



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 02:42 PM UTC

PDB ID : 8APQ / pdb_00008apq
Title : CaMct - Mesoacetyl-CoA C1:C4 CoA Transferase of *Chloroflexus aurantiacus*
Authors : Pfister, P.; Zarzycki, J.; Erb, T.J.
Deposited on : 2022-08-10
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

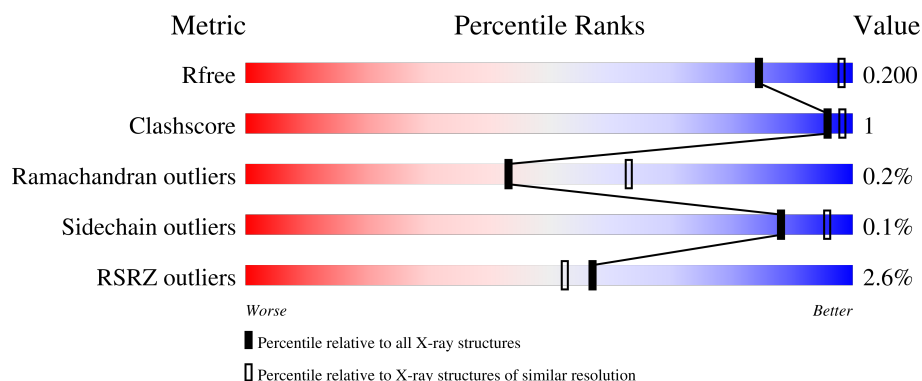
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

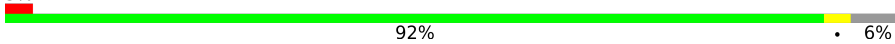
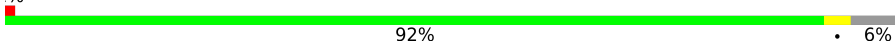
The reported resolution of this entry is 2.49 Å.

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.



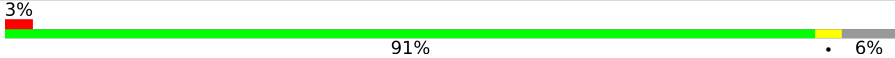
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	430	
1	B	430	
1	C	430	
1	D	430	
1	E	430	

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Mol	Chain	Length	Quality of chain
1	F	430	 A horizontal bar chart showing the quality of chain 1. The bar is green, indicating a high quality. The chart is labeled with '3%' at the start, '91%' in the middle, and '6%' at the end. The bar is divided into three segments: a small red segment at the beginning, a large green segment in the middle, and a small yellow segment at the end.

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
4	MEZ	B	502	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20187 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 2-methylfumaryl-CoA isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3134	1989	565	565	15			
1	B	406	Total	C	N	O	S	0	0	0
			3134	1989	565	565	15			
1	C	406	Total	C	N	O	S	0	0	0
			3134	1989	565	565	15			
1	D	406	Total	C	N	O	S	0	0	0
			3133	1989	565	564	15			
1	E	405	Total	C	N	O	S	0	0	0
			3126	1984	564	564	14			
1	F	406	Total	C	N	O	S	0	0	0
			3134	1989	565	565	15			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A9WC36
A	-19	GLY	-	expression tag	UNP A9WC36
A	-18	HIS	-	expression tag	UNP A9WC36
A	-17	HIS	-	expression tag	UNP A9WC36
A	-16	HIS	-	expression tag	UNP A9WC36
A	-15	HIS	-	expression tag	UNP A9WC36
A	-14	HIS	-	expression tag	UNP A9WC36
A	-13	HIS	-	expression tag	UNP A9WC36
A	-12	HIS	-	expression tag	UNP A9WC36
A	-11	HIS	-	expression tag	UNP A9WC36
A	-10	HIS	-	expression tag	UNP A9WC36
A	-9	HIS	-	expression tag	UNP A9WC36
A	-8	SER	-	expression tag	UNP A9WC36
A	-7	SER	-	expression tag	UNP A9WC36
A	-6	GLY	-	expression tag	UNP A9WC36
A	-5	HIS	-	expression tag	UNP A9WC36
A	-4	ILE	-	expression tag	UNP A9WC36

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP A9WC36
A	-2	GLY	-	expression tag	UNP A9WC36
A	-1	ARG	-	expression tag	UNP A9WC36
A	0	HIS	-	expression tag	UNP A9WC36
B	-20	MET	-	initiating methionine	UNP A9WC36
B	-19	GLY	-	expression tag	UNP A9WC36
B	-18	HIS	-	expression tag	UNP A9WC36
B	-17	HIS	-	expression tag	UNP A9WC36
B	-16	HIS	-	expression tag	UNP A9WC36
B	-15	HIS	-	expression tag	UNP A9WC36
B	-14	HIS	-	expression tag	UNP A9WC36
B	-13	HIS	-	expression tag	UNP A9WC36
B	-12	HIS	-	expression tag	UNP A9WC36
B	-11	HIS	-	expression tag	UNP A9WC36
B	-10	HIS	-	expression tag	UNP A9WC36
B	-9	HIS	-	expression tag	UNP A9WC36
B	-8	SER	-	expression tag	UNP A9WC36
B	-7	SER	-	expression tag	UNP A9WC36
B	-6	GLY	-	expression tag	UNP A9WC36
B	-5	HIS	-	expression tag	UNP A9WC36
B	-4	ILE	-	expression tag	UNP A9WC36
B	-3	GLU	-	expression tag	UNP A9WC36
B	-2	GLY	-	expression tag	UNP A9WC36
B	-1	ARG	-	expression tag	UNP A9WC36
B	0	HIS	-	expression tag	UNP A9WC36
C	-20	MET	-	initiating methionine	UNP A9WC36
C	-19	GLY	-	expression tag	UNP A9WC36
C	-18	HIS	-	expression tag	UNP A9WC36
C	-17	HIS	-	expression tag	UNP A9WC36
C	-16	HIS	-	expression tag	UNP A9WC36
C	-15	HIS	-	expression tag	UNP A9WC36
C	-14	HIS	-	expression tag	UNP A9WC36
C	-13	HIS	-	expression tag	UNP A9WC36
C	-12	HIS	-	expression tag	UNP A9WC36
C	-11	HIS	-	expression tag	UNP A9WC36
C	-10	HIS	-	expression tag	UNP A9WC36
C	-9	HIS	-	expression tag	UNP A9WC36
C	-8	SER	-	expression tag	UNP A9WC36
C	-7	SER	-	expression tag	UNP A9WC36
C	-6	GLY	-	expression tag	UNP A9WC36
C	-5	HIS	-	expression tag	UNP A9WC36
C	-4	ILE	-	expression tag	UNP A9WC36

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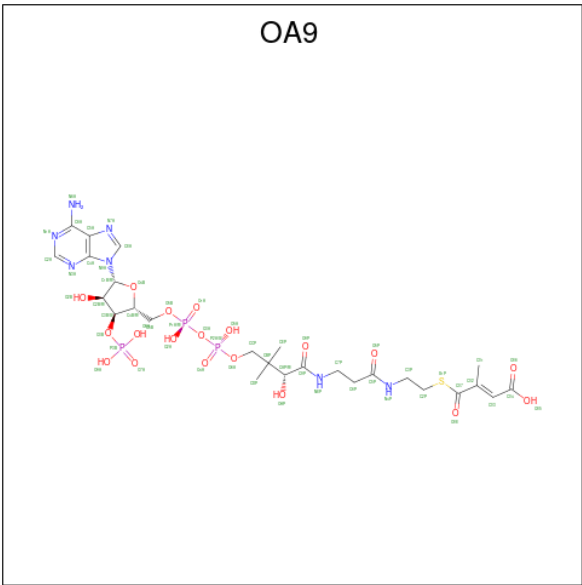
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP A9WC36
C	-2	GLY	-	expression tag	UNP A9WC36
C	-1	ARG	-	expression tag	UNP A9WC36
C	0	HIS	-	expression tag	UNP A9WC36
D	-20	MET	-	initiating methionine	UNP A9WC36
D	-19	GLY	-	expression tag	UNP A9WC36
D	-18	HIS	-	expression tag	UNP A9WC36
D	-17	HIS	-	expression tag	UNP A9WC36
D	-16	HIS	-	expression tag	UNP A9WC36
D	-15	HIS	-	expression tag	UNP A9WC36
D	-14	HIS	-	expression tag	UNP A9WC36
D	-13	HIS	-	expression tag	UNP A9WC36
D	-12	HIS	-	expression tag	UNP A9WC36
D	-11	HIS	-	expression tag	UNP A9WC36
D	-10	HIS	-	expression tag	UNP A9WC36
D	-9	HIS	-	expression tag	UNP A9WC36
D	-8	SER	-	expression tag	UNP A9WC36
D	-7	SER	-	expression tag	UNP A9WC36
D	-6	GLY	-	expression tag	UNP A9WC36
D	-5	HIS	-	expression tag	UNP A9WC36
D	-4	ILE	-	expression tag	UNP A9WC36
D	-3	GLU	-	expression tag	UNP A9WC36
D	-2	GLY	-	expression tag	UNP A9WC36
D	-1	ARG	-	expression tag	UNP A9WC36
D	0	HIS	-	expression tag	UNP A9WC36
E	-20	MET	-	initiating methionine	UNP A9WC36
E	-19	GLY	-	expression tag	UNP A9WC36
E	-18	HIS	-	expression tag	UNP A9WC36
E	-17	HIS	-	expression tag	UNP A9WC36
E	-16	HIS	-	expression tag	UNP A9WC36
E	-15	HIS	-	expression tag	UNP A9WC36
E	-14	HIS	-	expression tag	UNP A9WC36
E	-13	HIS	-	expression tag	UNP A9WC36
E	-12	HIS	-	expression tag	UNP A9WC36
E	-11	HIS	-	expression tag	UNP A9WC36
E	-10	HIS	-	expression tag	UNP A9WC36
E	-9	HIS	-	expression tag	UNP A9WC36
E	-8	SER	-	expression tag	UNP A9WC36
E	-7	SER	-	expression tag	UNP A9WC36
E	-6	GLY	-	expression tag	UNP A9WC36
E	-5	HIS	-	expression tag	UNP A9WC36
E	-4	ILE	-	expression tag	UNP A9WC36

