W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 11:22 pm GMT

PDB ID	:	6S83
Title	:	Crystal structure of methionine adenosyltransferase from Pyrococcus furiosus in complex with AMPPCP, SAM, and PCP
Authors	:	Degano, M.; Minici, C.; Porcelli, M.
Deposited on	:	2019-07-08
Resolution	:	2.34 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, 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 ⓘ

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

The reported resolution of this entry is 2.34 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.
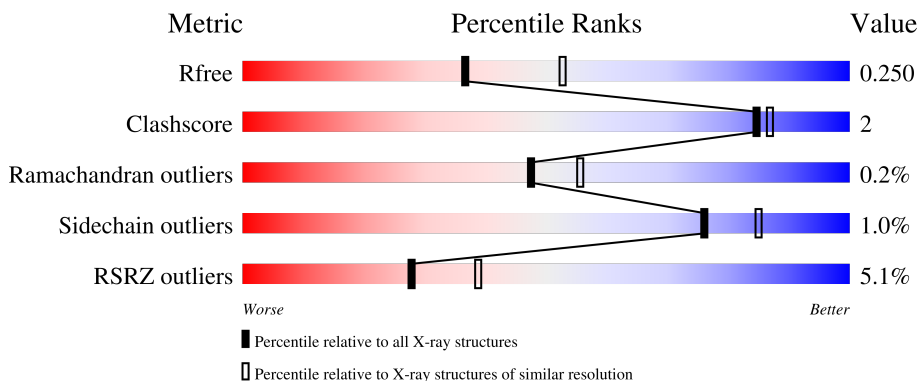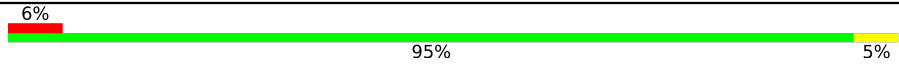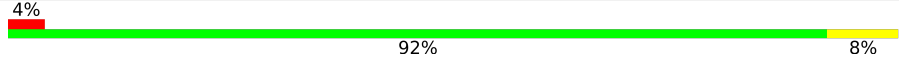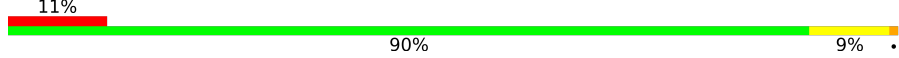

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	401	3% / 94% / 6%
1	B	401	4% / 94% / 5%
1	C	401	4% / 93% / 6%
1	D	401	2% / 93% / 7%
1	E	401	5% / 92% / 8%

Continued on next page...

Continued from previous page...

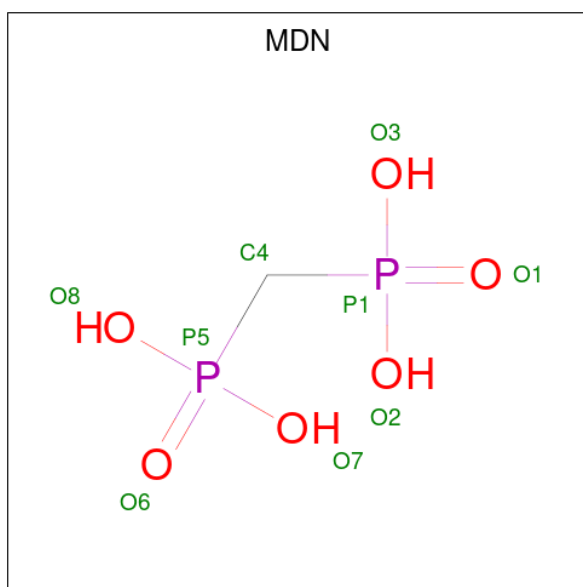| Mol	Chain	Length	Quality of chain
1	F	401	6% 95% 5%
1	G	401	4% 92% 8%
1	H	401	11% 90% 9%

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 51213 atoms, of which 25546 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	400	Total	C	H	N	O	S	0	1	0
			6296	1971	3180	540	598	7			
1	B	400	Total	C	H	N	O	S	0	1	0
			6292	1970	3178	539	597	8			
1	C	400	Total	C	H	N	O	S	0	0	0
			6280	1966	3171	539	597	7			
1	D	400	Total	C	H	N	O	S	0	0	0
			6280	1966	3171	539	597	7			
1	E	400	Total	C	H	N	O	S	0	3	0
			6315	1978	3187	543	600	7			
1	F	400	Total	C	H	N	O	S	0	2	0
			6311	1975	3189	542	597	8			
1	G	400	Total	C	H	N	O	S	0	3	0
			6310	1976	3184	541	602	7			
1	H	400	Total	C	H	N	O	S	0	1	0
			6292	1970	3178	539	597	8			

- Molecule 2 is METHYLENEDIPHOSPHONIC ACID (three-letter code: MDN) (formula: $CH_6O_6P_2$) (labeled as "Ligand of Interest" by depositor).
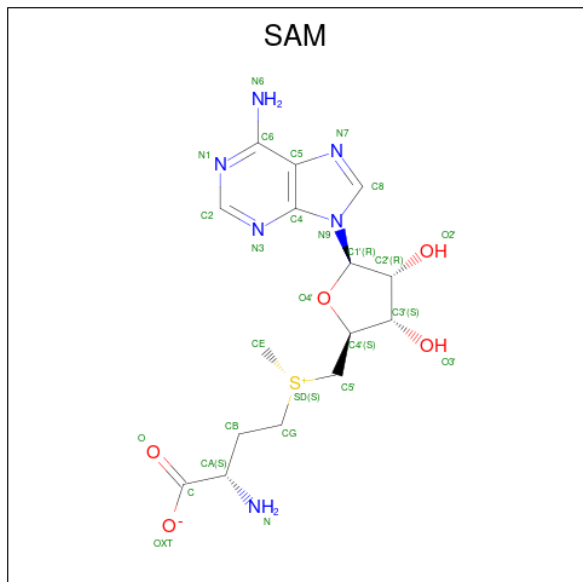
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	C	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	E	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	H	1	Total	C	H	O	P	0	0
			11	1	2	6	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	4	Total	Mg	0	0
			4	4		
3	C	1	Total	Mg	0	0
			1	1		
3	D	4	Total	Mg	0	0
			4	4		
3	E	1	Total	Mg	0	0
			1	1		
3	F	4	Total	Mg	0	0
			4	4		
3	G	1	Total	Mg	0	0
			1	1		
3	H	4	Total	Mg	0	0
			4	4		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).
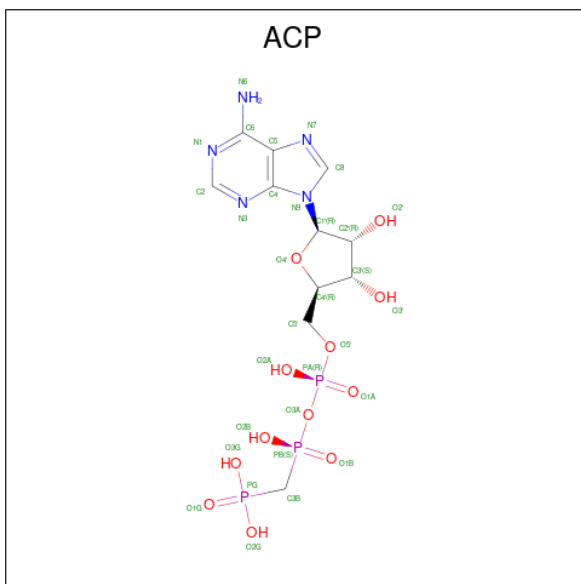

