



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:14 PM UTC

PDB ID : 5M45 / pdb_00005m45
Title : Structure of Acetone Carboxylase purified from Xanthobacter autotrophicus
Authors : Kabasakal, B.V.; Wells, J.N.; Nwaobi, B.C.; Eilers, B.J.; Peters, J.W.; Murray, J.W.
Deposited on : 2016-10-18
Resolution : 1.87 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

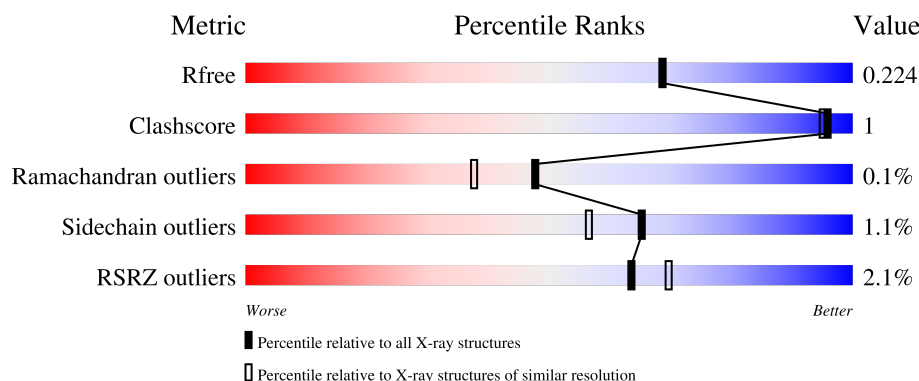
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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.



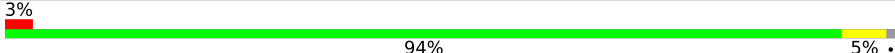
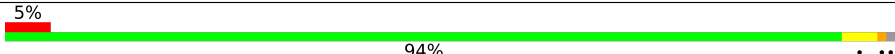
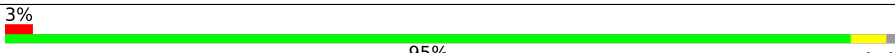
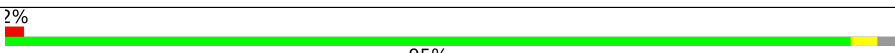
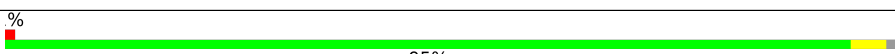
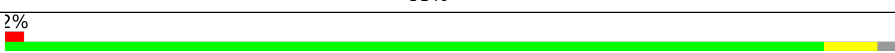
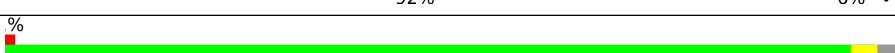
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	776	% 96% ..
1	D	776	96% ..
1	G	776	96% ..
1	J	776	% 95% ..
2	B	717	5% 95% ..

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Mol	Chain	Length	Quality of chain
2	E	717	 3% 94% 5% .
2	H	717	 5% 94% . .
2	K	717	 3% 95% . .
3	C	168	 2% 95% . .
3	F	168	 % 95% . .
3	I	168	 2% 92% 6% .
3	L	168	 % 95% . .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 56067 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 Acetone carboxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	0	0
			5990	3782	1049	1125	34			
1	D	762	Total	C	N	O	S	0	0	0
			5990	3782	1049	1125	34			
1	G	762	Total	C	N	O	S	0	0	0
			5990	3782	1049	1125	34			
1	J	762	Total	C	N	O	S	0	0	0
			5990	3782	1049	1125	34			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	674	THR	ALA	conflict	UNP Q8RM03
A	675	ALA	GLY	conflict	UNP Q8RM03
A	737	ASP	SER	conflict	UNP Q8RM03
D	674	THR	ALA	conflict	UNP Q8RM03
D	675	ALA	GLY	conflict	UNP Q8RM03
D	737	ASP	SER	conflict	UNP Q8RM03
G	674	THR	ALA	conflict	UNP Q8RM03
G	675	ALA	GLY	conflict	UNP Q8RM03
G	737	ASP	SER	conflict	UNP Q8RM03
J	674	THR	ALA	conflict	UNP Q8RM03
J	675	ALA	GLY	conflict	UNP Q8RM03
J	737	ASP	SER	conflict	UNP Q8RM03

- Molecule 2 is a protein called Acetone carboxylase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	709	Total	C	N	O	S	0	0	0
			5463	3439	953	1046	25			
2	E	709	Total	C	N	O	S	0	0	0
			5463	3439	953	1046	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	709	Total	C	N	O	S	0	0	0
			5463	3439	953	1046	25			
2	K	709	Total	C	N	O	S	0	0	0
			5463	3439	953	1046	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	151	MET	ILE	conflict	UNP Q8RM04
B	190	VAL	GLU	conflict	UNP Q8RM04
E	151	MET	ILE	conflict	UNP Q8RM04
E	190	VAL	GLU	conflict	UNP Q8RM04
H	151	MET	ILE	conflict	UNP Q8RM04
H	190	VAL	GLU	conflict	UNP Q8RM04
K	151	MET	ILE	conflict	UNP Q8RM04
K	190	VAL	GLU	conflict	UNP Q8RM04

- Molecule 3 is a protein called Acetone carboxylase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	165	Total	C	N	O	S	0	0	0
			1375	891	230	245	9			
3	F	165	Total	C	N	O	S	0	0	0
			1375	891	230	245	9			
3	I	165	Total	C	N	O	S	0	0	0
			1375	891	230	245	9			
3	L	165	Total	C	N	O	S	0	0	0
			1375	891	230	245	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	HIS	SER	conflict	UNP Q8RM02
F	90	HIS	SER	conflict	UNP Q8RM02
I	90	HIS	SER	conflict	UNP Q8RM02
L	90	HIS	SER	conflict	UNP Q8RM02

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

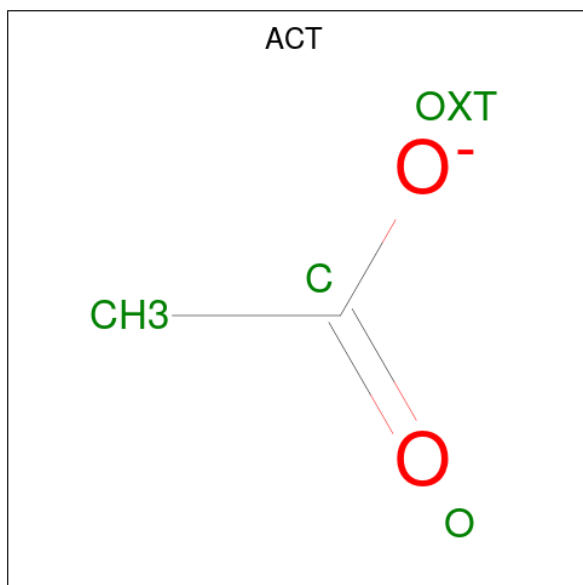
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mn	0	0
			1	1		
4	G	1	Total	Mn	0	0
			1	1		
4	J	1	Total	Mn	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



