Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 06:16 PM EDT

PDB ID	:	7UUL
Title	:	Crystal structure of aminoglycoside resistance enzyme ApmA, complex with kanamycin B and coenzyme A
Authors	:	Stogios, P.J.; Evdokimova, E.; Di Leo, R.; Bordeleau, E.; Wright, G.D.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID); Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on	:	2022-04-28
Resolution	:	2.26 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:

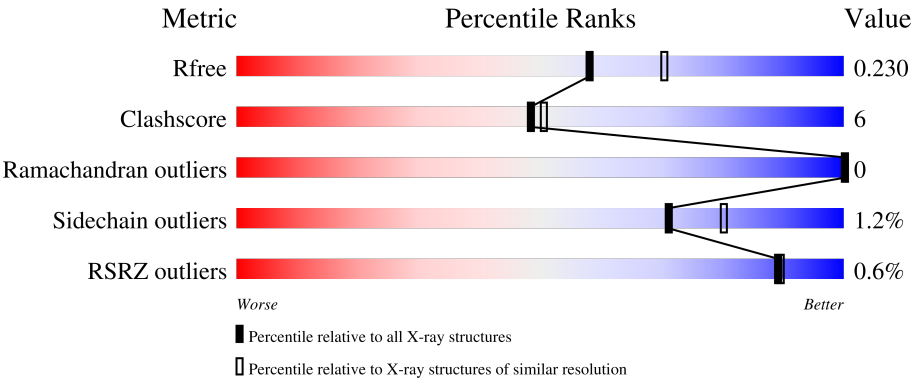
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	276	86% 13%
1	B	276	% 88% 11%
1	C	276	% 89% 9%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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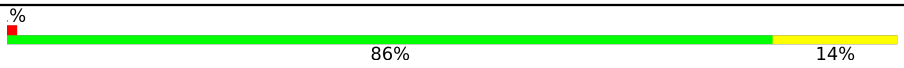
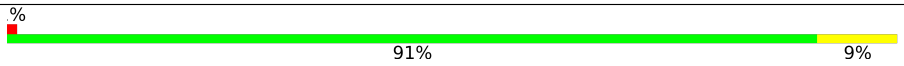
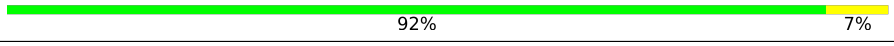
Mol	Chain	Length	Quality of chain
1	D	276	
1	E	276	
1	F	276	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COA	A	302	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15641 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.

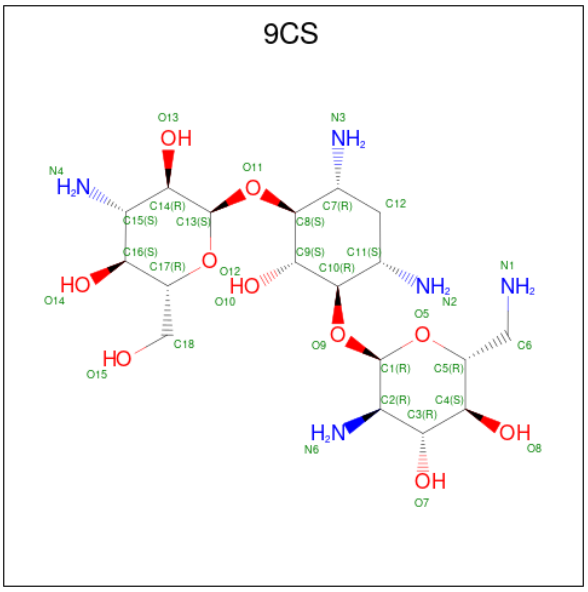
- Molecule 1 is a protein called Aminocyclitol acetyltransferase ApmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	2	0
			2201	1406	368	418	9			
1	B	275	Total	C	N	O	S	0	1	0
			2208	1410	373	416	9			
1	C	273	Total	C	N	O	S	0	1	0
			2194	1403	369	413	9			
1	D	275	Total	C	N	O	S	0	0	0
			2200	1406	369	416	9			
1	E	276	Total	C	N	O	S	0	1	0
			2214	1414	371	420	9			
1	F	275	Total	C	N	O	S	0	0	0
			2200	1405	370	416	9			

There are 12 discrepancies between the modelled and reference sequences:

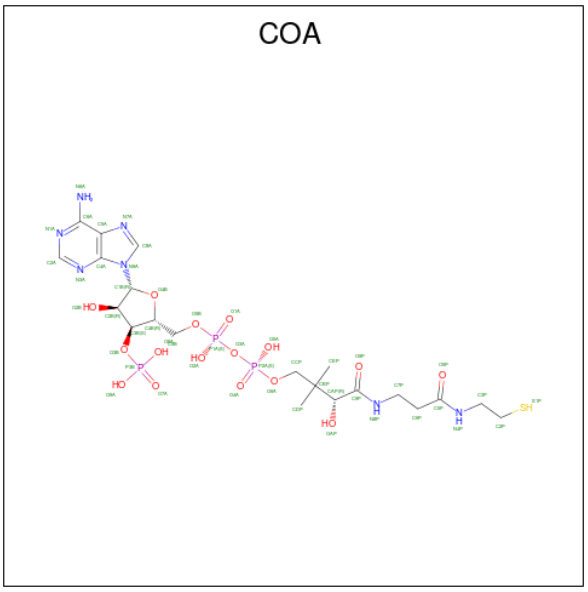
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP A0A1D0AST6
A	0	GLY	-	expression tag	UNP A0A1D0AST6
B	-1	GLN	-	expression tag	UNP A0A1D0AST6
B	0	GLY	-	expression tag	UNP A0A1D0AST6
C	-1	GLN	-	expression tag	UNP A0A1D0AST6
C	0	GLY	-	expression tag	UNP A0A1D0AST6
D	-1	GLN	-	expression tag	UNP A0A1D0AST6
D	0	GLY	-	expression tag	UNP A0A1D0AST6
E	-1	GLN	-	expression tag	UNP A0A1D0AST6
E	0	GLY	-	expression tag	UNP A0A1D0AST6
F	-1	GLN	-	expression tag	UNP A0A1D0AST6
F	0	GLY	-	expression tag	UNP A0A1D0AST6

- Molecule 2 is (1R,2S,3S,4R,6S)-4,6-DIAMINO-3-[(3-AMINO-3-DEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-2-HYDROXYCYCLOHEXYL 2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: 9CS) (formula: $C_{18}H_{37}N_5O_{10}$) (labeled as "Ligand of Interest" by depositor).



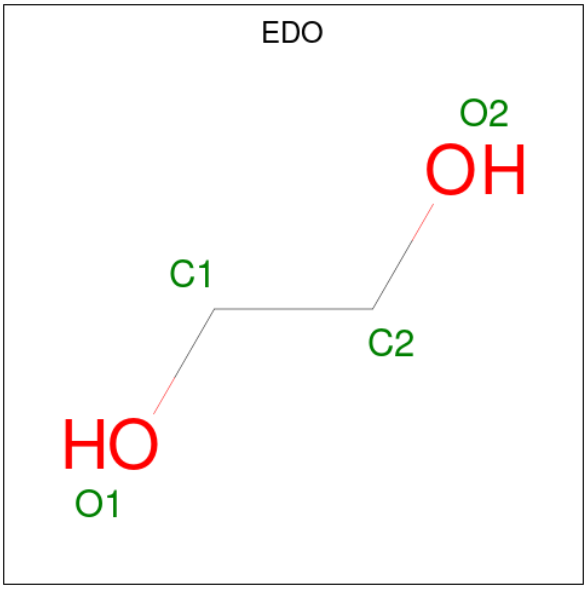
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 33 18 5 10	0	0
2	B	1	Total C N O 33 18 5 10	0	0
2	C	1	Total C N O 33 18 5 10	0	0
2	C	1	Total C N O 33 18 5 10	0	0
2	D	1	Total C N O 33 18 5 10	0	0
2	E	1	Total C N O 33 18 5 10	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



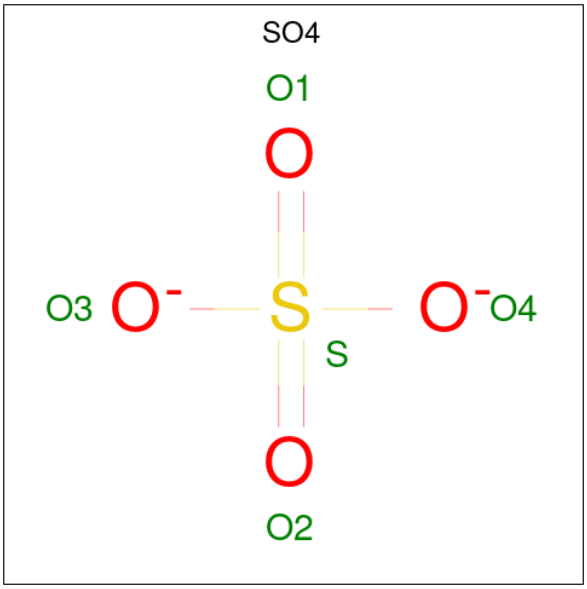
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is water.

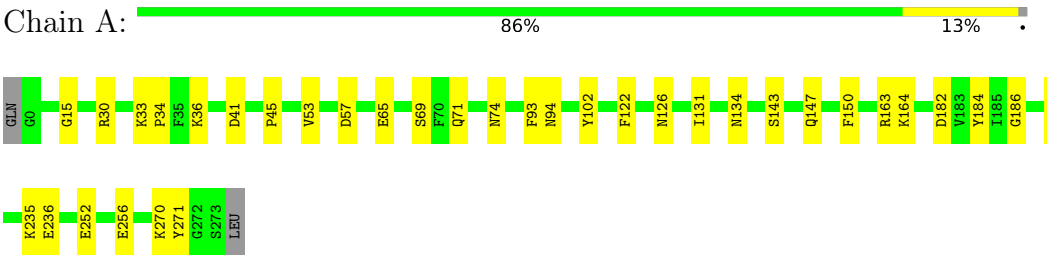
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	323	Total O 337 337	0	14
7	B	307	Total O 314 314	0	7
7	C	348	Total O 361 361	0	13
7	D	281	Total O 294 294	0	13
7	E	309	Total O 321 321	0	12
7	F	261	Total O 273 273	0	12

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.

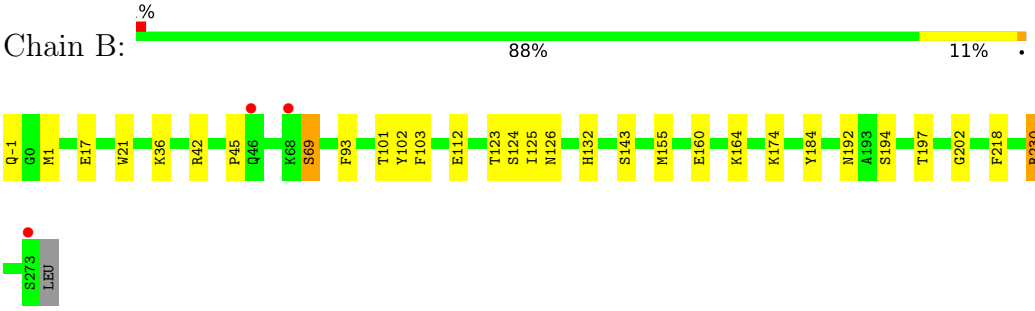
• Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain A:



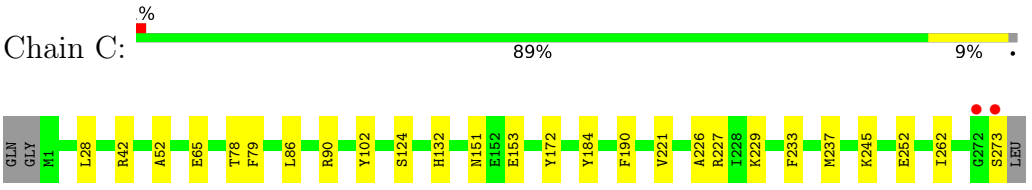
• Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain B:



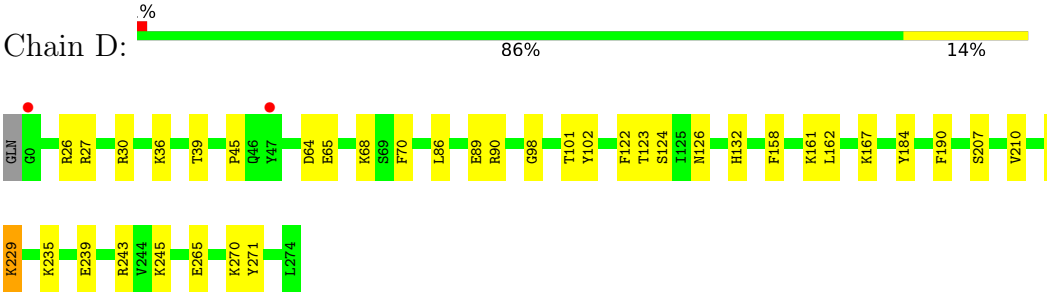
• Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain C:



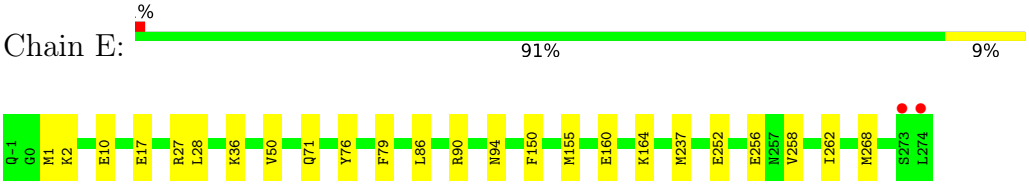
• Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain D:



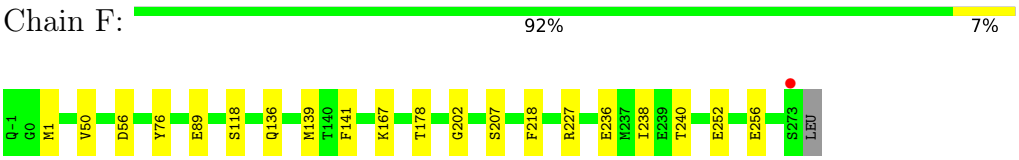
• Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain E:



• Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.09Å 131.69Å 157.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.47 – 2.26 29.47 – 2.25	Depositor EDS
% Data completeness (in resolution range)	83.3 (29.47-2.26) 88.4 (29.47-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.172 , 0.232 0.172 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15641	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9CS, EDO, SO4, CL, COA

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	0.43	0/2261	0.60	0/3065
1	B	0.44	0/2265	0.61	0/3069
1	C	0.43	0/2252	0.60	0/3053
1	D	0.43	0/2254	0.60	0/3054
1	E	0.41	0/2271	0.59	0/3077
1	F	0.40	0/2254	0.59	0/3055
All	All	0.42	0/13557	0.60	0/18373

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	2201	0	2132	33	0
1	B	2208	0	2145	39	0
1	C	2194	0	2128	20	0
1	D	2200	0	2135	37	0
1	E	2214	0	2147	14	0
1	F	2200	0	2132	15	0
2	A	33	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	33	0	37	3	0
2	C	66	0	74	2	0
2	D	33	0	37	2	0
2	E	33	0	37	1	0
3	A	48	0	32	24	0
3	B	48	0	32	15	0
3	C	48	0	32	3	0
3	D	48	0	32	11	0
3	E	48	0	32	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	16	0	24	1	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	F	8	0	12	0	0
5	A	10	0	0	1	0
5	B	15	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	D	1	0	0	0	0
7	A	337	0	0	4	0
7	B	314	0	0	2	0
7	C	361	0	0	4	0
7	D	294	0	0	4	0
7	E	321	0	0	2	0
7	F	273	0	0	2	0
All	All	15641	0	13261	161	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 6.