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		
4	E	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
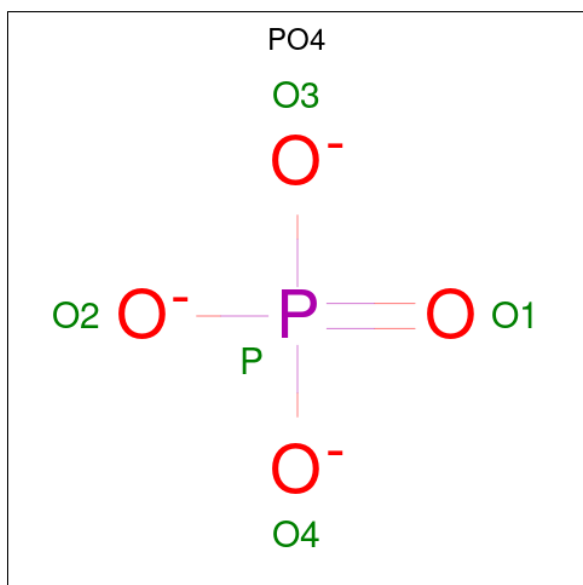
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	P 1	0	0
5	B	1	Total 5	O 4	P 1	0	0
5	C	1	Total 5	O 4	P 1	0	0
5	D	1	Total 5	O 4	P 1	0	0
5	F	1	Total 5	O 4	P 1	0	0
5	F	1	Total 5	O 4	P 1	0	0
5	G	1	Total 5	O 4	P 1	0	0
5	H	1	Total 5	O 4	P 1	0	0

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 45	C 11	H 14	N 5	O 12	P 3	0	0
6	D	1	Total 45	C 11	H 14	N 5	O 12	P 3	0	0
6	F	1	Total 45	C 11	H 14	N 5	O 12	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
6	H	1	45	11	14	5	12	3	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	52	Total 52	O 52	0	0
7	B	72	Total 72	O 72	0	0
7	C	57	Total 57	O 57	0	0
7	D	68	Total 68	O 68	0	0
7	E	62	Total 62	O 62	0	0
7	F	59	Total 59	O 59	0	0
7	G	46	Total 46	O 46	0	0
7	H	38	Total 38	O 38	0	0

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.

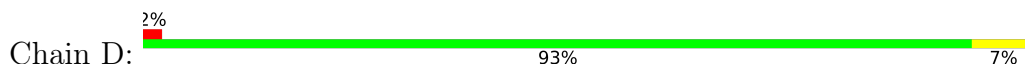• Molecule 1: S-adenosylmethionine synthase
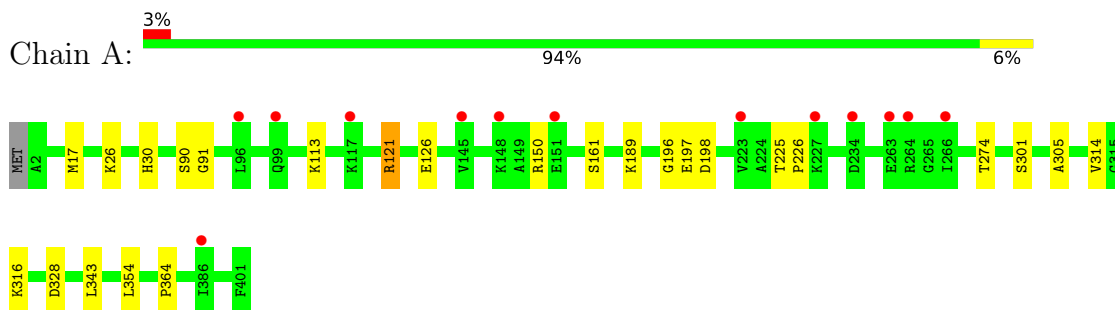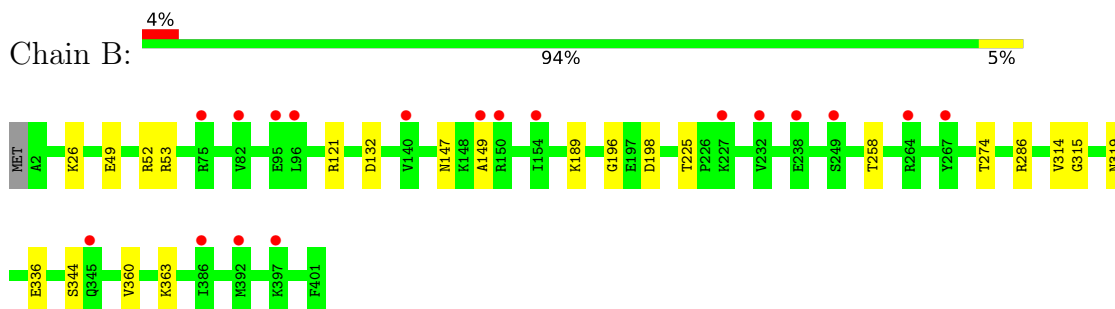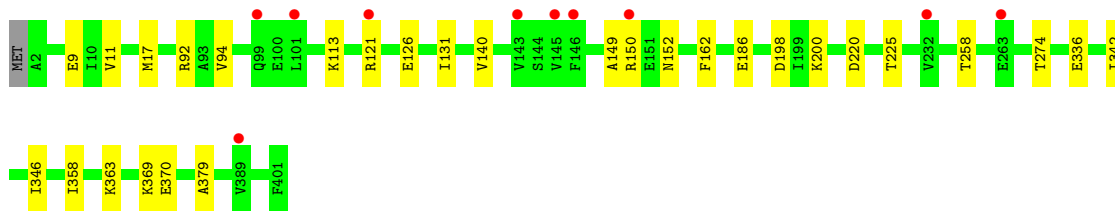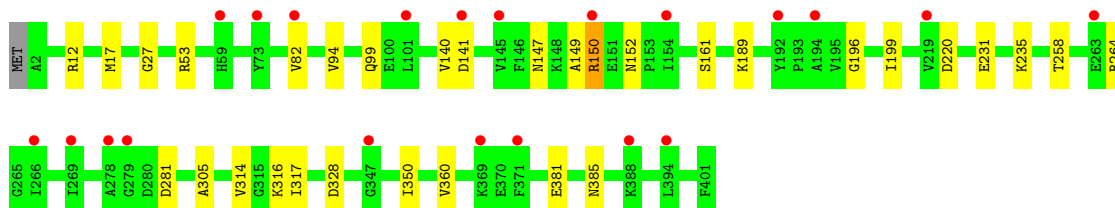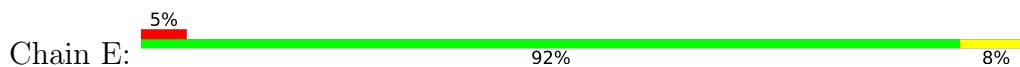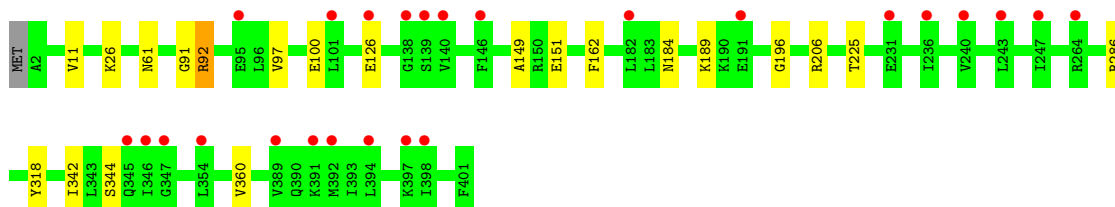

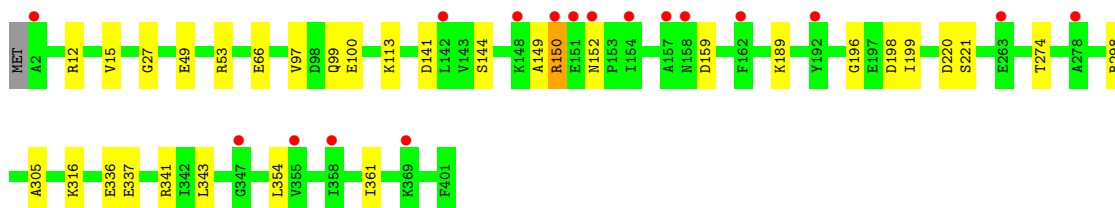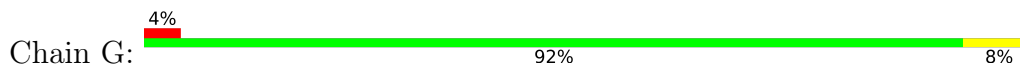• Molecule 1: S-adenosylmethionine synthase

