Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2020 – 03:33 pm GMT

PDB ID	:	6Y7O
Title	:	The complex between the eight-bladed symmetrical designer protein Tako8 and the silicotungstic acid Keggin (STA)
Authors	:	Vandebroek, L.; Noguchi, H.; Parac-Vogt, T.N.; Van Meervelt, L.; Voet, A.R.D.
Deposited on	:	2020-03-02
Resolution	:	2.30 Å(reported)

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

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

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

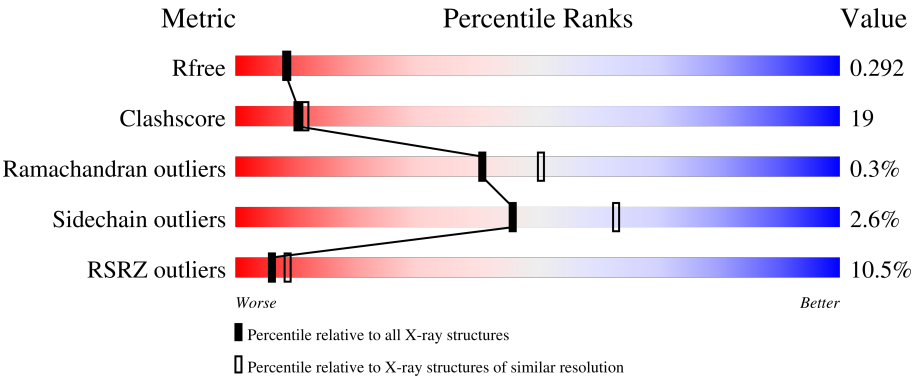
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.15.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	324	11% 72% 26%
1	B	324	6% 75% 22%
1	C	324	14% 71% 24%

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	SIW	A	407	-	-	X	-
2	SIW	B	401[B]	-	-	X	-
2	SIW	B	403	-	-	X	-
2	SIW	C	401[A]	-	-	X	-
2	SIW	C	401[B]	-	-	X	-
2	SIW	C	403[B]	-	-	X	-
2	SIW	C	404	-	-	X	-

2 Entry composition (i)

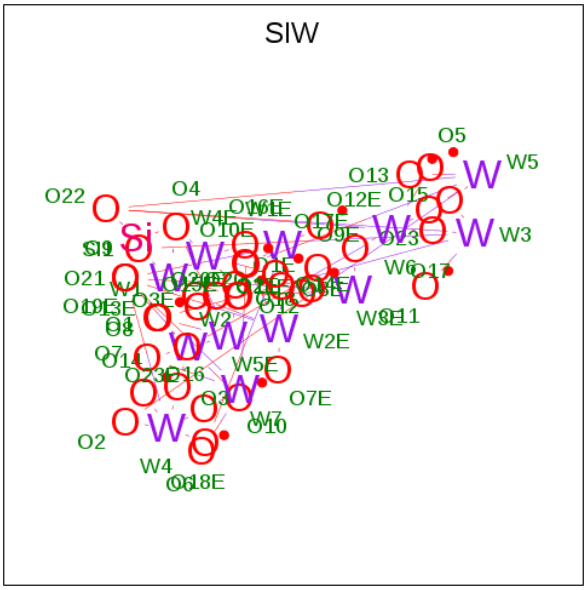
There are 3 unique types of molecules in this entry. The entry contains 8347 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tako8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	0	0	0
			2419	1481	429	509			
1	B	318	Total	C	N	O	0	0	0
			2419	1481	429	509			
1	C	313	Total	C	N	O	0	0	0
			2384	1461	422	501			

- Molecule 2 is Keggin (STA) (three-letter code: SIW) (formula: $O_{40}SiW_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	Si	W	0	1
			106	80	2	24		
2	A	1	Total	O	Si	W	0	1
			106	80	2	24		
2	A	1	Total	O	Si	W	0	0
			53	40	1	12		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	Si	W	0	0
			53	40	1	12		
2	A	1	Total	O	Si	W	0	0
			53	40	1	12		
2	A	1	Total	O	Si	W	0	0
			53	40	1	12		
2	A	1	Total	O	Si	W	0	0
			53	40	1	12		
2	B	1	Total	O	Si	W	0	1
			106	80	2	24		
2	B	1	Total	O	Si	W	0	0
			53	40	1	12		
2	B	1	Total	O	Si	W	0	0
			53	40	1	12		
2	C	1	Total	O	Si	W	0	1
			106	80	2	24		
2	C	1	Total	O	Si	W	0	1
			106	80	2	24		
2	C	1	Total	O	Si	W	0	1
			106	80	2	24		
2	C	1	Total	O	Si	W	0	0
			53	40	1	12		

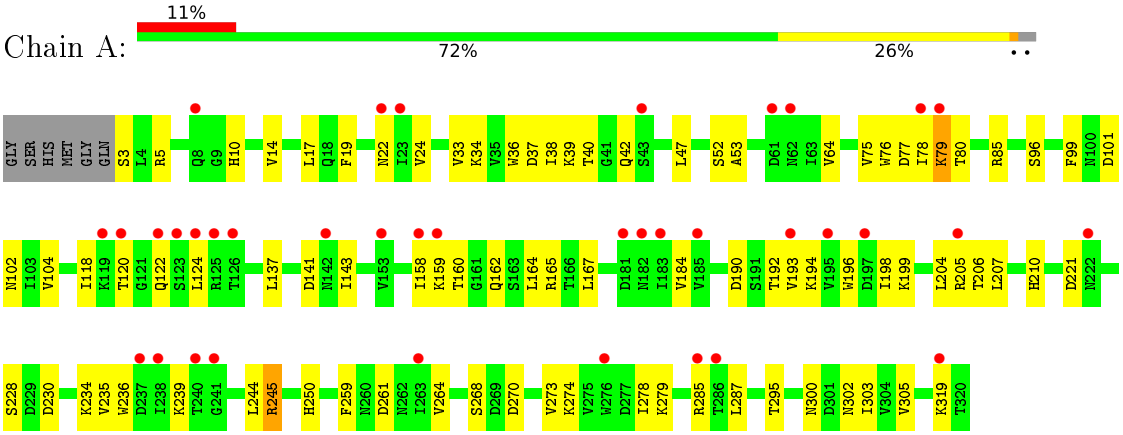
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	18	Total	O	0	0
			18	18		
3	C	21	Total	O	0	1
			22	22		

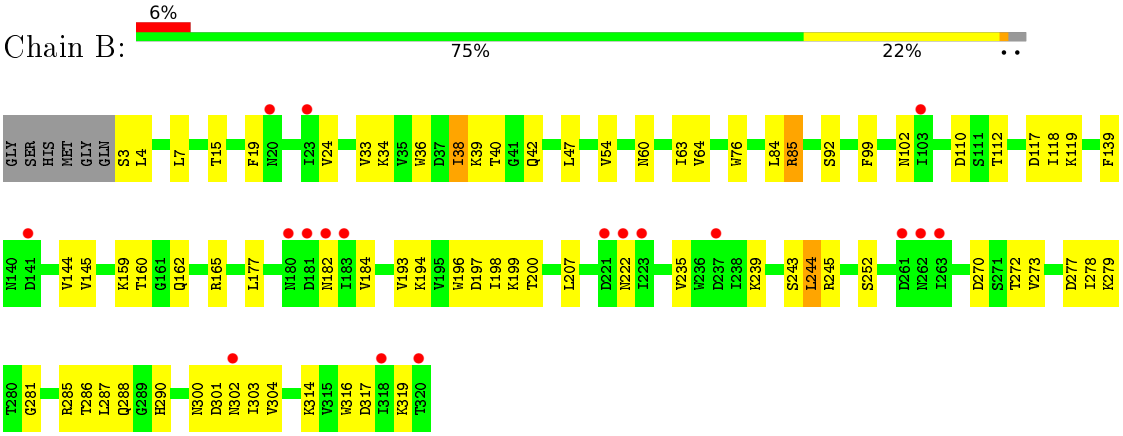
3 Residue-property plots (i)

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.

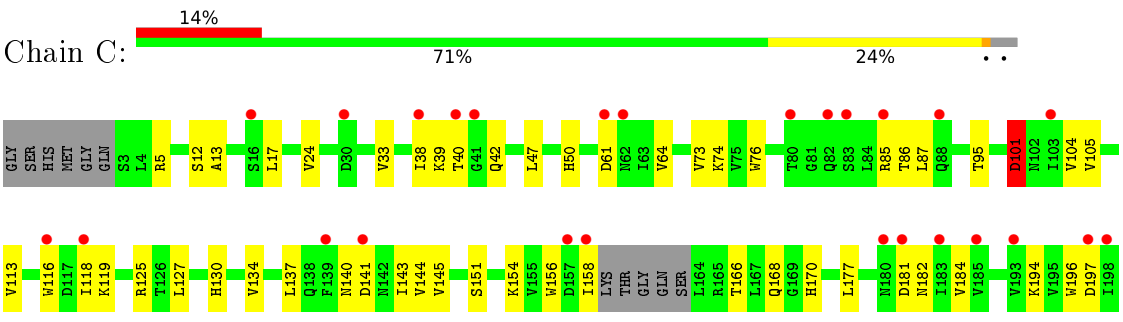
- Molecule 1: Tako8

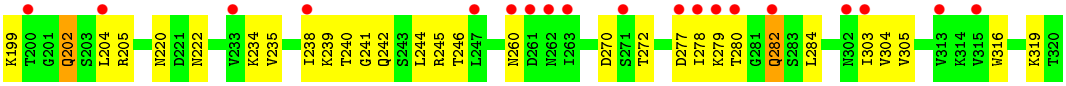


- Molecule 1: Tako8



- Molecule 1: Tako8




K199
T200
G201
Q202
S203
L204
R205
N220
D221
N222
V233
K234
V235
I238
K239
T240
G241
Q242
S243
L244
R245
T246
L247
N260
D261
N262
I263
D270
S271
T272
D277
I278
K279
T280
G281
Q282
S283
L284
N302
I303
V304
V305
V313
K314
V315
W316
K319
T320

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.55Å 133.50Å 81.75Å 90.00° 125.27° 90.00°	Depositor
Resolution (Å)	47.20 – 2.30 47.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.20-2.30) 99.6 (47.28-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.241 , 0.293 0.241 , 0.292	Depositor DCC
R_{free} test set	1912 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 3.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.457 for -1/2*h+1/2*k-l,3/2*h+1/2*k+l,1/2*h-1/2*k 0.450 for 1/2*h-1/2*k+l,-1/2*h+1/2*k+l,-h-l 0.438 for 1/2*h+1/2*k+l,1/2*h+1/2*k-l,-h-l 0.436 for -1/2*h-1/2*k-l,-3/2*h+1/2*k-l,1/2*h+1/2*k 0.469 for -h,-h-2*l,1/2*h-1/2*k 0.469 for -h,h+2*l,1/2*h+1/2*k 0.437 for 1/2*h+1/2*k+l,3/2*h-1/2*k+l,-l 0.457 for 1/2*h-1/2*k+l,-3/2*h-1/2*k-l,-l 0.456 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2*h-1/2*k 0.438 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/2*h+1/2*k 0.477 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8347	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

[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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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	0.27	0/2450	0.55	0/3332
1	B	0.27	0/2450	0.57	1/3332 (0.0%)
1	C	0.26	0/2414	0.55	0/3283
All	All	0.27	0/7314	0.56	1/9947 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	LEU	CA-CB-CG	7.14	131.72	115.30

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	2419	0	2364	60	0
1	B	2419	0	2364	49	1
1	C	2384	0	2327	54	1
2	A	477	0	0	63	1
2	B	212	0	0	34	1
2	C	371	0	0	59	0
3	A	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	0	0
3	C	22	0	0	1	0
All	All	8347	0	7055	288	2

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 19.

