Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:00 PM EDT

PDB ID	:	6CI7
Title	:	The structure of YcaO from Methanopyrus kandleri bound with AMPPCP and Mg2+
Authors	:	Dong, S.-H.; Nair, S.K.
Deposited on	:	2018-02-23
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

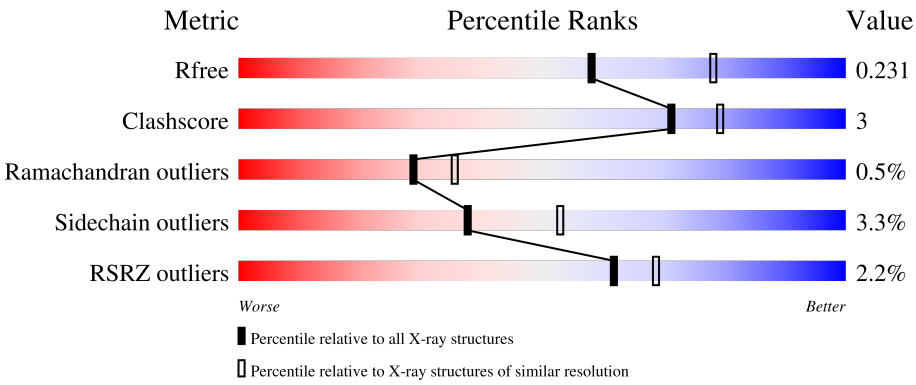
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	4%, 86%, 10%
1	B	377	2%, 86%, 9%
1	C	377	%, 86%, 9%
1	D	377	2%, 84%, 11%
1	E	377	2%, 86%, 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	377	2% 86% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19084 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

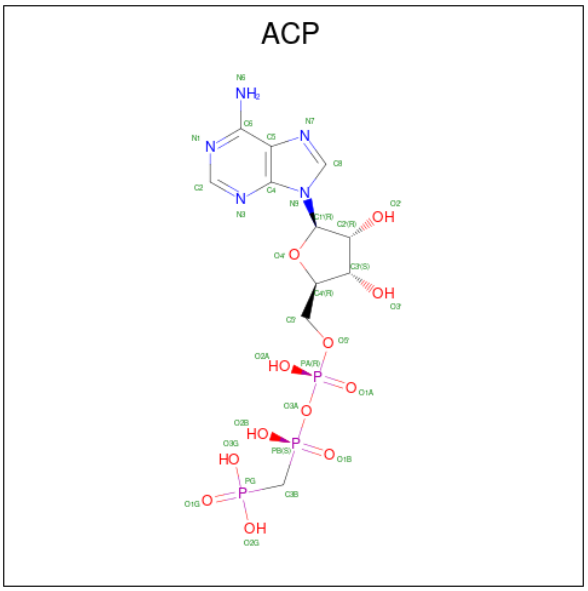
- Molecule 1 is a protein called YcaO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	365	2914	1832	525	549	1	7	0	0	0
1	B	364	2908	1828	524	548	1	7	0	0	0
1	C	361	2884	1811	520	545	1	7	0	0	0
1	D	362	2890	1817	521	544	1	7	0	0	0
1	E	364	2908	1828	524	548	1	7	0	0	0
1	F	362	2891	1816	521	546	1	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	-	initiating methionine	UNP Q8TZ25
B	2	MSE	-	initiating methionine	UNP Q8TZ25
C	2	MSE	-	initiating methionine	UNP Q8TZ25
D	2	MSE	-	initiating methionine	UNP Q8TZ25
E	2	MSE	-	initiating methionine	UNP Q8TZ25
F	2	MSE	-	initiating methionine	UNP Q8TZ25

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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

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

- Molecule 4 is water.

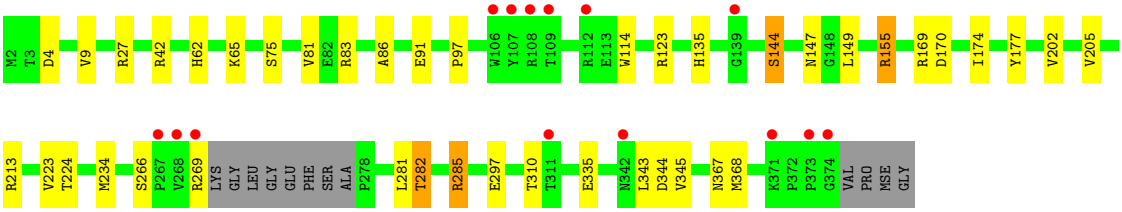
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	243	243	243	0	0
			Total	O		
4	B	286	286	286	0	0
			Total	O		
4	C	196	196	196	0	0
			Total	O		
4	D	198	198	198	0	0
			Total	O		
4	E	275	275	275	0	0
			Total	O		
4	F	299	299	299	0	0

3 Residue-property plots (i)

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

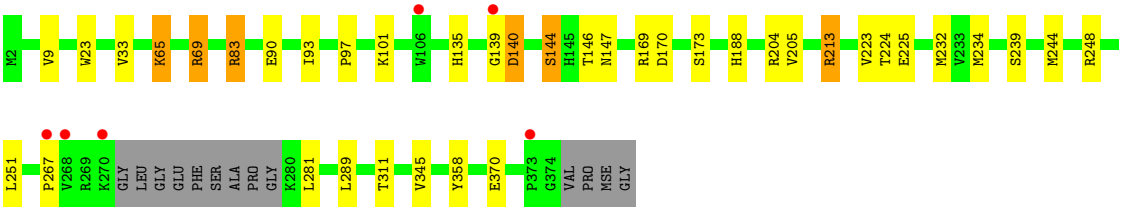
- Molecule 1: YcaO

Chain A:



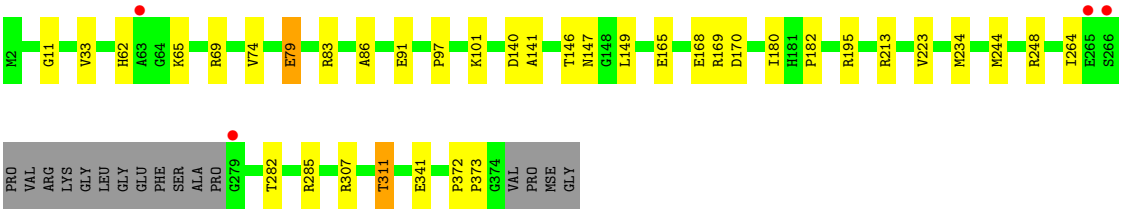
- Molecule 1: YcaO

Chain B:



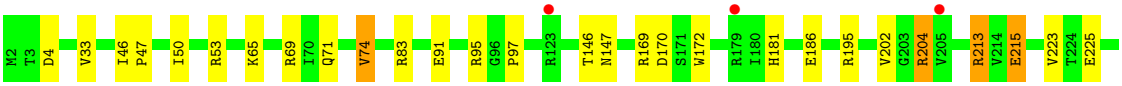
- Molecule 1: YcaO

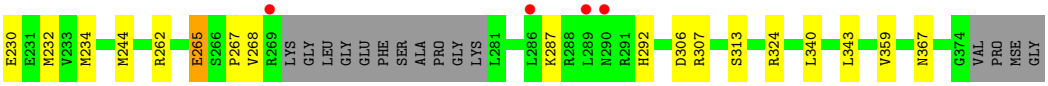
Chain C:



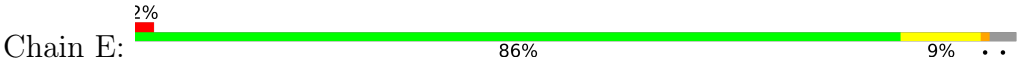
- Molecule 1: YcaO

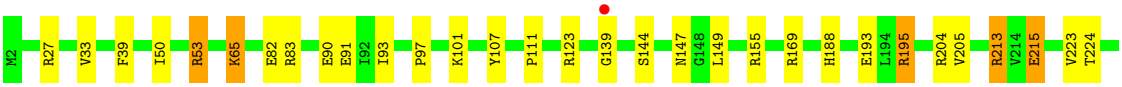
Chain D:

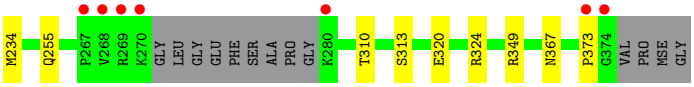




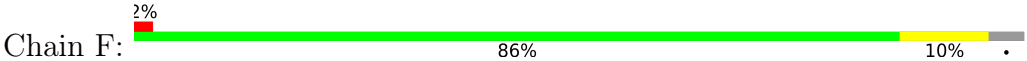
• Molecule 1: YcaO

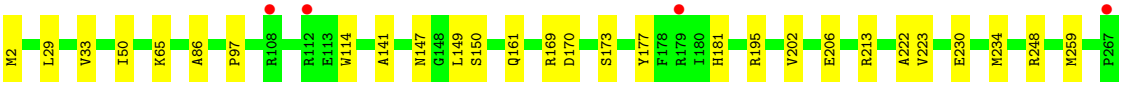


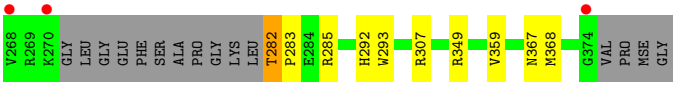




• Molecule 1: YcaO







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	123.19Å 106.75Å 141.45Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 137.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (25.00-2.30) 98.1 (137.45-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.185 , 0.226 0.193 , 0.231	Depositor DCC
R_{free} test set	7674 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19084	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7605e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/2967	0.72	1/4013 (0.0%)
1	B	0.50	0/2960	0.77	3/4004 (0.1%)
1	C	0.47	0/2935	0.69	0/3969
1	D	0.49	0/2942	0.72	2/3981 (0.1%)
1	E	0.51	0/2960	0.77	4/4004 (0.1%)
1	F	0.49	0/2943	0.73	0/3982
All	All	0.49	0/17707	0.73	10/23953 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	E	213	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	E	139	GLY	N-CA-C	6.20	128.59	113.10
1	B	213	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	42	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	E	53	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	D	69	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	83	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	213	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	E	53	ARG	NE-CZ-NH1	-5.17	117.71	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	310	THR	Peptide

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	2914	0	2901	21	0
1	B	2908	0	2892	21	0
1	C	2884	0	2864	18	0
1	D	2890	0	2873	20	0
1	E	2908	0	2892	21	0
1	F	2891	0	2868	23	0
2	A	31	0	14	1	0
2	B	31	0	14	1	0
2	C	31	0	14	0	0
2	D	31	0	14	0	0
2	E	31	0	14	0	0
2	F	31	0	14	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	243	0	0	1	0
4	B	286	0	0	2	0
4	C	196	0	0	4	0
4	D	198	0	0	3	0
4	E	275	0	0	5	0
4	F	299	0	0	4	0
All	All	19084	0	17374	122	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 3.