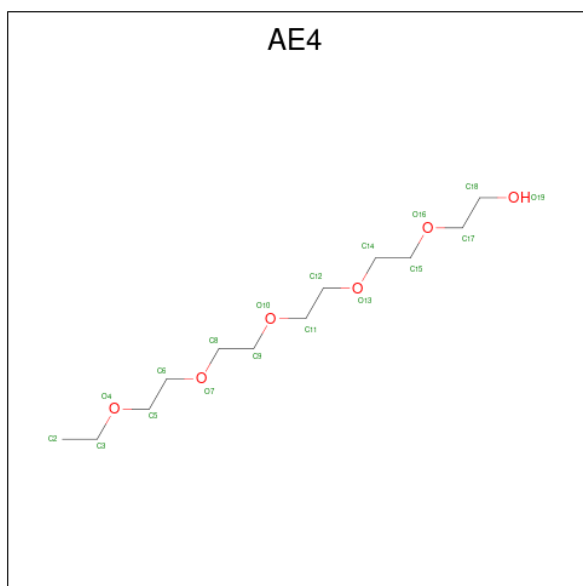
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 3,6,9,12,15-PENTAOXAHEPTADECAN-1-OL (CCD ID: AE4) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			18	12	6		
6	D	1	Total	C	O	0	0
			18	12	6		
6	G	1	Total	C	O	0	0
			18	12	6		
6	J	1	Total	C	O	0	0
			18	12	6		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

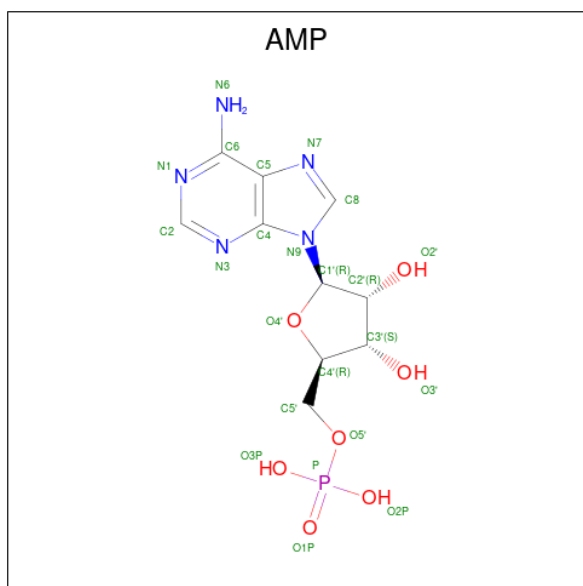
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total 4	Mg 4	0	0
7	D	2	Total 2	Mg 2	0	0
7	E	4	Total 4	Mg 4	0	0
7	G	2	Total 2	Mg 2	0	0
7	H	4	Total 4	Mg 4	0	0
7	J	2	Total 2	Mg 2	0	0
7	K	3	Total 3	Mg 3	0	0
7	L	1	Total 1	Mg 1	0	0

- Molecule 8 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
8	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
8	H	1	Total 23	C 10	N 5	O 7	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	K	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Zn	0	0
			1	1		
9	F	1	Total	Zn	0	0
			1	1		
9	I	1	Total	Zn	0	0
			1	1		
9	L	1	Total	Zn	0	0
			1	1		

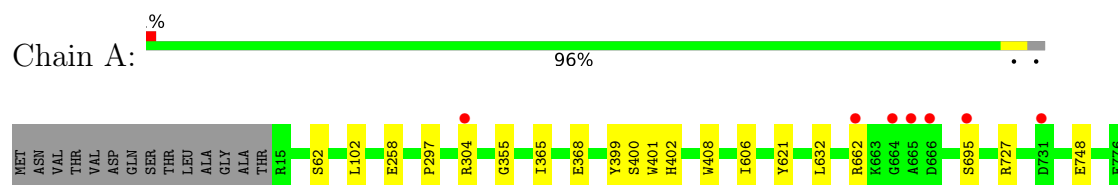
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	578	Total	O	0	0
			578	578		
10	B	391	Total	O	0	0
			391	391		
10	C	122	Total	O	0	0
			122	122		
10	D	598	Total	O	0	0
			598	598		
10	E	477	Total	O	0	0
			477	477		
10	F	134	Total	O	0	0
			134	134		
10	G	618	Total	O	0	0
			618	618		
10	H	376	Total	O	0	0
			376	376		
10	I	124	Total	O	0	0
			124	124		
10	J	573	Total	O	0	0
			573	573		
10	K	386	Total	O	0	0
			386	386		
10	L	134	Total	O	0	0
			134	134		

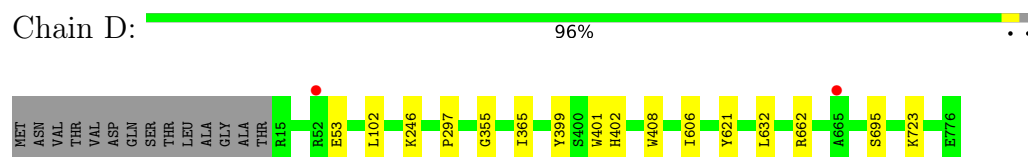
3 Residue-property plots

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

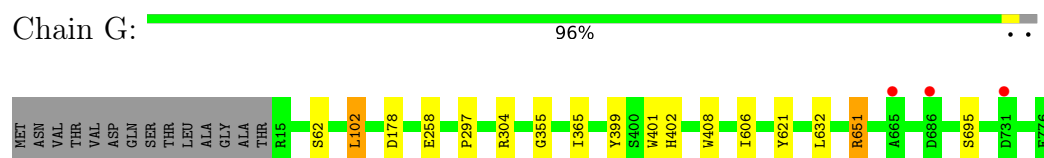
- Molecule 1: Acetone carboxylase alpha subunit



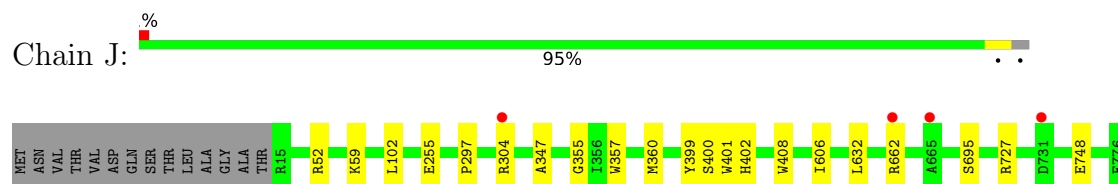
- Molecule 1: Acetone carboxylase alpha subunit



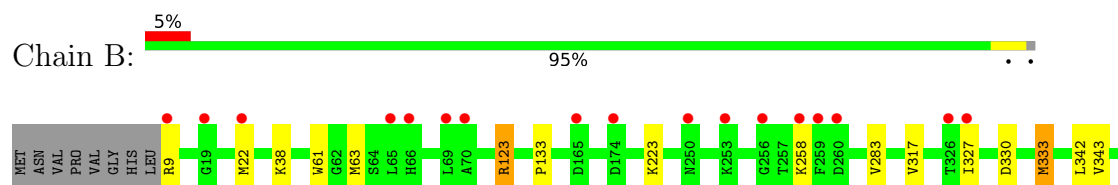
- Molecule 1: Acetone carboxylase alpha subunit

