Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:11 PM EDT

PDB ID	:	6X3C
Title	:	Crystal structure of streptogramin A acetyltransferase VatA from Staphylococcus aureus in complex with streptogramin analog F1037 (47)
Authors	:	Chaires, H.A.; Fraser, J.S.
Deposited on	:	2020-05-21
Resolution	:	3.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

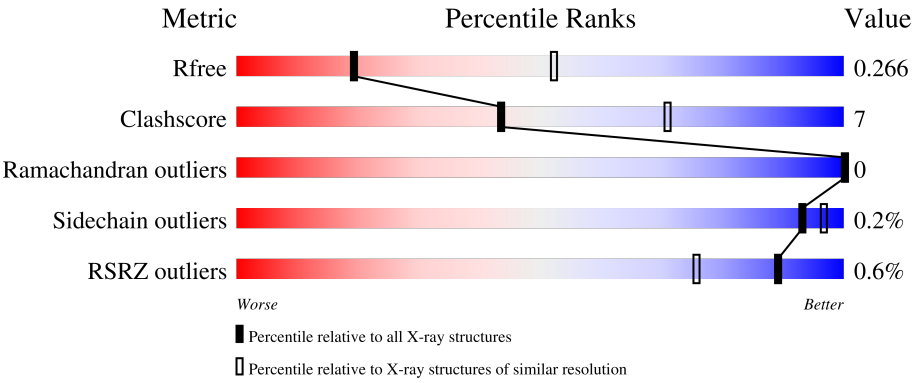
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	207	84% 15%
1	B	207	80% 19% .
1	C	207	88% 11% .
1	D	207	87% 12%
1	E	207	83% 15% .

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Mol	Chain	Length	Quality of chain
1	F	207	2% 88% 11%

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
2	SXA	A	301	X	-	-	-
2	SXA	B	301	X	-	-	-
2	SXA	B	303	X	-	-	-
2	SXA	C	301	X	-	-	-
2	SXA	E	301	X	-	-	-
2	SXA	F	301	X	-	-	-
4	PO4	B	306	-	-	X	-
4	PO4	C	304	-	-	X	-
4	PO4	E	306	-	-	X	-
4	PO4	F	303	-	-	X	-

2 Entry composition

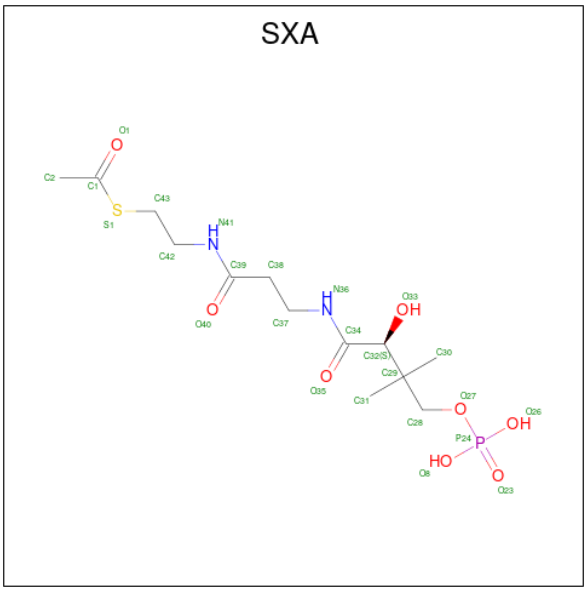
There are 8 unique types of molecules in this entry. The entry contains 20517 atoms, of which 10168 are hydrogens and 0 are deuteriums.

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 Virginiamycin A acetyltransferase.

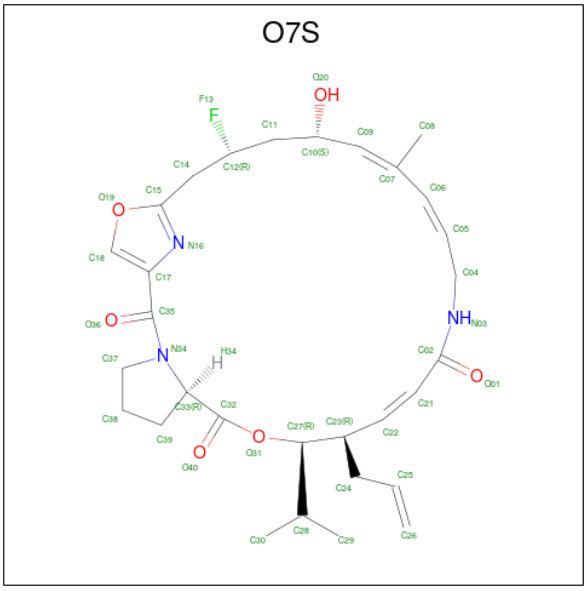
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	207	Total	C	H	N	O	S	0	0	0
			3314	1072	1654	281	299	8			
1	B	204	Total	C	H	N	O	S	0	0	0
			3242	1054	1613	271	296	8			
1	C	205	Total	C	H	N	O	S	0	0	0
			3270	1060	1630	275	297	8			
1	D	206	Total	C	H	N	O	S	0	0	0
			3294	1066	1645	277	298	8			
1	E	203	Total	C	H	N	O	S	0	0	0
			3219	1048	1599	269	295	8			
1	F	206	Total	C	H	N	O	S	0	0	0
			3292	1066	1643	277	298	8			

- Molecule 2 is THIOACETIC ACID S-{2-[3-(2-HYDROXY-3,3-DIMETHYL-4-PHOSPHONOOXY-BUTYRYLAMINO)-PROPIONYLAMINO]-ETHYL} ESTER (three-letter code: SXA) (formula: $C_{13}H_{25}N_2O_8PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			44	13	24	2	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			44	13	24	2	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			44	13	24	2	4	1		
2	C	1	Total	C	H	N	O	S	0	0
			44	13	24	2	4	1		
2	E	1	Total	C	H	N	O	S	0	0
			44	13	24	2	4	1		
2	F	1	Total	C	H	N	O	S	0	0
			44	13	24	2	4	1		

- Molecule 3 is (3R,4R,5E,10E,12E,14S,16R,26aR)-16-fluoro-14-hydroxy-12-methyl-3-(propan-2-yl)-4-(prop-2-en-1-yl)-3,4,8,9,14,15,16,17,24,25,26,26a-dodecahydro-1H,7H,22H-21,18-(azeno)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosine-1,7,22-trione (three-letter code: O7S) (formula: $C_{30}H_{40}FN_3O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	0	0
			80	30	1	40	3	6		
3	B	1	Total	C	F	H	N	O	0	0
			80	30	1	40	3	6		
3	C	1	Total	C	F	H	N	O	0	0
			80	30	1	40	3	6		
3	D	1	Total	C	F	H	N	O	0	0
			80	30	1	40	3	6		

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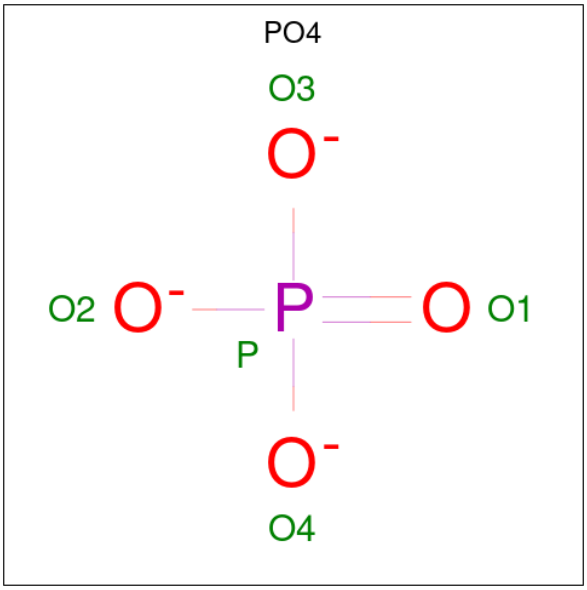
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C F H N O 80 30 1 40 3 6	0	0
3	F	1	Total C F H N O 80 30 1 40 3 6	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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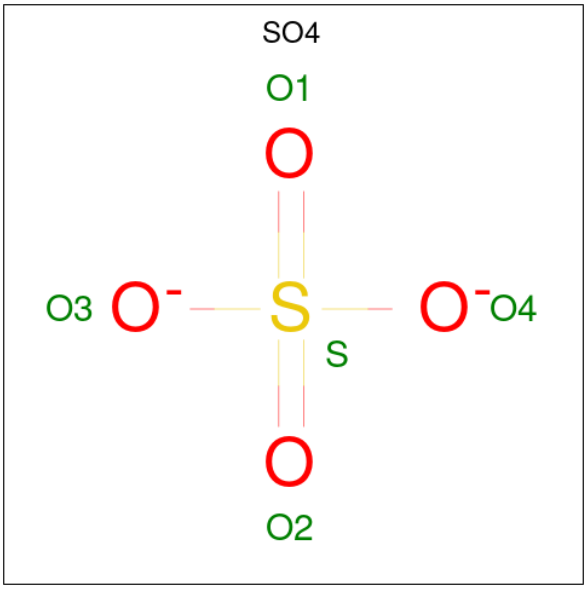
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- 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	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	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	A	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0
6	E	1	Total Cl 1 1	0	0
6	F	2	Total Cl 2 2	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	E	1	Total Mg 1 1	0	0

- Molecule 8 is water.

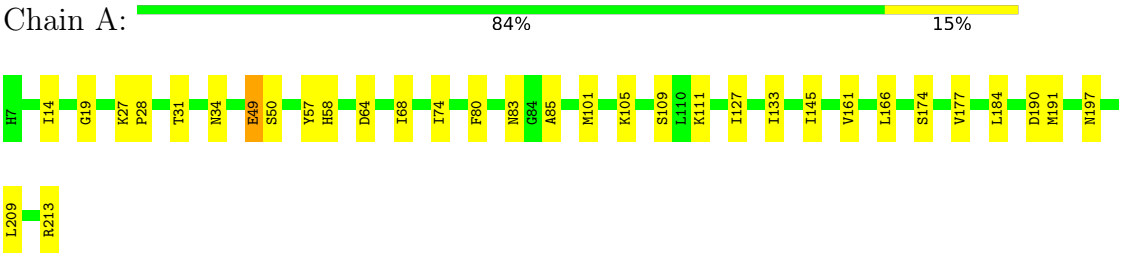
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	7	Total O 7 7	0	0
8	B	14	Total O 14 14	0	0
8	C	8	Total O 8 8	0	0
8	D	6	Total O 6 6	0	0
8	E	3	Total O 3 3	0	0
8	F	6	Total O 6 6	0	0

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.

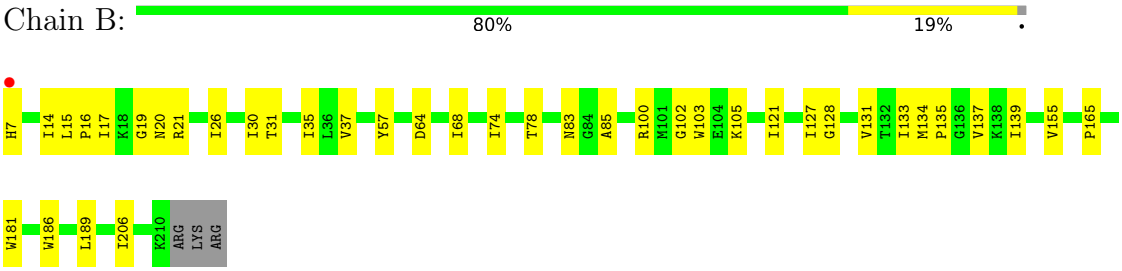
• Molecule 1: Virginiamycin A acetyltransferase

Chain A:



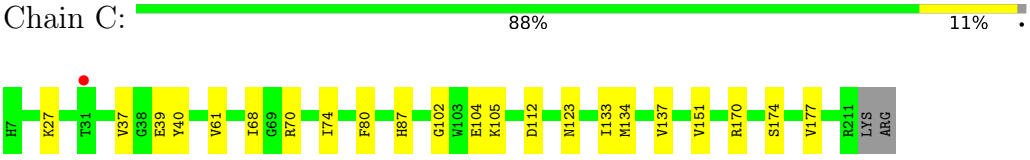
• Molecule 1: Virginiamycin A acetyltransferase

Chain B:



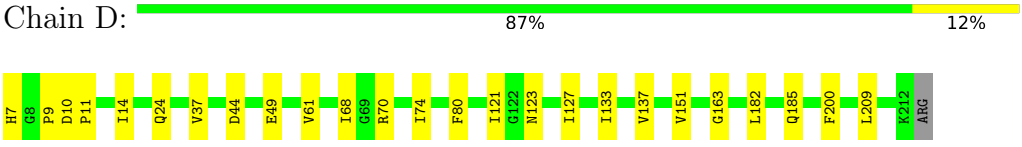
• Molecule 1: Virginiamycin A acetyltransferase

Chain C:



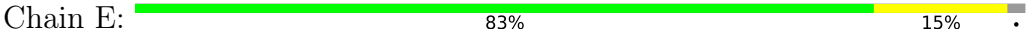
• Molecule 1: Virginiamycin A acetyltransferase

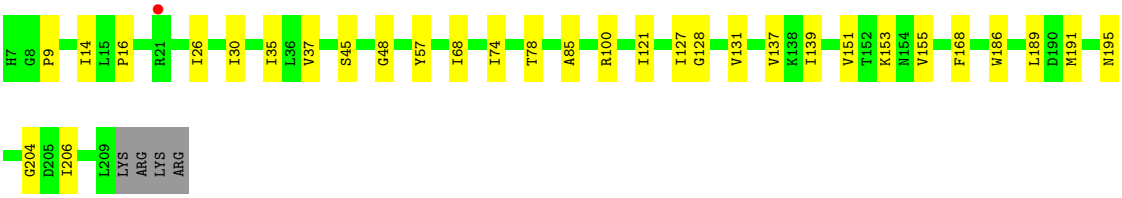
Chain D:



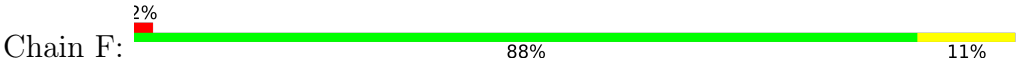
• Molecule 1: Virginiamycin A acetyltransferase

Chain E:





• Molecule 1: Virginiamycin A acetyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.54Å 105.62Å 178.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.14 – 3.05 89.10 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.14-3.05) 100.0 (89.10-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.234 , 0.266 0.234 , 0.266	Depositor DCC
R_{free} test set	1836 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20517	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: SXA, MG, PO4, CL, SO4, O7S

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	0.46	1/1702 (0.1%)	0.53	0/2303
1	B	0.43	0/1671	0.53	1/2264 (0.0%)
1	C	0.44	1/1682 (0.1%)	0.55	0/2278
1	D	0.32	0/1691	0.51	0/2289
1	E	0.29	0/1662	0.49	1/2253 (0.0%)
1	F	0.41	2/1691 (0.1%)	0.52	0/2289
All	All	0.40	4/10099 (0.0%)	0.52	2/13676 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLU	CD-OE1	-6.65	1.18	1.25
1	F	104	GLU	CD-OE2	-5.70	1.19	1.25
1	C	104	GLU	CD-OE2	-5.65	1.19	1.25
1	F	104	GLU	CD-OE1	-5.12	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	CB-CA-C	5.42	121.24	110.40
1	E	100	ARG	CB-CA-C	5.01	120.42	110.40

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	1660	1654	1654	28	1
1	B	1629	1613	1616	32	2
1	C	1640	1630	1629	19	1
1	D	1649	1645	1644	18	0
1	E	1620	1599	1600	21	0
1	F	1649	1643	1643	18	9
2	A	20	24	21	0	0
2	B	40	48	42	4	0
2	C	20	24	21	1	0
2	E	20	24	21	1	0
2	F	20	24	21	3	0
3	A	40	40	0	1	0
3	B	40	40	0	1	0
3	C	40	40	0	1	0
3	D	40	40	0	1	0
3	E	40	40	0	1	0
3	F	40	40	0	1	0
4	A	5	0	0	0	0
4	B	10	0	0	1	7
4	C	15	0	0	4	0
4	D	10	0	0	0	0
4	E	20	0	0	2	0
4	F	10	0	0	2	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	D	5	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	1	0
6	D	1	0	0	1	0
6	E	1	0	0	0	0
6	F	2	0	0	1	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
8	A	7	0	0	1	0
8	B	14	0	0	3	0
8	C	8	0	0	2	0
8	D	6	0	0	3	0
8	E	3	0	0	0	0
8	F	6	0	0	0	0
All	All	10349	10168	9912	136	10

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 7.

All (136) 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:7:HIS:CE1	1:C:102:GLY:HA3	1.69	1.27
1:E:153:LYS:NZ	4:E:306:PO4:O3	1.83	1.11
1:A:101:MET:SD	1:E:9:PRO:HA	1.94	1.07
1:D:44:ASP:OD2	8:D:501:HOH:O	1.86	0.90
1:A:31:THR:HG21	1:B:19:GLY:HA2	1.54	0.88
1:B:7:HIS:CE1	1:C:102:GLY:CA	2.57	0.84
1:D:70:ARG:N	1:D:123:ASN:OD1	2.10	0.82
4:C:304:PO4:O2	8:C:401:HOH:O	2.01	0.77
4:B:305:PO4:O2	8:D:501:HOH:O	2.05	0.75
1:B:7:HIS:HE1	1:C:102:GLY:HA3	1.43	0.75
1:D:68:ILE:HD13	1:D:74:ILE:HD11	1.70	0.73
1:F:170:ARG:HH12	2:F:301:SXA:H31B	1.55	0.72
1:C:68:ILE:HD13	1:C:74:ILE:HD11	1.73	0.71
8:A:405:HOH:O	6:F:305:CL:CL	2.46	0.70
1:F:170:ARG:HH12	2:F:301:SXA:C31	2.05	0.69
1:F:34:ASN:HB3	1:F:65:LYS:HG2	1.74	0.68
2:B:301:SXA:O35	8:B:401:HOH:O	2.10	0.68
1:F:200:PHE:HB2	1:F:209:LEU:HD21	1.74	0.68
1:A:31:THR:HG21	1:B:19:GLY:CA	2.23	0.68
1:E:45:SER:OG	1:E:48:GLY:HA2	1.94	0.67
1:A:31:THR:CG2	1:B:19:GLY:HA2	2.23	0.67
1:C:137:VAL:HG11	1:C:151:VAL:HG12	1.78	0.66
1:E:137:VAL:HG11	1:E:151:VAL:HG12	1.77	0.65
1:D:137:VAL:HG11	1:D:151:VAL:HG12	1.78	0.64
1:C:80:PHE:CE2	1:C:133:ILE:HD12	2.35	0.62
4:C:304:PO4:O2	8:C:402:HOH:O	2.16	0.61
1:D:80:PHE:CE2	1:D:133:ILE:HD12	2.36	0.60
1:B:57:TYR:CG	1:B:85:ALA:HB2	2.36	0.60
1:E:137:VAL:HG11	1:E:151:VAL:CG1	2.30	0.60
1:A:34:ASN:HB2	1:A:58:HIS:NE2	2.17	0.59
1:D:10:ASP:OD1	1:D:11:PRO:HD2	2.02	0.59
8:B:414:HOH:O	6:C:306:CL:CL	2.54	0.58
1:B:133:ILE:HG23	1:B:137:VAL:HG21	1.84	0.58
1:E:45:SER:OG	1:E:48:GLY:CA	2.52	0.57
1:A:197:ASN:HB3	1:A:209:LEU:CD2	2.37	0.54
1:A:184:LEU:HD21	1:A:209:LEU:HD13	1.88	0.54
1:A:213:ARG:HA	1:A:213:ARG:HE	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:TYR:CG	1:E:85:ALA:HB2	2.43	0.54
1:A:209:LEU:O	1:A:213:ARG:HG2	2.09	0.53
1:B:7:HIS:HE1	1:C:102:GLY:CA	2.08	0.53
1:A:197:ASN:HB3	1:A:209:LEU:HD21	1.89	0.53
1:C:137:VAL:HG11	1:C:151:VAL:CG1	2.39	0.53
1:A:57:TYR:CD2	1:A:85:ALA:HB2	2.43	0.53
1:B:57:TYR:CD2	1:B:85:ALA:HB2	2.43	0.53
1:B:102:GLY:HA3	1:D:7:HIS:NE2	2.23	0.52
1:F:68:ILE:HD13	1:F:74:ILE:HD11	1.92	0.51
1:D:137:VAL:HG11	1:D:151:VAL:CG1	2.40	0.51
1:A:68:ILE:HD13	1:A:74:ILE:HD11	1.92	0.51
1:C:27:LYS:NZ	4:C:303:PO4:O3	2.31	0.51
1:B:26:ILE:HB	1:B:37:VAL:HG11	1.92	0.51
1:A:14:ILE:HD12	1:B:15:LEU:HB2	1.92	0.50
1:E:168:PHE:N	4:E:306:PO4:O4	2.38	0.50
1:D:68:ILE:HD13	1:D:74:ILE:CD1	2.41	0.50
1:C:61:VAL:HG22	1:C:61:VAL:O	2.11	0.50
1:E:26:ILE:HB	1:E:37:VAL:HG11	1.94	0.49
1:E:139:ILE:HG23	1:E:155:VAL:HB	1.95	0.49
1:E:191:MET:O	1:E:195:ASN:ND2	2.45	0.49
1:F:200:PHE:HB2	1:F:209:LEU:CD2	2.43	0.49
1:C:170:ARG:HH12	2:C:301:SXA:C31	2.26	0.49
1:C:174:SER:OG	1:C:177:VAL:HG23	2.14	0.48
1:F:80:PHE:CE2	1:F:133:ILE:HD12	2.49	0.48
1:F:35:ILE:HG22	1:F:35:ILE:O	2.14	0.48
1:A:80:PHE:CE2	1:A:133:ILE:HD12	2.49	0.48
1:B:133:ILE:CG2	1:B:137:VAL:HG21	2.44	0.48
1:E:57:TYR:CD2	1:E:85:ALA:HB2	2.49	0.47
1:F:70:ARG:NH2	4:F:303:PO4:O1	2.38	0.47
1:E:30:ILE:HD12	1:E:35:ILE:HG21	1.96	0.47
1:F:57:TYR:CD2	1:F:85:ALA:HB2	2.50	0.47
1:A:101:MET:SD	1:E:9:PRO:CA	2.86	0.46
1:B:186:TRP:HA	1:B:189:LEU:HG	1.97	0.46
1:A:57:TYR:CG	1:A:85:ALA:HB2	2.50	0.46
1:A:213:ARG:HA	1:A:213:ARG:NE	2.31	0.46
1:E:204:GLY:O	1:E:206:ILE:N	2.47	0.46
1:C:68:ILE:HD13	1:C:74:ILE:CD1	2.44	0.46
1:D:61:VAL:O	1:D:61:VAL:HG22	2.16	0.45
1:D:37:VAL:HG13	1:D:68:ILE:HB	1.99	0.45
1:F:207:GLU:OE2	1:F:207:GLU:HA	2.15	0.45
1:B:121:ILE:HD13	1:B:127:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:O	1:C:40:TYR:HB2	2.17	0.45
1:C:70:ARG:N	1:C:123:ASN:OD1	2.21	0.45
1:D:14:ILE:O	1:D:24:GLN:HA	2.17	0.44
1:B:30:ILE:HD12	1:B:35:ILE:HG21	1.99	0.44
1:B:134:MET:O	1:B:137:VAL:HG22	2.18	0.44
1:B:21:ARG:O	1:B:21:ARG:HG2	2.17	0.44
6:D:405:CL:CL	8:D:506:HOH:O	2.58	0.44
1:E:186:TRP:HA	1:E:189:LEU:HG	2.00	0.43
1:B:68:ILE:HD13	1:B:74:ILE:HD11	1.98	0.43
1:A:161:VAL:HG21	1:A:166:LEU:HD21	2.00	0.43
1:B:128:GLY:HA2	2:B:301:SXA:H42	2.00	0.43
1:A:49:GLU:O	1:A:49:GLU:HG2	2.18	0.43
1:B:181:TRP:NE1	1:B:206:ILE:HD13	2.34	0.43
1:F:27:LYS:HB3	1:F:28:PRO:HD3	2.01	0.43
1:E:121:ILE:HD13	1:E:127:ILE:HD11	2.01	0.42
1:F:27:LYS:NZ	4:F:303:PO4:O4	2.52	0.42
1:A:190:ASP:OD1	1:A:191:MET:N	2.52	0.42
1:B:64:ASP:OD2	1:B:83:ASN:HB2	2.19	0.42
1:F:170:ARG:NH1	2:F:301:SXA:C31	2.79	0.42
1:A:127:ILE:HD13	1:A:133:ILE:HD11	2.01	0.42
2:B:303:SXA:H2	8:B:405:HOH:O	2.19	0.42
1:B:181:TRP:CZ2	1:B:206:ILE:HG21	2.55	0.42
1:E:78:THR:HA	1:E:131:VAL:O	2.20	0.42
1:A:68:ILE:HD13	1:A:74:ILE:CD1	2.50	0.42
1:E:128:GLY:HA2	2:E:301:SXA:H42	2.01	0.42
3:E:302:O7S:N16	3:E:302:O7S:C37	2.83	0.42
1:A:19:GLY:HA2	1:B:31:THR:HG21	2.02	0.42
1:B:14:ILE:O	1:B:16:PRO:HD3	2.20	0.42
1:C:37:VAL:HG13	1:C:68:ILE:HB	2.02	0.42
1:C:87:HIS:N	1:C:87:HIS:CD2	2.88	0.42
1:C:112:ASP:OD2	4:C:305:PO4:O4	2.38	0.42
1:E:68:ILE:HD13	1:E:74:ILE:HD11	2.02	0.42
1:D:121:ILE:HD13	1:D:127:ILE:HD11	2.01	0.41
3:D:401:O7S:N16	3:D:401:O7S:C37	2.83	0.41
1:B:165:PRO:HD3	1:D:163:GLY:HA3	2.02	0.41
3:B:302:O7S:N16	3:B:302:O7S:C37	2.83	0.41
1:F:145:ILE:HD13	1:F:161:VAL:HG22	2.03	0.41
1:B:17:ILE:HB	1:B:20:ASN:HB3	2.02	0.41
1:B:134:MET:HE3	1:B:135:PRO:HD3	2.02	0.41
1:A:64:ASP:OD2	1:A:83:ASN:HB2	2.21	0.41
1:B:103:TRP:CZ2	1:D:9:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLU:OE1	1:D:49:GLU:N	2.46	0.41
1:F:127:ILE:HD13	1:F:133:ILE:HD11	2.03	0.41
2:B:301:SXA:H37A	1:C:134:MET:CE	2.51	0.41
1:D:200:PHE:HB2	1:D:209:LEU:HD21	2.02	0.41
1:F:57:TYR:CG	1:F:85:ALA:HB2	2.56	0.41
3:C:302:O7S:N16	3:C:302:O7S:C37	2.84	0.41
1:E:14:ILE:O	1:E:16:PRO:HD3	2.20	0.41
1:A:27:LYS:HB3	1:A:28:PRO:HD3	2.03	0.40
1:A:145:ILE:HD13	1:A:161:VAL:HG22	2.03	0.40
3:A:302:O7S:N16	3:A:302:O7S:C37	2.84	0.40
1:B:78:THR:HA	1:B:131:VAL:O	2.21	0.40
1:F:161:VAL:HG21	1:F:166:LEU:HD21	2.03	0.40
1:D:182:LEU:O	1:D:185:GLN:HG3	2.22	0.40
3:F:302:O7S:N16	3:F:302:O7S:C37	2.83	0.40
1:A:174:SER:OG	1:A:177:VAL:HG23	2.21	0.40
1:B:139:ILE:HG23	1:B:155:VAL:HB	2.03	0.40
1:A:109:SER:OG	1:A:111:LYS:HG2	2.22	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:LYS:NZ	4:B:306:PO4:O4[3_544]	0.78	1.42
1:F:105:LYS:HZ3	4:B:306:PO4:O4[3_544]	0.78	0.82
1:F:105:LYS:HZ1	4:B:306:PO4:O4[3_544]	0.88	0.72
1:F:105:LYS:NZ	4:B:306:PO4:P[3_544]	1.70	0.50
1:A:105:LYS:HZ2	1:C:105:LYS:HZ3[4_455]	1.20	0.40
1:B:105:LYS:NZ	1:F:105:LYS:HZ2[3_554]	1.20	0.40
1:F:105:LYS:CE	4:B:306:PO4:O4[3_544]	1.81	0.39
1:F:105:LYS:HZ1	4:B:306:PO4:P[3_544]	1.35	0.25
1:B:105:LYS:NZ	1:F:105:LYS:NZ[3_554]	2.02	0.18
1:F:105:LYS:NZ	4:B:306:PO4:O2[3_544]	2.14	0.06