All (122) 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:B:244:MSE:SE	4:B:722:HOH:O	2.34	0.95
1:F:50:ILE:HG12	1:F:259:MSE:HE1	1.54	0.89
1:D:244:MSE:SE	4:D:717:HOH:O	2.45	0.85
1:E:82:GLU:OE2	1:E:83:ARG:NH1	2.20	0.73
1:D:204:ARG:HB2	1:D:225:GLU:HB2	1.71	0.72
1:B:83:ARG:CZ	1:B:146:THR:HG21	2.20	0.70
1:B:147:ASN:OD1	1:B:169:ARG:HG3	1.91	0.70
1:B:204:ARG:HB2	1:B:225:GLU:HB2	1.76	0.68
1:E:27:ARG:HD3	4:E:651:HOH:O	1.92	0.68
1:D:225:GLU:HA	1:D:232:MSE:HE3	1.78	0.66
1:D:213:ARG:NH2	1:D:367:ASN:O	2.22	0.65
1:F:223:VAL:HG12	1:F:234:MSE:HE3	1.78	0.64
1:D:223:VAL:HG12	1:D:234:MSE:HG2	1.79	0.63
1:A:223:VAL:HG12	1:A:234:MSE:HG2	1.80	0.62
1:D:215:GLU:HG2	1:D:324:ARG:NH1	2.15	0.62
1:E:213:ARG:NH2	1:E:367:ASN:O	2.22	0.61
1:B:170:ASP:OD2	1:B:213:ARG:HD3	2.02	0.60
1:F:50:ILE:CG1	1:F:259:MSE:HE1	2.30	0.60
1:D:147:ASN:OD1	1:D:169:ARG:HG3	2.02	0.59
1:F:234:MSE:HE1	1:F:293:TRP:CE2	2.37	0.59
1:E:223:VAL:HG12	1:E:234:MSE:HG2	1.88	0.56
1:F:223:VAL:CG1	1:F:234:MSE:HE3	2.36	0.55
1:F:282:THR:N	4:F:602:HOH:O	2.40	0.55
1:C:62:HIS:HB3	1:C:79:GLU:HG2	1.88	0.55
1:C:307:ARG:HH22	1:C:311:THR:HG22	1.72	0.54
1:A:285:ARG:HD2	1:E:195:ARG:NH2	2.23	0.53
1:E:205:VAL:HG22	1:E:224:THR:HG22	1.89	0.53
1:B:225:GLU:HA	1:B:232:MSE:HE2	1.90	0.53
1:F:170:ASP:OD2	1:F:213:ARG:HD3	2.08	0.53
1:B:135:HIS:ND1	1:B:144:SER:HB3	2.24	0.52
1:A:97:PRO:HG3	1:A:114:TRP:CD1	2.44	0.52
1:C:248:ARG:NH1	4:C:602:HOH:O	2.43	0.52
1:B:97:PRO:HG2	1:B:101:LYS:HE3	1.92	0.51
1:B:146:THR:O	1:B:146:THR:HG22	2.11	0.51
1:D:91:GLU:HB2	4:D:689:HOH:O	2.10	0.51
1:D:215:GLU:HG2	1:D:324:ARG:HH11	1.76	0.51
1:A:86:ALA:HB2	1:A:149:LEU:HD11	1.93	0.50
1:E:188:HIS:HE1	4:E:606:HOH:O	1.94	0.50
1:F:2:MSE:N	4:F:603:HOH:O	2.45	0.50
1:E:215:GLU:HG2	1:E:324:ARG:HH11	1.78	0.49
1:C:180:ILE:O	1:C:182:PRO:HD3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:MSE:O	1:B:248:ARG:HG3	2.14	0.48
1:E:91:GLU:HB2	4:E:822:HOH:O	2.12	0.48
1:A:170:ASP:OD2	1:A:213:ARG:HD3	2.13	0.48
1:D:265:GLU:HB2	1:D:267:PRO:HD3	1.96	0.48
1:A:62:HIS:CE1	1:A:83:ARG:HG3	2.49	0.47
1:E:147:ASN:OD1	1:E:169:ARG:HG3	2.14	0.47
1:A:155:ARG:NH1	1:A:335:GLU:OE1	2.47	0.47
1:A:27:ARG:HH22	1:A:344:ASP:HB3	1.80	0.47
1:C:91:GLU:HB2	4:C:749:HOH:O	2.15	0.47
1:B:244:MSE:HE3	1:B:248:ARG:HD2	1.97	0.47
1:E:97:PRO:HG2	1:E:101:LYS:HE3	1.96	0.47
1:E:215:GLU:HG2	1:E:324:ARG:NH1	2.29	0.46
1:F:349:ARG:NH1	4:F:604:HOH:O	2.47	0.46
1:B:223:VAL:HG12	1:B:234:MSE:HG2	1.98	0.46
1:A:205:VAL:HG22	1:A:224:THR:HG22	1.97	0.46
1:B:248:ARG:NH2	2:B:500:ACP:O1A	2.49	0.46
1:D:170:ASP:OD2	1:D:213:ARG:HD3	2.16	0.46
1:F:282:THR:HA	1:F:283:PRO:HD3	1.82	0.46
1:E:65:LYS:HD2	1:E:255:GLN:OE1	2.15	0.45
1:D:181:HIS:CE1	1:D:292:HIS:HA	2.51	0.45
1:E:107:TYR:CE2	1:E:111:PRO:HG3	2.51	0.45
1:B:239:SER:HB2	1:B:244:MSE:HE2	1.98	0.45
1:A:147:ASN:OD1	1:A:169:ARG:HG3	2.16	0.45
1:A:281:LEU:HD11	1:A:285:ARG:HG2	1.98	0.45
1:C:223:VAL:HG12	1:C:234:MSE:HG2	1.98	0.45
1:C:282:THR:HG23	1:C:285:ARG:H	1.82	0.45
1:A:135:HIS:ND1	1:A:144:SER:HB3	2.32	0.45
1:B:205:VAL:HG22	1:B:224:THR:HG22	1.98	0.44
1:E:39:PHE:HB2	1:E:50:ILE:HB	1.99	0.44
1:D:83:ARG:HD3	4:D:649:HOH:O	2.17	0.44
