Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 04:23 PM JST

PDB ID	:	6LRT
Title	:	Crystal structure of isocitrate lyase (Caur_3889) from Chloroflexus aurantiacus in complex with isocitrate and manganese ion
Authors	:	Lee, S.H.; Kim, K.J.
Deposited on	:	2020-01-16
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

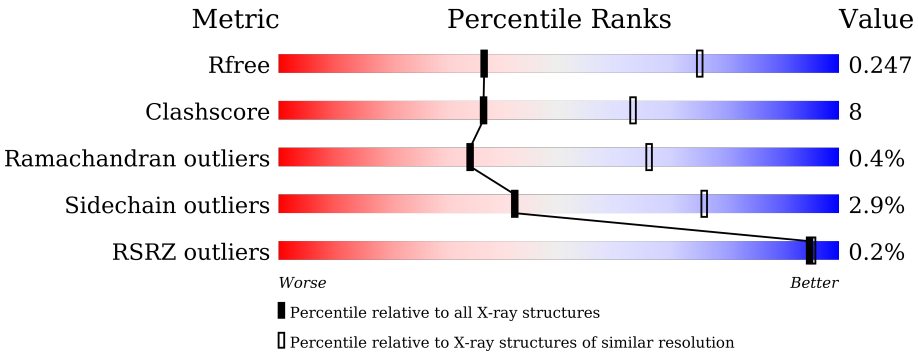
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	436	78% 18%
1	D	436	82% 14%
1	G	436	79% 17%
1	J	436	80% 16%
1	M	436	75% 21%
1	P	436	79% 18%

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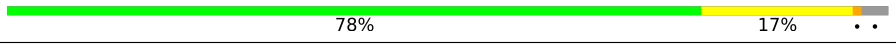
Mol	Chain	Length	Quality of chain
1	S	436	
1	V	436	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27179 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 Isocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	D	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	G	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	J	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	M	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	P	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	S	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			
1	V	423	Total	C	N	O	S	0	0	0
			3291	2077	579	620	15			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP A9WDE7
A	-10	ARG	-	expression tag	UNP A9WDE7
A	-9	GLY	-	expression tag	UNP A9WDE7
A	-8	SER	-	expression tag	UNP A9WDE7
A	-7	HIS	-	expression tag	UNP A9WDE7
A	-6	HIS	-	expression tag	UNP A9WDE7
A	-5	HIS	-	expression tag	UNP A9WDE7
A	-4	HIS	-	expression tag	UNP A9WDE7
A	-3	HIS	-	expression tag	UNP A9WDE7
A	-2	HIS	-	expression tag	UNP A9WDE7
A	-1	GLY	-	expression tag	UNP A9WDE7
A	0	SER	-	expression tag	UNP A9WDE7
D	-11	MET	-	initiating methionine	UNP A9WDE7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ARG	-	expression tag	UNP A9WDE7
D	-9	GLY	-	expression tag	UNP A9WDE7
D	-8	SER	-	expression tag	UNP A9WDE7
D	-7	HIS	-	expression tag	UNP A9WDE7
D	-6	HIS	-	expression tag	UNP A9WDE7
D	-5	HIS	-	expression tag	UNP A9WDE7
D	-4	HIS	-	expression tag	UNP A9WDE7
D	-3	HIS	-	expression tag	UNP A9WDE7
D	-2	HIS	-	expression tag	UNP A9WDE7
D	-1	GLY	-	expression tag	UNP A9WDE7
D	0	SER	-	expression tag	UNP A9WDE7
G	-11	MET	-	initiating methionine	UNP A9WDE7
G	-10	ARG	-	expression tag	UNP A9WDE7
G	-9	GLY	-	expression tag	UNP A9WDE7
G	-8	SER	-	expression tag	UNP A9WDE7
G	-7	HIS	-	expression tag	UNP A9WDE7
G	-6	HIS	-	expression tag	UNP A9WDE7
G	-5	HIS	-	expression tag	UNP A9WDE7
G	-4	HIS	-	expression tag	UNP A9WDE7
G	-3	HIS	-	expression tag	UNP A9WDE7
G	-2	HIS	-	expression tag	UNP A9WDE7
G	-1	GLY	-	expression tag	UNP A9WDE7
G	0	SER	-	expression tag	UNP A9WDE7
J	-11	MET	-	initiating methionine	UNP A9WDE7
J	-10	ARG	-	expression tag	UNP A9WDE7
J	-9	GLY	-	expression tag	UNP A9WDE7
J	-8	SER	-	expression tag	UNP A9WDE7
J	-7	HIS	-	expression tag	UNP A9WDE7
J	-6	HIS	-	expression tag	UNP A9WDE7
J	-5	HIS	-	expression tag	UNP A9WDE7
J	-4	HIS	-	expression tag	UNP A9WDE7
J	-3	HIS	-	expression tag	UNP A9WDE7
J	-2	HIS	-	expression tag	UNP A9WDE7
J	-1	GLY	-	expression tag	UNP A9WDE7
J	0	SER	-	expression tag	UNP A9WDE7
M	-11	MET	-	initiating methionine	UNP A9WDE7
M	-10	ARG	-	expression tag	UNP A9WDE7
M	-9	GLY	-	expression tag	UNP A9WDE7
M	-8	SER	-	expression tag	UNP A9WDE7
M	-7	HIS	-	expression tag	UNP A9WDE7
M	-6	HIS	-	expression tag	UNP A9WDE7
M	-5	HIS	-	expression tag	UNP A9WDE7

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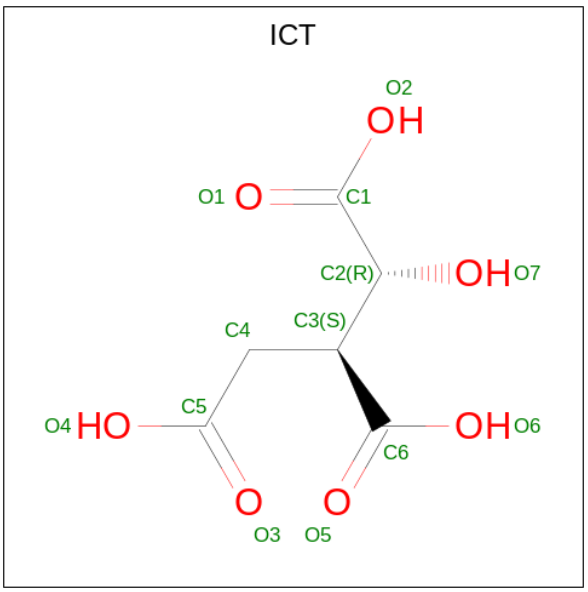
Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	HIS	-	expression tag	UNP A9WDE7
M	-3	HIS	-	expression tag	UNP A9WDE7
M	-2	HIS	-	expression tag	UNP A9WDE7
M	-1	GLY	-	expression tag	UNP A9WDE7
M	0	SER	-	expression tag	UNP A9WDE7
P	-11	MET	-	initiating methionine	UNP A9WDE7
P	-10	ARG	-	expression tag	UNP A9WDE7
P	-9	GLY	-	expression tag	UNP A9WDE7
P	-8	SER	-	expression tag	UNP A9WDE7
P	-7	HIS	-	expression tag	UNP A9WDE7
P	-6	HIS	-	expression tag	UNP A9WDE7
P	-5	HIS	-	expression tag	UNP A9WDE7
P	-4	HIS	-	expression tag	UNP A9WDE7
P	-3	HIS	-	expression tag	UNP A9WDE7
P	-2	HIS	-	expression tag	UNP A9WDE7
P	-1	GLY	-	expression tag	UNP A9WDE7
P	0	SER	-	expression tag	UNP A9WDE7
S	-11	MET	-	initiating methionine	UNP A9WDE7
S	-10	ARG	-	expression tag	UNP A9WDE7
S	-9	GLY	-	expression tag	UNP A9WDE7
S	-8	SER	-	expression tag	UNP A9WDE7
S	-7	HIS	-	expression tag	UNP A9WDE7
S	-6	HIS	-	expression tag	UNP A9WDE7
S	-5	HIS	-	expression tag	UNP A9WDE7
S	-4	HIS	-	expression tag	UNP A9WDE7
S	-3	HIS	-	expression tag	UNP A9WDE7
S	-2	HIS	-	expression tag	UNP A9WDE7
S	-1	GLY	-	expression tag	UNP A9WDE7
S	0	SER	-	expression tag	UNP A9WDE7
V	-11	MET	-	initiating methionine	UNP A9WDE7
V	-10	ARG	-	expression tag	UNP A9WDE7
V	-9	GLY	-	expression tag	UNP A9WDE7
V	-8	SER	-	expression tag	UNP A9WDE7
V	-7	HIS	-	expression tag	UNP A9WDE7
V	-6	HIS	-	expression tag	UNP A9WDE7
V	-5	HIS	-	expression tag	UNP A9WDE7
V	-4	HIS	-	expression tag	UNP A9WDE7
V	-3	HIS	-	expression tag	UNP A9WDE7
V	-2	HIS	-	expression tag	UNP A9WDE7
V	-1	GLY	-	expression tag	UNP A9WDE7
V	0	SER	-	expression tag	UNP A9WDE7

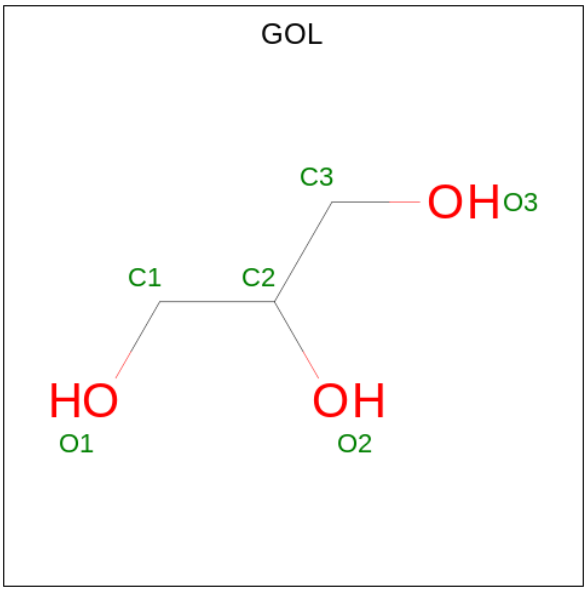
- Molecule 2 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0
2	M	1	Total C O 13 6 7	0	0
2	P	1	Total C O 13 6 7	0	0
2	S	1	Total C O 13 6 7	0	0
2	V	1	Total C O 13 6 7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	P	1	Total C O 6 3 3	0	0
3	S	1	Total C O 6 3 3	0	0
3	S	1	Total C O 6 3 3	0	0
3	S	1	Total C O 6 3 3	0	0
3	V	1	Total C O 6 3 3	0	0
3	V	1	Total C O 6 3 3	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0
4	G	1	Total Mn 1 1	0	0
4	J	1	Total Mn 1 1	0	0
4	M	1	Total Mn 1 1	0	0
4	P	1	Total Mn 1 1	0	0
4	S	1	Total Mn 1 1	0	0
4	V	1	Total Mn 1 1	0	0

- Molecule 5 is water.

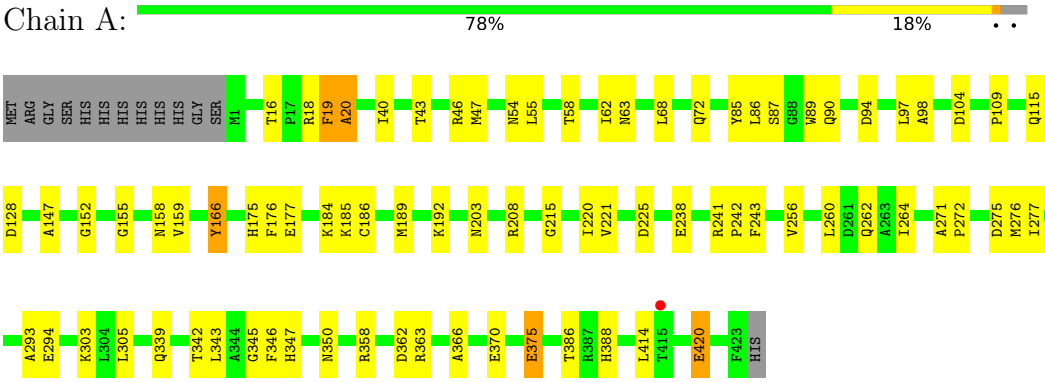
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	116	Total O 116 116	0	0
5	D	75	Total O 75 75	0	0
5	G	94	Total O 94 94	0	0
5	J	72	Total O 72 72	0	0
5	M	100	Total O 100 100	0	0
5	P	48	Total O 48 48	0	0
5	S	82	Total O 82 82	0	0
5	V	80	Total O 80 80	0	0

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.

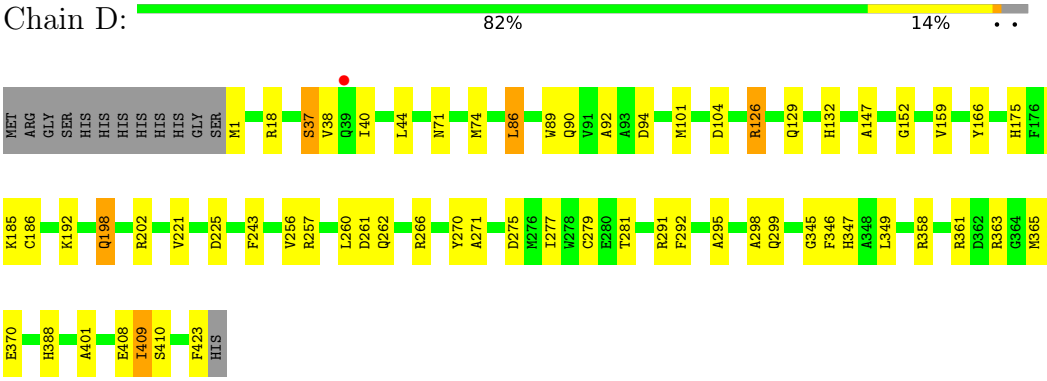
- Molecule 1: Isocitrate lyase

Chain A:



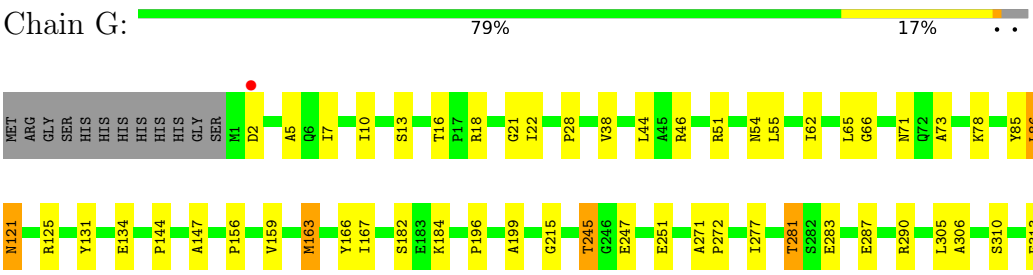
- Molecule 1: Isocitrate lyase

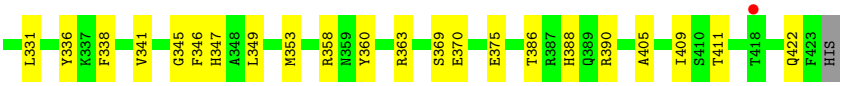
Chain D:



- Molecule 1: Isocitrate lyase

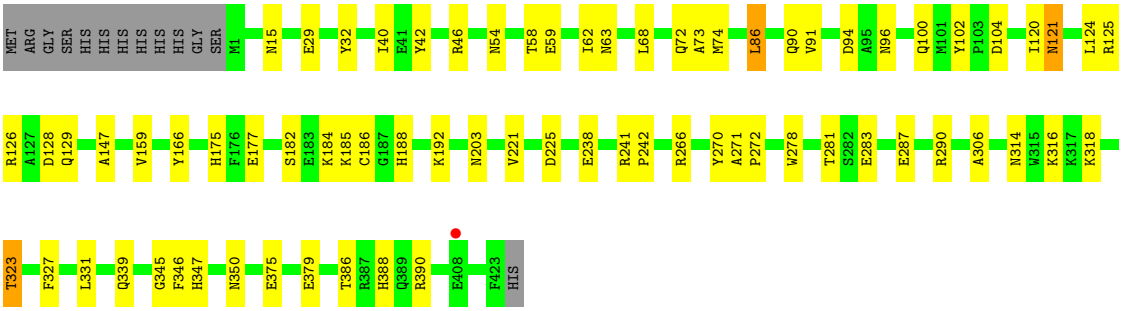
Chain G:





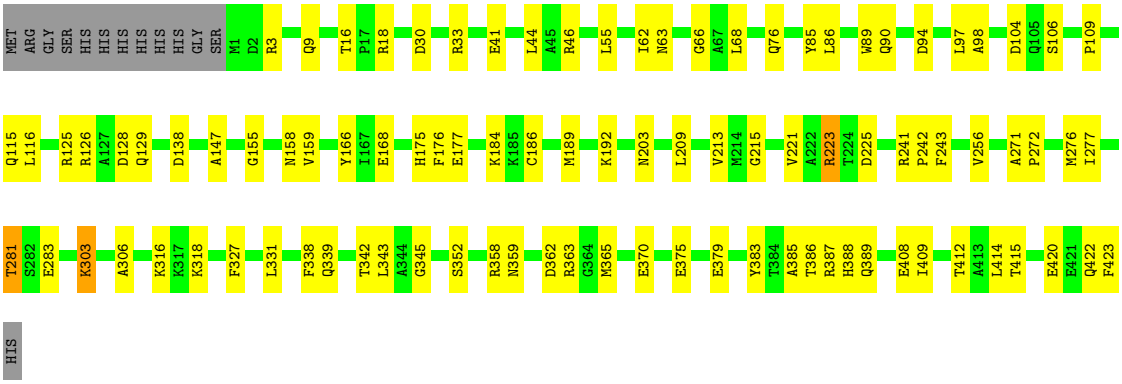
• Molecule 1: Isocitrate lyase

Chain J:



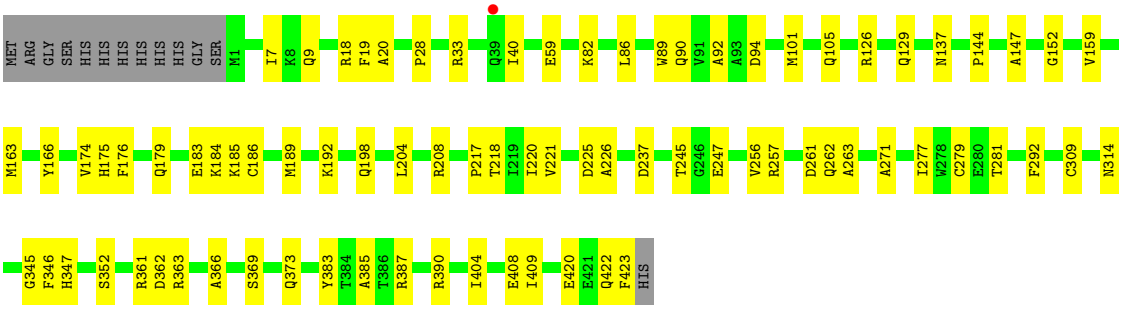
• Molecule 1: Isocitrate lyase

Chain M:



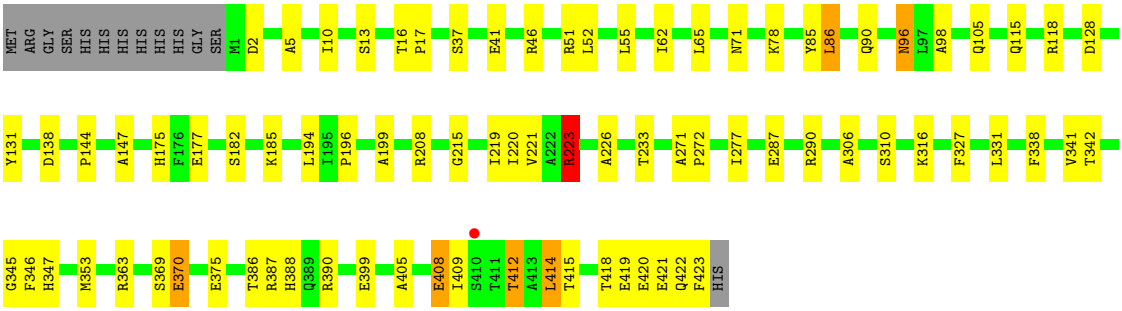
• Molecule 1: Isocitrate lyase

Chain P:



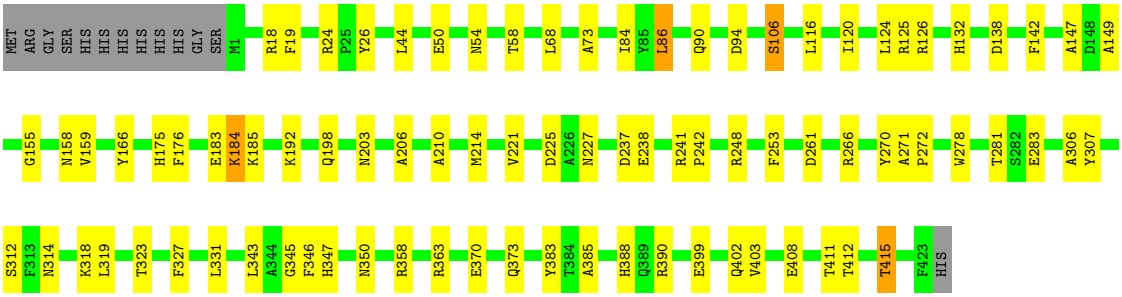
• Molecule 1: Isocitrate lyase

Chain S:



• Molecule 1: Isocitrate lyase

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	157.31Å 157.31Å 197.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.05 – 2.90 32.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (32.05-2.90) 95.9 (32.03-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.246 0.182 , 0.247	Depositor DCC
R_{free} test set	5601 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 19.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.457 for h,-h-k,-l 0.007 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27179	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, ICT

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	0.74	1/3364 (0.0%)	0.91	0/4562
1	D	0.75	1/3364 (0.0%)	0.94	0/4562
1	G	0.74	0/3364	0.93	0/4562
1	J	0.73	0/3364	0.90	1/4562 (0.0%)
1	M	0.73	0/3364	0.92	0/4562
1	P	0.74	0/3364	0.92	1/4562 (0.0%)
1	S	0.74	0/3364	0.94	1/4562 (0.0%)
1	V	0.72	0/3364	0.89	0/4562
All	All	0.74	2/26912 (0.0%)	0.92	3/36496 (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	G	0	1
1	P	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	GLU	CD-OE1	5.25	1.31	1.25
1	D	177	GLU	CD-OE1	5.20	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	223	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	P	387	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	J	15	ASN	CB-CA-C	5.13	120.66	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	PHE	Peptide
1	G	21	GLY	Peptide
1	P	20	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3291	0	3188	63	0
1	D	3291	0	3188	51	0
1	G	3291	0	3188	65	0
1	J	3291	0	3188	55	0
1	M	3291	0	3188	70	0
1	P	3291	0	3188	51	0
1	S	3291	0	3188	63	0
1	V	3291	0	3188	59	0
2	A	13	0	5	2	0
2	D	13	0	5	0	0
2	G	13	0	4	1	0
2	J	13	0	5	2	0
2	M	13	0	4	1	0
2	P	13	0	5	0	0
2	S	13	0	5	1	0
2	V	13	0	5	0	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
3	G	12	0	16	0	0
3	J	12	0	16	0	0
3	P	6	0	8	0	0
3	S	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	12	0	16	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
4	M	1	0	0	0	0
4	P	1	0	0	0	0
4	S	1	0	0	0	0
4	V	1	0	0	0	0
5	A	116	0	0	1	0
5	D	75	0	0	0	0
5	G	94	0	0	0	0
5	J	72	0	0	2	0
5	M	100	0	0	1	0
5	P	48	0	0	1	0
5	S	82	0	0	1	0
5	V	80	0	0	1	0
All	All	27179	0	25638	414	0