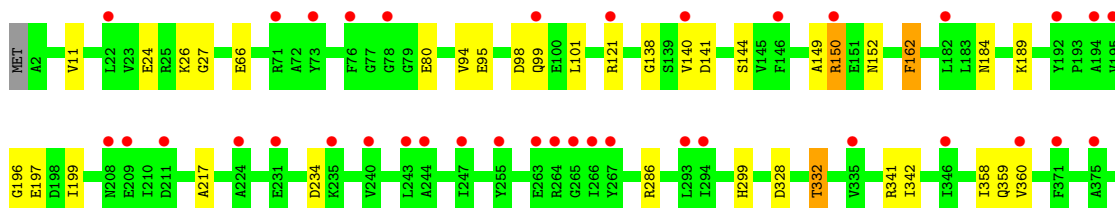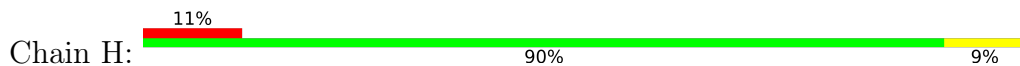• Molecule 1: S-adenosylmethionine synthase
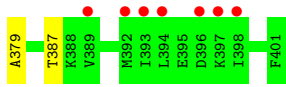

• Molecule 1: S-adenosylmethionine synthase

• Molecule 1: S-adenosylmethionine synthase

Chain E:

• Molecule 1: S-adenosylmethionine synthase

Chain F:

• Molecule 1: S-adenosylmethionine synthase

Chain G:

• Molecule 1: S-adenosylmethionine synthase

Chain H:
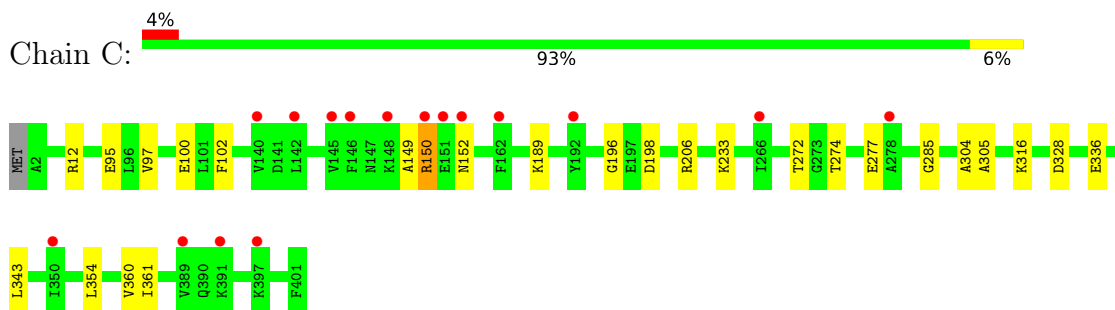
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.20Å 111.43Å 400.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.47 – 2.34 200.20 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.47-2.34) 100.0 (200.20-2.34)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.240 0.224 , 0.250	Depositor DCC
R_{free} test set	7504 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 39.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51213	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: ACP, MDN, SAM, MG, PO4

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	0.25	0/3165	0.44	0/4287
1	B	0.25	0/3166	0.43	0/4287
1	C	0.25	0/3158	0.44	0/4277
1	D	0.25	0/3158	0.43	0/4277
1	E	0.25	0/3184	0.44	0/4313
1	F	0.25	0/3177	0.44	0/4301
1	G	0.25	0/3181	0.44	0/4308
1	H	0.24	0/3166	0.43	0/4287
All	All	0.25	0/25355	0.44	0/34337

There are no bond length outliers.

There are no bond angle outliers.

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	3116	3180	3179	14	0
1	B	3114	3178	3180	11	0
1	C	3109	3171	3171	13	0
1	D	3109	3171	3171	16	0
1	E	3128	3187	3191	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3122	3189	3193	14	0
1	G	3126	3184	3187	19	0
1	H	3114	3178	3180	23	0
2	A	9	2	2	1	0
2	C	9	2	2	0	0
2	E	9	2	2	1	0
2	H	9	2	2	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
3	F	4	0	0	0	0
3	G	1	0	0	0	0
3	H	4	0	0	0	0
4	A	27	22	22	0	0
4	E	27	22	22	2	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	F	10	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
6	B	31	14	13	0	0
6	D	31	14	13	1	0
6	F	31	14	13	0	0
6	H	31	14	13	0	0
7	A	52	0	0	4	0
7	B	72	0	0	2	0
7	C	57	0	0	1	0
7	D	68	0	0	4	0
7	E	62	0	0	2	0
7	F	59	0	0	1	0
7	G	46	0	0	1	0
7	H	38	0	0	2	0
All	All	25667	25546	25556	119	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 2.

The worst 5 of 119 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:H:24:GLU:OE2	7:H:602:HOH:O	2.04	0.74
1:H:234:ASP:OD2	7:H:603:HOH:O	2.05	0.74
1:E:141:ASP:OD1	7:E:601:HOH:O	2.06	0.74
1:D:220:ASP:OD1	7:D:601:HOH:O	2.07	0.73
1:A:305:ALA:O	1:A:316:LYS:NZ	2.21	0.73

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/401 (100%)	388 (97%)	10 (2%)	1 (0%)	41	47
1	B	399/401 (100%)	389 (98%)	10 (2%)	0	100	100
1	C	398/401 (99%)	387 (97%)	10 (2%)	1 (0%)	41	47
1	D	398/401 (99%)	386 (97%)	11 (3%)	1 (0%)	41	47
1	E	401/401 (100%)	388 (97%)	12 (3%)	1 (0%)	47	55
1	F	400/401 (100%)	387 (97%)	13 (3%)	0	100	100
1	G	401/401 (100%)	391 (98%)	9 (2%)	1 (0%)	47	55
1	H	399/401 (100%)	389 (98%)	9 (2%)	1 (0%)	41	47
All	All	3195/3208 (100%)	3105 (97%)	84 (3%)	6 (0%)	47	55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	ARG
1	E	150	ARG
1	G	150	ARG
1	A	150	ARG
1	D	150	ARG

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	339/339 (100%)	336 (99%)	3 (1%)	78	87
1	B	339/339 (100%)	336 (99%)	3 (1%)	78	87
1	C	338/339 (100%)	335 (99%)	3 (1%)	78	87
1	D	338/339 (100%)	333 (98%)	5 (2%)	65	76
1	E	341/339 (101%)	337 (99%)	4 (1%)	71	82
1	F	340/339 (100%)	337 (99%)	3 (1%)	78	87
1	G	341/339 (101%)	340 (100%)	1 (0%)	92	96
1	H	339/339 (100%)	335 (99%)	4 (1%)	71	82
All	All	2715/2712 (100%)	2689 (99%)	26 (1%)	76	85

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	17	MET
1	E	360	VAL
1	H	360	VAL
1	E	328	ASP
1	F	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	99	GLN
1	H	345	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 39 ligands modelled in this entry, 21 are monoatomic - leaving 18 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	#$|Z| > 2$
2	MDN	A	501	3	6,8,8	1.16	1 (16%)	12,13,13	1.46	2 (16%)
2	MDN	E	501	3	6,8,8	1.15	1 (16%)	12,13,13	1.42	1 (8%)
5	PO4	C	502	3	4,4,4	0.89	0	6,6,6	0.37	0
5	PO4	F	501	3	4,4,4	0.90	0	6,6,6	0.41	0
5	PO4	F	505	3	4,4,4	0.89	0	6,6,6	0.41	0
5	PO4	G	501	3	4,4,4	0.88	0	6,6,6	0.41	0
5	PO4	H	505	3	4,4,4	0.88	0	6,6,6	0.47	0
6	ACP	B	504	3	27,33,33	4.69	10 (37%)	32,52,52	2.24	6 (18%)
6	ACP	D	503	3	27,33,33	4.68	10 (37%)	32,52,52	2.27	6 (18%)
2	MDN	C	501	3	6,8,8	1.29	2 (33%)	12,13,13	1.86	2 (16%)
6	ACP	H	504	3	27,33,33	4.69	9 (33%)	32,52,52	2.23	6 (18%)
5	PO4	D	504	3	4,4,4	0.90	0	6,6,6	0.42	0
6	ACP	F	504	3	27,33,33	4.69	10 (37%)	32,52,52	2.27	6 (18%)
4	SAM	A	503	-	24,29,29	1.21	3 (12%)	23,42,42	1.59	5 (21%)
5	PO4	B	505	3	4,4,4	0.88	0	6,6,6	0.45	0
2	MDN	H	501	3	6,8,8	0.95	0	12,13,13	1.02	0
5	PO4	B	501	3	4,4,4	0.86	0	6,6,6	0.44	0
4	SAM	E	503	-	24,29,29	1.21	3 (12%)	23,42,42	1.52	4 (17%)

