



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2021 – 10:11 PM JST

PDB ID : 7CX7
Title : Crystal structure of Arabinose isomerase from hybrid AI8
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Lee, S.H.
Deposited on : 2020-09-01
Resolution : 2.49 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

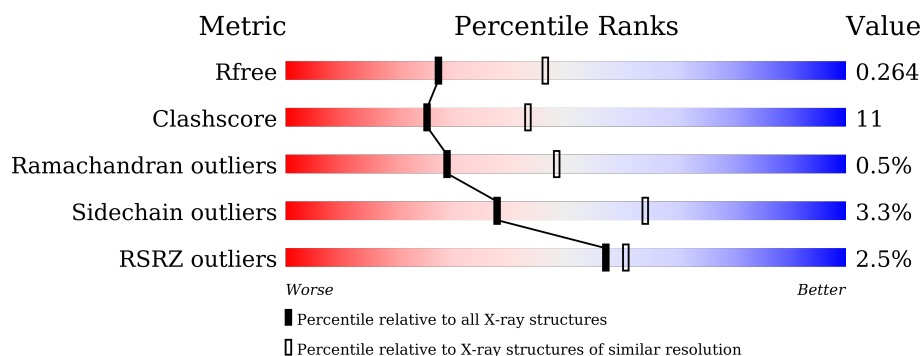
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	497	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 74%, yellow 74%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 74% 24% </div> </div>
1	B	497	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 74%, yellow 74%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 74% 25% </div> </div>
1	C	497	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 72%, yellow 72%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 27% </div> </div>
1	D	497	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 72%, yellow 72%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 26% </div> </div>
1	E	497	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 78%, yellow 78%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 78% 21% </div> </div>
1	F	497	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 73%, yellow 73%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 73% 24% </div> </div>

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	MPD	E	501	-	-	X	-
4	GOL	C	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23927 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.

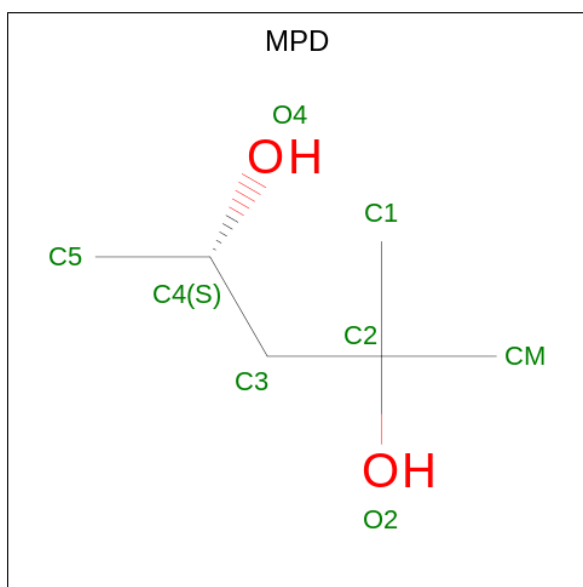
- Molecule 1 is a protein called L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3916	2486	692	714	24			
1	B	495	Total	C	N	O	S	0	0	0
			3916	2486	692	714	24			
1	C	495	Total	C	N	O	S	0	0	0
			3916	2486	692	714	24			
1	D	494	Total	C	N	O	S	0	0	0
			3904	2477	691	712	24			
1	E	495	Total	C	N	O	S	0	0	0
			3916	2486	692	714	24			
1	F	490	Total	C	N	O	S	0	0	0
			3872	2456	687	705	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q5KYP7
B	1	MET	-	initiating methionine	UNP Q5KYP7
C	1	MET	-	initiating methionine	UNP Q5KYP7
D	1	MET	-	initiating methionine	UNP Q5KYP7
E	1	MET	-	initiating methionine	UNP Q5KYP7
F	1	MET	-	initiating methionine	UNP Q5KYP7

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

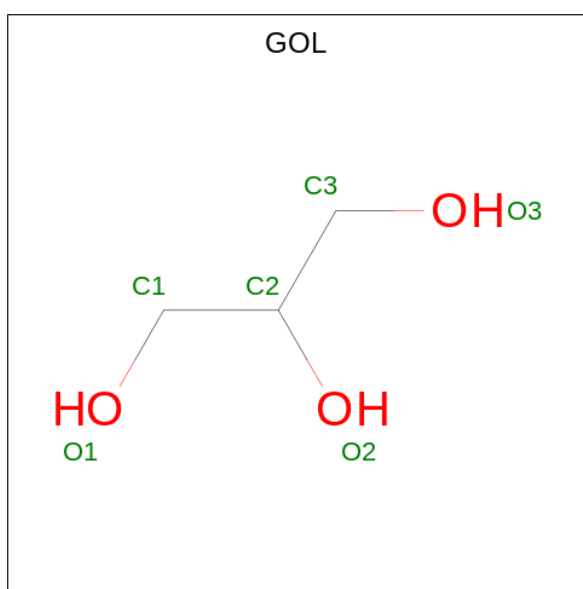
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mn	0	0
			2	2		
3	D	1	Total	Mn	0	0
			1	1		
3	E	2	Total	Mn	0	0
			2	2		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	72	Total	O	0	0
			72	72		
5	C	66	Total	O	0	0
			66	66		
5	D	59	Total	O	0	0
			59	59		

