



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:34 PM UTC

PDB ID : 6S83 / pdb_00006s83
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 types of validation reports are described at

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

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

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

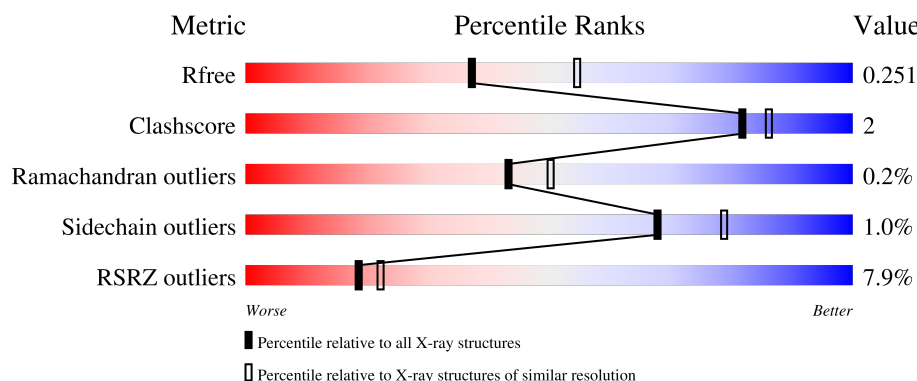
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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.



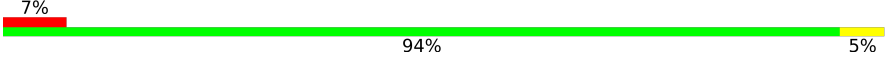
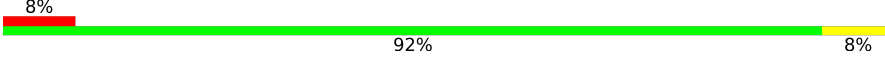
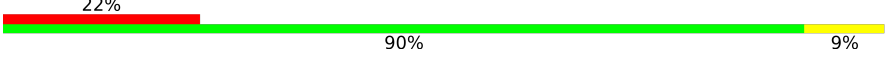
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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 $\leq 5\%$. 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	5% 93% 6%
1	B	401	4% 94% 6%
1	C	401	4% 93% 7%
1	D	401	4% 93% 6%
1	E	401	8% 92% 7%

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Mol	Chain	Length	Quality of chain
1	F	401	
1	G	401	
1	H	401	

2 Entry composition

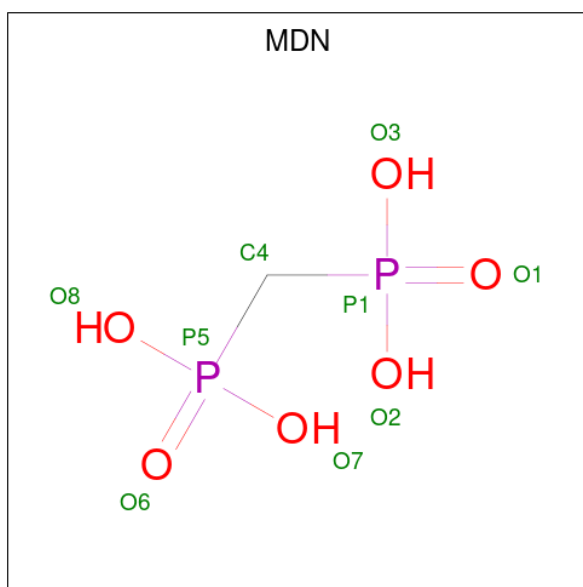
There are 7 unique types of molecules in this entry. The entry contains 51213 atoms, of which 25546 are hydrogens and 0 are deuteriums.

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 (CCD ID: MDN) (formula: $\text{CH}_6\text{O}_6\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

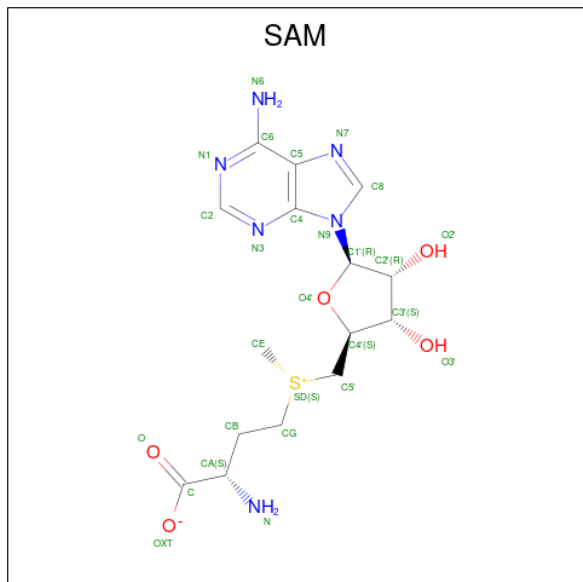


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	C	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	E	1	Total	C	H	O	P	0	0
			11	1	2	6	2		
2	H	1	Total	C	H	O	P	0	0
			11	1	2	6	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

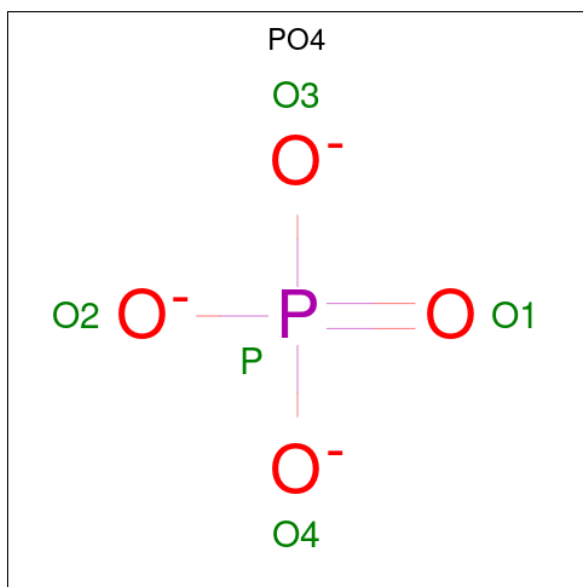
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	4	Total	Mg	0	0
			4	4		
3	C	1	Total	Mg	0	0
			1	1		
3	D	4	Total	Mg	0	0
			4	4		
3	E	1	Total	Mg	0	0
			1	1		
3	F	4	Total	Mg	0	0
			4	4		
3	G	1	Total	Mg	0	0
			1	1		
3	H	4	Total	Mg	0	0
			4	4		

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



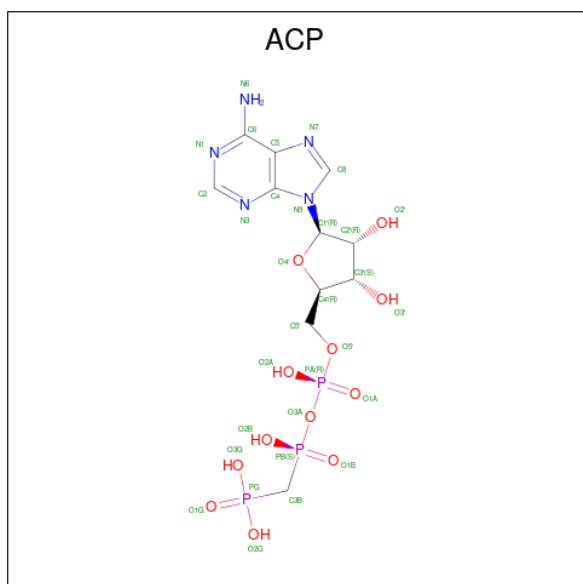
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		
4	E	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: 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 (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$) (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

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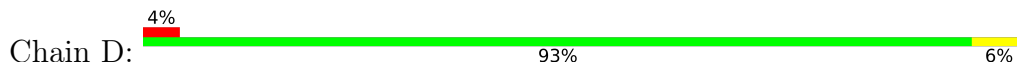
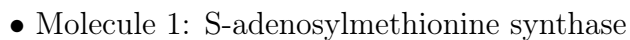
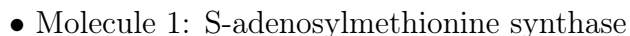
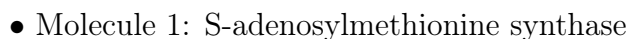
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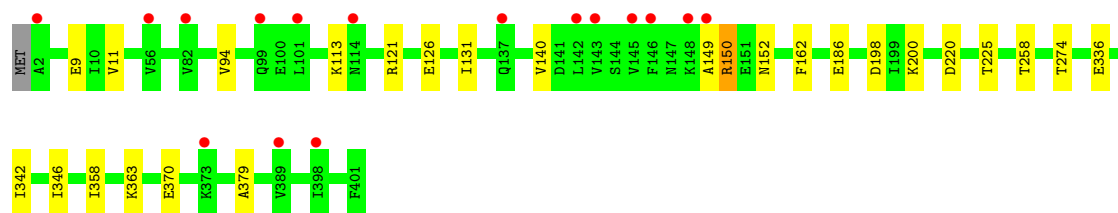
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	H	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 7 is water.

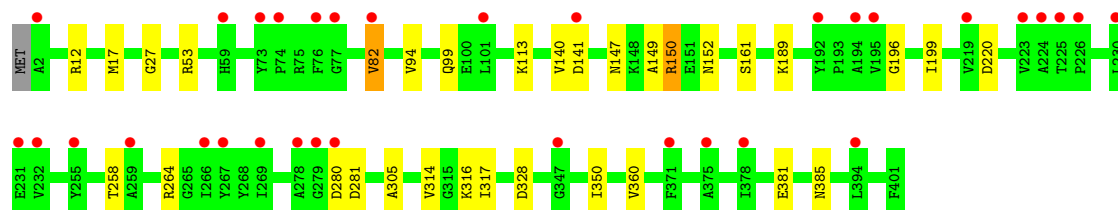
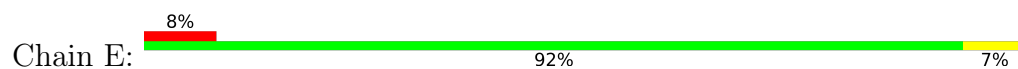
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	52	Total	O	0	0
			52	52		
7	B	72	Total	O	0	0
			72	72		
7	C	57	Total	O	0	0
			57	57		
7	D	68	Total	O	0	0
			68	68		
7	E	62	Total	O	0	0
			62	62		
7	F	59	Total	O	0	0
			59	59		
7	G	46	Total	O	0	0
			46	46		
7	H	38	Total	O	0	0
			38	38		

