



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2026 – 02:29 am BST

PDB ID : 9SLB / pdb_00009slb
Title : Zuzalysin active bi-pentamer
Authors : Rodriguez-Banqueri, A.; Eckhard, U.; Potempa, J.; Gomis Ruth, F.X.
Deposited on : 2025-09-03
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

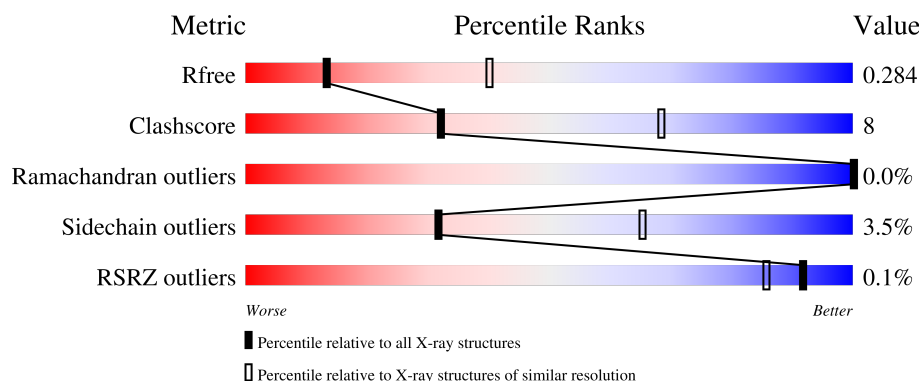
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	828	 74% 19% • 6%
1	B	828	 74% 17% •• 7%
1	C	828	 75% 17% • 7%
1	D	828	 72% 19% •• 7%
1	E	828	 76% 17% • 6%

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Mol	Chain	Length	Quality of chain
1	F	828	73%18%6%
1	G	828	75%17%6%
1	H	828	69%21%6%
1	I	828	70%21%7%
1	J	828	71%21%6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 63321 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 Zinc-dependent metalloprotease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	0	0	0
			6281	4005	1080	1167	29			
1	B	772	Total	C	N	O	S	0	0	0
			6228	3969	1074	1156	29			
1	C	774	Total	C	N	O	S	0	0	0
			6246	3982	1076	1159	29			
1	D	773	Total	C	N	O	S	0	0	0
			6235	3973	1075	1158	29			
1	E	779	Total	C	N	O	S	0	0	0
			6290	4011	1082	1168	29			
1	F	776	Total	C	N	O	S	0	0	0
			6266	3997	1078	1162	29			
1	G	776	Total	C	N	O	S	0	0	0
			6266	3997	1078	1162	29			
1	H	775	Total	C	N	O	S	0	0	0
			6258	3991	1077	1161	29			
1	I	772	Total	C	N	O	S	0	0	0
			6224	3964	1074	1157	29			
1	J	775	Total	C	N	O	S	0	0	0
			6259	3993	1077	1160	29			

There are 190 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0AAF0BD41
A	-12	HIS	-	expression tag	UNP A0AAF0BD41
A	-11	HIS	-	expression tag	UNP A0AAF0BD41
A	-10	HIS	-	expression tag	UNP A0AAF0BD41
A	-9	HIS	-	expression tag	UNP A0AAF0BD41
A	-8	HIS	-	expression tag	UNP A0AAF0BD41
A	-7	HIS	-	expression tag	UNP A0AAF0BD41
A	-6	GLU	-	expression tag	UNP A0AAF0BD41
A	-5	ASN	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP A0AAF0BD41
A	-3	TYR	-	expression tag	UNP A0AAF0BD41
A	-2	PHE	-	expression tag	UNP A0AAF0BD41
A	-1	GLN	-	expression tag	UNP A0AAF0BD41
A	197	MET	VAL	conflict	UNP A0AAF0BD41
A	298	PRO	LEU	conflict	UNP A0AAF0BD41
A	306	VAL	ILE	conflict	UNP A0AAF0BD41
A	751	HIS	TYR	conflict	UNP A0AAF0BD41
A	774	HIS	TYR	conflict	UNP A0AAF0BD41
A	805	ALA	SER	conflict	UNP A0AAF0BD41
B	-13	MET	-	initiating methionine	UNP A0AAF0BD41
B	-12	HIS	-	expression tag	UNP A0AAF0BD41
B	-11	HIS	-	expression tag	UNP A0AAF0BD41
B	-10	HIS	-	expression tag	UNP A0AAF0BD41
B	-9	HIS	-	expression tag	UNP A0AAF0BD41
B	-8	HIS	-	expression tag	UNP A0AAF0BD41
B	-7	HIS	-	expression tag	UNP A0AAF0BD41
B	-6	GLU	-	expression tag	UNP A0AAF0BD41
B	-5	ASN	-	expression tag	UNP A0AAF0BD41
B	-4	LEU	-	expression tag	UNP A0AAF0BD41
B	-3	TYR	-	expression tag	UNP A0AAF0BD41
B	-2	PHE	-	expression tag	UNP A0AAF0BD41
B	-1	GLN	-	expression tag	UNP A0AAF0BD41
B	197	MET	VAL	conflict	UNP A0AAF0BD41
B	298	PRO	LEU	conflict	UNP A0AAF0BD41
B	306	VAL	ILE	conflict	UNP A0AAF0BD41
B	751	HIS	TYR	conflict	UNP A0AAF0BD41
B	774	HIS	TYR	conflict	UNP A0AAF0BD41
B	805	ALA	SER	conflict	UNP A0AAF0BD41
C	-13	MET	-	initiating methionine	UNP A0AAF0BD41
C	-12	HIS	-	expression tag	UNP A0AAF0BD41
C	-11	HIS	-	expression tag	UNP A0AAF0BD41
C	-10	HIS	-	expression tag	UNP A0AAF0BD41
C	-9	HIS	-	expression tag	UNP A0AAF0BD41
C	-8	HIS	-	expression tag	UNP A0AAF0BD41
C	-7	HIS	-	expression tag	UNP A0AAF0BD41
C	-6	GLU	-	expression tag	UNP A0AAF0BD41
C	-5	ASN	-	expression tag	UNP A0AAF0BD41
C	-4	LEU	-	expression tag	UNP A0AAF0BD41
C	-3	TYR	-	expression tag	UNP A0AAF0BD41
C	-2	PHE	-	expression tag	UNP A0AAF0BD41
C	-1	GLN	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	197	MET	VAL	conflict	UNP A0AAF0BD41
C	298	PRO	LEU	conflict	UNP A0AAF0BD41
C	306	VAL	ILE	conflict	UNP A0AAF0BD41
C	751	HIS	TYR	conflict	UNP A0AAF0BD41
C	774	HIS	TYR	conflict	UNP A0AAF0BD41
C	805	ALA	SER	conflict	UNP A0AAF0BD41
D	-13	MET	-	initiating methionine	UNP A0AAF0BD41
D	-12	HIS	-	expression tag	UNP A0AAF0BD41
D	-11	HIS	-	expression tag	UNP A0AAF0BD41
D	-10	HIS	-	expression tag	UNP A0AAF0BD41
D	-9	HIS	-	expression tag	UNP A0AAF0BD41
D	-8	HIS	-	expression tag	UNP A0AAF0BD41
D	-7	HIS	-	expression tag	UNP A0AAF0BD41
D	-6	GLU	-	expression tag	UNP A0AAF0BD41
D	-5	ASN	-	expression tag	UNP A0AAF0BD41
D	-4	LEU	-	expression tag	UNP A0AAF0BD41
D	-3	TYR	-	expression tag	UNP A0AAF0BD41
D	-2	PHE	-	expression tag	UNP A0AAF0BD41
D	-1	GLN	-	expression tag	UNP A0AAF0BD41
D	197	MET	VAL	conflict	UNP A0AAF0BD41
D	298	PRO	LEU	conflict	UNP A0AAF0BD41
D	306	VAL	ILE	conflict	UNP A0AAF0BD41
D	751	HIS	TYR	conflict	UNP A0AAF0BD41
D	774	HIS	TYR	conflict	UNP A0AAF0BD41
D	805	ALA	SER	conflict	UNP A0AAF0BD41
E	-13	MET	-	initiating methionine	UNP A0AAF0BD41
E	-12	HIS	-	expression tag	UNP A0AAF0BD41
E	-11	HIS	-	expression tag	UNP A0AAF0BD41
E	-10	HIS	-	expression tag	UNP A0AAF0BD41
E	-9	HIS	-	expression tag	UNP A0AAF0BD41
E	-8	HIS	-	expression tag	UNP A0AAF0BD41
E	-7	HIS	-	expression tag	UNP A0AAF0BD41
E	-6	GLU	-	expression tag	UNP A0AAF0BD41
E	-5	ASN	-	expression tag	UNP A0AAF0BD41
E	-4	LEU	-	expression tag	UNP A0AAF0BD41
E	-3	TYR	-	expression tag	UNP A0AAF0BD41
E	-2	PHE	-	expression tag	UNP A0AAF0BD41
E	-1	GLN	-	expression tag	UNP A0AAF0BD41
E	197	MET	VAL	conflict	UNP A0AAF0BD41
E	298	PRO	LEU	conflict	UNP A0AAF0BD41
E	306	VAL	ILE	conflict	UNP A0AAF0BD41
E	751	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
E	774	HIS	TYR	conflict	UNP A0AAF0BD41
E	805	ALA	SER	conflict	UNP A0AAF0BD41
F	-13	MET	-	initiating methionine	UNP A0AAF0BD41
F	-12	HIS	-	expression tag	UNP A0AAF0BD41
F	-11	HIS	-	expression tag	UNP A0AAF0BD41
F	-10	HIS	-	expression tag	UNP A0AAF0BD41
F	-9	HIS	-	expression tag	UNP A0AAF0BD41
F	-8	HIS	-	expression tag	UNP A0AAF0BD41
F	-7	HIS	-	expression tag	UNP A0AAF0BD41
F	-6	GLU	-	expression tag	UNP A0AAF0BD41
F	-5	ASN	-	expression tag	UNP A0AAF0BD41
F	-4	LEU	-	expression tag	UNP A0AAF0BD41
F	-3	TYR	-	expression tag	UNP A0AAF0BD41
F	-2	PHE	-	expression tag	UNP A0AAF0BD41
F	-1	GLN	-	expression tag	UNP A0AAF0BD41
F	197	MET	VAL	conflict	UNP A0AAF0BD41
F	298	PRO	LEU	conflict	UNP A0AAF0BD41
F	306	VAL	ILE	conflict	UNP A0AAF0BD41
F	751	HIS	TYR	conflict	UNP A0AAF0BD41
F	774	HIS	TYR	conflict	UNP A0AAF0BD41
F	805	ALA	SER	conflict	UNP A0AAF0BD41
G	-13	MET	-	initiating methionine	UNP A0AAF0BD41
G	-12	HIS	-	expression tag	UNP A0AAF0BD41
G	-11	HIS	-	expression tag	UNP A0AAF0BD41
G	-10	HIS	-	expression tag	UNP A0AAF0BD41
G	-9	HIS	-	expression tag	UNP A0AAF0BD41
G	-8	HIS	-	expression tag	UNP A0AAF0BD41
G	-7	HIS	-	expression tag	UNP A0AAF0BD41
G	-6	GLU	-	expression tag	UNP A0AAF0BD41
G	-5	ASN	-	expression tag	UNP A0AAF0BD41
G	-4	LEU	-	expression tag	UNP A0AAF0BD41
G	-3	TYR	-	expression tag	UNP A0AAF0BD41
G	-2	PHE	-	expression tag	UNP A0AAF0BD41
G	-1	GLN	-	expression tag	UNP A0AAF0BD41
G	197	MET	VAL	conflict	UNP A0AAF0BD41
G	298	PRO	LEU	conflict	UNP A0AAF0BD41
G	306	VAL	ILE	conflict	UNP A0AAF0BD41
G	751	HIS	TYR	conflict	UNP A0AAF0BD41
G	774	HIS	TYR	conflict	UNP A0AAF0BD41
G	805	ALA	SER	conflict	UNP A0AAF0BD41
H	-13	MET	-	initiating methionine	UNP A0AAF0BD41
H	-12	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	HIS	-	expression tag	UNP A0AAF0BD41
H	-10	HIS	-	expression tag	UNP A0AAF0BD41
H	-9	HIS	-	expression tag	UNP A0AAF0BD41
H	-8	HIS	-	expression tag	UNP A0AAF0BD41
H	-7	HIS	-	expression tag	UNP A0AAF0BD41
H	-6	GLU	-	expression tag	UNP A0AAF0BD41
H	-5	ASN	-	expression tag	UNP A0AAF0BD41
H	-4	LEU	-	expression tag	UNP A0AAF0BD41
H	-3	TYR	-	expression tag	UNP A0AAF0BD41
H	-2	PHE	-	expression tag	UNP A0AAF0BD41
H	-1	GLN	-	expression tag	UNP A0AAF0BD41
H	197	MET	VAL	conflict	UNP A0AAF0BD41
H	298	PRO	LEU	conflict	UNP A0AAF0BD41
H	306	VAL	ILE	conflict	UNP A0AAF0BD41
H	751	HIS	TYR	conflict	UNP A0AAF0BD41
H	774	HIS	TYR	conflict	UNP A0AAF0BD41
H	805	ALA	SER	conflict	UNP A0AAF0BD41
I	-13	MET	-	initiating methionine	UNP A0AAF0BD41
I	-12	HIS	-	expression tag	UNP A0AAF0BD41
I	-11	HIS	-	expression tag	UNP A0AAF0BD41
I	-10	HIS	-	expression tag	UNP A0AAF0BD41
I	-9	HIS	-	expression tag	UNP A0AAF0BD41
I	-8	HIS	-	expression tag	UNP A0AAF0BD41
I	-7	HIS	-	expression tag	UNP A0AAF0BD41
I	-6	GLU	-	expression tag	UNP A0AAF0BD41
I	-5	ASN	-	expression tag	UNP A0AAF0BD41
I	-4	LEU	-	expression tag	UNP A0AAF0BD41
I	-3	TYR	-	expression tag	UNP A0AAF0BD41
I	-2	PHE	-	expression tag	UNP A0AAF0BD41
I	-1	GLN	-	expression tag	UNP A0AAF0BD41
I	197	MET	VAL	conflict	UNP A0AAF0BD41
I	298	PRO	LEU	conflict	UNP A0AAF0BD41
I	306	VAL	ILE	conflict	UNP A0AAF0BD41
I	751	HIS	TYR	conflict	UNP A0AAF0BD41
I	774	HIS	TYR	conflict	UNP A0AAF0BD41
I	805	ALA	SER	conflict	UNP A0AAF0BD41
J	-13	MET	-	initiating methionine	UNP A0AAF0BD41
J	-12	HIS	-	expression tag	UNP A0AAF0BD41
J	-11	HIS	-	expression tag	UNP A0AAF0BD41
J	-10	HIS	-	expression tag	UNP A0AAF0BD41
J	-9	HIS	-	expression tag	UNP A0AAF0BD41
J	-8	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-7	HIS	-	expression tag	UNP A0AAF0BD41
J	-6	GLU	-	expression tag	UNP A0AAF0BD41
J	-5	ASN	-	expression tag	UNP A0AAF0BD41
J	-4	LEU	-	expression tag	UNP A0AAF0BD41
J	-3	TYR	-	expression tag	UNP A0AAF0BD41
J	-2	PHE	-	expression tag	UNP A0AAF0BD41
J	-1	GLN	-	expression tag	UNP A0AAF0BD41
J	197	MET	VAL	conflict	UNP A0AAF0BD41
J	298	PRO	LEU	conflict	UNP A0AAF0BD41
J	306	VAL	ILE	conflict	UNP A0AAF0BD41
J	751	HIS	TYR	conflict	UNP A0AAF0BD41
J	774	HIS	TYR	conflict	UNP A0AAF0BD41
J	805	ALA	SER	conflict	UNP A0AAF0BD41

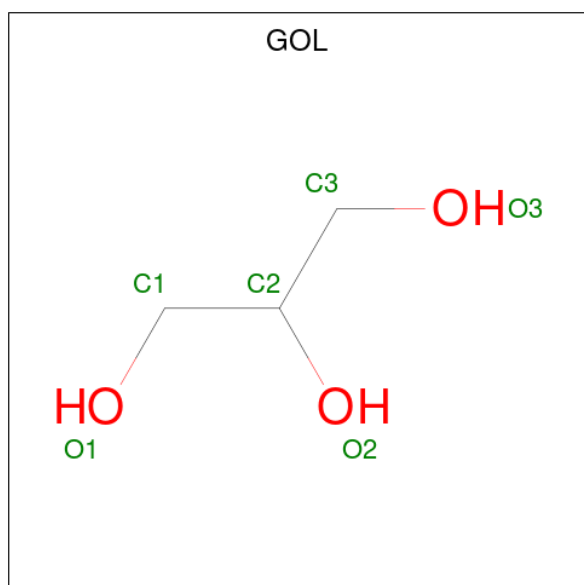
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



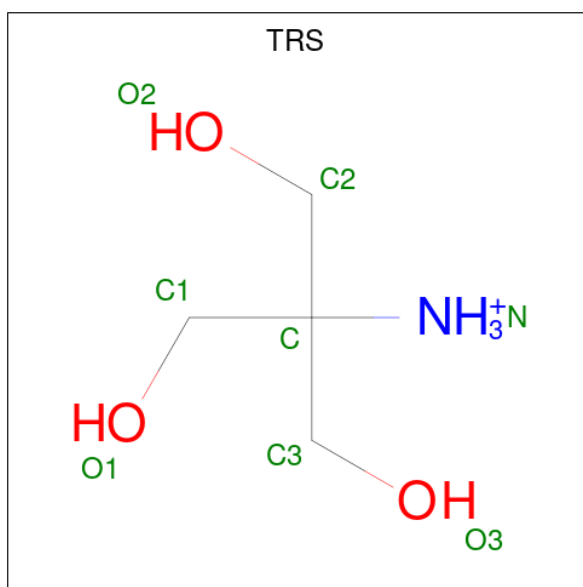
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	I	1	Total 6	C 3	O 3	0	0
4	J	1	Total 6	C 3	O 3	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

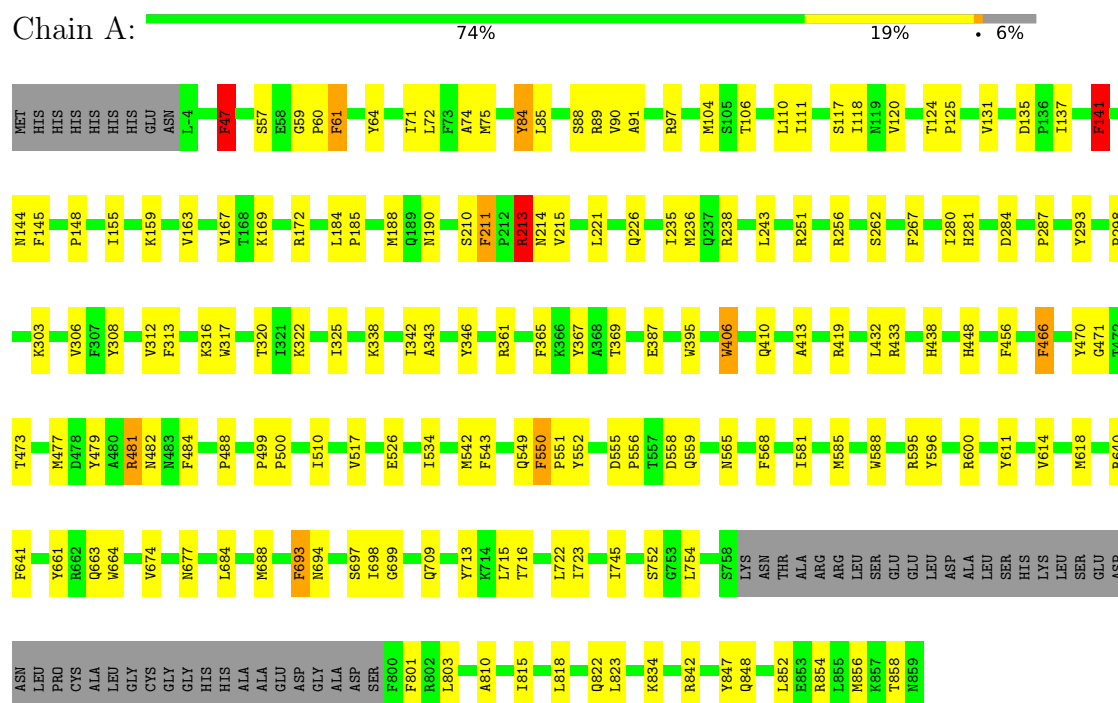
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	92	Total	O	0	0
			92	92		
6	B	99	Total	O	0	0
			99	99		
6	C	57	Total	O	0	0
			57	57		
6	D	69	Total	O	0	0
			69	69		
6	E	92	Total	O	0	0
			92	92		
6	F	59	Total	O	0	0
			59	59		
6	G	38	Total	O	0	0
			38	38		
6	H	23	Total	O	0	0
			23	23		
6	I	36	Total	O	0	0
			36	36		
6	J	49	Total	O	0	0
			49	49		

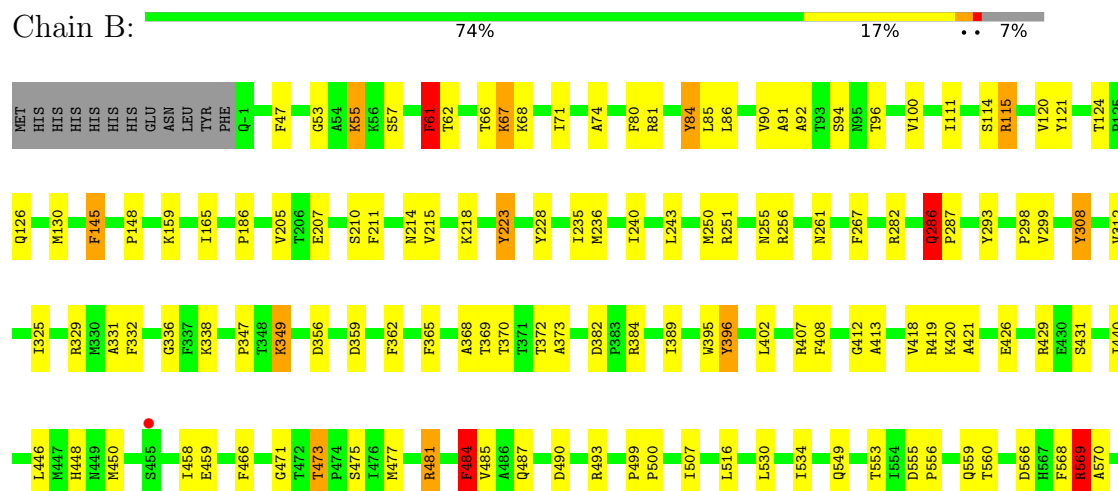
3 Residue-property plots

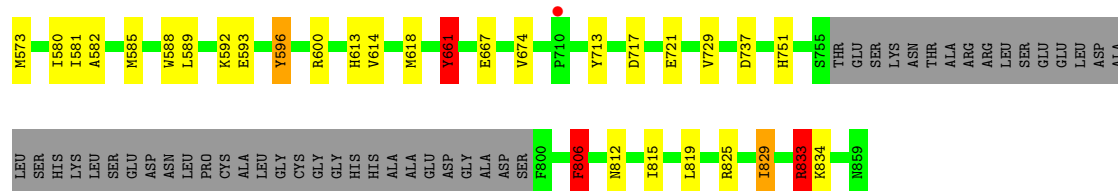
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Zinc-dependent metalloprotease



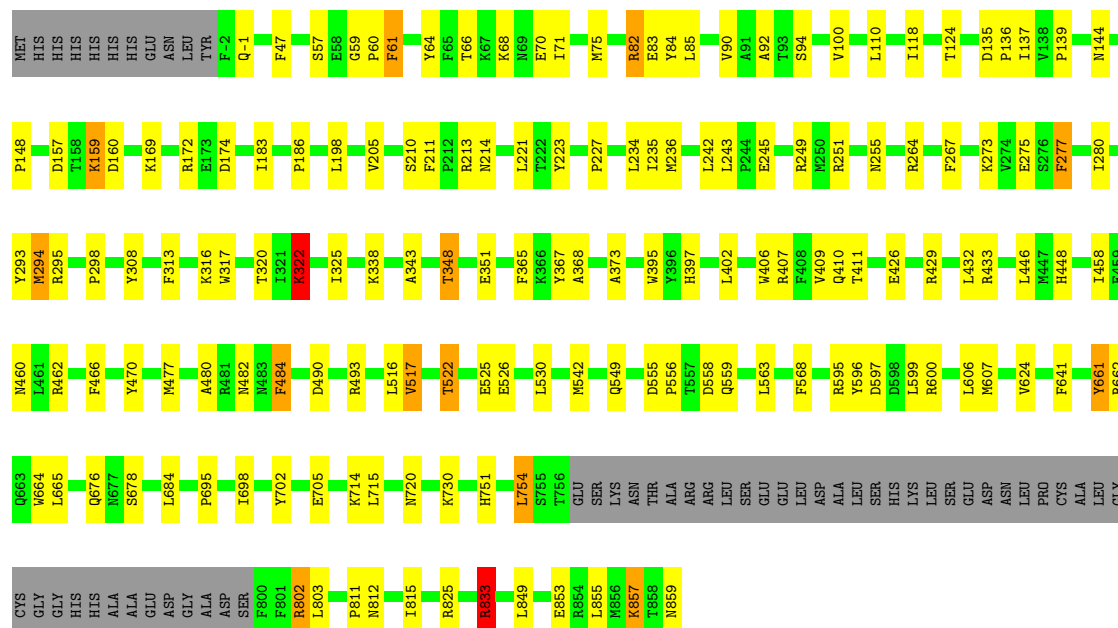
• Molecule 1: Zinc-dependent metalloprotease





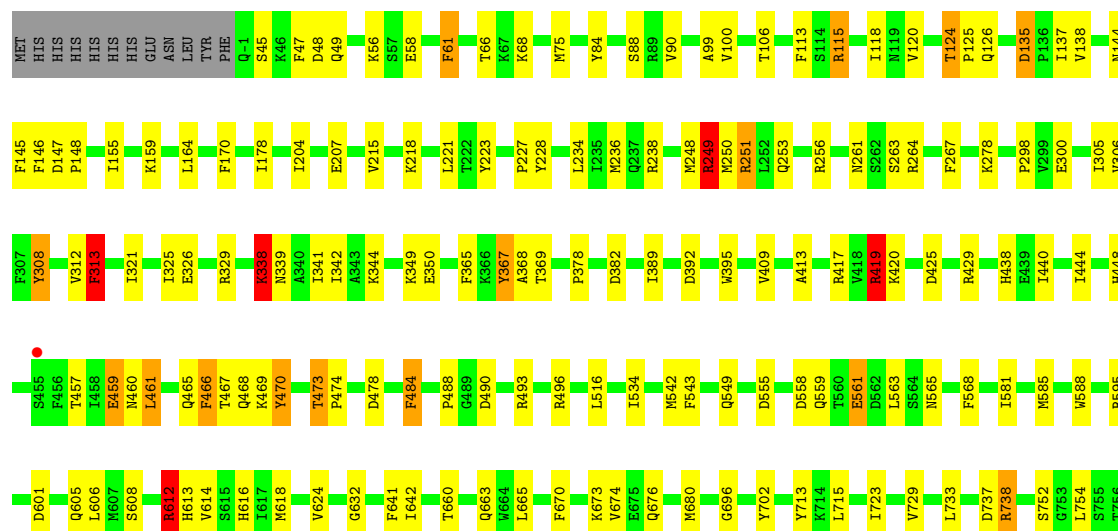
• Molecule 1: Zinc-dependent metalloprotease