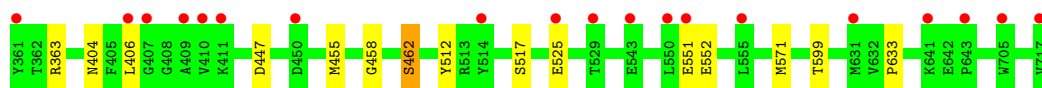


- Molecule 1: Acetone carboxylase alpha subunit

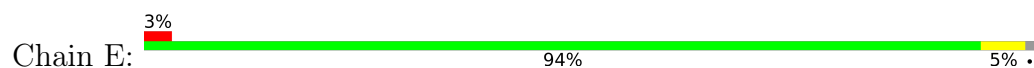


- Molecule 2: Acetone carboxylase beta subunit

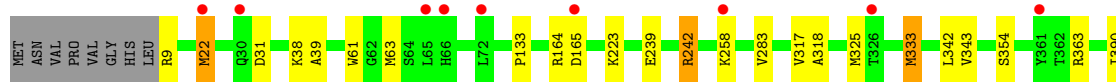
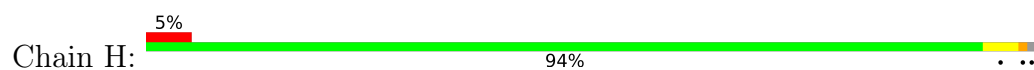




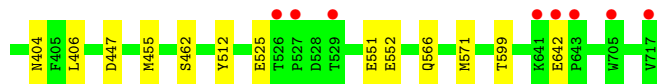
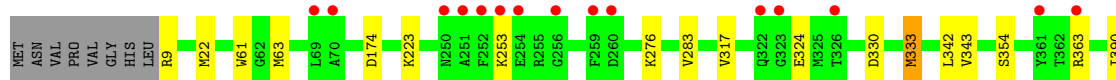
- Molecule 2: Acetone carboxylase beta subunit



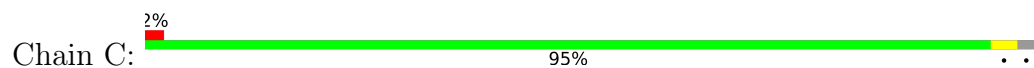
- Molecule 2: Acetone carboxylase beta subunit



- Molecule 2: Acetone carboxylase beta subunit



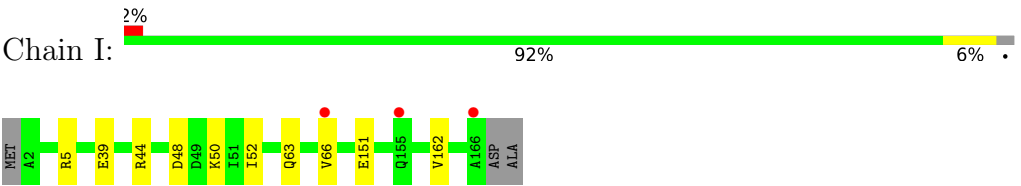
- Molecule 3: Acetone carboxylase gamma subunit



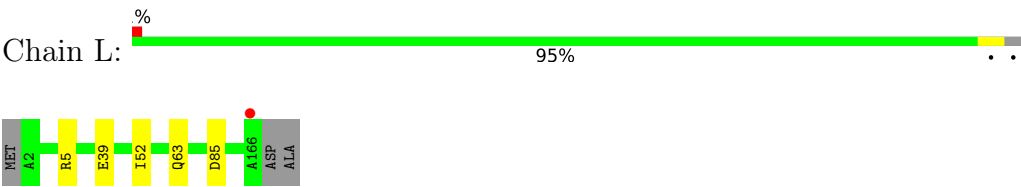
- Molecule 3: Acetone carboxylase gamma subunit



● Molecule 3: Acetone carboxylase gamma subunit



● Molecule 3: Acetone carboxylase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.92Å 139.73Å 165.83Å 65.89° 86.54° 88.69°	Depositor
Resolution (Å)	126.06 – 1.87 126.06 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.3 (126.06-1.87) 97.3 (126.06-1.87)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.192 , 0.217 0.201 , 0.224	Depositor DCC
R_{free} test set	28101 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.079 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	56067	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AE4, AMP, MN, ZN, ACT, MG

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	0.96	0/6143	0.92	5/8324 (0.1%)
1	D	0.97	0/6143	0.93	3/8324 (0.0%)
1	G	0.97	0/6143	0.93	7/8324 (0.1%)
1	J	0.96	1/6143 (0.0%)	0.92	5/8324 (0.1%)
2	B	0.93	2/5578 (0.0%)	0.94	1/7561 (0.0%)
2	E	0.95	2/5578 (0.0%)	0.95	1/7561 (0.0%)
2	H	0.94	1/5578 (0.0%)	0.96	2/7561 (0.0%)
2	K	0.93	1/5578 (0.0%)	0.93	0/7561
3	C	0.92	0/1423	0.94	0/1943
3	F	0.94	0/1423	0.94	0/1943
3	I	0.93	0/1423	0.94	0/1943
3	L	0.92	0/1423	0.91	0/1943
All	All	0.95	7/52576 (0.0%)	0.93	24/71312 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	ASP	C-O	-7.56	1.20	1.23
2	E	133	PRO	CA-C	7.26	1.55	1.51
2	H	133	PRO	CA-C	7.05	1.55	1.51
2	K	330	ASP	C-O	-5.66	1.21	1.23
2	B	133	PRO	CA-C	5.49	1.54	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	123	ARG	CB-CG-CD	9.26	132.59	111.30
1	D	662	ARG	CG-CD-NE	-7.40	95.72	112.00
1	G	651	ARG	CG-CD-NE	6.46	126.22	112.00
1	G	651	ARG	CA-CB-CG	6.33	126.76	114.10
1	G	102	LEU	CA-CB-CG	6.21	138.05	116.30

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	5990	0	5745	9	0
1	D	5990	0	5745	6	0
1	G	5990	0	5745	6	0
1	J	5990	0	5745	8	0
2	B	5463	0	5381	16	0
2	E	5463	0	5381	21	0
2	H	5463	0	5381	17	0
2	K	5463	0	5381	14	1
3	C	1375	0	1335	3	0
3	F	1375	0	1335	2	0
3	I	1375	0	1335	6	0
3	L	1375	0	1335	3	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
5	A	8	0	6	0	0
5	B	4	0	3	0	0
5	D	8	0	6	0	0
5	E	4	0	3	0	0
5	G	8	0	6	0	0
5	H	4	0	3	0	0
5	J	8	0	6	0	0
5	K	4	0	3	0	0
6	A	18	0	26	0	0
6	D	18	0	26	1	0
6	G	18	0	26	1	0
6	J	18	0	26	0	0
7	A	2	0	0	0	0
7	B	4	0	0	0	0
7	D	2	0	0	0	0
7	E	4	0	0	0	0
7	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	4	0	0	0	0
7	J	2	0	0	0	0
7	K	3	0	0	0	0
7	L	1	0	0	0	0
8	B	23	0	12	0	0
8	E	23	0	12	0	0
8	H	23	0	12	0	0
8	K	23	0	12	0	0
9	C	1	0	0	0	0
9	F	1	0	0	0	0
9	I	1	0	0	0	0
9	L	1	0	0	0	0
10	A	578	0	0	2	0
10	B	391	0	0	1	0
10	C	122	0	0	1	0
10	D	598	0	0	1	0
10	E	477	0	0	3	1
10	F	134	0	0	0	0
10	G	618	0	0	1	0
10	H	376	0	0	0	0
10	I	124	0	0	3	0
10	J	573	0	0	1	0
10	K	386	0	0	2	0
10	L	134	0	0	1	0
All	All	56067	0	50032	110	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 110 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)
2:H:571:MET:HE1	2:H:599:THR:HG22	1.58	0.86
2:E:571:MET:HE1	2:E:599:THR:HG22	1.59	0.85
2:K:571:MET:HE1	2:K:599:THR:HG22	1.59	0.83
2:B:571:MET:HE1	2:B:599:THR:HG22	1.67	0.75
2:B:22:MET:SD	2:B:406:LEU:HD13	2.32	0.70