All (288) 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:A:204:LEU:O	1:A:205:ARG:HD2	1.38	1.19
1:B:199:LYS:NZ	2:B:401[B]:SIW:O11E	1.92	1.01
1:B:199:LYS:NZ	2:B:401[A]:SIW:O14E	1.94	0.99
1:A:204:LEU:O	1:A:205:ARG:NH1	1.98	0.97
1:C:199:LYS:NZ	2:C:403[B]:SIW:O14E	2.02	0.92
1:B:199:LYS:NZ	2:B:401[B]:SIW:O15E	2.03	0.90
2:A:407:SIW:O15E	2:C:404:SIW:O10	1.98	0.81
2:A:402[A]:SIW:O13E	2:A:402[A]:SIW:SI1	2.71	0.79
1:B:285:ARG:NH1	1:B:317:ASP:O	2.16	0.77
1:B:300:ASN:HB2	1:B:303:ILE:HG22	1.68	0.76
1:A:122:GLN:HE22	1:A:124:LEU:HG	1.50	0.76
1:A:319:LYS:NZ	2:A:405:SIW:O14	2.19	0.75
1:A:300:ASN:ND2	2:C:401[B]:SIW:O13	2.18	0.75
1:A:204:LEU:O	1:A:205:ARG:CD	2.30	0.72
1:A:264:VAL:HG23	1:A:278:ILE:HG12	1.72	0.71
1:A:79:LYS:HD2	1:A:80:THR:HG23	1.73	0.71
1:C:222:ASN:ND2	2:C:401[B]:SIW:O7	2.27	0.67
2:A:407:SIW:O13E	2:C:404:SIW:O1	2.13	0.67
1:A:17:LEU:HD11	1:A:305:VAL:HG12	1.78	0.66
1:A:120:THR:OG1	1:A:122:GLN:HG3	1.96	0.66
1:C:145:VAL:HG12	1:C:177:LEU:HD21	1.79	0.64
1:A:279:LYS:HD2	1:B:165:ARG:HH22	1.61	0.64
1:C:238:ILE:HG23	1:C:239:LYS:HE3	1.79	0.63
1:A:3:SER:N	3:A:501:HOH:O	2.30	0.63
1:A:37:ASP:HB3	1:A:42:GLN:HG2	1.81	0.63
1:B:199:LYS:HZ3	1:B:199:LYS:HB2	1.63	0.62
1:B:102:ASN:ND2	1:B:117:ASP:OD1	2.31	0.61
1:A:235:VAL:HG12	1:A:244:LEU:HD12	1.83	0.60
2:A:403:SIW:O21	2:A:403:SIW:O16	2.20	0.60
1:C:220:ASN:ND2	2:C:401[B]:SIW:O14E	2.25	0.59
1:A:159:LYS:HE3	2:A:403:SIW:O13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HB	1:A:207:LEU:HB2	1.85	0.59
1:C:279:LYS:HD2	2:C:401[A]:SIW:O5	2.03	0.59
1:A:19:PHE:HB2	1:A:24:VAL:HG22	1.85	0.59
1:B:4:LEU:HD21	1:B:317:ASP:HB2	1.85	0.58
1:A:261:ASP:O	2:B:401[B]:SIW:O11	2.20	0.58
1:A:19:PHE:CE2	1:A:303:ILE:HD11	2.37	0.58
1:A:210:HIS:CE1	1:A:234:LYS:HD2	2.37	0.58
1:A:239:LYS:HD2	2:B:403:SIW:O10	2.04	0.58
1:A:205:ARG:HA	1:A:205:ARG:CZ	2.33	0.57
1:A:64:VAL:HB	1:A:76:TRP:HB2	1.86	0.57
1:C:140:ASN:ND2	2:C:403[B]:SIW:O10	2.37	0.56
1:A:158:ILE:HG23	1:A:159:LYS:HE2	1.86	0.56
1:A:184:VAL:HG13	1:A:196:TRP:HB2	1.88	0.56
1:C:197:ASP:OD2	1:C:199:LYS:HB2	2.06	0.56
1:B:304:VAL:HB	1:B:316:TRP:HB2	1.87	0.55
2:A:401[B]:SIW:O18	2:A:401[B]:SIW:O4	2.24	0.55
1:C:277:ASP:OD1	1:C:280:THR:HG22	2.06	0.55
1:B:278:ILE:HD12	1:B:278:ILE:H	1.72	0.55
1:C:240:THR:HG23	1:C:242:GLN:H	1.71	0.55
1:C:304:VAL:HB	1:C:316:TRP:HB2	1.89	0.54
1:B:182:ASN:O	1:B:198:ILE:HG13	2.08	0.54
2:A:402[A]:SIW:O18	2:A:402[A]:SIW:O4	2.25	0.54
1:B:184:VAL:HG13	1:B:196:TRP:HB2	1.88	0.54
1:C:270:ASP:OD1	1:C:272:THR:HG22	2.07	0.54
2:A:402[A]:SIW:O16	2:A:402[A]:SIW:O21	2.26	0.53
1:A:205:ARG:NH1	1:A:205:ARG:HA	2.23	0.53
1:C:130:HIS:CE1	1:C:154:LYS:HD2	2.43	0.53
1:B:19:PHE:HB2	1:B:24:VAL:HG22	1.90	0.53
1:C:33:VAL:HB	1:C:47:LEU:HB2	1.90	0.53
1:A:190:ASP:OD1	1:A:192:THR:HG22	2.08	0.52
1:A:250:HIS:CE1	1:A:274:LYS:HG3	2.44	0.52
1:B:199:LYS:NZ	2:B:401[A]:SIW:O2E	2.43	0.52
2:A:402[B]:SIW:O18	2:A:402[B]:SIW:O4	2.27	0.52
1:B:270:ASP:OD1	1:B:272:THR:HG22	2.10	0.52
1:B:34:LYS:HD3	1:B:36:TRP:CZ2	2.45	0.51
1:C:181:ASP:HA	2:C:403[A]:SIW:O10E	2.11	0.51
2:A:403:SIW:O4	2:A:403:SIW:O20	2.28	0.51
1:A:10:HIS:CE1	1:A:34:LYS:HG3	2.46	0.51
1:A:184:VAL:HG12	1:A:198:ILE:HG12	1.91	0.51
2:C:401[A]:SIW:O16	2:C:401[A]:SIW:O21	2.28	0.51
2:A:401[B]:SIW:O19E	2:A:401[B]:SIW:O9E	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:402[A]:SIW:O4	2:C:402[A]:SIW:O18	2.29	0.51
2:C:402[A]:SIW:O16	2:C:402[A]:SIW:O21	2.29	0.51
2:B:401[B]:SIW:O21	2:B:401[B]:SIW:O16	2.28	0.51
1:B:15:THR:OG1	1:B:54:VAL:O	2.23	0.51
1:B:117:ASP:OD2	1:B:119:LYS:HG2	2.10	0.50
1:B:239:LYS:NZ	2:B:403:SIW:O23E	2.40	0.50
1:A:228:SER:OG	1:A:230:ASP:OD1	2.29	0.50
2:A:401[A]:SIW:O9E	2:A:401[A]:SIW:O19E	2.29	0.50
2:B:401[A]:SIW:O18	2:B:401[A]:SIW:O4	2.30	0.50
2:C:401[B]:SIW:O18	2:C:401[B]:SIW:O4	2.29	0.50
2:A:405:SIW:O18	2:A:405:SIW:O4	2.29	0.50
2:B:403:SIW:O19E	2:B:403:SIW:O9E	2.30	0.50
1:C:24:VAL:HG23	1:C:38:ILE:HG12	1.92	0.50
1:C:144:VAL:HG23	1:C:158:ILE:HD11	1.93	0.50
2:C:403[B]:SIW:O4	2:C:403[B]:SIW:O18	2.30	0.50
2:A:404:SIW:O18	2:A:404:SIW:O4	2.30	0.50
2:A:405:SIW:O16	2:A:405:SIW:O21	2.30	0.50
1:C:39:LYS:HD3	2:C:402[A]:SIW:O20	2.12	0.50
2:B:403:SIW:O18	2:B:403:SIW:O4	2.30	0.50
2:C:404:SIW:O4	2:C:404:SIW:O18	2.30	0.50
2:C:402[A]:SIW:O19E	2:C:402[A]:SIW:O9E	2.29	0.50
1:B:139:PHE:HB3	1:B:144:VAL:HG22	1.94	0.50
2:C:401[B]:SIW:O19E	2:C:401[B]:SIW:O9E	2.29	0.49
2:C:403[B]:SIW:O21	2:C:403[B]:SIW:O16	2.29	0.49
2:A:401[A]:SIW:O18	2:A:401[A]:SIW:O4	2.30	0.49
2:A:402[B]:SIW:O9E	2:A:402[B]:SIW:O19E	2.30	0.49
2:A:406:SIW:O18	2:A:406:SIW:O4	2.30	0.49
2:A:407:SIW:O18	2:A:407:SIW:O4	2.30	0.49
1:B:60:ASN:ND2	2:C:402[B]:SIW:O12E	2.46	0.49
1:B:19:PHE:CB	1:B:24:VAL:HG22	2.43	0.49
1:B:235:VAL:HG21	1:B:278:ILE:HG23	1.93	0.49
2:B:402:SIW:O21	2:B:402:SIW:O16	2.29	0.49
2:C:403[A]:SIW:O16	2:C:403[A]:SIW:O21	2.30	0.49
2:C:403[A]:SIW:O19E	2:C:403[A]:SIW:O9E	2.31	0.49
2:A:407:SIW:O11E	2:C:404:SIW:O3	2.30	0.49
2:B:401[B]:SIW:O18	2:B:401[B]:SIW:O4	2.30	0.49
2:A:404:SIW:O21	2:A:404:SIW:O16	2.31	0.49
2:A:405:SIW:O3	2:A:406:SIW:O14E	2.30	0.49
2:C:404:SIW:O9E	2:C:404:SIW:O19E	2.31	0.49
1:B:290:HIS:CE1	1:B:314:LYS:HD2	2.48	0.49
2:B:401[A]:SIW:O19E	2:B:401[A]:SIW:O9E	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:403[A]:SIW:O4	2:C:403[A]:SIW:O18	2.30	0.49
1:A:143:ILE:HD11	1:A:164:LEU:HD12	1.94	0.49
2:A:405:SIW:O9E	2:A:405:SIW:O19E	2.31	0.49
2:A:406:SIW:O21	2:A:406:SIW:O16	2.30	0.49
2:C:402[B]:SIW:O21	2:C:402[B]:SIW:O16	2.31	0.49
2:B:402:SIW:O20	2:B:402:SIW:O4	2.31	0.49
1:B:64:VAL:HB	1:B:76:TRP:HB2	1.94	0.49
2:A:403:SIW:O4	2:A:403:SIW:O18	2.31	0.48
1:C:202:GLN:OE1	1:C:204:LEU:HD13	2.12	0.48
2:C:402[B]:SIW:O9E	2:C:402[B]:SIW:O19E	2.31	0.48
1:C:50:HIS:CE1	1:C:74:LYS:HG3	2.48	0.48
2:C:401[A]:SIW:O9E	2:C:401[A]:SIW:O19E	2.32	0.48
2:B:402:SIW:O18	2:B:402:SIW:O4	2.31	0.48
1:C:280:THR:HG21	1:C:282:GLN:HG2	1.94	0.48
2:A:402[A]:SIW:O22	2:A:402[A]:SIW:O23	2.32	0.48
2:B:401[B]:SIW:O9E	2:B:401[B]:SIW:O19E	2.32	0.48
1:C:184:VAL:HB	1:C:196:TRP:HB2	1.94	0.48
1:C:17:LEU:HD11	1:C:305:VAL:HG12	1.96	0.48
2:C:403[B]:SIW:O9E	2:C:403[B]:SIW:O19E	2.31	0.48
2:A:407:SIW:O9E	2:A:407:SIW:O19E	2.31	0.48
2:B:401[A]:SIW:O21	2:B:401[A]:SIW:O16	2.32	0.48
2:C:402[A]:SIW:O22	2:C:402[A]:SIW:O23	2.32	0.48
2:A:402[B]:SIW:O21	2:A:402[B]:SIW:O16	2.31	0.48
2:A:402[B]:SIW:O22	2:A:402[B]:SIW:O23	2.32	0.48
2:B:403:SIW:O16	2:B:403:SIW:O21	2.31	0.48
2:C:401[A]:SIW:O4	2:C:401[A]:SIW:O18	2.31	0.48
2:C:404:SIW:O21	2:C:404:SIW:O16	2.31	0.48
2:C:401[B]:SIW:O16	2:C:401[B]:SIW:O21	2.32	0.48
2:C:401[A]:SIW:O17	2:C:401[A]:SIW:O22	2.32	0.48
2:C:402[B]:SIW:O18	2:C:402[B]:SIW:O4	2.31	0.48