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	205/207 (99%)	199 (97%)	6 (3%)	0	100	100
1	B	202/207 (98%)	194 (96%)	8 (4%)	0	100	100
1	C	203/207 (98%)	193 (95%)	10 (5%)	0	100	100
1	D	204/207 (99%)	193 (95%)	11 (5%)	0	100	100
1	E	201/207 (97%)	192 (96%)	9 (4%)	0	100	100
1	F	204/207 (99%)	196 (96%)	8 (4%)	0	100	100
All	All	1219/1242 (98%)	1167 (96%)	52 (4%)	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	179/179 (100%)	178 (99%)	1 (1%)	86	93
1	B	176/179 (98%)	176 (100%)	0	100	100
1	C	177/179 (99%)	177 (100%)	0	100	100
1	D	178/179 (99%)	178 (100%)	0	100	100
1	E	175/179 (98%)	175 (100%)	0	100	100
1	F	178/179 (99%)	177 (99%)	1 (1%)	86	93
All	All	1063/1074 (99%)	1061 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	F	101	MET

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

Mol	Chain	Res	Type
1	B	7	HIS
1	D	13	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 8 are 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	$\#\|Z\| > 2$
4	PO4	B	306	-	4,4,4	0.93	0	6,6,6	0.48	0
3	O7S	E	302	-	36,42,42	1.28	3 (8%)	42,57,57	1.00	3 (7%)
4	PO4	C	304	-	4,4,4	0.93	0	6,6,6	0.35	0
2	SXA	B	301	-	18,19,24	1.63	1 (5%)	23,25,33	1.22	3 (13%)
4	PO4	E	307	-	4,4,4	0.88	0	6,6,6	0.40	0
4	PO4	F	303	-	4,4,4	0.89	0	6,6,6	0.51	0
3	O7S	F	302	-	36,42,42	1.28	2 (5%)	42,57,57	0.94	2 (4%)
4	PO4	C	305	-	4,4,4	0.91	0	6,6,6	0.46	0
3	O7S	B	302	-	36,42,42	1.32	3 (8%)	42,57,57	1.05	3 (7%)
4	PO4	D	403	-	4,4,4	0.87	0	6,6,6	0.51	0
3	O7S	D	401	-	36,42,42	1.28	2 (5%)	42,57,57	0.92	3 (7%)
4	PO4	B	305	-	4,4,4	0.89	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SXA	F	301	-	18,19,24	1.75	1 (5%)	23,25,33	1.26	4 (17%)
2	SXA	E	301	-	18,19,24	1.64	1 (5%)	23,25,33	1.20	3 (13%)
2	SXA	A	301	-	18,19,24	1.72	1 (5%)	23,25,33	1.31	4 (17%)
2	SXA	C	301	-	18,19,24	1.79	1 (5%)	23,25,33	1.26	4 (17%)
4	PO4	D	402	-	4,4,4	0.87	0	6,6,6	0.46	0
4	PO4	F	304	-	4,4,4	0.87	0	6,6,6	0.44	0
3	O7S	A	302	-	36,42,42	1.28	2 (5%)	42,57,57	0.93	2 (4%)
5	SO4	B	307	-	4,4,4	0.13	0	6,6,6	0.17	0
4	PO4	E	305	-	4,4,4	0.89	0	6,6,6	0.40	0
4	PO4	E	306	-	4,4,4	0.87	0	6,6,6	0.43	0
5	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.16	0
5	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.14	0
4	PO4	E	304	-	4,4,4	0.93	0	6,6,6	0.35	0
5	SO4	B	308	-	4,4,4	0.17	0	6,6,6	0.04	0
4	PO4	A	303	-	4,4,4	0.85	0	6,6,6	0.43	0
4	PO4	C	303	-	4,4,4	0.92	0	6,6,6	0.44	0
2	SXA	B	303	-	18,19,24	1.78	1 (5%)	23,25,33	1.21	4 (17%)
3	O7S	C	302	-	36,42,42	1.24	2 (5%)	42,57,57	0.88	2 (4%)

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
3	O7S	B	302	-	-	6/45/61/61	0/2/3/3
3	O7S	D	401	-	-	1/45/61/61	0/2/3/3
2	SXA	F	301	-	1/1/7/8	10/23/23/30	-
2	SXA	E	301	-	1/1/7/8	11/23/23/30	-
2	SXA	A	301	-	1/1/7/8	10/23/23/30	-
2	SXA	C	301	-	1/1/7/8	11/23/23/30	-
3	O7S	E	302	-	-	5/45/61/61	0/2/3/3
3	O7S	A	302	-	-	1/45/61/61	0/2/3/3
2	SXA	B	301	-	1/1/7/8	11/23/23/30	-
2	SXA	B	303	-	1/1/7/8	10/23/23/30	-
3	O7S	C	302	-	-	1/45/61/61	0/2/3/3
3	O7S	F	302	-	-	1/45/61/61	0/2/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SXA	C29-C32	6.70	1.59	1.55
2	B	303	SXA	C29-C32	6.69	1.59	1.55
2	F	301	SXA	C29-C32	6.49	1.59	1.55
2	A	301	SXA	C29-C32	6.39	1.59	1.55
2	E	301	SXA	C29-C32	5.96	1.59	1.55
2	B	301	SXA	C29-C32	5.96	1.59	1.55
3	B	302	O7S	C14-C15	3.96	1.52	1.49
3	D	401	O7S	C14-C15	3.78	1.51	1.49
3	A	302	O7S	C14-C15	3.75	1.51	1.49
3	F	302	O7S	C14-C15	3.62	1.51	1.49
3	E	302	O7S	C14-C15	3.46	1.51	1.49
3	C	302	O7S	C14-C15	3.18	1.51	1.49
3	E	302	O7S	C17-C35	-3.17	1.45	1.50
3	B	302	O7S	C17-C35	-3.15	1.45	1.50
3	F	302	O7S	C17-C35	-3.09	1.45	1.50
3	C	302	O7S	C17-C35	-3.06	1.45	1.50
3	A	302	O7S	C17-C35	-2.97	1.45	1.50
3	D	401	O7S	C17-C35	-2.92	1.45	1.50
3	E	302	O7S	C21-C02	-2.18	1.43	1.48
3	B	302	O7S	C21-C02	-2.14	1.43	1.48

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	SXA	C37-N36-C34	2.84	127.66	122.59
2	A	301	SXA	C43-C42-N41	2.79	118.29	112.42
2	E	301	SXA	C37-N36-C34	2.74	127.48	122.59
2	A	301	SXA	C37-N36-C34	2.65	127.31	122.59
2	F	301	SXA	C43-C42-N41	2.64	117.96	112.42
2	B	301	SXA	C37-C38-C39	2.62	116.72	112.36
2	E	301	SXA	C37-C38-C39	2.52	116.55	112.36
3	B	302	O7S	C04-N03-C02	2.48	126.04	122.03
2	F	301	SXA	C37-N36-C34	2.42	126.91	122.59
2	B	303	SXA	C38-C37-N36	2.41	116.77	111.90
3	F	302	O7S	C04-N03-C02	2.39	125.90	122.03
2	A	301	SXA	C37-C38-C39	2.38	116.33	112.36
3	E	302	O7S	C04-N03-C02	2.36	125.85	122.03
2	B	301	SXA	C43-C42-N41	2.36	117.38	112.42
2	C	301	SXA	C38-C37-N36	2.32	116.57	111.90
2	F	301	SXA	C37-C38-C39	2.27	116.14	112.36
2	C	301	SXA	C43-C42-N41	2.27	117.18	112.42
3	A	302	O7S	C04-N03-C02	2.23	125.64	122.03
2	C	301	SXA	C37-N36-C34	2.21	126.53	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	SXA	C37-C38-C39	2.21	116.03	112.36
3	C	302	O7S	C04-N03-C02	2.18	125.56	122.03
3	D	401	O7S	C04-N03-C02	2.17	125.54	122.03
3	B	302	O7S	C38-C37-N34	2.16	107.03	103.25
2	E	301	SXA	C43-C42-N41	2.15	116.94	112.42
3	D	401	O7S	C38-C37-N34	2.14	107.00	103.25
3	A	302	O7S	C38-C37-N34	2.11	106.95	103.25
3	F	302	O7S	C38-C37-N34	2.10	106.93	103.25
3	E	302	O7S	C38-C37-N34	2.08	106.90	103.25
3	E	302	O7S	C27-O31-C32	2.08	121.35	117.78
3	B	302	O7S	C08-C07-C06	2.07	121.34	118.08
3	C	302	O7S	C38-C37-N34	2.06	106.87	103.25
2	B	303	SXA	C37-N36-C34	2.06	126.26	122.59
2	A	301	SXA	C38-C37-N36	2.05	116.04	111.90
3	D	401	O7S	C08-C07-C06	2.04	121.29	118.08
2	B	303	SXA	C43-C42-N41	2.04	116.69	112.42
2	B	303	SXA	C37-C38-C39	2.03	115.73	112.36
2	F	301	SXA	C38-C37-N36	2.01	115.96	111.90

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	SXA	C32
2	B	301	SXA	C32
2	B	303	SXA	C32
2	C	301	SXA	C32
2	E	301	SXA	C32
2	F	301	SXA	C32

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SXA	C28-C29-C32-O33
2	A	301	SXA	C28-C29-C32-C34
2	A	301	SXA	C30-C29-C32-O33
2	A	301	SXA	C30-C29-C32-C34
2	A	301	SXA	C31-C29-C32-O33
2	A	301	SXA	C31-C29-C32-C34
2	B	301	SXA	C28-C29-C32-O33
2	B	301	SXA	C28-C29-C32-C34
2	B	301	SXA	C30-C29-C32-O33
2	B	301	SXA	C30-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
2	B	301	SXA	C31-C29-C32-O33
2	B	301	SXA	C31-C29-C32-C34
2	B	303	SXA	C28-C29-C32-O33
2	B	303	SXA	C28-C29-C32-C34
2	B	303	SXA	C30-C29-C32-O33
2	B	303	SXA	C30-C29-C32-C34
2	B	303	SXA	C31-C29-C32-O33
2	B	303	SXA	C31-C29-C32-C34
2	C	301	SXA	C28-C29-C32-O33
2	C	301	SXA	C28-C29-C32-C34
2	C	301	SXA	C30-C29-C32-O33
2	C	301	SXA	C30-C29-C32-C34
2	C	301	SXA	C31-C29-C32-O33
2	C	301	SXA	C31-C29-C32-C34
2	E	301	SXA	C28-C29-C32-O33
2	E	301	SXA	C28-C29-C32-C34
2	E	301	SXA	C30-C29-C32-O33
2	E	301	SXA	C30-C29-C32-C34
2	E	301	SXA	C31-C29-C32-O33
2	E	301	SXA	C31-C29-C32-C34
2	E	301	SXA	O1-C1-S1-C43
2	E	301	SXA	C2-C1-S1-C43
2	F	301	SXA	C28-C29-C32-O33
2	F	301	SXA	C28-C29-C32-C34
2	F	301	SXA	C30-C29-C32-O33
2	F	301	SXA	C30-C29-C32-C34
2	F	301	SXA	C31-C29-C32-O33
2	F	301	SXA	C31-C29-C32-C34
3	A	302	O7S	C21-C22-C23-C24
3	B	302	O7S	C21-C22-C23-C24
3	B	302	O7S	C21-C22-C23-C27
3	B	302	O7S	C11-C12-C14-C15
3	C	302	O7S	C21-C22-C23-C24
3	D	401	O7S	C21-C22-C23-C24
3	F	302	O7S	C21-C22-C23-C24
3	E	302	O7S	O01-C02-C21-C22
3	E	302	O7S	N03-C02-C21-C22
3	B	302	O7S	O01-C02-C21-C22
3	B	302	O7S	N03-C02-C21-C22
2	A	301	SXA	O1-C1-S1-C43
2	A	301	SXA	C2-C1-S1-C43
2	B	301	SXA	O1-C1-S1-C43

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Mol	Chain	Res	Type	Atoms
2	B	301	SXA	C2-C1-S1-C43
2	B	303	SXA	O1-C1-S1-C43
2	B	303	SXA	C2-C1-S1-C43
2	C	301	SXA	O1-C1-S1-C43
2	C	301	SXA	C2-C1-S1-C43
2	F	301	SXA	O1-C1-S1-C43
2	F	301	SXA	C2-C1-S1-C43
3	E	302	O7S	C21-C22-C23-C27
3	E	302	O7S	C21-C22-C23-C24
2	B	303	SXA	C42-C43-S1-C1
2	E	301	SXA	C42-C43-S1-C1
2	A	301	SXA	N36-C37-C38-C39
2	B	303	SXA	N36-C37-C38-C39
2	C	301	SXA	N36-C37-C38-C39
2	E	301	SXA	C43-C42-N41-C39
2	B	301	SXA	N36-C37-C38-C39
2	E	301	SXA	N36-C37-C38-C39
2	F	301	SXA	N36-C37-C38-C39
2	B	301	SXA	C43-C42-N41-C39
2	A	301	SXA	C42-C43-S1-C1
2	B	301	SXA	C42-C43-S1-C1
2	C	301	SXA	C42-C43-S1-C1
2	F	301	SXA	C42-C43-S1-C1
2	C	301	SXA	C43-C42-N41-C39
3	B	302	O7S	C22-C23-C24-C25
3	E	302	O7S	C22-C23-C24-C25

There are no ring outliers.