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)
2:K:642:GLU:OE1	10:E:901:HOH:O[1_545]	2.19	0.01

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	760/776 (98%)	738 (97%)	21 (3%)	1 (0%)	48	37
1	D	760/776 (98%)	737 (97%)	22 (3%)	1 (0%)	48	37
1	G	760/776 (98%)	737 (97%)	22 (3%)	1 (0%)	48	37
1	J	760/776 (98%)	736 (97%)	24 (3%)	0	100	100
2	B	707/717 (99%)	691 (98%)	15 (2%)	1 (0%)	48	37
2	E	707/717 (99%)	689 (98%)	17 (2%)	1 (0%)	48	37
2	H	707/717 (99%)	690 (98%)	16 (2%)	1 (0%)	48	37
2	K	707/717 (99%)	692 (98%)	14 (2%)	1 (0%)	48	37
3	C	163/168 (97%)	159 (98%)	4 (2%)	0	100	100
3	F	163/168 (97%)	159 (98%)	4 (2%)	0	100	100
3	I	163/168 (97%)	159 (98%)	4 (2%)	0	100	100
3	L	163/168 (97%)	159 (98%)	4 (2%)	0	100	100
All	All	6520/6644 (98%)	6346 (97%)	167 (3%)	7 (0%)	48	37

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	LYS
2	E	223	LYS
2	H	223	LYS
2	K	223	LYS
1	A	365	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/623 (98%)	609 (100%)	3 (0%)	81	76
1	D	612/623 (98%)	608 (99%)	4 (1%)	76	69
1	G	612/623 (98%)	607 (99%)	5 (1%)	73	68
1	J	612/623 (98%)	609 (100%)	3 (0%)	81	76
2	B	573/580 (99%)	564 (98%)	9 (2%)	55	43
2	E	573/580 (99%)	564 (98%)	9 (2%)	55	43
2	H	573/580 (99%)	561 (98%)	12 (2%)	47	32
2	K	573/580 (99%)	563 (98%)	10 (2%)	53	40
3	C	154/156 (99%)	154 (100%)	0	100	100
3	F	154/156 (99%)	152 (99%)	2 (1%)	61	50
3	I	154/156 (99%)	153 (99%)	1 (1%)	78	72
3	L	154/156 (99%)	154 (100%)	0	100	100
All	All	5356/5436 (98%)	5298 (99%)	58 (1%)	65	56

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	178	ASP
2	K	462	SER
2	H	242	ARG
2	K	447	ASP
2	K	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	193	GLN
1	J	434	ASN
2	K	404	ASN
1	D	772	GLN

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Mol	Chain	Res	Type
1	D	598	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 32 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$
5	ACT	A	802	4	3,3,3	0.85	0	3,3,3	0.89	0
8	AMP	E	801	7	25,25,25	1.56	5 (20%)	37,38,38	1.91	10 (27%)
8	AMP	H	801	7	25,25,25	1.56	4 (16%)	37,38,38	1.71	8 (21%)
5	ACT	E	805	7	3,3,3	0.78	0	3,3,3	0.73	0
6	AE4	G	804	-	17,17,17	0.62	0	16,16,16	0.63	0
5	ACT	G	803	-	3,3,3	0.83	0	3,3,3	0.68	0
8	AMP	B	801	7	25,25,25	1.47	5 (20%)	37,38,38	1.84	11 (29%)
5	ACT	H	806	7	3,3,3	0.86	0	3,3,3	0.71	0
8	AMP	K	801	7	25,25,25	1.48	5 (20%)	37,38,38	1.93	11 (29%)
5	ACT	D	803	-	3,3,3	0.95	0	3,3,3	0.67	0
5	ACT	J	802	4	3,3,3	0.74	0	3,3,3	0.91	0
5	ACT	D	802	4	3,3,3	0.74	0	3,3,3	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	AE4	D	804	-	17,17,17	0.68	0	16,16,16	0.53	0
5	ACT	A	803	-	3,3,3	0.86	0	3,3,3	0.96	0
5	ACT	G	802	4	3,3,3	0.78	0	3,3,3	1.00	0
6	AE4	A	804	-	17,17,17	0.53	0	16,16,16	0.37	0
6	AE4	J	804	-	17,17,17	0.64	0	16,16,16	0.44	0
5	ACT	B	805	7	3,3,3	0.78	0	3,3,3	0.76	0
5	ACT	J	803	-	3,3,3	0.93	0	3,3,3	0.55	0
5	ACT	K	805	7	3,3,3	0.85	0	3,3,3	0.55	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
6	AE4	A	804	-	-	4/15/15/15	-
8	AMP	K	801	7	-	1/10/26/26	0/3/3/3
6	AE4	J	804	-	-	6/15/15/15	-
8	AMP	E	801	7	-	2/10/26/26	0/3/3/3
8	AMP	B	801	7	-	0/10/26/26	0/3/3/3
8	AMP	H	801	7	-	1/10/26/26	0/3/3/3
6	AE4	D	804	-	-	6/15/15/15	-
6	AE4	G	804	-	-	7/15/15/15	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	801	AMP	C5-C4	5.06	1.48	1.39
8	H	801	AMP	C5-C4	4.76	1.47	1.39
8	K	801	AMP	C5-C4	4.72	1.47	1.39
8	B	801	AMP	C5-C4	4.48	1.47	1.39
8	H	801	AMP	C4-N9	-2.79	1.31	1.37

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	801	AMP	C5-C4-N3	-4.99	119.85	126.72
8	B	801	AMP	C5-C4-N3	-4.48	120.55	126.72
8	E	801	AMP	C5-C4-N3	-4.39	120.67	126.72
8	K	801	AMP	N3-C4-N9	4.25	134.39	127.17
8	H	801	AMP	C5-C4-N3	-4.09	121.08	126.72

