:H	1:C:287:MET:CE	2.29	0.46
1:D:194:PRO:HD2	1:D:235:ASN:ND2	2.31	0.46
1:F:165:TRP:N	1:F:172:ASN:OD1	2.47	0.46
1:G:155:LYS:HA	1:G:174:TRP:NE1	2.31	0.46
1:H:75:TRP:HB2	1:H:77:GLU:O	2.16	0.46
1:K:270:PRO:HG2	1:K:286:PHE:CD2	2.50	0.46
1:K:274:HIS:O	1:K:284:ASP:N	2.47	0.46
1:L:99:ARG:HB2	1:L:101:LEU:HG	1.97	0.46
1:L:212:THR:HA	1:L:221:ASP:O	2.16	0.46
1:N:75:TRP:HB2	1:N:77:GLU:O	2.16	0.46
1:N:99:ARG:HB2	1:N:101:LEU:HG	1.97	0.46
1:C:75:TRP:HB2	1:C:77:GLU:O	2.15	0.46
1:C:192:GLN:OE1	1:C:200:THR:OG1	2.21	0.46
1:D:32:LEU:HB3	1:D:38:TYR:CE2	2.51	0.46
1:D:112:TRP:CD2	1:D:285:MET:HE2	2.51	0.46
1:E:249:PRO:O	1:E:252:ARG:HG3	2.16	0.46
1:F:75:TRP:CG	1:F:81:ASN:HB2	2.50	0.46
1:G:90:GLN:NE2	1:G:223:GLY:O	2.45	0.46
1:H:99:ARG:NH1	1:H:118:ASP:HB2	2.30	0.46
1:J:230:ILE:O	1:J:233:TRP:N	2.45	0.46
1:M:249:PRO:O	1:M:252:ARG:HG3	2.16	0.46
1:N:32:LEU:HB3	1:N:38:TYR:CE2	2.51	0.46
1:B:32:LEU:HB3	1:B:38:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:GLN:O	1:B:309:VAL:HG23	2.15	0.45
1:C:189:GLY:HA3	1:C:205:ILE:HD13	1.97	0.45
1:C:322:ALA:O	1:E:34:ARG:NH1	2.50	0.45
1:H:32:LEU:HB3	1:H:38:TYR:CE2	2.50	0.45
1:H:212:THR:HA	1:H:221:ASP:O	2.16	0.45
1:I:287:MET:H	1:I:287:MET:CE	2.29	0.45
1:J:300:MET:HE2	1:J:300:MET:HB2	1.87	0.45
1:L:249:PRO:O	1:L:252:ARG:HG3	2.16	0.45
1:M:75:TRP:CG	1:M:81:ASN:HB2	2.52	0.45
1:A:38:TYR:HD1	1:A:196:GLY:HA2	1.81	0.45
1:B:38:TYR:HD1	1:B:196:GLY:HA2	1.81	0.45
1:D:157:ALA:HA	1:D:161:GLY:O	2.17	0.45
1:F:109:PRO:HD2	1:F:287:MET:SD	2.56	0.45
1:F:212:THR:HA	1:F:221:ASP:O	2.17	0.45
1:G:309:VAL:O	1:G:313:LEU:HG	2.16	0.45
1:H:98:PHE:CE1	1:H:227:THR:HG23	2.52	0.45
1:I:274:HIS:O	1:I:284:ASP:N	2.45	0.45
1:N:165:TRP:N	1:N:172:ASN:OD1	2.46	0.45
1:A:90:GLN:NE2	1:A:223:GLY:O	2.50	0.45
1:A:99:ARG:HB2	1:A:101:LEU:HG	1.97	0.45
1:A:155:LYS:HA	1:A:174:TRP:NE1	2.31	0.45
1:A:238:HIS:O	1:A:254:ASP:HB3	2.17	0.45
1:B:309:VAL:HG12	1:B:313:LEU:HD21	1.98	0.45
1:D:90:GLN:HE22	1:D:223:GLY:C	2.25	0.45
1:F:99:ARG:HB2	1:F:101:LEU:HG	1.98	0.45
1:G:165:TRP:N	1:G:172:ASN:OD1	2.45	0.45
1:H:34:ARG:NH1	1:J:322:ALA:O	2.49	0.45
1:K:21:ARG:NH1	1:K:225:THR:HG23	2.31	0.45
1:K:75:TRP:HB2	1:K:77:GLU:O	2.16	0.45
1:L:86:GLN:O	1:L:89:SER:OG	2.33	0.45
1:M:218:PRO:HA	1:M:220:PHE:N	2.29	0.45
1:B:94:LEU:O	1:B:98:PHE:HD1	1.99	0.45
1:D:249:PRO:O	1:D:252:ARG:HG3	2.17	0.45
1:G:86:GLN:O	1:G:89:SER:OG	2.32	0.45
1:K:38:TYR:HD1	1:K:196:GLY:HA2	1.82	0.45
1:M:21:ARG:NH1	1:M:225:THR:HG23	2.31	0.45
1:A:220:PHE:HB3	1:A:225:THR:OG1	2.16	0.45
1:D:201:ASP:OD1	1:D:317:ARG:NH2	2.34	0.45
1:A:94:LEU:O	1:A:98:PHE:HD1	1.99	0.45
1:G:157:ALA:HA	1:G:161:GLY:O	2.17	0.45
1:H:270:PRO:HG2	1:H:286:PHE:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:PRO:HD2	1:K:235:ASN:ND2	2.32	0.45
1:N:26:MET:HE3	1:N:244:LEU:HD23	1.98	0.45
1:F:305:GLN:O	1:F:309:VAL:HG23	2.17	0.45
1:G:194:PRO:HA	1:G:317:ARG:NH2	2.32	0.45
1:I:68:PRO:HB2	1:I:170:TYR:CD1	2.52	0.45
1:J:309:VAL:HG12	1:J:313:LEU:HD21	1.99	0.45
1:L:109:PRO:HD2	1:L:287:MET:SD	2.56	0.45
1:M:68:PRO:HB2	1:M:170:TYR:CD1	2.51	0.45
1:B:21:ARG:NH1	1:B:225:THR:HG23	2.31	0.45
1:B:98:PHE:CE1	1:B:227:THR:HG23	2.52	0.45
1:B:220:PHE:HB3	1:B:225:THR:OG1	2.16	0.45
1:C:181:SER:OG	1:C:183:ILE:HG12	2.16	0.45
1:E:75:TRP:HB2	1:E:77:GLU:O	2.16	0.45
1:E:322:ALA:O	1:G:34:ARG:NH1	2.50	0.45
1:I:94:LEU:O	1:I:98:PHE:HD1	2.00	0.45
1:J:112:TRP:CD2	1:J:285:MET:HE2	2.51	0.45
1:J:189:GLY:HA3	1:J:205:ILE:HD13	1.99	0.45
1:J:220:PHE:HB3	1:J:225:THR:OG1	2.16	0.45
1:K:109:PRO:HD2	1:K:287:MET:SD	2.57	0.45
1:M:38:TYR:HD1	1:M:196:GLY:HA2	1.82	0.45
1:N:21:ARG:NH1	1:N:225:THR:HG23	2.32	0.45
1:N:38:TYR:HD1	1:N:196:GLY:HA2	1.80	0.45
1:B:199:GLU:H	1:B:199:GLU:HG3	1.57	0.45
1:C:194:PRO:HD2	1:C:235:ASN:ND2	2.32	0.45
1:C:220:PHE:HB3	1:C:225:THR:OG1	2.16	0.45
1:F:220:PHE:HB3	1:F:225:THR:OG1	2.17	0.45
1:G:220:PHE:HB3	1:G:225:THR:OG1	2.17	0.45
1:H:65:VAL:HG21	1:H:321:LEU:HD22	1.97	0.45
1:H:199:GLU:H	1:H:199:GLU:HG3	1.55	0.45
1:H:220:PHE:HB3	1:H:225:THR:OG1	2.16	0.45
1:H:238:HIS:O	1:H:254:ASP:HB3	2.17	0.45
1:K:189:GLY:HA3	1:K:205:ILE:HD13	1.98	0.45
1:K:230:ILE:O	1:K:233:TRP:N	2.48	0.45
1:L:26:MET:HE3	1:L:244:LEU:HD23	1.99	0.45
1:A:165:TRP:N	1:A:172:ASN:OD1	2.47	0.45
1:B:230:ILE:O	1:B:233:TRP:N	2.48	0.45
1:E:112:TRP:CD2	1:E:285:MET:HE2	2.52	0.45
1:F:36:ALA:HA	1:F:39:VAL:HB	1.99	0.45
1:G:189:GLY:HA3	1:G:205:ILE:HD13	1.99	0.45
1:G:199:GLU:H	1:G:199:GLU:HG3	1.56	0.45
1:H:194:PRO:HA	1:H:317:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:TRP:HB2	1:J:77:GLU:O	2.17	0.45
1:J:155:LYS:HA	1:J:174:TRP:NE1	2.31	0.45
1:K:75:TRP:CG	1:K:81:ASN:HB2	2.52	0.45
1:K:157:ALA:HA	1:K:161:GLY:O	2.17	0.45
1:L:230:ILE:O	1:L:233:TRP:N	2.48	0.45
1:C:90:GLN:NE2	1:C:223:GLY:O	2.50	0.44
1:F:189:GLY:HA3	1:F:205:ILE:HD13	1.99	0.44
1:G:109:PRO:HD2	1:G:287:MET:SD	2.57	0.44
1:J:42:ARG:NH1	1:J:235:ASN:HD21	2.15	0.44
1:N:249:PRO:O	1:N:252:ARG:HG3	2.16	0.44
1:C:300:MET:HE2	1:C:300:MET:HB2	1.89	0.44
1:F:21:ARG:HG3	1:F:188:LEU:HD12	1.99	0.44
1:F:270:PRO:HG2	1:F:286:PHE:CD2	2.53	0.44
1:J:68:PRO:HB2	1:J:170:TYR:CD1	2.52	0.44
1:K:212:THR:HA	1:K:221:ASP:O	2.18	0.44
1:L:157:ALA:HA	1:L:161:GLY:O	2.16	0.44
1:L:194:PRO:HA	1:L:317:ARG:NH2	2.32	0.44
1:M:90:GLN:NE2	1:M:223:GLY:O	2.50	0.44
1:N:98:PHE:CE1	1:N:227:THR:HG23	2.51	0.44
1:C:38:TYR:HD1	1:C:196:GLY:HA2	1.82	0.44
1:C:129:ASP:HB3	1:C:135:THR:HB	2.00	0.44
1:C:165:TRP:N	1:C:172:ASN:OD1	2.50	0.44
1:F:194:PRO:HD2	1:F:235:ASN:ND2	2.33	0.44
1:G:98:PHE:CE1	1:G:227:THR:HG23	2.53	0.44
1:J:274:HIS:O	1:J:284:ASP:N	2.46	0.44
1:L:36:ALA:HA	1:L:39:VAL:HB	1.99	0.44
1:M:199:GLU:H	1:M:199:GLU:HG3	1.58	0.44
1:N:212:THR:HA	1:N:221:ASP:O	2.17	0.44
1:D:305:GLN:O	1:D:309:VAL:HG23	2.16	0.44
1:J:38:TYR:CE2	1:J:42:ARG:HG3	2.52	0.44
1:N:36:ALA:HA	1:N:39:VAL:HB	2.00	0.44
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.80	0.44
1:D:269:CYS:HA	1:D:270:PRO:HD3	1.83	0.44
1:E:38:TYR:HD1	1:E:196:GLY:HA2	1.82	0.44
1:H:155:LYS:HA	1:H:174:TRP:NE1	2.33	0.44
1:K:249:PRO:O	1:K:252:ARG:HG3	2.18	0.44
1:K:300:MET:HE2	1:K:300:MET:HB2	1.85	0.44
1:M:26:MET:HE3	1:M:244:LEU:HD23	1.99	0.44
1:M:270:PRO:HG2	1:M:286:PHE:CB	2.48	0.44
1:D:181:SER:OG	1:D:183:ILE:HG12	2.18	0.44
1:D:220:PHE:HB3	1:D:225:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:SER:OG	1:F:183:ILE:HG12	2.17	0.44
1:I:165:TRP:O	1:I:172:ASN:ND2	2.46	0.44
1:I:249:PRO:O	1:I:252:ARG:HG3	2.17	0.44
1:J:157:ALA:HA	1:J:161:GLY:O	2.17	0.44
1:L:90:GLN:HE22	1:L:223:GLY:C	2.24	0.44
1:L:201:ASP:OD1	1:L:317:ARG:NH2	2.35	0.44
1:A:21:ARG:NH1	1:A:225:THR:HG23	2.32	0.44
1:A:157:ALA:HA	1:A:161:GLY:O	2.17	0.44
1:B:65:VAL:HG21	1:B:321:LEU:HD22	2.00	0.44
1:C:309:VAL:HG12	1:C:313:LEU:HD21	1.98	0.44
1:D:98:PHE:CE1	1:D:227:THR:HG23	2.52	0.44
1:F:157:ALA:HA	1:F:161:GLY:O	2.17	0.44
1:H:102:ASN:OD1	1:H:102:ASN:N	2.51	0.44
1:K:90:GLN:NE2	1:K:223:GLY:O	2.50	0.44
1:L:192:GLN:OE1	1:L:200:THR:OG1	2.21	0.44
1:N:220:PHE:HB3	1:N:225:THR:OG1	2.17	0.44
1:A:98:PHE:CE1	1:A:227:THR:HG23	2.53	0.44
1:D:65:VAL:HG21	1:D:321:LEU:HD22	1.99	0.44
1:D:75:TRP:HB2	1:D:77:GLU:O	2.17	0.44
1:E:102:ASN:OD1	1:E:102:ASN:N	2.51	0.44
1:H:30:HIS:ND1	1:H:30:HIS:C	2.76	0.44
1:K:220:PHE:HB3	1:K:225:THR:OG1	2.17	0.44
1:M:36:ALA:HA	1:M:39:VAL:HB	1.99	0.44
1:M:238:HIS:O	1:M:254:ASP:HB3	2.18	0.44
1:N:189:GLY:HA3	1:N:205:ILE:HD13	1.99	0.44
1:E:238:HIS:O	1:E:254:ASP:HB3	2.17	0.44
1:F:38:TYR:HD1	1:F:196:GLY:HA2	1.82	0.44
1:F:206:VAL:HG13	1:F:208:ALA:H	1.83	0.44
1:G:273:PRO:HB2	1:G:283:GLY:HA3	1.99	0.44
1:E:157:ALA:HA	1:E:161:GLY:O	2.17	0.43
1:E:212:THR:HA	1:E:221:ASP:O	2.17	0.43
1:F:21:ARG:NH1	1:F:225:THR:HG23	2.33	0.43
1:G:26:MET:HE3	1:G:244:LEU:HD23	2.00	0.43
1:C:249:PRO:O	1:C:252:ARG:HG3	2.18	0.43
1:D:84:ASP:OD1	1:D:140:ARG:NH2	2.40	0.43
1:D:189:GLY:HA3	1:D:205:ILE:HD13	2.00	0.43
1:E:220:PHE:HB3	1:E:225:THR:OG1	2.18	0.43
1:E:309:VAL:HG12	1:E:313:LEU:HD21	1.99	0.43
1:I:38:TYR:HD1	1:I:196:GLY:HA2	1.83	0.43
1:J:206:VAL:HG13	1:J:208:ALA:H	1.83	0.43
1:L:21:ARG:NH1	1:L:225:THR:HG23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:OD1	1:A:140:ARG:NH2	2.39	0.43
1:H:90:GLN:HE22	1:H:223:GLY:C	2.26	0.43
1:H:309:VAL:HG12	1:H:313:LEU:HD21	2.00	0.43
1:K:272:TYR:HA	1:K:273:PRO:HA	1.87	0.43
1:M:65:VAL:HG21	1:M:321:LEU:HD22	2.00	0.43
1:N:84:ASP:OD1	1:N:140:ARG:NH2	2.42	0.43
1:E:98:PHE:CE1	1:E:227:THR:HG23	2.53	0.43
1:I:65:VAL:HG21	1:I:321:LEU:HD22	2.00	0.43
1:I:269:CYS:HA	1:I:270:PRO:HD3	1.83	0.43
1:L:309:VAL:HG12	1:L:313:LEU:HD21	1.99	0.43
1:N:181:SER:OG	1:N:183:ILE:HG12	2.19	0.43
1:A:279:ASN:O	1:B:278:SER:HB2	2.19	0.43
1:B:34:ARG:NH2	1:D:323:ARG:C	2.76	0.43
1:B:270:PRO:HG2	1:B:286:PHE:CB	2.49	0.43
1:C:270:PRO:HG2	1:C:286:PHE:CB	2.48	0.43
1:E:108:VAL:CG2	1:E:300:MET:HG2	2.48	0.43
1:G:62:MET:C	1:I:246:PHE:HB3	2.44	0.43
1:I:86:GLN:O	1:I:89:SER:OG	2.36	0.43
1:K:68:PRO:HB2	1:K:170:TYR:CD1	2.53	0.43
1:A:46:GLU:HB3	1:B:50:LEU:HD21	2.00	0.43
1:B:112:TRP:CD2	1:B:285:MET:HE2	2.54	0.43
1:B:155:LYS:HA	1:B:174:TRP:NE1	2.33	0.43
1:D:109:PRO:HD2	1:D:287:MET:SD	2.58	0.43
1:F:102:ASN:N	1:F:102:ASN:OD1	2.51	0.43
1:G:129:ASP:HB3	1:G:135:THR:HB	2.01	0.43
1:G:249:PRO:O	1:G:252:ARG:HG3	2.18	0.43
1:I:109:PRO:HD2	1:I:287:MET:SD	2.59	0.43
1:I:249:PRO:HB2	1:I:263:ALA:CB	2.46	0.43
1:J:108:VAL:CG2	1:J:300:MET:HG2	2.49	0.43
1:J:165:TRP:N	1:J:172:ASN:OD1	2.45	0.43
1:K:224:ARG:HD2	1:K:289:TYR:CE1	2.40	0.43
1:M:112:TRP:CD2	1:M:285:MET:HE2	2.54	0.43
1:A:75:TRP:CG	1:A:81:ASN:HB2	2.53	0.43
1:B:90:GLN:HE22	1:B:223:GLY:C	2.27	0.43
1:C:305:GLN:O	1:C:309:VAL:HG23	2.17	0.43
1:D:21:ARG:HG3	1:D:188:LEU:HD12	2.01	0.43
1:D:270:PRO:HG2	1:D:286:PHE:CB	2.49	0.43
1:F:269:CYS:HA	1:F:270:PRO:HD3	1.82	0.43
1:H:179:LEU:HD23	1:H:179:LEU:HA	1.78	0.43
1:I:90:GLN:HE22	1:I:223:GLY:C	2.27	0.43
1:I:90:GLN:NE2	1:I:223:GLY:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:ASP:OD2	1:K:155:LYS:NZ	2.45	0.43
1:K:155:LYS:HA	1:K:174:TRP:NE1	2.33	0.43
1:L:165:TRP:N	1:L:172:ASN:OD1	2.49	0.43
1:M:75:TRP:HB2	1:M:77:GLU:O	2.19	0.43
1:N:300:MET:HE2	1:N:300:MET:HB2	1.84	0.43
1:A:192:GLN:OE1	1:A:200:THR:OG1	2.22	0.43
1:C:65:VAL:HG21	1:C:321:LEU:HD22	2.01	0.43
1:G:65:VAL:HG21	1:G:321:LEU:HD22	2.00	0.43
1:G:68:PRO:HB2	1:G:170:TYR:CD1	2.53	0.43
1:G:75:TRP:HB2	1:G:77:GLU:O	2.19	0.43
1:I:309:VAL:HG12	1:I:313:LEU:HD21	1.99	0.43
1:J:180:LYS:HB3	1:J:180:LYS:HE2	1.76	0.43
1:K:36:ALA:HA	1:K:39:VAL:HB	2.01	0.43
1:M:194:PRO:HD2	1:M:235:ASN:ND2	2.34	0.43
1:N:102:ASN:N	1:N:102:ASN:OD1	2.52	0.43
1:N:199:GLU:H	1:N:199:GLU:HG3	1.55	0.43
1:A:199:GLU:H	1:A:199:GLU:HG3	1.59	0.43
1:B:36:ALA:HA	1:B:39:VAL:HB	2.01	0.43
1:F:194:PRO:HA	1:F:317:ARG:NH2	2.34	0.43
1:H:21:ARG:NH1	1:H:225:THR:HG23	2.34	0.43
1:H:192:GLN:NE2	1:H:196:GLY:HA3	2.34	0.43
1:L:314:ASP:O	1:L:318:SER:HB3	2.18	0.43
1:N:68:PRO:HB2	1:N:170:TYR:CD1	2.54	0.43
1:B:165:TRP:N	1:B:172:ASN:OD1	2.49	0.43
1:D:102:ASN:OD1	1:D:102:ASN:N	2.52	0.43
1:E:270:PRO:HG2	1:E:286:PHE:CB	2.49	0.43
1:H:38:TYR:HD1	1:H:196:GLY:HA2	1.82	0.43
1:K:129:ASP:HB3	1:K:135:THR:HB	2.01	0.43
1:L:180:LYS:HB3	1:L:180:LYS:HE2	1.75	0.43
1:N:270:PRO:HG2	1:N:286:PHE:CB	2.49	0.43
1:A:112:TRP:CD2	1:A:285:MET:HE2	2.53	0.42
1:A:309:VAL:HG12	1:A:313:LEU:HD21	2.00	0.42
1:B:75:TRP:HB2	1:B:77:GLU:O	2.19	0.42
1:B:165:TRP:O	1:B:172:ASN:ND2	2.47	0.42
1:D:155:LYS:HA	1:D:174:TRP:NE1	2.34	0.42
1:D:274:HIS:O	1:D:284:ASP:N	2.47	0.42
1:A:26:MET:HE3	1:A:244:LEU:HD23	2.01	0.42
1:A:152:ASP:OD2	1:A:155:LYS:NZ	2.41	0.42
1:D:180:LYS:HE2	1:D:180:LYS:HB3	1.75	0.42
1:E:194:PRO:HD2	1:E:235:ASN:ND2	2.34	0.42
1:F:155:LYS:HA	1:F:174:TRP:NE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:TYR:HA	1:H:273:PRO:HA	1.88	0.42
1:I:194:PRO:HD2	1:I:235:ASN:ND2	2.35	0.42
1:K:95:ASN:O	1:K:101:LEU:HD12	2.19	0.42
1:M:108:VAL:CG2	1:M:300:MET:HG2	2.49	0.42
1:N:90:GLN:HE22	1:N:223:GLY:C	2.26	0.42
1:A:109:PRO:HD2	1:A:287:MET:SD	2.59	0.42
1:B:224:ARG:HD2	1:B:289:TYR:CE1	2.42	0.42
1:C:238:HIS:O	1:C:254:ASP:HB3	2.19	0.42
1:D:165:TRP:N	1:D:172:ASN:OD1	2.50	0.42
1:E:65:VAL:HG21	1:E:321:LEU:HD22	2.01	0.42
1:I:270:PRO:HG2	1:I:286:PHE:CB	2.49	0.42
1:D:108:VAL:CG2	1:D:300:MET:HG2	2.49	0.42
1:F:249:PRO:O	1:F:252:ARG:HG3	2.19	0.42
1:H:84:ASP:OD1	1:H:140:ARG:NH2	2.42	0.42
1:H:300:MET:HE2	1:H:300:MET:HB2	1.83	0.42
1:J:26:MET:HE3	1:J:244:LEU:HD23	2.01	0.42
1:J:90:GLN:HE22	1:J:223:GLY:C	2.27	0.42
1:J:238:HIS:O	1:J:254:ASP:HB3	2.20	0.42
1:L:38:TYR:HD1	1:L:196:GLY:HA2	1.83	0.42
1:L:102:ASN:OD1	1:L:102:ASN:N	2.52	0.42
1:A:36:ALA:HA	1:A:39:VAL:HB	2.00	0.42
1:A:194:PRO:HA	1:A:317:ARG:NH2	2.34	0.42
1:C:245:ARG:HD3	1:C:245:ARG:N	2.33	0.42
1:D:36:ALA:HA	1:D:39:VAL:HB	2.00	0.42
1:E:26:MET:HE3	1:E:244:LEU:HD23	2.01	0.42
1:E:165:TRP:N	1:E:172:ASN:OD1	2.46	0.42
1:F:68:PRO:HB2	1:F:170:TYR:CD1	2.54	0.42
1:G:21:ARG:NH1	1:G:225:THR:HG23	2.35	0.42
1:I:238:HIS:O	1:I:254:ASP:HB3	2.19	0.42
1:N:180:LYS:HB3	1:N:180:LYS:HE2	1.75	0.42
1:A:90:GLN:HE22	1:A:223:GLY:C	2.28	0.42
1:B:269:CYS:HA	1:B:270:PRO:HD3	1.83	0.42
1:C:157:ALA:HA	1:C:161:GLY:O	2.19	0.42
1:E:68:PRO:HB2	1:E:170:TYR:CD1	2.53	0.42
1:F:29:HIS:O	1:F:33:LEU:HG	2.19	0.42
1:F:222:LYS:HB3	1:F:224:ARG:HG2	2.01	0.42
1:J:201:ASP:OD1	1:J:317:ARG:NH2	2.33	0.42
1:K:165:TRP:O	1:K:172:ASN:ND2	2.47	0.42
1:L:270:PRO:HG2	1:L:286:PHE:CB	2.50	0.42
1:M:181:SER:OG	1:M:183:ILE:HG12	2.19	0.42
1:A:230:ILE:O	1:A:233:TRP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:C	1:C:34:ARG:HH22	2.28	0.42
1:C:68:PRO:HB2	1:C:170:TYR:CD1	2.54	0.42
1:G:238:HIS:O	1:G:254:ASP:HB3	2.20	0.42
1:H:112:TRP:CD2	1:H:285:MET:HE2	2.55	0.42
1:I:29:HIS:O	1:I:33:LEU:HG	2.20	0.42
1:I:206:VAL:HG13	1:I:208:ALA:H	1.84	0.42
1:J:249:PRO:O	1:J:252:ARG:HG3	2.20	0.42
1:K:108:VAL:CG2	1:K:300:MET:HG2	2.50	0.42
1:L:220:PHE:HB3	1:L:225:THR:OG1	2.19	0.42
1:L:305:GLN:O	1:L:309:VAL:HG23	2.19	0.42
1:A:68:PRO:HB2	1:A:170:TYR:CD1	2.54	0.42
1:A:165:TRP:O	1:A:172:ASN:ND2	2.47	0.42
1:C:102:ASN:OD1	1:C:102:ASN:N	2.52	0.42
1:D:26:MET:HE3	1:D:244:LEU:HD23	2.02	0.42
1:E:70:VAL:HG21	1:E:165:TRP:CE2	2.55	0.42
1:F:224:ARG:HD2	1:F:289:TYR:CE1	2.43	0.42
1:G:112:TRP:CD2	1:G:285:MET:HE2	2.54	0.42
1:I:36:ALA:HA	1:I:39:VAL:HB	2.01	0.42
1:K:238:HIS:O	1:K:254:ASP:HB3	2.19	0.42
1:M:129:ASP:HB3	1:M:135:THR:HB	2.00	0.42
1:N:201:ASP:OD1	1:N:317:ARG:NH2	2.37	0.42
1:A:245:ARG:N	1:A:245:ARG:HD3	2.35	0.42
1:B:129:ASP:HB3	1:B:135:THR:HB	2.02	0.42
1:F:179:LEU:HD23	1:F:179:LEU:HA	1.76	0.42
1:G:300:MET:HE2	1:G:300:MET:HB2	1.83	0.42
1:I:21:ARG:NH1	1:I:225:THR:HG23	2.35	0.42
1:J:36:ALA:HA	1:J:39:VAL:HB	2.01	0.42
1:J:70:VAL:HG21	1:J:165:TRP:CE2	2.55	0.42
1:J:129:ASP:HB3	1:J:135:THR:HB	2.01	0.42
1:K:26:MET:HE3	1:K:244:LEU:HD23	2.02	0.42
1:K:102:ASN:OD1	1:K:102:ASN:N	2.53	0.42
1:K:194:PRO:HA	1:K:317:ARG:NH2	2.35	0.42
1:N:129:ASP:HB3	1:N:135:THR:HB	2.02	0.42
1:N:222:LYS:HB3	1:N:224:ARG:HG2	2.02	0.42
1:A:274:HIS:O	1:A:284:ASP:N	2.46	0.42
1:C:36:ALA:HA	1:C:39:VAL:HB	2.02	0.42
1:E:62:MET:C	1:G:246:PHE:HB3	2.45	0.42
1:G:90:GLN:HE22	1:G:223:GLY:C	2.27	0.42
1:G:180:LYS:HE2	1:G:180:LYS:HB3	1.76	0.42
1:G:270:PRO:HG2	1:G:286:PHE:CB	2.50	0.42
1:J:194:PRO:HA	1:J:317:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:PRO:HG2	1:J:286:PHE:CB	2.50	0.42
1:K:309:VAL:HG12	1:K:313:LEU:HD21	2.01	0.42
1:N:112:TRP:CD2	1:N:285:MET:HE2	2.55	0.42
1:A:222:LYS:HB3	1:A:224:ARG:HG2	2.02	0.41
1:B:164:ALA:HB2	1:B:174:TRP:HZ2	1.84	0.41
1:D:21:ARG:NH1	1:D:225:THR:HG23	2.35	0.41
1:E:32:LEU:HD22	1:E:38:TYR:CE1	2.55	0.41
1:F:34:ARG:HH22	1:H:323:ARG:C	2.27	0.41
1:F:112:TRP:CD2	1:F:285:MET:HE2	2.55	0.41
1:F:300:MET:HE2	1:F:300:MET:HB2	1.82	0.41
1:I:194:PRO:HA	1:I:317:ARG:NH2	2.35	0.41
1:J:102:ASN:OD1	1:J:102:ASN:N	2.53	0.41
1:J:181:SER:OG	1:J:183:ILE:HG12	2.20	0.41
1:N:164:ALA:HB2	1:N:174:TRP:HZ2	1.84	0.41
1:A:108:VAL:HG12	1:A:109:PRO:O	2.21	0.41
1:A:129:ASP:HB3	1:A:135:THR:HB	2.02	0.41
1:B:109:PRO:HD2	1:B:287:MET:SD	2.60	0.41
1:C:155:LYS:HA	1:C:174:TRP:NE1	2.36	0.41
1:C:269:CYS:HA	1:C:270:PRO:HD3	1.84	0.41
1:F:230:ILE:O	1:F:233:TRP:N	2.51	0.41
1:G:30:HIS:HB2	1:G:244:LEU:CD1	2.50	0.41
1:G:108:VAL:HG12	1:G:109:PRO:O	2.20	0.41
1:J:32:LEU:HB3	1:J:38:TYR:CD2	2.56	0.41
1:L:245:ARG:HD3	1:L:245:ARG:N	2.36	0.41
1:A:50:LEU:HD11	1:A:54:GLN:OE1	2.21	0.41
1:A:206:VAL:HG13	1:A:208:ALA:H	1.86	0.41
1:I:129:ASP:HB3	1:I:135:THR:HB	2.03	0.41
1:I:165:TRP:N	1:I:172:ASN:OD1	2.49	0.41
1:L:129:ASP:HB3	1:L:135:THR:HB	2.01	0.41
1:L:273:PRO:HB2	1:L:283:GLY:HA3	2.03	0.41
1:B:108:VAL:HG12	1:B:109:PRO:O	2.20	0.41
1:C:70:VAL:HG21	1:C:165:TRP:CE2	2.56	0.41
1:H:36:ALA:HA	1:H:39:VAL:HB	2.02	0.41
1:H:109:PRO:HD2	1:H:287:MET:SD	2.60	0.41
1:K:70:VAL:HG21	1:K:165:TRP:CE2	2.56	0.41
1:L:65:VAL:HG21	1:L:321:LEU:HD22	2.02	0.41
1:N:108:VAL:CG2	1:N:300:MET:HG2	2.50	0.41
1:B:108:VAL:CG2	1:B:300:MET:HG2	2.51	0.41
1:B:249:PRO:HA	1:B:252:ARG:NE	2.35	0.41
1:G:50:LEU:HD21	1:H:46:GLU:HB3	2.02	0.41
1:H:108:VAL:CG2	1:H:300:MET:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:LYS:HB3	1:H:224:ARG:HG2	2.01	0.41
1:I:249:PRO:HA	1:I:252:ARG:NE	2.36	0.41
1:J:29:HIS:O	1:J:33:LEU:HG	2.21	0.41
1:J:165:TRP:O	1:J:172:ASN:ND2	2.44	0.41
1:K:65:VAL:HG21	1:K:321:LEU:HD22	2.02	0.41
1:M:279:ASN:C	1:N:278:SER:HB2	2.46	0.41
1:D:273:PRO:HB2	1:D:283:GLY:HA3	2.02	0.41
1:G:279:ASN:C	1:H:278:SER:HB2	2.46	0.41
1:H:129:ASP:HB3	1:H:135:THR:HB	2.03	0.41
1:H:194:PRO:HD2	1:H:235:ASN:ND2	2.35	0.41
1:J:38:TYR:HD1	1:J:196:GLY:HA2	1.83	0.41
1:A:270:PRO:HG2	1:A:286:PHE:CB	2.50	0.41
1:B:102:ASN:OD1	1:B:102:ASN:N	2.53	0.41
1:B:273:PRO:HB2	1:B:283:GLY:HA3	2.02	0.41
1:F:32:LEU:HB3	1:F:38:TYR:CD2	2.56	0.41
1:F:129:ASP:HB3	1:F:135:THR:HB	2.03	0.41
1:I:70:VAL:HG21	1:I:165:TRP:CE2	2.56	0.41
1:I:201:ASP:OD1	1:I:317:ARG:NH2	2.35	0.41
1:K:165:TRP:N	1:K:172:ASN:OD1	2.50	0.41
1:L:249:PRO:HA	1:L:252:ARG:NE	2.36	0.41
1:M:179:LEU:HA	1:M:179:LEU:HD23	1.79	0.41
1:N:249:PRO:HA	1:N:252:ARG:NE	2.36	0.41
1:A:181:SER:OG	1:A:183:ILE:HG12	2.20	0.41
1:D:129:ASP:HB3	1:D:135:THR:HB	2.02	0.41
1:D:313:LEU:HA	1:D:317:ARG:HB2	2.03	0.41
1:H:68:PRO:HB2	1:H:170:TYR:CD1	2.55	0.41
1:H:206:VAL:HG13	1:H:208:ALA:H	1.85	0.41
1:L:181:SER:OG	1:L:183:ILE:HG12	2.20	0.41
1:M:269:CYS:HA	1:M:270:PRO:HD3	1.84	0.41
1:N:273:PRO:HB2	1:N:283:GLY:HA3	2.03	0.41
1:A:65:VAL:HG21	1:A:321:LEU:HD22	2.02	0.41
1:A:86:GLN:O	1:A:89:SER:OG	2.39	0.41
1:A:278:SER:HB2	1:B:279:ASN:O	2.21	0.41
1:B:180:LYS:HB3	1:B:180:LYS:HE2	1.73	0.41
1:C:95:ASN:O	1:C:101:LEU:HD12	2.21	0.41
1:C:194:PRO:HG2	1:C:235:ASN:HB2	2.03	0.41
1:C:206:VAL:HG13	1:C:208:ALA:H	1.86	0.41
1:C:272:TYR:HA	1:C:273:PRO:HA	1.89	0.41
1:E:189:GLY:HA3	1:E:205:ILE:HD13	2.02	0.41
1:E:249:PRO:HB2	1:E:263:ALA:CB	2.48	0.41
1:F:86:GLN:O	1:F:89:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:LYS:HB3	1:F:180:LYS:HE2	1.76	0.41
1:F:227:THR:O	1:F:230:ILE:HB	2.21	0.41
1:F:270:PRO:HG2	1:F:286:PHE:CB	2.51	0.41
1:F:272:TYR:HA	1:F:286:PHE:HZ	1.86	0.41
1:G:36:ALA:HA	1:G:39:VAL:HB	2.02	0.41
1:G:102:ASN:N	1:G:102:ASN:OD1	2.53	0.41
1:G:165:TRP:O	1:G:172:ASN:ND2	2.49	0.41
1:H:26:MET:HE3	1:H:244:LEU:HD23	2.03	0.41
1:H:180:LYS:HB3	1:H:180:LYS:HE2	1.78	0.41
1:H:273:PRO:HB2	1:H:283:GLY:HA3	2.03	0.41
1:I:313:LEU:HA	1:I:317:ARG:HB2	2.03	0.41
1:L:222:LYS:HB3	1:L:224:ARG:HG2	2.03	0.41
1:M:29:HIS:O	1:M:33:LEU:HG	2.21	0.41
1:N:152:ASP:OD2	1:N:155:LYS:NZ	2.42	0.41
1:N:245:ARG:HD3	1:N:245:ARG:N	2.36	0.41
1:A:257:ASP:HB3	1:B:251:SER:HA	2.02	0.41
1:D:68:PRO:HB3	1:D:126:ALA:HB2	2.03	0.41
1:E:129:ASP:HB3	1:E:135:THR:HB	2.03	0.41
1:F:249:PRO:HB2	1:F:263:ALA:CB	2.46	0.41
1:I:180:LYS:HE2	1:I:180:LYS:HB3	1.74	0.41
1:I:222:LYS:HB3	1:I:224:ARG:HG2	2.03	0.41
1:M:50:LEU:HD21	1:N:46:GLU:HB3	2.01	0.41
1:A:95:ASN:O	1:A:101:LEU:HD12	2.21	0.40
1:C:29:HIS:O	1:C:33:LEU:HG	2.21	0.40
1:C:90:GLN:HE22	1:C:223:GLY:C	2.29	0.40
1:D:61:ARG:O	1:D:61:ARG:HG2	2.21	0.40
1:D:224:ARG:HD2	1:D:289:TYR:CE1	2.44	0.40
1:E:86:GLN:O	1:E:89:SER:OG	2.39	0.40
1:H:29:HIS:O	1:H:33:LEU:HG	2.20	0.40
1:H:76:ASN:HB3	1:H:80:GLU:OE2	2.21	0.40
1:H:230:ILE:O	1:H:233:TRP:N	2.51	0.40
1:J:32:LEU:HD22	1:J:38:TYR:CE1	2.56	0.40
1:K:29:HIS:O	1:K:33:LEU:HG	2.22	0.40
1:L:194:PRO:HD2	1:L:235:ASN:HD22	1.87	0.40
1:M:165:TRP:O	1:M:172:ASN:ND2	2.48	0.40
1:N:194:PRO:HA	1:N:317:ARG:NH2	2.36	0.40
1:B:181:SER:OG	1:B:183:ILE:HG12	2.22	0.40
1:E:30:HIS:HB2	1:E:244:LEU:CD1	2.51	0.40
1:F:26:MET:HE3	1:F:244:LEU:HD23	2.02	0.40
1:F:108:VAL:CG2	1:F:300:MET:HG2	2.50	0.40
1:G:269:CYS:HA	1:G:270:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:SER:OG	1:K:183:ILE:HG12	2.20	0.40
1:K:313:LEU:HA	1:K:317:ARG:HB2	2.03	0.40
1:M:21:ARG:HG3	1:M:188:LEU:HD12	2.02	0.40
1:M:102:ASN:N	1:M:102:ASN:OD1	2.52	0.40
1:A:300:MET:HB2	1:A:300:MET:HE2	1.84	0.40
1:B:246:PHE:HB2	1:D:64:ILE:HG22	2.03	0.40
1:B:272:TYR:HA	1:B:273:PRO:HA	1.88	0.40
1:C:32:LEU:HB3	1:C:38:TYR:CD2	2.56	0.40
1:C:222:LYS:HB3	1:C:224:ARG:HG2	2.03	0.40
1:D:35:SER:C	1:D:37:SER:N	2.80	0.40
1:J:249:PRO:HB2	1:J:263:ALA:CB	2.48	0.40
1:K:64:ILE:HG22	1:M:246:PHE:HB2	2.03	0.40
1:K:270:PRO:HG2	1:K:286:PHE:CB	2.51	0.40
1:M:109:PRO:HD2	1:M:287:MET:SD	2.62	0.40
1:N:164:ALA:HB2	1:N:174:TRP:CZ2	2.57	0.40
1:A:70:VAL:HG21	1:A:165:TRP:CE2	2.57	0.40
1:A:249:PRO:O	1:A:252:ARG:HG3	2.21	0.40
1:A:322:ALA:O	1:C:34:ARG:NH1	2.54	0.40
1:C:180:LYS:HE2	1:C:180:LYS:HB3	1.77	0.40
1:E:95:ASN:O	1:E:101:LEU:HD12	2.21	0.40
1:F:313:LEU:HA	1:F:317:ARG:HB2	2.04	0.40
1:H:313:LEU:HA	1:H:317:ARG:HB2	2.04	0.40
1:I:32:LEU:HB3	1:I:38:TYR:CD2	2.57	0.40
1:J:164:ALA:HB2	1:J:174:TRP:HZ2	1.86	0.40
1:J:245:ARG:N	1:J:245:ARG:HD3	2.37	0.40
1:M:249:PRO:HA	1:M:252:ARG:NE	2.35	0.40
1:B:26:MET:HE3	1:B:244:LEU:HD23	2.04	0.40
1:D:300:MET:HB2	1:D:300:MET:HE2	1.86	0.40
1:E:32:LEU:HB3	1:E:38:TYR:CD2	2.56	0.40
1:E:165:TRP:O	1:E:172:ASN:ND2	2.49	0.40
1:F:245:ARG:HD3	1:F:245:ARG:N	2.36	0.40
1:F:273:PRO:HB2	1:F:283:GLY:HA3	2.03	0.40
1:G:127:THR:HG22	1:G:134:GLN:HG3	2.04	0.40
1:K:179:LEU:HD23	1:K:179:LEU:HA	1.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:OG	1:B:113:SER:OG[4_566]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/360 (84%)	286 (94%)	18 (6%)	0	100	100
1	B	304/360 (84%)	287 (94%)	17 (6%)	0	100	100
1	C	304/360 (84%)	289 (95%)	15 (5%)	0	100	100
1	D	304/360 (84%)	289 (95%)	15 (5%)	0	100	100
1	E	304/360 (84%)	286 (94%)	18 (6%)	0	100	100
1	F	304/360 (84%)	287 (94%)	17 (6%)	0	100	100
1	G	304/360 (84%)	288 (95%)	16 (5%)	0	100	100
1	H	304/360 (84%)	287 (94%)	17 (6%)	0	100	100
1	I	304/360 (84%)	287 (94%)	17 (6%)	0	100	100
1	J	304/360 (84%)	289 (95%)	15 (5%)	0	100	100
1	K	304/360 (84%)	288 (95%)	16 (5%)	0	100	100
1	L	304/360 (84%)	288 (95%)	16 (5%)	0	100	100
1	M	304/360 (84%)	288 (95%)	16 (5%)	0	100	100
1	N	304/360 (84%)	287 (94%)	17 (6%)	0	100	100
All	All	4256/5040 (84%)	4026 (95%)	230 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	262/310 (84%)	230 (88%)	32 (12%)	5	18
1	B	262/310 (84%)	229 (87%)	33 (13%)	4	17
1	C	262/310 (84%)	229 (87%)	33 (13%)	4	17
1	D	262/310 (84%)	231 (88%)	31 (12%)	5	19
1	E	262/310 (84%)	228 (87%)	34 (13%)	4	16
1	F	262/310 (84%)	230 (88%)	32 (12%)	5	18
1	G	262/310 (84%)	229 (87%)	33 (13%)	4	17
1	H	262/310 (84%)	226 (86%)	36 (14%)	3	15
1	I	262/310 (84%)	231 (88%)	31 (12%)	5	19
1	J	262/310 (84%)	231 (88%)	31 (12%)	5	19
1	K	262/310 (84%)	229 (87%)	33 (13%)	4	17
1	L	262/310 (84%)	230 (88%)	32 (12%)	5	18
1	M	262/310 (84%)	230 (88%)	32 (12%)	5	18
1	N	262/310 (84%)	229 (87%)	33 (13%)	4	17
All	All	3668/4340 (84%)	3212 (88%)	456 (12%)	4	18