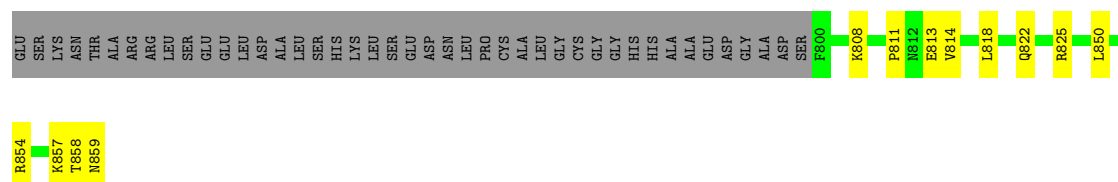
Chain C: 75% 17% 7%



• Molecule 1: Zinc-dependent metalloprotease

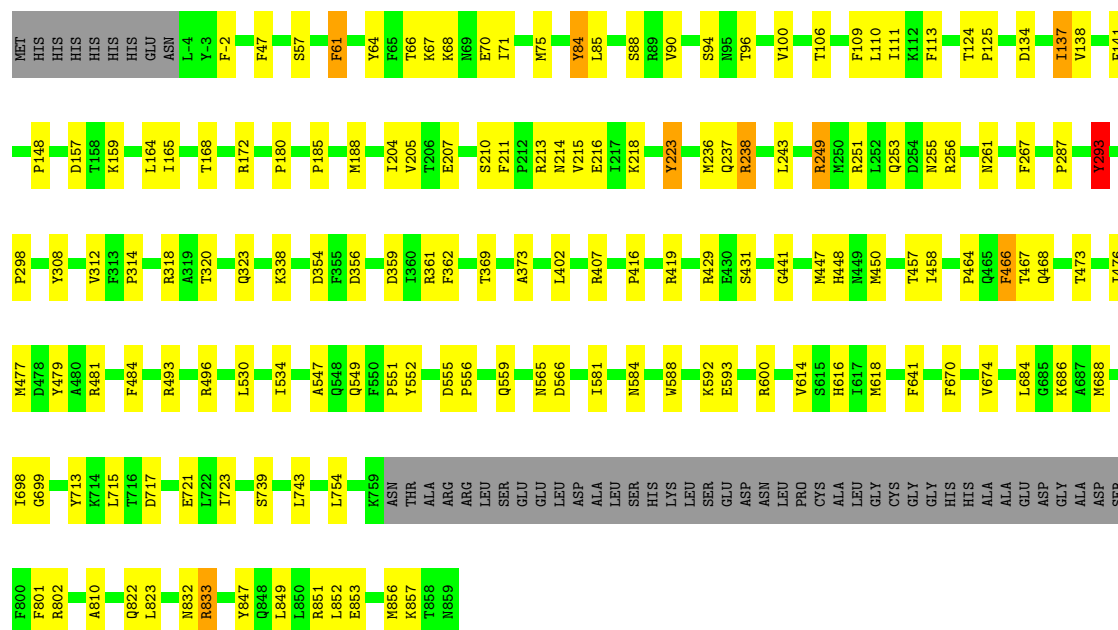
Chain D: 72% 19% 7%





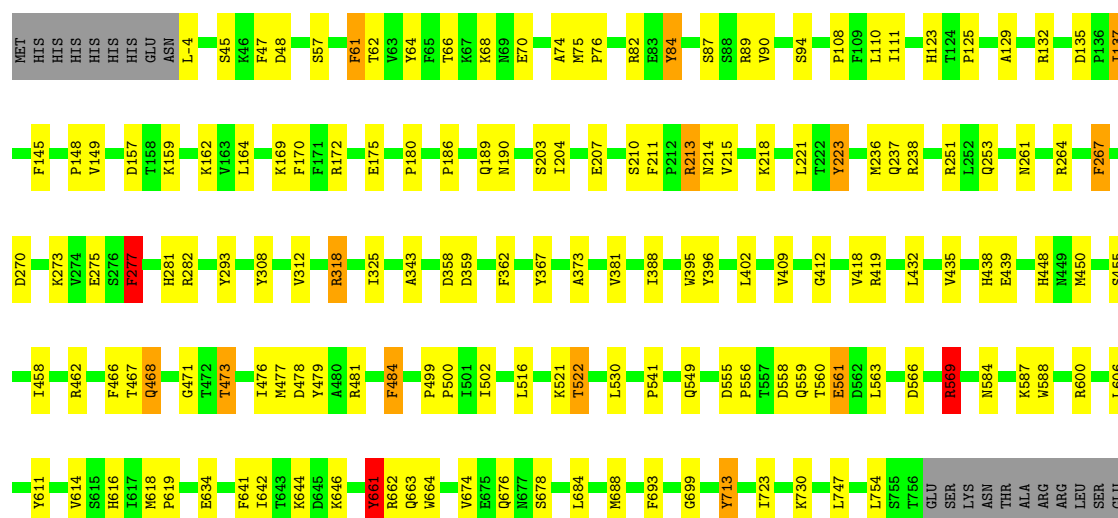
- Molecule 1: Zinc-dependent metalloprotease

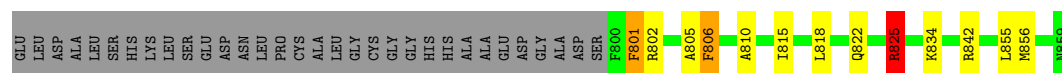
Chain E: 76% 17% 6%



- Molecule 1: Zinc-dependent metalloprotease

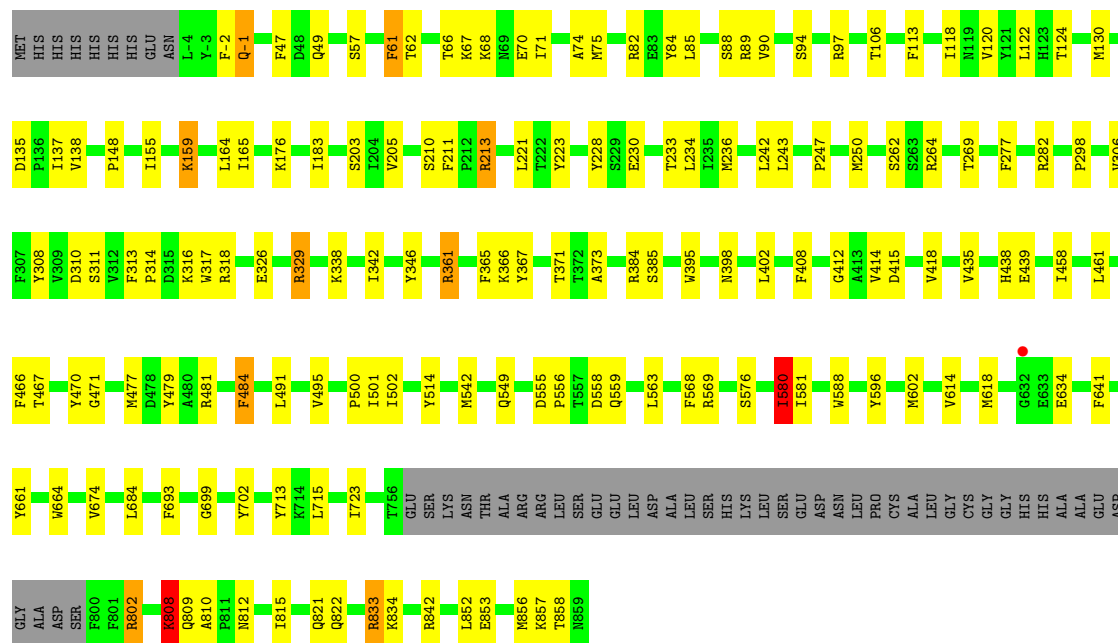
Chain F: 73% 18% 6%





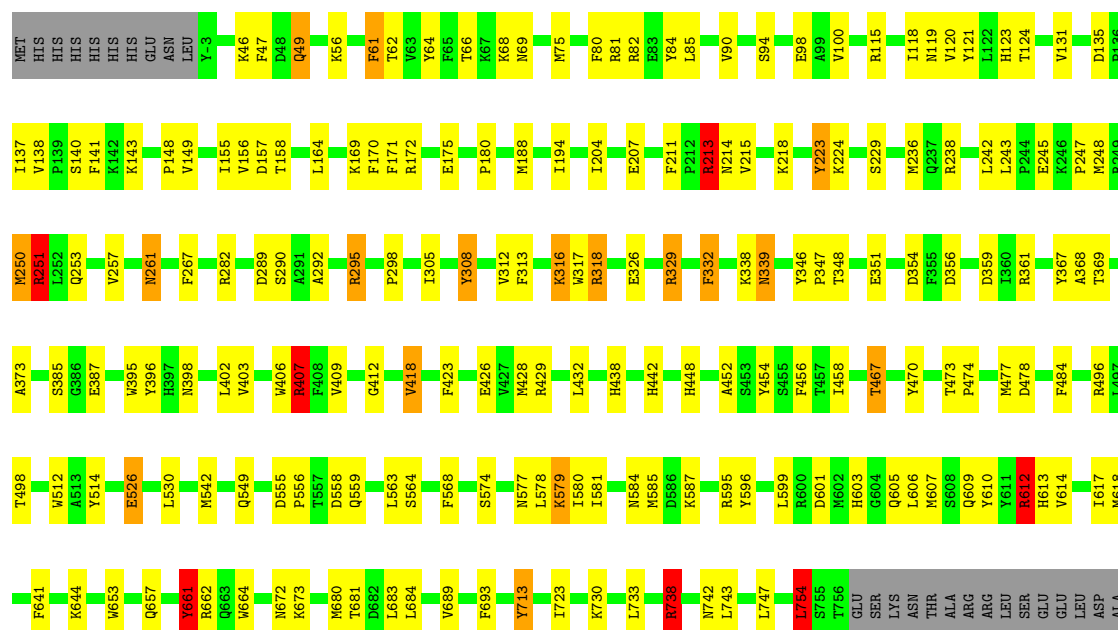
• Molecule 1: Zinc-dependent metalloprotease

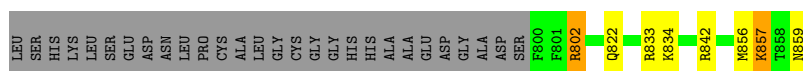
Chain G: 75% 17% 6%



• Molecule 1: Zinc-dependent metalloprotease

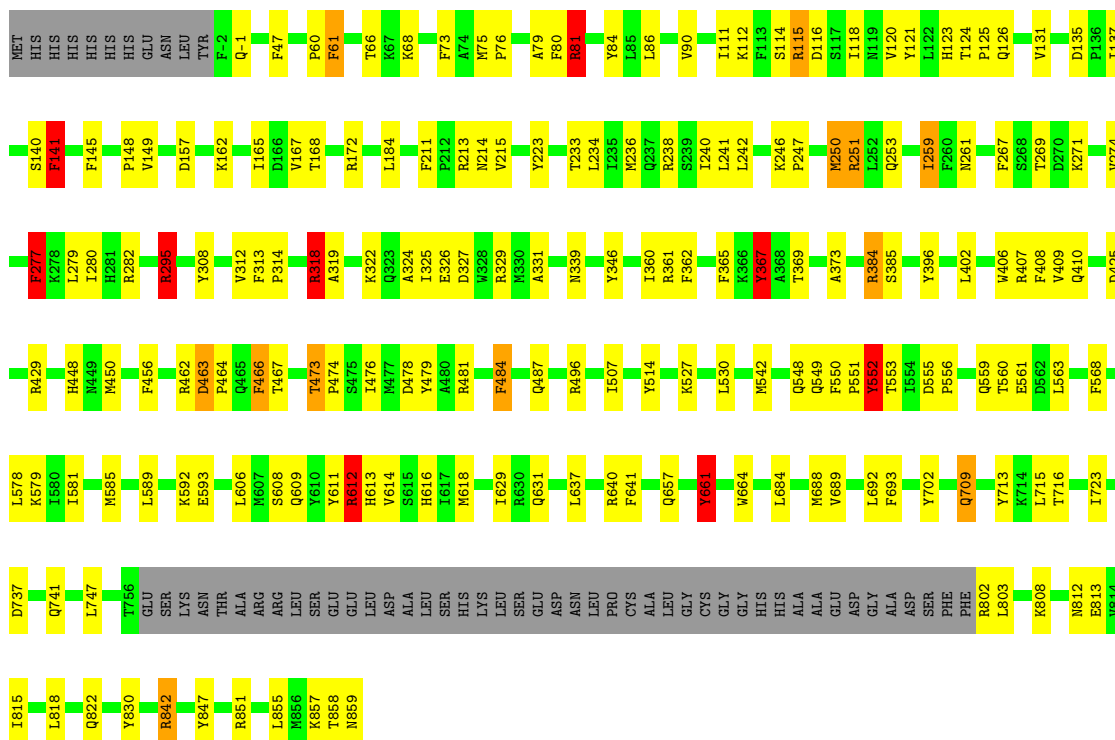
Chain H: 69% 21% 6%





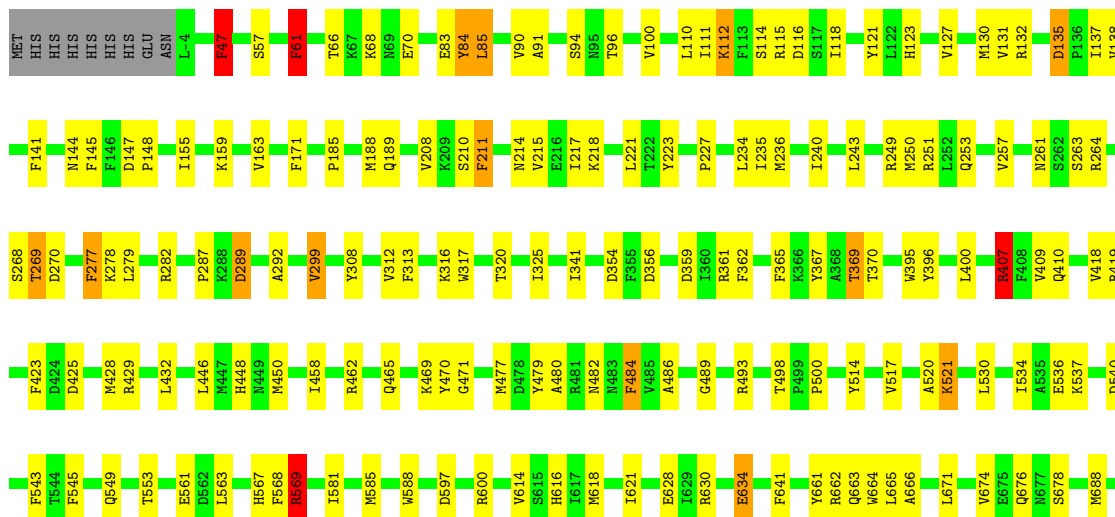
• Molecule 1: Zinc-dependent metalloprotease

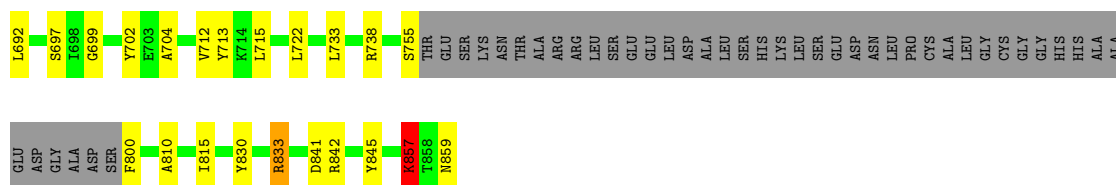
Chain I: 70% 21% 7%



• Molecule 1: Zinc-dependent metalloprotease

Chain J: 71% 21% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	129.80Å 129.40Å 188.50Å 98.20° 104.70° 115.10°	Depositor
Resolution (Å)	84.16 – 3.00 84.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (84.16-3.00) 96.5 (84.16-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX 2.0rc1_5617	Depositor
R, R_{free}	0.257 , 0.296 0.257 , 0.284	Depositor DCC
R_{free} test set	998 reflections (0.48%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.158 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	63321	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, GOL, CA, ZN

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	0.46	0/6432	0.84	13/8708 (0.1%)
1	B	0.47	0/6377	0.87	15/8633 (0.2%)
1	C	0.46	1/6396 (0.0%)	0.84	6/8659 (0.1%)
1	D	0.51	4/6384 (0.1%)	0.91	21/8643 (0.2%)
1	E	0.48	1/6441 (0.0%)	0.83	10/8719 (0.1%)
1	F	0.48	2/6417 (0.0%)	0.87	22/8688 (0.3%)
1	G	0.45	4/6417 (0.1%)	0.82	12/8688 (0.1%)
1	H	0.51	3/6409 (0.0%)	0.93	24/8677 (0.3%)
1	I	0.55	3/6372 (0.0%)	0.93	17/8627 (0.2%)
1	J	0.48	2/6410 (0.0%)	0.91	17/8678 (0.2%)
All	All	0.49	20/64055 (0.0%)	0.88	157/86720 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
1	C	0	5
1	D	0	6
1	E	0	3
1	F	0	8
1	G	0	4
1	H	0	7
1	I	0	10
1	J	0	3
All	All	0	54

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	329	ARG	CZ-NH1	9.46	1.46	1.32
1	E	138	VAL	CA-CB	9.31	1.60	1.53
1	I	259	ILE	CG1-CD1	9.20	1.87	1.51
1	J	138	VAL	CA-CB	7.63	1.59	1.53
1	F	825	ARG	CZ-NH1	7.34	1.43	1.32
1	G	329	ARG	CB-CG	-7.10	1.31	1.52
1	F	318	ARG	CB-CG	-6.92	1.31	1.52
1	H	738	ARG	NE-CZ	6.77	1.40	1.33
1	D	264	ARG	CZ-NH1	6.68	1.42	1.32
1	G	329	ARG	NE-CZ	6.42	1.40	1.33
1	G	138	VAL	CA-CB	6.33	1.58	1.53
1	H	738	ARG	CZ-NH1	6.32	1.41	1.32
1	H	138	VAL	CA-CB	6.08	1.58	1.53
1	D	264	ARG	NE-CZ	6.01	1.39	1.33
1	D	251	ARG	CZ-NH2	5.86	1.41	1.33
1	I	318	ARG	CG-CD	-5.73	1.35	1.52
1	C	517	VAL	CA-C	-5.50	1.48	1.53
1	D	138	VAL	CA-CB	5.46	1.57	1.53
1	J	830	TYR	CB-CG	-5.10	1.40	1.51
1	I	271	LYS	CE-NZ	-5.07	1.34	1.49

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	521	LYS	CB-CG-CD	-14.71	77.46	111.30
1	G	329	ARG	CG-CD-NE	-12.87	83.69	112.00
1	H	857	LYS	CD-CE-NZ	-11.66	74.58	111.90
1	F	825	ARG	CA-CB-CG	-10.99	92.13	114.10
1	E	249	ARG	CG-CD-NE	-10.35	89.23	112.00
1	B	55	LYS	CA-CB-CG	-10.06	93.97	114.10
1	F	468	GLN	CA-CB-CG	9.84	133.79	114.10
1	C	517	VAL	CA-C-O	9.14	124.54	119.15
1	H	612	ARG	CB-CG-CD	-9.06	90.47	111.30
1	F	825	ARG	CD-NE-CZ	-8.62	112.33	124.40
1	I	318	ARG	CA-CB-CG	-8.44	97.22	114.10
1	G	-1	GLN	CA-CB-CG	-8.07	97.96	114.10
1	F	318	ARG	CG-CD-NE	-7.84	94.75	112.00
1	J	521	LYS	CG-CD-CE	7.80	129.24	111.30
1	H	49	GLN	CA-CB-CG	7.78	129.66	114.10
1	J	521	LYS	CD-CE-NZ	-7.77	87.03	111.90
1	G	329	ARG	CB-CA-C	-7.60	98.17	110.79
1	H	661	TYR	CA-CB-CG	7.54	127.48	113.90
1	B	833	ARG	CG-CD-NE	7.53	128.55	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	561	GLU	CA-CB-CG	7.44	128.98	114.10
1	J	289	ASP	CB-CA-C	7.19	122.51	110.79
1	H	213	ARG	CG-CD-NE	7.19	127.81	112.00
1	J	407	ARG	CB-CG-CD	-7.16	94.83	111.30
1	D	419	ARG	CA-CB-CG	7.05	128.20	114.10
1	J	569	ARG	CB-CG-CD	-7.05	95.09	111.30
1	B	661	TYR	CA-CB-CG	7.02	126.54	113.90
1	A	550	PHE	CB-CA-C	7.00	118.75	109.65
1	D	338	LYS	N-CA-C	-6.98	99.17	110.20
1	D	468	GLN	CA-CB-CG	-6.93	100.23	114.10
1	B	286	GLN	CA-CB-CG	6.92	127.94	114.10
1	E	584	ASN	OD1-CG-ND2	6.86	129.46	122.60
1	F	661	TYR	CA-CB-CG	6.86	126.25	113.90
1	B	481	ARG	CA-CB-CG	-6.79	100.52	114.10
1	H	250	MET	CB-CG-SD	6.79	133.05	112.70
1	J	634	GLU	CB-CG-CD	6.73	124.04	112.60
1	D	250	MET	CA-C-N	-6.73	112.13	122.62
1	D	250	MET	C-N-CA	-6.73	112.13	122.62
1	H	213	ARG	CB-CG-CD	6.69	126.69	111.30
1	J	833	ARG	CB-CG-CD	-6.66	95.98	111.30
1	H	316	LYS	CD-CE-NZ	-6.59	90.80	111.90
1	H	730	LYS	CA-CB-CG	-6.57	100.96	114.10
1	B	349	LYS	CG-CD-CE	6.56	126.38	111.30
1	D	49	GLN	CA-CB-CG	6.46	127.02	114.10
1	A	858	THR	CA-C-N	6.45	133.30	121.70
1	A	858	THR	C-N-CA	6.45	133.30	121.70
1	J	520	ALA	CA-C-N	-6.44	111.92	122.54
1	J	520	ALA	C-N-CA	-6.44	111.92	122.54
1	F	466	PHE	CB-CA-C	6.43	123.02	110.67
1	D	466	PHE	CA-CB-CG	6.43	120.23	113.80
1	H	251	ARG	CB-CA-C	6.42	121.31	109.70
1	H	329	ARG	CA-CB-CG	6.40	126.91	114.10
1	J	112	LYS	CG-CD-CE	6.38	125.98	111.30
1	H	407	ARG	CG-CD-NE	-6.36	98.02	112.00
1	I	326	GLU	CA-CB-CG	-6.32	101.45	114.10
1	G	580	ILE	CG1-CB-CG2	-6.30	91.80	110.70
1	F	318	ARG	CB-CA-C	-6.29	100.97	110.90
1	F	277	PHE	CA-CB-CG	6.25	120.05	113.80
1	J	830	TYR	CB-CA-C	-6.20	100.32	110.85
1	F	801	PHE	CA-CB-CG	6.19	119.99	113.80
1	H	407	ARG	CA-CB-CG	-6.19	101.73	114.10
1	A	303	LYS	CD-CE-NZ	-6.16	92.19	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	TRP	CA-CB-CG	6.10	125.19	113.60
1	H	738	ARG	CB-CG-CD	-6.08	97.30	111.30
1	B	349	LYS	CB-CG-CD	6.08	125.28	111.30
1	G	833	ARG	CG-CD-NE	6.07	125.34	112.00
1	I	552	TYR	CA-CB-CG	6.06	124.81	113.90
1	G	809	GLN	CA-CB-CG	-6.03	102.04	114.10
1	J	634	GLU	CA-CB-CG	6.01	126.13	114.10
1	G	326	GLU	CA-CB-CG	-6.00	102.09	114.10
1	C	322	LYS	CB-CG-CD	5.99	125.08	111.30
1	F	468	GLN	CB-CG-CD	5.98	122.76	112.60
1	F	467	THR	CA-C-N	-5.96	110.56	120.68
1	F	467	THR	C-N-CA	-5.96	110.56	120.68
1	I	277	PHE	CA-CB-CG	5.95	119.75	113.80
1	F	801	PHE	CB-CA-C	5.91	118.87	110.24
1	D	349	LYS	CA-CB-CG	5.90	125.89	114.10
1	D	858	THR	CA-C-N	5.90	132.32	121.70
1	D	858	THR	C-N-CA	5.90	132.32	121.70
1	I	661	TYR	CA-CB-CG	5.89	124.51	113.90
1	F	560	THR	CA-C-N	5.87	135.35	125.02
1	F	560	THR	C-N-CA	5.87	135.35	125.02
1	H	289	ASP	CA-C-N	5.84	128.10	120.28
1	H	289	ASP	C-N-CA	5.84	128.10	120.28
1	I	367	TYR	CA-CB-CG	5.84	124.40	113.90
1	D	419	ARG	CB-CG-CD	-5.79	97.97	111.30
1	J	857	LYS	CA-CB-CG	-5.78	102.55	114.10
1	H	188	MET	CB-CA-C	-5.74	104.10	111.22
1	F	825	ARG	N-CA-CB	5.71	118.51	110.12
1	H	329	ARG	CB-CG-CD	-5.71	98.18	111.30
1	I	141	PHE	CA-CB-CG	5.69	119.49	113.80
1	I	466	PHE	CB-CA-C	5.67	121.56	110.67
1	D	367	TYR	CA-CB-CG	5.64	124.05	113.90
1	A	226	GLN	CA-CB-CG	5.63	125.37	114.10
1	B	481	ARG	CB-CG-CD	5.62	124.22	111.30
1	E	138	VAL	N-CA-CB	-5.61	106.96	110.50
1	E	832	ASN	CA-C-N	5.61	130.09	120.72
1	E	832	ASN	C-N-CA	5.61	130.09	120.72
1	J	112	LYS	CD-CE-NZ	-5.61	93.94	111.90
1	B	223	TYR	CA-CB-CG	5.60	123.98	113.90
1	D	249	ARG	N-CA-CB	5.60	118.20	109.97
1	F	569	ARG	CG-CD-NE	-5.60	99.69	112.00
1	B	55	LYS	N-CA-CB	5.56	118.14	109.85
1	D	466	PHE	CB-CA-C	5.55	121.58	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	295	ARG	CG-CD-NE	-5.54	99.80	112.00
1	B	466	PHE	CB-CA-C	5.54	121.31	110.67
1	G	821	GLN	CA-CB-CG	5.53	125.17	114.10
1	E	584	ASN	CB-CA-C	-5.50	101.86	110.94
1	C	857	LYS	CA-CB-CG	-5.50	103.10	114.10
1	G	49	GLN	CA-CB-CG	5.50	125.09	114.10
1	E	466	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	484	PHE	CB-CA-C	5.46	121.41	109.99
1	H	526	GLU	CA-C-N	5.45	126.90	120.09
1	H	526	GLU	C-N-CA	5.45	126.90	120.09
1	A	466	PHE	CA-CB-CG	5.45	119.25	113.80
1	D	313	PHE	CA-CB-CG	5.44	119.24	113.80
1	H	754	LEU	CB-CG-CD1	5.43	126.98	110.70
1	I	81	ARG	CG-CD-NE	-5.38	100.16	112.00
1	E	137	ILE	CA-C-N	-5.36	116.86	120.24
1	E	137	ILE	C-N-CA	-5.36	116.86	120.24
1	A	141	PHE	CA-CB-CG	5.34	119.14	113.80
1	D	313	PHE	N-CA-CB	5.31	118.41	110.02
1	A	47	PHE	CA-CB-CG	5.30	119.11	113.80
1	H	738	ARG	NH1-CZ-NH2	-5.30	112.41	119.30
1	I	463	ASP	CB-CA-C	5.28	117.92	109.62
1	D	561	GLU	CA-C-N	5.27	128.57	120.82
1	D	561	GLU	C-N-CA	5.27	128.57	120.82
1	J	61	PHE	CB-CA-C	5.27	120.12	109.68
1	H	250	MET	CA-CB-CG	-5.27	103.57	114.10
1	I	277	PHE	CB-CA-C	5.27	120.59	109.79
1	C	406	TRP	CA-CB-CG	5.26	123.59	113.60
1	F	561	GLU	N-CA-CB	5.24	121.36	113.65
1	D	264	ARG	NH1-CZ-NH2	-5.24	112.49	119.30
1	A	406	TRP	CB-CA-C	-5.23	102.68	110.88
1	B	61	PHE	CB-CA-C	5.22	120.02	109.68
1	A	190	ASN	N-CA-C	5.21	118.43	111.75
1	G	802	ARG	CA-CB-CG	5.20	124.51	114.10
1	D	612	ARG	CB-CG-CD	5.19	123.23	111.30
1	B	829	ILE	CG1-CB-CG2	-5.18	95.17	110.70
1	I	250	MET	CA-CB-CG	5.17	124.44	114.10
1	G	808	LYS	CA-C-N	5.15	129.03	120.94
1	G	808	LYS	C-N-CA	5.15	129.03	120.94
1	I	808	LYS	CG-CD-CE	-5.15	99.46	111.30
1	F	856	MET	CB-CG-SD	-5.15	97.26	112.70
1	B	667	GLU	CA-CB-CG	-5.10	103.91	114.10
1	E	293	TYR	CA-CB-CG	5.09	123.06	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	466	PHE	CA-CB-CG	5.08	118.89	113.80
1	F	805	ALA	CA-C-N	5.08	131.25	121.54
1	F	805	ALA	C-N-CA	5.08	131.25	121.54
1	I	250	MET	CG-SD-CE	-5.07	89.75	100.90
1	A	97	ARG	CA-CB-CG	5.06	124.22	114.10
1	D	170	PHE	CB-CA-C	5.05	120.38	110.67
1	C	294	MET	CA-C-N	-5.05	114.72	122.60
1	C	294	MET	C-N-CA	-5.05	114.72	122.60
1	H	612	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	A	466	PHE	CB-CA-C	5.04	120.36	110.67
1	J	47	PHE	CA-CB-CG	5.01	118.81	113.80
1	I	612	ARG	CG-CD-NE	5.00	123.01	112.00