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

All (414) 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:G:310:SER:OG	2:G:501:ICT:O3	1.87	0.93
1:A:177:GLU:OE2	1:A:184:LYS:HE2	1.71	0.90
1:S:46:ARG:NH1	1:S:215:GLY:O	2.09	0.86
1:S:418:THR:HG22	1:V:312:SER:O	1.82	0.79
1:S:90:GLN:HE22	1:S:345:GLY:H	1.30	0.77
1:G:71:ASN:HD22	1:J:350:ASN:HD21	1.31	0.77
1:G:55:LEU:HB3	1:G:62:ILE:HD11	1.67	0.76
1:S:363:ARG:NH2	1:S:370:GLU:OE1	2.18	0.75
1:S:310:SER:OG	2:S:501:ICT:O4	2.03	0.75
1:S:90:GLN:HE22	1:S:345:GLY:N	1.85	0.74
1:M:33:ARG:NH2	1:S:399:GLU:OE1	2.21	0.73
1:S:375:GLU:HB3	1:S:386:THR:HB	1.70	0.73
1:M:177:GLU:OE2	1:M:184:LYS:HE2	1.88	0.72
1:M:3:ARG:NH1	5:M:601:HOH:O	2.23	0.72
1:S:347:HIS:NE2	1:V:388:HIS:HD2	1.88	0.71
1:D:37:SER:HB3	1:J:128:ASP:OD1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:179:GLN:HE22	1:P:185:LYS:H	1.40	0.69
1:M:168:GLU:OE2	1:S:118:ARG:NH1	2.26	0.69
1:A:90:GLN:HE22	1:A:345:GLY:N	1.90	0.69
1:D:363:ARG:NH2	1:D:370:GLU:OE2	2.26	0.69
1:D:179:GLN:HE22	1:D:185:LYS:H	1.41	0.69
1:S:55:LEU:HB3	1:S:62:ILE:HD11	1.75	0.68
1:J:29:GLU:HB2	5:J:630:HOH:O	1.93	0.68
1:A:90:GLN:HE22	1:A:345:GLY:H	1.39	0.68
1:P:86:LEU:HB3	1:P:147:ALA:HA	1.75	0.68
1:S:418:THR:CG2	1:V:312:SER:O	2.42	0.68
1:A:126:ARG:NH2	1:D:101:MET:O	2.26	0.67
1:D:86:LEU:HB3	1:D:147:ALA:HA	1.77	0.67
1:D:363:ARG:HH22	1:D:370:GLU:CD	1.98	0.67
1:G:90:GLN:HE22	1:G:345:GLY:H	1.42	0.66
1:A:192:LYS:CE	1:A:225:ASP:HB3	2.25	0.66
1:G:10:ILE:O	1:G:13:SER:OG	2.08	0.66
1:M:16:THR:O	1:M:18:ARG:O	2.13	0.66
1:M:412:THR:HB	1:M:415:THR:CG2	2.25	0.66
1:J:188:HIS:HD2	2:J:501:ICT:O4	1.78	0.65
1:V:132:HIS:HD2	5:V:648:HOH:O	1.79	0.65
1:G:46:ARG:NH1	1:G:215:GLY:O	2.29	0.65
1:A:90:GLN:NE2	1:A:346:PHE:H	1.94	0.65
1:P:390:ARG:NH2	1:P:420:GLU:OE1	2.29	0.65
1:G:71:ASN:HD21	1:J:346:PHE:HE1	1.43	0.65
1:S:347:HIS:NE2	1:V:388:HIS:CD2	2.65	0.65
1:D:256:VAL:HG21	1:D:262:GLN:HE22	1.62	0.64
1:G:90:GLN:HE22	1:G:345:GLY:N	1.94	0.64
1:D:358:ARG:NH2	1:D:361:ARG:HH21	1.95	0.64
1:J:379:GLU:OE2	1:J:386:THR:HG21	1.98	0.64
1:D:358:ARG:NH2	1:D:361:ARG:NH2	2.46	0.64
1:G:86:LEU:HB3	1:G:147:ALA:HA	1.80	0.64
1:G:375:GLU:HB3	1:G:386:THR:HB	1.78	0.64
1:A:85:TYR:HH	1:A:175:HIS:HE2	1.45	0.63
1:S:86:LEU:HB3	1:S:147:ALA:HA	1.79	0.63
1:J:86:LEU:HB3	1:J:147:ALA:HA	1.81	0.63
1:A:271:ALA:HA	1:A:277:ILE:HD11	1.79	0.62
1:M:192:LYS:CE	1:M:225:ASP:HB3	2.29	0.62
1:M:46:ARG:NH2	1:M:215:GLY:O	2.32	0.62
1:M:412:THR:HB	1:M:415:THR:HG21	1.81	0.62
1:S:177:GLU:HB3	1:S:223:ARG:HD2	1.81	0.62
1:A:342:THR:HG21	2:A:501:ICT:H42	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:327:PHE:CE2	1:S:331:LEU:HD11	2.34	0.62
1:M:271:ALA:HA	1:M:277:ILE:HD11	1.80	0.62
1:G:196:PRO:O	1:G:199:ALA:HB3	2.00	0.61
1:A:350:ASN:HD21	1:D:71:ASN:HD22	1.49	0.60
1:V:54:ASN:O	1:V:58:THR:HG23	2.00	0.60
1:V:238:GLU:HG3	1:V:241:ARG:HH12	1.66	0.60
1:S:185:LYS:HE2	1:V:411:THR:O	2.01	0.60
1:A:155:GLY:H	1:A:158:ASN:HD22	1.50	0.60
1:D:192:LYS:CE	1:D:225:ASP:HB3	2.31	0.60
1:J:177:GLU:OE2	1:J:184:LYS:HE2	2.02	0.60
1:J:375:GLU:HB3	1:J:386:THR:HB	1.84	0.59
1:A:192:LYS:HE3	1:A:225:ASP:HB3	1.84	0.59
1:G:363:ARG:NH2	1:G:370:GLU:OE1	2.33	0.59
1:M:375:GLU:HB3	1:M:386:THR:HB	1.83	0.59
1:S:71:ASN:HD22	1:V:350:ASN:HD21	1.50	0.59
1:J:54:ASN:O	1:J:58:THR:HG23	2.02	0.59
1:D:256:VAL:CG2	1:D:262:GLN:HE22	2.14	0.59
1:G:405:ALA:CB	1:G:409:ILE:HG23	2.32	0.59
1:P:192:LYS:CE	1:P:225:ASP:HB3	2.33	0.59
1:P:279:CYS:HB2	1:P:292:PHE:CZ	2.38	0.59
1:D:198:GLN:HE22	1:G:251:GLU:HA	1.67	0.58
1:A:86:LEU:HD21	1:A:116:LEU:HD23	1.85	0.58
1:J:90:GLN:NE2	1:J:346:PHE:H	2.01	0.58
1:J:126:ARG:NH2	1:J:129:GLN:OE1	2.36	0.58
1:P:390:ARG:NH1	5:P:601:HOH:O	2.35	0.58
1:P:126:ARG:NH2	1:P:129:GLN:OE1	2.33	0.58
1:V:50:GLU:HG2	3:V:503:GOL:H31	1.85	0.58
1:G:71:ASN:ND2	1:J:346:PHE:CE1	2.71	0.58
1:G:287:GLU:OE1	1:G:290:ARG:NH1	2.36	0.58
1:A:366:ALA:O	1:A:370:GLU:HG3	2.04	0.57
1:G:281:THR:CG2	1:G:283:GLU:O	2.52	0.57
1:G:405:ALA:HB2	1:G:409:ILE:HG23	1.86	0.57
1:P:404:ILE:HD13	1:V:206:ALA:HB2	1.85	0.57
1:S:90:GLN:NE2	1:S:346:PHE:H	2.02	0.57
1:G:90:GLN:NE2	1:G:346:PHE:H	2.02	0.57
1:M:408:GLU:HG2	5:S:633:HOH:O	2.04	0.57
1:P:408:GLU:O	1:P:408:GLU:HG3	2.06	0.56
1:S:405:ALA:CB	1:S:409:ILE:HG23	2.36	0.56
1:G:16:THR:O	1:G:18:ARG:O	2.23	0.56
1:M:147:ALA:HB1	1:M:166:TYR:CE1	2.41	0.56
1:M:90:GLN:HE22	1:M:345:GLY:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:THR:OG1	1:G:247:GLU:HG3	2.06	0.55
1:D:192:LYS:HE2	1:D:225:ASP:HB3	1.89	0.55
1:V:278:TRP:HB2	1:V:306:ALA:HB3	1.89	0.55
1:G:147:ALA:HB1	1:G:166:TYR:CE1	2.41	0.55
1:A:363:ARG:HH22	1:A:370:GLU:CD	2.08	0.55
1:M:271:ALA:O	1:M:303:LYS:HE2	2.06	0.55
1:A:243:PHE:O	1:A:256:VAL:HA	2.06	0.55
1:M:126:ARG:NH2	1:P:101:MET:O	2.40	0.55
1:M:192:LYS:HE3	1:M:225:ASP:HB3	1.88	0.55
1:A:350:ASN:HD21	1:D:71:ASN:ND2	2.05	0.54
1:D:147:ALA:HB1	1:D:166:TYR:CE1	2.42	0.54
1:J:159:VAL:HG11	1:J:203:ASN:O	2.07	0.54
1:G:347:HIS:NE2	1:J:388:HIS:HD2	2.05	0.54
1:M:30:ASP:OD1	1:M:33:ARG:NH1	2.41	0.54
1:M:422:GLN:NE2	1:P:314:ASN:H	2.04	0.54
1:S:96:ASN:HD22	1:S:98:ALA:H	1.54	0.54
1:P:192:LYS:HE3	1:P:225:ASP:HB3	1.90	0.53
1:G:422:GLN:HE22	1:J:314:ASN:H	1.56	0.53
1:M:128:ASP:OD1	1:S:37:SER:OG	2.26	0.53
1:D:18:ARG:HH12	1:D:275:ASP:CG	2.12	0.53
1:G:422:GLN:NE2	1:J:314:ASN:H	2.07	0.53
1:S:41:GLU:OE1	1:S:46:ARG:NH2	2.42	0.53
1:D:260:LEU:CD2	1:D:291:ARG:HD2	2.39	0.53
1:J:287:GLU:OE2	1:J:290:ARG:NH1	2.41	0.53
1:M:155:GLY:H	1:M:158:ASN:HD22	1.55	0.53
1:P:90:GLN:NE2	1:P:346:PHE:H	2.06	0.53
1:A:40:ILE:HD12	1:G:125:ARG:CZ	2.39	0.53
1:P:175:HIS:HA	1:P:221:VAL:O	2.07	0.53
1:D:271:ALA:HA	1:D:277:ILE:HD11	1.90	0.53
1:P:361:ARG:NH1	1:P:362:ASP:OD1	2.41	0.53
1:J:40:ILE:HG22	1:J:42:TYR:CZ	2.44	0.53
1:M:85:TYR:HH	1:M:175:HIS:HE2	1.57	0.52
1:M:129:GLN:HE21	3:S:504:GOL:H11	1.73	0.52
1:M:177:GLU:HB3	1:M:223:ARG:HD2	1.91	0.52
1:P:245:THR:HA	1:P:257:ARG:NH2	2.25	0.52
1:S:115:GLN:HA	1:S:115:GLN:NE2	2.25	0.52
1:G:44:LEU:HD11	1:G:125:ARG:HD2	1.90	0.52
1:S:10:ILE:O	1:S:13:SER:OG	2.19	0.52
1:S:287:GLU:OE2	1:S:290:ARG:NH1	2.42	0.52
1:V:210:ALA:O	1:V:214:MET:HG2	2.09	0.52
1:M:243:PHE:O	1:M:256:VAL:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:271:ALA:HA	1:P:277:ILE:HD11	1.91	0.52
1:A:375:GLU:HB3	1:A:386:THR:HB	1.92	0.52
1:G:71:ASN:ND2	1:J:350:ASN:HD21	2.03	0.52
1:M:316:LYS:HE2	1:P:373:GLN:HG3	1.90	0.52
1:A:54:ASN:O	1:A:58:THR:HG23	2.10	0.52
1:G:71:ASN:HB2	1:J:94:ASP:OD2	2.10	0.51
1:A:152:GLY:HA3	1:A:159:VAL:HG22	1.93	0.51
1:P:383:TYR:CZ	1:P:385:ALA:HB3	2.45	0.51
1:V:90:GLN:NE2	1:V:346:PHE:H	2.09	0.51
1:A:238:GLU:HG3	1:A:241:ARG:HH21	1.74	0.51
1:J:73:ALA:CB	1:J:120:ILE:HG23	2.40	0.51
1:S:96:ASN:ND2	1:S:98:ALA:HB3	2.25	0.51
1:A:72:GLN:HG3	1:D:349:LEU:HD21	1.93	0.51
1:A:89:TRP:CD1	1:A:104:ASP:HB2	2.46	0.51
1:G:51:ARG:HD3	1:G:144:PRO:HD3	1.93	0.51
1:G:245:THR:OG1	1:G:247:GLU:CG	2.59	0.51
1:M:358:ARG:NH2	1:M:362:ASP:OD2	2.44	0.51
1:D:365:MET:HE3	1:D:368:TYR:HB3	1.93	0.51
1:M:186:CYS:HB3	1:M:189:MET:HG3	1.92	0.51
1:M:375:GLU:OE2	1:P:347:HIS:ND1	2.25	0.51
1:S:405:ALA:HB2	1:S:409:ILE:HG23	1.93	0.51
1:V:283:GLU:OE1	1:V:318:LYS:NZ	2.44	0.51
1:J:59:GLU:HG3	1:J:62:ILE:HD11	1.93	0.50
1:M:359:ASN:OD1	1:M:363:ARG:NH1	2.45	0.50
1:P:408:GLU:O	1:P:408:GLU:CG	2.59	0.50
1:V:183:GLU:O	1:V:185:LYS:HE2	2.11	0.50
1:S:196:PRO:O	1:S:199:ALA:HB3	2.11	0.50
1:G:347:HIS:NE2	1:J:388:HIS:CD2	2.79	0.50
1:S:65:LEU:HD23	1:S:341:VAL:HB	1.94	0.50
1:G:281:THR:HG23	1:G:283:GLU:O	2.11	0.50
1:G:78:LYS:HE3	1:G:131:TYR:OH	2.11	0.50
1:A:256:VAL:HG21	1:A:262:GLN:HE22	1.76	0.50
1:P:186:CYS:HB3	1:P:189:MET:SD	2.52	0.50
1:A:271:ALA:HB3	1:A:272:PRO:HD3	1.94	0.49
1:M:89:TRP:CD1	1:M:104:ASP:HB2	2.48	0.49
1:V:18:ARG:O	1:V:19:PHE:HB2	2.12	0.49
1:A:280:GLU:OE2	2:A:501:ICT:O6	2.30	0.49
5:A:686:HOH:O	1:D:410:SER:HB3	2.12	0.49
1:P:89:TRP:O	1:P:92:ALA:HB3	2.12	0.49
1:J:271:ALA:N	1:J:272:PRO:CD	2.75	0.49
1:J:278:TRP:HB2	1:J:306:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:LEU:HB3	1:G:62:ILE:CD1	2.40	0.49
1:A:358:ARG:NH1	1:A:362:ASP:OD2	2.44	0.49
1:D:104:ASP:HB3	1:D:186:CYS:HB2	1.95	0.48
1:A:184:LYS:HD3	1:A:185:LYS:N	2.28	0.48
1:S:71:ASN:HB2	1:V:94:ASP:OD2	2.13	0.48
1:S:388:HIS:HD2	1:V:347:HIS:NE2	2.10	0.48
1:J:327:PHE:CE2	1:J:331:LEU:HD11	2.48	0.48
1:A:420:GLU:O	1:A:420:GLU:HG2	2.13	0.48
1:D:175:HIS:HA	1:D:221:VAL:O	2.14	0.48
1:D:89:TRP:O	1:D:92:ALA:HB3	2.14	0.48
1:D:147:ALA:HB1	1:D:166:TYR:CZ	2.48	0.48
1:A:46:ARG:NH2	1:A:215:GLY:O	2.44	0.48
1:D:279:CYS:HB2	1:D:292:PHE:CZ	2.49	0.48
1:A:86:LEU:HB3	1:A:147:ALA:HA	1.95	0.48
1:D:40:ILE:HD12	1:J:125:ARG:HD3	1.96	0.48
1:M:90:GLN:HE22	1:M:345:GLY:N	2.12	0.48
1:V:120:ILE:O	1:V:124:LEU:HG	2.14	0.47
1:D:243:PHE:O	1:D:257:ARG:HG3	2.14	0.47
1:M:318:LYS:HD3	1:P:422:GLN:NE2	2.29	0.47
1:A:159:VAL:HG11	1:A:203:ASN:O	2.14	0.47
1:A:388:HIS:HD2	1:D:347:HIS:NE2	2.12	0.47
1:G:73:ALA:CB	1:G:120:ILE:HG23	2.45	0.47
1:M:221:VAL:HG22	1:M:276:MET:HB3	1.97	0.47
1:J:46:ARG:NH2	5:J:602:HOH:O	2.47	0.47
1:D:409:ILE:O	1:D:409:ILE:HG23	2.15	0.47
1:M:44:LEU:HD11	1:M:125:ARG:HD2	1.97	0.47
1:M:383:TYR:CZ	1:M:385:ALA:HB3	2.49	0.47
1:P:40:ILE:HD11	1:V:44:LEU:HD21	1.96	0.47
1:A:94:ASP:OD2	1:D:71:ASN:HB2	2.15	0.47
1:M:388:HIS:HD2	1:P:347:HIS:NE2	2.13	0.47
1:V:86:LEU:HB3	1:V:147:ALA:HA	1.97	0.47
1:G:271:ALA:N	1:G:272:PRO:CD	2.78	0.46
1:G:327:PHE:CE2	1:G:331:LEU:HD11	2.50	0.46
1:P:179:GLN:NE2	1:P:185:LYS:H	2.11	0.46
1:S:16:THR:HB	1:S:17:PRO:CD	2.45	0.46
1:V:155:GLY:H	1:V:158:ASN:HD22	1.62	0.46
1:A:271:ALA:N	1:A:272:PRO:CD	2.78	0.46
1:G:271:ALA:HA	1:G:277:ILE:HD11	1.97	0.46
1:M:41:GLU:HG2	1:S:41:GLU:HB3	1.96	0.46
1:S:96:ASN:HD22	1:S:98:ALA:N	2.13	0.46
1:S:422:GLN:NE2	1:V:314:ASN:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7:ILE:HG23	1:P:28:PRO:HB2	1.98	0.46
1:V:192:LYS:HE2	1:V:225:ASP:HB3	1.98	0.46
1:S:412:THR:HB	1:S:415:THR:CG2	2.46	0.46
1:M:271:ALA:N	1:M:272:PRO:CD	2.79	0.46
1:V:266:ARG:HB3	1:V:270:TYR:CE2	2.51	0.46
1:D:295:ALA:O	1:D:298:ALA:HB3	2.16	0.46
1:S:387:ARG:NH2	1:S:423:PHE:HB3	2.31	0.46
1:V:159:VAL:HG11	1:V:203:ASN:O	2.16	0.46
1:V:271:ALA:N	1:V:272:PRO:CD	2.78	0.46
1:G:375:GLU:OE2	1:J:347:HIS:ND1	2.46	0.46
1:P:404:ILE:HD13	1:V:206:ALA:CB	2.46	0.46
1:S:2:ASP:HA	1:S:5:ALA:HB3	1.97	0.46
1:S:388:HIS:CD2	1:V:347:HIS:NE2	2.84	0.46
1:A:241:ARG:N	1:A:242:PRO:HD2	2.31	0.46
1:M:86:LEU:HB3	1:M:147:ALA:HA	1.98	0.46
1:S:306:ALA:HA	1:S:338:PHE:O	2.16	0.46
1:J:283:GLU:OE1	1:J:318:LYS:NZ	2.48	0.46
1:S:177:GLU:CB	1:S:223:ARG:HD2	2.44	0.46
1:A:104:ASP:O	1:A:185:LYS:HA	2.16	0.45
1:A:90:GLN:HE22	1:A:345:GLY:CA	2.30	0.45
1:D:126:ARG:NH1	1:D:129:GLN:OE1	2.50	0.45
1:G:283:GLU:HB2	1:G:318:LYS:HE2	1.97	0.45
1:M:55:LEU:HB3	1:M:62:ILE:HD11	1.98	0.45
1:V:192:LYS:CE	1:V:225:ASP:HB3	2.47	0.45
1:A:159:VAL:HG13	1:A:176:PHE:CE1	2.52	0.45
1:A:184:LYS:HD3	1:A:184:LYS:C	2.37	0.45
1:G:54:ASN:N	1:G:54:ASN:HD22	2.15	0.45
1:G:71:ASN:HD22	1:J:350:ASN:ND2	2.07	0.45
1:G:369:SER:OG	1:J:316:LYS:HE3	2.16	0.45
1:P:90:GLN:HE22	1:P:345:GLY:N	2.15	0.45
1:G:65:LEU:HD23	1:G:341:VAL:HB	1.99	0.45
1:M:241:ARG:HB2	1:M:242:PRO:HD3	1.98	0.45
1:M:363:ARG:HH22	1:M:370:GLU:CD	2.19	0.45
1:V:73:ALA:HB1	1:V:84:ILE:HD13	1.97	0.45
1:M:63:ASN:HA	1:M:339:GLN:O	2.16	0.45
1:P:208:ARG:CZ	1:P:220:ILE:HD12	2.47	0.45
1:A:86:LEU:C	1:A:86:LEU:HD13	2.37	0.45
1:J:104:ASP:HB3	1:J:186:CYS:HB2	1.99	0.45
1:V:266:ARG:HD2	1:V:270:TYR:OH	2.17	0.45
1:V:319:LEU:HD22	1:V:323:THR:HG21	1.99	0.45
1:M:365:MET:SD	1:P:309:CYS:HB3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLU:OE2	1:D:347:HIS:ND1	2.34	0.45
1:P:256:VAL:HG21	1:P:262:GLN:HE22	1.81	0.45
1:G:349:LEU:HD21	1:J:72:GLN:HG2	1.98	0.44
1:P:33:ARG:NE	1:V:399:GLU:OE1	2.45	0.44
1:S:90:GLN:HE21	1:S:346:PHE:H	1.65	0.44
1:G:134:GLU:OE1	1:G:390:ARG:NH2	2.50	0.44
1:P:90:GLN:HE22	1:P:345:GLY:H	1.64	0.44
1:J:147:ALA:HB1	1:J:166:TYR:CE1	2.52	0.44
1:J:241:ARG:N	1:J:242:PRO:HD2	2.33	0.44
1:S:71:ASN:ND2	1:V:350:ASN:HD21	2.15	0.44
1:P:175:HIS:HB3	1:P:221:VAL:HB	1.97	0.44
1:S:271:ALA:HA	1:S:277:ILE:HD11	2.00	0.44
1:D:198:GLN:NE2	1:D:202:ARG:HH22	2.15	0.44
1:V:18:ARG:O	1:V:19:PHE:CB	2.65	0.44
1:D:266:ARG:HD2	1:D:270:TYR:OH	2.18	0.44
1:G:66:GLY:HA2	1:G:85:TYR:O	2.18	0.44
1:S:175:HIS:HA	1:S:221:VAL:O	2.17	0.44
1:V:106:SER:HB2	1:V:184:LYS:HG2	2.00	0.44
1:D:40:ILE:CD1	1:J:125:ARG:HD3	2.48	0.44
1:J:175:HIS:HA	1:J:221:VAL:O	2.18	0.44
1:M:342:THR:HB	2:M:501:ICT:O1	2.18	0.44
1:S:55:LEU:HB3	1:S:62:ILE:CD1	2.44	0.44
1:A:347:HIS:NE2	1:D:388:HIS:HD2	2.16	0.44
1:M:97:LEU:HD21	1:M:115:GLN:HG2	2.00	0.44
1:P:422:GLN:HE21	1:P:422:GLN:HB3	1.60	0.44
1:S:52:LEU:HD23	1:S:219:ILE:HD13	2.00	0.44
1:A:55:LEU:HB3	1:A:62:ILE:HD11	2.00	0.43
2:J:501:ICT:O5	2:J:501:ICT:C5	2.66	0.43
1:M:86:LEU:HD21	1:M:116:LEU:HD23	1.99	0.43
1:A:19:PHE:O	1:A:20:ALA:C	2.56	0.43
1:M:209:LEU:O	1:M:213:VAL:HG23	2.18	0.43
1:A:18:ARG:HA	1:A:18:ARG:HD2	1.93	0.43
1:A:63:ASN:HA	1:A:339:GLN:O	2.19	0.43
1:A:208:ARG:HA	1:A:220:ILE:HD11	2.00	0.43
1:J:91:VAL:O	1:J:96:ASN:HB3	2.19	0.43
1:J:241:ARG:N	1:J:242:PRO:CD	2.81	0.43
1:P:18:ARG:O	1:P:19:PHE:CB	2.66	0.43
1:S:271:ALA:N	1:S:272:PRO:CD	2.82	0.43
1:M:177:GLU:CB	1:M:223:ARG:HD2	2.48	0.43
1:S:115:GLN:NE2	1:S:115:GLN:CA	2.82	0.43
1:S:208:ARG:HA	1:S:220:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ASN:HD22	1:J:124:LEU:HD12	1.84	0.43
1:M:241:ARG:N	1:M:242:PRO:HD2	2.33	0.43
1:M:316:LYS:HD2	1:P:369:SER:HB2	2.01	0.43
1:V:198:GLN:HG2	1:V:237:ASP:OD2	2.19	0.43
1:D:152:GLY:HA3	1:D:159:VAL:HG22	2.01	0.43
1:D:363:ARG:O	1:D:366:ALA:HB3	2.19	0.43
1:S:85:TYR:CE2	1:S:342:THR:HG22	2.54	0.43
1:V:363:ARG:NH2	1:V:370:GLU:OE1	2.51	0.43
1:A:293:ALA:HA	1:A:305:LEU:HD11	2.00	0.43
1:V:399:GLU:O	1:V:403:VAL:HG23	2.19	0.43
1:V:408:GLU:HG3	1:V:408:GLU:O	2.19	0.43
1:A:186:CYS:HB3	1:A:189:MET:HG3	2.00	0.42
1:G:411:THR:O	1:J:185:LYS:HE2	2.17	0.42
1:M:352:SER:HB3	1:P:352:SER:HB3	2.00	0.42
1:J:100:GLN:HB2	1:J:102:TYR:CE2	2.53	0.42
1:M:327:PHE:CE2	1:M:331:LEU:HD11	2.54	0.42
1:V:175:HIS:HA	1:V:221:VAL:O	2.19	0.42
1:V:281:THR:HG21	1:V:307:TYR:OH	2.20	0.42
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.93	0.42
1:M:90:GLN:HE22	1:M:345:GLY:CA	2.32	0.42
1:V:24:ARG:O	1:V:26:TYR:N	2.50	0.42
1:V:125:ARG:HG2	1:V:142:PHE:HE1	1.84	0.42
1:V:383:TYR:CZ	1:V:385:ALA:HB3	2.55	0.42
1:J:192:LYS:HE3	1:J:225:ASP:HB3	2.02	0.42
1:M:379:GLU:HA	1:M:383:TYR:O	2.19	0.42
1:D:90:GLN:HE22	1:D:345:GLY:N	2.17	0.42
1:D:260:LEU:HD23	1:D:291:ARG:HD2	2.01	0.42
1:V:175:HIS:HB3	1:V:221:VAL:HB	2.01	0.42
1:A:47:MET:HE1	1:G:38:VAL:HG21	2.02	0.42
1:G:349:LEU:HD21	1:J:72:GLN:CG	2.50	0.42
1:J:238:GLU:HA	1:J:241:ARG:HH11	1.84	0.42
1:M:414:LEU:HD23	1:M:414:LEU:HA	1.92	0.42
1:P:183:GLU:O	1:P:185:LYS:HE2	2.19	0.42
1:S:353:MET:CE	1:V:345:GLY:HA2	2.50	0.42
1:V:327:PHE:CE2	1:V:331:LEU:HD11	2.54	0.42
1:P:152:GLY:HA3	1:P:159:VAL:HG22	2.01	0.42
1:S:13:SER:HB2	3:S:503:GOL:H32	2.01	0.42
1:S:327:PHE:HE2	1:S:331:LEU:HD11	1.83	0.42
1:J:266:ARG:HD2	1:J:270:TYR:OH	2.19	0.42
1:J:323:THR:O	1:J:327:PHE:N	2.53	0.42
1:M:66:GLY:O	1:M:76:GLN:NE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD21	1:A:115:GLN:HG2	2.01	0.42
1:A:260:LEU:O	1:A:264:ILE:HG13	2.19	0.42
1:G:7:ILE:HG23	1:G:28:PRO:HB2	2.00	0.42
1:G:156:PRO:O	1:G:159:VAL:HB	2.19	0.42
1:S:51:ARG:HD3	1:S:144:PRO:HD3	2.01	0.42
1:A:43:THR:HG22	1:A:47:MET:SD	2.59	0.42
1:A:147:ALA:HB1	1:A:166:TYR:CE1	2.54	0.42
1:M:389:GLN:OE1	1:M:389:GLN:HA	2.20	0.42
1:S:414:LEU:HD23	1:S:414:LEU:HA	1.85	0.42
1:G:2:ASP:HA	1:G:5:ALA:HB3	2.02	0.41
1:M:159:VAL:HG11	1:M:203:ASN:O	2.19	0.41
1:M:175:HIS:HA	1:M:221:VAL:O	2.20	0.41
1:M:241:ARG:N	1:M:242:PRO:CD	2.84	0.41
1:P:390:ARG:CZ	1:P:390:ARG:HB2	2.50	0.41
1:A:16:THR:O	1:A:18:ARG:O	2.38	0.41
1:G:281:THR:HG22	1:G:313:PHE:CZ	2.56	0.41
1:D:179:GLN:NE2	1:D:185:LYS:H	2.12	0.41
1:G:121:ASN:HD22	1:G:121:ASN:HA	1.67	0.41
1:G:163:MET:O	1:G:167:ILE:HG13	2.21	0.41
1:G:353:MET:CE	1:J:345:GLY:HA2	2.49	0.41
1:S:194:LEU:HD11	1:S:226:ALA:HA	2.01	0.41
1:V:68:LEU:HA	1:V:116:LEU:HD21	2.02	0.41
1:M:86:LEU:C	1:M:86:LEU:HD13	2.40	0.41
1:P:174:VAL:HG12	1:P:176:PHE:CE2	2.55	0.41
1:D:401:ALA:HB1	1:D:409:ILE:CD1	2.50	0.41
1:J:63:ASN:HA	1:J:339:GLN:O	2.20	0.41
1:M:90:GLN:HE22	1:M:345:GLY:HA3	1.85	0.41
1:V:147:ALA:HB1	1:V:166:TYR:CE1	2.55	0.41
1:G:22:ILE:HD12	1:G:22:ILE:C	2.41	0.41
1:A:18:ARG:HH21	1:A:275:ASP:CG	2.23	0.41
1:D:71:ASN:O	1:D:74:MET:HB3	2.20	0.41
1:S:194:LEU:O	1:S:233:THR:HG23	2.21	0.41
1:S:408:GLU:O	1:S:408:GLU:HG2	2.20	0.41
1:V:90:GLN:HE21	1:V:346:PHE:H	1.69	0.41
1:V:248:ARG:HA	1:V:253:PHE:O	2.20	0.41
1:A:98:ALA:HB2	1:A:109:PRO:HD3	2.03	0.41
1:A:290:ARG:NH1	1:A:294:GLU:OE2	2.53	0.41
1:D:44:LEU:HD21	1:J:40:ILE:HD11	2.02	0.41
1:D:90:GLN:NE2	1:D:346:PHE:H	2.18	0.41
1:M:281:THR:CG2	1:M:283:GLU:O	2.68	0.41
1:P:18:ARG:O	1:P:19:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:226:ALA:HB3	1:P:263:ALA:HA	2.02	0.41
1:A:221:VAL:HG22	1:A:276:MET:HB3	2.01	0.41
1:D:89:TRP:CD1	1:D:104:ASP:HB2	2.56	0.41
1:G:283:GLU:CB	1:G:318:LYS:HE2	2.51	0.41
1:G:305:LEU:O	1:G:336:TYR:HA	2.21	0.41
1:G:306:ALA:HA	1:G:338:PHE:O	2.21	0.41
1:G:360:TYR:OH	1:J:63:ASN:HB2	2.21	0.41
1:M:98:ALA:HB2	1:M:109:PRO:HD3	2.03	0.41
1:P:198:GLN:HG2	1:P:237:ASP:OD2	2.20	0.41
1:G:388:HIS:CD2	1:J:347:HIS:NE2	2.89	0.41
1:M:283:GLU:CB	1:M:318:LYS:HE2	2.51	0.41
1:S:316:LYS:HZ2	1:V:373:GLN:HE21	1.69	0.41
1:V:155:GLY:N	1:V:158:ASN:HD22	2.19	0.41
1:V:412:THR:HG22	1:V:415:THR:HB	2.02	0.41
1:D:1:MET:O	1:D:1:MET:HG2	2.21	0.40
1:P:363:ARG:O	1:P:366:ALA:HB3	2.20	0.40
1:S:78:LYS:HE3	1:S:131:TYR:OH	2.21	0.40
1:D:132:HIS:HE1	1:J:32:TYR:O	2.04	0.40
1:M:306:ALA:HA	1:M:338:PHE:O	2.21	0.40
1:M:387:ARG:NH2	1:M:423:PHE:C	2.75	0.40
1:P:82:LYS:O	1:P:144:PRO:HD2	2.21	0.40
1:P:204:LEU:HD23	1:P:204:LEU:HA	1.89	0.40
1:V:149:ALA:HB1	1:V:176:PHE:CE1	2.56	0.40
1:A:68:LEU:HA	1:A:116:LEU:HD21	2.03	0.40
1:G:358:ARG:HD2	1:G:358:ARG:O	2.22	0.40
1:M:159:VAL:HG13	1:M:176:PHE:CE1	2.57	0.40
1:P:245:THR:OG1	1:P:247:GLU:HG2	2.21	0.40
1:S:327:PHE:CE2	1:S:331:LEU:CD1	3.03	0.40
1:V:241:ARG:N	1:V:242:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	421/436 (97%)	401 (95%)	19 (4%)	1 (0%)	47 78
1	D	421/436 (97%)	401 (95%)	17 (4%)	3 (1%)	22 54
1	G	421/436 (97%)	399 (95%)	21 (5%)	1 (0%)	47 78
1	J	421/436 (97%)	395 (94%)	26 (6%)	0	100 100
1	M	421/436 (97%)	398 (94%)	20 (5%)	3 (1%)	22 54
1	P	421/436 (97%)	394 (94%)	25 (6%)	2 (0%)	29 61
1	S	421/436 (97%)	403 (96%)	17 (4%)	1 (0%)	47 78
1	V	421/436 (97%)	400 (95%)	20 (5%)	1 (0%)	47 78
All	All	3368/3488 (97%)	3191 (95%)	165 (5%)	12 (0%)	34 66

