



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:20 PM JST

PDB ID : 7CH3  
Title : Crystal structure of Arabinose isomerase from hyper thermophilic bacterium  
Thermotoga maritima (TMAI) triple mutant (K264A, E265A, K266A)  
Authors : Cao, T.P.; Dhanasingh, I.; Sung, J.Y.; Shin, S.M.; Lee, D.W.; Lee, S.H.  
Deposited on : 2020-07-04  
Resolution : 3.61 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](mailto: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.

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

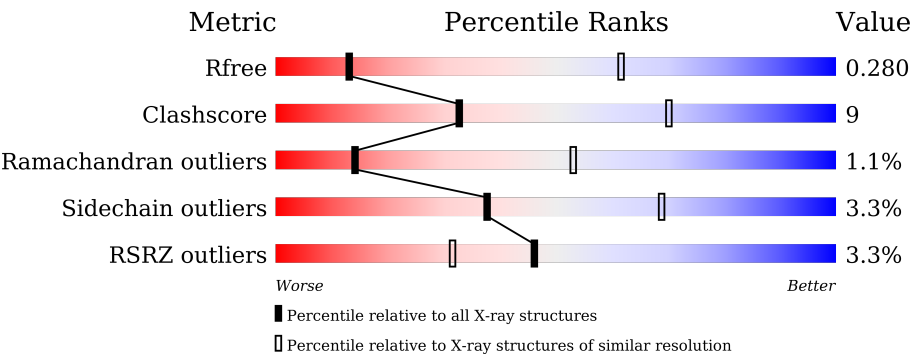
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.61 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))
$R_{free}$	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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  $\geq 3$ , 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	496	<div><div>3%</div><div><div></div><div>69%</div><div>25%</div><div>• 5%</div></div></div>
1	B	496	<div><div>%</div><div><div></div><div>73%</div><div>24%</div><div>•</div></div></div>
1	C	496	<div><div>4%</div><div><div></div><div>73%</div><div>26%</div><div>•</div></div></div>
1	D	496	<div><div>3%</div><div><div></div><div>78%</div><div>20%</div><div>•</div></div></div>
1	E	496	<div><div>2%</div><div><div></div><div>76%</div><div>22%</div><div>•</div></div></div>
1	F	496	<div><div>2%</div><div><div></div><div>77%</div><div>22%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain	
1	G	496		•
1	H	496		•
1	I	496		•
1	J	496		•
1	K	496		•
1	L	496		•

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	J	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47435 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3739	2402	642	677	18			
1	B	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	C	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	D	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	E	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	F	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	G	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	H	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	I	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	J	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	K	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			
1	L	495	Total	C	N	O	S	0	0	0
			3969	2549	677	724	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	ALA	LYS	engineered mutation	UNP Q9WYB3
A	265	ALA	GLU	engineered mutation	UNP Q9WYB3
A	266	ALA	LYS	engineered mutation	UNP Q9WYB3
B	264	ALA	LYS	engineered mutation	UNP Q9WYB3
B	265	ALA	GLU	engineered mutation	UNP Q9WYB3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	266	ALA	LYS	engineered mutation	UNP Q9WYB3
C	264	ALA	LYS	engineered mutation	UNP Q9WYB3
C	265	ALA	GLU	engineered mutation	UNP Q9WYB3
C	266	ALA	LYS	engineered mutation	UNP Q9WYB3
D	264	ALA	LYS	engineered mutation	UNP Q9WYB3
D	265	ALA	GLU	engineered mutation	UNP Q9WYB3
D	266	ALA	LYS	engineered mutation	UNP Q9WYB3
E	264	ALA	LYS	engineered mutation	UNP Q9WYB3
E	265	ALA	GLU	engineered mutation	UNP Q9WYB3
E	266	ALA	LYS	engineered mutation	UNP Q9WYB3
F	264	ALA	LYS	engineered mutation	UNP Q9WYB3
F	265	ALA	GLU	engineered mutation	UNP Q9WYB3
F	266	ALA	LYS	engineered mutation	UNP Q9WYB3
G	264	ALA	LYS	engineered mutation	UNP Q9WYB3
G	265	ALA	GLU	engineered mutation	UNP Q9WYB3
G	266	ALA	LYS	engineered mutation	UNP Q9WYB3
H	264	ALA	LYS	engineered mutation	UNP Q9WYB3
H	265	ALA	GLU	engineered mutation	UNP Q9WYB3
H	266	ALA	LYS	engineered mutation	UNP Q9WYB3
I	264	ALA	LYS	engineered mutation	UNP Q9WYB3
I	265	ALA	GLU	engineered mutation	UNP Q9WYB3
I	266	ALA	LYS	engineered mutation	UNP Q9WYB3
J	264	ALA	LYS	engineered mutation	UNP Q9WYB3
J	265	ALA	GLU	engineered mutation	UNP Q9WYB3
J	266	ALA	LYS	engineered mutation	UNP Q9WYB3
K	264	ALA	LYS	engineered mutation	UNP Q9WYB3
K	265	ALA	GLU	engineered mutation	UNP Q9WYB3
K	266	ALA	LYS	engineered mutation	UNP Q9WYB3
L	264	ALA	LYS	engineered mutation	UNP Q9WYB3
L	265	ALA	GLU	engineered mutation	UNP Q9WYB3
L	266	ALA	LYS	engineered mutation	UNP Q9WYB3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	1	Total Mn 1 1	0	0
2	C	2	Total Mn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Mn 1	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0
2	G	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	J	2	Total 2	Mn 2	0	0
2	K	1	Total 1	Mn 1	0	0
2	L	2	Total 2	Mn 2	0	0

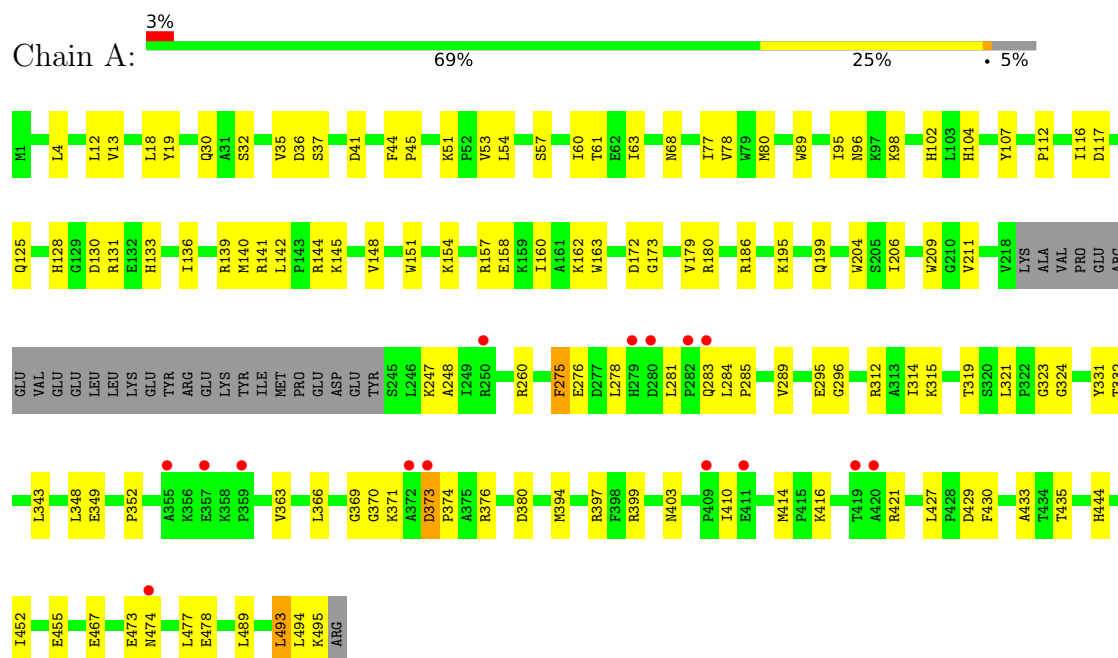
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	3	Total 3	O 3	0	0
3	C	2	Total 2	O 2	0	0
3	D	3	Total 3	O 3	0	0
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	K	2	Total 2	O 2	0	0

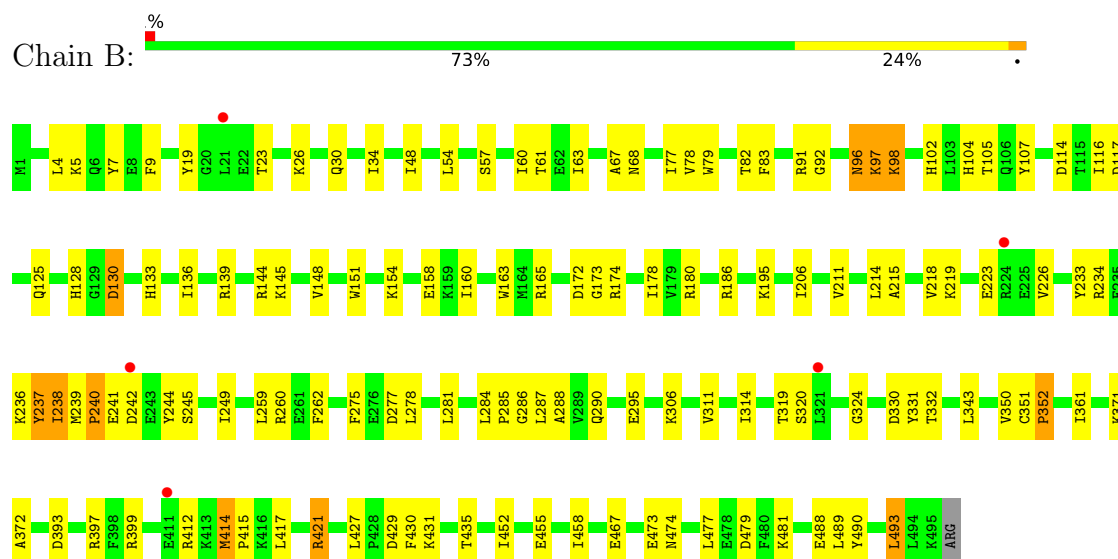
### 3 Residue-property plots [i](#)

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

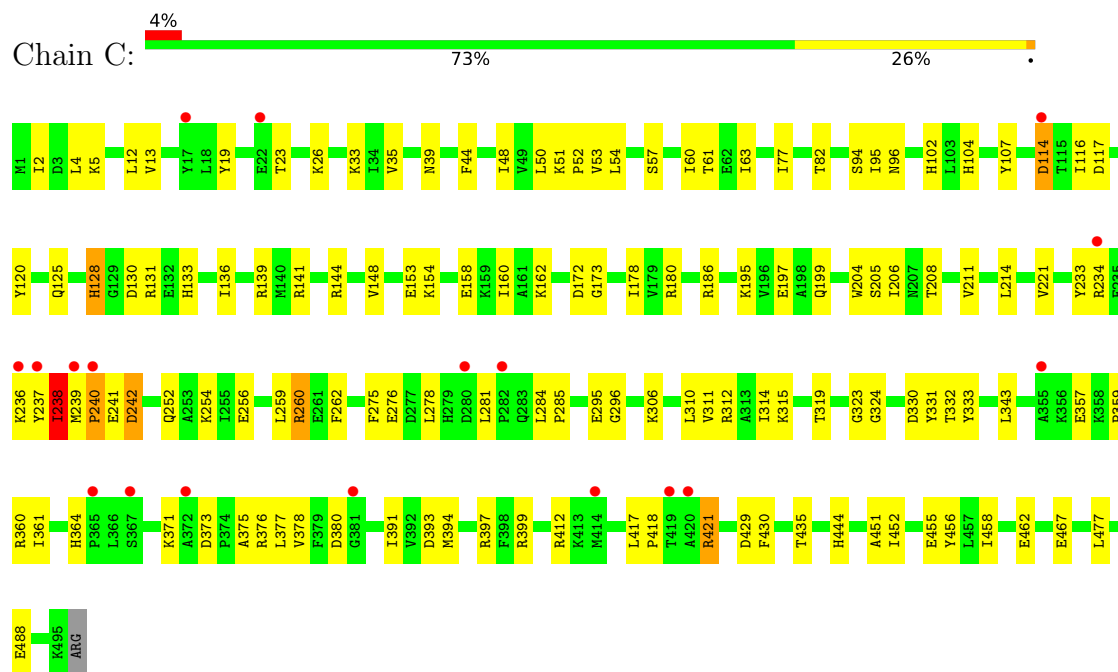
#### • Molecule 1: L-arabinose isomerase



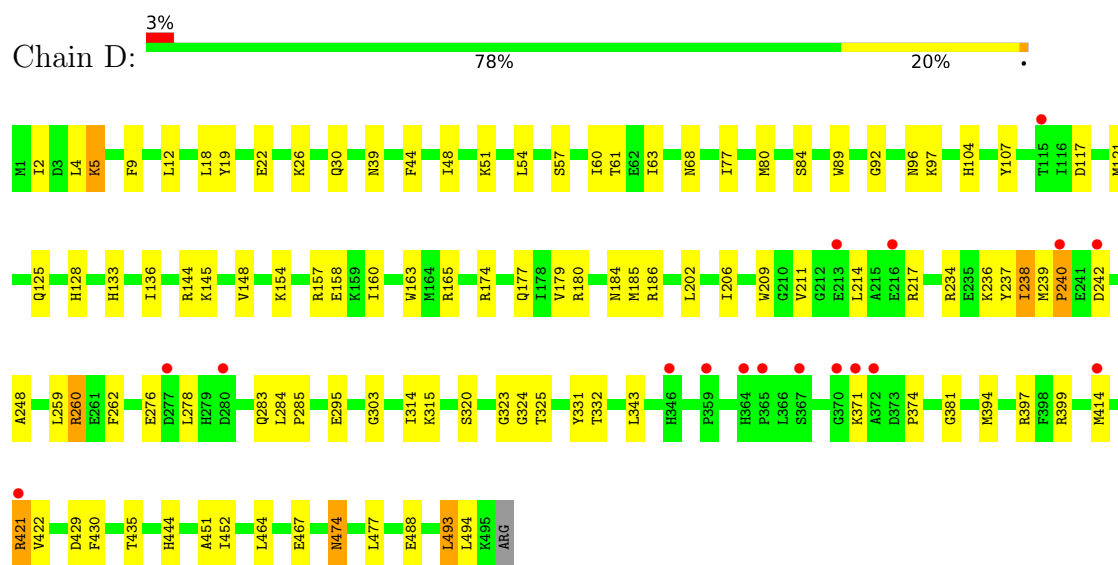
#### • Molecule 1: L-arabinose isomerase



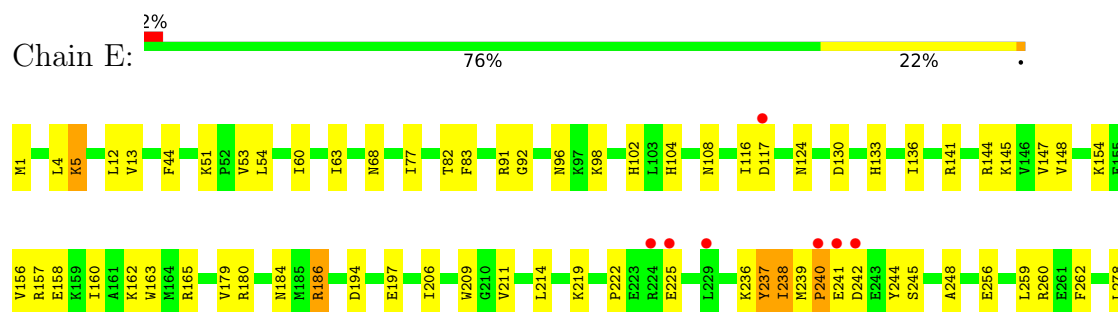
• Molecule 1: L-arabinose isomerase



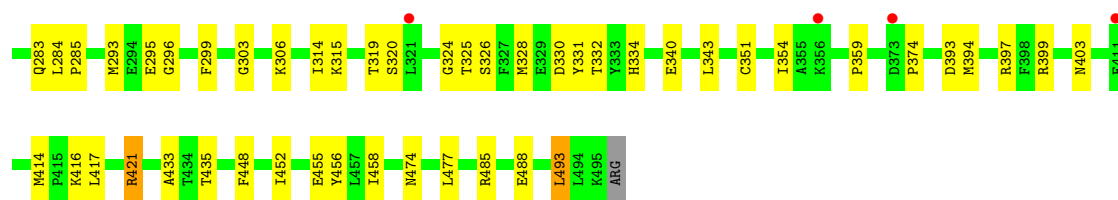
• Molecule 1: L-arabinose isomerase



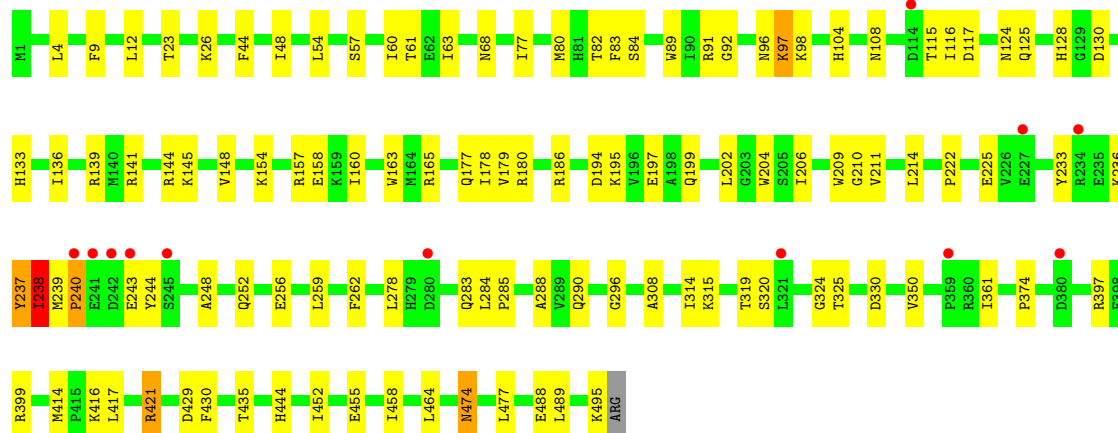
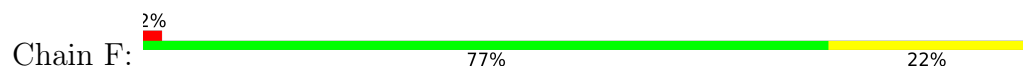
• Molecule 1: L-arabinose isomerase



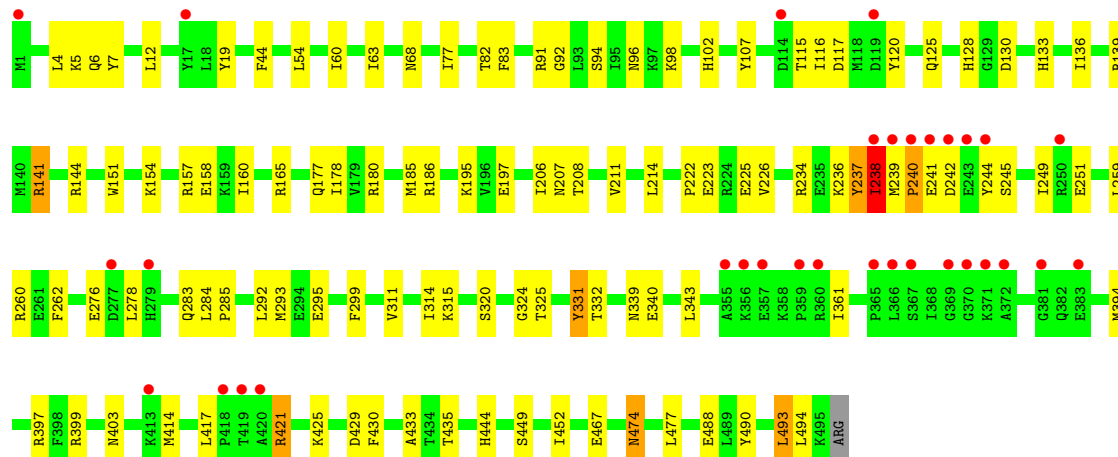
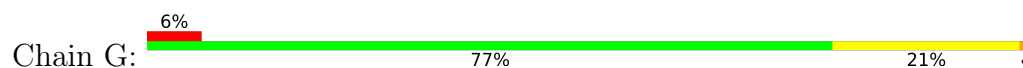