18 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	306	PO4	0	7
3	E	302	O7S	1	0
4	C	304	PO4	2	0
2	B	301	SXA	3	0
4	F	303	PO4	2	0
3	F	302	O7S	1	0
4	C	305	PO4	1	0
3	B	302	O7S	1	0
3	D	401	O7S	1	0
4	B	305	PO4	1	0
2	F	301	SXA	3	0

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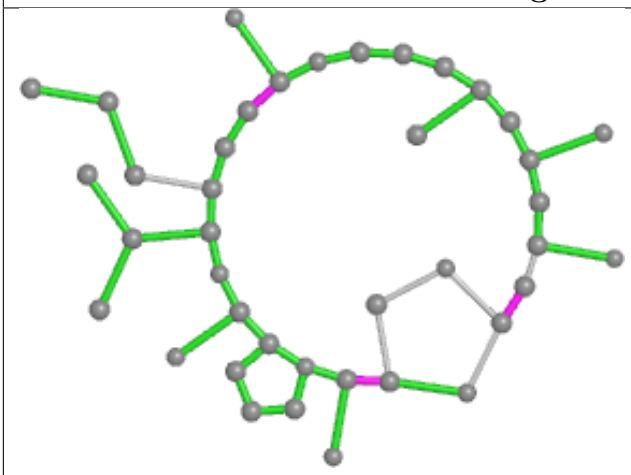
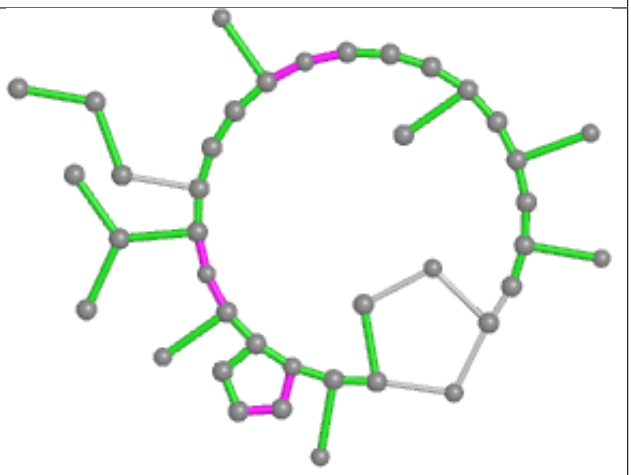
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	SXA	1	0
2	C	301	SXA	1	0
3	A	302	O7S	1	0
4	E	306	PO4	2	0
4	C	303	PO4	1	0
2	B	303	SXA	1	0
3	C	302	O7S	1	0

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.

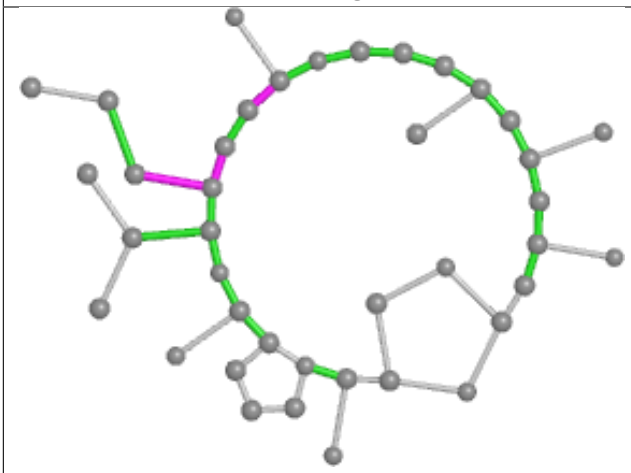
Ligand O7S E 302



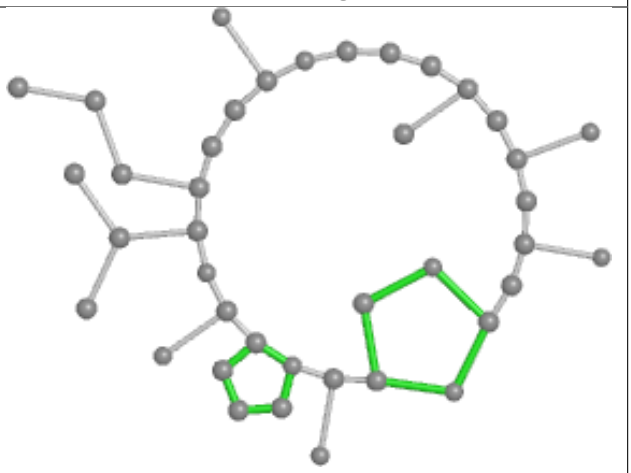
Bond lengths



Bond angles

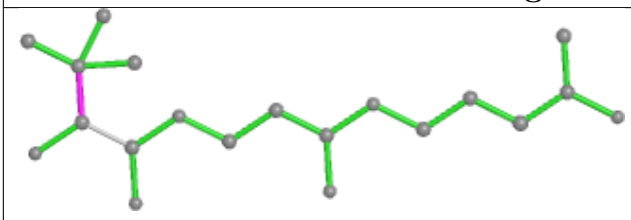


Torsions



Rings

Ligand SXA B 301



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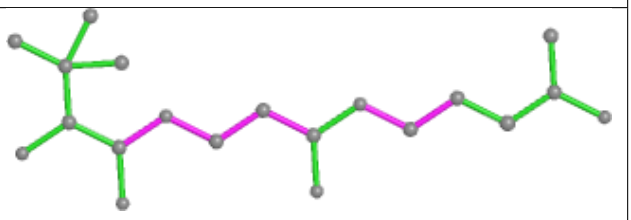
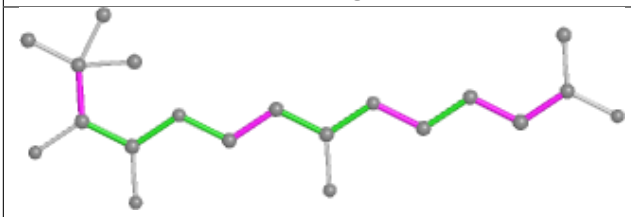


Bond angles



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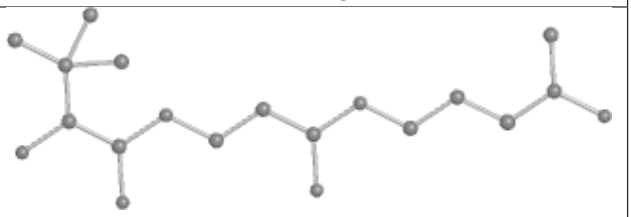
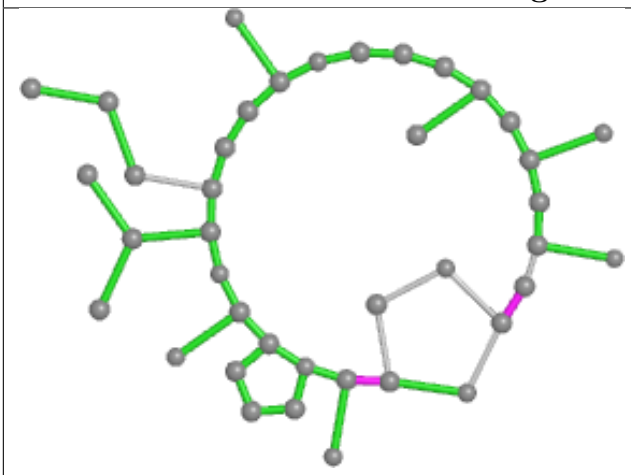
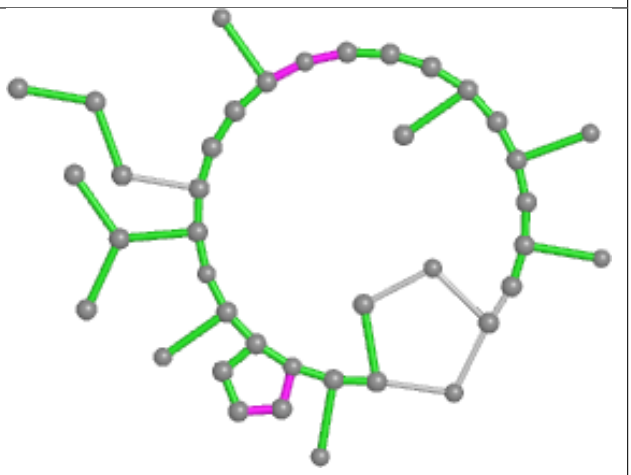


Rings

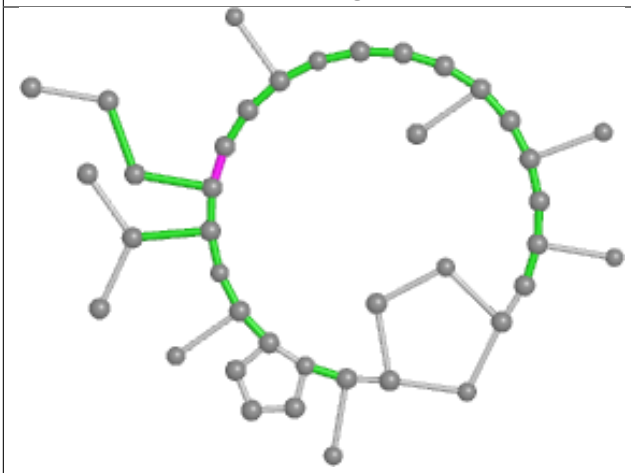
Ligand O7S F 302



Bond lengths



Bond angles



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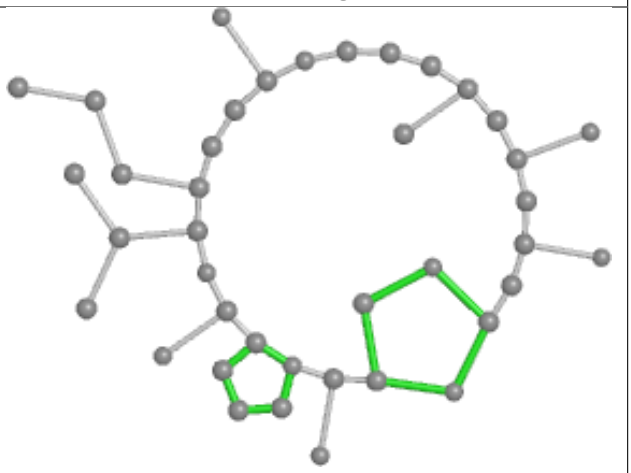
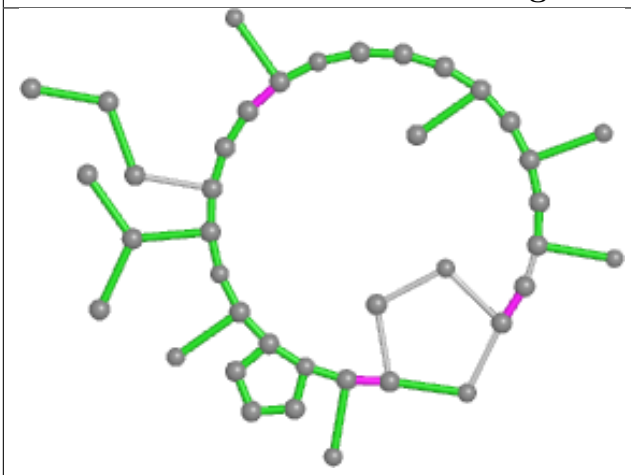
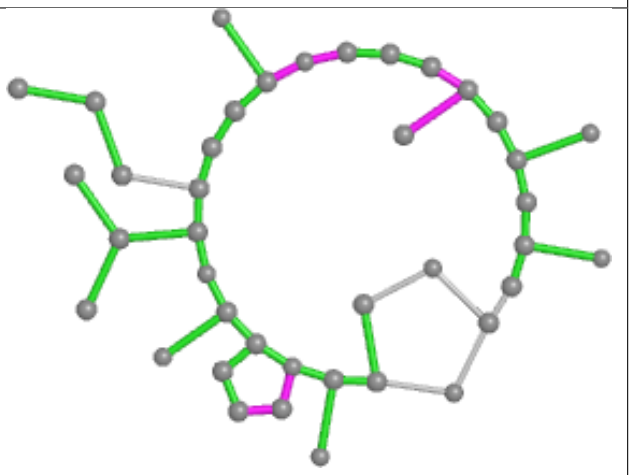