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	37	SER
1	A	54	GLN
1	A	59	ILE
1	A	61	ARG
1	A	63	GLU
1	A	64	ILE
1	A	69	VAL
1	A	78	GLU
1	A	93	ILE
1	A	105	VAL
1	A	106	SER
1	A	123	PHE
1	A	125	LEU
1	A	128	LYS
1	A	141	THR
1	A	145	VAL
1	A	149	THR
1	A	150	THR

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Mol	Chain	Res	Type
1	A	153	GLU
1	A	156	PHE
1	A	192	GLN
1	A	220	PHE
1	A	239	ILE
1	A	247	GLU
1	A	248	ASP
1	A	252	ARG
1	A	259	THR
1	A	267	PHE
1	A	286	PHE
1	A	287	MET
1	A	299	VAL
1	B	37	SER
1	B	54	GLN
1	B	59	ILE
1	B	61	ARG
1	B	63	GLU
1	B	64	ILE
1	B	69	VAL
1	B	72	HIS
1	B	78	GLU
1	B	93	ILE
1	B	105	VAL
1	B	106	SER
1	B	123	PHE
1	B	125	LEU
1	B	128	LYS
1	B	141	THR
1	B	145	VAL
1	B	149	THR
1	B	150	THR
1	B	153	GLU
1	B	156	PHE
1	B	169	ARG
1	B	192	GLN
1	B	220	PHE
1	B	239	ILE
1	B	247	GLU
1	B	248	ASP
1	B	252	ARG
1	B	259	THR

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Mol	Chain	Res	Type
1	B	267	PHE
1	B	286	PHE
1	B	287	MET
1	B	299	VAL
1	C	37	SER
1	C	54	GLN
1	C	59	ILE
1	C	61	ARG
1	C	63	GLU
1	C	64	ILE
1	C	69	VAL
1	C	72	HIS
1	C	78	GLU
1	C	93	ILE
1	C	105	VAL
1	C	106	SER
1	C	123	PHE
1	C	125	LEU
1	C	128	LYS
1	C	141	THR
1	C	145	VAL
1	C	149	THR
1	C	150	THR
1	C	153	GLU
1	C	156	PHE
1	C	169	ARG
1	C	192	GLN
1	C	220	PHE
1	C	239	ILE
1	C	247	GLU
1	C	248	ASP
1	C	252	ARG
1	C	259	THR
1	C	267	PHE
1	C	286	PHE
1	C	287	MET
1	C	299	VAL
1	D	37	SER
1	D	54	GLN
1	D	59	ILE
1	D	61	ARG
1	D	63	GLU

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Mol	Chain	Res	Type
1	D	64	ILE
1	D	69	VAL
1	D	72	HIS
1	D	93	ILE
1	D	105	VAL
1	D	106	SER
1	D	123	PHE
1	D	125	LEU
1	D	128	LYS
1	D	141	THR
1	D	145	VAL
1	D	149	THR
1	D	150	THR
1	D	153	GLU
1	D	156	PHE
1	D	192	GLN
1	D	220	PHE
1	D	239	ILE
1	D	247	GLU
1	D	248	ASP
1	D	252	ARG
1	D	259	THR
1	D	267	PHE
1	D	286	PHE
1	D	287	MET
1	D	299	VAL
1	E	30	HIS
1	E	37	SER
1	E	54	GLN
1	E	59	ILE
1	E	61	ARG
1	E	63	GLU
1	E	64	ILE
1	E	69	VAL
1	E	78	GLU
1	E	93	ILE
1	E	105	VAL
1	E	106	SER
1	E	123	PHE
1	E	125	LEU
1	E	128	LYS
1	E	141	THR