All (161) 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)
3:A:302:COA:HN4	1:B:132:HIS:CB	1.69	1.06
1:B:126:ASN:HB2	3:B:302:COA:H22	1.38	1.01
3:A:302:COA:HN4	1:B:132:HIS:HB3	1.27	1.00
3:A:302:COA:N4P	1:B:132:HIS:CB	2.26	0.97
3:A:302:COA:H31	1:B:132:HIS:CG	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:COA:N4P	1:B:132:HIS:HB3	1.82	0.91
3:B:302:COA:H61	1:D:190:PHE:CZ	2.08	0.88
3:A:302:COA:C3P	1:B:132:HIS:CB	2.53	0.87
3:A:302:COA:N4P	1:B:132:HIS:HB2	1.90	0.86
3:A:302:COA:H31	1:B:132:HIS:CD2	2.12	0.85
1:D:65:GLU:HA	1:D:68:LYS:HE3	1.63	0.79
1:A:126:ASN:HD22	3:A:302:COA:H22	1.48	0.78
1:C:262:ILE:HA	1:F:139:MET:HE3	1.66	0.76
1:D:126:ASN:HB2	3:D:302:COA:H22	1.68	0.75
3:A:302:COA:H32	7:A:404:HOH:O	1.87	0.74
3:A:302:COA:C3P	1:B:132:HIS:CG	2.72	0.72
3:A:302:COA:C3P	1:B:132:HIS:HB3	2.19	0.71
1:E:252:GLU:H	1:E:252:GLU:CD	1.94	0.70
2:B:301:9CS:N6	3:B:302:COA:S1P	2.65	0.70
3:A:302:COA:H31	1:B:132:HIS:CB	2.20	0.69
3:B:302:COA:H61	1:D:190:PHE:HZ	1.55	0.69
1:D:227:ARG:NE	1:D:229:LYS:HE3	2.07	0.69
3:A:302:COA:HN4	1:B:132:HIS:HB2	1.47	0.68
1:A:34:PRO:HG3	1:E:10:GLU:HA	1.77	0.66
1:A:126:ASN:ND2	3:A:302:COA:H22	2.12	0.65
1:E:17:GLU:HG2	1:E:36:LYS:HB2	1.79	0.65
1:D:270:LYS:HD2	1:D:271:TYR:CZ	2.31	0.65
1:D:229:LYS:HA	1:D:229:LYS:HE2	1.77	0.65
1:C:233:PHE:HB3	1:C:237:MET:HG2	1.80	0.64
3:B:302:COA:H32	1:D:132:HIS:CG	2.35	0.61
1:D:207:SER:OG	3:D:302:COA:H72	2.02	0.60
1:D:235:LYS:NZ	1:D:239:GLU:OE2	2.35	0.59
1:B:230:ARG:NH1	3:B:302:COA:O4A	2.36	0.58
1:E:237:MET:HG3	1:E:268:MET:SD	2.43	0.58
1:F:252:GLU:O	1:F:256:GLU:HG3	2.03	0.58
1:E:258:VAL:HG22	1:E:262:ILE:HD12	1.86	0.58
1:D:86:LEU:HD12	1:D:90:ARG:HD2	1.84	0.57
1:D:126:ASN:HB2	3:D:302:COA:C2P	2.35	0.57
1:A:71:GLN:HG2	1:A:74:ASN:HB2	1.86	0.57
1:C:86:LEU:HD12	1:C:90:ARG:HD3	1.86	0.56
1:E:1:MET:SD	1:E:94:ASN:HB2	2.45	0.55
3:A:302:COA:H21	3:A:302:COA:O5P	2.07	0.55
1:C:42:ARG:HG3	7:C:709:HOH:O	2.06	0.55
1:A:190:PHE:CZ	3:D:302:COA:H61	2.42	0.54
1:B:252:GLU:CD	1:B:252:GLU:H	2.11	0.54
1:E:86:LEU:HD12	1:E:90:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLU:HG2	1:B:36:LYS:HB3	1.90	0.53
1:D:227:ARG:HE	1:D:229:LYS:HE3	1.73	0.53
3:D:302:COA:H52A	3:D:302:COA:H8A	1.91	0.53
1:B:102:TYR:CZ	2:B:301:9CS:H11	2.44	0.52
1:D:126:ASN:HD22	3:D:302:COA:C3P	2.21	0.52
3:A:302:COA:H4B	3:A:302:COA:O8A	2.09	0.52
2:E:301:9CS:N6	3:E:302:COA:S1P	2.82	0.52
2:D:301:9CS:N6	3:D:302:COA:S1P	2.83	0.52
1:D:89:GLU:HG2	1:D:98:GLY:HA2	1.92	0.52
1:D:126:ASN:HD22	3:D:302:COA:H32	1.74	0.52
1:A:270:LYS:HD3	1:A:271:TYR:CZ	2.45	0.51
1:A:134:ASN:OD1	3:D:302:COA:H10	2.11	0.51
1:A:252:GLU:O	1:A:256:GLU:HG3	2.10	0.51
1:B:45:PRO:HG3	1:B:69:SER:HB2	1.92	0.51
1:A:102:TYR:CZ	2:A:301:9CS:H11	2.45	0.51
7:B:596:HOH:O	1:D:167:LYS:HD3	2.10	0.51
1:A:65:GLU:CD	1:F:89:GLU:HG3	2.32	0.50
1:A:102:TYR:CE2	2:A:301:9CS:H11	2.45	0.50
1:C:102:TYR:CZ	2:C:302:9CS:H11	2.46	0.50
1:E:28:LEU:HD13	1:E:79:PHE:CD1	2.47	0.50
1:A:94:ASN:ND2	7:A:408:HOH:O	2.43	0.50
1:A:164:LYS:NZ	7:A:410:HOH:O	2.44	0.50
1:A:71:GLN:CG	1:A:74:ASN:HB2	2.41	0.50
1:D:210:VAL:HG23	1:D:224:VAL:HG22	1.92	0.50
1:F:236:GLU:O	1:F:240:THR:HG22	2.12	0.49
1:B:202:GLY:HA3	1:B:218:PHE:CD1	2.48	0.49
1:B:-1:GLN:HB3	1:B:1:MET:H	1.78	0.49
1:A:15:GLY:O	1:E:36:LYS:HE3	2.13	0.49
1:A:126:ASN:HD22	3:A:302:COA:C2P	2.22	0.48
1:A:186:GLY:HA2	3:A:302:COA:H21	1.94	0.48
1:B:102:TYR:OH	1:B:124:SER:HB3	2.12	0.48
1:A:143:SER:HB2	1:D:122:PHE:O	2.13	0.48
3:B:302:COA:H32	1:D:132:HIS:CD2	2.48	0.48
1:D:27:ARG:HD2	7:D:620:HOH:O	2.12	0.48
1:B:126:ASN:ND2	3:B:302:COA:H31	2.29	0.48
1:D:243:ARG:HH11	1:D:243:ARG:HG2	1.79	0.48
1:A:30:ARG:NH2	1:D:64:ASP:OD2	2.36	0.48
1:B:126:ASN:HD22	3:B:302:COA:H31	1.79	0.47
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.79	0.47
1:E:90:ARG:NH1	7:E:415:HOH:O	2.48	0.46
1:A:236:GLU:H	1:A:236:GLU:CD	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HA	1:C:227:ARG:O	2.16	0.46
3:B:302:COA:O8A	3:B:302:COA:H4B	2.16	0.45
1:F:218:PHE:CD2	1:F:238:ILE:HG13	2.51	0.45
1:C:252:GLU:OE1	1:C:252:GLU:N	2.45	0.45
1:A:36:LYS:HE2	1:A:36:LYS:HB2	1.81	0.45
3:B:302:COA:C6P	1:D:190:PHE:CZ	2.93	0.45
1:D:229:LYS:HA	1:D:229:LYS:CE	2.43	0.45
1:F:202:GLY:HA3	1:F:218:PHE:CD1	2.51	0.45
1:B:184:TYR:CE1	3:B:302:COA:H71	2.52	0.45
7:C:706:HOH:O	1:F:167:LYS:HD3	2.16	0.45
1:C:262:ILE:CA	1:F:139:MET:HE3	2.42	0.45
1:C:221:VAL:HB	1:C:226:ALA:HB1	1.99	0.44
1:B:126:ASN:HD22	3:B:302:COA:C3P	2.30	0.44
1:A:184:TYR:HE1	3:A:302:COA:H71	1.82	0.44
1:A:122:PHE:O	1:B:143:SER:HB2	2.17	0.44
1:D:65:GLU:O	1:D:68:LYS:HG2	2.17	0.44
3:A:302:COA:C3P	1:B:132:HIS:HB2	2.35	0.44
1:B:101:THR:HA	1:B:123:THR:O	2.18	0.44
2:C:301:9CS:H1	2:C:301:9CS:O10	2.18	0.44
3:A:302:COA:H31	1:B:132:HIS:HB2	1.99	0.44
1:C:102:TYR:CZ	1:C:124:SER:HB3	2.52	0.44
1:A:126:ASN:HB2	3:A:302:COA:S1P	2.57	0.44
1:A:147:GLN:HA	1:A:150:PHE:CD2	2.53	0.44
3:B:302:COA:C9P	7:B:441:HOH:O	2.65	0.43
1:A:93:PHE:O	1:A:94:ASN:HB2	2.17	0.43
1:A:41:ASP:HB3	7:A:566:HOH:O	2.17	0.43
1:A:182:ASP:O	1:A:202:GLY:HA2	2.19	0.43
1:B:102:TYR:CZ	1:B:124:SER:HB3	2.53	0.43
1:C:52:ALA:O	1:C:78:THR:HA	2.19	0.43
1:C:102:TYR:OH	1:C:124:SER:HB3	2.17	0.43
1:B:21:TRP:CD1	1:D:26:ARG:HD3	2.53	0.43
1:D:207:SER:OG	3:D:302:COA:O5P	2.37	0.43
1:D:245:LYS:NZ	7:D:411:HOH:O	2.51	0.43
1:D:45:PRO:HD3	1:D:70:PHE:CE1	2.54	0.43
1:A:45:PRO:HG3	1:A:69:SER:HB2	2.00	0.43
1:B:160:GLU:O	1:B:164:LYS:HG3	2.19	0.43
1:C:65:GLU:HG2	7:C:580[A]:HOH:O	2.19	0.43
1:D:39:THR:HG23	7:D:437:HOH:O	2.19	0.43
1:D:101:THR:HA	1:D:123:THR:O	2.19	0.43
1:A:131:ILE:HG12	1:A:191:ILE:HB	2.01	0.43
1:B:192:ASN:OD1	1:B:194:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:GLU:O	1:E:164:LYS:HG3	2.19	0.43
1:C:172:TYR:OH	4:C:307:EDO:H21	2.19	0.42
1:C:184:TYR:CE2	3:C:303:COA:H71	2.54	0.42
1:D:158:PHE:CE2	1:D:162:LEU:HD11	2.54	0.42
1:B:174:LYS:HE2	1:B:197:THR:HG22	2.01	0.42
1:C:132[B]:HIS:CE1	1:C:190:PHE:CE1	3.07	0.42
1:B:265:GLU:H	1:B:265:GLU:CD	2.23	0.42
1:B:184:TYR:OH	3:B:302:COA:N4P	2.53	0.42
1:E:71:GLN:HG3	7:E:628:HOH:O	2.18	0.42
1:E:150:PHE:HD2	1:E:155:MET:HE1	1.83	0.42
1:F:252:GLU:CD	1:F:252:GLU:H	2.23	0.42
1:A:184:TYR:OH	3:A:302:COA:H62	2.20	0.42
1:D:102:TYR:OH	1:D:124:SER:HB3	2.20	0.42
1:F:1:MET:HB3	1:F:1:MET:HE2	1.85	0.42
1:F:50:VAL:O	1:F:76:TYR:HA	2.20	0.42
1:C:229:LYS:HG2	3:C:303:COA:H52A	2.01	0.41
1:C:245:LYS:HE2	7:C:690:HOH:O	2.20	0.41
1:A:163:ARG:HA	1:A:163:ARG:HD3	1.89	0.41
1:C:151:ASN:OD1	1:C:153:GLU:HG2	2.20	0.41
3:C:303:COA:O5B	3:C:303:COA:H8A	2.20	0.41
1:F:178:THR:HG23	7:F:469:HOH:O	2.21	0.41
1:A:53:VAL:HB	1:A:57:ASP:OD2	2.20	0.41
1:B:102:TYR:CE2	2:B:301:9CS:H11	2.56	0.41
1:D:161:LYS:HG2	7:D:418:HOH:O	2.20	0.41
1:B:103:PHE:HB3	1:B:125:ILE:HB	2.02	0.41
5:A:304:SO4:O1	2:D:301:9CS:N2	2.53	0.41
1:F:139:MET:HE2	1:F:141:PHE:CZ	2.56	0.41
1:F:136:GLN:HG3	1:F:139:MET:SD	2.61	0.41
1:B:93:PHE:CE2	1:B:112:GLU:HB2	2.56	0.40
1:C:28:LEU:HD13	1:C:79:PHE:CG	2.57	0.40
1:D:184:TYR:OH	3:D:302:COA:N4P	2.55	0.40
1:E:50:VAL:O	1:E:76:TYR:HA	2.22	0.40
1:F:118:SER:OG	7:F:401:HOH:O	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	274/276 (99%)	271 (99%)	3 (1%)	0	100	100
1	B	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	C	272/276 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
1	E	275/276 (100%)	269 (98%)	6 (2%)	0	100	100
1	F	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
All	All	1641/1656 (99%)	1603 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	238/238 (100%)	236 (99%)	2 (1%)	81	88
1	B	238/238 (100%)	233 (98%)	5 (2%)	53	62
1	C	237/238 (100%)	236 (100%)	1 (0%)	91	94
1	D	237/238 (100%)	233 (98%)	4 (2%)	60	71
1	E	239/238 (100%)	236 (99%)	3 (1%)	69	79
1	F	237/238 (100%)	234 (99%)	3 (1%)	69	79
All	All	1426/1428 (100%)	1408 (99%)	18 (1%)	71	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	235	LYS
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	69	SER
1	B	155	MET
1	B	230	ARG
1	C	273	SER
1	D	30	ARG
1	D	36	LYS
1	D	229	LYS
1	D	265	GLU
1	E	2	LYS
1	E	27	ARG
1	E	256	GLU
1	F	56	ASP
1	F	207	SER
1	F	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	9CS	E	301	-	35,35,35	1.51	6 (17%)	46,52,52	1.33	6 (13%)
5	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.43	0
4	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.58	0
5	SO4	B	305	-	4,4,4	0.33	0	6,6,6	0.49	0
2	9CS	B	301	-	35,35,35	1.43	4 (11%)	46,52,52	1.20	3 (6%)
4	EDO	B	303	-	3,3,3	0.46	0	2,2,2	0.43	0
5	SO4	C	308	-	4,4,4	0.22	0	6,6,6	0.11	0
2	9CS	C	302	-	35,35,35	1.60	6 (17%)	46,52,52	1.30	6 (13%)
4	EDO	C	307	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.14	0
4	EDO	E	303	-	3,3,3	0.45	0	2,2,2	0.57	0
4	EDO	C	305	-	3,3,3	0.42	0	2,2,2	0.60	0
5	SO4	D	304	-	4,4,4	0.18	0	6,6,6	0.45	0
4	EDO	F	301	-	3,3,3	0.48	0	2,2,2	0.21	0
2	9CS	A	301	-	35,35,35	1.40	4 (11%)	46,52,52	1.22	6 (13%)
3	COA	A	302	-	41,50,50	0.93	1 (2%)	52,75,75	1.45	6 (11%)
2	9CS	D	301	-	35,35,35	1.61	5 (14%)	46,52,52	1.25	6 (13%)
5	SO4	F	303	-	4,4,4	0.24	0	6,6,6	0.32	0
4	EDO	F	302	-	3,3,3	0.35	0	2,2,2	0.64	0
3	COA	D	302	-	41,50,50	1.07	4 (9%)	52,75,75	1.58	7 (13%)
3	COA	C	303	-	41,50,50	1.08	3 (7%)	52,75,75	1.31	6 (11%)
3	COA	B	302	-	41,50,50	1.17	3 (7%)	52,75,75	2.08	16 (30%)
5	SO4	A	304	-	4,4,4	0.19	0	6,6,6	0.42	0
5	SO4	B	306	-	4,4,4	0.18	0	6,6,6	0.36	0
5	SO4	E	304	-	4,4,4	0.25	0	6,6,6	0.44	0
4	EDO	D	303	-	3,3,3	0.49	0	2,2,2	0.40	0
3	COA	E	302	-	41,50,50	0.89	1 (2%)	52,75,75	1.25	6 (11%)
2	9CS	C	301	-	35,35,35	1.44	5 (14%)	46,52,52	1.15	3 (6%)
4	EDO	C	304	-	3,3,3	0.40	0	2,2,2	0.14	0
5	SO4	A	305	-	4,4,4	0.19	0	6,6,6	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9CS	E	301	-	-	2/12/72/72	0/3/3/3
4	EDO	A	303	-	-	1/1/1/1	-
2	9CS	B	301	-	-	3/12/72/72	0/3/3/3
4	EDO	B	303	-	-	1/1/1/1	-
2	9CS	C	302	-	-	3/12/72/72	0/3/3/3
4	EDO	C	307	-	-	0/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	C	305	-	-	1/1/1/1	-
4	EDO	F	301	-	-	0/1/1/1	-
2	9CS	A	301	-	-	2/12/72/72	0/3/3/3
3	COA	A	302	-	-	15/44/64/64	0/3/3/3
2	9CS	D	301	-	-	3/12/72/72	0/3/3/3
4	EDO	F	302	-	-	0/1/1/1	-
3	COA	D	302	-	-	11/44/64/64	0/3/3/3
3	COA	C	303	-	-	9/44/64/64	0/3/3/3
3	COA	B	302	-	-	15/44/64/64	0/3/3/3
4	EDO	D	303	-	-	0/1/1/1	-
3	COA	E	302	-	-	16/44/64/64	0/3/3/3
2	9CS	C	301	-	-	3/12/72/72	0/3/3/3
4	EDO	C	304	-	-	1/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	9CS	C15-N4	-3.75	1.41	1.47
2	D	301	9CS	C15-N4	-3.65	1.41	1.47
2	A	301	9CS	C2-N6	-3.57	1.41	1.47
2	B	301	9CS	C15-N4	-3.54	1.41	1.47
2	C	302	9CS	C2-N6	-3.31	1.42	1.47
2	D	301	9CS	C16-C15	-3.19	1.49	1.53
2	E	301	9CS	C3-C2	-3.11	1.49	1.53
2	E	301	9CS	C14-C15	-3.07	1.49	1.53
2	C	301	9CS	C2-N6	-3.07	1.42	1.47
2	A	301	9CS	C3-C2	-3.00	1.49	1.53
2	B	301	9CS	C2-N6	-2.98	1.42	1.47
2	E	301	9CS	C15-N4	-2.96	1.42	1.47
2	C	301	9CS	C15-N4	-2.89	1.42	1.47
3	B	302	COA	C6P-C5P	2.84	1.56	1.51
2	C	301	9CS	C16-C15	-2.74	1.50	1.53
2	B	301	9CS	C14-C15	-2.68	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	9CS	C2-N6	-2.60	1.43	1.47
2	A	301	9CS	C15-N4	-2.54	1.43	1.47
2	D	301	9CS	C2-N6	-2.49	1.43	1.47
3	D	302	COA	O5P-C5P	-2.47	1.18	1.23
3	B	302	COA	C5A-C4A	2.46	1.47	1.40
3	A	302	COA	C5A-C4A	2.46	1.47	1.40
3	D	302	COA	C5A-C4A	2.40	1.47	1.40
3	E	302	COA	C5A-C4A	2.38	1.47	1.40
2	C	301	9CS	C14-C15	-2.38	1.50	1.53
2	E	301	9CS	O12-C17	-2.35	1.38	1.44
2	C	302	9CS	O12-C17	-2.29	1.38	1.44
2	D	301	9CS	C14-C15	-2.28	1.50	1.53
3	D	302	COA	C2B-C1B	-2.28	1.50	1.53
3	C	303	COA	C2B-C1B	-2.26	1.50	1.53
3	D	302	COA	O4B-C1B	2.23	1.44	1.41
2	D	301	9CS	O11-C8	-2.23	1.38	1.43
2	C	302	9CS	O11-C8	-2.19	1.38	1.43
2	C	302	9CS	C4-C5	-2.16	1.48	1.53
2	E	301	9CS	C4-C5	-2.15	1.48	1.53
3	C	303	COA	C5A-N7A	-2.13	1.32	1.39
3	B	302	COA	C2B-C1B	-2.12	1.50	1.53
2	C	302	9CS	C3-C2	-2.12	1.50	1.53
2	B	301	9CS	O12-C17	-2.12	1.39	1.44
3	C	303	COA	P3B-O9A	-2.11	1.46	1.54
2	A	301	9CS	O12-C17	-2.05	1.39	1.44
2	C	301	9CS	C3-C2	-2.02	1.51	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	COA	C3P-N4P-C5P	6.65	135.18	122.84
3	B	302	COA	C6P-C7P-N8P	6.04	124.08	111.90
3	A	302	COA	O6A-CCP-CBP	5.14	118.82	110.55
2	E	301	9CS	C4-C3-C2	-4.96	102.55	111.07
3	B	302	COA	O6A-CCP-CBP	4.91	118.44	110.55
3	D	302	COA	C2P-C3P-N4P	4.60	122.83	112.31
3	B	302	COA	C2P-C3P-N4P	3.99	121.42	112.31
2	C	302	9CS	C6-C5-C4	-3.90	105.43	113.10
3	C	303	COA	N3A-C2A-N1A	-3.86	122.64	128.68
3	D	302	COA	O6A-CCP-CBP	3.74	116.56	110.55
3	B	302	COA	C4A-C5A-N7A	-3.57	105.68	109.40
2	E	301	9CS	C6-C5-C4	-3.56	106.09	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	9CS	O14-C16-C15	-3.51	103.91	110.22
3	D	302	COA	C3P-N4P-C5P	3.37	129.09	122.84
3	C	303	COA	O6A-CCP-CBP	3.33	115.91	110.55
3	C	303	COA	P2A-O3A-P1A	-3.25	121.66	132.83
2	D	301	9CS	O7-C3-C4	-3.23	102.87	110.35
3	E	302	COA	N3A-C2A-N1A	-3.22	123.64	128.68
3	D	302	COA	C4A-C5A-N7A	-3.20	106.06	109.40
3	B	302	COA	CDP-CBP-CCP	3.19	113.44	108.23
2	C	302	9CS	O9-C10-C11	-3.15	101.65	109.18
3	A	302	COA	C4A-C5A-N7A	-2.95	106.32	109.40
2	D	301	9CS	C11-C12-C7	-2.93	105.17	111.18
2	D	301	9CS	C6-C5-C4	-2.89	107.41	113.10
2	E	301	9CS	O5-C5-C6	2.87	111.35	106.01
3	E	302	COA	P2A-O3A-P1A	-2.86	123.00	132.83
3	B	302	COA	O3B-P3B-O7A	-2.86	98.36	109.39
2	A	301	9CS	O12-C13-C14	-2.85	104.32	110.35
3	A	302	COA	N3A-C2A-N1A	-2.82	124.27	128.68
2	A	301	9CS	C6-C5-C4	-2.82	107.56	113.10
2	B	301	9CS	C6-C5-C4	-2.81	107.57	113.10
2	A	301	9CS	O5-C5-C6	2.77	111.16	106.01
3	B	302	COA	C7P-C6P-C5P	2.73	116.90	112.36
2	B	301	9CS	C1-C2-N6	-2.71	105.33	110.20
2	A	301	9CS	C10-C9-C8	2.68	114.52	108.96
2	A	301	9CS	C4-C3-C2	-2.68	106.47	111.07
2	B	301	9CS	O9-C10-C9	2.65	114.33	107.28
3	B	302	COA	N3A-C2A-N1A	-2.64	124.55	128.68
2	D	301	9CS	O9-C10-C9	2.56	114.10	107.28
3	C	303	COA	C6P-C7P-N8P	2.51	116.97	111.90
3	B	302	COA	P2A-O3A-P1A	-2.50	124.24	132.83
3	E	302	COA	C2A-N1A-C6A	2.50	123.03	118.75
2	D	301	9CS	O14-C16-C15	-2.44	105.84	110.22
2	C	302	9CS	O7-C3-C4	-2.40	104.80	110.35
3	E	302	COA	C4A-C5A-N7A	-2.39	106.91	109.40
2	C	302	9CS	C18-C17-C16	2.37	118.56	113.00
2	C	302	9CS	O5-C5-C6	2.37	110.42	106.01
3	C	303	COA	C4A-C5A-N7A	-2.35	106.95	109.40
3	B	302	COA	CDP-CBP-CAP	2.35	112.90	108.82
3	B	302	COA	C2A-N1A-C6A	2.34	122.76	118.75
3	A	302	COA	P2A-O3A-P1A	-2.33	124.82	132.83
3	D	302	COA	O5A-P2A-O4A	2.31	123.66	112.24
3	D	302	COA	N3A-C2A-N1A	-2.27	125.13	128.68
2	E	301	9CS	O9-C10-C9	2.24	113.25	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	302	COA	O6A-CCP-CBP	2.23	114.14	110.55
3	D	302	COA	O8A-P3B-O7A	2.23	119.40	110.68
3	C	303	COA	C2A-N1A-C6A	2.21	122.53	118.75
3	B	302	COA	C7P-N8P-C9P	2.20	126.52	122.59
2	C	302	9CS	C10-C9-C8	2.19	113.50	108.96
2	C	301	9CS	O9-C10-C11	-2.18	103.98	109.18
3	B	302	COA	C3B-C2B-C1B	2.17	104.70	99.89
3	E	302	COA	O5A-P2A-O4A	2.15	122.89	112.24
3	A	302	COA	C2A-N1A-C6A	2.14	122.42	118.75
2	E	301	9CS	C10-C9-C8	2.13	113.38	108.96
2	A	301	9CS	O9-C10-C9	2.12	112.92	107.28
2	C	301	9CS	C10-C9-C8	2.12	113.35	108.96
2	D	301	9CS	C4-C3-C2	-2.11	107.44	111.07
2	E	301	9CS	O12-C13-C14	-2.11	105.89	110.35
3	B	302	COA	C5A-C6A-N1A	-2.07	115.66	120.35
3	B	302	COA	C5A-C6A-N6A	2.03	123.43	120.35
3	A	302	COA	C3P-N4P-C5P	-2.01	119.10	122.84