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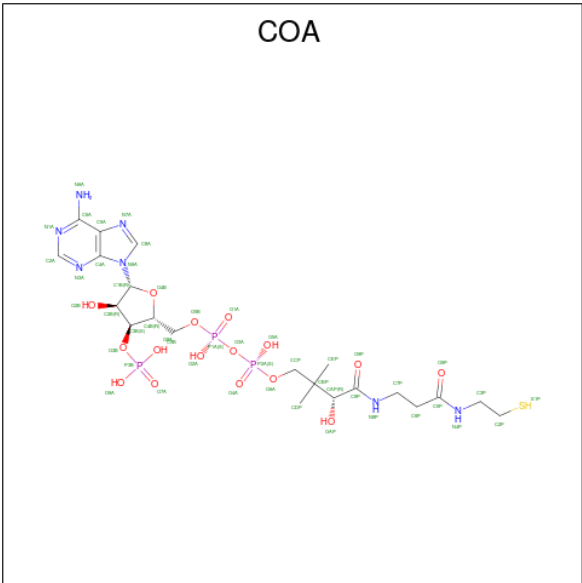
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLU	-	expression tag	UNP A9WC36
E	-2	GLY	-	expression tag	UNP A9WC36
E	-1	ARG	-	expression tag	UNP A9WC36
E	0	HIS	-	expression tag	UNP A9WC36
F	-20	MET	-	initiating methionine	UNP A9WC36
F	-19	GLY	-	expression tag	UNP A9WC36
F	-18	HIS	-	expression tag	UNP A9WC36
F	-17	HIS	-	expression tag	UNP A9WC36
F	-16	HIS	-	expression tag	UNP A9WC36
F	-15	HIS	-	expression tag	UNP A9WC36
F	-14	HIS	-	expression tag	UNP A9WC36
F	-13	HIS	-	expression tag	UNP A9WC36
F	-12	HIS	-	expression tag	UNP A9WC36
F	-11	HIS	-	expression tag	UNP A9WC36
F	-10	HIS	-	expression tag	UNP A9WC36
F	-9	HIS	-	expression tag	UNP A9WC36
F	-8	SER	-	expression tag	UNP A9WC36
F	-7	SER	-	expression tag	UNP A9WC36
F	-6	GLY	-	expression tag	UNP A9WC36
F	-5	HIS	-	expression tag	UNP A9WC36
F	-4	ILE	-	expression tag	UNP A9WC36
F	-3	GLU	-	expression tag	UNP A9WC36
F	-2	GLY	-	expression tag	UNP A9WC36
F	-1	ARG	-	expression tag	UNP A9WC36
F	0	HIS	-	expression tag	UNP A9WC36

- Molecule 2 is Mesoacetyl Coenzyme A (CCD ID: OA9) (formula: $C_{26}H_{40}N_7O_{19}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



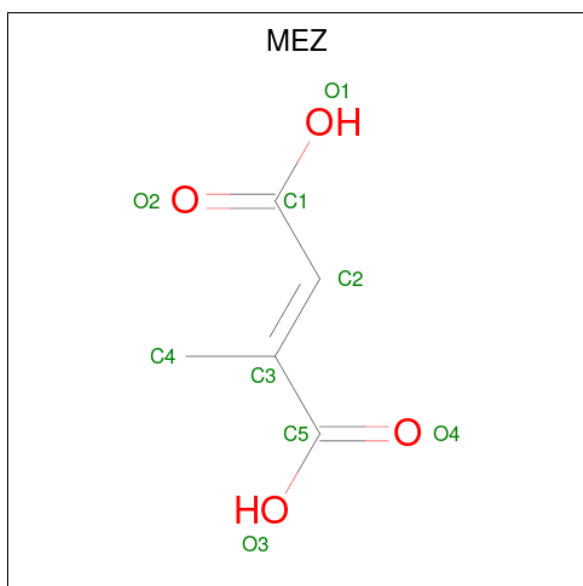
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is (2E)-2-METHYLBUT-2-ENEDIOIC ACID (CCD ID: MEZ) (formula: C₅H₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	5	3		
4	C	1	Total	C	O	0	0
			8	5	3		
4	D	1	Total	C	O	0	0
			9	5	4		
4	E	1	Total	C	O	0	0
			8	5	3		
4	F	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		

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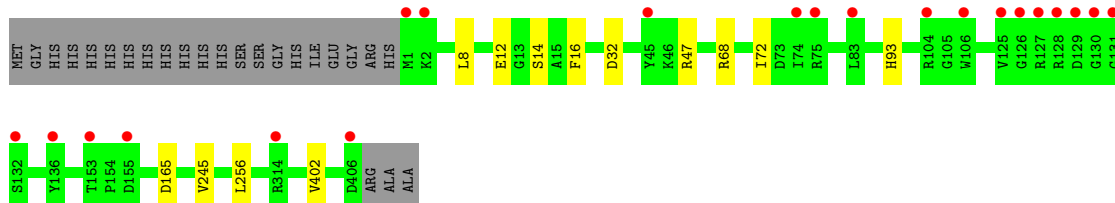
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	151	Total 151	O 151	0	0
5	C	172	Total 172	O 172	0	0
5	D	177	Total 177	O 177	0	0
5	E	185	Total 185	O 185	0	0
5	F	197	Total 197	O 197	0	0

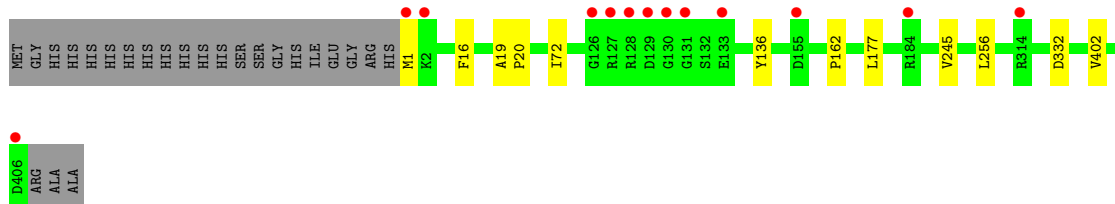
- Molecule 1: 2-methylfumaryl-CoA isomerase

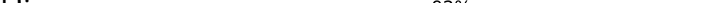


- Chain B: 5% 91% 6%



- Chain C: 3% 92% 6%



- Chain D:  92% 6%



- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

MET
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
HIS
ILE
GLU
GLY
ARG
HIS
MET
K2
F16
R78
G126
D129
G130
G131
Y136
L174
L177
H184
V245
D250
L256
L383
L388
D406
A08
ALA
ALA

Chain F: 3% 91% 6%

Sequence logo for the 1000bp upstream region of the H19 gene. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions from -1000 to +1000. The logo highlights several key motifs: a T361 site at position -980, a L366 site at position -960, a L383 site at position -940, an E384 site at position -920, a L388 site at position -900, a V402 site at position -880, a D406 site at position -860, an ARG site at position -840, an ALA site at position -820, and an ALA site at position -800. The H19 gene structure is shown below the logo, with exons represented by yellow boxes and introns by grey lines. The H19 gene starts at position -1000 and ends at position +1000.

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.84Å 193.84Å 251.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.69 – 2.49 29.69 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.69-2.49) 99.7 (29.69-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.200 0.185 , 0.200	Depositor DCC
R_{free} test set	1998 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20187	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 2.04% 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: OA9, COA, MEZ

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	0.09	0/3205	0.25	0/4350
1	B	0.13	0/3205	0.28	1/4350 (0.0%)
1	C	0.11	0/3205	0.27	0/4350
1	D	0.09	0/3204	0.25	0/4348
1	E	0.09	0/3197	0.26	0/4340
1	F	0.11	0/3205	0.27	0/4350
All	All	0.10	0/19221	0.26	1/26088 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASP	CA-CB-CG	6.57	119.17	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3134	0	3141	6	0
1	B	3134	0	3141	6	0
1	C	3134	0	3141	8	0
1	D	3133	0	3141	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3126	0	3129	4	1
1	F	3134	0	3141	10	0
2	A	56	0	0	0	0
3	B	48	0	32	0	0
3	C	48	0	32	0	0
3	D	48	0	31	1	0
3	E	48	0	32	0	0
3	F	48	0	32	1	0
4	B	8	0	4	1	0
4	C	8	0	4	2	0
4	D	9	0	4	1	0
4	E	8	0	4	1	0
4	F	8	0	4	1	0
5	A	173	0	0	0	0
5	B	151	0	0	0	0
5	C	172	0	0	3	0
5	D	177	0	0	1	1
5	E	185	0	0	0	0
5	F	197	0	0	3	0
All	All	20187	0	19013	41	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 41 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:C:332:ASP:OD2	5:C:601:HOH:O	2.13	0.66
1:F:72:ILE:HD13	1:F:402:VAL:HG12	1.77	0.66
1:D:245:VAL:HG21	1:D:256:LEU:HD13	1.81	0.63
1:F:245:VAL:HG21	1:F:256:LEU:HD13	1.85	0.59
1:E:245:VAL:HG21	1:E:256:LEU:HD13	1.86	0.58

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ARG:NH2	5:D:644:HOH:O[2_564]	2.17	0.03