- Molecule 1: S-adenosylmethionine synthase

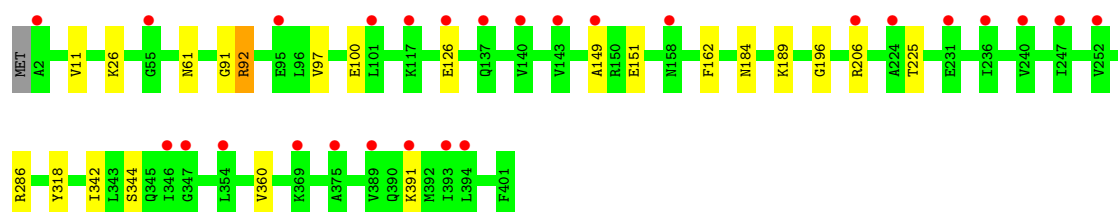




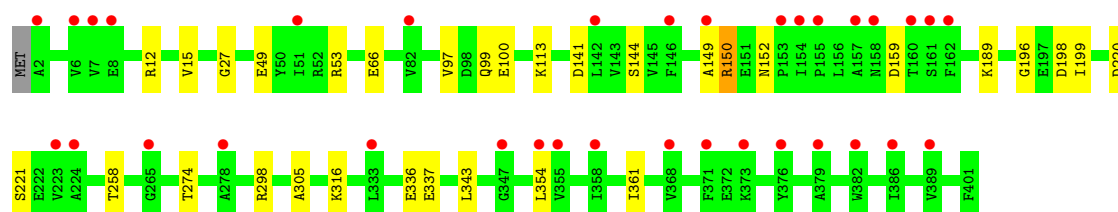
• Molecule 1: S-adenosylmethionine synthase



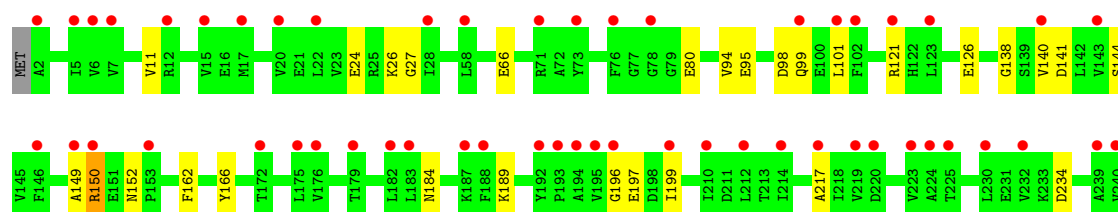
• Molecule 1: S-adenosylmethionine synthase

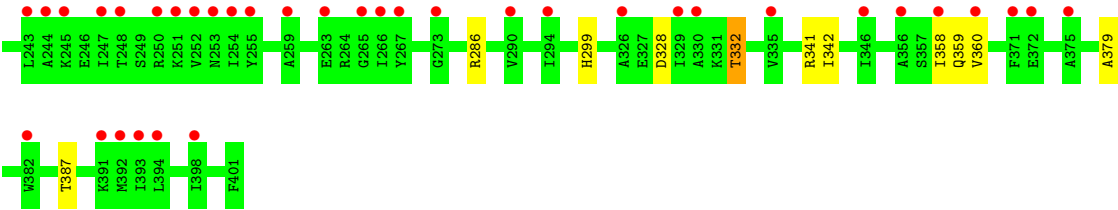


• Molecule 1: S-adenosylmethionine synthase



• 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 74.47 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.47-2.34) 100.0 (74.47-2.34)	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 0.226 , 0.251	Depositor DCC
R_{free} test set	7504 reflections (5.02%)	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 , 37.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MDN, MG, ACP, 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	0.12	0/3165	0.30	0/4287
1	B	0.11	0/3166	0.28	0/4287
1	C	0.11	0/3158	0.27	0/4277
1	D	0.11	0/3158	0.28	0/4277
1	E	0.12	0/3184	0.29	0/4313
1	F	0.11	0/3177	0.29	0/4301
1	G	0.11	0/3181	0.28	0/4308
1	H	0.11	0/3166	0.28	0/4287
All	All	0.11	0/25355	0.28	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	15	0
1	B	3114	3178	3180	12	0
1	C	3109	3171	3171	14	0
1	D	3109	3171	3171	16	0
1	E	3128	3187	3191	22	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	25	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	1	0
4	E	27	22	22	3	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	1	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	3	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	125	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 (125) 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:A:113:LYS:NZ	1:D:126:GLU:O	2.32	0.61
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
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:E:280:ASP:OD2	4:E:503:SAM:O3'	2.27	0.51
1:F:206[B]:ARG:NH1	7:F:608:HOH:O	2.43	0.51
1:E:53:ARG:NH2	1:H:80:GLU:OE1	2.42	0.51
1:G:149:ALA:O	1:G:152:ASN:N	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:E:189:LYS:NZ	1:E: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:C:308:LYS:NZ	5:D:504:PO4:O3	2.48	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:149:ALA:O	1:G:150:ARG:C	2.59	0.45
1:C:149:ALA:O	1:C:150:ARG:C	2.60	0.45
1:G:66:GLU:HG3	1:H:66:GLU:HB2	1.98	0.45
1:H:149:ALA:O	1:H:150:ARG:C	2.59	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
4:A:503:SAM:HE3	1:B:159:ASP:CG	2.43	0.43
1:C:272:THR:N	1:C:277:GLU:OE1	2.47	0.43
1:E:149:ALA:O	1:E:150:ARG:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:113:LYS:NZ	1:H:126:GLU:O	2.43	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
1:A:149:ALA:O	1:A:150:ARG:C	2.62	0.42
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:149:ALA:O	1:D:150:ARG:C	2.63	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: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:H:166:TYR:CD1	1:H:166:TYR:C	2.99	0.40
1:A:90:SER:OG	1:A:91:GLY:N	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:LYS:NZ	1:H:196:GLY:O	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/401 (100%)	388 (97%)	10 (2%)	1 (0%)	36	41
1	B	399/401 (100%)	389 (98%)	10 (2%)	0	100	100
1	C	398/401 (99%)	387 (97%)	10 (2%)	1 (0%)	36	41
1	D	398/401 (99%)	386 (97%)	11 (3%)	1 (0%)	36	41
1	E	401/401 (100%)	388 (97%)	12 (3%)	1 (0%)	43	50
1	F	400/401 (100%)	387 (97%)	13 (3%)	0	100	100
1	G	401/401 (100%)	391 (98%)	9 (2%)	1 (0%)	43	50
1	H	399/401 (100%)	389 (98%)	9 (2%)	1 (0%)	36	41
All	All	3195/3208 (100%)	3105 (97%)	84 (3%)	6 (0%)	43	50

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%)	70	80
1	B	339/339 (100%)	335 (99%)	4 (1%)	63	75
1	C	338/339 (100%)	334 (99%)	4 (1%)	63	75
1	D	338/339 (100%)	335 (99%)	3 (1%)	70	80
1	E	341/339 (101%)	336 (98%)	5 (2%)	57	69
1	F	340/339 (100%)	336 (99%)	4 (1%)	63	75
1	G	341/339 (101%)	340 (100%)	1 (0%)	86	91
1	H	339/339 (100%)	336 (99%)	3 (1%)	70	80
All	All	2715/2712 (100%)	2688 (99%)	27 (1%)	68	79

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	328	ASP
1	A	346	ILE
1	B	225	THR
1	B	258	THR
1	B	360	VAL
1	B	387	THR
1	C	206	ARG
1	C	360	VAL
1	C	387	THR
1	C	391	LYS
1	D	225	THR
1	D	258	THR
1	D	346	ILE
1	E	17	MET
1	E	82	VAL
1	E	258	THR
1	E	328	ASP
1	E	360	VAL

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Mol	Chain	Res	Type
1	F	92	ARG
1	F	225	THR
1	F	360	VAL
1	F	391	LYS
1	G	258	THR
1	H	332	THR
1	H	360	VAL
1	H	387	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	118	ASN
1	B	19	GLN
1	B	118	ASN
1	B	366	HIS
1	D	99	GLN
1	D	118	ASN
1	D	345	GLN
1	D	352	GLN
1	E	19	GLN
1	E	64	GLN
1	E	122	HIS
1	E	128	HIS
1	E	152	ASN
1	F	118	ASN
1	F	366	HIS
1	G	137	GLN
1	G	152	ASN
1	G	366	HIS
1	G	385	ASN
1	H	345	GLN
1	H	352	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
5	PO4	B	501	3	4,4,4	0.90	0	6,6,6	0.47	0
5	PO4	F	505	3	4,4,4	0.93	0	6,6,6	0.44	0
2	MDN	A	501	3	6,8,8	1.21	1 (16%)	12,13,13	1.48	2 (16%)
4	SAM	E	503	-	27,29,29	1.12	4 (14%)	34,42,42	1.94	8 (23%)
6	ACP	B	504	3	31,33,33	3.17	11 (35%)	47,52,52	1.98	12 (25%)
6	ACP	H	504	3	31,33,33	3.20	10 (32%)	47,52,52	1.99	12 (25%)
5	PO4	H	505	3	4,4,4	0.92	0	6,6,6	0.50	0
5	PO4	B	505	3	4,4,4	0.92	0	6,6,6	0.48	0
5	PO4	G	501	3	4,4,4	0.92	0	6,6,6	0.44	0
6	ACP	D	503	3	31,33,33	3.19	10 (32%)	47,52,52	1.98	12 (25%)
6	ACP	F	504	3	31,33,33	3.17	10 (32%)	47,52,52	1.99	12 (25%)
2	MDN	E	501	3	6,8,8	1.19	1 (16%)	12,13,13	1.45	2 (16%)
5	PO4	F	501	3	4,4,4	0.94	0	6,6,6	0.44	0
5	PO4	D	504	3	4,4,4	0.94	0	6,6,6	0.45	0
5	PO4	C	502	3	4,4,4	0.94	0	6,6,6	0.40	0
4	SAM	A	503	-	27,29,29	1.11	3 (11%)	34,42,42	1.98	9 (26%)
2	MDN	H	501	3	6,8,8	0.98	0	12,13,13	1.04	0
2	MDN	C	501	3	6,8,8	1.34	2 (33%)	12,13,13	1.90	3 (25%)