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	481	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	569	ARG	Sidechain
1	B	661	TYR	Sidechain
1	B	806	PHE	Peptide
1	B	833	ARG	Sidechain
1	C	295	ARG	Peptide,Sidechain
1	C	802	ARG	Sidechain
1	C	82	ARG	Sidechain
1	C	833	ARG	Sidechain
1	D	115	ARG	Sidechain
1	D	249	ARG	Sidechain
1	D	338	LYS	Peptide
1	D	419	ARG	Sidechain
1	D	612	ARG	Sidechain
1	D	738	ARG	Sidechain
1	E	213	ARG	Sidechain
1	E	238	ARG	Sidechain
1	E	833	ARG	Sidechain
1	F	213	ARG	Sidechain
1	F	238	ARG	Sidechain
1	F	318	ARG	Sidechain
1	F	569	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	661	TYR	Sidechain
1	F	662	ARG	Sidechain
1	F	802	ARG	Sidechain
1	F	825	ARG	Sidechain
1	G	213	ARG	Sidechain
1	G	329	ARG	Sidechain
1	G	833	ARG	Sidechain
1	G	97	ARG	Sidechain
1	H	213	ARG	Sidechain
1	H	238	ARG	Sidechain
1	H	251	ARG	Sidechain
1	H	295	ARG	Sidechain
1	H	407	ARG	Sidechain
1	H	738	ARG	Sidechain
1	H	802	ARG	Sidechain
1	I	114	SER	Peptide
1	I	115	ARG	Sidechain
1	I	238	ARG	Sidechain
1	I	251	ARG	Sidechain
1	I	318	ARG	Sidechain
1	I	407	ARG	Sidechain
1	I	552	TYR	Sidechain
1	I	612	ARG	Sidechain
1	I	81	ARG	Sidechain
1	I	842	ARG	Sidechain
1	J	114	SER	Peptide
1	J	115	ARG	Sidechain
1	J	569	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6281	0	6216	96	0
1	B	6228	0	6169	94	0
1	C	6246	0	6185	93	0
1	D	6235	0	6176	106	0
1	E	6290	0	6229	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	6266	0	6205	100	0
1	G	6266	0	6205	85	0
1	H	6258	0	6194	140	0
1	I	6224	0	6167	129	0
1	J	6259	0	6198	119	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
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
3	J	1	0	0	0	0
4	A	18	0	22	0	0
4	B	6	0	6	0	0
4	C	18	0	22	0	0
4	D	12	0	14	0	0
4	E	24	0	30	0	0
4	F	18	0	22	1	0
4	G	12	0	14	0	0
4	H	6	0	6	0	0
4	I	6	0	6	0	0
4	J	6	0	6	0	0
5	B	8	0	12	0	0
6	A	92	0	0	0	0
6	B	99	0	0	0	0
6	C	57	0	0	0	0
6	D	69	0	0	0	0
6	E	92	0	0	0	0
6	F	59	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	38	0	0	0	0
6	H	23	0	0	0	0
6	I	36	0	0	0	0
6	J	49	0	0	0	0
All	All	63321	0	62104	995	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (995) 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:I:259:ILE:CD1	1:I:259:ILE:CG1	1.87	1.48
1:J:407:ARG:HH12	1:J:498:THR:HG22	1.34	0.91
1:C:66:THR:HG22	1:C:68:LYS:H	1.37	0.90
1:B:829:ILE:HG22	1:B:833:ARG:HD2	1.55	0.88
1:H:733:LEU:HB2	1:H:738:ARG:HH21	1.40	0.87
1:H:403:VAL:HA	1:H:406:TRP:HD1	1.40	0.85
1:J:66:THR:HG22	1:J:68:LYS:H	1.41	0.85
1:D:561:GLU:HG3	1:D:612:ARG:HE	1.43	0.83
1:I:250:MET:HB2	1:I:279:LEU:HD13	1.62	0.81
1:H:644:LYS:HE3	1:H:713:TYR:HA	1.63	0.81
1:I:126:GLN:HG2	1:I:145:PHE:HB3	1.61	0.81
1:F:132:ARG:HB3	1:F:135:ASP:HB2	1.64	0.79
1:I:66:THR:HG22	1:I:68:LYS:H	1.48	0.78
1:H:406:TRP:HZ3	1:H:612:ARG:HH12	1.31	0.78
1:E:47:PHE:HB2	1:E:157:ASP:HB3	1.67	0.77
1:E:549:GLN:HE22	1:E:555:ASP:HB3	1.49	0.77
1:I:556:PRO:HA	1:I:559:GLN:HE21	1.49	0.77
1:J:127:VAL:HG12	1:J:264:ARG:HH12	1.50	0.77
1:F:549:GLN:HE22	1:F:555:ASP:HB3	1.50	0.76
1:B:556:PRO:HA	1:B:559:GLN:HE21	1.49	0.76
1:G:311:SER:HA	1:G:318:ARG:HH12	1.51	0.76
1:I:251:ARG:HB2	1:I:280:ILE:HG12	1.68	0.75
1:H:251:ARG:HH11	1:H:530:LEU:HD21	1.51	0.75
1:C:859:ASN:HB3	1:D:857:LYS:HE2	1.68	0.74
1:B:420:LYS:HD3	1:B:421:ALA:H	1.52	0.74
1:I:247:PRO:HB2	1:I:385:SER:HB3	1.69	0.74
1:G:298:PRO:HB2	1:G:338:LYS:HG3	1.67	0.74
1:H:247:PRO:HB2	1:H:385:SER:HB3	1.69	0.74
1:G:556:PRO:HA	1:G:559:GLN:HE21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:ARG:HH12	1:H:242:LEU:HB3	1.52	0.73
1:D:75:MET:HE1	1:D:120:VAL:HG11	1.69	0.73
1:H:607:MET:HE1	1:H:681:THR:HG22	1.70	0.73
1:F:458:ILE:HD11	1:F:566:ASP:HB3	1.69	0.72
1:C:47:PHE:HB2	1:C:157:ASP:HB3	1.70	0.72
1:F:556:PRO:HA	1:F:559:GLN:HE21	1.54	0.72
1:F:169:LYS:HG2	1:F:172:ARG:HH21	1.55	0.71
1:F:66:THR:HG22	1:F:68:LYS:H	1.55	0.71
1:F:476:ILE:HD11	1:F:502:ILE:HA	1.72	0.71
1:C:135:ASP:HB3	1:C:137:ILE:HG12	1.73	0.70
1:B:287:PRO:HB3	1:B:299:VAL:HG21	1.71	0.70
1:I:80:PHE:HD2	1:I:115:ARG:HD3	1.56	0.70
1:F:47:PHE:HB2	1:F:157:ASP:HB3	1.73	0.70
1:F:699:GLY:HA2	1:F:810:ALA:HB2	1.73	0.70
1:A:550:PHE:HD1	1:A:551:PRO:HA	1.57	0.70
1:J:857:LYS:O	1:J:857:LYS:HG3	1.91	0.70
1:H:204:ILE:HD11	1:I:118:ILE:HD13	1.72	0.69
1:I:76:PRO:HA	1:I:162:LYS:HG2	1.74	0.69
1:G:549:GLN:HE22	1:G:555:ASP:HB3	1.57	0.69
1:A:221:LEU:HD12	1:A:236:MET:HG3	1.75	0.69
1:D:409:VAL:HG23	1:D:606:LEU:HD23	1.75	0.69
1:G:71:ILE:HD11	1:G:205:VAL:HG11	1.75	0.68
1:C:407:ARG:HG3	1:C:482:ASN:HD21	1.57	0.68
1:H:312:VAL:HB	1:I:137:ILE:HA	1.76	0.67
1:H:66:THR:HG22	1:H:68:LYS:H	1.59	0.67
1:H:316:LYS:HG3	1:H:317:TRP:CD1	2.29	0.67
1:J:112:LYS:HB3	1:J:123:HIS:HB2	1.75	0.67
1:F:45:SER:H	1:F:48:ASP:HB2	1.59	0.67
1:C:273:LYS:HE3	1:C:275:GLU:HG2	1.77	0.67
1:I:549:GLN:NE2	1:I:553:THR:HG23	2.09	0.67
1:G:66:THR:HG22	1:G:68:LYS:H	1.59	0.66
1:J:282:ARG:HB2	1:J:514:TYR:HE1	1.59	0.66
1:B:365:PHE:HE1	1:B:395:TRP:HB2	1.60	0.66
1:H:75:MET:HE1	1:H:120:VAL:HG11	1.77	0.66
1:C:556:PRO:HA	1:C:559:GLN:HE21	1.59	0.66
1:D:561:GLU:HG3	1:D:612:ARG:NE	2.10	0.66
1:J:85:LEU:HD13	1:J:243:LEU:HD11	1.78	0.66
1:D:859:ASN:HB3	1:E:857:LYS:HE2	1.77	0.66
1:F:409:VAL:HG13	1:F:606:LEU:HD23	1.78	0.66
1:J:354:ASP:HB3	1:J:361:ARG:HH22	1.61	0.66
1:D:61:PHE:HE1	1:D:215:VAL:HG21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:THR:HG22	1:E:68:LYS:H	1.60	0.66
1:H:549:GLN:HG2	1:H:802:ARG:HD3	1.78	0.66
1:E:419:ARG:HH11	1:E:588:TRP:CD1	2.13	0.66
1:D:470:TYR:HD2	1:D:542:MET:HE1	1.60	0.65
1:A:75:MET:HE1	1:A:120:VAL:HG11	1.77	0.65
1:D:137:ILE:HA	1:E:312:VAL:HB	1.79	0.65
1:E:236:MET:HB3	1:E:238:ARG:HE	1.60	0.65
1:H:61:PHE:HD2	1:H:75:MET:HG2	1.61	0.65
1:G:247:PRO:HB2	1:G:385:SER:HB3	1.78	0.65
1:F:137:ILE:HA	1:J:312:VAL:HB	1.79	0.65
1:F:723:ILE:HG13	1:F:822:GLN:HB3	1.79	0.65
1:C:446:LEU:HB2	1:C:477:MET:HE3	1.79	0.65
1:E:581:ILE:HA	1:E:588:TRP:HZ3	1.61	0.65
1:I:135:ASP:HB3	1:I:137:ILE:HG12	1.79	0.65
1:C:448:HIS:HA	1:C:477:MET:HB3	1.77	0.64
1:H:85:LEU:HD13	1:H:243:LEU:HD11	1.78	0.64
1:I:47:PHE:HB2	1:I:157:ASP:HB3	1.80	0.64
1:J:251:ARG:HH11	1:J:530:LEU:HD21	1.62	0.64
1:J:733:LEU:HD21	1:J:833:ARG:HH22	1.62	0.64
1:A:169:LYS:HG2	1:A:172:ARG:HH21	1.62	0.63
1:H:369:THR:HG21	1:I:141:PHE:HB2	1.80	0.63
1:H:614:VAL:HG12	1:H:618:MET:HE3	1.80	0.63
1:A:549:GLN:HE22	1:A:555:ASP:HB3	1.63	0.63
1:G:282:ARG:HB2	1:G:514:TYR:HE1	1.64	0.63
1:H:556:PRO:HA	1:H:559:GLN:HE21	1.63	0.63
1:H:579:LYS:HG3	1:H:664:TRP:CE3	2.34	0.63
1:J:112:LYS:HE2	1:J:147:ASP:OD2	1.98	0.63
1:J:676:GLN:HG2	1:J:678:SER:H	1.62	0.63
1:J:448:HIS:HA	1:J:477:MET:HB3	1.79	0.63
1:B:592:LYS:HG2	1:B:593:GLU:HG3	1.80	0.63
1:E:457:THR:HG23	1:E:565:ASN:HD21	1.64	0.62
1:H:90:VAL:HG22	1:H:236:MET:HE1	1.81	0.62
1:C:221:LEU:HD12	1:C:236:MET:HG3	1.81	0.62
1:B:66:THR:HG22	1:B:68:LYS:H	1.63	0.62
1:I:549:GLN:HB3	1:I:802:ARG:HD3	1.82	0.62
1:I:408:PHE:HE2	1:I:589:LEU:HD11	1.65	0.62
1:J:263:SER:HA	1:J:278:LYS:HG2	1.82	0.62
1:F:90:VAL:HG22	1:F:236:MET:HE1	1.81	0.62
1:H:47:PHE:HB2	1:H:157:ASP:HB3	1.82	0.62
1:C:411:THR:HG23	1:C:482:ASN:HD22	1.65	0.61
1:G:90:VAL:HG22	1:G:236:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:PHE:CE1	1:A:367:TYR:HB2	2.34	0.61
1:G:549:GLN:HE21	1:G:558:ASP:HB2	1.64	0.61
1:A:90:VAL:HG22	1:A:236:MET:HE1	1.83	0.61
1:A:699:GLY:HA2	1:A:810:ALA:HB2	1.83	0.61
1:E:556:PRO:HA	1:E:559:GLN:HE21	1.65	0.61
1:F:273:LYS:HE3	1:F:275:GLU:HG2	1.81	0.61
1:I:593:GLU:HA	1:J:630:ARG:HB3	1.83	0.61
1:C:186:PRO:HD3	1:D:227:PRO:HG3	1.82	0.61
1:H:409:VAL:HG13	1:H:606:LEU:HD23	1.83	0.61
1:I:282:ARG:HB2	1:I:514:TYR:CE1	2.36	0.60
1:E:686:LYS:HE2	1:E:743:LEU:HD11	1.83	0.60
1:J:320:THR:HG21	1:J:429:ARG:HB3	1.83	0.60
1:D:61:PHE:HD2	1:D:75:MET:HG2	1.67	0.60
1:E:441:GLY:HA3	1:E:477:MET:HE1	1.83	0.60
1:F:47:PHE:CD2	1:F:159:LYS:HB3	2.37	0.60
1:D:66:THR:HG22	1:D:68:LYS:H	1.66	0.60
1:G:221:LEU:HD12	1:G:236:MET:HG3	1.84	0.60
1:H:207:GLU:HB3	1:H:218:LYS:HB2	1.83	0.60
1:C:47:PHE:CD2	1:C:159:LYS:HB3	2.37	0.60
1:B:148:PRO:HG3	1:C:94:SER:HB2	1.84	0.59
1:E:823:LEU:HB3	1:E:856:MET:HE1	1.84	0.59
1:B:256:ARG:HD2	1:B:534:ILE:HG21	1.84	0.59
1:E:723:ILE:HG13	1:E:822:GLN:HB3	1.84	0.59
1:A:185:PRO:HD2	1:A:188:MET:HB2	1.84	0.59
1:D:90:VAL:HG22	1:D:236:MET:HE1	1.83	0.59
1:E:581:ILE:HA	1:E:588:TRP:CZ3	2.38	0.59
1:D:549:GLN:NE2	1:D:555:ASP:HB3	2.17	0.59
1:F:312:VAL:HB	1:G:137:ILE:HA	1.84	0.59
1:C:322:LYS:HG2	1:C:343:ALA:HB3	1.84	0.59
1:E:57:SER:HB3	1:E:210:SER:HB3	1.85	0.59
1:H:61:PHE:HE1	1:H:215:VAL:HG21	1.66	0.59
1:G:85:LEU:HD13	1:G:243:LEU:HD11	1.85	0.59
1:H:140:SER:HA	1:H:143:LYS:HE2	1.84	0.59
1:J:90:VAL:HG22	1:J:236:MET:HE1	1.83	0.59
1:D:614:VAL:HG12	1:D:618:MET:HE3	1.84	0.59
1:H:298:PRO:HB2	1:H:338:LYS:HB2	1.85	0.59
1:H:356:ASP:HB3	1:H:359:ASP:HB2	1.83	0.59
1:H:467:THR:HB	1:H:496:ARG:HB3	1.84	0.58
1:I:314:PRO:HG2	1:J:269:THR:HG21	1.84	0.58
1:I:716:THR:HG22	1:I:818:LEU:HD13	1.85	0.58
1:C:676:GLN:HE21	1:C:678:SER:HB3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:373:ALA:HB1	1:I:402:LEU:HB2	1.84	0.58
1:H:213:ARG:NH1	1:H:242:LEU:HB3	2.17	0.58
1:B:812:ASN:HA	1:B:815:ILE:HG22	1.86	0.58
1:G:57:SER:HB3	1:G:210:SER:HB3	1.86	0.58
1:I:168:THR:O	1:I:172:ARG:HG2	2.03	0.58
1:H:484:PHE:HE1	1:H:563:LEU:HB2	1.69	0.57
1:I:410:GLN:HE21	1:I:609:GLN:HE22	1.52	0.57
1:E:207:GLU:HB3	1:E:218:LYS:HB3	1.87	0.57
1:H:458:ILE:HG13	1:H:564:SER:HB2	1.86	0.57
1:A:614:VAL:HG12	1:A:618:MET:HE3	1.87	0.57
1:G:66:THR:HB	1:G:70:GLU:H	1.69	0.57
1:H:155:ILE:HD11	1:H:158:THR:HG23	1.86	0.57
1:I:702:TYR:HB2	1:I:715:LEU:HD22	1.85	0.57
1:I:369:THR:HG21	1:J:141:PHE:HB2	1.85	0.57
1:F:203:SER:HB2	1:F:221:LEU:HD23	1.87	0.57
1:H:456:PHE:CE1	1:H:542:MET:HE3	2.40	0.57
1:C:66:THR:HB	1:C:70:GLU:H	1.69	0.57
1:E:90:VAL:HG22	1:E:236:MET:HE1	1.86	0.57
1:G:203:SER:HB2	1:G:221:LEU:HD23	1.87	0.57
1:A:854:ARG:HH12	1:E:754:LEU:HD11	1.70	0.56
1:E:185:PRO:HD2	1:E:188:MET:HB2	1.87	0.56
1:J:83:GLU:HB3	1:J:110:LEU:HD11	1.87	0.56
1:A:131:VAL:HB	1:A:141:PHE:CD2	2.40	0.56
1:A:456:PHE:HE1	1:A:542:MET:HE3	1.70	0.56
1:C:159:LYS:HG3	1:C:160:ASP:N	2.20	0.56
1:G:467:THR:HG21	1:G:495:VAL:HG13	1.87	0.56
1:I:406:TRP:CE3	1:I:481:ARG:HG2	2.40	0.56
1:D:559:GLN:NE2	1:D:616:HIS:HA	2.21	0.56
1:H:412:GLY:HA2	1:H:418:VAL:HG21	1.85	0.56
1:D:702:TYR:HB2	1:D:715:LEU:HD22	1.87	0.56
1:E:85:LEU:HD13	1:E:243:LEU:HD11	1.87	0.56
1:H:584:ASN:HA	1:H:587:LYS:HE3	1.87	0.56
1:I:76:PRO:HD2	1:I:79:ALA:HB2	1.86	0.56
1:B:370:THR:HG21	1:B:396:TYR:HD2	1.69	0.56
1:G:576:SER:O	1:G:580:ILE:HG12	2.05	0.56
1:G:415:ASP:HA	1:G:491:LEU:HD22	1.88	0.56
1:G:581:ILE:HA	1:G:588:TRP:CZ3	2.41	0.55
1:G:834:LYS:HG3	1:G:842:ARG:HG3	1.87	0.55
1:H:80:PHE:CD2	1:H:115:ARG:HD2	2.42	0.55
1:J:458:ILE:O	1:J:462:ARG:HG2	2.06	0.55
1:A:64:TYR:HB2	1:A:72:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HD11	1:B:570:ALA:HB2	1.89	0.55
1:E:168:THR:HG22	1:E:172:ARG:HG2	1.88	0.55
1:D:382:ASP:HB2	1:D:389:ILE:HD11	1.89	0.55
1:E:458:ILE:HD11	1:E:566:ASP:HB3	1.89	0.55
1:E:467:THR:HG22	1:E:496:ARG:HB3	1.88	0.55
1:H:438:HIS:CD2	1:H:442:HIS:NE2	2.75	0.55
1:H:131:VAL:HB	1:H:141:PHE:HD2	1.71	0.55
1:I:90:VAL:HG22	1:I:236:MET:HE1	1.88	0.55
1:I:282:ARG:HB2	1:I:514:TYR:HE1	1.71	0.55
1:J:738:ARG:HH12	1:J:841:ASP:HA	1.71	0.55
1:F:293:TYR:HE2	1:F:516:LEU:HD23	1.72	0.55
1:F:438:HIS:HD1	1:F:477:MET:HA	1.71	0.55
1:H:403:VAL:HA	1:H:406:TRP:CD1	2.32	0.55
1:H:661:TYR:CE2	1:H:684:LEU:HB3	2.42	0.55
1:J:407:ARG:NH1	1:J:498:THR:HG22	2.14	0.55
1:J:484:PHE:CD1	1:J:563:LEU:HD12	2.42	0.55
1:B:91:ALA:HB3	1:B:235:ILE:HG22	1.88	0.55
1:G:471:GLY:HA3	1:G:500:PRO:HD3	1.88	0.55
1:J:446:LEU:HB2	1:J:477:MET:HE3	1.89	0.55
1:E:61:PHE:HE1	1:E:215:VAL:HG21	1.71	0.54
1:F:549:GLN:HE21	1:F:558:ASP:HB2	1.71	0.54
1:C:90:VAL:HG22	1:C:236:MET:HE1	1.88	0.54
1:E:256:ARG:HB2	1:E:534:ILE:HD13	1.89	0.54
1:F:549:GLN:NE2	1:F:555:ASP:HB3	2.21	0.54
1:H:857:LYS:NZ	1:I:859:ASN:HA	2.21	0.54
1:A:88:SER:HB3	1:A:106:THR:HB	1.88	0.54
1:D:126:GLN:HG2	1:D:145:PHE:HB3	1.88	0.54
1:E:686:LYS:HG3	1:E:743:LEU:HD21	1.88	0.54
1:H:585:MET:HG2	1:H:599:LEU:HD11	1.88	0.54
1:C:348:THR:HG22	1:C:351:GLU:H	1.72	0.54
1:C:549:GLN:NE2	1:C:555:ASP:HB3	2.22	0.54
1:G:581:ILE:HA	1:G:588:TRP:HZ3	1.72	0.54
1:J:536:GLU:HG2	1:J:537:LYS:HE3	1.90	0.54
1:B:286:GLN:HE21	1:B:286:GLN:HA	1.71	0.54
1:H:282:ARG:HB2	1:H:514:TYR:HE1	1.72	0.54
1:A:556:PRO:HA	1:A:559:GLN:HE21	1.73	0.54
1:C:549:GLN:HE22	1:C:555:ASP:HB3	1.73	0.54
1:C:812:ASN:HA	1:C:815:ILE:HG22	1.90	0.54
1:G:282:ARG:HB2	1:G:514:TYR:CE1	2.42	0.54
1:H:224:LYS:HE3	1:H:229:SER:HB3	1.89	0.54
1:A:47:PHE:CE2	1:A:159:LYS:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:PHE:HE2	1:B:589:LEU:HD11	1.73	0.54
1:D:45:SER:HB2	1:D:159:LYS:HD2	1.90	0.54
1:D:549:GLN:HE22	1:D:555:ASP:HB3	1.73	0.54
1:H:857:LYS:HG3	1:H:859:ASN:H	1.71	0.54
1:J:287:PRO:HB3	1:J:299:VAL:HG21	1.90	0.54
1:B:57:SER:HB3	1:B:210:SER:HB3	1.89	0.54
1:I:857:LYS:HE2	1:I:859:ASN:HB2	1.90	0.54
1:A:640:ARG:HA	1:A:709:GLN:HE22	1.73	0.54
1:J:462:ARG:HH12	1:J:486:ALA:HA	1.71	0.54
1:B:407:ARG:HD2	1:B:431:SER:OG	2.08	0.54
1:C:47:PHE:CE2	1:C:159:LYS:HB3	2.43	0.54
1:G:484:PHE:CD1	1:G:563:LEU:HD12	2.43	0.54
1:H:248:MET:HG2	1:H:385:SER:HB2	1.90	0.53
1:H:423:PHE:HB2	1:H:428:MET:HE2	1.89	0.53
1:C:705:GLU:HG3	1:C:714:LYS:HG2	1.89	0.53
1:G:228:TYR:HB2	1:G:230:GLU:HG3	1.90	0.53
1:A:698:ILE:HG23	1:A:715:LEU:HD11	1.89	0.53
1:B:84:TYR:HB2	1:B:111:ILE:HG13	1.90	0.53
1:B:420:LYS:HD3	1:B:421:ALA:N	2.21	0.53
1:H:834:LYS:HG3	1:H:842:ARG:HG3	1.91	0.53
1:I:555:ASP:HB2	1:I:802:ARG:HH22	1.73	0.53
1:J:251:ARG:HH12	1:J:517:VAL:HG23	1.73	0.53
1:D:308:TYR:CE2	1:D:344:LYS:HE2	2.44	0.53
1:F:325:ILE:HB	1:F:343:ALA:HB2	1.89	0.53
1:F:484:PHE:CD1	1:F:563:LEU:HD12	2.43	0.53
1:G:47:PHE:CD2	1:G:159:LYS:HB3	2.44	0.53
1:F:135:ASP:OD2	1:F:137:ILE:HG12	2.08	0.53
1:G:852:LEU:HB3	1:G:856:MET:HE2	1.90	0.53
1:H:723:ILE:HG13	1:H:822:GLN:HB3	1.90	0.53
1:H:754:LEU:HD22	1:H:856:MET:HA	1.88	0.53
1:A:57:SER:HB3	1:A:210:SER:HB3	1.90	0.53
1:F:754:LEU:HG	1:F:855:LEU:HG	1.90	0.53
1:J:395:TRP:HZ2	1:J:432:LEU:HD22	1.73	0.53
1:D:461:LEU:HD21	1:D:563:LEU:HB3	1.91	0.53
1:F:484:PHE:CE1	1:F:563:LEU:HB2	2.44	0.53
1:J:57:SER:HB3	1:J:210:SER:HB3	1.90	0.53
1:E:600:ARG:HB2	1:E:674:VAL:HB	1.91	0.53
1:H:316:LYS:O	1:H:429:ARG:HD3	2.09	0.53
1:I:80:PHE:CD2	1:I:115:ARG:HD3	2.40	0.53
1:I:60:PRO:HB3	1:I:242:LEU:HD13	1.90	0.52
1:I:112:LYS:HB3	1:I:123:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:640:ARG:HA	1:I:709:GLN:HE22	1.73	0.52
1:A:549:GLN:NE2	1:A:555:ASP:HB3	2.23	0.52
1:H:69:ASN:OD1	1:I:118:ILE:HD11	2.09	0.52
1:G:130:MET:HE1	1:G:250:MET:HE1	1.91	0.52
1:G:596:TYR:HB3	1:G:674:VAL:HG12	1.90	0.52
1:H:693:PHE:HB2	1:H:747:LEU:HD13	1.91	0.52
1:F:207:GLU:HB3	1:F:218:LYS:HB3	1.91	0.52
1:F:251:ARG:HH21	1:F:282:ARG:HH12	1.56	0.52
1:F:642:ILE:HG23	1:F:646:LYS:HE3	1.91	0.52
1:I:312:VAL:HB	1:J:137:ILE:HA	1.92	0.52
1:I:474:PRO:HB3	1:I:542:MET:HB3	1.90	0.52
1:J:699:GLY:HA2	1:J:810:ALA:HB2	1.92	0.52
1:A:470:TYR:CD1	1:A:542:MET:HE1	2.44	0.52
1:B:368:ALA:HB3	1:B:396:TYR:HA	1.92	0.52
1:F:395:TRP:HZ2	1:F:432:LEU:HD22	1.75	0.52
1:H:131:VAL:HB	1:H:141:PHE:CD2	2.45	0.52
1:I:331:ALA:HA	1:I:507:ILE:HG23	1.91	0.52
1:I:484:PHE:CD1	1:I:563:LEU:HD12	2.44	0.52
1:A:84:TYR:HB2	1:A:111:ILE:HG13	1.91	0.52
1:A:110:LEU:HD23	1:A:125:PRO:HB2	1.92	0.52
1:D:752:SER:HB2	1:D:754:LEU:HD13	1.91	0.52
1:G:723:ILE:HG13	1:G:822:GLN:HB3	1.91	0.52
1:H:180:PRO:HD2	1:H:223:TYR:OH	2.10	0.52
1:H:603:HIS:CE1	1:H:607:MET:HE3	2.45	0.52
1:H:673:LYS:HB2	1:I:629:ILE:HD11	1.92	0.52
1:J:842:ARG:HA	1:J:845:TYR:CD2	2.45	0.52
1:H:81:ARG:HH12	1:H:115:ARG:HH22	1.58	0.52
1:H:329:ARG:HG3	1:H:339:ASN:HA	1.92	0.52
1:G:614:VAL:HG12	1:G:618:MET:HE3	1.91	0.52
1:H:253:GLN:HG3	1:H:261:ASN:HB3	1.92	0.52
1:H:448:HIS:HA	1:H:477:MET:HB3	1.91	0.52
1:H:657:GLN:O	1:H:661:TYR:HB3	2.09	0.52
1:C:234:LEU:HD13	1:C:236:MET:HE3	1.92	0.52
1:E:320:THR:HG21	1:E:429:ARG:HB3	1.91	0.52
1:F:834:LYS:HG3	1:F:842:ARG:HG2	1.92	0.52
1:I:280:ILE:HD11	1:I:282:ARG:HD3	1.92	0.52
1:D:100:VAL:HG21	1:D:368:ALA:HB1	1.91	0.51
1:D:465:GLN:O	1:D:469:LYS:HG3	2.09	0.51
1:G:213:ARG:HD3	1:G:242:LEU:HB3	1.92	0.51
1:I:86:LEU:HB2	1:I:111:ILE:HD13	1.91	0.51
1:J:141:PHE:CE1	1:J:145:PHE:HD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:PRO:HD2	1:D:392:ASP:HB2	1.92	0.51
1:E:251:ARG:NH1	1:E:530:LEU:HD21	2.24	0.51
1:H:395:TRP:HZ2	1:H:432:LEU:HD22	1.75	0.51
1:I:527:LYS:HA	1:I:530:LEU:HD12	1.92	0.51
1:I:608:SER:O	1:I:612:ARG:HG3	2.09	0.51
1:A:614:VAL:HG11	1:A:688:MET:HE2	1.92	0.51
1:C:169:LYS:HG2	1:C:172:ARG:HH21	1.76	0.51
1:C:249:ARG:HH22	1:C:516:LEU:HD23	1.76	0.51
1:I:325:ILE:HD11	1:I:365:PHE:HD2	1.75	0.51
1:J:614:VAL:HG12	1:J:618:MET:HE3	1.92	0.51
1:H:308:TYR:HD2	1:H:347:PRO:HD3	1.75	0.51
1:J:600:ARG:HB3	1:J:674:VAL:HB	1.92	0.51
1:A:148:PRO:HG3	1:B:94:SER:HB2	1.93	0.51
1:D:148:PRO:HG3	1:E:94:SER:OG	2.11	0.51
1:E:373:ALA:HB1	1:E:402:LEU:HB2	1.91	0.51
1:I:131:VAL:HB	1:I:141:PHE:CD2	2.46	0.51
1:I:609:GLN:HG3	1:I:613:HIS:CE1	2.45	0.51
1:J:66:THR:HB	1:J:70:GLU:H	1.74	0.51
1:C:676:GLN:NE2	1:C:678:SER:HB3	2.25	0.51
1:G:88:SER:HB3	1:G:106:THR:HB	1.92	0.51
1:A:322:LYS:HG3	1:A:343:ALA:HB3	1.92	0.51
1:C:373:ALA:HB1	1:C:402:LEU:HB2	1.91	0.51
1:E:699:GLY:HA2	1:E:810:ALA:HB2	1.91	0.51
1:H:98:GLU:HG3	1:H:194:ILE:HD12	1.93	0.51
1:H:689:VAL:HB	1:H:743:LEU:HD23	1.93	0.51
1:I:614:VAL:HG12	1:I:618:MET:HE3	1.93	0.51
1:D:457:THR:OG1	1:D:459:GLU:HG2	2.11	0.51
1:G:61:PHE:HD2	1:G:75:MET:HG2	1.76	0.51
1:H:452:ALA:HB1	1:H:474:PRO:HB2	1.92	0.51
1:H:549:GLN:HE22	1:H:555:ASP:HB3	1.76	0.51
1:I:81:ARG:NH2	1:I:115:ARG:HH21	2.08	0.51
1:I:581:ILE:O	1:I:585:MET:HB2	2.11	0.51
1:J:489:GLY:O	1:J:493:ARG:HB2	2.10	0.51
1:B:80:PHE:CD2	1:B:115:ARG:HD2	2.46	0.51
1:B:298:PRO:HB2	1:B:338:LYS:HE3	1.91	0.51
1:D:221:LEU:HD12	1:D:236:MET:HG3	1.92	0.51
1:F:204:ILE:HD11	1:G:118:ILE:HD13	1.92	0.51
1:H:402:LEU:HG	1:H:406:TRP:NE1	2.26	0.51
1:I:479:TYR:HB3	1:I:561:GLU:OE2	2.11	0.51
1:A:471:GLY:HA3	1:A:500:PRO:HD3	1.92	0.50
1:B:382:ASP:HB2	1:B:389:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASP:HB2	1:C:198:LEU:HD22	1.93	0.50
1:E:852:LEU:O	1:E:856:MET:HG2	2.11	0.50
1:H:354:ASP:HB3	1:H:361:ARG:HH12	1.75	0.50
1:J:662:ARG:HG3	1:J:666:ALA:HB3	1.93	0.50
1:B:85:LEU:HD13	1:B:243:LEU:HD11	1.93	0.50
1:B:717:ASP:O	1:B:721:GLU:HG3	2.10	0.50
1:B:825:ARG:O	1:B:829:ILE:HG13	2.10	0.50
1:D:440:ILE:O	1:D:444:ILE:HG12	2.11	0.50
1:J:257:VAL:HG23	1:J:534:ILE:HD11	1.93	0.50
1:A:91:ALA:HB3	1:A:235:ILE:HG22	1.94	0.50
1:A:410:GLN:OE1	1:A:482:ASN:HB2	2.10	0.50
1:G:414:VAL:HG12	1:G:491:LEU:HB2	1.94	0.50
1:I:737:ASP:O	1:I:741:GLN:HB2	2.12	0.50
1:A:61:PHE:HE1	1:A:215:VAL:HG21	1.76	0.50
1:C:490:ASP:HA	1:C:493:ARG:HB2	1.92	0.50
1:E:287:PRO:HB3	1:E:293:TYR:HD2	1.76	0.50
1:I:61:PHE:HE1	1:I:215:VAL:HG21	1.75	0.50
1:I:723:ILE:HG13	1:I:822:GLN:HB3	1.94	0.50
1:J:208:VAL:HG22	1:J:217:ILE:HG23	1.94	0.50
1:F:57:SER:HB3	1:F:210:SER:HB3	1.92	0.50
1:D:484:PHE:CD1	1:D:563:LEU:HD12	2.47	0.50
1:F:611:TYR:HD1	1:F:684:LEU:HD23	1.76	0.50
1:H:857:LYS:HZ1	1:I:859:ASN:HA	1.76	0.50
1:I:247:PRO:HG3	1:I:384:ARG:HG3	1.92	0.50
1:J:359:ASP:HB3	1:J:362:PHE:HD2	1.77	0.50
1:B:419:ARG:HD2	1:B:588:TRP:CD2	2.47	0.50
1:E:847:TYR:CZ	1:E:851:ARG:HD2	2.47	0.50
1:H:549:GLN:NE2	1:H:555:ASP:HB3	2.27	0.50
1:I:253:GLN:HG3	1:I:261:ASN:HD22	1.76	0.49
1:C:695:PRO:HG3	1:C:751:HIS:CD2	2.48	0.49
1:D:234:LEU:HB3	1:D:236:MET:HE3	1.94	0.49
1:J:661:TYR:HD2	1:J:665:LEU:HD12	1.77	0.49
1:B:600:ARG:HB3	1:B:674:VAL:HB	1.94	0.49
1:J:91:ALA:HB3	1:J:235:ILE:HG22	1.92	0.49
1:A:298:PRO:HB2	1:A:338:LYS:HB2	1.93	0.49
1:D:490:ASP:HA	1:D:493:ARG:HB2	1.94	0.49
1:F:373:ALA:HB1	1:F:402:LEU:HB2	1.94	0.49
1:B:100:VAL:HG21	1:B:368:ALA:HB1	1.93	0.49
1:A:852:LEU:O	1:A:856:MET:HG2	2.12	0.49
1:C:118:ILE:HD13	1:D:204:ILE:HD11	1.94	0.49
1:C:596:TYR:HD1	1:C:599:LEU:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ILE:O	1:H:155:ILE:HG22	2.12	0.49
1:J:96:THR:HG23	1:J:100:VAL:HG23	1.95	0.49
1:E:253:GLN:HG3	1:E:261:ASN:HD22	1.78	0.49
1:F:123:HIS:CE1	1:F:149:VAL:HG22	2.47	0.49
1:I:548:GLN:O	1:I:802:ARG:HG2	2.12	0.49
1:J:116:ASP:HB2	1:J:121:TYR:HE2	1.78	0.49
1:G:549:GLN:NE2	1:G:555:ASP:HB3	2.25	0.49
1:H:46:LYS:HE2	1:H:156:VAL:HG13	1.95	0.49
1:G:62:THR:HB	1:G:74:ALA:HB3	1.95	0.49
1:I:657:GLN:O	1:I:661:TYR:HB3	2.13	0.49
1:F:76:PRO:HG3	1:F:162:LYS:HE2	1.94	0.49
1:H:733:LEU:HD21	1:H:833:ARG:HH22	1.77	0.49
1:B:446:LEU:HB2	1:B:477:MET:HE2	1.95	0.48
1:D:305:ILE:HB	1:D:341:ILE:HD12	1.94	0.48
1:E:407:ARG:HD2	1:E:431:SER:OG	2.12	0.48
1:H:438:HIS:CD2	1:H:442:HIS:HE2	2.19	0.48
1:I:484:PHE:CE1	1:I:563:LEU:HB2	2.47	0.48
1:B:207:GLU:HB3	1:B:218:LYS:HB2	1.95	0.48
1:F:264:ARG:HB2	1:F:277:PHE:CD1	2.48	0.48
1:F:412:GLY:HA2	1:F:418:VAL:HG21	1.94	0.48
1:H:123:HIS:CD2	1:H:149:VAL:HG22	2.48	0.48
1:H:312:VAL:HG23	1:H:367:TYR:HD2	1.78	0.48
1:B:61:PHE:HE1	1:B:215:VAL:HG21	1.78	0.48
1:F:614:VAL:HG11	1:F:688:MET:HE2	1.94	0.48
1:A:448:HIS:HA	1:A:477:MET:HB3	1.95	0.48
1:F:132:ARG:NH1	1:F:270:ASP:H	2.11	0.48
1:F:221:LEU:HD12	1:F:236:MET:HG3	1.96	0.48
1:F:481:ARG:O	1:F:499:PRO:HD3	2.13	0.48
1:H:211:PHE:HB2	1:H:214:ASN:OD1	2.13	0.48
1:J:407:ARG:HB3	1:J:423:PHE:HZ	1.77	0.48
1:J:118:ILE:O	1:J:155:ILE:HG22	2.12	0.48
1:C:702:TYR:CD2	1:C:811:PRO:HG3	2.49	0.48
1:D:118:ILE:HD13	1:E:204:ILE:HD11	1.95	0.48
1:F:264:ARG:HH12	4:F:905:GOL:H32	1.78	0.48
1:J:234:LEU:HB3	1:J:236:MET:HE2	1.95	0.48
1:J:480:ALA:HB1	1:J:563:LEU:HD23	1.94	0.48
1:A:745:ILE:HD12	1:A:848:GLN:OE1	2.14	0.48
1:B:356:ASP:HB3	1:B:359:ASP:HB2	1.96	0.48
1:C:100:VAL:HG21	1:C:368:ALA:HB1	1.95	0.48
1:F:614:VAL:HG12	1:F:618:MET:HE3	1.95	0.48
1:I:213:ARG:HE	1:I:361:ARG:CZ	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:676:GLN:HG2	1:J:678:SER:N	2.28	0.48
1:B:211:PHE:HB2	1:B:214:ASN:OD1	2.13	0.48
1:D:549:GLN:HE21	1:D:558:ASP:HB2	1.79	0.48
1:F:211:PHE:HB2	1:F:214:ASN:OD1	2.13	0.48
1:G:438:HIS:HD1	1:G:477:MET:HA	1.78	0.48
1:D:251:ARG:HH22	1:D:516:LEU:HA	1.78	0.48
1:H:373:ALA:HB1	1:H:402:LEU:HB2	1.95	0.48
1:H:549:GLN:HE21	1:H:558:ASP:HB2	1.79	0.48
1:J:325:ILE:HG23	1:J:341:ILE:HG12	1.96	0.48
1:J:618:MET:HE2	1:J:688:MET:HA	1.95	0.48
1:B:47:PHE:CD2	1:B:159:LYS:HB3	2.49	0.48
1:B:126:GLN:HG2	1:B:145:PHE:HB3	1.96	0.48
1:B:614:VAL:HG12	1:B:618:MET:HE3	1.95	0.48
1:D:306:VAL:HG22	1:D:342:ILE:HB	1.96	0.48
1:D:467:THR:HB	1:D:496:ARG:HB3	1.95	0.48
1:E:96:THR:HG23	1:E:100:VAL:HG23	1.96	0.48
1:F:66:THR:HB	1:F:70:GLU:H	1.79	0.48
1:G:501:ILE:HG22	1:G:502:ILE:HG12	1.96	0.48
1:A:213:ARG:CZ	1:A:361:ARG:HD3	2.43	0.47
1:A:481:ARG:O	1:A:499:PRO:HD3	2.14	0.47
1:E:549:GLN:HA	1:E:802:ARG:O	2.13	0.47
1:F:359:ASP:HB3	1:F:362:PHE:HD2	1.79	0.47
1:H:609:GLN:HA	1:H:612:ARG:HD2	1.96	0.47
1:J:407:ARG:CD	1:J:482:ASN:ND2	2.77	0.47
1:J:857:LYS:HE3	1:J:859:ASN:O	2.14	0.47
1:C:298:PRO:HB2	1:C:338:LYS:HE3	1.95	0.47
1:D:298:PRO:O	1:D:338:LYS:HE3	2.14	0.47
1:F:87:SER:HB3	1:F:108:PRO:HG3	1.96	0.47
1:H:100:VAL:HG21	1:H:368:ALA:HB1	1.96	0.47
1:E:551:PRO:HG2	1:E:552:TYR:CE2	2.50	0.47
1:F:693:PHE:HB2	1:F:747:LEU:HD13	1.95	0.47
1:G:412:GLY:HA2	1:G:418:VAL:HG21	1.96	0.47
1:B:114:SER:HB3	1:B:121:TYR:HB2	1.95	0.47
1:F:419:ARG:HD2	1:F:588:TRP:CD2	2.50	0.47
1:H:135:ASP:HB3	1:H:137:ILE:HG12	1.96	0.47
1:J:84:TYR:HB2	1:J:111:ILE:HG13	1.96	0.47
1:A:262:SER:HB2	1:A:281:HIS:NE2	2.28	0.47
1:A:694:ASN:HB3	1:A:697:SER:HB2	1.97	0.47
1:B:412:GLY:HA2	1:B:418:VAL:HG21	1.97	0.47