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	404/430 (94%)	394 (98%)	9 (2%)	1 (0%)	43	63
1	B	404/430 (94%)	394 (98%)	9 (2%)	1 (0%)	43	63
1	C	404/430 (94%)	395 (98%)	8 (2%)	1 (0%)	43	63
1	D	404/430 (94%)	393 (97%)	10 (2%)	1 (0%)	43	63
1	E	403/430 (94%)	391 (97%)	11 (3%)	1 (0%)	43	63
1	F	404/430 (94%)	392 (97%)	11 (3%)	1 (0%)	43	63
All	All	2423/2580 (94%)	2359 (97%)	58 (2%)	6 (0%)	43	63

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	PHE
1	C	16	PHE
1	D	16	PHE
1	E	16	PHE
1	F	16	PHE

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	323/342 (94%)	322 (100%)	1 (0%)	86	94
1	B	323/342 (94%)	323 (100%)	0	100	100
1	C	323/342 (94%)	323 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	323/342 (94%)	322 (100%)	1 (0%)	86	94
1	E	322/342 (94%)	322 (100%)	0	100	100
1	F	323/342 (94%)	323 (100%)	0	100	100
All	All	1937/2052 (94%)	1935 (100%)	2 (0%)	88	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	D	165	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	159	HIS
1	F	115	HIS
1	D	170	GLN
1	F	123	ASN
1	E	288	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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	MEZ	D	502	-	8,8,8	1.54	3 (37%)	10,10,10	1.40	1 (10%)
4	MEZ	E	502	1	7,7,8	2.14	2 (28%)	7,8,10	4.14	2 (28%)
4	MEZ	F	502	1	7,7,8	1.44	1 (14%)	7,8,10	2.50	2 (28%)
3	COA	B	501	-	47,50,50	2.01	6 (12%)	69,75,75	1.48	11 (15%)
4	MEZ	C	502	1	7,7,8	2.01	2 (28%)	7,8,10	2.01	2 (28%)
4	MEZ	B	502	1	7,7,8	2.91	4 (57%)	7,8,10	6.51	3 (42%)
3	COA	D	501	1	47,50,50	1.83	6 (12%)	69,75,75	1.55	12 (17%)
3	COA	E	501	-	47,50,50	1.99	6 (12%)	69,75,75	1.47	11 (15%)
3	COA	F	501	-	47,50,50	1.96	6 (12%)	69,75,75	1.73	14 (20%)
3	COA	C	501	-	47,50,50	1.58	6 (12%)	69,75,75	1.69	14 (20%)
2	OA9	A	500	-	54,58,58	1.91	16 (29%)	76,86,86	1.98	14 (18%)

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	MEZ	D	502	-	-	2/8/8/8	-
4	MEZ	E	502	1	-	4/6/6/8	-
4	MEZ	F	502	1	-	3/7/7/8	-
3	COA	B	501	-	-	13/48/64/64	0/3/3/3
4	MEZ	C	502	1	-	1/7/7/8	-
4	MEZ	B	502	1	-	2/6/6/8	-
3	COA	D	501	1	-	8/48/64/64	0/3/3/3
3	COA	E	501	-	-	13/48/64/64	0/3/3/3
3	COA	F	501	-	-	7/48/64/64	0/3/3/3
3	COA	C	501	-	-	13/48/64/64	0/3/3/3
2	OA9	A	500	-	-	26/57/75/75	0/3/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	COA	P1A-O3A	10.54	1.70	1.59
3	E	501	COA	P1A-O3A	10.47	1.70	1.59
3	F	501	COA	P1A-O3A	9.69	1.70	1.59
3	D	501	COA	P1A-O3A	8.46	1.68	1.59
3	C	501	COA	P1A-O3A	6.66	1.66	1.59

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	MEZ	O4-C5-C3	-15.90	108.87	125.11
2	A	500	OA9	C2P-S1P-C07	11.12	112.95	99.85
4	E	502	MEZ	O4-C5-C3	-9.62	115.29	125.11
4	F	502	MEZ	O2-C1-C2	-5.95	115.69	123.68
4	B	502	MEZ	C1-C2-C3	-5.35	120.43	128.40

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	OA9	C02-C07-S1P-C2P
2	A	500	OA9	O08-C07-S1P-C2P
2	A	500	OA9	S1P-C2P-C3P-N4P
2	A	500	OA9	C3P-C2P-S1P-C07
2	A	500	OA9	N8P-C9P-CAP-OAP

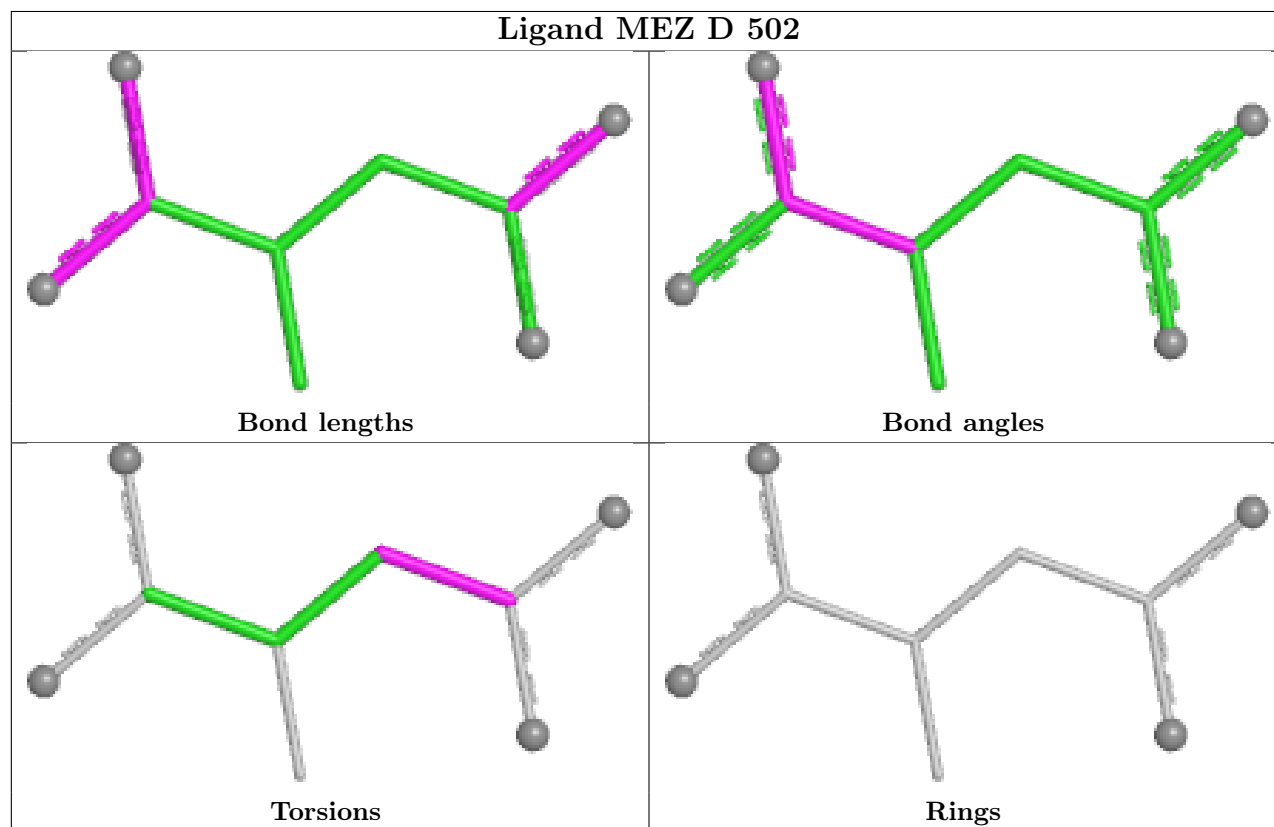
There are no ring outliers.