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

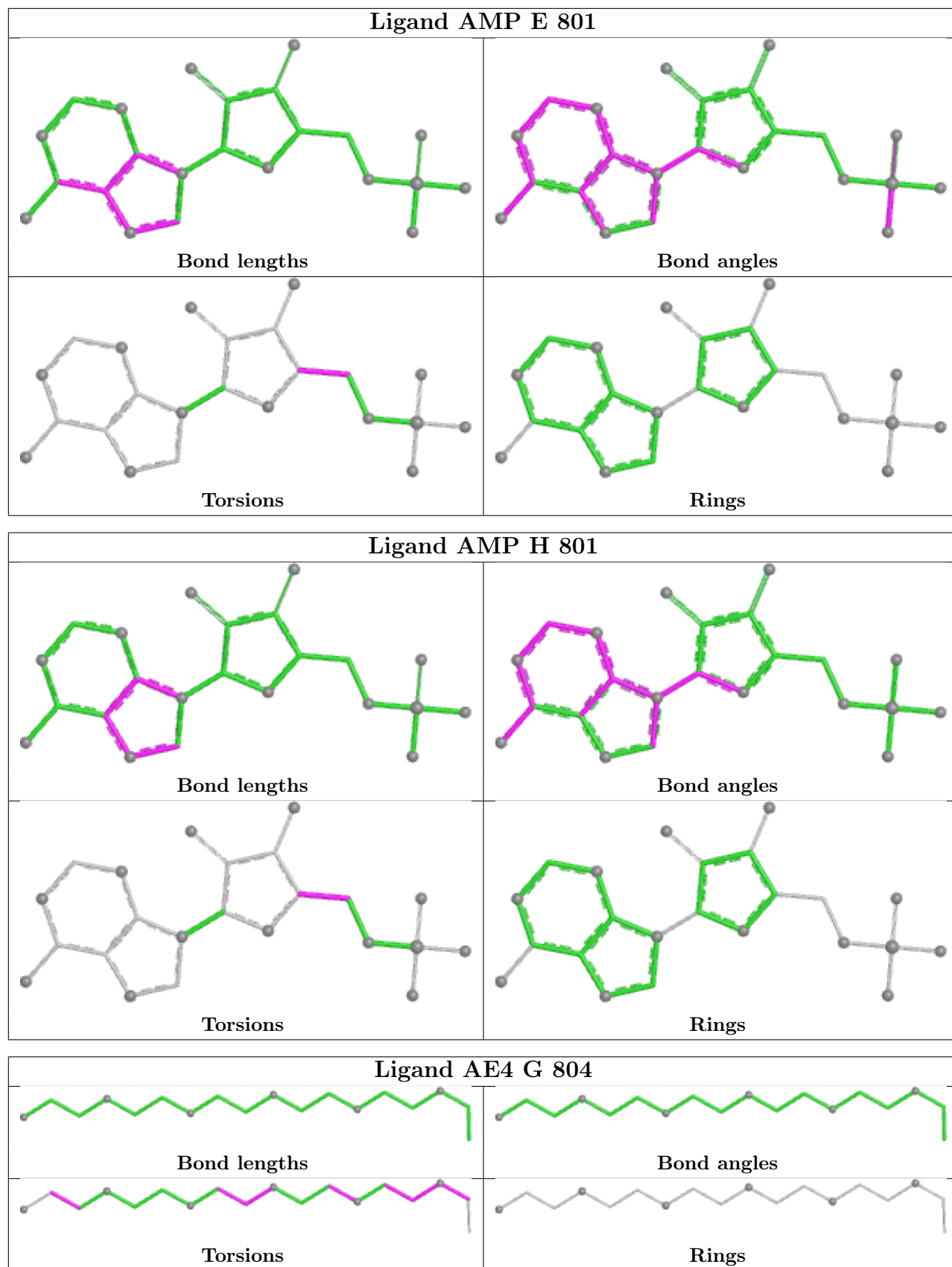
Mol	Chain	Res	Type	Atoms
6	J	804	AE4	O4-C5-C6-O7
6	J	804	AE4	O10-C11-C12-O13
6	A	804	AE4	O4-C5-C6-O7
6	G	804	AE4	O4-C5-C6-O7
8	E	801	AMP	C3'-C4'-C5'-O5'

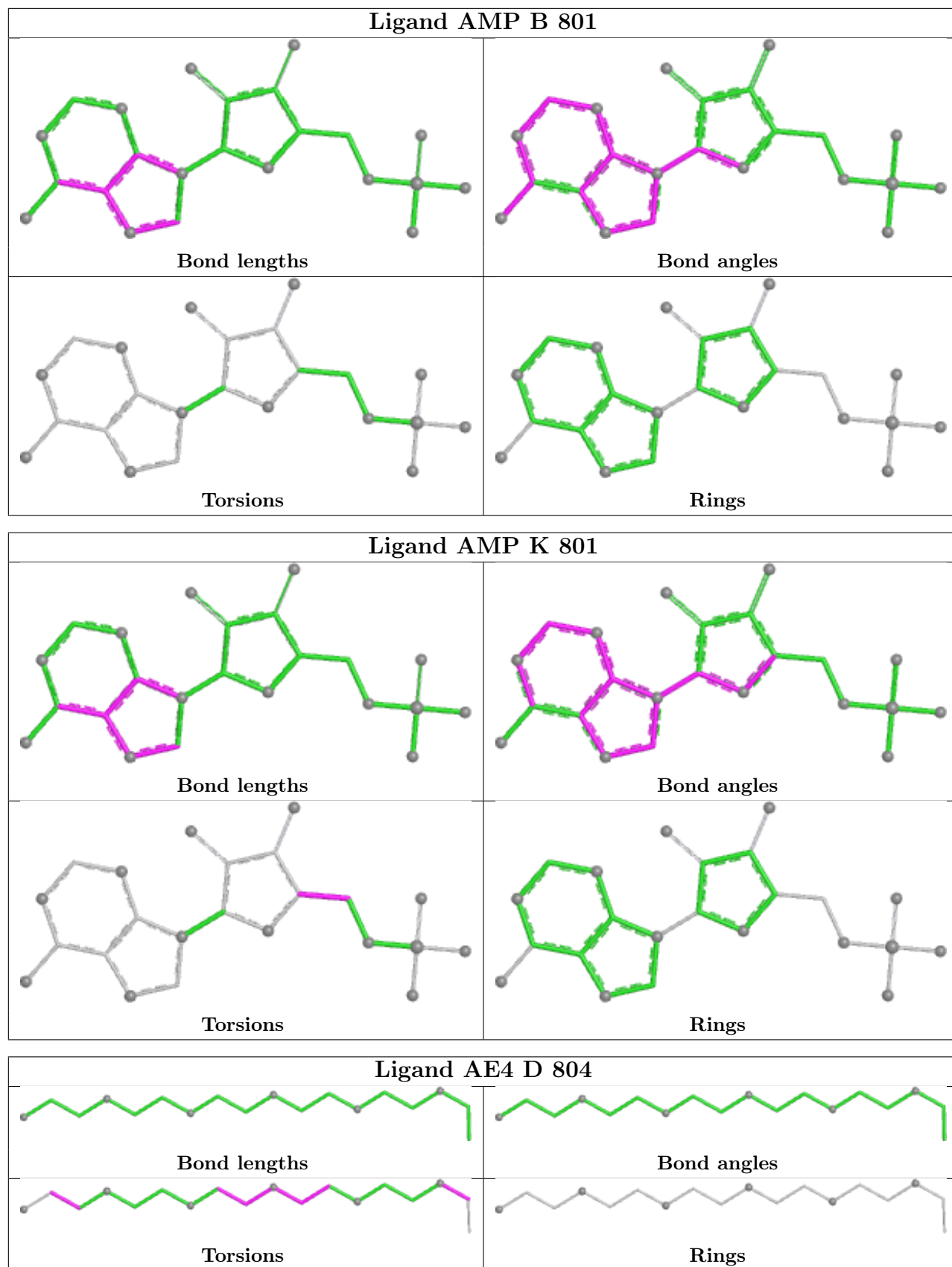
There are no ring outliers.