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	COA	C5B-O5B-P1A-O2A
3	A	302	COA	CCP-O6A-P2A-O3A
3	A	302	COA	CCP-O6A-P2A-O4A
3	A	302	COA	CCP-O6A-P2A-O5A
3	A	302	COA	CDP-CBP-CCP-O6A
3	A	302	COA	CEP-CBP-CCP-O6A
3	A	302	COA	CAP-CBP-CCP-O6A
3	A	302	COA	C6P-C5P-N4P-C3P
3	A	302	COA	C2P-C3P-N4P-C5P
3	A	302	COA	S1P-C2P-C3P-N4P
3	B	302	COA	C4B-C3B-O3B-P3B
3	B	302	COA	C5B-O5B-P1A-O2A
3	B	302	COA	C5B-O5B-P1A-O3A
3	B	302	COA	CCP-O6A-P2A-O5A
3	B	302	COA	CAP-CBP-CCP-O6A
3	B	302	COA	S1P-C2P-C3P-N4P
3	C	303	COA	CAP-CBP-CCP-O6A
3	C	303	COA	S1P-C2P-C3P-N4P
3	D	302	COA	C5B-O5B-P1A-O3A
3	D	302	COA	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
3	D	302	COA	S1P-C2P-C3P-N4P
3	E	302	COA	CCP-O6A-P2A-O3A
3	E	302	COA	CCP-O6A-P2A-O5A
3	E	302	COA	OAP-CAP-CBP-CCP
3	E	302	COA	C9P-CAP-CBP-CCP
3	E	302	COA	OAP-CAP-CBP-CDP
3	E	302	COA	S1P-C2P-C3P-N4P
3	A	302	COA	O5P-C5P-N4P-C3P
3	B	302	COA	C3B-C4B-C5B-O5B
3	D	302	COA	O4B-C4B-C5B-O5B
3	B	302	COA	O4B-C4B-C5B-O5B
2	A	301	9CS	O5-C1-O9-C10
3	C	303	COA	CDP-CBP-CCP-O6A
3	C	303	COA	CEP-CBP-CCP-O6A
3	D	302	COA	CDP-CBP-CCP-O6A
3	D	302	COA	CEP-CBP-CCP-O6A
2	C	301	9CS	C9-C10-O9-C1
3	D	302	COA	C3B-C4B-C5B-O5B
4	A	303	EDO	O1-C1-C2-O2
2	C	302	9CS	O5-C1-O9-C10
2	B	301	9CS	C9-C10-O9-C1
2	E	301	9CS	C9-C10-O9-C1
3	E	302	COA	O4B-C4B-C5B-O5B
3	B	302	COA	CDP-CBP-CCP-O6A
3	E	302	COA	CDP-CBP-CCP-O6A
3	E	302	COA	CEP-CBP-CCP-O6A
3	A	302	COA	C2B-C3B-O3B-P3B
3	E	302	COA	C2B-C3B-O3B-P3B
3	E	302	COA	OAP-CAP-CBP-CEP
3	D	302	COA	P2A-O3A-P1A-O1A
2	D	301	9CS	C9-C10-O9-C1
2	C	302	9CS	C9-C10-O9-C1
2	D	301	9CS	O5-C1-O9-C10
2	A	301	9CS	C9-C10-O9-C1
2	B	301	9CS	O5-C1-O9-C10
2	E	301	9CS	O5-C1-O9-C10
4	C	306	EDO	O1-C1-C2-O2
3	E	302	COA	C3B-C4B-C5B-O5B
3	B	302	COA	CEP-CBP-CCP-O6A
3	E	302	COA	C9P-CAP-CBP-CDP
3	A	302	COA	C5B-O5B-P1A-O3A
3	B	302	COA	CCP-O6A-P2A-O3A

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Mol	Chain	Res	Type	Atoms
3	B	302	COA	P1A-O3A-P2A-O5A
2	B	301	9CS	C11-C10-O9-C1
2	C	301	9CS	C11-C10-O9-C1
2	C	302	9CS	C11-C10-O9-C1
2	D	301	9CS	C11-C10-O9-C1
3	A	302	COA	C5B-O5B-P1A-O1A
3	B	302	COA	C5B-O5B-P1A-O1A
3	B	302	COA	CCP-O6A-P2A-O4A
3	D	302	COA	C5B-O5B-P1A-O1A
3	D	302	COA	C5B-O5B-P1A-O2A
3	E	302	COA	CCP-O6A-P2A-O4A
3	A	302	COA	C4B-C3B-O3B-P3B
2	C	301	9CS	O5-C1-O9-C10
4	B	303	EDO	O1-C1-C2-O2
3	D	302	COA	P2A-O3A-P1A-O2A
3	B	302	COA	P1A-O3A-P2A-O4A
3	C	303	COA	P1A-O3A-P2A-O5A
4	C	305	EDO	O1-C1-C2-O2
3	E	302	COA	C4B-C3B-O3B-P3B
3	C	303	COA	O9P-C9P-CAP-OAP
3	C	303	COA	C2B-C3B-O3B-P3B
4	C	304	EDO	O1-C1-C2-O2
3	C	303	COA	P1A-O3A-P2A-O4A
3	E	302	COA	P1A-O3A-P2A-O4A
3	C	303	COA	C4B-C3B-O3B-P3B

There are no ring outliers.

13 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	9CS	1	0
2	B	301	9CS	3	0
2	C	302	9CS	1	0
4	C	307	EDO	1	0
2	A	301	9CS	2	0
3	A	302	COA	24	0
2	D	301	9CS	2	0
3	D	302	COA	11	0
3	C	303	COA	3	0
3	B	302	COA	15	0
5	A	304	SO4	1	0
3	E	302	COA	1	0

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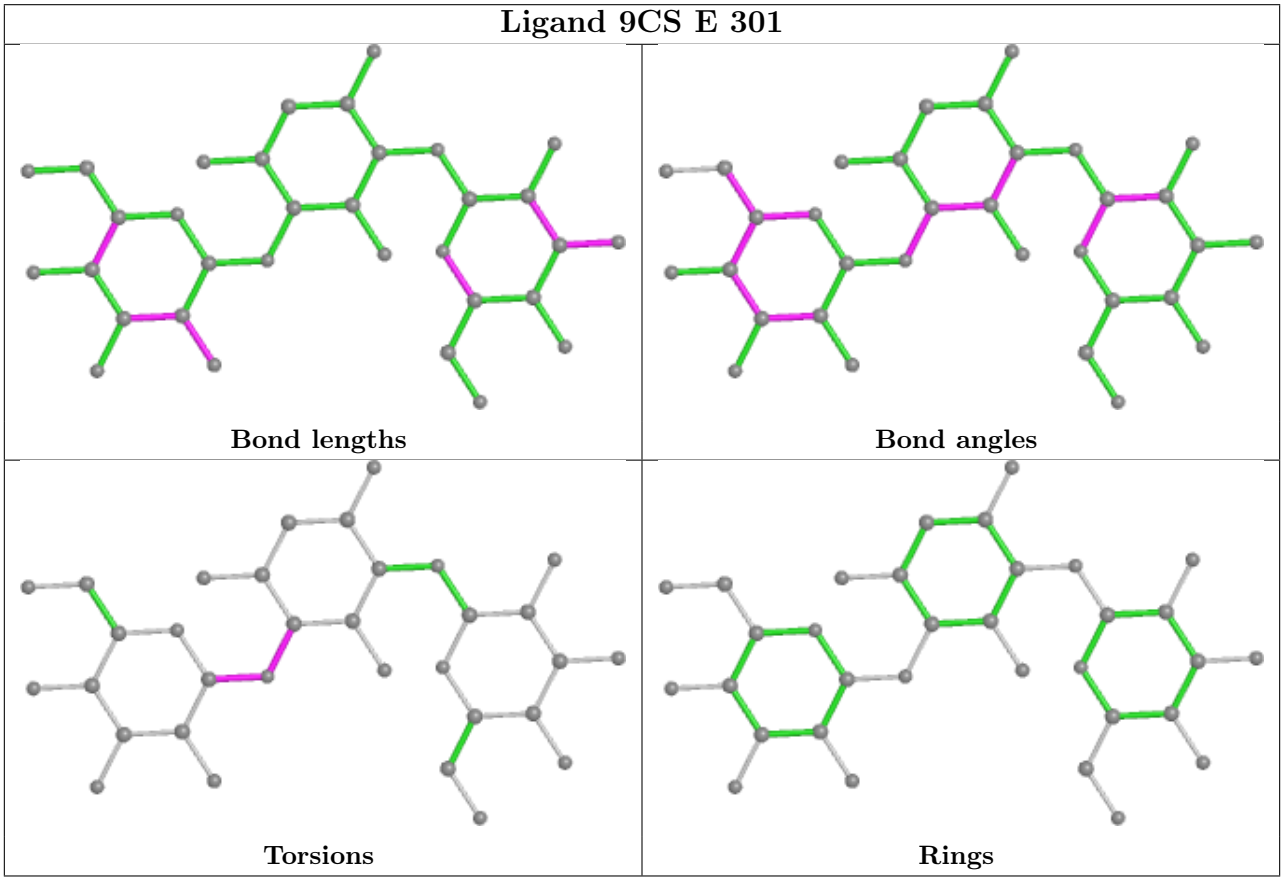
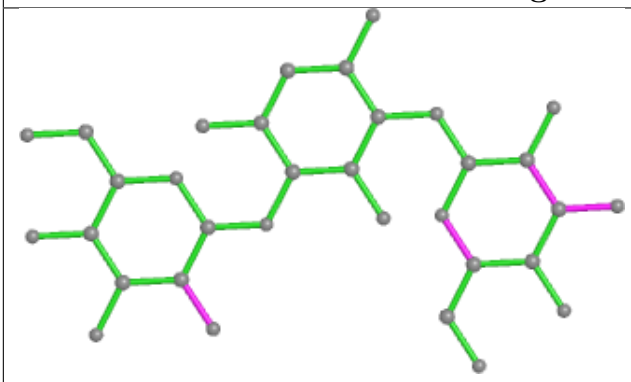
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	9CS	1	0