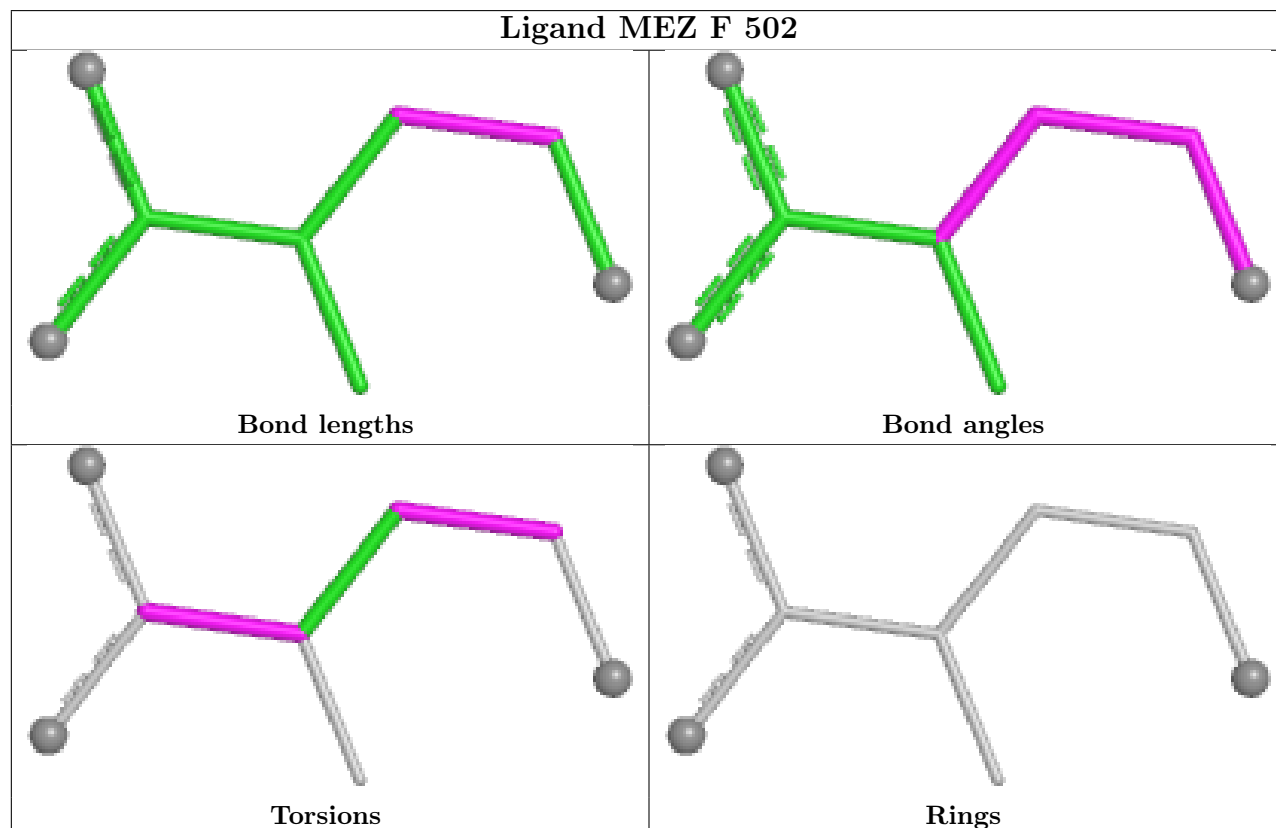
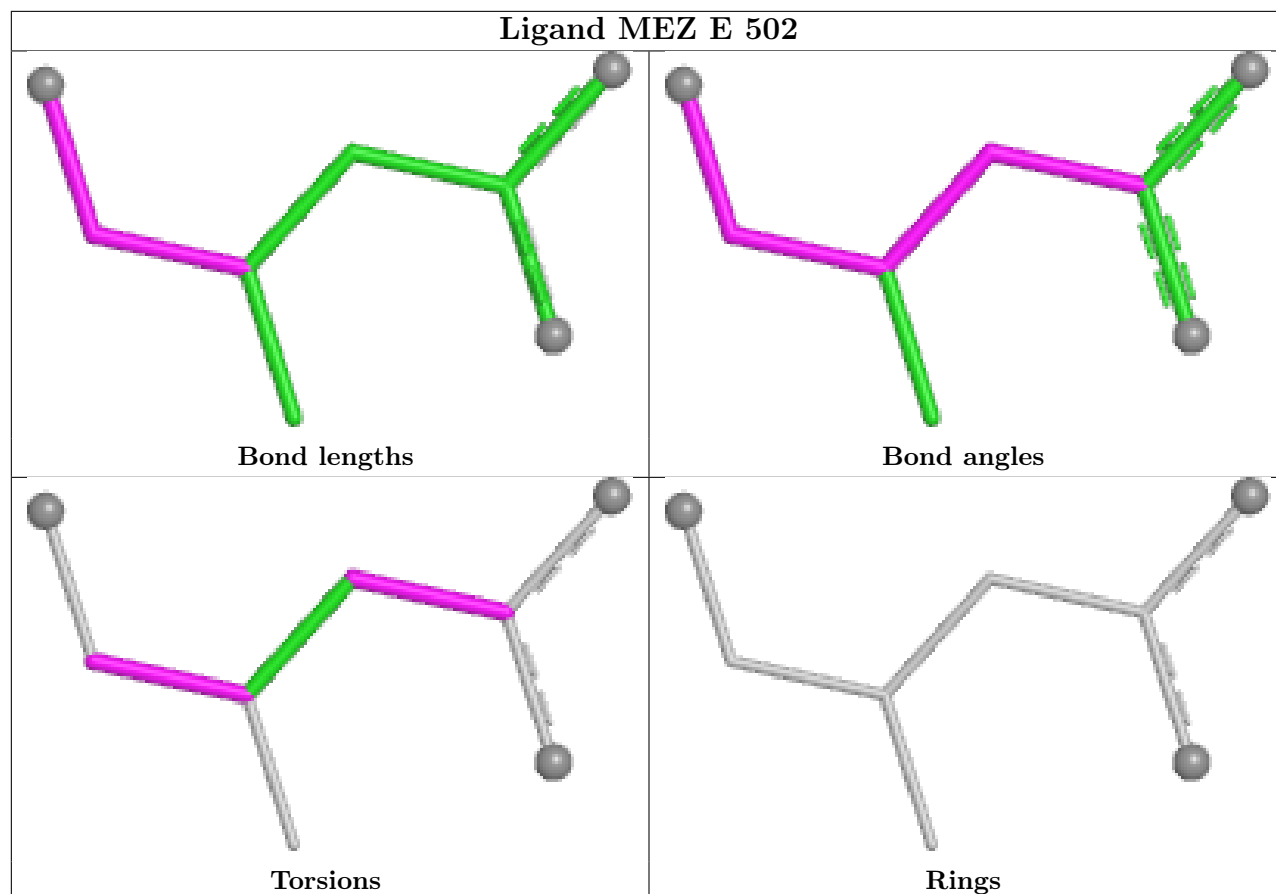
7 monomers are involved in 7 short contacts:

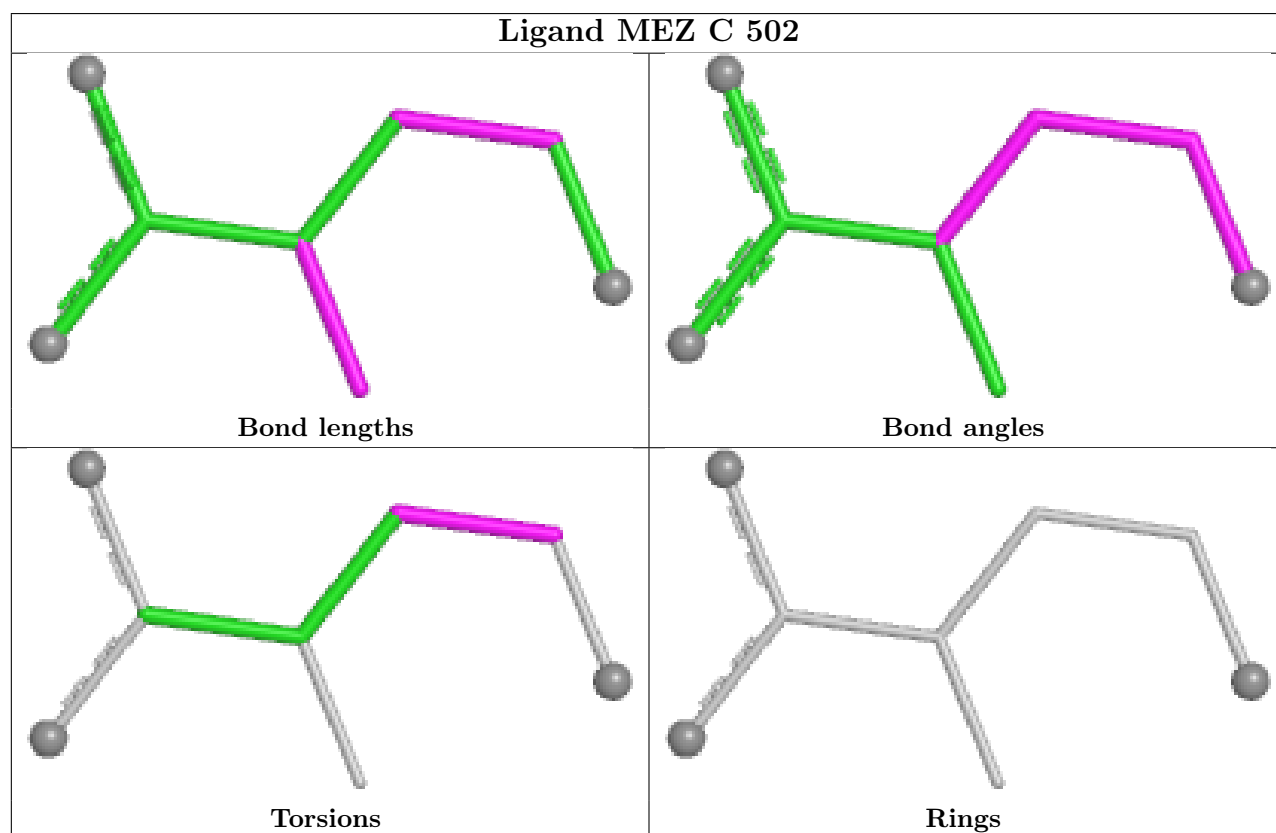
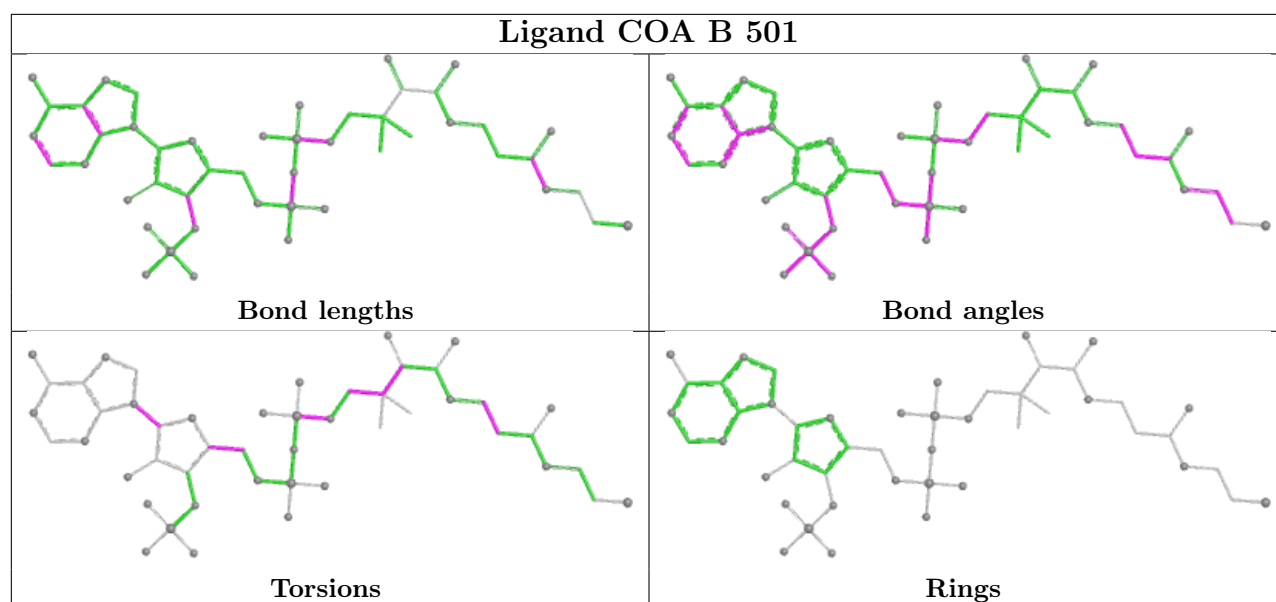
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	502	MEZ	1	0
4	E	502	MEZ	1	0
4	F	502	MEZ	1	0
4	C	502	MEZ	2	0
4	B	502	MEZ	1	0
3	D	501	COA	1	0
3	F	501	COA	1	0