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	-
4	SAM	E	503	-	-	6/17/33/33	0/3/3/3
6	ACP	B	504	3	-	5/19/38/38	0/3/3/3
6	ACP	H	504	3	-	8/19/38/38	0/3/3/3
6	ACP	D	503	3	-	7/19/38/38	0/3/3/3
6	ACP	F	504	3	-	5/19/38/38	0/3/3/3
2	MDN	E	501	3	-	1/6/6/6	-
4	SAM	A	503	-	-	5/17/33/33	0/3/3/3
2	MDN	H	501	3	-	0/6/6/6	-
2	MDN	C	501	3	-	0/6/6/6	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	504	ACP	O4'-C1'	8.92	1.62	1.42
6	B	504	ACP	O4'-C1'	8.88	1.62	1.42
6	D	503	ACP	O4'-C1'	8.87	1.62	1.42
6	F	504	ACP	O4'-C1'	8.85	1.62	1.42
6	F	504	ACP	C2'-C1'	-7.09	1.31	1.53
6	B	504	ACP	C2'-C1'	-7.07	1.31	1.53
6	D	503	ACP	C2'-C1'	-7.05	1.31	1.53
6	H	504	ACP	C2'-C1'	-7.01	1.31	1.53
6	H	504	ACP	PB-O3A	6.40	1.65	1.58
6	D	503	ACP	PB-O3A	6.35	1.65	1.58
6	B	504	ACP	PB-O3A	6.27	1.65	1.58
6	F	504	ACP	PB-O3A	6.22	1.65	1.58
6	B	504	ACP	O4'-C4'	-6.18	1.31	1.45
6	D	503	ACP	O4'-C4'	-6.15	1.31	1.45
6	H	504	ACP	O4'-C4'	-6.14	1.31	1.45
6	F	504	ACP	O4'-C4'	-6.12	1.31	1.45
6	H	504	ACP	PA-O3A	5.74	1.65	1.59
6	D	503	ACP	PA-O3A	5.63	1.65	1.59
6	F	504	ACP	PA-O3A	5.35	1.65	1.59
6	B	504	ACP	PA-O3A	5.16	1.65	1.59
6	F	504	ACP	C6-N6	4.45	1.45	1.34
6	H	504	ACP	C6-N6	4.45	1.45	1.34
6	B	504	ACP	C6-N6	4.44	1.45	1.34
6	D	503	ACP	C6-N6	4.43	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	504	ACP	C5-C4	-2.91	1.33	1.39
6	D	503	ACP	C5-C4	-2.89	1.33	1.39
6	F	504	ACP	C5-C4	-2.86	1.34	1.39
6	B	504	ACP	C5-C4	-2.85	1.34	1.39
6	B	504	ACP	O2'-C2'	2.85	1.50	1.43
6	D	503	ACP	O2'-C2'	2.81	1.49	1.43
6	F	504	ACP	O2'-C2'	2.81	1.49	1.43
6	H	504	ACP	O2'-C2'	2.79	1.49	1.43
6	F	504	ACP	O3'-C3'	-2.74	1.36	1.43
6	B	504	ACP	O3'-C3'	-2.72	1.36	1.43
6	D	503	ACP	O3'-C3'	-2.71	1.36	1.43
6	F	504	ACP	C5-N7	-2.67	1.34	1.39
6	H	504	ACP	O3'-C3'	-2.67	1.36	1.43
4	E	503	SAM	C2-N1	2.66	1.38	1.33
4	A	503	SAM	C2-N1	2.64	1.38	1.33
4	A	503	SAM	C2-N3	2.64	1.38	1.33
6	D	503	ACP	C5-N7	-2.62	1.34	1.39
4	E	503	SAM	C2-N3	2.61	1.38	1.33
6	H	504	ACP	C5-N7	-2.60	1.34	1.39
6	B	504	ACP	C5-N7	-2.60	1.34	1.39
4	E	503	SAM	OXT-C	-2.23	1.23	1.30
2	C	501	MDN	P5-O6	2.20	1.54	1.50
4	A	503	SAM	OXT-C	-2.20	1.23	1.30
2	A	501	MDN	P1-O1	2.18	1.54	1.50
2	E	501	MDN	P1-O1	2.15	1.54	1.50
2	C	501	MDN	P1-O1	2.09	1.54	1.50
6	B	504	ACP	PB-O2B	-2.01	1.51	1.56
4	E	503	SAM	C5-N7	-2.00	1.35	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	504	ACP	N3-C2-N1	-5.71	119.93	128.58
6	B	504	ACP	N3-C2-N1	-5.71	119.94	128.58
6	D	503	ACP	N3-C2-N1	-5.66	120.02	128.58
4	A	503	SAM	N3-C2-N1	-5.63	120.06	128.58
6	H	504	ACP	N3-C2-N1	-5.62	120.07	128.58
4	E	503	SAM	N3-C2-N1	-5.50	120.25	128.58
6	D	503	ACP	N6-C6-N1	-5.22	106.74	118.38
6	B	504	ACP	N6-C6-N1	-5.16	106.89	118.38
6	F	504	ACP	N6-C6-N1	-5.16	106.89	118.38
6	H	504	ACP	N6-C6-N1	-5.15	106.90	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	504	ACP	C5-C4-N3	-5.07	119.73	126.72
6	B	504	ACP	C5-C4-N3	-5.02	119.80	126.72
6	D	503	ACP	C5-C4-N3	-4.93	119.93	126.72
6	F	504	ACP	C5-C4-N3	-4.91	119.95	126.72
4	E	503	SAM	C5-C4-N3	-4.70	120.25	126.72
4	A	503	SAM	C5-C4-N3	-4.50	120.52	126.72
6	D	503	ACP	C5-C6-N6	4.07	133.37	123.29
6	F	504	ACP	C5-C6-N6	4.00	133.19	123.29
6	F	504	ACP	N9-C8-N7	-3.98	108.29	113.94
6	B	504	ACP	C5-C6-N6	3.96	133.10	123.29
6	D	503	ACP	N9-C8-N7	-3.96	108.31	113.94
6	H	504	ACP	N9-C8-N7	-3.96	108.32	113.94
6	B	504	ACP	N9-C8-N7	-3.95	108.33	113.94
6	H	504	ACP	C5-C6-N6	3.94	133.05	123.29
4	A	503	SAM	N9-C8-N7	-3.73	108.64	113.94
4	E	503	SAM	N9-C8-N7	-3.62	108.80	113.94
4	E	503	SAM	C2-N3-C4	3.45	120.26	111.83
6	B	504	ACP	C2-N3-C4	3.44	120.23	111.83
6	H	504	ACP	C2-N3-C4	3.43	120.21	111.83
4	A	503	SAM	C2-N3-C4	3.41	120.15	111.83
6	D	503	ACP	C2-N3-C4	3.38	120.10	111.83
6	F	504	ACP	C2-N3-C4	3.38	120.09	111.83
4	E	503	SAM	C5-N7-C8	3.37	108.75	103.45
4	A	503	SAM	C5-N7-C8	3.30	108.63	103.45
4	A	503	SAM	N3-C4-N9	3.11	132.46	127.17
4	E	503	SAM	N3-C4-N9	3.07	132.39	127.17
6	H	504	ACP	N3-C4-N9	2.92	132.14	127.17
6	F	504	ACP	C5-N7-C8	2.91	108.02	103.45
6	B	504	ACP	N3-C4-N9	2.90	132.10	127.17
6	H	504	ACP	C5-N7-C8	2.90	108.00	103.45
6	D	503	ACP	C5-N7-C8	2.86	107.94	103.45
6	B	504	ACP	C5-N7-C8	2.82	107.89	103.45
6	D	503	ACP	N3-C4-N9	2.79	131.92	127.17
6	F	504	ACP	N3-C4-N9	2.79	131.91	127.17
4	A	503	SAM	OXT-C-O	-2.62	118.14	124.08
2	C	501	MDN	O6-P5-C4	-2.61	105.68	111.37
6	B	504	ACP	PB-O3A-PA	-2.58	123.96	132.37
4	E	503	SAM	OXT-C-O	-2.57	118.25	124.08
6	F	504	ACP	PB-O3A-PA	-2.54	124.09	132.37
4	A	503	SAM	CG-SD-C5'	-2.46	97.41	103.43
2	C	501	MDN	O1-P1-C4	-2.45	106.02	111.37
6	H	504	ACP	PB-O3A-PA	-2.37	124.65	132.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	MDN	O1-P1-C4	-2.35	106.25	111.37
6	D	503	ACP	PB-O3A-PA	-2.31	124.84	132.37
6	F	504	ACP	C4-C5-N7	-2.29	107.96	110.58
4	E	503	SAM	C4-C5-N7	-2.28	107.98	110.58
6	D	503	ACP	C4-C5-N7	-2.26	108.00	110.58
6	H	504	ACP	C4-C5-N7	-2.26	108.00	110.58
2	A	501	MDN	O1-P1-C4	-2.21	106.55	111.37
6	B	504	ACP	C4-C5-N7	-2.21	108.06	110.58
6	D	503	ACP	C5-C4-N9	2.14	108.15	105.81
2	A	501	MDN	O2-P1-O3	2.14	114.07	107.96
6	F	504	ACP	C5-C4-N9	2.13	108.14	105.81
6	H	504	ACP	C5-C4-N9	2.13	108.13	105.81
6	H	504	ACP	C6-C5-C4	2.11	120.06	117.18
6	B	504	ACP	C5-C4-N9	2.10	108.10	105.81
4	A	503	SAM	C4-C5-N7	-2.09	108.20	110.58
2	C	501	MDN	O2-P1-O3	2.05	113.79	107.96
6	B	504	ACP	C6-C5-C4	2.03	119.95	117.18
6	F	504	ACP	C6-C5-C4	2.03	119.95	117.18
2	E	501	MDN	O2-P1-O3	2.03	113.73	107.96
6	D	503	ACP	C6-C5-C4	2.01	119.93	117.18

There are no chirality outliers.

All (38) 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'
6	F	504	ACP	C3'-C4'-C5'-O5'
6	B	504	ACP	O4'-C4'-C5'-O5'
4	E	503	SAM	OXT-C-CA-N
6	D	503	ACP	C3'-C4'-C5'-O5'
4	E	503	SAM	C2'-C1'-N9-C8
6	B	504	ACP	C2'-C1'-N9-C8
6	F	504	ACP	C2'-C1'-N9-C8
6	H	504	ACP	C2'-C1'-N9-C8
4	A	503	SAM	N-CA-CB-CG
4	A	503	SAM	CA-CB-CG-SD
4	A	503	SAM	O-C-CA-CB
4	A	503	SAM	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	E	503	SAM	CB-CG-SD-C5'
6	D	503	ACP	C5'-O5'-PA-O2A
6	D	503	ACP	C5'-O5'-PA-O3A
6	H	504	ACP	C5'-O5'-PA-O2A
4	E	503	SAM	C-CA-CB-CG
6	F	504	ACP	C4'-C5'-O5'-PA
6	D	503	ACP	O4'-C4'-C5'-O5'
6	F	504	ACP	O4'-C4'-C5'-O5'
6	B	504	ACP	O4'-C1'-N9-C8
6	H	504	ACP	O4'-C1'-N9-C8
6	H	504	ACP	PG-C3B-PB-O1B
6	F	504	ACP	O4'-C1'-N9-C8
2	A	501	MDN	P5-C4-P1-O1
2	E	501	MDN	P5-C4-P1-O1
6	D	503	ACP	PB-C3B-PG-O1G
4	A	503	SAM	C2'-C1'-N9-C8
6	D	503	ACP	C2'-C1'-N9-C8
6	H	504	ACP	PB-O3A-PA-O2A
4	E	503	SAM	O4'-C1'-N9-C8
6	B	504	ACP	C2'-C1'-N9-C4
6	H	504	ACP	C2'-C1'-N9-C4