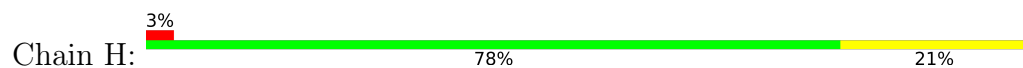
• Molecule 1: L-arabinose isomerase

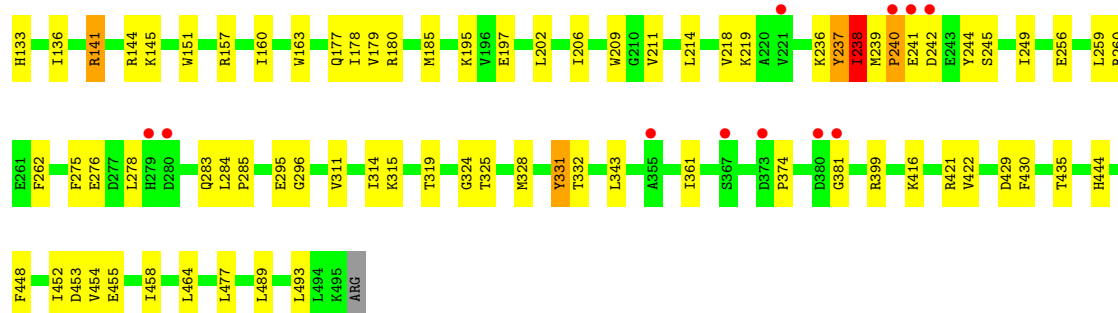


• Molecule 1: L-arabinose isomerase

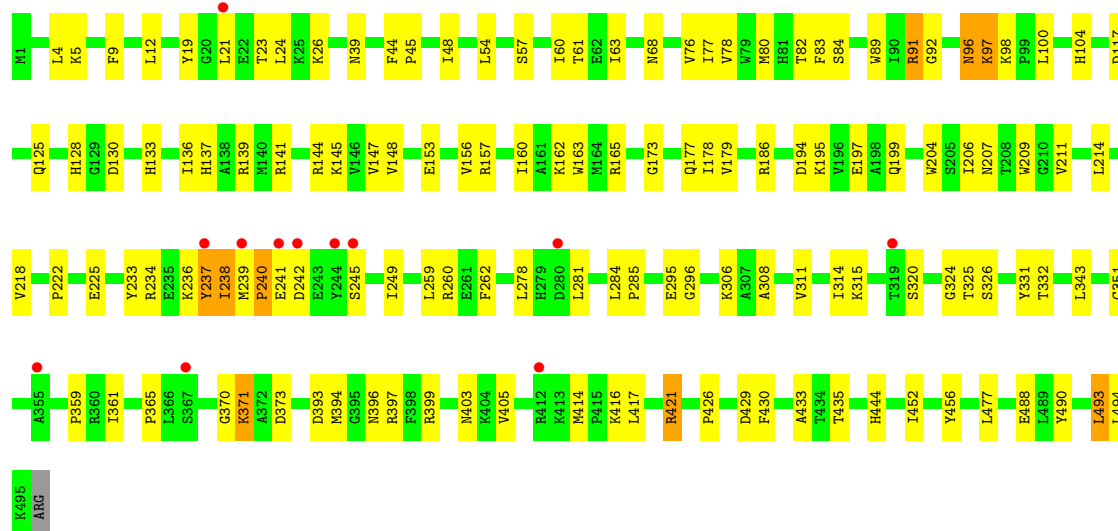


• Molecule 1: L-arabinose isomerase

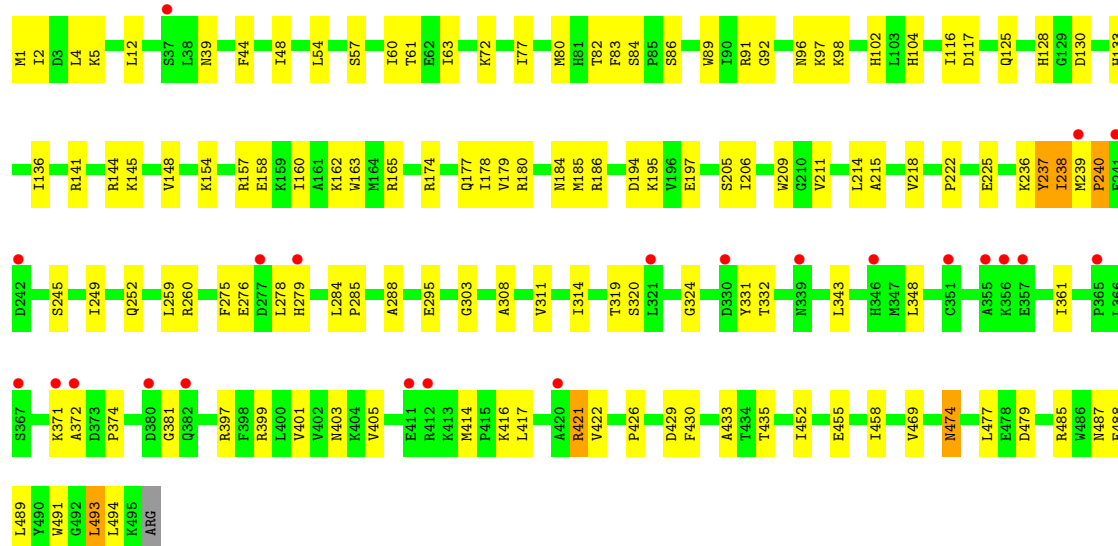
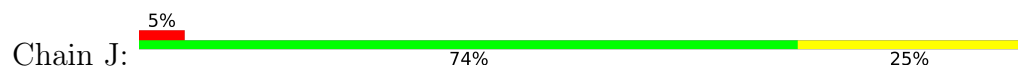




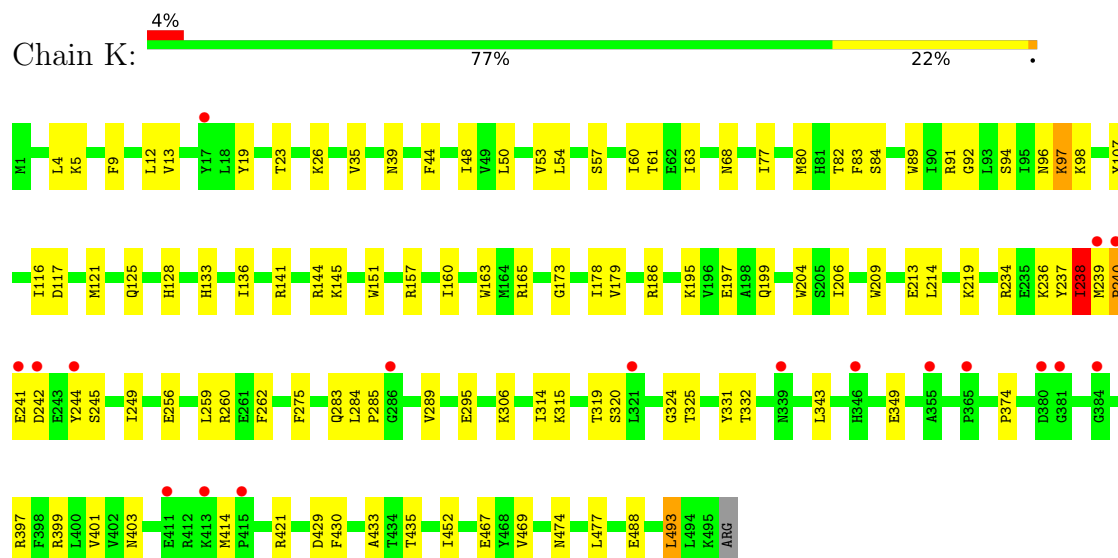
• Molecule 1: L-arabinose isomerase



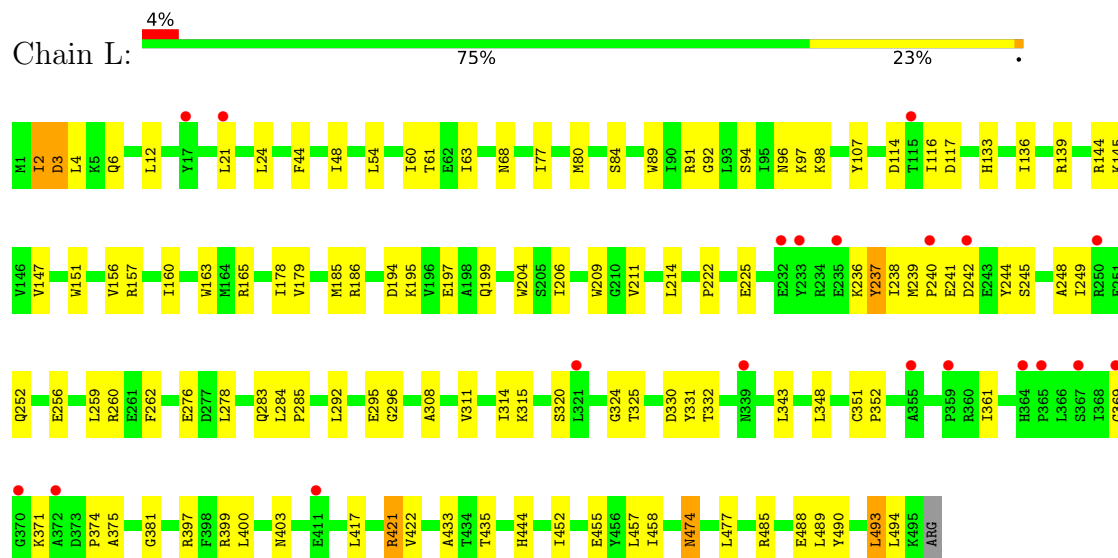
• Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.42Å 113.91Å 160.83Å 81.08° 81.15° 88.89°	Depositor
Resolution (Å)	33.11 – 3.61 33.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	96.1 (33.11-3.61) 96.1 (33.11-3.61)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.01 (at 3.65Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.232 , 0.280 0.232 , 0.280	Depositor DCC
$R_{free}$ test set	3336 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	47435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN

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	0.26	0/3828	0.50	0/5183
1	B	0.26	0/4064	0.48	0/5502
1	C	0.28	0/4064	0.50	1/5502 (0.0%)
1	D	0.26	0/4064	0.49	0/5502
1	E	0.26	0/4064	0.48	1/5502 (0.0%)
1	F	0.28	0/4064	0.49	1/5502 (0.0%)
1	G	0.26	0/4064	0.48	1/5502 (0.0%)
1	H	0.27	0/4064	0.49	1/5502 (0.0%)
1	I	0.26	0/4064	0.47	0/5502
1	J	0.26	0/4064	0.47	0/5502
1	K	0.26	0/4064	0.47	1/5502 (0.0%)
1	L	0.25	0/4064	0.47	0/5502
All	All	0.26	0/48532	0.48	6/65705 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	238	ILE	C-N-CA	8.28	142.41	121.70
1	G	238	ILE	C-N-CA	6.88	138.91	121.70
1	C	238	ILE	C-N-CA	6.40	137.71	121.70
1	F	238	ILE	C-N-CA	6.15	137.07	121.70
1	K	238	ILE	C-N-CA	6.10	136.96	121.70
1	E	238	ILE	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3739	0	3756	80	0
1	B	3969	0	3980	85	0
1	C	3969	0	3980	84	0
1	D	3969	0	3980	63	0
1	E	3969	0	3980	73	0
1	F	3969	0	3980	74	0
1	G	3969	0	3980	71	0
1	H	3969	0	3980	63	0
1	I	3969	0	3980	90	0
1	J	3969	0	3980	78	0
1	K	3969	0	3980	67	0
1	L	3969	0	3980	73	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	2	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	2	0	0	0	0
2	K	1	0	0	0	0
2	L	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
3	C	2	0	0	0	0
3	D	3	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	2	0	0	0	0
All	All	47435	0	47536	829	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 9.

