



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:03 pm BST

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)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

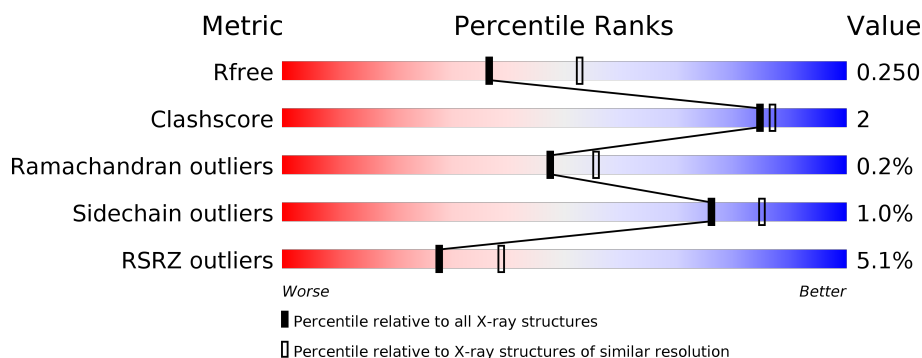
1 Overall quality at a glance

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 on 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	401	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	401	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	C	401	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	D	401	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	E	401	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	F	401	<div> <div>6%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	401	<div><div></div><div>4%</div><div>92%</div><div>8%</div></div>
1	H	401	<div><div></div><div>11%</div><div>90%</div><div>9%</div></div>

2 Entry composition

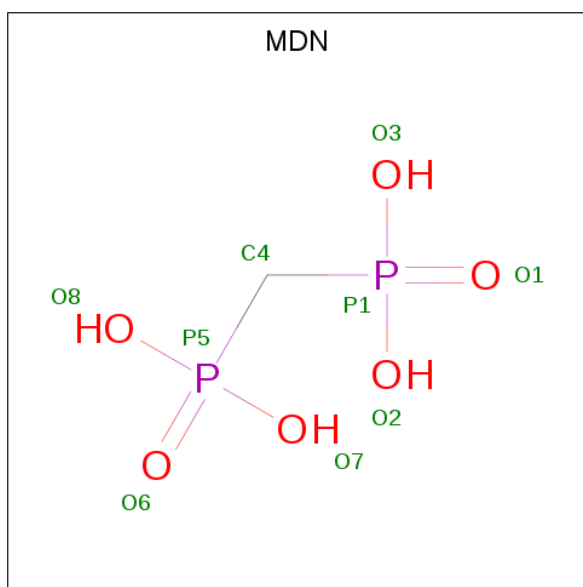
There are 7 unique types of molecules in this entry. The entry contains 51213 atoms, of which 25546 are hydrogens and 0 are deuteriums.

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: $\text{CH}_6\text{O}_6\text{P}_2$) (labeled as "Ligand of Interest" by author).

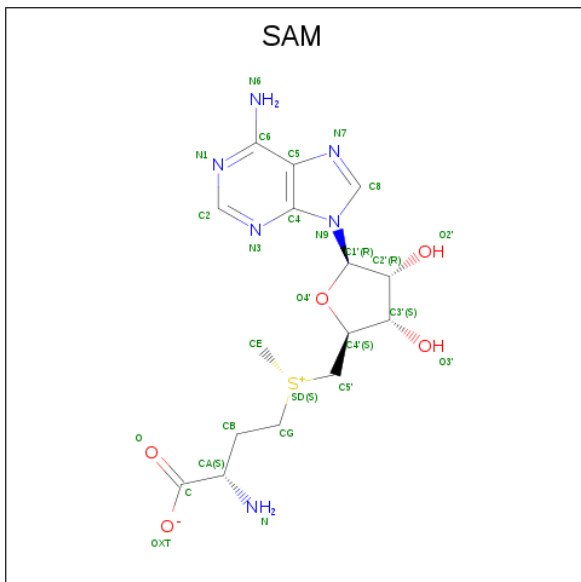


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	C	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	E	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	H	1	Total	C	H	O	P	0	0
			11	1	2	6	2		

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

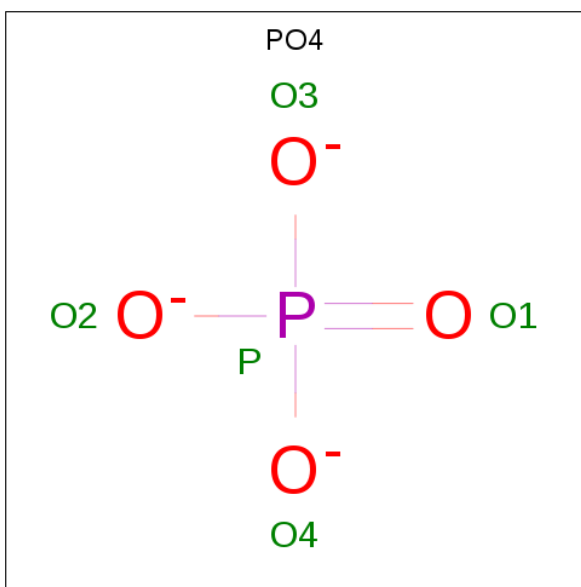
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	4	Total	Mg	0	0
			4	4		
3	E	1	Total	Mg	0	0
			1	1		
3	H	4	Total	Mg	0	0
			4	4		
3	B	4	Total	Mg	0	0
			4	4		
3	C	1	Total	Mg	0	0
			1	1		
3	A	2	Total	Mg	0	0
			2	2		
3	F	4	Total	Mg	0	0
			4	4		

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



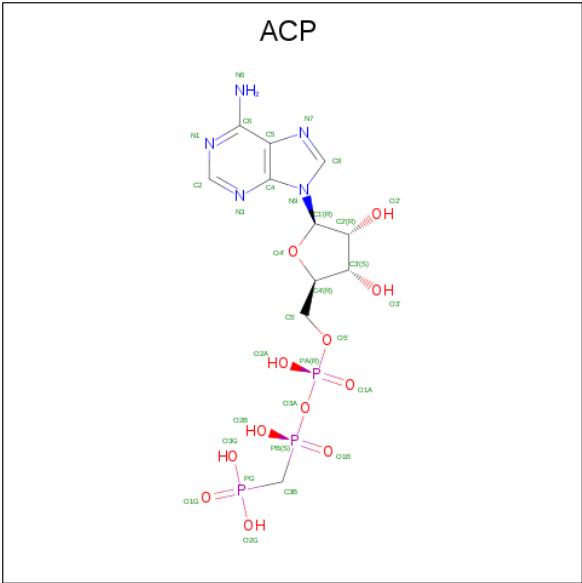
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		
4	E	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by author).



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

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

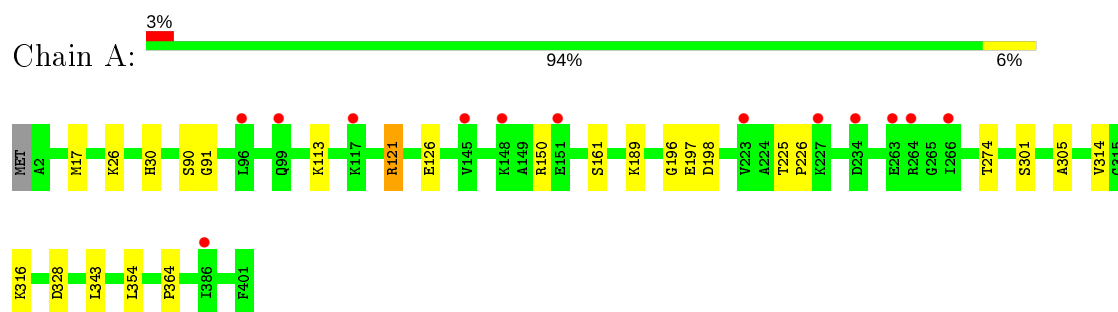
- Molecule 7 is water.

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

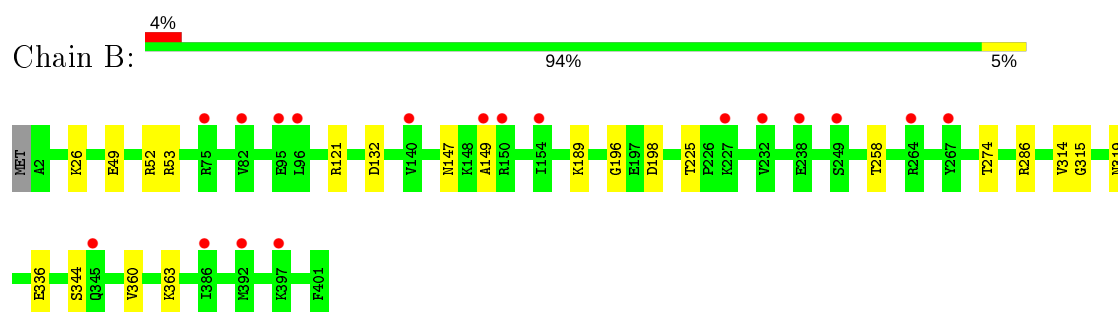
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

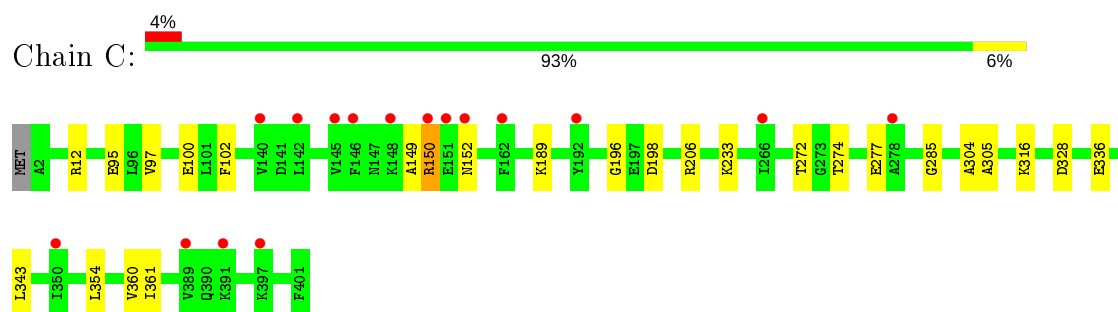
- Molecule 1: S-adenosylmethionine synthase