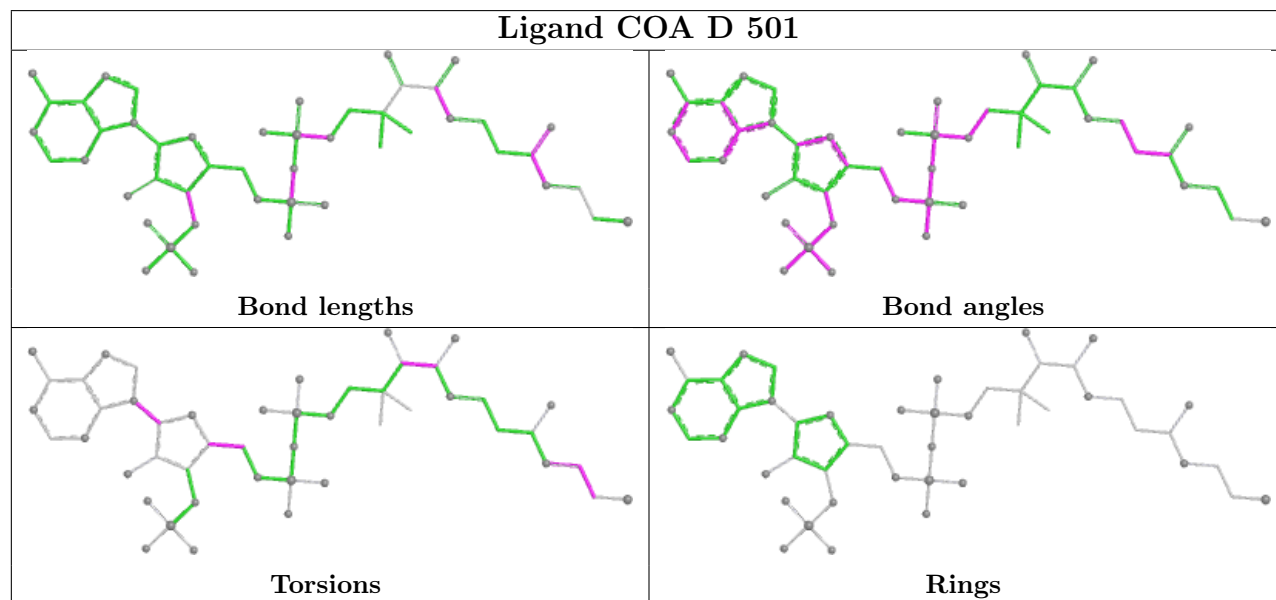
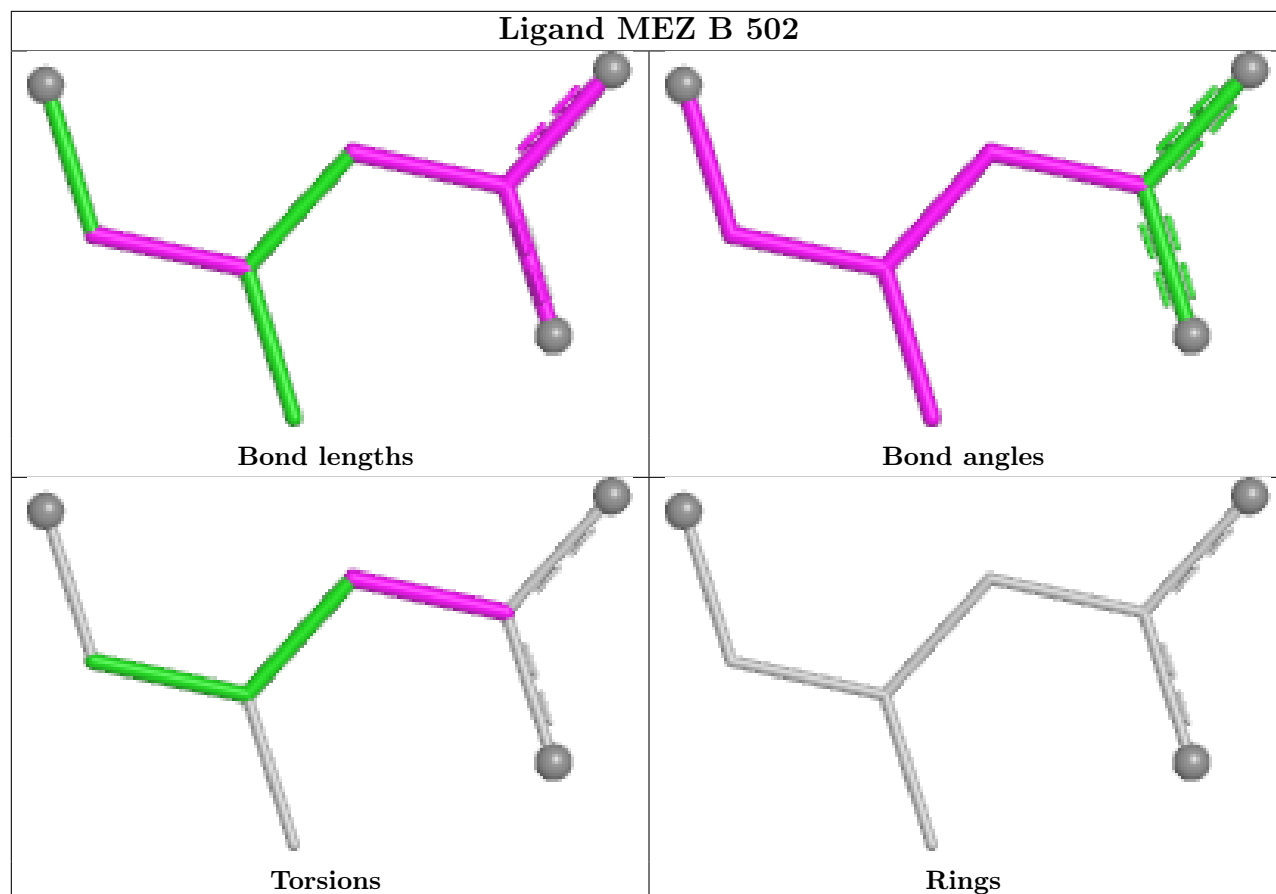
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

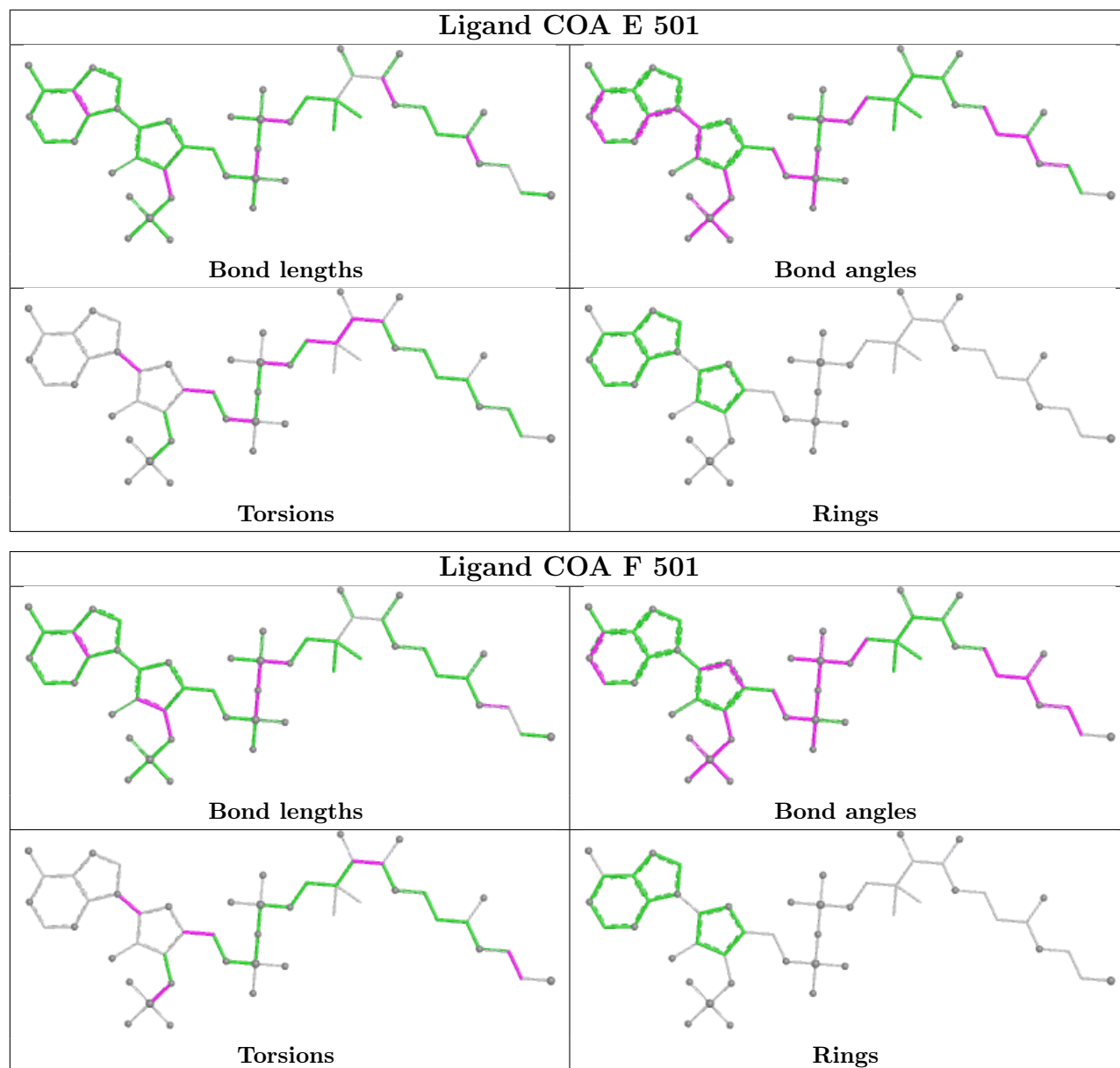
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