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Mol	Chain	Res	Type
1	E	145	VAL
1	E	149	THR
1	E	150	THR
1	E	153	GLU
1	E	156	PHE
1	E	169	ARG
1	E	192	GLN
1	E	212	THR
1	E	220	PHE
1	E	239	ILE
1	E	247	GLU
1	E	248	ASP
1	E	252	ARG
1	E	259	THR
1	E	267	PHE
1	E	286	PHE
1	E	287	MET
1	E	299	VAL
1	F	37	SER
1	F	54	GLN
1	F	59	ILE
1	F	61	ARG
1	F	63	GLU
1	F	64	ILE
1	F	69	VAL
1	F	78	GLU
1	F	93	ILE
1	F	105	VAL
1	F	106	SER
1	F	123	PHE
1	F	125	LEU
1	F	128	LYS
1	F	141	THR
1	F	145	VAL
1	F	149	THR
1	F	150	THR
1	F	153	GLU
1	F	156	PHE
1	F	169	ARG
1	F	192	GLN
1	F	220	PHE
1	F	239	ILE

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Mol	Chain	Res	Type
1	F	247	GLU
1	F	248	ASP
1	F	252	ARG
1	F	259	THR
1	F	267	PHE
1	F	286	PHE
1	F	287	MET
1	F	299	VAL
1	G	37	SER
1	G	54	GLN
1	G	59	ILE
1	G	61	ARG
1	G	63	GLU
1	G	64	ILE
1	G	69	VAL
1	G	72	HIS
1	G	78	GLU
1	G	93	ILE
1	G	105	VAL
1	G	106	SER
1	G	123	PHE
1	G	125	LEU
1	G	128	LYS
1	G	141	THR
1	G	145	VAL
1	G	149	THR
1	G	150	THR
1	G	153	GLU
1	G	156	PHE
1	G	169	ARG
1	G	192	GLN
1	G	220	PHE
1	G	239	ILE
1	G	247	GLU
1	G	248	ASP
1	G	252	ARG
1	G	259	THR
1	G	267	PHE
1	G	286	PHE
1	G	287	MET
1	G	299	VAL
1	H	30	HIS

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Mol	Chain	Res	Type
1	H	37	SER
1	H	54	GLN
1	H	59	ILE
1	H	61	ARG
1	H	63	GLU
1	H	64	ILE
1	H	69	VAL
1	H	70	VAL
1	H	72	HIS
1	H	78	GLU
1	H	93	ILE
1	H	105	VAL
1	H	106	SER
1	H	123	PHE
1	H	125	LEU
1	H	128	LYS
1	H	141	THR
1	H	145	VAL
1	H	149	THR
1	H	150	THR
1	H	153	GLU
1	H	156	PHE
1	H	169	ARG
1	H	192	GLN
1	H	212	THR
1	H	220	PHE
1	H	239	ILE
1	H	247	GLU
1	H	248	ASP
1	H	252	ARG
1	H	259	THR
1	H	267	PHE
1	H	286	PHE
1	H	287	MET
1	H	299	VAL
1	I	37	SER
1	I	54	GLN
1	I	59	ILE
1	I	61	ARG
1	I	63	GLU
1	I	64	ILE
1	I	69	VAL

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Mol	Chain	Res	Type
1	I	78	GLU
1	I	93	ILE
1	I	105	VAL
1	I	106	SER
1	I	123	PHE
1	I	125	LEU
1	I	128	LYS
1	I	141	THR
1	I	145	VAL
1	I	149	THR
1	I	150	THR
1	I	153	GLU
1	I	156	PHE
1	I	169	ARG
1	I	192	GLN
1	I	220	PHE
1	I	239	ILE
1	I	247	GLU
1	I	248	ASP
1	I	252	ARG
1	I	267	PHE
1	I	286	PHE
1	I	287	MET
1	I	299	VAL
1	J	37	SER
1	J	54	GLN
1	J	59	ILE
1	J	61	ARG
1	J	63	GLU
1	J	64	ILE
1	J	69	VAL
1	J	93	ILE
1	J	105	VAL
1	J	106	SER
1	J	123	PHE
1	J	125	LEU
1	J	128	LYS
1	J	141	THR
1	J	145	VAL
1	J	149	THR
1	J	150	THR
1	J	153	GLU

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Mol	Chain	Res	Type
1	J	156	PHE
1	J	169	ARG
1	J	192	GLN
1	J	220	PHE
1	J	239	ILE
1	J	247	GLU
1	J	248	ASP
1	J	252	ARG
1	J	259	THR
1	J	267	PHE
1	J	286	PHE
1	J	287	MET
1	J	299	VAL
1	K	30	HIS
1	K	37	SER
1	K	54	GLN
1	K	59	ILE
1	K	61	ARG
1	K	63	GLU
1	K	64	ILE
1	K	69	VAL
1	K	78	GLU
1	K	93	ILE
1	K	105	VAL
1	K	106	SER
1	K	123	PHE
1	K	125	LEU
1	K	128	LYS
1	K	141	THR
1	K	145	VAL
1	K	149	THR
1	K	150	THR
1	K	153	GLU
1	K	156	PHE
1	K	169	ARG
1	K	192	GLN
1	K	220	PHE
1	K	239	ILE
1	K	247	GLU
1	K	248	ASP
1	K	252	ARG
1	K	259	THR

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Mol	Chain	Res	Type
1	K	267	PHE
1	K	286	PHE
1	K	287	MET
1	K	299	VAL
1	L	37	SER
1	L	54	GLN
1	L	59	ILE
1	L	61	ARG
1	L	63	GLU
1	L	64	ILE
1	L	69	VAL
1	L	78	GLU
1	L	93	ILE
1	L	105	VAL
1	L	106	SER
1	L	123	PHE
1	L	125	LEU
1	L	128	LYS
1	L	141	THR
1	L	145	VAL
1	L	149	THR
1	L	150	THR
1	L	153	GLU
1	L	156	PHE
1	L	169	ARG
1	L	192	GLN
1	L	220	PHE
1	L	239	ILE
1	L	247	GLU
1	L	248	ASP
1	L	252	ARG
1	L	259	THR
1	L	267	PHE
1	L	286	PHE
1	L	287	MET
1	L	299	VAL
1	M	37	SER
1	M	54	GLN
1	M	59	ILE
1	M	61	ARG
1	M	63	GLU
1	M	64	ILE

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Mol	Chain	Res	Type
1	M	69	VAL
1	M	78	GLU
1	M	93	ILE
1	M	105	VAL
1	M	106	SER
1	M	123	PHE
1	M	125	LEU
1	M	128	LYS
1	M	141	THR
1	M	145	VAL
1	M	149	THR
1	M	150	THR
1	M	153	GLU
1	M	156	PHE
1	M	169	ARG
1	M	192	GLN
1	M	220	PHE
1	M	239	ILE
1	M	247	GLU
1	M	248	ASP
1	M	252	ARG
1	M	259	THR
1	M	267	PHE
1	M	286	PHE
1	M	287	MET
1	M	299	VAL
1	N	37	SER
1	N	54	GLN
1	N	59	ILE
1	N	61	ARG
1	N	63	GLU
1	N	64	ILE
1	N	69	VAL
1	N	72	HIS
1	N	78	GLU
1	N	93	ILE
1	N	105	VAL
1	N	106	SER
1	N	123	PHE
1	N	125	LEU
1	N	128	LYS
1	N	141	THR

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Mol	Chain	Res	Type
1	N	145	VAL
1	N	149	THR
1	N	150	THR
1	N	153	GLU
1	N	156	PHE
1	N	169	ARG
1	N	192	GLN
1	N	220	PHE
1	N	239	ILE
1	N	247	GLU
1	N	248	ASP
1	N	252	ARG
1	N	259	THR
1	N	267	PHE
1	N	286	PHE
1	N	287	MET
1	N	299	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	88	GLN
1	A	235	ASN
1	B	29	HIS
1	B	72	HIS
1	B	134	GLN
1	B	235	ASN
1	C	72	HIS
1	C	88	GLN
1	C	235	ASN
1	D	72	HIS
1	D	235	ASN
1	E	72	HIS
1	E	235	ASN
1	F	72	HIS
1	F	88	GLN
1	F	235	ASN
1	G	72	HIS
1	G	88	GLN
1	G	235	ASN
1	H	72	HIS

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Mol	Chain	Res	Type
1	H	88	GLN
1	H	235	ASN
1	I	72	HIS
1	I	88	GLN
1	I	235	ASN
1	J	72	HIS
1	J	235	ASN
1	K	72	HIS
1	K	88	GLN
1	K	235	ASN
1	L	72	HIS
1	L	88	GLN
1	L	235	ASN
1	M	72	HIS
1	M	134	GLN
1	M	235	ASN
1	N	72	HIS
1	N	76	ASN
1	N	88	GLN
1	N	235	ASN

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 ⓘ

Of 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	306/360 (85%)	1.49	84 (27%) 1 5	164, 186, 210, 221	0
1	B	306/360 (85%)	1.45	77 (25%) 1 5	151, 170, 187, 204	0
1	C	306/360 (85%)	1.46	78 (25%) 1 5	159, 184, 207, 220	0
1	D	306/360 (85%)	1.49	83 (27%) 1 5	147, 169, 191, 214	0
1	E	306/360 (85%)	1.56	94 (30%) 1 4	145, 166, 188, 221	0
1	F	306/360 (85%)	1.64	93 (30%) 1 4	143, 166, 187, 209	0
1	G	306/360 (85%)	1.72	103 (33%) 1 4	143, 160, 180, 200	0
1	H	306/360 (85%)	1.58	88 (28%) 1 4	120, 149, 164, 190	0
1	I	306/360 (85%)	1.58	90 (29%) 1 4	142, 172, 199, 219	0
1	J	306/360 (85%)	1.47	83 (27%) 1 5	137, 160, 184, 198	0
1	K	306/360 (85%)	1.45	81 (26%) 1 5	159, 186, 211, 228	0
1	L	306/360 (85%)	1.38	73 (23%) 2 5	144, 168, 193, 208	0
1	M	306/360 (85%)	1.58	86 (28%) 1 4	160, 180, 200, 220	0
1	N	306/360 (85%)	1.47	78 (25%) 1 5	141, 163, 182, 193	0
All	All	4284/5040 (85%)	1.52	1191 (27%) 1 5	120, 170, 200, 228	0

All (1191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	21	ARG	8.6
1	F	188	LEU	8.3
1	G	210	PHE	8.2
1	M	112	TRP	8.2
1	I	210	PHE	7.9
1	H	21	ARG	7.9
1	K	210	PHE	7.7
1	B	21	ARG	7.4