Rings

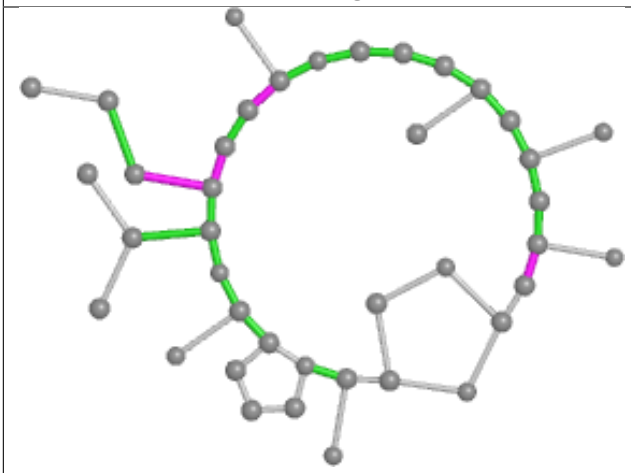
Ligand O7S B 302



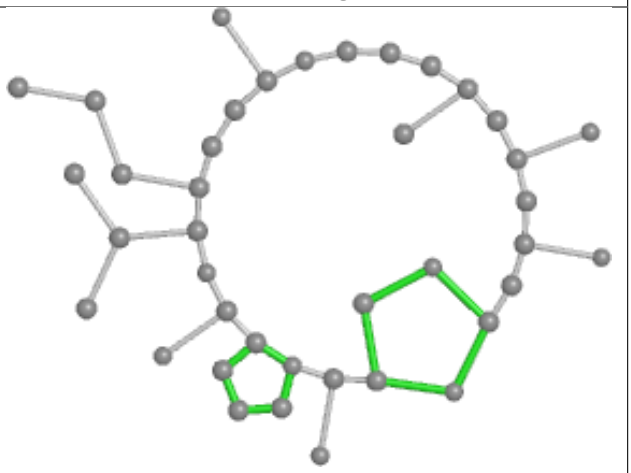
Bond lengths



Bond angles

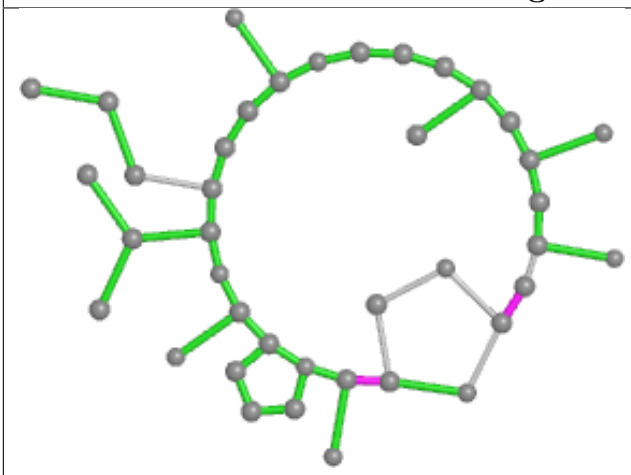


Torsions

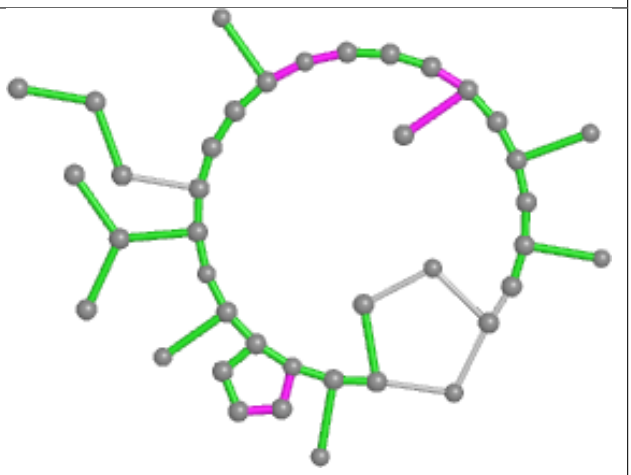


Rings

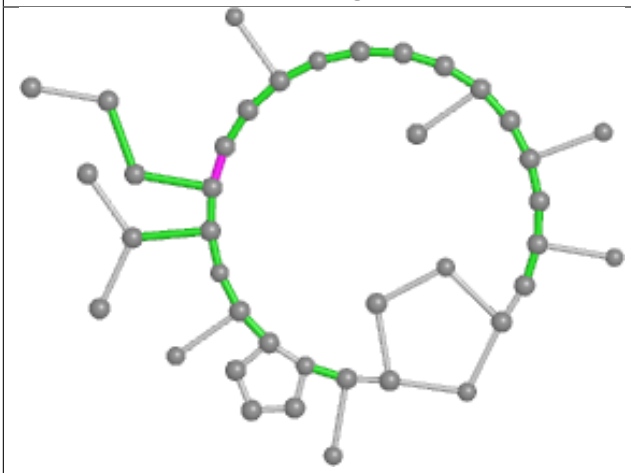
Ligand O7S D 401



Bond lengths



Bond angles



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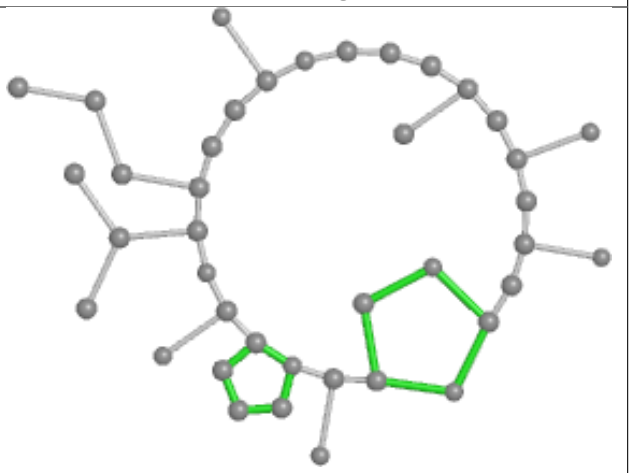
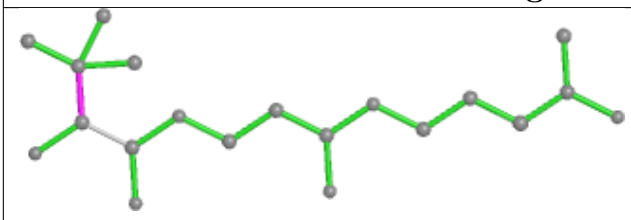


Rings

Ligand SXA F 301



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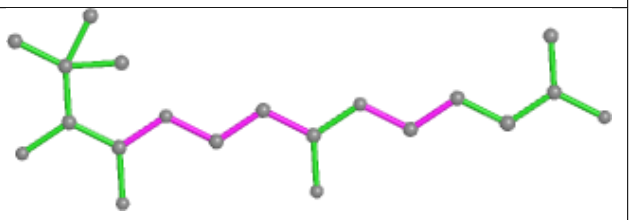
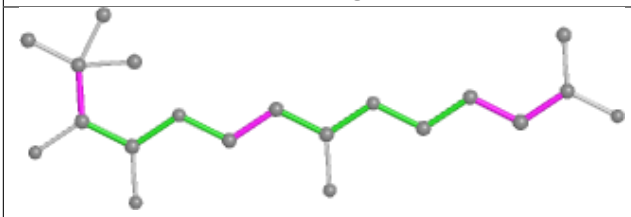


Bond angles



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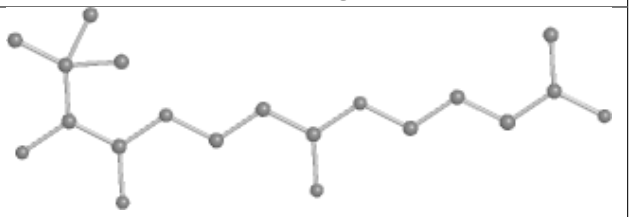
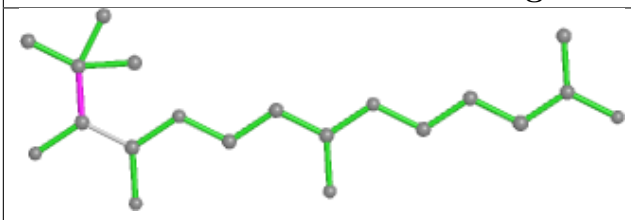


Rings

Ligand SXA E 301



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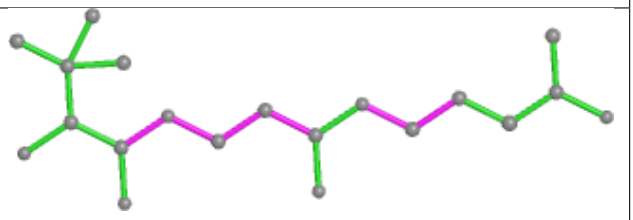

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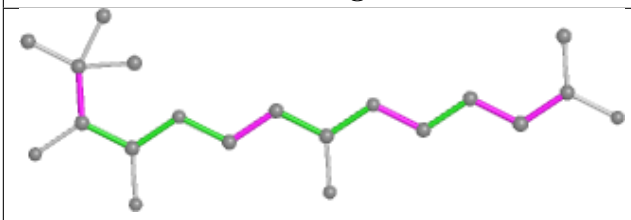

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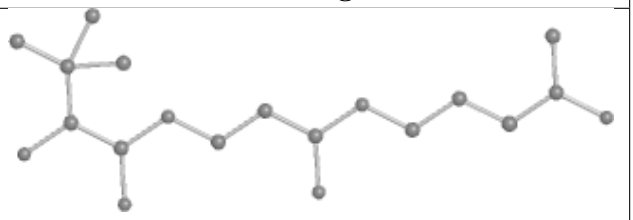
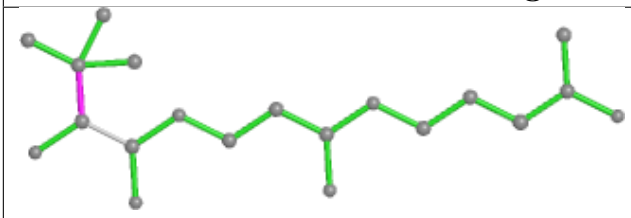


Rings

Ligand SXA A 301



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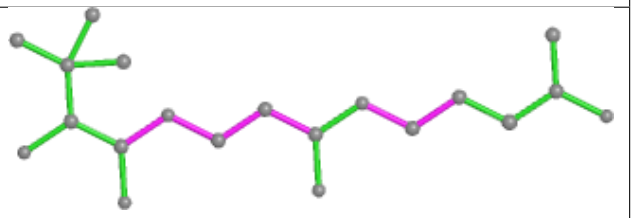

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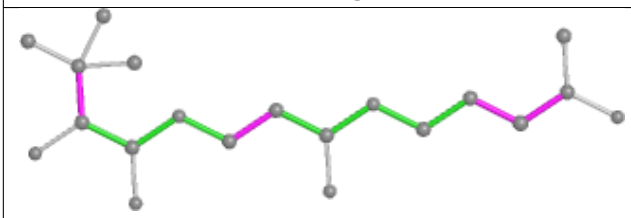

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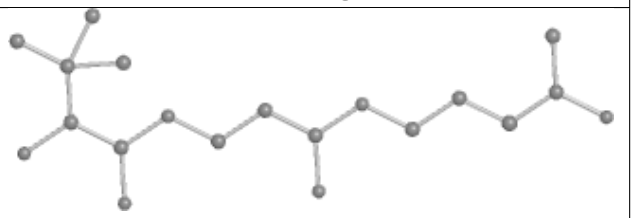
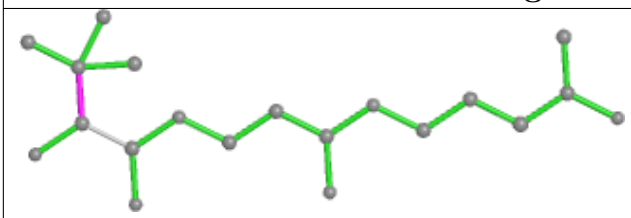
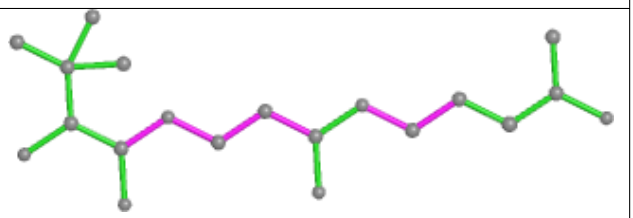