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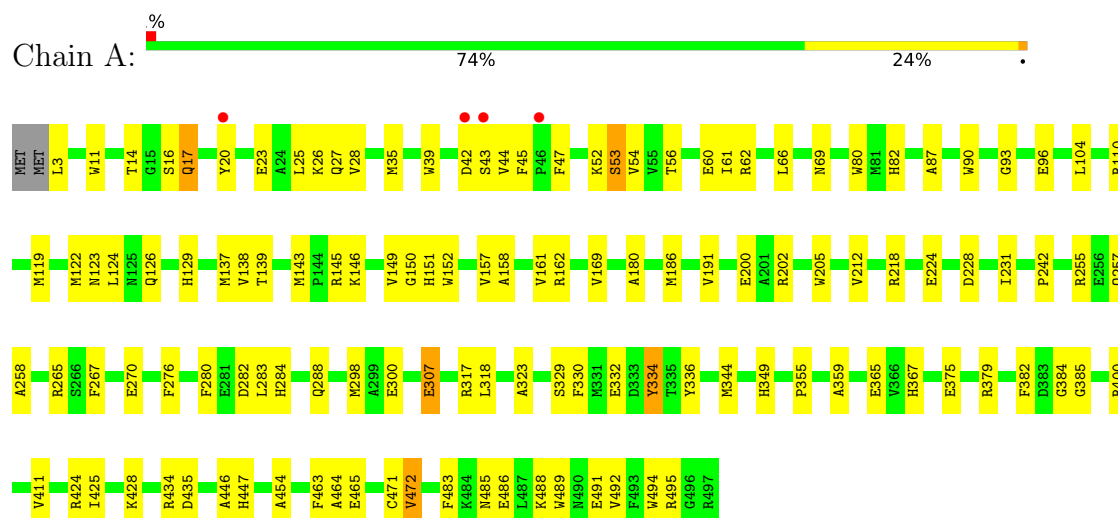
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	47	Total	O	0	0
			47	47		
5	F	52	Total	O	0	0
			52	52		

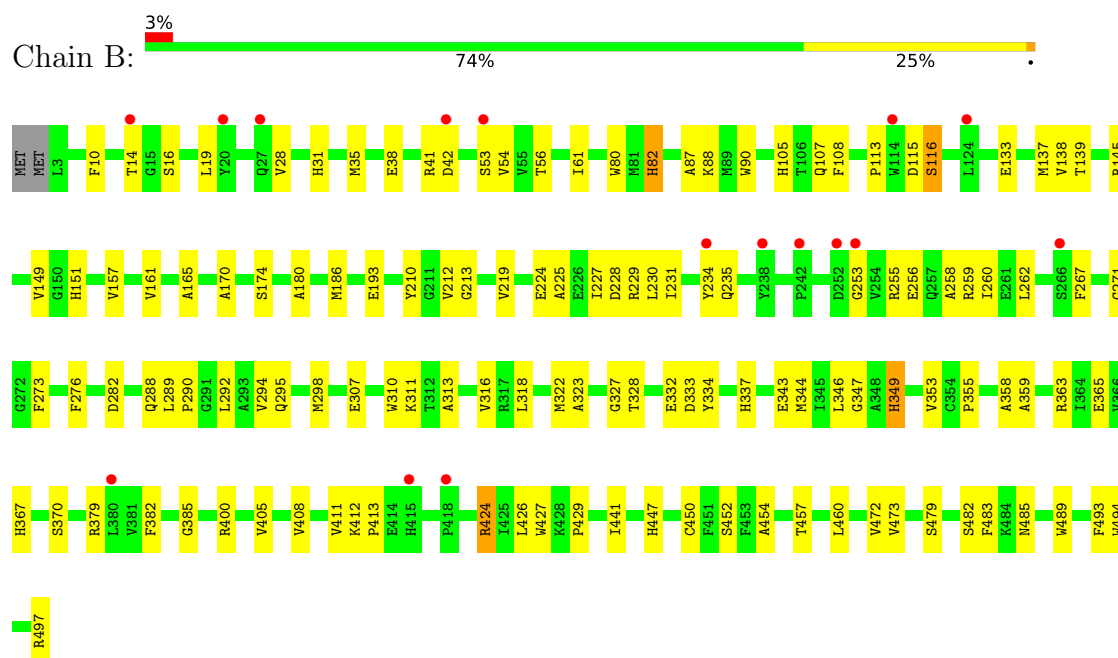
3 Residue-property plots

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.