1:C:86:ALA:HB2	1:C:149:LEU:HD11	1.99	0.44
1:E:149:LEU:HD22	4:E:611:HOH:O	2.17	0.44
1:F:206:GLU:O	1:F:222:ALA:HA	2.18	0.44
1:B:83:ARG:NH1	1:B:146:THR:HG21	2.31	0.44
1:F:150:SER:OG	1:F:161:GLN:HG2	2.17	0.44
1:D:340:LEU:O	1:D:343:LEU:O	2.36	0.43
1:A:213:ARG:NH2	1:A:367:ASN:O	2.40	0.43
1:F:282:THR:HG23	1:F:285:ARG:HB3	2.00	0.43
1:F:248:ARG:NH2	2:F:500:ACP:O1A	2.51	0.43
1:A:81:VAL:HG11	1:A:345:VAL:HG11	1.99	0.43
1:A:266:SER:HB2	1:A:269:ARG:H	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:ARG:NH1	4:E:611:HOH:O	2.50	0.43
1:E:320:GLU:O	1:E:324:ARG:HG2	2.18	0.42
1:A:27:ARG:HH12	1:A:344:ASP:H	1.68	0.42
1:D:46:ILE:HA	1:D:47:PRO:HD2	1.94	0.42
1:D:95:ARG:O	1:D:97:PRO:HD3	2.19	0.42
1:B:140:ASP:N	4:B:612:HOH:O	2.52	0.42
1:C:140:ASP:HB3	1:C:141:ALA:H	1.69	0.42
1:C:170:ASP:OD2	1:C:213:ARG:HD3	2.19	0.42
1:F:213:ARG:NH2	1:F:367:ASN:O	2.51	0.42
1:C:165:GLU:O	1:C:168:GLU:HB3	2.20	0.42
1:C:372:PRO:HA	1:C:373:PRO:HD2	1.89	0.42
1:D:71:GLN:HA	1:D:74:VAL:HG13	2.01	0.42
1:F:147:ASN:OD1	1:F:169:ARG:HG3	2.20	0.42
1:A:282:THR:HG22	1:A:285:ARG:H	1.85	0.42
1:A:174:ILE:HG12	1:A:213:ARG:HD2	2.02	0.41
1:B:173:SER:HB3	1:B:358:TYR:HB3	2.02	0.41
1:C:97:PRO:HG2	1:C:101:LYS:HE3	2.02	0.41
1:F:173:SER:HA	1:F:359:VAL:HG13	2.02	0.41
2:A:500:ACP:H3B1	4:A:678:HOH:O	2.20	0.41
1:B:65:LYS:HG3	1:B:251:LEU:HB3	2.03	0.41
1:D:230:GLU:CD	1:D:230:GLU:H	2.24	0.41
1:C:146:THR:HA	4:C:610:HOH:O	2.20	0.41
1:C:147:ASN:OD1	1:C:169:ARG:HG3	2.21	0.41
1:B:90:GLU:HA	1:B:93:ILE:HD12	2.03	0.41
1:B:23:TRP:CH2	1:B:345:VAL:HG22	2.56	0.41
1:D:172:TRP:CG	1:D:359:VAL:HG11	2.56	0.41
1:F:2:MSE:N	4:F:609:HOH:O	2.54	0.41
1:F:97:PRO:HG3	1:F:114:TRP:CD1	2.56	0.41
1:A:285:ARG:CD	1:E:195:ARG:NH2	2.84	0.41
1:C:62:HIS:CE1	1:C:83:ARG:HG3	2.56	0.41
1:C:149:LEU:HD22	4:C:610:HOH:O	2.20	0.41
1:D:50:ILE:HD13	1:D:262:ARG:HD2	2.03	0.41
1:F:86:ALA:HB2	1:F:149:LEU:HD21	2.03	0.40
1:A:177:TYR:CG	1:A:368:MSE:HE3	2.57	0.40
1:F:177:TYR:CG	1:F:368:MSE:HE3	2.56	0.40
1:F:181:HIS:CE1	1:F:292:HIS:HA	2.57	0.40
1:C:11:GLY:HA2	1:C:244:MSE:CE	2.51	0.40
1:E:90:GLU:HA	1:E:93:ILE:HD12	2.02	0.40
1:A:285:ARG:HD2	1:E:195:ARG:HH22	1.86	0.40
1:F:29:LEU:O	1:F:33:VAL:HB	2.20	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	361/377 (96%)	350 (97%)	9 (2%)	2 (1%)	25	31
1	B	360/377 (96%)	346 (96%)	10 (3%)	4 (1%)	14	15
1	C	357/377 (95%)	346 (97%)	11 (3%)	0	100	100
1	D	358/377 (95%)	342 (96%)	15 (4%)	1 (0%)	41	50
1	E	360/377 (96%)	348 (97%)	11 (3%)	1 (0%)	41	50
1	F	358/377 (95%)	346 (97%)	10 (3%)	2 (1%)	25	31
All	All	2154/2262 (95%)	2078 (96%)	66 (3%)	10 (0%)	29	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	139	GLY
1	B	140	ASP
1	E	373	PRO
1	F	141	ALA
1	F	202	VAL
1	B	9	VAL
1	D	202	VAL
1	A	9	VAL
1	A	202	VAL
1	B	267	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/312 (100%)	299 (96%)	12 (4%)	32	46
1	B	310/312 (99%)	301 (97%)	9 (3%)	42	58
1	C	307/312 (98%)	298 (97%)	9 (3%)	42	58
1	D	308/312 (99%)	292 (95%)	16 (5%)	23	32
1	E	310/312 (99%)	299 (96%)	11 (4%)	36	50
1	F	308/312 (99%)	303 (98%)	5 (2%)	62	78
All	All	1854/1872 (99%)	1792 (97%)	62 (3%)	38	53

