Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 04:42 pm GMT

PDB ID	:	2WZY
Title	:	Crystal structure of A-AChBP in complex with 13-desmethyl spirolide C
Authors	:	Bourne, Y.; Radic, Z.; Araoz, R.; Talley, T.T.; Benoit, E.; Servent, D.; Taylor, P.; Molgo, J.; Marchot, P.
Deposited on	:	2009-12-03
Resolution	:	2.51 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:

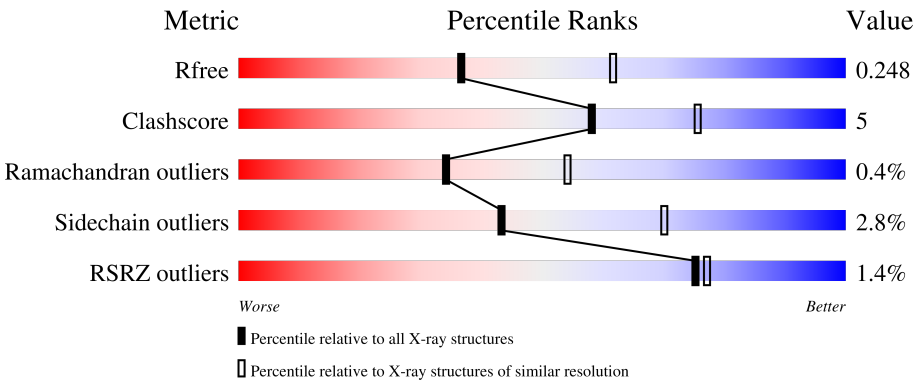
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	228	.% 84% 7% • 7%
1	B	228	.% 87% 7% 7%
1	C	228	.% 86% 7% 7%
1	D	228	.% 77% 14% • 7%
1	E	228	2% 79% 12% • 8%

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Mol	Chain	Length	Quality of chain
1	F	228	% 80% 11% 9%
1	G	228	2% 80% 13% 7%
1	H	228	82% 11% 7%
1	I	228	% 81% 11% 8%
1	J	228	2% 82% 11% • 7%

2 Entry composition (i)

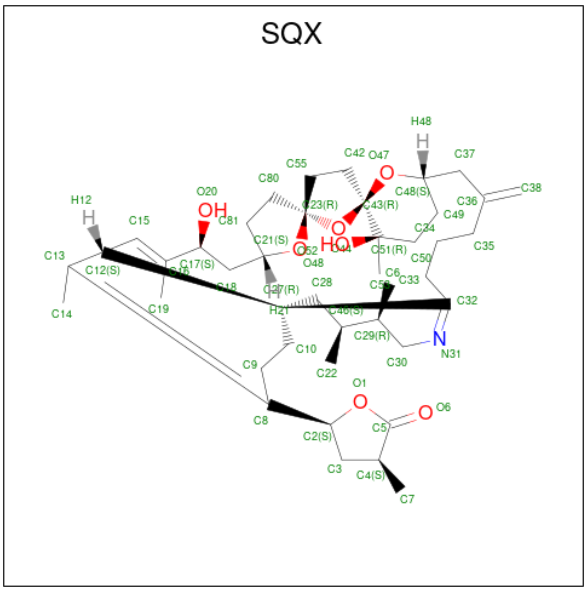
There are 3 unique types of molecules in this entry. The entry contains 18450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SOLUBLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1724	1090	285	339	10	0	4	0
1	B	213	1716	1082	286	339	9	0	3	0
1	C	213	1702	1076	282	334	10	0	3	0
1	D	211	1701	1074	286	332	9	0	3	0
1	E	210	1698	1074	284	331	9	0	3	0
1	F	208	1680	1062	280	329	9	0	3	0
1	G	212	1710	1080	282	337	11	0	3	0
1	H	211	1695	1071	282	333	9	0	2	0
1	I	209	1703	1079	282	332	10	0	5	0
1	J	212	1713	1081	285	337	10	0	3	0

- Molecule 2 is 13-DESMETHYL SPIROLIDE C (three-letter code: SQX) (formula: $C_{42}H_{63}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	50	42	1	7	0	0
2	B	1	50	42	1	7	0	0
2	C	1	50	42	1	7	0	0
2	D	1	50	42	1	7	0	0
2	E	1	50	42	1	7	0	0
2	F	1	50	42	1	7	0	0
2	G	1	50	42	1	7	0	0
2	H	1	50	42	1	7	0	0
2	I	1	50	42	1	7	0	0
2	J	1	50	42	1	7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0
3	B	95	95	95	0	0

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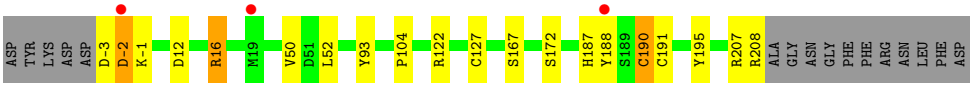
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	99	99	99	0	0
			Total	O		
3	D	102	102	102	0	0
			Total	O		
3	E	79	79	79	0	0
			Total	O		
3	F	95	95	95	0	0
			Total	O		
3	G	78	78	78	0	0
			Total	O		
3	H	95	95	95	0	0
			Total	O		
3	I	108	108	108	0	0
			Total	O		
3	J	99	99	99	0	0

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.

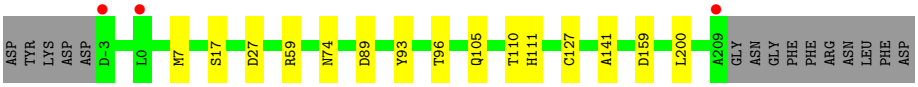
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain A:



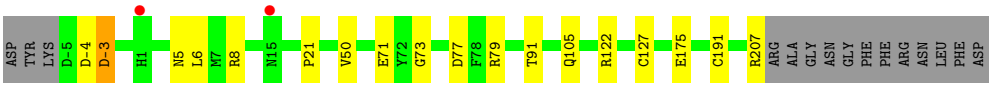
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain B:



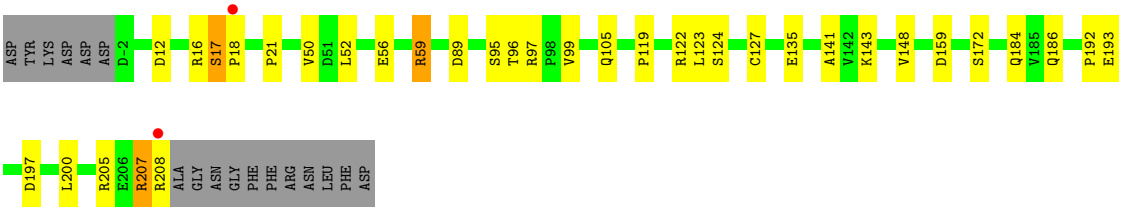
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain C:



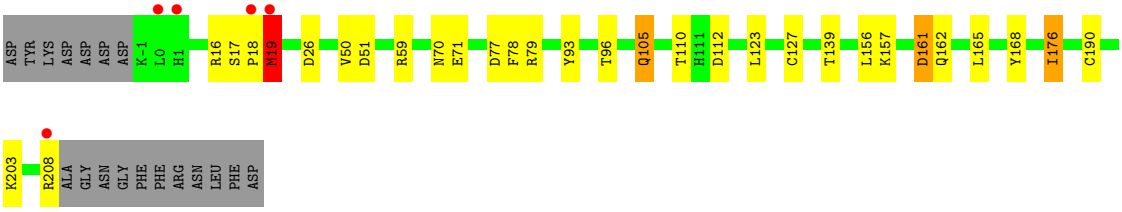
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain D:



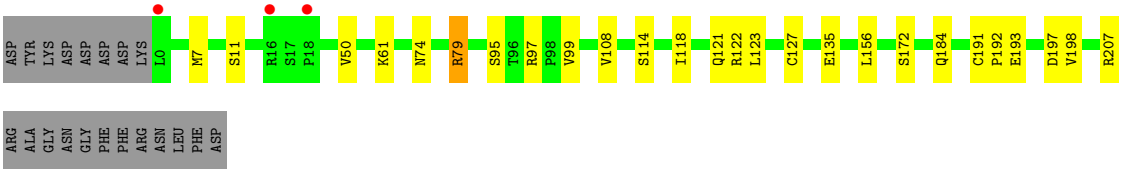
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain E:



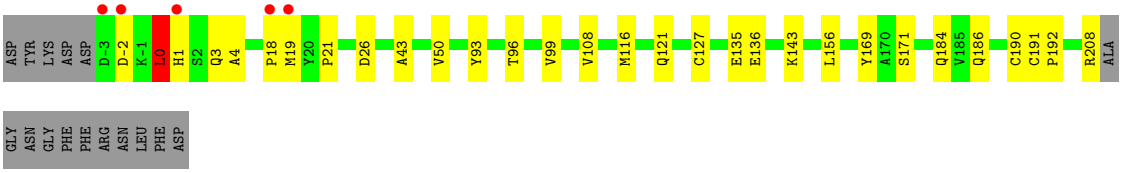
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain F:



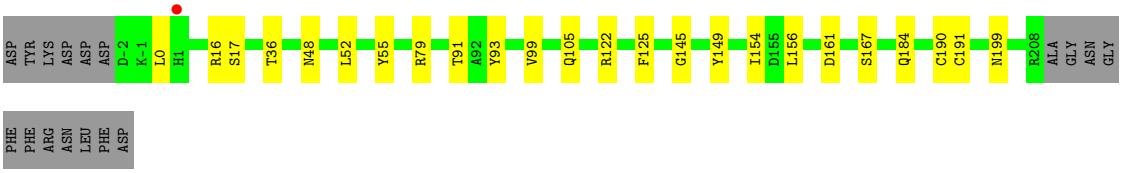
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain G:



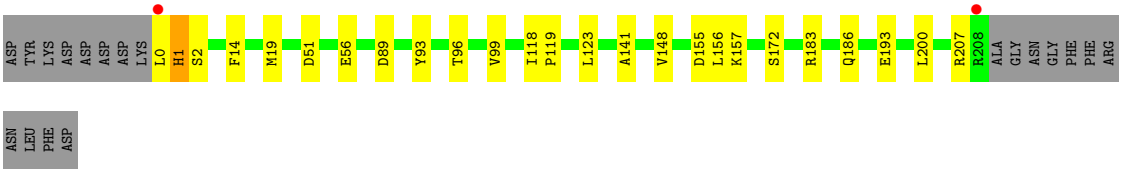
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain H:



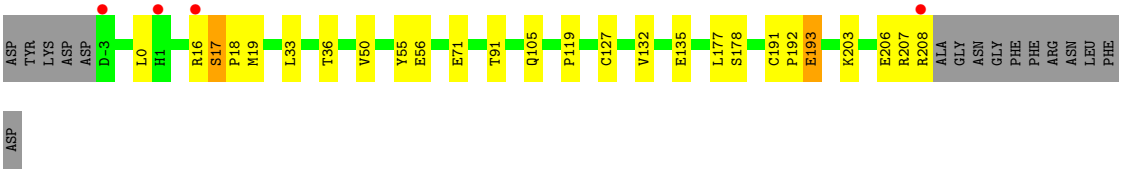
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain I:



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain J:


ASP
TYR
LYS
ASP
ASP
D-3
LO
H1
R16
S17
P18
M19
L33
T36
V50
Y55
E56
E71
T91
Q105
P119
C127
V132
E135
L177
S178
C191
P192
E193
K203
E206
R207
R208
ALA
GLY
ASN
GLY
PHE
PHE
ARG
ASN
LEU
PHE

ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.63Å 131.75Å 125.59Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	20.00 – 2.51 19.97 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.51) 98.6 (19.97-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.237 0.189 , 0.248	Depositor DCC
R_{free} test set	1705 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 23.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.014 for -h,l,k 0.108 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18450	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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 (i)

5.1 Standard geometry (i)

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

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	0/1776	0.59	0/2420
1	B	0.44	0/1766	0.58	0/2406
1	C	0.44	0/1751	0.62	0/2386
1	D	0.46	0/1751	0.64	2/2386 (0.1%)
1	E	0.44	0/1748	0.60	0/2380
1	F	0.44	0/1729	0.60	0/2355
1	G	0.44	0/1760	0.60	0/2397
1	H	0.48	0/1742	0.60	0/2374
1	I	0.45	0/1760	0.63	0/2398
1	J	0.48	0/1763	0.60	0/2401
All	All	0.45	0/17546	0.61	2/23903 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	207[A]	ARG	C-N-CA	5.57	135.63	121.70
1	D	207[B]	ARG	C-N-CA	5.57	135.63	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	190	CYS	Peptide
1	G	190	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1658	19	0
1	B	1716	0	1657	15	0
1	C	1702	0	1632	15	0
1	D	1701	0	1643	21	0
1	E	1698	0	1652	19	0
1	F	1680	0	1626	17	0
1	G	1710	0	1652	16	0
1	H	1695	0	1638	12	0
1	I	1703	0	1652	22	0
1	J	1713	0	1656	10	0
2	A	50	0	63	4	0
2	B	50	0	63	2	0
2	C	50	0	63	2	0
2	D	50	0	63	2	0
2	E	50	0	63	2	0
2	F	50	0	63	2	0
2	G	50	0	63	3	0
2	H	50	0	63	2	0
2	I	50	0	63	2	0
2	J	50	0	63	3	0
3	A	58	0	0	0	0
3	B	95	0	0	1	0
3	C	99	0	0	0	0
3	D	102	0	0	0	0
3	E	79	0	0	1	0
3	F	95	0	0	2	0
3	G	78	0	0	0	0
3	H	95	0	0	0	0
3	I	108	0	0	2	0
3	J	99	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18450	0	17096	166	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 5.