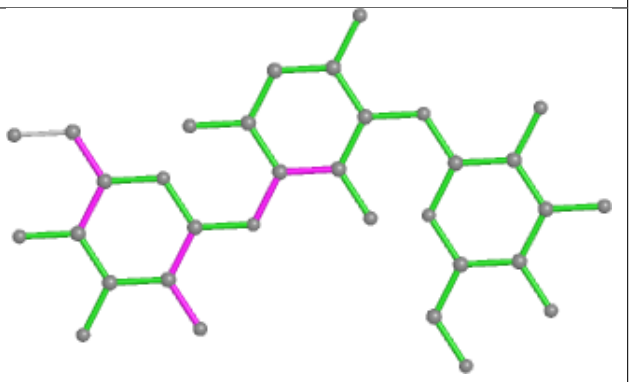
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



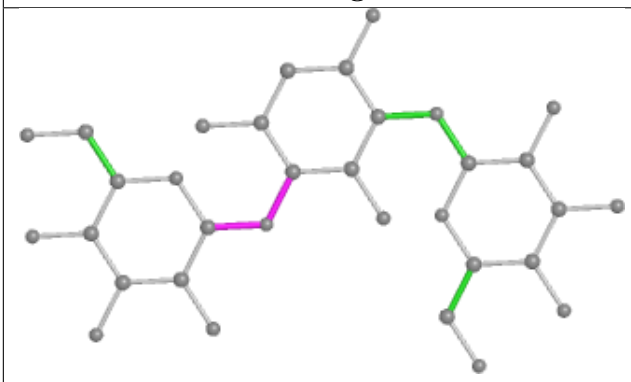
Ligand 9CS B 301



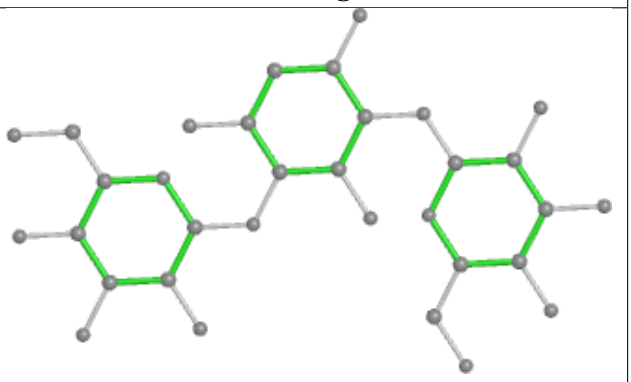
Bond lengths



Bond angles

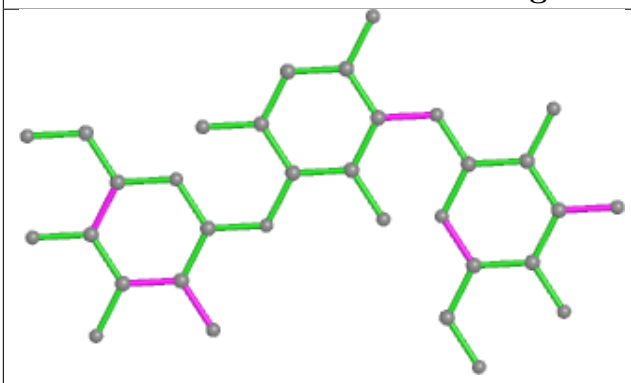


Torsions

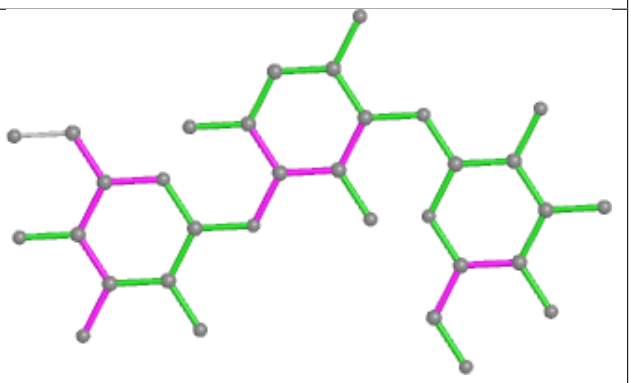


Rings

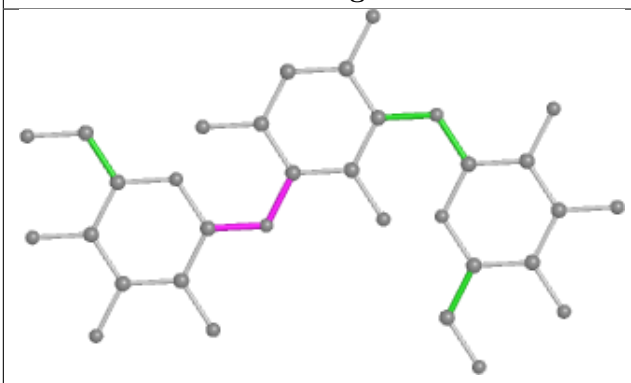
Ligand 9CS C 302



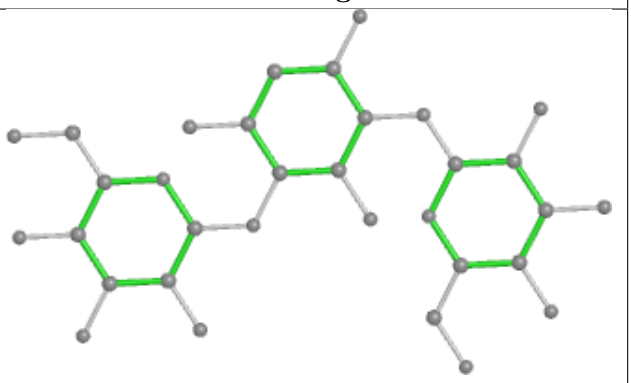
Bond lengths



Bond angles

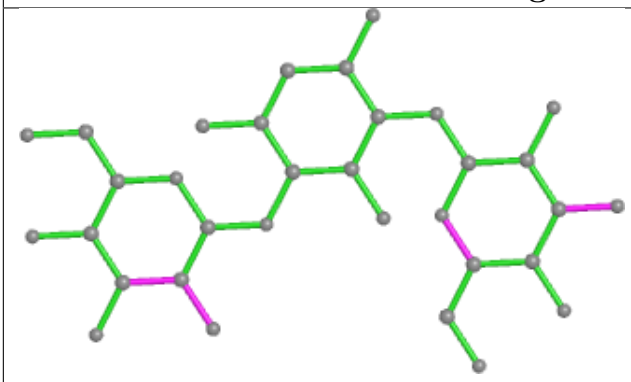


Torsions

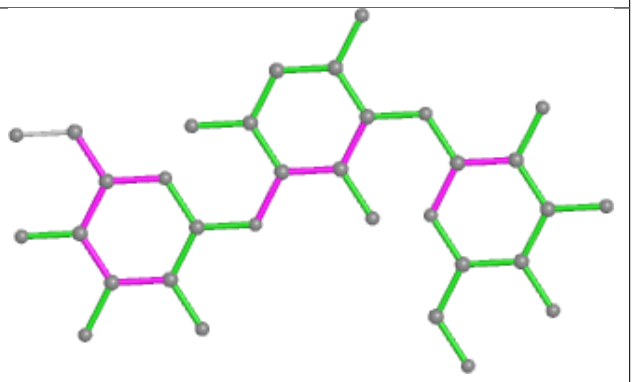


Rings

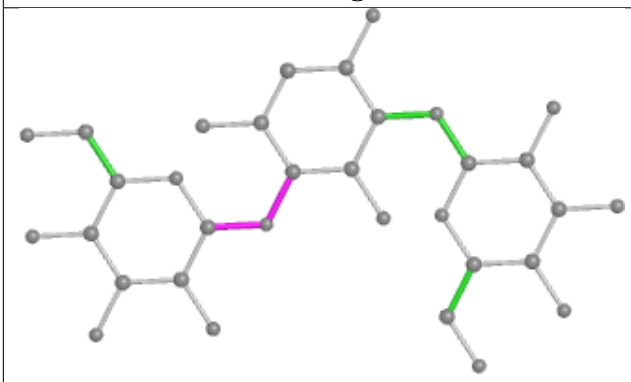
Ligand 9CS A 301



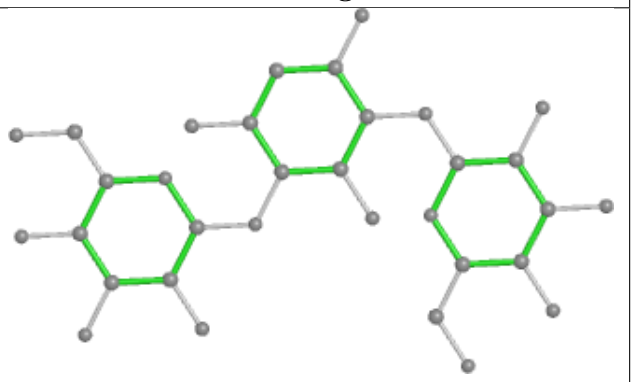
Bond lengths



Bond angles

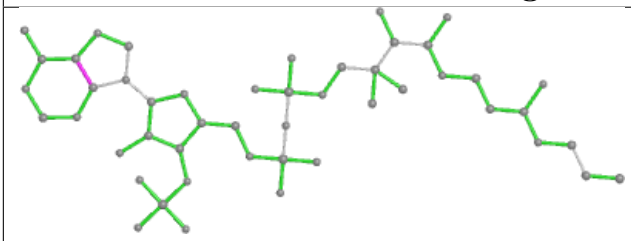


Torsions

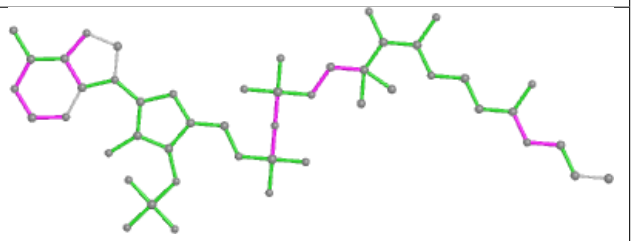


Rings

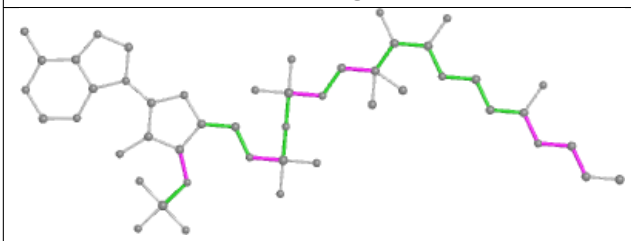
Ligand COA A 302



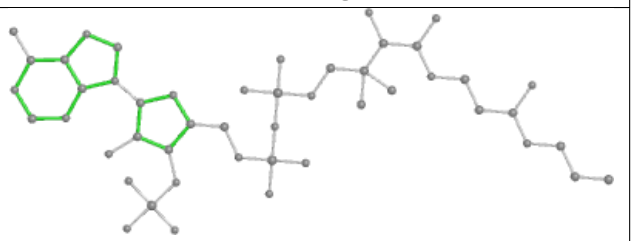
Bond lengths



Bond angles

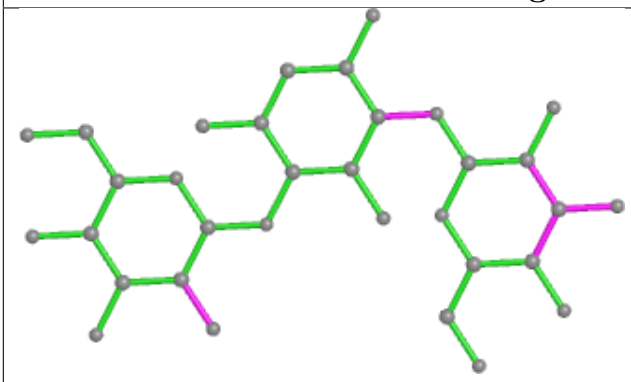


Torsions

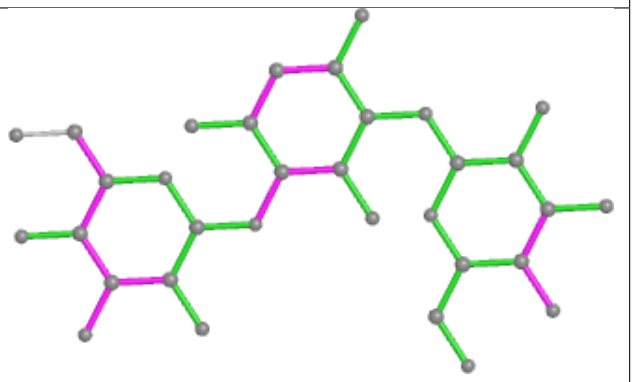


Rings

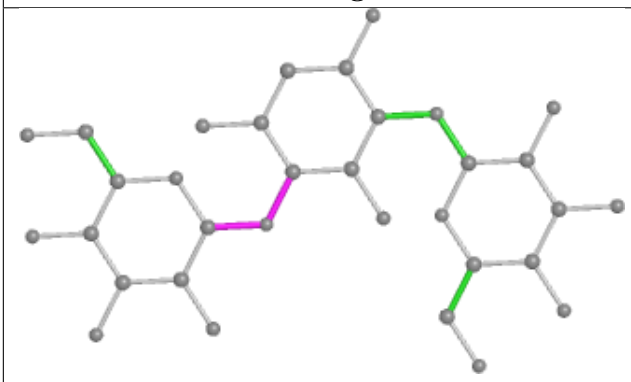
Ligand 9CS D 301



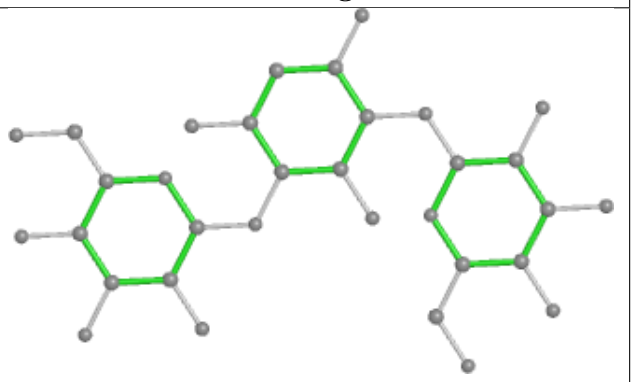
Bond lengths



Bond angles

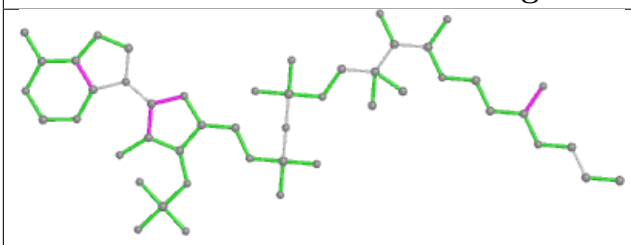


Torsions

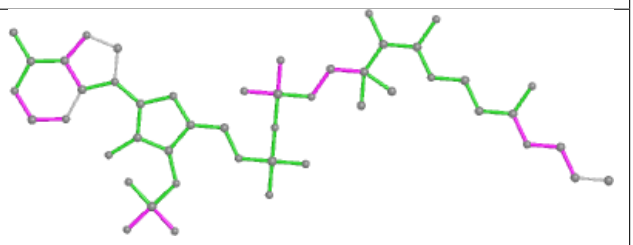


Rings

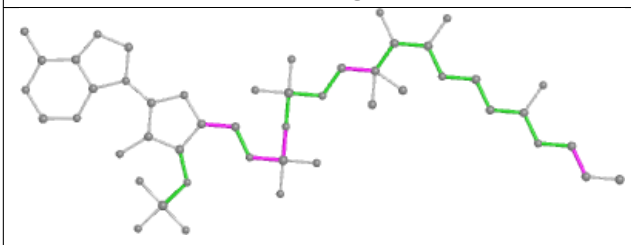
Ligand COA D 302



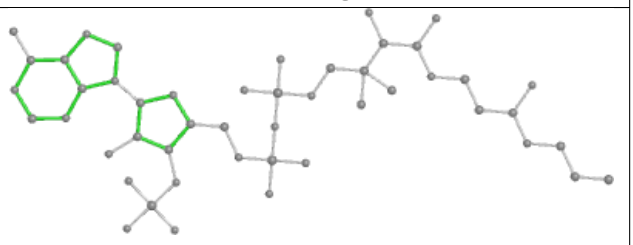
Bond lengths



Bond angles