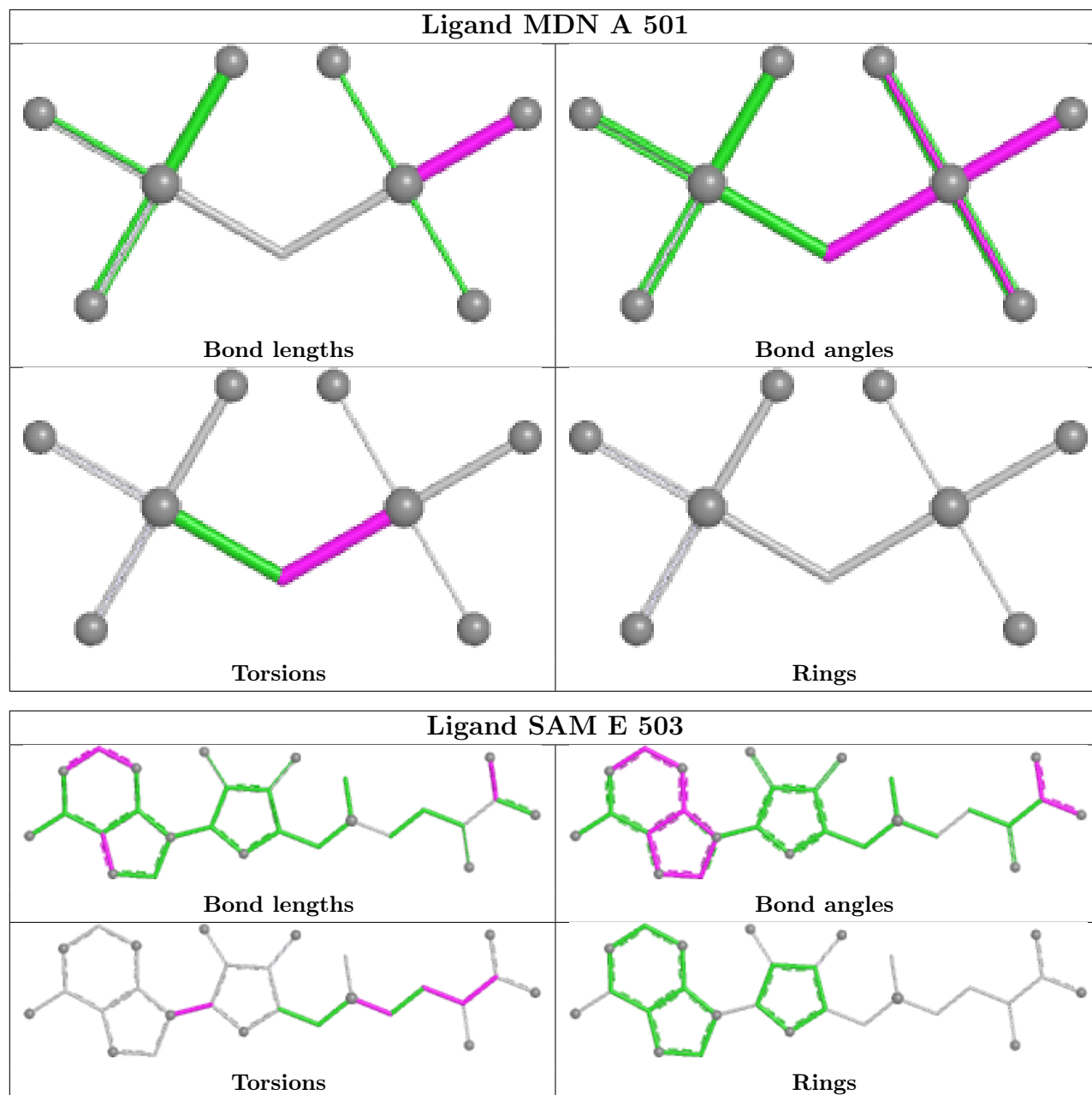
There are no ring outliers.

6 monomers are involved in 7 short contacts:

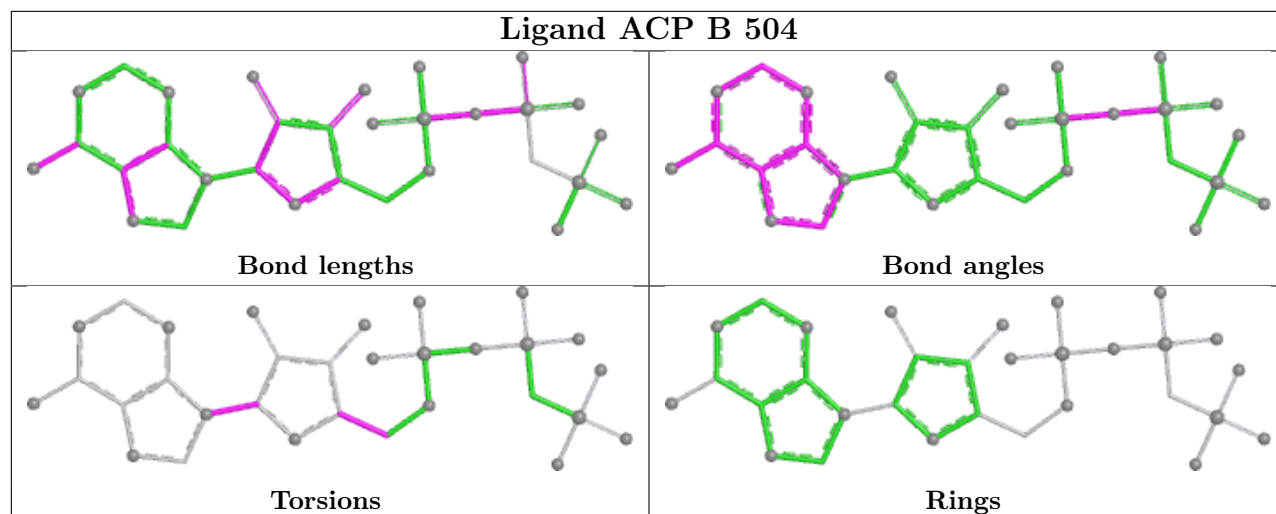
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MDN	1	0
4	E	503	SAM	3	0
6	D	503	ACP	1	0
2	E	501	MDN	1	0
5	D	504	PO4	1	0
4	A	503	SAM	1	0

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

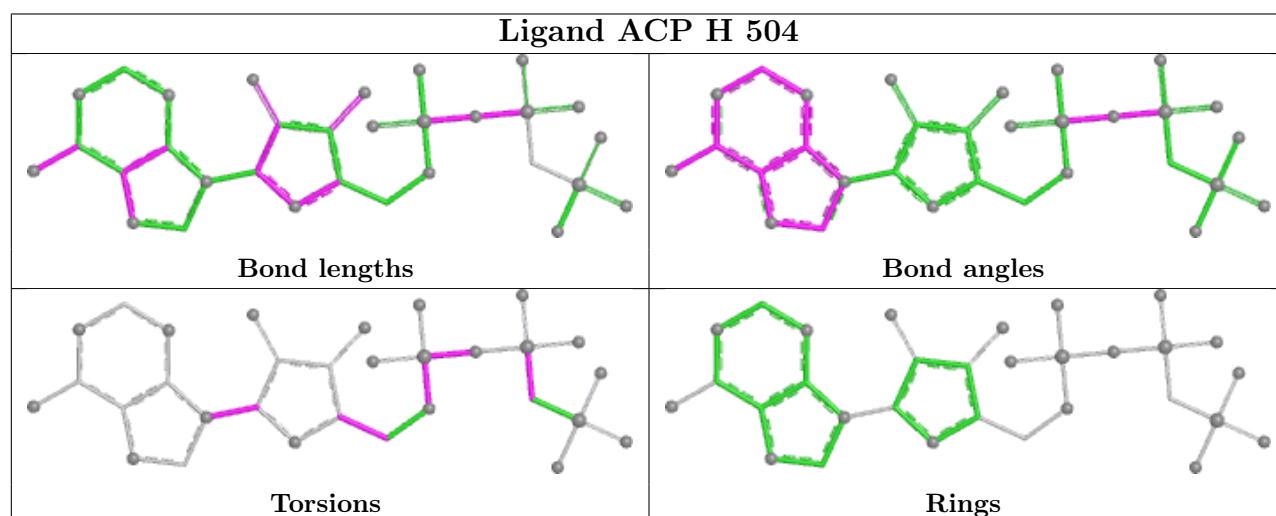
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