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Mol	Chain	Res	Type	RSRZ
1	M	111	VAL	7.3
1	F	189	GLY	7.3
1	A	210	PHE	7.3
1	D	272	TYR	7.2
1	F	237	TYR	7.1
1	B	210	PHE	6.9
1	A	188	LEU	6.8
1	N	188	LEU	6.8
1	I	112	TRP	6.6
1	J	237	TYR	6.6
1	N	285	MET	6.4
1	M	18	PRO	6.4
1	M	113	SER	6.3
1	D	261	ASN	6.3
1	F	261	ASN	6.2
1	N	112	TRP	6.2
1	L	210	PHE	6.2
1	J	234	LEU	6.2
1	F	210	PHE	6.1
1	D	54	GLN	6.1
1	G	237	TYR	6.1
1	H	190	TYR	6.0
1	B	188	LEU	5.8
1	I	255	GLU	5.8
1	G	87	ILE	5.8
1	A	285	MET	5.8
1	E	112	TRP	5.7
1	L	237	TYR	5.7
1	J	210	PHE	5.7
1	G	234	LEU	5.7
1	I	287	MET	5.7
1	I	237	TYR	5.6
1	F	321	LEU	5.6
1	D	210	PHE	5.6
1	G	225	THR	5.6
1	C	237	TYR	5.6
1	H	220	PHE	5.5
1	I	188	LEU	5.5
1	J	21	ARG	5.5
1	C	261	ASN	5.5
1	E	111	VAL	5.4
1	M	234	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	234	LEU	5.3
1	E	261	ASN	5.3
1	E	301	PHE	5.3
1	L	301	PHE	5.3
1	H	261	ASN	5.3
1	N	114	ASN	5.3
1	A	234	LEU	5.3
1	M	301	PHE	5.3
1	K	234	LEU	5.2
1	I	21	ARG	5.2
1	H	237	TYR	5.2
1	C	210	PHE	5.2
1	K	112	TRP	5.2
1	M	237	TYR	5.2
1	E	281	PRO	5.1
1	D	188	LEU	5.1
1	N	210	PHE	5.1
1	F	308	ARG	5.1
1	H	188	LEU	5.1
1	G	308	ARG	5.1
1	B	112	TRP	5.1
1	C	18	PRO	5.1
1	J	272	TYR	5.1
1	L	308	ARG	5.1
1	H	167	ALA	5.0
1	F	54	GLN	5.0
1	I	108	VAL	5.0
1	C	195	GLY	5.0
1	K	237	TYR	5.0
1	E	18	PRO	5.0
1	G	18	PRO	4.9
1	E	54	GLN	4.9
1	G	193	PHE	4.9
1	M	258	ASP	4.9
1	C	308	ARG	4.9
1	H	112	TRP	4.9
1	A	112	TRP	4.9
1	L	188	LEU	4.9
1	E	239	ILE	4.9
1	N	267	PHE	4.8
1	I	87	ILE	4.8
1	A	167	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	M	114	ASN	4.8
1	J	111	VAL	4.8
1	A	18	PRO	4.8
1	M	305	GLN	4.8
1	J	136	THR	4.8
1	A	235	ASN	4.7
1	D	18	PRO	4.7
1	A	305	GLN	4.7
1	G	112	TRP	4.7
1	M	239	ILE	4.7
1	K	245	ARG	4.7
1	H	210	PHE	4.7
1	B	54	GLN	4.6
1	D	119	LEU	4.6
1	K	179	LEU	4.6
1	B	123	PHE	4.6
1	I	261	ASN	4.6
1	C	234	LEU	4.6
1	G	191	ALA	4.6
1	B	111	VAL	4.6
1	G	188	LEU	4.6
1	H	308	ARG	4.6
1	H	191	ALA	4.6
1	E	210	PHE	4.5
1	L	112	TRP	4.5
1	B	199	GLU	4.5
1	F	69	VAL	4.5
1	B	291	ASP	4.5
1	E	169	ARG	4.5
1	H	234	LEU	4.5
1	M	291	ASP	4.5
1	N	21	ARG	4.5
1	G	285	MET	4.5
1	F	220	PHE	4.5
1	I	305	GLN	4.5
1	N	59	ILE	4.5
1	F	285	MET	4.4
1	L	234	LEU	4.4
1	J	271	SER	4.4
1	F	258	ASP	4.4
1	I	234	LEU	4.4
1	E	308	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	282	ASN	4.4
1	D	185	GLN	4.4
1	F	60	SER	4.4
1	M	66	LYS	4.4
1	B	108	VAL	4.4
1	L	98	PHE	4.4
1	E	305	GLN	4.4
1	H	291	ASP	4.3
1	D	136	THR	4.3
1	A	237	TYR	4.3
1	F	234	LEU	4.3
1	E	258	ASP	4.3
1	G	221	ASP	4.3
1	C	98	PHE	4.3
1	D	234	LEU	4.3
1	C	112	TRP	4.3
1	A	98	PHE	4.3
1	G	286	PHE	4.3
1	K	94	LEU	4.3
1	L	179	LEU	4.3
1	J	281	PRO	4.2
1	B	179	LEU	4.2
1	G	220	PHE	4.2
1	M	136	THR	4.2
1	L	119	LEU	4.2
1	M	59	ILE	4.2
1	C	301	PHE	4.2
1	B	103	SER	4.2
1	C	103	SER	4.2
1	I	107	GLN	4.2
1	B	234	LEU	4.2
1	M	222	LYS	4.2
1	M	272	TYR	4.2
1	D	258	ASP	4.1
1	I	189	GLY	4.1
1	A	103	SER	4.1
1	H	123	PHE	4.1
1	A	281	PRO	4.1
1	G	222	LYS	4.1
1	J	305	GLN	4.1
1	D	190	TYR	4.1
1	H	193	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	123	PHE	4.1
1	C	272	TYR	4.1
1	F	199	GLU	4.1
1	D	179	LEU	4.1
1	M	103	SER	4.1
1	G	272	TYR	4.1
1	H	312	CYS	4.1
1	E	103	SER	4.1
1	C	316	PRO	4.0
1	K	272	TYR	4.0
1	C	138	ILE	4.0
1	F	191	ALA	4.0
1	C	281	PRO	4.0
1	I	199	GLU	4.0
1	K	123	PHE	4.0
1	A	255	GLU	4.0
1	G	108	VAL	4.0
1	F	301	PHE	4.0
1	M	285	MET	4.0
1	N	234	LEU	4.0
1	L	305	GLN	4.0
1	K	103	SER	4.0
1	C	188	LEU	3.9
1	M	188	LEU	3.9
1	B	56	PHE	3.9
1	N	305	GLN	3.9
1	E	198	ALA	3.9
1	H	18	PRO	3.9
1	C	59	ILE	3.9
1	J	301	PHE	3.9
1	F	59	ILE	3.9
1	D	112	TRP	3.9
1	J	112	TRP	3.9
1	F	187	ILE	3.9
1	F	245	ARG	3.9
1	A	108	VAL	3.9
1	F	225	THR	3.8
1	K	59	ILE	3.8
1	G	190	TYR	3.8
1	M	245	ARG	3.8
1	M	60	SER	3.8
1	J	18	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	321	LEU	3.8
1	F	61	ARG	3.8
1	F	119	LEU	3.8
1	D	98	PHE	3.8
1	L	103	SER	3.8
1	N	146	THR	3.8
1	N	82	ILE	3.8
1	G	74	VAL	3.8
1	B	18	PRO	3.8
1	H	199	GLU	3.8
1	E	288	ASN	3.8
1	H	103	SER	3.8
1	D	285	MET	3.8
1	F	286	PHE	3.8
1	J	123	PHE	3.8
1	C	255	GLU	3.8
1	M	288	ASN	3.8
1	I	54	GLN	3.8
1	D	237	TYR	3.8
1	K	258	ASP	3.8
1	M	115	LEU	3.8
1	E	123	PHE	3.7
1	H	204	VAL	3.7
1	I	69	VAL	3.7
1	A	198	ALA	3.7
1	N	27	GLU	3.7
1	F	137	GLY	3.7
1	M	210	PHE	3.7
1	E	285	MET	3.7
1	G	287	MET	3.7
1	D	103	SER	3.7
1	E	119	LEU	3.7
1	M	119	LEU	3.7
1	M	236	LEU	3.7
1	G	69	VAL	3.7
1	J	119	LEU	3.7
1	J	308	ARG	3.7
1	G	67	ILE	3.7
1	B	113	SER	3.7
1	I	123	PHE	3.7
1	I	285	MET	3.7
1	M	90	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	245	ARG	3.7
1	F	272	TYR	3.7
1	J	24	GLY	3.6
1	G	167	ALA	3.6
1	D	308	ARG	3.6
1	D	158	SER	3.6
1	G	261	ASN	3.6
1	F	138	ILE	3.6
1	J	190	TYR	3.6
1	D	115	LEU	3.6
1	L	94	LEU	3.6
1	I	220	PHE	3.6
1	G	171	LEU	3.6
1	J	94	LEU	3.6
1	I	173	ILE	3.6
1	G	19	THR	3.6
1	G	199	GLU	3.6
1	F	305	GLN	3.6
1	J	98	PHE	3.6
1	C	305	GLN	3.6
1	I	296	LYS	3.6
1	E	220	PHE	3.6
1	B	114	ASN	3.6
1	H	282	ASN	3.6
1	J	110	SER	3.6
1	J	258	ASP	3.5
1	E	171	LEU	3.5
1	H	176	CYS	3.5
1	H	245	ARG	3.5
1	L	21	ARG	3.5
1	A	157	ALA	3.5
1	N	108	VAL	3.5
1	E	144	SER	3.5
1	K	60	SER	3.5
1	D	301	PHE	3.5
1	E	21	ARG	3.5
1	I	198	ALA	3.5
1	E	158	SER	3.5
1	H	305	GLN	3.5
1	F	236	LEU	3.5
1	N	308	ARG	3.5
1	C	109	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	157	ALA	3.5
1	F	314	ASP	3.5
1	I	158	SER	3.5
1	J	54	GLN	3.5
1	G	82	ILE	3.5
1	H	271	SER	3.5
1	D	245	ARG	3.5
1	E	98	PHE	3.5
1	G	98	PHE	3.5
1	I	167	ALA	3.5
1	F	243	GLU	3.5
1	H	60	SER	3.5
1	C	71	VAL	3.5
1	M	308	ARG	3.5
1	B	190	TYR	3.5
1	G	301	PHE	3.5
1	N	301	PHE	3.5
1	N	261	ASN	3.5
1	D	160	GLY	3.4
1	I	308	ARG	3.4
1	L	30	HIS	3.4
1	E	60	SER	3.4
1	J	90	GLN	3.4
1	H	298	MET	3.4
1	E	247	GLU	3.4
1	F	103	SER	3.4
1	N	54	GLN	3.4
1	C	236	LEU	3.4
1	A	96	LYS	3.4
1	M	230	ILE	3.4
1	A	21	ARG	3.4
1	J	204	VAL	3.4
1	N	199	GLU	3.4
1	G	54	GLN	3.4
1	K	90	GLN	3.4
1	N	90	GLN	3.4
1	K	190	TYR	3.4
1	I	98	PHE	3.4
1	A	59	ILE	3.4
1	K	230	ILE	3.4
1	G	66	LYS	3.4
1	N	282	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	313	LEU	3.4
1	I	321	LEU	3.4
1	L	321	LEU	3.4
1	E	136	THR	3.4
1	G	136	THR	3.4
1	I	119	LEU	3.4
1	K	115	LEU	3.4
1	H	57	ARG	3.3
1	A	187	ILE	3.3
1	D	230	ILE	3.3
1	D	57	ARG	3.3
1	M	98	PHE	3.3
1	K	108	VAL	3.3
1	D	262	GLN	3.3
1	F	185	GLN	3.3
1	K	54	GLN	3.3
1	C	230	ILE	3.3
1	N	221	ASP	3.3
1	B	115	LEU	3.3
1	I	297	CYS	3.3
1	D	60	SER	3.3
1	N	212	THR	3.3
1	E	66	LYS	3.3
1	D	157	ALA	3.3
1	D	111	VAL	3.3
1	N	79	GLU	3.3
1	C	179	LEU	3.3
1	C	253	SER	3.3
1	I	60	SER	3.3
1	I	18	PRO	3.3
1	K	301	PHE	3.3
1	B	119	LEU	3.3
1	C	119	LEU	3.3
1	K	119	LEU	3.3
1	F	112	TRP	3.3
1	I	144	SER	3.3
1	I	281	PRO	3.3
1	M	271	SER	3.3
1	J	312	CYS	3.2
1	K	282	ASN	3.2
1	H	24	GLY	3.2
1	J	167	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	18	PRO	3.2
1	D	123	PHE	3.2
1	J	56	PHE	3.2
1	J	65	VAL	3.2
1	N	115	LEU	3.2
1	K	136	THR	3.2
1	D	94	LEU	3.2
1	G	312	CYS	3.2
1	K	185	GLN	3.2
1	K	146	THR	3.2
1	A	31	ARG	3.2
1	C	61	ARG	3.2
1	E	191	ALA	3.2
1	L	60	SER	3.2
1	L	69	VAL	3.2
1	M	225	THR	3.2
1	F	66	LYS	3.2
1	L	96	LYS	3.2
1	D	236	LEU	3.2
1	J	203	VAL	3.2
1	K	61	ARG	3.2
1	F	157	ALA	3.2
1	G	60	SER	3.2
1	N	103	SER	3.2
1	N	167	ALA	3.2
1	B	305	GLN	3.2
1	H	321	LEU	3.2
1	M	190	TYR	3.2
1	C	220	PHE	3.2
1	H	239	ILE	3.2
1	L	36	ALA	3.2
1	N	147	PHE	3.1
1	E	233	TRP	3.1
1	C	69	VAL	3.1
1	D	30	HIS	3.1
1	J	103	SER	3.1
1	J	185	GLN	3.1
1	L	54	GLN	3.1
1	N	321	LEU	3.1
1	A	220	PHE	3.1
1	F	98	PHE	3.1
1	J	57	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	94	LEU	3.1
1	I	258	ASP	3.1
1	I	301	PHE	3.1
1	B	292	TYR	3.1
1	I	157	ALA	3.1
1	H	243	GLU	3.1
1	B	136	THR	3.1
1	G	103	SER	3.1
1	H	225	THR	3.1
1	K	18	PRO	3.1
1	A	100	LYS	3.1
1	A	261	ASN	3.1
1	D	59	ILE	3.1
1	G	173	ILE	3.1
1	I	91	ILE	3.1
1	K	236	LEU	3.1
1	F	312	CYS	3.1
1	B	94	LEU	3.1
1	B	167	ALA	3.1
1	L	123	PHE	3.1
1	G	46	GLU	3.1
1	N	145	VAL	3.1
1	A	258	ASP	3.1
1	K	110	SER	3.1
1	J	179	LEU	3.1
1	J	313	LEU	3.1
1	D	114	ASN	3.1
1	C	21	ARG	3.1
1	G	111	VAL	3.1
1	I	82	ILE	3.1
1	A	146	THR	3.0
1	H	235	ASN	3.0
1	A	69	VAL	3.0
1	M	255	GLU	3.0
1	B	236	LEU	3.0
1	L	90	GLN	3.0
1	I	146	THR	3.0
1	A	286	PHE	3.0
1	B	220	PHE	3.0
1	F	266	ASN	3.0
1	L	82	ILE	3.0
1	I	236	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	122	GLU	3.0
1	J	236	LEU	3.0
1	C	108	VAL	3.0
1	B	261	ASN	3.0
1	L	59	ILE	3.0
1	L	282	ASN	3.0
1	L	312	CYS	3.0
1	M	281	PRO	3.0
1	C	247	GLU	3.0
1	F	123	PHE	3.0
1	J	193	PHE	3.0
1	I	96	LYS	3.0
1	H	61	ARG	3.0
1	L	236	LEU	3.0
1	A	199	GLU	3.0
1	C	79	GLU	3.0
1	D	79	GLU	3.0
1	F	193	PHE	3.0
1	I	66	LYS	3.0
1	J	286	PHE	3.0
1	L	198	ALA	3.0
1	C	251	SER	3.0
1	N	271	SER	3.0
1	F	198	ALA	3.0
1	H	182	GLU	3.0
1	K	305	GLN	3.0
1	G	71	VAL	3.0
1	D	239	ILE	3.0
1	J	230	ILE	3.0
1	E	50	LEU	3.0
1	G	321	LEU	3.0
1	H	50	LEU	3.0
1	N	19	THR	3.0
1	L	281	PRO	3.0
1	I	59	ILE	2.9
1	A	158	SER	2.9
1	B	258	ASP	2.9
1	F	19	THR	2.9
1	F	18	PRO	2.9
1	I	260	PRO	2.9
1	L	56	PHE	2.9
1	M	177	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	198	ALA	2.9
1	H	111	VAL	2.9
1	J	255	GLU	2.9
1	M	21	ARG	2.9
1	L	285	MET	2.9
1	G	146	THR	2.9
1	M	109	PRO	2.9
1	N	237	TYR	2.9
1	H	198	ALA	2.9
1	K	30	HIS	2.9
1	D	282	ASN	2.9
1	E	62	MET	2.9
1	H	285	MET	2.9
1	L	46	GLU	2.9
1	A	272	TYR	2.9
1	B	147	PHE	2.9
1	L	18	PRO	2.9
1	K	104	ASP	2.9
1	M	264	ASP	2.9
1	B	308	ARG	2.9
1	C	198	ALA	2.9
1	C	323	ARG	2.9
1	F	71	VAL	2.9
1	K	191	ALA	2.9
1	G	182	GLU	2.9
1	A	250	CYS	2.9
1	K	137	GLY	2.9
1	L	193	PHE	2.9
1	A	144	SER	2.9
1	H	108	VAL	2.9
1	H	313	LEU	2.9
1	I	103	SER	2.9
1	J	226	ALA	2.9
1	J	309	VAL	2.9
1	C	199	GLU	2.9
1	A	90	GLN	2.9
1	K	66	LYS	2.9
1	A	147	PHE	2.9
1	I	160	GLY	2.9
1	A	239	ILE	2.9
1	D	269	CYS	2.9
1	M	157	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	60	SER	2.9
1	B	110	SER	2.9
1	F	307	THR	2.9
1	J	60	SER	2.9
1	A	291	ASP	2.9
1	J	109	PRO	2.9
1	K	316	PRO	2.9
1	N	245	ARG	2.9
1	F	146	THR	2.9
1	I	225	THR	2.9
1	H	264	ASP	2.9
1	K	255	GLU	2.9
1	K	98	PHE	2.9
1	E	115	LEU	2.9
1	I	217	LEU	2.9
1	K	188	LEU	2.9
1	D	187	ILE	2.8
1	F	250	CYS	2.8
1	N	158	SER	2.8
1	B	321	LEU	2.8
1	G	175	VAL	2.8
1	J	61	ARG	2.8
1	K	56	PHE	2.8
1	N	119	LEU	2.8
1	G	57	ARG	2.8
1	H	230	ILE	2.8
1	I	187	ILE	2.8
1	B	285	MET	2.8
1	E	56	PHE	2.8
1	C	60	SER	2.8
1	C	57	ARG	2.8
1	C	258	ASP	2.8
1	G	294	ASP	2.8
1	D	281	PRO	2.8
1	K	321	LEU	2.8
1	J	267	PHE	2.8
1	N	220	PHE	2.8
1	A	87	ILE	2.8
1	A	309	VAL	2.8
1	G	91	ILE	2.8
1	I	253	SER	2.8
1	G	262	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	171	LEU	2.8
1	N	95	ASN	2.8
1	N	236	LEU	2.8
1	G	123	PHE	2.8
1	H	287	MET	2.8
1	C	271	SER	2.8
1	D	305	GLN	2.8
1	M	58	ALA	2.8
1	L	87	ILE	2.8
1	N	67	ILE	2.8
1	B	30	HIS	2.8
1	F	177	HIS	2.8
1	B	222	LYS	2.8
1	B	144	SER	2.8
1	N	225	THR	2.8
1	H	236	LEU	2.8
1	A	45	ILE	2.7
1	N	87	ILE	2.7
1	F	115	LEU	2.7
1	H	98	PHE	2.7
1	M	220	PHE	2.7
1	L	91	ILE	2.7
1	N	239	ILE	2.7
1	F	57	ARG	2.7
1	B	287	MET	2.7
1	E	167	ALA	2.7
1	H	170	TYR	2.7
1	L	255	GLU	2.7
1	I	271	SER	2.7
1	F	108	VAL	2.7
1	D	96	LYS	2.7
1	A	236	LEU	2.7
1	H	94	LEU	2.7
1	G	233	TRP	2.7
1	E	193	PHE	2.7
1	D	90	GLN	2.7
1	F	260	PRO	2.7
1	D	21	ARG	2.7
1	K	158	SER	2.7
1	A	94	LEU	2.7
1	D	24	GLY	2.7
1	C	123	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	98	PHE	2.7
1	H	255	GLU	2.7
1	B	245	ARG	2.7
1	F	144	SER	2.7
1	D	50	LEU	2.7
1	G	160	GLY	2.7
1	M	261	ASN	2.7
1	M	260	PRO	2.7
1	A	61	ARG	2.7
1	H	54	GLN	2.7
1	K	312	CYS	2.7
1	F	50	LEU	2.7
1	F	94	LEU	2.7
1	E	35	SER	2.7
1	M	56	PHE	2.7
1	K	91	ILE	2.7
1	H	309	VAL	2.7
1	F	255	GLU	2.7
1	B	50	LEU	2.7
1	I	179	LEU	2.7
1	E	104	ASP	2.6
1	J	157	ALA	2.6
1	N	157	ALA	2.6
1	B	96	LYS	2.6
1	E	69	VAL	2.6
1	G	29	HIS	2.6
1	G	245	ARG	2.6
1	I	282	ASN	2.6
1	J	282	ASN	2.6
1	N	287	MET	2.6
1	E	188	LEU	2.6
1	E	321	LEU	2.6
1	H	27	GLU	2.6
1	J	199	GLU	2.6
1	M	44	GLN	2.6
1	I	312	CYS	2.6
1	K	157	ALA	2.6
1	E	237	TYR	2.6
1	L	230	ILE	2.6
1	J	108	VAL	2.6
1	D	321	LEU	2.6
1	H	290	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	122	GLU	2.6
1	K	122	GLU	2.6
1	A	117	ALA	2.6
1	D	191	ALA	2.6
1	A	277	CYS	2.6
1	A	119	LEU	2.6
1	M	179	LEU	2.6
1	A	67	ILE	2.6
1	E	230	ILE	2.6
1	G	121	ILE	2.6
1	G	239	ILE	2.6
1	A	115	LEU	2.6
1	I	309	VAL	2.6
1	C	158	SER	2.6
1	J	188	LEU	2.6
1	L	40	ARG	2.6
1	B	301	PHE	2.6
1	D	124	PHE	2.6
1	K	107	GLN	2.6
1	C	137	GLY	2.6
1	B	67	ILE	2.6
1	E	71	VAL	2.6
1	M	198	ALA	2.6
1	I	57	ARG	2.6
1	A	149	THR	2.6
1	D	109	PRO	2.6
1	D	291	ASP	2.6
1	B	156	PHE	2.6
1	H	301	PHE	2.6
1	A	46	GLU	2.6
1	C	96	LYS	2.6
1	E	96	LYS	2.6
1	G	255	GLU	2.6
1	I	41	GLU	2.6
1	B	91	ILE	2.6
1	F	173	ILE	2.6
1	F	179	LEU	2.6
1	G	298	MET	2.6
1	K	21	ARG	2.6
1	E	302	THR	2.6
1	C	168	ASP	2.6
1	D	27	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	205	ILE	2.6
1	D	171	LEU	2.6
1	E	236	LEU	2.6
1	G	50	LEU	2.6
1	J	261	ASN	2.6
1	K	111	VAL	2.6
1	N	323	ARG	2.6
1	G	96	LYS	2.5
1	K	220	PHE	2.5
1	A	116	ILE	2.5
1	F	230	ILE	2.5
1	N	230	ILE	2.5
1	J	74	VAL	2.5
1	M	203	VAL	2.5
1	C	250	CYS	2.5
1	E	272	TYR	2.5
1	C	19	THR	2.5
1	F	156	PHE	2.5
1	K	147	PHE	2.5
1	M	50	LEU	2.5
1	C	309	VAL	2.5
1	H	71	VAL	2.5
1	G	264	ASP	2.5
1	J	169	ARG	2.5
1	N	198	ALA	2.5
1	E	94	LEU	2.5
1	F	82	ILE	2.5
1	M	67	ILE	2.5
1	M	121	ILE	2.5
1	B	35	SER	2.5
1	F	160	GLY	2.5
1	H	195	GLY	2.5
1	K	167	ALA	2.5
1	E	163	ASP	2.5
1	N	96	LYS	2.5
1	I	56	PHE	2.5
1	K	193	PHE	2.5
1	F	39	VAL	2.5
1	F	309	VAL	2.5
1	G	232	HIS	2.5
1	I	137	GLY	2.5
1	K	19	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	169	ARG	2.5
1	C	185	GLN	2.5
1	L	272	TYR	2.5
1	K	124	PHE	2.5
1	H	119	LEU	2.5
1	B	230	ILE	2.5
1	D	173	ILE	2.5
1	F	67	ILE	2.5
1	H	91	ILE	2.5
1	H	288	ASN	2.5
1	J	91	ILE	2.5
1	G	323	ARG	2.5
1	N	211	GLY	2.5
1	E	29	HIS	2.5
1	G	209	ALA	2.5
1	G	226	ALA	2.5
1	H	164	ALA	2.5
1	I	30	HIS	2.5
1	K	226	ALA	2.5
1	B	66	LYS	2.5
1	C	20	GLN	2.5
1	C	66	LYS	2.5
1	D	303	GLN	2.5
1	F	46	GLU	2.5
1	K	296	LYS	2.5
1	E	67	ILE	2.5
1	G	22	ARG	2.5
1	L	137	GLY	2.5
1	I	176	CYS	2.5
1	G	212	THR	2.5
1	N	113	SER	2.5
1	B	90	GLN	2.5
1	G	119	LEU	2.5
1	H	179	LEU	2.5
1	C	197	PRO	2.5
1	H	323	ARG	2.5
1	L	108	VAL	2.5
1	M	108	VAL	2.5
1	E	241	GLY	2.5
1	K	195	GLY	2.5
1	K	261	ASN	2.5
1	M	100	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	302	THR	2.4
1	D	56	PHE	2.4
1	I	136	THR	2.4
1	M	286	PHE	2.4
1	A	91	ILE	2.4
1	C	190	TYR	2.4
1	L	309	VAL	2.4
1	N	281	PRO	2.4
1	I	323	ARG	2.4
1	E	222	LYS	2.4
1	H	296	LYS	2.4
1	H	115	LEU	2.4
1	D	286	PHE	2.4
1	G	156	PHE	2.4
1	B	146	THR	2.4
1	M	52	TYR	2.4
1	G	113	SER	2.4
1	K	285	MET	2.4
1	F	100	LYS	2.4
1	K	132	GLY	2.4
1	M	96	LYS	2.4
1	G	313	LEU	2.4
1	M	94	LEU	2.4
1	I	147	PHE	2.4
1	C	30	HIS	2.4
1	C	46	GLU	2.4
1	C	245	ARG	2.4
1	D	69	VAL	2.4
1	D	309	VAL	2.4
1	G	309	VAL	2.4
1	J	42	ARG	2.4
1	J	107	GLN	2.4
1	L	62	MET	2.4
1	L	314	ASP	2.4
1	B	116	ILE	2.4
1	D	91	ILE	2.4
1	N	116	ILE	2.4
1	B	145	VAL	2.4
1	A	136	THR	2.4
1	E	212	THR	2.4
1	F	40	ARG	2.4
1	L	111	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	60	SER	2.4
1	M	296	LYS	2.4
1	A	312	CYS	2.4
1	C	160	GLY	2.4
1	G	179	LEU	2.4
1	C	56	PHE	2.4
1	E	221	ASP	2.4
1	G	291	ASP	2.4
1	J	257	ASP	2.4
1	F	45	ILE	2.4
1	G	138	ILE	2.4
1	G	105	VAL	2.4
1	D	19	THR	2.4
1	E	19	THR	2.4
1	J	41	GLU	2.4
1	M	106	SER	2.4
1	N	94	LEU	2.4
1	B	198	ALA	2.4
1	H	226	ALA	2.4
1	B	82	ILE	2.4
1	E	59	ILE	2.4
1	A	168	ASP	2.4
1	C	186	ASP	2.4
1	B	52	TYR	2.4
1	F	31	ARG	2.4
1	J	287	MET	2.4
1	F	96	LYS	2.4
1	H	66	LYS	2.4
1	E	197	PRO	2.4
1	M	197	PRO	2.4
1	N	60	SER	2.4
1	B	59	ILE	2.4
1	M	173	ILE	2.4
1	N	187	ILE	2.4
1	G	62	MET	2.4
1	M	323	ARG	2.4
1	C	171	LEU	2.4
1	L	29	HIS	2.4
1	H	172	ASN	2.4
1	H	197	PRO	2.3
1	N	197	PRO	2.3
1	I	79	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	142	GLN	2.3
1	C	157	ALA	2.3
1	F	36	ALA	2.3
1	H	19	THR	2.3
1	H	87	ILE	2.3
1	D	287	MET	2.3
1	H	265	PRO	2.3
1	K	281	PRO	2.3
1	A	230	ILE	2.3
1	D	227	THR	2.3
1	H	62	MET	2.3
1	I	53	LYS	2.3
1	N	179	LEU	2.3
1	D	163	ASP	2.3
1	N	294	ASP	2.3
1	G	270	PRO	2.3
1	J	29	HIS	2.3
1	K	197	PRO	2.3
1	A	214	GLY	2.3
1	I	67	ILE	2.3
1	I	230	ILE	2.3
1	J	198	ALA	2.3
1	B	19	THR	2.3
1	B	323	ARG	2.3
1	L	105	VAL	2.3
1	L	313	LEU	2.3
1	M	233	TRP	2.3
1	D	257	ASP	2.3
1	J	220	PHE	2.3
1	L	195	GLY	2.3
1	B	78	GLU	2.3
1	L	114	ASN	2.3
1	E	39	VAL	2.3
1	K	309	VAL	2.3
1	N	74	VAL	2.3
1	C	285	MET	2.3
1	D	62	MET	2.3
1	A	173	ILE	2.3
1	L	197	PRO	2.3
1	E	291	ASP	2.3
1	M	241	GLY	2.3
1	E	322	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	2.3
1	D	40	ARG	2.3
1	E	269	CYS	2.3
1	E	312	CYS	2.3
1	H	262	GLN	2.3
1	J	175	VAL	2.3
1	J	176	CYS	2.3
1	L	79	GLU	2.3
1	L	271	SER	2.3
1	H	109	PRO	2.3
1	H	281	PRO	2.3
1	F	284	ASP	2.3
1	A	54	GLN	2.3
1	E	313	LEU	2.3
1	G	20	GLN	2.3
1	L	162	GLU	2.3
1	M	54	GLN	2.3
1	A	56	PHE	2.3
1	B	225	THR	2.3
1	E	286	PHE	2.3
1	G	267	PHE	2.3
1	B	239	ILE	2.3
1	I	45	ILE	2.3
1	L	187	ILE	2.3
1	M	273	PRO	2.3
1	N	166	PRO	2.3
1	N	270	PRO	2.3
1	E	36	ALA	2.3
1	J	222	LYS	2.3
1	E	61	ARG	2.3
1	K	257	ASP	2.3
1	J	243	GLU	2.2
1	L	122	GLU	2.2
1	B	282	ASN	2.2
1	G	56	PHE	2.2
1	H	289	TYR	2.2
1	L	220	PHE	2.2
1	N	190	TYR	2.2
1	C	45	ILE	2.2
1	L	173	ILE	2.2
1	M	187	ILE	2.2
1	D	36	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	175	VAL	2.2
1	E	32	LEU	2.2
1	E	179	LEU	2.2
1	M	321	LEU	2.2
1	N	36	ALA	2.2
1	E	290	MET	2.2
1	J	323	ARG	2.2
1	K	290	MET	2.2
1	A	201	ASP	2.2
1	F	142	GLN	2.2
1	G	79	GLU	2.2
1	A	123	PHE	2.2
1	F	116	ILE	2.2
1	H	173	ILE	2.2
1	I	156	PHE	2.2
1	J	114	ASN	2.2
1	L	261	ASN	2.2
1	E	296	LYS	2.2
1	A	105	VAL	2.2
1	A	154	VAL	2.2
1	D	167	ALA	2.2
1	I	316	PRO	2.2
1	E	271	SER	2.2
1	F	158	SER	2.2
1	H	232	HIS	2.2
1	K	168	ASP	2.2
1	M	199	GLU	2.2
1	J	321	LEU	2.2
1	N	288	ASN	2.2
1	B	135	THR	2.2
1	E	105	VAL	2.2
1	C	58	ALA	2.2
1	G	157	ALA	2.2
1	G	317	ARG	2.2
1	L	42	ARG	2.2
1	J	158	SER	2.2
1	L	106	SER	2.2
1	A	243	GLU	2.2
1	B	185	GLN	2.2
1	E	121	ILE	2.2
1	E	138	ILE	2.2
1	G	142	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	59	ILE	2.2
1	L	121	ILE	2.2
1	N	193	PHE	2.2
1	A	50	LEU	2.2
1	I	115	LEU	2.2
1	J	115	LEU	2.2
1	J	292	TYR	2.2
1	C	131	ASN	2.2
1	D	132	GLY	2.2
1	E	74	VAL	2.2
1	F	317	ARG	2.2
1	I	29	HIS	2.2
1	B	193	PHE	2.2
1	J	53	LYS	2.2
1	K	96	LYS	2.2
1	A	247	GLU	2.2
1	B	171	LEU	2.2
1	G	236	LEU	2.2
1	L	217	LEU	2.2
1	F	226	ALA	2.2
1	G	114	ASN	2.2
1	G	125	LEU	2.2
1	M	32	LEU	2.2
1	E	20	GLN	2.2
1	G	134	GLN	2.2
1	I	272	TYR	2.2
1	C	275	VAL	2.2
1	C	40	ARG	2.2
1	C	257	ASP	2.2
1	E	22	ARG	2.2
1	E	287	MET	2.2
1	I	195	GLY	2.2
1	C	173	ILE	2.2
1	C	239	ILE	2.2
1	G	135	THR	2.2
1	N	173	ILE	2.2
1	H	30	HIS	2.2
1	E	42	ARG	2.2
1	F	27	GLU	2.2
1	H	175	VAL	2.2
1	G	25	ALA	2.1
1	G	260	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	118	ASP	2.1
1	M	43	ASP	2.1
1	M	221	ASP	2.1
1	F	56	PHE	2.1
1	A	114	ASN	2.1
1	I	50	LEU	2.1
1	K	173	ILE	2.1
1	C	146	THR	2.1
1	E	141	THR	2.1
1	I	212	THR	2.1
1	K	29	HIS	2.1
1	A	142	GLN	2.1
1	H	272	TYR	2.1
1	D	199	GLU	2.1
1	A	160	GLY	2.1
1	F	233	TRP	2.1
1	J	160	GLY	2.1
1	M	132	GLY	2.1
1	A	301	PHE	2.1
1	G	94	LEU	2.1
1	G	203	VAL	2.1
1	K	178	VAL	2.1
1	K	206	VAL	2.1
1	E	173	ILE	2.1
1	G	48	LEU	2.1
1	H	222	LYS	2.1
1	K	67	ILE	2.1
1	L	239	ILE	2.1
1	N	250	CYS	2.1
1	H	307	THR	2.1
1	L	19	THR	2.1
1	M	135	THR	2.1
1	B	157	ALA	2.1
1	F	122	GLU	2.1
1	I	27	GLU	2.1
1	M	322	ALA	2.1
1	E	91	ILE	2.1
1	K	93	ILE	2.1
1	B	312	CYS	2.1
1	N	258	ASP	2.1
1	N	175	VAL	2.1
1	E	323	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	30	HIS	2.1
1	K	225	THR	2.1
1	B	20	GLN	2.1
1	A	78	GLU	2.1
1	B	87	ILE	2.1
1	F	121	ILE	2.1
1	G	271	SER	2.1
1	M	303	GLN	2.1
1	B	109	PRO	2.1
1	D	233	TRP	2.1
1	H	156	PHE	2.1
1	J	147	PHE	2.1
1	K	239	ILE	2.1
1	C	62	MET	2.1
1	K	323	ARG	2.1
1	E	259	THR	2.1
1	F	161	GLY	2.1
1	I	226	ALA	2.1
1	J	146	THR	2.1
1	C	187	ILE	2.1
1	C	182	GLU	2.1
1	E	37	SER	2.1
1	G	158	SER	2.1
1	N	35	SER	2.1
1	L	300	MET	2.1
1	N	50	LEU	2.1
1	N	272	TYR	2.1
1	F	30	HIS	2.1
1	D	198	ALA	2.1
1	E	282	ASN	2.1
1	G	198	ALA	2.1
1	M	82	ILE	2.1
1	M	267	PHE	2.1
1	G	305	GLN	2.1
1	I	90	GLN	2.1
1	B	271	SER	2.1
1	G	41	GLU	2.1
1	L	199	GLU	2.1
1	C	203	VAL	2.1
1	A	42	ARG	2.0
1	H	96	LYS	2.0
1	L	118	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	160	GLY	2.0
1	J	121	ILE	2.0
1	M	24	GLY	2.0
1	N	123	PHE	2.0
1	A	133	ASN	2.0
1	F	262	GLN	2.0
1	F	281	PRO	2.0
1	J	135	THR	2.0
1	C	243	GLU	2.0
1	L	27	GLU	2.0
1	D	74	VAL	2.0
1	E	110	SER	2.0
1	F	271	SER	2.0
1	H	74	VAL	2.0
1	J	105	VAL	2.0
1	M	69	VAL	2.0
1	M	169	ARG	2.0
1	A	321	LEU	2.0
1	J	50	LEU	2.0
1	K	222	LYS	2.0
1	F	91	ILE	2.0
1	K	187	ILE	2.0
1	M	91	ILE	2.0
1	A	137	GLY	2.0
1	A	189	GLY	2.0
1	F	29	HIS	2.0
1	B	233	TRP	2.0
1	D	247	GLU	2.0
1	G	42	ARG	2.0
1	I	243	GLU	2.0
1	L	323	ARG	2.0
1	A	251	SER	2.0
1	D	144	SER	2.0
1	B	121	ILE	2.0
1	E	82	ILE	2.0
1	D	189	GLY	2.0
1	K	36	ALA	2.0
1	A	75	TRP	2.0
1	B	74	VAL	2.0
1	D	197	PRO	2.0
1	I	219	PRO	2.0
1	F	44	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	266	ASN	2.0
1	E	199	GLU	2.0
1	I	131	ASN	2.0
1	J	227	THR	2.0
1	M	287	MET	2.0
1	N	125	LEU	2.0
1	L	37	SER	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	L	402	1/1	0.88	0.10	162,162,162,162	0
3	CA	J	402	1/1	0.89	0.09	163,163,163,163	0
3	CA	B	402	1/1	0.89	0.17	183,183,183,183	0
3	CA	D	402	1/1	0.91	0.09	168,168,168,168	0
3	CA	G	402	1/1	0.94	0.16	162,162,162,162	0
3	CA	E	402	1/1	0.94	0.06	177,177,177,177	0
3	CA	F	402	1/1	0.94	0.09	172,172,172,172	0
3	CA	K	402	1/1	0.95	0.07	191,191,191,191	0
3	CA	C	402	1/1	0.96	0.08	188,188,188,188	0
3	CA	M	402	1/1	0.96	0.10	190,190,190,190	0
2	ZN	G	401	1/1	0.97	0.12	159,159,159,159	0
2	ZN	N	401	1/1	0.97	0.08	159,159,159,159	0
3	CA	A	402	1/1	0.97	0.10	193,193,193,193	0
3	CA	I	402	1/1	0.97	0.04	171,171,171,171	0
2	ZN	D	401	1/1	0.98	0.07	156,156,156,156	0
2	ZN	C	401	1/1	0.98	0.08	180,180,180,180	0