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
2	MDN	A	501	3	-	1/6/6/6	-
2	MDN	E	501	3	-	1/6/6/6	-
6	ACP	D	503	3	-	6/15/38/38	0/3/3/3
6	ACP	B	504	3	-	2/15/38/38	0/3/3/3
2	MDN	C	501	3	-	0/6/6/6	-
6	ACP	H	504	3	-	6/15/38/38	0/3/3/3
6	ACP	F	504	3	-	3/15/38/38	0/3/3/3
4	SAM	A	503	-	-	4/12/33/33	0/3/3/3
2	MDN	H	501	3	-	0/6/6/6	-
4	SAM	E	503	-	-	5/12/33/33	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	504	ACP	O4'-C1'	15.44	1.62	1.41
6	B	504	ACP	O4'-C1'	15.37	1.62	1.41
6	D	503	ACP	O4'-C1'	15.35	1.62	1.41
6	F	504	ACP	O4'-C1'	15.32	1.62	1.41
6	F	504	ACP	C2'-C1'	-14.88	1.31	1.53

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	503	ACP	C5-C6-N6	8.56	133.37	120.35
6	F	504	ACP	C5-C6-N6	8.45	133.19	120.35
6	B	504	ACP	C5-C6-N6	8.39	133.10	120.35
6	H	504	ACP	C5-C6-N6	8.35	133.05	120.35
6	D	503	ACP	N6-C6-N1	-5.70	106.74	118.57

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

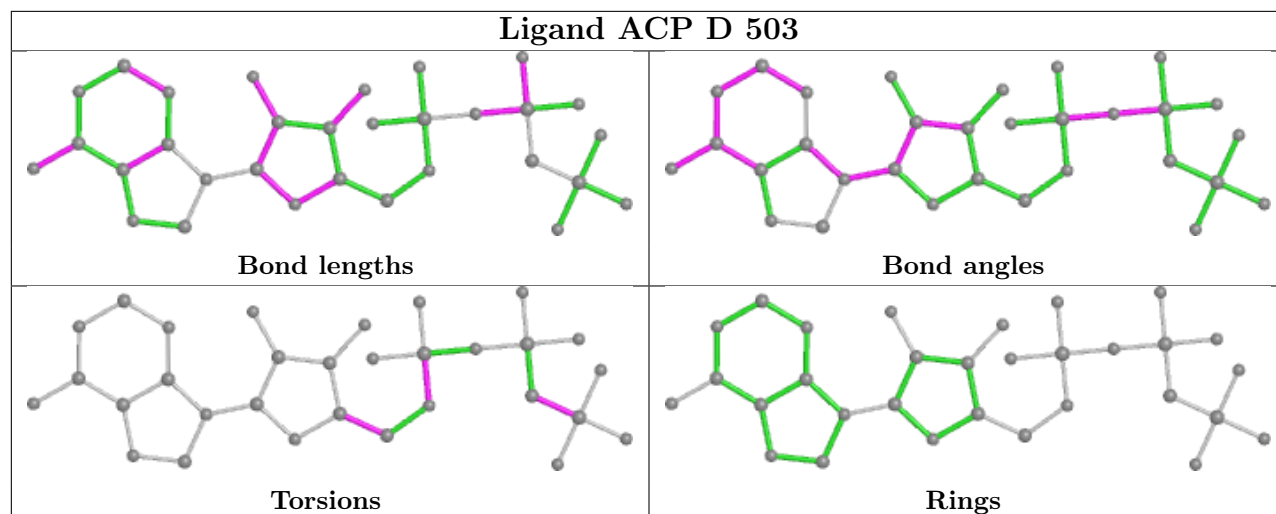| Mol	Chain	Res	Type	Atoms
4	E	503	SAM	CB-CG-SD-CE
6	D	503	ACP	C5'-O5'-PA-O1A
6	H	504	ACP	C3'-C4'-C5'-O5'
6	B	504	ACP	C3'-C4'-C5'-O5'
6	H	504	ACP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:
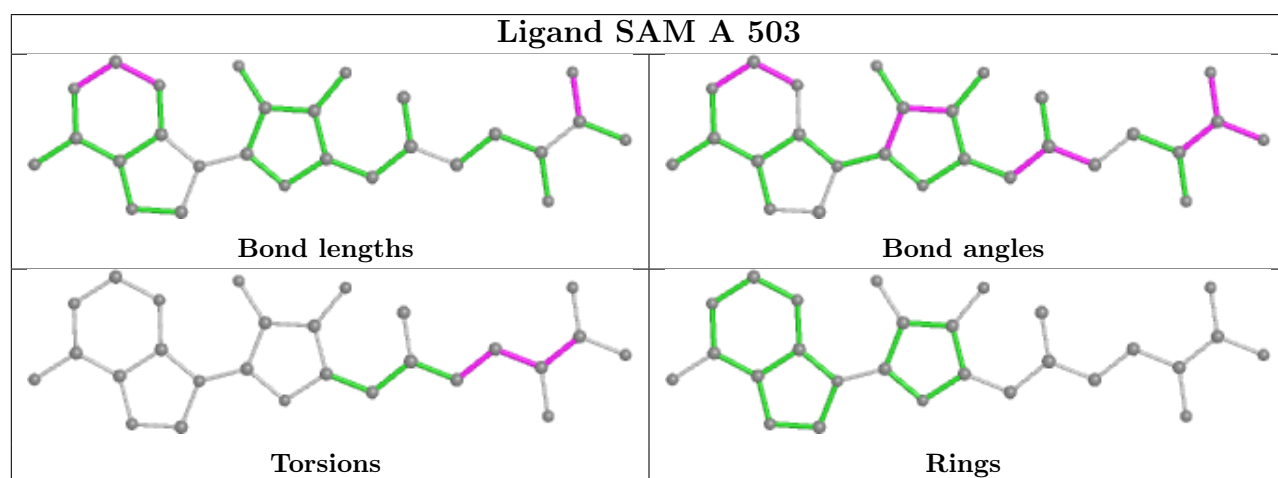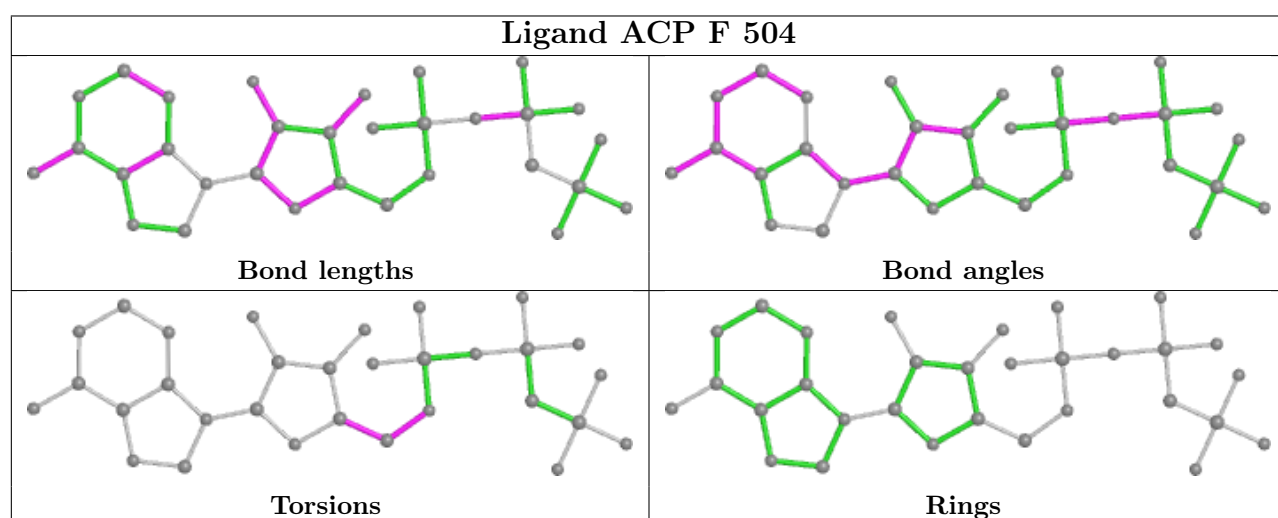
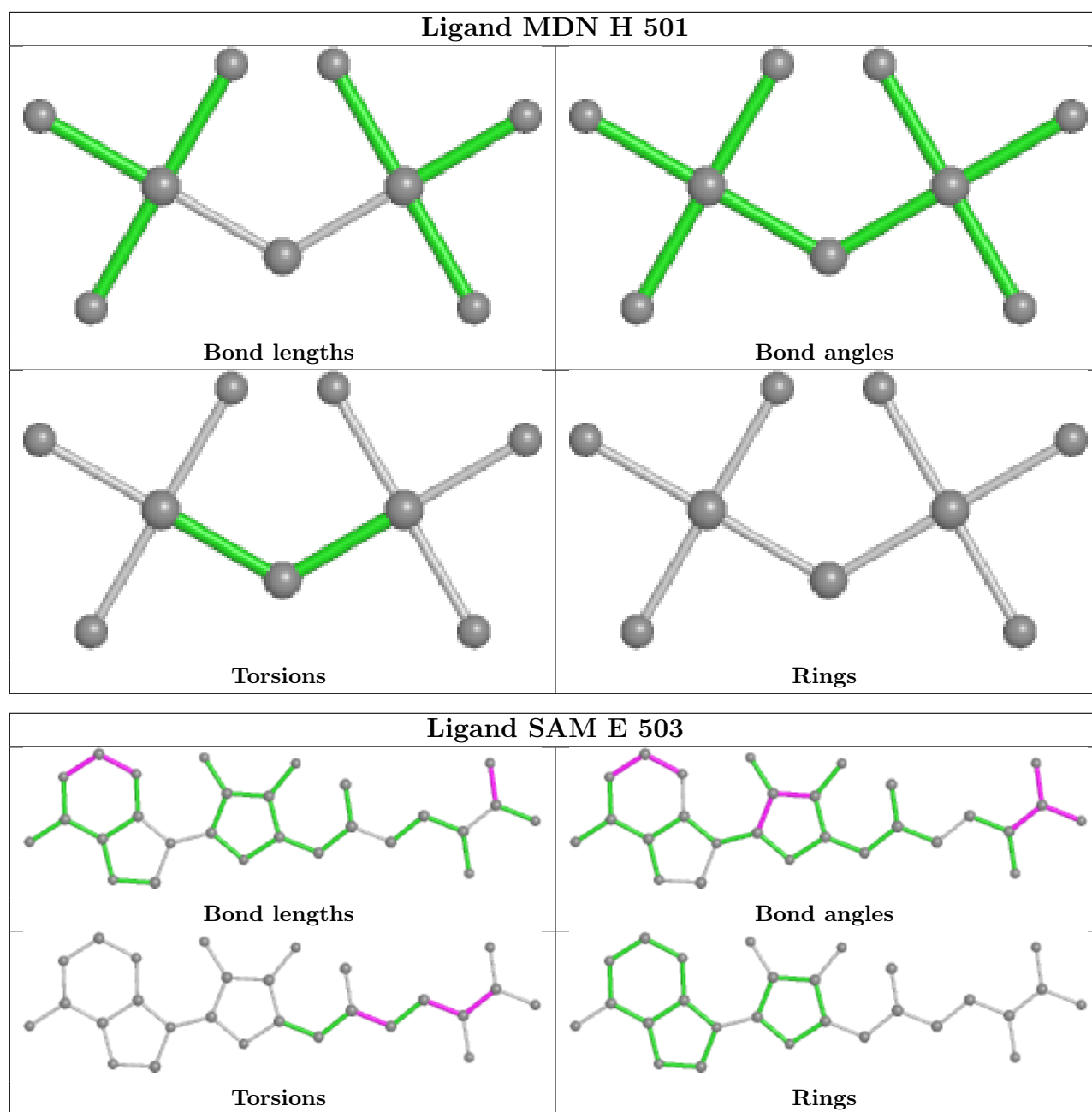| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MDN	1	0
2	E	501	MDN	1	0
6	D	503	ACP	1	0
4	E	503	SAM	2	0