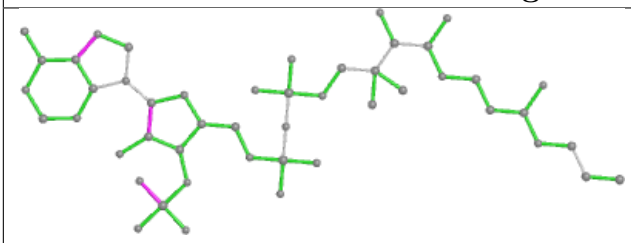


Torsions

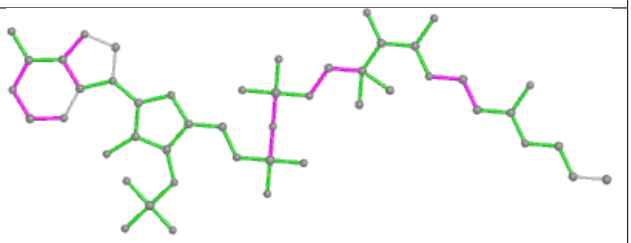


Rings

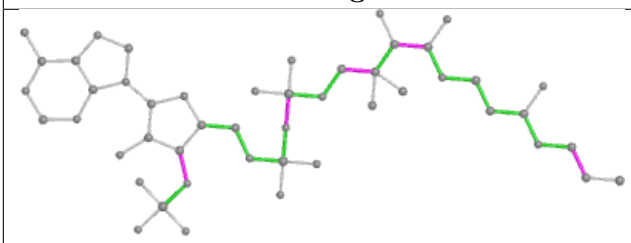
Ligand COA C 303



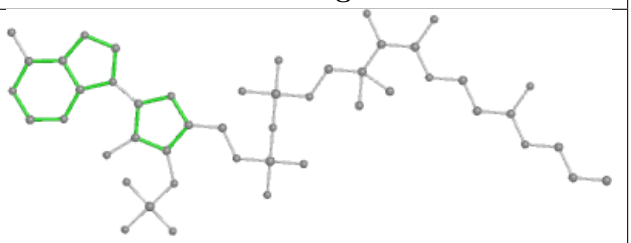
Bond lengths



Bond angles

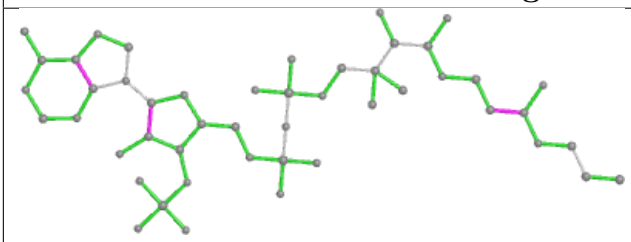


Torsions

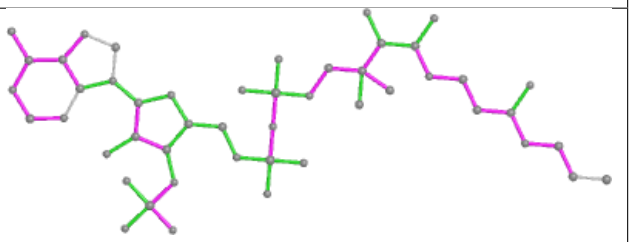


Rings

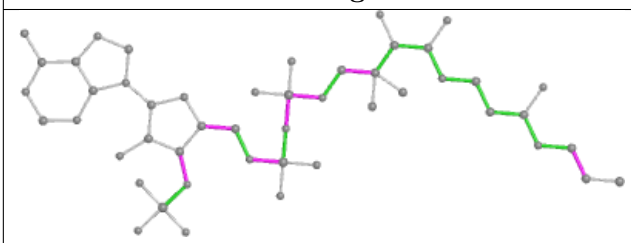
Ligand COA B 302



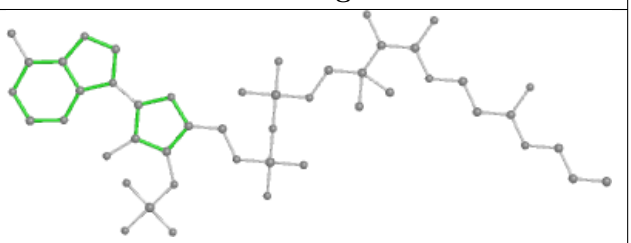
Bond lengths



Bond angles

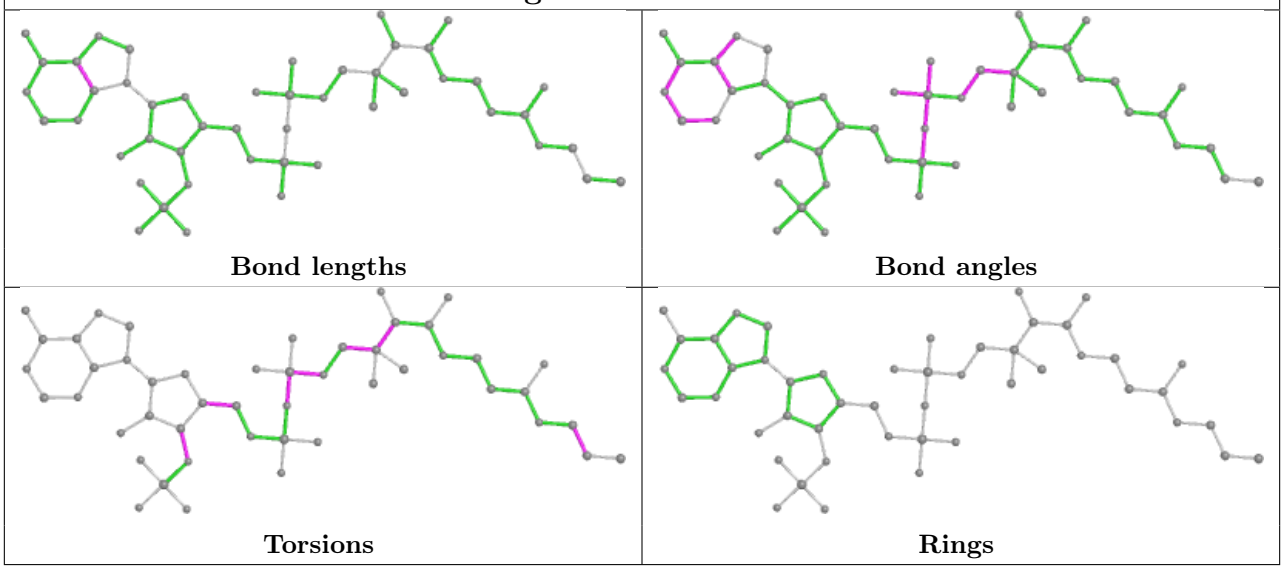


Torsions

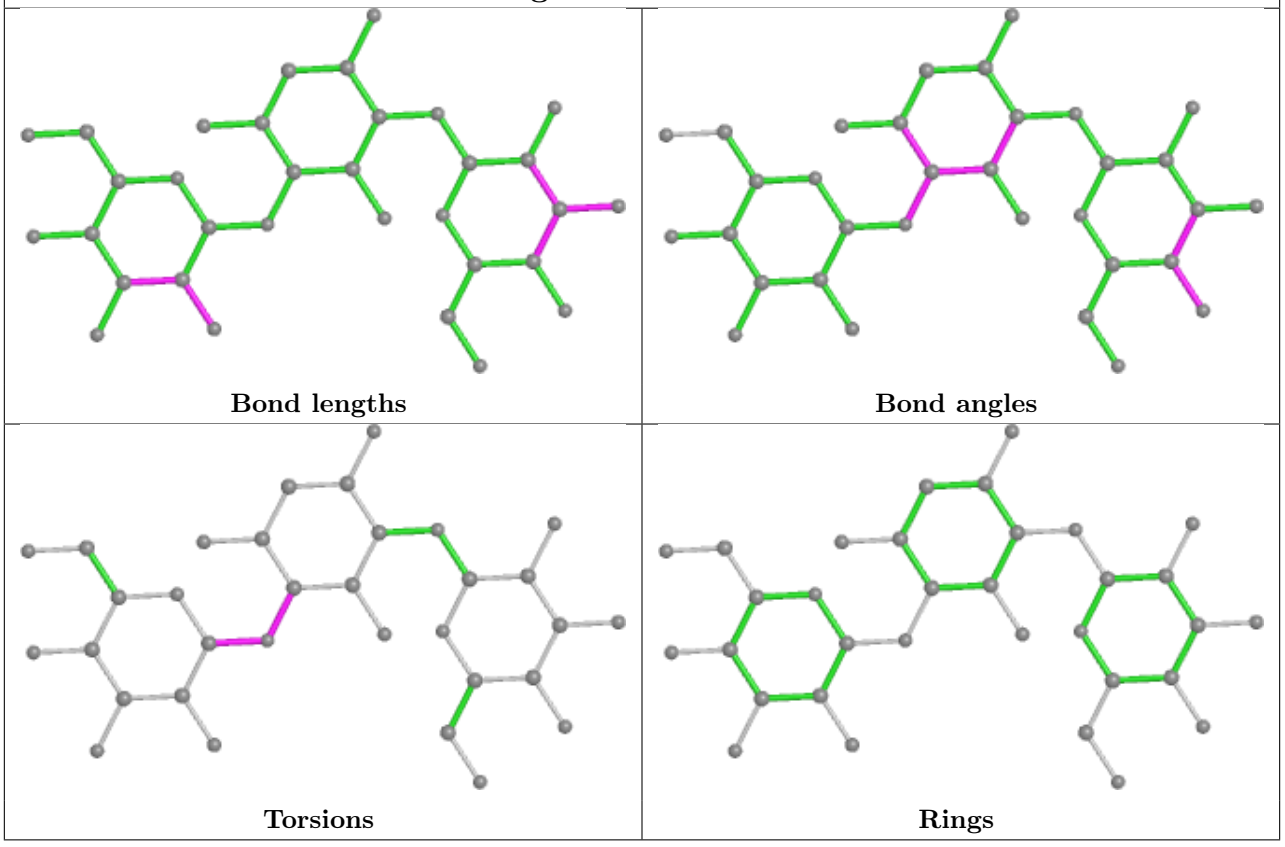


Rings

Ligand COA E 302



Ligand 9CS C 301



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, 95^{th} 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	274/276 (99%)	-0.46	0 100 100	24, 34, 49, 65	0
1	B	275/276 (99%)	-0.32	3 (1%) 80 82	24, 34, 58, 86	0
1	C	273/276 (98%)	-0.52	2 (0%) 87 88	24, 32, 50, 77	0
1	D	275/276 (99%)	-0.35	2 (0%) 87 88	24, 36, 58, 94	0
1	E	276/276 (100%)	-0.32	2 (0%) 87 88	26, 37, 57, 90	0
1	F	275/276 (99%)	-0.40	1 (0%) 92 93	25, 36, 70, 103	0
All	All	1648/1656 (99%)	-0.39	10 (0%) 89 89	24, 35, 58, 103	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	GLY	4.3
1	E	274	LEU	4.1
1	E	273	SER	3.1
1	F	273	SER	3.1
1	B	273	SER	2.8
1	C	273	SER	2.5
1	D	47	TYR	2.5
1	B	68	LYS	2.2
1	B	46	GLN	2.2
1	C	272	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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)