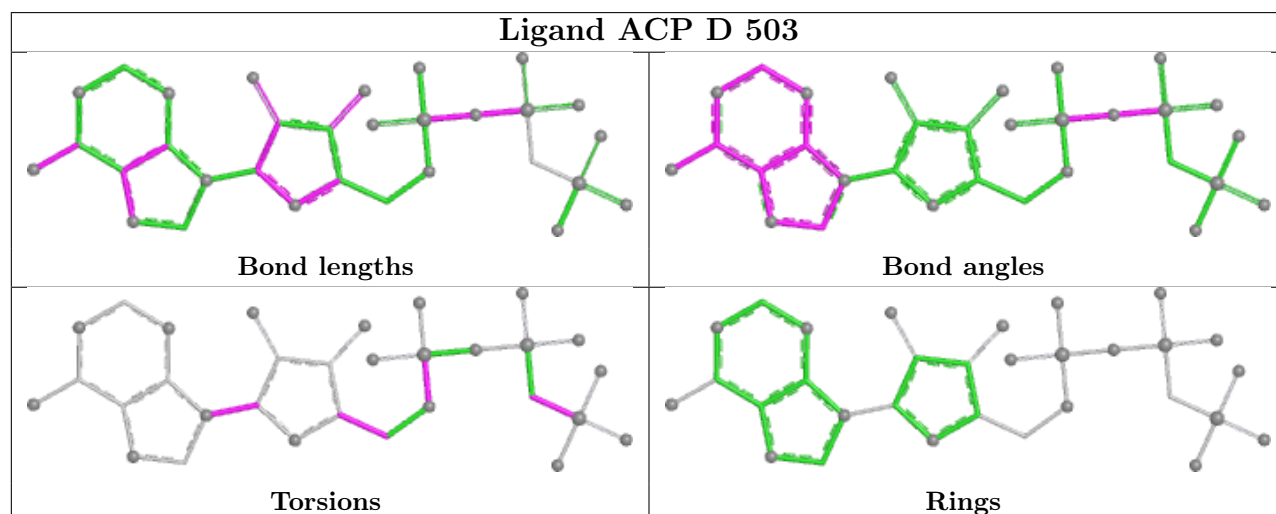
Ligand ACP B 504



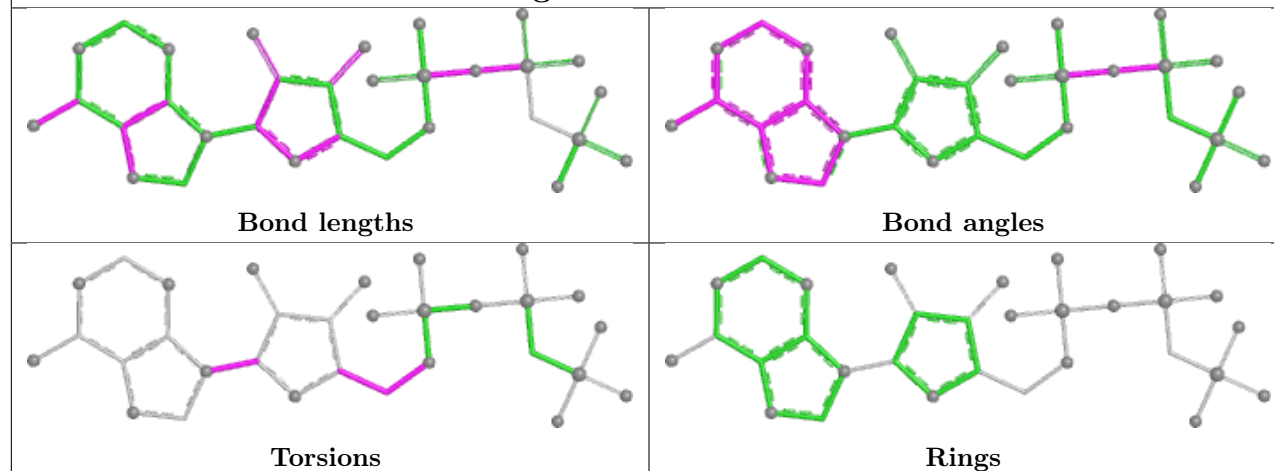
Ligand ACP H 504



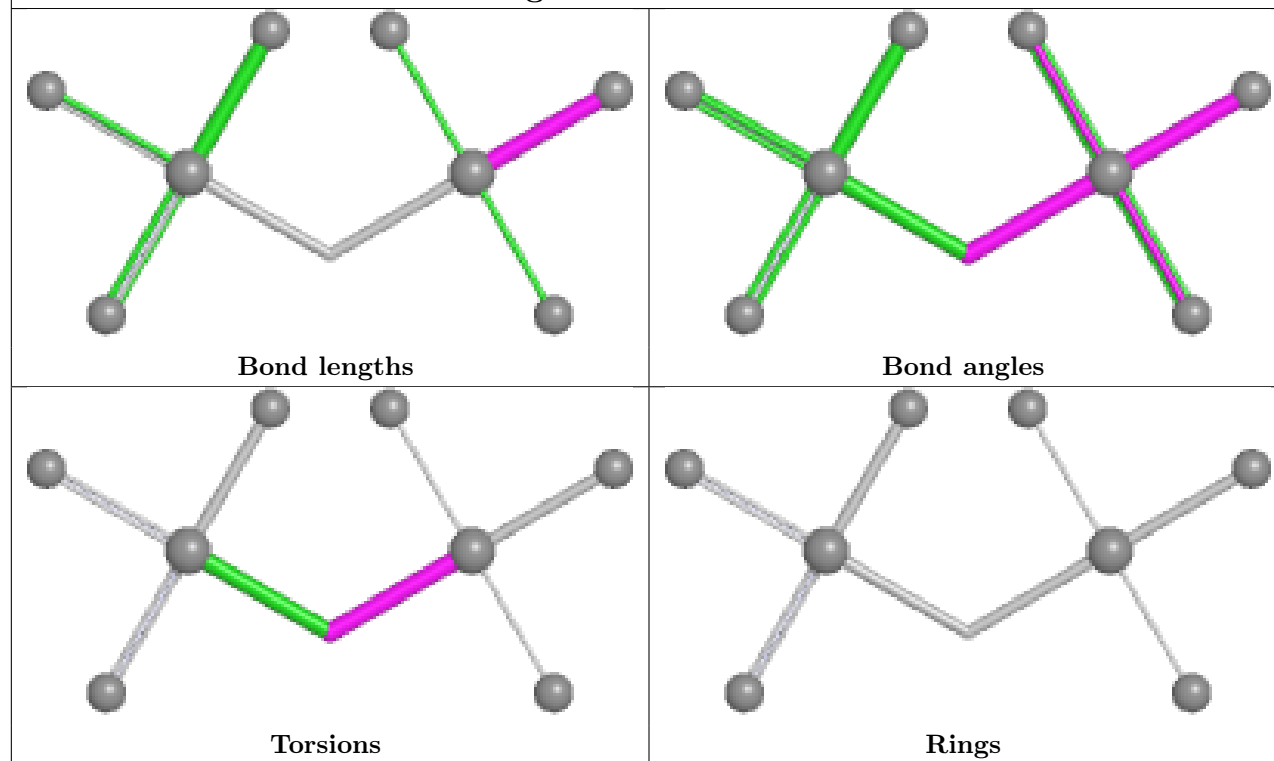
Ligand ACP D 503



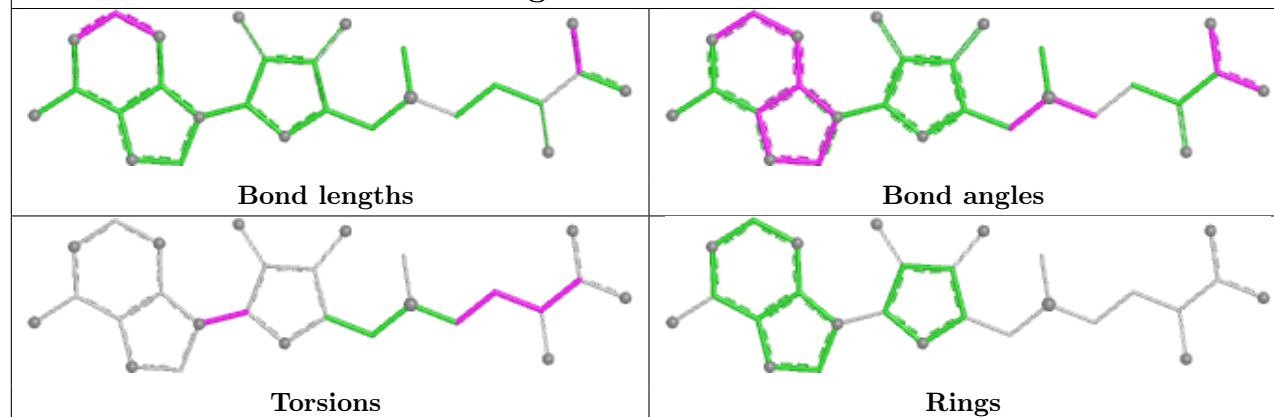
Ligand ACP F 504

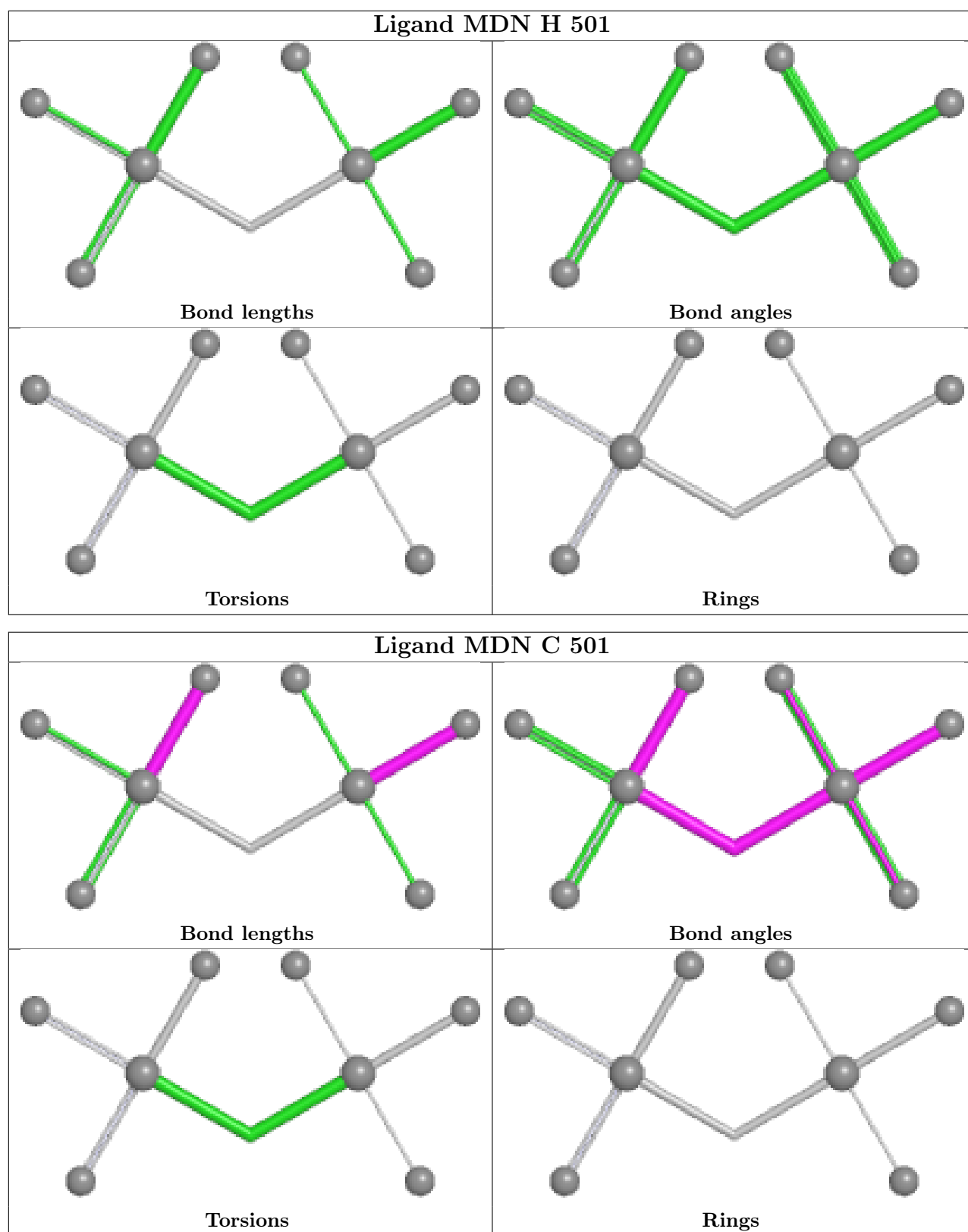


Ligand MDN E 501



Ligand SAM A 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.48	19 (4%)	35	42	28, 65, 102, 139	1 (0%)
1	B	400/401 (99%)	0.59	18 (4%)	38	44	27, 61, 103, 168	1 (0%)
1	C	400/401 (99%)	0.43	18 (4%)	38	44	37, 59, 96, 157	0
1	D	400/401 (99%)	0.37	16 (4%)	42	48	38, 56, 92, 160	0
1	E	400/401 (99%)	0.73	33 (8%)	17	20	36, 62, 102, 142	3 (0%)
1	F	400/401 (99%)	0.80	27 (6%)	23	27	29, 67, 112, 151	2 (0%)
1	G	400/401 (99%)	0.73	34 (8%)	16	20	30, 66, 116, 161	3 (0%)
1	H	400/401 (99%)	1.33	89 (22%)	2	2	35, 81, 120, 160	1 (0%)
All	All	3200/3208 (99%)	0.68	254 (7%)	18	22	27, 64, 109, 168	11 (0%)