All (166) 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:I:0:LEU:N	1:I:1:HIS:HB2	1.82	0.93
1:A:-3:ASP:H2	1:A:-1:LYS:N	1.73	0.86
1:C:207[A]:ARG:HH21	1:C:207[A]:ARG:HB3	1.45	0.81
1:E:168:TYR:CG	1:E:176:ILE:HD11	2.14	0.81
1:A:-3:ASP:H3	1:A:-2:ASP:HB2	1.45	0.80
1:D:17:SER:HB2	1:D:18:PRO:HA	1.62	0.80
1:B:59[B]:ARG:HH11	1:B:59[B]:ARG:HB2	1.51	0.76
2:J:301:SQX:H331	2:J:301:SQX:H192	1.69	0.74
2:D:301:SQX:H331	2:D:301:SQX:H192	1.67	0.74
2:E:301:SQX:H331	2:E:301:SQX:H192	1.70	0.73
1:E:18:PRO:HA	1:E:19:MET:HB2	1.71	0.72
1:G:99:VAL:HG11	1:G:121:GLN:HE21	1.57	0.69
1:E:105:GLN:HE21	1:E:105:GLN:HA	1.58	0.69
2:B:301:SQX:H331	2:B:301:SQX:H192	1.76	0.67
1:I:0:LEU:H3	1:I:1:HIS:HB2	1.60	0.66
2:F:301:SQX:H331	2:F:301:SQX:H192	1.76	0.66
1:B:59[B]:ARG:HB2	1:B:59[B]:ARG:NH1	2.10	0.66
1:J:206:GLU:HB3	1:J:208:ARG:HB2	1.78	0.65
1:H:190:CYS:HG	1:H:191:CYS:HG	0.67	0.65
1:A:-3:ASP:N	1:A:-2:ASP:HB2	2.12	0.65
1:F:172:SER:O	1:F:207[A]:ARG:HD3	1.98	0.63
1:I:0:LEU:CA	1:I:1:HIS:HB2	2.29	0.63
1:A:-3:ASP:H2	1:A:-1:LYS:H	1.46	0.62
1:D:172:SER:O	1:D:207[A]:ARG:HD2	1.98	0.62
1:E:18:PRO:HA	1:E:19:MET:CB	2.29	0.62
1:G:135:GLU:HG2	1:G:208:ARG:HH12	1.64	0.61
1:E:17:SER:HB2	1:E:18:PRO:HD2	1.83	0.61
1:E:168:TYR:CD2	1:E:176:ILE:HD11	2.36	0.60
1:D:59[B]:ARG:NH1	1:D:159:ASP:OD1	2.33	0.60
1:H:122:ARG:HD2	1:I:96:THR:O	2.01	0.60
2:I:301:SQX:H331	2:I:301:SQX:H192	1.84	0.60
1:I:0:LEU:H2	1:I:1:HIS:HB2	1.65	0.59
1:G:93:TYR:HB3	2:G:301:SQX:H72C	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:NZ	1:D:184:GLN:HE22	2.01	0.59
1:D:122:ARG:HD2	1:E:96:THR:O	2.03	0.58
2:A:301:SQX:H331	2:A:301:SQX:H192	1.86	0.58
1:A:207:ARG:O	1:A:208:ARG:HB2	2.03	0.58
2:H:301:SQX:H331	2:H:301:SQX:H192	1.86	0.57
1:I:0:LEU:H2	1:I:1:HIS:CB	2.18	0.56
1:C:6:LEU:HD23	1:D:21:PRO:HB2	1.86	0.56
1:I:89:ASP:OD2	1:I:148:VAL:HG22	2.05	0.56
1:G:135:GLU:HG2	1:G:208:ARG:NH1	2.20	0.56
1:E:105:GLN:HA	1:E:105:GLN:NE2	2.19	0.56
1:F:192:PRO:HD2	1:F:193:GLU:OE1	2.05	0.56
1:F:7:MET:HE2	1:G:21:PRO:HD3	1.88	0.55
1:H:93:TYR:HB3	2:H:301:SQX:H72C	1.88	0.55
1:G:108:VAL:HB	1:G:116[B]:MET:CG	2.36	0.55
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.47	0.55
1:A:-3:ASP:N	1:A:-1:LYS:N	2.52	0.55
1:E:157:LYS:NZ	3:E:2052:HOH:O	2.39	0.55
1:B:59[B]:ARG:NH2	1:B:159:ASP:OD2	2.40	0.54
1:A:-3:ASP:N	1:A:-1:LYS:H	2.05	0.54
1:A:12:ASP:HA	1:A:16:ARG:HG2	1.88	0.54
1:I:93:TYR:HB3	2:I:301:SQX:H72C	1.90	0.54
1:C:122:ARG:HD2	1:D:96:THR:O	2.07	0.54
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.48	0.54
2:G:301:SQX:H331	2:G:301:SQX:H192	1.89	0.54
1:B:93:TYR:HB3	2:B:301:SQX:H72C	1.90	0.53
1:H:105:GLN:HE21	1:H:105:GLN:HA	1.73	0.53
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.49	0.52
1:D:184:GLN:NE2	1:D:197:ASP:OD1	2.37	0.52
1:G:108:VAL:HB	1:G:116[B]:MET:HG2	1.92	0.52
1:H:105:GLN:HA	1:H:105:GLN:NE2	2.25	0.52
1:B:105:GLN:HE21	1:B:105:GLN:HA	1.75	0.52
1:A:93:TYR:HB3	2:A:301:SQX:H72C	1.92	0.52
1:A:172:SER:O	1:A:207:ARG:HD3	2.09	0.52
1:C:5:ASN:HD22	1:C:73:GLY:HA3	1.75	0.52
1:F:122:ARG:HD2	1:G:96:THR:O	2.10	0.52
1:G:1:HIS:HA	1:G:4:ALA:HB3	1.92	0.51
1:C:77:ASP:OD1	1:C:79:ARG:NH2	2.41	0.51
1:J:105:GLN:HE21	1:J:105:GLN:HA	1.76	0.51
1:F:74:ASN:ND2	3:F:2026:HOH:O	2.42	0.51
1:F:184:GLN:NE2	1:F:197:ASP:OD1	2.41	0.50
1:H:184:GLN:NE2	1:H:199:ASN:HB2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ASP:OD2	1:D:148:VAL:HG22	2.11	0.50
1:F:7:MET:SD	1:G:18:PRO:HB2	2.52	0.50
1:D:143:LYS:HZ3	1:D:184:GLN:HE22	1.58	0.50
1:E:165:LEU:HD22	1:E:176:ILE:HD13	1.94	0.49
1:D:135:GLU:O	1:D:205:ARG:NH2	2.45	0.49
1:I:118:ILE:HD12	2:J:301:SQX:H352	1.94	0.49
1:I:0:LEU:N	1:I:1:HIS:CB	2.63	0.48
2:C:301:SQX:H331	2:C:301:SQX:H192	1.95	0.48
1:I:193:GLU:HG2	3:I:2007:HOH:O	2.12	0.48
1:B:105:GLN:HA	1:B:105:GLN:NE2	2.28	0.48
1:H:52:LEU:HG	1:H:125:PHE:HE2	1.79	0.47
1:D:17:SER:CB	1:D:18:PRO:HA	2.37	0.47
1:I:172:SER:HB3	1:I:207[B]:ARG:HH12	1.79	0.47
1:C:5:ASN:ND2	1:C:73:GLY:HA3	2.29	0.47
1:D:12:ASP:HA	1:D:16:ARG:HB2	1.96	0.47
1:G:171:SER:O	1:H:48:ASN:ND2	2.47	0.47
1:C:79:ARG:NH1	2:D:301:SQX:H531	2.29	0.47
1:J:56:GLU:O	1:J:119:PRO:HD2	2.15	0.46
1:E:161:ASP:HB3	1:E:162:GLN:HE21	1.81	0.46
1:A:195:TYR:CZ	2:A:301:SQX:H802	2.51	0.46
1:I:0:LEU:H2	1:I:2:SER:H	1.62	0.46
1:D:56:GLU:O	1:D:119:PRO:HD2	2.16	0.46
1:I:172:SER:HB3	1:I:207[B]:ARG:NH1	2.30	0.46
1:F:156:LEU:HD13	1:F:198:VAL:HG23	1.98	0.46
1:A:-1:LYS:HG3	1:B:27:ASP:OD2	2.16	0.45
1:I:155:ASP:OD2	1:I:157:LYS:NZ	2.49	0.45
1:I:156:LEU:O	1:I:183:ARG:HD2	2.17	0.45
1:D:105:GLN:HE21	1:D:105:GLN:HA	1.81	0.45
1:G:0:LEU:O	1:G:3:GLN:HB2	2.16	0.45
1:B:7:MET:HG3	1:C:21:PRO:HG3	1.99	0.45
1:C:-4:ASP:O	1:C:-3:ASP:CB	2.65	0.45
1:C:105:GLN:HA	1:C:105:GLN:HE21	1.82	0.45
1:A:195:TYR:OH	2:A:301:SQX:H802	2.16	0.45
1:E:110:THR:HG22	1:E:112:ASP:H	1.82	0.45
1:J:36:THR:HB	1:J:55:TYR:HB2	1.98	0.45
1:F:99:VAL:HG11	1:F:121:GLN:OE1	2.18	0.44
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.57	0.44
1:E:17:SER:HB2	1:E:18:PRO:CD	2.46	0.44
1:E:139:THR:HG23	1:E:203[A]:LYS:HG2	1.99	0.44
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.58	0.44
1:C:8:ARG:NH2	1:C:71:GLU:O	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:CYS:HA	1:G:192:PRO:HD3	1.87	0.44
1:J:191:CYS:HB3	1:J:193:GLU:OE1	2.18	0.44
1:A:187[B]:HIS:ND1	1:A:187[B]:HIS:N	2.66	0.44
1:I:51:ASP:HA	1:I:123:LEU:O	2.18	0.44
1:A:188[C]:TYR:HB3	1:A:190:CYS:HB3	1.99	0.43
1:I:141:ALA:HA	1:I:200:LEU:O	2.19	0.43
1:G:143:LYS:HE3	1:G:184:GLN:NE2	2.33	0.43
1:C:191:CYS:SG	2:C:301:SQX:H801	2.59	0.43
1:F:193:GLU:H	1:F:193:GLU:CD	2.21	0.43
1:B:74:ASN:ND2	3:B:2030:HOH:O	2.45	0.43
1:C:207[A]:ARG:HH21	1:C:207[A]:ARG:CB	2.24	0.43
1:D:141:ALA:HA	1:D:200:LEU:O	2.19	0.43
1:H:149:TYR:CD2	1:H:154:ILE:HD12	2.54	0.43
1:B:110:THR:HG22	1:B:111:HIS:N	2.32	0.42
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.59	0.42
1:E:78:PHE:C	1:E:79:ARG:HD2	2.38	0.42
1:I:56:GLU:O	1:I:119:PRO:HD2	2.18	0.42
1:C:175:GLU:OE1	1:C:207[B]:ARG:HD3	2.20	0.42
1:G:169:TYR:CZ	1:G:171:SER:HB2	2.54	0.42
1:H:36:THR:HB	1:H:55:TYR:HB2	2.01	0.42
1:I:99:VAL:HG23	3:I:2051:HOH:O	2.18	0.42
1:D:97[B]:ARG:HD3	1:D:124:SER:CB	2.49	0.42
1:F:95:SER:HB3	1:F:123:LEU:HD11	2.01	0.42
1:F:191:CYS:HA	1:F:192:PRO:HD3	1.89	0.42
1:H:145:GLY:HA2	1:H:156:LEU:HD11	2.01	0.42
1:F:193:GLU:HG2	3:F:2058:HOH:O	2.20	0.42
1:B:141:ALA:HA	1:B:200:LEU:O	2.20	0.42
2:F:301:SQX:H331	2:F:301:SQX:H12	1.84	0.41
1:H:0:LEU:H	1:H:0:LEU:HD22	1.85	0.41
1:A:52:LEU:O	1:A:122:ARG:HA	2.21	0.41
1:A:122:ARG:HD2	1:B:96:THR:O	2.20	0.41
1:F:79:ARG:HD2	1:F:108:VAL:HG22	2.01	0.41
1:E:77:ASP:OD1	1:E:79:ARG:NH2	2.43	0.41
1:E:93:TYR:HB3	2:E:301:SQX:H72C	2.02	0.41
1:A:104:PRO:HG2	1:B:89:ASP:HB2	2.03	0.41
1:D:95:SER:HB3	1:D:123:LEU:HD11	2.03	0.41
1:I:14:PHE:HD2	1:I:19:MET:SD	2.44	0.41
1:B:110:THR:CG2	1:B:111:HIS:N	2.84	0.41
1:F:61:LYS:HA	1:F:114:SER:HA	2.03	0.41
1:B:59[B]:ARG:NH1	1:B:59[B]:ARG:CB	2.83	0.41
1:D:192:PRO:HD2	1:D:193:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ILE:HD12	2:G:301:SQX:H352	2.02	0.41
1:J:177:LEU:HB2	1:J:203:LYS:HG2	2.03	0.41
1:J:191:CYS:HA	1:J:192:PRO:HD3	1.90	0.41
1:D:105:GLN:HA	1:D:105:GLN:NE2	2.36	0.40
2:J:301:SQX:H4	3:J:2018:HOH:O	2.21	0.40
1:G:43:ALA:HA	1:G:50:VAL:HG22	2.03	0.40
1:E:51:ASP:HA	1:E:123:LEU:O	2.20	0.40
1:I:99:VAL:HG22	1:I:123:LEU:HD13	2.02	0.40
1:J:207[A]:ARG:HB3	1:J:208:ARG:HA	2.03	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	214/228 (94%)	210 (98%)	3 (1%)	1 (0%)	29	48
1	B	214/228 (94%)	211 (99%)	3 (1%)	0	100	100
1	C	213/228 (93%)	203 (95%)	9 (4%)	1 (0%)	29	48
1	D	212/228 (93%)	208 (98%)	3 (1%)	1 (0%)	29	48
1	E	211/228 (92%)	206 (98%)	4 (2%)	1 (0%)	29	48
1	F	208/228 (91%)	201 (97%)	7 (3%)	0	100	100
1	G	213/228 (93%)	209 (98%)	3 (1%)	1 (0%)	29	48
1	H	211/228 (92%)	206 (98%)	5 (2%)	0	100	100
1	I	212/228 (93%)	207 (98%)	4 (2%)	1 (0%)	29	48
1	J	213/228 (93%)	209 (98%)	2 (1%)	2 (1%)	17	31
All	All	2121/2280 (93%)	2070 (98%)	43 (2%)	8 (0%)	34	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	1	HIS
1	C	-3	ASP
1	D	17	SER
1	A	-2	ASP
1	E	19	MET
1	J	17	SER
1	G	0	LEU
1	J	18	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/206 (96%)	193 (98%)	4 (2%)	55	79
1	B	196/206 (95%)	194 (99%)	2 (1%)	76	90
1	C	192/206 (93%)	191 (100%)	1 (0%)	88	96
1	D	193/206 (94%)	187 (97%)	6 (3%)	40	67
1	E	194/206 (94%)	183 (94%)	11 (6%)	20	39
1	F	192/206 (93%)	187 (97%)	5 (3%)	46	72
1	G	196/206 (95%)	188 (96%)	8 (4%)	30	55
1	H	193/206 (94%)	186 (96%)	7 (4%)	35	61
1	I	195/206 (95%)	193 (99%)	2 (1%)	76	90
1	J	196/206 (95%)	185 (94%)	11 (6%)	21	40
All	All	1944/2060 (94%)	1887 (97%)	57 (3%)	43	69