All (829) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:MET:HG2	1:E:240:PRO:CD	1.98	0.94
1:E:239:MET:HG2	1:E:240:PRO:HD3	1.49	0.92
1:F:239:MET:HG2	1:F:240:PRO:HD2	1.53	0.90
1:K:68:ASN:HD21	1:K:96:ASN:HA	1.39	0.87
1:B:286:GLY:O	1:B:288:ALA:N	2.06	0.86
1:E:68:ASN:HD21	1:E:96:ASN:HA	1.42	0.83
1:I:370:GLY:C	1:I:371:LYS:HD2	1.99	0.82
1:H:239:MET:HG2	1:H:240:PRO:HD2	1.59	0.81
1:B:4:LEU:HD21	1:B:319:THR:HG21	1.64	0.80
1:A:95:ILE:HD11	1:D:68:ASN:HB3	1.66	0.77
1:A:380:ASP:HB3	1:A:410:ILE:HD13	1.66	0.77
1:D:117:ASP:HB3	1:H:416:LYS:HD2	1.66	0.77
1:E:239:MET:SD	1:E:245:SER:HB3	2.25	0.76
1:F:68:ASN:HD21	1:F:96:ASN:HA	1.49	0.75
1:H:68:ASN:HD21	1:H:96:ASN:HA	1.50	0.75
1:G:5:LYS:O	1:G:7:TYR:N	2.18	0.74
1:L:3:ASP:OD2	1:L:6:GLN:NE2	2.18	0.74
1:B:4:LEU:H	1:B:4:LEU:HD23	1.53	0.74
1:I:315:LYS:HD2	1:I:325:THR:HB	1.71	0.73
1:A:145:LYS:HE2	1:A:163:TRP:HB2	1.71	0.72
1:L:68:ASN:HD21	1:L:96:ASN:HA	1.54	0.72
1:A:275:PHE:CE1	1:A:276:GLU:OE1	2.43	0.71
1:D:488:GLU:OE2	1:F:141:ARG:NH2	2.24	0.71
1:K:77:ILE:HD13	1:K:160:ILE:HD11	1.73	0.70
1:A:12:LEU:HD11	1:A:63:ILE:HG21	1.72	0.70
1:C:417:LEU:HD23	1:C:421:ARG:HE	1.57	0.70
1:C:397:ARG:NH1	1:C:467:GLU:OE1	2.25	0.70
1:I:370:GLY:O	1:I:371:LYS:HD2	1.93	0.69
1:L:315:LYS:HD2	1:L:325:THR:HB	1.75	0.69
1:B:77:ILE:HD13	1:B:160:ILE:HD11	1.76	0.68
1:C:94:SER:O	1:F:97:LYS:NZ	2.27	0.68
1:A:284:LEU:HD12	1:A:285:PRO:HD2	1.75	0.68
1:G:284:LEU:HD12	1:G:285:PRO:HD2	1.75	0.68
1:K:97:LYS:NZ	1:L:94:SER:O	2.27	0.68
1:I:54:LEU:HD21	1:I:63:ILE:HG13	1.76	0.67
1:G:94:SER:O	1:I:97:LYS:NZ	2.27	0.67
1:L:77:ILE:HD13	1:L:160:ILE:HD11	1.75	0.67
1:E:91:ARG:NH1	1:J:174:ARG:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LYS:HD2	1:E:325:THR:HB	1.76	0.67
1:H:315:LYS:HD2	1:H:325:THR:HB	1.75	0.67
1:A:278:LEU:O	1:A:371:LYS:NZ	2.21	0.67
1:I:284:LEU:HD12	1:I:285:PRO:HD2	1.76	0.67
1:F:315:LYS:HD2	1:F:325:THR:HB	1.77	0.67
1:E:414:MET:HG2	1:G:116:ILE:HD11	1.75	0.67
1:F:284:LEU:HD12	1:F:285:PRO:HD2	1.76	0.66
1:K:284:LEU:HD12	1:K:285:PRO:HD2	1.76	0.66
1:A:141:ARG:NH1	1:C:488:GLU:OE1	2.29	0.66
1:D:77:ILE:HD13	1:D:160:ILE:HD11	1.78	0.66
1:C:284:LEU:HD12	1:C:285:PRO:HD2	1.76	0.65
1:H:284:LEU:HD12	1:H:285:PRO:HD2	1.78	0.65
1:K:12:LEU:HD11	1:K:63:ILE:HG21	1.78	0.65
1:F:488:GLU:OE2	1:H:141:ARG:NH2	2.29	0.65
1:E:54:LEU:HD13	1:E:60:ILE:HD13	1.79	0.65
1:I:12:LEU:HD11	1:I:63:ILE:HG21	1.79	0.65
1:C:162:LYS:HE3	1:C:456:TYR:CE1	2.32	0.65
1:K:54:LEU:HD13	1:K:60:ILE:HD13	1.79	0.65
1:E:12:LEU:HD11	1:E:63:ILE:HG21	1.79	0.65
1:F:54:LEU:HD13	1:F:60:ILE:HD13	1.79	0.65
1:D:22:GLU:HG3	1:D:26:LYS:HE3	1.78	0.64
1:D:284:LEU:HD12	1:D:285:PRO:HD2	1.77	0.64
1:L:284:LEU:HD12	1:L:285:PRO:HD2	1.79	0.64
1:B:488:GLU:OE2	1:C:141:ARG:NH2	2.27	0.64
1:E:116:ILE:HD11	1:K:414:MET:HG2	1.80	0.64
1:C:54:LEU:HD21	1:C:63:ILE:HG13	1.79	0.64
1:G:54:LEU:HD21	1:G:63:ILE:HG13	1.79	0.64
1:J:403:ASN:HD21	1:J:433:ALA:HB1	1.63	0.64
1:J:77:ILE:HD13	1:J:160:ILE:HD11	1.79	0.64
1:B:34:ILE:HD11	1:B:107:TYR:HB3	1.80	0.64
1:C:205:SER:HB2	1:F:91:ARG:HH12	1.63	0.64
1:J:54:LEU:HD21	1:J:63:ILE:HG13	1.80	0.64
1:G:54:LEU:HD13	1:G:60:ILE:HD13	1.80	0.64
1:E:239:MET:SD	1:E:245:SER:CB	2.86	0.64
1:G:197:GLU:OE2	1:I:139:ARG:NH1	2.31	0.63
1:L:60:ILE:HG22	1:L:92:GLY:HA3	1.81	0.63
1:A:180:ARG:HD2	1:A:206:ILE:HD11	1.80	0.63
1:A:104:HIS:ND1	1:A:130:ASP:OD1	2.24	0.63
1:B:54:LEU:HD13	1:B:60:ILE:HD13	1.81	0.63
1:E:104:HIS:ND1	1:E:130:ASP:OD2	2.32	0.63
1:A:260:ARG:NH1	1:A:295:GLU:OE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLY:O	1:A:371:LYS:N	2.31	0.63
1:D:145:LYS:HD3	1:D:163:TRP:HB2	1.80	0.63
1:H:332:THR:HG22	1:H:343:LEU:HB3	1.81	0.63
1:H:54:LEU:HD13	1:H:60:ILE:HD13	1.81	0.62
1:J:54:LEU:HD13	1:J:60:ILE:HD13	1.79	0.62
1:D:54:LEU:HD21	1:D:63:ILE:HG13	1.81	0.62
1:K:44:PHE:HE1	1:K:160:ILE:HG23	1.63	0.62
1:D:239:MET:HG2	1:D:240:PRO:HD2	1.82	0.62
1:H:4:LEU:CD2	1:H:319:THR:HG21	2.29	0.62
1:I:54:LEU:HD13	1:I:60:ILE:HD13	1.82	0.62
1:J:284:LEU:HD12	1:J:285:PRO:HD2	1.81	0.62
1:K:315:LYS:HD2	1:K:325:THR:HB	1.81	0.62
1:A:77:ILE:HD13	1:A:160:ILE:HD11	1.82	0.62
1:A:116:ILE:O	1:A:116:ILE:HD12	2.00	0.62
1:B:214:LEU:HD11	1:B:259:LEU:HD22	1.82	0.61
1:E:256:GLU:OE2	1:E:260:ARG:NH2	2.32	0.61
1:B:427:LEU:HD13	1:B:473:GLU:HG3	1.82	0.61
1:C:77:ILE:HD13	1:C:160:ILE:HD11	1.80	0.61
1:F:12:LEU:HD11	1:F:63:ILE:HG21	1.81	0.61
1:H:214:LEU:HD11	1:H:259:LEU:HD22	1.81	0.61
1:E:260:ARG:NH1	1:E:295:GLU:OE2	2.34	0.61
1:I:394:MET:O	1:J:141:ARG:NH1	2.34	0.61
1:G:417:LEU:HD23	1:G:421:ARG:HE	1.66	0.60
1:L:54:LEU:HD21	1:L:63:ILE:HG13	1.81	0.60
1:A:131:ARG:NH1	1:C:330:ASP:OD2	2.34	0.60
1:C:4:LEU:HD21	1:C:319:THR:HG21	1.83	0.60
1:C:214:LEU:HD11	1:C:259:LEU:HD22	1.83	0.60
1:D:12:LEU:HD11	1:D:63:ILE:HG21	1.83	0.60
1:G:332:THR:HG22	1:G:343:LEU:HB3	1.82	0.60
1:K:54:LEU:HD21	1:K:63:ILE:HG13	1.82	0.60
1:C:360:ARG:HG2	1:C:378:VAL:HB	1.82	0.60
1:A:4:LEU:HD11	1:A:45:PRO:HB2	1.84	0.60
1:E:54:LEU:HD21	1:E:63:ILE:HG13	1.83	0.60
1:E:284:LEU:HD12	1:E:285:PRO:HD2	1.82	0.60
1:F:115:THR:HG22	1:F:115:THR:O	2.02	0.60
1:G:331:TYR:HE2	1:K:121:MET:HB3	1.66	0.60
1:H:453:ASP:OD1	1:H:454:VAL:N	2.34	0.60
1:C:221:VAL:HG21	1:C:254:LYS:HB2	1.83	0.60
1:A:332:THR:HG22	1:A:343:LEU:HB3	1.84	0.60
1:C:54:LEU:HD13	1:C:60:ILE:HD13	1.83	0.60
1:B:102:HIS:HE1	1:B:130:ASP:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:LEU:HD11	1:G:63:ILE:HG21	1.84	0.59
1:A:54:LEU:HD13	1:A:60:ILE:HD13	1.85	0.59
1:J:474:ASN:O	1:J:474:ASN:ND2	2.35	0.59
1:L:12:LEU:HD11	1:L:63:ILE:HG21	1.84	0.59
1:K:35:VAL:HG21	1:K:50:LEU:HB2	1.84	0.59
1:F:77:ILE:HD13	1:F:160:ILE:HD11	1.85	0.59
1:G:195:LYS:HG3	1:G:206:ILE:HD13	1.84	0.59
1:K:35:VAL:HG11	1:K:50:LEU:HD23	1.84	0.59
1:B:330:ASP:OD2	1:C:131:ARG:NH1	2.36	0.59
1:L:417:LEU:HD23	1:L:421:ARG:HE	1.68	0.59
1:G:77:ILE:HD13	1:G:160:ILE:HD11	1.85	0.59
1:G:260:ARG:NH1	1:G:295:GLU:OE2	2.32	0.59
1:I:214:LEU:HD11	1:I:259:LEU:HD22	1.84	0.59
1:L:222:PRO:HB2	1:L:225:GLU:HG3	1.85	0.59
1:B:97:LYS:NZ	1:H:94:SER:O	2.36	0.58
1:C:332:THR:HG22	1:C:343:LEU:HB3	1.84	0.58
1:F:474:ASN:O	1:F:474:ASN:ND2	2.36	0.58
1:A:18:LEU:HD21	1:C:186:ARG:HH12	1.67	0.58
1:A:19:TYR:OH	1:A:125:GLN:OE1	2.19	0.58
1:G:474:ASN:O	1:G:474:ASN:ND2	2.34	0.58
1:J:12:LEU:HD11	1:J:63:ILE:HG21	1.86	0.58
1:B:54:LEU:HD21	1:B:63:ILE:HG13	1.84	0.58
1:D:211:VAL:HG11	1:D:278:LEU:HA	1.83	0.58
1:L:80:MET:SD	1:L:84:SER:OG	2.60	0.58
1:C:44:PHE:HE1	1:C:160:ILE:HG23	1.69	0.58
1:C:195:LYS:HG2	1:C:206:ILE:HD13	1.84	0.58
1:E:60:ILE:HG22	1:E:92:GLY:HA3	1.84	0.58
1:H:260:ARG:NH1	1:H:295:GLU:OE2	2.37	0.58
1:I:211:VAL:HG11	1:I:278:LEU:HA	1.86	0.58
1:H:256:GLU:OE2	1:H:260:ARG:NH2	2.37	0.58
1:D:248:ALA:HB1	1:D:283:GLN:HE22	1.69	0.58
1:H:104:HIS:ND1	1:H:130:ASP:OD1	2.37	0.58
1:L:474:ASN:O	1:L:474:ASN:ND2	2.36	0.58
1:K:260:ARG:NH1	1:K:295:GLU:OE2	2.36	0.57
1:B:397:ARG:NH1	1:B:467:GLU:OE1	2.33	0.57
1:A:78:VAL:HG11	1:A:133:HIS:HE1	1.68	0.57
1:D:4:LEU:O	1:D:5:LYS:HB2	2.04	0.57
1:D:474:ASN:ND2	1:D:474:ASN:O	2.37	0.57
1:G:133:HIS:O	1:G:136:ILE:HG22	2.05	0.57
1:F:211:VAL:HG11	1:F:278:LEU:HA	1.86	0.57
1:A:410:ILE:HD12	1:A:410:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:PRO:HB2	1:E:225:GLU:HG3	1.87	0.57
1:F:82:THR:HA	1:F:125:GLN:HB2	1.86	0.57
1:K:403:ASN:HD21	1:K:433:ALA:HB1	1.69	0.57
1:C:237:TYR:HB3	1:C:361:ILE:HG13	1.86	0.57
1:G:315:LYS:HD2	1:G:325:THR:HB	1.87	0.57
1:H:195:LYS:HG3	1:H:206:ILE:HD13	1.86	0.57
1:E:239:MET:HG2	1:E:240:PRO:HD2	1.82	0.57
1:I:416:LYS:HD2	1:J:117:ASP:HB3	1.86	0.57
1:J:194:ASP:HB3	1:J:197:GLU:HG2	1.87	0.56
1:C:252:GLN:HG3	1:C:375:ALA:HB3	1.87	0.56
1:G:222:PRO:HB2	1:G:225:GLU:HG3	1.87	0.56
1:J:211:VAL:HG11	1:J:278:LEU:HA	1.85	0.56
1:A:116:ILE:CD1	1:C:417:LEU:HB2	2.35	0.56
1:A:133:HIS:O	1:A:136:ILE:HG22	2.06	0.56
1:E:332:THR:HG22	1:E:343:LEU:HB3	1.86	0.56
1:K:94:SER:O	1:L:97:LYS:NZ	2.30	0.56
1:L:61:THR:HG21	1:L:91:ARG:HE	1.69	0.56
1:E:180:ARG:HD2	1:E:206:ILE:HD11	1.88	0.56
1:C:95:ILE:HD11	1:F:68:ASN:HB3	1.87	0.56
1:L:214:LEU:HD11	1:L:259:LEU:HD22	1.88	0.56
1:L:332:THR:HG22	1:L:343:LEU:HB3	1.87	0.56
1:D:185:MET:HG3	1:D:276:GLU:OE1	2.05	0.56
1:I:417:LEU:HD23	1:I:421:ARG:HE	1.71	0.56
1:A:54:LEU:HD21	1:A:63:ILE:HG13	1.88	0.56
1:L:239:MET:HG3	1:L:361:ILE:O	2.06	0.56
1:I:19:TYR:OH	1:I:125:GLN:OE1	2.22	0.56
1:I:403:ASN:HD21	1:I:433:ALA:HB1	1.71	0.56
1:E:214:LEU:HD11	1:E:259:LEU:HD22	1.88	0.56
1:L:54:LEU:HD13	1:L:60:ILE:HD13	1.86	0.56
1:B:284:LEU:HD12	1:B:285:PRO:HD2	1.87	0.56
1:D:180:ARG:HD2	1:D:206:ILE:HD11	1.87	0.56
1:K:256:GLU:OE2	1:K:260:ARG:NH2	2.39	0.56
1:B:455:GLU:O	1:B:458:ILE:HG22	2.05	0.55
1:A:36:ASP:OD1	1:A:37:SER:N	2.39	0.55
1:G:177:GLN:OE1	1:G:207:ASN:ND2	2.38	0.55
1:C:12:LEU:HD11	1:C:63:ILE:HG21	1.87	0.55
1:D:332:THR:HG22	1:D:343:LEU:HB3	1.88	0.55
1:E:4:LEU:HD21	1:E:319:THR:HG21	1.89	0.55
1:K:397:ARG:NH1	1:K:467:GLU:OE1	2.38	0.55
1:K:133:HIS:O	1:K:136:ILE:HG22	2.07	0.55
1:K:214:LEU:HD11	1:K:259:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:ILE:HG22	1:J:206:ILE:HA	1.89	0.55
1:B:239:MET:HG3	1:B:361:ILE:O	2.07	0.55
1:L:133:HIS:O	1:L:136:ILE:HG22	2.06	0.55
1:I:177:GLN:NE2	1:I:178:ILE:O	2.40	0.55
1:B:133:HIS:O	1:B:136:ILE:HG22	2.06	0.54
1:E:108:ASN:OD1	1:E:124:ASN:ND2	2.40	0.54
1:H:133:HIS:O	1:H:136:ILE:HG22	2.07	0.54
1:J:405:VAL:HG12	1:J:426:PRO:HA	1.88	0.54
1:B:211:VAL:HG11	1:B:278:LEU:HA	1.89	0.54
1:F:214:LEU:HD11	1:F:259:LEU:HD22	1.89	0.54
1:L:245:SER:O	1:L:249:ILE:HG12	2.07	0.54
1:B:145:LYS:HD3	1:B:163:TRP:HB2	1.90	0.54
1:B:234:ARG:HA	1:B:238:ILE:HG13	1.89	0.54
1:I:4:LEU:HD11	1:I:45:PRO:HB2	1.89	0.54
1:I:195:LYS:HG3	1:I:206:ILE:HD13	1.90	0.54
1:C:19:TYR:OH	1:C:125:GLN:OE1	2.25	0.54
1:G:214:LEU:HD11	1:G:259:LEU:HD22	1.88	0.54
1:H:107:TYR:HA	1:H:151:TRP:HE1	1.71	0.54
1:J:381:GLY:HA3	1:J:422:VAL:HG13	1.89	0.54
1:E:417:LEU:HD23	1:E:421:ARG:HE	1.72	0.54
1:H:12:LEU:HD11	1:H:63:ILE:HG21	1.89	0.54
1:F:177:GLN:NE2	1:F:178:ILE:O	2.41	0.54
1:A:30:GLN:HG2	1:A:107:TYR:CD2	2.43	0.54
1:C:417:LEU:HB3	1:C:421:ARG:HH21	1.72	0.54
1:D:19:TYR:OH	1:D:125:GLN:OE1	2.24	0.54
1:H:178:ILE:HG22	1:H:206:ILE:HA	1.90	0.54
1:A:403:ASN:HD21	1:A:433:ALA:HB1	1.72	0.53
1:J:239:MET:HG3	1:J:361:ILE:O	2.08	0.53
1:I:133:HIS:O	1:I:136:ILE:HG22	2.09	0.53
1:B:79:TRP:NE1	1:B:105:THR:O	2.42	0.53
1:D:381:GLY:HA3	1:D:422:VAL:HG13	1.89	0.53
1:I:239:MET:HG3	1:I:361:ILE:O	2.08	0.53
1:J:222:PRO:HB2	1:J:225:GLU:HG3	1.89	0.53
1:J:493:LEU:HD23	1:J:493:LEU:H	1.74	0.53
1:D:414:MET:HG2	1:F:116:ILE:HD11	1.90	0.53
1:E:394:MET:HG3	1:G:141:ARG:HH21	1.74	0.53
1:F:23:THR:HA	1:F:26:LYS:HD2	1.91	0.53
1:F:195:LYS:HG3	1:F:206:ILE:HD13	1.91	0.53
1:G:60:ILE:HG22	1:G:92:GLY:HA3	1.90	0.53
1:K:332:THR:HG22	1:K:343:LEU:HB3	1.91	0.53
1:F:314:ILE:HD11	1:F:452:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:HIS:CE1	1:B:130:ASP:HB2	2.43	0.53
1:B:107:TYR:HA	1:B:151:TRP:HE1	1.73	0.53
1:C:4:LEU:HD23	1:C:4:LEU:H	1.74	0.53
1:D:54:LEU:HD13	1:D:60:ILE:HD13	1.89	0.53
1:E:133:HIS:O	1:E:136:ILE:HG22	2.08	0.53
1:A:41:ASP:OD2	1:A:157:ARG:NH1	2.42	0.53
1:D:234:ARG:HA	1:D:238:ILE:HB	1.90	0.53
1:G:44:PHE:HE1	1:G:160:ILE:HG23	1.74	0.53
1:G:397:ARG:NH2	1:G:488:GLU:HA	2.24	0.53
1:H:54:LEU:HD21	1:H:63:ILE:HG13	1.91	0.53
1:J:489:LEU:HD13	1:L:489:LEU:HD11	1.90	0.53
1:L:403:ASN:HD21	1:L:433:ALA:HB1	1.74	0.53
1:B:332:THR:HG22	1:B:343:LEU:HB3	1.91	0.53
1:F:180:ARG:HD2	1:F:206:ILE:HD11	1.91	0.53
1:C:133:HIS:O	1:C:136:ILE:HG22	2.09	0.52
1:A:315:LYS:O	1:A:319:THR:OG1	2.27	0.52
1:B:211:VAL:HG21	1:B:277:ASP:O	2.10	0.52
1:F:54:LEU:HD21	1:F:63:ILE:HG13	1.90	0.52
1:I:78:VAL:HG11	1:I:133:HIS:HE1	1.73	0.52
1:I:130:ASP:OD1	1:I:130:ASP:N	2.40	0.52
1:C:23:THR:HA	1:C:26:LYS:HD2	1.91	0.52
1:E:165:ARG:NH2	1:E:320:SER:HB2	2.25	0.52
1:B:493:LEU:HD23	1:B:493:LEU:H	1.75	0.52
1:L:48:ILE:HD11	1:L:77:ILE:HD12	1.90	0.52
1:I:23:THR:HA	1:I:26:LYS:HD2	1.92	0.52
1:L:260:ARG:NH1	1:L:295:GLU:OE2	2.43	0.52
1:A:18:LEU:HD11	1:C:186:ARG:HH22	1.73	0.52
1:D:60:ILE:HG22	1:D:92:GLY:HA3	1.92	0.52
1:F:80:MET:SD	1:F:84:SER:OG	2.63	0.52
1:K:48:ILE:HD11	1:K:77:ILE:HD12	1.91	0.52
1:A:489:LEU:HD11	1:B:490:TYR:HD1	1.75	0.52
1:D:314:ILE:HD11	1:D:452:ILE:HD11	1.91	0.52
1:H:4:LEU:HD21	1:H:319:THR:HG21	1.92	0.52
1:H:44:PHE:HE1	1:H:160:ILE:HG23	1.74	0.52
1:L:381:GLY:HA3	1:L:422:VAL:HG13	1.92	0.52
1:D:104:HIS:HB3	1:D:148:VAL:HG22	1.92	0.52
1:G:325:THR:HG1	1:G:449:SER:HG	1.55	0.52
1:I:44:PHE:HE1	1:I:160:ILE:HG23	1.75	0.52
1:I:429:ASP:OD1	1:I:430:PHE:N	2.42	0.52
1:B:429:ASP:OD1	1:B:430:PHE:N	2.43	0.51
1:D:493:LEU:H	1:D:493:LEU:HD23	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ILE:HG21	1:F:89:TRP:HA	1.92	0.51
1:H:13:VAL:HB	1:H:53:VAL:HG22	1.91	0.51
1:I:493:LEU:HD23	1:I:493:LEU:H	1.76	0.51
1:D:260:ARG:NH1	1:D:295:GLU:OE1	2.43	0.51
1:E:397:ARG:HH21	1:E:488:GLU:HA	1.74	0.51
1:F:104:HIS:ND1	1:F:130:ASP:OD2	2.43	0.51
1:J:397:ARG:HH21	1:J:488:GLU:HA	1.75	0.51
1:K:178:ILE:HG22	1:K:206:ILE:HA	1.92	0.51
1:B:330:ASP:O	1:C:128:HIS:HB3	2.11	0.51
1:C:323:GLY:HA2	1:C:451:ALA:HB2	1.91	0.51
1:D:397:ARG:NH1	1:D:467:GLU:OE1	2.39	0.51
1:F:417:LEU:HD23	1:F:421:ARG:HE	1.75	0.51
1:L:397:ARG:NH2	1:L:488:GLU:HA	2.25	0.51
1:A:140:MET:HB3	1:A:142:LEU:HD23	1.92	0.51
1:G:239:MET:HG3	1:G:361:ILE:O	2.10	0.51
1:I:397:ARG:NH2	1:I:488:GLU:HA	2.25	0.51
1:J:44:PHE:HE1	1:J:160:ILE:HG23	1.75	0.51
1:J:332:THR:HG22	1:J:343:LEU:HB3	1.93	0.51
1:E:184:ASN:HA	1:E:303:GLY:HA3	1.93	0.51
1:F:414:MET:HG2	1:H:116:ILE:HD11	1.93	0.51
1:I:179:VAL:HG13	1:I:209:TRP:CE3	2.46	0.51
1:C:429:ASP:OD1	1:C:430:PHE:N	2.45	0.50
1:E:493:LEU:HD23	1:E:493:LEU:H	1.75	0.50
1:F:194:ASP:HB3	1:F:197:GLU:HG2	1.93	0.50
1:G:211:VAL:HG11	1:G:278:LEU:HA	1.94	0.50
1:L:493:LEU:HD23	1:L:493:LEU:H	1.75	0.50
1:C:178:ILE:HG22	1:C:206:ILE:HA	1.93	0.50
1:E:293:MET:SD	1:E:299:PHE:HB3	2.51	0.50
1:F:44:PHE:HE1	1:F:160:ILE:HG23	1.76	0.50
1:C:311:VAL:O	1:C:315:LYS:HB2	2.11	0.50
1:G:444:HIS:HB2	1:K:128:HIS:HB2	1.94	0.50
1:L:314:ILE:HD11	1:L:452:ILE:HD11	1.93	0.50
1:D:133:HIS:O	1:D:136:ILE:HG22	2.11	0.50
1:K:493:LEU:H	1:K:493:LEU:HD23	1.77	0.50
1:A:211:VAL:HG11	1:A:278:LEU:HA	1.93	0.50
1:A:248:ALA:HB1	1:A:283:GLN:HE22	1.76	0.50
1:D:51:LYS:HD3	1:D:63:ILE:HD12	1.94	0.50
1:I:100:LEU:HD23	1:I:137:HIS:HE1	1.76	0.50
1:J:195:LYS:HG3	1:J:206:ILE:HD13	1.92	0.50
1:J:133:HIS:O	1:J:136:ILE:HG22	2.12	0.50
1:L:195:LYS:HG3	1:L:206:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG13	1:A:209:TRP:CE3	2.47	0.50
1:C:162:LYS:HE2	1:C:455:GLU:HG2	1.94	0.50
1:D:80:MET:SD	1:D:84:SER:OG	2.59	0.50
1:D:179:VAL:HG13	1:D:209:TRP:CE3	2.47	0.50
1:D:214:LEU:HD11	1:D:259:LEU:HD22	1.94	0.50
1:L:21:LEU:HD12	1:L:24:LEU:HD12	1.94	0.50
1:B:154:LYS:O	1:B:158:GLU:HG3	2.12	0.49
1:D:429:ASP:OD1	1:D:430:PHE:N	2.45	0.49
1:C:239:MET:HG3	1:C:361:ILE:O	2.12	0.49
1:E:82:THR:OG1	1:E:83:PHE:N	2.46	0.49
1:F:199:GLN:HG2	1:F:204:TRP:O	2.11	0.49
1:E:179:VAL:HG13	1:E:209:TRP:CE3	2.47	0.49
1:K:23:THR:HA	1:K:26:LYS:HD2	1.94	0.49
1:A:57:SER:O	1:A:61:THR:HG23	2.11	0.49
1:A:128:HIS:HB2	1:C:444:HIS:HB2	1.94	0.49
1:F:248:ALA:HB1	1:F:283:GLN:HE22	1.77	0.49
1:J:429:ASP:OD1	1:J:430:PHE:N	2.46	0.49
1:K:239:MET:HG2	1:K:240:PRO:HD3	1.93	0.49
1:E:194:ASP:HB3	1:E:197:GLU:HG2	1.94	0.49
1:L:194:ASP:HB3	1:L:197:GLU:HG2	1.95	0.49
1:L:248:ALA:HB1	1:L:283:GLN:HE22	1.77	0.49
1:A:102:HIS:NE2	1:A:130:ASP:HB3	2.28	0.49
1:G:493:LEU:HD23	1:G:493:LEU:H	1.77	0.49
1:L:2:ILE:HD12	1:L:2:ILE:O	2.13	0.49
1:A:80:MET:HB2	1:A:130:ASP:OD2	2.13	0.49
1:A:366:LEU:HD23	1:A:376:ARG:HH22	1.78	0.49
1:G:397:ARG:HH21	1:G:488:GLU:HA	1.77	0.49
1:I:178:ILE:HG22	1:I:206:ILE:HA	1.94	0.49
1:K:107:TYR:HA	1:K:151:TRP:HE1	1.77	0.49
1:D:128:HIS:HB2	1:H:444:HIS:HB2	1.95	0.49
1:D:394:MET:HG3	1:F:141:ARG:NH1	2.27	0.49
1:G:178:ILE:HG22	1:G:206:ILE:HA	1.94	0.49
1:I:245:SER:O	1:I:249:ILE:HG12	2.13	0.49
1:I:314:ILE:HD11	1:I:452:ILE:HD11	1.95	0.49
1:A:195:LYS:HG3	1:A:206:ILE:HD13	1.94	0.49
1:G:429:ASP:OD1	1:G:430:PHE:N	2.46	0.49
1:I:9:PHE:HB2	1:I:48:ILE:HD12	1.94	0.49
1:I:104:HIS:ND1	1:I:130:ASP:OD2	2.45	0.49
1:I:332:THR:HG22	1:I:343:LEU:HB3	1.94	0.49
1:J:278:LEU:HB2	1:J:371:LYS:HE2	1.95	0.49
1:K:397:ARG:NH2	1:K:488:GLU:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:ILE:HD11	1:I:77:ILE:HD12	1.95	0.48
1:E:248:ALA:HB1	1:E:283:GLN:HE22	1.78	0.48
1:E:403:ASN:HD21	1:E:433:ALA:HB1	1.79	0.48
1:F:222:PRO:HB2	1:F:225:GLU:HG3	1.94	0.48
1:I:234:ARG:HA	1:I:238:ILE:CG1	2.42	0.48
1:I:241:GLU:HG2	1:I:242:ASP:H	1.77	0.48
1:K:197:GLU:HG2	1:L:139:ARG:NH1	2.28	0.48
1:B:68:ASN:HD22	1:B:98:LYS:HD3	1.78	0.48
1:G:165:ARG:NH2	1:G:320:SER:HB2	2.28	0.48
1:K:283:GLN:NE2	1:K:374:PRO:HA	2.29	0.48
1:L:60:ILE:HG21	1:L:89:TRP:HA	1.95	0.48
1:L:252:GLN:HG3	1:L:375:ALA:HB3	1.95	0.48
1:I:78:VAL:HG11	1:I:133:HIS:CE1	2.48	0.48
1:I:371:LYS:HD2	1:I:371:LYS:N	2.28	0.48
1:K:234:ARG:HA	1:K:238:ILE:HG13	1.94	0.48
1:I:414:MET:HG2	1:J:116:ILE:HD11	1.95	0.48
1:J:4:LEU:HD21	1:J:319:THR:HG21	1.94	0.48
1:H:429:ASP:OD1	1:H:430:PHE:N	2.47	0.48
1:H:180:ARG:HD2	1:H:206:ILE:HD11	1.96	0.48
1:C:237:TYR:HD1	1:C:359:PRO:O	1.97	0.48
1:D:184:ASN:HA	1:D:303:GLY:HA3	1.96	0.48
1:L:435:THR:HG23	1:L:477:LEU:HD21	1.94	0.48
1:B:180:ARG:HD2	1:B:206:ILE:HD11	1.95	0.48
1:J:245:SER:O	1:J:249:ILE:HG12	2.14	0.48
1:A:162:LYS:HD2	1:A:455:GLU:HG2	1.96	0.48
1:B:19:TYR:OH	1:B:125:GLN:OE1	2.29	0.48
1:C:102:HIS:NE2	1:C:130:ASP:HB2	2.29	0.48
1:D:435:THR:HG23	1:D:477:LEU:HD21	1.96	0.48
1:D:444:HIS:HB2	1:F:128:HIS:HB2	1.95	0.48
1:H:86:SER:HB3	1:H:136:ILE:HB	1.94	0.48
1:J:60:ILE:HG21	1:J:89:TRP:HA	1.96	0.48
1:J:184:ASN:HA	1:J:303:GLY:HA3	1.94	0.48
1:K:314:ILE:HD11	1:K:452:ILE:HD11	1.95	0.48
1:L:44:PHE:HE1	1:L:160:ILE:HG23	1.78	0.48
1:B:343:LEU:HD11	1:B:421:ARG:HB2	1.96	0.47
1:I:21:LEU:HD12	1:I:24:LEU:HD12	1.95	0.47
1:C:211:VAL:HG11	1:C:278:LEU:HA	1.95	0.47
1:J:145:LYS:HD3	1:J:163:TRP:HB2	1.95	0.47
1:D:278:LEU:HB2	1:D:371:LYS:HE2	1.95	0.47
1:I:60:ILE:HG21	1:I:89:TRP:HA	1.96	0.47
1:J:214:LEU:HD11	1:J:259:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:SER:O	1:B:61:THR:HG23	2.14	0.47
1:B:195:LYS:HG3	1:B:206:ILE:HD13	1.96	0.47
1:C:35:VAL:HG21	1:C:50:LEU:HB2	1.96	0.47
1:E:51:LYS:HD3	1:E:63:ILE:HD12	1.96	0.47
1:G:397:ARG:NH1	1:G:467:GLU:OE1	2.43	0.47
1:J:455:GLU:O	1:J:458:ILE:HG22	2.14	0.47
1:L:237:TYR:CB	1:L:361:ILE:HG13	2.44	0.47
1:A:478:GLU:CD	1:B:458:ILE:HD11	2.34	0.47
1:B:260:ARG:NH1	1:B:295:GLU:OE2	2.48	0.47
1:D:44:PHE:HE1	1:D:160:ILE:HG23	1.78	0.47
1:E:68:ASN:ND2	1:E:96:ASN:HA	2.21	0.47
1:E:77:ILE:HD13	1:E:160:ILE:HD11	1.96	0.47
1:J:260:ARG:NH1	1:J:295:GLU:OE2	2.47	0.47
1:K:429:ASP:OD1	1:K:430:PHE:N	2.47	0.47