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	ALA	6.2
1	A	2	ALA	5.4
1	B	149	ALA	5.3
1	A	146	PHE	5.2
1	G	162	PHE	5.1
1	F	394	LEU	5.0
1	H	192	TYR	4.6
1	C	2	ALA	4.5
1	D	146	PHE	4.5
1	B	145	VAL	4.5
1	D	2	ALA	4.5
1	E	59[A]	HIS	4.4
1	H	240	VAL	4.4
1	H	195	VAL	4.4
1	E	2	ALA	4.2
1	A	386	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	219	VAL	4.1
1	F	393	ILE	4.0
1	H	224	ALA	3.9
1	E	76	PHE	3.8
1	E	223	VAL	3.8
1	F	347	GLY	3.7
1	H	394	LEU	3.6
1	E	73	TYR	3.6
1	F	375	ALA	3.6
1	H	194	ALA	3.6
1	B	140	VAL	3.6
1	B	158	ASN	3.5
1	G	154	ILE	3.4
1	H	335	VAL	3.4
1	H	243	LEU	3.3
1	H	267	TYR	3.3
1	H	212	LEU	3.3
1	G	153	PRO	3.3
1	H	247	ILE	3.3
1	B	394	LEU	3.2
1	H	73	TYR	3.2
1	H	22	LEU	3.2
1	B	153	PRO	3.2
1	G	7	VAL	3.2
1	B	96	LEU	3.1
1	E	194	ALA	3.1
1	F	240	VAL	3.1
1	B	2	ALA	3.0
1	G	224	ALA	3.0
1	D	398	ILE	3.0
1	H	121	ARG	3.0
1	A	279	GLY	3.0
1	H	244	ALA	3.0
1	F	389	VAL	3.0
1	C	224	ALA	3.0
1	G	355	VAL	3.0
1	H	232	VAL	3.0
1	H	199	ILE	3.0
1	E	192	TYR	2.9
1	E	259	ALA	2.9
1	H	239	ALA	2.9
1	E	255	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	82	VAL	2.9
1	H	254	ILE	2.9
1	H	346	ILE	2.9
1	G	265	GLY	2.9
1	G	389	VAL	2.9
1	H	140	VAL	2.9
1	E	269	ILE	2.9
1	H	265	GLY	2.8
1	F	149	ALA	2.8
1	H	210	ILE	2.8
1	H	193	PRO	2.8
1	H	255	TYR	2.8
1	F	346	ILE	2.8
1	H	78	GLY	2.8
1	G	2	ALA	2.8
1	H	371	PHE	2.8
1	E	77	GLY	2.8
1	C	142	LEU	2.8
1	G	157	ALA	2.8
1	E	378	ILE	2.7
1	G	386	ILE	2.7
1	H	188	PHE	2.7
1	A	223	VAL	2.7
1	H	223	VAL	2.7
1	H	360	VAL	2.7
1	D	143	VAL	2.7
1	E	195	VAL	2.7
1	G	158	ASN	2.7
1	A	263	GLU	2.7
1	G	8[A]	GLU	2.7
1	H	398	ILE	2.7
1	F	2	ALA	2.6
1	H	326	ALA	2.6
1	B	150	ARG	2.6
1	C	149	ALA	2.6
1	E	371	PHE	2.6
1	H	225	THR	2.6
1	H	273	GLY	2.6
1	F	247	ILE	2.6
1	H	393	ILE	2.6
1	E	375	ALA	2.6
1	H	356	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	350	ILE	2.6
1	E	230	LEU	2.6
1	G	333	LEU	2.6
1	H	217	ALA	2.6
1	G	146	PHE	2.6
1	E	266	ILE	2.6
1	G	373	LYS	2.6
1	B	345	GLN	2.5
1	A	394	LEU	2.5
1	H	382	TRP	2.5
1	A	225	THR	2.5
1	C	153	PRO	2.5
1	E	74	PRO	2.5
1	E	279	GLY	2.5
1	D	145	VAL	2.5
1	H	266	ILE	2.5
1	A	73	TYR	2.5
1	H	196	GLY	2.5
1	G	382	TRP	2.5
1	C	278	ALA	2.5
1	E	226	PRO	2.5
1	F	126	GLU	2.5
1	H	102	PHE	2.5
1	H	358	ILE	2.5
1	A	343	LEU	2.5
1	E	224	ALA	2.5
1	G	379	ALA	2.5
1	C	266	ILE	2.4
1	G	6	VAL	2.4
1	F	354	LEU	2.4
1	H	58	LEU	2.4
1	H	182	LEU	2.4
1	A	149	ALA	2.4
1	G	155	PRO	2.4
1	H	259	ALA	2.4
1	D	101	LEU	2.4
1	G	354	LEU	2.4
1	H	175	LEU	2.4
1	H	12	ARG	2.4
1	D	389	VAL	2.4
1	F	140	VAL	2.4
1	H	6	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	143	VAL	2.4
1	H	252	VAL	2.4
1	A	190	LYS	2.4
1	E	225	THR	2.4
1	A	162	PHE	2.4
1	D	82	VAL	2.4
1	E	82	VAL	2.4
1	H	263	GLU	2.4
1	H	172	THR	2.3
1	G	358	ILE	2.3
1	A	59	HIS	2.3
1	B	53	ARG	2.3
1	H	375	ALA	2.3
1	A	145	VAL	2.3
1	D	99	GLN	2.3
1	E	232	VAL	2.3
1	H	146	PHE	2.3
1	E	141	ASP	2.3
1	H	220	ASP	2.3
1	C	279	GLY	2.3
1	H	17	MET	2.3
1	G	161	SER	2.3
1	C	263	GLU	2.3
1	C	398	ILE	2.3
1	H	5	ILE	2.3
1	C	223	VAL	2.3
1	G	82	VAL	2.3
1	H	219	VAL	2.3
1	H	245	LYS	2.3
1	F	236	ILE	2.3
1	H	214	ILE	2.3
1	C	82	VAL	2.3
1	C	145	VAL	2.3
1	G	371	PHE	2.2
1	H	183	LEU	2.2
1	F	158	ASN	2.2
1	B	267	TYR	2.2
1	E	267	TYR	2.2
1	E	278	ALA	2.2
1	B	373	LYS	2.2
1	D	148	LYS	2.2
1	D	373	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	369	LYS	2.2
1	E	394	LEU	2.2
1	H	15	VAL	2.2
1	H	20	VAL	2.2
1	H	101	LEU	2.2
1	D	114	ASN	2.2
1	F	206[A]	ARG	2.2
1	E	347	GLY	2.2
1	H	179	THR	2.2
1	F	101	LEU	2.2
1	F	55	GLY	2.2
1	F	117	LYS	2.2
1	G	160	THR	2.2
1	H	248	THR	2.2
1	A	266	ILE	2.2
1	H	329	ILE	2.2
1	D	56	VAL	2.2
1	E	280	ASP	2.2
1	H	392	MET	2.2
1	F	95	GLU	2.2
1	C	154	ILE	2.1
1	F	143	VAL	2.1
1	F	252	VAL	2.1
1	G	368	VAL	2.1
1	H	76	PHE	2.1
1	H	391	LYS	2.1
1	B	249	SER	2.1
1	F	224	ALA	2.1
1	G	149	ALA	2.1
1	H	149	ALA	2.1
1	H	150	ARG	2.1
1	B	393	ILE	2.1
1	F	391	LYS	2.1
1	H	251	LYS	2.1
1	H	294	ILE	2.1
1	H	253	ASN	2.1
1	H	372	GLU	2.1
1	C	97	VAL	2.1
1	G	223	VAL	2.1
1	H	176	VAL	2.1
1	H	99	GLN	2.1
1	B	75	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	149	ALA	2.1
1	H	187	LYS	2.1
1	D	142	LEU	2.1
1	E	101	LEU	2.1
1	B	141	ASP	2.1
1	G	347	GLY	2.1
1	H	71	ARG	2.1
1	G	278	ALA	2.1
1	H	330	ALA	2.1
1	E	231	GLU	2.1
1	F	231	GLU	2.1
1	A	99	GLN	2.1
1	G	142	LEU	2.1
1	H	28	ILE	2.1
1	G	376	TYR	2.1
1	H	153	PRO	2.1
1	C	56	VAL	2.1
1	C	28	ILE	2.0
1	G	51	ILE	2.0
1	H	7	VAL	2.0
1	H	290	VAL	2.0
1	D	137	GLN	2.0
1	F	137	GLN	2.0
1	H	123	LEU	2.0
1	H	230	LEU	2.0
1	A	342	ILE	2.0
1	H	250	ARG	2.0
1	A	373	LYS	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 oligosaccharides 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.