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	167	SER
1	A	190	CYS
1	A	191	CYS
1	B	17	SER
1	B	127	CYS

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Mol	Chain	Res	Type
1	C	91	THR
1	D	52	LEU
1	D	59[A]	ARG
1	D	59[B]	ARG
1	D	99	VAL
1	D	186	GLN
1	D	208	ARG
1	E	16	ARG
1	E	19	MET
1	E	26	ASP
1	E	59	ARG
1	E	70	ASN
1	E	71	GLU
1	E	105	GLN
1	E	156	LEU
1	E	161	ASP
1	E	176	ILE
1	E	208	ARG
1	F	11	SER
1	F	79	ARG
1	F	97[A]	ARG
1	F	97[B]	ARG
1	F	135	GLU
1	G	-2	ASP
1	G	0	LEU
1	G	19	MET
1	G	26	ASP
1	G	127	CYS
1	G	136	GLU
1	G	156	LEU
1	G	186	GLN
1	H	16	ARG
1	H	17	SER
1	H	79	ARG
1	H	91	THR
1	H	99	VAL
1	H	161	ASP
1	H	167	SER
1	I	186[A]	GLN
1	I	186[B]	GLN
1	J	0	LEU
1	J	16	ARG

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Mol	Chain	Res	Type
1	J	17	SER
1	J	19	MET
1	J	33	LEU
1	J	71	GLU
1	J	91	THR
1	J	132	VAL
1	J	135	GLU
1	J	178	SER
1	J	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	199	ASN
1	B	105	GLN
1	C	3	GLN
1	C	74	ASN
1	C	105	GLN
1	C	111	HIS
1	C	187	HIS
1	D	3	GLN
1	D	105	GLN
1	D	121	GLN
1	D	184	GLN
1	D	186	GLN
1	D	199	ASN
1	E	105	GLN
1	E	162	GLN
1	E	184	GLN
1	F	15	ASN
1	F	70	ASN
1	F	74	ASN
1	F	186	GLN
1	F	199	ASN
1	G	57	GLN
1	G	63	ASN
1	G	121	GLN
1	G	162	GLN
1	G	184	GLN
1	H	3	GLN
1	H	38	GLN

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Mol	Chain	Res	Type
1	H	105	GLN
1	H	184	GLN
1	I	184	GLN
1	I	199	ASN
1	J	105	GLN
1	J	121	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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	SQX	H	301	-	50,56,56	1.10	1 (2%)	52,88,88	1.43	8 (15%)
2	SQX	A	301	-	50,56,56	1.13	2 (4%)	52,88,88	1.57	9 (17%)
2	SQX	E	301	-	50,56,56	1.14	1 (2%)	52,88,88	1.72	10 (19%)
2	SQX	D	301	-	50,56,56	1.10	2 (4%)	52,88,88	1.31	9 (17%)
2	SQX	B	301	-	50,56,56	1.12	2 (4%)	52,88,88	1.49	8 (15%)
2	SQX	J	301	-	50,56,56	1.16	1 (2%)	52,88,88	1.60	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SQX	F	301	-	50,56,56	1.14	2 (4%)	52,88,88	1.51	8 (15%)
2	SQX	G	301	-	50,56,56	1.16	2 (4%)	52,88,88	1.47	8 (15%)
2	SQX	I	301	-	50,56,56	1.19	2 (4%)	52,88,88	1.42	8 (15%)
2	SQX	C	301	-	50,56,56	1.11	2 (4%)	52,88,88	1.78	11 (21%)

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	SQX	H	301	-	-	4/23/122/122	1/6/7/7
2	SQX	A	301	-	-	2/23/122/122	1/6/7/7
2	SQX	E	301	-	-	2/23/122/122	1/6/7/7
2	SQX	D	301	-	-	1/23/122/122	1/6/7/7
2	SQX	B	301	-	-	0/23/122/122	1/6/7/7
2	SQX	J	301	-	-	2/23/122/122	1/6/7/7
2	SQX	F	301	-	-	2/23/122/122	1/6/7/7
2	SQX	G	301	-	-	1/23/122/122	1/6/7/7
2	SQX	I	301	-	-	2/23/122/122	1/6/7/7
2	SQX	C	301	-	-	3/23/122/122	1/6/7/7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	SQX	O1-C5	7.01	1.45	1.35
2	J	301	SQX	O1-C5	6.90	1.45	1.35
2	E	301	SQX	O1-C5	6.80	1.45	1.35
2	A	301	SQX	O1-C5	6.69	1.45	1.35
2	D	301	SQX	O1-C5	6.49	1.44	1.35
2	G	301	SQX	O1-C5	6.44	1.44	1.35
2	F	301	SQX	O1-C5	6.39	1.44	1.35
2	H	301	SQX	O1-C5	6.38	1.44	1.35
2	C	301	SQX	O1-C5	6.33	1.44	1.35
2	B	301	SQX	O1-C5	6.28	1.44	1.35
2	G	301	SQX	C13-C8	3.12	1.36	1.33
2	C	301	SQX	O1-C2	-2.56	1.42	1.46
2	I	301	SQX	C13-C8	2.42	1.36	1.33
2	B	301	SQX	C13-C8	2.34	1.36	1.33
2	A	301	SQX	C13-C8	2.19	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	SQX	C13-C8	2.05	1.35	1.33
2	D	301	SQX	C13-C8	2.03	1.35	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	SQX	C2-O1-C5	-6.37	105.42	110.41
2	E	301	SQX	C2-O1-C5	-6.00	105.71	110.41
2	C	301	SQX	O1-C2-C3	4.87	108.03	104.11
2	E	301	SQX	O1-C2-C3	4.76	107.94	104.11
2	J	301	SQX	O1-C2-C3	4.76	107.93	104.11
2	B	301	SQX	C2-O1-C5	-4.71	106.72	110.41
2	J	301	SQX	C2-O1-C5	-4.70	106.73	110.41
2	I	301	SQX	C2-O1-C5	-4.42	106.95	110.41
2	H	301	SQX	O1-C2-C3	4.42	107.66	104.11
2	A	301	SQX	O47-C48-C37	4.24	109.83	105.78
2	D	301	SQX	C2-O1-C5	-3.92	107.34	110.41
2	C	301	SQX	O1-C5-C4	3.92	114.41	110.41
2	A	301	SQX	O1-C2-C3	3.89	107.24	104.11
2	F	301	SQX	C2-O1-C5	-3.89	107.37	110.41
2	A	301	SQX	C2-O1-C5	-3.88	107.37	110.41
2	E	301	SQX	O1-C5-C4	3.84	114.33	110.41
2	E	301	SQX	O6-C5-C4	-3.77	123.97	128.56
2	H	301	SQX	C2-O1-C5	-3.76	107.47	110.41
2	G	301	SQX	O1-C2-C3	3.73	107.11	104.11
2	I	301	SQX	O1-C2-C3	3.71	107.09	104.11
2	G	301	SQX	O47-C48-C37	3.68	109.30	105.78
2	G	301	SQX	C2-O1-C5	-3.66	107.55	110.41
2	A	301	SQX	O6-C5-C4	-3.65	124.11	128.56
2	B	301	SQX	O1-C5-C4	3.65	114.13	110.41
2	F	301	SQX	O1-C2-C3	3.64	107.04	104.11
2	B	301	SQX	O6-C5-C4	-3.60	124.17	128.56
2	C	301	SQX	C3-C4-C5	-3.54	99.33	102.59
2	I	301	SQX	O6-C5-C4	-3.50	124.29	128.56
2	J	301	SQX	O47-C48-C37	3.32	108.95	105.78
2	A	301	SQX	O1-C5-C4	3.30	113.78	110.41
2	B	301	SQX	O1-C2-C3	3.26	106.73	104.11
2	F	301	SQX	C19-C16-C17	3.08	120.86	115.22
2	J	301	SQX	C14-C13-C8	-3.08	118.21	123.86
2	F	301	SQX	C50-C49-C48	2.96	115.37	110.33
2	J	301	SQX	C19-C16-C17	2.93	120.58	115.22
2	E	301	SQX	C19-C16-C17	2.81	120.37	115.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	SQX	C14-C13-C8	-2.79	118.75	123.86
2	A	301	SQX	C19-C16-C17	2.78	120.31	115.22
2	G	301	SQX	O6-C5-C4	-2.77	125.19	128.56
2	C	301	SQX	O6-C5-C4	-2.76	125.20	128.56
2	G	301	SQX	C19-C16-C17	2.73	120.21	115.22
2	J	301	SQX	O6-C5-C4	-2.73	125.24	128.56
2	C	301	SQX	C14-C13-C8	-2.68	118.95	123.86
2	H	301	SQX	C55-C42-C43	2.65	107.23	103.28
2	G	301	SQX	O1-C5-C4	2.62	113.09	110.41
2	C	301	SQX	O47-C48-C37	2.57	108.23	105.78
2	F	301	SQX	O6-C5-C4	-2.56	125.44	128.56
2	H	301	SQX	C14-C13-C8	-2.53	119.22	123.86
2	D	301	SQX	O1-C2-C3	2.52	106.13	104.11
2	F	301	SQX	O1-C5-C4	2.50	112.96	110.41
2	I	301	SQX	C55-C42-C43	2.50	107.01	103.28
2	D	301	SQX	C55-C42-C43	2.41	106.88	103.28
2	D	301	SQX	C49-C50-C51	2.40	115.77	113.25
2	H	301	SQX	O1-C5-C4	2.40	112.86	110.41
2	H	301	SQX	O6-C5-C4	-2.39	125.65	128.56
2	F	301	SQX	C9-C10-C27	2.38	115.90	112.02
2	D	301	SQX	C21-C18-C17	-2.38	109.36	114.44
2	J	301	SQX	O1-C5-C4	2.37	112.83	110.41
2	B	301	SQX	C18-C21-C81	-2.36	110.88	114.64
2	G	301	SQX	C50-C49-C48	2.33	114.29	110.33
2	E	301	SQX	C55-C42-C43	2.32	106.74	103.28
2	I	301	SQX	C19-C16-C17	2.31	119.45	115.22
2	A	301	SQX	C55-C42-C43	2.31	106.73	103.28
2	D	301	SQX	C14-C13-C8	-2.31	119.63	123.86
2	I	301	SQX	O1-C5-C4	2.30	112.76	110.41
2	E	301	SQX	C50-C49-C48	2.30	114.25	110.33
2	H	301	SQX	C49-C48-C37	-2.29	108.92	113.21
2	J	301	SQX	C55-C42-C43	2.26	106.65	103.28
2	D	301	SQX	C19-C16-C17	2.26	119.35	115.22
2	G	301	SQX	C55-C42-C43	2.24	106.62	103.28
2	E	301	SQX	C14-C13-C8	-2.23	119.78	123.86
2	E	301	SQX	C3-C4-C5	-2.22	100.54	102.59
2	C	301	SQX	C42-C55-C23	2.20	105.61	103.14
2	A	301	SQX	C14-C13-C8	-2.17	119.88	123.86
2	B	301	SQX	C19-C16-C17	2.15	119.15	115.22
2	C	301	SQX	C18-C21-C81	-2.13	111.25	114.64
2	F	301	SQX	O47-C43-C51	2.11	112.58	110.21
2	B	301	SQX	C3-C4-C5	-2.11	100.64	102.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	SQX	C19-C16-C17	2.11	119.07	115.22
2	A	301	SQX	C4-C3-C2	2.10	107.95	103.66
2	D	301	SQX	O6-C5-C4	-2.09	126.02	128.56
2	J	301	SQX	C50-C49-C48	2.09	113.88	110.33
2	B	301	SQX	C42-C55-C23	2.09	105.48	103.14
2	I	301	SQX	C3-C4-C5	-2.07	100.68	102.59
2	C	301	SQX	C55-C42-C43	2.06	106.35	103.28
2	D	301	SQX	O1-C5-C4	2.05	112.50	110.41
2	H	301	SQX	C19-C16-C17	2.03	118.94	115.22
2	E	301	SQX	O48-C21-C18	-2.01	107.23	110.47