- Molecule 1: S-adenosylmethionine synthase

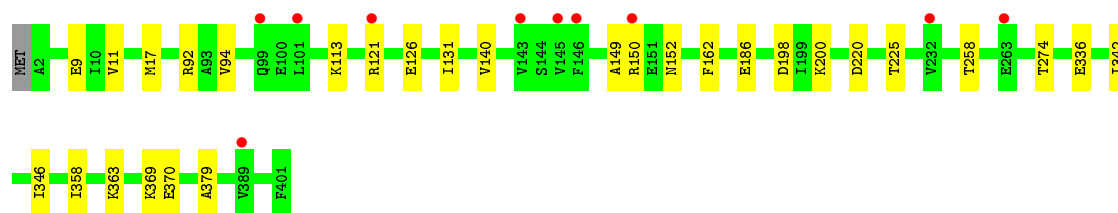


- Molecule 1: S-adenosylmethionine synthase

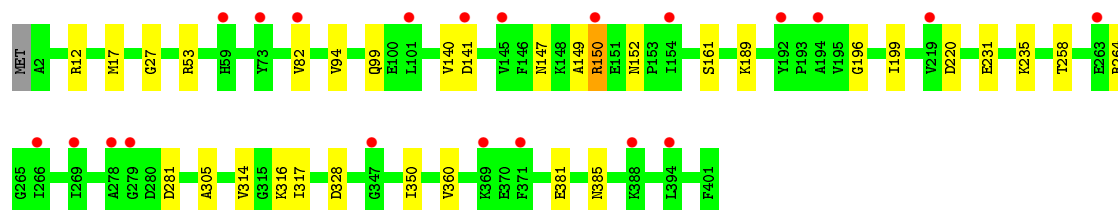


- Molecule 1: S-adenosylmethionine synthase

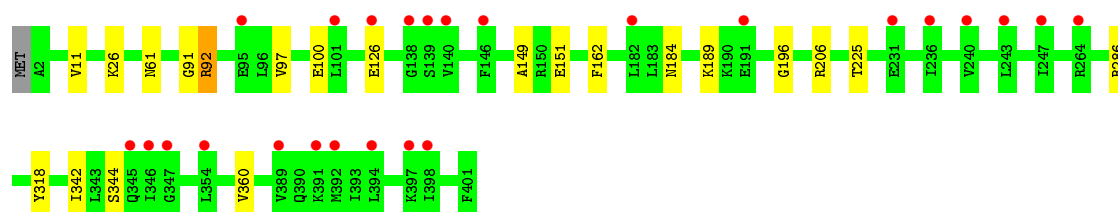




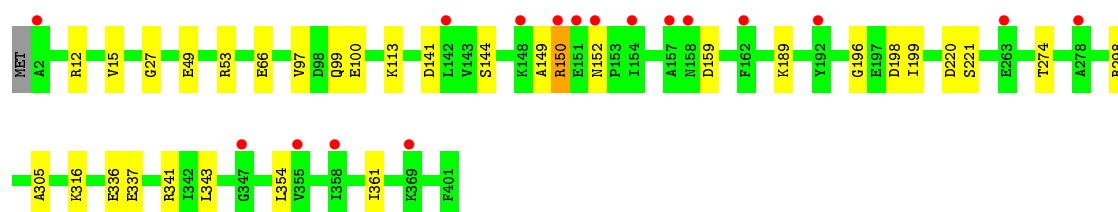
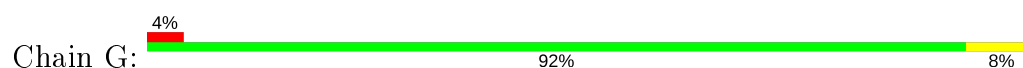
- Molecule 1: S-adenosylmethionine synthase



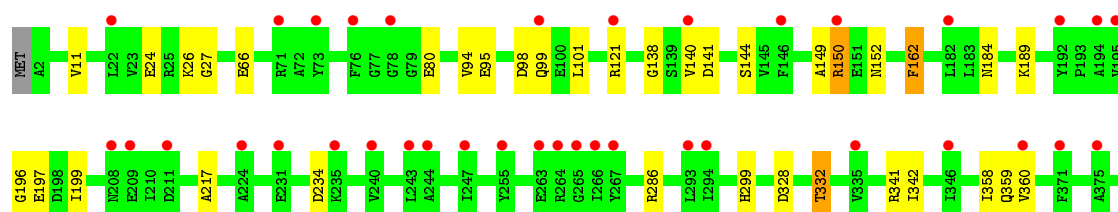
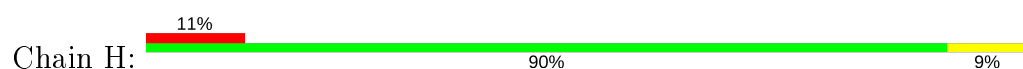
- Molecule 1: S-adenosylmethionine synthase

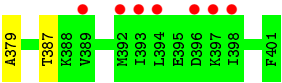


- Molecule 1: S-adenosylmethionine synthase



- Molecule 1: S-adenosylmethionine synthase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: MG, ACP, MDN, PO4, SAM

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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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.

All (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
1:B:132:ASP:OD2	7:B:601:HOH:O	2.07	0.72
1:H:328:ASP:O	1:H:332:THR:OG1	2.06	0.72
1:H:121:ARG:NH1	1:H:197:GLU:OE2	2.24	0.71
1:G:159:ASP:OD2	7:G:601:HOH:O	2.09	0.70
1:A:91:GLY:O	7:A:601:HOH:O	2.09	0.70
1:E:305:ALA:O	1:E:316:LYS:NZ	2.27	0.67
4:E:503:SAM:OXT	1:F:61:ASN:ND2	2.26	0.67
1:G:305:ALA:O	1:G:316:LYS:NZ	2.28	0.67
1:D:370:GLU:OE1	7:D:602:HOH:O	2.12	0.66
1:E:220:ASP:OD1	7:E:602:HOH:O	2.11	0.66
1:A:364:PRO:O	7:A:602:HOH:O	2.15	0.65
1:E:264:ARG:NH1	1:F:151:GLU:OE2	2.31	0.64
1:D:9:GLU:O	7:D:603:HOH:O	2.16	0.60
1:F:189:LYS:NZ	1:F:196:GLY:O	2.35	0.60
1:F:126:GLU:O	1:G:113:LYS:NZ	2.36	0.59
1:A:126:GLU:O	1:D:113:LYS:NZ	2.31	0.57
1:C:305:ALA:O	1:C:316:LYS:NZ	2.37	0.57
2:A:501:MDN:O1	7:A:603:HOH:O	2.17	0.56
1:F:91:GLY:O	1:F:92:ARG:NH1	2.38	0.55
1:B:49:GLU:OE2	1:B:52:ARG:NH1	2.40	0.55
1:A:113:LYS:NZ	1:D:126:GLU:O	2.32	0.54
2:E:501:MDN:O1	4:E:503:SAM:N	2.40	0.54
1:F:26:LYS:NZ	1:F:286:ARG:O	2.41	0.54
1:C:189:LYS:NZ	1:C:196:GLY:O	2.42	0.53
1:G:298:ARG:O	1:H:299:HIS:ND1	2.39	0.52
1:E:149:ALA:O	1:E:152:ASN:N	2.42	0.52
1:F:206[B]:ARG:NH1	7:F:608:HOH:O	2.43	0.51
1:G:149:ALA:O	1:G:152:ASN:N	2.42	0.51
1:E:53:ARG:NH2	1:H:80:GLU:OE1	2.42	0.51
1:H:196:GLY:N	1:H:217:ALA:O	2.40	0.50
1:E:27:GLY:N	1:E:199:ILE:O	2.43	0.50
1:E:381:GLU:O	1:E:385:ASN:ND2	2.41	0.49
1:G:189:LYS:NZ	1:G:196:GLY:O	2.46	0.49
1:C:343:LEU:O	1:C:354:LEU:N	2.46	0.48
1:H:141:ASP:OD2	1:H:144:SER:OG	2.31	0.48
1:C:233:LYS:NZ	7:C:611:HOH:O	2.46	0.48
1:A:189:LYS:NZ	1:A:196:GLY:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:ALA:O	1:H:152:ASN:N	2.45	0.48
1:G:12:ARG:HA	1:H:11:VAL:O	2.14	0.48
1:E:189:LYS:NZ	1:E:196:GLY:O	2.46	0.48
1:A:301:SER:OG	7:A:604:HOH:O	2.20	0.47
1:G:15:VAL:N	1:G:337:GLU:OE2	2.41	0.47
1:B:189:LYS:NZ	1:B:196:GLY:O	2.47	0.47
1:G:198:ASP:HB2	1:G:274:THR:HA	1.96	0.47
1:D:369:LYS:NZ	7:D:614:HOH:O	2.47	0.47
1:E:94:VAL:HG11	1:E:140:VAL:HG22	1.97	0.46
1:G:97:VAL:O	1:G:100:GLU:HG2	2.15	0.46
1:G:343:LEU:O	1:G:354:LEU:N	2.48	0.46
1:F:184:ASN:HA	1:F:189:LYS:HE2	1.98	0.46
1:B:26:LYS:NZ	1:B:286:ARG:O	2.49	0.46
1:F:318:TYR:CE1	1:F:344:SER:HB3	2.51	0.46
1:B:49:GLU:OE2	1:B:53:ARG:NE	2.49	0.45
1:A:161:SER:CB	1:A:314[A]:VAL:HG23	2.46	0.45
1:D:94:VAL:HG11	1:D:140:VAL:HG22	1.99	0.45
1:G:66:GLU:HG3	1:H:66:GLU:HB2	1.98	0.45
1:D:198:ASP:HB2	1:D:274:THR:HA	1.98	0.44
1:A:198:ASP:HB2	1:A:274:THR:HA	1.98	0.44
1:G:220:ASP:OD1	1:G:221:SER:N	2.51	0.44
1:G:141:ASP:O	1:G:144:SER:N	2.45	0.44
1:H:27:GLY:N	1:H:199:ILE:O	2.46	0.44
1:F:149:ALA:O	1:F:151:GLU:N	2.47	0.44
1:E:147:ASN:OD1	1:E:150:ARG:NH2	2.51	0.44
1:D:162:PHE:HA	1:D:342:ILE:O	2.18	0.44
1:C:272:THR:N	1:C:277:GLU:OE1	2.47	0.43
1:H:184:ASN:HA	1:H:189:LYS:HE2	2.00	0.43
1:H:341:ARG:NH1	1:H:359:GLN:OE1	2.46	0.43
1:E:12:ARG:HA	1:F:11:VAL:O	2.19	0.43
1:B:315:GLY:O	1:B:319:ASN:ND2	2.52	0.43
1:B:121:ARG:NH2	7:B:618:HOH:O	2.51	0.43
1:H:94:VAL:HG11	1:H:140:VAL:HG22	2.00	0.43
1:E:314:VAL:HG12	1:E:350:ILE:HG21	2.01	0.43
1:B:198:ASP:HB2	1:B:274:THR:HA	2.01	0.43
1:C:12:ARG:HA	1:D:11:VAL:O	2.18	0.43
1:A:343:LEU:O	1:A:354:LEU:N	2.52	0.43
1:G:49:GLU:OE2	1:G:53:ARG:NE	2.46	0.43
1:G:27:GLY:N	1:G:199:ILE:O	2.49	0.42
1:B:336:GLU:HG2	1:B:363:LYS:HA	2.01	0.42
1:H:162:PHE:HA	1:H:342:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ASP:HB2	1:C:274:THR:HA	2.02	0.42
1:E:82:VAL:HG11	1:H:101:LEU:HB3	2.00	0.42
1:H:26:LYS:NZ	1:H:286:ARG:O	2.53	0.42
1:H:358:ILE:HD11	1:H:379:ALA:HB2	2.02	0.42
1:C:336:GLU:N	1:C:361:ILE:O	2.50	0.42
1:F:162:PHE:HA	1:F:342:ILE:O	2.20	0.42
1:D:121:ARG:NH2	1:D:186:GLU:OE1	2.51	0.42
1:E:99:GLN:OE1	1:G:99:GLN:NE2	2.46	0.42
1:E:281:ASP:OD2	1:F:92:ARG:HD2	2.19	0.42
1:A:121:ARG:HG2	1:A:197:GLU:OE2	2.19	0.42
1:D:149:ALA:O	1:D:152:ASN:N	2.51	0.42
1:A:225:THR:OG1	1:A:226:PRO:HD2	2.20	0.41
1:C:149:ALA:O	1:C:152:ASN:N	2.53	0.41
1:H:98:ASP:O	1:H:99:GLN:HB2	2.20	0.41
1:D:336:GLU:HG2	1:D:363:LYS:HA	2.03	0.41
1:B:147:ASN:O	1:B:149:ALA:N	2.53	0.41
1:D:358:ILE:HD11	1:D:379:ALA:HB2	2.02	0.41
1:C:97:VAL:O	1:C:100:GLU:HG2	2.20	0.41
1:B:314:VAL:HG21	1:B:344:SER:OG	2.21	0.41
1:D:113:LYS:HG3	1:D:131:ILE:HD12	2.02	0.41
1:D:200:LYS:NZ	6:D:503:ACP:O3G	2.43	0.41
1:E:231:GLU:OE2	1:E:235:LYS:NZ	2.50	0.41
1:E:161[A]:SER:CB	1:E:314:VAL:HG23	2.50	0.41
1:E:314:VAL:HA	1:E:317:ILE:HG22	2.02	0.41
1:A:26:LYS:HE2	1:A:30:HIS:CE1	2.56	0.41
1:C:95:GLU:HA	1:C:102:PHE:HB3	2.03	0.40
1:G:149:ALA:O	1:G:150:ARG:C	2.59	0.40
1:A:90:SER:OG	1:A:91:GLY:N	2.54	0.40
1:C:149:ALA:O	1:C:150:ARG:C	2.60	0.40
1:F:97:VAL:O	1:F:100:GLU:HG2	2.21	0.40
1:H:95:GLU:OE1	1:H:138:GLY:N	2.55	0.40
1:H:149:ALA:O	1:H:150:ARG:C	2.59	0.40
1:C:285:GLY:HA3	1:C:304:ALA:HB2	2.03	0.40
1:E:161[B]:SER:CB	1:E:314:VAL:HG23	2.51	0.40
1:G:336:GLU:N	1:G:361:ILE:O	2.53	0.40
1:H:189:LYS:NZ	1:H:196:GLY:O	2.52	0.40