1:B:85:ARG:HH11	1:C:5:ARG:HH12	1.61	0.48
2:A:407:SIW:O16	2:A:407:SIW:O21	2.31	0.48
2:C:401[B]:SIW:O22	2:C:401[B]:SIW:O23	2.32	0.47
1:B:160:THR:HG23	1:B:162:GLN:H	1.79	0.47
1:B:273:VAL:HB	1:B:287:LEU:HB2	1.96	0.47
2:A:401[B]:SIW:O21	2:A:401[B]:SIW:O16	2.32	0.47
2:A:403:SIW:O17	2:A:403:SIW:O22	2.32	0.47
2:A:404:SIW:O9E	2:A:404:SIW:O19E	2.31	0.47
2:A:406:SIW:O9E	2:A:406:SIW:O19E	2.31	0.47
1:B:222:ASN:HB2	2:B:402:SIW:O14	2.14	0.47
2:B:401[A]:SIW:O20	2:B:401[A]:SIW:O4	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:SIW:O22	2:B:402:SIW:O17	2.31	0.47
1:C:245:ARG:HD2	1:C:278:ILE:O	2.14	0.47
1:B:33:VAL:HB	1:B:47:LEU:HB2	1.97	0.47
2:C:404:SIW:O17	2:C:404:SIW:O22	2.33	0.47
2:A:406:SIW:O23	2:A:406:SIW:O22	2.33	0.47
2:C:403[A]:SIW:O23	2:C:403[A]:SIW:O22	2.33	0.47
2:A:406:SIW:O22	2:A:406:SIW:O17	2.33	0.47
1:C:125:ARG:NH2	3:C:502[A]:HOH:O	2.48	0.47
2:C:404:SIW:O23	2:C:404:SIW:O22	2.33	0.47
1:A:259:PHE:HB3	1:A:264:VAL:HG22	1.97	0.47
1:A:24:VAL:HG23	1:A:38:ILE:HB	1.96	0.47
2:A:401[A]:SIW:O16	2:A:401[A]:SIW:O21	2.32	0.47
1:B:38:ILE:O	1:B:39:LYS:HD2	2.15	0.47
2:A:403:SIW:O22	2:A:403:SIW:O23	2.33	0.47
1:B:245:ARG:HG2	1:B:281:GLY:HA3	1.97	0.47
1:A:24:VAL:HB	1:A:36:TRP:HB2	1.96	0.46
2:A:407:SIW:O23	2:A:407:SIW:O22	2.33	0.46
2:B:403:SIW:O17	2:B:403:SIW:O22	2.33	0.46
1:C:205:ARG:HE	1:C:241:GLY:HA3	1.79	0.46
1:C:235:VAL:HG21	1:C:278:ILE:HG23	1.97	0.46
2:A:401[B]:SIW:O22	2:A:401[B]:SIW:O23	2.32	0.46
2:A:405:SIW:O22	2:A:405:SIW:O23	2.33	0.46
2:C:403[A]:SIW:O17	2:C:403[A]:SIW:O22	2.33	0.46
1:C:104:VAL:HG23	1:C:118:ILE:HG12	1.97	0.46
1:C:166:THR:HG22	1:C:168:GLN:HG3	1.96	0.46
2:C:403[B]:SIW:O22	2:C:403[B]:SIW:O23	2.33	0.46
2:A:401[B]:SIW:O22	2:A:401[B]:SIW:O17	2.34	0.46
2:A:401[A]:SIW:O4	2:A:401[A]:SIW:O20	2.33	0.46
2:A:404:SIW:O23	2:A:404:SIW:O22	2.33	0.46
1:B:110:ASP:OD1	1:B:112:THR:HG22	2.15	0.46
1:C:197:ASP:HB2	1:C:204:LEU:HD21	1.96	0.46
1:B:193:VAL:HB	1:B:207:LEU:HB2	1.97	0.46
2:B:401[A]:SIW:O22	2:B:401[A]:SIW:O17	2.34	0.46
2:B:401[B]:SIW:O22	2:B:401[B]:SIW:O17	2.33	0.46
1:C:39:LYS:HD3	2:C:402[B]:SIW:O2E	2.15	0.46
2:C:403[A]:SIW:O4	2:C:403[A]:SIW:O20	2.34	0.46
2:A:402[B]:SIW:O22	2:A:402[B]:SIW:O17	2.33	0.46
1:C:280:THR:HG23	1:C:282:GLN:H	1.81	0.46
2:C:402[B]:SIW:O22	2:C:402[B]:SIW:O23	2.33	0.46
1:A:302:ASN:OD1	2:C:401[A]:SIW:O11E	2.34	0.46
2:A:401[A]:SIW:O17	2:A:401[A]:SIW:O22	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:SIW:O23	2:B:403:SIW:O22	2.33	0.46
2:A:401[A]:SIW:O23	2:A:401[A]:SIW:O22	2.34	0.45
2:A:405:SIW:O17	2:A:405:SIW:O22	2.34	0.45
2:A:407:SIW:O17	2:A:407:SIW:O22	2.34	0.45
2:A:402[A]:SIW:O9E	2:A:402[A]:SIW:O19E	2.34	0.45
2:C:401[A]:SIW:O23	2:C:401[A]:SIW:O22	2.34	0.45
2:C:402[B]:SIW:O22	2:C:402[B]:SIW:O17	2.34	0.45
2:C:403[B]:SIW:O22	2:C:403[B]:SIW:O17	2.33	0.45
2:B:401[A]:SIW:O22	2:B:401[A]:SIW:O23	2.33	0.45
1:C:64:VAL:HB	1:C:76:TRP:HB2	1.98	0.45
1:B:286:THR:HG22	1:B:288:GLN:HG3	1.98	0.45
1:A:40:THR:HG22	1:C:244:LEU:HD22	1.99	0.45
2:B:403:SIW:O4	2:B:403:SIW:O20	2.35	0.45
1:B:99:PHE:HB2	1:B:118:ILE:HD11	1.97	0.45
1:C:74:LYS:NZ	1:C:86:THR:OG1	2.45	0.45
2:A:402[A]:SIW:O17	2:A:402[A]:SIW:O22	2.34	0.45
2:A:404:SIW:O22	2:A:404:SIW:O17	2.34	0.45
2:B:402:SIW:O9E	2:B:402:SIW:O19E	2.35	0.45
1:A:245:ARG:HD2	1:A:278:ILE:O	2.16	0.45
1:B:40:THR:HG23	1:B:42:GLN:H	1.81	0.45
1:A:22:ASN:N	1:A:22:ASN:OD1	2.47	0.45
2:A:403:SIW:O9E	2:A:403:SIW:O19E	2.35	0.45
1:C:40:THR:HG22	1:C:42:GLN:HB2	1.99	0.45
2:A:405:SIW:O20	2:A:405:SIW:O4	2.34	0.45
2:A:406:SIW:O4	2:A:406:SIW:O20	2.34	0.45
1:B:159:LYS:HA	1:B:159:LYS:HD3	1.76	0.45
2:B:401[B]:SIW:O23	2:B:401[B]:SIW:O22	2.33	0.45
1:B:63:ILE:HD11	1:B:84:LEU:HD12	1.99	0.45
1:C:73:VAL:HB	1:C:87:LEU:HB2	1.99	0.44
1:A:101:ASP:OD1	2:A:401[A]:SIW:O5	2.35	0.44
2:B:402:SIW:O22	2:B:402:SIW:O23	2.35	0.44
2:A:404:SIW:O4	2:A:404:SIW:O20	2.34	0.44
1:C:303:ILE:HG12	2:C:402[A]:SIW:O11	2.16	0.44
2:C:401[B]:SIW:O17	2:C:401[B]:SIW:O22	2.35	0.44
2:C:401[A]:SIW:O4	2:C:401[A]:SIW:O20	2.35	0.44
2:C:402[A]:SIW:O4	2:C:402[A]:SIW:O20	2.35	0.44
2:C:401[B]:SIW:O20	2:C:401[B]:SIW:O4	2.35	0.44
2:C:402[B]:SIW:O4	2:C:402[B]:SIW:O20	2.36	0.44
1:A:77:ASP:OD2	1:A:80:THR:OG1	2.28	0.44
1:C:143:ILE:HG23	2:C:403[B]:SIW:O11	2.17	0.44
2:A:402[B]:SIW:O20	2:A:402[B]:SIW:O4	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:407:SIW:O4	2:A:407:SIW:O20	2.36	0.44
1:B:194:LYS:HB3	1:B:196:TRP:NE1	2.33	0.44
2:C:404:SIW:O4	2:C:404:SIW:O20	2.35	0.44
1:A:160:THR:OG1	1:A:162:GLN:HG2	2.18	0.43
1:C:182:ASN:ND2	1:C:197:ASP:OD1	2.51	0.43
1:B:199:LYS:NZ	1:B:199:LYS:HB2	2.30	0.43
2:C:402[A]:SIW:O17	2:C:402[A]:SIW:O22	2.34	0.43
1:A:99:PHE:HB3	1:A:104:VAL:HG22	2.00	0.43
1:C:105:VAL:HG12	1:C:137:LEU:HD11	2.00	0.43
1:C:113:VAL:HB	1:C:127:LEU:HB2	2.01	0.43
1:A:234:LYS:HD3	1:A:236:TRP:CZ2	2.54	0.43
1:B:197:ASP:OD1	1:B:200:THR:HG22	2.19	0.43
2:A:401[B]:SIW:O20	2:A:401[B]:SIW:O4	2.36	0.43
1:A:5:ARG:HH22	1:A:39:LYS:NZ	2.16	0.43
1:A:159:LYS:HA	1:A:159:LYS:HD3	1.24	0.43
1:C:85:ARG:HH22	1:C:119:LYS:HZ2	1.65	0.43
2:B:401[B]:SIW:O20	2:B:401[B]:SIW:O4	2.36	0.42
1:C:12:SER:OG	1:C:13:ALA:N	2.52	0.42
1:A:34:LYS:HD2	1:A:36:TRP:CZ2	2.54	0.42
2:A:402[A]:SIW:O20	2:A:402[A]:SIW:O4	2.36	0.42
1:A:33:VAL:HB	1:A:47:LEU:HB2	2.00	0.42
2:C:403[B]:SIW:O20	2:C:403[B]:SIW:O4	2.36	0.42
1:A:64:VAL:HG23	1:A:78:ILE:HG23	2.00	0.42
1:C:127:LEU:HD13	1:C:156:TRP:CG	2.54	0.42
1:C:95:THR:OG1	1:C:134:VAL:O	2.31	0.42
1:B:85:ARG:HH12	1:C:39:LYS:CE	2.33	0.42
1:C:170:HIS:CE1	1:C:194:LYS:HG3	2.55	0.42
1:C:282:GLN:NE2	1:C:284:LEU:HD23	2.35	0.42
1:A:167:LEU:HB3	1:A:196:TRP:CE3	2.55	0.42
1:A:14:VAL:O	1:A:295:THR:OG1	2.34	0.42
1:A:96:SER:HB2	1:A:137:LEU:HG	2.02	0.42
1:B:277:ASP:OD1	1:B:279:LYS:HB3	2.20	0.42
1:C:87:LEU:HD13	1:C:116:TRP:CG	2.55	0.42
1:A:273:VAL:HB	1:A:287:LEU:HB2	2.01	0.41
2:B:402:SIW:O8E	2:B:402:SIW:O19E	2.38	0.41
1:A:52:SER:OG	1:A:53:ALA:N	2.52	0.41
1:B:244:LEU:HB2	1:B:245:ARG:H	1.43	0.41
1:B:145:VAL:HG12	1:B:177:LEU:HD11	2.01	0.41
1:C:74:LYS:HD2	1:C:76:TRP:CZ2	2.56	0.41
1:A:39:LYS:HD2	1:A:39:LYS:HA	1.80	0.41
1:B:7:LEU:HD13	1:B:36:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:SER:HB3	1:A:270:ASP:OD1	2.21	0.41
1:A:75:VAL:HG21	1:A:118:ILE:HG23	2.03	0.41
2:A:403:SIW:O8E	2:A:403:SIW:O19E	2.38	0.41
2:C:401[A]:SIW:O19E	2:C:401[A]:SIW:O8E	2.39	0.41
1:C:205:ARG:NE	1:C:241:GLY:HA3	2.36	0.40
1:C:234:LYS:NZ	1:C:246:THR:OG1	2.51	0.40
1:A:104:VAL:HG23	1:A:118:ILE:HD11	2.02	0.40
1:A:194:LYS:NZ	1:A:206:THR:OG1	2.48	0.40
1:B:3:SER:HB2	1:B:316:TRP:CZ3	2.56	0.40
1:A:160:THR:OG1	1:A:162:GLN:CD	2.59	0.40
2:B:401[B]:SIW:O8E	2:B:401[B]:SIW:O19E	2.39	0.40