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SQX	C17-C18-C21-C81
2	H	301	SQX	C17-C18-C21-C81
2	G	301	SQX	C32-C33-C34-C35
2	C	301	SQX	C32-C33-C34-C35
2	J	301	SQX	C32-C33-C34-C35
2	E	301	SQX	C32-C33-C34-C35
2	A	301	SQX	C17-C18-C21-O48
2	C	301	SQX	C17-C18-C21-O48
2	F	301	SQX	C17-C18-C21-O48
2	H	301	SQX	C17-C18-C21-O48
2	H	301	SQX	C32-C33-C34-C35
2	C	301	SQX	C17-C18-C21-C81
2	D	301	SQX	C17-C18-C21-C81
2	E	301	SQX	C17-C18-C21-C81
2	F	301	SQX	C17-C18-C21-C81
2	I	301	SQX	C17-C18-C21-C81
2	J	301	SQX	C17-C18-C21-C81
2	H	301	SQX	C38-C36-C37-C48
2	I	301	SQX	C32-C33-C34-C35

All (10) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	H	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	B	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	E	301	SQX	C27-C28-C29-C30-C32-C46-N31

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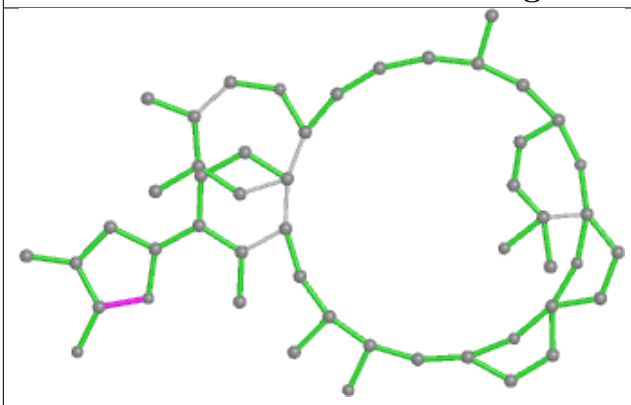
Mol	Chain	Res	Type	Atoms
2	G	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	F	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	I	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	D	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	C	301	SQX	C27-C28-C29-C30-C32-C46-N31
2	J	301	SQX	C27-C28-C29-C30-C32-C46-N31

10 monomers are involved in 24 short contacts:

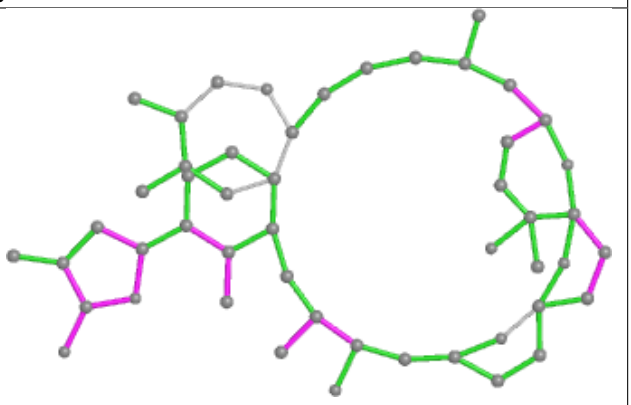
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	SQX	2	0
2	A	301	SQX	4	0
2	E	301	SQX	2	0
2	D	301	SQX	2	0
2	B	301	SQX	2	0
2	J	301	SQX	3	0
2	F	301	SQX	2	0
2	G	301	SQX	3	0
2	I	301	SQX	2	0
2	C	301	SQX	2	0