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

All (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
1	H	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

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	121	ARG
1	A	328	ASP
1	B	225	THR
1	B	258	THR
1	B	360	VAL
1	C	206	ARG
1	C	328	ASP
1	C	360	VAL
1	D	17	MET
1	D	92	ARG
1	D	225	THR
1	D	258	THR
1	D	346	ILE
1	E	17	MET
1	E	258	THR
1	E	328	ASP
1	E	360	VAL
1	F	92	ARG
1	F	225	THR
1	F	360	VAL
1	G	341	ARG
1	H	162	PHE
1	H	332	THR
1	H	360	VAL
1	H	387	THR

Some 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 carbohydrates 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
6	ACP	D	503	3	27,33,33	4.68	10 (37%)	32,52,52	2.27	6 (18%)
5	PO4	H	505	3	4,4,4	0.88	0	6,6,6	0.47	0
5	PO4	G	501	3	4,4,4	0.88	0	6,6,6	0.41	0
6	ACP	F	504	3	27,33,33	4.69	10 (37%)	32,52,52	2.27	6 (18%)
5	PO4	D	504	3	4,4,4	0.90	0	6,6,6	0.42	0
5	PO4	B	501	3	4,4,4	0.86	0	6,6,6	0.44	0
5	PO4	F	505	3	4,4,4	0.89	0	6,6,6	0.41	0
6	ACP	B	504	3	27,33,33	4.69	10 (37%)	32,52,52	2.24	6 (18%)
2	MDN	E	501	3	6,8,8	1.15	1 (16%)	12,13,13	1.42	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	F	501	3	4,4,4	0.90	0	6,6,6	0.41	0
4	SAM	A	503	-	21,29,29	1.21	2 (9%)	18,42,42	1.60	3 (16%)
6	ACP	H	504	3	27,33,33	4.69	9 (33%)	32,52,52	2.23	6 (18%)
2	MDN	A	501	3	6,8,8	1.16	1 (16%)	12,13,13	1.46	2 (16%)
4	SAM	E	503	-	21,29,29	1.20	2 (9%)	18,42,42	1.51	2 (11%)
2	MDN	H	501	3	6,8,8	0.95	0	12,13,13	1.02	0
5	PO4	B	505	3	4,4,4	0.88	0	6,6,6	0.45	0
5	PO4	C	502	3	4,4,4	0.89	0	6,6,6	0.37	0
2	MDN	C	501	3	6,8,8	1.29	2 (33%)	12,13,13	1.86	2 (16%)

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	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
6	ACP	H	504	3	-	6/15/38/38	0/3/3/3
2	MDN	E	501	3	-	1/6/6/6	-
4	SAM	A	503	-	-	2/8/33/33	0/3/3/3
2	MDN	A	501	3	-	1/6/6/6	-
4	SAM	E	503	-	-	3/8/33/33	0/3/3/3
2	MDN	H	501	3	-	0/6/6/6	-
6	ACP	F	504	3	-	3/15/38/38	0/3/3/3
2	MDN	C	501	3	-	0/6/6/6	-

All (47) 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
6	B	504	ACP	C2'-C1'	-14.82	1.31	1.53
6	D	503	ACP	C2'-C1'	-14.78	1.31	1.53
6	H	504	ACP	C2'-C1'	-14.70	1.31	1.53
6	H	504	ACP	PB-O3A	6.41	1.65	1.58
6	D	503	ACP	PB-O3A	6.36	1.65	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	ACP	PB-O3A	6.28	1.65	1.58
6	F	504	ACP	PB-O3A	6.24	1.65	1.58
6	B	504	ACP	O4'-C4'	-6.15	1.31	1.45
6	D	503	ACP	O4'-C4'	-6.12	1.31	1.45
6	H	504	ACP	O4'-C4'	-6.11	1.31	1.45
6	F	504	ACP	O4'-C4'	-6.09	1.31	1.45
4	A	503	SAM	C2-N3	4.05	1.38	1.32
4	E	503	SAM	C2-N3	4.02	1.38	1.32
6	F	504	ACP	C6-N6	3.16	1.45	1.34
6	H	504	ACP	C6-N6	3.16	1.45	1.34
6	B	504	ACP	C6-N6	3.15	1.45	1.34
6	D	503	ACP	C6-N6	3.14	1.45	1.34
6	B	504	ACP	O2'-C2'	2.98	1.50	1.43
6	D	503	ACP	O2'-C2'	2.95	1.49	1.43
6	F	504	ACP	O2'-C2'	2.94	1.49	1.43
6	H	504	ACP	O2'-C2'	2.92	1.49	1.43
6	F	504	ACP	O3'-C3'	-2.89	1.36	1.43
6	B	504	ACP	O3'-C3'	-2.86	1.36	1.43
6	D	503	ACP	O3'-C3'	-2.86	1.36	1.43
6	H	504	ACP	O3'-C3'	-2.81	1.36	1.43
6	H	504	ACP	C5-C4	-2.66	1.33	1.40
6	D	503	ACP	C5-C4	-2.64	1.33	1.40
6	F	504	ACP	C5-C4	-2.62	1.34	1.40
6	B	504	ACP	C5-C4	-2.62	1.34	1.40
4	E	503	SAM	C2-N1	2.55	1.38	1.33
4	A	503	SAM	C2-N1	2.54	1.38	1.33
6	F	504	ACP	C2-N3	2.29	1.35	1.32
6	B	504	ACP	C2-N3	2.26	1.35	1.32
6	H	504	ACP	C2-N3	2.26	1.35	1.32
6	D	503	ACP	C2-N3	2.16	1.35	1.32
2	C	501	MDN	P5-O6	2.13	1.54	1.50
2	A	501	MDN	P1-O1	2.11	1.54	1.50
6	B	504	ACP	PB-O2B	-2.09	1.51	1.56
2	E	501	MDN	P1-O1	2.07	1.54	1.50
6	D	503	ACP	PB-O2B	-2.05	1.51	1.56
2	C	501	MDN	P1-O1	2.01	1.54	1.50
6	F	504	ACP	PB-O2B	-2.00	1.51	1.56