1:A:51:LYS:HD3	1:A:63:ILE:HD12	1.97	0.47
1:C:455:GLU:O	1:C:458:ILE:HG22	2.13	0.47
1:I:39:ASN:HD21	1:I:48:ILE:HG22	1.79	0.47
1:I:104:HIS:HB3	1:I:148:VAL:HG22	1.97	0.47
1:J:57:SER:O	1:J:61:THR:HG23	2.13	0.47
1:B:139:ARG:NH1	1:H:197:GLU:HG2	2.29	0.47
1:C:51:LYS:HB3	1:C:52:PRO:HD2	1.97	0.47
1:H:57:SER:O	1:H:61:THR:HG23	2.14	0.47
1:K:80:MET:SD	1:K:84:SER:OG	2.68	0.47
1:L:397:ARG:HH21	1:L:488:GLU:HA	1.78	0.47
1:C:234:ARG:HA	1:C:238:ILE:HG13	1.97	0.47
1:E:283:GLN:NE2	1:E:374:PRO:HA	2.29	0.47
1:E:397:ARG:NH2	1:E:488:GLU:HA	2.30	0.47
1:F:455:GLU:O	1:F:458:ILE:HG22	2.15	0.47
1:H:211:VAL:HG11	1:H:278:LEU:HA	1.97	0.47
1:I:60:ILE:HG22	1:I:92:GLY:HA3	1.97	0.47
1:E:165:ARG:HH21	1:E:320:SER:HB2	1.78	0.47
1:G:245:SER:O	1:G:249:ILE:HG12	2.15	0.47
1:B:78:VAL:HG11	1:B:133:HIS:CE1	2.50	0.47
1:H:435:THR:HG23	1:H:477:LEU:HD21	1.96	0.47
1:G:435:THR:HG23	1:G:477:LEU:HD21	1.97	0.46
1:H:381:GLY:HA3	1:H:422:VAL:HG13	1.97	0.46
1:J:80:MET:SD	1:J:84:SER:OG	2.62	0.46
1:J:397:ARG:NH2	1:J:488:GLU:HA	2.29	0.46
1:A:78:VAL:HG11	1:A:133:HIS:CE1	2.49	0.46
1:A:275:PHE:HE1	1:A:276:GLU:OE1	1.93	0.46
1:B:431:LYS:NZ	1:C:153:GLU:OE2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LYS:HE2	1:C:462:GLU:OE2	2.16	0.46
1:E:416:LYS:HG3	1:G:117:ASP:HB3	1.97	0.46
1:H:145:LYS:HD3	1:H:163:TRP:HB2	1.96	0.46
1:I:61:THR:HG21	1:I:91:ARG:HE	1.80	0.46
1:I:100:LEU:CD2	1:I:137:HIS:HE1	2.29	0.46
1:K:195:LYS:HG3	1:K:206:ILE:HD13	1.96	0.46
1:A:107:TYR:HA	1:A:151:TRP:HE1	1.81	0.46
1:L:256:GLU:OE2	1:L:260:ARG:NH2	2.48	0.46
1:A:314:ILE:HD11	1:A:452:ILE:HD11	1.97	0.46
1:B:233:TYR:C	1:B:238:ILE:HG12	2.36	0.46
1:B:241:GLU:HG2	1:B:242:ASP:H	1.81	0.46
1:G:19:TYR:OH	1:G:125:GLN:OE1	2.31	0.46
1:I:260:ARG:NH1	1:I:295:GLU:OE2	2.48	0.46
1:J:61:THR:HG21	1:J:91:ARG:HE	1.80	0.46
1:J:279:HIS:NE2	1:K:213:GLU:HG2	2.30	0.46
1:A:429:ASP:OD1	1:A:430:PHE:N	2.48	0.46
1:H:82:THR:OG1	1:H:83:PHE:N	2.49	0.46
1:J:165:ARG:NH2	1:J:320:SER:HB2	2.31	0.46
1:L:165:ARG:NH2	1:L:320:SER:HB2	2.31	0.46
1:A:321:LEU:HA	1:A:321:LEU:HD12	1.59	0.46
1:B:82:THR:OG1	1:B:83:PHE:N	2.49	0.46
1:F:435:THR:HG23	1:F:477:LEU:HD21	1.98	0.46
1:I:76:VAL:HB	1:I:100:LEU:HD12	1.96	0.46
1:I:165:ARG:NH2	1:I:320:SER:HB2	2.31	0.46
1:D:30:GLN:HG2	1:D:107:TYR:CD2	2.49	0.46
1:D:283:GLN:NE2	1:D:374:PRO:HA	2.30	0.46
1:F:57:SER:O	1:F:61:THR:HG23	2.16	0.46
1:F:108:ASN:OD1	1:F:124:ASN:ND2	2.48	0.46
1:F:444:HIS:HB2	1:H:128:HIS:HB2	1.97	0.46
1:I:77:ILE:HD13	1:I:160:ILE:HD11	1.98	0.46
1:D:117:ASP:N	1:D:117:ASP:OD1	2.48	0.46
1:E:314:ILE:HD11	1:E:452:ILE:HD11	1.98	0.46
1:G:314:ILE:HD11	1:G:452:ILE:HD11	1.98	0.46
1:B:7:TYR:OH	1:B:172:ASP:OD1	2.26	0.46
1:B:237:TYR:CB	1:B:361:ILE:HG13	2.46	0.46
1:C:275:PHE:CE1	1:C:276:GLU:OE1	2.69	0.46
1:F:60:ILE:HG22	1:F:92:GLY:HA3	1.96	0.46
1:H:60:ILE:HG22	1:H:92:GLY:HA3	1.98	0.46
1:I:80:MET:SD	1:I:84:SER:OG	2.65	0.46
1:I:145:LYS:HD3	1:I:163:TRP:HB2	1.98	0.46
1:J:179:VAL:HG13	1:J:209:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:MET:HG2	1:L:116:ILE:HD11	1.97	0.46
1:L:348:LEU:HD21	1:L:374:PRO:HG2	1.97	0.46
1:A:416:LYS:HG3	1:B:117:ASP:HB3	1.98	0.46
1:B:48:ILE:HD11	1:B:77:ILE:HD12	1.97	0.46
1:C:180:ARG:HD2	1:C:206:ILE:HD11	1.97	0.46
1:D:9:PHE:HB2	1:D:48:ILE:HD12	1.98	0.46
1:E:239:MET:SD	1:E:245:SER:OG	2.74	0.46
1:G:117:ASP:OD1	1:G:117:ASP:N	2.49	0.46
1:G:394:MET:HG3	1:K:141:ARG:NH2	2.31	0.46
1:B:68:ASN:OD1	1:B:96:ASN:HA	2.16	0.45
1:F:48:ILE:HD11	1:F:77:ILE:HD12	1.97	0.45
1:G:237:TYR:CB	1:G:361:ILE:HG13	2.45	0.45
1:G:414:MET:HG2	1:K:116:ILE:HD11	1.97	0.45
1:A:112:PRO:HG2	1:A:116:ILE:HG23	1.98	0.45
1:A:172:ASP:OD2	1:A:312:ARG:NH2	2.47	0.45
1:B:78:VAL:HG11	1:B:133:HIS:HE1	1.80	0.45
1:B:178:ILE:HG22	1:B:206:ILE:HA	1.98	0.45
1:C:260:ARG:NH1	1:C:295:GLU:OE2	2.49	0.45
1:E:186:ARG:HG2	1:I:207:ASN:HB3	1.98	0.45
1:I:178:ILE:HD11	1:I:308:ALA:HB3	1.97	0.45
1:J:82:THR:OG1	1:J:83:PHE:N	2.50	0.45
1:J:252:GLN:NE2	1:J:288:ALA:H	2.14	0.45
1:J:416:LYS:HD2	1:L:117:ASP:HB3	1.97	0.45
1:C:435:THR:HG23	1:C:477:LEU:HD21	1.98	0.45
1:H:237:TYR:HB2	1:H:238:ILE:H	1.57	0.45
1:I:57:SER:O	1:I:61:THR:HG23	2.16	0.45
1:K:57:SER:O	1:K:61:THR:HG23	2.17	0.45
1:B:214:LEU:HD21	1:B:259:LEU:HD21	1.98	0.45
1:D:48:ILE:HD11	1:D:77:ILE:HD12	1.97	0.45
1:E:117:ASP:OD1	1:E:117:ASP:N	2.48	0.45
1:F:68:ASN:ND2	1:F:96:ASN:HA	2.26	0.45
1:G:102:HIS:NE2	1:G:130:ASP:HB2	2.31	0.45
1:H:117:ASP:OD1	1:H:117:ASP:N	2.49	0.45
1:J:82:THR:HA	1:J:125:GLN:HB2	1.98	0.45
1:K:117:ASP:N	1:K:117:ASP:OD1	2.50	0.45
1:B:23:THR:HA	1:B:26:LYS:HD2	1.98	0.45
1:C:394:MET:CE	1:C:399:ARG:HD2	2.47	0.45
1:K:82:THR:OG1	1:K:83:PHE:N	2.50	0.45
1:E:104:HIS:HB3	1:E:148:VAL:HG22	1.98	0.45
1:E:162:LYS:HG2	1:E:456:TYR:CZ	2.52	0.45
1:E:474:ASN:O	1:E:474:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:MET:HG2	1:G:240:PRO:HD2	1.98	0.45
1:I:128:HIS:HB3	1:L:330:ASP:O	2.16	0.45
1:A:154:LYS:O	1:A:158:GLU:HG3	2.16	0.45
1:F:133:HIS:O	1:F:136:ILE:HG22	2.17	0.45
1:K:4:LEU:HD21	1:K:319:THR:HG21	1.98	0.45
1:K:241:GLU:HG2	1:K:242:ASP:H	1.81	0.45
1:B:60:ILE:HG22	1:B:92:GLY:HA3	1.99	0.45
1:B:233:TYR:O	1:B:238:ILE:HG12	2.17	0.45
1:F:157:ARG:HA	1:F:160:ILE:HG22	1.99	0.45
1:G:259:LEU:HB3	1:G:292:LEU:HD21	1.99	0.45
1:A:199:GLN:HG2	1:A:204:TRP:O	2.17	0.45
1:B:215:ALA:HA	1:B:218:VAL:HG22	1.98	0.45
1:F:179:VAL:HG13	1:F:209:TRP:CE3	2.52	0.45
1:I:39:ASN:ND2	1:I:48:ILE:HG22	2.32	0.45
1:I:162:LYS:HG2	1:I:456:TYR:CZ	2.52	0.45
1:A:131:ARG:NH2	1:C:333:TYR:OH	2.45	0.44
1:C:57:SER:O	1:C:61:THR:HG23	2.17	0.44
1:C:82:THR:HA	1:C:125:GLN:HB2	1.99	0.44
1:C:197:GLU:HG2	1:F:139:ARG:NH1	2.32	0.44
1:H:157:ARG:HA	1:H:160:ILE:HG22	1.98	0.44
1:I:153:GLU:HB3	1:I:156:VAL:HG12	2.00	0.44
1:J:314:ILE:HD11	1:J:452:ILE:HD11	1.99	0.44
1:B:414:MET:HG3	1:B:417:LEU:HB3	1.99	0.44
1:D:57:SER:O	1:D:61:THR:HG23	2.16	0.44
1:D:343:LEU:HD11	1:D:421:ARG:HB2	1.99	0.44
1:E:13:VAL:HB	1:E:53:VAL:HG22	1.99	0.44
1:F:283:GLN:NE2	1:F:374:PRO:HA	2.32	0.44
1:G:241:GLU:HG2	1:G:242:ASP:H	1.82	0.44
1:K:39:ASN:ND2	1:K:48:ILE:HG22	2.31	0.44
1:L:145:LYS:HD3	1:L:163:TRP:HB2	2.00	0.44
1:H:245:SER:O	1:H:249:ILE:HG12	2.16	0.44
1:I:326:SER:HB2	1:I:351:CYS:HB3	2.00	0.44
1:K:145:LYS:HD3	1:K:163:TRP:HB2	1.99	0.44
1:B:435:THR:HG23	1:B:477:LEU:HD21	2.00	0.44
1:C:233:TYR:OH	1:C:256:GLU:OE1	2.33	0.44
1:C:343:LEU:HD11	1:C:421:ARG:HG3	1.98	0.44
1:D:39:ASN:OD1	1:D:48:ILE:HG22	2.17	0.44
1:K:401:VAL:HA	1:K:469:VAL:HG23	1.99	0.44
1:D:60:ILE:HG21	1:D:89:TRP:HA	2.00	0.44
1:H:237:TYR:CB	1:H:361:ILE:HG13	2.47	0.44
1:A:474:ASN:O	1:A:474:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:LYS:O	1:D:158:GLU:HG3	2.18	0.44
1:F:397:ARG:NH2	1:F:488:GLU:HA	2.32	0.44
1:J:487:ASN:O	1:J:491:TRP:HD1	2.01	0.44
1:L:199:GLN:HG2	1:L:204:TRP:O	2.18	0.44
1:C:13:VAL:HB	1:C:53:VAL:HG22	1.99	0.44
1:C:39:ASN:HD21	1:C:48:ILE:HG22	1.83	0.44
1:E:330:ASP:O	1:G:128:HIS:HB3	2.17	0.44
1:H:455:GLU:O	1:H:458:ILE:HG22	2.17	0.44
1:K:39:ASN:HD21	1:K:48:ILE:HG22	1.83	0.44
1:L:185:MET:HG3	1:L:276:GLU:OE2	2.18	0.44
1:A:247:LYS:HD2	1:A:247:LYS:HA	1.62	0.44
1:A:363:VAL:HB	1:A:373:ASP:OD1	2.18	0.44
1:B:9:PHE:HB2	1:B:48:ILE:HD12	1.99	0.44
1:F:117:ASP:N	1:F:117:ASP:OD1	2.51	0.44
1:G:185:MET:HG3	1:G:276:GLU:OE2	2.17	0.44
1:K:61:THR:HG21	1:K:91:ARG:HE	1.81	0.44
1:H:241:GLU:HG2	1:H:242:ASP:H	1.82	0.44
1:H:311:VAL:HA	1:H:314:ILE:HG22	2.00	0.44
1:J:104:HIS:HB3	1:J:148:VAL:HG22	2.00	0.44
1:J:348:LEU:HD21	1:J:374:PRO:HG2	1.99	0.44
1:K:199:GLN:HG2	1:K:204:TRP:O	2.18	0.44
1:I:68:ASN:OD1	1:I:96:ASN:HA	2.17	0.43
1:I:490:TYR:CZ	1:L:485:ARG:HB2	2.53	0.43
1:J:215:ALA:HA	1:J:218:VAL:HG22	2.00	0.43
1:L:117:ASP:OD1	1:L:117:ASP:N	2.50	0.43
1:C:310:LEU:HD22	1:C:391:ILE:HG13	2.00	0.43
1:C:364:HIS:O	1:C:376:ARG:NH2	2.51	0.43
1:D:97:LYS:HB2	1:D:97:LYS:HE2	1.77	0.43
1:E:145:LYS:HD3	1:E:163:TRP:HB2	1.99	0.43
1:G:154:LYS:O	1:G:158:GLU:HG3	2.18	0.43
1:J:97:LYS:HB2	1:J:97:LYS:HE2	1.80	0.43
1:C:314:ILE:HD11	1:C:452:ILE:HD11	1.99	0.43
1:E:4:LEU:HD12	1:E:5:LYS:N	2.33	0.43
1:E:334:HIS:O	1:E:340:GLU:HA	2.18	0.43
1:G:82:THR:OG1	1:G:83:PHE:N	2.51	0.43
1:J:60:ILE:HG22	1:J:92:GLY:HA3	2.01	0.43
1:A:444:HIS:HB2	1:B:128:HIS:HB2	2.00	0.43
1:A:489:LEU:HD22	1:B:489:LEU:HD12	2.00	0.43
1:B:165:ARG:NH2	1:B:320:SER:HB2	2.33	0.43
1:B:234:ARG:HA	1:B:238:ILE:CG1	2.49	0.43
1:B:245:SER:O	1:B:249:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:HD11	1:B:452:ILE:HD11	2.01	0.43
1:E:314:ILE:HG23	1:E:325:THR:HG21	2.00	0.43
1:G:180:ARG:HB2	1:G:208:THR:HA	1.99	0.43
1:H:102:HIS:NE2	1:H:130:ASP:HB2	2.34	0.43
1:L:211:VAL:HG11	1:L:278:LEU:HA	2.00	0.43
1:L:241:GLU:HG2	1:L:242:ASP:H	1.83	0.43
1:A:414:MET:HG2	1:B:116:ILE:HD11	2.01	0.43
1:C:278:LEU:O	1:C:371:LYS:HE2	2.18	0.43
1:E:102:HIS:NE2	1:E:130:ASP:HB2	2.33	0.43
1:E:328:MET:HB2	1:E:448:PHE:HB2	2.00	0.43
1:E:485:ARG:HB2	1:G:490:TYR:CZ	2.53	0.43
1:F:82:THR:OG1	1:F:83:PHE:N	2.51	0.43
1:F:233:TYR:OH	1:F:256:GLU:OE1	2.34	0.43
1:J:117:ASP:OD1	1:J:117:ASP:N	2.50	0.43
1:K:13:VAL:HB	1:K:53:VAL:HG22	2.00	0.43
1:K:60:ILE:HG21	1:K:89:TRP:HA	2.00	0.43
1:D:165:ARG:NH2	1:D:320:SER:HB2	2.34	0.43
1:D:202:LEU:HD22	1:D:464:LEU:HD13	2.01	0.43
1:E:435:THR:HG23	1:E:477:LEU:HD21	2.00	0.43
1:F:165:ARG:NH2	1:F:320:SER:HB2	2.34	0.43
1:K:435:THR:HG23	1:K:477:LEU:HD21	2.01	0.43
1:G:223:GLU:O	1:G:226:VAL:HG22	2.18	0.43
1:G:234:ARG:HA	1:G:238:ILE:HG13	2.00	0.43
1:I:157:ARG:HA	1:I:160:ILE:HG22	2.01	0.43
1:B:277:ASP:OD1	1:F:210:GLY:HA3	2.18	0.43
1:F:416:LYS:HG3	1:H:117:ASP:HB3	2.00	0.43
1:J:180:ARG:HD2	1:J:206:ILE:HD11	2.01	0.43
1:J:417:LEU:HD23	1:J:421:ARG:HE	1.84	0.43
1:L:114:ASP:OD1	1:L:114:ASP:N	2.48	0.43
1:B:493:LEU:HD13	1:H:493:LEU:HD13	2.01	0.43
1:F:145:LYS:HD3	1:F:163:TRP:HB2	2.01	0.43
1:I:239:MET:HG2	1:I:240:PRO:HD2	2.01	0.43
1:L:107:TYR:HA	1:L:151:TRP:HE1	1.83	0.43
1:L:179:VAL:HG13	1:L:209:TRP:CE3	2.54	0.43
1:E:241:GLU:HG2	1:E:242:ASP:H	1.83	0.43
1:E:306:LYS:HZ1	1:E:393:ASP:N	2.17	0.43
1:F:178:ILE:HD11	1:F:308:ALA:HB3	2.01	0.43
1:F:237:TYR:HB2	1:F:238:ILE:H	1.58	0.43
1:G:68:ASN:OD1	1:G:96:ASN:HA	2.18	0.43
1:H:283:GLN:NE2	1:H:374:PRO:HA	2.33	0.43
1:L:311:VAL:HA	1:L:314:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:O	1:A:495:LYS:HG3	2.19	0.42
1:F:136:ILE:HD12	1:F:136:ILE:HA	1.95	0.42
1:I:444:HIS:HB2	1:J:128:HIS:HB2	1.99	0.42
1:J:185:MET:HG3	1:J:276:GLU:OE1	2.19	0.42
1:K:179:VAL:HG13	1:K:209:TRP:CE3	2.54	0.42
1:L:369:GLY:O	1:L:371:LYS:NZ	2.36	0.42
1:B:174:ARG:O	3:B:601:HOH:O	2.22	0.42
1:B:415:PRO:HD2	1:C:114:ASP:HA	2.00	0.42
1:I:233:TYR:C	1:I:238:ILE:HG12	2.39	0.42
1:B:239:MET:HG2	1:B:240:PRO:HD2	2.02	0.42
1:I:147:VAL:CG1	1:I:156:VAL:HG23	2.49	0.42
1:I:222:PRO:HB2	1:I:225:GLU:HG3	2.00	0.42
1:L:178:ILE:HD11	1:L:308:ALA:HB3	2.00	0.42
1:C:180:ARG:HB2	1:C:208:THR:HA	2.02	0.42
1:D:493:LEU:HG	1:D:494:LEU:H	1.85	0.42
1:E:44:PHE:HE1	1:E:160:ILE:HG23	1.84	0.42
1:E:211:VAL:HG11	1:E:278:LEU:HA	2.00	0.42
1:G:237:TYR:HB2	1:G:238:ILE:H	1.56	0.42
1:J:239:MET:HG2	1:J:240:PRO:HD2	2.02	0.42
1:J:493:LEU:HG	1:J:494:LEU:H	1.85	0.42
1:A:44:PHE:HE1	1:A:160:ILE:HG23	1.84	0.42
1:A:348:LEU:HD11	1:A:374:PRO:HB2	2.02	0.42
1:F:237:TYR:CB	1:F:361:ILE:HG13	2.49	0.42
1:F:243:GLU:HB3	1:F:244:TYR:H	1.73	0.42
1:G:251:GLU:OE1	1:G:283:GLN:HG2	2.19	0.42
1:J:278:LEU:HD11	1:J:284:LEU:HD13	2.01	0.42
1:D:18:LEU:O	1:D:18:LEU:HD23	2.20	0.42
1:I:311:VAL:HA	1:I:314:ILE:HG22	2.01	0.42
1:I:365:PRO:HA	1:I:373:ASP:OD1	2.20	0.42
1:I:435:THR:HG23	1:I:477:LEU:HD21	2.02	0.42
1:B:117:ASP:OD1	1:B:117:ASP:N	2.51	0.42
1:C:117:ASP:OD1	1:C:117:ASP:N	2.51	0.42
1:D:237:TYR:O	1:D:238:ILE:HG22	2.20	0.42
1:E:157:ARG:HA	1:E:160:ILE:HG22	2.02	0.42
1:E:326:SER:HB2	1:E:351:CYS:HB3	2.02	0.42
1:H:314:ILE:HD11	1:H:452:ILE:HD11	2.01	0.42
1:I:117:ASP:OD1	1:I:117:ASP:N	2.50	0.42
1:I:128:HIS:HB2	1:L:444:HIS:HB2	2.01	0.42
1:J:157:ARG:HA	1:J:160:ILE:HG22	2.02	0.42
1:J:401:VAL:HA	1:J:469:VAL:HG23	2.01	0.42
1:K:60:ILE:HG22	1:K:92:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLN:HG2	1:B:107:TYR:CD1	2.54	0.42
1:B:290:GLN:HE21	1:B:350:VAL:H	1.68	0.42
1:C:104:HIS:HB3	1:C:148:VAL:HG22	2.01	0.42
1:F:154:LYS:O	1:F:158:GLU:HG3	2.19	0.42
1:H:237:TYR:HB2	1:H:361:ILE:HG13	2.01	0.42
1:J:485:ARG:HB2	1:L:490:TYR:CZ	2.55	0.42
1:K:4:LEU:O	1:K:5:LYS:HB2	2.20	0.42
1:F:104:HIS:HB3	1:F:148:VAL:HG22	2.02	0.42
1:G:82:THR:HA	1:G:125:GLN:HB2	2.01	0.42
1:I:214:LEU:O	1:I:218:VAL:HG13	2.20	0.42
1:K:165:ARG:NH2	1:K:320:SER:HB2	2.34	0.42
1:A:116:ILE:HD11	1:C:417:LEU:HB2	2.02	0.42
1:B:104:HIS:HB3	1:B:148:VAL:HG22	2.02	0.42
1:C:237:TYR:CB	1:C:361:ILE:HG13	2.49	0.42
1:C:281:LEU:HD23	1:C:281:LEU:HA	1.90	0.42
1:E:237:TYR:CD1	1:E:359:PRO:HB2	2.54	0.42
1:F:214:LEU:HD21	1:F:259:LEU:HD21	2.02	0.42
1:I:306:LYS:HZ1	1:I:393:ASP:N	2.18	0.42
1:K:9:PHE:HB2	1:K:48:ILE:HD12	2.02	0.42
1:C:199:GLN:HG2	1:C:204:TRP:O	2.18	0.41
1:E:147:VAL:CG1	1:E:156:VAL:HG23	2.50	0.41
1:G:403:ASN:HD21	1:G:433:ALA:HB1	1.85	0.41
1:C:241:GLU:HG2	1:C:242:ASP:H	1.85	0.41
1:D:323:GLY:HA2	1:D:451:ALA:HB2	2.02	0.41
1:G:339:ASN:OD1	1:G:425:LYS:HE2	2.20	0.41
1:H:61:THR:HG21	1:H:91:ARG:HE	1.84	0.41
1:H:82:THR:HA	1:H:125:GLN:HB2	2.02	0.41
1:J:177:GLN:HG2	1:J:205:SER:HB3	2.01	0.41
1:K:289:VAL:HG11	1:K:349:GLU:HG2	2.02	0.41
1:L:259:LEU:HB3	1:L:292:LEU:HD21	2.01	0.41
1:A:13:VAL:HB	1:A:53:VAL:HG22	2.02	0.41
1:A:32:SER:HA	1:A:35:VAL:HG22	2.02	0.41
1:B:223:GLU:O	1:B:226:VAL:HG22	2.20	0.41
1:C:359:PRO:HB2	1:C:377:LEU:HD22	2.02	0.41
1:F:202:LEU:HD22	1:F:464:LEU:HD13	2.02	0.41
1:H:179:VAL:HG13	1:H:209:TRP:CE3	2.54	0.41
1:I:12:LEU:HD12	1:I:12:LEU:HA	1.87	0.41
1:K:474:ASN:O	1:K:474:ASN:ND2	2.53	0.41
1:B:371:LYS:HB3	1:B:372:ALA:H	1.76	0.41
1:H:185:MET:HG3	1:H:276:GLU:OE1	2.20	0.41
1:I:82:THR:OG1	1:I:83:PHE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:TYR:OH	1:K:125:GLN:OE1	2.37	0.41
1:L:147:VAL:CG1	1:L:156:VAL:HG23	2.51	0.41
1:F:330:ASP:OD1	1:F:330:ASP:N	2.54	0.41
1:I:493:LEU:HG	1:I:494:LEU:H	1.85	0.41
1:K:245:SER:O	1:K:249:ILE:HG12	2.20	0.41
1:A:493:LEU:HD23	1:A:493:LEU:H	1.85	0.41
1:C:172:ASP:OD2	1:C:312:ARG:NE	2.49	0.41
1:D:121:MET:HB3	1:H:331:TYR:HE2	1.85	0.41
1:G:493:LEU:HG	1:G:494:LEU:H	1.86	0.41
1:J:39:ASN:OD1	1:J:48:ILE:HG22	2.21	0.41
1:L:178:ILE:HG22	1:L:206:ILE:HA	2.03	0.41
1:A:289:VAL:HG11	1:A:349:GLU:HG2	2.03	0.41
1:A:397:ARG:NH1	1:A:467:GLU:OE1	2.44	0.41
1:A:427:LEU:HD13	1:A:473:GLU:HG3	2.03	0.41
1:B:4:LEU:HD23	1:B:4:LEU:N	2.30	0.41
1:B:67:ALA:O	1:B:98:LYS:NZ	2.45	0.41
1:C:33:LYS:HD2	1:C:107:TYR:HE1	1.85	0.41
1:J:154:LYS:O	1:J:158:GLU:HG3	2.21	0.41
1:J:311:VAL:HA	1:J:314:ILE:HG22	2.03	0.41
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.95	0.41
1:B:351:CYS:HA	1:B:352:PRO:HD3	1.93	0.41
1:C:239:MET:HG2	1:C:240:PRO:HD2	2.02	0.41
1:D:157:ARG:HA	1:D:160:ILE:HG22	2.02	0.41
1:F:4:LEU:HD21	1:F:319:THR:HG21	2.02	0.41
1:G:107:TYR:HA	1:G:151:TRP:HE1	1.86	0.41
1:G:157:ARG:HA	1:G:160:ILE:HG22	2.03	0.41
1:G:311:VAL:HA	1:G:314:ILE:HG22	2.03	0.41
1:G:340:GLU:H	1:G:340:GLU:HG2	1.76	0.41
1:H:328:MET:HB2	1:H:448:PHE:HB2	2.02	0.41
1:J:104:HIS:ND1	1:J:130:ASP:OD2	2.51	0.41
1:J:237:TYR:HB2	1:J:238:ILE:H	1.58	0.41
1:B:306:LYS:HZ1	1:B:393:ASP:HB2	1.86	0.41
1:B:311:VAL:HA	1:B:314:ILE:HG22	2.02	0.41
1:C:154:LYS:O	1:C:158:GLU:HG3	2.21	0.41
1:C:306:LYS:HZ1	1:C:393:ASP:N	2.19	0.41
1:D:315:LYS:HZ3	1:D:325:THR:HB	1.85	0.41
1:E:154:LYS:O	1:E:158:GLU:HG3	2.21	0.41
1:G:116:ILE:HG22	1:G:120:TYR:CD2	2.56	0.41
1:G:136:ILE:HD12	1:G:136:ILE:HA	1.96	0.41
1:H:77:ILE:HD13	1:H:160:ILE:HD11	2.03	0.41
1:H:202:LEU:HD22	1:H:464:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:GLN:HG2	1:I:204:TRP:O	2.20	0.41
1:J:86:SER:HB3	1:J:136:ILE:HB	2.03	0.41
1:J:102:HIS:NE2	1:J:130:ASP:HB2	2.36	0.41
1:L:455:GLU:O	1:L:458:ILE:HG22	2.21	0.41
1:A:68:ASN:OD1	1:A:96:ASN:HA	2.21	0.41
1:A:321:LEU:C	1:A:323:GLY:H	2.24	0.41
1:A:435:THR:HG23	1:A:477:LEU:HD21	2.02	0.41
1:C:116:ILE:HG22	1:C:120:TYR:CD2	2.56	0.41
1:D:174:ARG:O	3:D:601:HOH:O	2.21	0.41
1:E:12:LEU:HD12	1:E:12:LEU:HA	1.88	0.41
1:F:252:GLN:NE2	1:F:288:ALA:H	2.19	0.41
1:F:429:ASP:OD1	1:F:430:PHE:N	2.54	0.41
1:G:293:MET:SD	1:G:299:PHE:HB3	2.61	0.41
1:I:194:ASP:HB3	1:I:197:GLU:HB2	2.02	0.41
1:L:400:LEU:HD21	1:L:457:LEU:HD22	2.02	0.41
1:L:493:LEU:HG	1:L:494:LEU:H	1.86	0.41
1:A:104:HIS:HB3	1:A:148:VAL:HG22	2.02	0.40
1:A:117:ASP:N	1:A:117:ASP:OD1	2.54	0.40
1:F:290:GLN:HE21	1:F:350:VAL:H	1.69	0.40
1:G:115:THR:O	1:G:115:THR:HG22	2.22	0.40
1:I:68:ASN:HD21	1:I:97:LYS:H	1.68	0.40
1:I:396:ASN:OD1	1:I:396:ASN:N	2.52	0.40
1:I:405:VAL:HG12	1:I:426:PRO:HA	2.04	0.40
1:J:371:LYS:HB3	1:J:372:ALA:H	1.78	0.40
1:K:157:ARG:HA	1:K:160:ILE:HG22	2.03	0.40
1:L:157:ARG:HA	1:L:160:ILE:HG22	2.03	0.40
1:L:351:CYS:HA	1:L:352:PRO:HD3	1.92	0.40
1:C:376:ARG:HD2	1:C:418:PRO:HB2	2.03	0.40
1:E:354:ILE:H	1:E:354:ILE:HG13	1.71	0.40
1:F:489:LEU:HD23	1:H:489:LEU:CD1	2.52	0.40
1:I:237:TYR:CD1	1:I:359:PRO:HB2	2.57	0.40
1:K:151:TRP:O	1:K:157:ARG:NE	2.54	0.40
1:K:197:GLU:HG2	1:L:139:ARG:HH12	1.85	0.40
1:L:283:GLN:NE2	1:L:374:PRO:HA	2.35	0.40
1:C:39:ASN:ND2	1:C:48:ILE:HG22	2.36	0.40
1:F:489:LEU:HD12	1:F:489:LEU:HA	1.77	0.40
1:I:233:TYR:HB3	1:I:238:ILE:HD11	2.04	0.40
1:I:281:LEU:HD23	1:I:281:LEU:HA	1.97	0.40
1:K:239:MET:HG2	1:K:240:PRO:CD	2.51	0.40
1:E:455:GLU:O	1:E:458:ILE:HG22	2.22	0.40
1:F:9:PHE:HB2	1:F:48:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:ARG:NH1	1:I:197:GLU:HG2	2.37	0.40
1:H:214:LEU:O	1:H:218:VAL:HG13	2.20	0.40
1:J:178:ILE:HD11	1:J:308:ALA:HB3	2.03	0.40
1:K:306:LYS:H	1:K:306:LYS:HG2	1.69	0.40
1:L:4:LEU:HD12	1:L:4:LEU:HA	1.86	0.40
1:A:80:MET:HE3	1:A:89:TRP:CZ2	2.57	0.40
1:B:278:LEU:O	1:B:281:LEU:HB2	2.21	0.40
1:D:39:ASN:HD21	1:D:48:ILE:H	1.69	0.40
1:H:23:THR:HA	1:H:26:LYS:HD2	2.04	0.40
1:J:162:LYS:HD2	1:J:455:GLU:HG2	2.03	0.40
1:J:238:ILE:HD13	1:J:238:ILE:HA	1.96	0.40
1:J:435:THR:HG23	1:J:477:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/496 (94%)	431 (93%)	30 (6%)	4 (1%)	17	56
1	B	493/496 (99%)	454 (92%)	33 (7%)	6 (1%)	13	51
1	C	493/496 (99%)	448 (91%)	35 (7%)	10 (2%)	7	41
1	D	493/496 (99%)	453 (92%)	34 (7%)	6 (1%)	13	51
1	E	493/496 (99%)	451 (92%)	37 (8%)	5 (1%)	15	54
1	F	493/496 (99%)	456 (92%)	33 (7%)	4 (1%)	19	58
1	G	493/496 (99%)	451 (92%)	37 (8%)	5 (1%)	15	54
1	H	493/496 (99%)	451 (92%)	37 (8%)	5 (1%)	15	54
1	I	493/496 (99%)	453 (92%)	34 (7%)	6 (1%)	13	51
1	J	493/496 (99%)	449 (91%)	39 (8%)	5 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	493/496 (99%)	455 (92%)	34 (7%)	4 (1%)	19	58
1	L	493/496 (99%)	452 (92%)	35 (7%)	6 (1%)	13	51
All	All	5888/5952 (99%)	5404 (92%)	418 (7%)	66 (1%)	14	53