All (2) 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:B:319:LYS:NZ	2:B:403:SIW:O16E[2_655]	2.17	0.03
1:C:101:ASP:O	2:A:401[B]:SIW:O14E[2_655]	2.18	0.02

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	316/324 (98%)	288 (91%)	27 (8%)	1 (0%)	41	50
1	B	316/324 (98%)	286 (90%)	29 (9%)	1 (0%)	41	50
1	C	309/324 (95%)	283 (92%)	25 (8%)	1 (0%)	41	50
All	All	941/972 (97%)	857 (91%)	81 (9%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	C	101	ASP
1	B	38	ILE

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	287/291 (99%)	279 (97%)	8 (3%)	43	60
1	B	287/291 (99%)	281 (98%)	6 (2%)	53	70
1	C	283/291 (97%)	275 (97%)	8 (3%)	43	60
All	All	857/873 (98%)	835 (97%)	22 (3%)	46	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	A	85	ARG
1	A	141	ASP
1	A	165	ARG
1	A	199	LYS
1	A	221	ASP
1	A	245	ARG
1	A	285	ARG
1	B	85	ARG
1	B	92	SER
1	B	243	SER
1	B	252	SER
1	B	301	ASP
1	B	302	ASN
1	C	61	ASP
1	C	101	ASP
1	C	141	ASP
1	C	151	SER
1	C	202	GLN
1	C	260	ASN

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Mol	Chain	Res	Type
1	C	282	GLN
1	C	319	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	B	222	ASN
1	C	8	GLN

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

20 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	SIW	A	402[B]	-	16,76,76	3.72	13 (81%)	0,234,234	0.00	-
2	SIW	A	401[B]	1	16,76,76	3.78	13 (81%)	0,234,234	0.00	-
2	SIW	A	404	2	16,76,76	3.71	13 (81%)	0,234,234	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SIW	C	402[A]	-	16,76,76	3.73	13 (81%)	0,234,234	0.00	-
2	SIW	A	401[A]	1	16,76,76	3.81	13 (81%)	0,234,234	0.00	-
2	SIW	C	401[A]	-	16,76,76	3.75	13 (81%)	0,234,234	0.00	-
2	SIW	A	405	1	16,76,76	3.73	13 (81%)	0,234,234	0.00	-
2	SIW	A	406	-	16,76,76	3.70	13 (81%)	0,234,234	0.00	-
2	SIW	B	402	-	16,76,76	3.78	13 (81%)	0,234,234	0.00	-
2	SIW	A	407	2	16,76,76	3.71	13 (81%)	0,234,234	0.00	-
2	SIW	C	404	2	16,76,76	3.70	13 (81%)	0,234,234	0.00	-
2	SIW	C	403[B]	1	16,76,76	3.73	13 (81%)	0,234,234	0.00	-
2	SIW	A	403	1,2	16,76,76	3.69	14 (87%)	0,234,234	0.00	-
2	SIW	C	403[A]	-	16,76,76	3.72	13 (81%)	0,234,234	0.00	-
2	SIW	B	401[A]	1	16,76,76	3.71	13 (81%)	0,234,234	0.00	-
2	SIW	B	401[B]	1	16,76,76	3.75	13 (81%)	0,234,234	0.00	-
2	SIW	C	402[B]	-	16,76,76	3.74	13 (81%)	0,234,234	0.00	-
2	SIW	C	401[B]	1	16,76,76	3.70	13 (81%)	0,234,234	0.00	-
2	SIW	A	402[A]	-	16,76,76	3.75	12 (75%)	0,234,234	0.00	-
2	SIW	B	403	1	16,76,76	3.68	13 (81%)	0,234,234	0.00	-