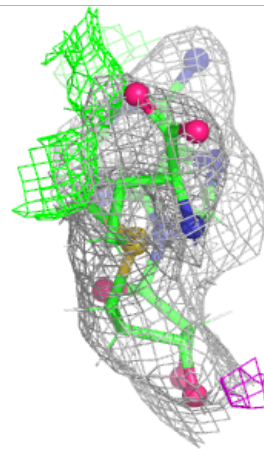
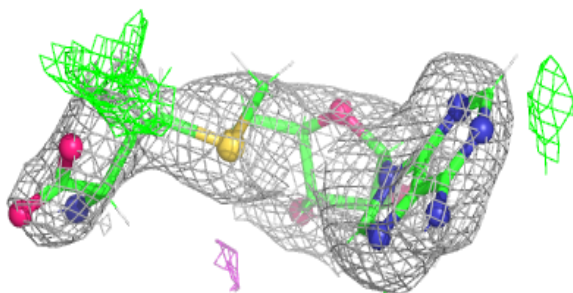
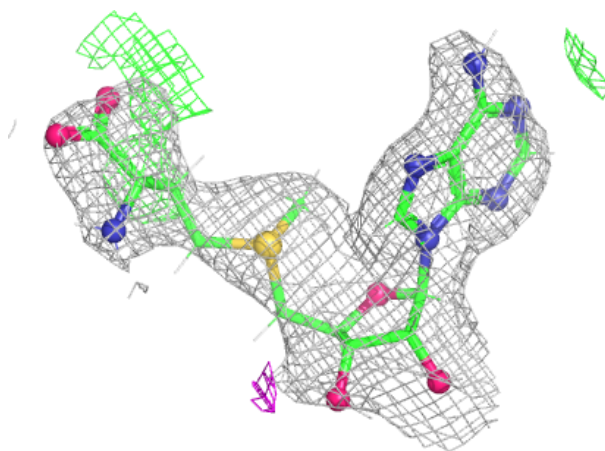
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SAM	A	503	27/27	0.83	0.15	79,90,106,108	0
4	SAM	E	503	27/27	0.83	0.15	82,96,114,117	0
6	ACP	H	504	31/31	0.86	0.12	61,102,124,124	0
6	ACP	B	504	31/31	0.89	0.09	50,75,91,91	0
5	PO4	F	501	5/5	0.90	0.13	52,55,62,64	0
3	MG	F	503	1/1	0.90	0.06	45,45,45,45	0
6	ACP	D	503	31/31	0.90	0.10	53,84,104,105	0
3	MG	H	503	1/1	0.90	0.12	44,44,44,44	0
3	MG	D	506	1/1	0.91	0.08	75,75,75,75	0
5	PO4	D	504	5/5	0.91	0.11	57,63,65,65	0
6	ACP	F	504	31/31	0.92	0.09	49,67,80,81	0
3	MG	B	503	1/1	0.92	0.20	49,49,49,49	0
3	MG	D	502	1/1	0.93	0.10	39,39,39,39	0
5	PO4	C	502	5/5	0.94	0.14	57,65,66,67	0
2	MDN	H	501	9/9	0.94	0.08	59,63,75,75	0
5	PO4	B	501	5/5	0.94	0.13	52,66,67,67	0
5	PO4	H	505	5/5	0.94	0.09	59,60,65,66	0
5	PO4	G	501	5/5	0.95	0.10	62,63,72,73	0
2	MDN	C	501	9/9	0.95	0.07	47,53,64,64	0
3	MG	H	507	1/1	0.95	0.09	71,71,71,71	0
5	PO4	B	505	5/5	0.96	0.07	47,47,50,51	0
3	MG	F	507	1/1	0.97	0.04	66,66,66,66	0
5	PO4	F	505	5/5	0.97	0.06	43,50,52,52	0
2	MDN	E	501	9/9	0.97	0.06	49,52,63,63	0
2	MDN	A	501	9/9	0.97	0.06	42,49,60,60	0
3	MG	G	502	1/1	0.98	0.04	54,54,54,54	0
3	MG	H	502	1/1	0.98	0.06	56,56,56,56	0
3	MG	A	504	1/1	0.98	0.10	58,58,58,58	0
3	MG	F	502	1/1	0.98	0.03	43,43,43,43	0
3	MG	D	501	1/1	0.98	0.05	46,46,46,46	0
3	MG	B	502	1/1	0.98	0.04	42,42,42,42	0
3	MG	F	506	1/1	0.99	0.03	43,43,43,43	0
3	MG	B	506	1/1	0.99	0.03	41,41,41,41	0
3	MG	D	505	1/1	0.99	0.03	49,49,49,49	0
3	MG	B	507	1/1	0.99	0.02	75,75,75,75	0
3	MG	C	503	1/1	0.99	0.07	50,50,50,50	0
3	MG	H	506	1/1	0.99	0.04	52,52,52,52	0
3	MG	A	502	1/1	0.99	0.03	40,40,40,40	0
3	MG	E	502	1/1	1.00	0.07	44,44,44,44	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.

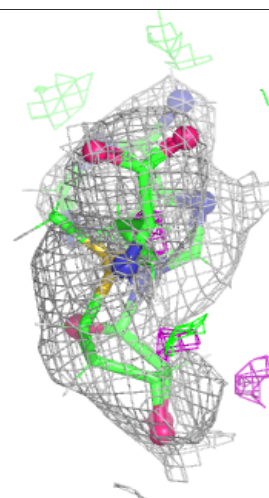
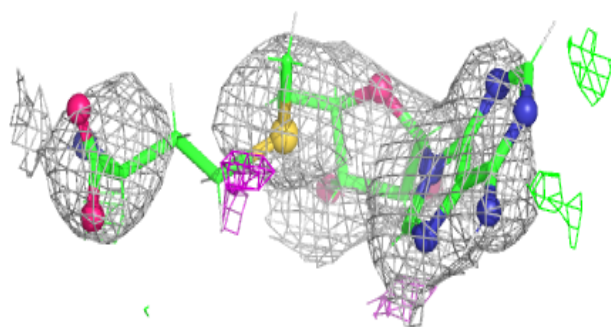
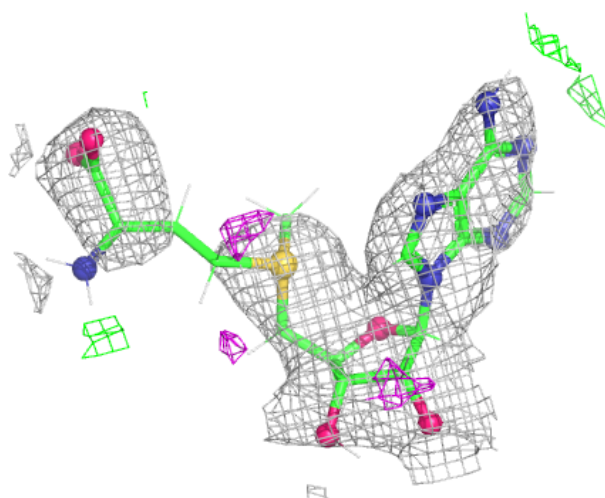
Electron density around SAM A 503:

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



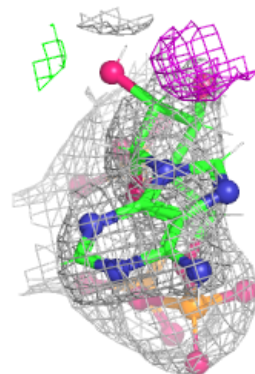
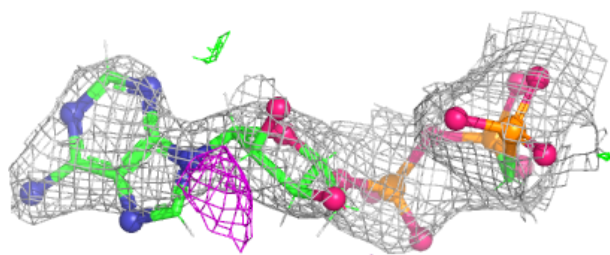
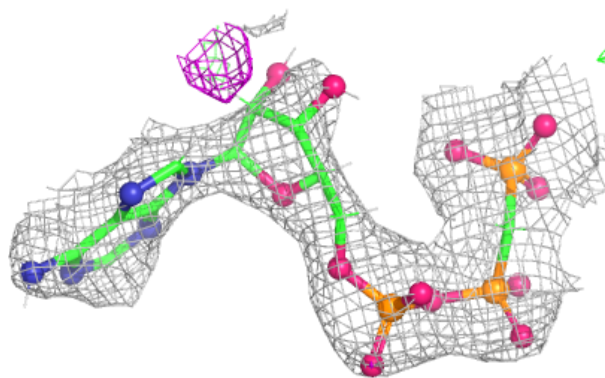
Electron density around SAM E 503:

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

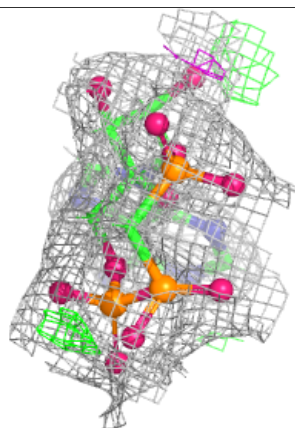
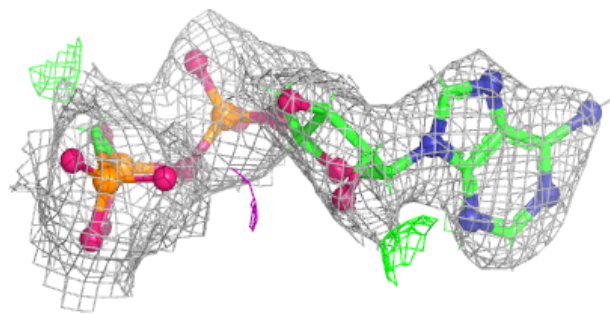
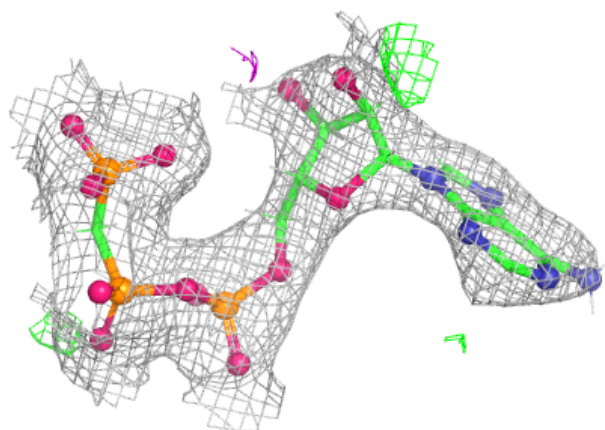


Electron density around ACP H 504:

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

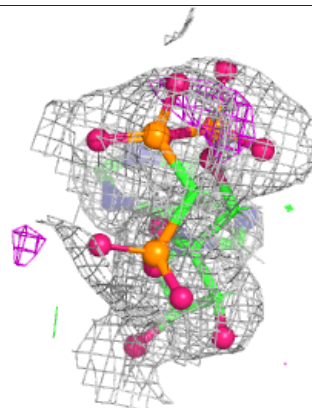
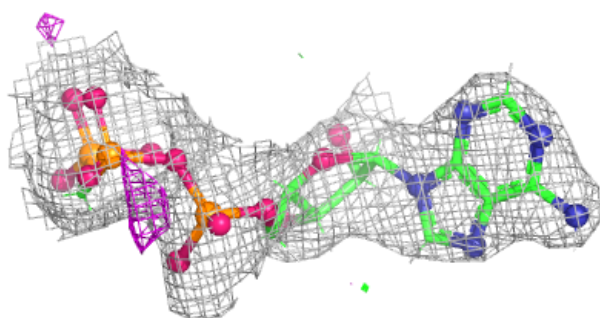
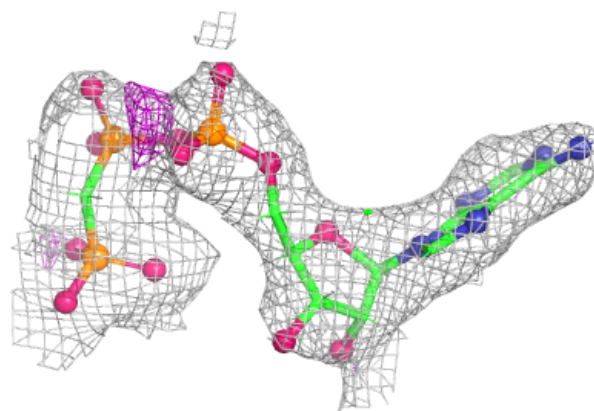
**Electron density around ACP B 504:**