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLY
1	B	240	PRO
1	B	287	LEU
1	C	240	PRO
1	D	2	ILE
1	D	238	ILE
1	D	240	PRO
1	F	240	PRO
1	G	240	PRO
1	H	240	PRO
1	I	240	PRO
1	J	240	PRO
1	L	240	PRO
1	B	238	ILE
1	C	5	LYS
1	C	238	ILE
1	D	5	LYS
1	D	242	ASP
1	E	238	ILE
1	F	238	ILE
1	G	6	GLN
1	G	238	ILE
1	H	5	LYS
1	H	238	ILE
1	I	238	ILE
1	J	238	ILE
1	K	238	ILE
1	L	238	ILE
1	C	242	ASP
1	E	240	PRO
1	G	4	LEU
1	I	5	LYS
1	K	240	PRO
1	B	5	LYS

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Mol	Chain	Res	Type
1	C	357	GLU
1	C	373	ASP
1	E	5	LYS
1	J	5	LYS
1	A	324	GLY
1	F	324	GLY
1	G	324	GLY
1	K	324	GLY
1	L	3	ASP
1	C	324	GLY
1	D	324	GLY
1	E	324	GLY
1	H	324	GLY
1	I	324	GLY
1	J	324	GLY
1	L	324	GLY
1	B	324	GLY
1	L	2	ILE
1	C	2	ILE
1	J	2	ILE
1	E	296	GLY
1	A	173	GLY
1	A	296	GLY
1	B	173	GLY
1	C	173	GLY
1	C	296	GLY
1	F	296	GLY
1	H	296	GLY
1	I	173	GLY
1	I	296	GLY
1	K	173	GLY
1	L	296	GLY

### 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	397/423 (94%)	385 (97%)	12 (3%)	41	71
1	B	422/423 (100%)	399 (94%)	23 (6%)	21	56
1	C	422/423 (100%)	410 (97%)	12 (3%)	43	72
1	D	422/423 (100%)	409 (97%)	13 (3%)	40	70
1	E	422/423 (100%)	408 (97%)	14 (3%)	38	69
1	F	422/423 (100%)	411 (97%)	11 (3%)	46	73
1	G	422/423 (100%)	408 (97%)	14 (3%)	38	69
1	H	422/423 (100%)	409 (97%)	13 (3%)	40	70
1	I	422/423 (100%)	407 (96%)	15 (4%)	35	67
1	J	422/423 (100%)	407 (96%)	15 (4%)	35	67
1	K	422/423 (100%)	408 (97%)	14 (3%)	38	69
1	L	422/423 (100%)	410 (97%)	12 (3%)	43	72
All	All	5039/5076 (99%)	4871 (97%)	168 (3%)	38	69

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LYS
1	A	139	ARG
1	A	144	ARG
1	A	186	ARG
1	A	275	PHE
1	A	331	TYR
1	A	352	PRO
1	A	373	ASP
1	A	394	MET
1	A	399	ARG
1	A	421	ARG
1	A	493	LEU
1	B	91	ARG
1	B	96	ASN
1	B	97	LYS
1	B	98	LYS
1	B	114	ASP
1	B	130	ASP
1	B	144	ARG
1	B	186	ARG
1	B	219	LYS
1	B	236	LYS

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Mol	Chain	Res	Type
1	B	237	TYR
1	B	244	TYR
1	B	262	PHE
1	B	275	PHE
1	B	331	TYR
1	B	352	PRO
1	B	399	ARG
1	B	412	ARG
1	B	414	MET
1	B	421	ARG
1	B	474	ASN
1	B	479	ASP
1	B	493	LEU
1	C	96	ASN
1	C	114	ASP
1	C	128	HIS
1	C	139	ARG
1	C	144	ARG
1	C	236	LYS
1	C	260	ARG
1	C	262	PHE
1	C	331	TYR
1	C	380	ASP
1	C	412	ARG
1	C	421	ARG
1	D	96	ASN
1	D	144	ARG
1	D	177	GLN
1	D	186	ARG
1	D	217	ARG
1	D	236	LYS
1	D	260	ARG
1	D	262	PHE
1	D	331	TYR
1	D	399	ARG
1	D	421	ARG
1	D	474	ASN
1	D	493	LEU
1	E	1	MET
1	E	98	LYS
1	E	141	ARG
1	E	144	ARG

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Mol	Chain	Res	Type
1	E	186	ARG
1	E	219	LYS
1	E	236	LYS
1	E	237	TYR
1	E	244	TYR
1	E	262	PHE
1	E	331	TYR
1	E	399	ARG
1	E	421	ARG
1	E	493	LEU
1	F	97	LYS
1	F	98	LYS
1	F	144	ARG
1	F	186	ARG
1	F	236	LYS
1	F	237	TYR
1	F	262	PHE
1	F	399	ARG
1	F	421	ARG
1	F	474	ASN
1	F	495	LYS
1	G	91	ARG
1	G	98	LYS
1	G	141	ARG
1	G	144	ARG
1	G	186	ARG
1	G	236	LYS
1	G	237	TYR
1	G	244	TYR
1	G	262	PHE
1	G	331	TYR
1	G	399	ARG
1	G	421	ARG
1	G	474	ASN
1	G	493	LEU
1	H	98	LYS
1	H	141	ARG
1	H	144	ARG
1	H	177	GLN
1	H	219	LYS
1	H	236	LYS
1	H	237	TYR

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Mol	Chain	Res	Type
1	H	244	TYR
1	H	262	PHE
1	H	275	PHE
1	H	331	TYR
1	H	399	ARG
1	H	421	ARG
1	I	91	ARG
1	I	96	ASN
1	I	97	LYS
1	I	98	LYS
1	I	141	ARG
1	I	144	ARG
1	I	186	ARG
1	I	236	LYS
1	I	237	TYR
1	I	262	PHE
1	I	331	TYR
1	I	371	LYS
1	I	399	ARG
1	I	421	ARG
1	I	493	LEU
1	J	1	MET
1	J	72	LYS
1	J	96	ASN
1	J	98	LYS
1	J	144	ARG
1	J	186	ARG
1	J	236	LYS
1	J	237	TYR
1	J	275	PHE
1	J	331	TYR
1	J	399	ARG
1	J	421	ARG
1	J	474	ASN
1	J	479	ASP
1	J	493	LEU
1	K	97	LYS
1	K	98	LYS
1	K	144	ARG
1	K	186	ARG
1	K	219	LYS
1	K	236	LYS