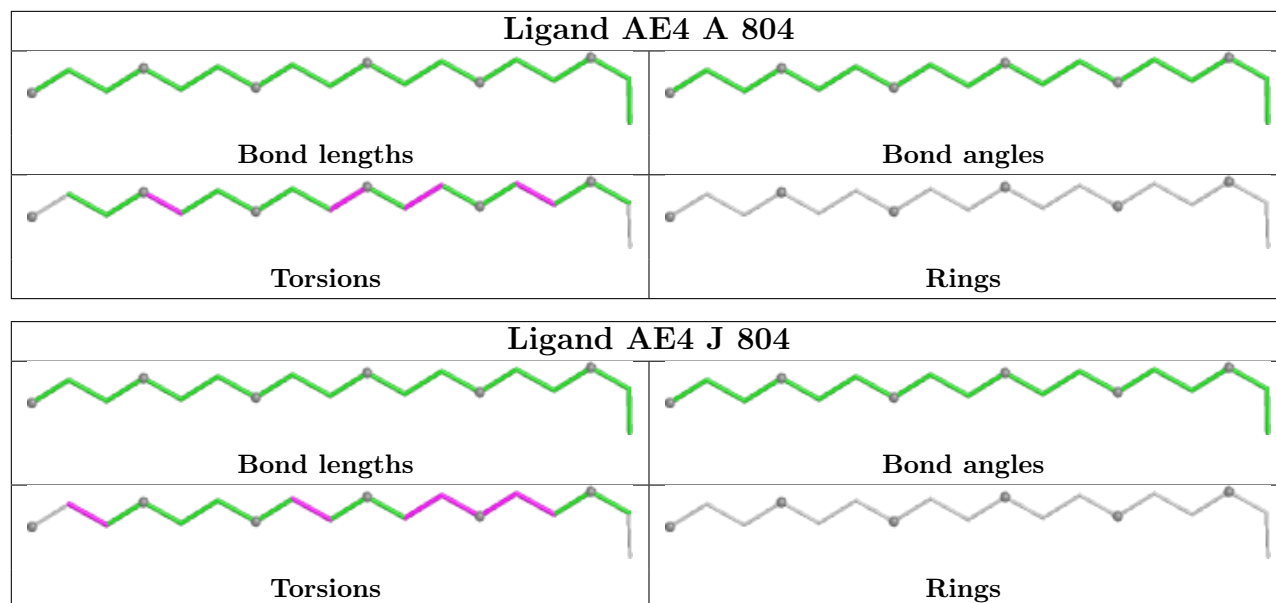
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	804	AE4	1	0
6	D	804	AE4	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	762/776 (98%)	-0.24	7 (0%) 81 85	10, 15, 25, 62	0
1	D	762/776 (98%)	-0.26	2 (0%) 90 93	10, 14, 23, 40	0
1	G	762/776 (98%)	-0.26	3 (0%) 88 92	11, 14, 24, 40	0
1	J	762/776 (98%)	-0.22	4 (0%) 87 90	10, 15, 27, 61	0
2	B	709/717 (98%)	0.44	36 (5%) 33 35	12, 24, 43, 61	0
2	E	709/717 (98%)	0.22	21 (2%) 52 57	12, 21, 36, 73	0
2	H	709/717 (98%)	0.38	33 (4%) 36 38	12, 23, 41, 57	0
2	K	709/717 (98%)	0.32	23 (3%) 50 55	13, 22, 38, 53	0
3	C	165/168 (98%)	0.04	3 (1%) 67 73	12, 20, 34, 38	0
3	F	165/168 (98%)	0.01	2 (1%) 76 81	12, 18, 32, 39	0
3	I	165/168 (98%)	0.15	3 (1%) 67 73	12, 20, 35, 41	0
3	L	165/168 (98%)	0.09	1 (0%) 85 89	13, 21, 33, 41	0
All	All	6544/6644 (98%)	0.04	138 (2%) 63 70	10, 18, 35, 73	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	66	HIS	5.1
2	E	529	THR	4.7
2	B	529	THR	4.5
2	K	529	THR	4.4
2	E	65	LEU	4.3

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 ⓘ

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
5	ACT	E	805	4/4	0.73	0.22	40,43,44,45	0
7	MG	H	804	1/1	0.77	0.14	45,45,45,45	0
5	ACT	K	805	4/4	0.84	0.16	37,39,40,42	0
5	ACT	D	803	4/4	0.84	0.15	29,29,31,31	0
5	ACT	B	805	4/4	0.85	0.17	40,41,42,42	0
6	AE4	D	804	18/18	0.85	0.18	21,33,61,62	0
5	ACT	J	803	4/4	0.85	0.15	34,34,36,37	0
5	ACT	H	806	4/4	0.86	0.16	41,41,42,43	0
6	AE4	G	804	18/18	0.90	0.14	17,30,57,57	0
6	AE4	J	804	18/18	0.90	0.15	20,33,59,61	0
6	AE4	A	804	18/18	0.90	0.14	18,34,58,60	0
7	MG	H	805	1/1	0.90	0.07	27,27,27,27	0
7	MG	E	804	1/1	0.92	0.07	30,30,30,30	0
7	MG	G	806	1/1	0.94	0.08	33,33,33,33	0
7	MG	B	806	1/1	0.95	0.08	31,31,31,31	0
7	MG	D	806	1/1	0.95	0.07	32,32,32,32	0
7	MG	K	804	1/1	0.95	0.05	25,25,25,25	0
8	AMP	B	801	23/23	0.95	0.07	20,25,28,28	0
8	AMP	H	801	23/23	0.95	0.07	22,25,27,30	0
5	ACT	G	803	4/4	0.96	0.06	19,20,20,21	0
5	ACT	G	802	4/4	0.96	0.07	13,14,14,14	0
8	AMP	E	801	23/23	0.96	0.06	18,19,25,29	0
7	MG	A	806	1/1	0.96	0.05	23,23,23,23	0
8	AMP	K	801	23/23	0.96	0.06	20,21,24,26	0
7	MG	J	805	1/1	0.97	0.04	19,19,19,19	0
7	MG	J	806	1/1	0.97	0.03	20,20,20,20	0
5	ACT	D	802	4/4	0.97	0.05	14,14,15,15	0
5	ACT	A	803	4/4	0.97	0.06	17,19,20,20	0
5	ACT	A	802	4/4	0.97	0.06	13,13,13,13	0
5	ACT	J	802	4/4	0.97	0.06	15,15,15,15	0
7	MG	D	805	1/1	0.97	0.04	19,19,19,19	0
7	MG	H	803	1/1	0.98	0.03	11,11,11,11	0