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	408	GLU
1	D	409	ILE
1	G	245	THR
1	M	409	ILE
1	P	94	ASP
1	A	20	ALA
1	S	408	GLU
1	V	138	ASP
1	D	94	ASP
1	P	137	ASN
1	M	94	ASP
1	M	106	SER

5.3.2 Protein sidechains (i)

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	324/335 (97%)	318 (98%)	6 (2%)	57 84
1	D	324/335 (97%)	315 (97%)	9 (3%)	43 76
1	G	324/335 (97%)	318 (98%)	6 (2%)	57 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	324/335 (97%)	316 (98%)	8 (2%)	47 78
1	M	324/335 (97%)	316 (98%)	8 (2%)	47 78
1	P	324/335 (97%)	312 (96%)	12 (4%)	34 68
1	S	324/335 (97%)	309 (95%)	15 (5%)	27 60
1	V	324/335 (97%)	313 (97%)	11 (3%)	37 71
All	All	2592/2680 (97%)	2517 (97%)	75 (3%)	42 76

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	128	ASP
1	A	166	TYR
1	A	303	LYS
1	A	343	LEU
1	A	420	GLU
1	D	37	SER
1	D	38	VAL
1	D	86	LEU
1	D	126	ARG
1	D	198	GLN
1	D	261	ASP
1	D	281	THR
1	D	299	GLN
1	D	423	PHE
1	G	86	LEU
1	G	121	ASN
1	G	163	MET
1	G	182	SER
1	G	184	LYS
1	G	281	THR
1	J	68	LEU
1	J	74	MET
1	J	86	LEU
1	J	121	ASN
1	J	182	SER
1	J	281	THR
1	J	323	THR
1	J	390	ARG
1	M	9	GLN

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Mol	Chain	Res	Type
1	M	68	LEU
1	M	138	ASP
1	M	223	ARG
1	M	281	THR
1	M	303	LYS
1	M	343	LEU
1	M	420	GLU
1	P	9	GLN
1	P	59	GLU
1	P	105	GLN
1	P	163	MET
1	P	166	TYR
1	P	184	LYS
1	P	217	PRO
1	P	218	THR
1	P	261	ASP
1	P	281	THR
1	P	409	ILE
1	P	423	PHE
1	S	86	LEU
1	S	96	ASN
1	S	105	GLN
1	S	128	ASP
1	S	138	ASP
1	S	182	SER
1	S	223	ARG
1	S	369	SER
1	S	370	GLU
1	S	390	ARG
1	S	412	THR
1	S	414	LEU
1	S	419	GLU
1	S	420	GLU
1	S	421	GLU
1	V	86	LEU
1	V	106	SER
1	V	126	ARG
1	V	184	LYS
1	V	227	ASN
1	V	261	ASP
1	V	343	LEU
1	V	358	ARG

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Mol	Chain	Res	Type
1	V	390	ARG
1	V	402	GLN
1	V	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	90	GLN
1	A	132	HIS
1	A	137	ASN
1	A	158	ASN
1	A	179	GLN
1	A	188	HIS
1	A	198	GLN
1	A	262	GLN
1	A	373	GLN
1	A	388	HIS
1	D	15	ASN
1	D	54	ASN
1	D	63	ASN
1	D	71	ASN
1	D	90	GLN
1	D	132	HIS
1	D	179	GLN
1	D	198	GLN
1	D	262	GLN
1	D	328	GLN
1	D	388	HIS
1	D	402	GLN
1	G	54	ASN
1	G	63	ASN
1	G	71	ASN
1	G	76	GLN
1	G	90	GLN
1	G	121	ASN
1	G	132	HIS
1	G	158	ASN
1	G	179	GLN
1	G	198	GLN
1	G	388	HIS
1	G	422	GLN

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Mol	Chain	Res	Type
1	J	54	ASN
1	J	71	ASN
1	J	90	GLN
1	J	105	GLN
1	J	115	GLN
1	J	121	ASN
1	J	158	ASN
1	J	179	GLN
1	J	188	HIS
1	J	262	GLN
1	J	373	GLN
1	J	388	HIS
1	J	422	GLN
1	M	54	ASN
1	M	90	GLN
1	M	121	ASN
1	M	137	ASN
1	M	158	ASN
1	M	179	GLN
1	M	188	HIS
1	M	198	GLN
1	M	262	GLN
1	M	388	HIS
1	M	422	GLN
1	P	9	GLN
1	P	54	ASN
1	P	57	HIS
1	P	90	GLN
1	P	121	ASN
1	P	132	HIS
1	P	158	ASN
1	P	179	GLN
1	P	262	GLN
1	P	373	GLN
1	P	388	HIS
1	P	422	GLN
1	S	9	GLN
1	S	54	ASN
1	S	71	ASN
1	S	90	GLN
1	S	96	ASN
1	S	115	GLN

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Mol	Chain	Res	Type
1	S	132	HIS
1	S	158	ASN
1	S	179	GLN
1	S	227	ASN
1	S	388	HIS
1	S	422	GLN
1	V	54	ASN
1	V	71	ASN
1	V	90	GLN
1	V	105	GLN
1	V	132	HIS
1	V	158	ASN
1	V	179	GLN
1	V	198	GLN
1	V	227	ASN
1	V	262	GLN
1	V	388	HIS
1	V	422	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
3	GOL	S	502	-	5,5,5	0.17	0	5,5,5	0.50	0
3	GOL	P	502	-	5,5,5	0.19	0	5,5,5	0.38	0
3	GOL	V	502	-	5,5,5	0.16	0	5,5,5	0.55	0
3	GOL	G	503	-	5,5,5	0.11	0	5,5,5	0.22	0
3	GOL	D	502	-	5,5,5	0.17	0	5,5,5	0.36	0
3	GOL	S	504	-	5,5,5	0.27	0	5,5,5	0.56	0
3	GOL	A	502	-	5,5,5	0.23	0	5,5,5	0.67	0
3	GOL	J	503	-	5,5,5	0.11	0	5,5,5	0.30	0
3	GOL	V	503	-	5,5,5	0.20	0	5,5,5	0.28	0
2	ICT	A	501	4	12,12,12	1.17	2 (16%)	13,16,16	1.42	1 (7%)
2	ICT	M	501	4	12,12,12	1.00	1 (8%)	13,16,16	1.48	2 (15%)
2	ICT	D	501	4	12,12,12	1.16	0	13,16,16	1.21	1 (7%)
3	GOL	J	502	-	5,5,5	0.12	0	5,5,5	0.35	0
2	ICT	G	501	4	12,12,12	1.21	2 (16%)	13,16,16	1.29	0
3	GOL	S	503	-	5,5,5	0.10	0	5,5,5	0.34	0
2	ICT	P	501	4	12,12,12	1.26	1 (8%)	13,16,16	0.98	0
2	ICT	S	501	4	12,12,12	1.33	2 (16%)	13,16,16	1.11	1 (7%)
3	GOL	G	502	-	5,5,5	0.09	0	5,5,5	0.20	0
2	ICT	V	501	4	12,12,12	1.10	0	13,16,16	1.21	1 (7%)
2	ICT	J	501	4	12,12,12	1.13	0	13,16,16	1.31	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
3	GOL	S	502	-	-	0/4/4/4	-
3	GOL	P	502	-	-	2/4/4/4	-
3	GOL	V	502	-	-	0/4/4/4	-
3	GOL	G	503	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	S	504	-	-	4/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	J	503	-	-	2/4/4/4	-
3	GOL	V	503	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ICT	A	501	4	-	12/16/16/16	-
2	ICT	M	501	4	-	4/16/16/16	-
2	ICT	D	501	4	-	8/16/16/16	-
3	GOL	J	502	-	-	2/4/4/4	-
2	ICT	G	501	4	-	5/16/16/16	-
3	GOL	S	503	-	-	2/4/4/4	-
2	ICT	P	501	4	-	6/16/16/16	-
2	ICT	S	501	4	-	12/16/16/16	-
3	GOL	G	502	-	-	2/4/4/4	-
2	ICT	V	501	4	-	4/16/16/16	-
2	ICT	J	501	4	-	7/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	501	ICT	O5-C6	2.61	1.30	1.22
2	P	501	ICT	O4-C5	-2.52	1.22	1.30
2	G	501	ICT	O2-C1	-2.50	1.22	1.30
2	S	501	ICT	O2-C1	-2.14	1.23	1.30
2	M	501	ICT	O2-C1	-2.12	1.23	1.30
2	A	501	ICT	O2-C1	-2.08	1.23	1.30
2	A	501	ICT	O4-C5	-2.06	1.23	1.30
2	G	501	ICT	O4-C5	-2.01	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	501	ICT	C4-C3-C2	2.69	117.84	110.29
2	M	501	ICT	O5-C6-C3	-2.31	117.15	122.95
2	V	501	ICT	O5-C6-C3	-2.26	117.28	122.95
2	D	501	ICT	O5-C6-C3	-2.16	117.54	122.95
2	A	501	ICT	O5-C6-C3	-2.12	117.64	122.95
2	S	501	ICT	O7-C2-C3	-2.02	105.66	110.58

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ICT	O7-C2-C3-C6

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Mol	Chain	Res	Type	Atoms
2	A	501	ICT	C6-C3-C4-C5
2	D	501	ICT	C6-C3-C4-C5
2	J	501	ICT	C2-C3-C4-C5
2	J	501	ICT	C6-C3-C4-C5
2	M	501	ICT	C1-C2-C3-C4
2	M	501	ICT	C6-C3-C4-C5
2	P	501	ICT	C1-C2-C3-C4
2	P	501	ICT	C6-C3-C4-C5
2	S	501	ICT	C1-C2-C3-C4
2	S	501	ICT	O7-C2-C3-C4
2	S	501	ICT	C2-C3-C4-C5
2	S	501	ICT	C6-C3-C4-C5
2	V	501	ICT	C2-C3-C4-C5
2	V	501	ICT	C6-C3-C4-C5
3	D	502	GOL	C1-C2-C3-O3
3	D	502	GOL	O2-C2-C3-O3
3	G	502	GOL	O1-C1-C2-C3
3	J	502	GOL	O1-C1-C2-C3
3	S	504	GOL	O1-C1-C2-C3
3	S	504	GOL	C1-C2-C3-O3
3	V	503	GOL	C1-C2-C3-O3
2	J	501	ICT	O1-C1-C2-O7
2	J	501	ICT	O2-C1-C2-O7
2	A	501	ICT	O1-C1-C2-O7
2	A	501	ICT	O2-C1-C2-O7
2	P	501	ICT	O1-C1-C2-O7
3	A	502	GOL	O1-C1-C2-C3
3	G	503	GOL	O1-C1-C2-C3
3	J	503	GOL	O1-C1-C2-C3
3	P	502	GOL	O1-C1-C2-C3
2	P	501	ICT	O2-C1-C2-O7
3	A	502	GOL	O1-C1-C2-O2
3	G	502	GOL	O1-C1-C2-O2
3	J	502	GOL	O1-C1-C2-O2
3	S	504	GOL	O2-C2-C3-O3
3	V	503	GOL	O2-C2-C3-O3
2	S	501	ICT	O2-C1-C2-O7
2	A	501	ICT	C1-C2-C3-C6
2	S	501	ICT	C1-C2-C3-C6
3	G	503	GOL	O1-C1-C2-O2
3	S	504	GOL	O1-C1-C2-O2
2	A	501	ICT	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	G	501	ICT	O7-C2-C3-C6
2	S	501	ICT	O7-C2-C3-C6
2	D	501	ICT	C2-C3-C4-C5
2	A	501	ICT	O1-C1-C2-C3
2	A	501	ICT	C4-C3-C6-O6
3	J	503	GOL	O1-C1-C2-O2
3	P	502	GOL	O1-C1-C2-O2
3	V	503	GOL	O1-C1-C2-O2
2	S	501	ICT	O1-C1-C2-O7
2	D	501	ICT	O1-C1-C2-O7
2	D	501	ICT	O1-C1-C2-C3
2	S	501	ICT	O1-C1-C2-C3
2	D	501	ICT	C3-C4-C5-O3
2	D	501	ICT	C3-C4-C5-O4
2	V	501	ICT	C3-C4-C5-O3
2	P	501	ICT	O1-C1-C2-C3
2	S	501	ICT	O2-C1-C2-C3
3	S	503	GOL	O1-C1-C2-C3
3	V	503	GOL	O1-C1-C2-C3
2	M	501	ICT	C3-C4-C5-O4
2	D	501	ICT	O2-C1-C2-O7
2	D	501	ICT	O2-C1-C2-C3
2	A	501	ICT	C3-C4-C5-O3
2	V	501	ICT	C3-C4-C5-O4
2	M	501	ICT	C3-C4-C5-O3
2	P	501	ICT	O2-C1-C2-C3
2	A	501	ICT	C4-C3-C6-O5
2	G	501	ICT	C4-C3-C6-O5
2	S	501	ICT	C4-C3-C6-O5
2	S	501	ICT	C4-C3-C6-O6
3	S	503	GOL	O1-C1-C2-O2
2	A	501	ICT	C3-C4-C5-O4
2	J	501	ICT	C3-C4-C5-O4
2	A	501	ICT	O7-C2-C3-C4
2	J	501	ICT	O2-C1-C2-C3
2	G	501	ICT	C3-C4-C5-O4
2	G	501	ICT	O2-C1-C2-C3
2	G	501	ICT	C3-C4-C5-O3
2	J	501	ICT	C3-C4-C5-O3

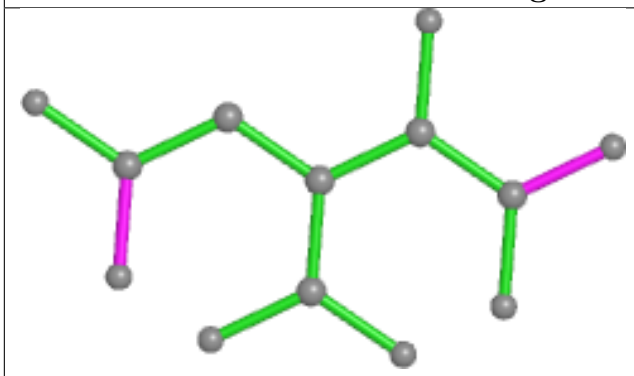
There are no ring outliers.

8 monomers are involved in 10 short contacts:

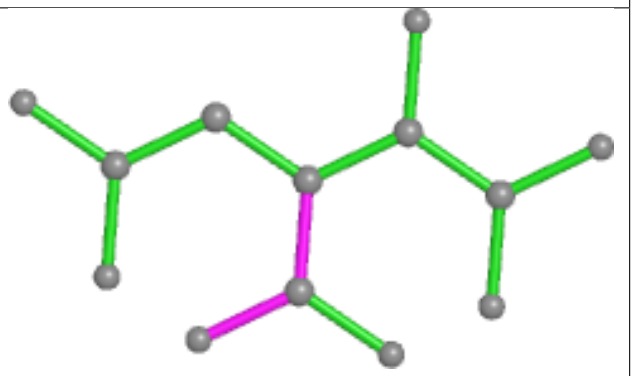
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	504	GOL	1	0
3	V	503	GOL	1	0
2	A	501	ICT	2	0
2	M	501	ICT	1	0
2	G	501	ICT	1	0
3	S	503	GOL	1	0
2	S	501	ICT	1	0
2	J	501	ICT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