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	65	LYS
1	A	75	SER
1	A	91	GLU
1	A	123	ARG
1	A	144	SER
1	A	155	ARG
1	A	282	THR
1	A	285	ARG
1	A	297	GLU
1	A	310	THR
1	A	343	LEU
1	B	33	VAL
1	B	65	LYS
1	B	69	ARG
1	B	144	SER
1	B	188	HIS
1	B	281	LEU
1	B	289	LEU
1	B	311	THR
1	B	370	GLU
1	C	33	VAL
1	C	65	LYS
1	C	69	ARG
1	C	74	VAL
1	C	79	GLU
1	C	195	ARG
1	C	264	ILE
1	C	311	THR
1	C	341	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4	ASP
1	D	33	VAL
1	D	53	ARG
1	D	65	LYS
1	D	74	VAL
1	D	146	THR
1	D	186	GLU
1	D	195	ARG
1	D	204	ARG
1	D	215	GLU
1	D	265	GLU
1	D	268	VAL
1	D	287	LYS
1	D	306	ASP
1	D	307	ARG
1	D	313	SER
1	E	33	VAL
1	E	53	ARG
1	E	65	LYS
1	E	123	ARG
1	E	144	SER
1	E	155	ARG
1	E	193	GLU
1	E	195	ARG
1	E	204	ARG
1	E	215	GLU
1	E	313	SER
1	F	65	LYS
1	F	195	ARG
1	F	230	GLU
1	F	282	THR
1	F	307	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	56	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACP	C	500	3	27,33,33	1.94	7 (25%)	32,52,52	1.24	4 (12%)
2	ACP	D	500	3	27,33,33	1.93	8 (29%)	32,52,52	1.08	2 (6%)
2	ACP	F	500	3	27,33,33	2.19	9 (33%)	32,52,52	1.32	4 (12%)
2	ACP	A	500	3	27,33,33	2.21	8 (29%)	32,52,52	1.20	3 (9%)
2	ACP	E	500	3	27,33,33	1.68	7 (25%)	32,52,52	1.21	2 (6%)
2	ACP	B	500	3	27,33,33	2.14	9 (33%)	32,52,52	1.22	2 (6%)

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	ACP	C	500	3	-	3/15/38/38	0/3/3/3
2	ACP	D	500	3	-	4/15/38/38	0/3/3/3
2	ACP	F	500	3	-	1/15/38/38	0/3/3/3
2	ACP	A	500	3	-	4/15/38/38	0/3/3/3
2	ACP	E	500	3	-	4/15/38/38	0/3/3/3
2	ACP	B	500	3	-	5/15/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	ACP	PG-O1G	5.64	1.62	1.50
2	A	500	ACP	PG-O1G	5.56	1.61	1.50
2	C	500	ACP	PG-O1G	5.52	1.61	1.50
2	F	500	ACP	PG-O1G	5.51	1.61	1.50
2	F	500	ACP	PB-O3A	5.32	1.64	1.58
2	B	500	ACP	PG-O1G	5.30	1.61	1.50
2	A	500	ACP	PB-O3A	4.99	1.63	1.58
2	C	500	ACP	PB-O3A	4.82	1.63	1.58
2	B	500	ACP	PB-O3A	4.76	1.63	1.58
2	D	500	ACP	PB-O3A	4.55	1.63	1.58
2	E	500	ACP	PB-O3A	4.55	1.63	1.58
2	B	500	ACP	PB-O1B	4.54	1.62	1.51
2	A	500	ACP	PB-O1B	4.41	1.62	1.51
2	F	500	ACP	PB-O1B	4.37	1.62	1.51
2	A	500	ACP	PB-O2B	-3.34	1.48	1.56
2	C	500	ACP	PG-O3G	3.26	1.62	1.54
2	B	500	ACP	PB-O2B	-3.25	1.48	1.56
2	F	500	ACP	PB-O2B	-3.15	1.49	1.56
2	E	500	ACP	PG-O3G	3.09	1.62	1.54
2	D	500	ACP	PG-O3G	3.06	1.61	1.54
2	A	500	ACP	PG-O3G	-3.05	1.47	1.54
2	E	500	ACP	PG-O2G	2.93	1.61	1.54
2	F	500	ACP	PG-O2G	2.83	1.61	1.54
2	A	500	ACP	PG-O2G	2.82	1.61	1.54
2	B	500	ACP	PG-O3G	-2.81	1.48	1.54
2	F	500	ACP	PG-O3G	-2.79	1.48	1.54
2	C	500	ACP	PG-O2G	-2.77	1.48	1.54
2	E	500	ACP	C5-C4	2.76	1.48	1.40
2	B	500	ACP	PG-O2G	2.71	1.61	1.54
2	F	500	ACP	C5-C4	2.68	1.48	1.40
2	D	500	ACP	PG-O2G	-2.67	1.48	1.54
2	C	500	ACP	C2-N3	2.60	1.36	1.32
2	A	500	ACP	C5-C4	2.54	1.47	1.40
2	B	500	ACP	C5-C4	2.46	1.47	1.40
2	E	500	ACP	PB-O2B	2.41	1.62	1.56
2	C	500	ACP	C5-C4	2.40	1.47	1.40
2	B	500	ACP	O4'-C1'	2.39	1.44	1.41
2	C	500	ACP	PB-O2B	2.38	1.62	1.56
2	A	500	ACP	C2-N3	2.37	1.35	1.32
2	E	500	ACP	O4'-C1'	2.36	1.44	1.41
2	D	500	ACP	C5-C4	2.34	1.47	1.40
2	D	500	ACP	O4'-C1'	2.33	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	ACP	C2-N3	2.31	1.35	1.32
2	D	500	ACP	PB-O2B	2.29	1.61	1.56
2	B	500	ACP	C2-N3	2.10	1.35	1.32
2	F	500	ACP	O4'-C1'	2.09	1.44	1.41
2	F	500	ACP	C2-N3	2.04	1.35	1.32
2	D	500	ACP	C2-N3	2.01	1.35	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	ACP	N3-C2-N1	-3.77	122.78	128.68
2	C	500	ACP	N3-C2-N1	-3.60	123.04	128.68
2	E	500	ACP	N3-C2-N1	-3.39	123.38	128.68
2	B	500	ACP	N3-C2-N1	-3.38	123.40	128.68
2	A	500	ACP	N3-C2-N1	-3.15	123.75	128.68
2	F	500	ACP	N3-C2-N1	-3.13	123.78	128.68
2	C	500	ACP	O3G-PG-C3B	3.02	113.72	106.40
2	E	500	ACP	O3G-PG-C3B	2.32	112.03	106.40
2	F	500	ACP	O2G-PG-C3B	2.31	112.00	106.40
2	C	500	ACP	C4-C5-N7	-2.23	107.07	109.40
2	F	500	ACP	O2G-PG-O1G	-2.22	106.52	112.39
2	B	500	ACP	C4-C5-N7	-2.19	107.12	109.40
2	A	500	ACP	C4-C5-N7	-2.14	107.17	109.40
2	F	500	ACP	C4-C5-N7	-2.12	107.19	109.40
2	A	500	ACP	PB-O3A-PA	-2.11	125.87	132.56
2	C	500	ACP	O4'-C1'-C2'	-2.03	103.96	106.93
2	D	500	ACP	C2-N1-C6	2.02	122.20	118.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ACP	PB-O3A-PA-O5'
2	A	500	ACP	C5'-O5'-PA-O2A
2	B	500	ACP	C5'-O5'-PA-O2A
2	C	500	ACP	PB-C3B-PG-O1G
2	C	500	ACP	PB-C3B-PG-O2G
2	C	500	ACP	PB-C3B-PG-O3G
2	B	500	ACP	PB-O3A-PA-O5'
2	D	500	ACP	PB-O3A-PA-O5'
2	E	500	ACP	PB-O3A-PA-O5'
2	F	500	ACP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	500	ACP	C5'-O5'-PA-O3A
2	B	500	ACP	C5'-O5'-PA-O3A
2	E	500	ACP	C5'-O5'-PA-O3A
2	A	500	ACP	C5'-O5'-PA-O1A
2	B	500	ACP	C5'-O5'-PA-O1A
2	E	500	ACP	C5'-O5'-PA-O2A
2	D	500	ACP	C3'-C4'-C5'-O5'
2	E	500	ACP	PB-C3B-PG-O1G
2	D	500	ACP	O4'-C4'-C5'-O5'
2	D	500	ACP	PB-O3A-PA-O2A
2	B	500	ACP	C3'-C4'-C5'-O5'