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

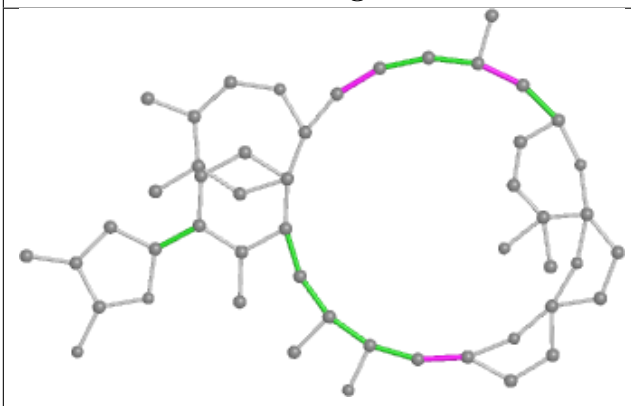
Ligand SQX H 301



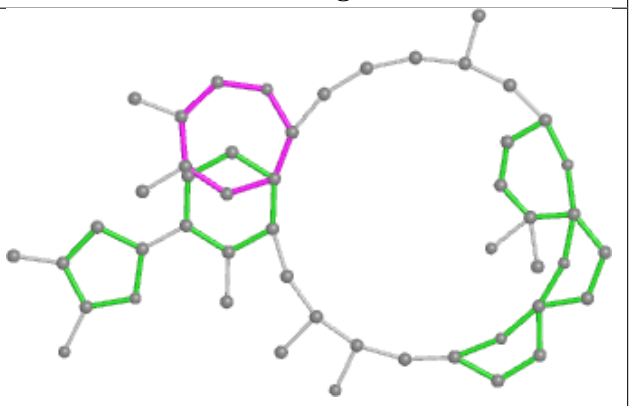
Bond lengths



Bond angles

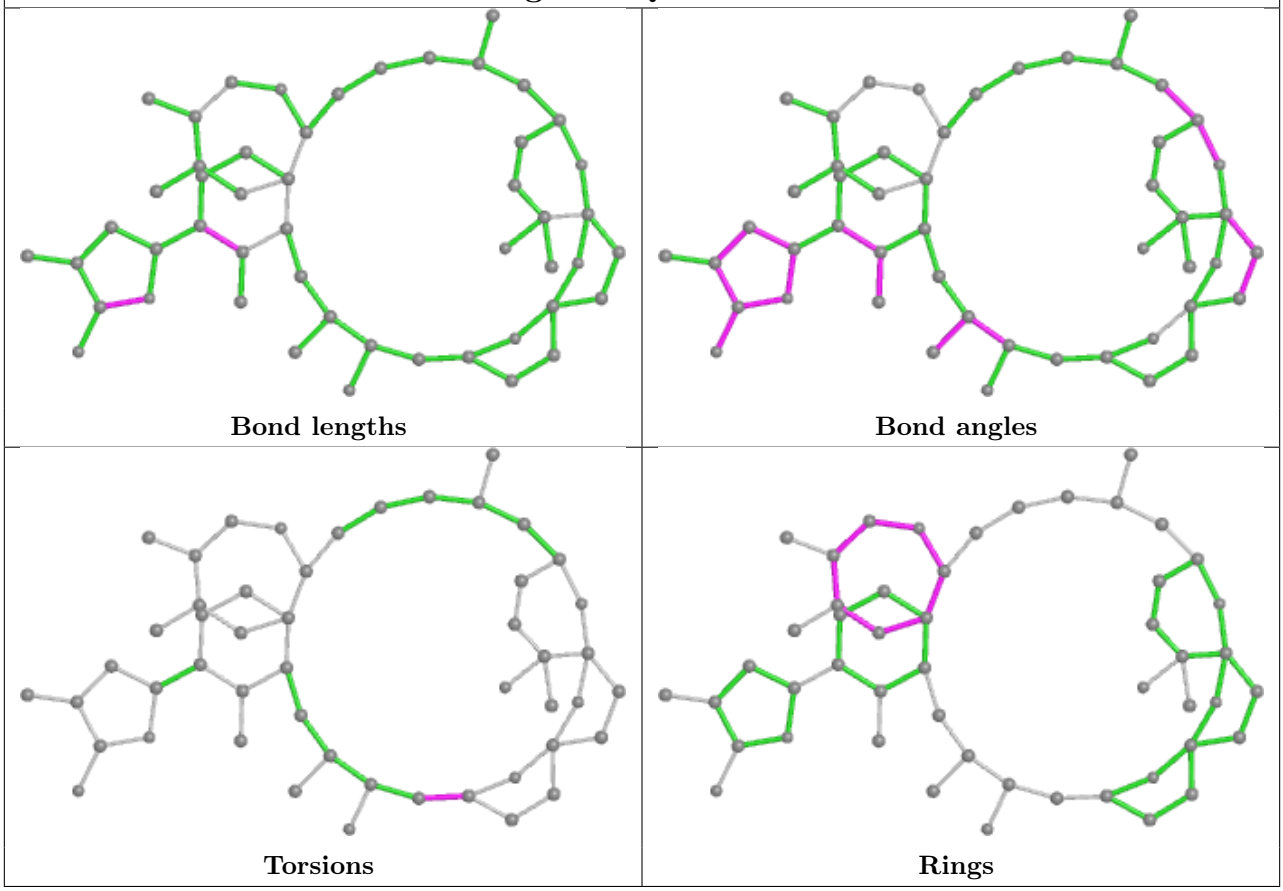


Torsions

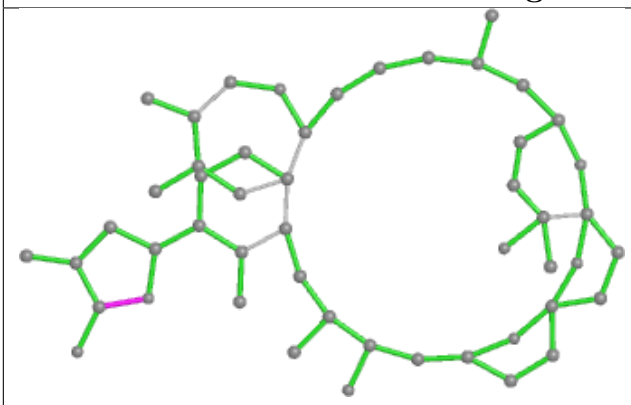


Rings

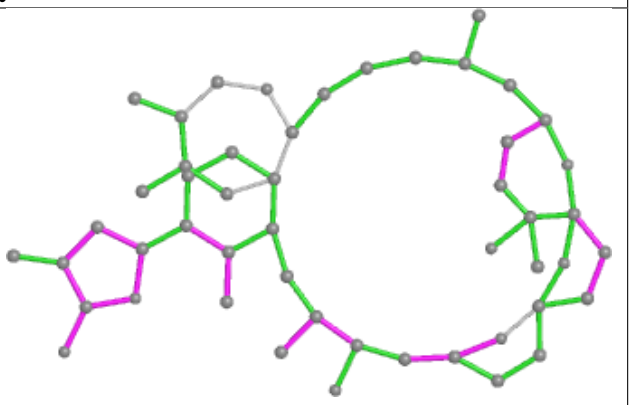
Ligand SQX A 301



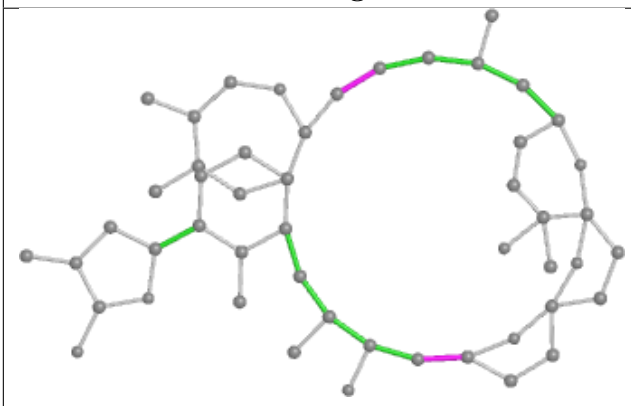
Ligand SQX E 301



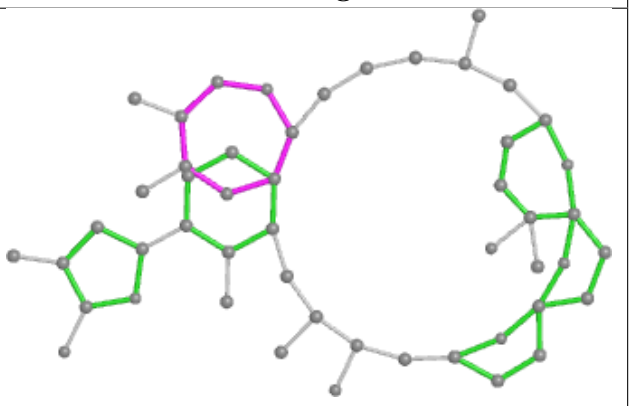
Bond lengths



Bond angles

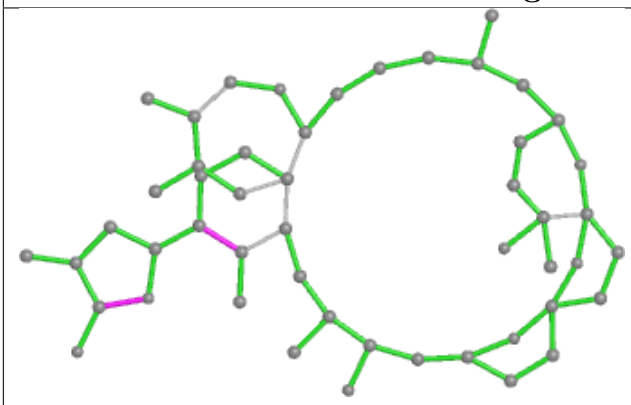


Torsions

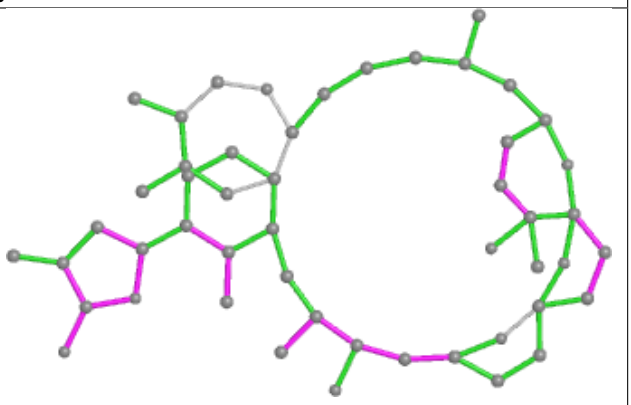


Rings

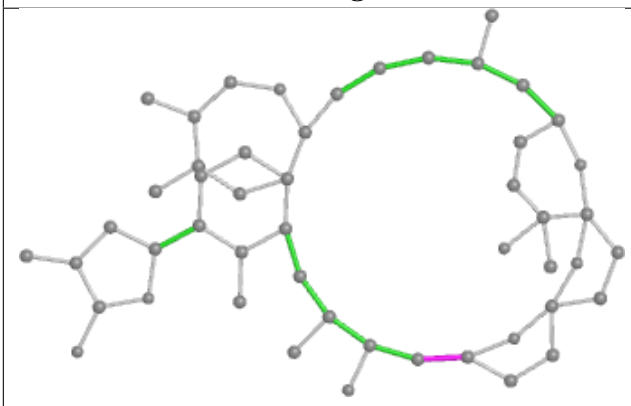
Ligand SQX D 301



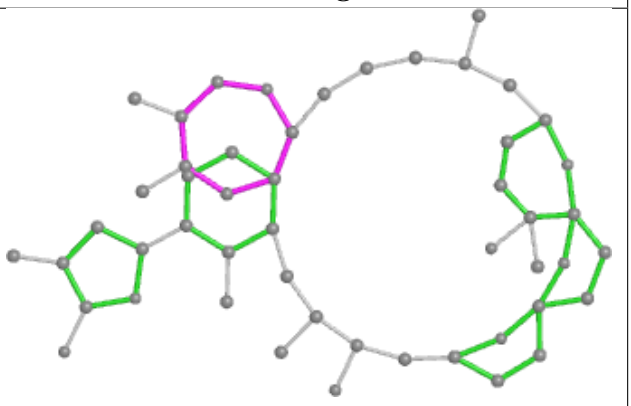
Bond lengths



Bond angles

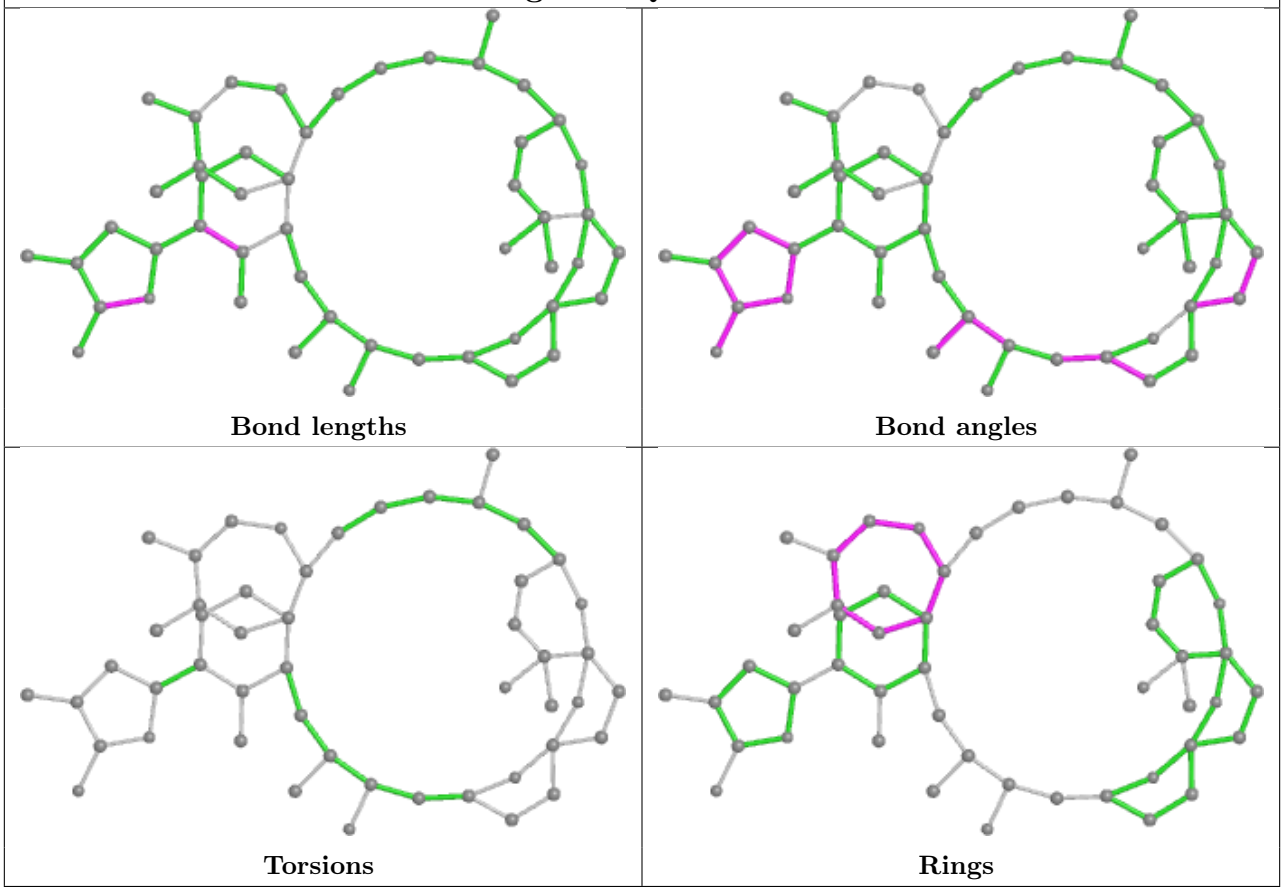


Torsions

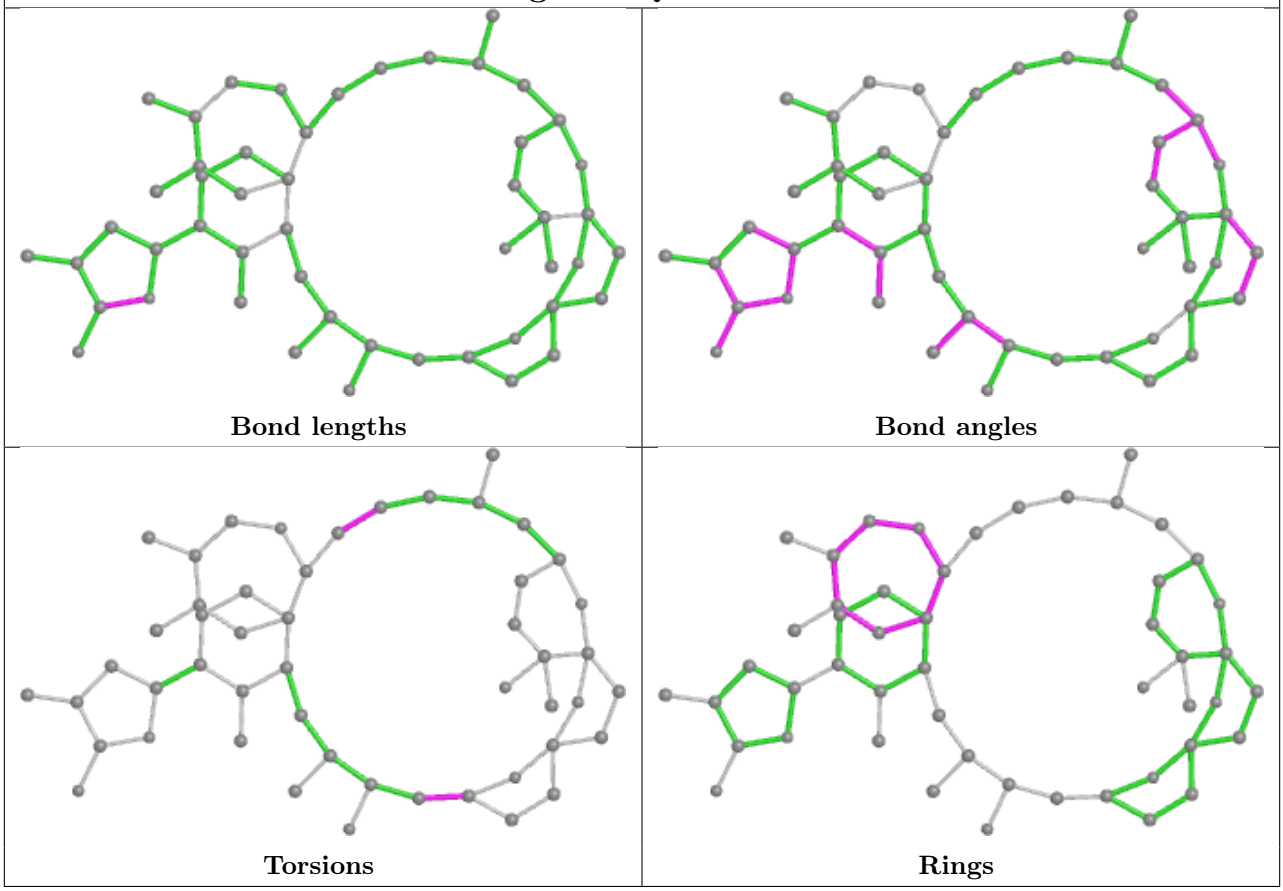


Rings

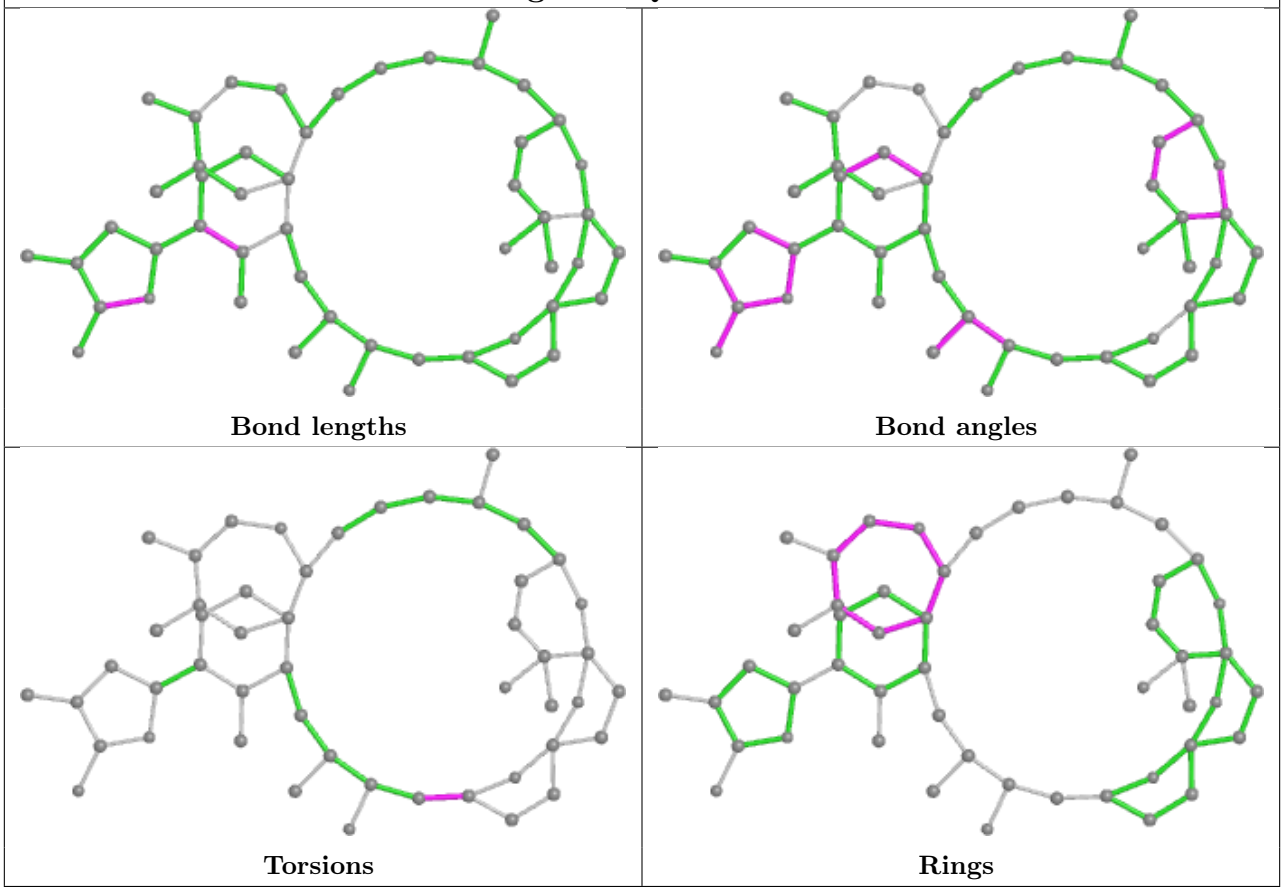
Ligand SQX B 301



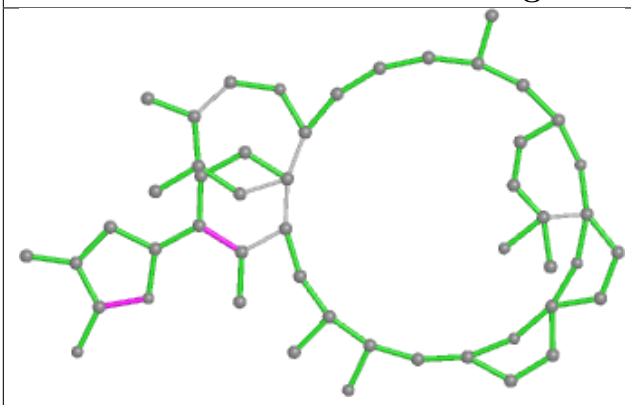
Ligand SQX J 301



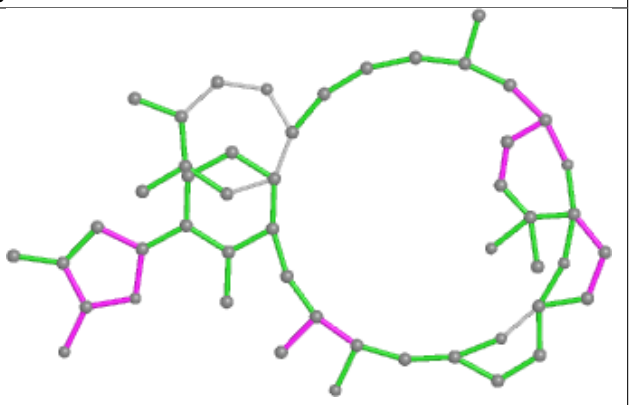
Ligand SQX F 301



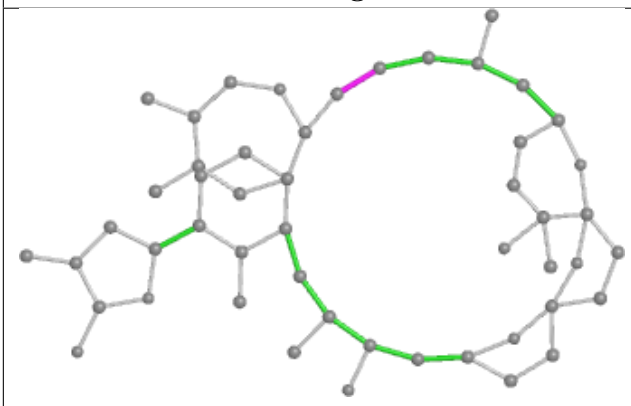
Ligand SQX G 301



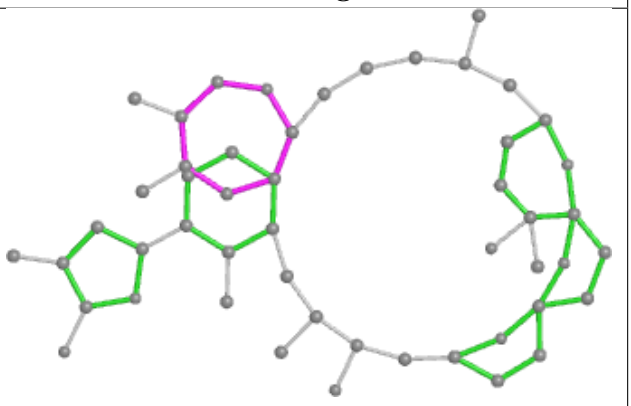
Bond lengths



Bond angles

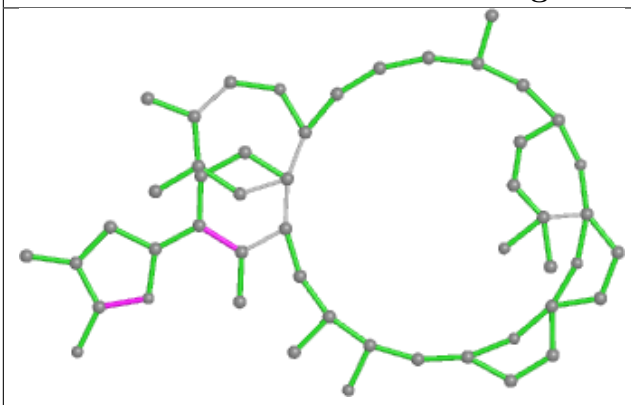


Torsions

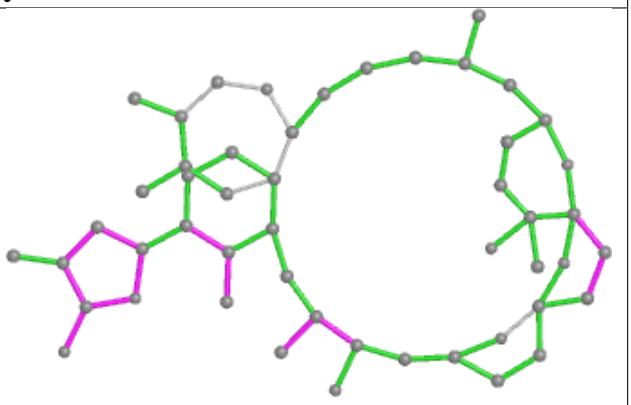


Rings

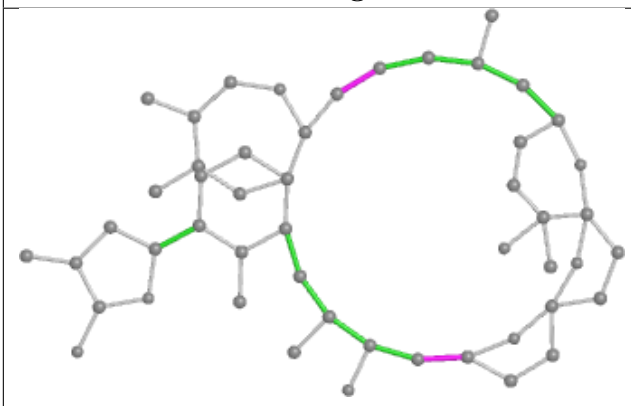
Ligand SQX I 301



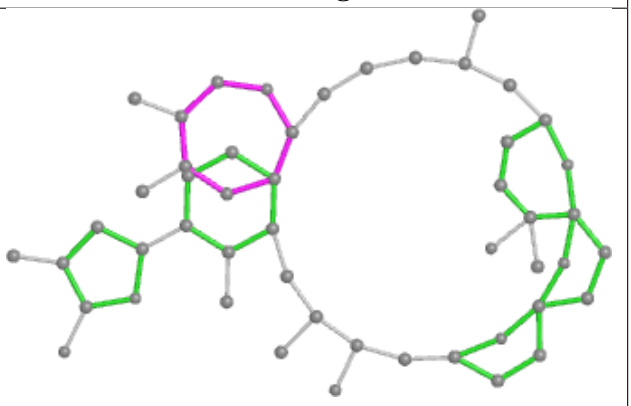
Bond lengths



Bond angles

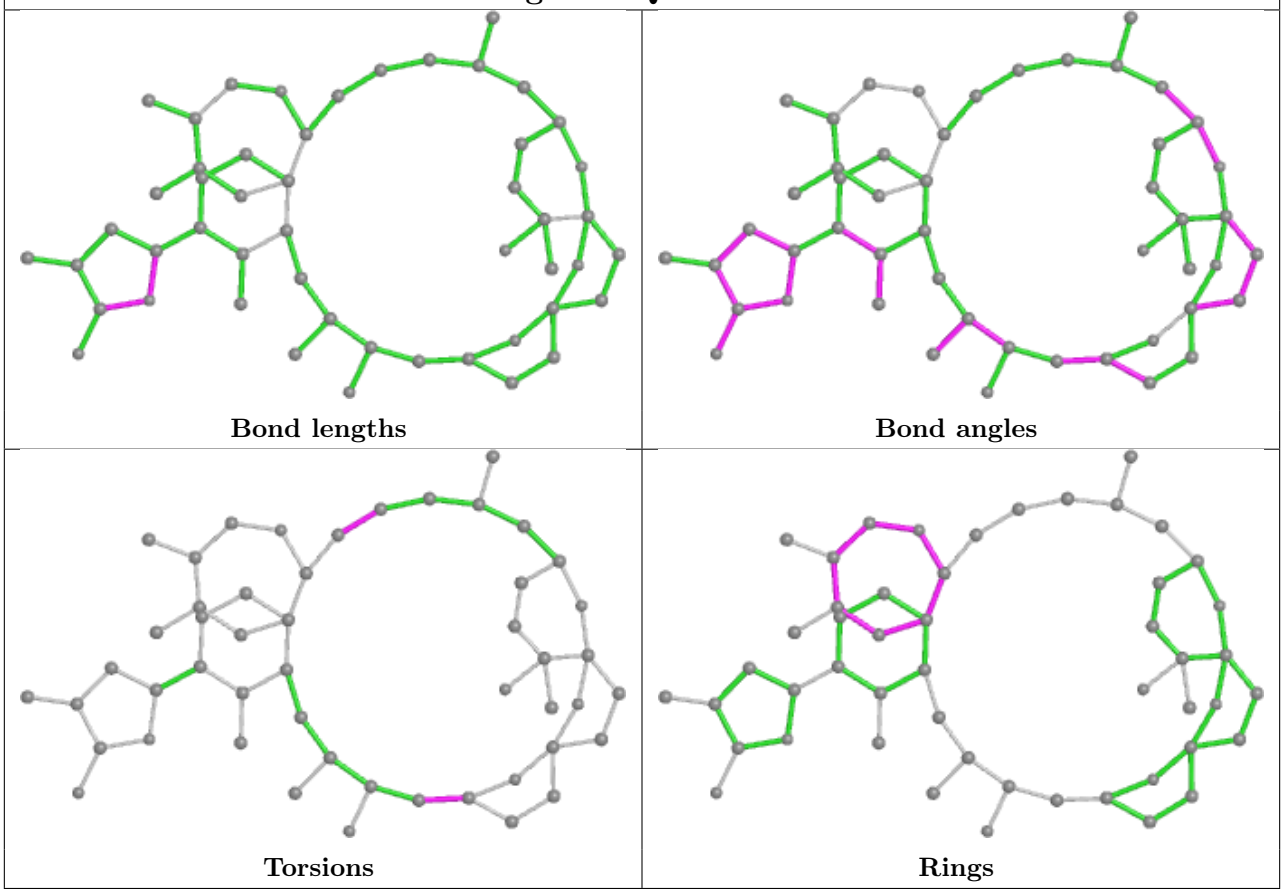


Torsions



Rings

Ligand SQX 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	212/228 (92%)	-0.31	3 (1%)	75	77	32, 49, 81, 104	0
1	B	213/228 (93%)	-0.48	3 (1%)	75	77	30, 43, 66, 91	0
1	C	213/228 (93%)	-0.52	2 (0%)	84	86	26, 41, 78, 102	0