All (260) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	SIW	SI1-O19E	-9.38	1.45	1.62
2	A	401[A]	SIW	SI1-O19E	-9.34	1.45	1.62
2	A	401[B]	SIW	SI1-O19E	-9.33	1.45	1.62
2	C	401[A]	SIW	SI1-O19E	-9.32	1.45	1.62
2	A	402[A]	SIW	SI1-O19E	-9.26	1.45	1.62
2	B	401[B]	SIW	SI1-O19E	-9.18	1.46	1.62
2	C	403[A]	SIW	SI1-O19E	-9.17	1.46	1.62
2	C	402[A]	SIW	SI1-O19E	-9.17	1.46	1.62
2	A	405	SIW	SI1-O19E	-9.16	1.46	1.62
2	B	401[A]	SIW	SI1-O19E	-9.16	1.46	1.62
2	A	402[B]	SIW	SI1-O19E	-9.14	1.46	1.62
2	C	402[B]	SIW	SI1-O19E	-9.12	1.46	1.62
2	C	403[B]	SIW	SI1-O19E	-9.12	1.46	1.62
2	A	407	SIW	SI1-O19E	-9.09	1.46	1.62
2	C	404	SIW	SI1-O19E	-9.09	1.46	1.62
2	A	404	SIW	SI1-O19E	-9.06	1.46	1.62
2	A	406	SIW	SI1-O19E	-9.06	1.46	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	SIW	SI1-O19E	-9.04	1.46	1.62
2	C	401[B]	SIW	SI1-O19E	-9.04	1.46	1.62
2	A	403	SIW	SI1-O19E	-8.87	1.46	1.62
2	A	401[A]	SIW	SI1-O4	-8.46	1.47	1.62
2	A	402[A]	SIW	SI1-O4	-8.38	1.47	1.62
2	A	401[B]	SIW	SI1-O4	-8.28	1.47	1.62
2	A	403	SIW	SI1-O4	-8.25	1.47	1.62
2	B	402	SIW	SI1-O4	-8.18	1.47	1.62
2	C	403[B]	SIW	SI1-O4	-8.17	1.47	1.62
2	A	402[B]	SIW	SI1-O4	-8.16	1.47	1.62
2	B	401[B]	SIW	SI1-O4	-8.16	1.47	1.62
2	C	402[A]	SIW	SI1-O4	-8.16	1.47	1.62
2	B	401[A]	SIW	SI1-O4	-8.13	1.48	1.62
2	A	405	SIW	SI1-O4	-8.12	1.48	1.62
2	C	402[B]	SIW	SI1-O4	-8.12	1.48	1.62
2	A	404	SIW	SI1-O4	-8.07	1.48	1.62
2	C	401[A]	SIW	SI1-O4	-8.07	1.48	1.62
2	C	403[A]	SIW	SI1-O4	-8.05	1.48	1.62
2	A	407	SIW	SI1-O4	-8.02	1.48	1.62
2	C	404	SIW	SI1-O4	-8.02	1.48	1.62
2	C	401[B]	SIW	SI1-O4	-8.00	1.48	1.62
2	A	406	SIW	SI1-O4	-7.98	1.48	1.62
2	B	403	SIW	SI1-O4	-7.93	1.48	1.62
2	C	402[B]	SIW	SI1-O21	3.60	1.69	1.62
2	A	402[A]	SIW	SI1-O22	3.51	1.69	1.62
2	B	401[B]	SIW	SI1-O21	3.49	1.69	1.62
2	C	401[B]	SIW	SI1-O21	3.48	1.69	1.62
2	A	401[A]	SIW	SI1-O21	3.46	1.69	1.62
2	A	407	SIW	SI1-O21	3.44	1.68	1.62
2	A	401[B]	SIW	SI1-O21	3.43	1.68	1.62
2	A	406	SIW	SI1-O21	3.41	1.68	1.62
2	A	404	SIW	SI1-O21	3.41	1.68	1.62
2	B	402	SIW	SI1-O21	3.40	1.68	1.62
2	C	403[B]	SIW	SI1-O21	3.39	1.68	1.62
2	C	403[A]	SIW	SI1-O21	3.37	1.68	1.62
2	A	405	SIW	SI1-O21	3.35	1.68	1.62
2	B	403	SIW	SI1-O21	3.31	1.68	1.62
2	C	402[A]	SIW	SI1-O21	3.28	1.68	1.62
2	C	404	SIW	SI1-O21	3.24	1.68	1.62
2	A	402[B]	SIW	SI1-O21	3.20	1.68	1.62
2	C	401[A]	SIW	SI1-O21	3.19	1.68	1.62
2	A	403	SIW	SI1-O21	3.08	1.68	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[A]	SIW	SI1-O21	3.05	1.68	1.62
2	C	401[A]	SIW	SI1-O22	3.03	1.68	1.62
2	A	406	SIW	SI1-O22	2.95	1.68	1.62
2	C	402[B]	SIW	SI1-O22	2.94	1.68	1.62
2	B	401[B]	SIW	SI1-O22	2.91	1.68	1.62
2	A	404	SIW	SI1-O22	2.91	1.68	1.62
2	C	403[B]	SIW	SI1-O22	2.91	1.68	1.62
2	B	402	SIW	SI1-O22	2.90	1.68	1.62
2	C	402[A]	SIW	SI1-O22	2.90	1.68	1.62
2	C	403[A]	SIW	SI1-O22	2.89	1.67	1.62
2	A	405	SIW	SI1-O22	2.89	1.67	1.62
2	A	407	SIW	SI1-O22	2.87	1.67	1.62
2	A	401[A]	SIW	SI1-O22	2.87	1.67	1.62
2	B	401[A]	SIW	SI1-O22	2.86	1.67	1.62
2	C	404	SIW	SI1-O22	2.86	1.67	1.62
2	A	402[B]	SIW	SI1-O22	2.85	1.67	1.62
2	A	403	SIW	SI1-O22	2.85	1.67	1.62
2	A	401[B]	SIW	SI1-O22	2.83	1.67	1.62
2	C	401[B]	SIW	SI1-O22	2.80	1.67	1.62
2	B	403	SIW	SI1-O22	2.76	1.67	1.62
2	C	401[A]	SIW	W6-O5	-2.47	1.58	2.16
2	A	401[A]	SIW	W6-O5	-2.45	1.58	2.16
2	B	402	SIW	W6-O5	-2.43	1.59	2.16
2	B	401[B]	SIW	W6-O5	-2.42	1.59	2.16
2	B	401[A]	SIW	W6-O5	-2.42	1.59	2.16
2	C	404	SIW	W6-O5	-2.42	1.59	2.16
2	C	402[A]	SIW	W6-O5	-2.41	1.59	2.16
2	A	406	SIW	W6-O5	-2.41	1.59	2.16
2	C	403[A]	SIW	W6-O5	-2.41	1.59	2.16
2	A	402[B]	SIW	W6-O5	-2.41	1.59	2.16
2	A	404	SIW	W6-O5	-2.41	1.59	2.16
2	A	402[A]	SIW	W6-O5	-2.41	1.59	2.16
2	A	401[B]	SIW	W6-O5	-2.41	1.59	2.16
2	A	403	SIW	W6-O5	-2.41	1.59	2.16
2	C	401[B]	SIW	W6-O5	-2.41	1.59	2.16
2	B	403	SIW	W6-O5	-2.41	1.59	2.16
2	C	402[B]	SIW	W6-O5	-2.41	1.59	2.16
2	A	405	SIW	W6-O5	-2.41	1.59	2.16
2	C	403[B]	SIW	W6-O5	-2.41	1.59	2.16
2	A	407	SIW	W6-O5	-2.41	1.59	2.16
2	A	401[A]	SIW	W1-O12	-2.32	1.61	2.16
2	B	402	SIW	W1E-O12E	-2.30	1.61	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	403[B]	SIW	W1-O12	-2.29	1.62	2.16
2	C	403[A]	SIW	W1E-O12E	-2.29	1.62	2.16
2	A	401[A]	SIW	W1E-O12E	-2.29	1.62	2.16
2	A	402[B]	SIW	W1E-O12E	-2.29	1.62	2.16
2	C	401[A]	SIW	W1-O12	-2.29	1.62	2.16
2	B	401[B]	SIW	W1-O12	-2.29	1.62	2.16
2	A	405	SIW	W1E-O12E	-2.29	1.62	2.16
2	A	402[A]	SIW	W1E-O12E	-2.29	1.62	2.16
2	B	401[A]	SIW	W1E-O12E	-2.28	1.62	2.16
2	B	401[A]	SIW	W1-O12	-2.28	1.62	2.16
2	A	407	SIW	W1E-O12E	-2.28	1.62	2.16
2	B	401[B]	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	402[A]	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	402[A]	SIW	W1-O12	-2.28	1.62	2.16
2	A	403	SIW	W1-O12	-2.28	1.62	2.16
2	C	401[B]	SIW	W1-O12	-2.28	1.62	2.16
2	C	403[A]	SIW	W1-O12	-2.28	1.62	2.16
2	A	406	SIW	W1E-O12E	-2.28	1.62	2.16
2	A	402[B]	SIW	W1-O12	-2.28	1.62	2.16
2	A	404	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	402[B]	SIW	W1-O12	-2.28	1.62	2.16
2	C	404	SIW	W1-O12	-2.28	1.62	2.16
2	A	401[B]	SIW	W1-O12	-2.28	1.62	2.16
2	A	402[A]	SIW	W1-O12	-2.28	1.62	2.16
2	A	405	SIW	W1-O12	-2.28	1.62	2.16
2	A	406	SIW	W1-O12	-2.28	1.62	2.16
2	A	401[B]	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	401[B]	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	402[B]	SIW	W1E-O12E	-2.28	1.62	2.16
2	A	407	SIW	W1-O12	-2.28	1.62	2.16
2	B	403	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	403[B]	SIW	W1E-O12E	-2.28	1.62	2.16
2	C	404	SIW	W1E-O12E	-2.28	1.62	2.16
2	B	403	SIW	W1-O12	-2.28	1.62	2.16
2	A	404	SIW	W1-O12	-2.28	1.62	2.16
2	B	402	SIW	W1-O12	-2.28	1.62	2.16
2	C	401[A]	SIW	W1E-O12E	-2.28	1.62	2.16
2	A	403	SIW	W1E-O12E	-2.26	1.62	2.16
2	C	401[B]	SIW	W3-O11	-2.20	1.64	2.16
2	C	403[B]	SIW	W3-O11	-2.18	1.64	2.16
2	C	402[A]	SIW	W3-O11	-2.18	1.64	2.16
2	C	401[B]	SIW	W3E-O11E	-2.17	1.65	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401[A]	SIW	W3E-O11E	-2.17	1.65	2.16
2	C	403[B]	SIW	W3E-O11E	-2.16	1.65	2.16
2	A	406	SIW	W3-O11	-2.16	1.65	2.16
2	B	401[B]	SIW	W3-O11	-2.16	1.65	2.16
2	A	403	SIW	W3E-O11E	-2.16	1.65	2.16
2	A	401[A]	SIW	W3E-O11E	-2.16	1.65	2.16
2	C	403[A]	SIW	W3-O11	-2.16	1.65	2.16
2	A	402[A]	SIW	W3E-O11E	-2.16	1.65	2.16
2	C	403[A]	SIW	W3E-O11E	-2.16	1.65	2.16
2	A	405	SIW	W3E-O11E	-2.16	1.65	2.16
2	C	402[A]	SIW	W3E-O11E	-2.16	1.65	2.16
2	B	403	SIW	W3-O11	-2.16	1.65	2.16
2	B	403	SIW	W3E-O11E	-2.16	1.65	2.16
2	A	405	SIW	W3-O11	-2.16	1.65	2.16
2	C	404	SIW	W3E-O11E	-2.16	1.65	2.16
2	C	401[A]	SIW	W3-O11	-2.16	1.65	2.16
2	B	401[B]	SIW	W3E-O11E	-2.16	1.65	2.16
2	B	402	SIW	W3-O11	-2.16	1.65	2.16
2	B	401[A]	SIW	W3-O11	-2.16	1.65	2.16
2	A	402[B]	SIW	W3-O11	-2.16	1.65	2.16
2	A	401[B]	SIW	W3E-O11E	-2.16	1.65	2.16
2	C	402[B]	SIW	W3-O11	-2.16	1.65	2.16
2	B	401[A]	SIW	W3E-O11E	-2.16	1.65	2.16
2	A	401[B]	SIW	W3-O11	-2.16	1.65	2.16
2	A	404	SIW	W3-O11	-2.15	1.65	2.16
2	C	402[B]	SIW	W3E-O11E	-2.15	1.65	2.16
2	A	402[B]	SIW	W3E-O11E	-2.15	1.65	2.16
2	A	404	SIW	W3E-O11E	-2.15	1.65	2.16
2	C	404	SIW	W3-O11	-2.15	1.65	2.16
2	A	407	SIW	W3-O11	-2.15	1.65	2.16
2	A	406	SIW	W3E-O11E	-2.15	1.65	2.16
2	A	402[A]	SIW	W3-O11	-2.15	1.65	2.16
2	A	402[A]	SIW	W5E-O13E	-2.15	1.65	2.16
2	B	402	SIW	W3E-O11E	-2.15	1.65	2.16
2	A	403	SIW	W3-O11	-2.15	1.65	2.16
2	A	407	SIW	W3E-O11E	-2.15	1.65	2.16
2	A	401[A]	SIW	W3-O11	-2.15	1.65	2.16
2	A	403	SIW	W4-O14	-2.15	1.65	2.16
2	A	401[B]	SIW	W4E-O14E	-2.14	1.65	2.16
2	B	402	SIW	W4-O14	-2.13	1.66	2.16
2	C	403[B]	SIW	W4E-O14E	-2.13	1.66	2.16
2	A	401[A]	SIW	W4-O14	-2.12	1.66	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	SIW	W4E-O14E	-2.12	1.66	2.16
2	C	402[B]	SIW	W4E-O14E	-2.12	1.66	2.16
2	A	405	SIW	W4E-O14E	-2.12	1.66	2.16
2	A	405	SIW	W4-O14	-2.12	1.66	2.16
2	C	401[A]	SIW	W4-O14	-2.12	1.66	2.16
2	A	406	SIW	W4E-O14E	-2.12	1.66	2.16
2	C	401[B]	SIW	W4E-O14E	-2.12	1.66	2.16
2	B	402	SIW	W4E-O14E	-2.12	1.66	2.16
2	B	401[A]	SIW	W4-O14	-2.12	1.66	2.16
2	A	402[B]	SIW	W4-O14	-2.12	1.66	2.16
2	B	403	SIW	W4-O14	-2.11	1.66	2.16
2	C	402[A]	SIW	W4E-O14E	-2.11	1.66	2.16
2	C	404	SIW	W4-O14	-2.11	1.66	2.16
2	B	401[B]	SIW	W4E-O14E	-2.11	1.66	2.16
2	A	402[A]	SIW	W4-O14	-2.11	1.66	2.16
2	A	406	SIW	W4-O14	-2.11	1.66	2.16
2	C	403[A]	SIW	W4E-O14E	-2.11	1.66	2.16
2	C	402[A]	SIW	W4-O14	-2.11	1.66	2.16
2	A	407	SIW	W4E-O14E	-2.11	1.66	2.16
2	A	404	SIW	W4-O14	-2.11	1.66	2.16
2	C	402[B]	SIW	W4-O14	-2.11	1.66	2.16
2	B	401[B]	SIW	W4-O14	-2.11	1.66	2.16
2	A	401[B]	SIW	W4-O14	-2.11	1.66	2.16
2	C	404	SIW	W4E-O14E	-2.11	1.66	2.16
2	C	403[A]	SIW	W4-O14	-2.11	1.66	2.16
2	A	407	SIW	W4-O14	-2.11	1.66	2.16
2	B	403	SIW	W4E-O14E	-2.11	1.66	2.16
2	C	401[B]	SIW	W4-O14	-2.11	1.66	2.16
2	A	402[B]	SIW	W4E-O14E	-2.11	1.66	2.16
2	A	404	SIW	W4E-O14E	-2.11	1.66	2.16
2	A	402[A]	SIW	W4E-O14E	-2.11	1.66	2.16
2	C	401[A]	SIW	W4E-O14E	-2.11	1.66	2.16
2	C	403[B]	SIW	W4-O14	-2.11	1.66	2.16
2	B	401[A]	SIW	W4E-O14E	-2.11	1.66	2.16
2	A	403	SIW	W4E-O14E	-2.10	1.66	2.16
2	B	402	SIW	W5E-O13E	-2.08	1.67	2.16
2	A	403	SIW	W7-O6	-2.07	1.67	2.16
2	A	401[B]	SIW	W5E-O13E	-2.05	1.68	2.16
2	A	402[A]	SIW	W5-O13	-2.04	1.68	2.16
2	C	401[B]	SIW	W5-O13	-2.04	1.68	2.16
2	C	402[A]	SIW	W5E-O13E	-2.04	1.68	2.16
2	B	402	SIW	W5-O13	-2.03	1.68	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	402[B]	SIW	W5-O13	-2.03	1.68	2.16
2	C	403[A]	SIW	W5-O13	-2.03	1.68	2.16
2	A	404	SIW	W5E-O13E	-2.03	1.68	2.16
2	C	403[A]	SIW	W5E-O13E	-2.03	1.68	2.16
2	C	402[B]	SIW	W5-O13	-2.03	1.68	2.16
2	A	405	SIW	W5E-O13E	-2.03	1.68	2.16
2	C	403[B]	SIW	W5-O13	-2.03	1.68	2.16
2	A	403	SIW	W5E-O13E	-2.03	1.68	2.16
2	C	404	SIW	W5-O13	-2.03	1.68	2.16
2	A	407	SIW	W5-O13	-2.03	1.68	2.16
2	B	401[A]	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	401[B]	SIW	W5-O13	-2.03	1.68	2.16
2	C	401[B]	SIW	W5E-O13E	-2.03	1.68	2.16
2	B	403	SIW	W5-O13	-2.03	1.68	2.16
2	C	402[A]	SIW	W5-O13	-2.03	1.68	2.16
2	A	401[A]	SIW	W5E-O13E	-2.03	1.68	2.16
2	C	403[B]	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	403	SIW	W5-O13	-2.03	1.68	2.16
2	A	407	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	401[A]	SIW	W5-O13	-2.03	1.68	2.16
2	B	403	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	406	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	406	SIW	W5-O13	-2.03	1.68	2.16
2	B	401[B]	SIW	W5-O13	-2.03	1.68	2.16
2	C	402[B]	SIW	W5E-O13E	-2.03	1.68	2.16
2	C	401[A]	SIW	W5E-O13E	-2.03	1.68	2.16
2	A	405	SIW	W5-O13	-2.03	1.68	2.16
2	A	404	SIW	W5-O13	-2.03	1.68	2.16
2	C	404	SIW	W5E-O13E	-2.03	1.68	2.16
2	B	401[A]	SIW	W5-O13	-2.03	1.68	2.16
2	A	402[B]	SIW	W5E-O13E	-2.02	1.68	2.16
2	C	401[A]	SIW	W5-O13	-2.02	1.68	2.16