Rings

Ligand SXA C 301



Bond lengths



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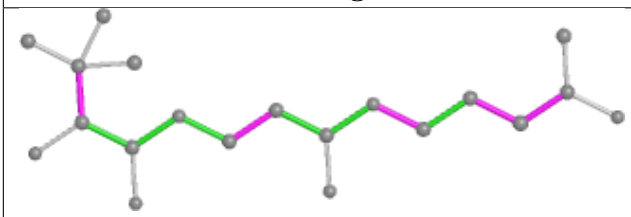
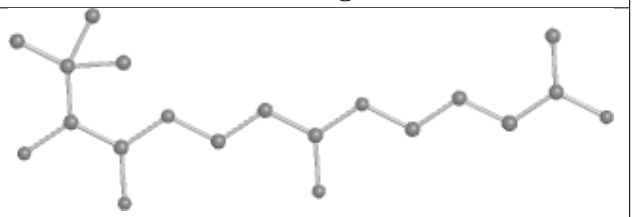
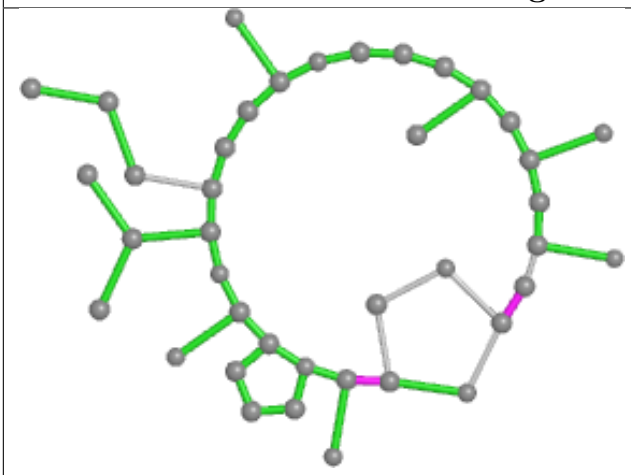


Torsions



Rings

Ligand O7S A 302



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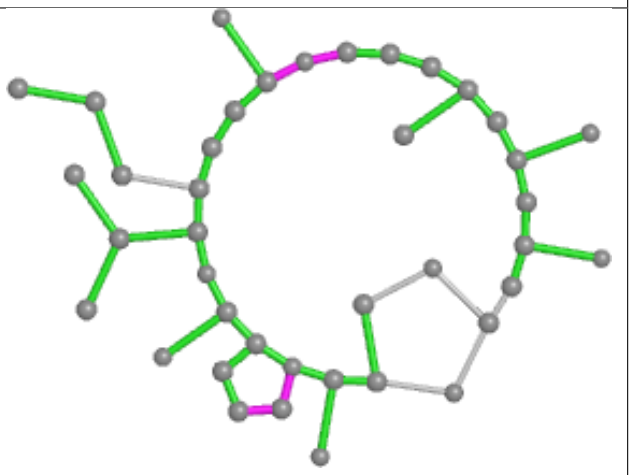
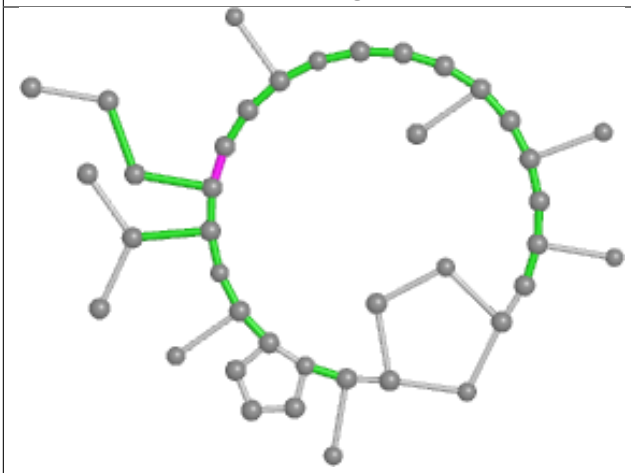
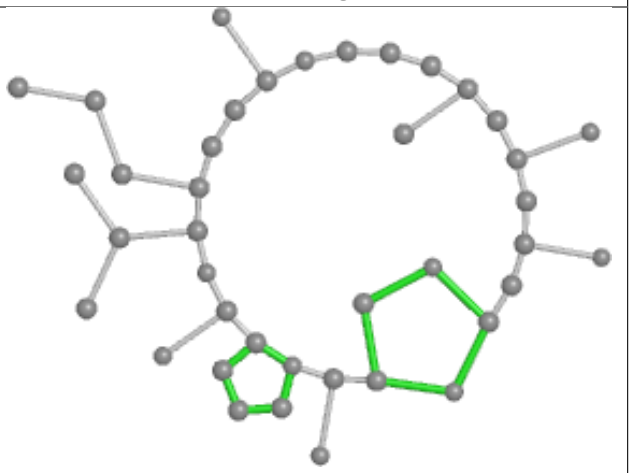


Bond angles

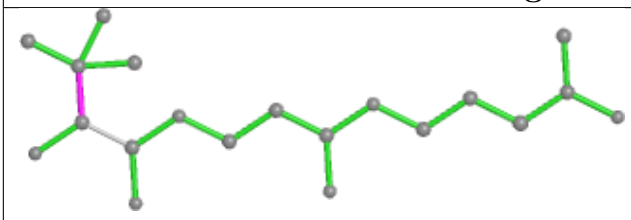


Torsions

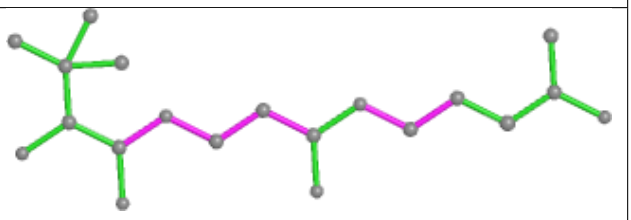


Rings

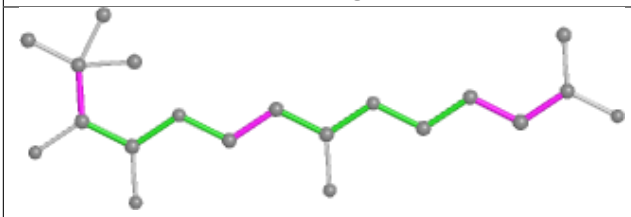
Ligand SXA B 303



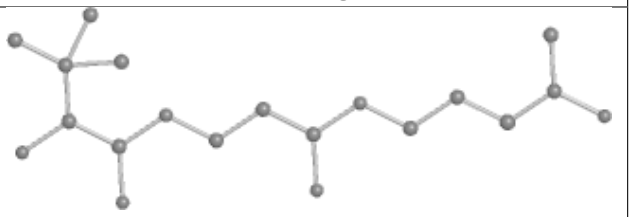
Bond lengths



Bond angles

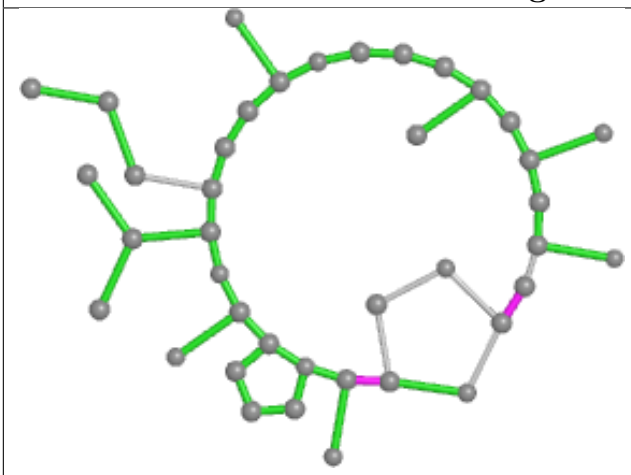


Torsions

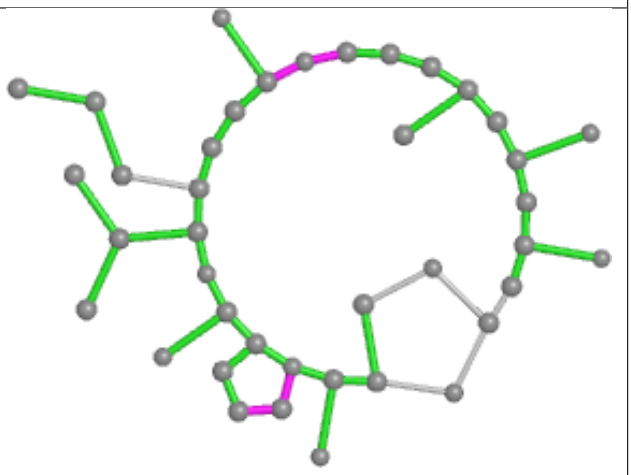


Rings

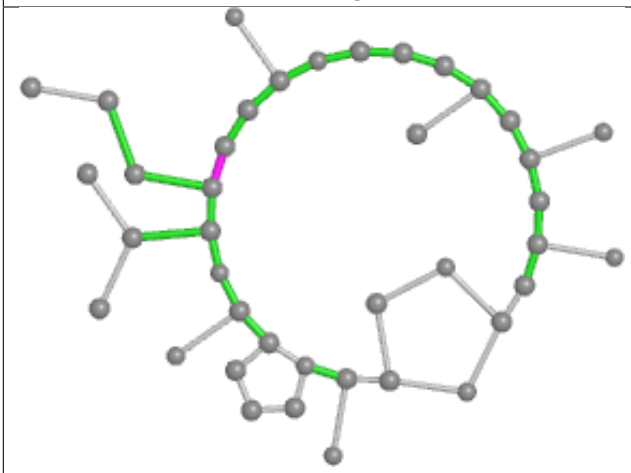
Ligand O7S C 302



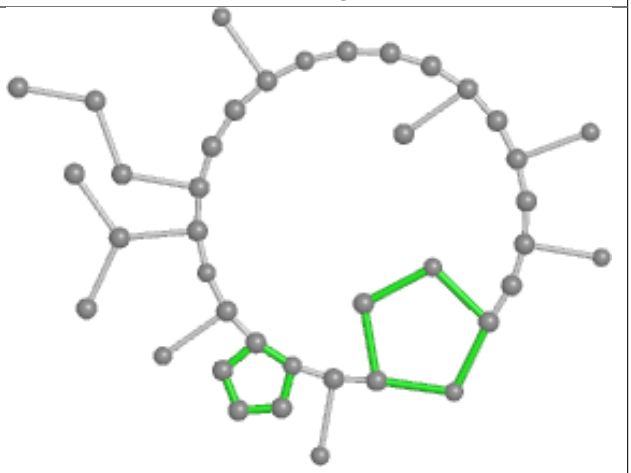
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	207/207 (100%)	0.15	0 100 100	33, 52, 83, 112	0
1	B	204/207 (98%)	0.12	1 (0%) 91 79	35, 54, 81, 109	0
1	C	205/207 (99%)	0.20	1 (0%) 91 79	42, 64, 98, 142	0
1	D	206/207 (99%)	0.03	0 100 100	37, 62, 95, 123	0
1	E	203/207 (98%)	0.09	1 (0%) 91 79	39, 63, 90, 117	0
1	F	206/207 (99%)	0.20	4 (1%) 66 43	36, 65, 106, 134	0
All	All	1231/1242 (99%)	0.13	7 (0%) 89 76	33, 60, 95, 142	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	35	ILE	3.0
1	F	32	ASN	2.9
1	F	31	THR	2.8
1	F	34	ASN	2.4
1	B	7	HIS	2.2
1	C	31	THR	2.2
1	E	21	ARG	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

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
4	PO4	C	304	5/5	0.74	0.25	34,34,34,34	5
2	SXA	B	303	20/25	0.82	0.39	23,93,225,311	0
2	SXA	F	301	20/25	0.84	0.42	23,93,225,311	0
2	SXA	A	301	20/25	0.84	0.44	23,93,225,311	0
2	SXA	B	301	20/25	0.86	0.37	23,93,225,311	0
2	SXA	E	301	20/25	0.86	0.36	23,93,225,311	0
4	PO4	E	305	5/5	0.86	0.22	33,33,33,33	5
4	PO4	E	307	5/5	0.86	0.22	34,34,34,34	5
2	SXA	C	301	20/25	0.87	0.36	23,93,225,311	0
4	PO4	D	402	5/5	0.87	0.29	33,33,33,33	5
6	CL	F	306	1/1	0.87	0.14	34,34,34,34	1
6	CL	A	305	1/1	0.88	0.15	34,34,34,34	1
4	PO4	C	305	5/5	0.88	0.29	34,34,34,34	5
6	CL	E	308	1/1	0.89	0.14	34,34,34,34	1
4	PO4	B	306	5/5	0.89	0.20	34,34,34,34	5
4	PO4	A	303	5/5	0.91	0.16	33,33,33,33	5
3	O7S	D	401	40/40	0.92	0.33	36,66,112,138	0
4	PO4	F	304	5/5	0.92	0.17	34,34,34,34	5
4	PO4	D	403	5/5	0.92	0.17	34,34,34,34	5
3	O7S	E	302	40/40	0.92	0.36	36,66,112,138	0
4	PO4	E	306	5/5	0.92	0.16	34,34,34,34	5
6	CL	D	405	1/1	0.93	0.18	34,34,34,34	1
5	SO4	B	307	5/5	0.93	0.24	34,34,34,34	5
6	CL	F	305	1/1	0.93	0.16	34,34,34,34	1
4	PO4	F	303	5/5	0.93	0.20	33,33,33,33	5
7	MG	E	303	1/1	0.93	0.06	33,33,33,33	0
4	PO4	C	303	5/5	0.94	0.20	33,33,33,33	5
3	O7S	B	302	40/40	0.94	0.32	36,66,112,138	0
5	SO4	A	304	5/5	0.94	0.23	34,34,34,34	5
4	PO4	B	305	5/5	0.94	0.25	34,34,34,34	5
7	MG	B	304	1/1	0.94	0.12	33,33,33,33	0
3	O7S	C	302	40/40	0.94	0.34	36,66,112,138	0
5	SO4	B	308	5/5	0.95	0.16	34,34,34,34	5
3	O7S	F	302	40/40	0.95	0.27	36,66,112,138	0
4	PO4	E	304	5/5	0.95	0.18	33,33,33,33	5
3	O7S	A	302	40/40	0.95	0.30	36,66,112,138	0
5	SO4	D	404	5/5	0.97	0.19	34,34,34,34	5