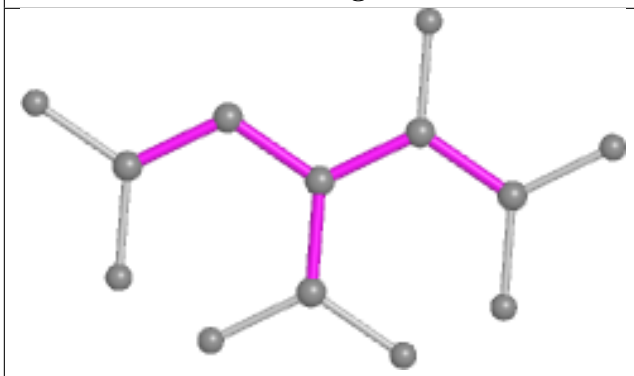
Ligand ICT A 501



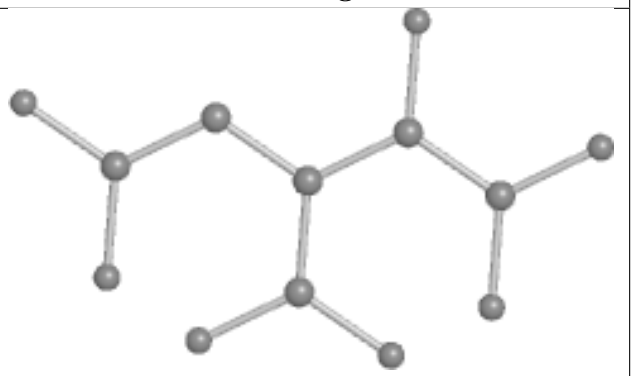
Bond lengths



Bond angles

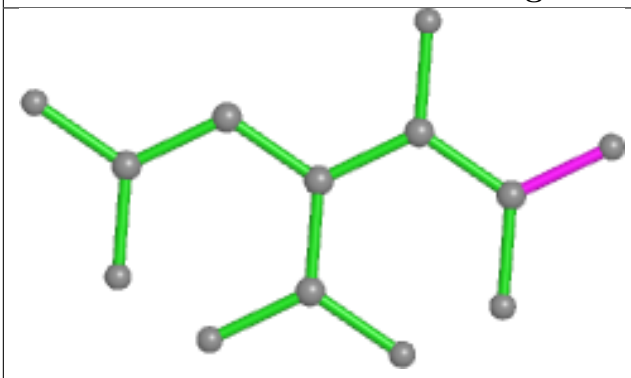


Torsions



Rings

Ligand ICT M 501



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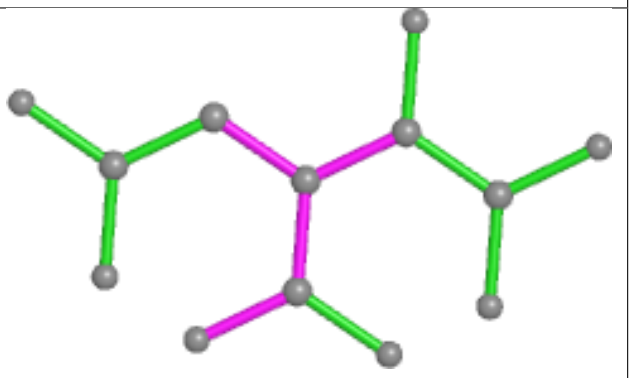
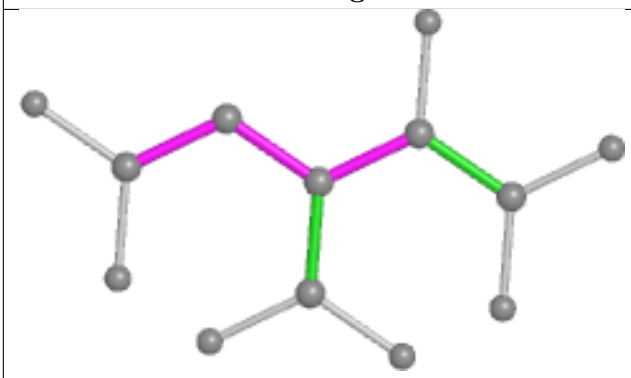
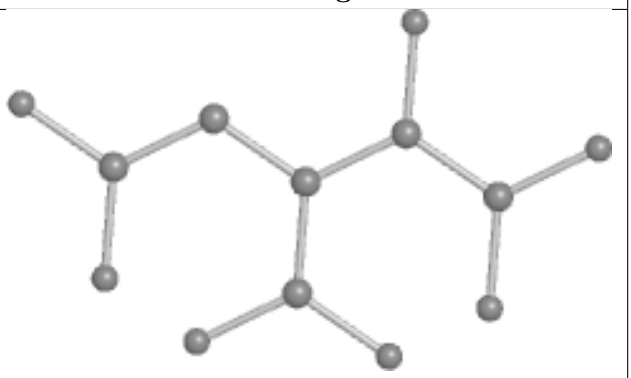


Bond angles

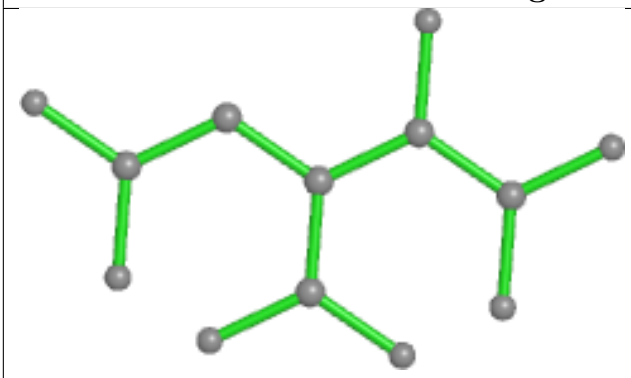


Torsions

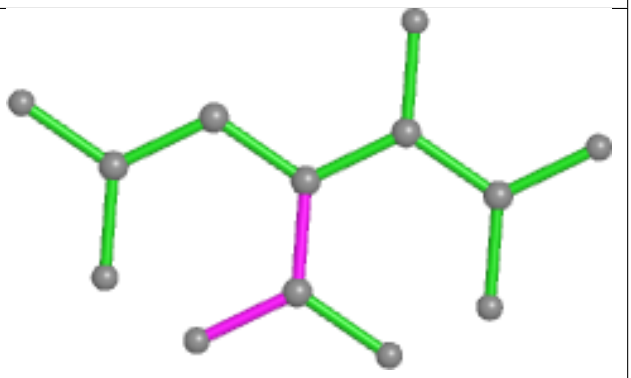


Rings

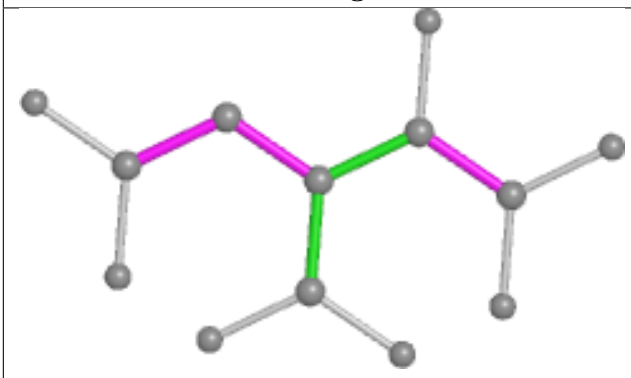
Ligand ICT D 501



Bond lengths



Bond angles



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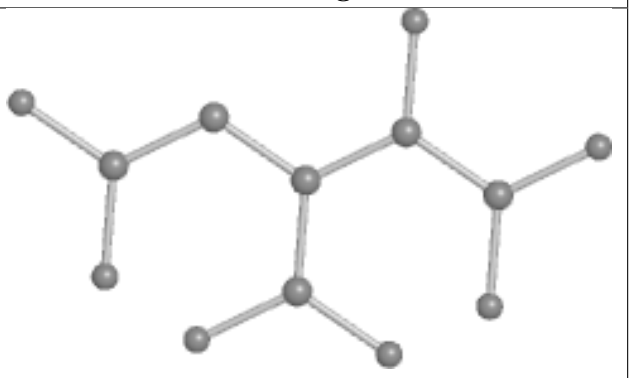
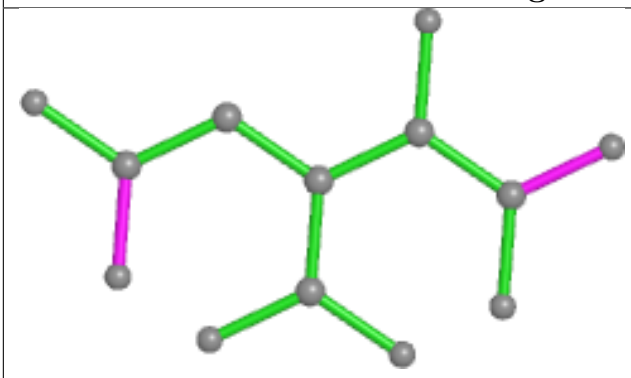
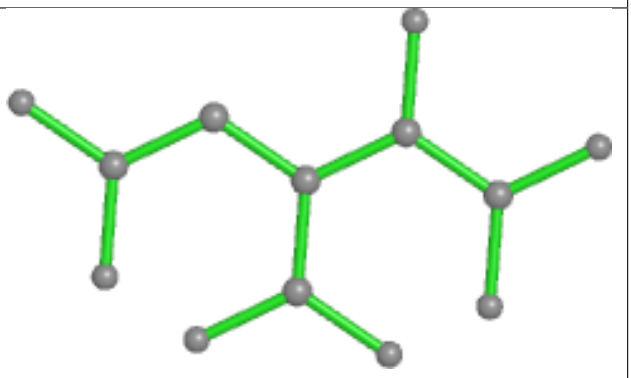


Rings

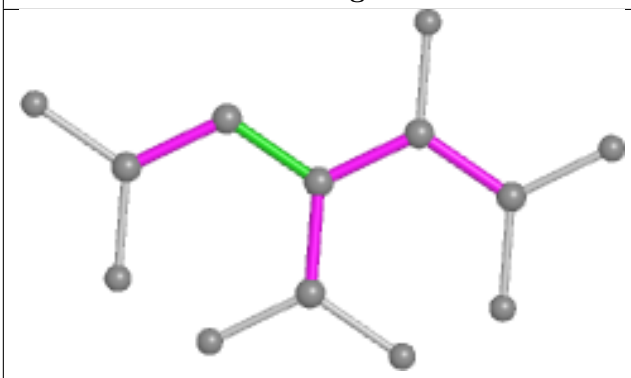
Ligand ICT G 501



Bond lengths



Bond angles



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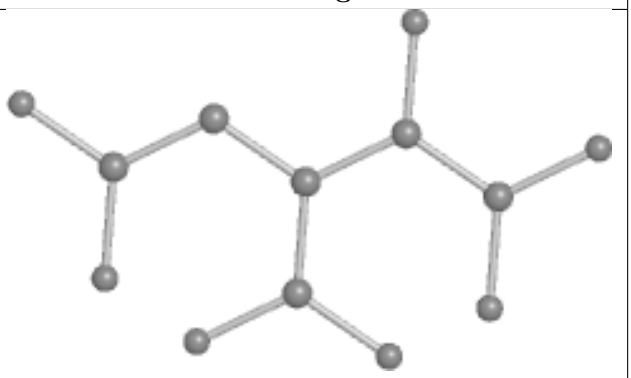
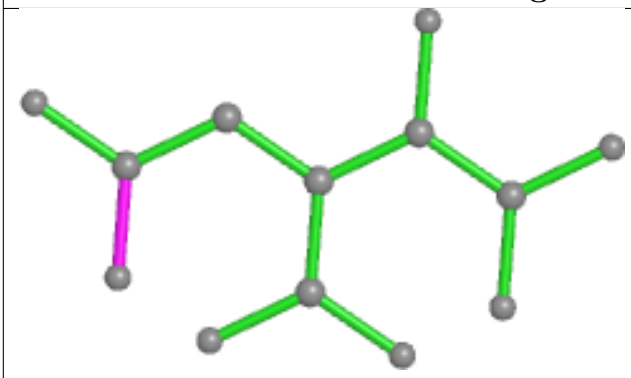
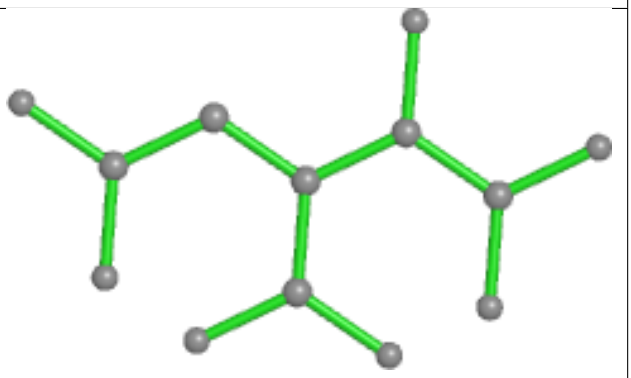


Rings

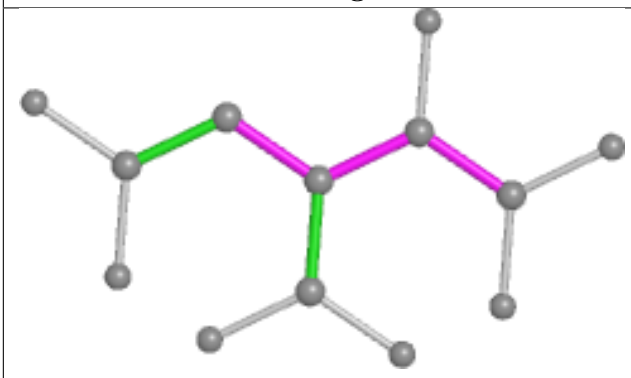
Ligand ICT P 501



Bond lengths



Bond angles



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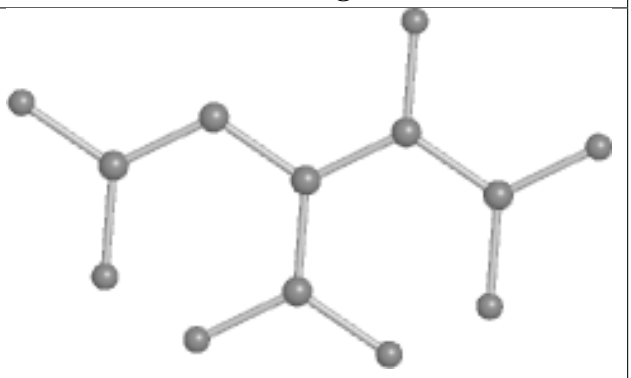
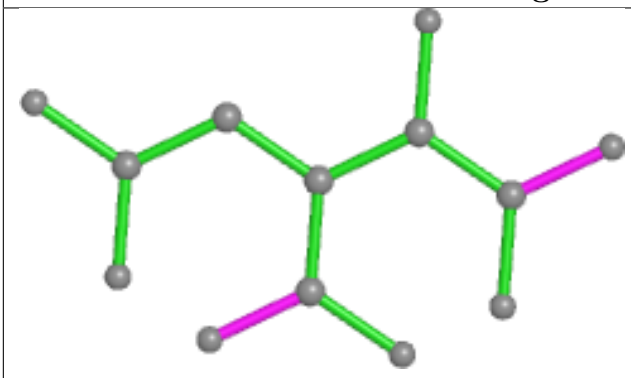
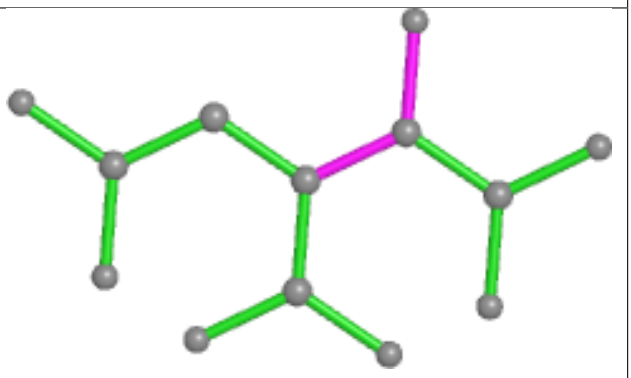