1:B:471:GLY:HA3	1:B:500:PRO:HD3	1.96	0.47
1:D:660:THR:O	1:D:663:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:THR:O	1:E:148:PRO:HD2	2.14	0.47
1:G:365:PHE:HE1	1:G:395:TRP:HB2	1.80	0.47
1:G:373:ALA:HB1	1:G:402:LEU:HB2	1.95	0.47
1:H:82:ARG:HH12	1:H:245:GLU:HG2	1.79	0.47
1:J:111:ILE:HD11	1:J:240:ILE:HG23	1.97	0.47
1:J:289:ASP:OD1	1:J:292:ALA:HB3	2.15	0.47
1:B:582:ALA:HA	1:B:585:MET:HE2	1.97	0.47
1:B:596:TYR:HB3	1:B:674:VAL:HG12	1.97	0.47
1:D:45:SER:H	1:D:48:ASP:HB2	1.80	0.47
1:D:90:VAL:HG21	1:D:99:ALA:HB1	1.96	0.47
1:D:256:ARG:HD2	1:D:534:ILE:HG21	1.96	0.47
1:G:367:TYR:CD1	1:G:395:TRP:HD1	2.33	0.47
1:I:847:TYR:CZ	1:I:851:ARG:HD2	2.50	0.47
1:J:250:MET:HG2	1:J:279:LEU:HD22	1.97	0.47
1:J:410:GLN:OE1	1:J:482:ASN:HB2	2.15	0.47
1:A:413:ALA:HB1	1:A:488:PRO:HG3	1.97	0.47
1:I:234:LEU:HD13	1:I:236:MET:HE3	1.96	0.47
1:B:90:VAL:HG22	1:B:236:MET:HE1	1.97	0.47
1:B:829:ILE:O	1:B:833:ARG:HG3	2.14	0.47
1:H:398:ASN:HD21	1:I:274:VAL:HB	1.79	0.47
1:H:402:LEU:HG	1:H:406:TRP:HE1	1.80	0.47
1:I:329:ARG:HD3	1:I:339:ASN:OD1	2.15	0.47
1:B:293:TYR:HE2	1:B:516:LEU:HB2	1.80	0.46
1:I:111:ILE:HD11	1:I:240:ILE:HG23	1.97	0.46
1:A:456:PHE:CE1	1:A:542:MET:HE3	2.49	0.46
1:C:859:ASN:HB3	1:D:857:LYS:CE	2.42	0.46
1:D:178:ILE:HD12	1:D:238:ARG:HD3	1.97	0.46
1:I:456:PHE:HE1	1:I:542:MET:HE3	1.80	0.46
1:I:549:GLN:HE22	1:I:553:THR:HG23	1.79	0.46
1:C:294:MET:HB3	1:C:294:MET:HE2	1.63	0.46
1:D:263:SER:HA	1:D:278:LYS:HG2	1.97	0.46
1:D:702:TYR:CE2	1:D:811:PRO:HG2	2.50	0.46
1:F:170:PHE:HA	1:F:175:GLU:HG3	1.97	0.46
1:A:85:LEU:HD13	1:A:243:LEU:HD11	1.97	0.46
1:D:733:LEU:HB3	1:D:737:ASP:HB3	1.96	0.46
1:E:547:ALA:HB1	1:E:801:PHE:HA	1.96	0.46
1:G:135:ASP:HB3	1:G:137:ILE:HG12	1.97	0.46
1:H:170:PHE:CE1	1:H:175:GLU:HG2	2.50	0.46
1:H:456:PHE:HE1	1:H:542:MET:HE3	1.80	0.46
1:I:259:ILE:CD1	1:I:259:ILE:CB	2.87	0.46
1:J:540:ASP:HB3	1:J:543:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LYS:HE3	1:A:317:TRP:CE2	2.50	0.46
1:B:806:PHE:HD1	1:B:806:PHE:H	1.62	0.46
1:D:365:PHE:HE1	1:D:395:TRP:HB2	1.81	0.46
1:I:241:LEU:HB2	1:I:360:ILE:HD13	1.97	0.46
1:J:407:ARG:HD3	1:J:482:ASN:ND2	2.31	0.46
1:A:406:TRP:CH2	1:A:481:ARG:HG2	2.50	0.46
1:F:438:HIS:ND1	1:F:477:MET:HA	2.31	0.46
1:H:82:ARG:HG2	1:H:242:LEU:HD11	1.98	0.46
1:I:124:THR:O	1:I:148:PRO:HD2	2.15	0.46
1:J:621:ILE:HG22	1:J:697:SER:HB3	1.98	0.46
1:B:293:TYR:HE1	1:B:336:GLY:HA3	1.81	0.46
1:D:613:HIS:HA	1:D:616:HIS:ND1	2.31	0.46
1:E:211:PHE:HB2	1:E:214:ASN:OD1	2.15	0.46
1:G:461:LEU:HD21	1:G:563:LEU:HB3	1.98	0.46
1:E:216:GLU:HB3	1:E:237:GLN:HE22	1.80	0.46
1:J:316:LYS:HE2	1:J:317:TRP:CE2	2.51	0.46
1:D:417:ARG:O	1:D:420:LYS:HE2	2.15	0.46
1:G:470:TYR:HD1	1:G:542:MET:HE1	1.81	0.46
1:I:211:PHE:HB2	1:I:214:ASN:OD1	2.16	0.46
1:C:754:LEU:HD12	1:C:855:LEU:O	2.15	0.46
1:F:458:ILE:O	1:F:462:ARG:HG2	2.16	0.46
1:H:326:GLU:HG2	1:H:329:ARG:NH2	2.31	0.46
1:J:663:GLN:HG3	1:J:664:TRP:N	2.31	0.46
1:C:211:PHE:HB2	1:C:214:ASN:OD1	2.16	0.45
1:G:853:GLU:HG2	1:G:857:LYS:NZ	2.31	0.45
1:I:812:ASN:HA	1:I:815:ILE:HG22	1.98	0.45
1:J:581:ILE:HA	1:J:588:TRP:CZ3	2.51	0.45
1:A:369:THR:HG21	1:E:141:PHE:HA	1.98	0.45
1:B:120:VAL:HB	1:B:165:ILE:HG21	1.98	0.45
1:E:47:PHE:CD1	1:E:164:LEU:HD22	2.51	0.45
1:F:82:ARG:HB2	1:F:84:TYR:HE1	1.81	0.45
1:H:326:GLU:HG2	1:H:329:ARG:HH21	1.81	0.45
1:A:823:LEU:HB3	1:A:856:MET:HE1	1.98	0.45
1:B:256:ARG:HB2	1:B:534:ILE:HD13	1.98	0.45
1:B:448:HIS:HB3	1:B:450:MET:HE2	1.99	0.45
1:C:661:TYR:CE2	1:C:662:ARG:HG3	2.51	0.45
1:D:300:GLU:HA	1:D:338:LYS:O	2.15	0.45
1:I:112:LYS:HB2	1:I:125:PRO:HG3	1.99	0.45
1:E:448:HIS:HB3	1:E:450:MET:HE2	1.99	0.45
1:F:253:GLN:HG3	1:F:261:ASN:HD22	1.81	0.45
1:H:318:ARG:HB2	1:H:318:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:407:ARG:O	1:H:407:ARG:HG3	2.14	0.45
1:H:484:PHE:CD1	1:H:563:LEU:HD12	2.51	0.45
1:I:369:THR:H	1:J:144:ASN:ND2	2.14	0.45
1:J:365:PHE:HE1	1:J:395:TRP:HB2	1.80	0.45
1:B:251:ARG:HD2	1:B:530:LEU:HD11	1.99	0.45
1:E:684:LEU:O	1:E:688:MET:HG3	2.16	0.45
1:F:644:LYS:HE2	1:F:713:TYR:HA	1.98	0.45
1:A:325:ILE:HD11	1:A:365:PHE:HD2	1.81	0.45
1:A:693:PHE:CE1	1:A:722:LEU:HD21	2.52	0.45
1:B:71:ILE:HD11	1:B:205:VAL:HG11	1.98	0.45
1:B:419:ARG:HD2	1:B:588:TRP:CE3	2.52	0.45
1:D:125:PRO:HA	1:D:147:ASP:HB3	1.97	0.45
1:G:243:LEU:HB3	1:G:384:ARG:NH2	2.31	0.45
1:J:409:VAL:HG13	1:J:410:GLN:HG3	1.97	0.45
1:B:490:ASP:HA	1:B:493:ARG:HB3	1.98	0.45
1:C:600:ARG:HB3	1:C:676:GLN:OE1	2.15	0.45
1:C:607:MET:HA	1:C:665:LEU:HD21	1.97	0.45
1:E:47:PHE:CE2	1:E:159:LYS:HB3	2.52	0.45
1:E:448:HIS:HA	1:E:477:MET:HB3	1.98	0.45
1:F:62:THR:HB	1:F:74:ALA:HB3	1.99	0.45
1:I:409:VAL:HG11	1:I:606:LEU:HA	1.99	0.45
1:I:473:THR:HG21	1:I:478:ASP:HB3	1.98	0.45
1:I:614:VAL:HG11	1:I:688:MET:HE2	1.98	0.45
1:C:367:TYR:CD1	1:C:395:TRP:HD1	2.35	0.45
1:I:123:HIS:CE1	1:I:149:VAL:HG22	2.52	0.45
1:A:89:ARG:HA	1:A:104:MET:HA	1.99	0.45
1:A:118:ILE:O	1:A:155:ILE:HG22	2.17	0.45
1:A:716:THR:HG22	1:A:818:LEU:HD13	1.97	0.45
1:D:326:GLU:O	1:D:329:ARG:HG2	2.16	0.45
1:D:474:PRO:HG3	1:D:542:MET:HE3	1.98	0.45
1:E:66:THR:HB	1:E:70:GLU:H	1.82	0.45
1:E:88:SER:HB3	1:E:106:THR:HB	1.99	0.45
1:F:251:ARG:HH11	1:F:530:LEU:HD21	1.81	0.45
1:J:425:ASP:HB3	1:J:429:ARG:NH1	2.32	0.45
1:B:325:ILE:HG12	1:B:440:ILE:HG13	1.99	0.45
1:C:316:LYS:HE3	1:C:317:TRP:CE2	2.52	0.45
1:D:88:SER:HB3	1:D:106:THR:HB	1.99	0.45
1:E:110:LEU:HD23	1:E:125:PRO:HB2	1.99	0.45
1:H:282:ARG:O	1:H:387:GLU:HA	2.17	0.45
1:H:609:GLN:HG3	1:H:613:HIS:CE1	2.52	0.45
1:I:408:PHE:CE2	1:I:589:LEU:HD11	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:LEU:HD12	1:J:110:LEU:HA	1.99	0.45
1:J:448:HIS:HB3	1:J:450:MET:HE2	1.99	0.45
1:J:704:ALA:HB1	1:J:712:VAL:HG11	1.98	0.45
1:B:251:ARG:HB2	1:B:282:ARG:CZ	2.47	0.44
1:C:57:SER:HB3	1:C:210:SER:HB3	1.98	0.44
1:C:144:ASN:ND2	1:D:369:THR:H	2.15	0.44
1:F:61:PHE:CE2	1:F:75:MET:HE2	2.52	0.44
1:F:367:TYR:CD1	1:F:395:TRP:HD1	2.35	0.44
1:F:810:ALA:HB3	1:F:815:ILE:HD11	1.99	0.44
1:H:305:ILE:HD12	1:H:332:PHE:HE2	1.82	0.44
1:I:462:ARG:HH12	1:I:487:GLN:H	1.65	0.44
1:A:214:ASN:HD21	1:A:361:ARG:NE	2.15	0.44
1:C:85:LEU:HD13	1:C:243:LEU:HD11	1.99	0.44
1:D:608:SER:HA	1:D:680:MET:HE1	1.99	0.44
1:E:457:THR:HG23	1:E:565:ASN:ND2	2.32	0.44
1:F:661:TYR:HA	1:F:664:TRP:NE1	2.31	0.44
1:H:742:ASN:HD22	1:I:813:GLU:HB3	1.82	0.44
1:A:320:THR:HG23	1:A:433:ARG:HB2	1.98	0.44
1:B:86:LEU:HB2	1:B:111:ILE:HD13	1.98	0.44
1:C:661:TYR:HE1	1:C:684:LEU:HB2	1.82	0.44
1:D:425:ASP:HB3	1:D:429:ARG:NH1	2.33	0.44
1:E:698:ILE:HG23	1:E:715:LEU:HD11	1.99	0.44
1:F:584:ASN:HA	1:F:587:LYS:HE2	1.99	0.44
1:H:119:ASN:HB2	1:H:121:TYR:CZ	2.53	0.44
1:H:596:TYR:CE2	1:I:631:GLN:HG2	2.52	0.44
1:B:81:ARG:HD2	1:B:81:ARG:HA	1.76	0.44
1:C:549:GLN:HE21	1:C:558:ASP:HB2	1.82	0.44
1:D:702:TYR:CZ	1:D:814:VAL:HG21	2.52	0.44
1:F:479:TYR:HA	1:F:481:ARG:NH1	2.33	0.44
1:G:316:LYS:HE3	1:G:317:TRP:CE2	2.53	0.44
1:I:120:VAL:HB	1:I:165:ILE:HG21	1.99	0.44
1:J:666:ALA:HB1	1:J:671:LEU:HD11	2.00	0.44
1:B:186:PRO:HD3	1:C:227:PRO:HB3	2.00	0.44
1:B:829:ILE:HG22	1:B:833:ARG:CD	2.38	0.44
1:C:213:ARG:HG3	1:C:242:LEU:HB3	2.00	0.44
1:C:460:ASN:HB3	1:C:466:PHE:CE2	2.51	0.44
1:D:248:MET:HG2	1:D:249:ARG:O	2.17	0.44
1:D:413:ALA:HB1	1:D:488:PRO:HG3	1.98	0.44
1:D:457:THR:O	1:D:460:ASN:HB2	2.18	0.44
1:D:581:ILE:O	1:D:585:MET:HG3	2.18	0.44
1:D:601:ASP:O	1:D:605:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:381:VAL:HG12	1:F:388:ILE:HG12	1.98	0.44
1:F:600:ARG:HB3	1:F:674:VAL:HB	1.99	0.44
1:G:549:GLN:NE2	1:G:558:ASP:HB2	2.31	0.44
1:I:560:THR:O	1:I:616:HIS:HE1	2.01	0.44
1:J:462:ARG:NH1	1:J:486:ALA:HA	2.32	0.44
1:J:597:ASP:O	1:J:600:ARG:HG2	2.18	0.44
1:A:213:ARG:NH1	1:A:361:ARG:HD3	2.33	0.44
1:C:92:ALA:HB3	1:C:235:ILE:HD12	1.99	0.44
1:E:359:ASP:HB3	1:E:362:PHE:HD2	1.82	0.44
1:G:310:ASP:HA	1:G:346:TYR:CD2	2.52	0.44
1:I:233:THR:HB	1:J:148:PRO:HA	1.99	0.44
1:I:448:HIS:HB3	1:I:450:MET:HE2	2.00	0.44
1:J:116:ASP:HB2	1:J:121:TYR:CE2	2.52	0.44
1:J:479:TYR:HB3	1:J:561:GLU:OE2	2.17	0.44
1:A:312:VAL:HB	1:E:137:ILE:HA	2.00	0.44
1:B:481:ARG:O	1:B:499:PRO:HD3	2.18	0.44
1:E:298:PRO:HB2	1:E:338:LYS:HG3	2.00	0.44
1:E:419:ARG:HD2	1:E:588:TRP:CD1	2.52	0.44
1:E:614:VAL:HG11	1:E:688:MET:HE2	1.99	0.44
1:F:730:LYS:HA	1:F:730:LYS:HD3	1.78	0.44
1:H:47:PHE:CD1	1:H:164:LEU:HD22	2.53	0.44
1:H:617:ILE:HG13	1:H:653:TRP:CE3	2.52	0.44
1:J:755:SER:HB2	1:J:857:LYS:NZ	2.33	0.44
1:E:356:ASP:HB3	1:E:359:ASP:HB2	1.99	0.44
1:H:680:MET:HA	1:H:683:LEU:HB3	1.99	0.44
1:I:803:LEU:H	1:I:803:LEU:HD23	1.83	0.44
1:A:211:PHE:HB2	1:A:214:ASN:OD1	2.18	0.44
1:A:752:SER:HB2	1:A:754:LEU:HD13	1.99	0.44
1:C:367:TYR:HE1	1:C:397:HIS:HA	1.83	0.44
1:C:484:PHE:HE1	1:C:563:LEU:HB2	1.82	0.44
1:F:47:PHE:CD1	1:F:164:LEU:HD22	2.53	0.44
1:F:521:LYS:HG3	1:F:522:THR:HG22	1.99	0.44
1:H:595:ARG:HD2	1:H:595:ARG:HA	1.72	0.44
1:H:738:ARG:HD3	1:H:738:ARG:N	2.32	0.44
1:J:581:ILE:O	1:J:585:MET:HB2	2.18	0.44
1:B:92:ALA:HB3	1:B:235:ILE:HB	2.00	0.43
1:C:365:PHE:HE1	1:C:395:TRP:HB2	1.81	0.43
1:D:329:ARG:CZ	1:D:339:ASN:HB3	2.48	0.43
1:G:661:TYR:HA	1:G:664:TRP:NE1	2.33	0.43
1:A:256:ARG:HD2	1:A:534:ILE:HG21	2.00	0.43
1:B:53:GLY:O	1:B:67:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:O	1:B:148:PRO:HD2	2.18	0.43
1:E:251:ARG:HH11	1:E:530:LEU:HD21	1.82	0.43
1:G:94:SER:HB3	1:H:148:PRO:HG3	2.01	0.43
1:G:314:PRO:O	1:G:318:ARG:HG3	2.17	0.43
1:I:684:LEU:O	1:I:688:MET:HG3	2.17	0.43
1:J:130:MET:HE2	1:J:130:MET:HB3	1.82	0.43
1:J:185:PRO:HD2	1:J:188:MET:HE3	1.99	0.43
1:J:419:ARG:HD3	1:J:588:TRP:CD2	2.53	0.43
1:A:124:THR:O	1:A:148:PRO:HD2	2.19	0.43
1:E:216:GLU:HB3	1:E:237:GLN:NE2	2.33	0.43
1:E:592:LYS:HG3	1:E:593:GLU:OE1	2.18	0.43
1:F:455:SER:HB2	1:F:541:PRO:HB2	2.00	0.43
1:G:-2:PHE:C	1:G:-1:GLN:HG2	2.42	0.43
1:G:435:VAL:O	1:G:439:GLU:HG2	2.18	0.43
1:H:56:LYS:HE3	1:H:62:THR:HG21	2.00	0.43
1:J:96:THR:HG21	1:J:370:THR:HB	2.00	0.43
1:A:213:ARG:H	1:A:213:ARG:HG3	1.49	0.43
1:B:96:THR:HG23	1:B:100:VAL:HG23	2.00	0.43
1:B:566:ASP:OD2	1:B:569:ARG:HG2	2.18	0.43
1:C:124:THR:O	1:C:148:PRO:HD2	2.19	0.43
1:F:267:PHE:CE2	1:J:369:THR:HG23	2.53	0.43
1:G:47:PHE:CE2	1:G:159:LYS:HB3	2.54	0.43
1:H:257:VAL:HG21	1:H:512:TRP:CD2	2.54	0.43
1:I:611:TYR:HB2	1:I:684:LEU:HD21	2.00	0.43
1:C:71:ILE:HD11	1:C:205:VAL:HG11	1.99	0.43
1:C:82:ARG:HE	1:C:245:GLU:HG3	1.83	0.43
1:C:251:ARG:HB3	1:C:280:ILE:HG12	2.01	0.43
1:C:409:VAL:HG13	1:C:606:LEU:HD23	1.99	0.43
1:C:426:GLU:CD	1:C:429:ARG:HH21	2.26	0.43
1:G:808:LYS:HB3	1:G:808:LYS:HE3	1.72	0.43
1:H:574:SER:HA	1:H:577:ASN:HD22	1.84	0.43
1:I:61:PHE:HD2	1:I:75:MET:HG2	1.84	0.43
1:I:251:ARG:O	1:I:279:LEU:HA	2.18	0.43
1:A:117:SER:HB3	1:F:-4:LEU:HB3	2.00	0.43
1:A:144:ASN:ND2	1:B:369:THR:H	2.16	0.43
1:A:595:ARG:HH12	1:E:255:ASN:HD22	1.67	0.43
1:C:137:ILE:HA	1:D:312:VAL:HB	2.00	0.43
1:C:730:LYS:HA	1:C:833:ARG:HH12	1.83	0.43
1:D:313:PHE:CE1	1:D:367:TYR:HB2	2.53	0.43
1:F:129:ALA:HB3	1:F:145:PHE:CE2	2.53	0.43
1:G:702:TYR:HB2	1:G:715:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:319:ALA:HA	1:I:322:LYS:HD2	2.00	0.43
1:I:609:GLN:HA	1:I:612:ARG:HD2	2.01	0.43
1:J:471:GLY:HA3	1:J:500:PRO:HD3	2.00	0.43
1:J:545:PHE:HE2	1:J:800:PHE:HB3	1.83	0.43
1:J:810:ALA:HB3	1:J:815:ILE:HD11	2.01	0.43
1:D:642:ILE:HD13	1:D:642:ILE:HA	1.92	0.43
1:F:180:PRO:HD2	1:F:223:TYR:OH	2.19	0.43
1:G:124:THR:O	1:G:148:PRO:HD2	2.19	0.43
1:H:585:MET:HE2	1:H:585:MET:HB3	1.86	0.43
1:I:329:ARG:HG3	1:I:339:ASN:HA	1.99	0.43
1:I:476:ILE:HD12	1:I:476:ILE:HA	1.91	0.43
1:I:579:LYS:HE2	1:I:664:TRP:CG	2.54	0.43
1:B:834:LYS:HB3	1:B:834:LYS:HE2	1.67	0.43
1:C:325:ILE:HG21	1:C:343:ALA:HB2	2.01	0.43
1:D:670:PHE:HA	1:D:673:LYS:HE2	2.01	0.43
1:E:354:ASP:HB3	1:E:361:ARG:HH22	1.83	0.43
1:E:464:PRO:HD3	1:E:493:ARG:NH2	2.34	0.43
1:J:313:PHE:CZ	1:J:367:TYR:HB2	2.54	0.43
1:D:253:GLN:HG3	1:D:261:ASN:HD22	1.83	0.43
1:E:416:PRO:O	1:E:419:ARG:HG2	2.19	0.43
1:H:484:PHE:HD2	1:H:613:HIS:HE2	1.66	0.43
1:I:661:TYR:HA	1:I:664:TRP:NE1	2.34	0.43
1:A:517:VAL:HB	1:A:526:GLU:HG2	2.01	0.43
1:B:473:THR:HB	1:B:475:SER:H	1.84	0.43
1:F:395:TRP:CZ2	1:F:432:LEU:HD22	2.54	0.43
1:I:640:ARG:HA	1:I:709:GLN:NE2	2.33	0.43
1:J:61:PHE:HE1	1:J:215:VAL:HG21	1.84	0.43
1:A:185:PRO:HG3	1:B:228:TYR:OH	2.19	0.42
1:D:813:GLU:OE1	1:E:739:SER:HA	2.20	0.42
1:J:47:PHE:CD2	1:J:159:LYS:HB3	2.55	0.42
1:A:135:ASP:OD2	1:A:137:ILE:HG12	2.19	0.42
1:A:611:TYR:HB2	1:A:684:LEU:HD21	2.01	0.42
1:D:118:ILE:O	1:D:155:ILE:HG12	2.19	0.42
1:F:186:PRO:HD3	1:J:227:PRO:HG3	2.01	0.42
1:F:471:GLY:HA3	1:F:500:PRO:HD3	2.01	0.42
1:G:234:LEU:HB3	1:G:236:MET:HE2	2.00	0.42
1:H:169:LYS:HD2	1:H:172:ARG:HH21	1.84	0.42
1:J:130:MET:HE1	1:J:250:MET:HE1	2.01	0.42
1:J:249:ARG:O	1:J:250:MET:HG3	2.19	0.42
1:A:551:PRO:HG2	1:A:552:TYR:CD2	2.54	0.42
1:D:124:THR:O	1:D:148:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ARG:HD2	1:F:358:ASP:HB3	2.01	0.42
1:F:616:HIS:O	1:F:619:PRO:HD2	2.18	0.42
1:H:61:PHE:CD2	1:H:75:MET:HG2	2.47	0.42
1:H:474:PRO:HG3	1:H:542:MET:HG2	2.01	0.42
1:H:644:LYS:CE	1:H:713:TYR:HA	2.42	0.42
1:H:738:ARG:HD3	1:H:738:ARG:H	1.83	0.42
1:I:550:PHE:CD1	1:I:551:PRO:HA	2.55	0.42
1:J:131:VAL:HB	1:J:141:PHE:CE2	2.53	0.42
1:A:438:HIS:HE1	1:A:448:HIS:CD2	2.37	0.42
1:D:146:PHE:O	1:E:94:SER:HA	2.19	0.42
1:D:325:ILE:HG12	1:D:440:ILE:HG13	2.01	0.42
1:I:313:PHE:HB2	1:I:318:ARG:CZ	2.49	0.42
1:J:423:PHE:HB2	1:J:428:MET:HE2	2.01	0.42
1:J:567:HIS:HB3	1:J:616:HIS:HB3	2.01	0.42
1:A:308:TYR:HB3	1:A:346:TYR:CD1	2.54	0.42
1:A:815:ILE:HD12	1:A:815:ILE:HA	1.89	0.42
1:B:426:GLU:CD	1:B:429:ARG:HH21	2.27	0.42
1:B:581:ILE:O	1:B:585:MET:HG3	2.19	0.42
1:D:144:ASN:ND2	1:E:369:THR:H	2.17	0.42
1:G:371:THR:HA	1:G:398:ASN:HD22	1.84	0.42
1:H:473:THR:HG21	1:H:478:ASP:HB3	2.02	0.42
1:H:484:PHE:HD1	1:H:563:LEU:HD12	1.84	0.42
1:J:132:ARG:O	1:J:135:ASP:HB2	2.19	0.42
1:J:218:LYS:HE3	1:J:218:LYS:HB2	1.75	0.42
1:J:277:PHE:H	1:J:277:PHE:HD2	1.67	0.42
1:A:448:HIS:HD2	1:A:477:MET:O	2.02	0.42
1:A:834:LYS:HG3	1:A:842:ARG:HG3	2.02	0.42
1:B:549:GLN:HG3	1:B:553:THR:HA	2.01	0.42
1:F:213:ARG:HA	1:F:213:ARG:HD3	1.74	0.42
1:G:89:ARG:HH21	1:G:366:LYS:NZ	2.18	0.42
1:G:479:TYR:HA	1:G:481:ARG:NH1	2.34	0.42
1:J:155:ILE:HD12	1:J:163:VAL:HG13	2.02	0.42
1:J:692:LEU:HD13	1:J:722:LEU:HD11	2.01	0.42
1:A:549:GLN:HE21	1:A:558:ASP:HB2	1.84	0.42
1:D:696:GLY:HA2	1:D:808:LYS:O	2.20	0.42
1:F:94:SER:OG	1:G:148:PRO:HG3	2.20	0.42
1:F:189:GLN:CD	1:F:190:ASN:H	2.28	0.42
1:G:853:GLU:HG2	1:G:857:LYS:HZ2	1.85	0.42
1:H:601:ASP:O	1:H:605:GLN:HG2	2.19	0.42
1:A:71:ILE:HB	1:A:167:VAL:HG23	2.01	0.42
1:A:141:PHE:HB2	1:B:369:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:661:TYR:HD2	1:F:688:MET:HE1	1.85	0.42
1:G:699:GLY:HA2	1:G:810:ALA:HB2	2.02	0.42
1:H:312:VAL:HG21	1:I:140:SER:HB2	2.02	0.42
1:H:610:TYR:OH	1:H:657:GLN:HB3	2.19	0.42
1:J:702:TYR:HB2	1:J:715:LEU:HD22	2.02	0.42
1:A:137:ILE:HA	1:B:312:VAL:HB	2.02	0.42
1:A:479:TYR:HB3	1:A:481:ARG:HE	1.85	0.42
1:B:729:VAL:HG21	1:B:737:ASP:OD2	2.20	0.42
1:C:661:TYR:HA	1:C:664:TRP:NE1	2.35	0.42
1:D:329:ARG:HH21	1:D:341:ILE:N	2.18	0.42
1:F:818:LEU:O	1:F:822:GLN:HG2	2.20	0.42
1:H:313:PHE:CZ	1:H:367:TYR:HB2	2.55	0.42
1:I:693:PHE:HB2	1:I:747:LEU:HD13	2.02	0.42
1:J:465:GLN:O	1:J:469:LYS:HG2	2.20	0.42
1:B:329:ARG:HA	1:B:332:PHE:HD2	1.83	0.42
1:C:251:ARG:HD2	1:C:530:LEU:HD11	2.01	0.42
1:C:410:GLN:OE1	1:C:482:ASN:HB2	2.20	0.42
1:C:542:MET:HE2	1:C:542:MET:HB3	1.79	0.42
1:D:555:ASP:HA	1:D:624:VAL:O	2.20	0.42
1:F:484:PHE:HE1	1:F:563:LEU:HB2	1.84	0.42
1:G:361:ARG:HE	1:G:361:ARG:HB2	1.77	0.42
1:H:661:TYR:HD1	1:H:662:ARG:N	2.17	0.42
1:H:661:TYR:HE2	1:H:684:LEU:HB3	1.84	0.42
1:I:75:MET:HE3	1:I:165:ILE:HD11	2.02	0.42
1:I:741:GLN:HG2	1:I:830:TYR:OH	2.19	0.42
1:J:253:GLN:HG3	1:J:261:ASN:HD22	1.84	0.42
1:A:684:LEU:O	1:A:688:MET:HG3	2.20	0.41
1:C:313:PHE:CZ	1:C:367:TYR:HB2	2.55	0.41
1:F:644:LYS:HG3	1:F:713:TYR:CD1	2.55	0.41
1:I:592:LYS:HG2	1:I:593:GLU:OE1	2.20	0.41
1:A:395:TRP:CZ2	1:A:432:LEU:HD22	2.55	0.41
1:A:661:TYR:HA	1:A:664:TRP:HE1	1.85	0.41
1:B:130:MET:HE1	1:B:250:MET:HE1	2.02	0.41
1:B:286:GLN:NE2	1:B:287:PRO:HD2	2.35	0.41
1:D:135:ASP:OD2	1:D:137:ILE:HG12	2.19	0.41
1:G:176:LYS:HG3	1:G:183:ILE:HD11	2.03	0.41
1:H:124:THR:O	1:H:148:PRO:HD2	2.20	0.41
1:I:406:TRP:O	1:I:410:GLN:HG3	2.21	0.41
1:A:596:TYR:HB3	1:A:674:VAL:HG12	2.01	0.41
1:B:86:LEU:HD13	1:B:240:ILE:HG12	2.02	0.41
1:B:487:GLN:HE21	1:B:573:MET:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:THR:HG23	1:C:525:GLU:HG3	2.03	0.41
1:G:82:ARG:HG2	1:G:242:LEU:HD11	2.02	0.41
1:G:233:THR:HB	1:H:148:PRO:HA	2.01	0.41
1:G:408:PHE:CE2	1:G:602:MET:HG2	2.56	0.41
1:I:184:LEU:HD23	1:I:184:LEU:HA	1.87	0.41
1:I:578:LEU:HD11	1:I:613:HIS:HE1	1.84	0.41
1:A:74:ALA:HA	1:A:163:VAL:O	2.21	0.41
1:A:581:ILE:O	1:A:585:MET:HB2	2.20	0.41
1:B:484:PHE:CD2	1:B:613:HIS:HE1	2.39	0.41
1:D:419:ARG:HD2	1:D:588:TRP:CD1	2.56	0.41
1:D:850:LEU:O	1:D:854:ARG:HG3	2.21	0.41
1:F:281:HIS:CG	1:F:381:VAL:HG11	2.55	0.41
1:G:306:VAL:HG22	1:G:342:ILE:HB	2.01	0.41
1:I:450:MET:SD	1:I:560:THR:HG22	2.60	0.41
1:A:723:ILE:HG13	1:A:822:GLN:HB3	2.03	0.41
1:C:183:ILE:HG21	1:D:228:TYR:HA	2.01	0.41
1:D:308:TYR:CZ	1:D:344:LYS:HE2	2.55	0.41
1:D:818:LEU:O	1:D:822:GLN:HG2	2.20	0.41
1:E:670:PHE:O	1:E:674:VAL:HG22	2.21	0.41
1:F:132:ARG:HH12	1:F:270:ASP:H	1.69	0.41
1:G:47:PHE:CD1	1:G:164:LEU:HD22	2.55	0.41
1:G:458:ILE:HG13	1:G:569:ARG:HH11	1.86	0.41
1:A:287:PRO:HG3	1:A:293:TYR:HD2	1.85	0.41
1:B:308:TYR:HD2	1:B:347:PRO:HD3	1.85	0.41
1:C:83:GLU:HB3	1:C:110:LEU:HD11	2.02	0.41
1:C:255:ASN:HD22	1:D:595:ARG:NH1	2.18	0.41
1:E:67:LYS:HB3	1:I:-1:GLN:HG3	2.03	0.41
1:E:84:TYR:HB2	1:E:111:ILE:HG13	2.03	0.41
1:E:559:GLN:OE1	1:E:616:HIS:HA	2.20	0.41
1:E:833:ARG:HH11	1:E:833:ARG:HD3	1.68	0.41
1:F:84:TYR:HB2	1:F:111:ILE:HG13	2.03	0.41
1:F:448:HIS:HB3	1:F:450:MET:HE2	2.02	0.41
1:G:313:PHE:CZ	1:G:367:TYR:HB2	2.56	0.41
1:J:221:LEU:HD12	1:J:236:MET:HG3	2.03	0.41
1:J:251:ARG:HB2	1:J:282:ARG:NH2	2.36	0.41
1:J:628:GLU:HB3	1:J:630:ARG:NH1	2.36	0.41
1:B:370:THR:HG23	1:B:372:THR:H	1.86	0.41
1:B:549:GLN:HE22	1:B:555:ASP:HB3	1.85	0.41
1:C:61:PHE:HD2	1:C:75:MET:HG2	1.84	0.41
1:C:480:ALA:HB1	1:C:563:LEU:HD21	2.02	0.41
1:C:555:ASP:HA	1:C:624:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:857:LYS:HE3	1:D:857:LYS:HB3	1.80	0.41
1:E:323:GLN:O	1:E:323:GLN:HG3	2.19	0.41
1:E:419:ARG:HH11	1:E:588:TRP:HD1	1.66	0.41
1:F:61:PHE:HE1	1:F:215:VAL:HG21	1.86	0.41
1:H:348:THR:HG22	1:H:351:GLU:HG3	2.03	0.41
1:I:689:VAL:HA	1:I:692:LEU:HD12	2.01	0.41
1:A:600:ARG:HB2	1:A:674:VAL:HB	2.03	0.41
1:B:331:ALA:HA	1:B:507:ILE:HG12	2.02	0.41
1:D:47:PHE:HD1	1:D:164:LEU:HD22	1.86	0.41
1:D:825:ARG:HA	1:D:825:ARG:HD2	1.81	0.41
1:E:71:ILE:HD11	1:E:205:VAL:HG11	2.03	0.41
1:E:476:ILE:HD13	1:E:476:ILE:HA	1.91	0.41
1:F:110:LEU:HD23	1:F:125:PRO:HB2	2.03	0.41
1:G:262:SER:HB3	1:G:264:ARG:NH1	2.36	0.41
1:I:251:ARG:HG2	1:I:282:ARG:CZ	2.51	0.41
1:I:467:THR:HB	1:I:496:ARG:HB3	2.02	0.41
1:J:400:LEU:HD23	1:J:432:LEU:HD21	2.02	0.41
1:B:255:ASN:ND2	1:C:595:ARG:HH12	2.19	0.41
1:C:136:PRO:O	1:C:139:PRO:HD2	2.20	0.41
1:C:264:ARG:HB2	1:C:277:PHE:CE2	2.56	0.41
1:E:468:GLN:OE1	1:E:496:ARG:HB2	2.21	0.41
1:F:148:PRO:HG3	1:J:94:SER:OG	2.20	0.41
1:H:292:ALA:HA	1:H:295:ARG:HE	1.86	0.41
1:H:580:ILE:H	1:H:580:ILE:HG12	1.73	0.41
1:H:661:TYR:CE1	1:H:662:ARG:HG3	2.55	0.41
1:I:131:VAL:HB	1:I:141:PHE:CE2	2.56	0.41
1:I:450:MET:HB3	1:I:559:GLN:O	2.21	0.41
1:A:59:GLY:HA3	1:A:60:PRO:HD2	1.97	0.41
1:A:184:LEU:HA	1:A:185:PRO:HD3	1.93	0.41
1:A:510:ILE:HD13	1:A:510:ILE:HA	1.93	0.41
1:B:484:PHE:HD1	1:B:485:VAL:N	2.18	0.41
1:C:458:ILE:O	1:C:462:ARG:HG2	2.20	0.41
1:D:312:VAL:HG23	1:D:367:TYR:CD2	2.56	0.41
1:D:674:VAL:HG23	1:D:676:GLN:HB2	2.03	0.41
1:E:180:PRO:HD2	1:E:223:TYR:OH	2.21	0.41
1:E:447:MET:HE2	1:E:447:MET:HB3	1.93	0.41
1:E:479:TYR:HA	1:E:481:ARG:NH1	2.35	0.41
1:E:614:VAL:HG12	1:E:618:MET:HE3	2.03	0.41
1:F:82:ARG:HB2	1:F:84:TYR:CE1	2.55	0.41
1:F:237:GLN:HG2	1:F:358:ASP:HB3	2.03	0.41
1:G:723:ILE:HD13	1:G:723:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:HB	1:B:74:ALA:HB3	2.02	0.40
1:C:597:ASP:HA	1:C:600:ARG:HE	1.85	0.40
1:D:61:PHE:CD2	1:D:75:MET:HG2	2.52	0.40
1:D:75:MET:HE3	1:D:75:MET:HB2	1.84	0.40
1:D:733:LEU:HB2	1:D:738:ARG:CZ	2.51	0.40
1:E:-2:PHE:HB2	1:J:155:ILE:HD13	2.03	0.40
1:F:435:VAL:O	1:F:439:GLU:HG2	2.21	0.40
1:G:812:ASN:HA	1:G:815:ILE:HG22	2.02	0.40
1:H:329:ARG:NH1	1:H:339:ASN:HB3	2.36	0.40
1:H:603:HIS:HE1	1:H:607:MET:HE3	1.86	0.40
1:I:312:VAL:HG23	1:I:367:TYR:CD2	2.56	0.40
1:J:356:ASP:HB3	1:J:359:ASP:HB2	2.03	0.40
1:A:141:PHE:CE1	1:A:145:PHE:HD2	2.39	0.40
1:B:286:GLN:HA	1:B:286:GLN:NE2	2.35	0.40
1:C:517:VAL:HB	1:C:526:GLU:HG3	2.04	0.40
1:C:849:LEU:O	1:C:853:GLU:HB2	2.21	0.40
1:D:308:TYR:CD2	1:D:344:LYS:HE2	2.56	0.40
1:E:314:PRO:O	1:E:318:ARG:HG3	2.22	0.40
1:H:316:LYS:HD2	1:H:317:TRP:CE2	2.56	0.40
1:I:73:PHE:CD2	1:I:167:VAL:HG11	2.57	0.40
1:I:277:PHE:CD1	1:I:277:PHE:C	2.99	0.40
1:I:295:ARG:NH1	1:I:295:ARG:HG3	2.35	0.40
1:I:324:ALA:HA	1:I:327:ASP:OD2	2.21	0.40
1:J:211:PHE:HB2	1:J:214:ASN:OD1	2.22	0.40
1:J:312:VAL:HG23	1:J:367:TYR:CD2	2.56	0.40
1:J:549:GLN:OE1	1:J:553:THR:HG23	2.20	0.40
1:A:306:VAL:HG22	1:A:342:ILE:HB	2.03	0.40
1:C:59:GLY:HA3	1:C:60:PRO:HD2	1.97	0.40
1:C:320:THR:HG23	1:C:433:ARG:HB2	2.03	0.40
1:C:395:TRP:CZ2	1:C:432:LEU:HD22	2.56	0.40
1:D:207:GLU:HB3	1:D:218:LYS:HB2	2.03	0.40
1:D:723:ILE:HG13	1:D:822:GLN:HB3	2.02	0.40
1:E:75:MET:HE3	1:E:165:ILE:HD11	2.04	0.40
1:H:94:SER:OG	1:I:148:PRO:HG3	2.21	0.40
1:H:578:LEU:HD11	1:H:613:HIS:HE1	1.86	0.40
1:H:857:LYS:HE2	1:H:859:ASN:OD1	2.21	0.40
1:A:251:ARG:HB3	1:A:280:ILE:HG12	2.04	0.40
1:A:284:ASP:HB2	1:A:387:GLU:HG3	2.03	0.40
1:A:419:ARG:HD2	1:A:588:TRP:CD2	2.57	0.40
1:A:847:TYR:HD2	1:A:848:GLN:HE21	1.70	0.40
1:C:-1:GLN:HG3	1:G:67:LYS:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:ASN:HA	1:C:825:ARG:HH12	1.86	0.40
1:D:438:HIS:HE1	1:D:448:HIS:CD2	2.39	0.40
1:D:473:THR:HG21	1:D:478:ASP:HB3	2.02	0.40
1:D:632:GLY:HA3	1:E:592:LYS:HD2	2.04	0.40
1:F:473:THR:HG21	1:F:478:ASP:HB3	2.03	0.40
1:F:676:GLN:HE21	1:F:678:SER:HB3	1.87	0.40
1:G:120:VAL:HG23	1:G:155:ILE:HG22	2.04	0.40
1:H:581:ILE:O	1:H:585:MET:HB2	2.22	0.40
1:H:672:ASN:ND2	1:I:637:LEU:HD12	2.36	0.40
1:J:289:ASP:OD1	1:J:299:VAL:HG11	2.20	0.40
1:B:373:ALA:HB1	1:B:402:LEU:HB2	2.03	0.40
1:B:413:ALA:HB1	1:B:580:ILE:HD11	2.04	0.40
1:B:751:HIS:HB2	1:B:819:LEU:HD11	2.03	0.40
1:C:698:ILE:HG23	1:C:715:LEU:HD11	2.02	0.40
1:D:56:LYS:HE3	1:D:58:GLU:OE2	2.20	0.40
1:D:321:ILE:HG23	1:D:365:PHE:CE2	2.56	0.40
1:E:717:ASP:O	1:E:721:GLU:HG3	2.22	0.40
1:E:849:LEU:O	1:E:853:GLU:HG3	2.22	0.40
1:G:113:PHE:CE1	1:G:122:LEU:HD13	2.57	0.40
1:G:155:ILE:HA	1:G:165:ILE:HG22	2.04	0.40
1:I:116:ASP:HB2	1:I:121:TYR:HE2	1.87	0.40
1:I:425:ASP:HB3	1:I:429:ARG:NH1	2.37	0.40
1:I:463:ASP:HA	1:I:464:PRO:HD3	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	774/828 (94%)	765 (99%)	9 (1%)	0	100	100
1	B	768/828 (93%)	757 (99%)	11 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	770/828 (93%)	757 (98%)	13 (2%)	0	100	100
1	D	769/828 (93%)	755 (98%)	14 (2%)	0	100	100
1	E	775/828 (94%)	763 (98%)	12 (2%)	0	100	100
1	F	772/828 (93%)	757 (98%)	14 (2%)	1 (0%)	48	80
1	G	772/828 (93%)	762 (99%)	10 (1%)	0	100	100
1	H	771/828 (93%)	757 (98%)	14 (2%)	0	100	100
1	I	768/828 (93%)	758 (99%)	10 (1%)	0	100	100
1	J	771/828 (93%)	759 (98%)	12 (2%)	0	100	100
All	All	7710/8280 (93%)	7590 (98%)	119 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	806	PHE