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

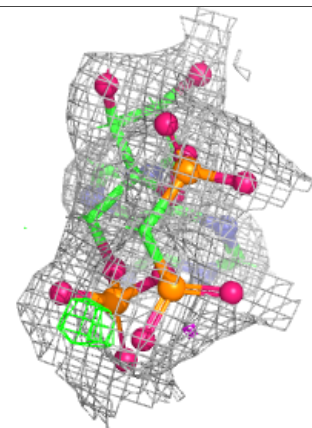
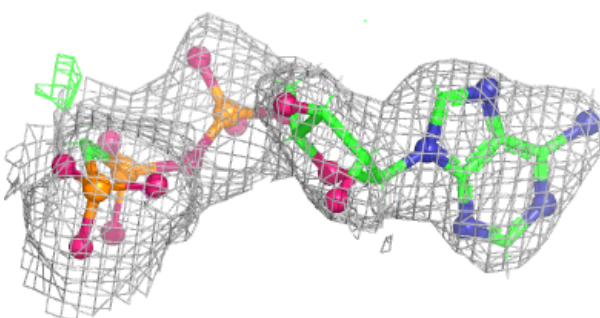
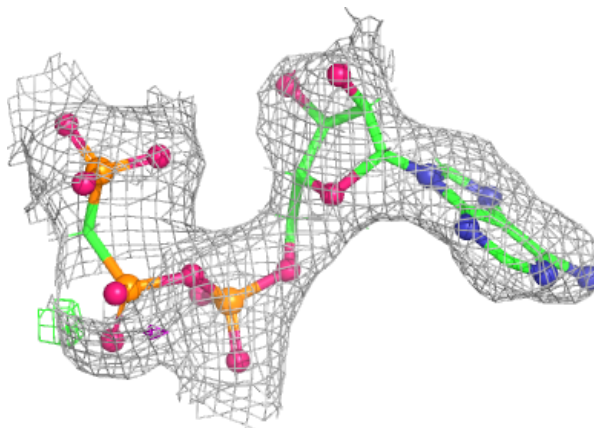


Electron density around ACP D 503:

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

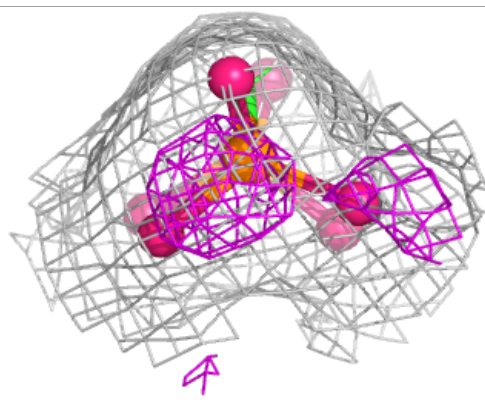
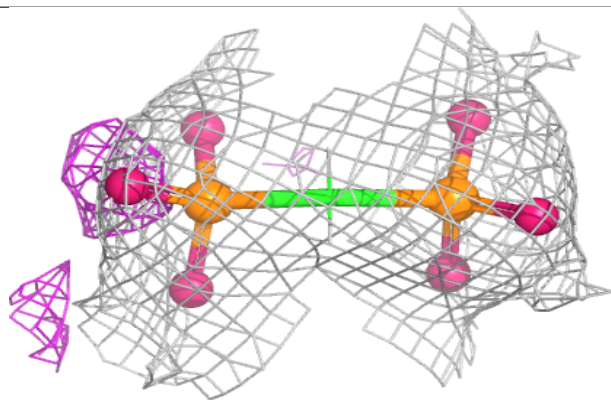
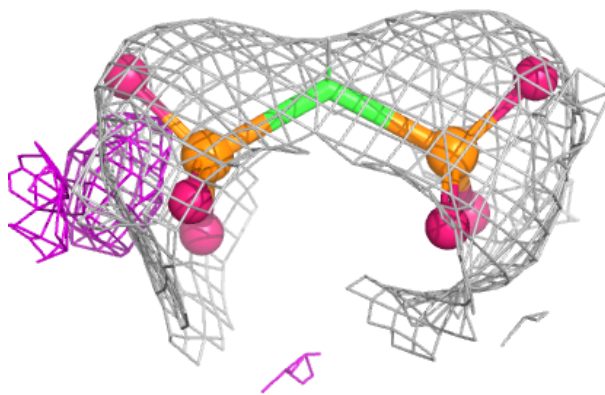
**Electron density around ACP F 504:**

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



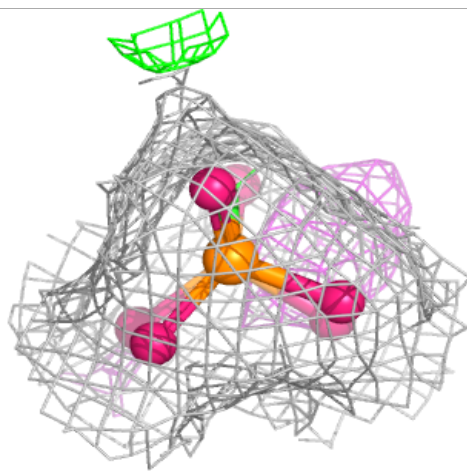
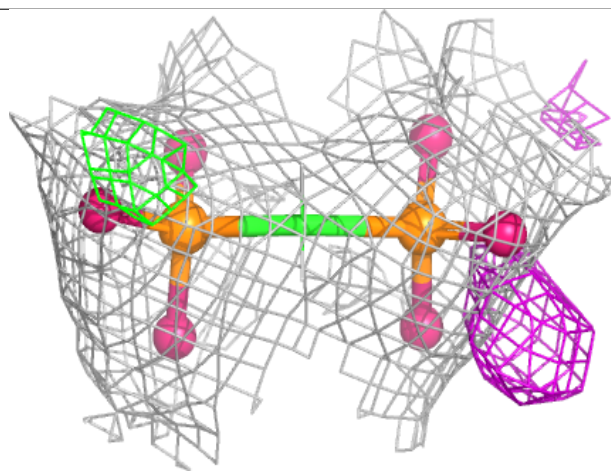
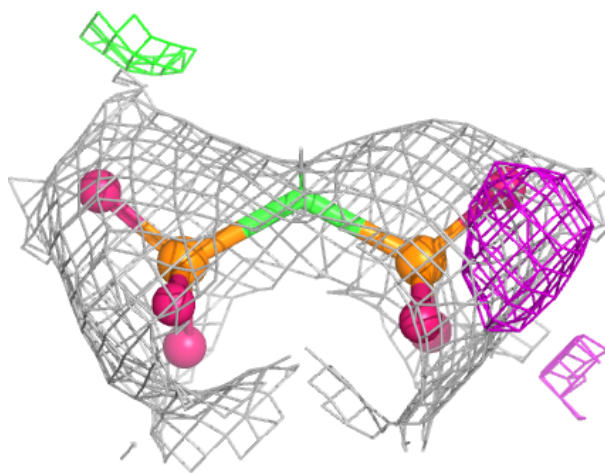
Electron density around MDN H 501:

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



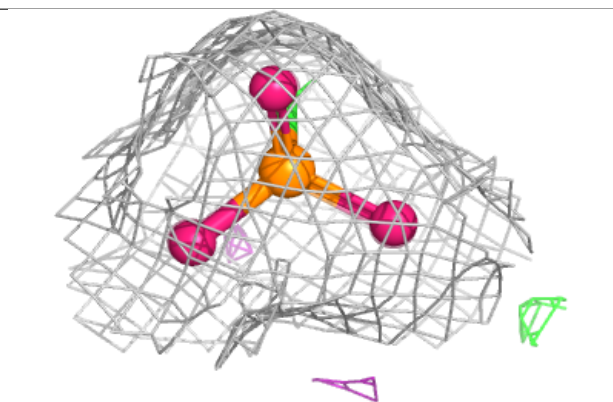
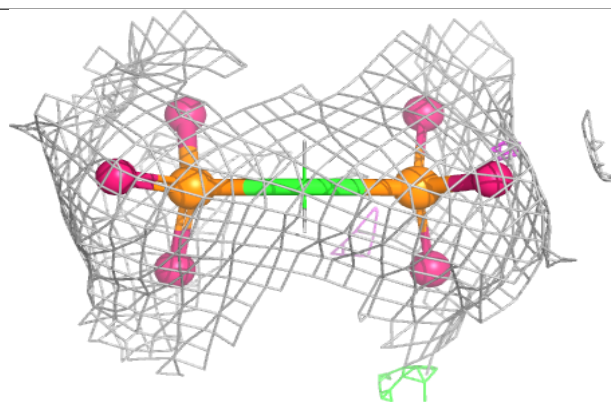
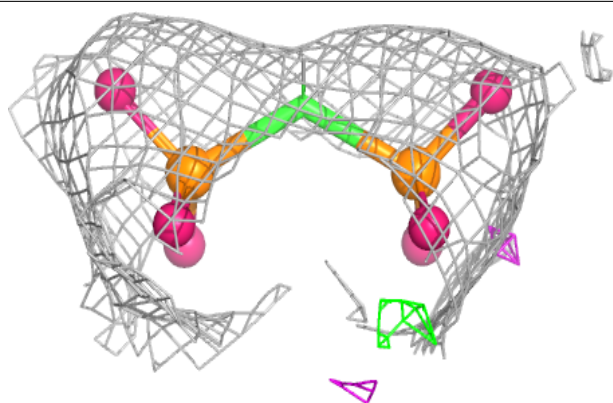
Electron density around MDN C 501:

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

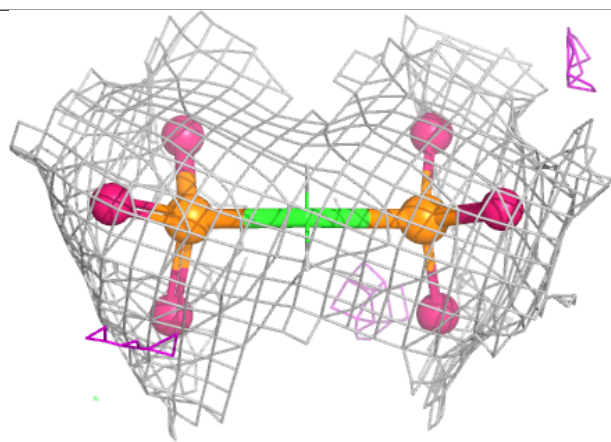
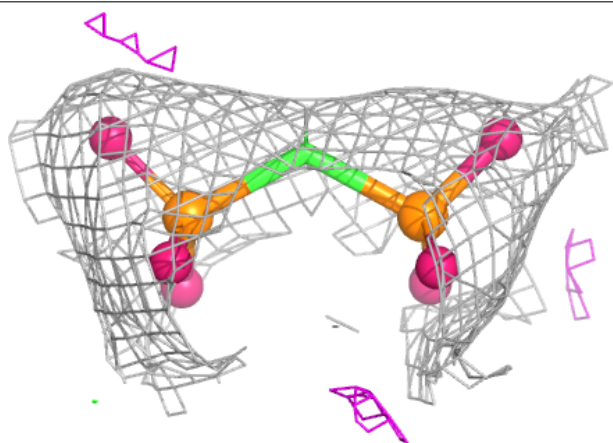


Electron density around MDN E 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.