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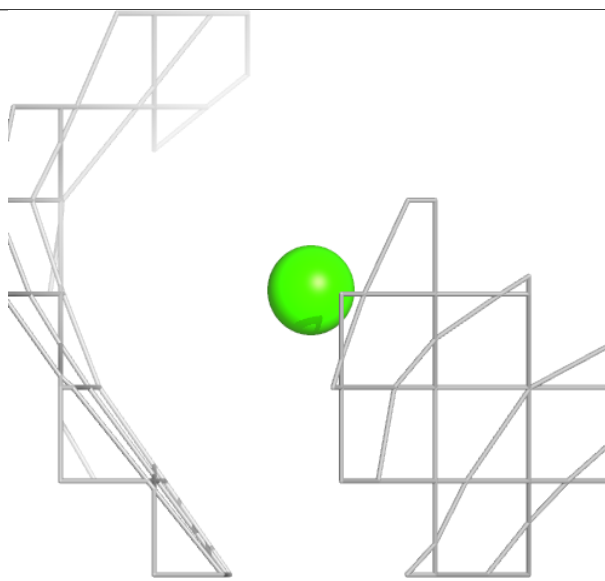
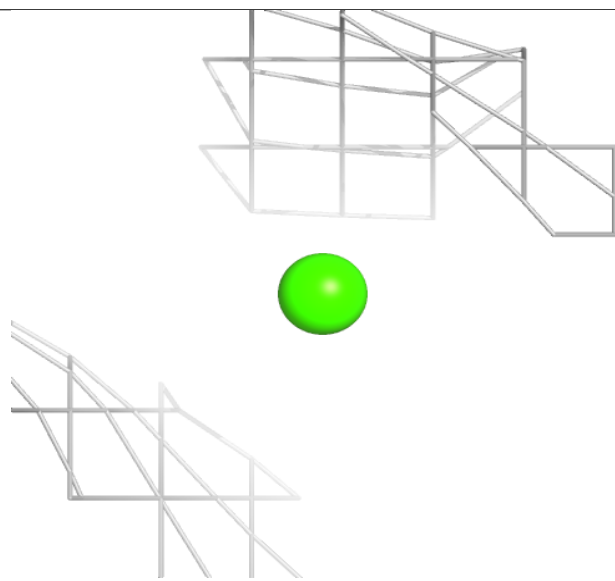
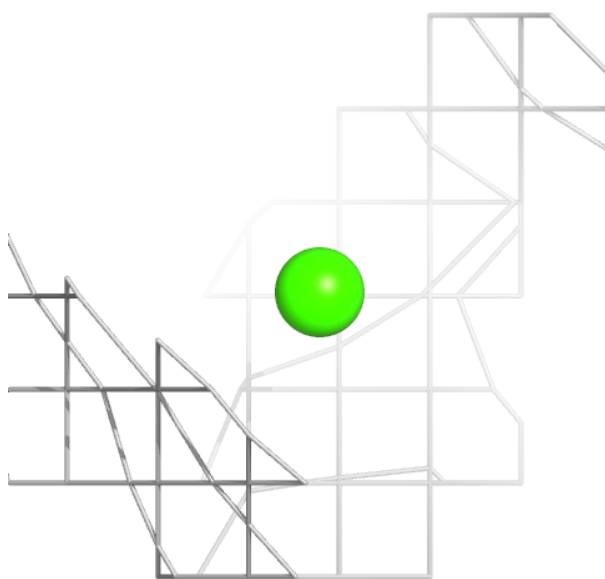
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	K	401	1/1	0.98	0.08	174,174,174,174	0
2	ZN	M	401	1/1	0.98	0.07	177,177,177,177	0
3	CA	H	402	1/1	0.98	0.10	159,159,159,159	0
2	ZN	F	401	1/1	0.99	0.08	140,140,140,140	0
2	ZN	A	401	1/1	0.99	0.08	179,179,179,179	0
2	ZN	H	401	1/1	0.99	0.06	136,136,136,136	0
2	ZN	I	401	1/1	0.99	0.05	142,142,142,142	0
2	ZN	B	401	1/1	0.99	0.04	149,149,149,149	0
2	ZN	L	401	1/1	0.99	0.09	145,145,145,145	0
2	ZN	E	401	1/1	0.99	0.06	152,152,152,152	0
3	CA	N	402	1/1	0.99	0.10	168,168,168,168	0
2	ZN	J	401	1/1	1.00	0.07	142,142,142,142	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.

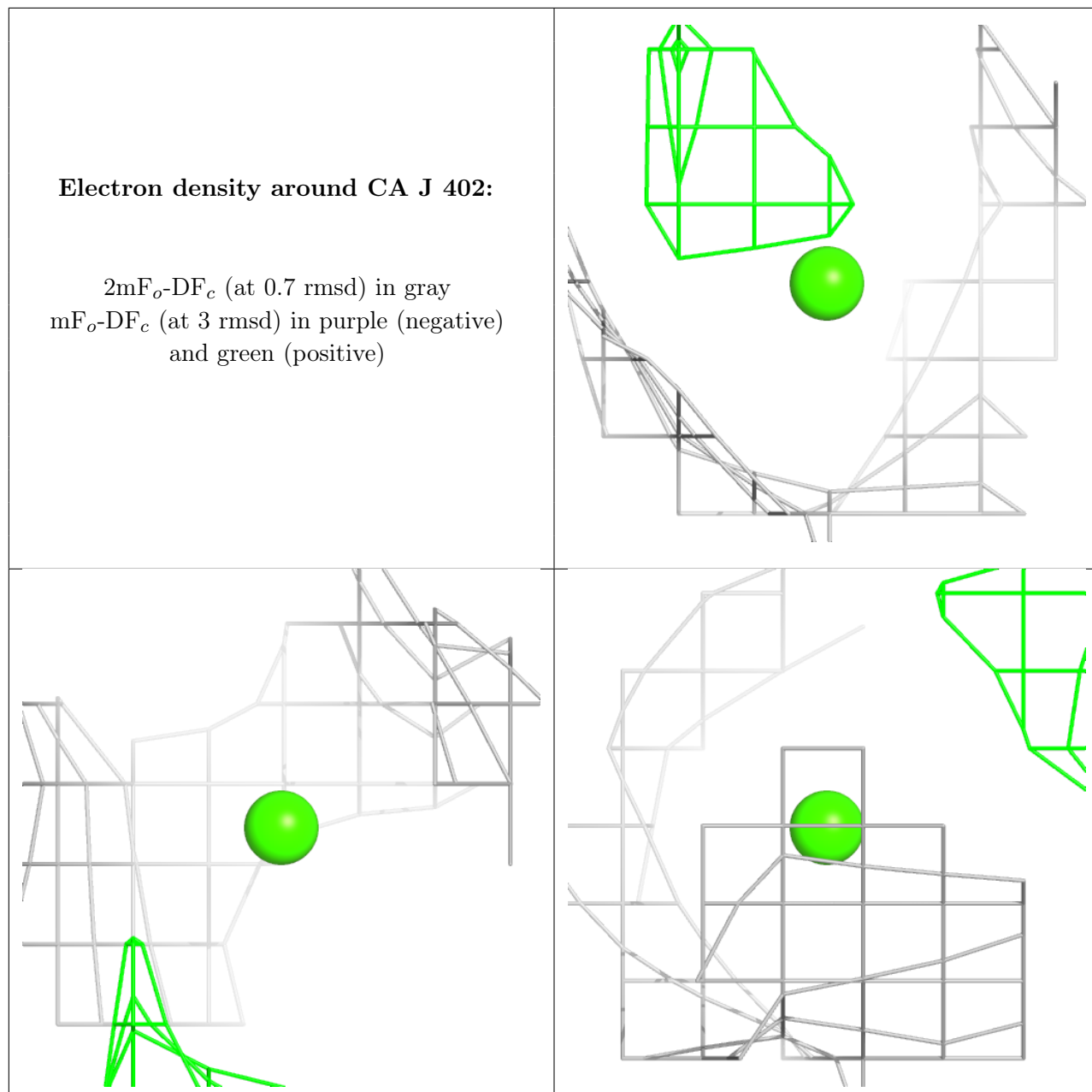
Electron density around CA L 402:

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



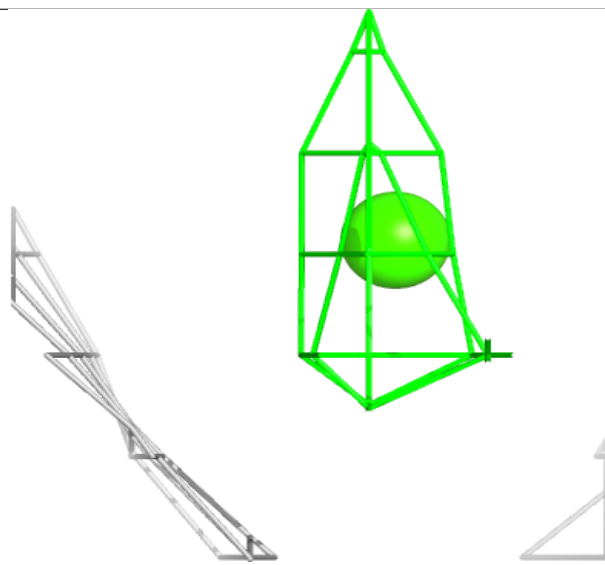
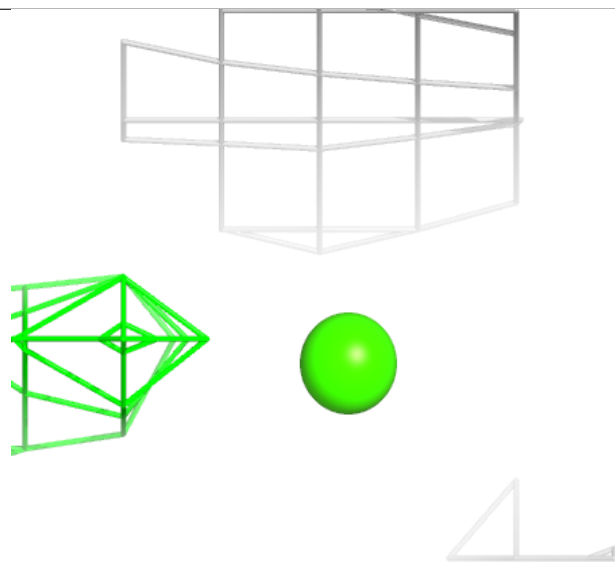
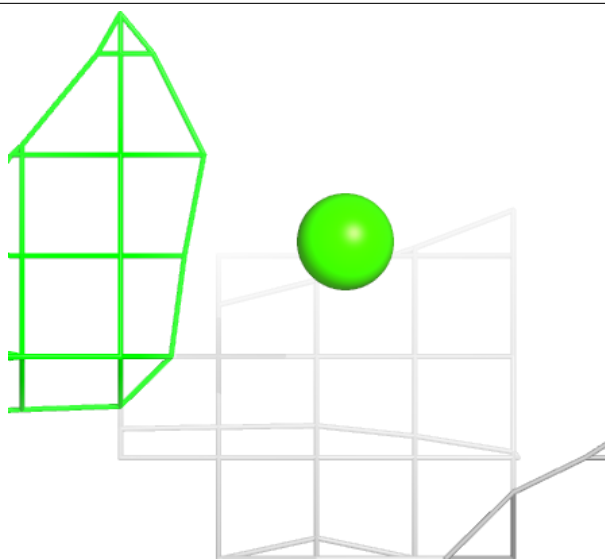
Electron density around CA J 402:

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



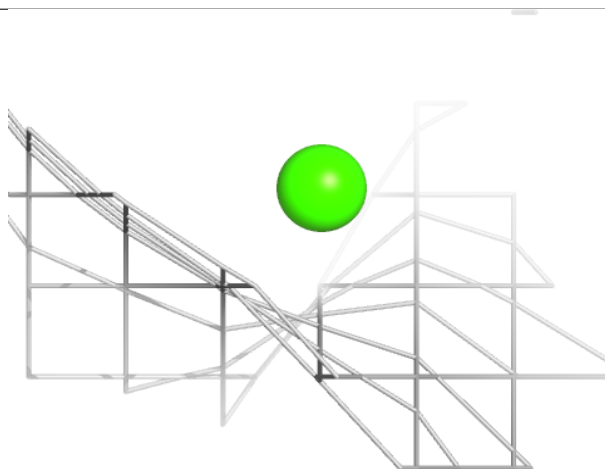
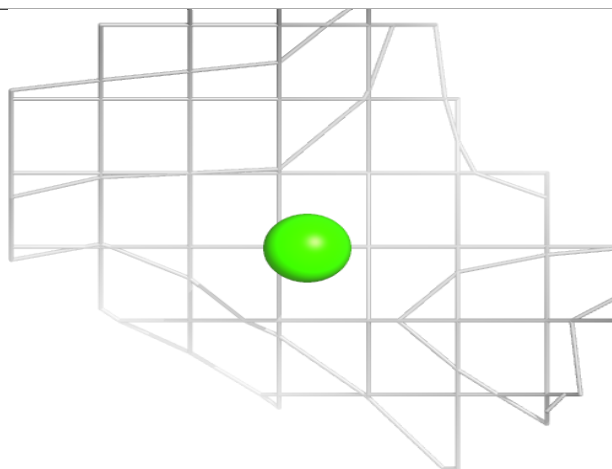
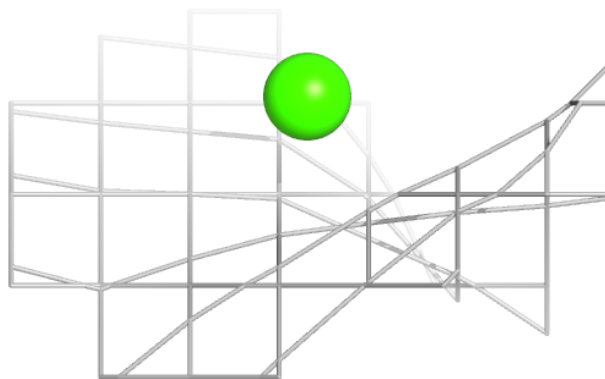
Electron density around CA B 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



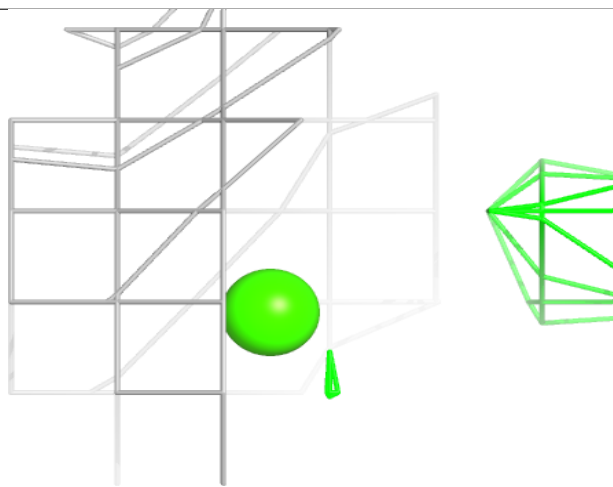
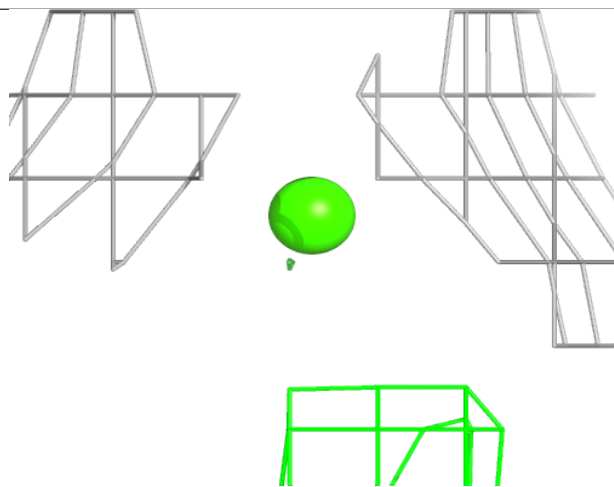
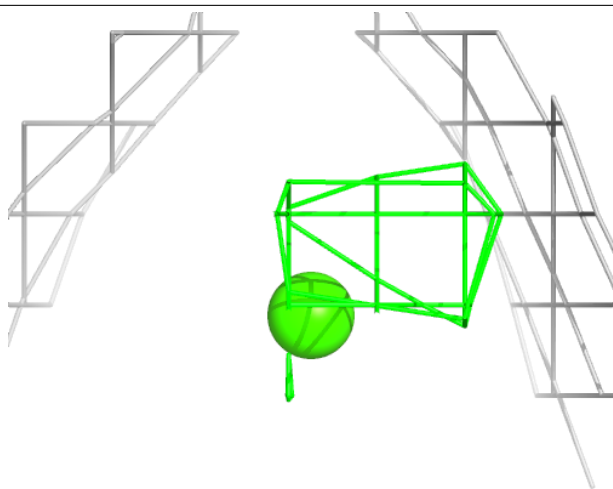
Electron density around CA D 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



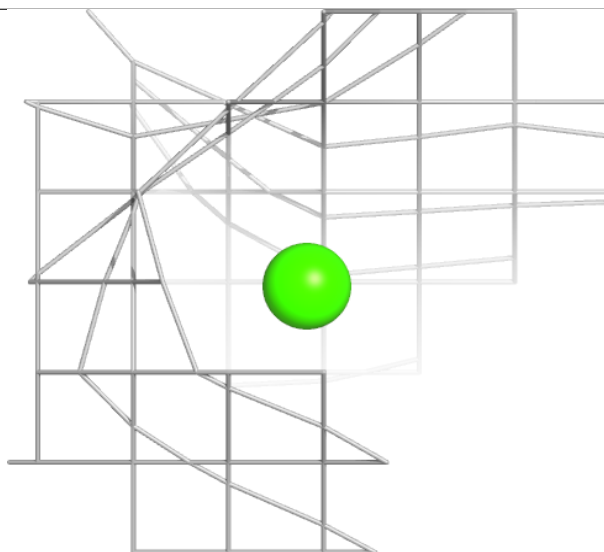
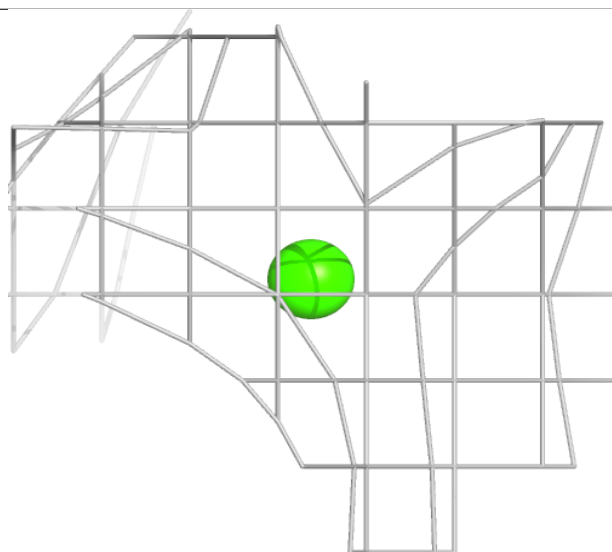
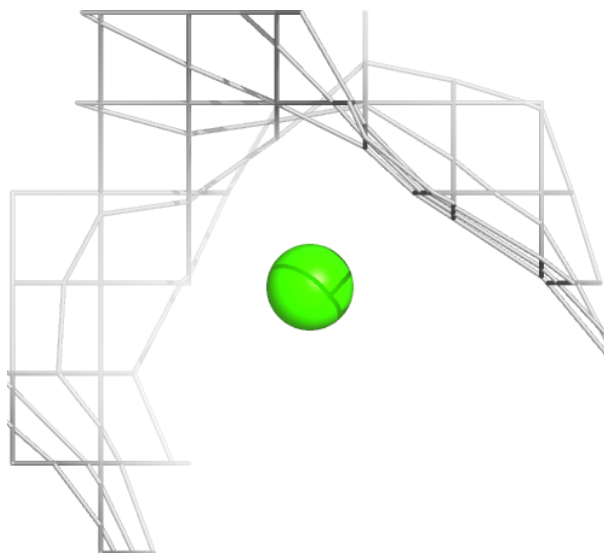
Electron density around CA G 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