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	682/722 (94%)	662 (97%)	20 (3%)	37	70
1	B	676/722 (94%)	651 (96%)	25 (4%)	30	64
1	C	678/722 (94%)	656 (97%)	22 (3%)	34	67
1	D	677/722 (94%)	651 (96%)	26 (4%)	29	63
1	E	683/722 (95%)	667 (98%)	16 (2%)	44	74
1	F	680/722 (94%)	657 (97%)	23 (3%)	32	66
1	G	680/722 (94%)	659 (97%)	21 (3%)	35	68
1	H	679/722 (94%)	647 (95%)	32 (5%)	23	58
1	I	676/722 (94%)	649 (96%)	27 (4%)	28	62
1	J	679/722 (94%)	651 (96%)	28 (4%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6790/7220 (94%)	6550 (96%)	240 (4%)	32 65

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	A	61	PHE
1	A	84	TYR
1	A	141	PHE
1	A	211	PHE
1	A	213	ARG
1	A	267	PHE
1	A	466	PHE
1	A	473	THR
1	A	484	PHE
1	A	543	PHE
1	A	565	ASN
1	A	568	PHE
1	A	641	PHE
1	A	663	GLN
1	A	677	ASN
1	A	693	PHE
1	A	713	TYR
1	A	801	PHE
1	A	803	LEU
1	B	55	LYS
1	B	61	PHE
1	B	67	LYS
1	B	84	TYR
1	B	145	PHE
1	B	223	TYR
1	B	261	ASN
1	B	267	PHE
1	B	286	GLN
1	B	308	TYR
1	B	349	LYS
1	B	362	PHE
1	B	384	ARG
1	B	396	TYR
1	B	459	GLU
1	B	473	THR
1	B	484	PHE