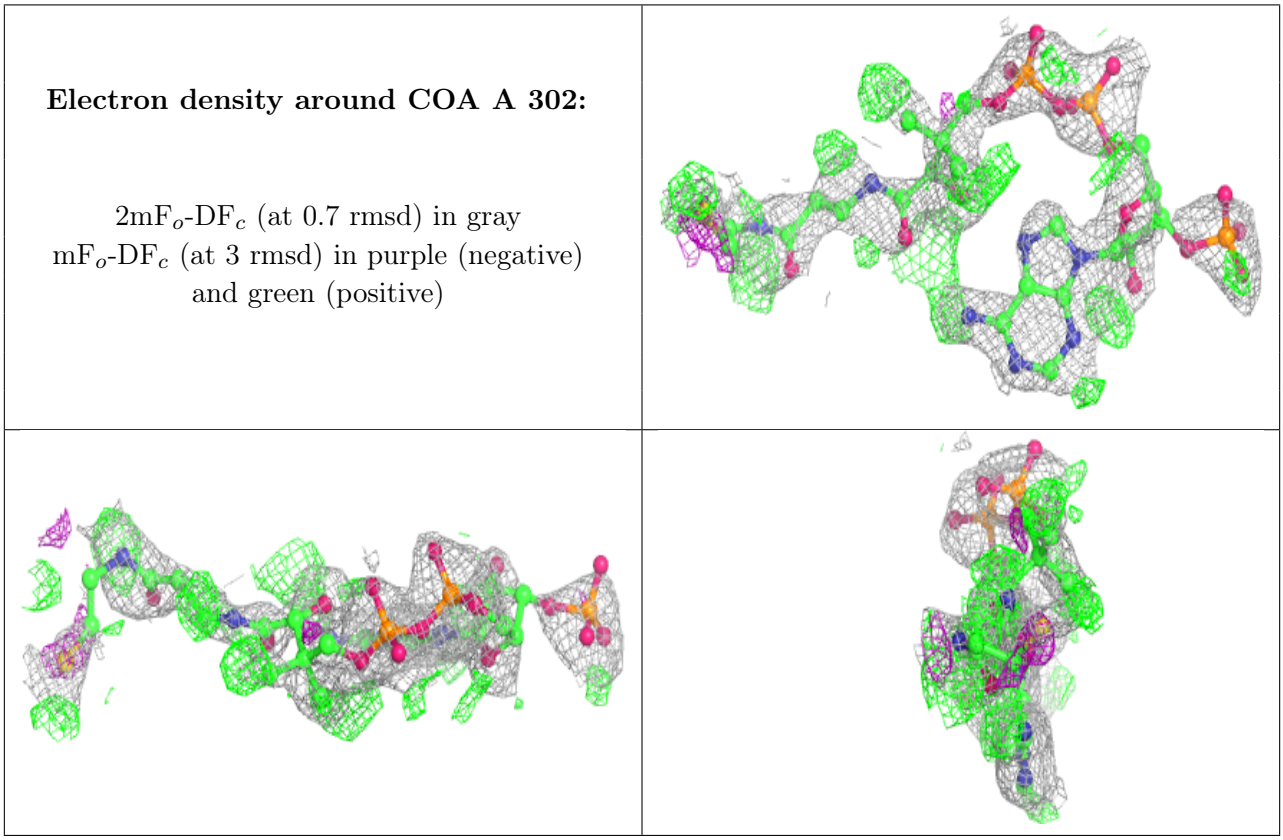
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	COA	A	302	48/48	0.72	0.29	30,39,50,56	48
3	COA	D	302	48/48	0.75	0.24	31,42,60,68	48
3	COA	E	302	48/48	0.80	0.23	35,43,53,58	48
4	EDO	C	304	4/4	0.82	0.19	40,48,48,53	0
4	EDO	C	306	4/4	0.85	0.25	51,53,53,54	0
6	CL	D	305	1/1	0.85	0.12	59,59,59,59	0
4	EDO	B	303	4/4	0.86	0.13	44,48,51,52	0
4	EDO	F	301	4/4	0.86	0.11	53,54,54,55	0
3	COA	B	302	48/48	0.86	0.19	27,38,47,51	48
5	SO4	B	306	5/5	0.87	0.37	47,48,62,66	0
3	COA	C	303	48/48	0.88	0.14	34,43,58,63	48
5	SO4	B	305	5/5	0.90	0.25	42,48,51,63	0
4	EDO	C	305	4/4	0.90	0.18	44,47,48,49	0
5	SO4	D	304	5/5	0.90	0.18	40,45,57,59	0
5	SO4	A	305	5/5	0.90	0.23	64,67,74,85	0
4	EDO	A	303	4/4	0.91	0.19	44,47,47,52	0
5	SO4	E	304	5/5	0.93	0.24	46,52,63,63	0
2	9CS	B	301	33/33	0.94	0.12	28,31,35,39	0
2	9CS	A	301	33/33	0.95	0.10	27,31,35,37	0
2	9CS	C	302	33/33	0.95	0.12	24,30,36,38	0
2	9CS	D	301	33/33	0.95	0.10	28,31,35,37	0
4	EDO	F	302	4/4	0.95	0.11	37,38,39,41	0
2	9CS	E	301	33/33	0.95	0.09	27,33,41,43	0
2	9CS	C	301	33/33	0.96	0.09	25,31,33,38	0
4	EDO	E	303	4/4	0.96	0.08	42,43,43,44	0
5	SO4	F	303	5/5	0.96	0.16	38,42,53,55	0
5	SO4	A	304	5/5	0.96	0.12	44,47,50,54	0
4	EDO	C	307	4/4	0.97	0.12	31,31,34,37	0
5	SO4	B	304	5/5	0.97	0.23	42,49,54,56	0
4	EDO	D	303	4/4	0.98	0.09	36,37,39,40	0
5	SO4	C	308	5/5	0.98	0.08	35,44,46,48	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.

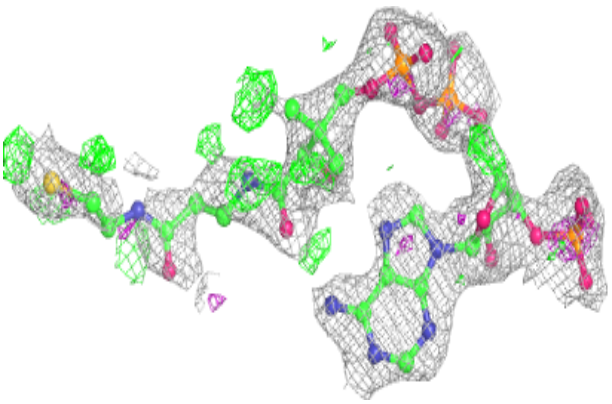
Electron density around COA A 302:

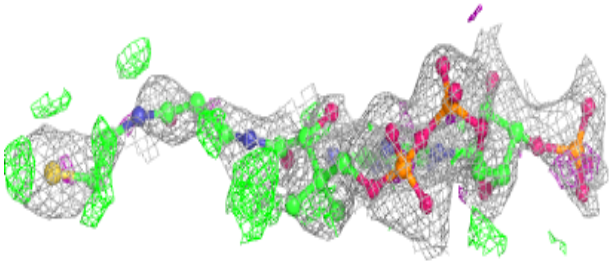
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

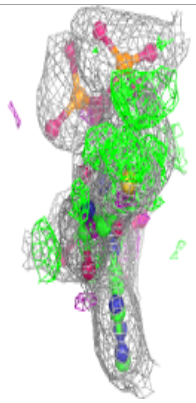


Electron density around COA D 302:

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

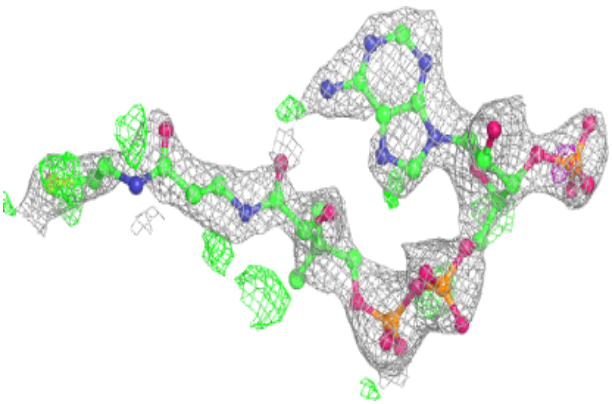


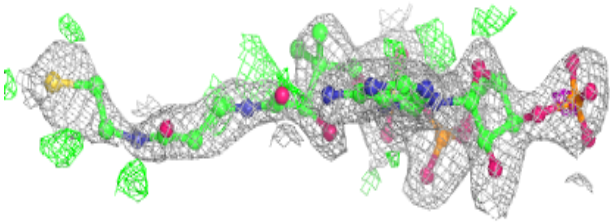


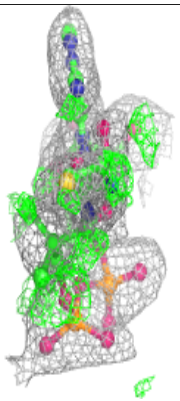


Electron density around COA E 302:

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

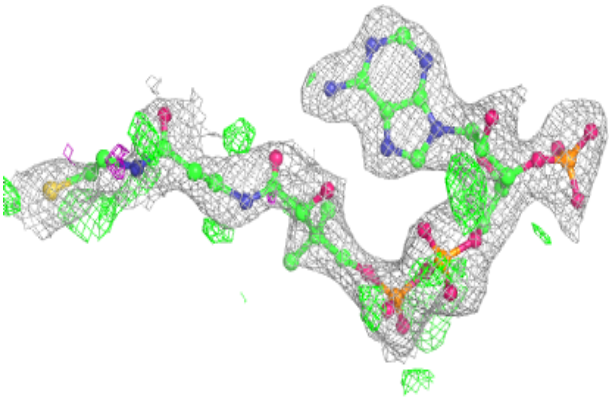


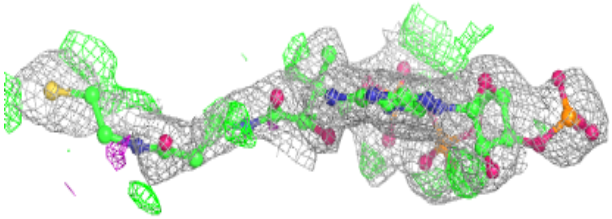


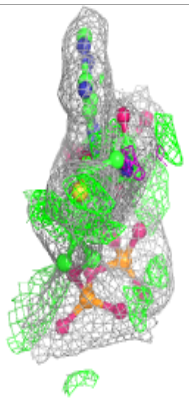


Electron density around COA B 302:

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

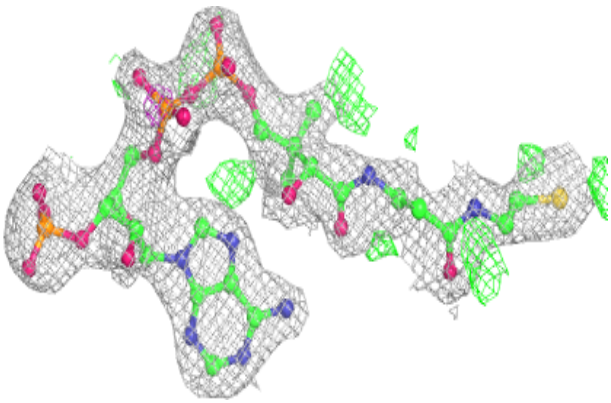


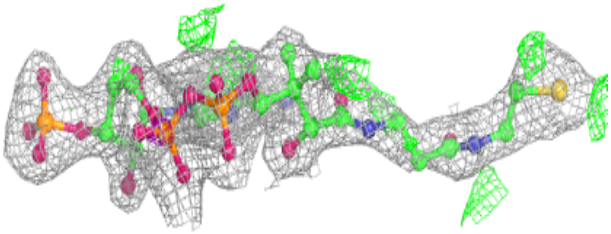


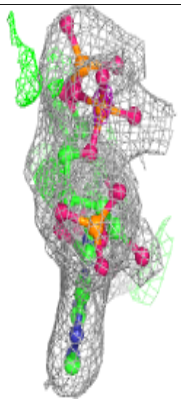


Electron density around COA C 303:

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

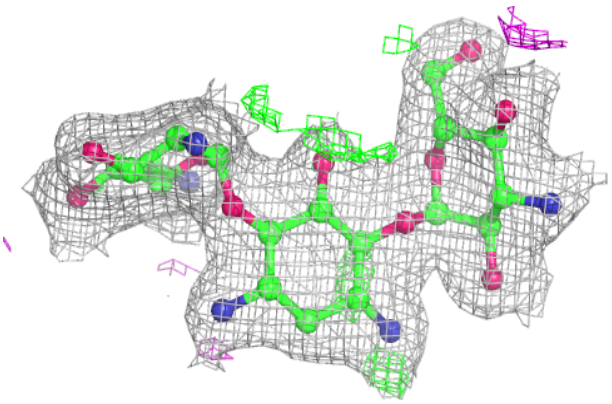


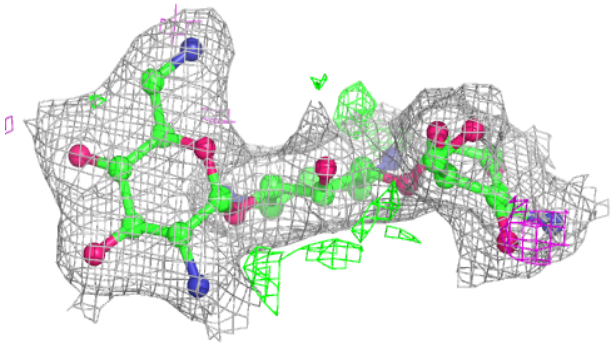


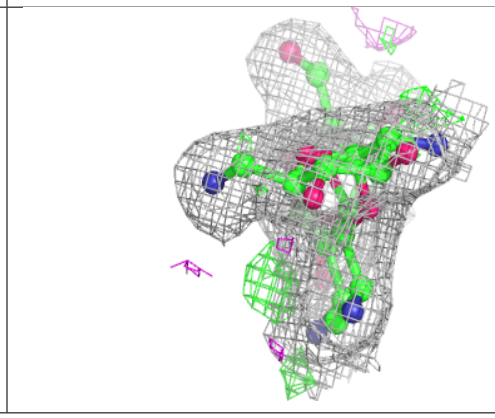


Electron density around 9CS B 301:

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

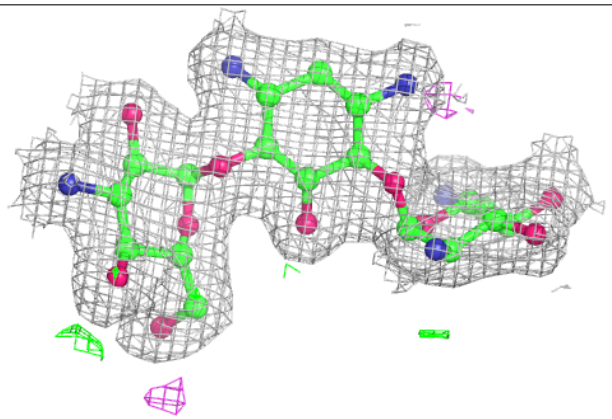


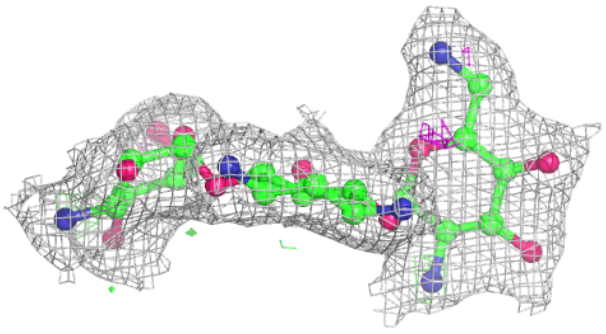


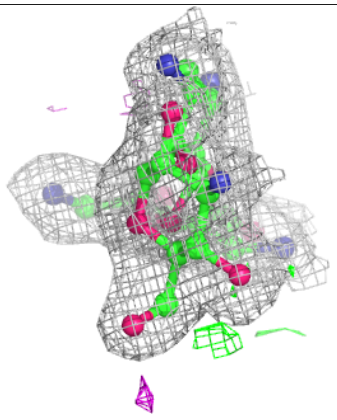


Electron density around 9CS A 301:

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

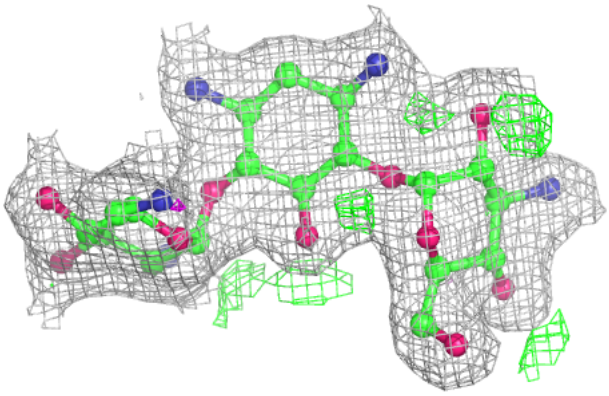


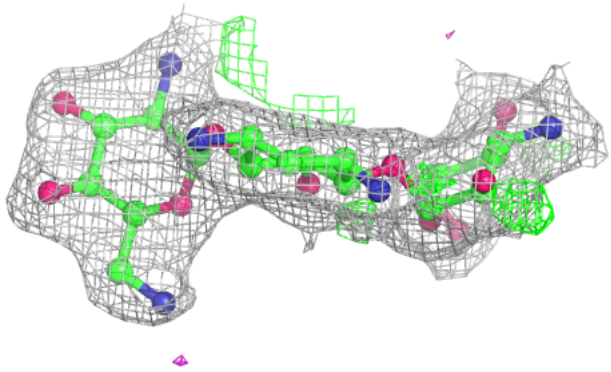


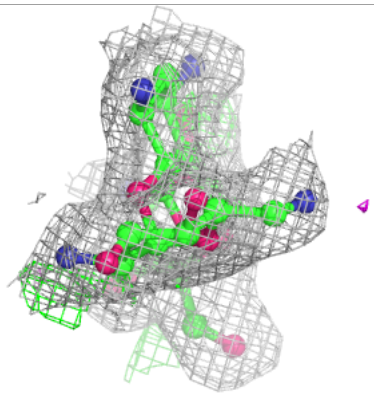


Electron density around 9CS C 302:

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

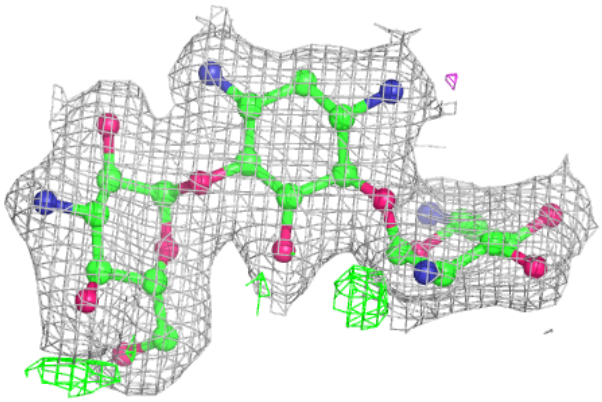


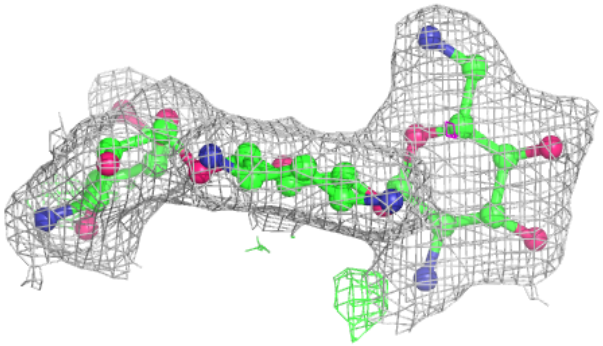


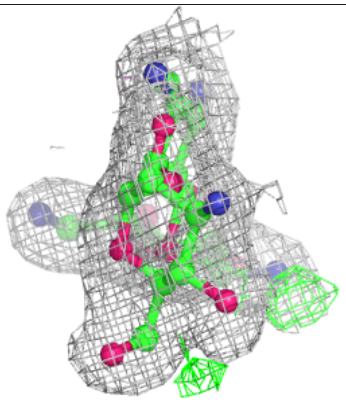


Electron density around 9CS D 301:

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

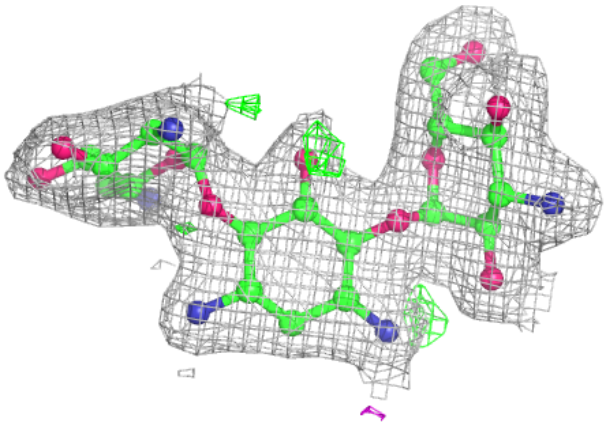


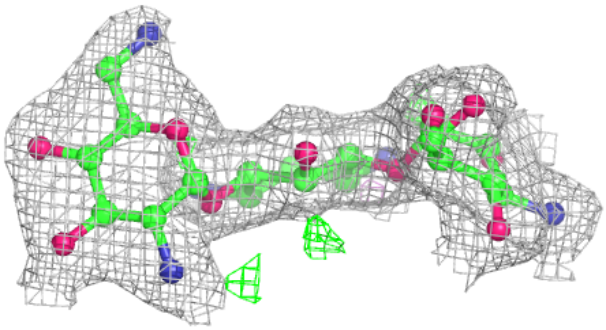


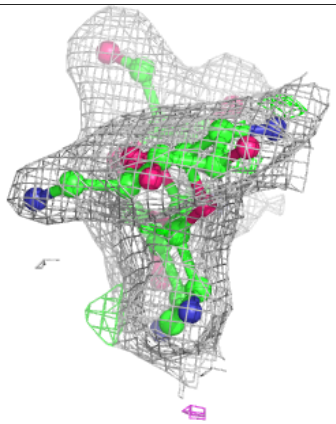


Electron density around 9CS E 301:

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

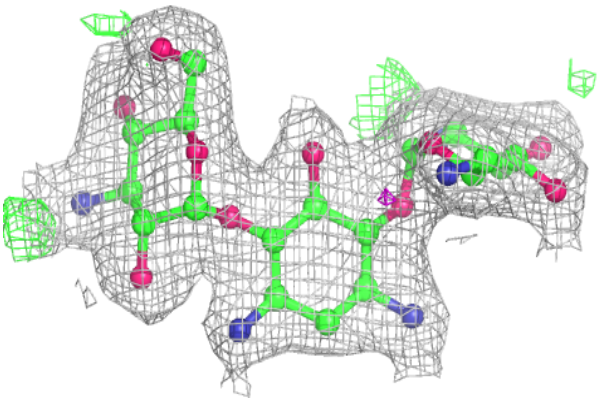


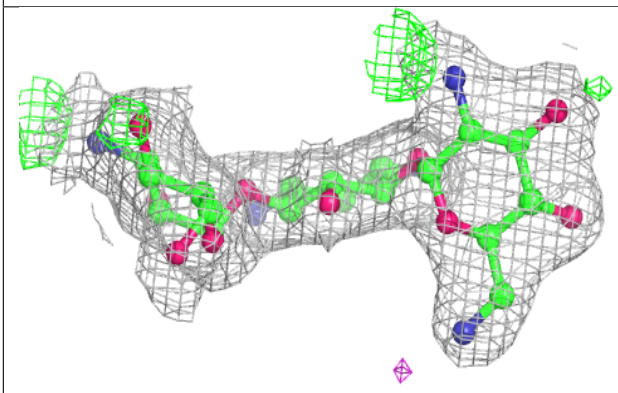


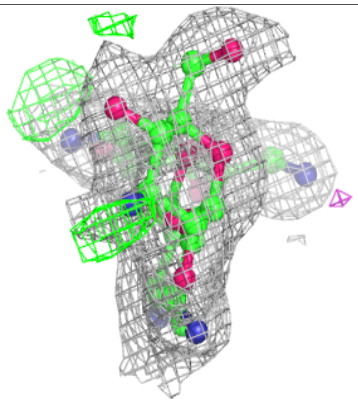


Electron density around 9CS C 301:

$2mF_o$-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.