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 MDN A 501

Bond lengths   Bond angles

Torsions   Rings

Ligand MDN E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP B 504

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP D 503	
Bond lengths	Bond angles
Torsions	Rings

Ligand MDN C 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand ACP H 504

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP F 504

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand MDN H 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM E 503

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 (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(Å²)	Q<0.9
1	A	400/401 (99%)	0.51	13 (3%)	46	57	35, 59, 92, 130	0
1	B	400/401 (99%)	0.55	18 (4%)	33	44	36, 56, 94, 150	0
1	C	400/401 (99%)	0.46	16 (4%)	38	49	34, 54, 86, 139	0
1	D	400/401 (99%)	0.42	10 (2%)	57	66	35, 51, 81, 141	0
1	E	400/401 (99%)	0.59	21 (5%)	26	37	34, 57, 94, 126	0
1	F	400/401 (99%)	0.65	25 (6%)	20	28	36, 61, 105, 140	0
1	G	400/401 (99%)	0.58	17 (4%)	35	46	36, 60, 103, 150	0
1	H	400/401 (99%)	0.90	44 (11%)	5	9	39, 73, 109, 145	0
All	All	3200/3208 (99%)	0.58	164 (5%)	28	39	34, 58, 99, 150	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	192	TYR	5.9
1	C	150	ARG	5.5
1	H	267	TYR	5.2
1	B	140	VAL	5.2
1	H	208	ASN	4.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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, 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($\mathring{A}^2$)	Q<0.9
3	MG	D	506	1/1	0.69	0.06	75,75,75,75	0