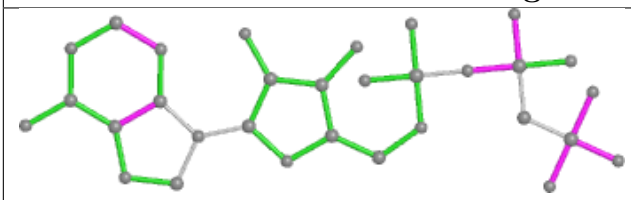
There are no ring outliers.

3 monomers are involved in 3 short contacts:

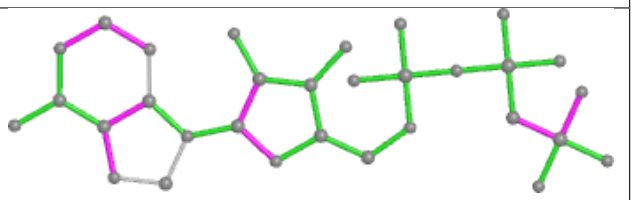
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	ACP	1	0
2	A	500	ACP	1	0
2	B	500	ACP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

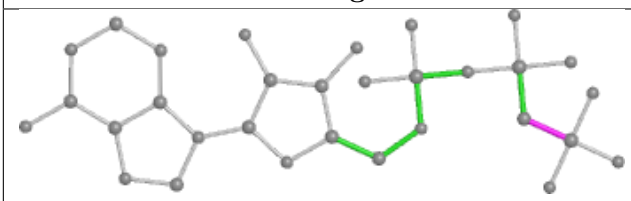
Ligand ACP C 500



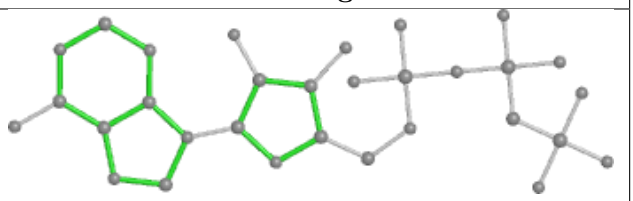
Bond lengths



Bond angles

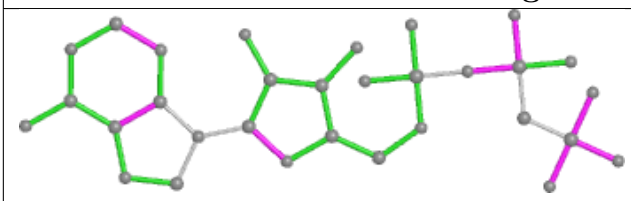


Torsions

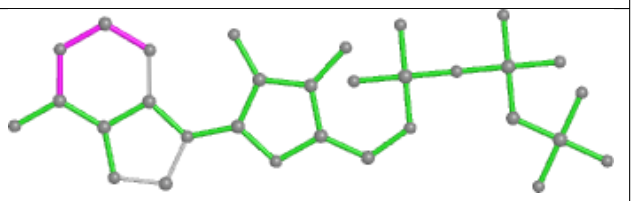


Rings

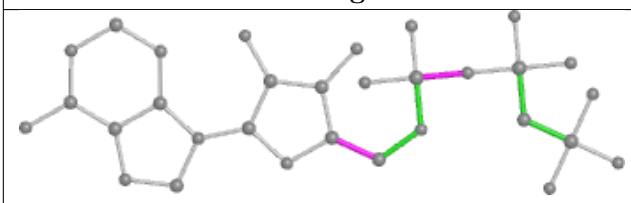
Ligand ACP D 500



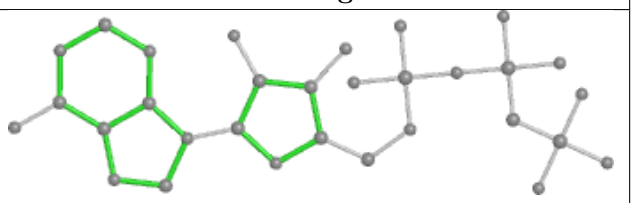
Bond lengths



Bond angles

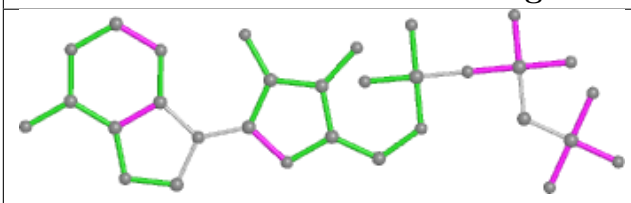


Torsions

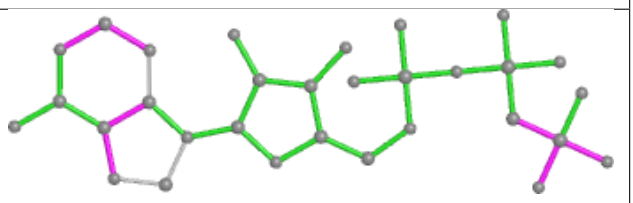


Rings

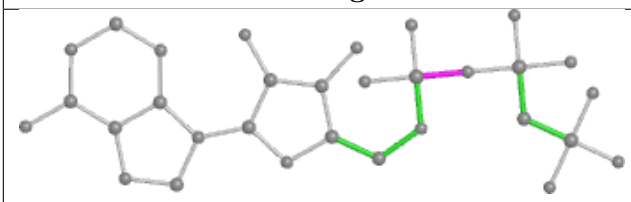
Ligand ACP F 500



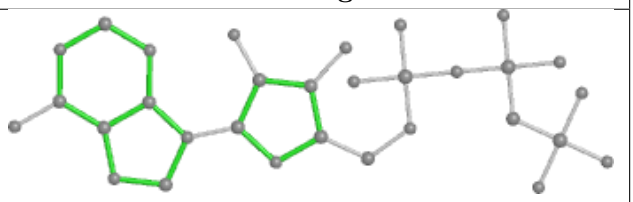
Bond lengths



Bond angles

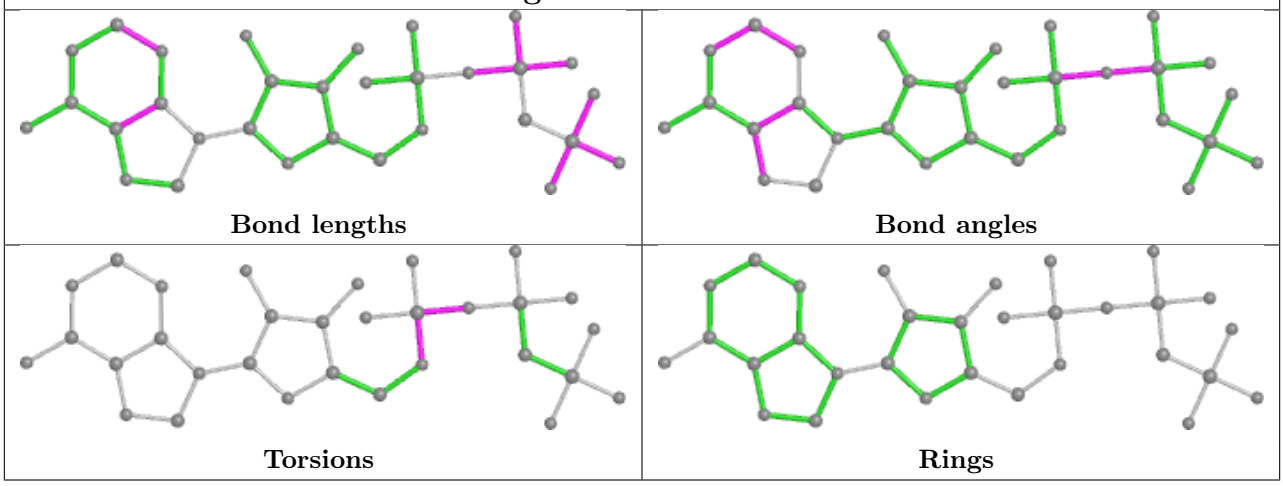


Torsions

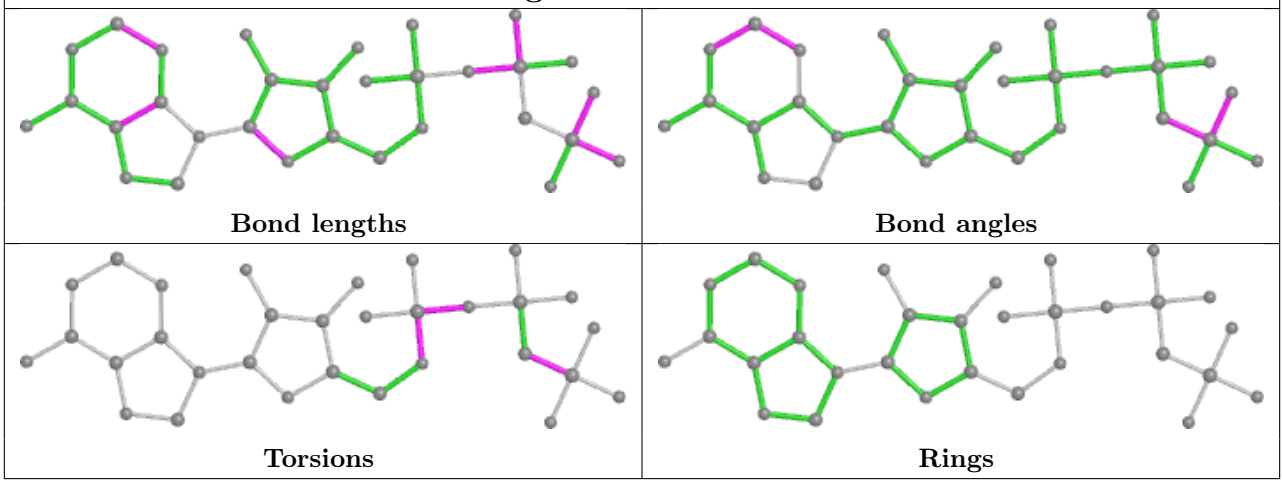


Rings

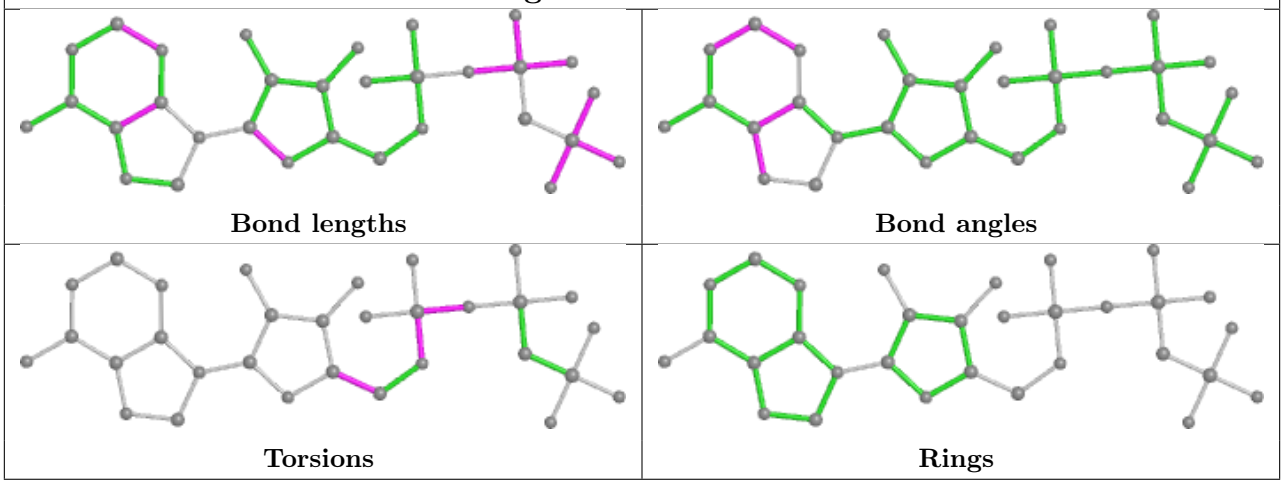
Ligand ACP A 500



Ligand ACP E 500



Ligand ACP B 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	358/377 (94%)	0.61	14 (3%)	39	46	39, 56, 99, 179	0
1	B	357/377 (94%)	0.44	6 (1%)	70	76	33, 48, 86, 144	0
1	C	354/377 (93%)	0.43	4 (1%)	80	85	44, 63, 100, 141	0
1	D	355/377 (94%)	0.43	7 (1%)	65	71	37, 57, 101, 126	0
1	E	357/377 (94%)	0.51	8 (2%)	62	69	33, 48, 83, 163	0
1	F	355/377 (94%)	0.47	7 (1%)	65	71	35, 51, 94, 138	0
All	All	2136/2262 (94%)	0.48	46 (2%)	62	69	33, 54, 98, 179	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	26.3
1	A	269	ARG	26.0
1	E	268	VAL	7.9
1	E	267	PRO	6.1
1	F	268	VAL	5.3
1	A	267	PRO	5.3