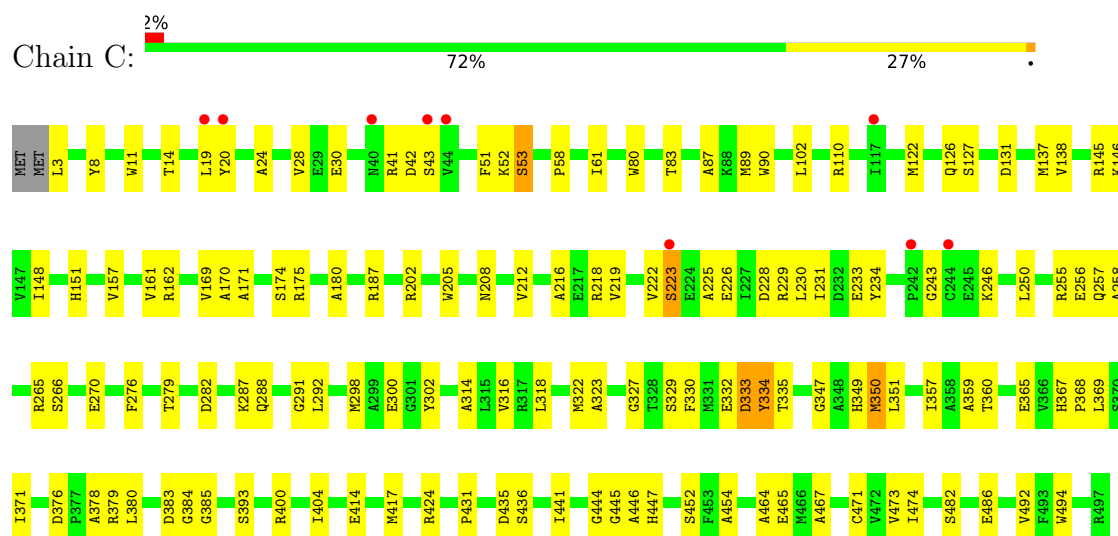
- Molecule 1: L-arabinose isomerase



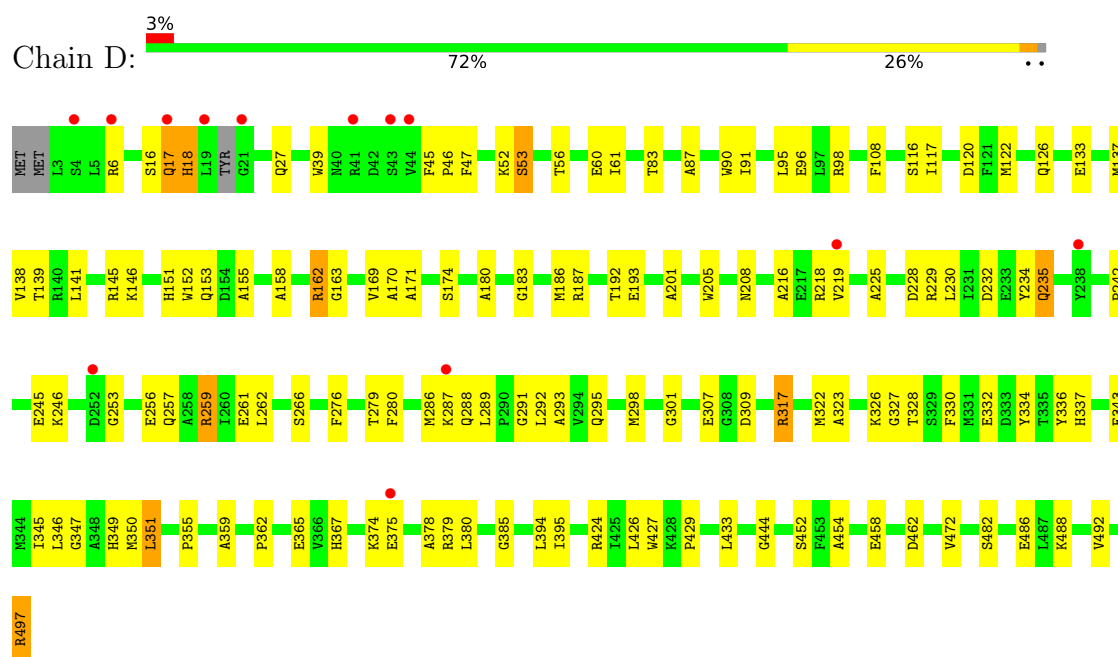
- Molecule 1: L-arabinose isomerase



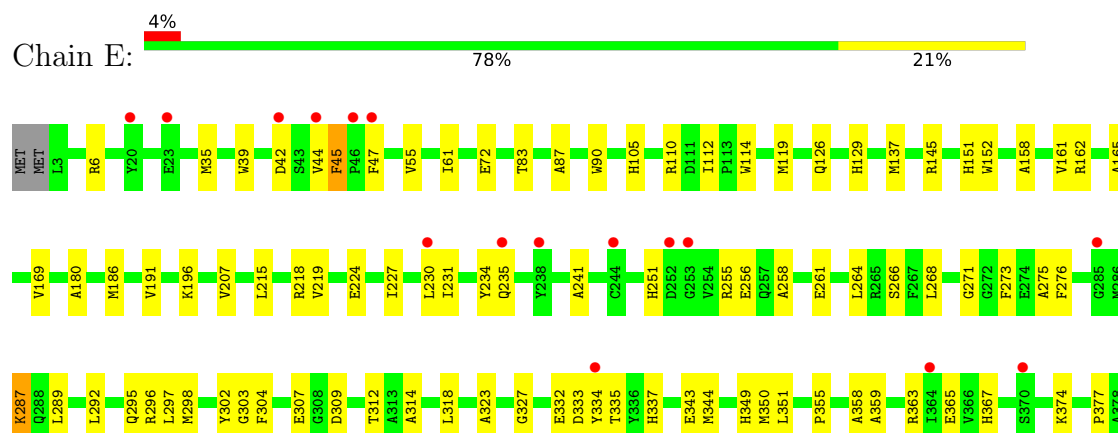
- Molecule 1: L-arabinose isomerase



• 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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.59Å 81.91Å 192.00Å 90.00° 117.90° 90.00°	Depositor
Resolution (Å)	48.59 – 2.49 48.54 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.59-2.49) 98.6 (48.54-2.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.268 0.193 , 0.264	Depositor DCC
R_{free} test set	4784 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23927	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: MPD, MN, GOL

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	0.68	0/4015	0.88	0/5433
1	B	0.68	0/4015	0.85	0/5433
1	C	0.68	0/4015	0.86	0/5433
1	D	0.69	0/4001	0.87	1/5412 (0.0%)
1	E	0.68	0/4015	0.85	0/5433
1	F	0.67	0/3967	0.86	0/5363
All	All	0.68	0/24028	0.86	1/32507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
1	F	0	4
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	ARG	NE-CZ-NH1	5.51	123.06	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	SER	Peptide
1	C	329	SER	Peptide
1	D	351	LEU	Peptide
1	D	53	SER	Peptide
1	F	53	SER	Peptide

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	3916	0	3804	88	0
1	B	3916	0	3804	82	0
1	C	3916	0	3804	103	0
1	D	3904	0	3794	87	0
1	E	3916	0	3804	68	0
1	F	3872	0	3767	88	0
2	A	16	0	28	7	0
2	B	8	0	14	0	0
2	C	16	0	28	6	0
2	E	16	0	28	7	0
2	F	16	0	28	3	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
4	C	6	0	8	4	0
5	A	104	0	0	6	0
5	B	72	0	0	3	0
5	C	66	0	0	2	0
5	D	59	0	0	3	0
5	E	47	0	0	1	0
5	F	52	0	0	1	0
All	All	23927	0	22911	496	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 11.

The worst 5 of 496 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:B:138:VAL:HG11	1:B:145:ARG:HD3	1.28	1.15
1:A:138:VAL:HG11	1:A:145:ARG:HD3	1.29	1.05
1:D:98:ARG:NH1	1:F:95:LEU:O	1.91	1.02
1:C:138:VAL:HG11	1:C:145:ARG:HD3	1.43	0.98
1:E:45:PHE:HB2	2:E:501:MPD:H51	1.48	0.92

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	493/497 (99%)	470 (95%)	20 (4%)	3 (1%)	25	43
1	B	493/497 (99%)	471 (96%)	21 (4%)	1 (0%)	47	68
1	C	493/497 (99%)	460 (93%)	30 (6%)	3 (1%)	25	43
1	D	490/497 (99%)	465 (95%)	22 (4%)	3 (1%)	25	43
1	E	493/497 (99%)	458 (93%)	34 (7%)	1 (0%)	47	68
1	F	484/497 (97%)	454 (94%)	27 (6%)	3 (1%)	25	43
All	All	2946/2982 (99%)	2778 (94%)	154 (5%)	14 (0%)	29	48