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Mol	Chain	Res	Type
1	B	560	THR
1	B	568	PHE
1	B	569	ARG
1	B	596	TYR
1	B	661	TYR
1	B	713	TYR
1	B	806	PHE
1	B	833	ARG
1	C	61	PHE
1	C	64	TYR
1	C	84	TYR
1	C	159	LYS
1	C	223	TYR
1	C	267	PHE
1	C	277	PHE
1	C	293	TYR
1	C	308	TYR
1	C	322	LYS
1	C	348	THR
1	C	470	TYR
1	C	484	PHE
1	C	522	THR
1	C	568	PHE
1	C	641	PHE
1	C	661	TYR
1	C	754	LEU
1	C	802	ARG
1	C	803	LEU
1	C	833	ARG
1	C	857	LYS
1	D	61	PHE
1	D	84	TYR
1	D	113	PHE
1	D	115	ARG
1	D	124	THR
1	D	135	ASP
1	D	223	TYR
1	D	249	ARG
1	D	267	PHE
1	D	308	TYR
1	D	313	PHE
1	D	350	GLU

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Mol	Chain	Res	Type
1	D	459	GLU
1	D	461	LEU
1	D	466	PHE
1	D	470	TYR
1	D	473	THR
1	D	484	PHE
1	D	543	PHE
1	D	565	ASN
1	D	568	PHE
1	D	612	ARG
1	D	641	PHE
1	D	665	LEU
1	D	713	TYR
1	D	729	VAL
1	E	61	PHE
1	E	64	TYR
1	E	84	TYR
1	E	109	PHE
1	E	113	PHE
1	E	134	ASP
1	E	223	TYR
1	E	249	ARG
1	E	267	PHE
1	E	293	TYR
1	E	308	TYR
1	E	466	PHE
1	E	473	THR
1	E	484	PHE
1	E	641	PHE
1	E	713	TYR
1	F	61	PHE
1	F	64	TYR
1	F	84	TYR
1	F	137	ILE
1	F	223	TYR
1	F	267	PHE
1	F	277	PHE
1	F	308	TYR
1	F	396	TYR
1	F	468	GLN
1	F	473	THR
1	F	484	PHE

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Mol	Chain	Res	Type
1	F	522	THR
1	F	561	GLU
1	F	569	ARG
1	F	634	GLU
1	F	641	PHE
1	F	661	TYR
1	F	663	GLN
1	F	713	TYR
1	F	801	PHE
1	F	806	PHE
1	F	825	ARG
1	G	61	PHE
1	G	84	TYR
1	G	159	LYS
1	G	211	PHE
1	G	223	TYR
1	G	269	THR
1	G	277	PHE
1	G	308	TYR
1	G	361	ARG
1	G	466	PHE
1	G	484	PHE
1	G	568	PHE
1	G	580	ILE
1	G	634	GLU
1	G	641	PHE
1	G	684	LEU
1	G	693	PHE
1	G	713	TYR
1	G	802	ARG
1	G	808	LYS
1	G	858	THR
1	H	49	GLN
1	H	61	PHE
1	H	64	TYR
1	H	84	TYR
1	H	171	PHE
1	H	213	ARG
1	H	223	TYR
1	H	250	MET
1	H	261	ASN
1	H	267	PHE

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Mol	Chain	Res	Type
1	H	290	SER
1	H	308	TYR
1	H	318	ARG
1	H	332	PHE
1	H	339	ASN
1	H	346	TYR
1	H	396	TYR
1	H	418	VAL
1	H	426	GLU
1	H	454	TYR
1	H	467	THR
1	H	470	TYR
1	H	498	THR
1	H	526	GLU
1	H	568	PHE
1	H	579	LYS
1	H	612	ARG
1	H	641	PHE
1	H	661	TYR
1	H	713	TYR
1	H	738	ARG
1	H	754	LEU
1	I	61	PHE
1	I	84	TYR
1	I	141	PHE
1	I	223	TYR
1	I	246	LYS
1	I	267	PHE
1	I	269	THR
1	I	277	PHE
1	I	295	ARG
1	I	308	TYR
1	I	346	TYR
1	I	362	PHE
1	I	367	TYR
1	I	384	ARG
1	I	396	TYR
1	I	466	PHE
1	I	473	THR
1	I	484	PHE
1	I	552	TYR
1	I	568	PHE

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Mol	Chain	Res	Type
1	I	641	PHE
1	I	661	TYR
1	I	709	GLN
1	I	713	TYR
1	I	842	ARG
1	I	855	LEU
1	I	858	THR
1	J	47	PHE
1	J	61	PHE
1	J	84	TYR
1	J	85	LEU
1	J	135	ASP
1	J	171	PHE
1	J	189	GLN
1	J	211	PHE
1	J	223	TYR
1	J	268	SER
1	J	269	THR
1	J	270	ASP
1	J	277	PHE
1	J	299	VAL
1	J	308	TYR
1	J	369	THR
1	J	396	TYR
1	J	407	ARG
1	J	418	VAL
1	J	470	TYR
1	J	484	PHE
1	J	521	LYS
1	J	568	PHE
1	J	569	ARG
1	J	634	GLU
1	J	641	PHE
1	J	713	TYR
1	J	857	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	487	GLN
1	B	286	GLN

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Mol	Chain	Res	Type
1	B	549	GLN
1	B	613	HIS
1	B	859	ASN
1	C	404	HIS
1	C	482	ASN
1	C	821	GLN
1	D	482	ASN
1	E	123	HIS
1	E	261	ASN
1	E	265	GLN
1	E	482	ASN
1	G	339	ASN
1	G	548	GLN
1	G	706	GLN
1	H	397	HIS
1	H	631	GLN
1	I	438	HIS
1	I	605	GLN
1	I	609	GLN
1	I	709	GLN
1	J	123	HIS
1	J	261	ASN
1	J	482	ASN
1	J	626	HIS
1	J	751	HIS
1	J	848	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 20 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	C	905	-	5,5,5	0.35	0	5,5,5	0.46	0
4	GOL	C	903	3	5,5,5	0.51	0	5,5,5	0.83	0
4	GOL	G	903	3	5,5,5	0.35	0	5,5,5	0.68	0
4	GOL	C	904	-	5,5,5	0.32	0	5,5,5	0.42	0
4	GOL	D	903	3	5,5,5	0.32	0	5,5,5	0.49	0
4	GOL	A	905	-	5,5,5	0.26	0	5,5,5	0.37	0
4	GOL	A	903	3	5,5,5	0.45	0	5,5,5	0.58	0
5	TRS	B	904	-	7,7,7	0.37	0	9,9,9	0.58	0
4	GOL	E	906	-	5,5,5	0.35	0	5,5,5	0.41	0
4	GOL	F	903	3	5,5,5	0.41	0	5,5,5	0.72	0
4	GOL	F	905	-	5,5,5	0.40	0	5,5,5	0.41	0
4	GOL	D	904	-	5,5,5	0.35	0	5,5,5	0.27	0
4	GOL	E	905	-	5,5,5	0.25	0	5,5,5	0.53	0
4	GOL	B	903	3	5,5,5	0.36	0	5,5,5	0.84	0
4	GOL	E	903	3	5,5,5	0.47	0	5,5,5	0.66	0
4	GOL	I	903	3	5,5,5	0.33	0	5,5,5	0.67	0
4	GOL	H	903	3	5,5,5	0.52	0	5,5,5	0.86	0
4	GOL	F	904	-	5,5,5	0.27	0	5,5,5	0.40	0
4	GOL	G	904	-	5,5,5	0.28	0	5,5,5	0.84	0
4	GOL	E	904	-	5,5,5	0.26	0	5,5,5	0.40	0
4	GOL	J	903	3	5,5,5	0.39	0	5,5,5	0.75	0
4	GOL	A	904	-	5,5,5	0.26	0	5,5,5	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	905	-	-	0/4/4/4	-
4	GOL	C	903	3	-	0/4/4/4	-
4	GOL	G	903	3	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	904	-	-	2/4/4/4	-
4	GOL	D	903	3	-	0/4/4/4	-
4	GOL	A	905	-	-	1/4/4/4	-
4	GOL	A	903	3	-	0/4/4/4	-
5	TRS	B	904	-	-	6/9/9/9	-
4	GOL	E	906	-	-	0/4/4/4	-
4	GOL	F	903	3	-	0/4/4/4	-
4	GOL	F	905	-	-	0/4/4/4	-
4	GOL	D	904	-	-	1/4/4/4	-
4	GOL	E	905	-	-	0/4/4/4	-
4	GOL	B	903	3	-	0/4/4/4	-
4	GOL	E	903	3	-	0/4/4/4	-
4	GOL	I	903	3	-	0/4/4/4	-
4	GOL	H	903	3	-	0/4/4/4	-
4	GOL	F	904	-	-	0/4/4/4	-
4	GOL	G	904	-	-	3/4/4/4	-
4	GOL	E	904	-	-	2/4/4/4	-
4	GOL	J	903	3	-	0/4/4/4	-
4	GOL	A	904	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	904	GOL	C1-C2-C3-O3
5	B	904	TRS	N-C-C2-O2
5	B	904	TRS	C1-C-C3-O3
5	B	904	TRS	C2-C-C3-O3
5	B	904	TRS	N-C-C3-O3
4	C	904	GOL	O1-C1-C2-C3
5	B	904	TRS	C3-C-C2-O2
4	E	904	GOL	O2-C2-C3-O3
4	C	904	GOL	O1-C1-C2-O2
4	G	904	GOL	O1-C1-C2-O2
4	G	904	GOL	O1-C1-C2-C3
5	B	904	TRS	C1-C-C2-O2
4	A	905	GOL	C1-C2-C3-O3
4	D	904	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	G	904	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	905	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	778/828 (93%)	-1.20	0 100 100	48, 75, 110, 160	0
1	B	772/828 (93%)	-0.97	2 (0%) 90 79	52, 89, 118, 227	0
1	C	774/828 (93%)	-1.08	0 100 100	57, 103, 137, 199	0
1	D	773/828 (93%)	-1.07	1 (0%) 92 86	61, 103, 143, 184	0
1	E	779/828 (94%)	-1.16	0 100 100	57, 81, 118, 187	0
1	F	776/828 (93%)	-1.09	0 100 100	55, 96, 134, 178	0
1	G	776/828 (93%)	-1.11	1 (0%) 92 86	66, 100, 138, 187	0
1	H	775/828 (93%)	-0.88	0 100 100	76, 122, 169, 230	0
1	I	772/828 (93%)	-0.62	0 100 100	74, 119, 155, 206	0
1	J	775/828 (93%)	-0.98	0 100 100	60, 110, 155, 200	0
All	All	7750/8280 (93%)	-1.02	4 (0%) 92 86	48, 99, 146, 230	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	455	SER	2.4
1	B	710	PRO	2.3
1	G	632	GLY	2.2
1	B	455	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	F	904	6/6	0.91	0.07	85,90,91,93	0
4	GOL	C	905	6/6	0.93	0.07	71,78,81,82	0
4	GOL	F	905	6/6	0.93	0.08	74,76,79,81	0
4	GOL	C	904	6/6	0.94	0.06	66,74,79,80	0
4	GOL	D	904	6/6	0.95	0.07	75,81,81,85	0
4	GOL	E	906	6/6	0.95	0.07	78,80,83,85	0
4	GOL	C	903	6/6	0.96	0.07	99,103,106,111	0
4	GOL	G	904	6/6	0.96	0.06	68,70,81,84	0
4	GOL	J	903	6/6	0.96	0.07	96,100,102,106	0
5	TRS	B	904	8/8	0.96	0.05	64,71,73,73	0
4	GOL	A	905	6/6	0.97	0.07	66,77,83,87	0
4	GOL	A	903	6/6	0.98	0.08	78,80,85,86	0
4	GOL	B	903	6/6	0.98	0.06	77,80,84,87	0
4	GOL	D	903	6/6	0.98	0.05	96,105,105,107	0
4	GOL	G	903	6/6	0.98	0.05	96,96,97,100	0
4	GOL	A	904	6/6	0.98	0.04	72,80,81,87	0
4	GOL	H	903	6/6	0.98	0.06	107,112,114,117	0
4	GOL	I	903	6/6	0.98	0.05	108,109,114,114	0
4	GOL	E	903	6/6	0.98	0.08	74,78,81,83	0
4	GOL	E	905	6/6	0.98	0.07	67,69,71,77	0
4	GOL	F	903	6/6	0.99	0.07	84,85,87,94	0
2	CA	B	901	1/1	0.99	0.04	89,89,89,89	0
4	GOL	E	904	6/6	0.99	0.04	67,78,84,85	0
2	CA	E	901	1/1	1.00	0.04	76,76,76,76	0
2	CA	F	901	1/1	1.00	0.01	88,88,88,88	0
2	CA	G	901	1/1	1.00	0.01	89,89,89,89	0
2	CA	H	901	1/1	1.00	0.04	117,117,117,117	0
2	CA	I	901	1/1	1.00	0.02	112,112,112,112	0
2	CA	J	901	1/1	1.00	0.02	132,132,132,132	0
3	ZN	A	902	1/1	1.00	0.03	88,88,88,88	0
3	ZN	B	902	1/1	1.00	0.02	92,92,92,92	0
3	ZN	C	902	1/1	1.00	0.02	115,115,115,115	0
3	ZN	D	902	1/1	1.00	0.01	98,98,98,98	0
3	ZN	E	902	1/1	1.00	0.02	81,81,81,81	0
3	ZN	F	902	1/1	1.00	0.02	81,81,81,81	0
3	ZN	G	902	1/1	1.00	0.01	94,94,94,94	0
3	ZN	H	902	1/1	1.00	0.02	115,115,115,115	0

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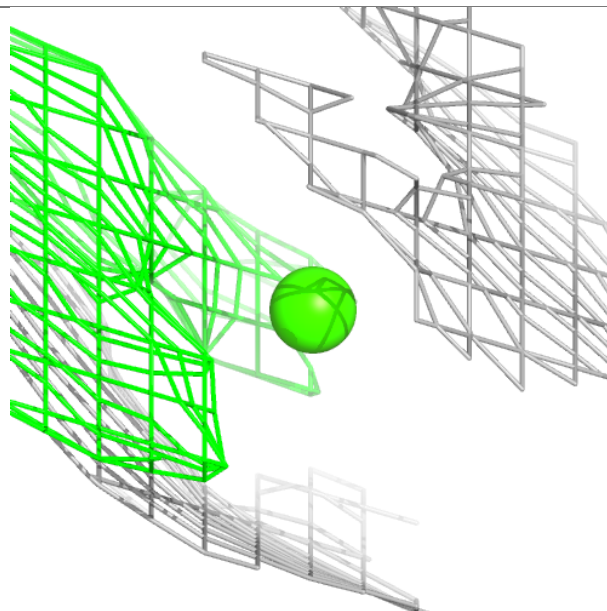
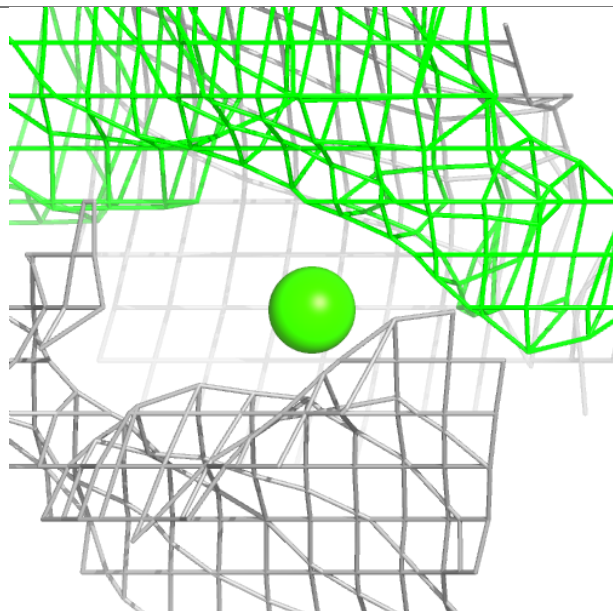
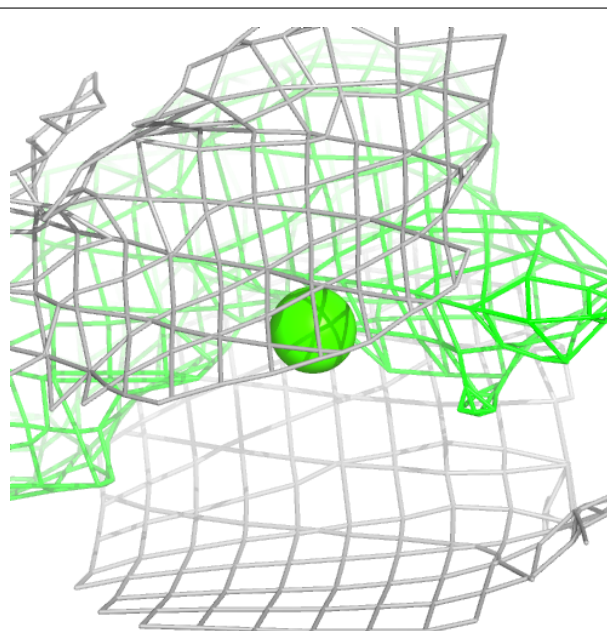
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	I	902	1/1	1.00	0.02	108,108,108,108	0
3	ZN	J	902	1/1	1.00	0.02	102,102,102,102	0
2	CA	A	901	1/1	1.00	0.01	79,79,79,79	0
2	CA	C	901	1/1	1.00	0.02	112,112,112,112	0
2	CA	D	901	1/1	1.00	0.02	106,106,106,106	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.

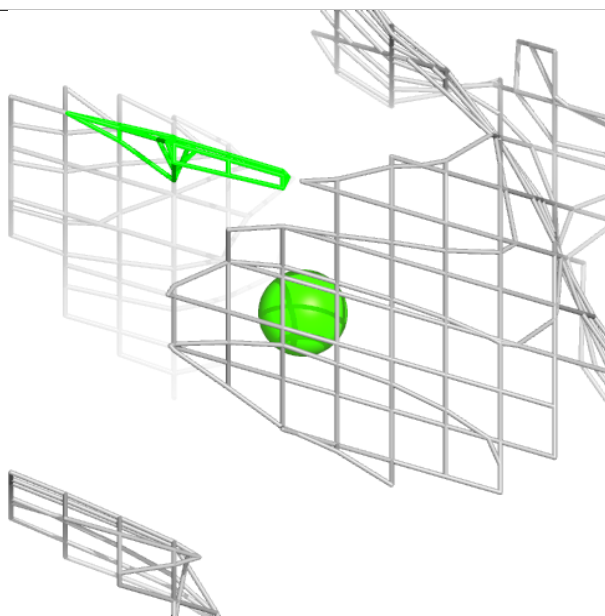
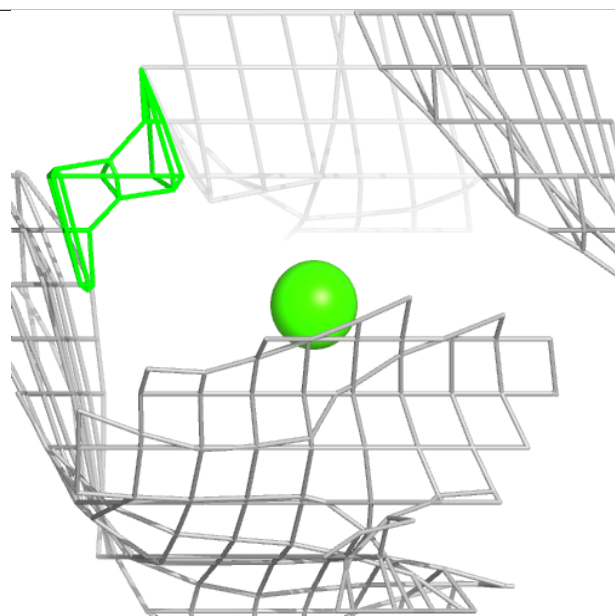
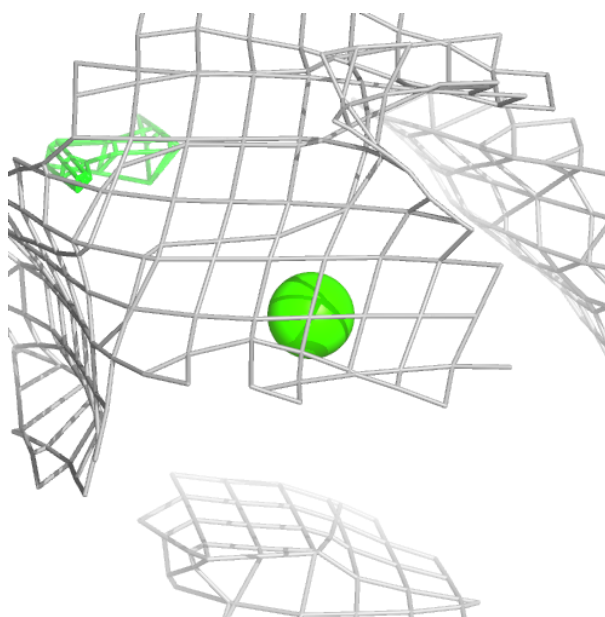
Electron density around CA B 901:

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



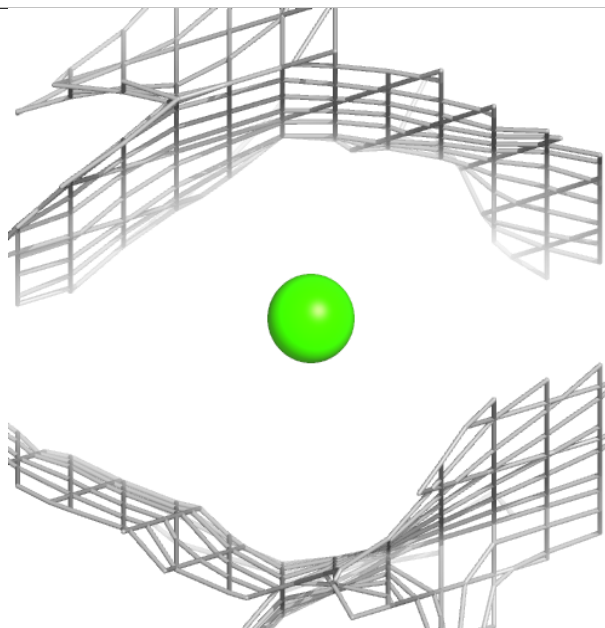
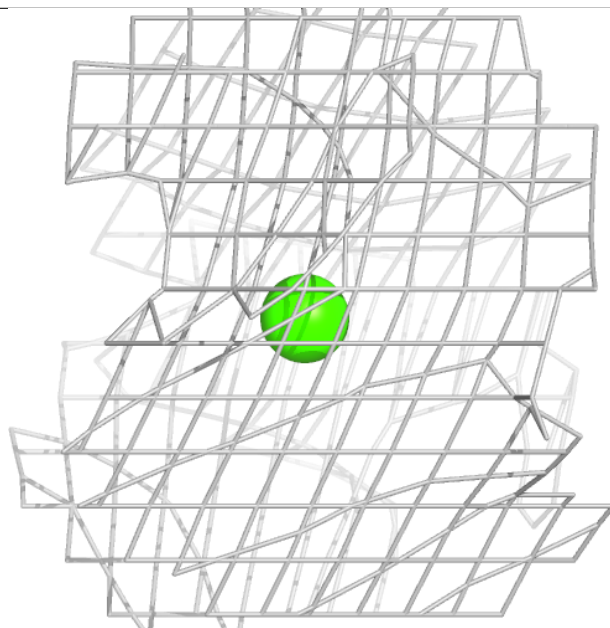
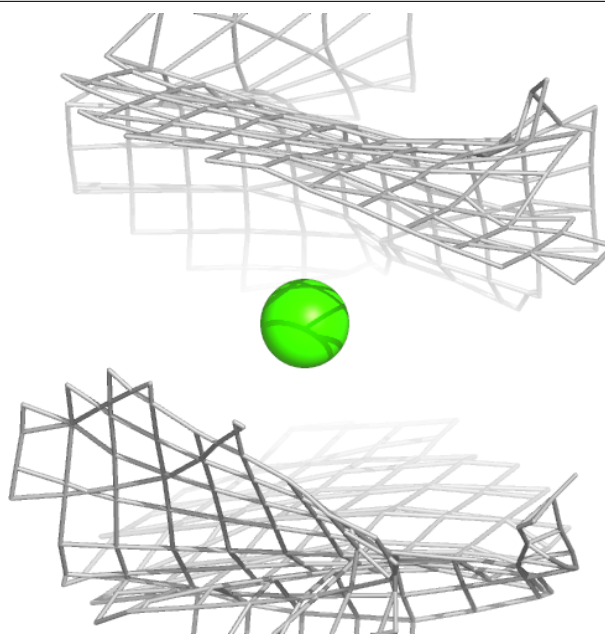
Electron density around CA E 901:

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and green (positive)



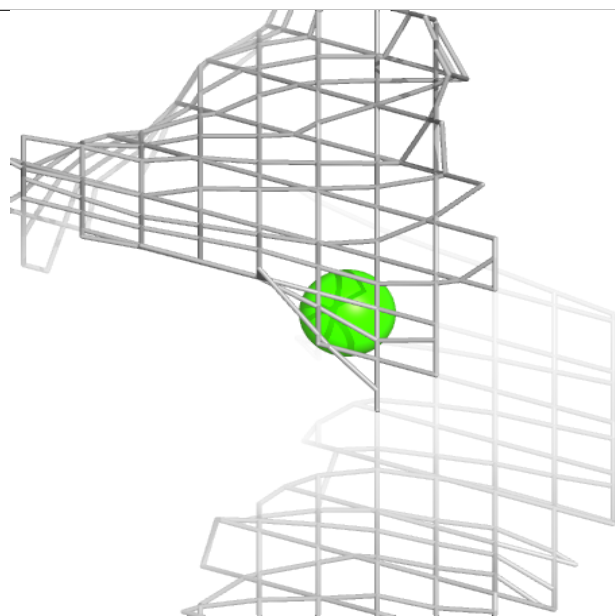
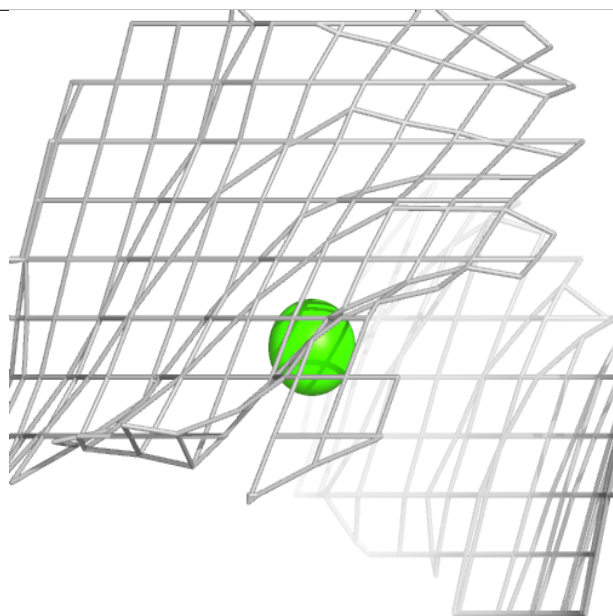
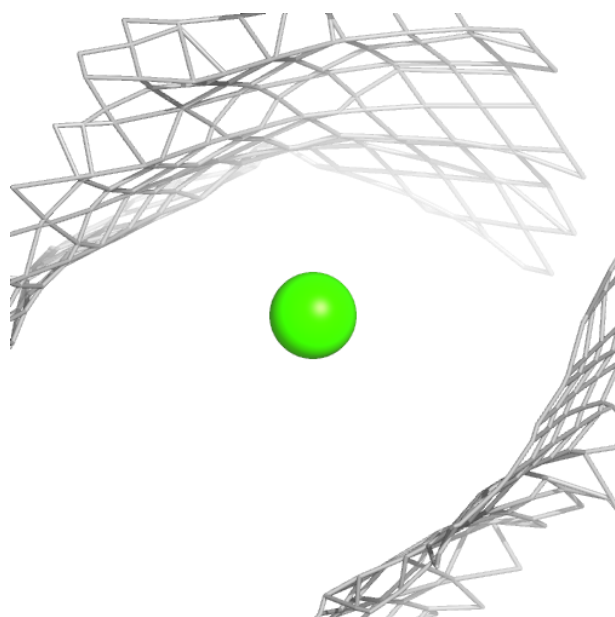
Electron density around CA F 901:

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and green (positive)



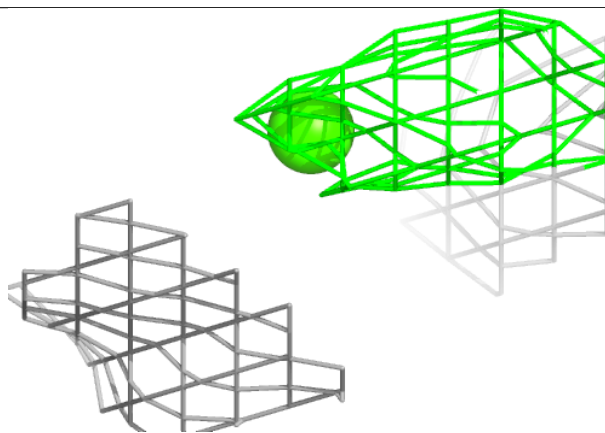
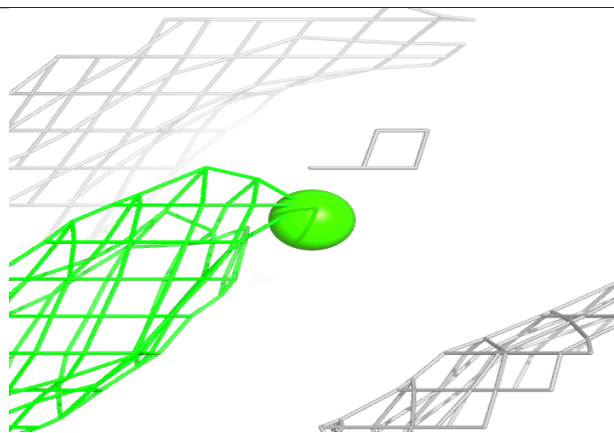
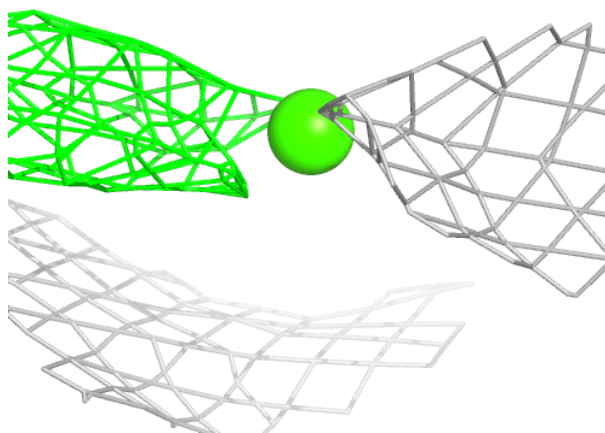
Electron density around CA G 901:

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and green (positive)



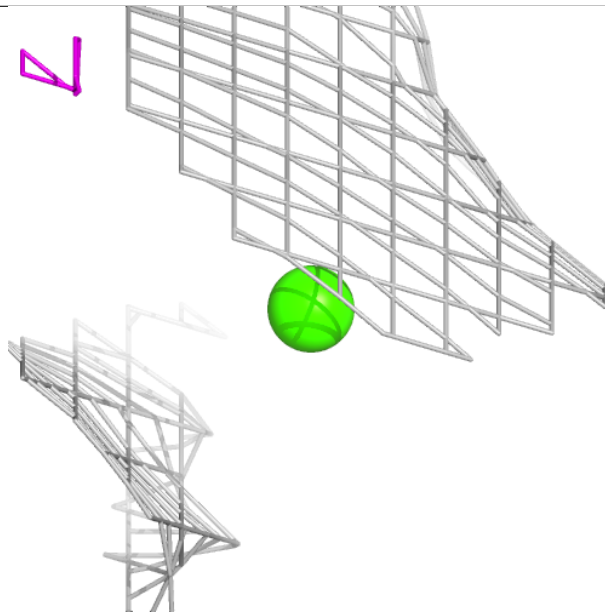
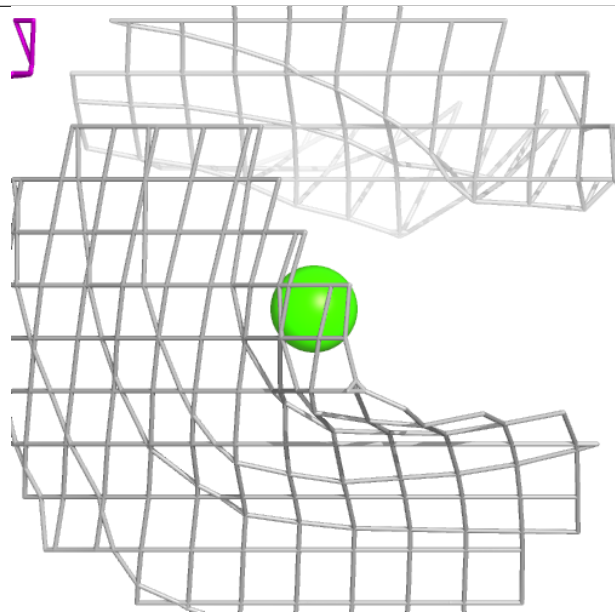
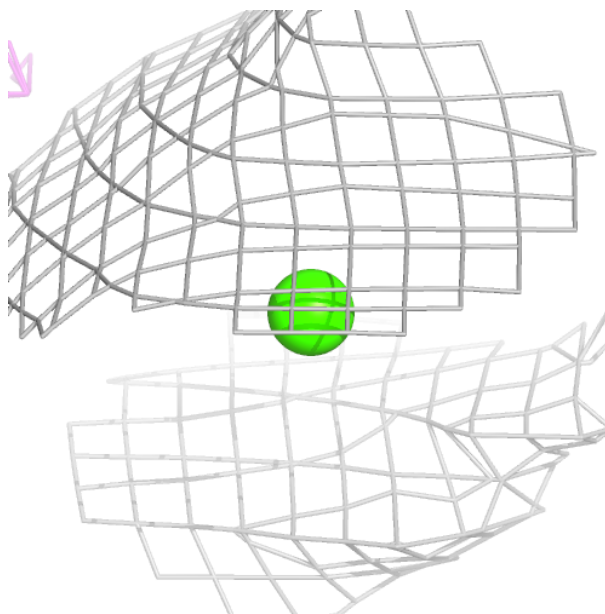
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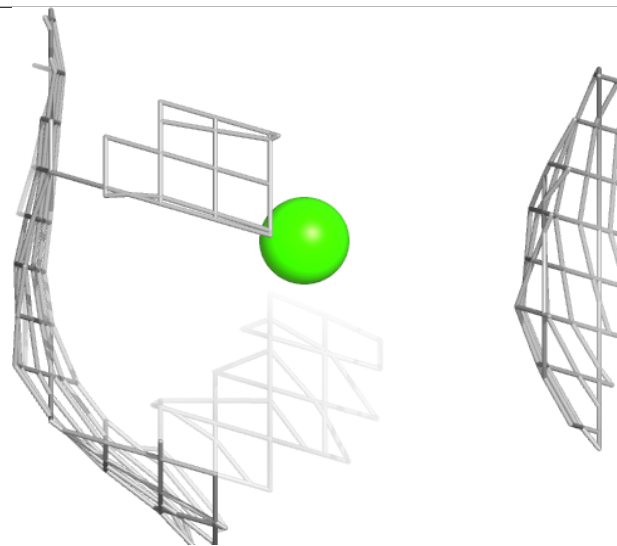
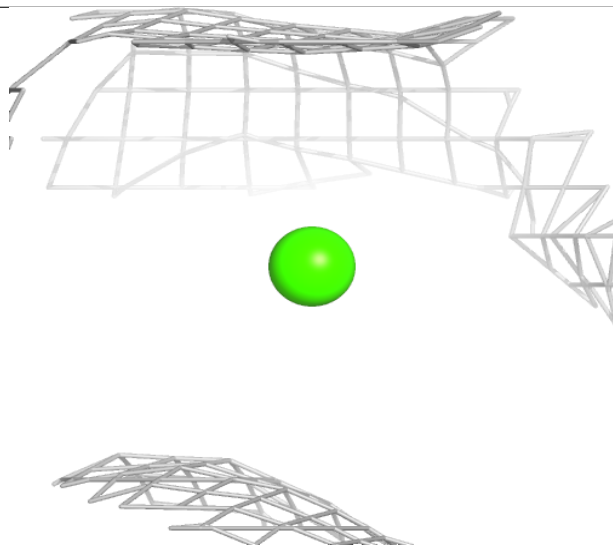
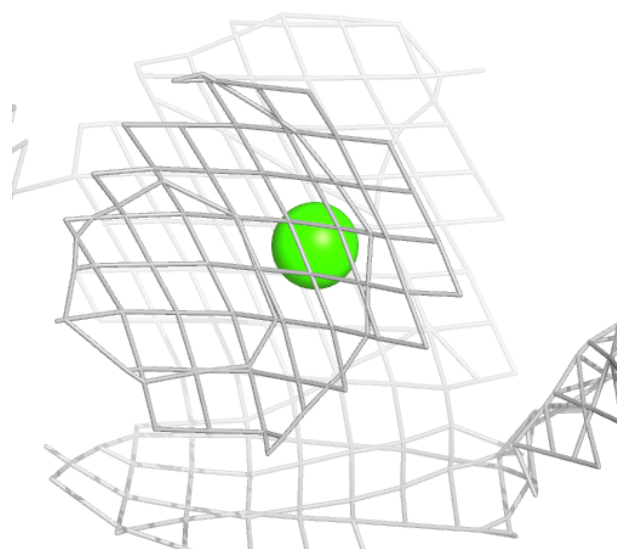
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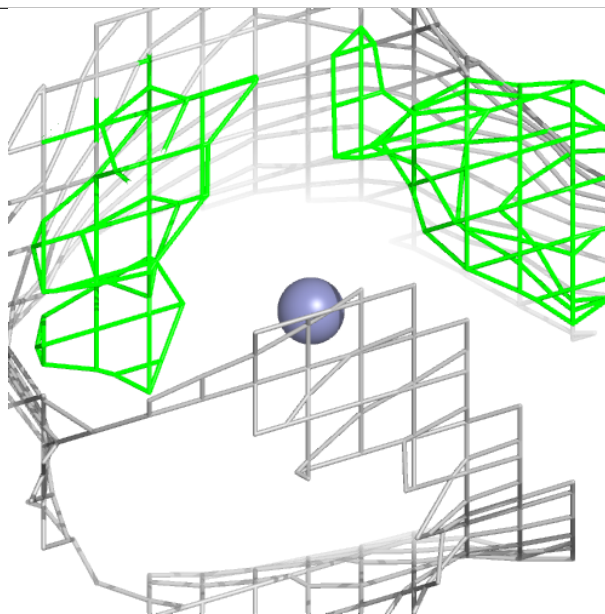
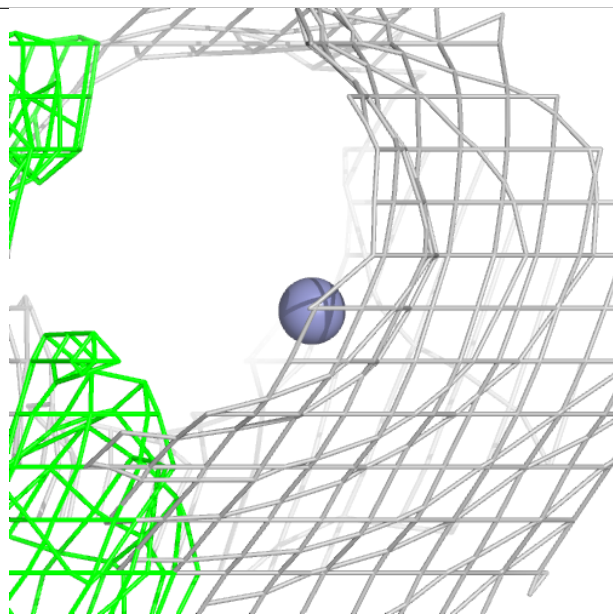
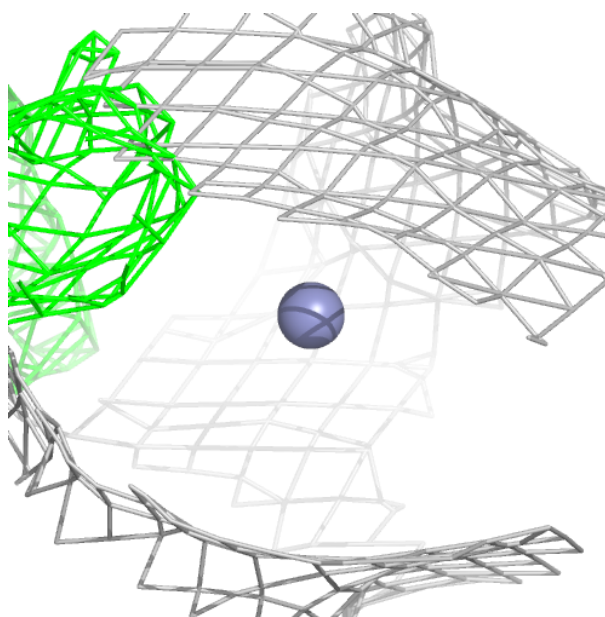
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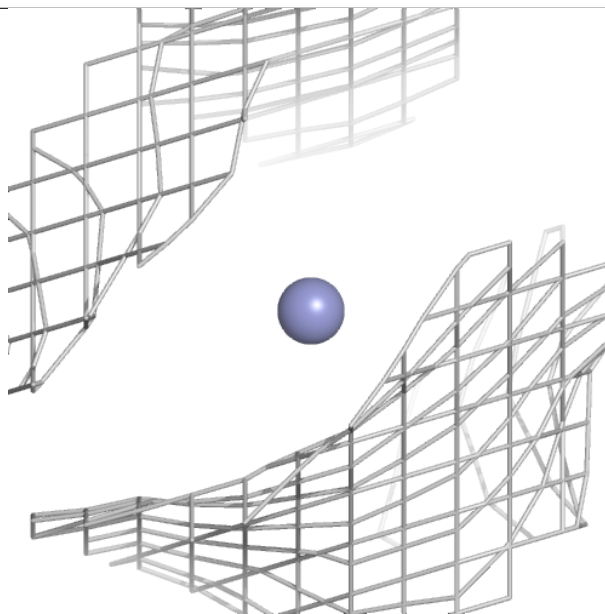
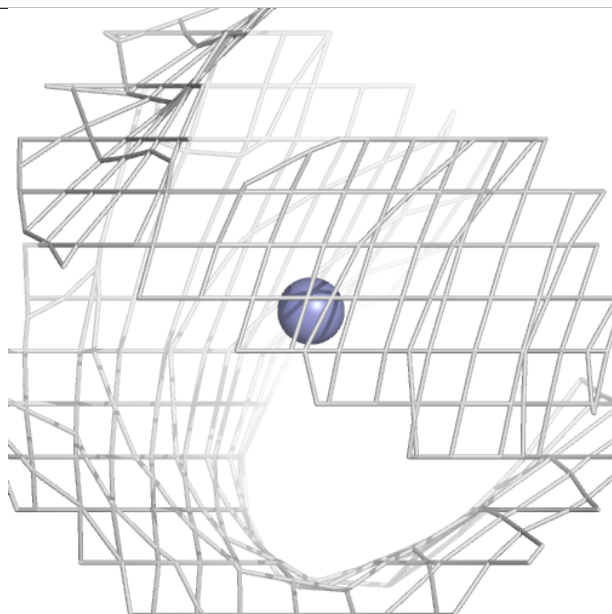
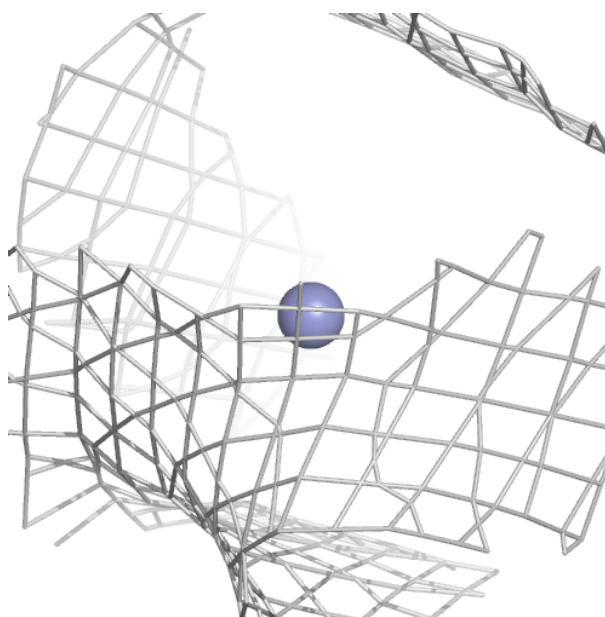
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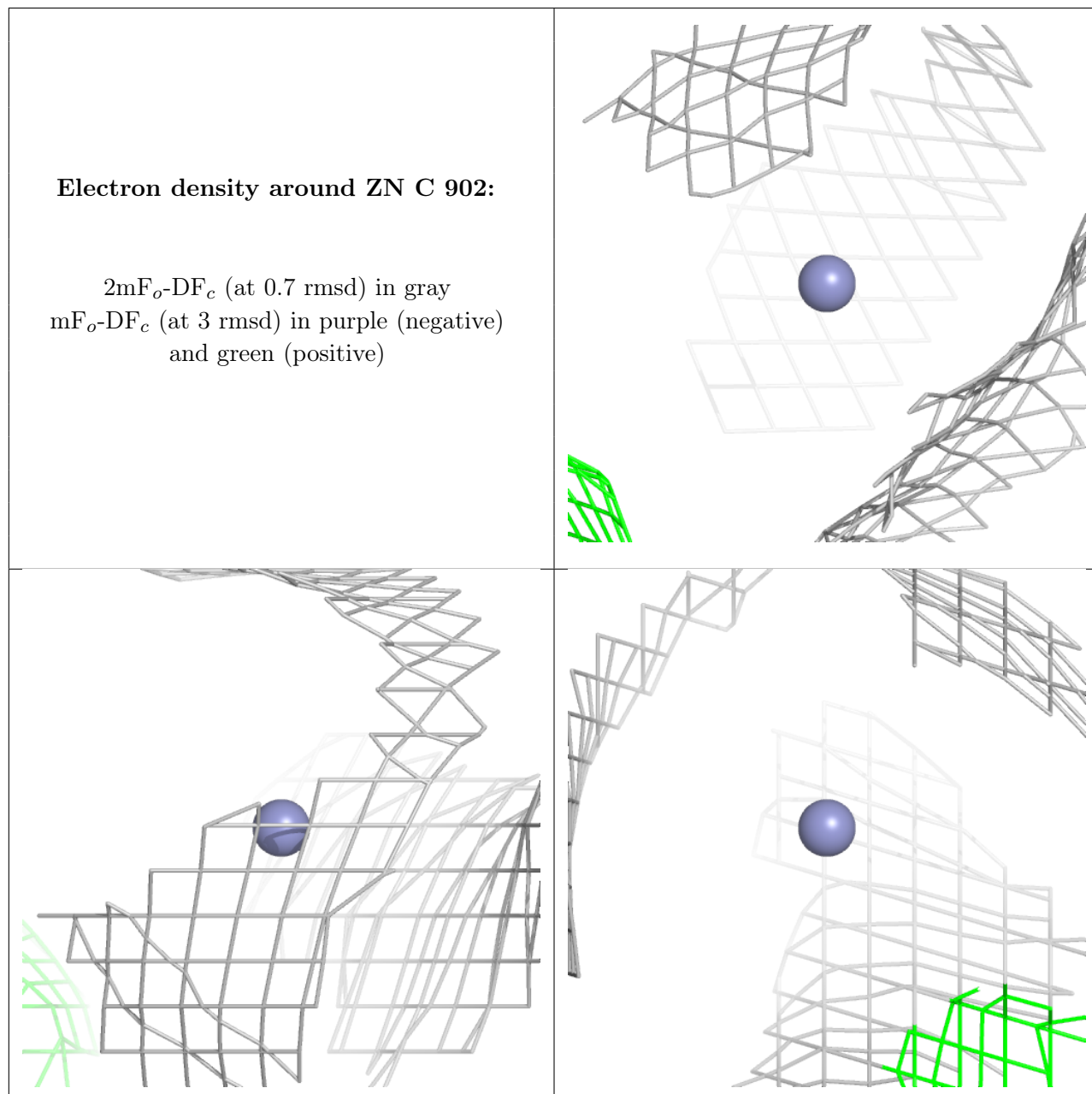
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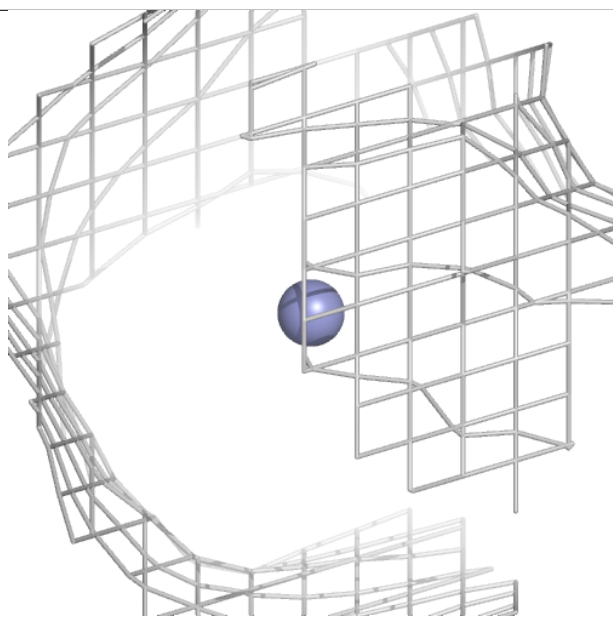
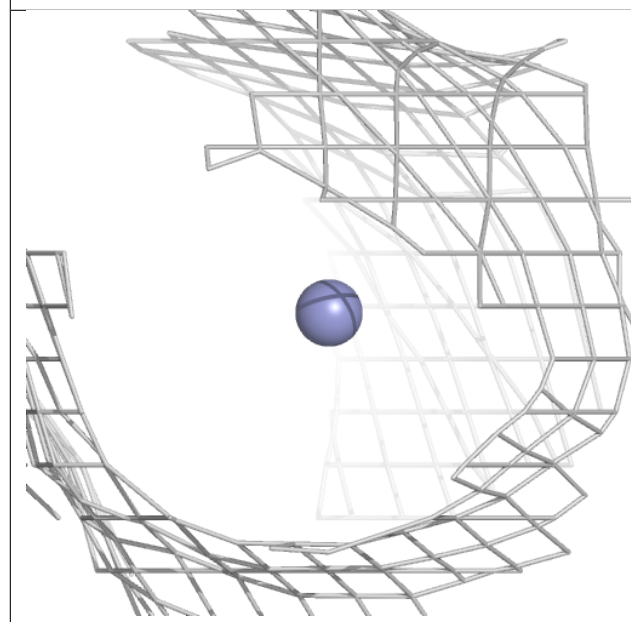
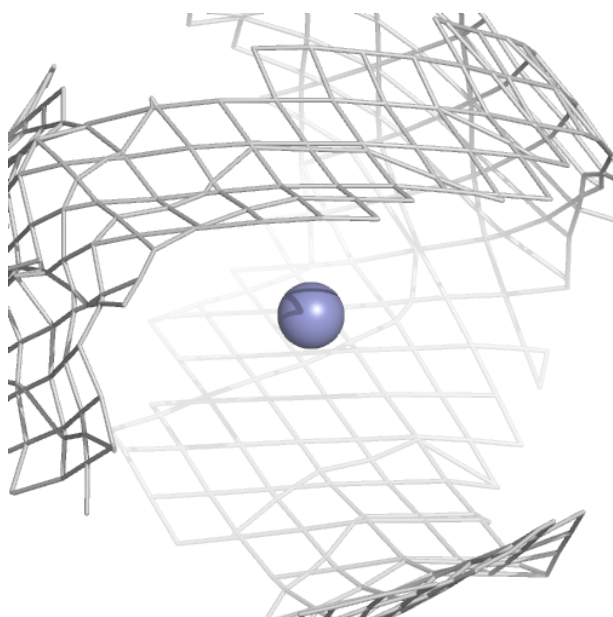
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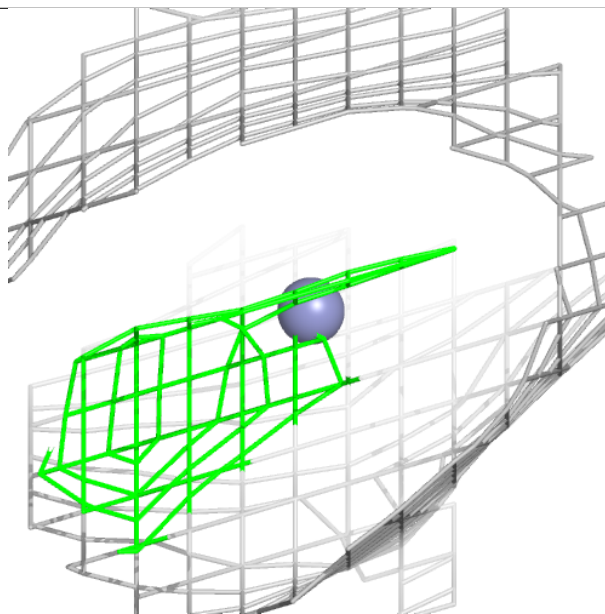
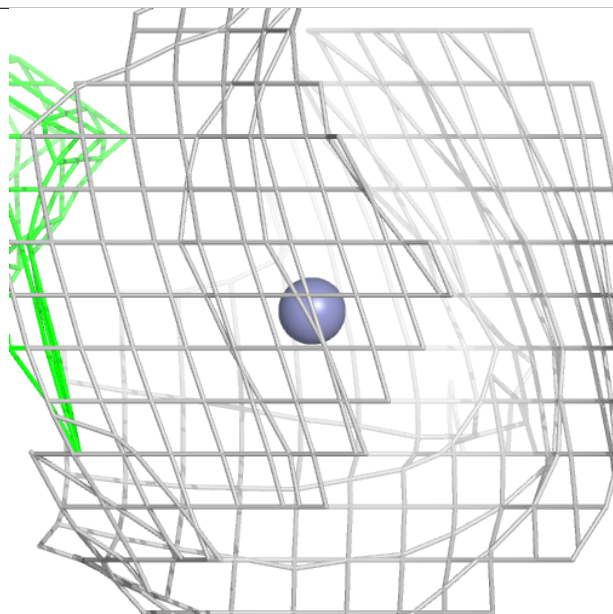
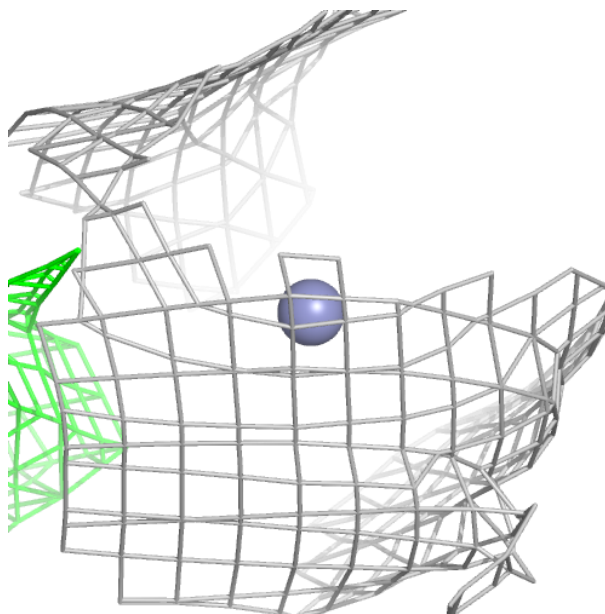
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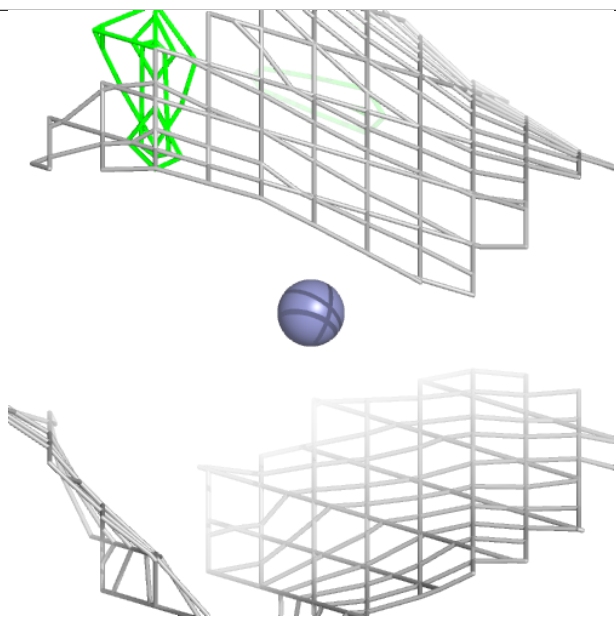
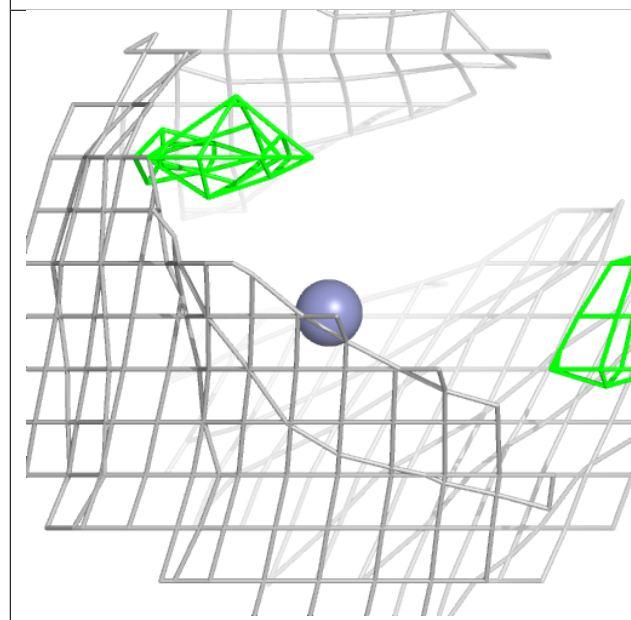
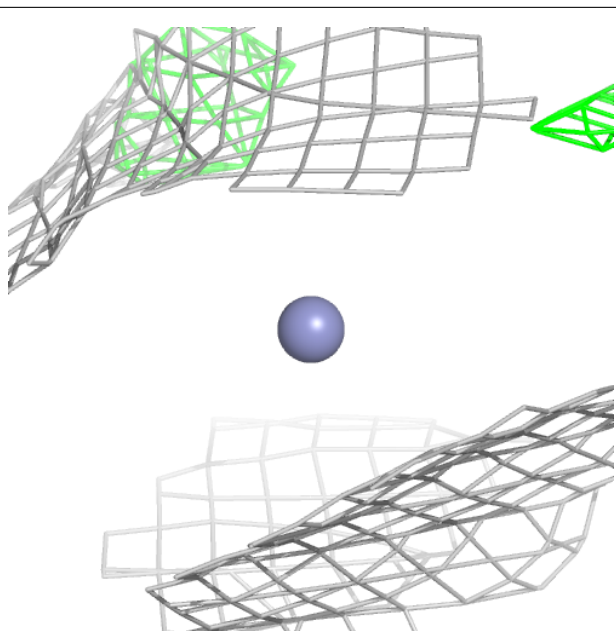
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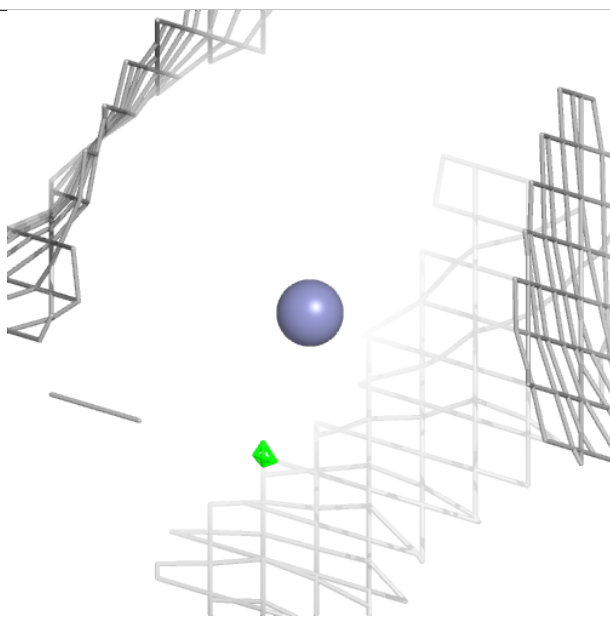
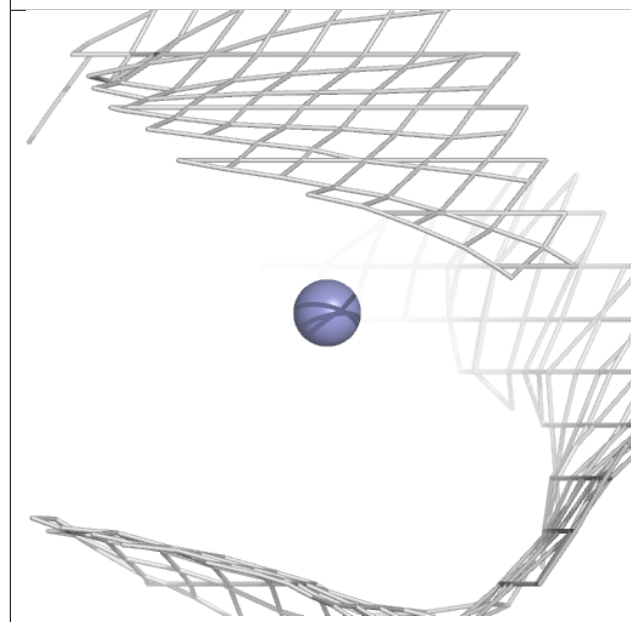
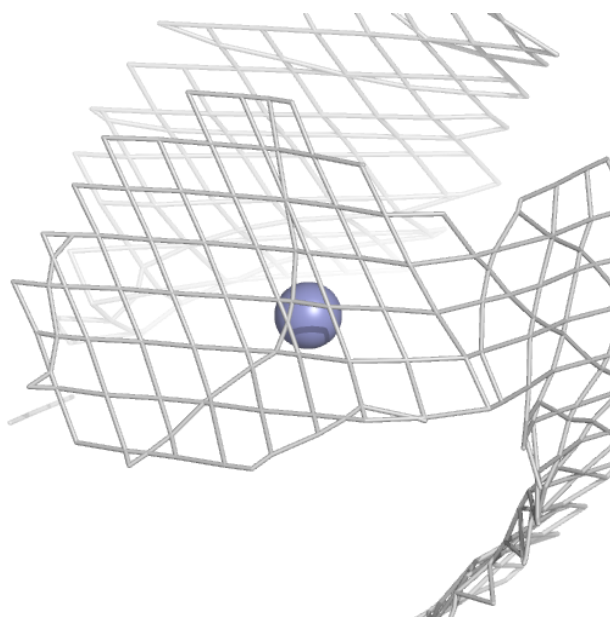
Electron density around ZN F 902:

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and green (positive)



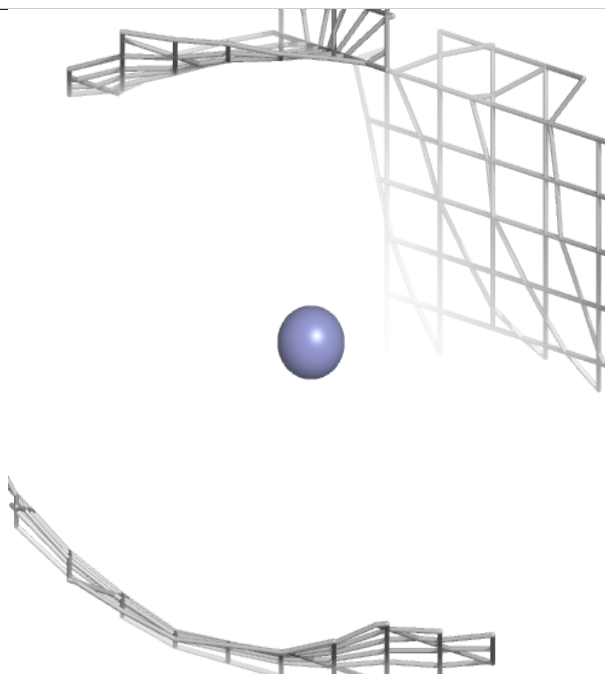
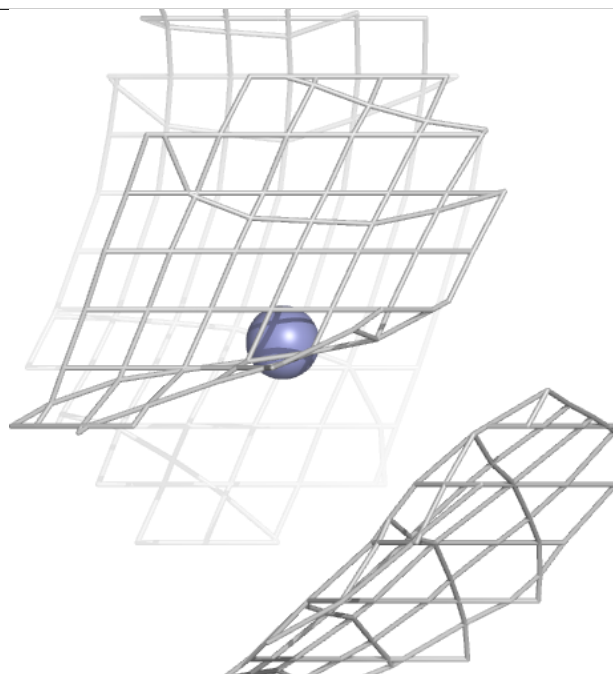
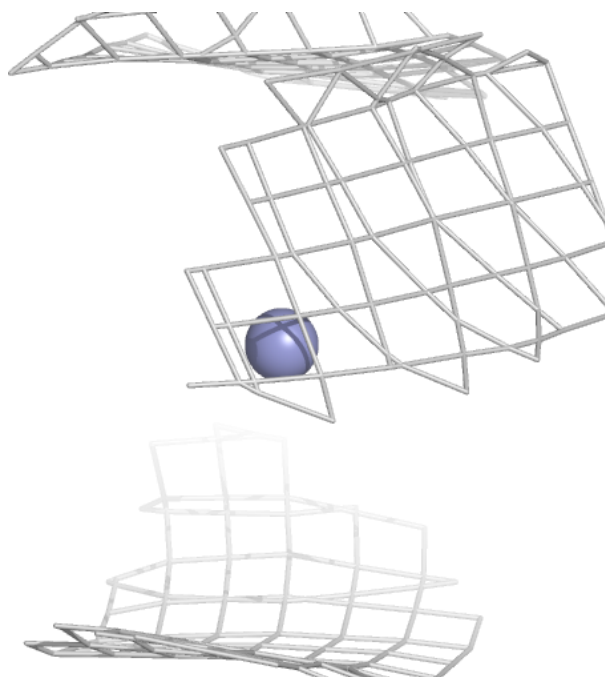
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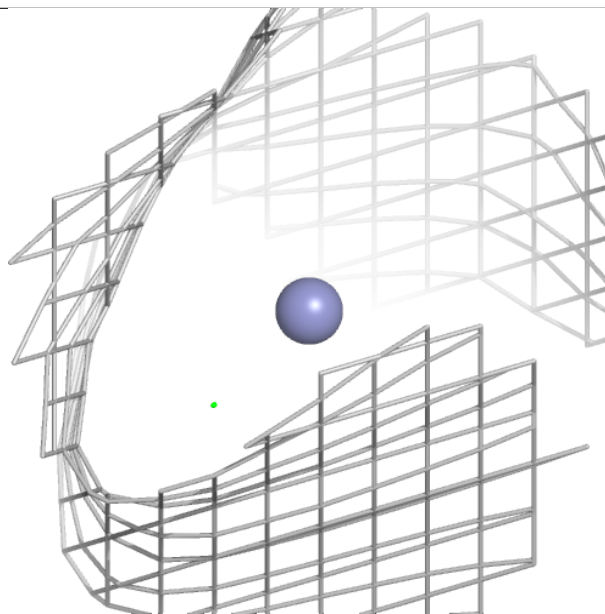
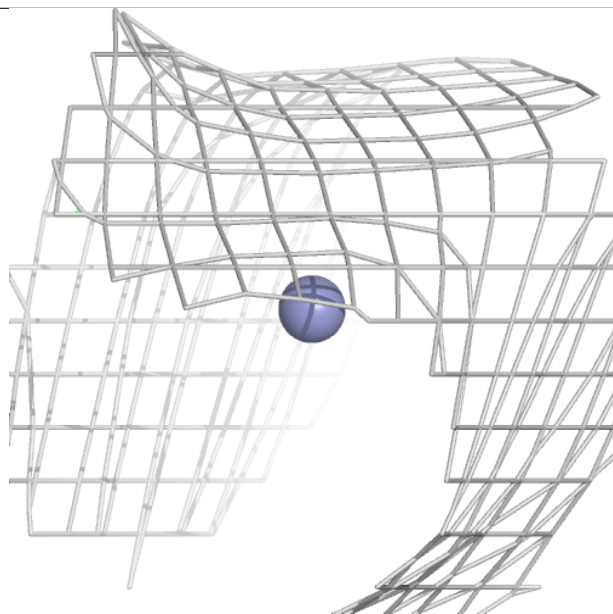
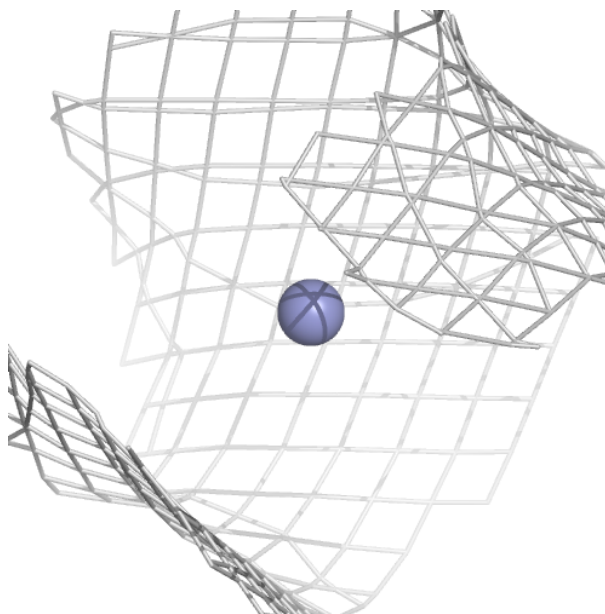
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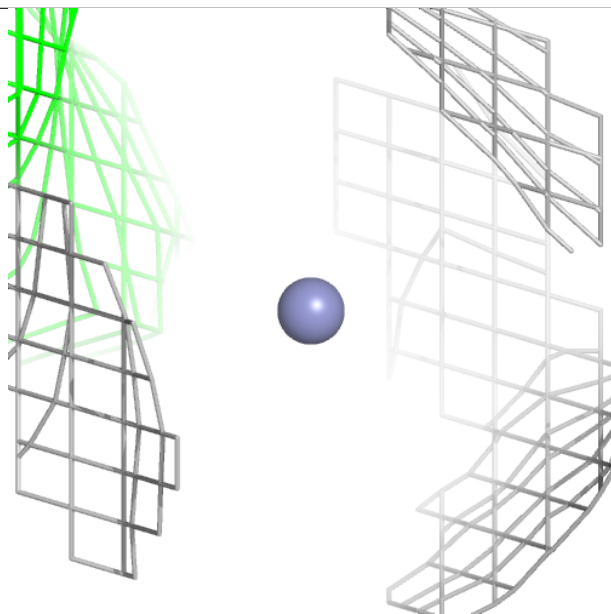
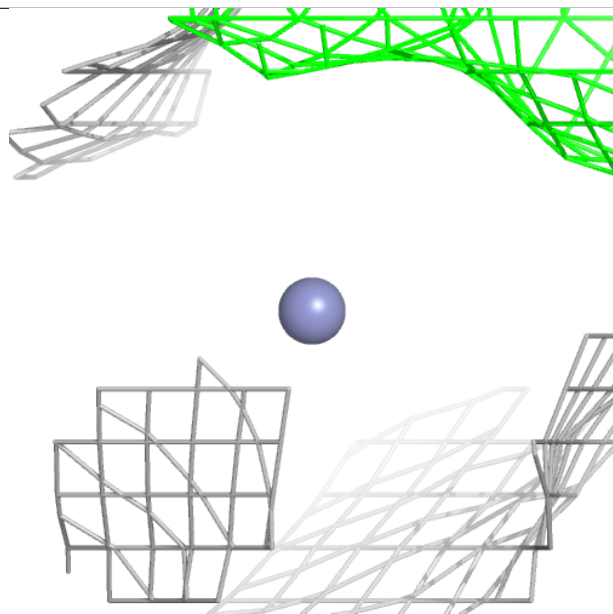
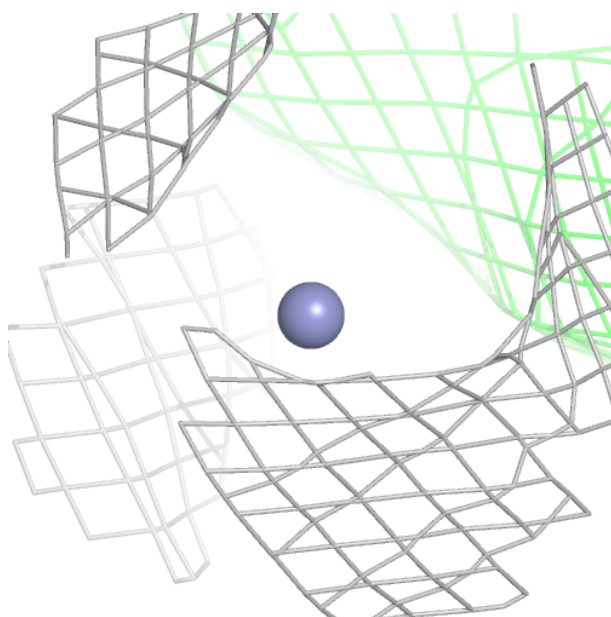
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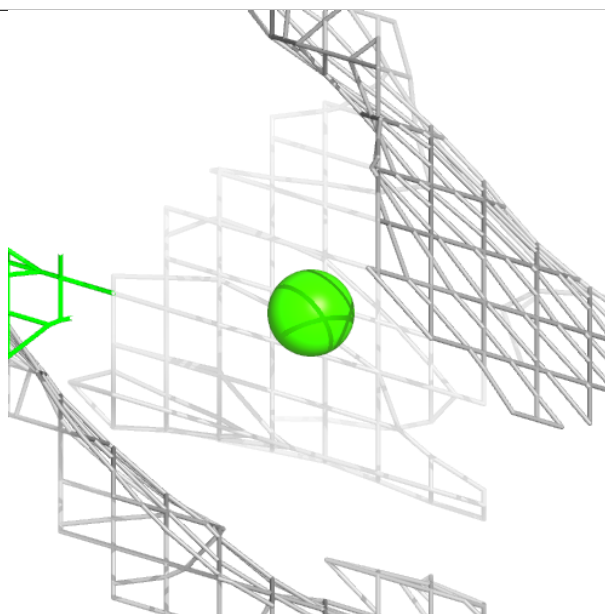
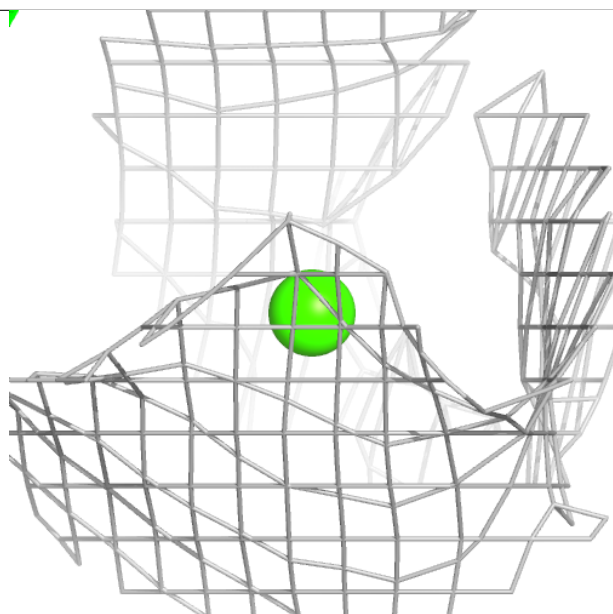
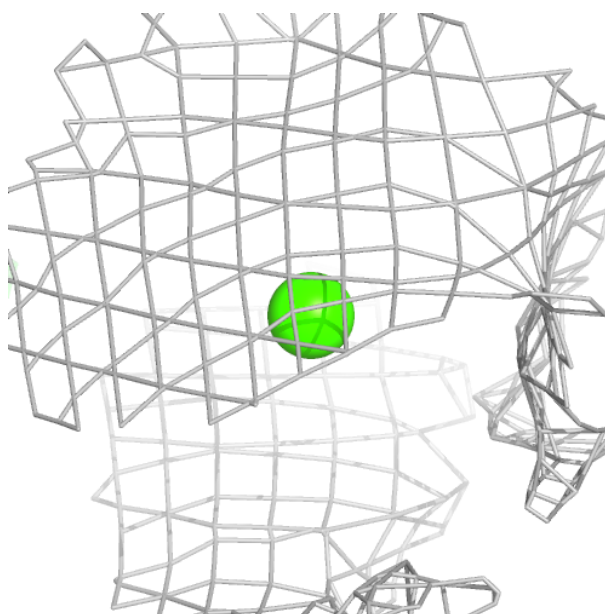
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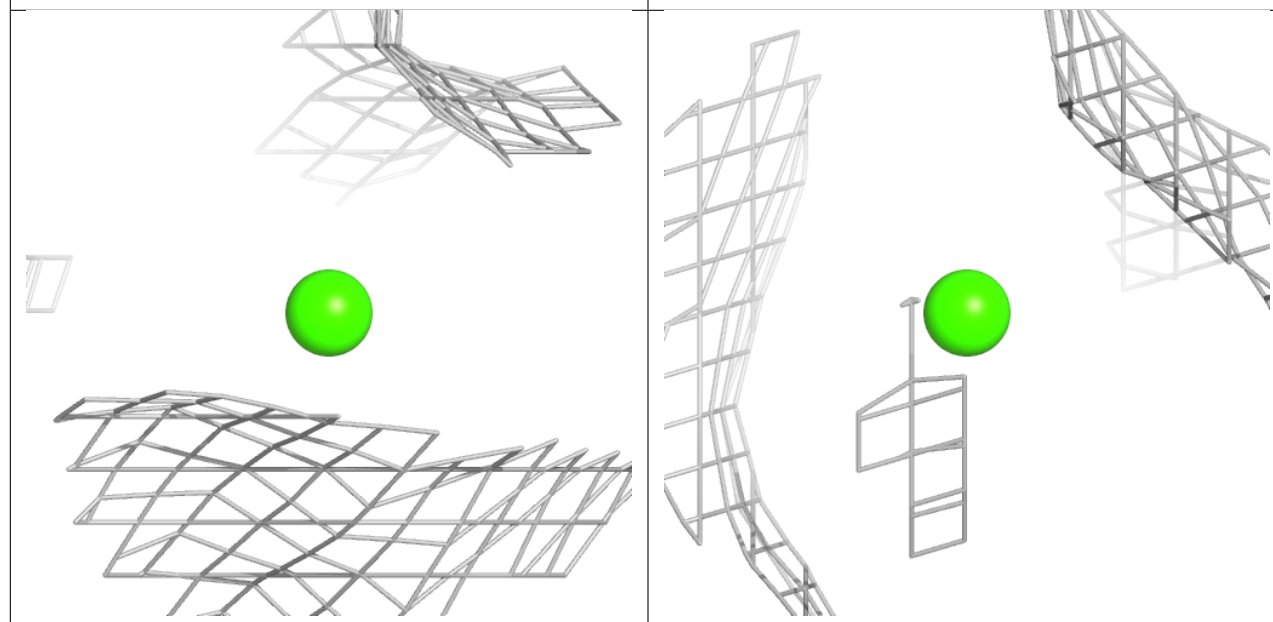
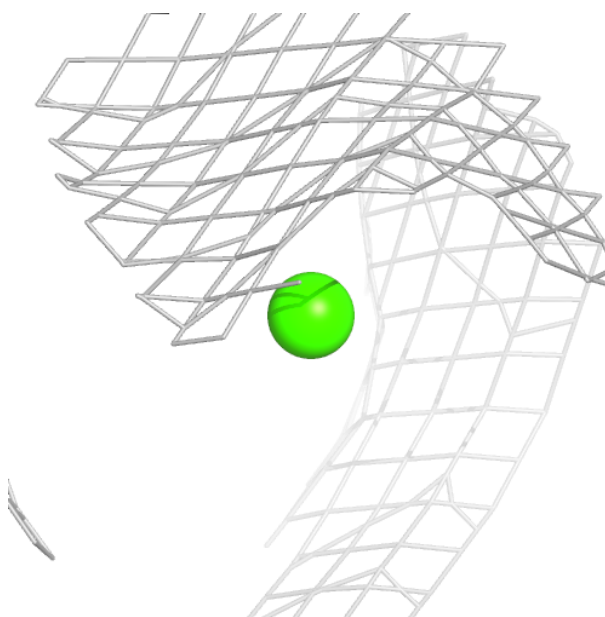
Electron density around CA A 901:

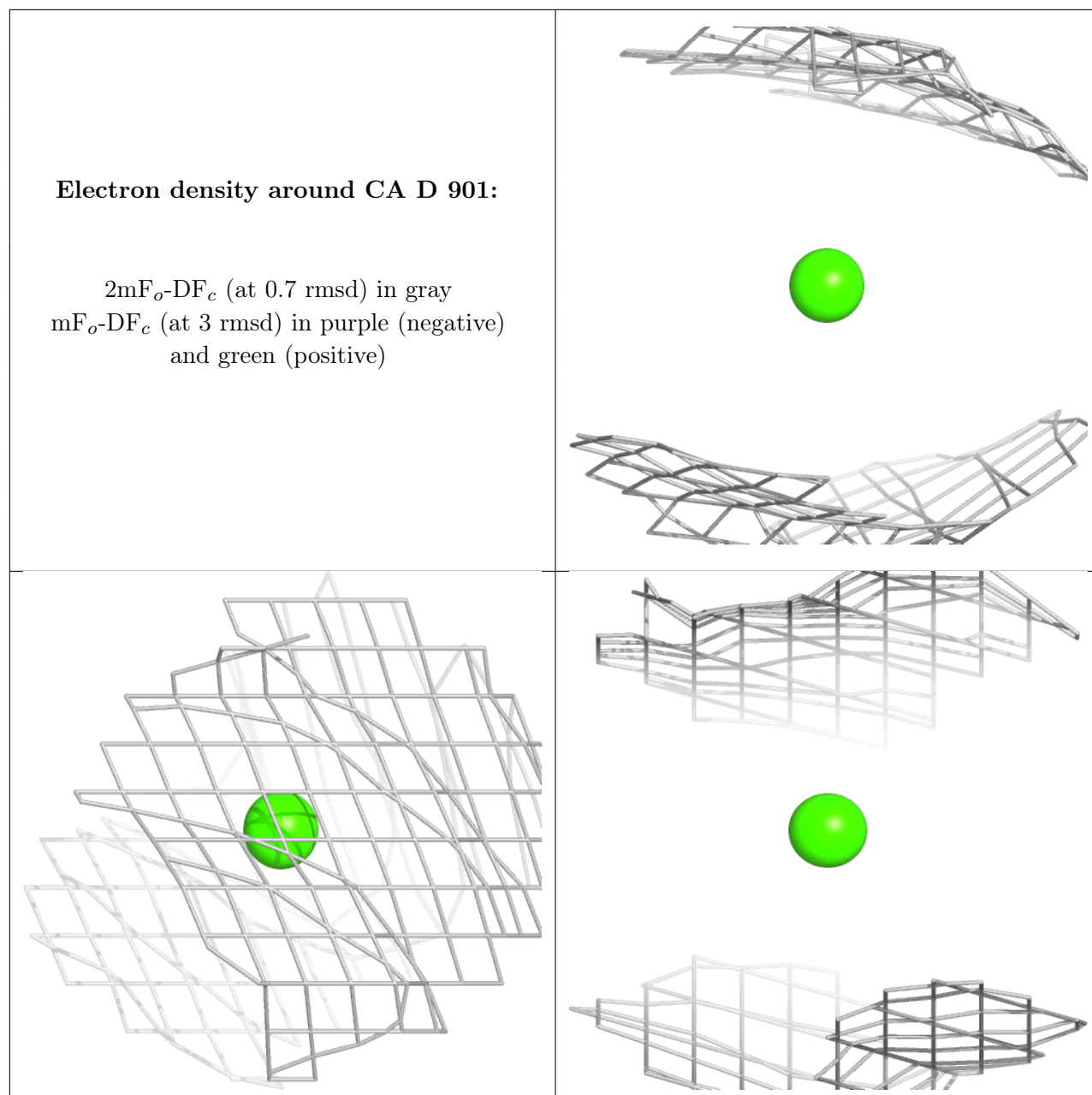
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA C 901:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.