1	D	211/228 (92%)	-0.48	2 (0%)	84	86	27, 42, 79, 93	0
1	E	210/228 (92%)	-0.43	5 (2%)	59	62	30, 44, 77, 96	0
1	F	208/228 (91%)	-0.52	3 (1%)	75	77	28, 42, 80, 96	0
1	G	212/228 (92%)	-0.41	5 (2%)	59	62	31, 44, 84, 111	0
1	H	211/228 (92%)	-0.60	1 (0%)	91	91	30, 41, 72, 88	0
1	I	209/228 (91%)	-0.63	2 (0%)	82	84	29, 40, 62, 70	0
1	J	212/228 (92%)	-0.56	4 (1%)	66	69	28, 39, 74, 100	0
All	All	2111/2280 (92%)	-0.49	30 (1%)	75	77	26, 42, 78, 111	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ALA	5.3
1	E	19	MET	4.6
1	A	19[A]	MET	4.4
1	G	19	MET	3.9
1	A	188[B]	TYR	3.7
1	J	1	HIS	3.7
1	E	0	LEU	3.4
1	G	1	HIS	3.3
1	E	18	PRO	3.1
1	F	0	LEU	3.1
1	G	-3	ASP	3.0
1	F	18	PRO	3.0
1	B	-3	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	208	ARG	2.9
1	E	1	HIS	2.8
1	A	-2	ASP	2.7
1	G	-2	ASP	2.7
1	C	1	HIS	2.7
1	J	208	ARG	2.7
1	G	18	PRO	2.6
1	J	-3	ASP	2.6
1	B	0	LEU	2.5
1	D	208	ARG	2.5
1	D	18	PRO	2.5
1	I	208	ARG	2.3
1	F	16	ARG	2.2
1	J	16	ARG	2.2
1	H	1	HIS	2.1
1	I	0	LEU	2.1
1	C	15	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SQX	A	301	50/50	0.94	0.12	46,50,53,54	0
2	SQX	C	301	50/50	0.96	0.12	31,38,41,42	0
2	SQX	D	301	50/50	0.96	0.12	33,36,37,38	0
2	SQX	F	301	50/50	0.96	0.12	33,39,41,43	0
2	SQX	G	301	50/50	0.96	0.12	37,44,46,47	0
2	SQX	I	301	50/50	0.96	0.11	34,38,41,44	0

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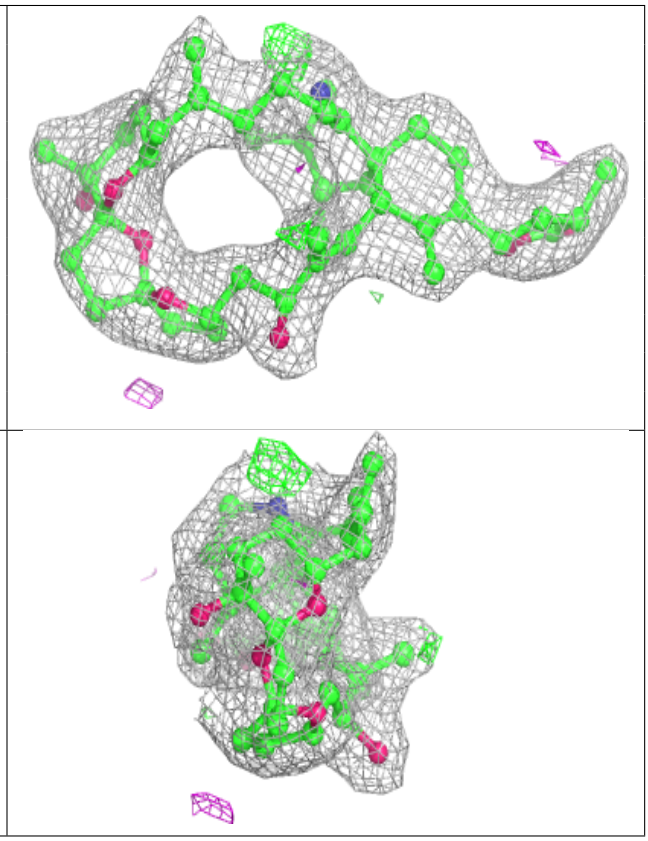
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SQX	J	301	50/50	0.96	0.11	31,35,39,41	0
2	SQX	H	301	50/50	0.97	0.10	32,37,39,40	0
2	SQX	B	301	50/50	0.97	0.12	37,42,45,45	0
2	SQX	E	301	50/50	0.97	0.11	36,39,41,43	0

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.