All (34) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
6	B	504	ACP	N6-C6-N1	-5.63	106.89	118.57
6	F	504	ACP	N6-C6-N1	-5.63	106.89	118.57
6	H	504	ACP	N6-C6-N1	-5.63	106.90	118.57
6	F	504	ACP	N3-C2-N1	-5.60	119.93	128.68
6	B	504	ACP	N3-C2-N1	-5.59	119.94	128.68
6	D	503	ACP	N3-C2-N1	-5.54	120.02	128.68
4	A	503	SAM	N3-C2-N1	-5.51	120.06	128.68
6	H	504	ACP	N3-C2-N1	-5.51	120.07	128.68
4	E	503	SAM	N3-C2-N1	-5.39	120.25	128.68
6	B	504	ACP	PA-O3A-PB	-2.71	123.96	132.56
6	F	504	ACP	PA-O3A-PB	-2.67	124.09	132.56
2	C	501	MDN	O6-P5-C4	-2.58	105.68	111.24
6	D	503	ACP	C3'-C2'-C1'	2.50	104.75	100.98
6	H	504	ACP	PA-O3A-PB	-2.49	124.65	132.56
6	F	504	ACP	C3'-C2'-C1'	2.47	104.70	100.98
6	D	503	ACP	PA-O3A-PB	-2.43	124.84	132.56
2	C	501	MDN	O1-P1-C4	-2.42	106.02	111.24
4	A	503	SAM	C5'-SD-CG	-2.35	97.41	103.40
6	H	504	ACP	C3'-C2'-C1'	2.32	104.47	100.98
2	E	501	MDN	O1-P1-C4	-2.32	106.25	111.24
4	E	503	SAM	C3'-C2'-C1'	2.28	104.41	100.98
6	B	504	ACP	C3'-C2'-C1'	2.25	104.36	100.98
2	A	501	MDN	O1-P1-C4	-2.18	106.55	111.24
4	A	503	SAM	C3'-C2'-C1'	2.17	104.24	100.98
6	B	504	ACP	C1'-N9-C4	-2.13	122.89	126.64
6	F	504	ACP	C1'-N9-C4	-2.13	122.90	126.64
2	A	501	MDN	O2-P1-O3	2.05	114.07	108.08
6	H	504	ACP	C1'-N9-C4	-2.04	123.05	126.64
6	D	503	ACP	C1'-N9-C4	-2.03	123.07	126.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
6	B	504	ACP	C3'-C4'-C5'-O5'
6	H	504	ACP	O4'-C4'-C5'-O5'
6	F	504	ACP	C3'-C4'-C5'-O5'
6	B	504	ACP	O4'-C4'-C5'-O5'
6	D	503	ACP	C5'-O5'-PA-O3A
4	A	503	SAM	N-CA-CB-CG
6	D	503	ACP	C3'-C4'-C5'-O5'
6	D	503	ACP	C5'-O5'-PA-O2A
6	H	504	ACP	C5'-O5'-PA-O2A
4	E	503	SAM	CB-CG-SD-C5'
4	A	503	SAM	CA-CB-CG-SD
6	F	504	ACP	C4'-C5'-O5'-PA
6	H	504	ACP	PG-C3B-PB-O1B
6	D	503	ACP	O4'-C4'-C5'-O5'
6	F	504	ACP	O4'-C4'-C5'-O5'
6	D	503	ACP	PB-C3B-PG-O1G
2	A	501	MDN	P5-C4-P1-O1
2	E	501	MDN	P5-C4-P1-O1
6	H	504	ACP	PB-O3A-PA-O2A
6	H	504	ACP	C5'-O5'-PA-O3A

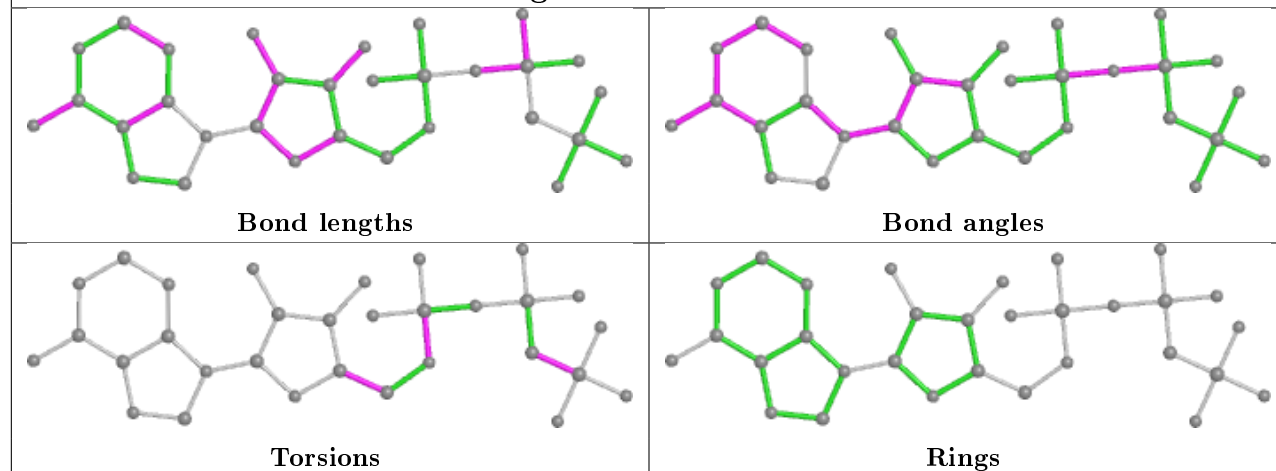
There are no ring outliers.

4 monomers are involved in 4 short contacts:

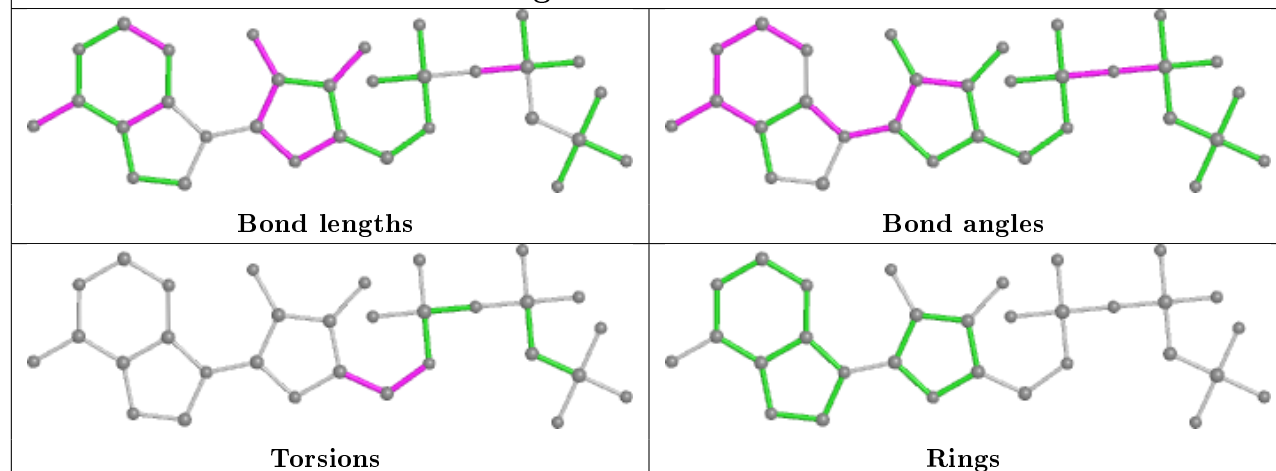
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	503	ACP	1	0
2	E	501	MDN	1	0
2	A	501	MDN	1	0
4	E	503	SAM	2	0

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 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.

Ligand ACP D 503

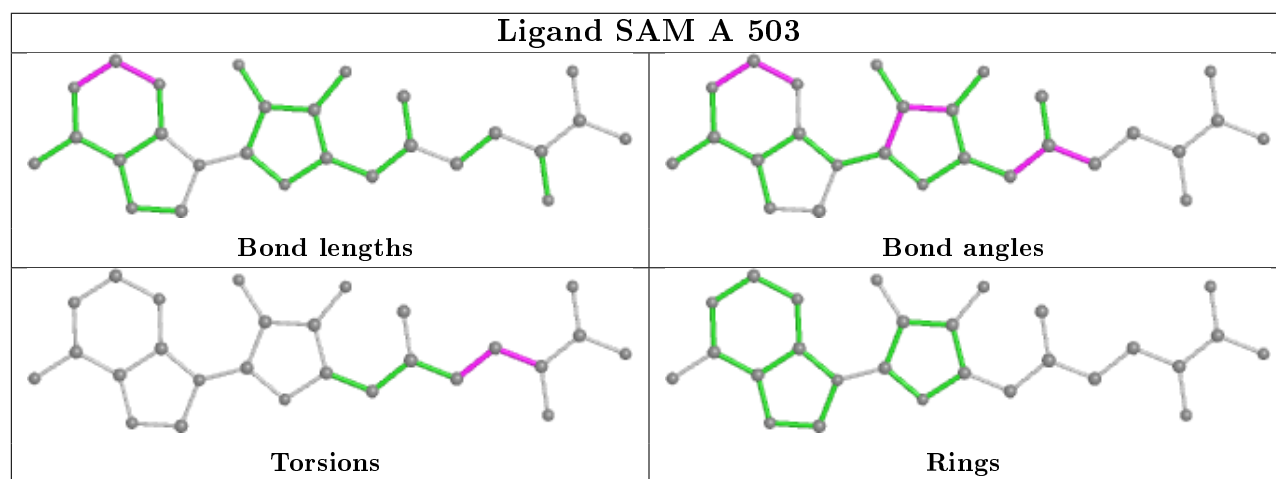
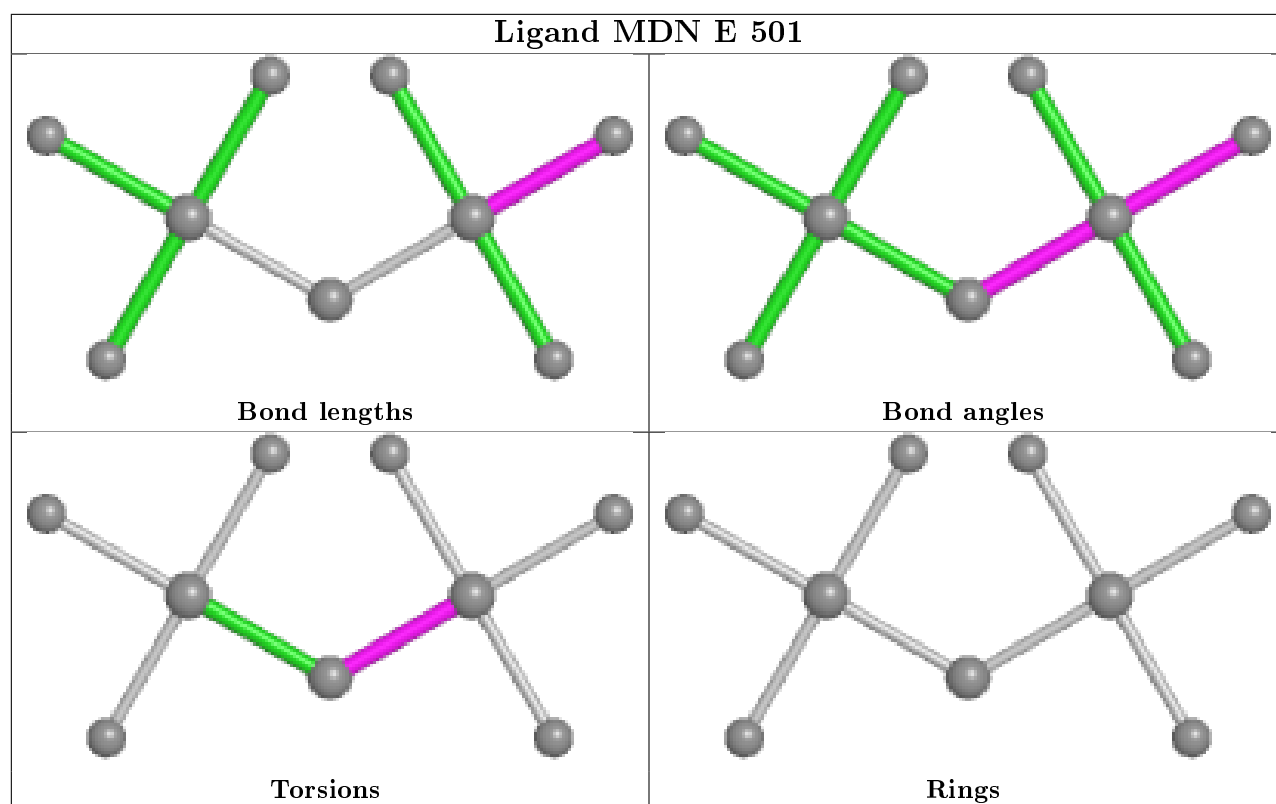