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

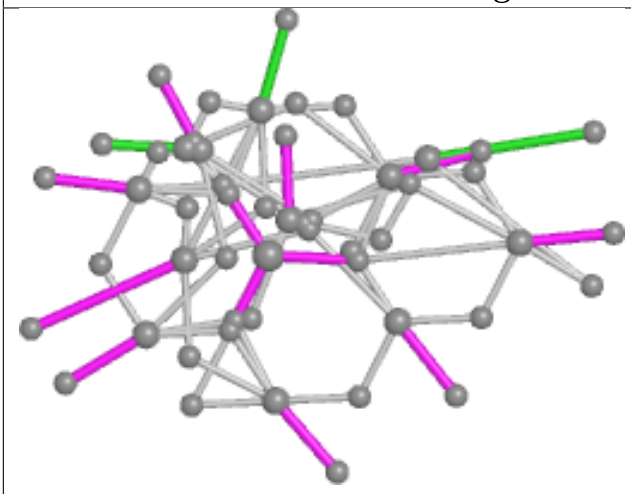
There are no ring outliers.

20 monomers are involved in 155 short contacts:

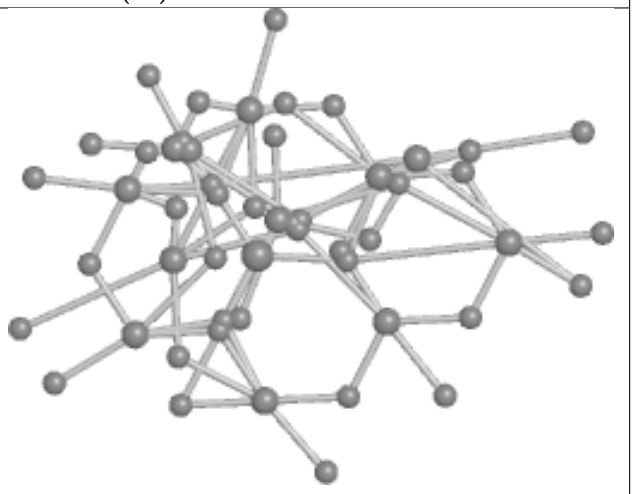
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402[B]	SIW	6	0
2	A	401[B]	SIW	6	1
2	A	404	SIW	6	0
2	C	402[A]	SIW	8	0
2	A	401[A]	SIW	7	0
2	C	401[A]	SIW	9	0
2	A	405	SIW	8	0
2	A	406	SIW	7	0
2	B	402	SIW	8	0
2	A	407	SIW	9	0
2	C	404	SIW	9	0
2	C	403[B]	SIW	9	0
2	A	403	SIW	8	0
2	C	403[A]	SIW	7	0
2	B	401[A]	SIW	8	0
2	B	401[B]	SIW	10	0
2	C	402[B]	SIW	8	0
2	C	401[B]	SIW	9	0
2	A	402[A]	SIW	7	0
2	B	403	SIW	8	1

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.

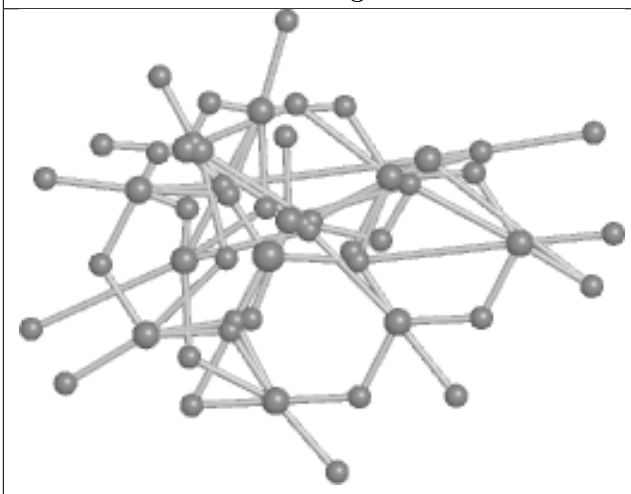
Ligand SIW A 402 (B)



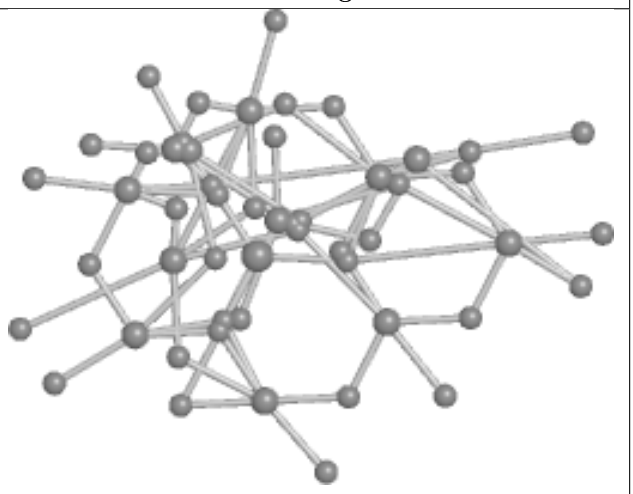
Bond lengths



Bond angles

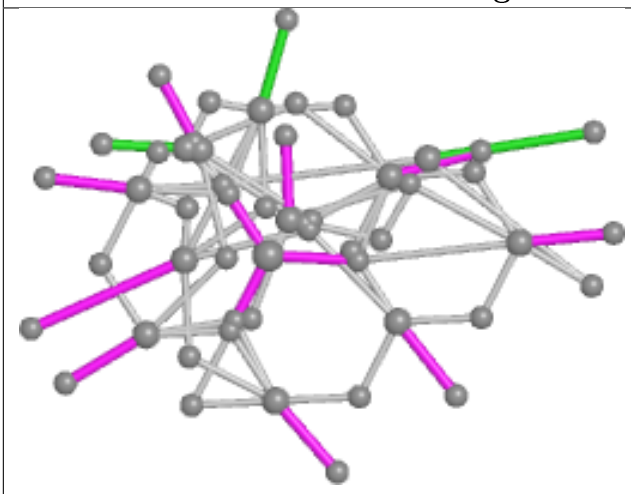


Torsions

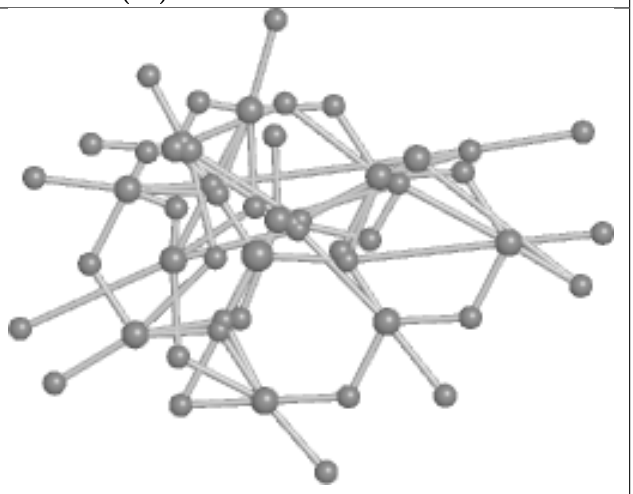


Rings

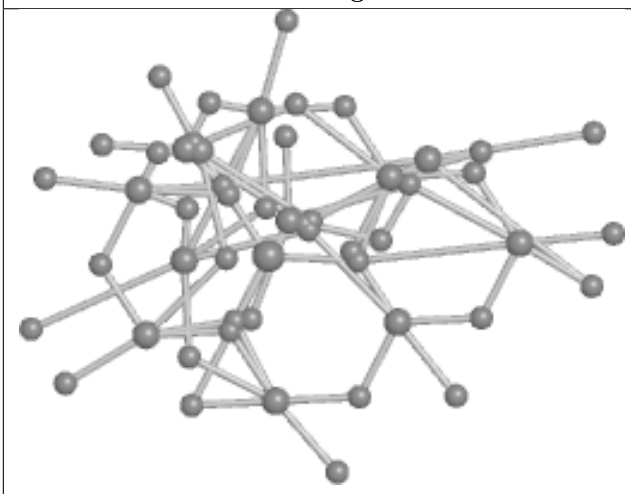
Ligand SIW A 401 (B)