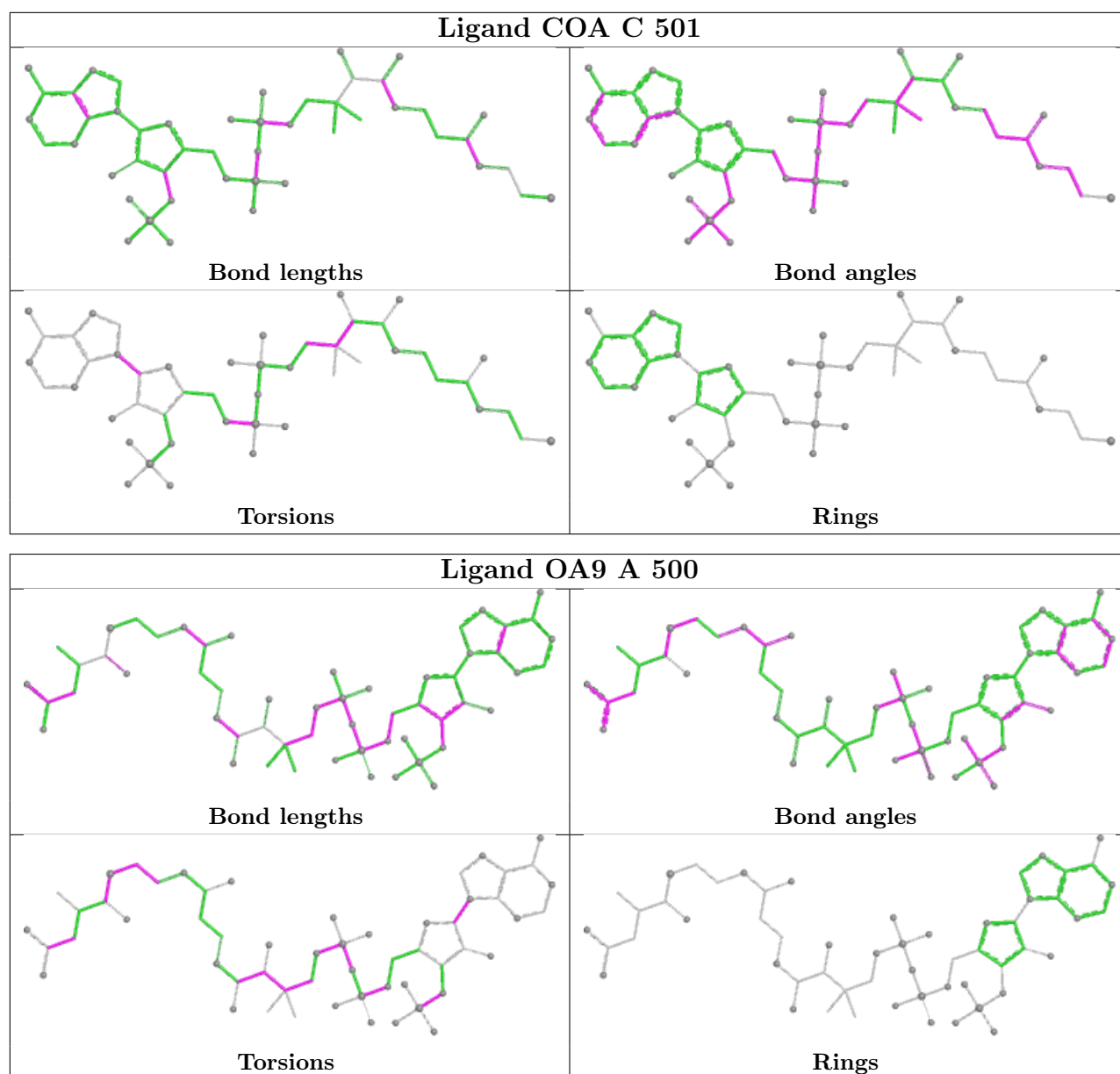












5.7 Other polymers [i](#)

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	406/430 (94%)	-0.21	2 (0%) 87 85	38, 49, 69, 102	0
1	B	406/430 (94%)	-0.01	21 (5%) 33 29	38, 50, 82, 106	0
1	C	406/430 (94%)	-0.13	13 (3%) 50 46	38, 47, 70, 105	0
1	D	406/430 (94%)	-0.29	5 (1%) 76 73	39, 46, 65, 94	0
1	E	405/430 (94%)	-0.23	8 (1%) 65 61	38, 45, 61, 90	0
1	F	406/430 (94%)	-0.17	14 (3%) 48 43	38, 46, 67, 114	0
All	All	2435/2580 (94%)	-0.17	63 (2%) 57 52	38, 47, 70, 114	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	4.7
1	B	74	ILE	4.5
1	C	1	MET	4.3
1	C	126	GLY	4.0
1	F	131	GLY	4.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

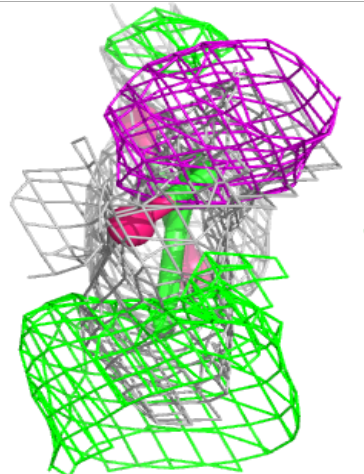
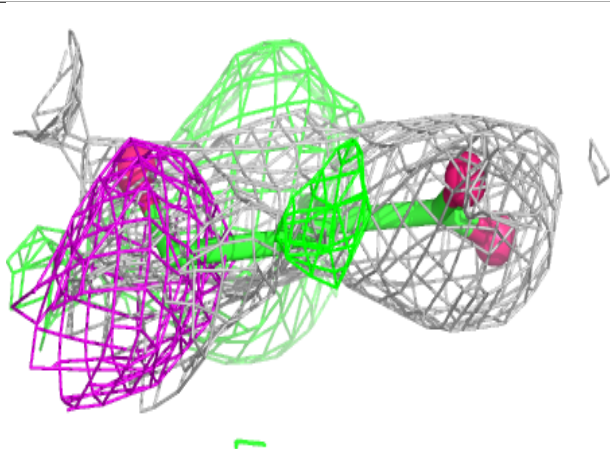
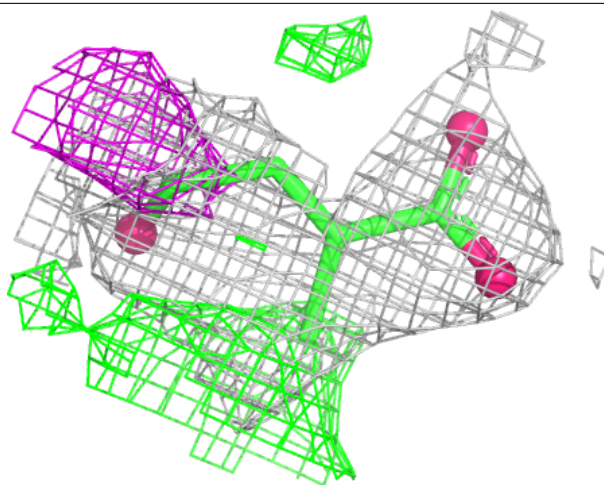
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MEZ	F	502	8/9	0.70	0.29	49,56,60,62	8
3	COA	B	501	48/48	0.73	0.27	79,93,114,118	48
4	MEZ	B	502	8/9	0.75	0.30	46,57,63,66	8
4	MEZ	C	502	8/9	0.76	0.20	67,74,76,78	0
4	MEZ	E	502	8/9	0.77	0.26	38,53,56,57	8
3	COA	F	501	48/48	0.78	0.24	69,82,105,107	48
4	MEZ	D	502	9/9	0.79	0.25	52,54,59,60	9
3	COA	C	501	48/48	0.82	0.19	65,76,100,102	48
3	COA	E	501	48/48	0.87	0.16	53,62,84,86	48
2	OA9	A	500	56/56	0.92	0.13	44,51,70,73	0
3	COA	D	501	48/48	0.94	0.10	38,47,64,68	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.