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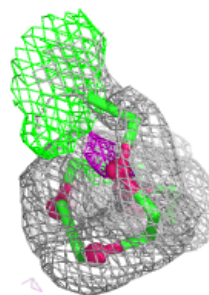
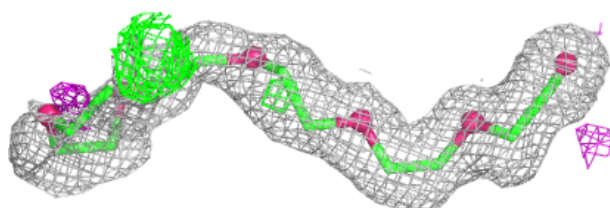
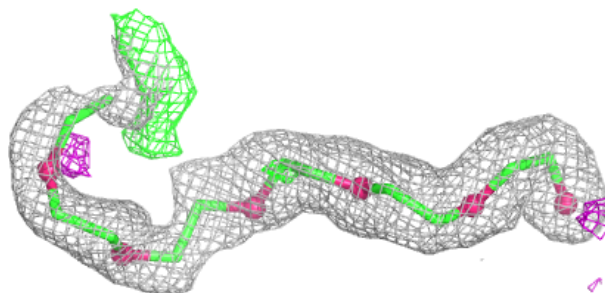
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	B	804	1/1	0.98	0.03	25,25,25,25	0
7	MG	E	806	1/1	0.98	0.03	21,21,21,21	0
7	MG	G	805	1/1	0.98	0.04	20,20,20,20	0
7	MG	B	802	1/1	0.98	0.03	16,16,16,16	0
4	MN	A	801	1/1	0.99	0.03	11,11,11,11	0
7	MG	A	805	1/1	0.99	0.02	18,18,18,18	0
7	MG	K	802	1/1	0.99	0.02	11,11,11,11	0
7	MG	K	803	1/1	0.99	0.02	11,11,11,11	0
4	MN	G	801	1/1	0.99	0.03	11,11,11,11	0
7	MG	L	202	1/1	0.99	0.03	23,23,23,23	0
7	MG	H	802	1/1	0.99	0.04	15,15,15,15	0
4	MN	J	801	1/1	0.99	0.02	13,13,13,13	0
7	MG	E	803	1/1	0.99	0.04	14,14,14,14	0
7	MG	B	803	1/1	0.99	0.02	16,16,16,16	0
9	ZN	C	201	1/1	0.99	0.07	28,28,28,28	0
9	ZN	F	201	1/1	0.99	0.06	28,28,28,28	0
9	ZN	I	201	1/1	0.99	0.06	26,26,26,26	0
9	ZN	L	201	1/1	0.99	0.06	30,30,30,30	0
7	MG	E	802	1/1	1.00	0.02	12,12,12,12	0
4	MN	D	801	1/1	1.00	0.02	11,11,11,11	0

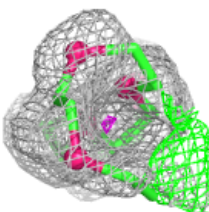
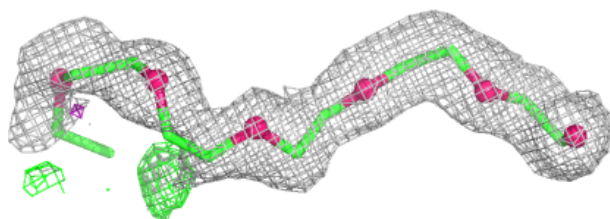
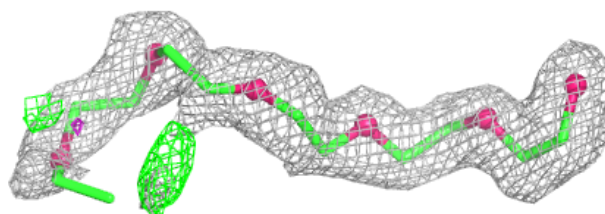
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AE4 D 804:

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

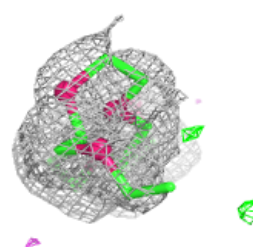
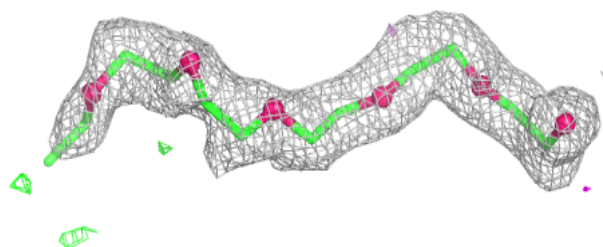
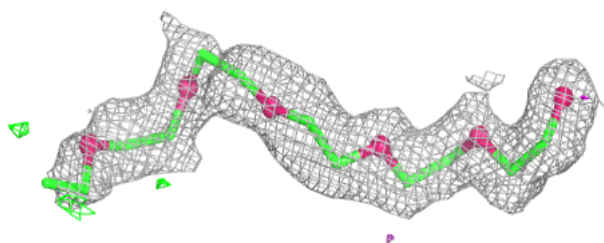
**Electron density around AE4 G 804:**

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

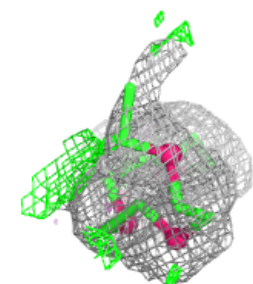
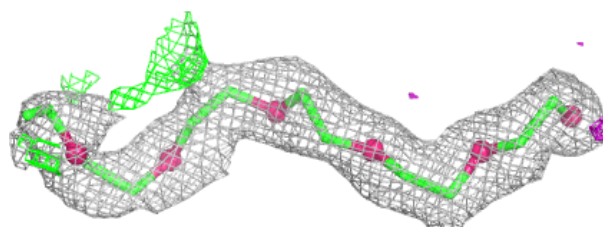
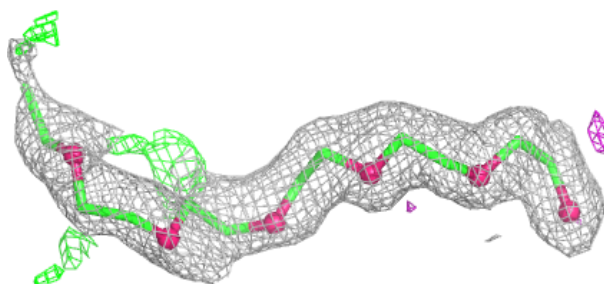


Electron density around AE4 J 804:

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

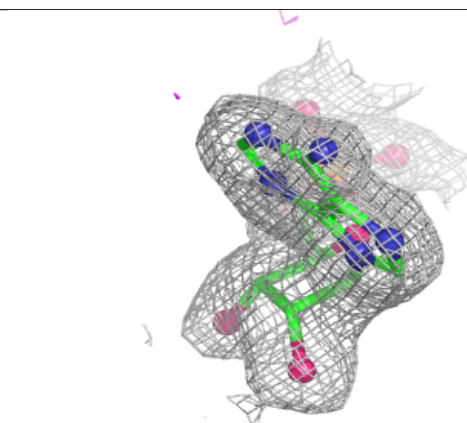
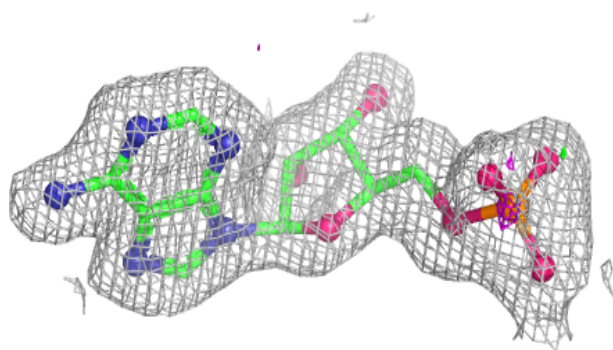
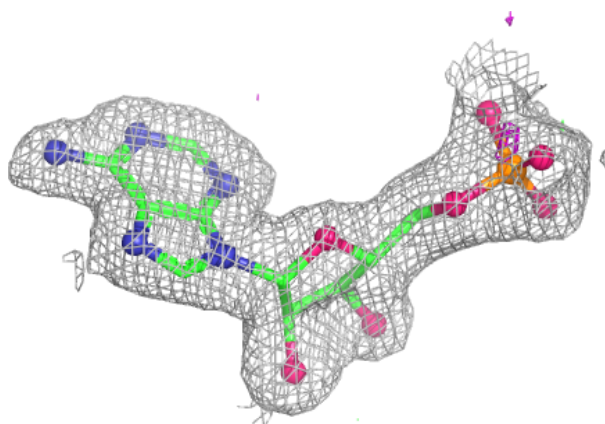
**Electron density around AE4 A 804:**