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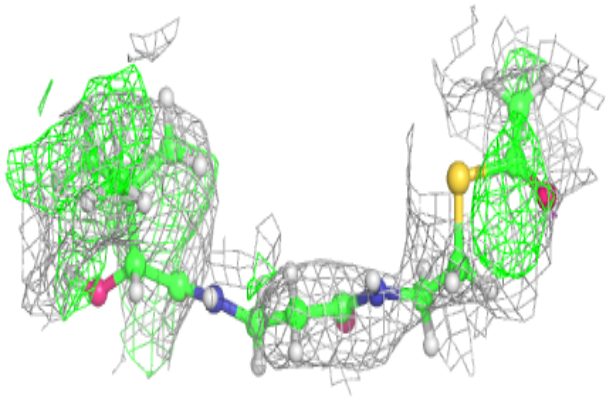
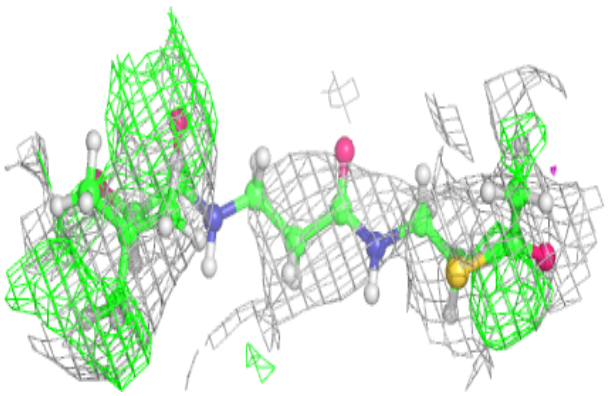
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	C	306	1/1	0.97	0.23	34,34,34,34	1

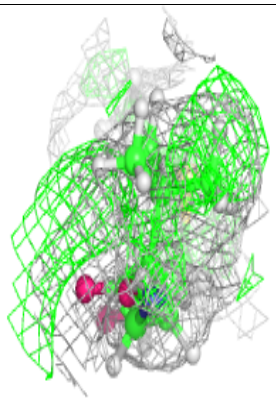
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SXA B 303:

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

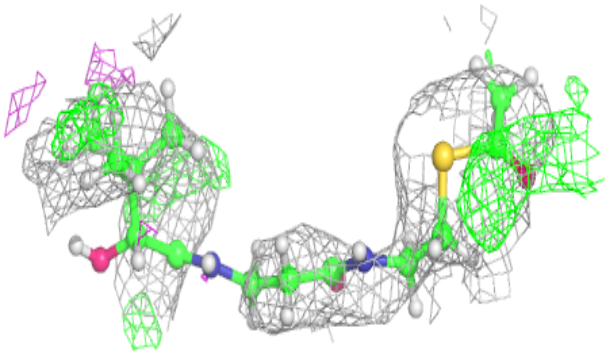


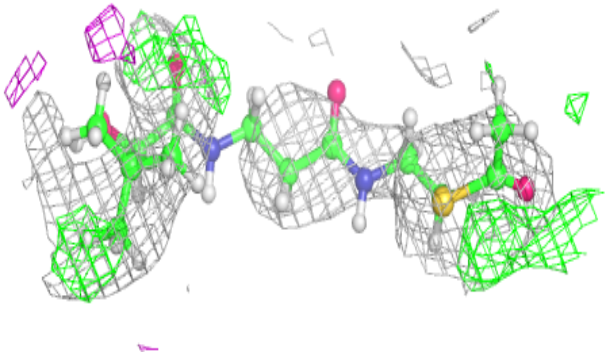


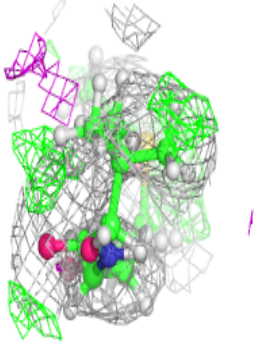


Electron density around SXA F 301:

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

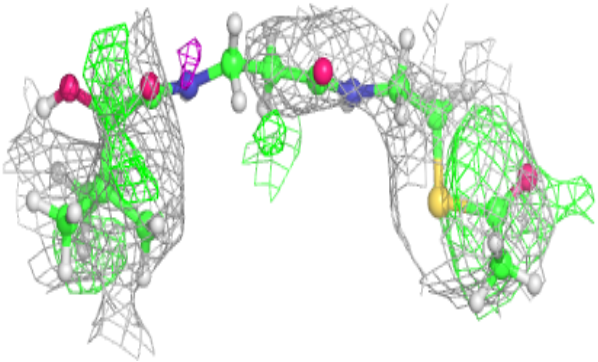


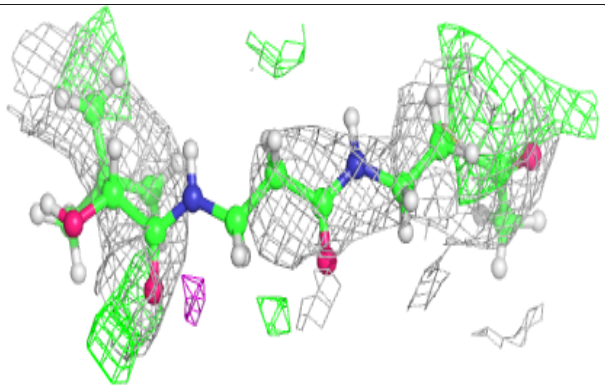


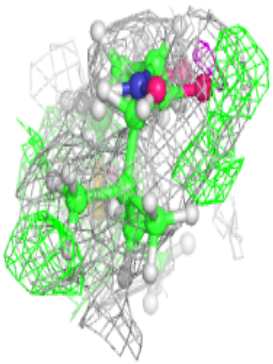


Electron density around SXA A 301:

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

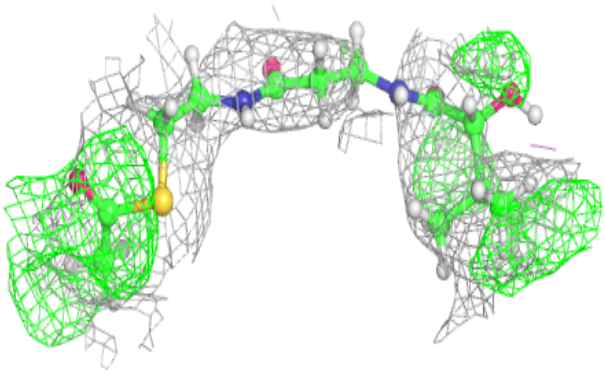


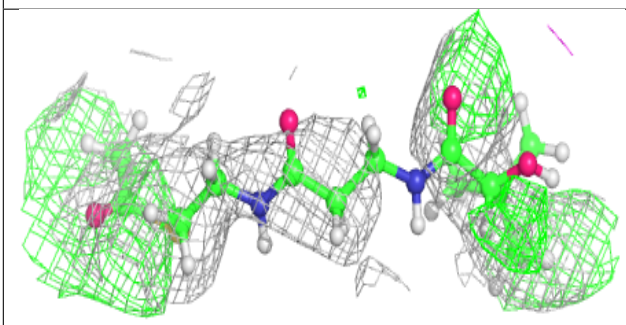


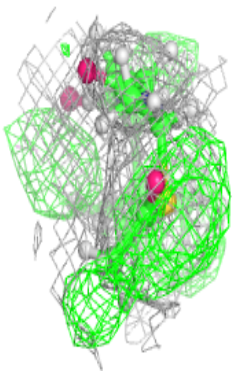


Electron density around SXA B 301:

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

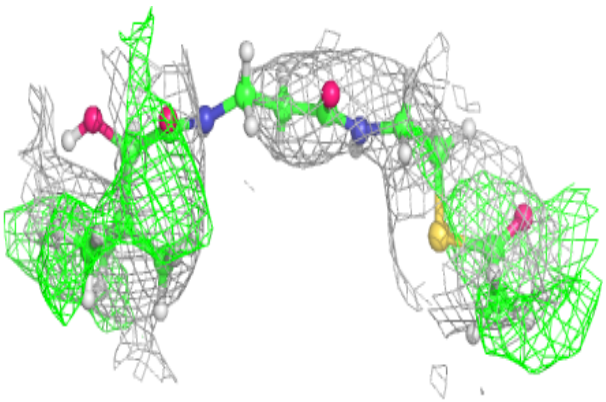


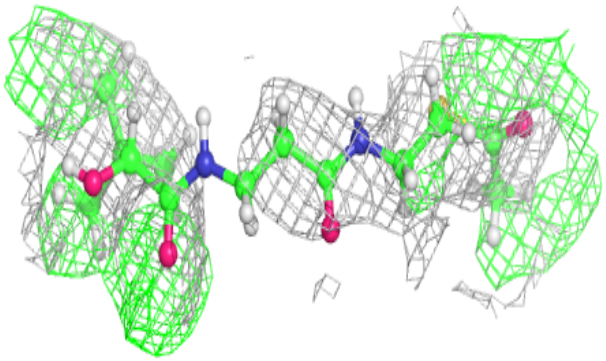


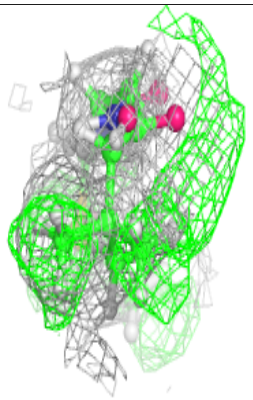


Electron density around SXA E 301:

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

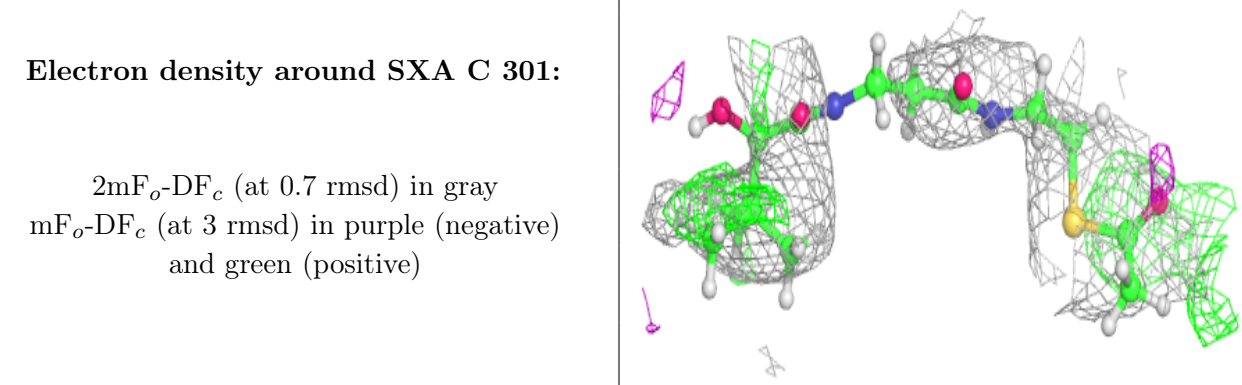


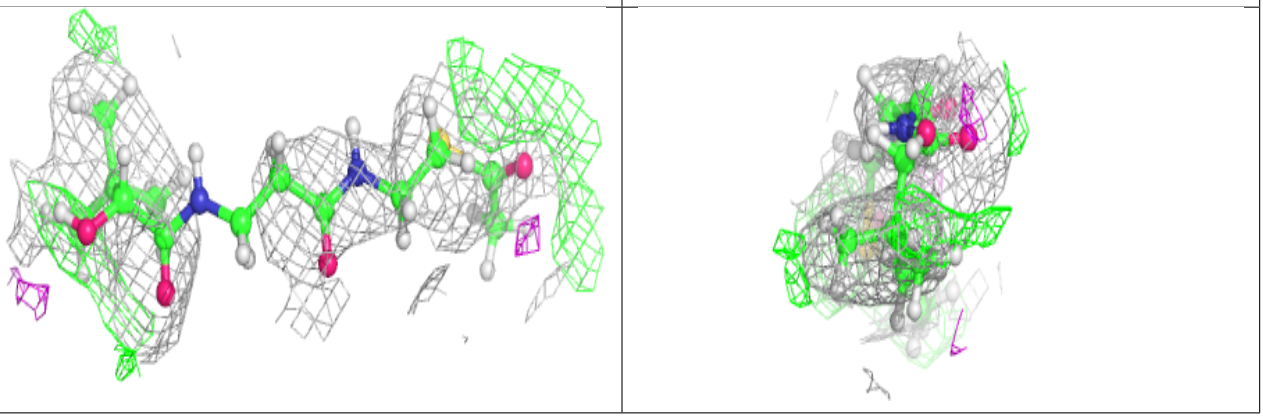




Electron density around SXA C 301:

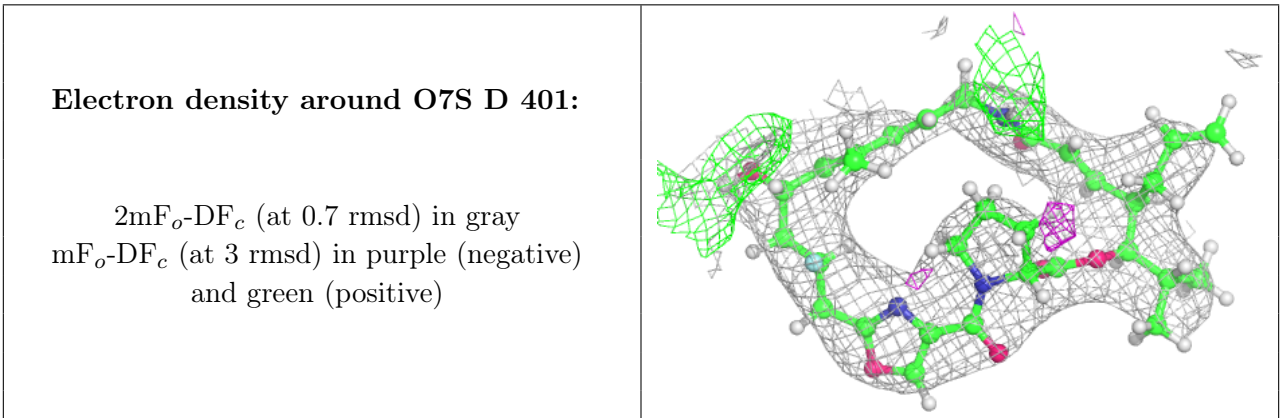
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

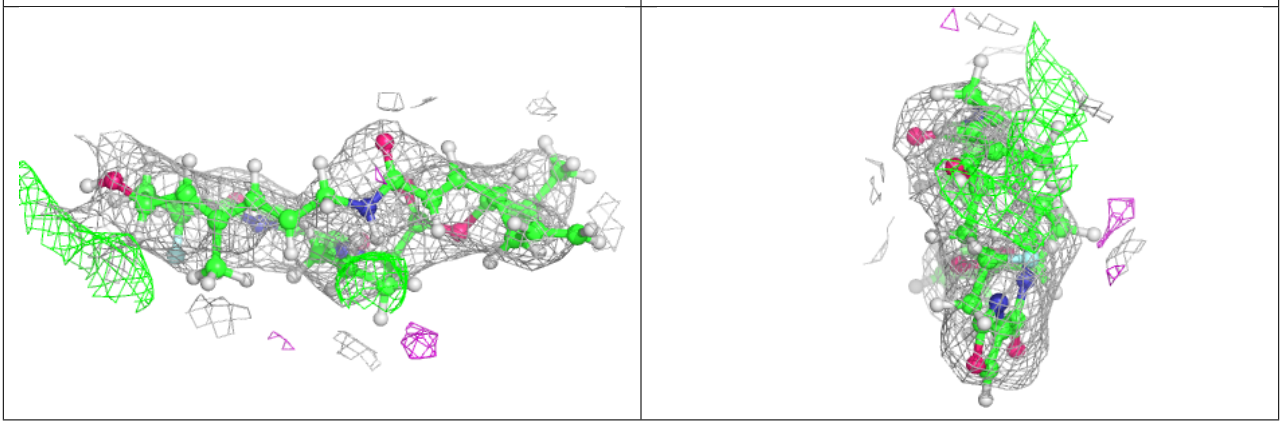




Electron density around O7S D 401:

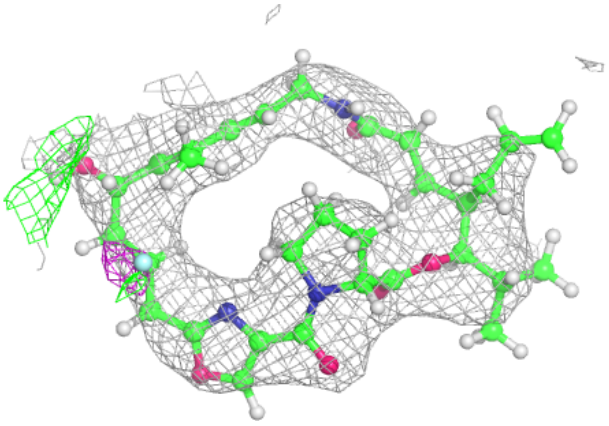
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

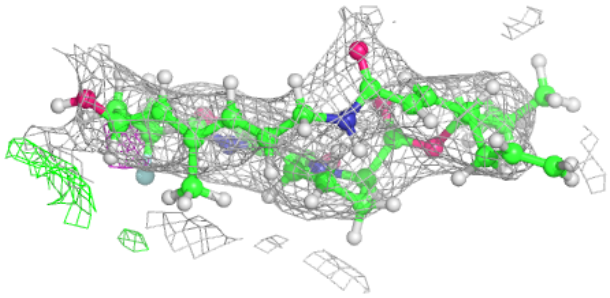


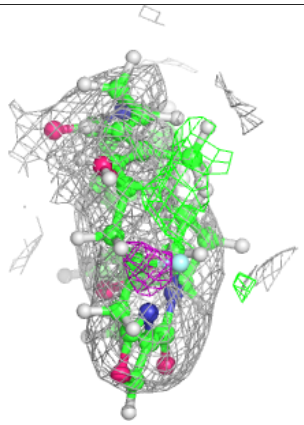


Electron density around O7S E 302:

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

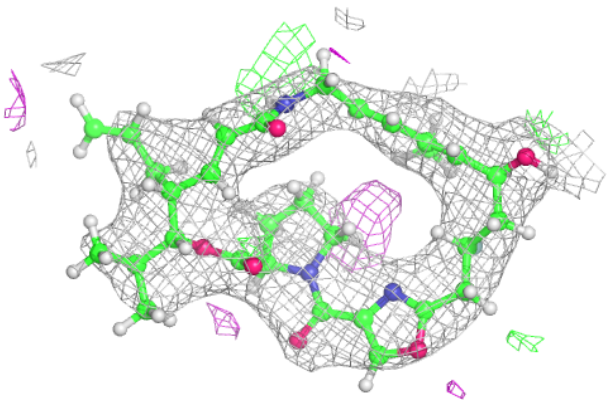


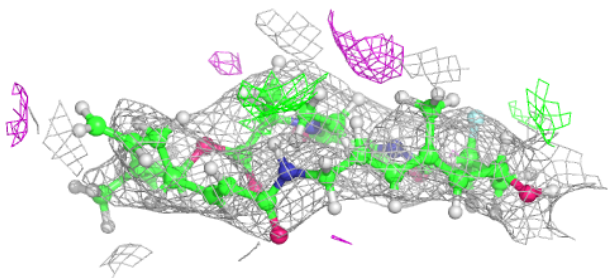


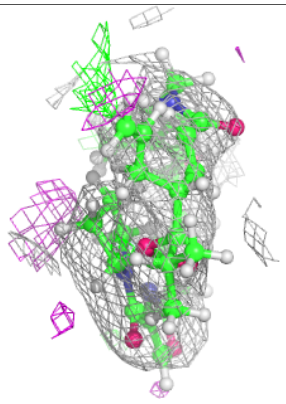


Electron density around O7S B 302:

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

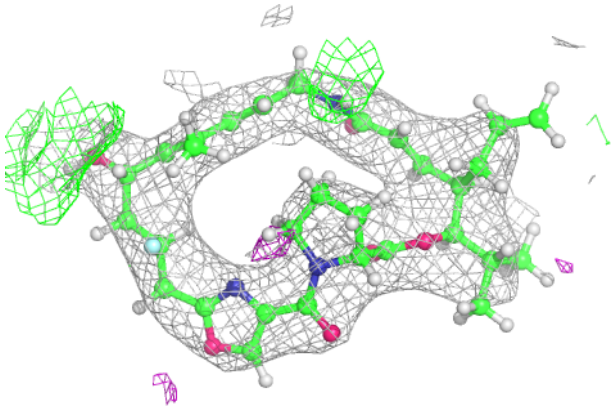


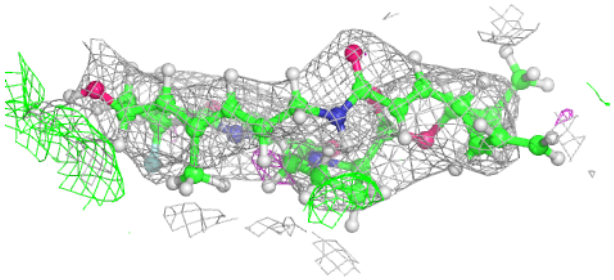


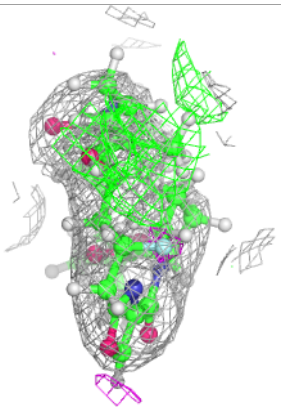


Electron density around O7S C 302:

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

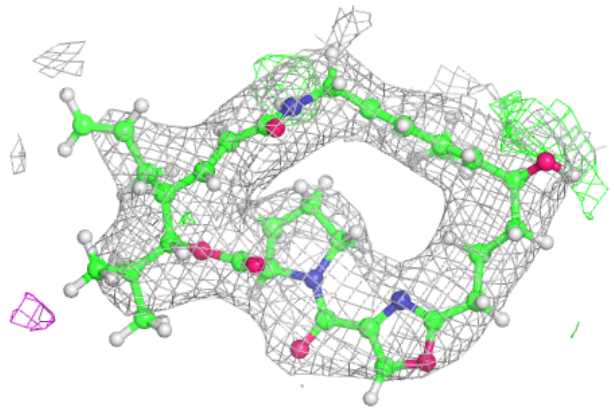


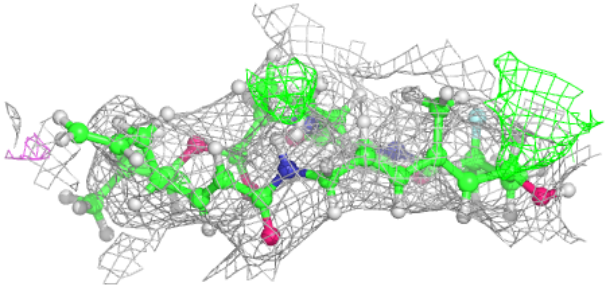


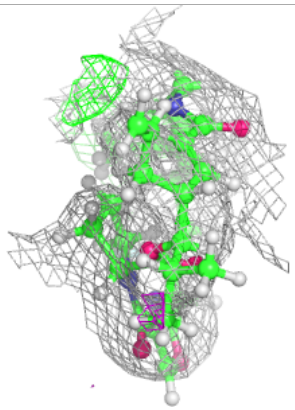


Electron density around O7S F 302:

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

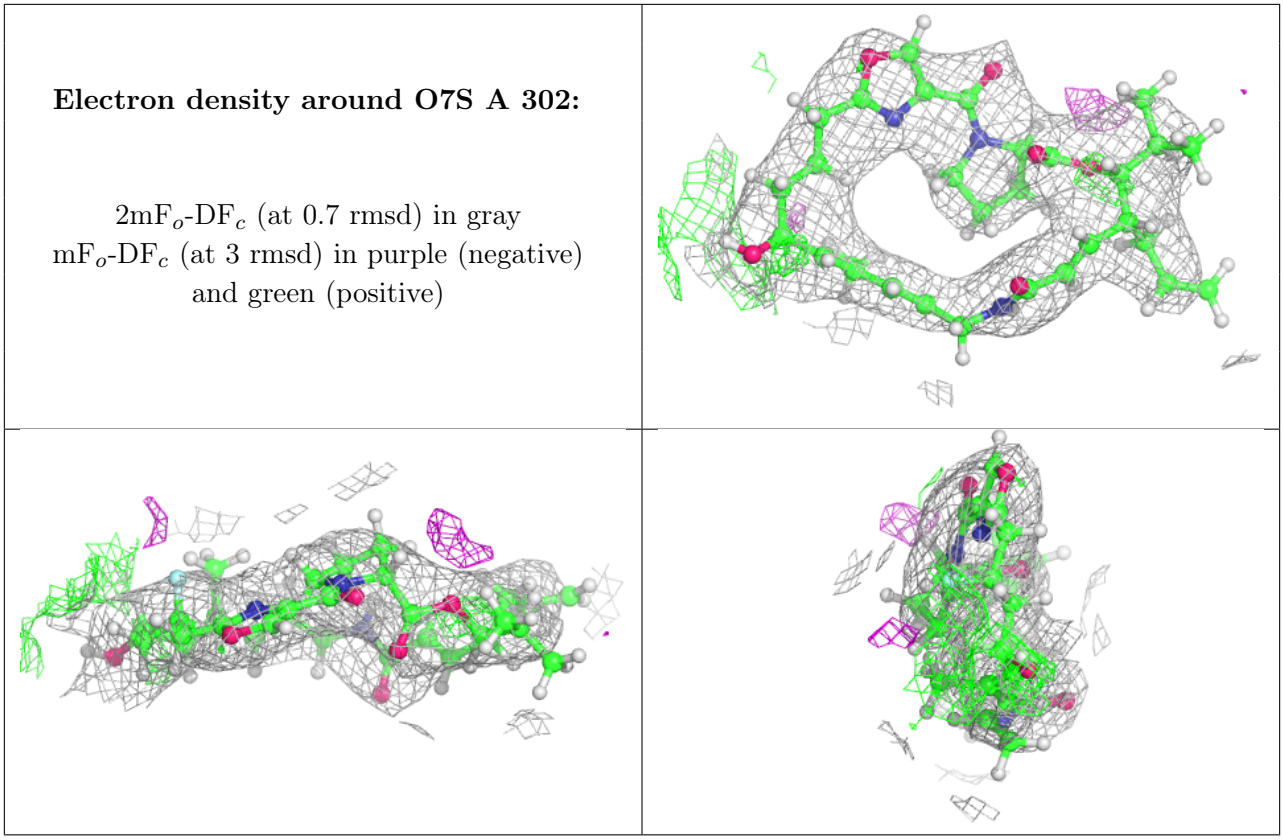






Electron density around O7S A 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.