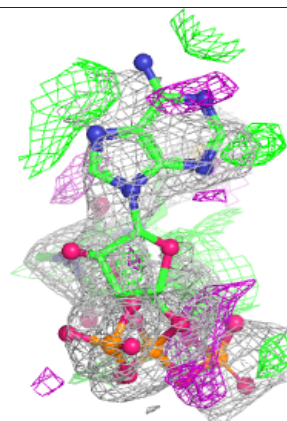
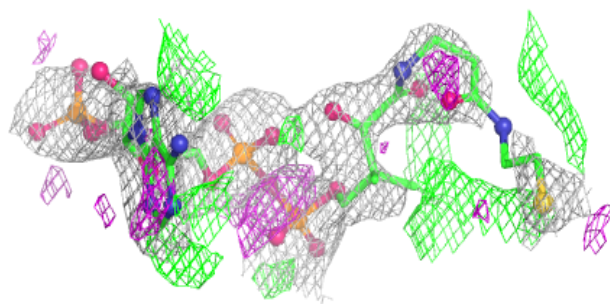
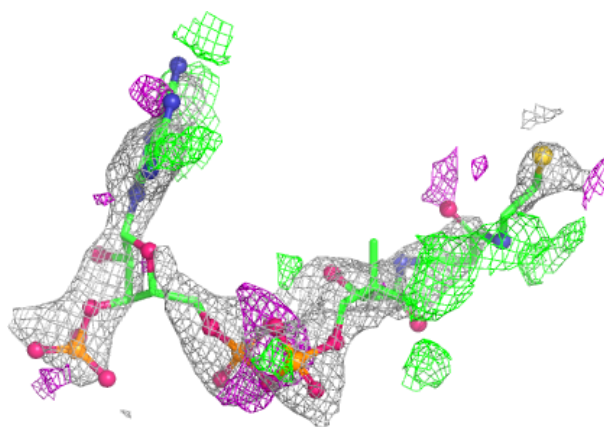
Electron density around MEZ F 502:

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



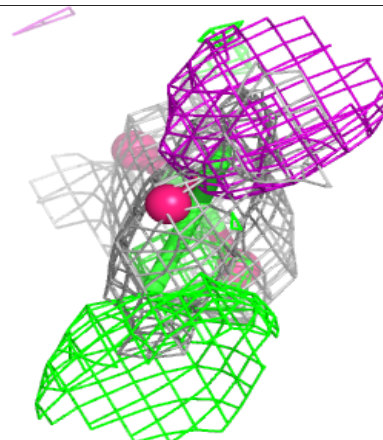
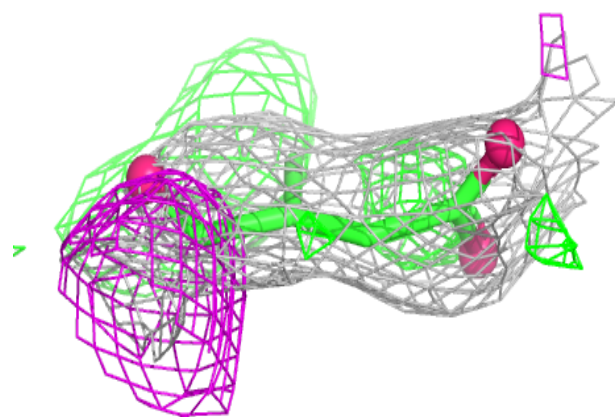
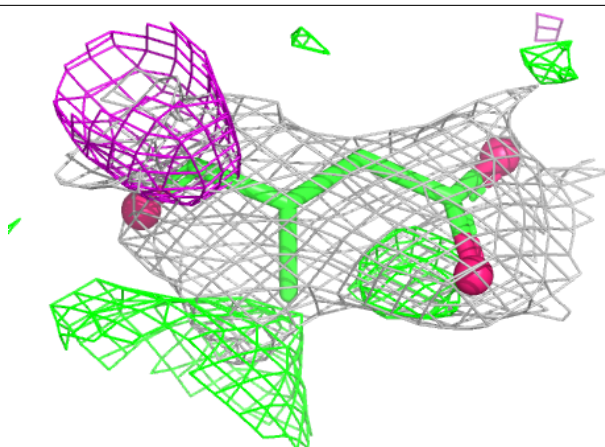
Electron density around COA B 501:

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

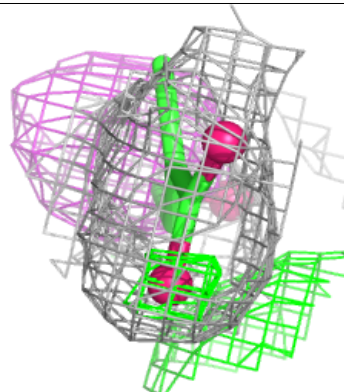
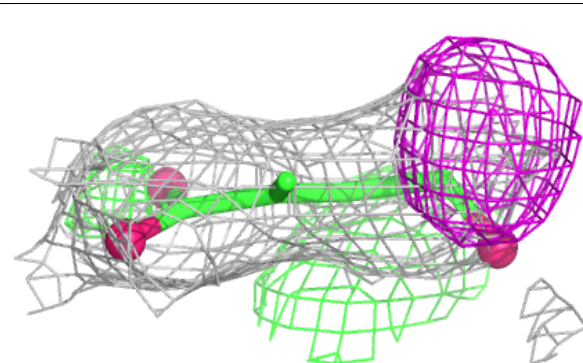
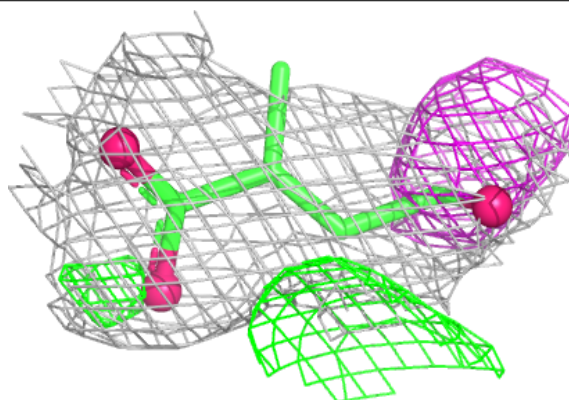


Electron density around MEZ B 502:

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and green (positive)

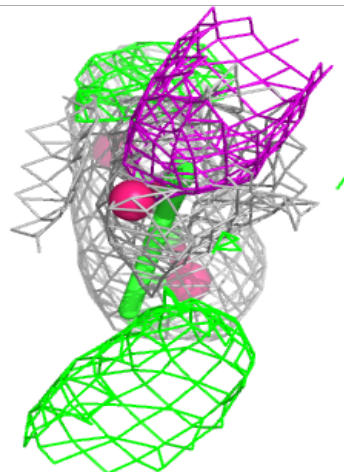
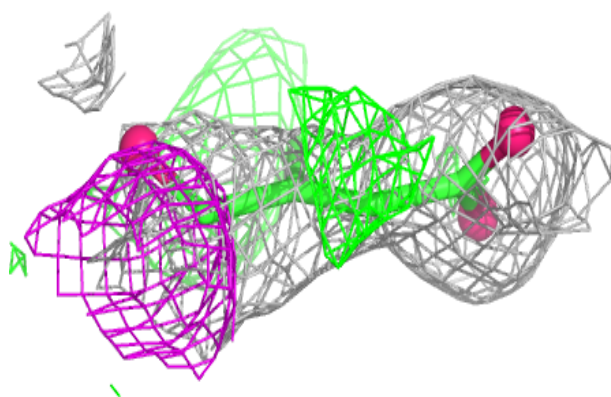
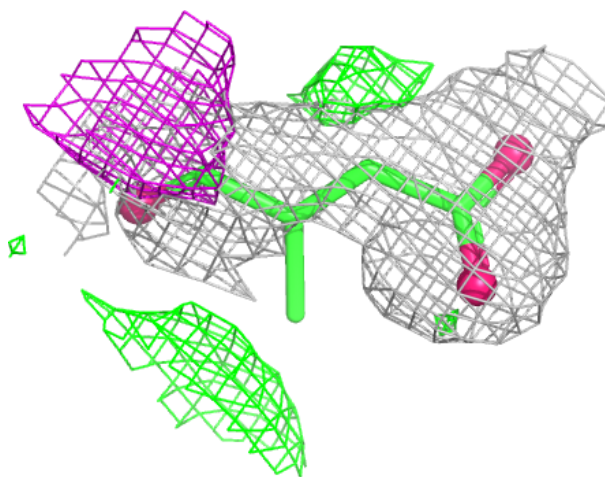
**Electron density around MEZ C 502:**

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and green (positive)



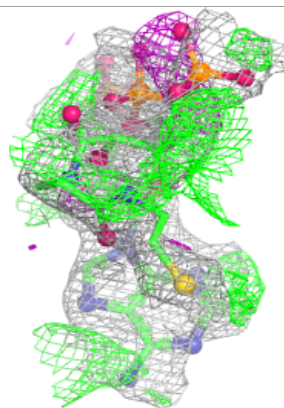
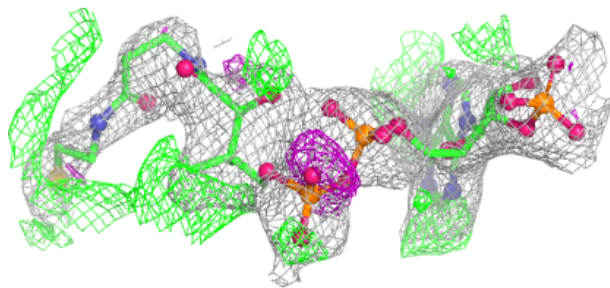
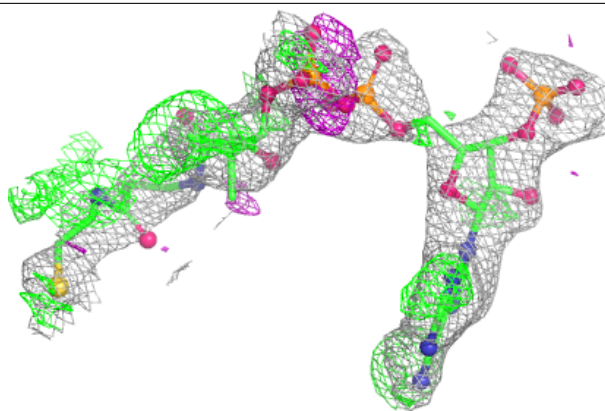
Electron density around MEZ E 502:

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and green (positive)



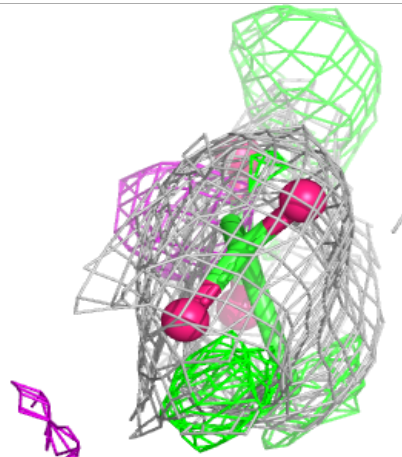
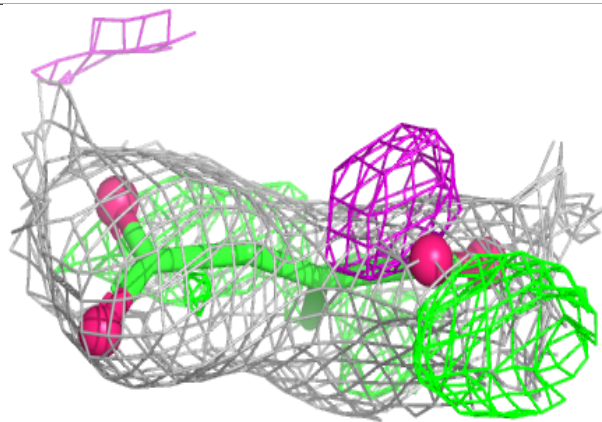
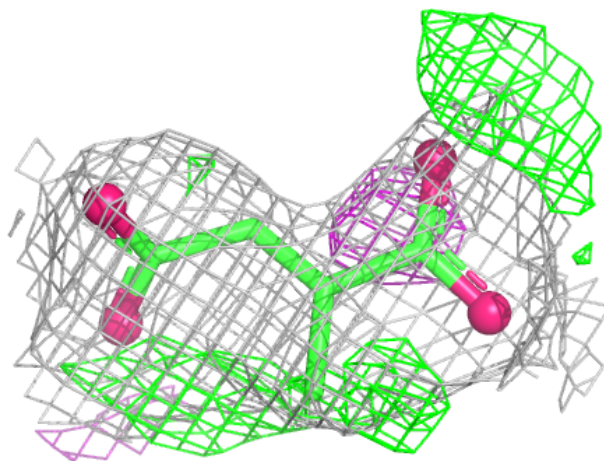
Electron density around COA F 501:

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



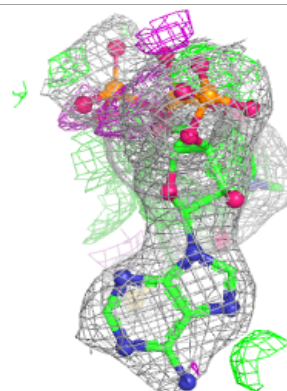
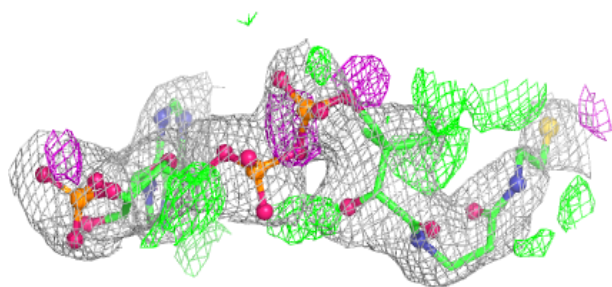
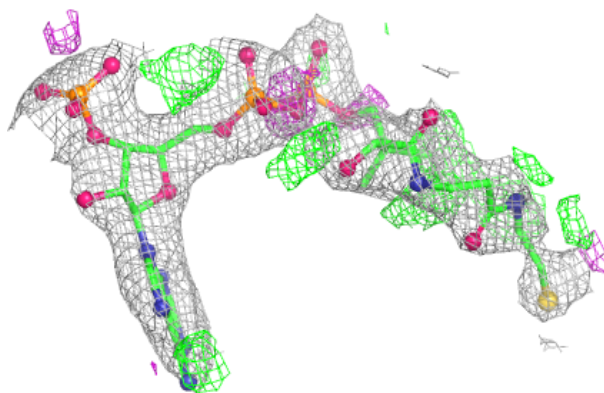
Electron density around MEZ D 502:

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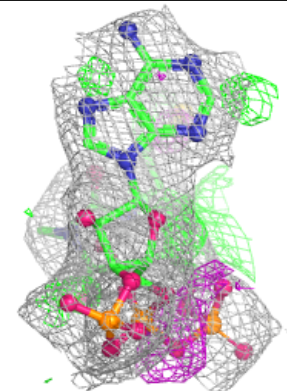
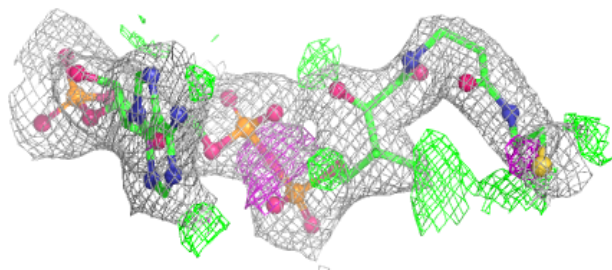
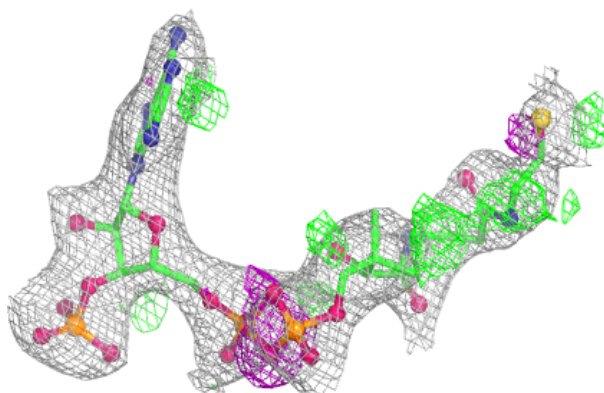


Electron density around COA C 501:

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and green (positive)

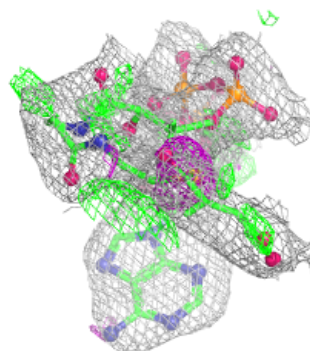
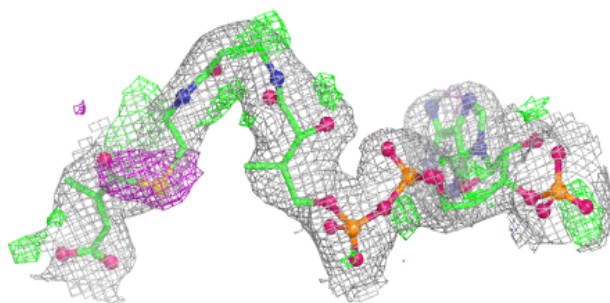
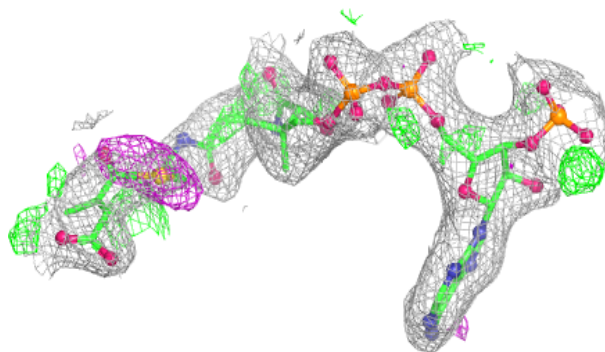
**Electron density around COA E 501:**

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and green (positive)

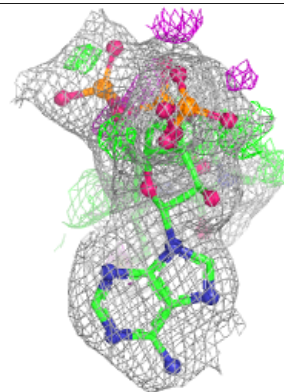
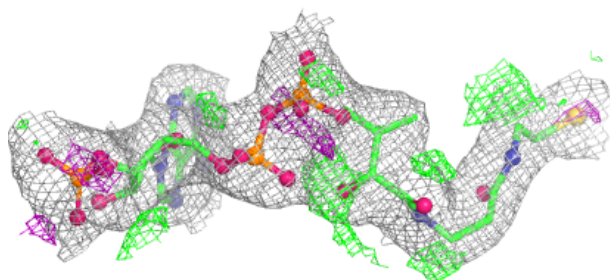
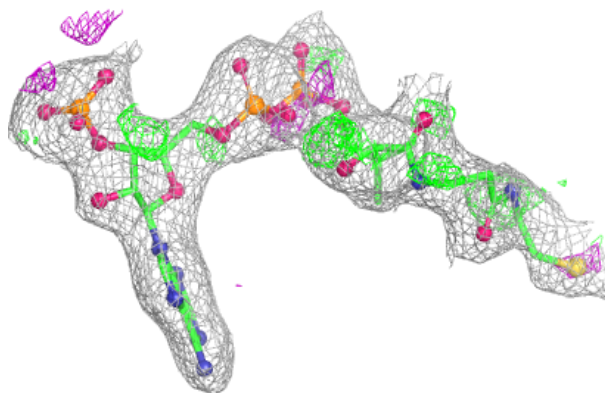


Electron density around OA9 A 500:

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

**Electron density around COA 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 [i](#)

There are no such residues in this entry.