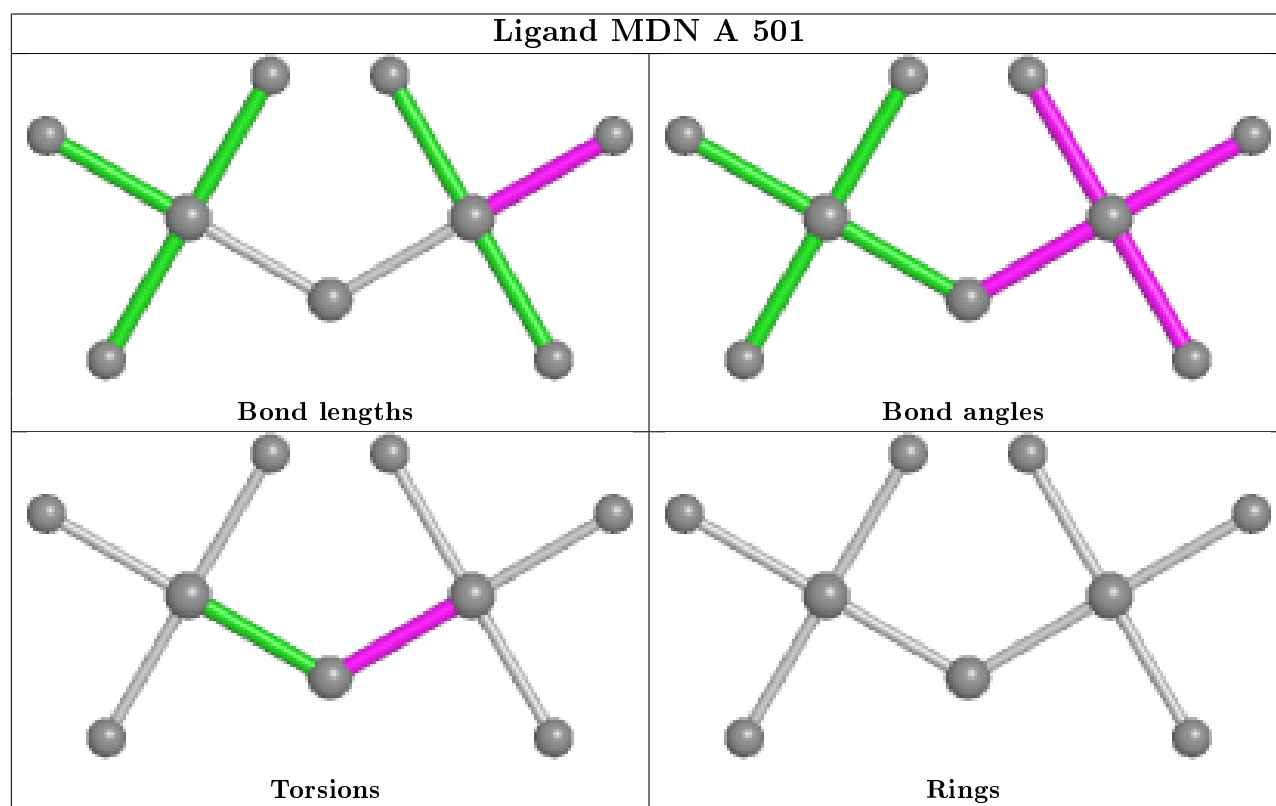
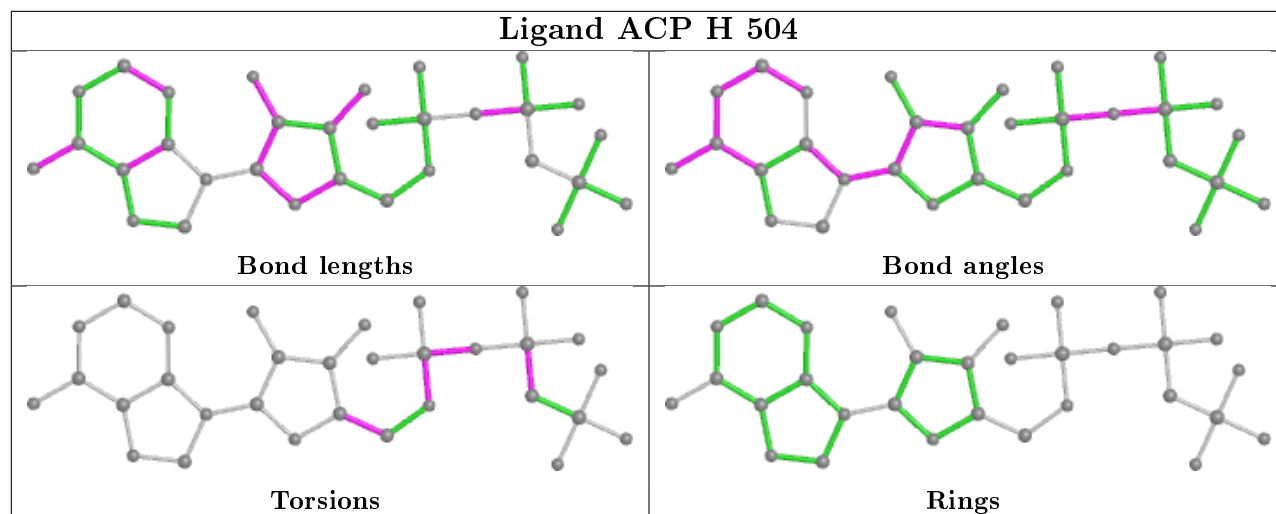
Ligand ACP F 504

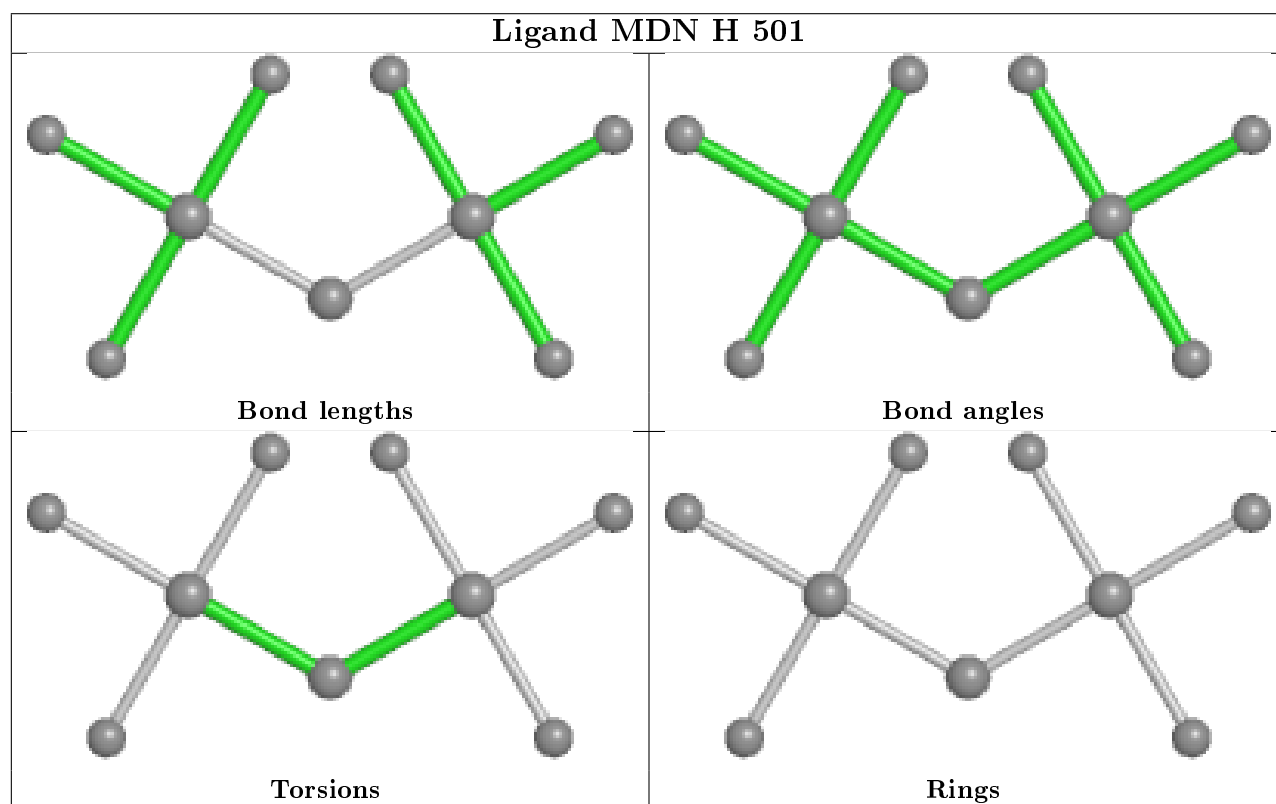
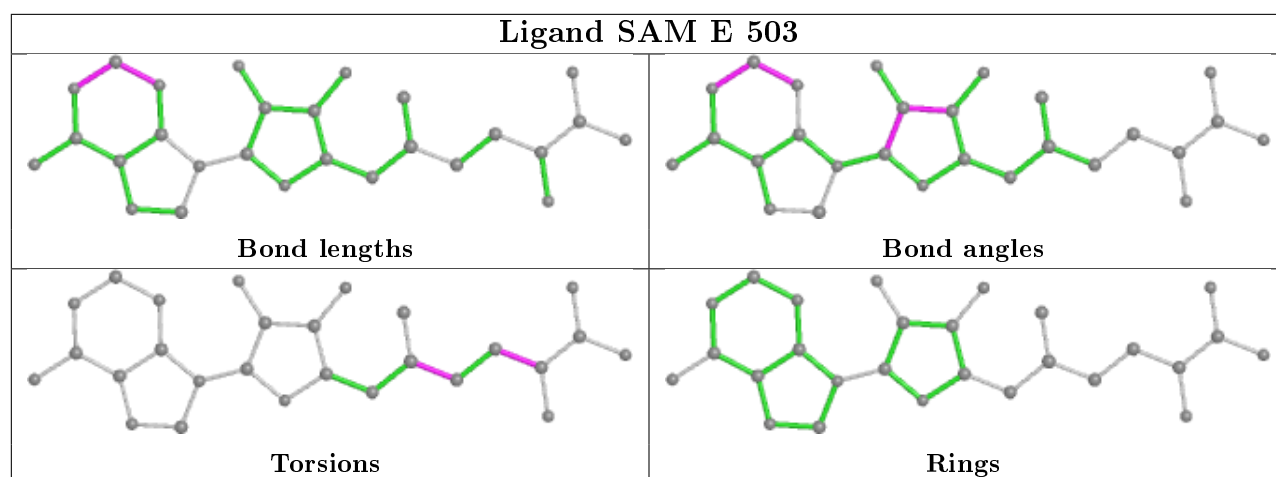