1	E	269	ARG	4.7
1	C	279	GLY	4.6
1	A	371	LYS	4.5
1	E	374	GLY	4.2
1	A	374	GLY	3.9
1	F	112	ARG	3.9
1	F	270	LYS	3.9
1	B	267	PRO	3.8
1	E	139	GLY	3.3
1	D	289	LEU	3.2
1	B	373	PRO	3.2
1	A	107	TYR	3.1
1	C	266	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	139	GLY	3.1
1	A	112	ARG	3.1
1	A	139	GLY	2.8
1	C	63	ALA	2.8
1	A	311	THR	2.8
1	D	179	ARG	2.7
1	A	106	TRP	2.7
1	A	373	PRO	2.6
1	A	108	ARG	2.6
1	F	108	ARG	2.6
1	F	267	PRO	2.6
1	E	280	LYS	2.6
1	C	265	GLU	2.5
1	D	286	LEU	2.5
1	F	179	ARG	2.4
1	A	109	THR	2.4
1	B	268	VAL	2.3
1	E	373	PRO	2.2
1	D	123	ARG	2.2
1	B	270	LYS	2.2
1	D	205	VAL	2.2
1	A	342	ASN	2.1
1	D	269	ARG	2.1
1	B	106	TRP	2.1
1	F	374	GLY	2.0
1	D	290	ASN	2.0
1	E	270	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 monosaccharides 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,

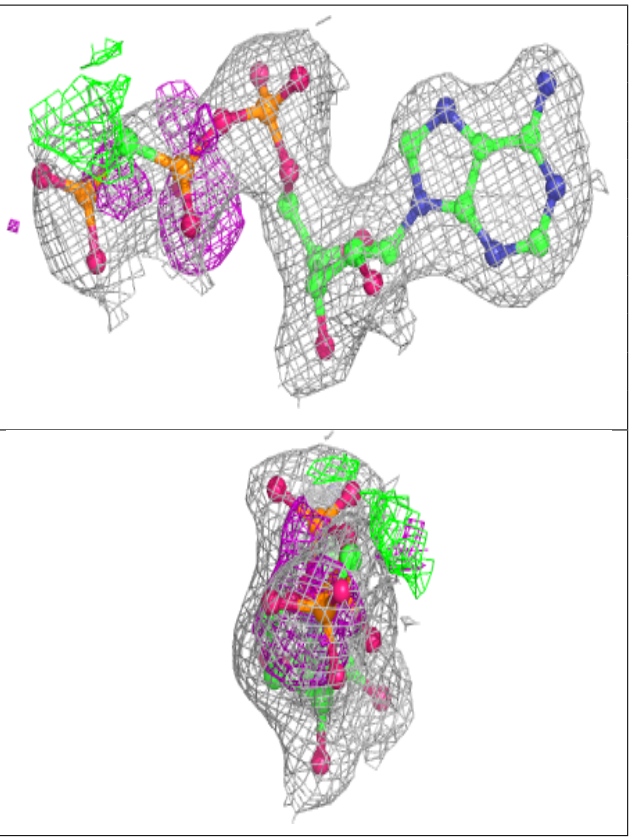
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	501	1/1	0.94	0.07	73,73,73,73	0
3	MG	D	501	1/1	0.94	0.04	74,74,74,74	0
3	MG	F	501	1/1	0.94	0.06	68,68,68,68	0
2	ACP	E	500	31/31	0.95	0.19	36,40,95,104	0
2	ACP	C	500	31/31	0.95	0.19	46,57,112,117	0
2	ACP	F	500	31/31	0.96	0.19	41,44,83,94	0
3	MG	A	501	1/1	0.96	0.08	53,53,53,53	0
3	MG	B	501	1/1	0.96	0.05	63,63,63,63	0
2	ACP	A	500	31/31	0.96	0.18	39,47,82,93	0
2	ACP	D	500	31/31	0.96	0.18	38,43,93,100	0
3	MG	E	501	1/1	0.96	0.05	59,59,59,59	0
2	ACP	B	500	31/31	0.96	0.18	36,40,78,84	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.

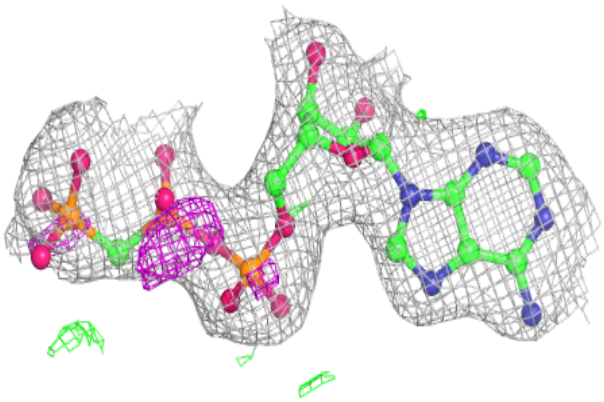
Electron density around ACP E 500:

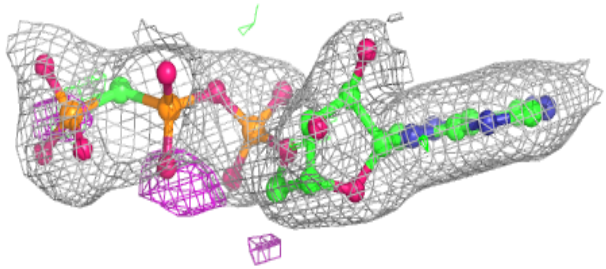
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

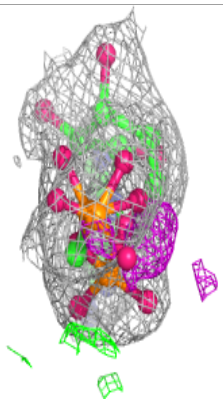


Electron density around ACP C 500:

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

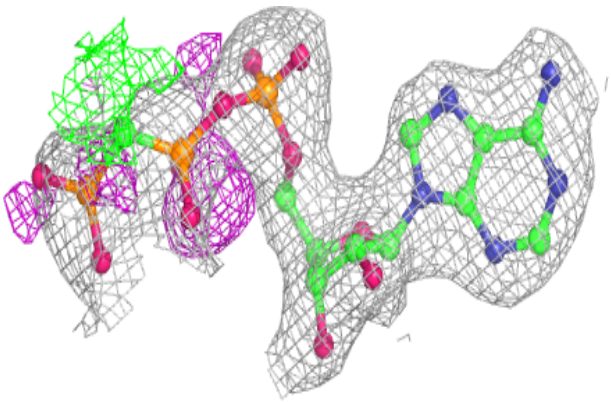


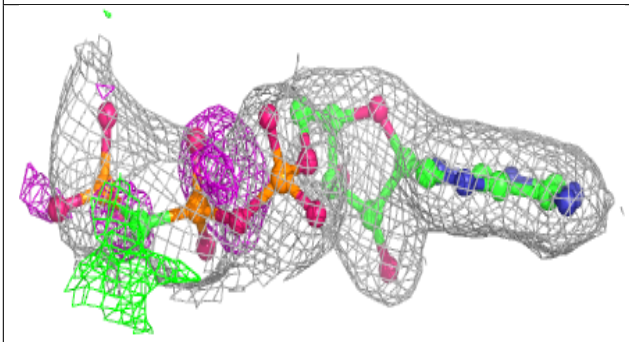


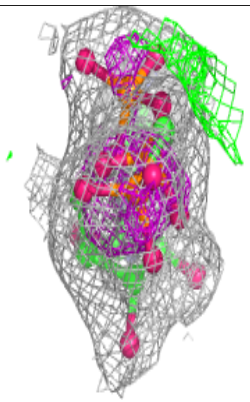


Electron density around ACP F 500:

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

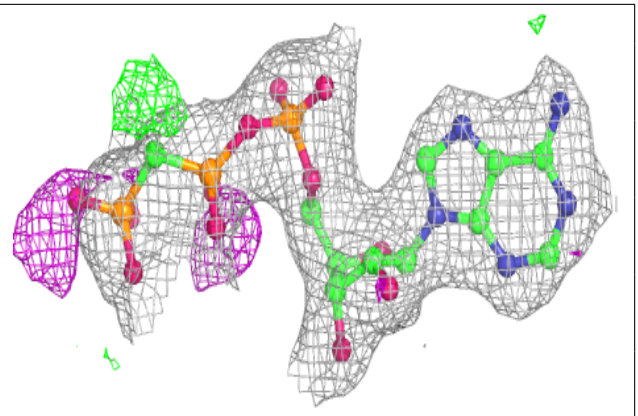


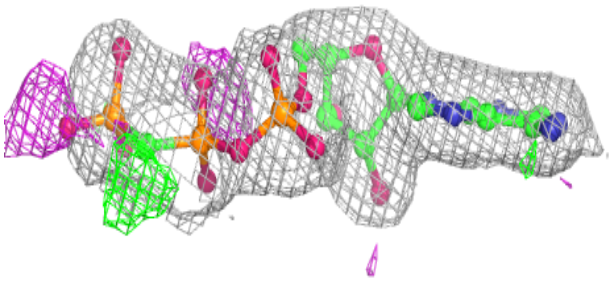


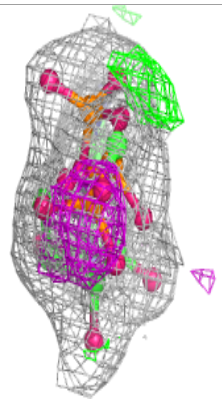


Electron density around ACP A 500:

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

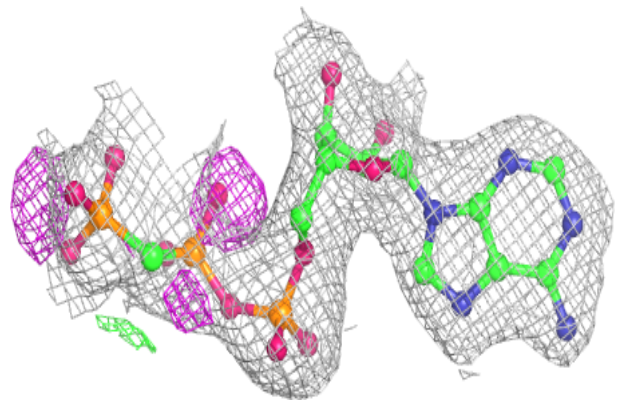


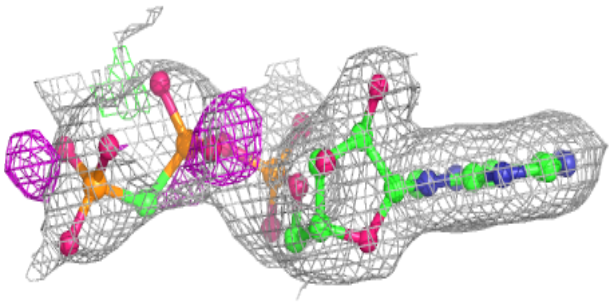


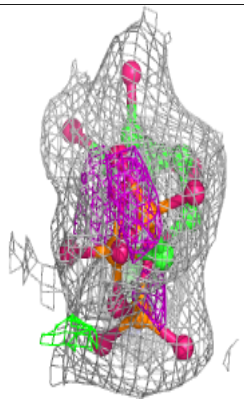


Electron density around ACP D 500:

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

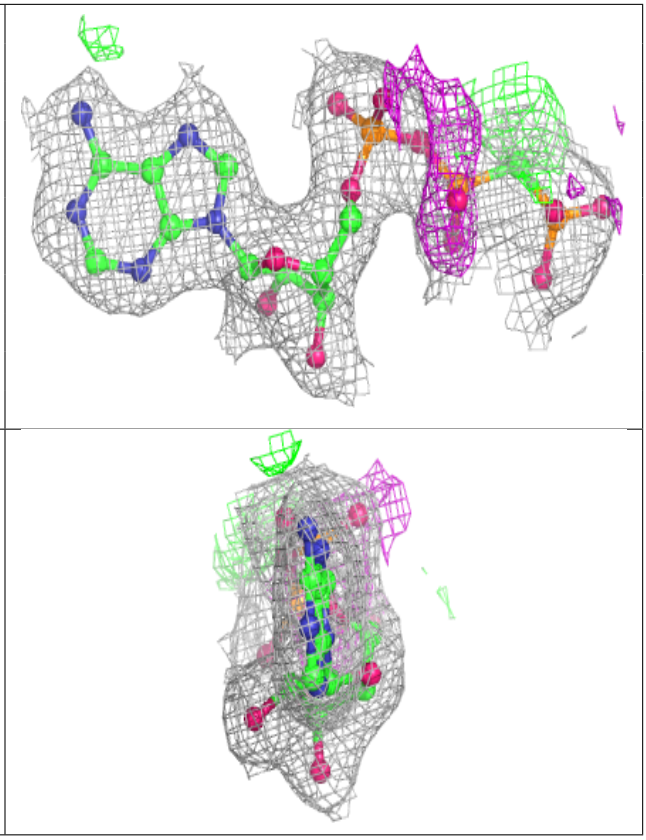






Electron density around ACP B 500:

$2mF_o$-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.