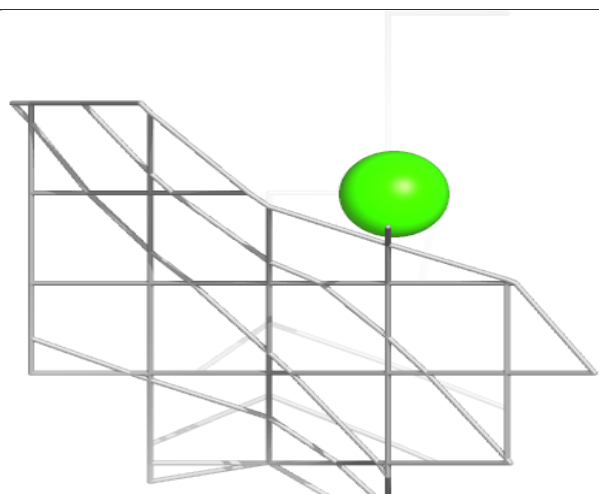
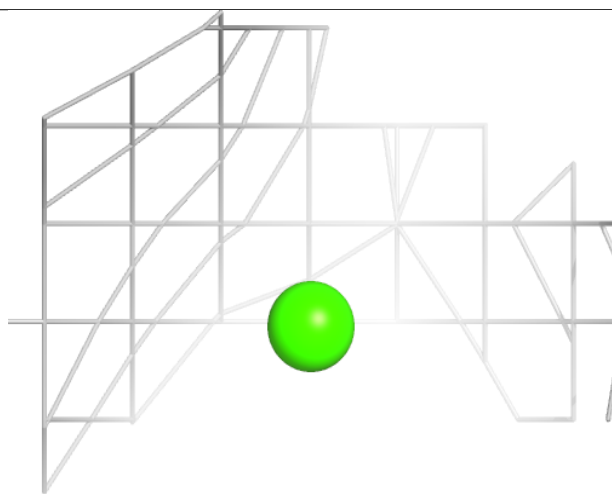
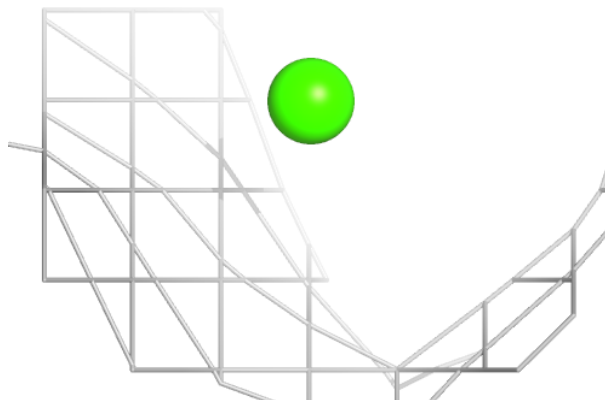
Electron density around CA E 402:

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



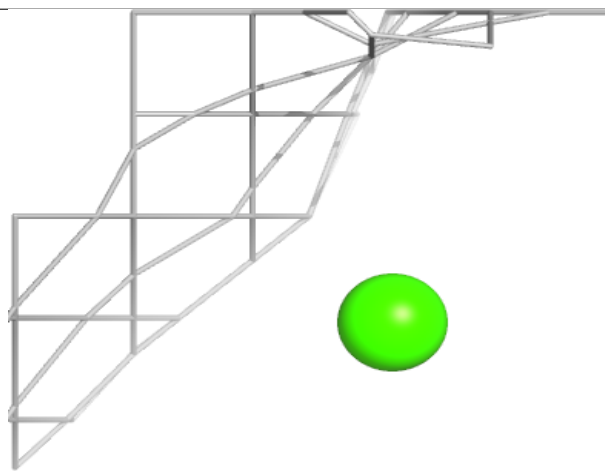
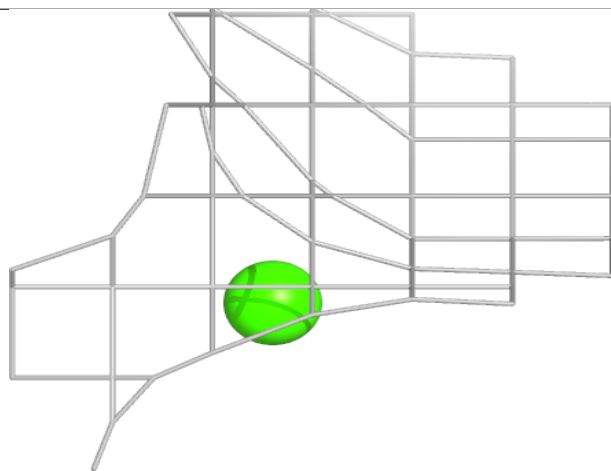
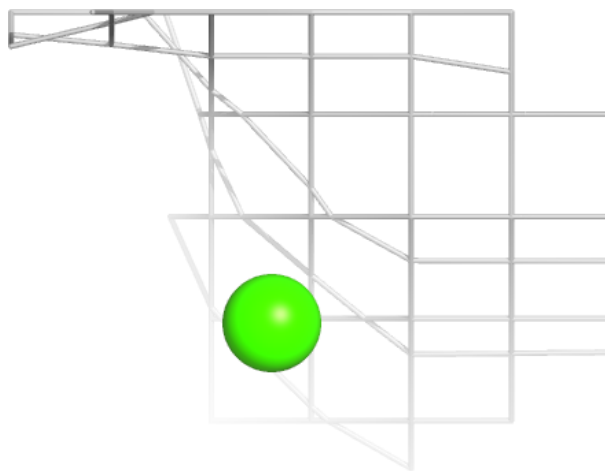
Electron density around CA F 402:

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



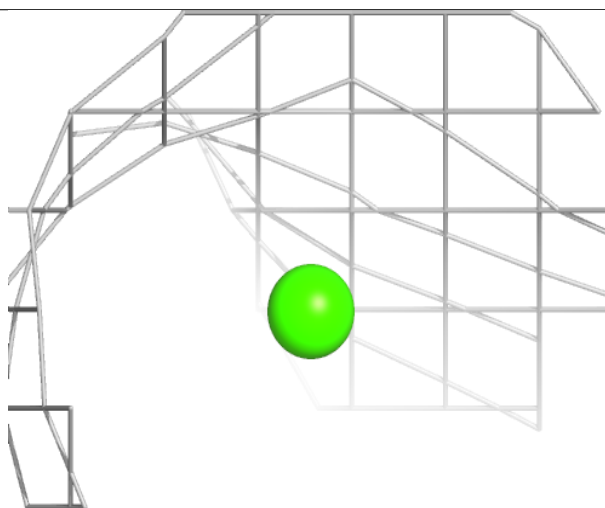
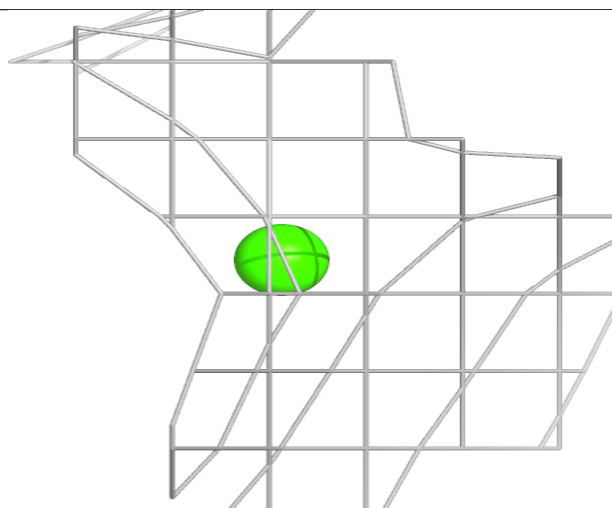
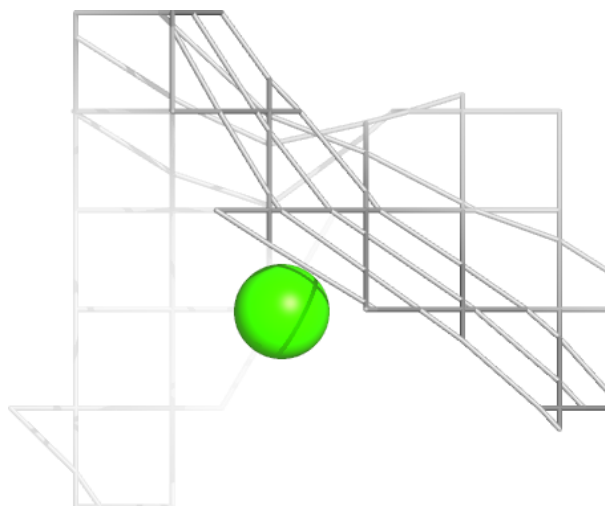
Electron density around CA K 402:

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



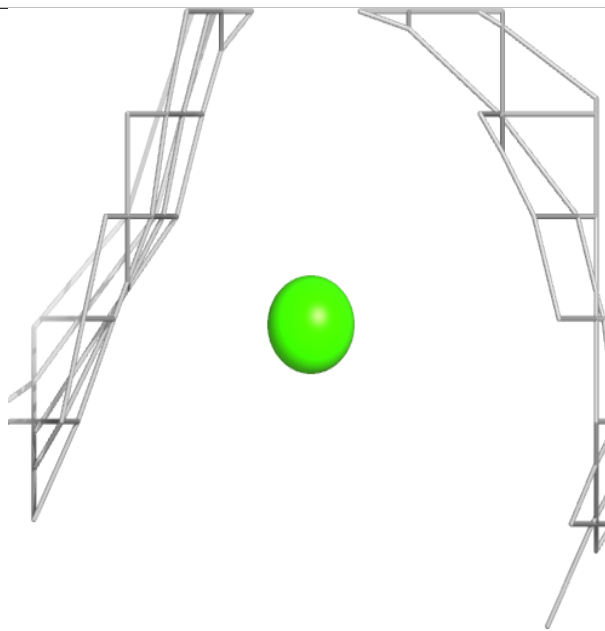
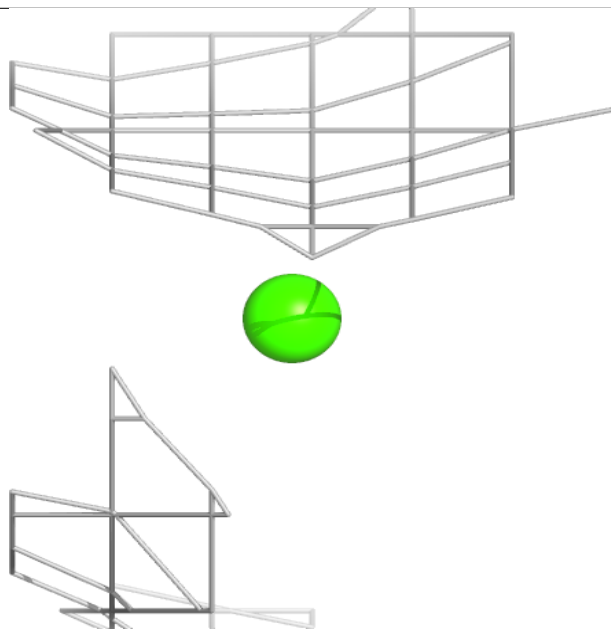
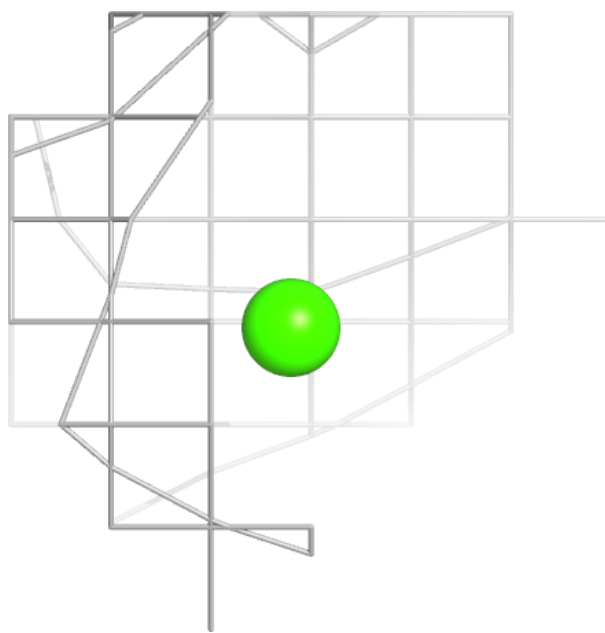
Electron density around CA C 402:

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



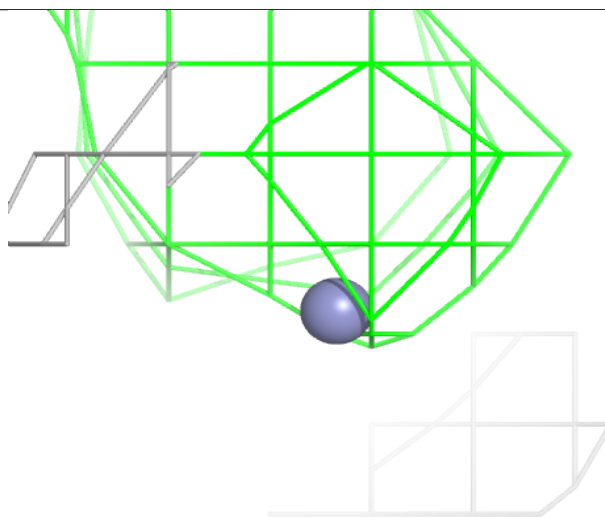
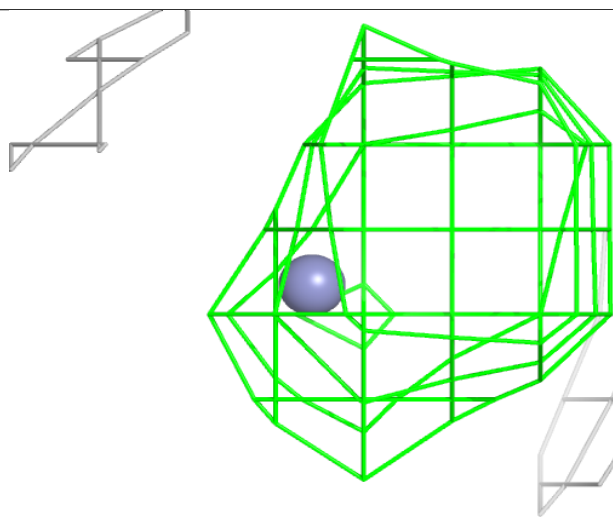
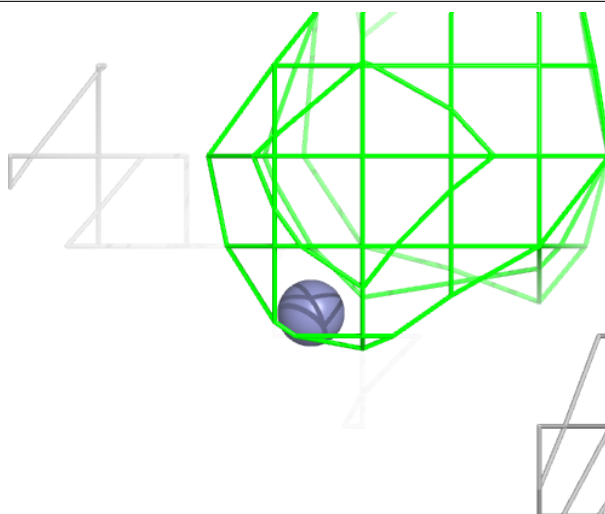
Electron density around CA M 402:

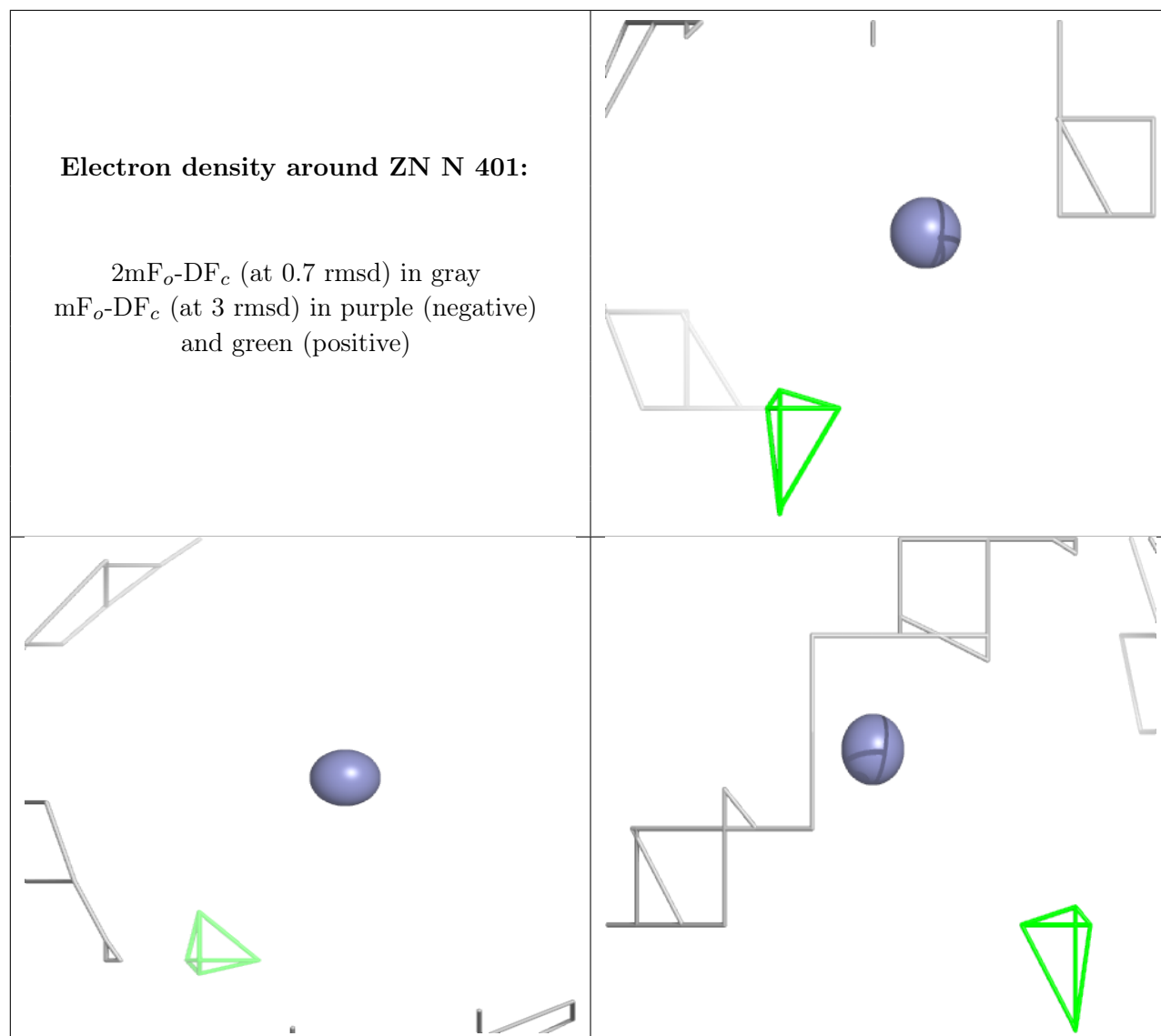
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN G 401:

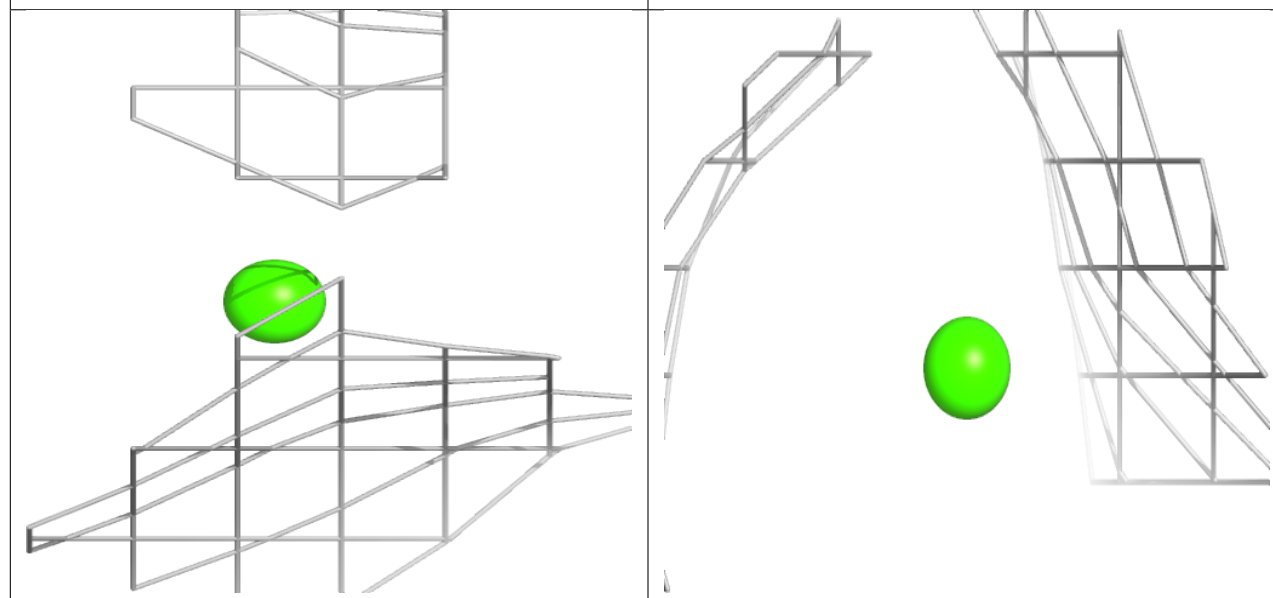
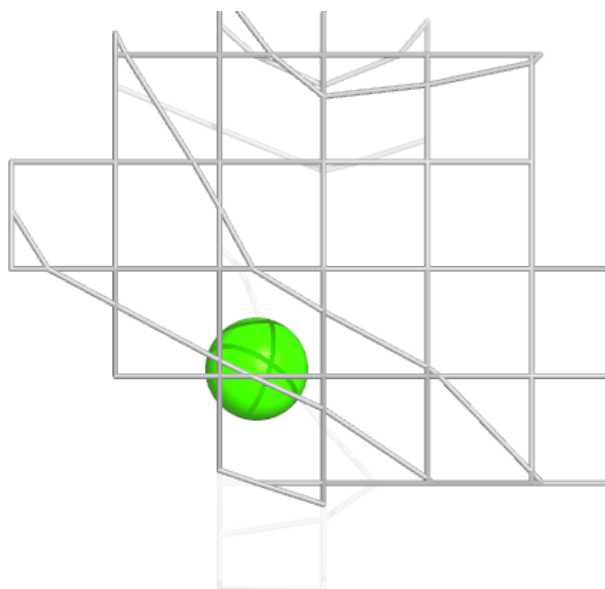
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