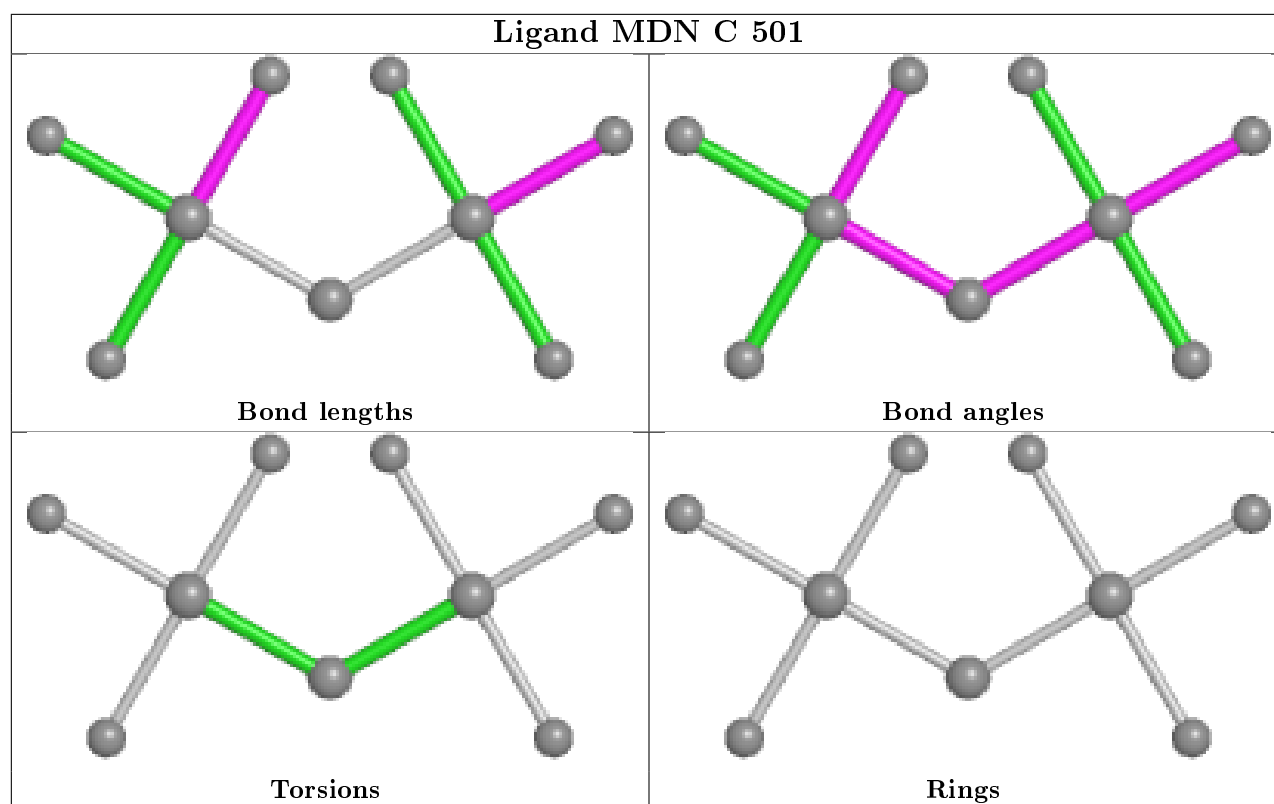
Ligand ACP B 504











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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	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

All (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
1	A	223	VAL	4.4
1	H	266	ILE	4.4
1	H	73	TYR	4.2
1	F	391	LYS	4.1
1	H	22	LEU	4.0
1	F	394	LEU	3.9
1	G	158	ASN	3.8
1	A	266	ILE	3.7
1	D	146	PHE	3.7
1	B	150	ARG	3.6
1	E	263	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	264	ARG	3.5
1	G	162	PHE	3.5
1	B	238	GLU	3.5
1	H	99	GLN	3.4
1	A	234	ASP	3.4
1	H	195	VAL	3.4
1	G	150	ARG	3.4
1	F	146	PHE	3.4
1	H	264	ARG	3.3
1	D	99	GLN	3.3
1	F	140	VAL	3.3
1	G	369	LYS	3.3
1	C	148	LYS	3.2
1	G	263	GLU	3.2
1	A	99	GLN	3.2
1	F	101	LEU	3.2
1	E	347	GLY	3.2
1	H	393	ILE	3.1
1	A	263	GLU	3.1
1	H	150	ARG	3.1
1	E	219	VAL	3.1
1	A	145	VAL	3.0
1	F	389	VAL	3.0
1	G	148	LYS	3.0
1	C	142	LEU	2.9
1	G	154	ILE	2.9
1	B	397	LYS	2.9
1	H	346	ILE	2.9
1	H	398	ILE	2.9
1	H	240	VAL	2.9
1	E	394	LEU	2.8
1	G	2	ALA	2.8
1	G	347	GLY	2.8
1	E	154	ILE	2.8
1	H	71	ARG	2.8
1	G	152	ASN	2.8
1	D	150	ARG	2.8
1	H	121	ARG	2.8
1	F	392	MET	2.8
1	B	82	VAL	2.7
1	H	194	ALA	2.7
1	E	82	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	266	ILE	2.7
1	A	151	GLU	2.7
1	D	101	LEU	2.7
1	E	141	ASP	2.6
1	C	397	LYS	2.6
1	G	358	ILE	2.6
1	F	95	GLU	2.6
1	F	126	GLU	2.6
1	A	148	LYS	2.6
1	A	386	ILE	2.6
1	D	143	VAL	2.6
1	H	224	ALA	2.6
1	F	138	GLY	2.5
1	G	355	VAL	2.5
1	H	371	PHE	2.5
1	H	392	MET	2.5
1	H	263	GLU	2.5
1	E	59[A]	HIS	2.5
1	D	389	VAL	2.5
1	G	151	GLU	2.5
1	A	227	LYS	2.5
1	H	265	GLY	2.5
1	F	240	VAL	2.5
1	H	360	VAL	2.5
1	H	235	LYS	2.4
1	B	267	TYR	2.4
1	B	386	ILE	2.4
1	C	350	ILE	2.4
1	C	389	VAL	2.4
1	G	142	LEU	2.4
1	F	247	ILE	2.4
1	H	294	ILE	2.4
1	B	154	ILE	2.4
1	H	231	GLU	2.4
1	F	397	LYS	2.4
1	F	191	GLU	2.4
1	H	247	ILE	2.4
1	E	279	GLY	2.4
1	B	95	GLU	2.4
1	H	76	PHE	2.4
1	F	236	ILE	2.3
1	F	182	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	243	LEU	2.3
1	H	335	VAL	2.3
1	F	231	GLU	2.3
1	B	96	LEU	2.3
1	H	394	LEU	2.3
1	H	78	GLY	2.3
1	E	101	LEU	2.3
1	E	388	LYS	2.3
1	A	117	LYS	2.3
1	G	278	ALA	2.3
1	E	278	ALA	2.3
1	F	139	SER	2.3
1	D	263	GLU	2.2
1	E	73	TYR	2.2
1	E	371	PHE	2.2
1	C	152	ASN	2.2
1	F	345	GLN	2.2
1	H	140	VAL	2.2
1	C	278	ALA	2.2
1	E	194	ALA	2.2
1	F	347	GLY	2.2
1	B	264	ARG	2.2
1	H	244	ALA	2.2
1	F	346	ILE	2.2
1	H	243	LEU	2.2
1	B	392	MET	2.2
1	B	249	SER	2.2
1	H	396	ASP	2.2
1	A	264	ARG	2.2
1	E	150	ARG	2.2
1	H	211	ASP	2.2
1	B	345	GLN	2.2
1	H	146	PHE	2.1
1	G	157	ALA	2.1
1	H	209	GLU	2.1
1	H	293	LEU	2.1
1	D	121	ARG	2.1
1	B	232	VAL	2.1
1	C	192	TYR	2.1
1	G	192	TYR	2.1
1	F	354	LEU	2.1
1	D	232	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	192	TYR	2.1
1	H	182	LEU	2.1
1	C	140	VAL	2.1
1	D	145	VAL	2.1
1	E	145	VAL	2.1
1	C	146	PHE	2.1
1	H	397	LYS	2.1
1	B	149	ALA	2.1
1	C	391	LYS	2.1
1	H	375	ALA	2.1
1	H	389	VAL	2.1
1	C	151	GLU	2.0
1	C	145	VAL	2.0
1	C	162	PHE	2.0
1	E	369	LYS	2.0
1	A	96	LEU	2.0
1	C	266	ILE	2.0
1	E	269	ILE	2.0
1	B	75	ARG	2.0
1	B	227	LYS	2.0
1	H	255	TYR	2.0
1	F	398	ILE	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	MG	D	506	1/1	0.69	0.06	75,75,75,75	0