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Mol	Chain	Res	Type
1	K	237	TYR
1	K	244	TYR
1	K	262	PHE
1	K	275	PHE
1	K	331	TYR
1	K	399	ARG
1	K	421	ARG
1	K	493	LEU
1	L	98	LYS
1	L	144	ARG
1	L	186	ARG
1	L	236	LYS
1	L	237	TYR
1	L	244	TYR
1	L	262	PHE
1	L	331	TYR
1	L	399	ARG
1	L	421	ARG
1	L	474	ASN
1	L	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	133	HIS
1	D	252	GLN
1	D	283	GLN
1	E	68	ASN
1	F	68	ASN
1	F	177	GLN
1	F	252	GLN
1	H	68	ASN
1	H	124	ASN
1	I	137	HIS
1	J	252	GLN
1	K	68	ASN
1	K	137	HIS
1	L	68	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	469/496 (94%)	-0.13	15 (3%) 47 32	18, 54, 130, 156	0
1	B	495/496 (99%)	-0.25	5 (1%) 82 70	16, 57, 112, 140	0
1	C	495/496 (99%)	-0.11	18 (3%) 42 29	22, 56, 135, 190	0
1	D	495/496 (99%)	-0.04	17 (3%) 45 31	29, 63, 137, 171	0
1	E	495/496 (99%)	-0.20	11 (2%) 62 46	20, 59, 116, 153	0
1	F	495/496 (99%)	-0.11	12 (2%) 59 43	26, 65, 135, 172	0
1	G	495/496 (99%)	0.04	32 (6%) 18 11	29, 63, 142, 190	0
1	H	495/496 (99%)	-0.09	13 (2%) 56 40	26, 64, 140, 176	0
1	I	495/496 (99%)	-0.08	12 (2%) 59 43	32, 69, 135, 164	0
1	J	495/496 (99%)	0.07	23 (4%) 32 21	31, 74, 155, 183	0
1	K	495/496 (99%)	0.04	18 (3%) 42 29	23, 80, 148, 182	0
1	L	495/496 (99%)	0.12	20 (4%) 38 25	39, 83, 143, 192	0
All	All	5914/5952 (99%)	-0.06	196 (3%) 46 31	16, 66, 138, 192	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	242	ASP	5.7
1	K	240	PRO	5.4
1	G	242	ASP	5.4
1	G	365	PRO	5.2
1	H	367	SER	5.1
1	G	419	THR	5.0
1	G	240	PRO	4.9
1	G	356	LYS	4.8
1	F	321	LEU	4.7
1	L	339	ASN	4.6
1	G	367	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	K	242	ASP	4.5
1	J	357	GLU	4.3
1	L	355	ALA	4.2
1	L	369	GLY	4.2
1	F	242	ASP	4.1
1	L	367	SER	4.0
1	C	420	ALA	4.0
1	L	321	LEU	4.0
1	A	355	ALA	4.0
1	D	240	PRO	3.9
1	C	365	PRO	3.8
1	B	242	ASP	3.8
1	C	240	PRO	3.8
1	J	277	ASP	3.7
1	E	321	LEU	3.7
1	A	282	PRO	3.7
1	J	380	ASP	3.7
1	G	418	PRO	3.7
1	G	1	MET	3.7
1	D	421	ARG	3.6
1	D	346	HIS	3.6
1	L	17	TYR	3.6
1	K	241	GLU	3.5
1	K	384	GLY	3.5
1	A	250	ARG	3.5
1	C	280	ASP	3.5
1	C	372	ALA	3.5
1	C	234	ARG	3.4
1	L	115	THR	3.4
1	H	280	ASP	3.3
1	C	367	SER	3.3
1	D	365	PRO	3.3
1	K	346	HIS	3.3
1	K	17	TYR	3.2
1	L	240	PRO	3.2
1	G	17	TYR	3.2
1	J	321	LEU	3.2
1	J	367	SER	3.2
1	D	371	LYS	3.1
1	H	380	ASP	3.1
1	C	239	MET	3.1
1	L	359	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	370	GLY	3.1
1	D	367	SER	3.1
1	G	372	ALA	3.1
1	J	411	GLU	3.1
1	K	413	LYS	3.0
1	H	221	VAL	3.0
1	H	242	ASP	3.0
1	G	383	GLU	3.0
1	F	380	ASP	3.0
1	E	242	ASP	3.0
1	J	242	ASP	2.9
1	K	415	PRO	2.9
1	L	411	GLU	2.9
1	D	242	ASP	2.9
1	E	356	LYS	2.9
1	H	355	ALA	2.9
1	C	419	THR	2.9
1	E	240	PRO	2.9
1	C	17	TYR	2.9
1	L	370	GLY	2.8
1	J	365	PRO	2.8
1	A	279	HIS	2.7
1	J	279	HIS	2.7
1	L	250	ARG	2.7
1	A	411	GLU	2.7
1	G	371	LYS	2.7
1	D	277	ASP	2.7
1	I	241	GLU	2.7
1	F	280	ASP	2.7
1	G	420	ALA	2.7
1	H	279	HIS	2.7
1	A	419	THR	2.7
1	K	355	ALA	2.7
1	A	359	PRO	2.7
1	A	372	ALA	2.7
1	J	356	LYS	2.7
1	A	280	ASP	2.6
1	K	286	GLY	2.6
1	L	232	GLU	2.6
1	I	319	THR	2.6
1	J	382	GLN	2.6
1	G	239	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	238	ILE	2.6
1	F	114	ASP	2.6
1	E	224	ARG	2.6
1	G	357	GLU	2.5
1	A	283	GLN	2.5
1	J	339	ASN	2.5
1	E	411	GLU	2.5
1	C	22	GLU	2.5
1	L	364	HIS	2.5
1	I	237	TYR	2.5
1	J	351	CYS	2.5
1	H	381	GLY	2.5
1	K	380	ASP	2.5
1	G	119	ASP	2.5
1	J	330	ASP	2.5
1	E	373	ASP	2.4
1	K	244	TYR	2.4
1	L	235	GLU	2.4
1	G	250	ARG	2.4
1	G	381	GLY	2.4
1	G	277	ASP	2.4
1	I	367	SER	2.4
1	A	474	ASN	2.4
1	J	346	HIS	2.4
1	D	364	HIS	2.4
1	K	381	GLY	2.4
1	F	234	ARG	2.4
1	I	245	SER	2.4
1	C	381	GLY	2.4
1	G	241	GLU	2.4
1	K	321	LEU	2.4
1	A	373	ASP	2.4
1	C	114	ASP	2.4
1	D	115	THR	2.4
1	G	244	TYR	2.4
1	H	20	GLY	2.3
1	C	237	TYR	2.3
1	E	241	GLU	2.3
1	K	365	PRO	2.3
1	D	372	ALA	2.3
1	L	372	ALA	2.3
1	F	240	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	411	GLU	2.3
1	G	114	ASP	2.3
1	F	243	GLU	2.2
1	J	241	GLU	2.2
1	G	243	GLU	2.2
1	G	359	PRO	2.2
1	G	369	GLY	2.2
1	C	355	ALA	2.2
1	H	3	ASP	2.2
1	J	412	ARG	2.2
1	K	339	ASN	2.2
1	A	420	ALA	2.2
1	J	372	ALA	2.2
1	A	357	GLU	2.2
1	G	279	HIS	2.2
1	F	227	GLU	2.2
1	F	245	SER	2.2
1	G	370	GLY	2.2
1	H	240	PRO	2.2
1	L	21	LEU	2.2
1	J	420	ALA	2.2
1	G	366	LEU	2.2
1	J	239	MET	2.2
1	C	282	PRO	2.2
1	E	117	ASP	2.2
1	D	280	ASP	2.2
1	I	242	ASP	2.2
1	E	225	GLU	2.2
1	G	355	ALA	2.1
1	A	409	PRO	2.1
1	I	244	TYR	2.1
1	E	229	LEU	2.1
1	I	355	ALA	2.1
1	C	414	MET	2.1
1	H	373	ASP	2.1
1	L	233	TYR	2.1
1	D	216	GLU	2.1
1	G	360	ARG	2.1
1	J	371	LYS	2.1
1	D	213	GLU	2.1
1	C	236	LYS	2.1
1	I	239	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	239	MET	2.1
1	F	241	GLU	2.1
1	L	365	PRO	2.1
1	I	280	ASP	2.1
1	B	411	GLU	2.0
1	B	321	LEU	2.0
1	I	412	ARG	2.0
1	D	359	PRO	2.0
1	D	414	MET	2.0
1	H	241	GLU	2.0
1	B	224	ARG	2.0
1	J	355	ALA	2.0
1	B	21	LEU	2.0
1	F	359	PRO	2.0
1	G	413	LYS	2.0
1	I	21	LEU	2.0
1	J	37	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	G	501	1/1	0.73	0.17	135,135,135,135	0
2	MN	J	501	1/1	0.79	0.54	144,144,144,144	0
2	MN	L	501	1/1	0.79	0.19	108,108,108,108	0
2	MN	K	501	1/1	0.85	0.23	124,124,124,124	0
2	MN	A	501	1/1	0.85	0.31	144,144,144,144	0
2	MN	C	501	1/1	0.87	0.18	116,116,116,116	0

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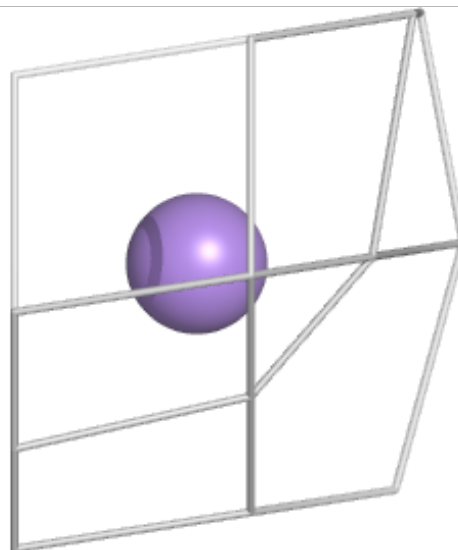
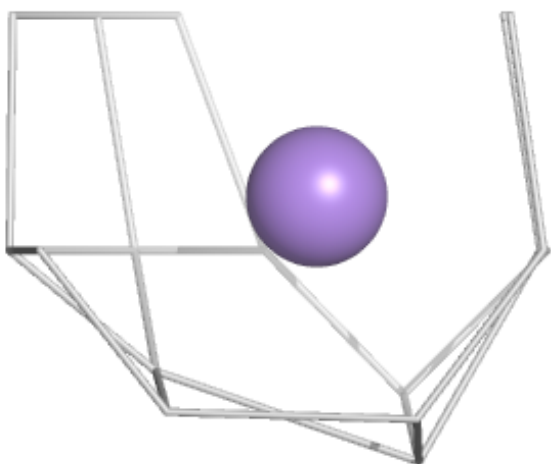
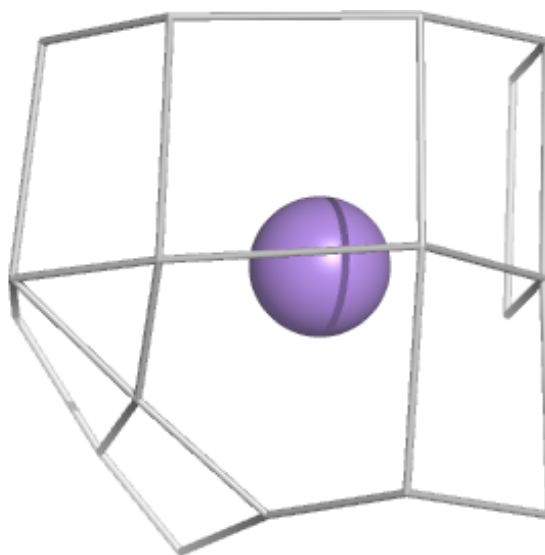
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	F	501	1/1	0.87	0.15	72,72,72,72	0
2	MN	E	502	1/1	0.91	0.07	51,51,51,51	0
2	MN	E	501	1/1	0.91	0.17	78,78,78,78	0
2	MN	I	501	1/1	0.94	0.17	121,121,121,121	0
2	MN	B	501	1/1	0.94	0.18	97,97,97,97	0
2	MN	A	502	1/1	0.96	0.09	41,41,41,41	0
2	MN	C	502	1/1	0.96	0.07	66,66,66,66	0
2	MN	D	501	1/1	0.97	0.16	71,71,71,71	0
2	MN	H	501	1/1	0.97	0.30	118,118,118,118	0
2	MN	L	502	1/1	0.97	0.06	43,43,43,43	0
2	MN	F	502	1/1	0.98	0.06	51,51,51,51	0
2	MN	J	502	1/1	0.99	0.08	47,47,47,47	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.

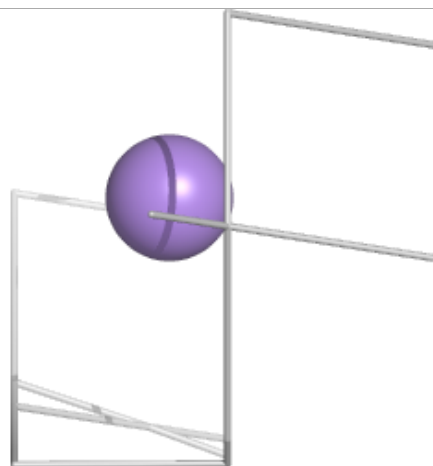
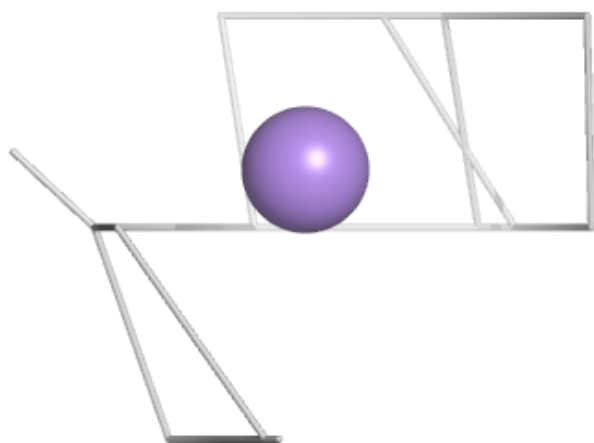
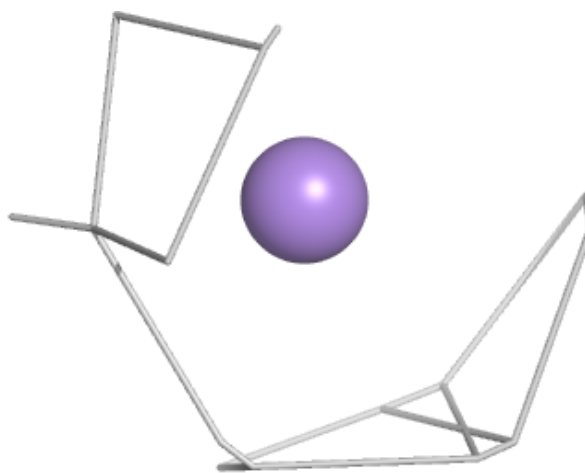
**Electron density around MN G 501:**

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



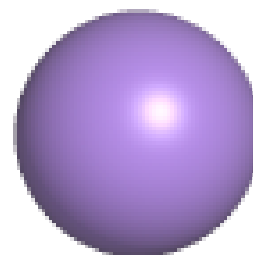
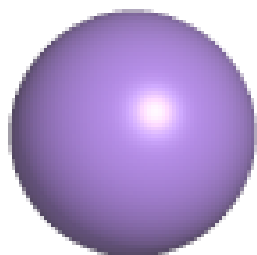
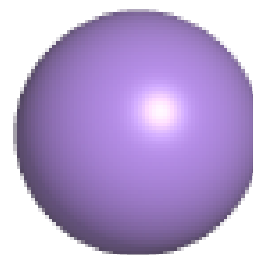
**Electron density around MN J 501:**

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



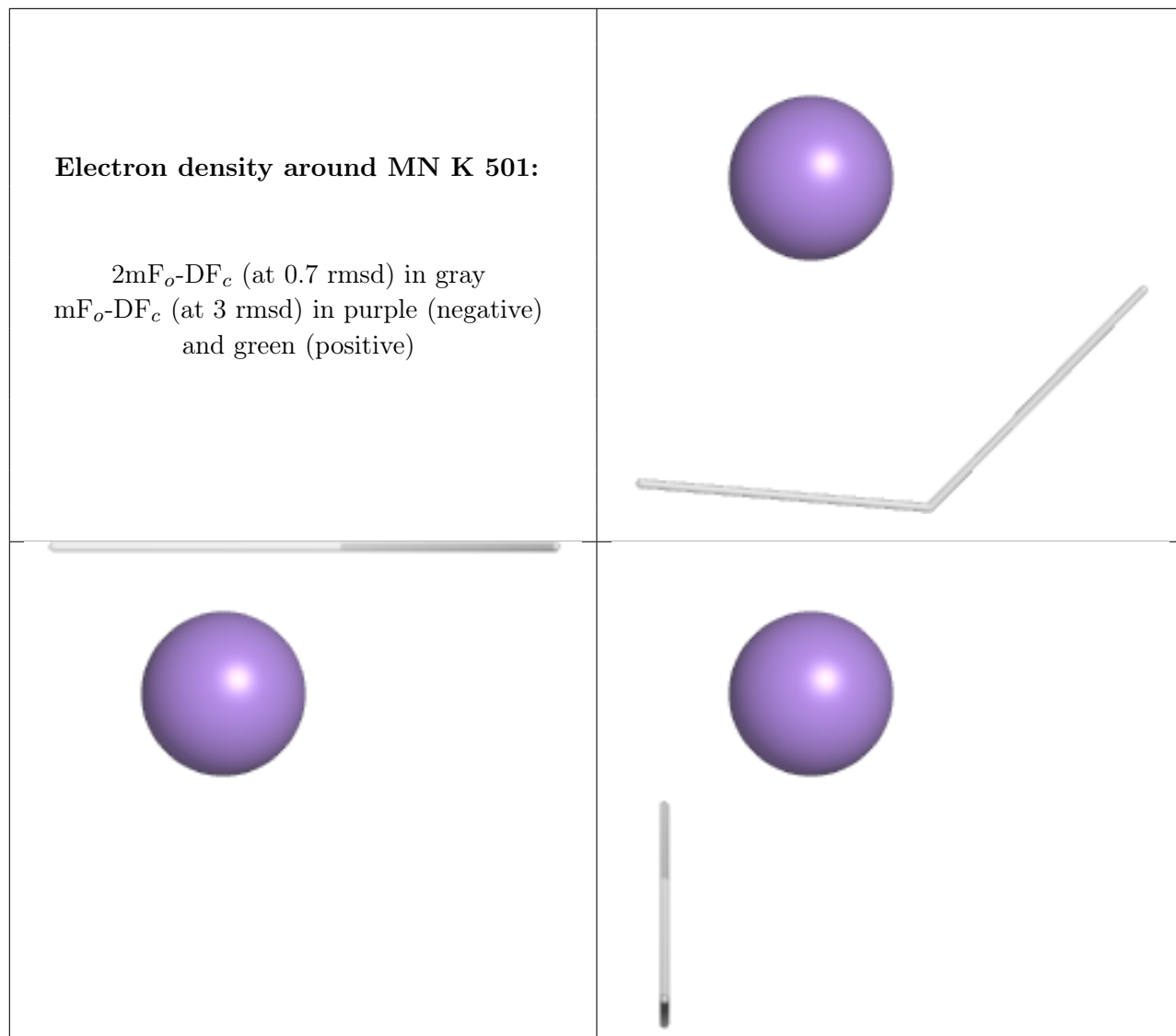
**Electron density around MN L 501:**

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



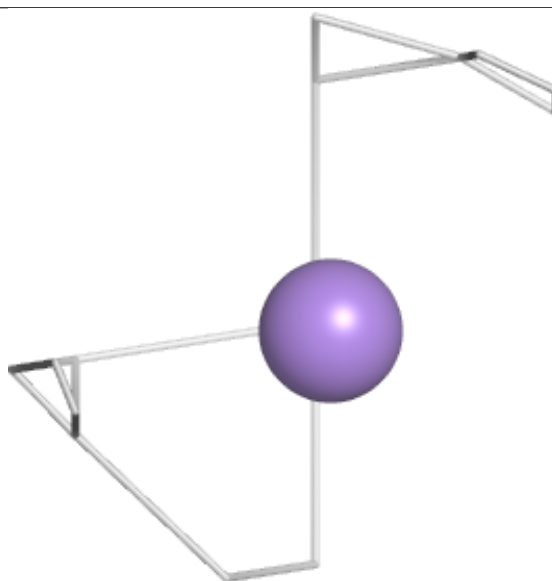
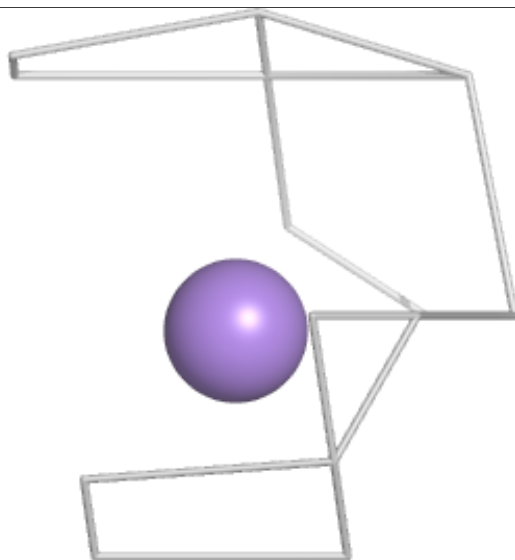
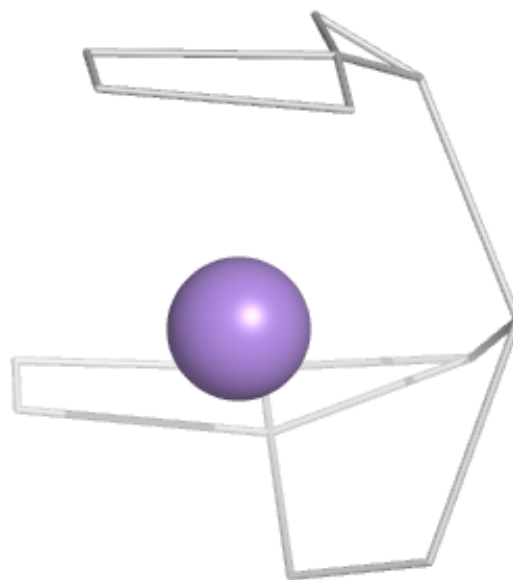
**Electron density around MN K 501:**