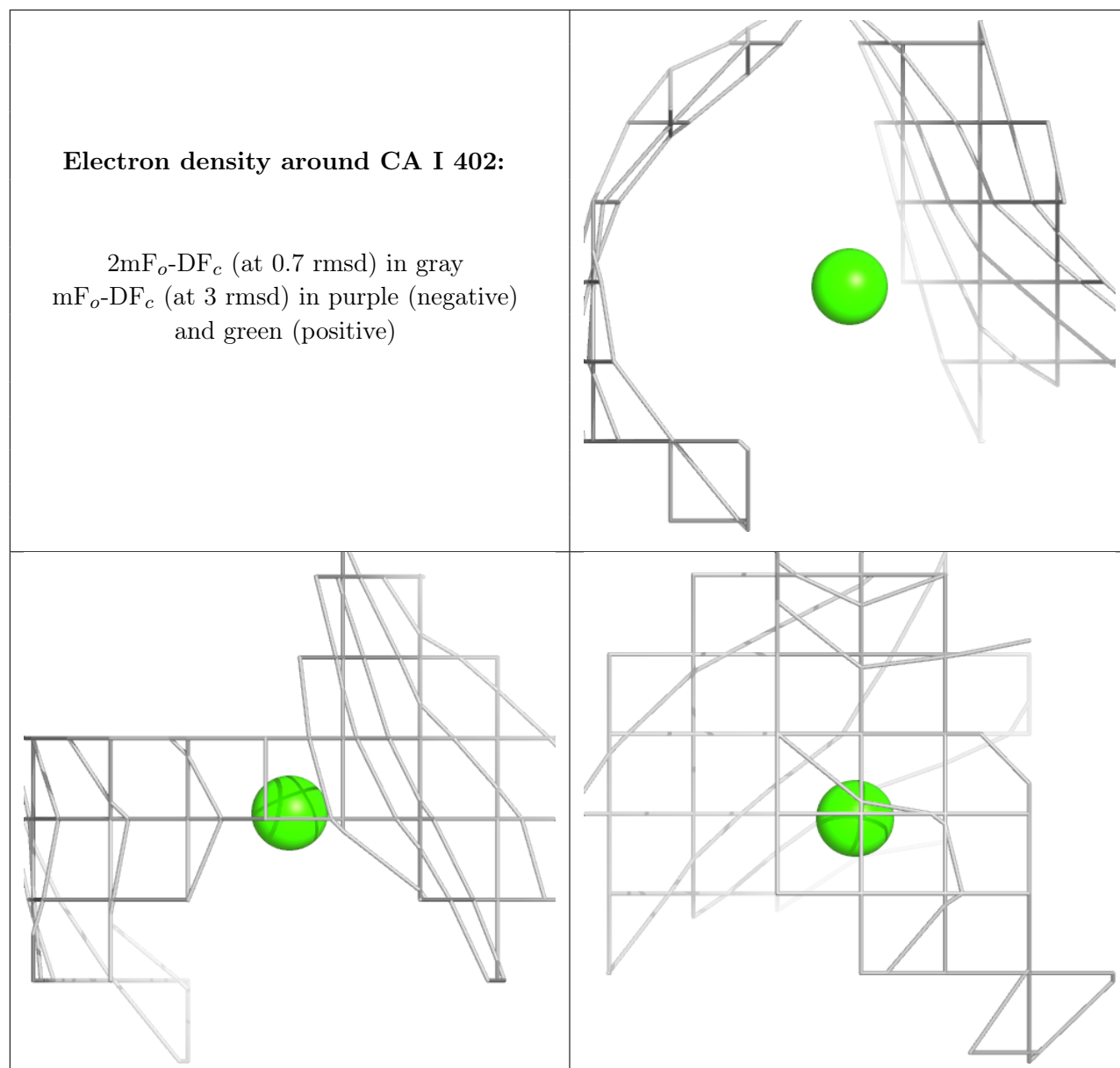


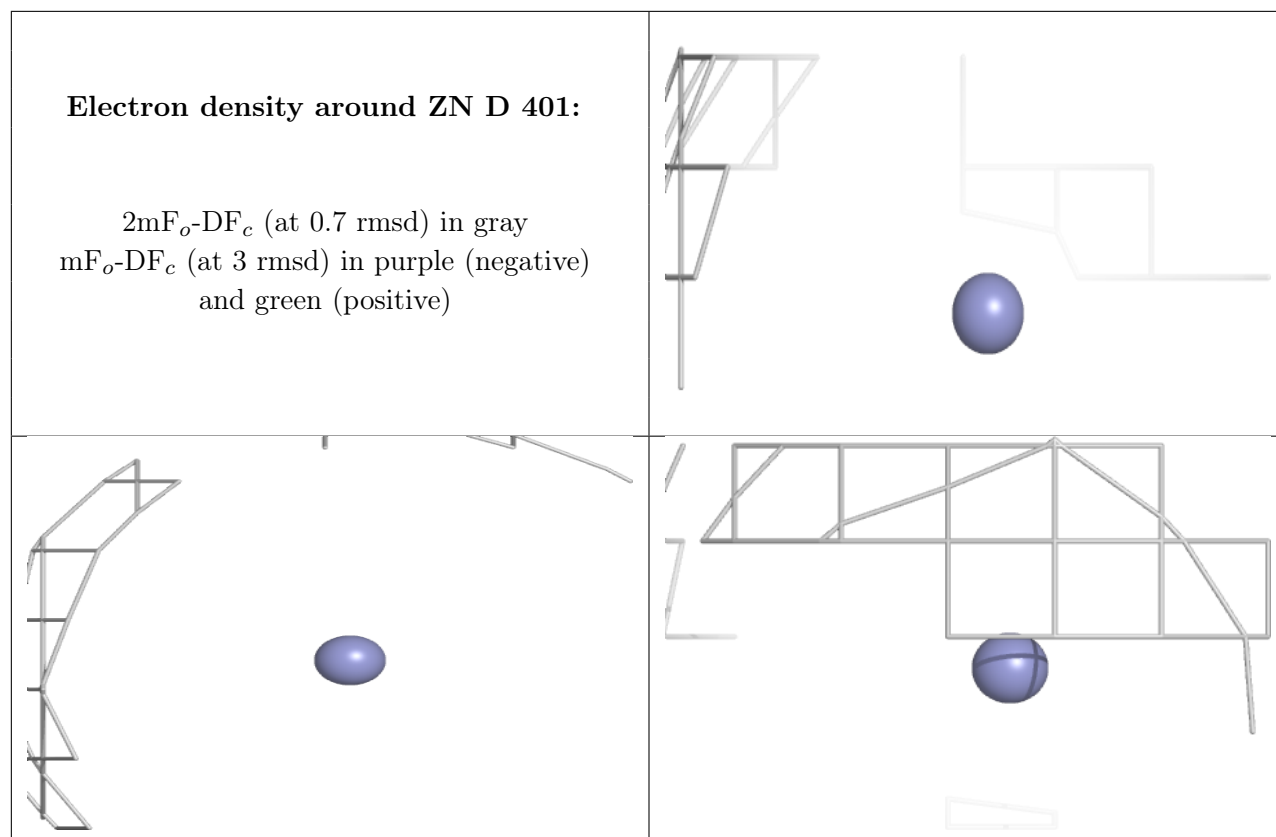


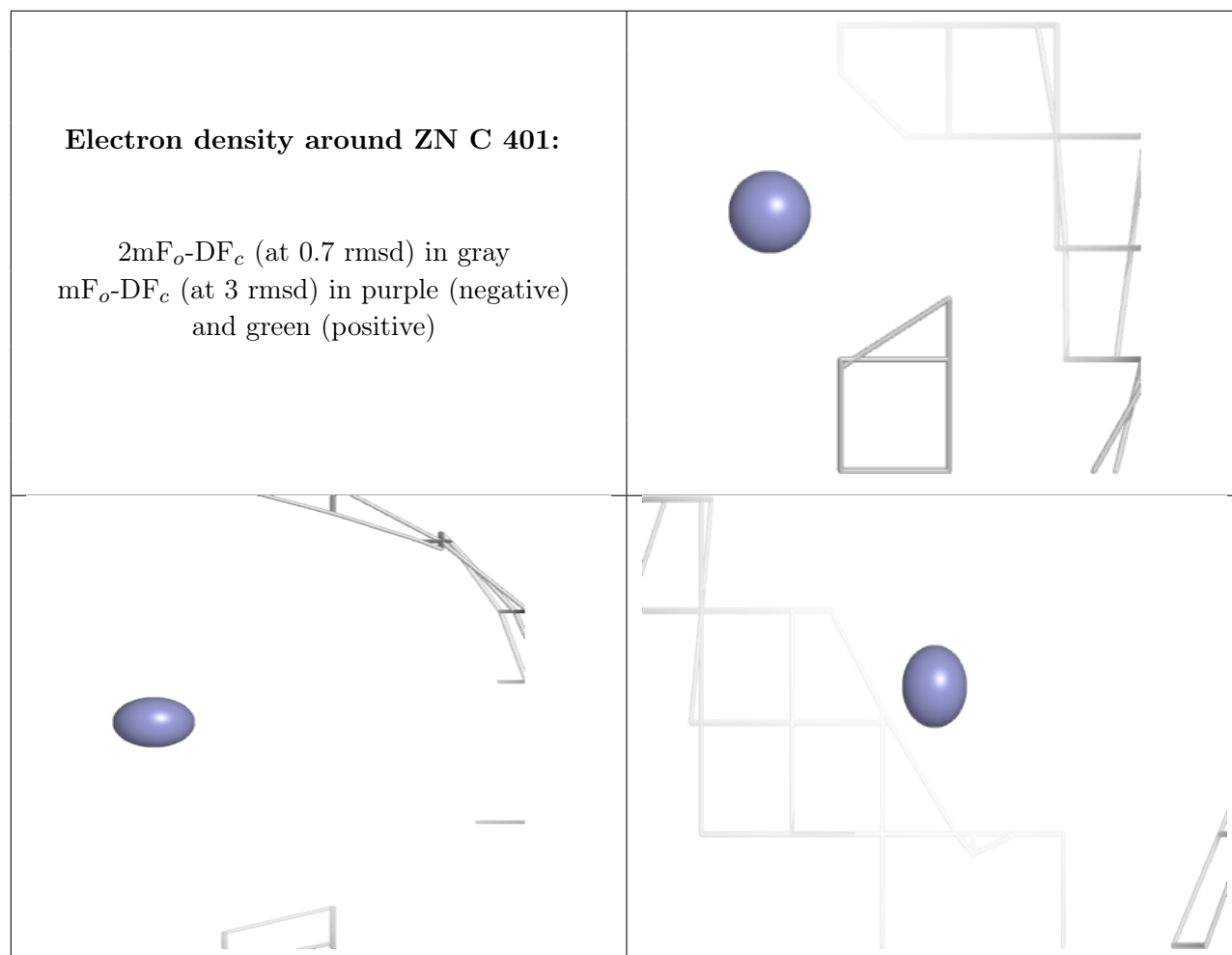
Electron density around CA A 402:

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



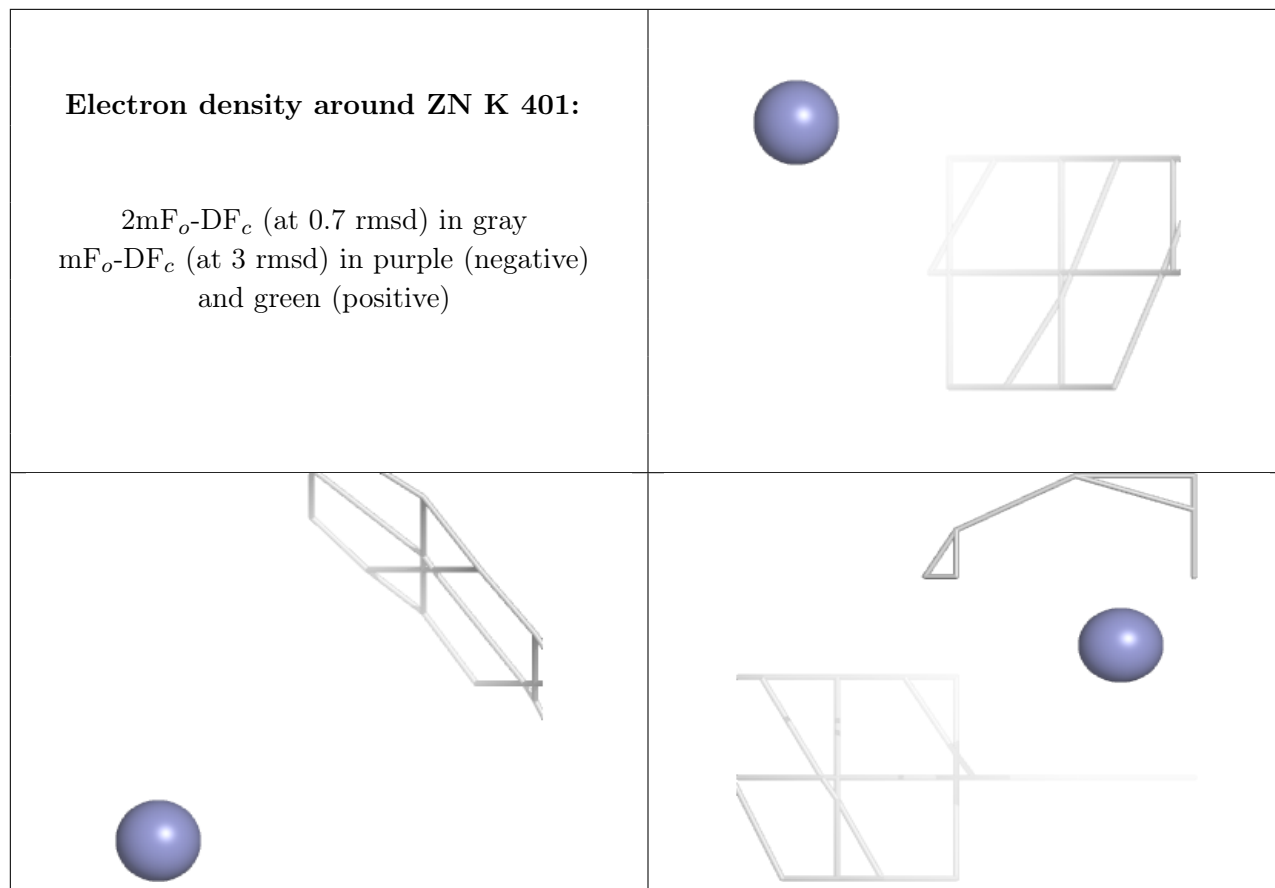




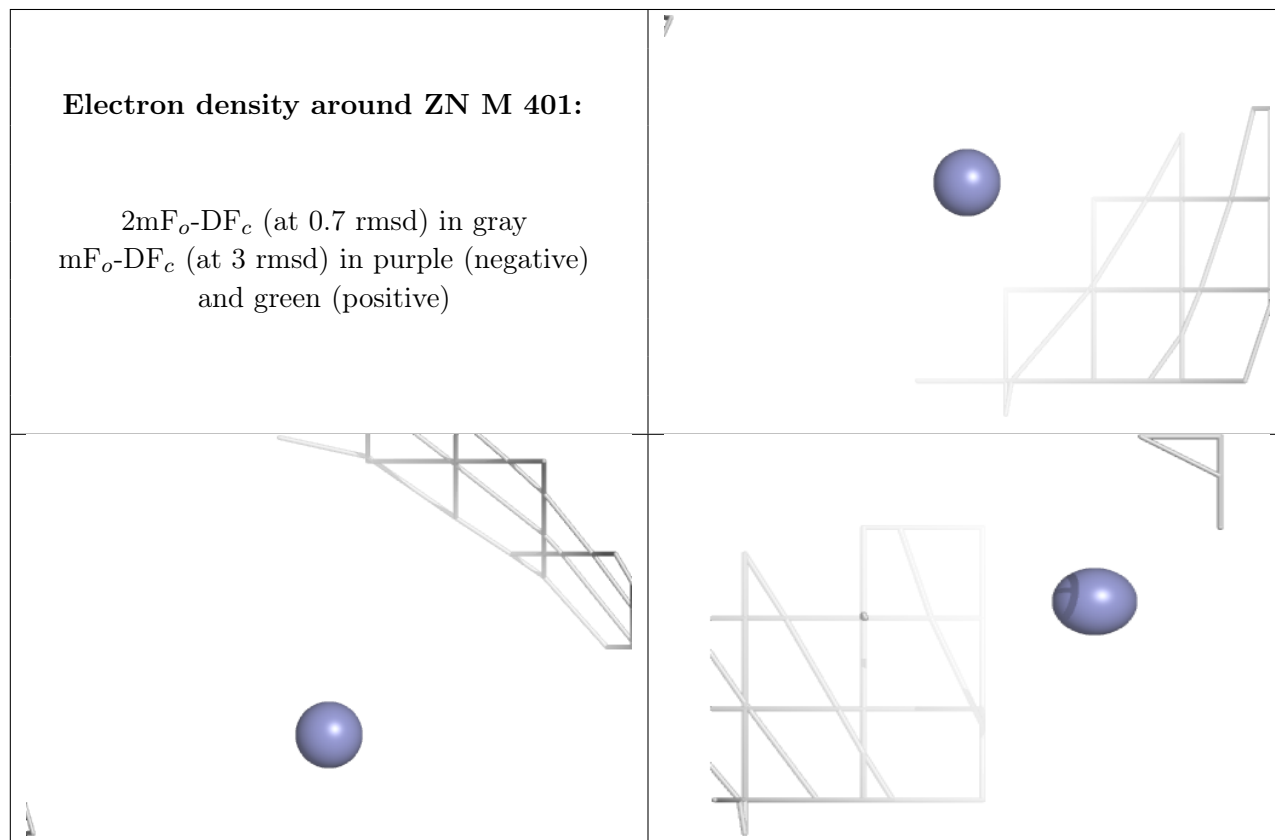


Electron density around ZN K 401:

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

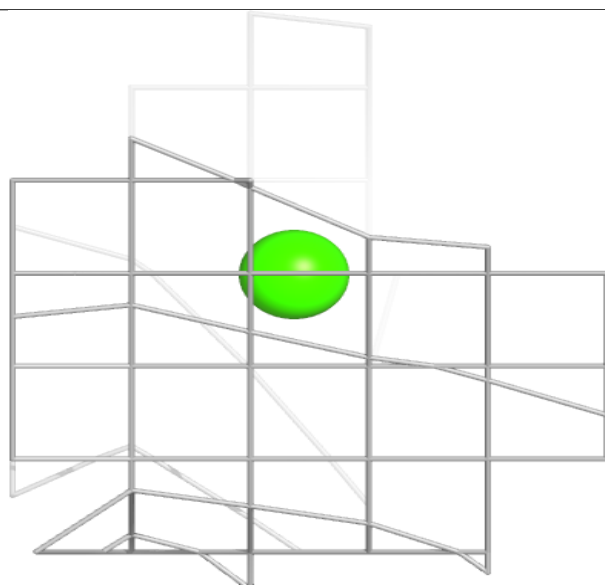
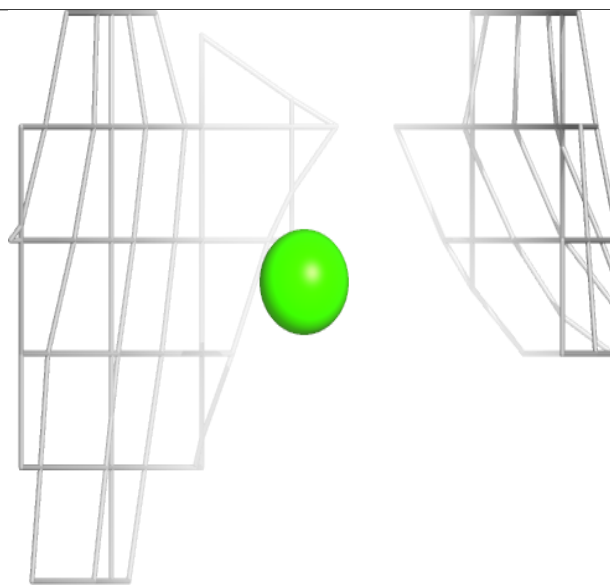
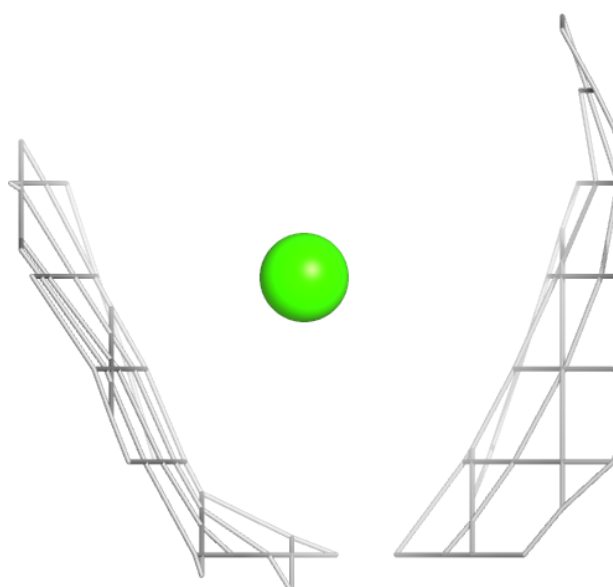
**Electron density around ZN M 401:**

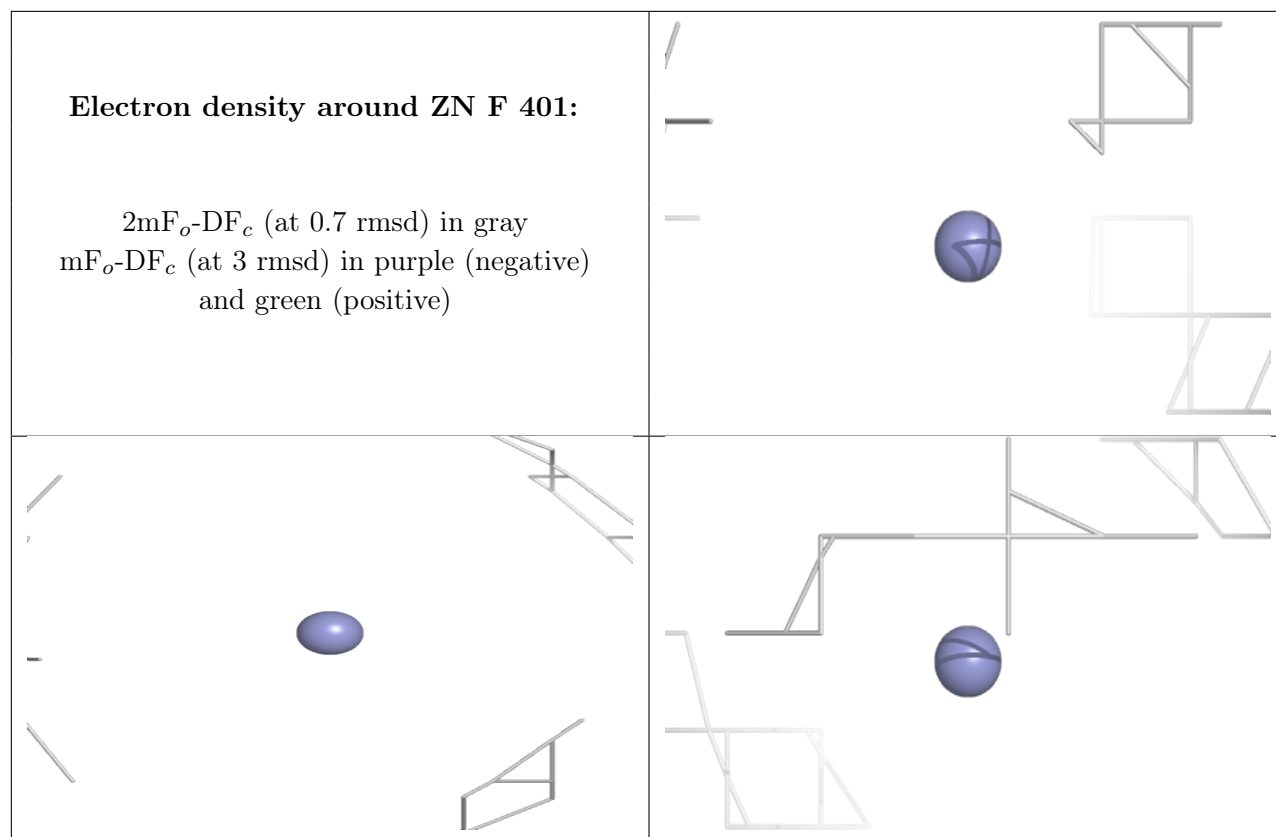
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA H 402:

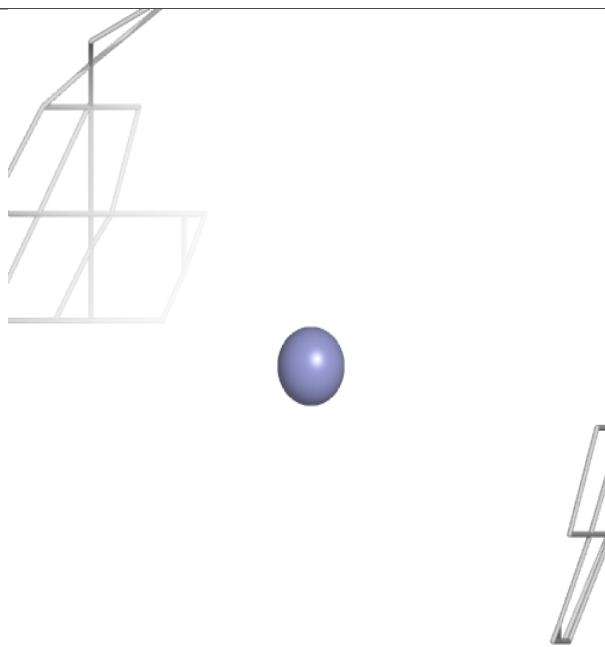
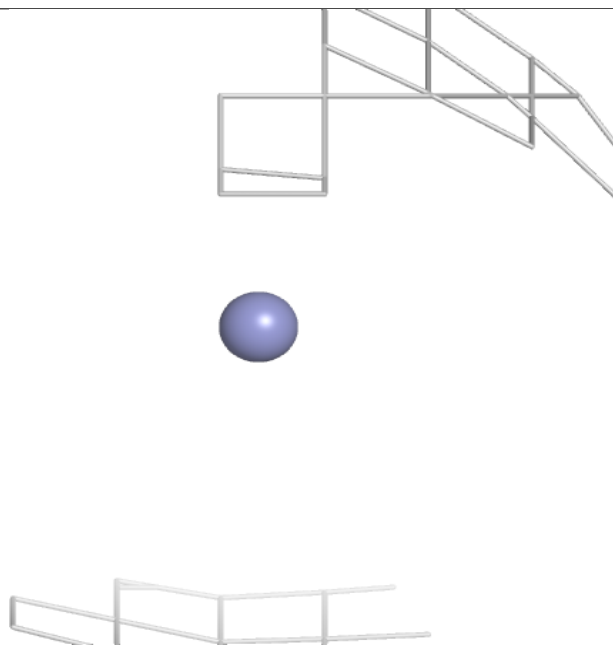
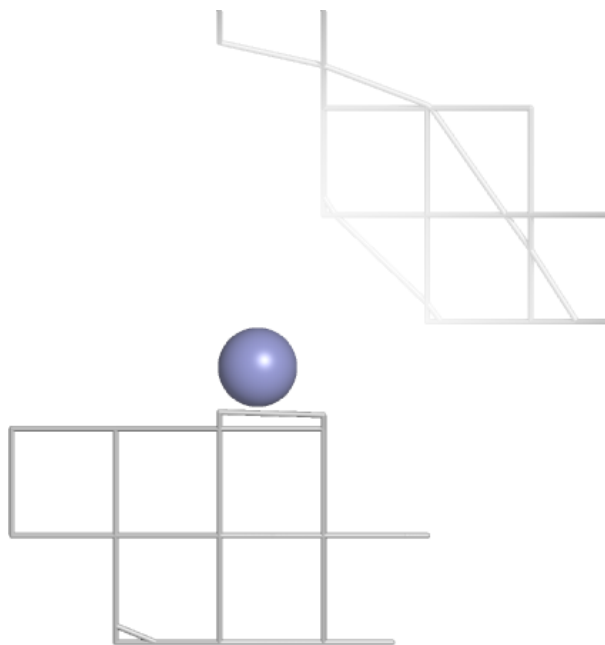
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





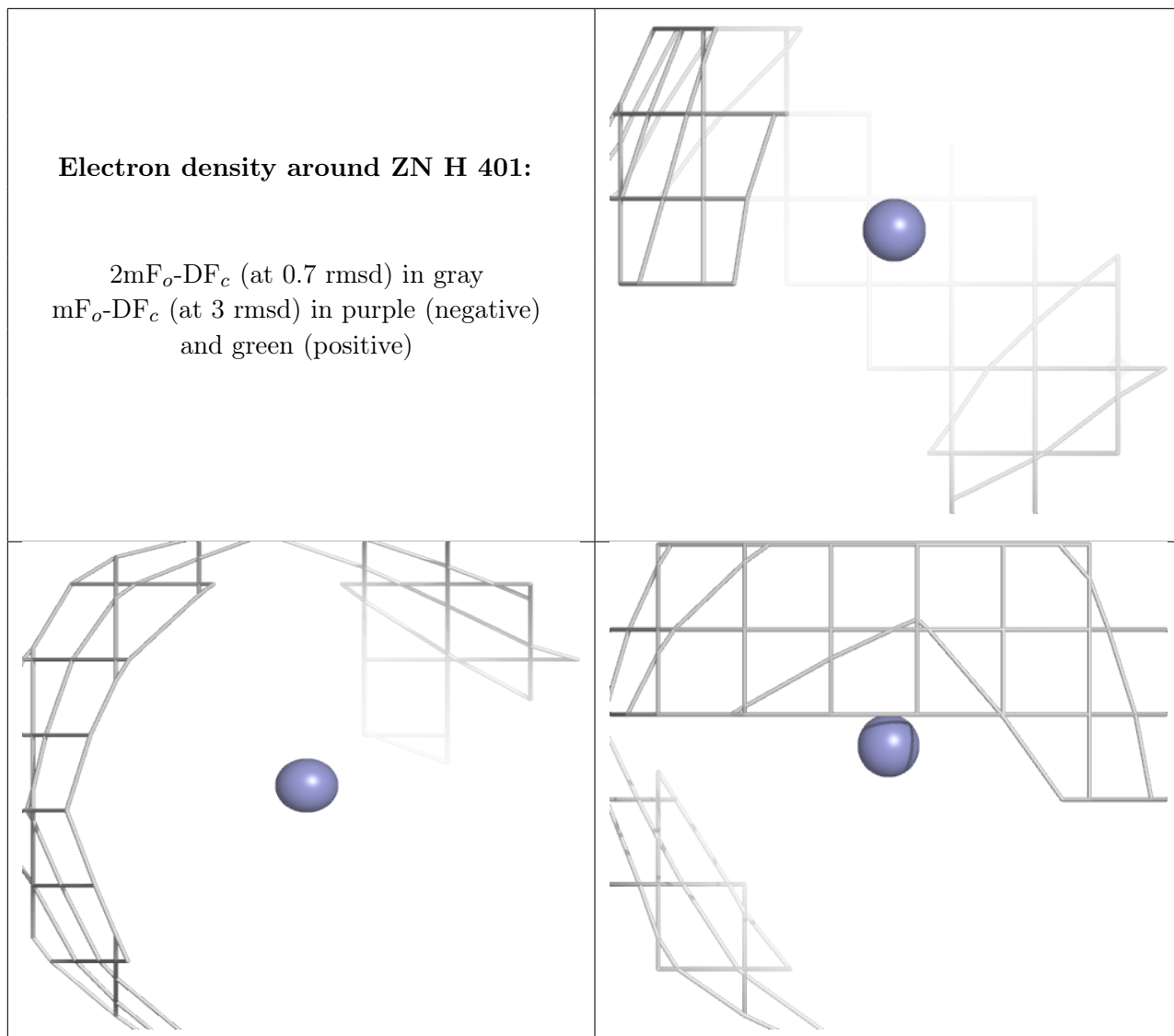
Electron density around ZN A 401:

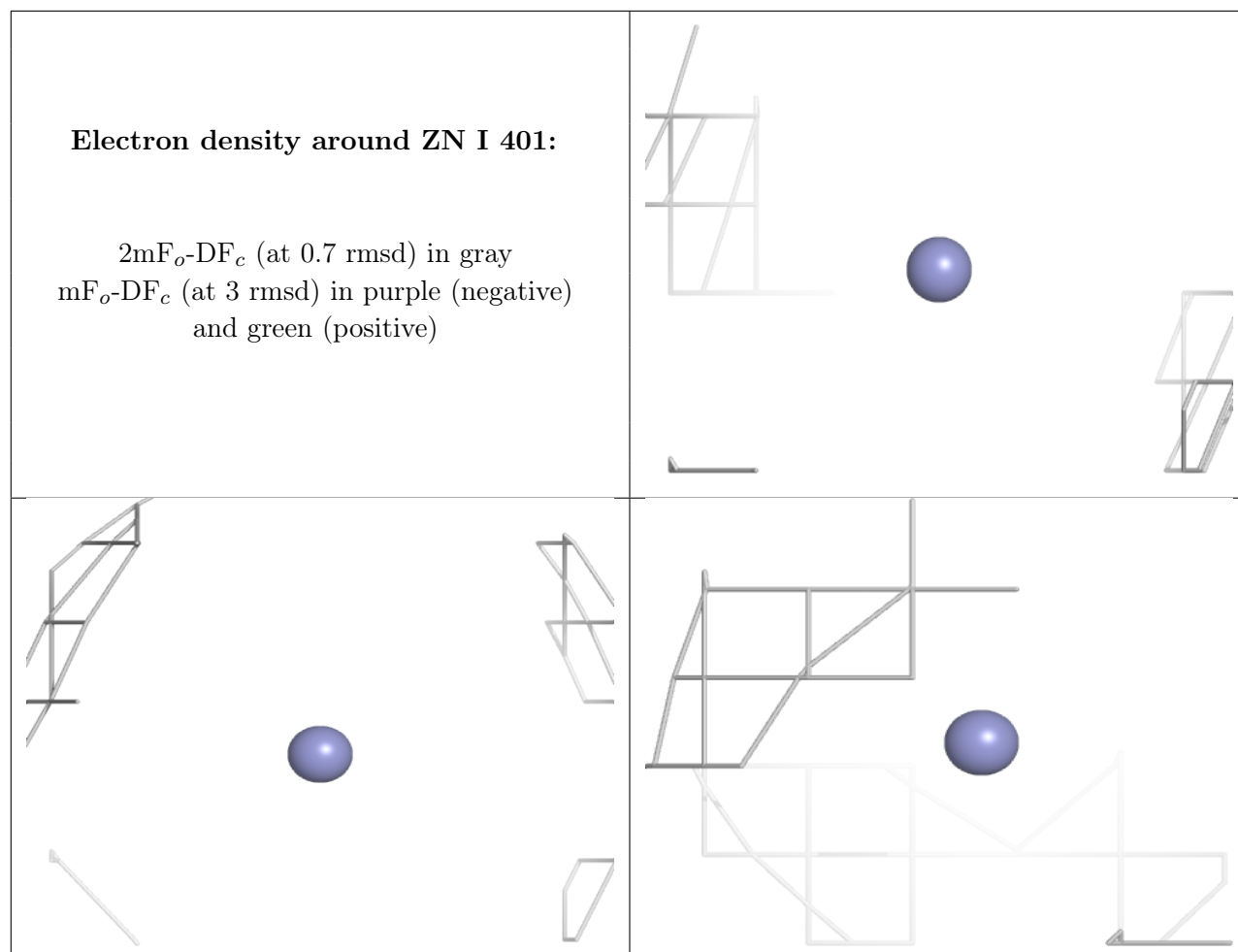
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN H 401:

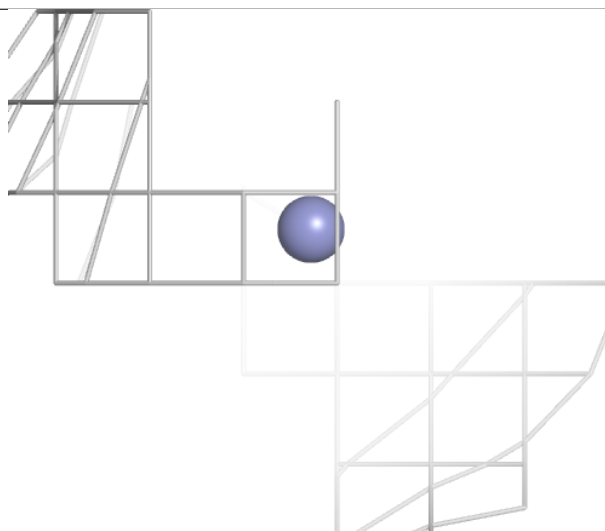
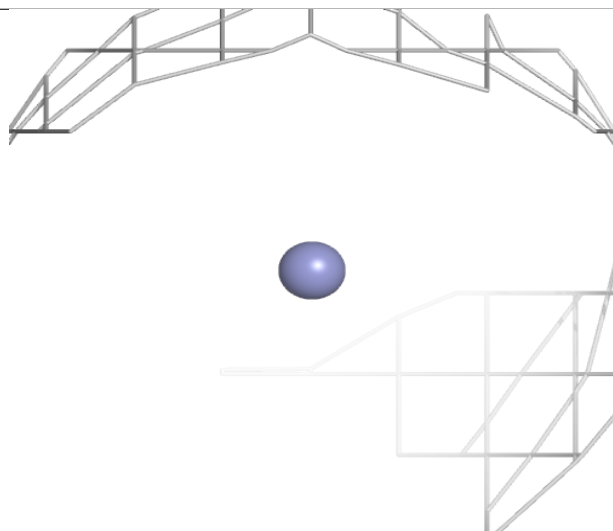
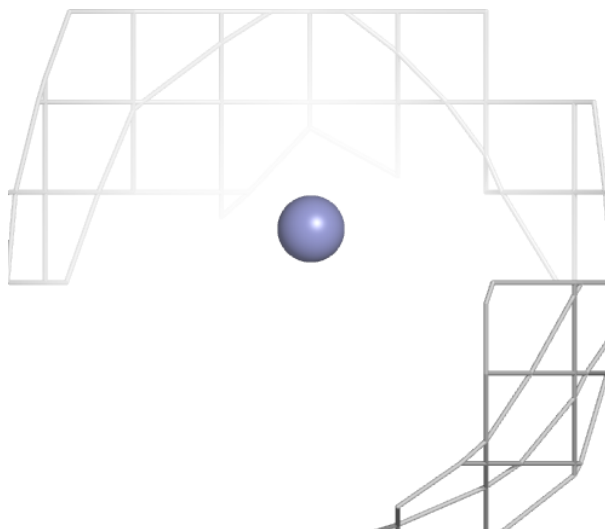
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

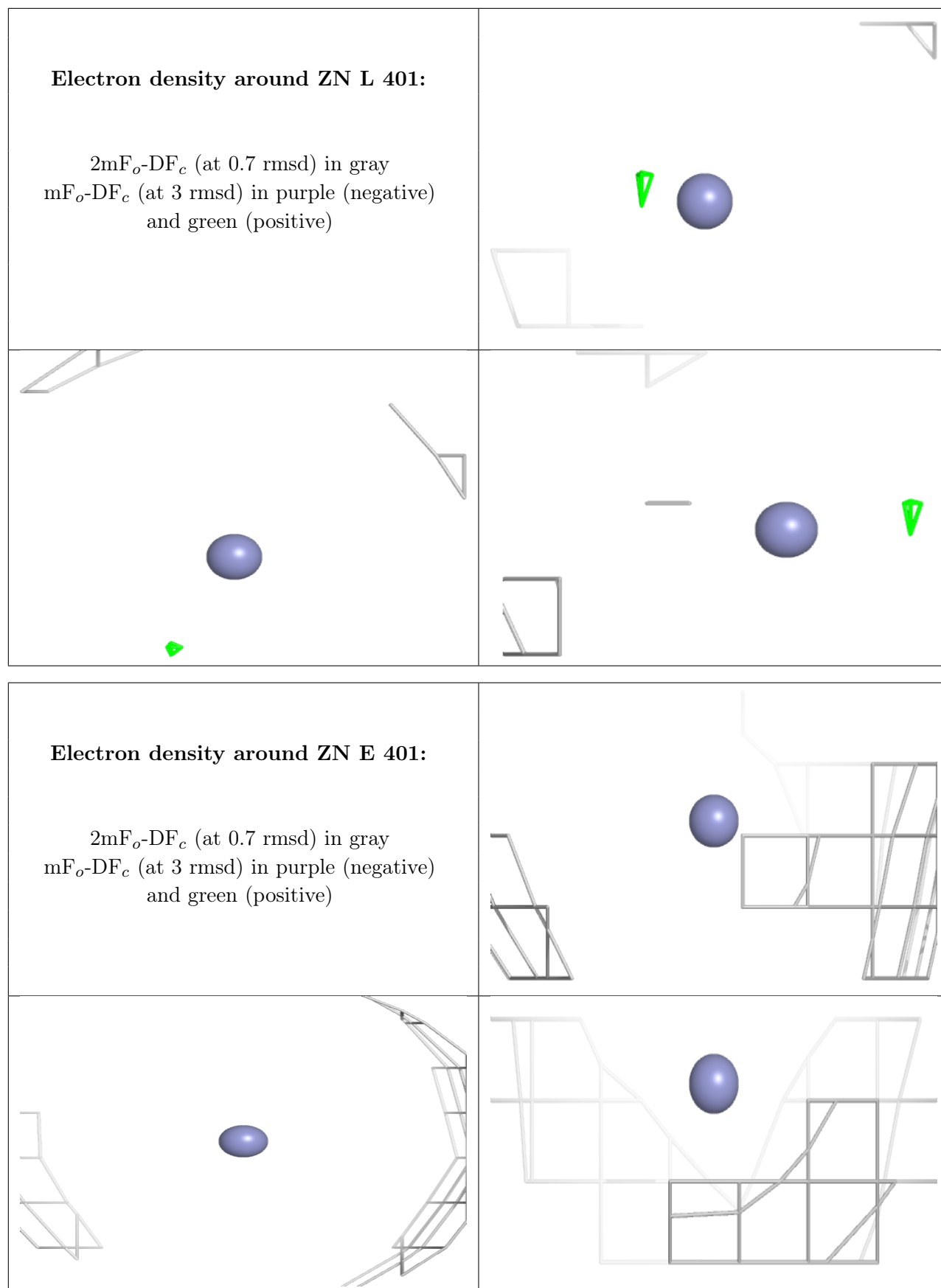




Electron density around ZN B 401:

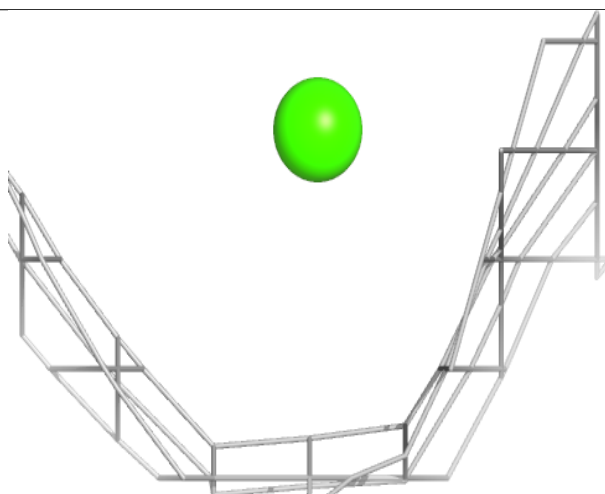
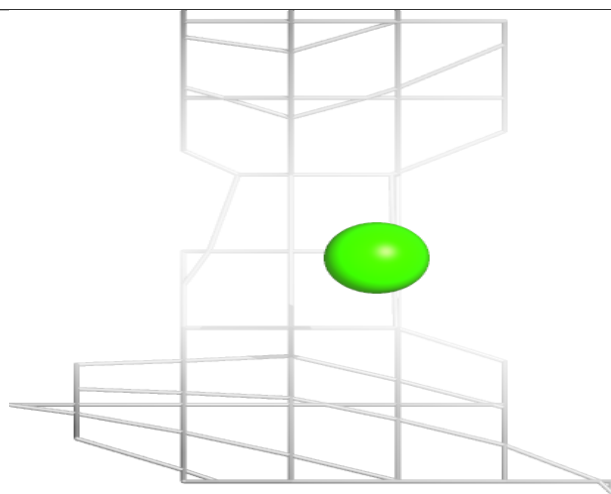
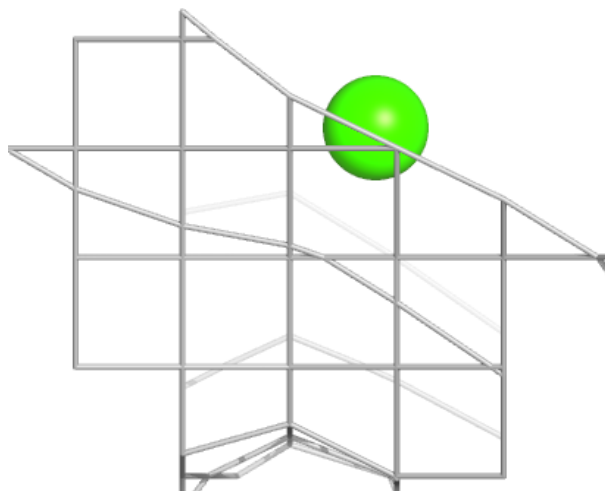
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

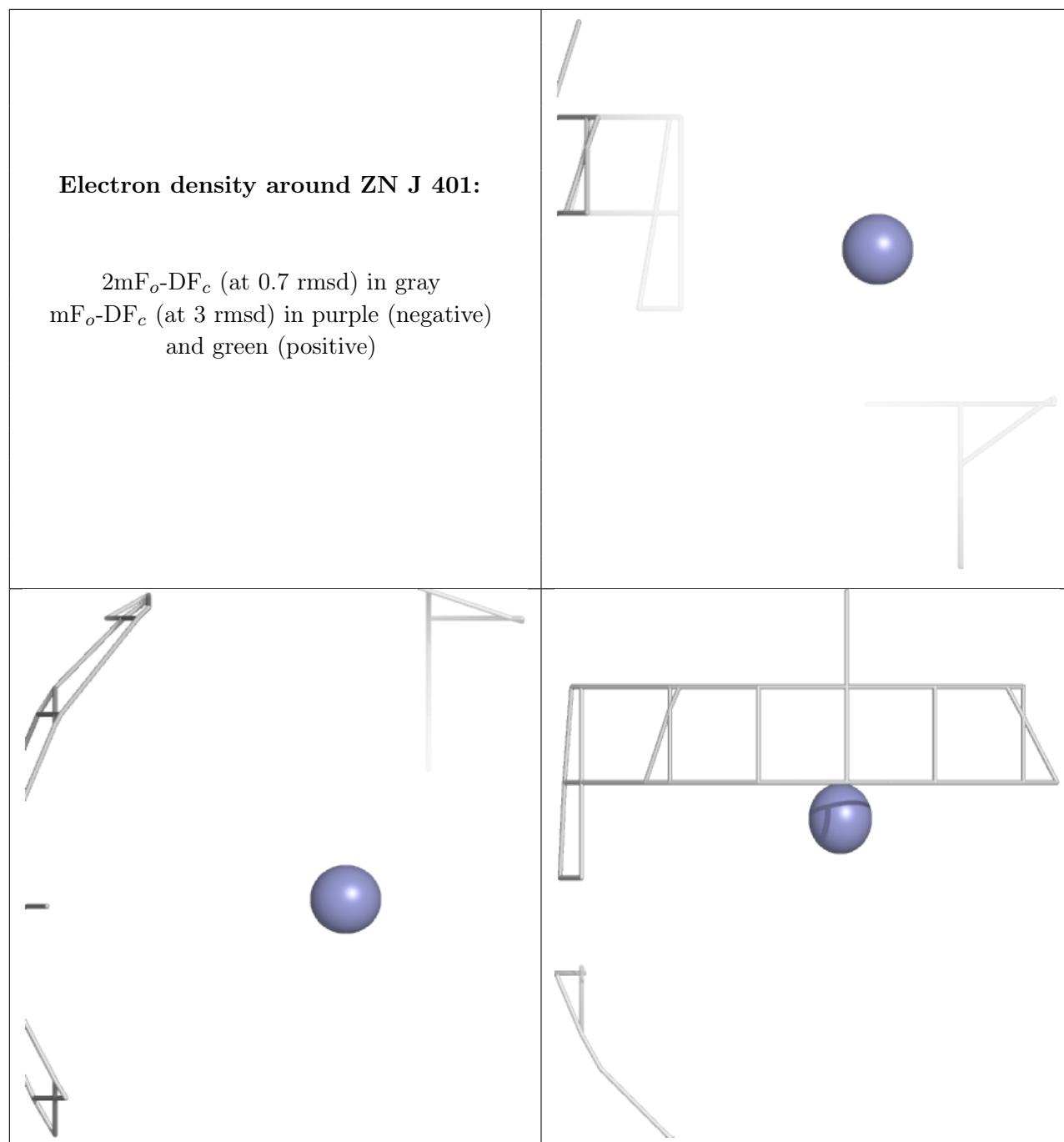




Electron density around CA N 402:

$2mF_o-DF_c$ (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.