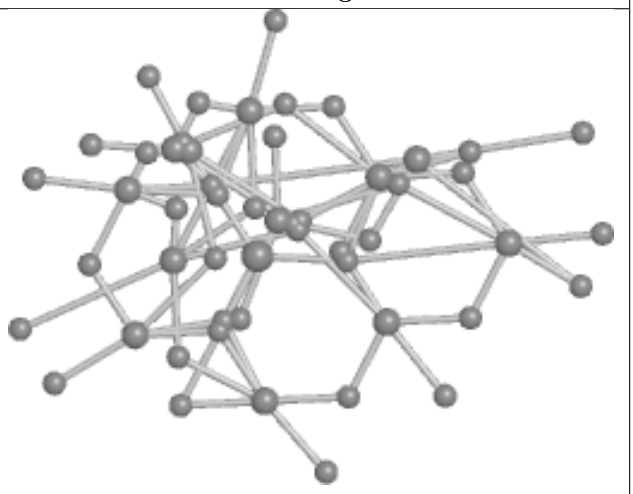
Bond lengths



Bond angles

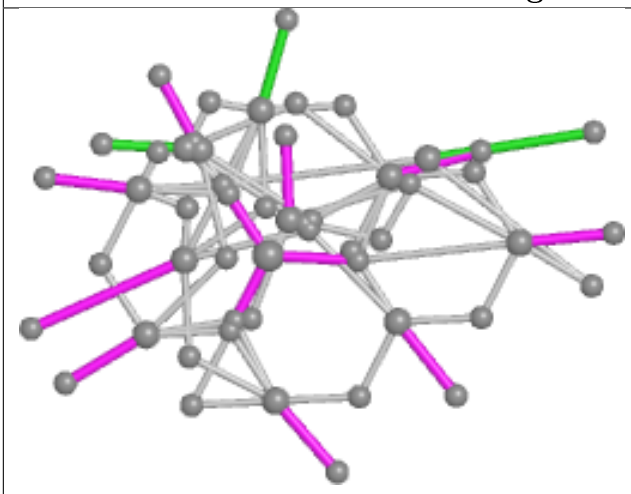


Torsions

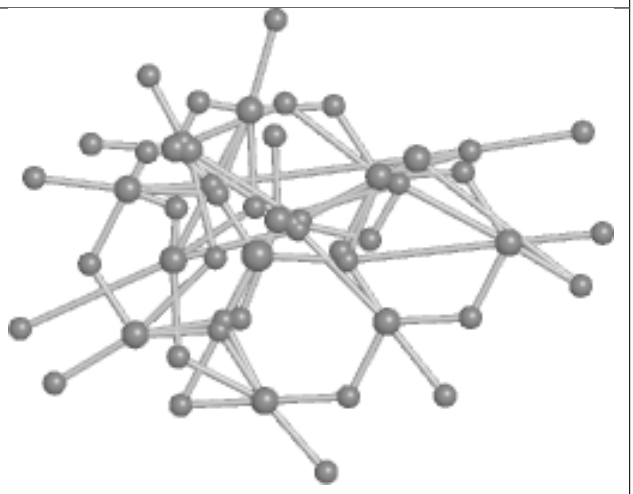


Rings

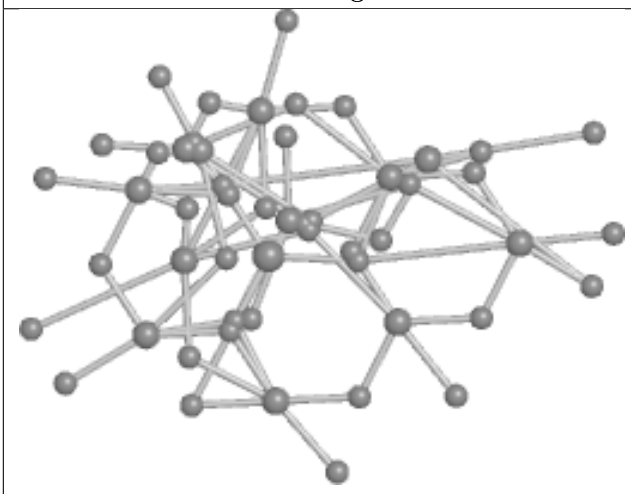
Ligand SIW A 404



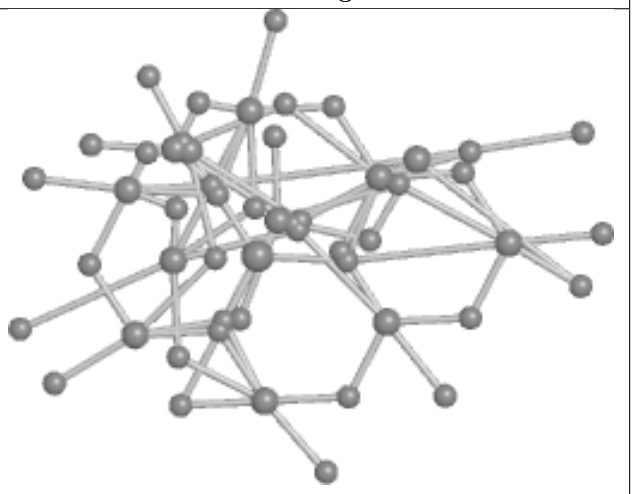
Bond lengths



Bond angles

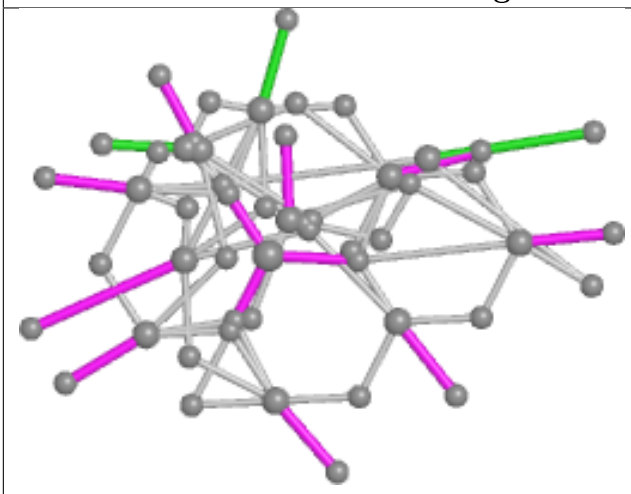


Torsions



Rings

Ligand SIW C 402 (A)



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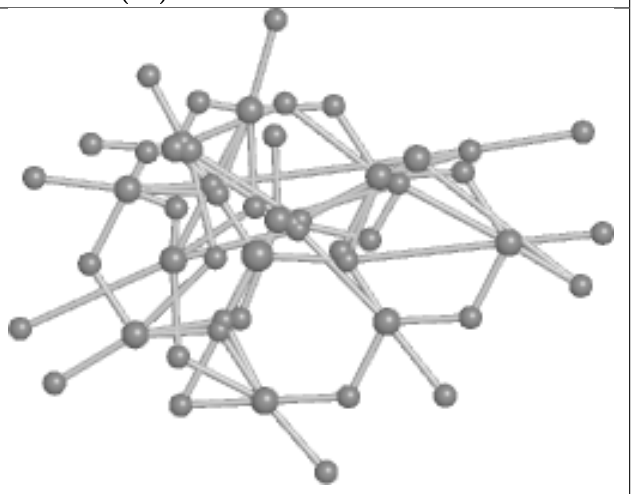
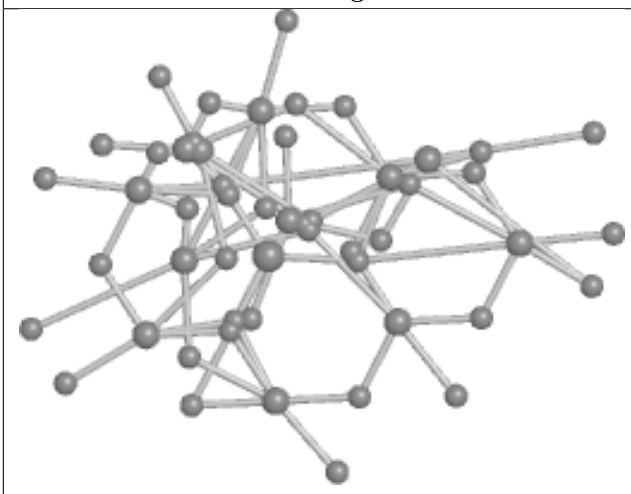
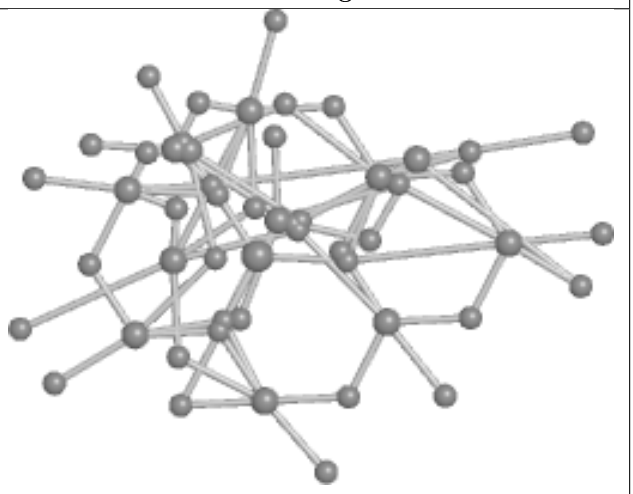