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



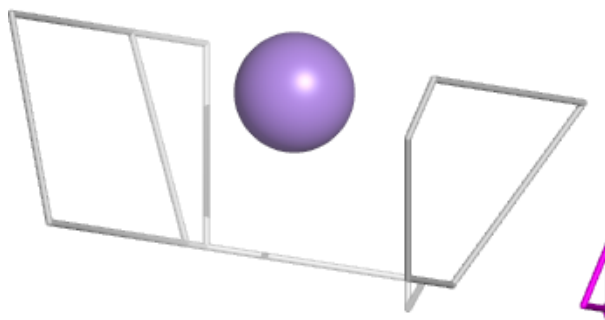
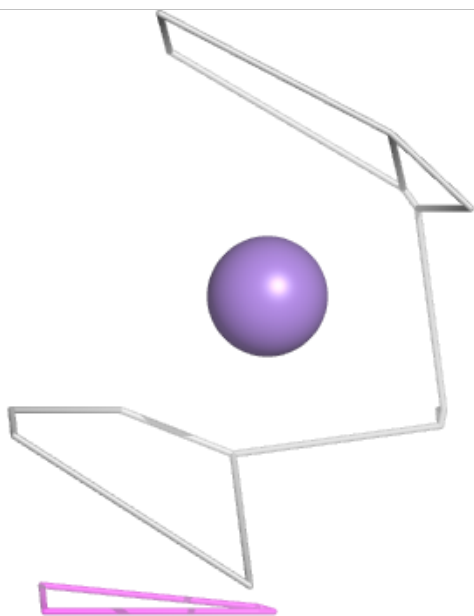
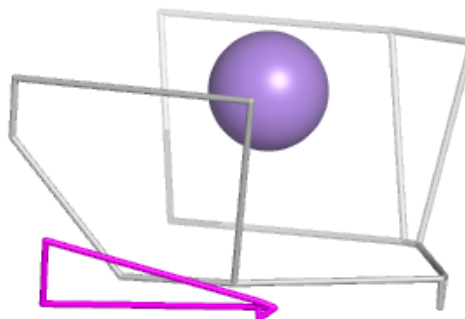
**Electron density around MN A 501:**

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and green (positive)



**Electron density around MN C 501:**

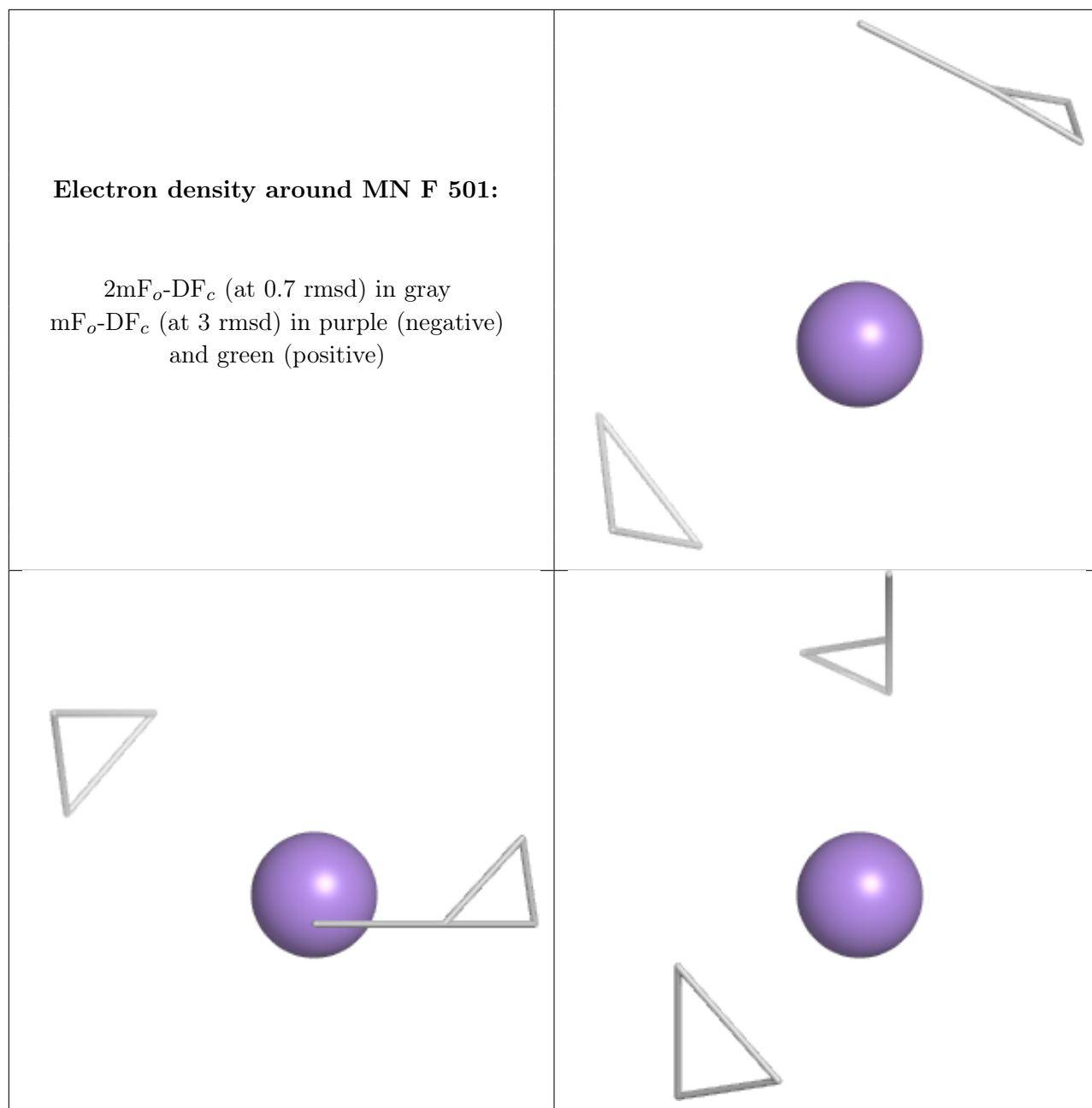
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





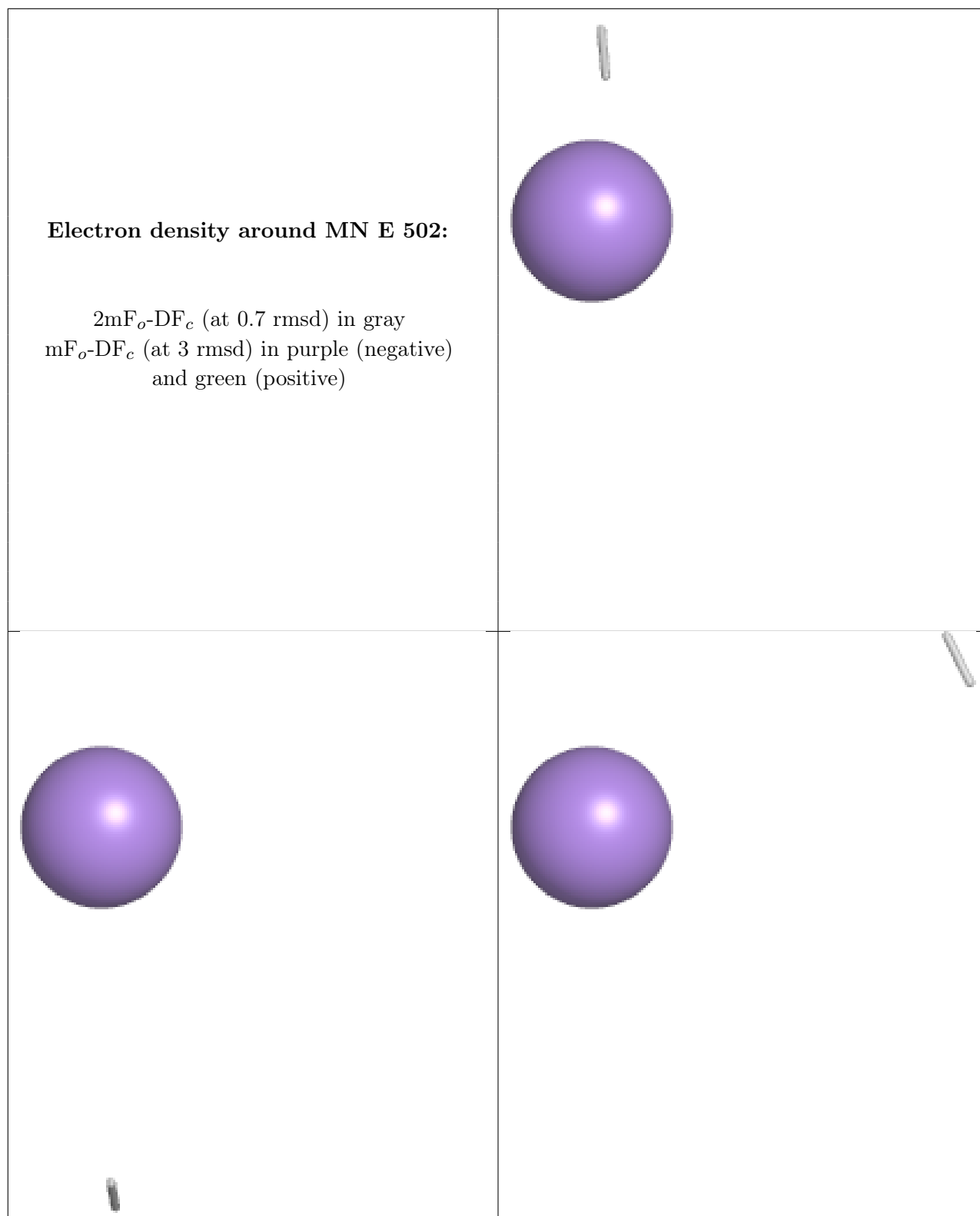
**Electron density around MN F 501:**

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



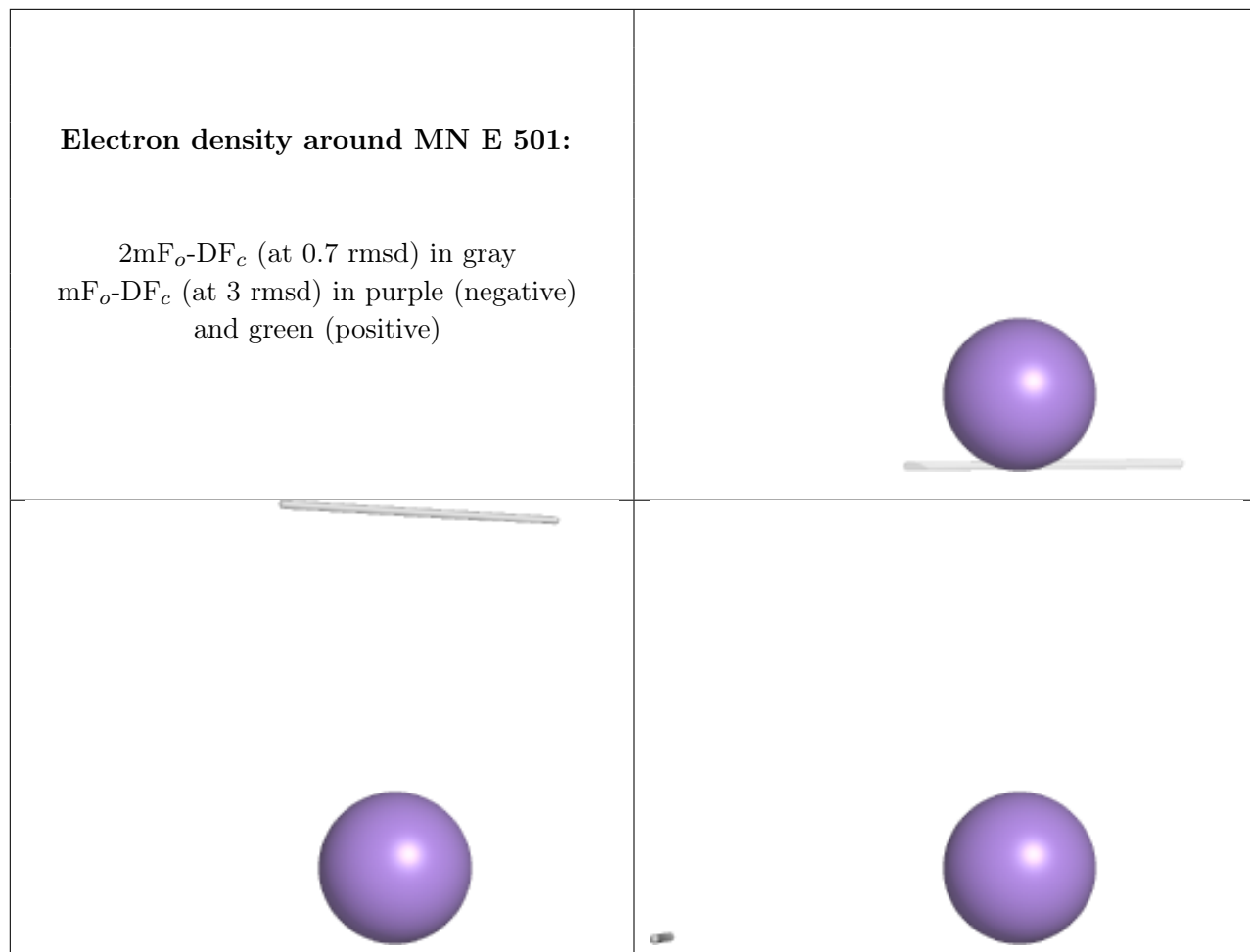
**Electron density around MN E 502:**

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



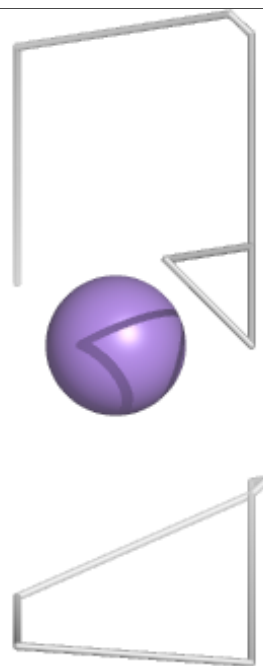
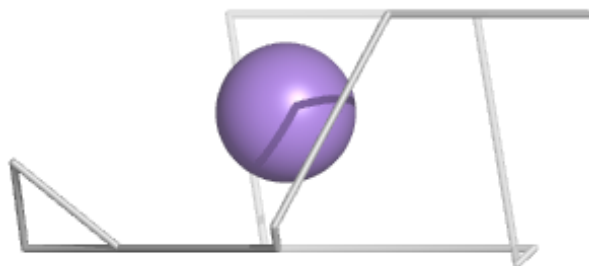
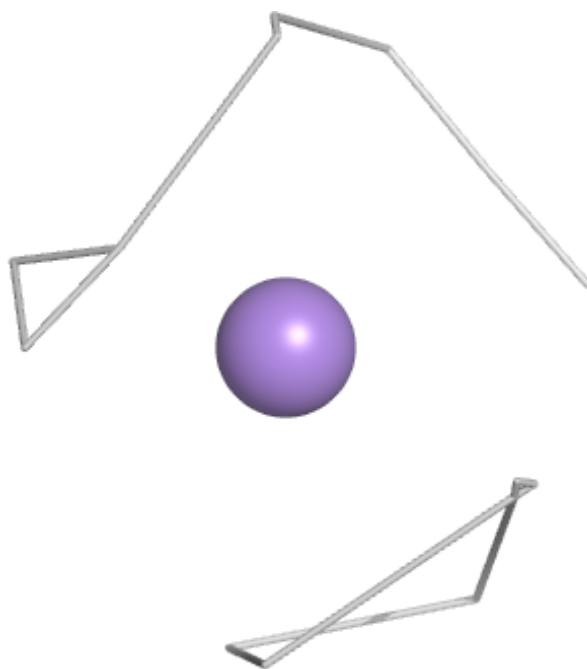
**Electron density around MN E 501:**

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



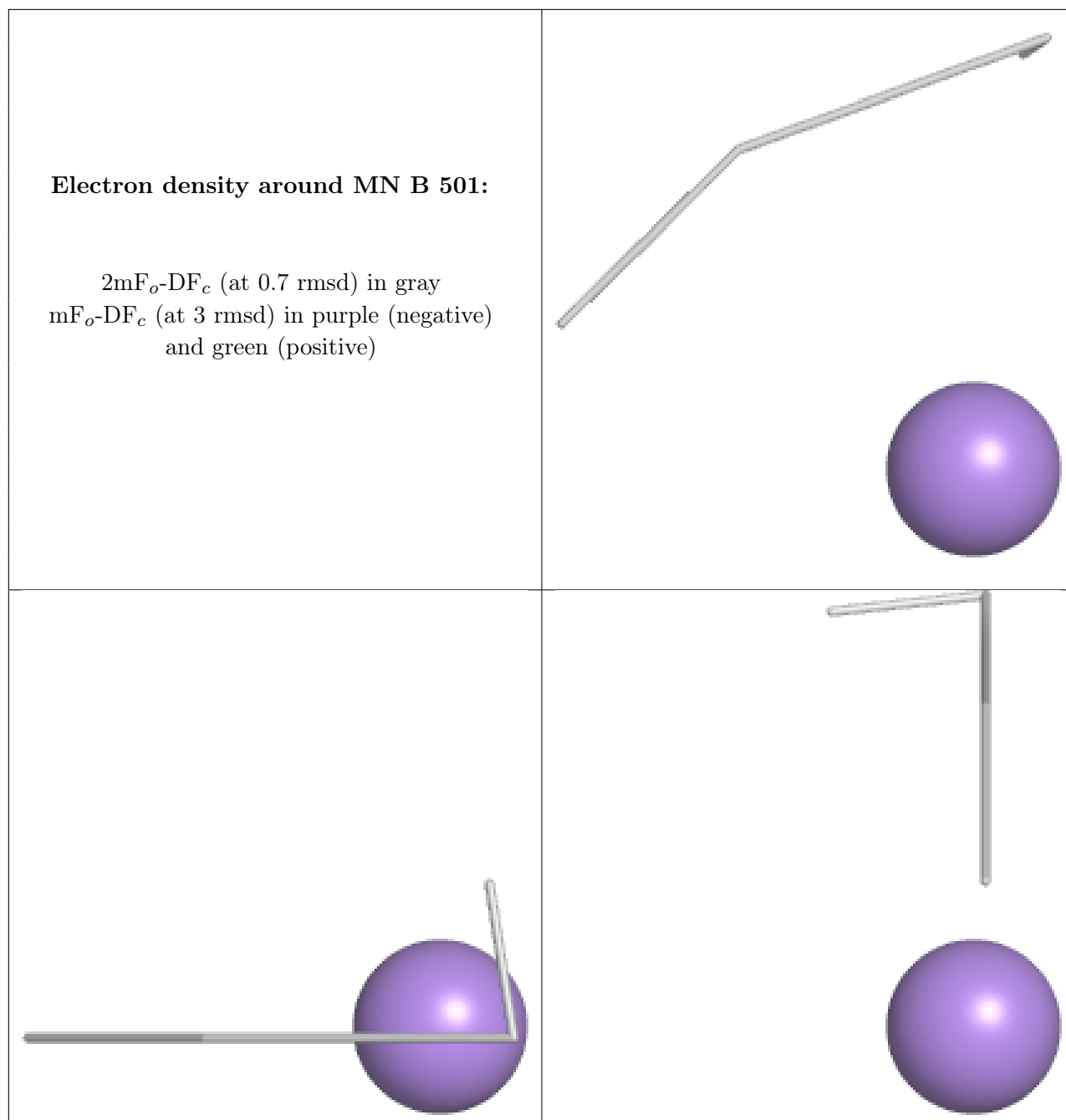
**Electron density around MN I 501:**

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and green (positive)