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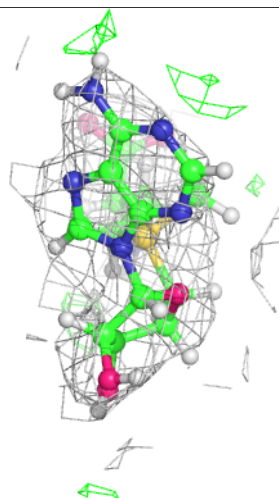
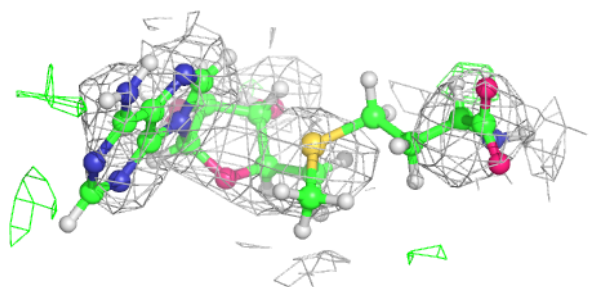
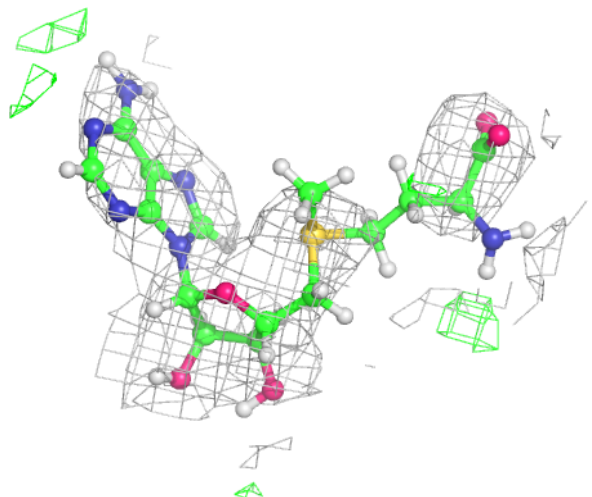
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SAM	E	503	27/27	0.84	0.22	82,96,114,117	0
3	MG	F	506	1/1	0.84	0.12	43,43,43,43	0
4	SAM	A	503	27/27	0.86	0.17	79,90,106,108	0
3	MG	B	503	1/1	0.88	0.17	49,49,49,49	0
3	MG	H	502	1/1	0.90	0.07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

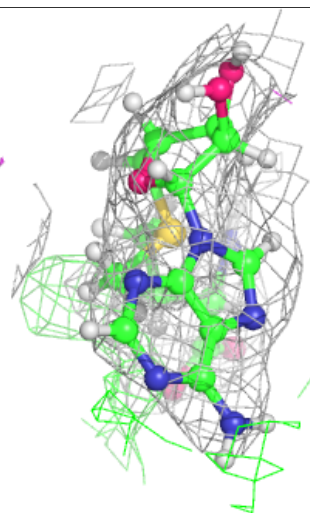
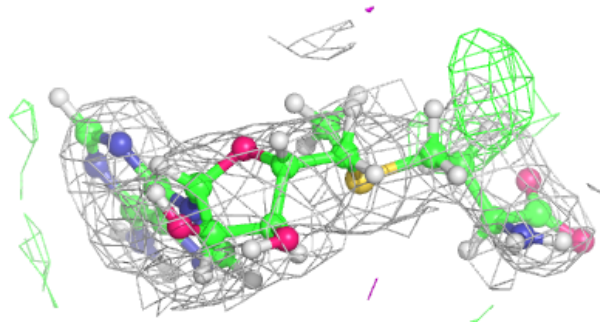
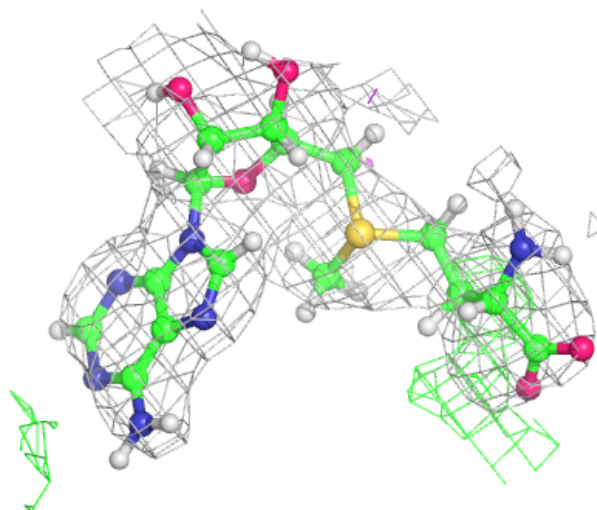
Electron density around SAM E 503:

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



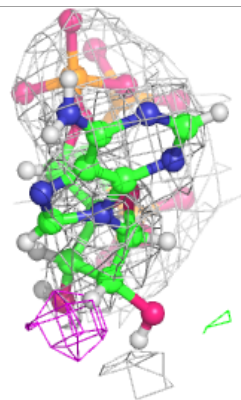
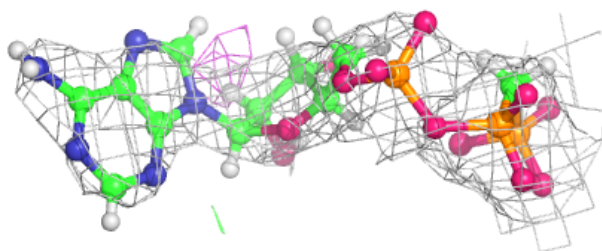
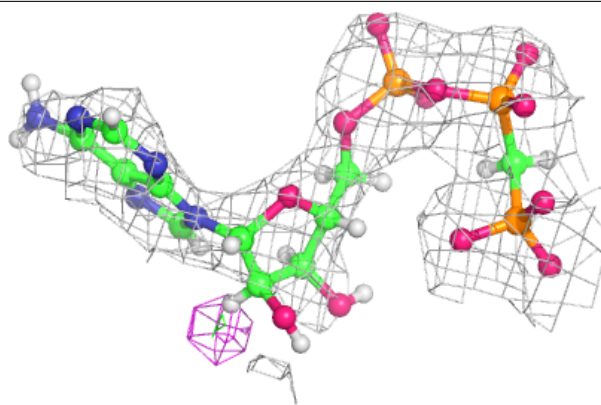
Electron density around SAM A 503:

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

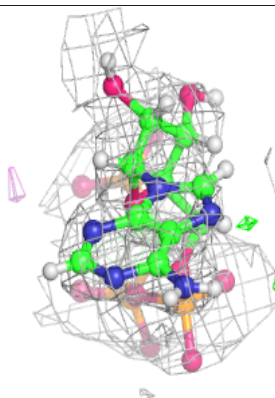
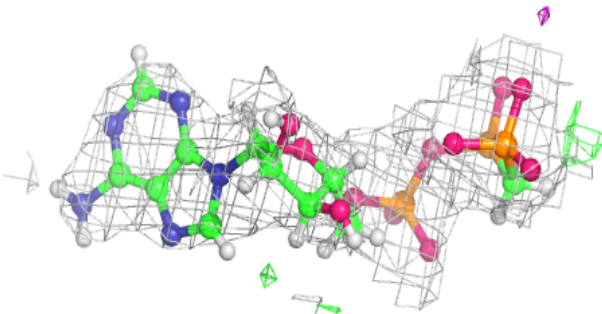
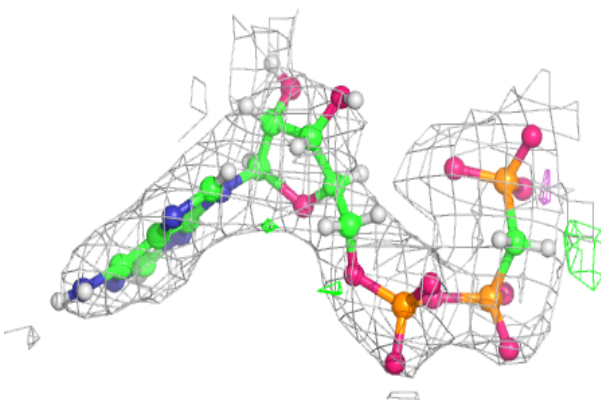


Electron density around ACP H 504:

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

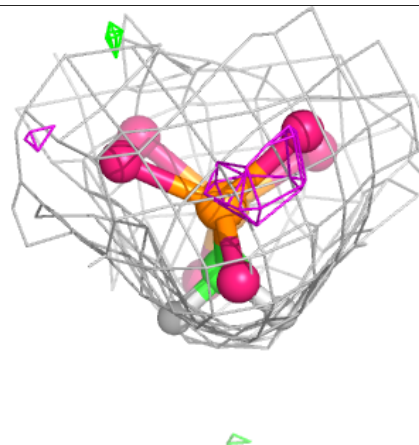
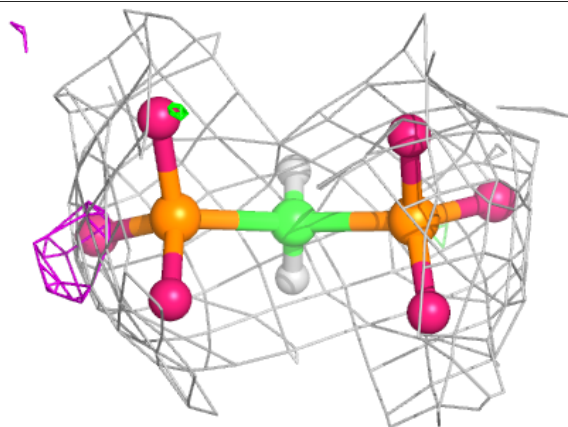
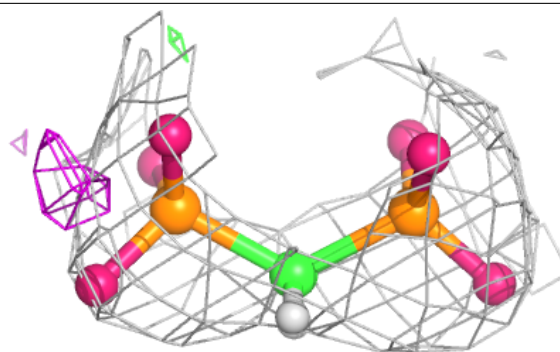
**Electron density around ACP D 503:**