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	ASP
1	C	246	LYS
1	F	53	SER
1	B	42	ASP
1	C	350	MET

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	406/408 (100%)	392 (97%)	14 (3%)	37	63
1	B	406/408 (100%)	393 (97%)	13 (3%)	39	65
1	C	406/408 (100%)	396 (98%)	10 (2%)	47	73
1	D	405/408 (99%)	385 (95%)	20 (5%)	25	47
1	E	406/408 (100%)	394 (97%)	12 (3%)	41	68
1	F	401/408 (98%)	390 (97%)	11 (3%)	44	71
All	All	2430/2448 (99%)	2350 (97%)	80 (3%)	38	64

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	45	PHE
1	F	162	ARG
1	E	145	ARG
1	E	374	LYS
1	F	376	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	185	ASN
1	F	123	ASN
1	D	126	GLN
1	C	288	GLN
1	D	151	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	503	-	5,5,5	0.12	0	5,5,5	0.31	0
2	MPD	A	501	-	7,7,7	0.24	0	9,10,10	0.67	0
2	MPD	C	501	-	7,7,7	0.19	0	9,10,10	0.73	0
2	MPD	F	501	-	7,7,7	0.24	0	9,10,10	0.59	0
2	MPD	F	502	-	7,7,7	0.29	0	9,10,10	0.70	0
2	MPD	E	502	-	7,7,7	0.18	0	9,10,10	0.49	0
2	MPD	C	502	-	7,7,7	0.21	0	9,10,10	0.41	0
2	MPD	A	502	-	7,7,7	0.19	0	9,10,10	0.68	0
2	MPD	B	501	-	7,7,7	0.09	0	9,10,10	0.73	0
2	MPD	E	501	-	7,7,7	0.19	0	9,10,10	0.40	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	503	-	-	4/4/4/4	-
2	MPD	A	501	-	-	4/5/5/5	-
2	MPD	C	501	-	-	3/5/5/5	-
2	MPD	F	501	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	F	502	-	-	2/5/5/5	-
2	MPD	E	502	-	-	0/5/5/5	-
2	MPD	C	502	-	-	0/5/5/5	-
2	MPD	A	502	-	-	1/5/5/5	-
2	MPD	B	501	-	-	2/5/5/5	-
2	MPD	E	501	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	MPD	C2-C3-C4-O4
4	C	503	GOL	O1-C1-C2-O2
4	C	503	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
4	C	503	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	GOL	4	0
2	A	501	MPD	5	0
2	C	501	MPD	4	0
2	F	501	MPD	2	0
2	F	502	MPD	1	0
2	C	502	MPD	2	0
2	A	502	MPD	2	0
2	E	501	MPD	7	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	495/497 (99%)	-0.22	4 (0%) 86 87	24, 39, 64, 99	0
1	B	495/497 (99%)	0.07	16 (3%) 47 51	26, 47, 76, 121	0
1	C	495/497 (99%)	-0.09	9 (1%) 68 71	26, 46, 76, 114	0
1	D	494/497 (99%)	0.03	13 (2%) 56 59	28, 47, 81, 101	0
1	E	495/497 (99%)	0.03	19 (3%) 40 43	28, 48, 88, 121	0
1	F	490/497 (98%)	0.05	13 (2%) 54 58	31, 52, 83, 126	0
All	All	2964/2982 (99%)	-0.02	74 (2%) 57 61	24, 46, 80, 126	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	248	GLY	7.6
1	C	44	VAL	6.0
1	E	252	ASP	4.8
1	E	285	GLY	4.6
1	F	423	ALA	4.6