3	MG	F	506	1/1	0.84	0.12	43,43,43,43	0
4	SAM	E	503	27/27	0.84	0.22	82,96,114,117	0
4	SAM	A	503	27/27	0.86	0.17	79,90,106,108	0
3	MG	B	503	1/1	0.88	0.17	49,49,49,49	0
3	MG	H	502	1/1	0.90	0.07	56,56,56,56	0
3	MG	D	502	1/1	0.91	0.09	39,39,39,39	0
3	MG	H	503	1/1	0.91	0.14	44,44,44,44	0
3	MG	F	503	1/1	0.91	0.07	45,45,45,45	0
3	MG	D	505	1/1	0.91	0.09	49,49,49,49	0
6	ACP	H	504	31/31	0.91	0.20	61,102,124,124	0
6	ACP	D	503	31/31	0.92	0.15	53,84,104,105	0
5	PO4	F	501	5/5	0.92	0.13	52,55,62,64	0
3	MG	H	507	1/1	0.93	0.10	71,71,71,71	0
5	PO4	G	501	5/5	0.93	0.08	62,63,72,73	0
3	MG	C	503	1/1	0.93	0.05	50,50,50,50	0
3	MG	B	502	1/1	0.93	0.10	42,42,42,42	0
3	MG	F	502	1/1	0.94	0.11	43,43,43,43	0
3	MG	A	504	1/1	0.94	0.20	58,58,58,58	0
3	MG	B	506	1/1	0.94	0.08	41,41,41,41	0
3	MG	A	502	1/1	0.94	0.10	40,40,40,40	0
2	MDN	H	501	9/9	0.95	0.14	59,63,75,75	0
6	ACP	B	504	31/31	0.95	0.14	50,75,91,91	0
3	MG	D	501	1/1	0.95	0.07	46,46,46,46	0
6	ACP	F	504	31/31	0.95	0.12	49,67,80,81	0
3	MG	F	507	1/1	0.95	0.07	66,66,66,66	0
3	MG	B	507	1/1	0.96	0.04	75,75,75,75	0
2	MDN	C	501	9/9	0.96	0.12	47,53,64,64	0
5	PO4	B	501	5/5	0.96	0.12	52,66,67,67	0
5	PO4	D	504	5/5	0.96	0.11	57,63,65,65	0
3	MG	G	502	1/1	0.96	0.09	54,54,54,54	0
5	PO4	H	505	5/5	0.97	0.09	59,60,65,66	0
5	PO4	C	502	5/5	0.97	0.12	57,65,66,67	0
2	MDN	E	501	9/9	0.97	0.13	49,52,63,63	0
2	MDN	A	501	9/9	0.97	0.14	42,49,60,60	0
5	PO4	B	505	5/5	0.97	0.12	47,47,50,51	0
3	MG	E	502	1/1	0.98	0.16	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	MG	H	506	1/1	0.98	0.11	52,52,52,52	0