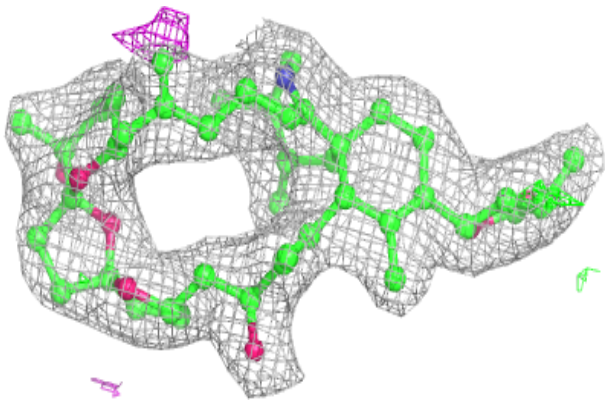
Electron density around SQX A 301:

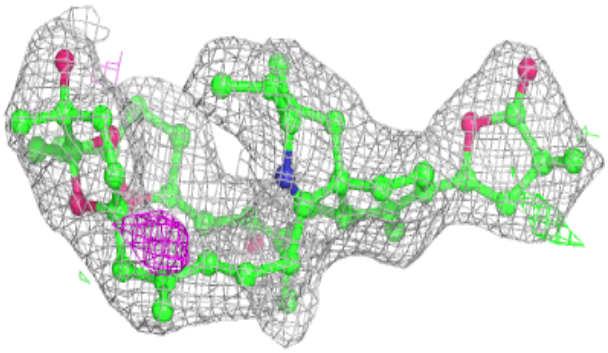
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

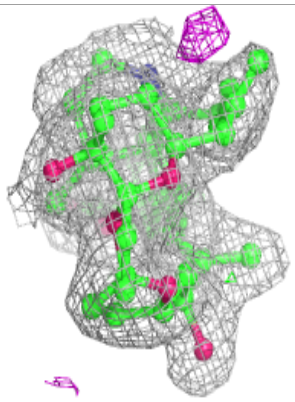


Electron density around SQX C 301:

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

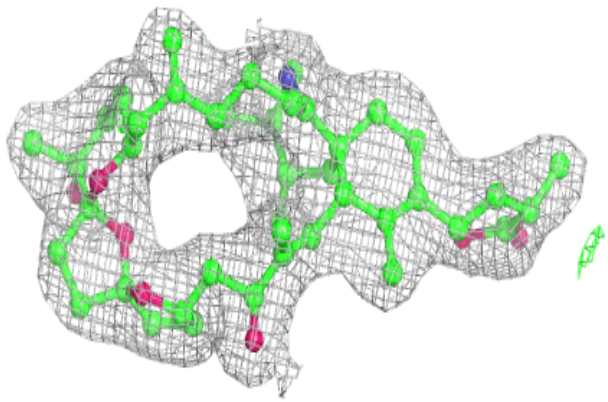


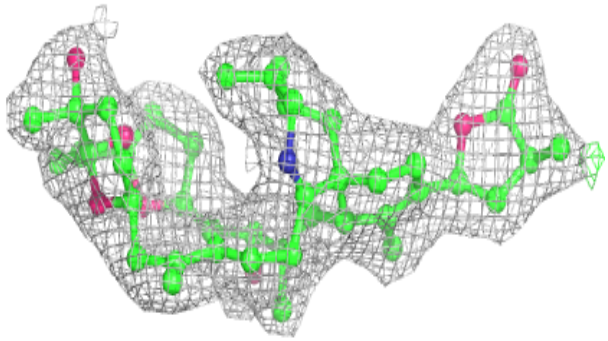


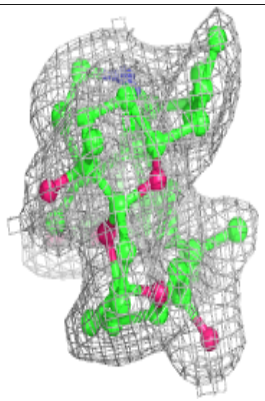


Electron density around SQX D 301:

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

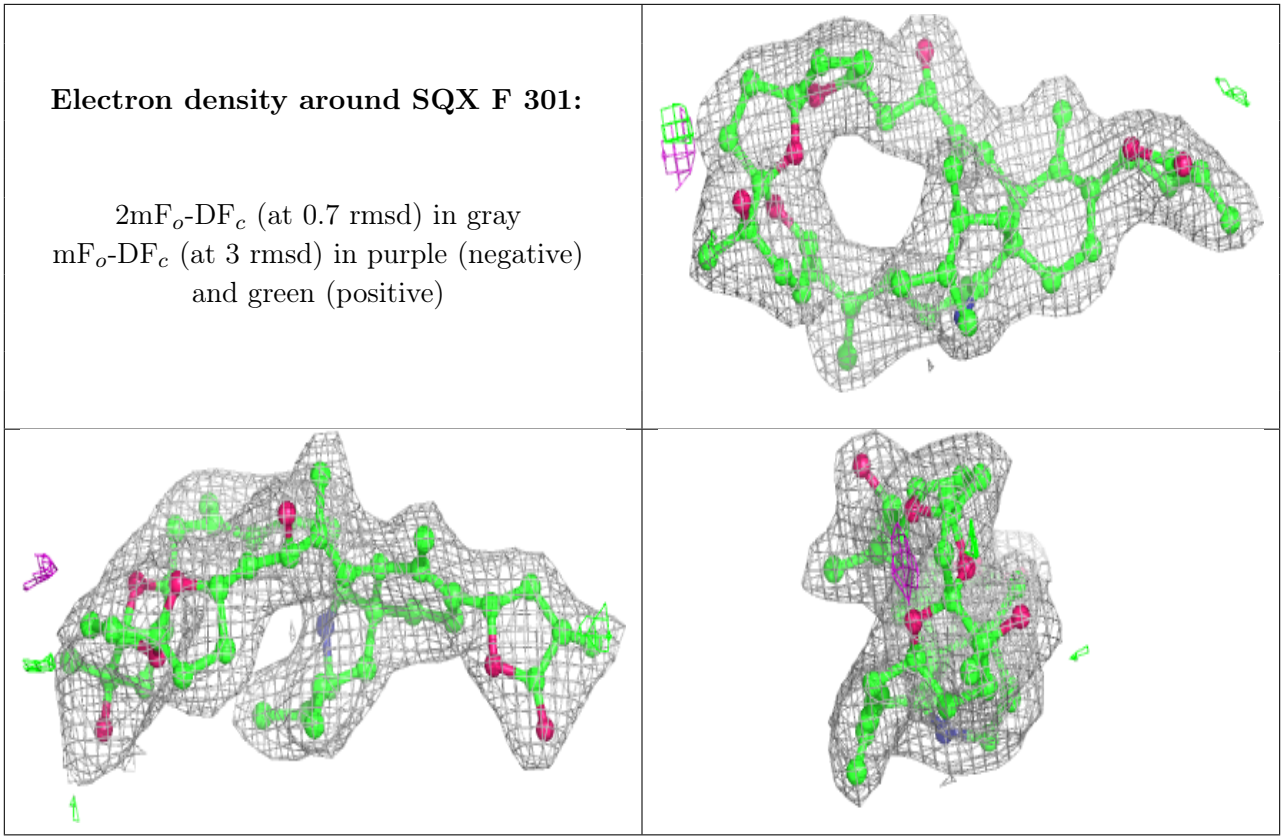






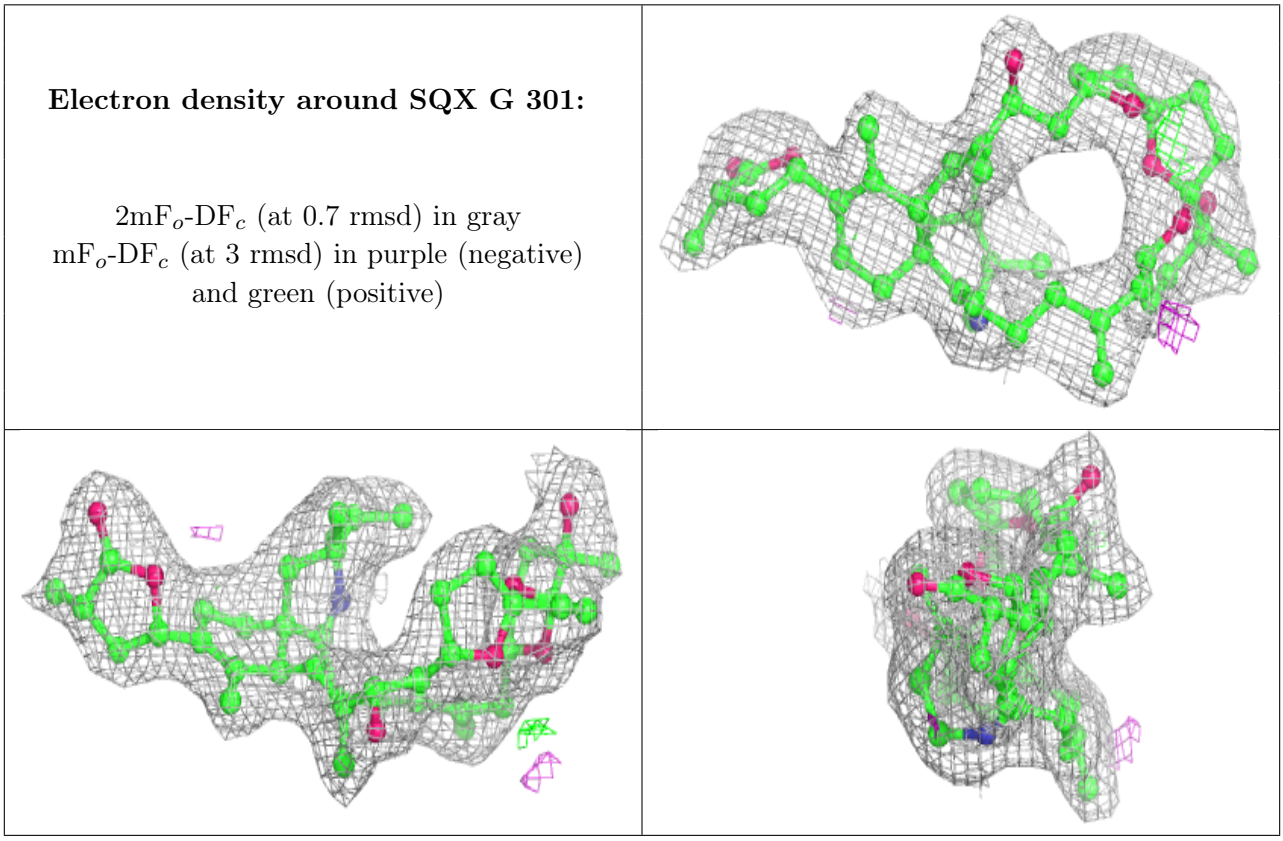
Electron density around SQX F 301:

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



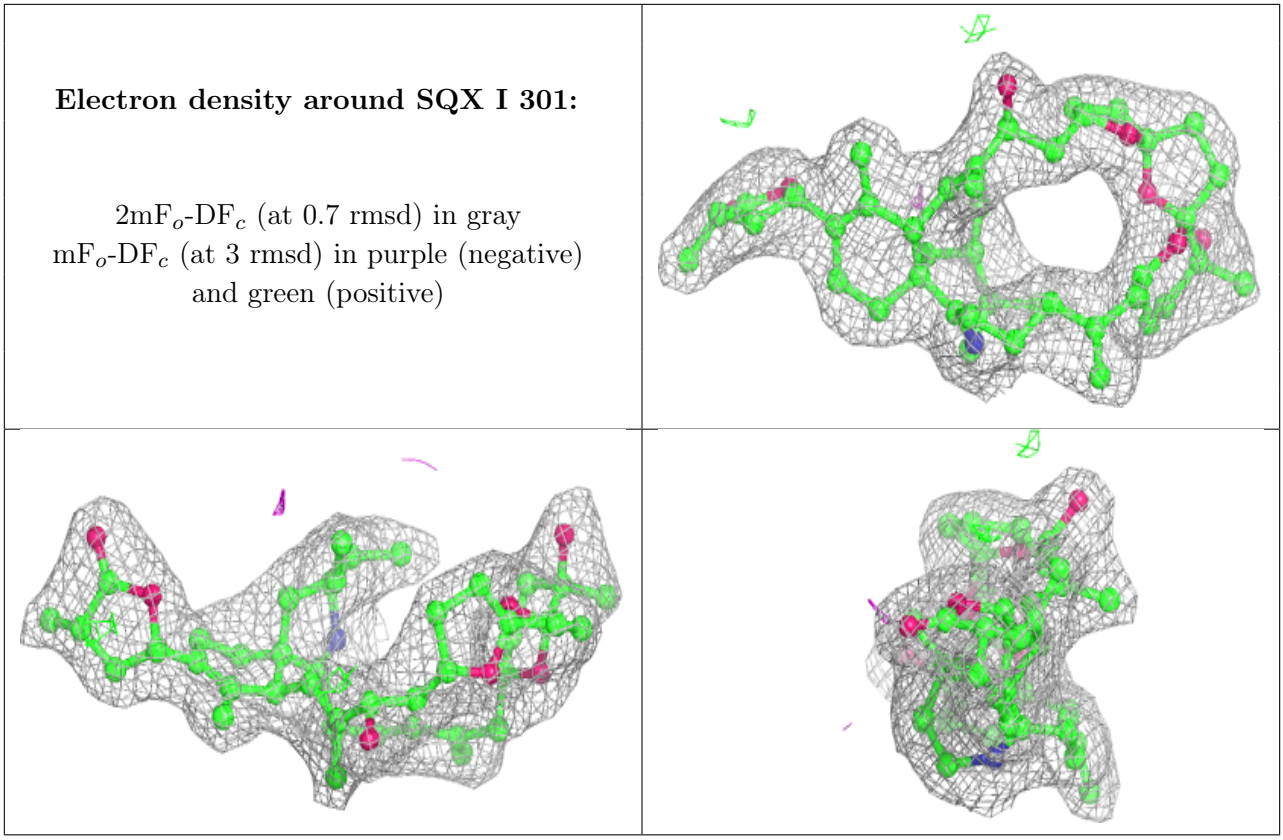
Electron density around SQX G 301:

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



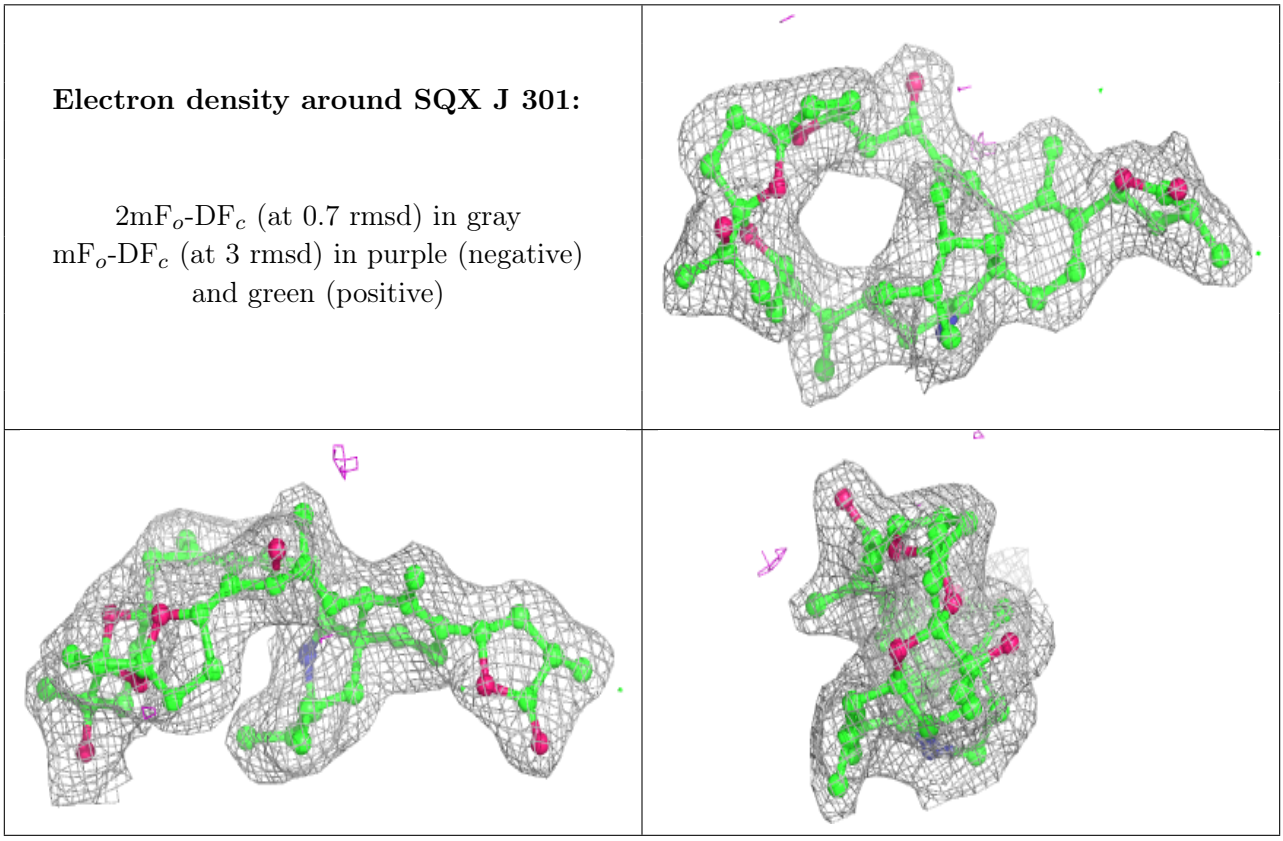
Electron density around SQX I 301:

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



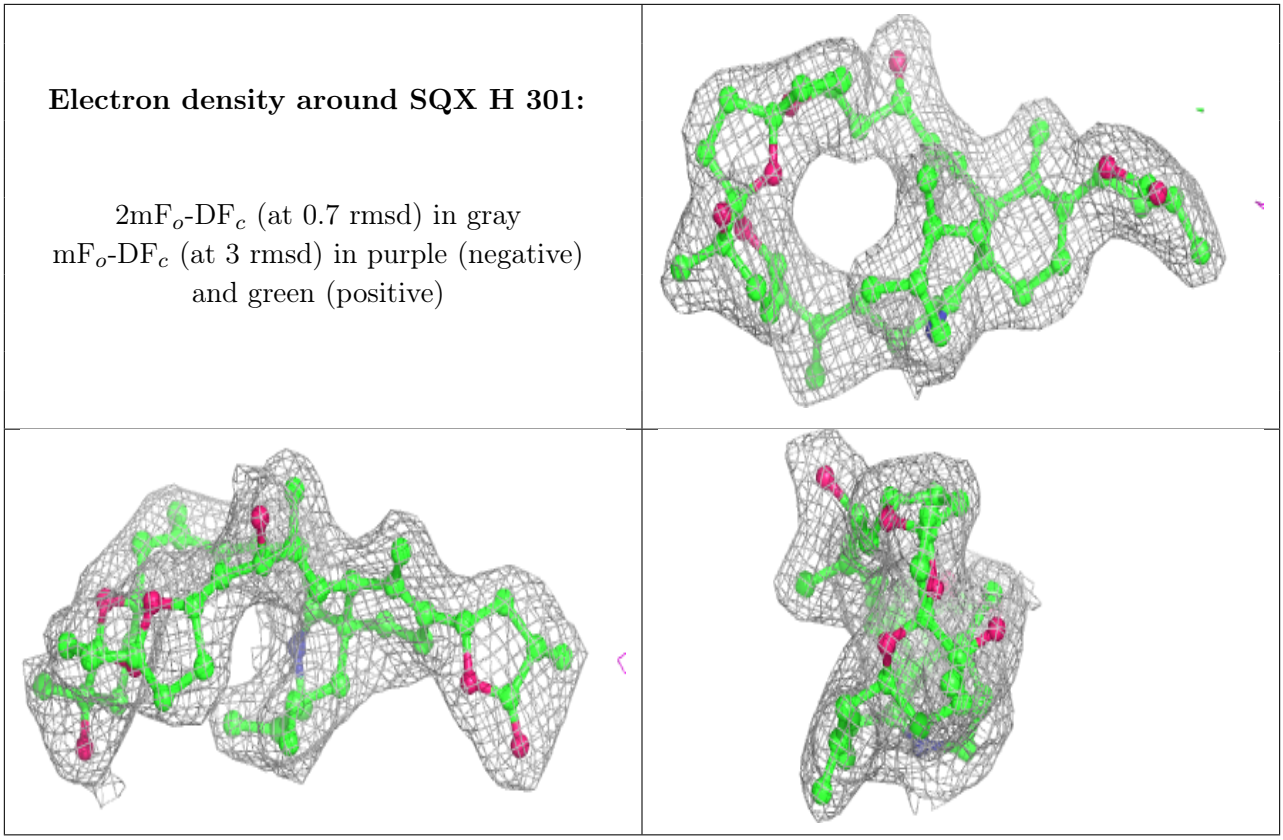
Electron density around SQX J 301:

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



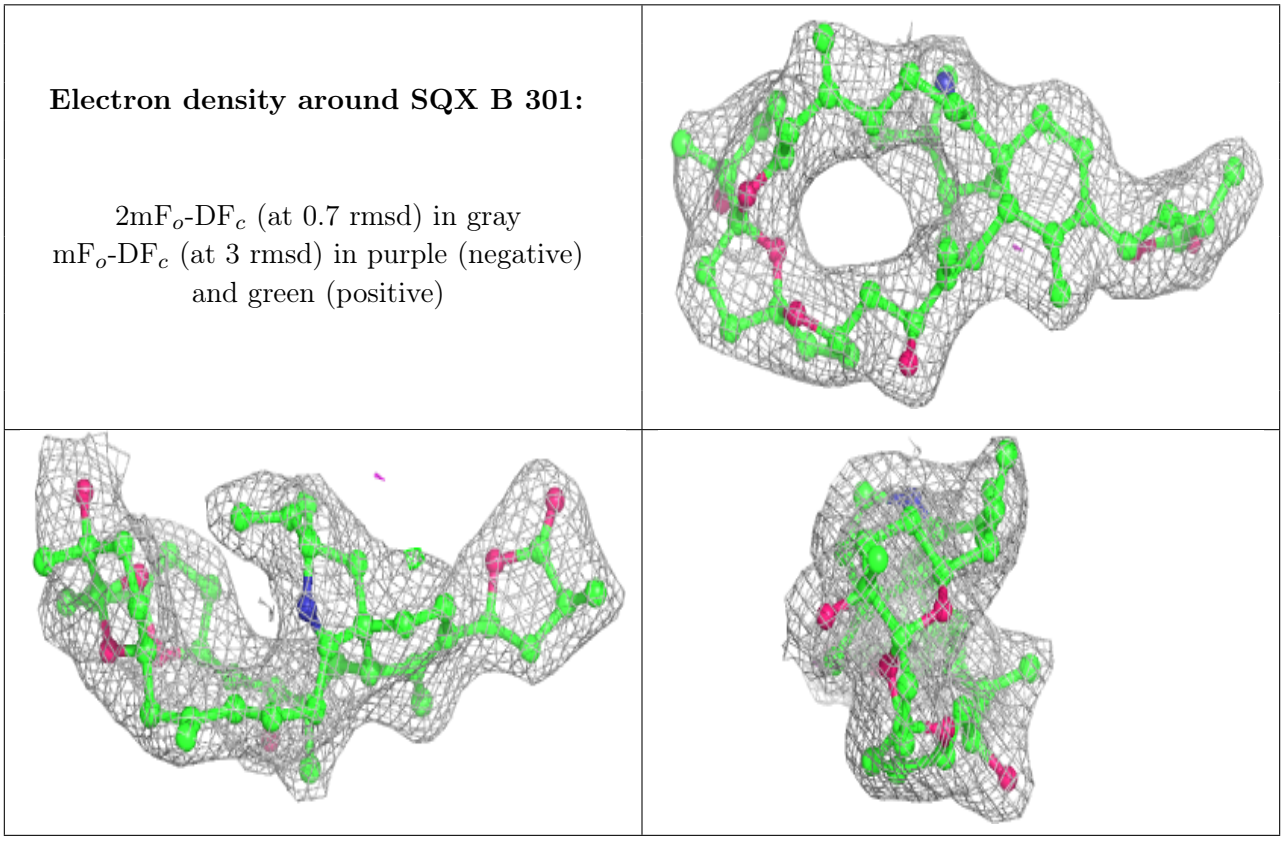
Electron density around SQX H 301:

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



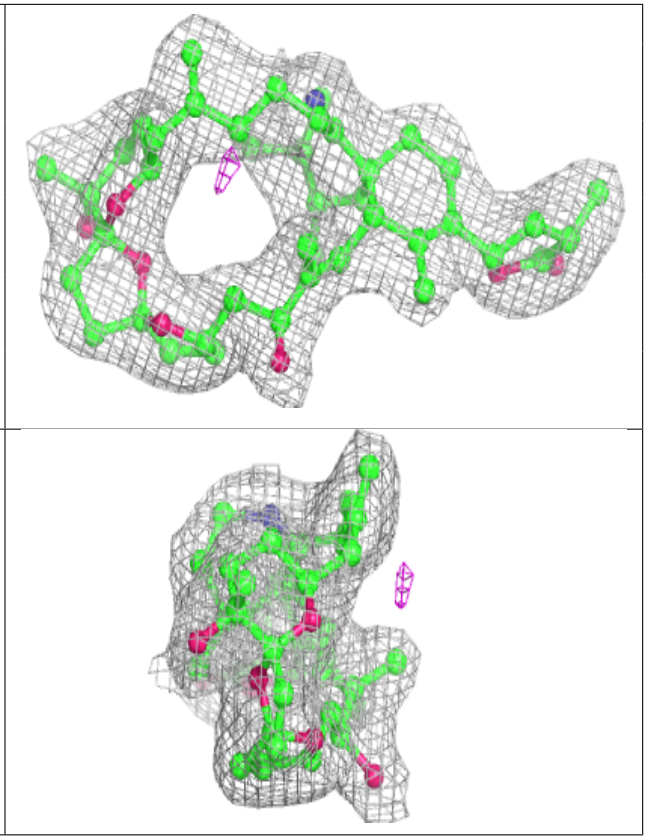
Electron density around SQX B 301:

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



Electron density around SQX 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)



6.5 Other polymers (i)

There are no such residues in this entry.