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

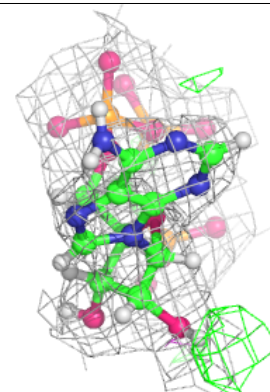
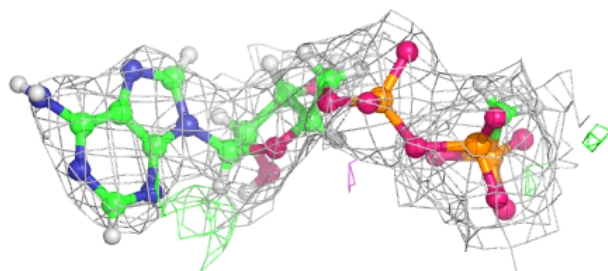
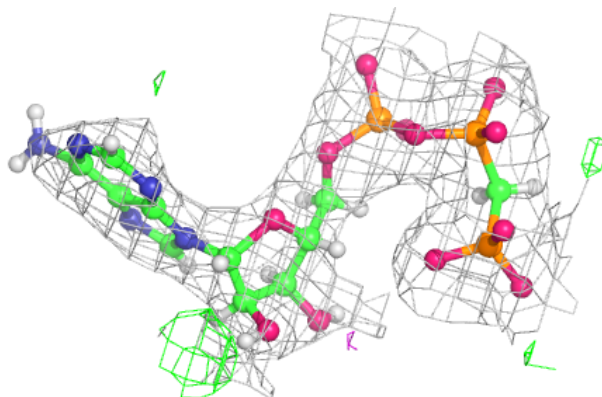


Electron density around MDN H 501:

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

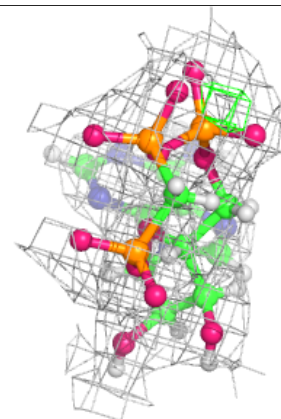
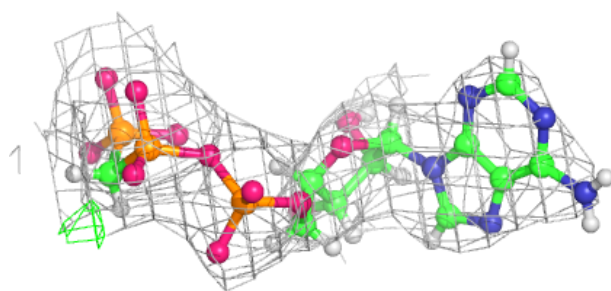
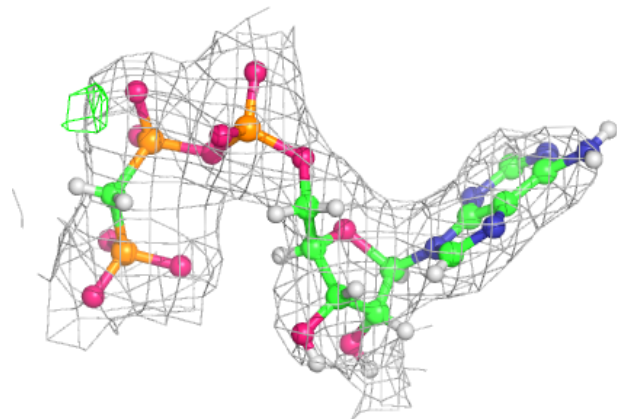
**Electron density around ACP B 504:**

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



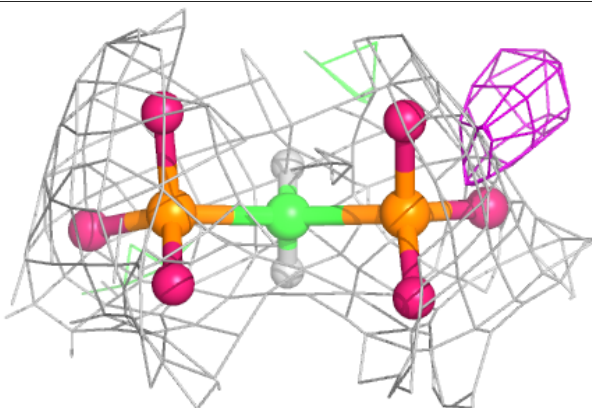
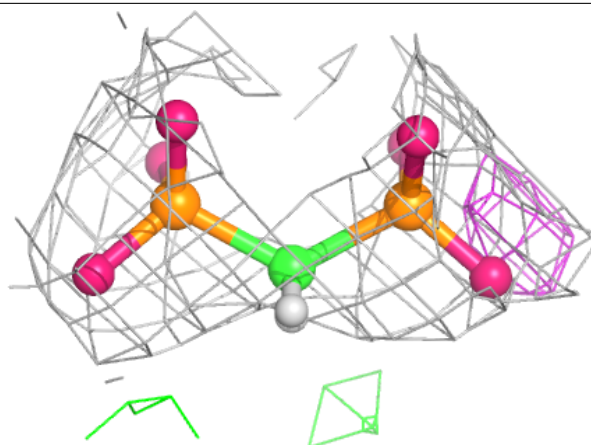
Electron density around ACP F 504:

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



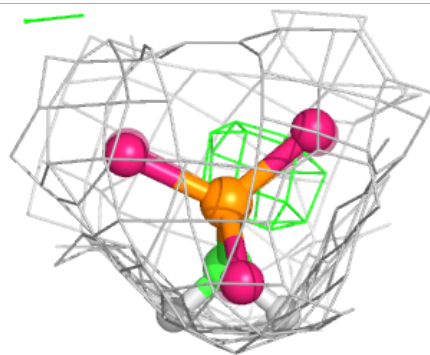
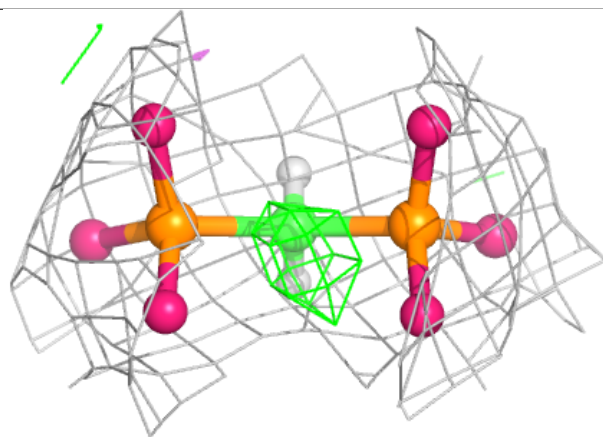
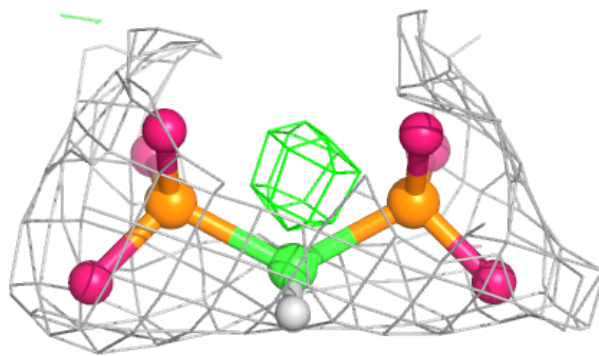
Electron density around MDN C 501:

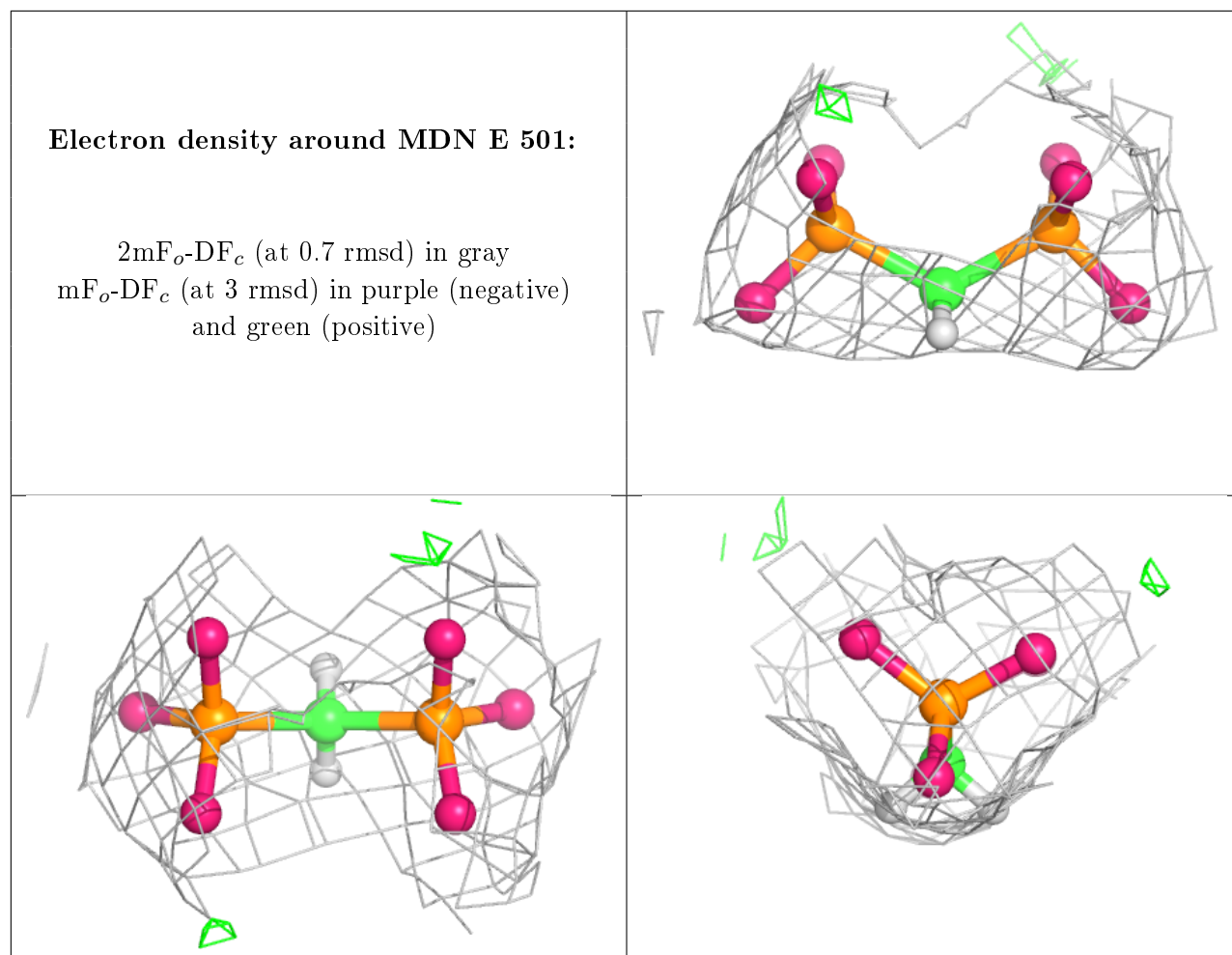
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MDN A 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.