5	PO4	F	505	5/5	0.98	0.14	43,50,52,52	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 SAM E 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
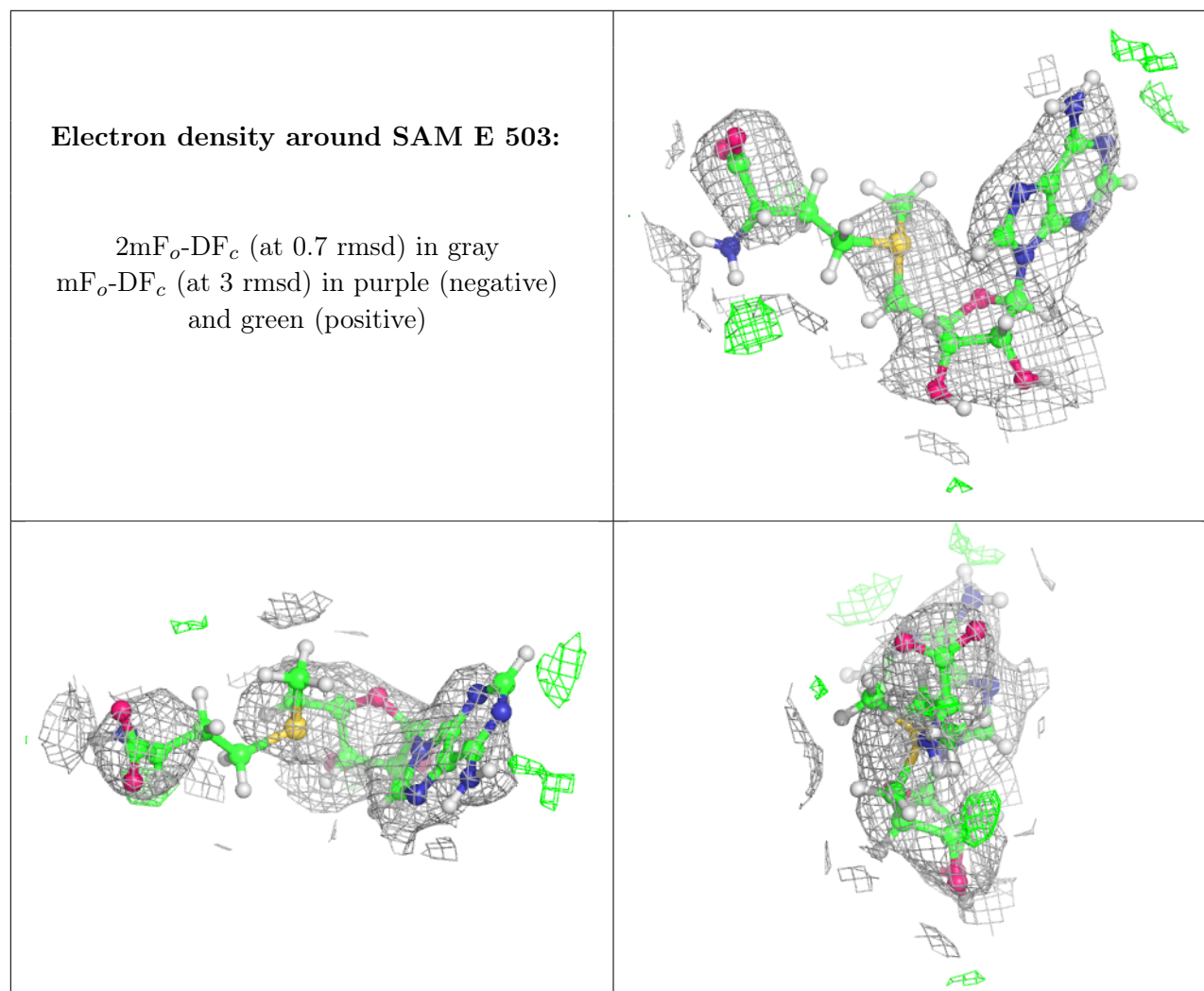
Electron density around SAM A 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
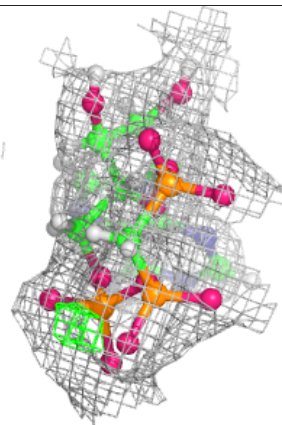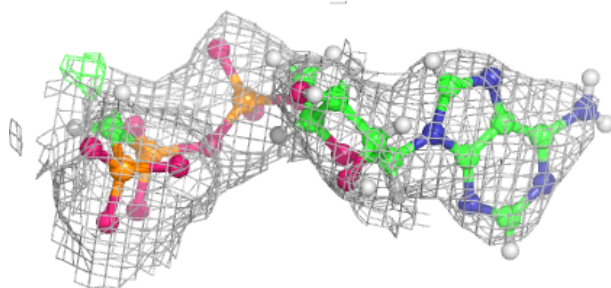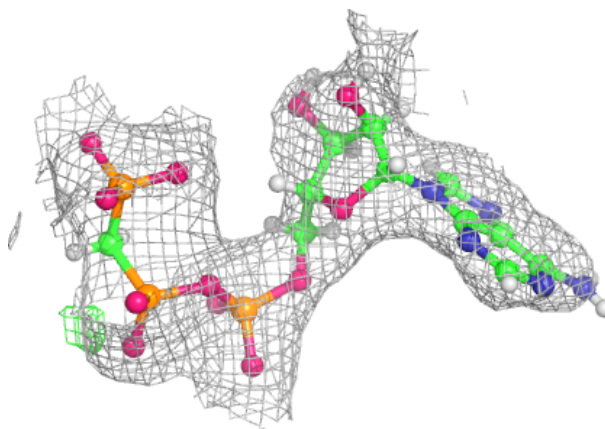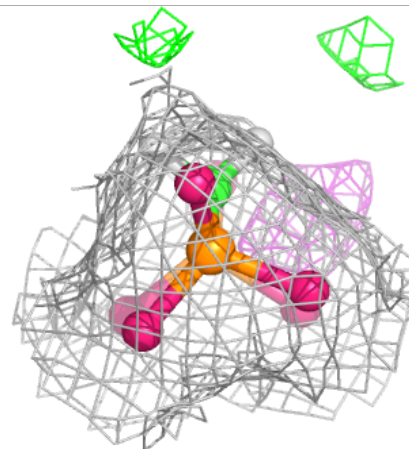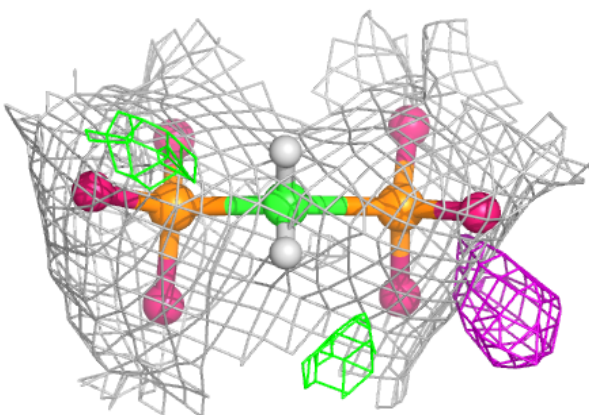and green (positive)
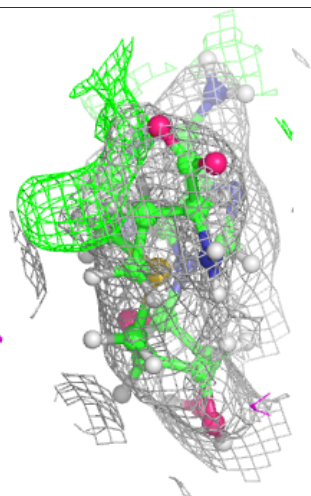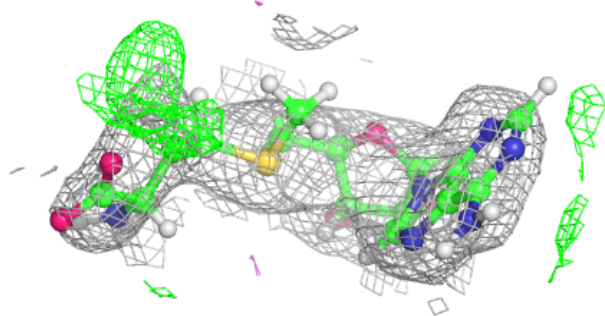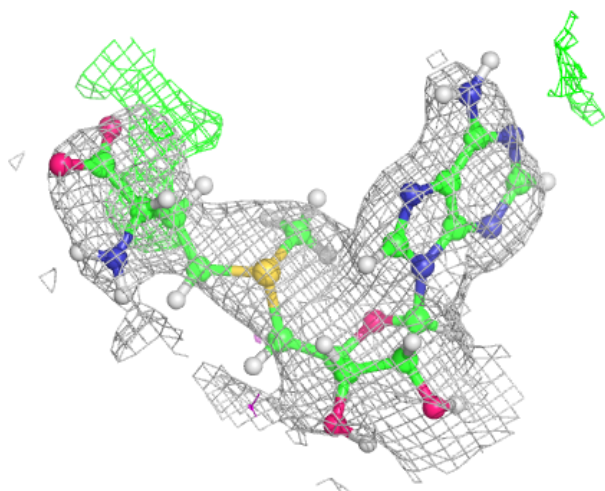
Electron density around ACP H 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
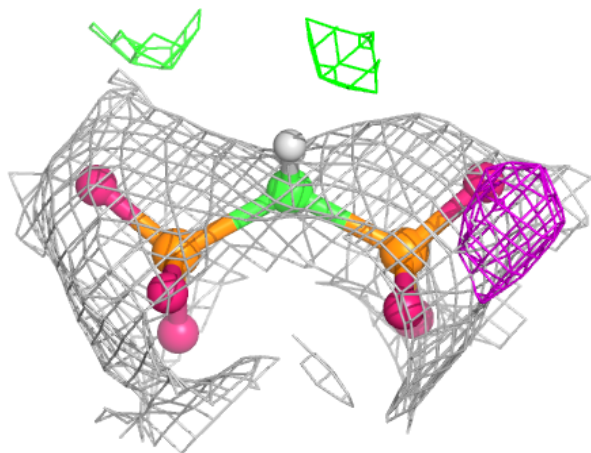mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
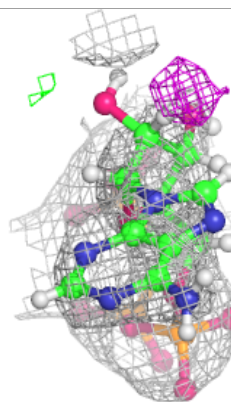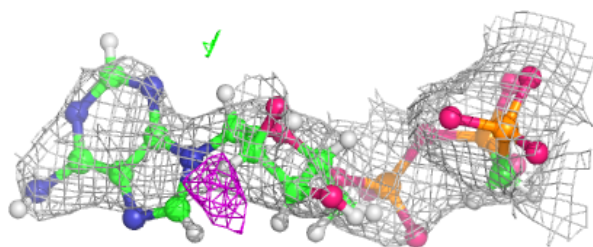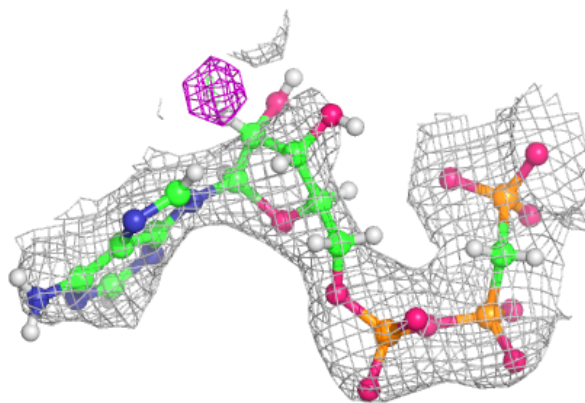
Electron density around ACP D 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
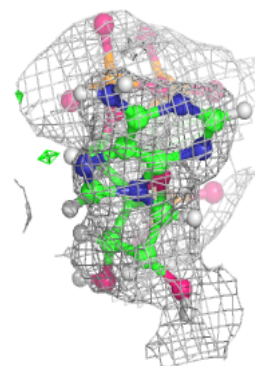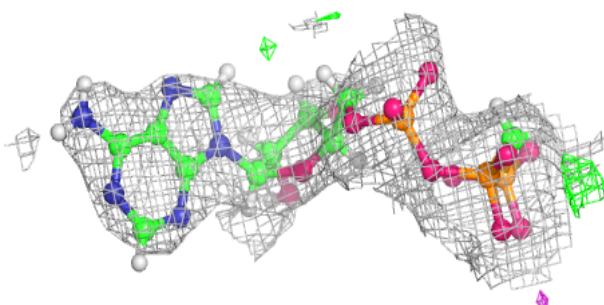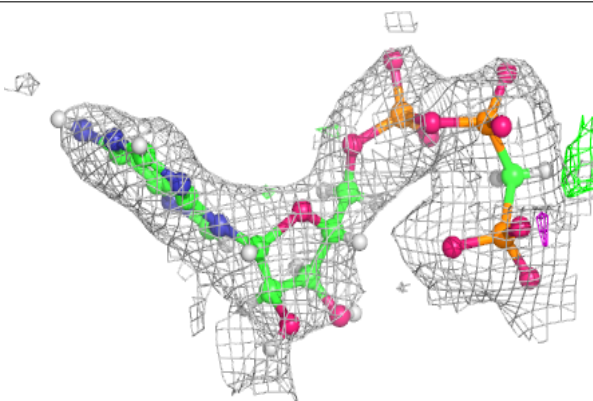
Electron density around MDN H 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
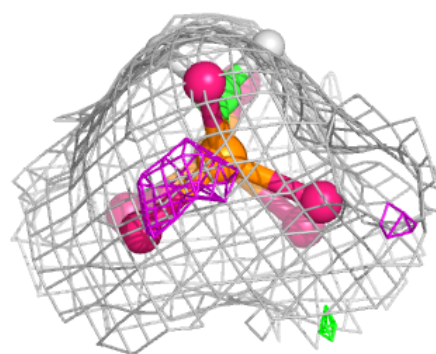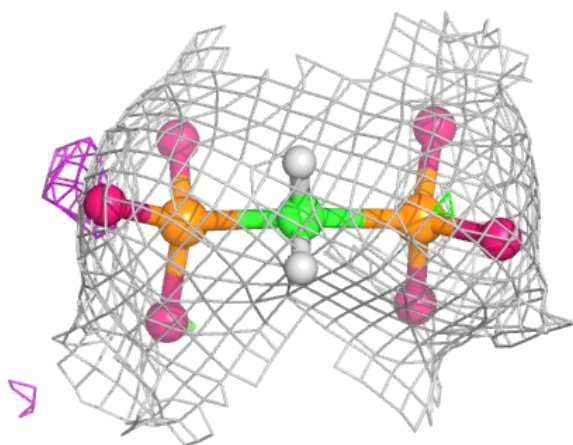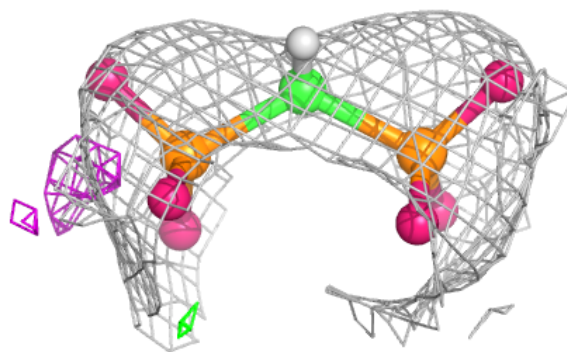
Electron density around ACP B 504:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
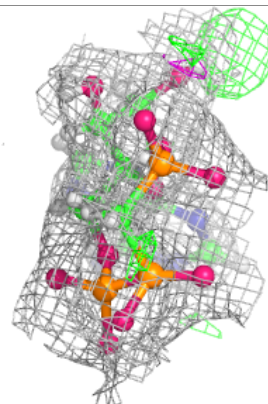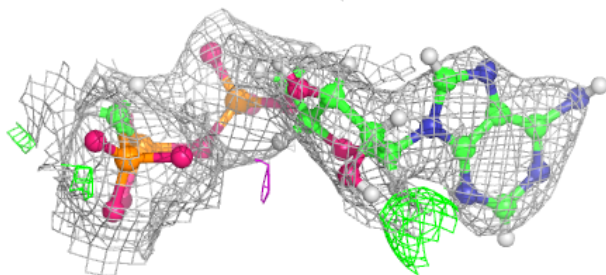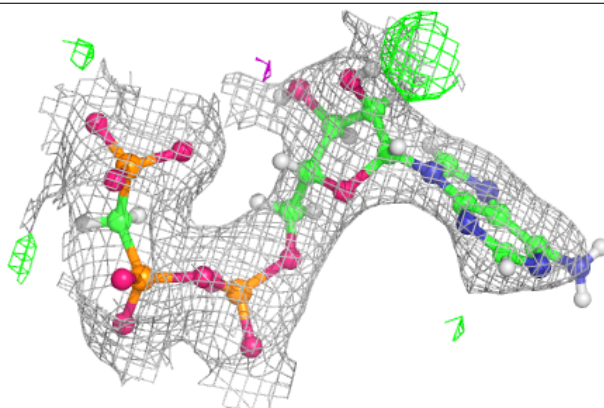
Electron density around ACP F 504:

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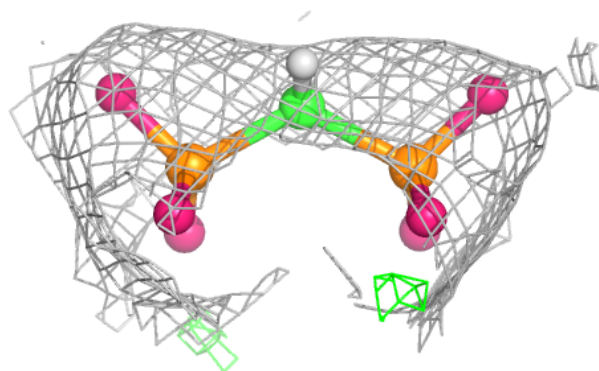and green (positive)

Electron density around MDN C 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 MDN E 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
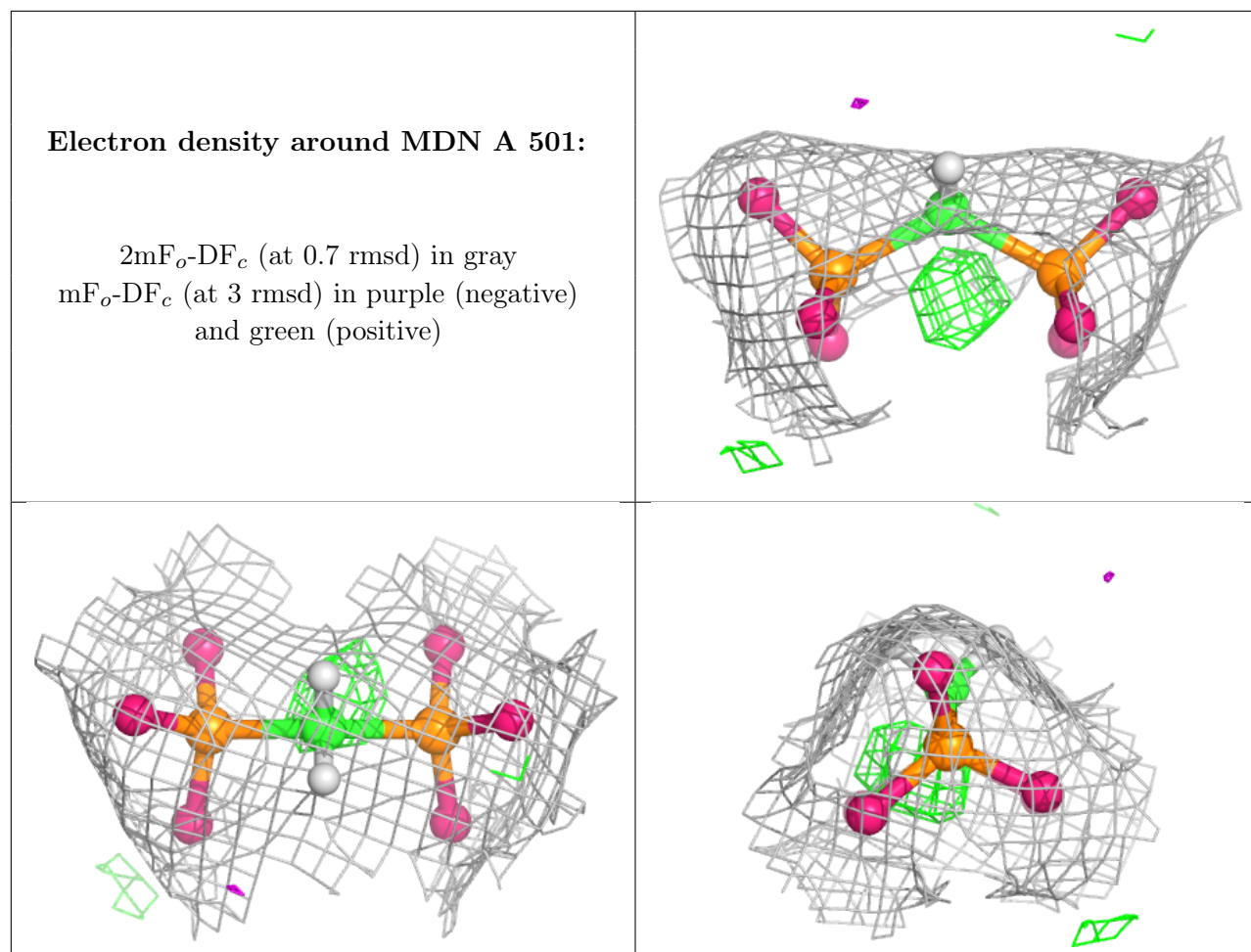
Electron density around MDN A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
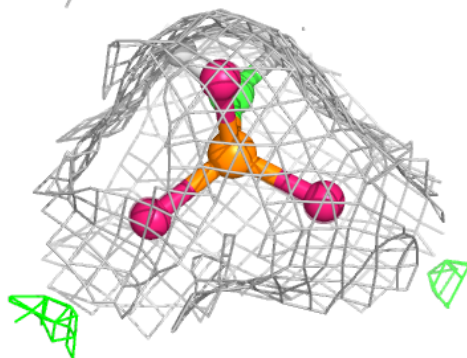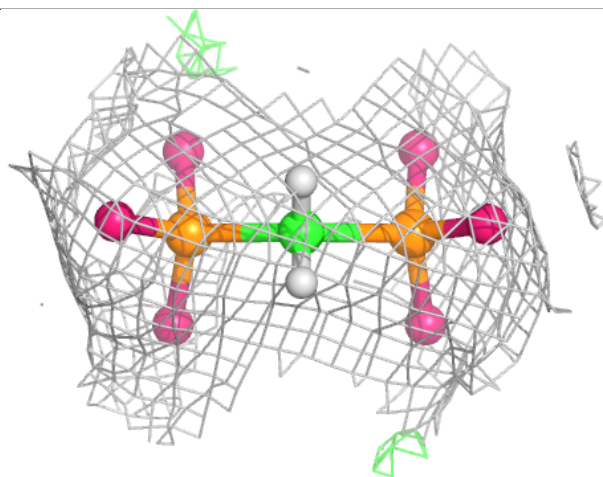
6.5 Other polymers (i)

There are no such residues in this entry.