Rings

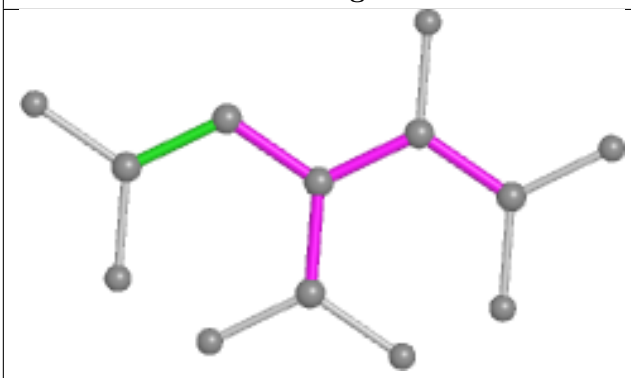
Ligand ICT S 501



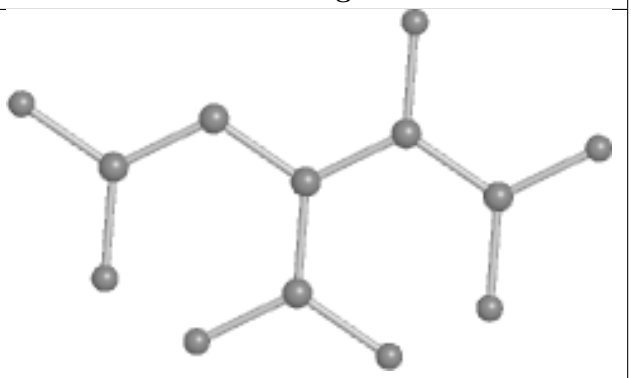
Bond lengths



Bond angles

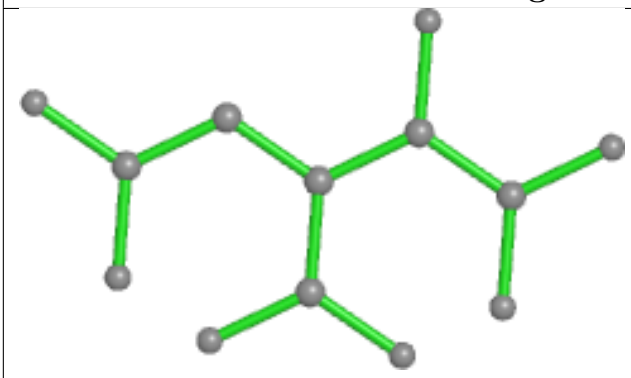


Torsions

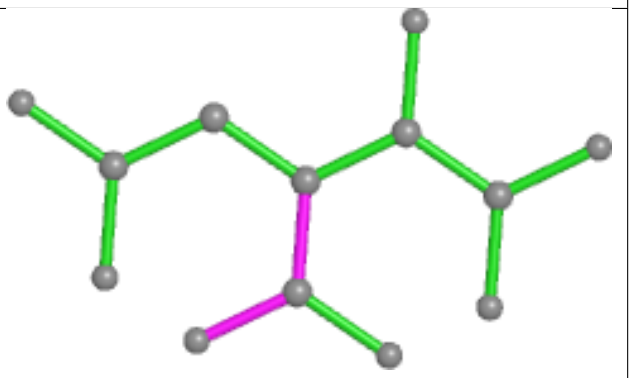


Rings

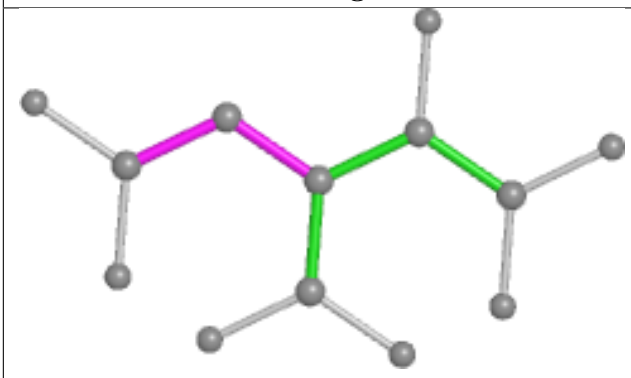
Ligand ICT V 501



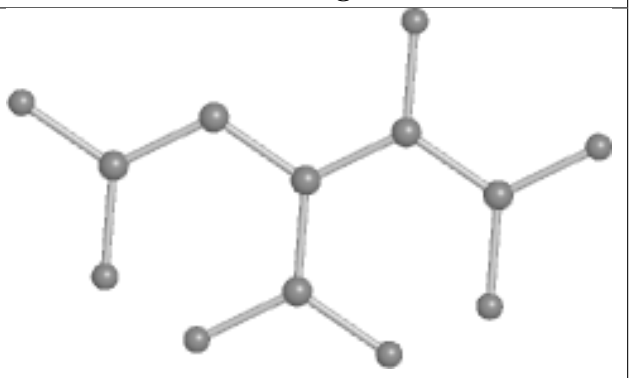
Bond lengths



Bond angles

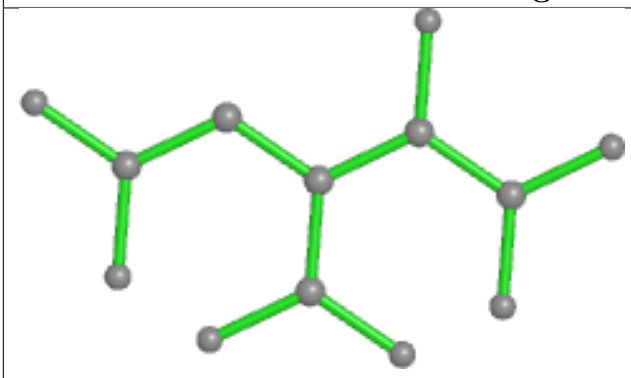


Torsions

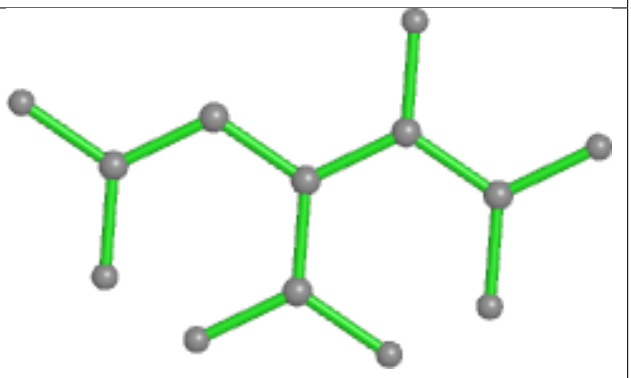


Rings

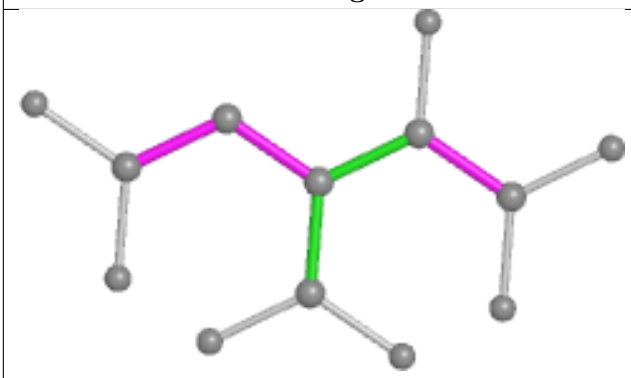
Ligand ICT J 501



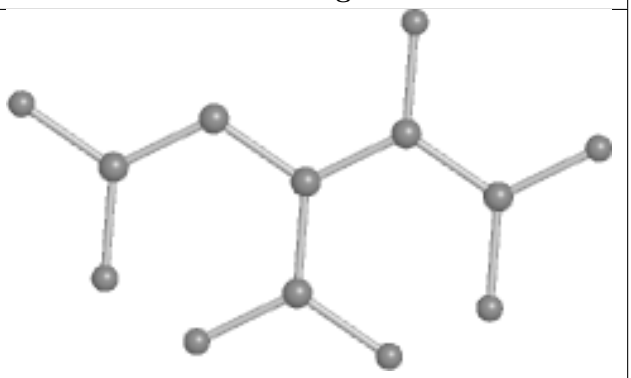
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	423/436 (97%)	-0.18	1 (0%) 95 95	22, 36, 58, 106	0
1	D	423/436 (97%)	-0.17	1 (0%) 95 95	24, 37, 56, 100	0
1	G	423/436 (97%)	-0.12	2 (0%) 91 91	23, 37, 59, 94	0
1	J	423/436 (97%)	-0.14	1 (0%) 95 95	25, 40, 60, 99	0
1	M	423/436 (97%)	-0.20	0 100 100	20, 36, 59, 86	0
1	P	423/436 (97%)	-0.15	1 (0%) 95 95	23, 37, 59, 107	0
1	S	423/436 (97%)	-0.13	1 (0%) 95 95	20, 38, 58, 102	0
1	V	423/436 (97%)	-0.13	0 100 100	24, 40, 60, 88	0
All	All	3384/3488 (97%)	-0.15	7 (0%) 95 95	20, 37, 59, 107	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	418	THR	2.5
1	D	39	GLN	2.4
1	S	410	SER	2.3
1	A	415	THR	2.2
1	G	2	ASP	2.1
1	J	408	GLU	2.1
1	P	39	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

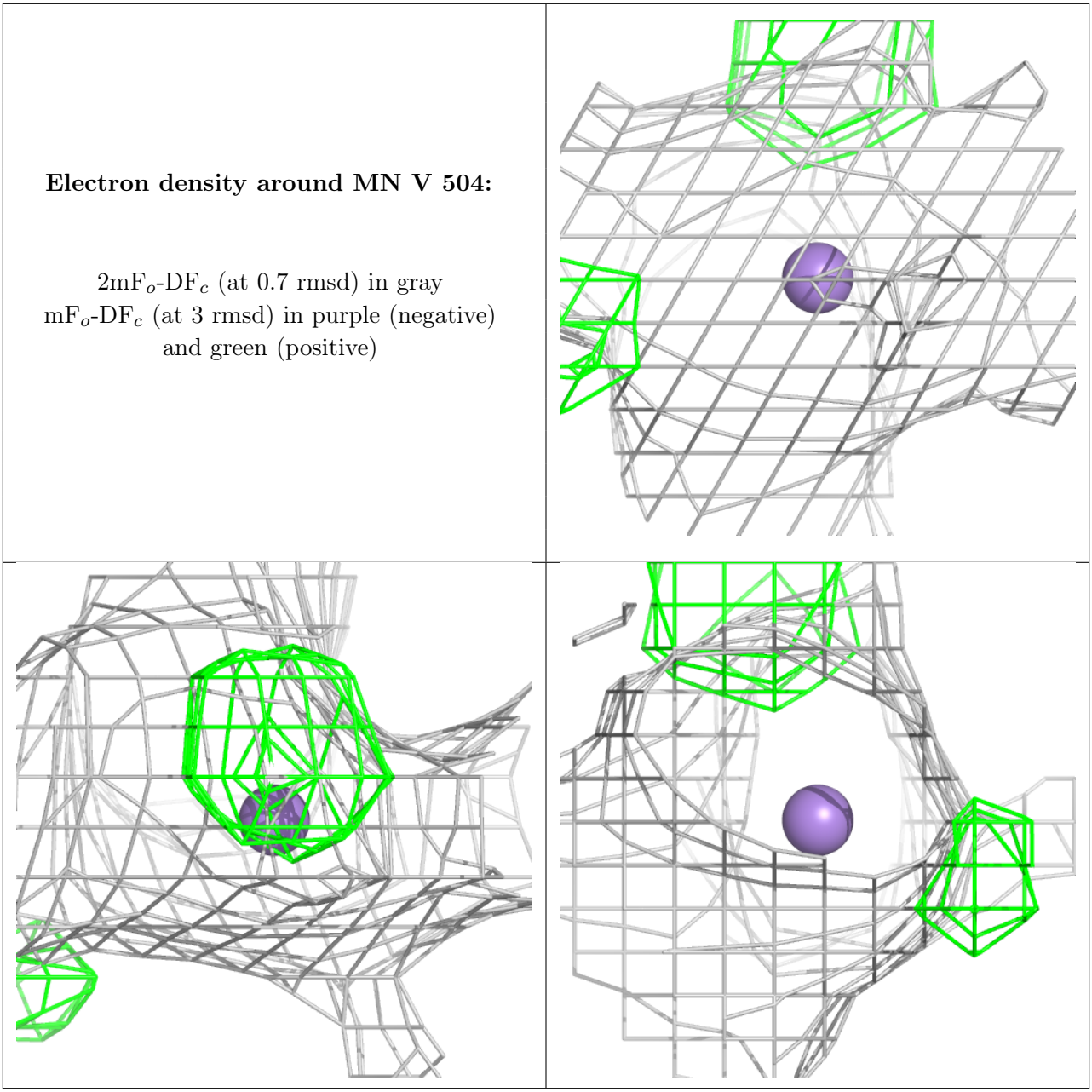
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	J	503	6/6	0.75	0.29	62,66,69,69	0
3	GOL	V	503	6/6	0.86	0.37	86,88,99,102	0
3	GOL	S	503	6/6	0.90	0.22	49,57,60,72	0
3	GOL	S	504	6/6	0.92	0.19	52,56,60,61	0
3	GOL	P	502	6/6	0.95	0.18	53,58,63,66	0
3	GOL	V	502	6/6	0.95	0.18	36,47,48,49	0
3	GOL	A	502	6/6	0.95	0.21	55,59,61,63	0
4	MN	V	504	1/1	0.95	0.10	84,84,84,84	0
4	MN	D	503	1/1	0.96	0.08	99,99,99,99	0
4	MN	G	504	1/1	0.96	0.07	99,99,99,99	0
4	MN	J	504	1/1	0.96	0.14	86,86,86,86	0
4	MN	M	502	1/1	0.96	0.06	85,85,85,85	0
2	ICT	S	501	13/13	0.96	0.18	35,42,49,50	0
3	GOL	J	502	6/6	0.97	0.26	61,65,68,69	0
2	ICT	V	501	13/13	0.97	0.14	36,45,56,58	0
4	MN	S	505	1/1	0.97	0.14	89,89,89,89	0
3	GOL	G	503	6/6	0.97	0.19	51,56,62,63	0
2	ICT	G	501	13/13	0.98	0.17	39,49,51,56	0
3	GOL	D	502	6/6	0.98	0.19	37,43,45,50	0
3	GOL	G	502	6/6	0.98	0.21	39,44,46,50	0
4	MN	A	503	1/1	0.98	0.07	86,86,86,86	0
2	ICT	J	501	13/13	0.98	0.15	28,37,47,51	0
2	ICT	M	501	13/13	0.98	0.16	32,46,55,56	0
2	ICT	P	501	13/13	0.98	0.21	38,54,65,66	0
2	ICT	A	501	13/13	0.98	0.20	39,46,54,60	0
4	MN	P	503	1/1	0.98	0.09	86,86,86,86	0
3	GOL	S	502	6/6	0.98	0.18	39,43,51,53	0
2	ICT	D	501	13/13	0.98	0.18	34,46,51,54	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.

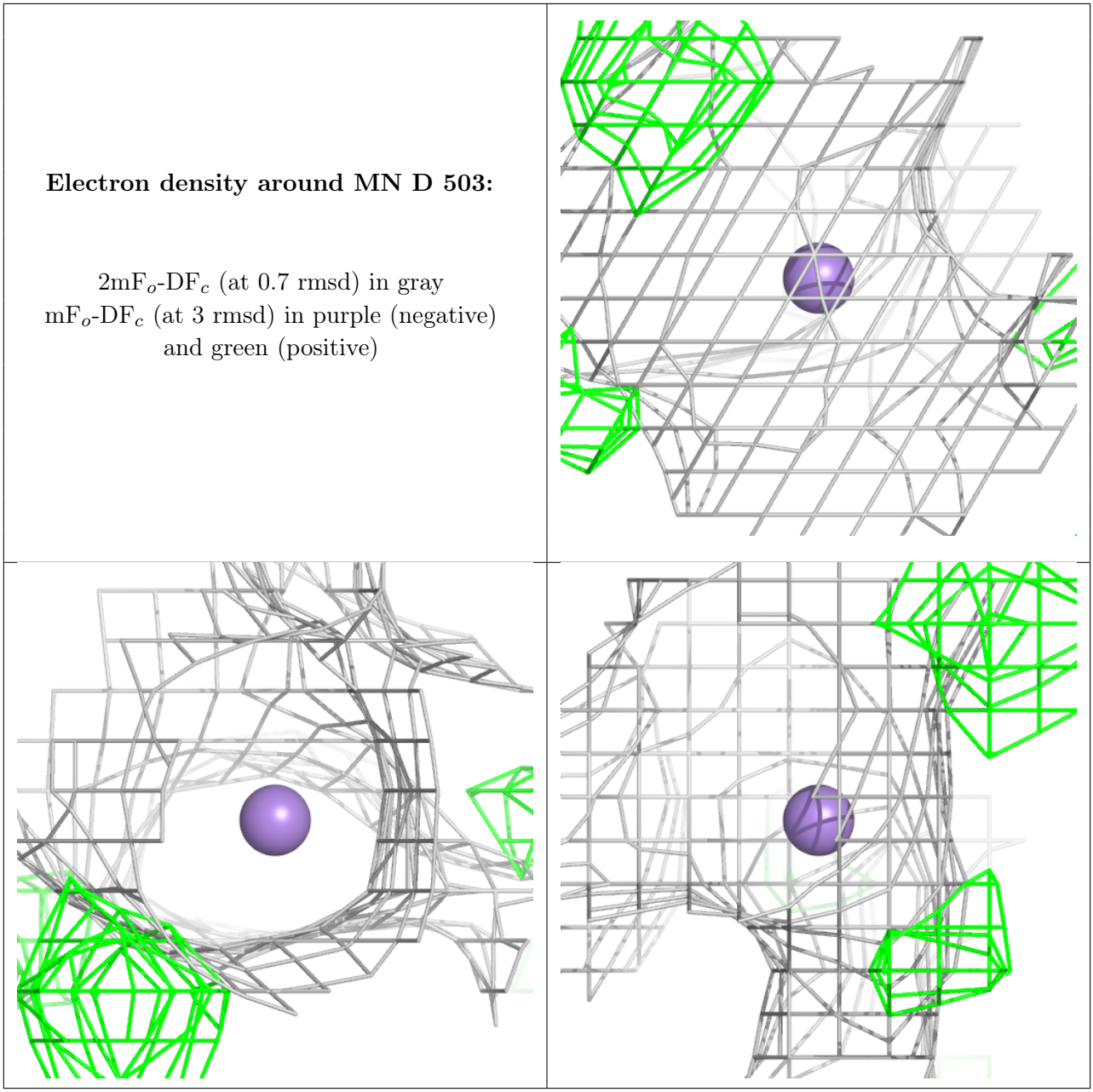
Electron density around MN V 504:

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



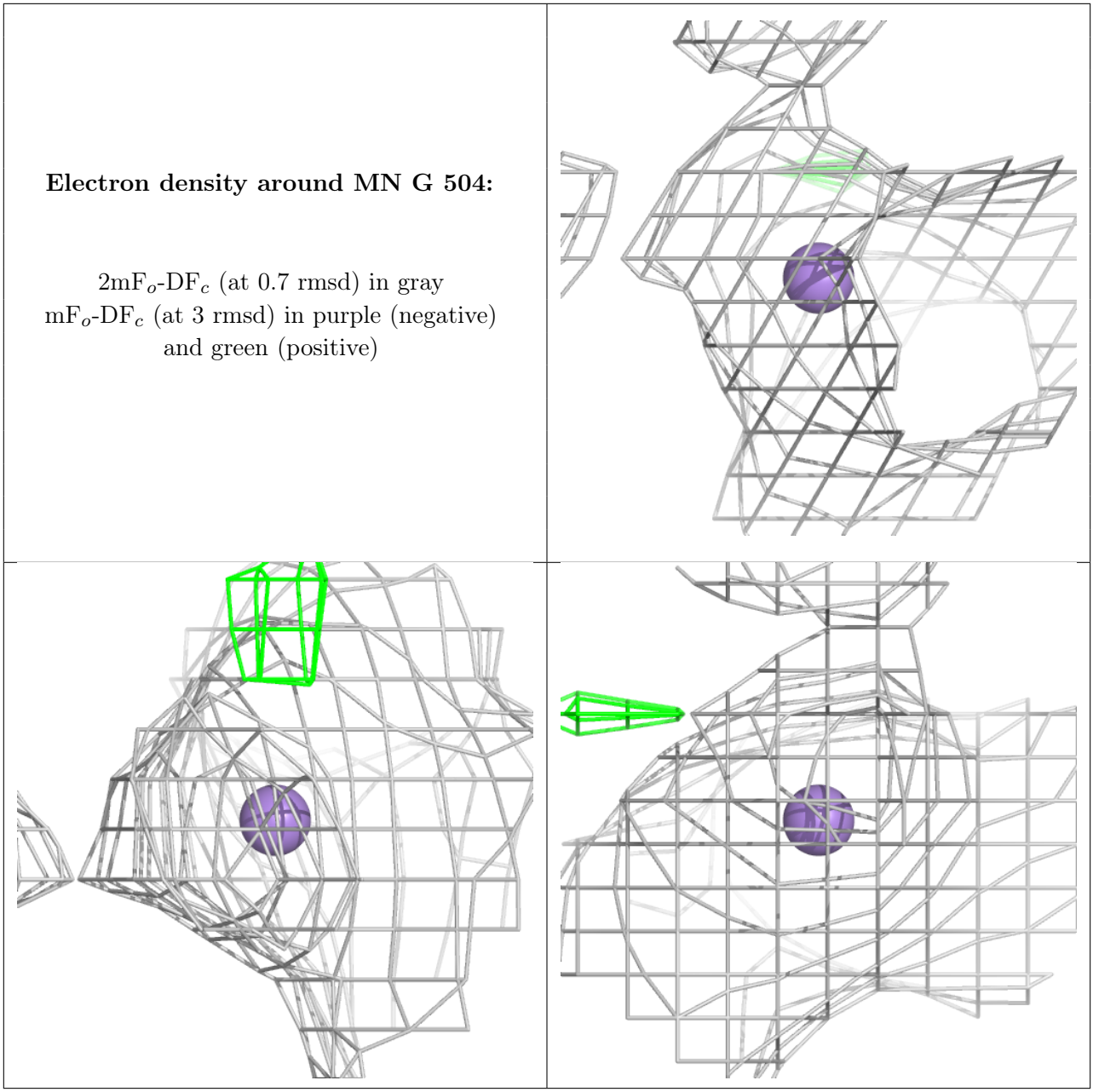
Electron density around MN D 503:

$2mF_o$-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 G 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 J 504:

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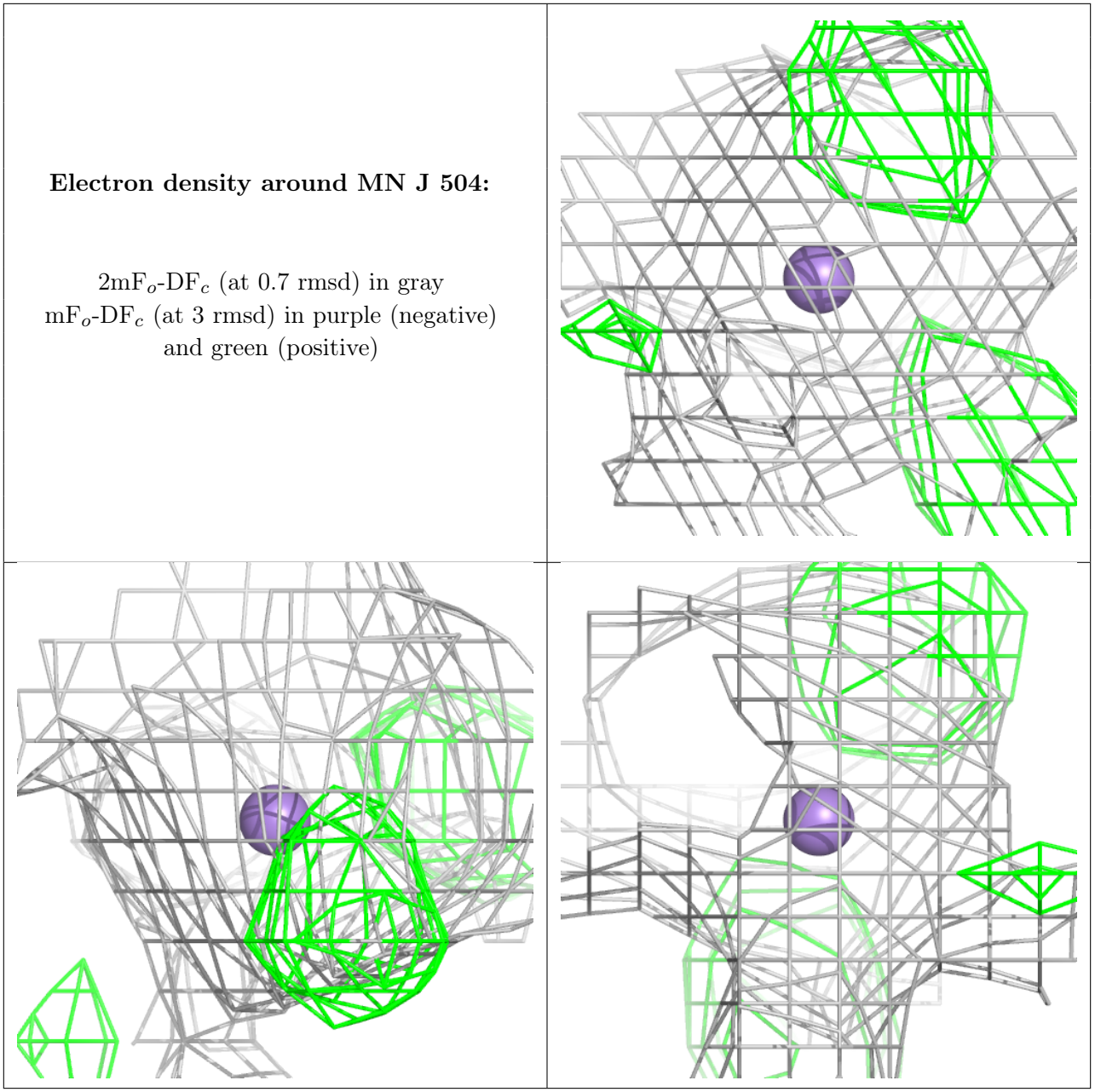
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN M 502:

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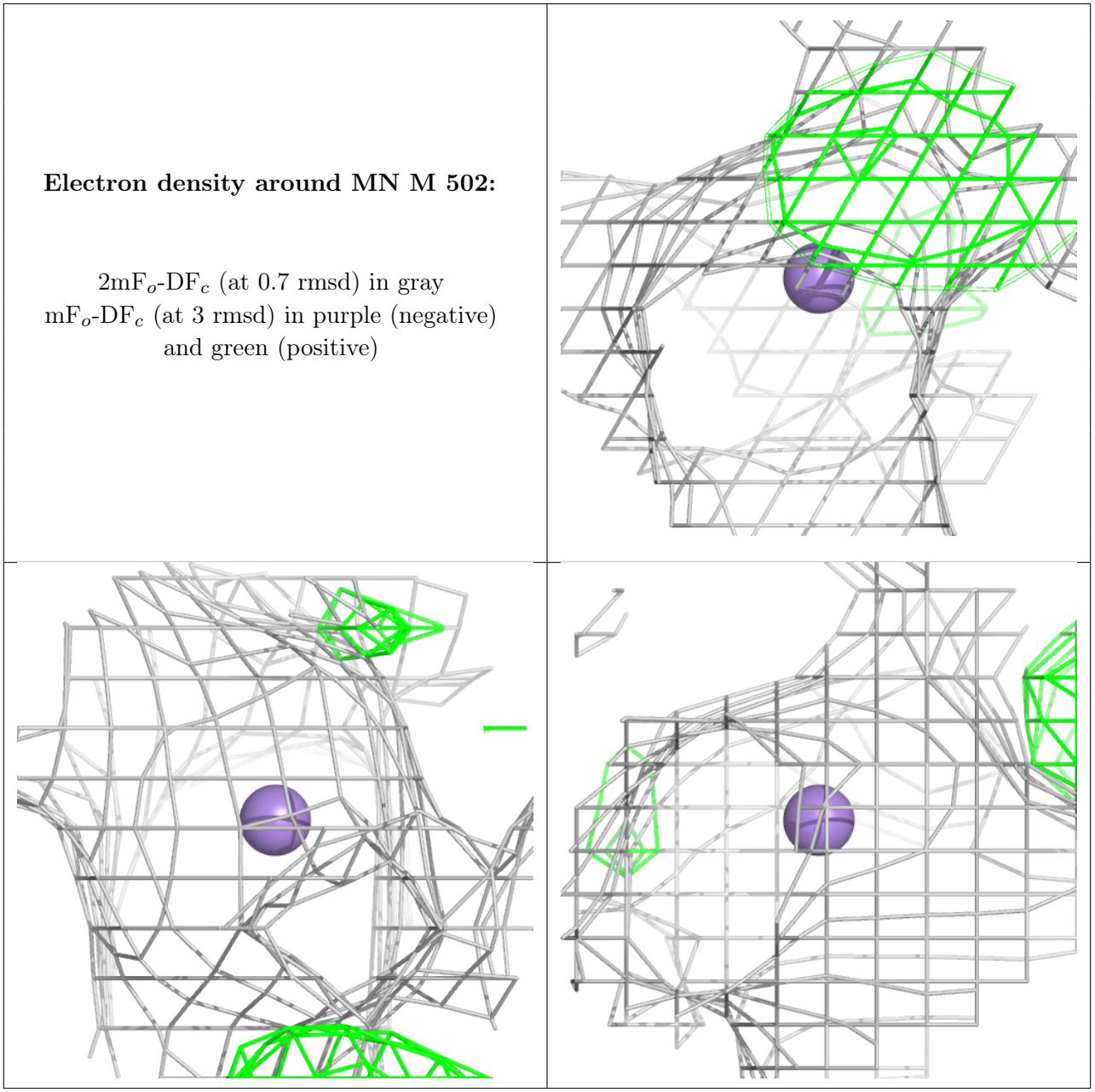
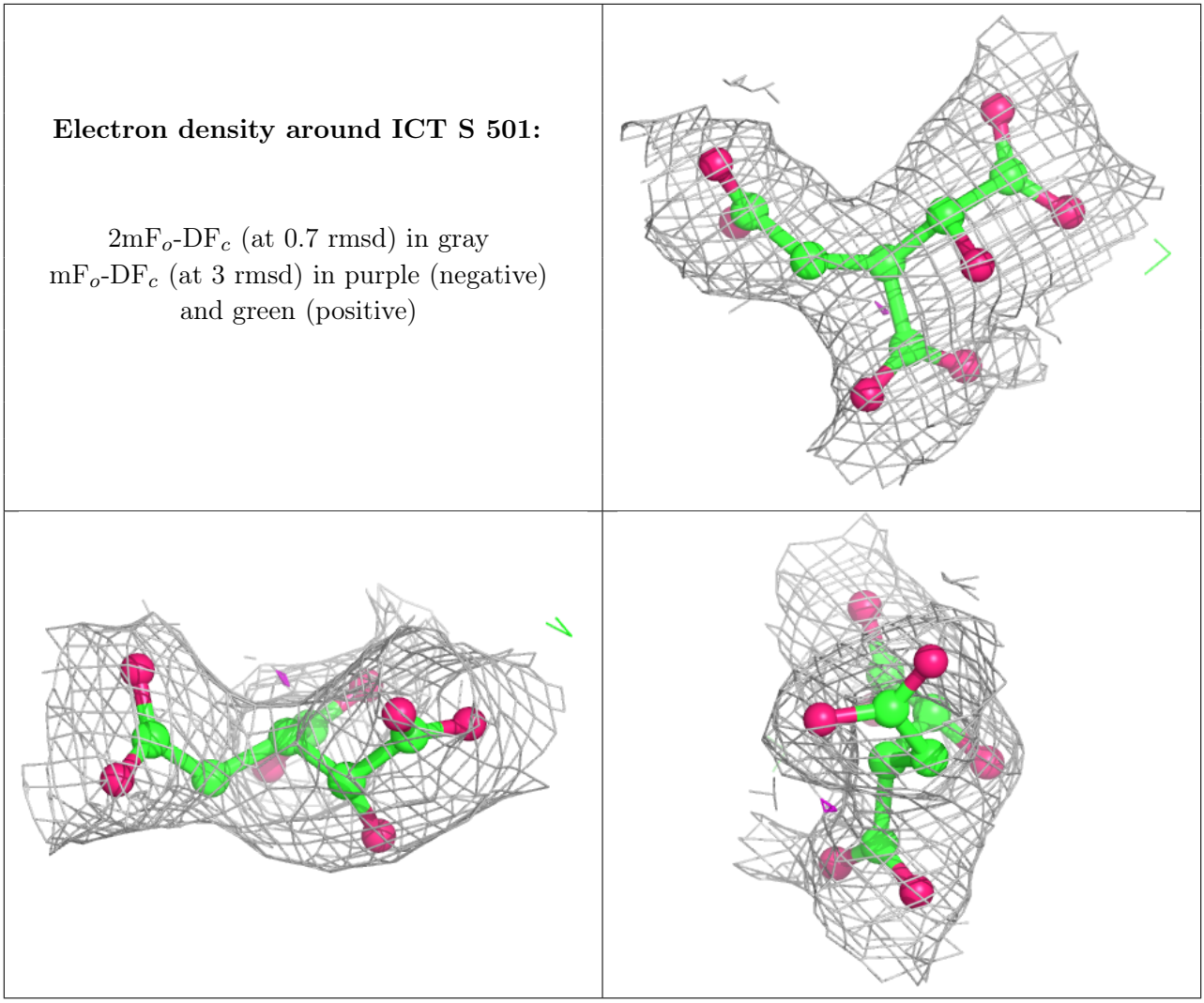
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ICT S 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 ICT V 501:

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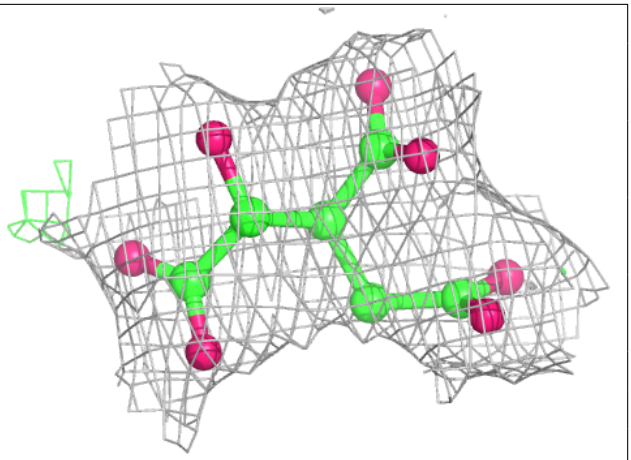
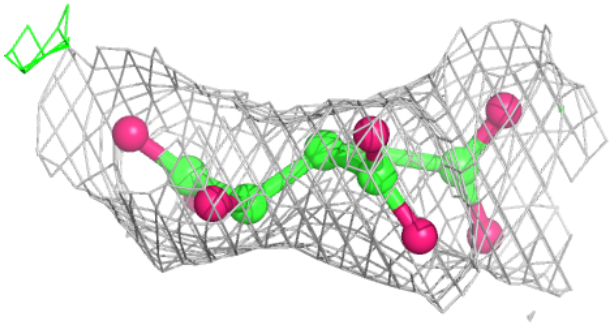
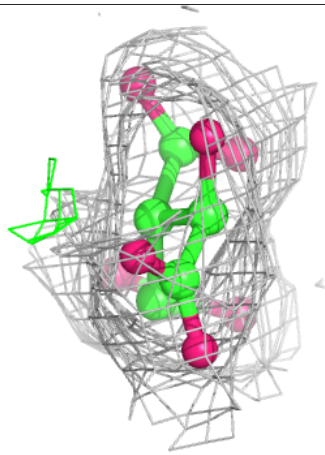
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around MN S 505:

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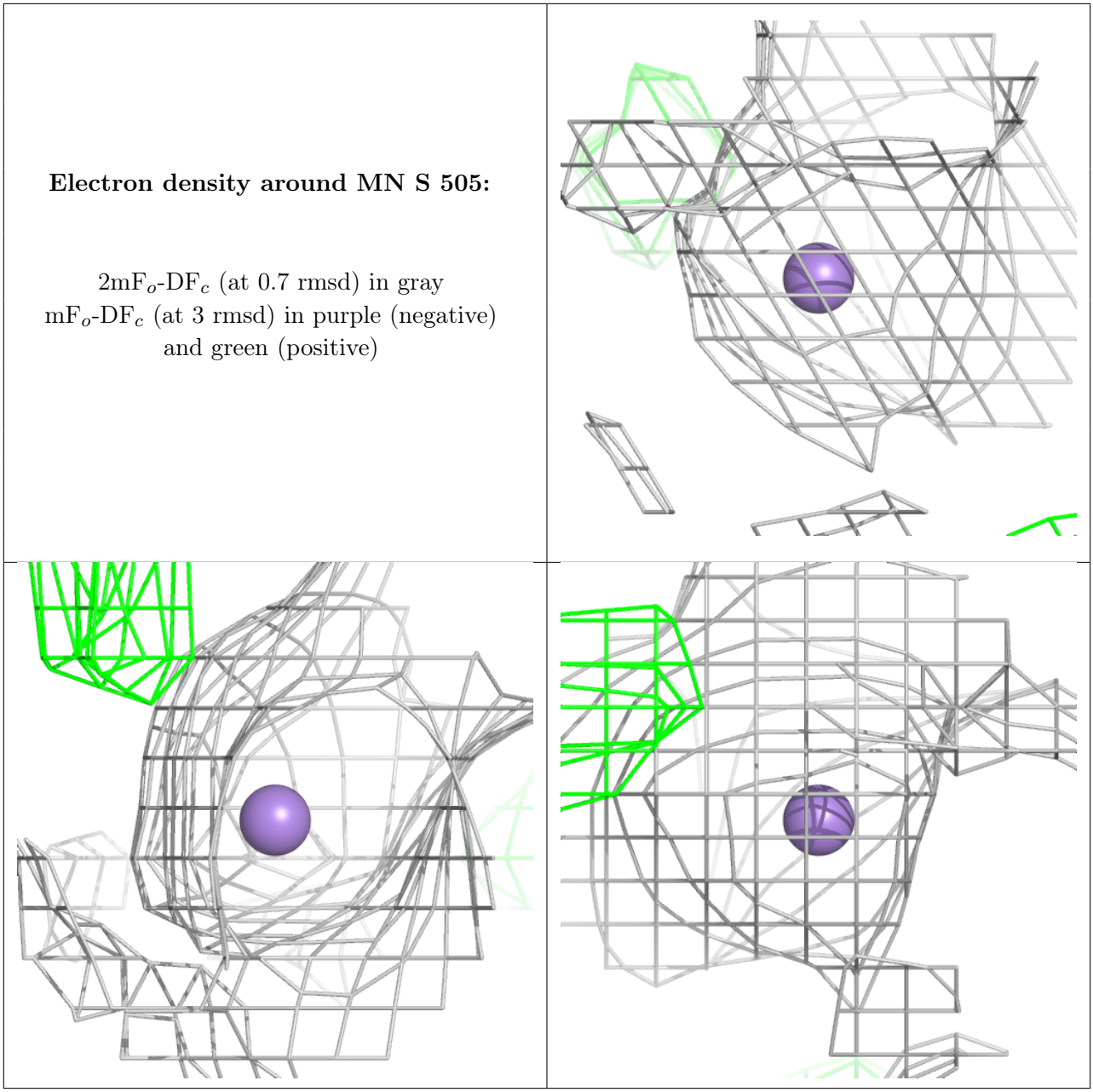
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ICT G 501:

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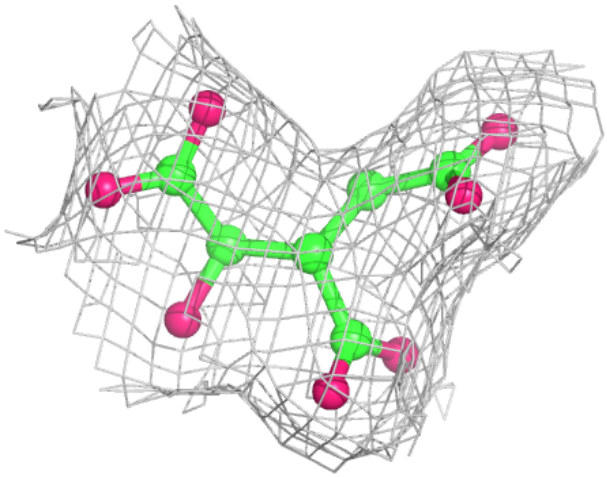
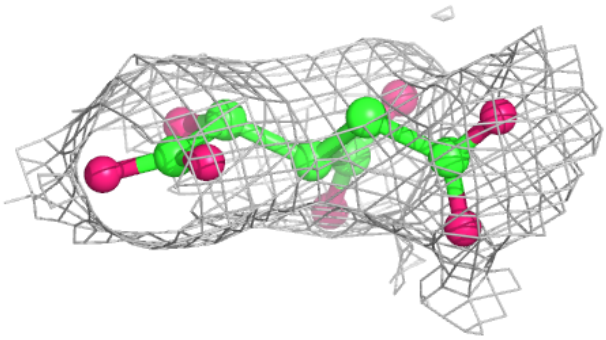
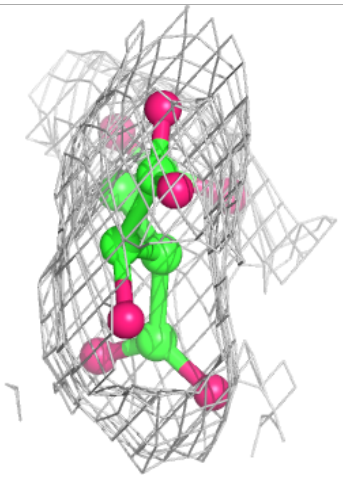
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around MN A 503:

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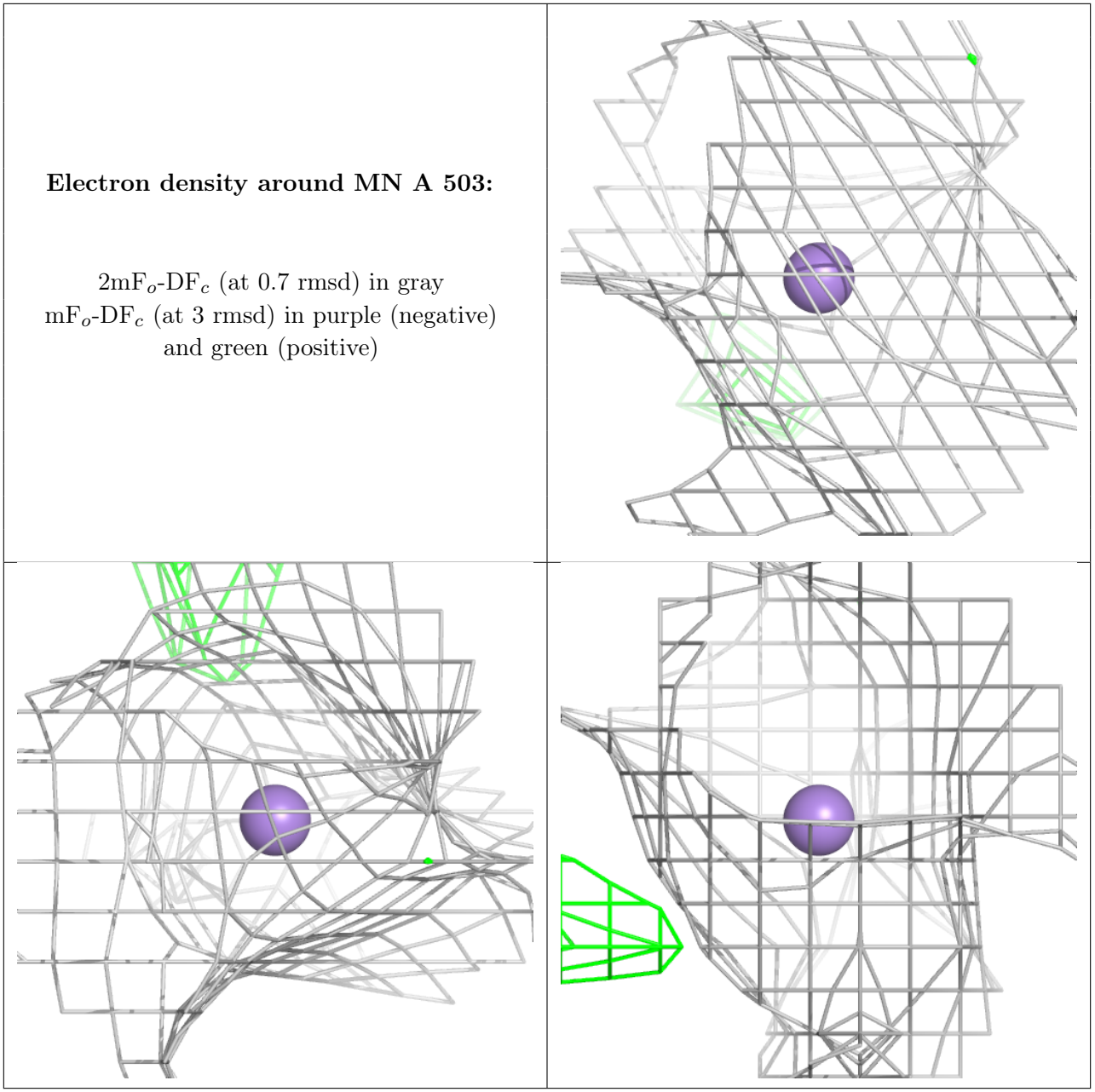
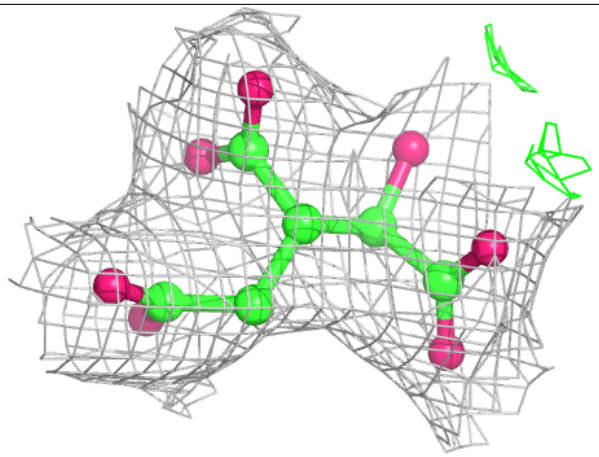
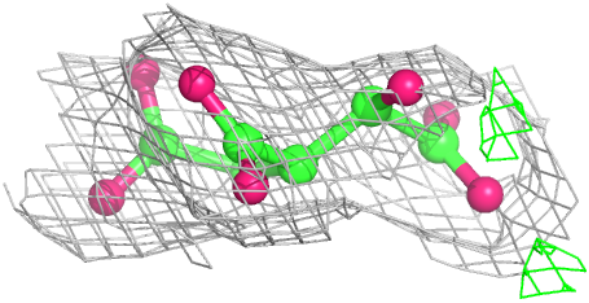
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

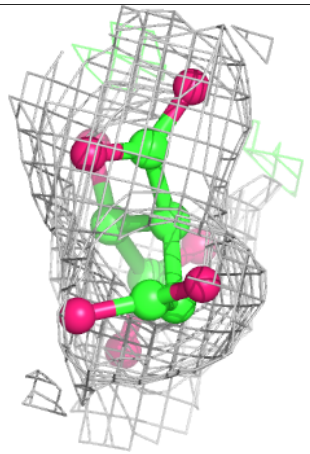


Electron density around ICT J 501:

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







Electron density around ICT M 501:

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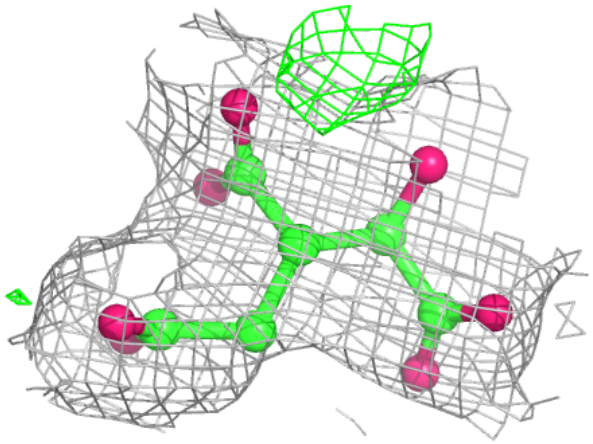
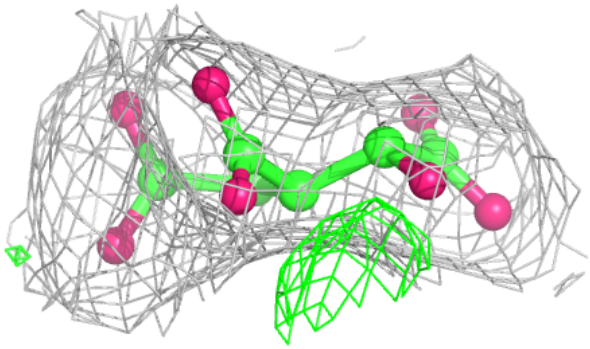
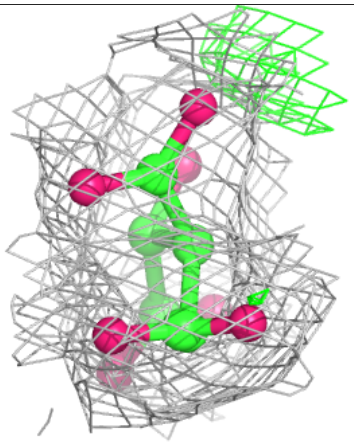
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

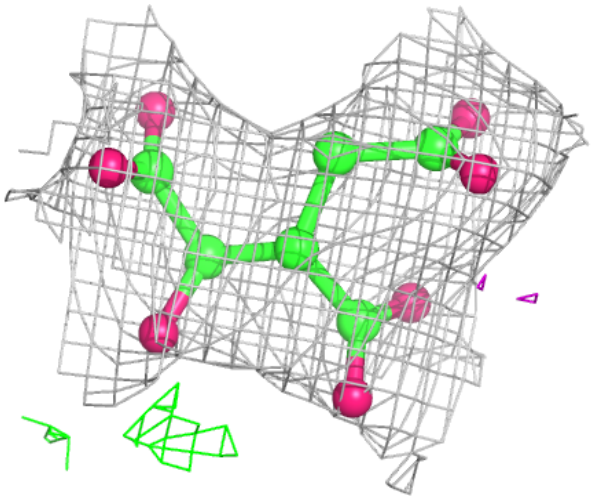


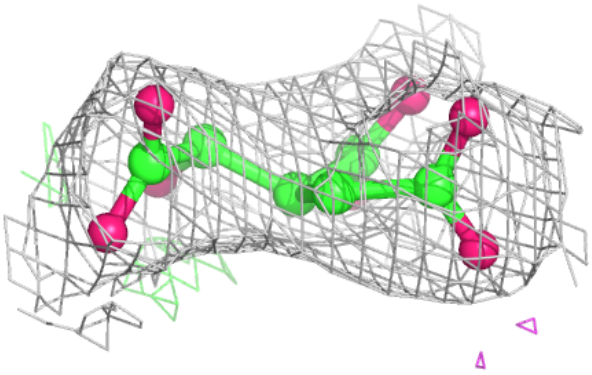


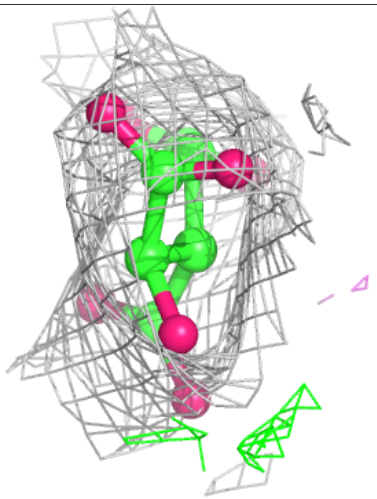


Electron density around ICT P 501:

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







Electron density around ICT A 501:

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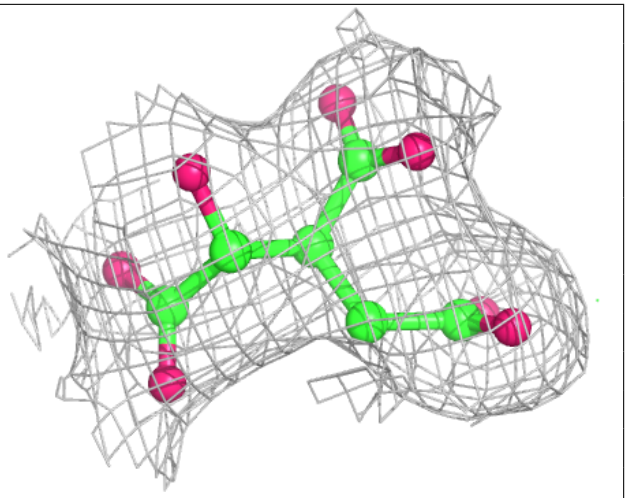
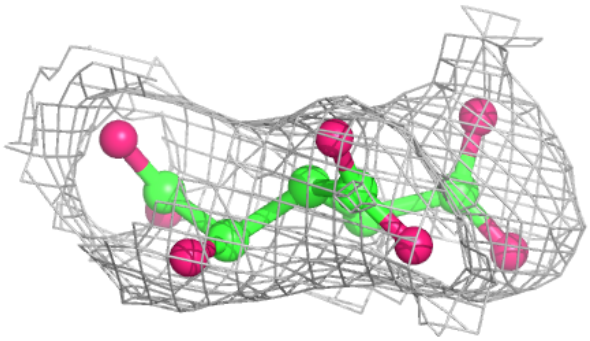
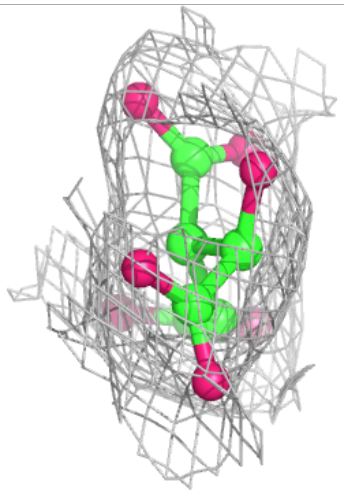
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

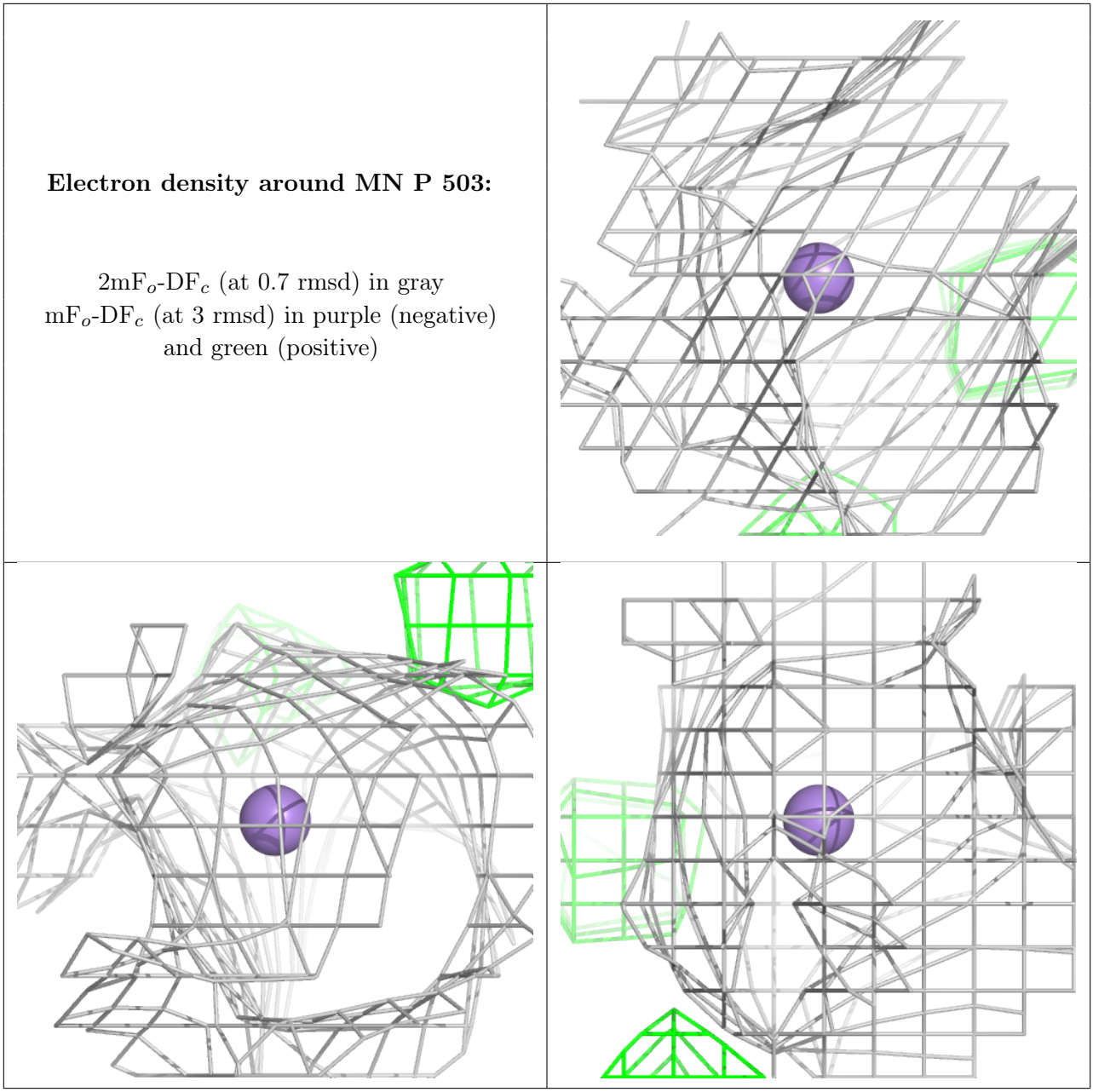






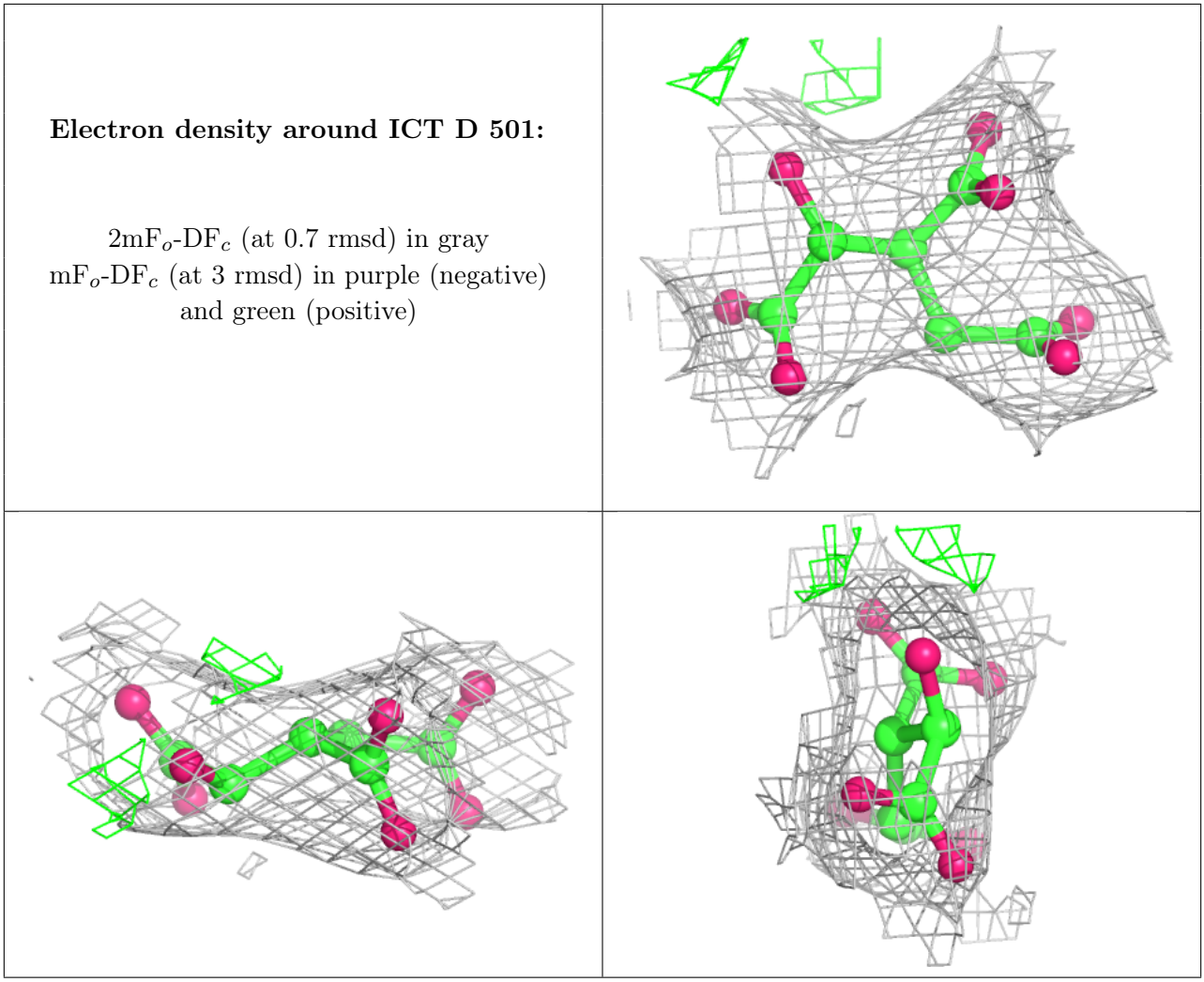
Electron density around MN P 503:

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



Electron density around ICT 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)



6.5 Other polymers

There are no such residues in this entry.