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 ⓘ

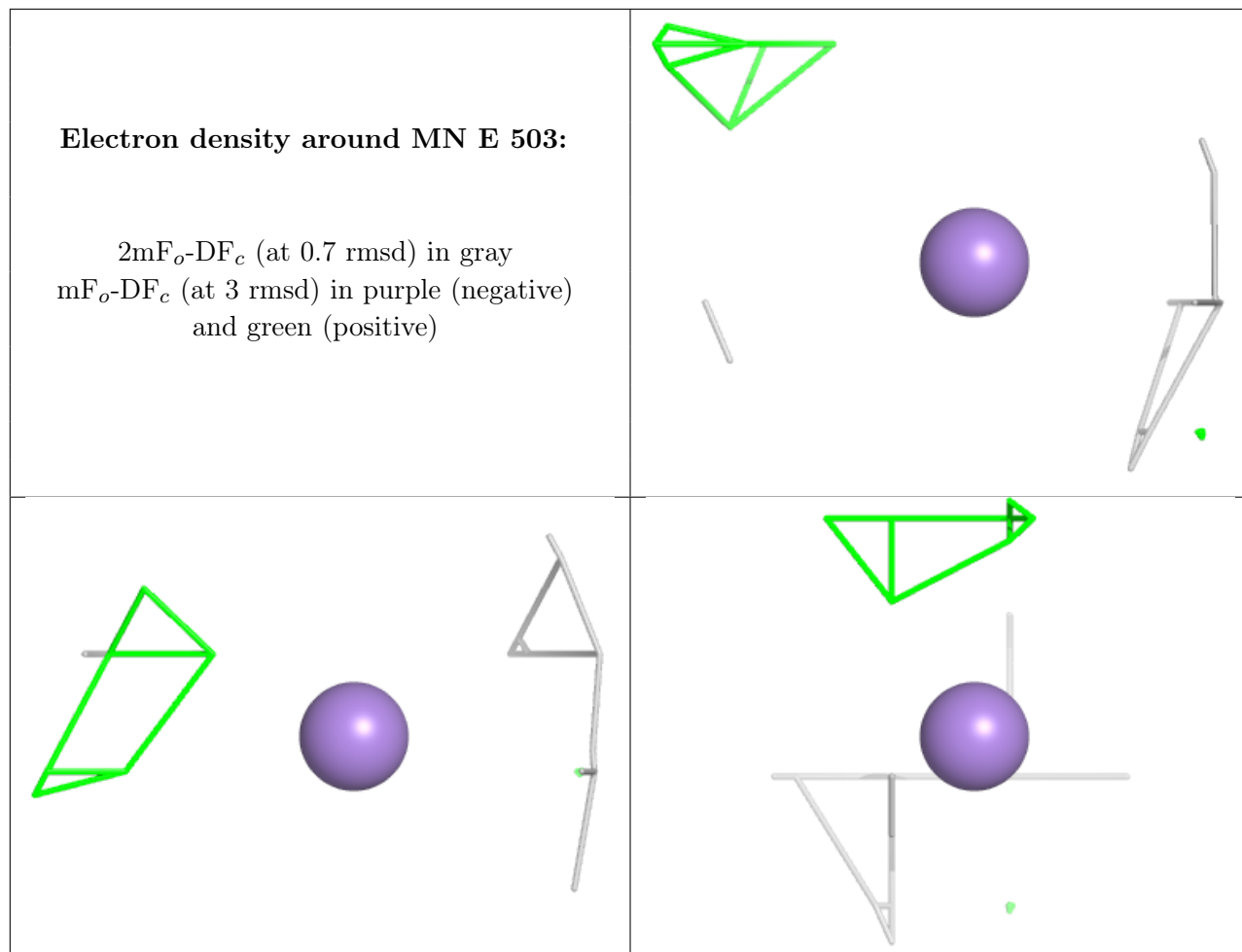
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MPD	C	501	8/8	0.70	0.29	73,86,92,95	0
2	MPD	A	501	8/8	0.88	0.25	73,79,85,89	0
2	MPD	E	502	8/8	0.88	0.27	59,68,83,83	0
2	MPD	F	501	8/8	0.88	0.41	73,88,107,110	0
2	MPD	A	502	8/8	0.90	0.23	56,60,63,64	0
2	MPD	C	502	8/8	0.91	0.22	57,60,66,71	0
2	MPD	E	501	8/8	0.91	0.35	80,83,88,89	0
2	MPD	F	502	8/8	0.91	0.26	59,64,72,76	0
3	MN	E	503	1/1	0.91	0.10	70,70,70,70	0
4	GOL	C	503	6/6	0.91	0.27	77,78,82,85	0
2	MPD	B	501	8/8	0.93	0.24	51,53,67,72	0
3	MN	E	504	1/1	0.97	0.09	58,58,58,58	0
3	MN	C	504	1/1	0.97	0.07	57,57,57,57	0
3	MN	F	503	1/1	0.98	0.09	53,53,53,53	0
3	MN	D	501	1/1	0.99	0.11	43,43,43,43	0
3	MN	A	504	1/1	0.99	0.17	61,61,61,61	0
3	MN	B	502	1/1	0.99	0.14	45,45,45,45	0
3	MN	A	503	1/1	0.99	0.12	40,40,40,40	0
3	MN	C	505	1/1	0.99	0.11	45,45,45,45	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.

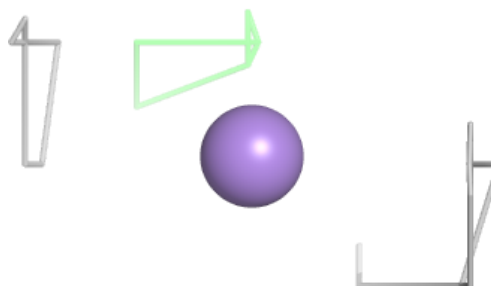
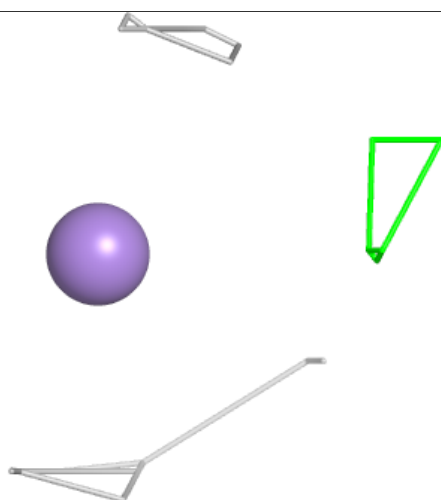
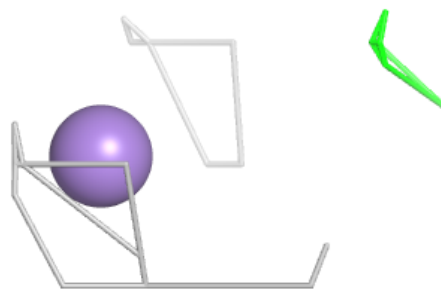
Electron density around MN E 503:

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



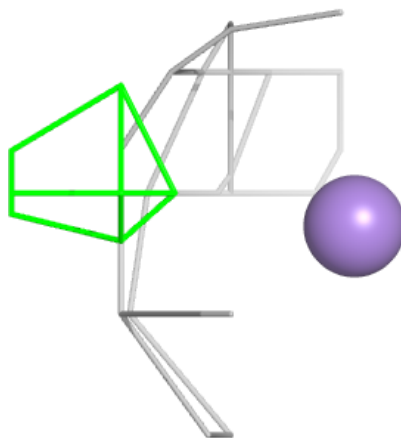
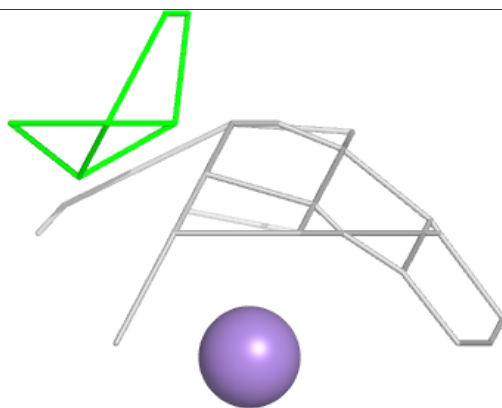
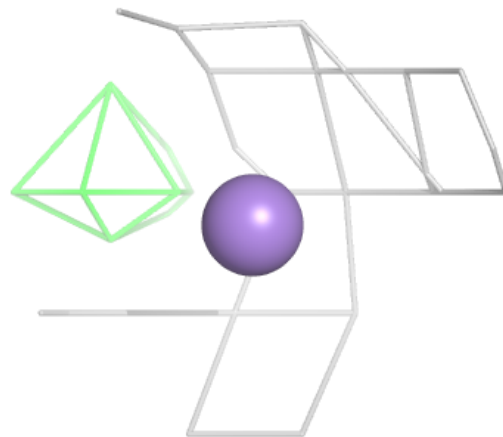
Electron density around MN E 504:

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



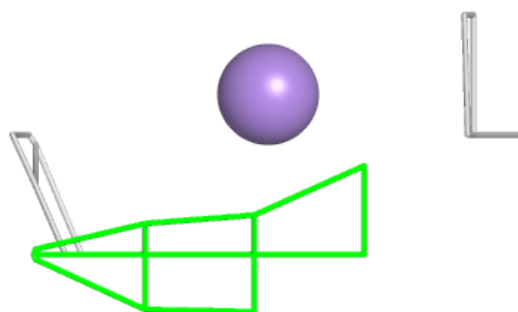
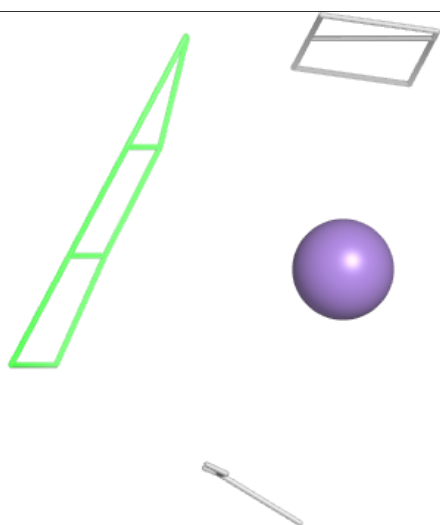
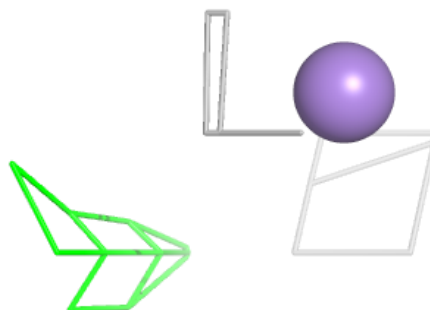
Electron density around MN C 504:

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



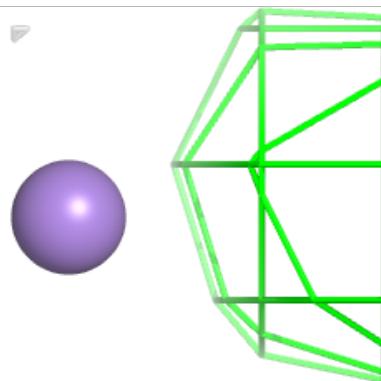
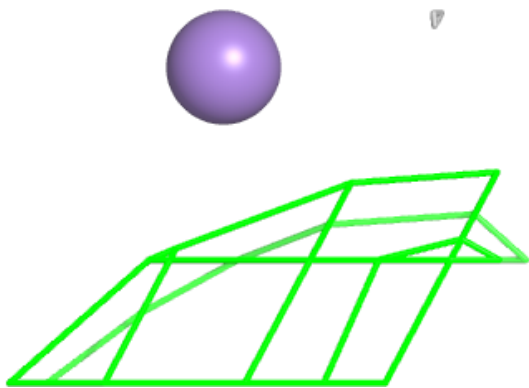
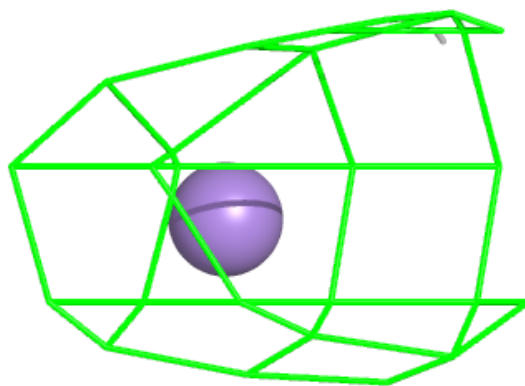
Electron density around MN F 503:

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



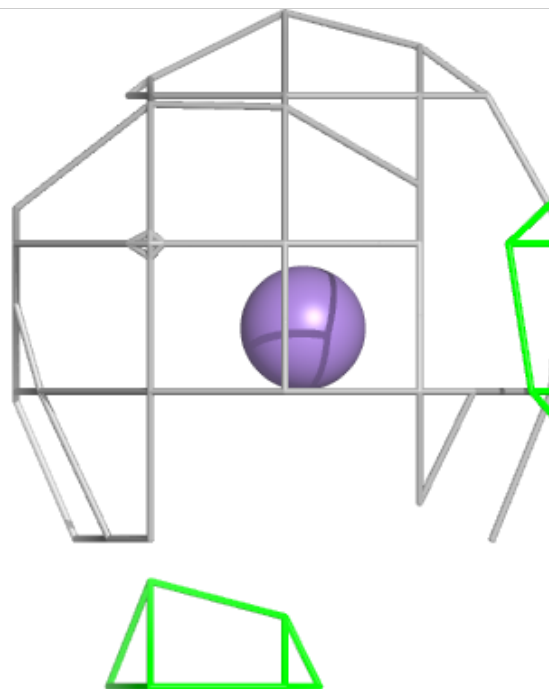
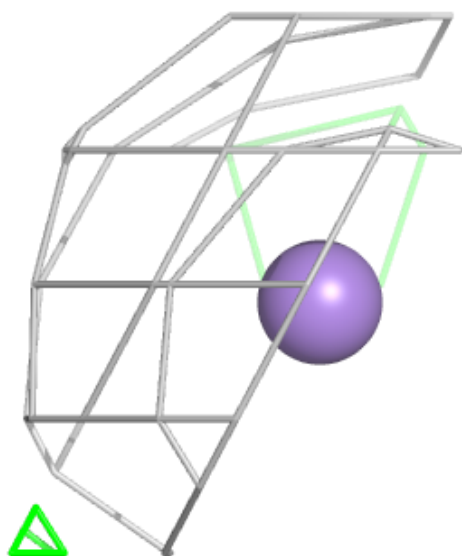
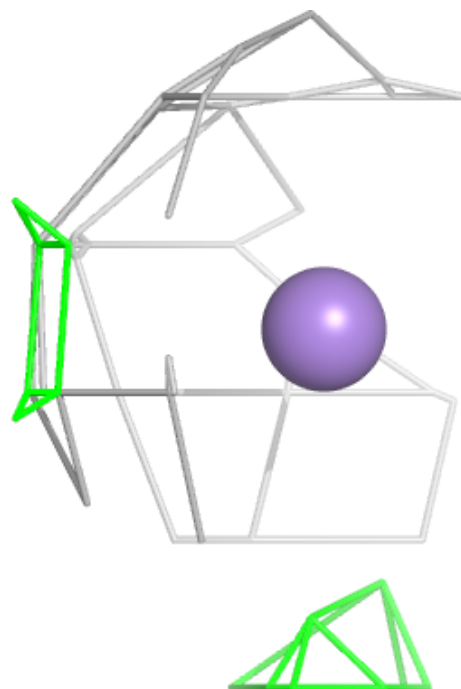
Electron density around MN D 501:

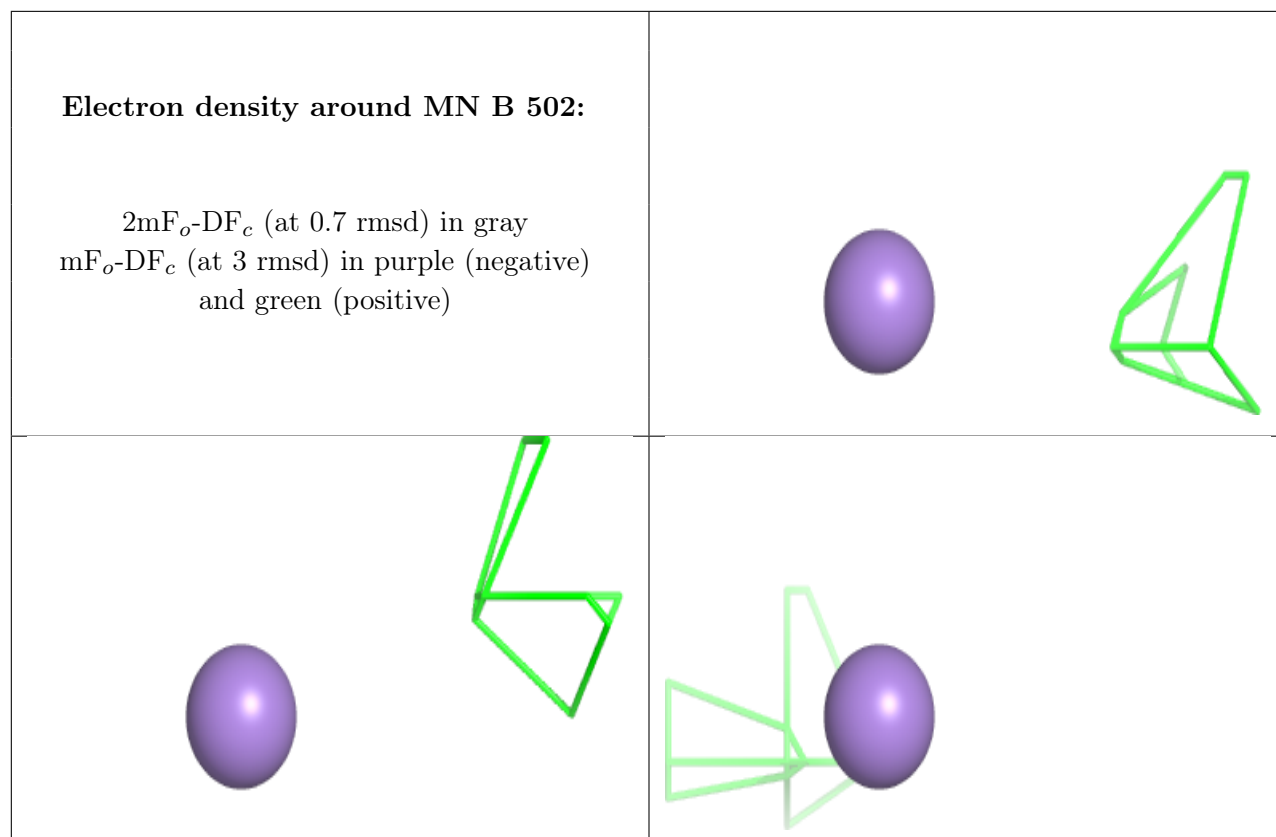
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 504:

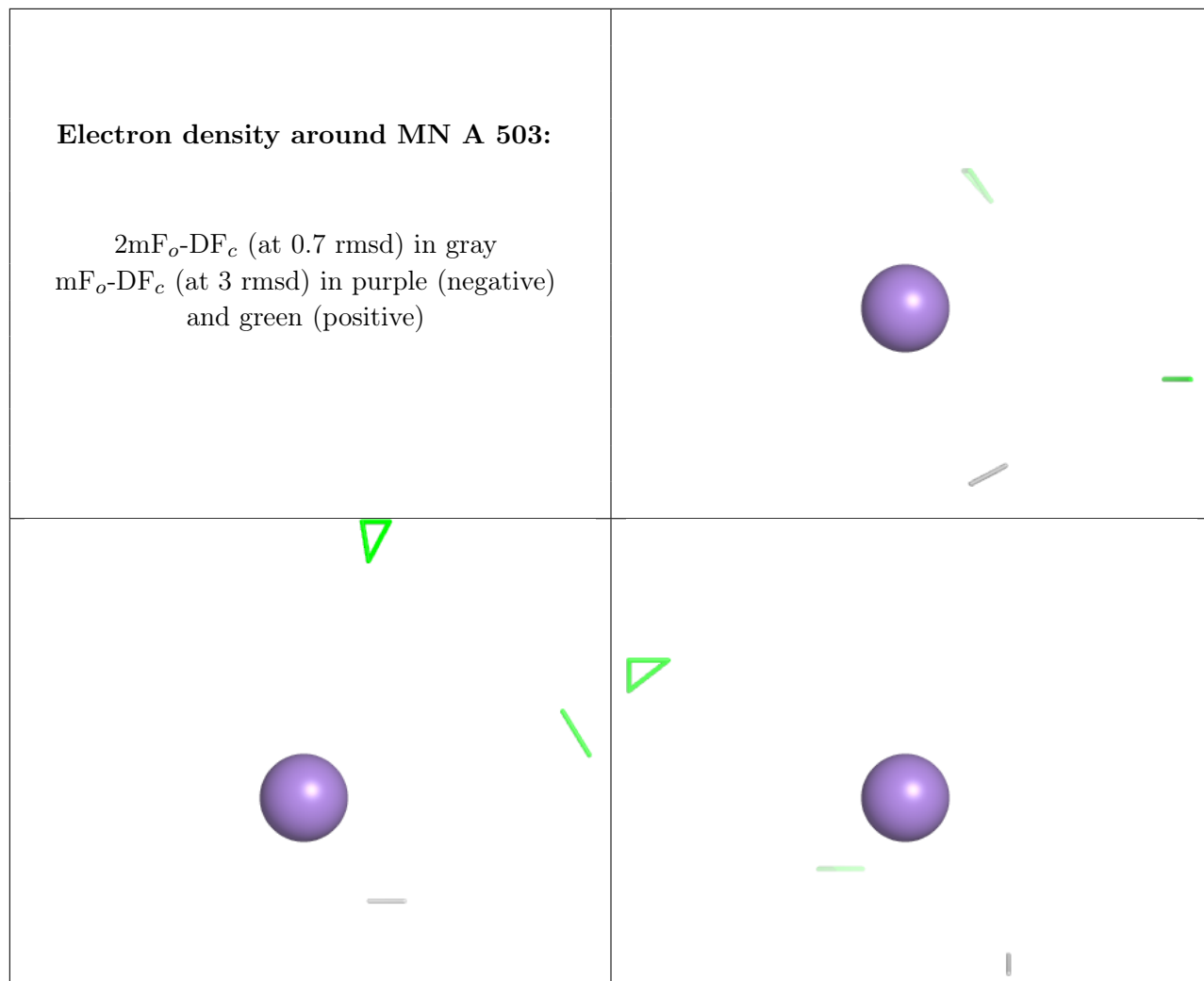
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

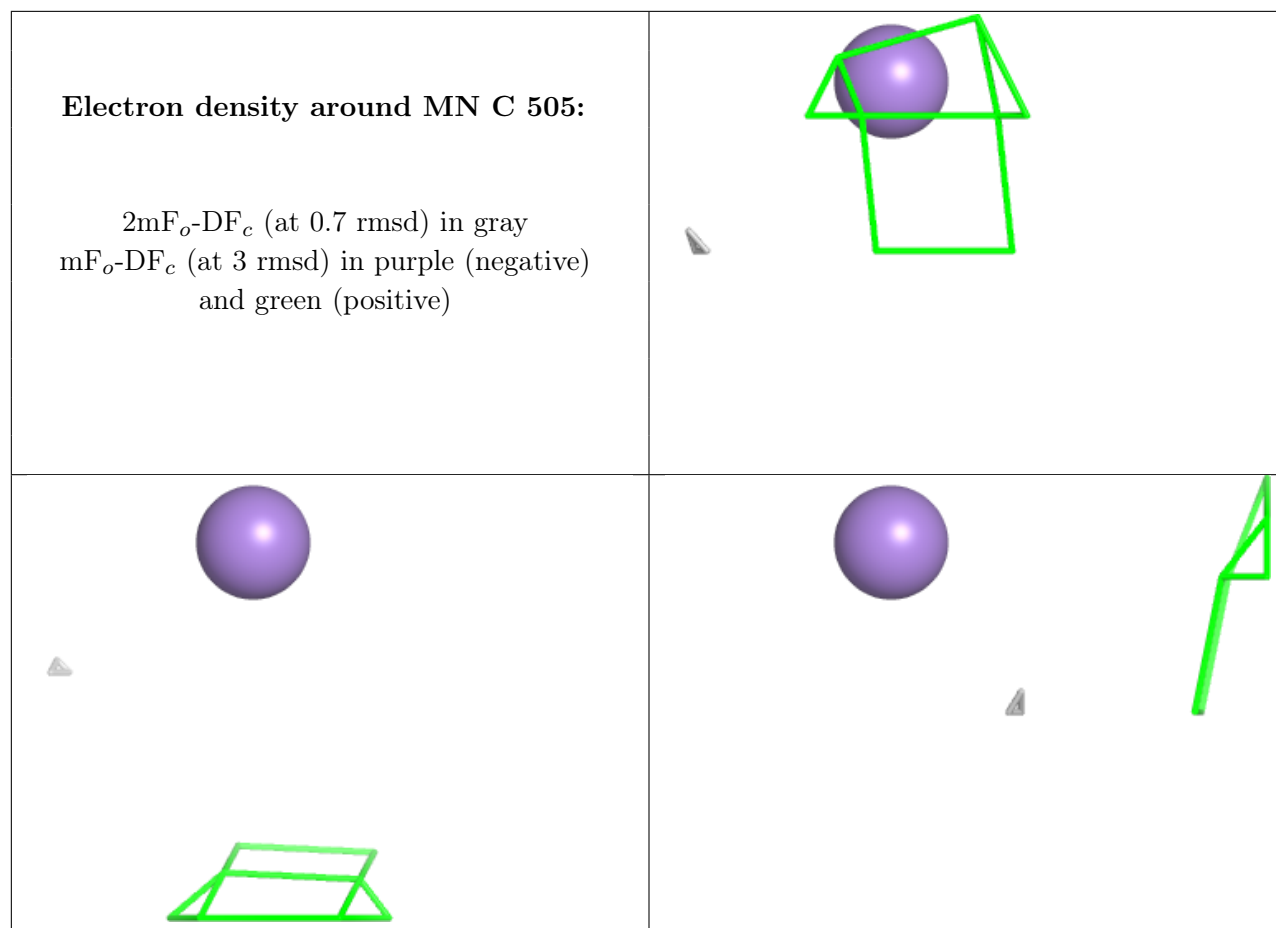




Electron density around MN A 503:

$2mF_o-DF_c$ (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.