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

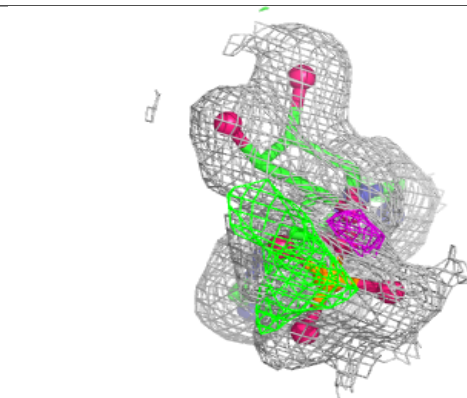
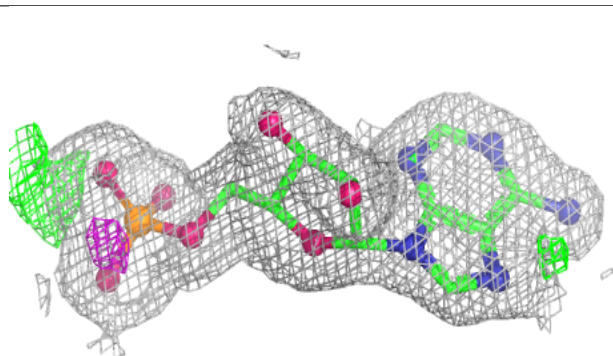
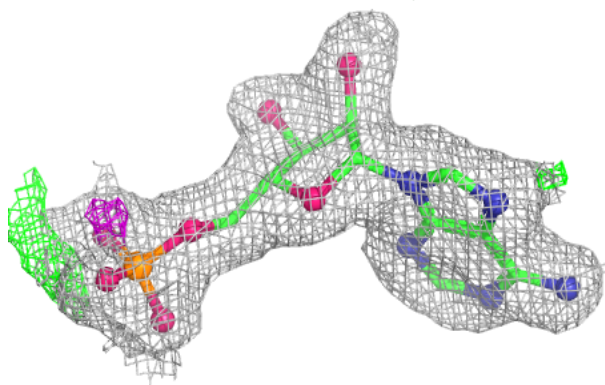


Electron density around AMP B 801:

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

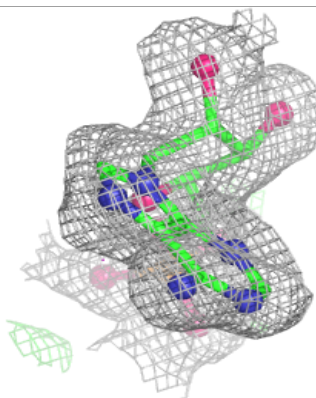
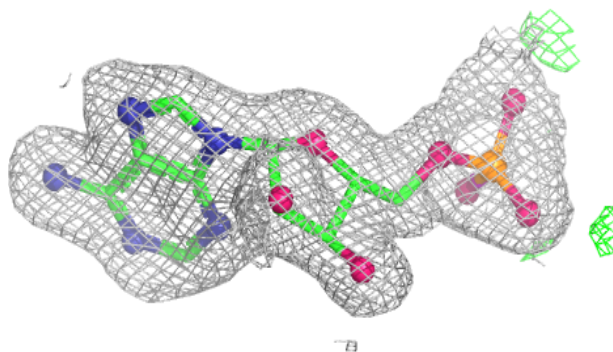
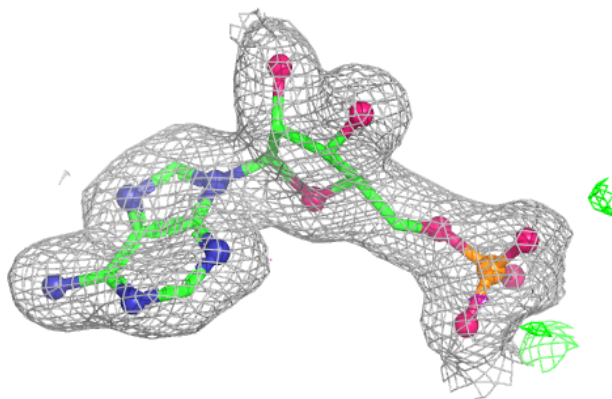
**Electron density around AMP H 801:**

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

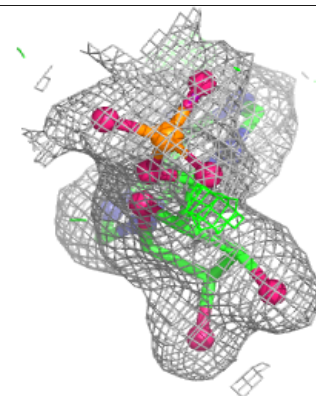
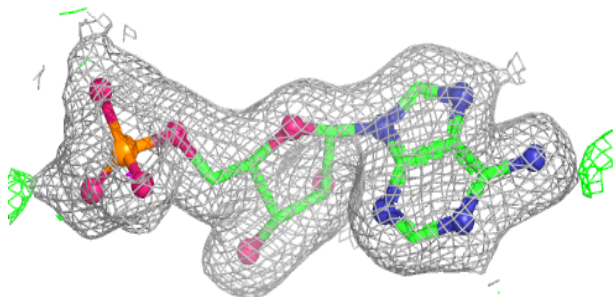
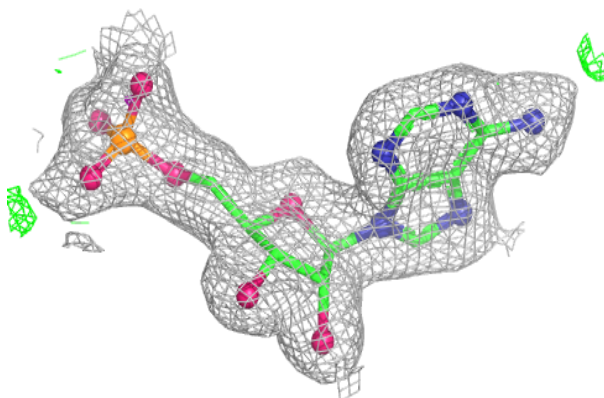


Electron density around AMP E 801:

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

**Electron density around AMP K 801:**

$2mF_o-DF_c$ (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.