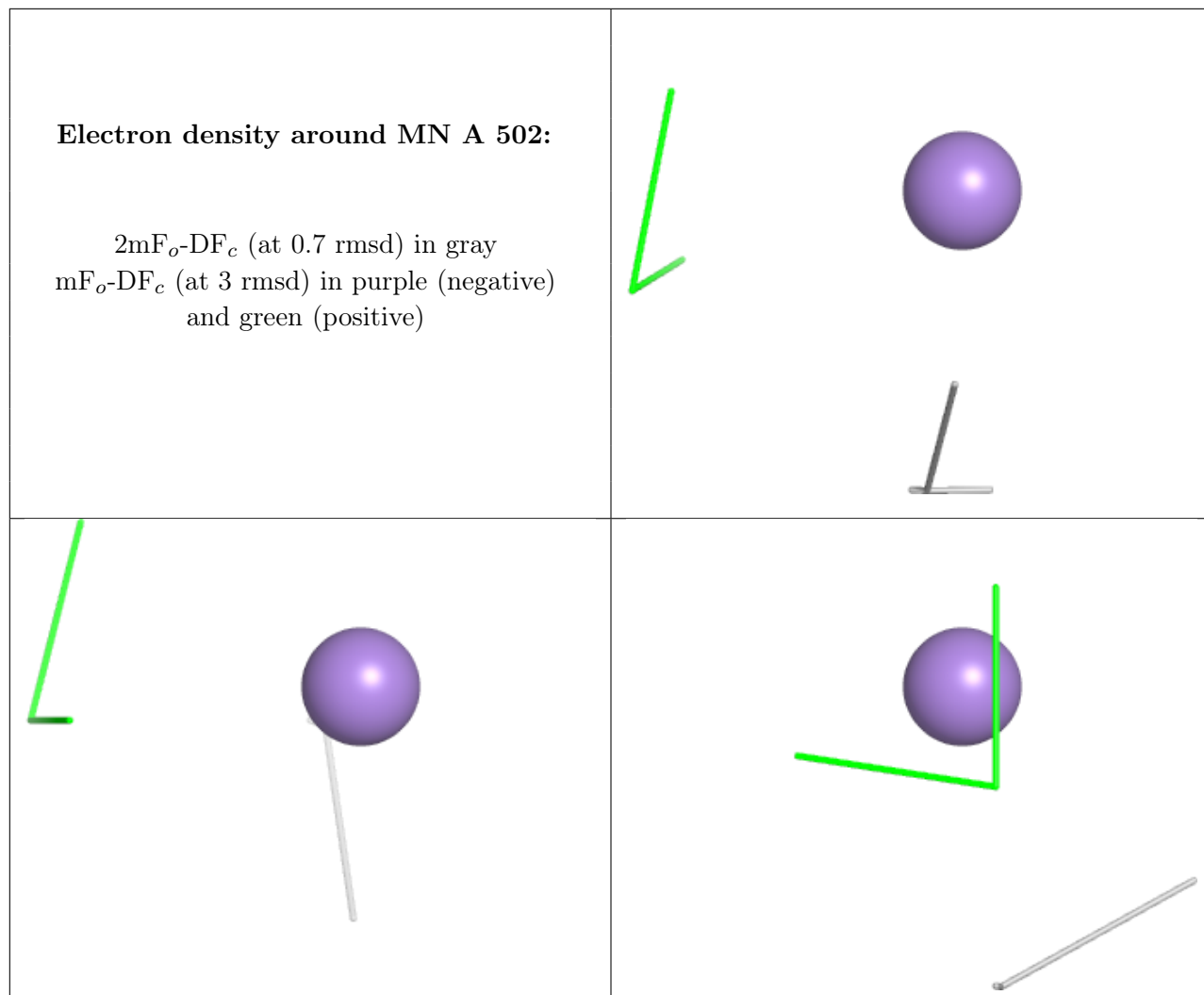
**Electron density around MN B 501:**

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and green (positive)



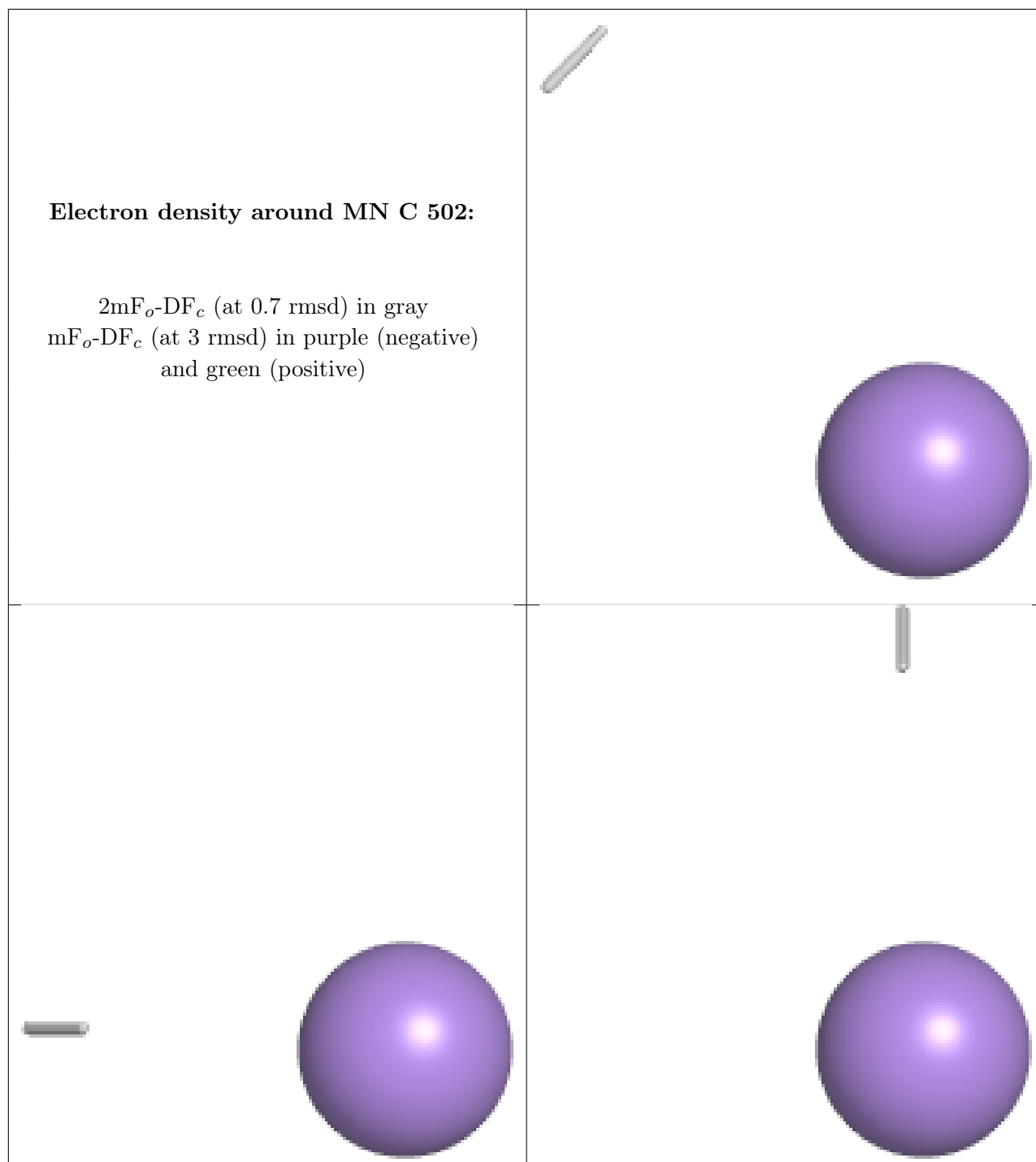
**Electron density around MN A 502:**

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



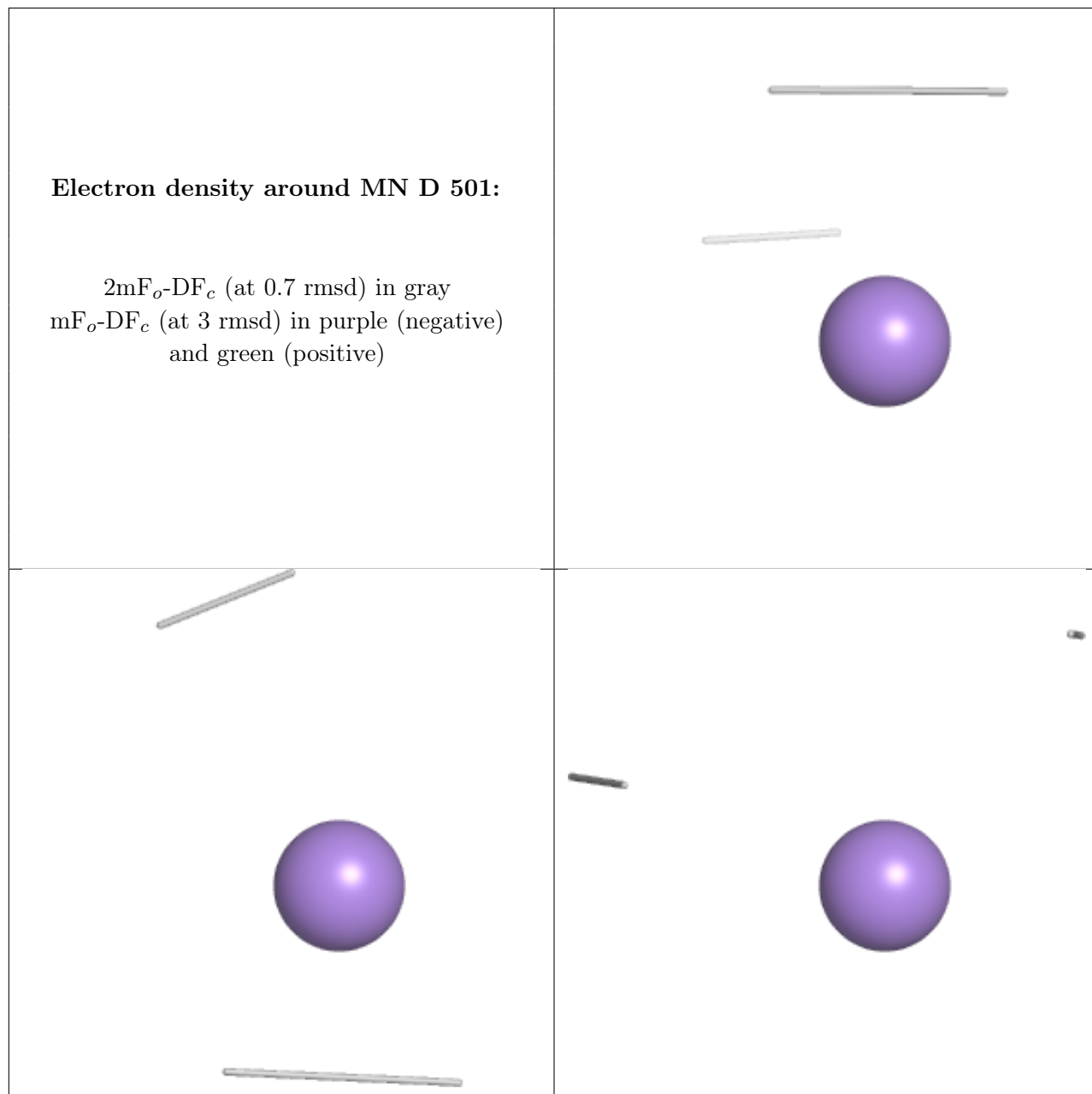
**Electron density around MN C 502:**

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



**Electron density around MN D 501:**

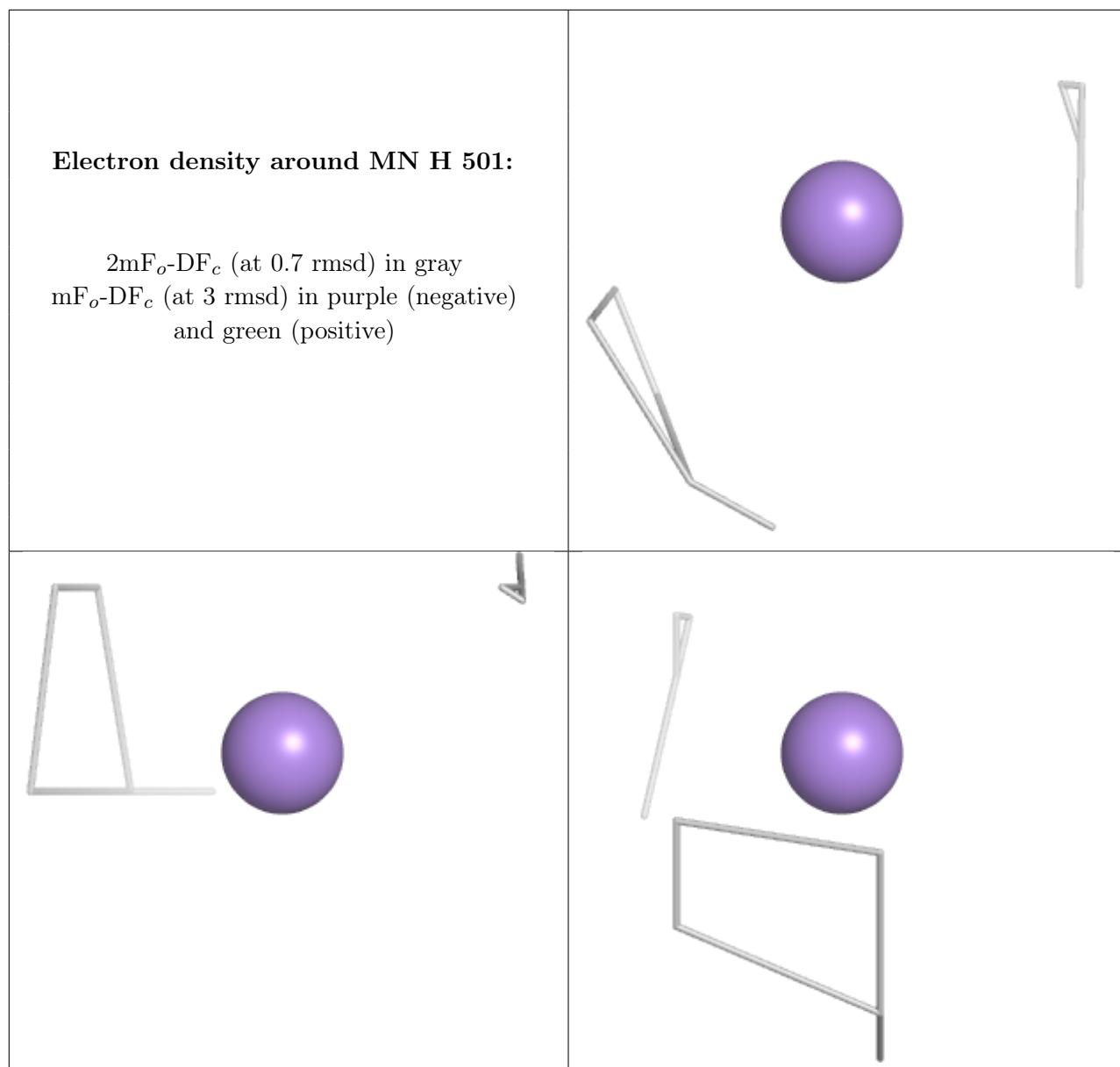
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

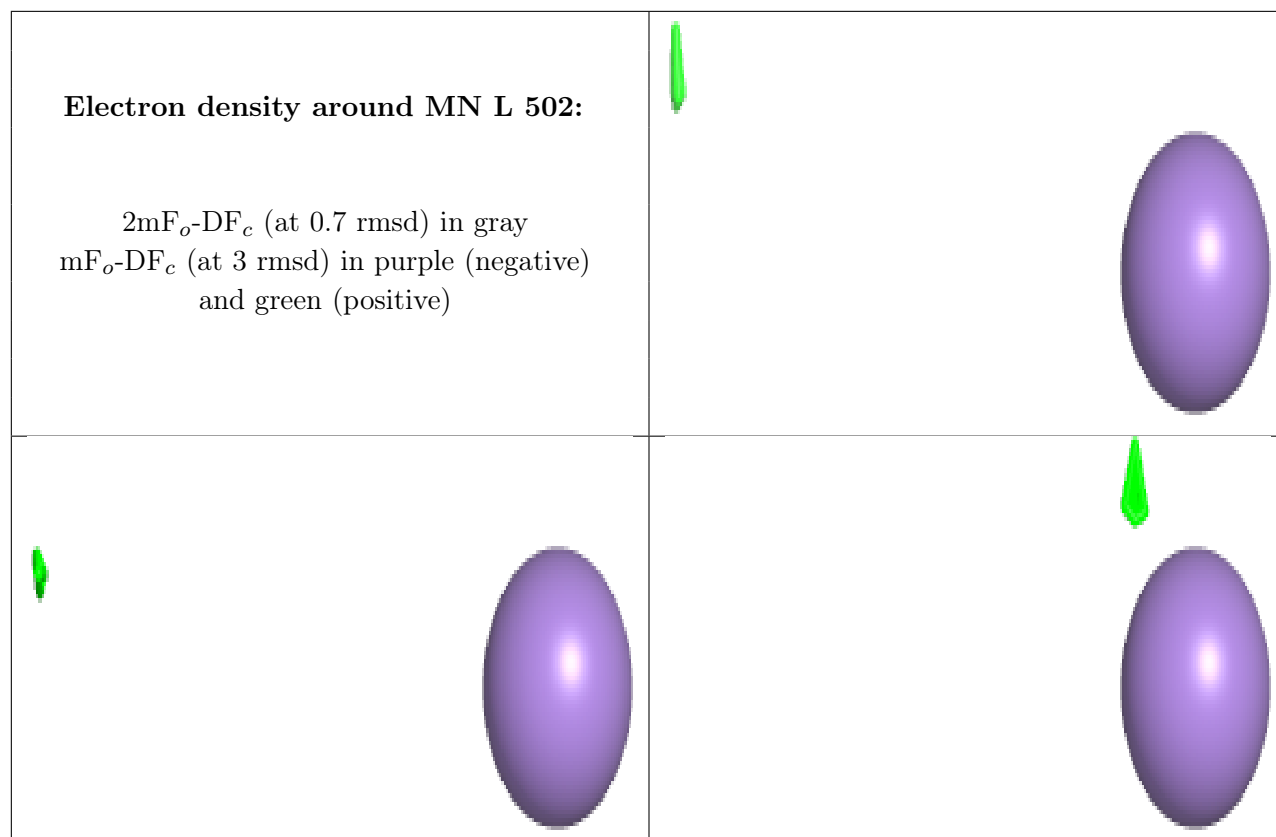




**Electron density around MN H 501:**

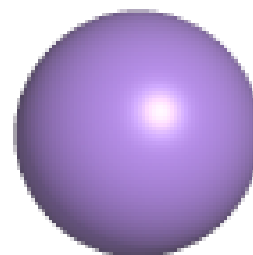
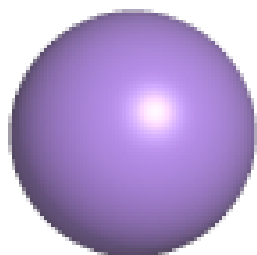
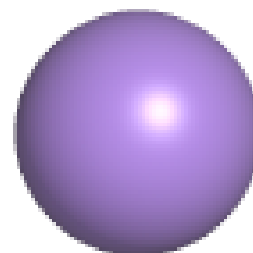
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

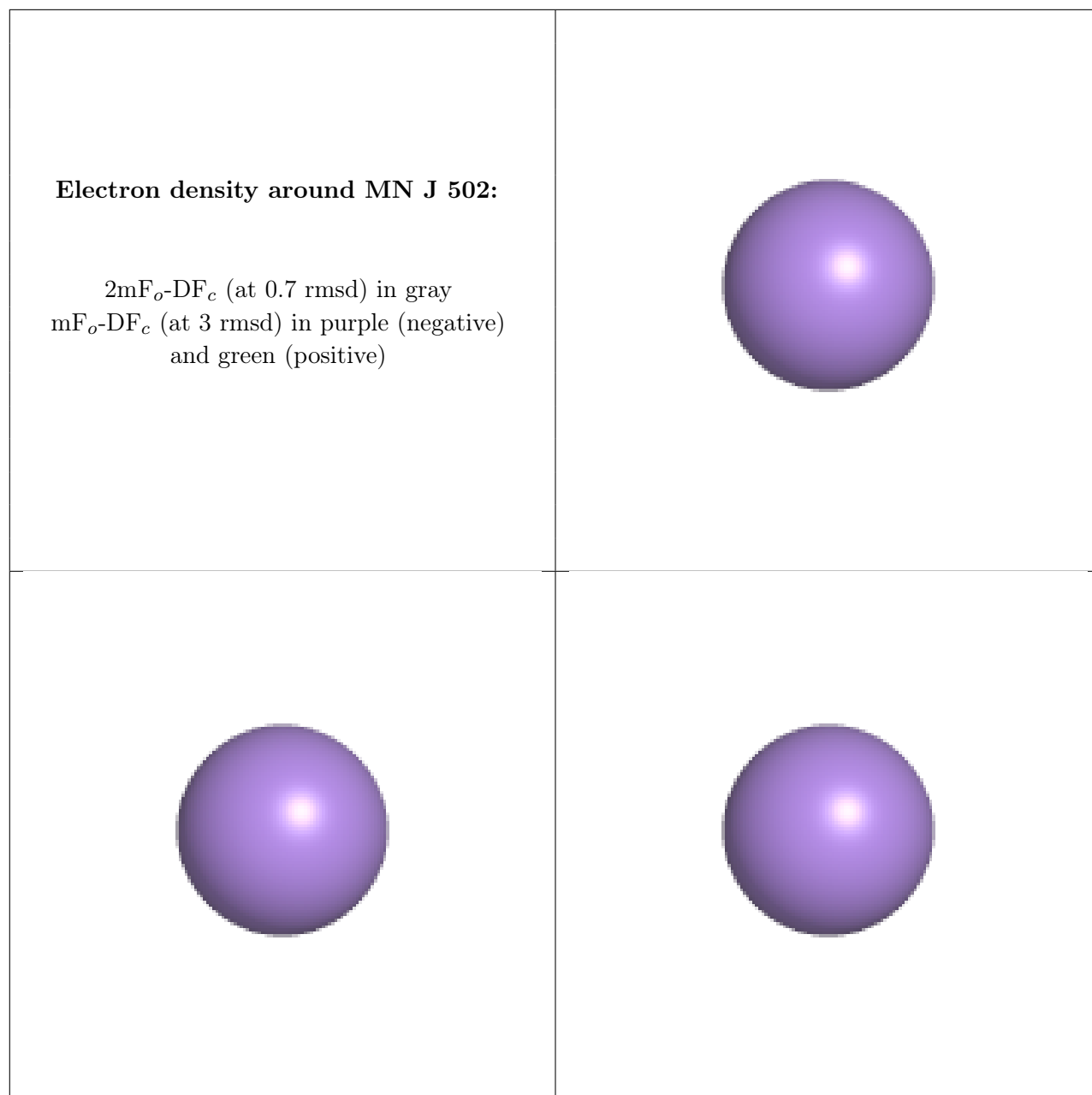




**Electron density around MN F 502:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.