Bond angles

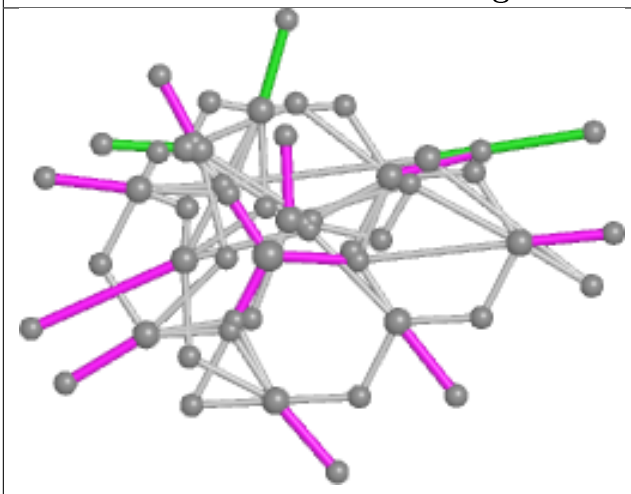


Torsions

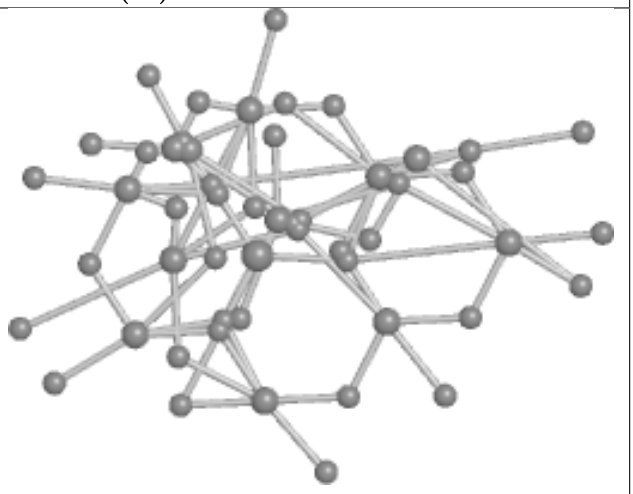


Rings

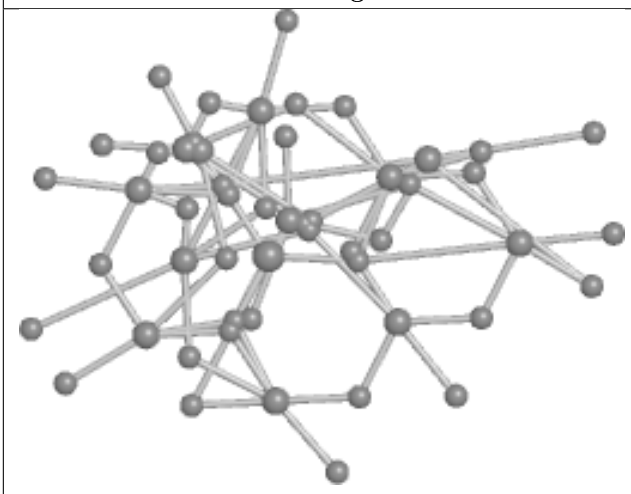
Ligand SIW A 401 (A)



Bond lengths



Bond angles



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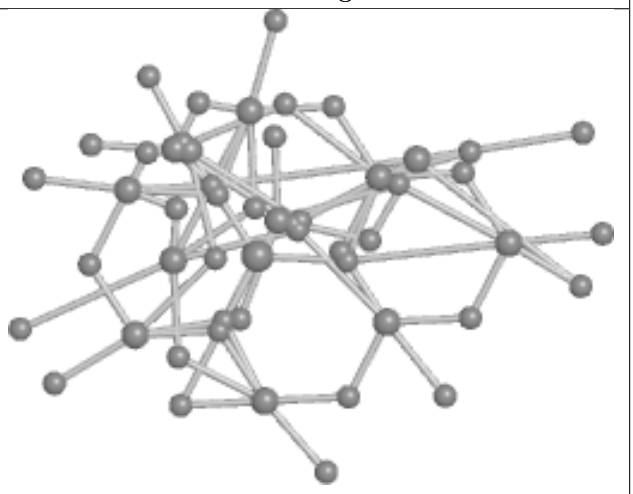
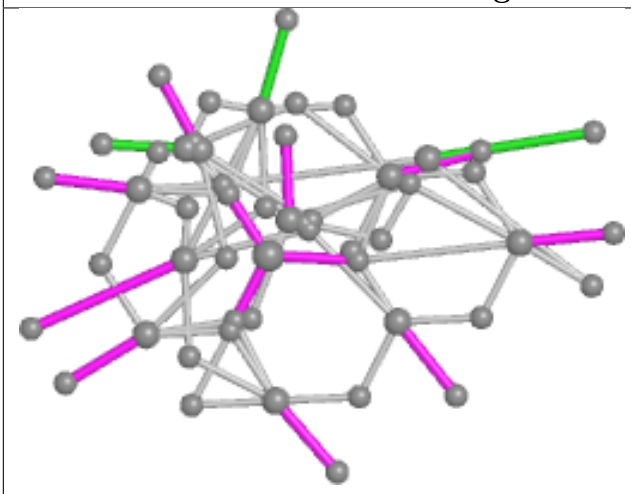


Rings

Ligand SIW C 401 (A)



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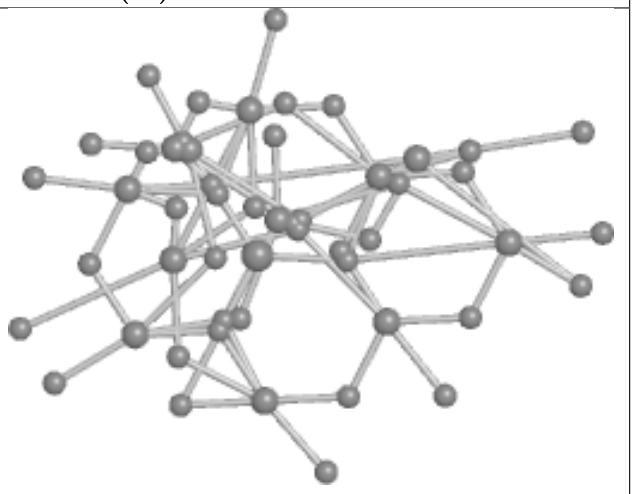
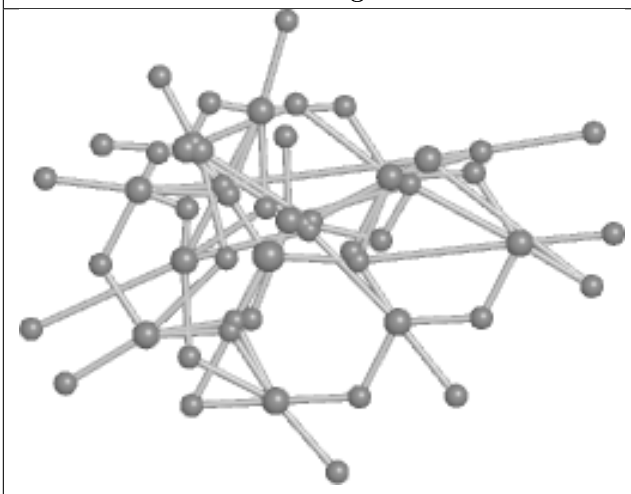
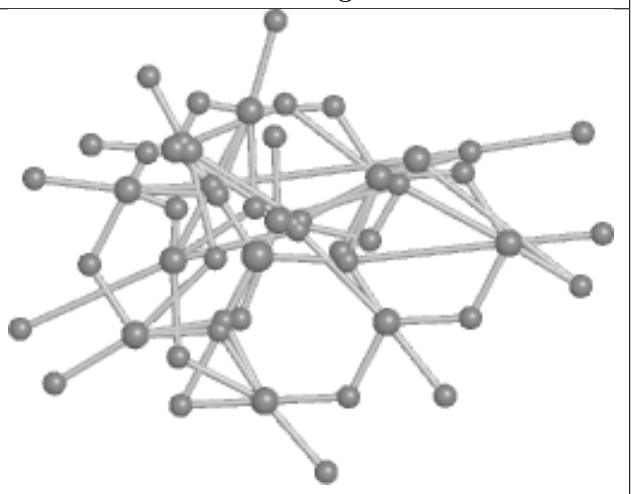


Bond angles

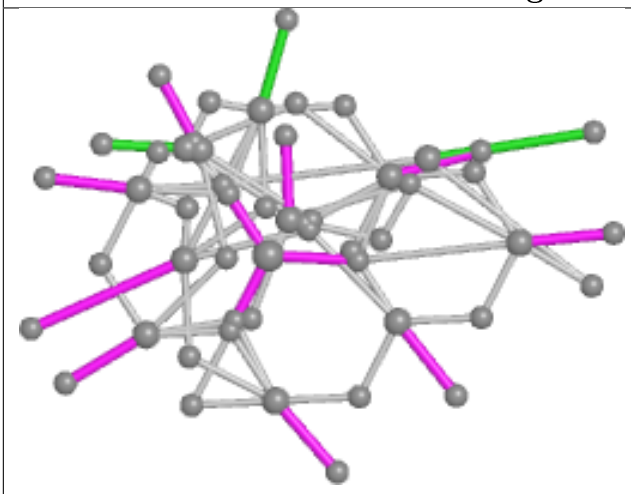


Torsions

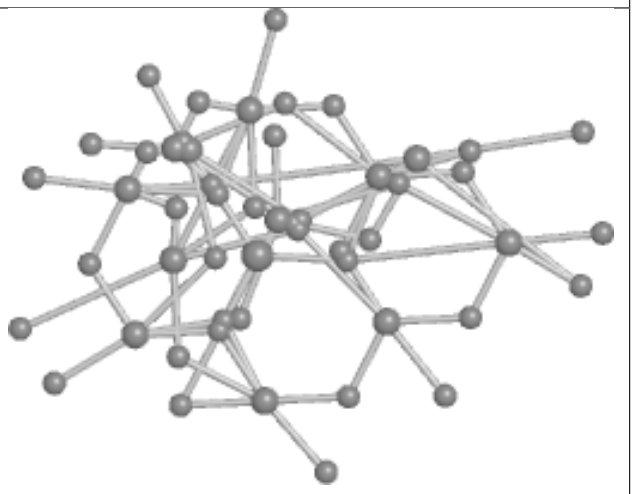


Rings

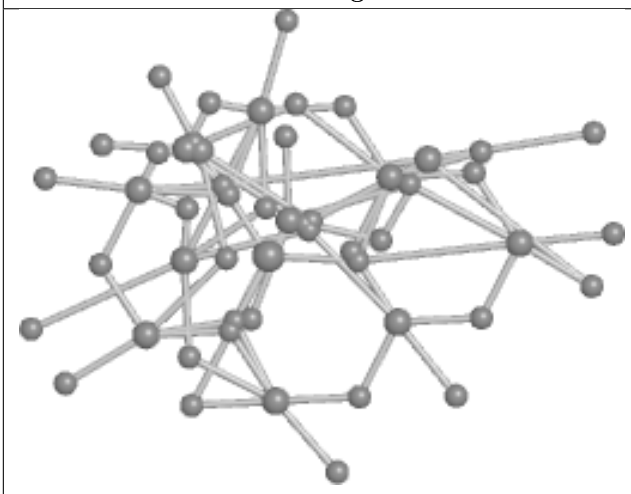
Ligand SIW A 405



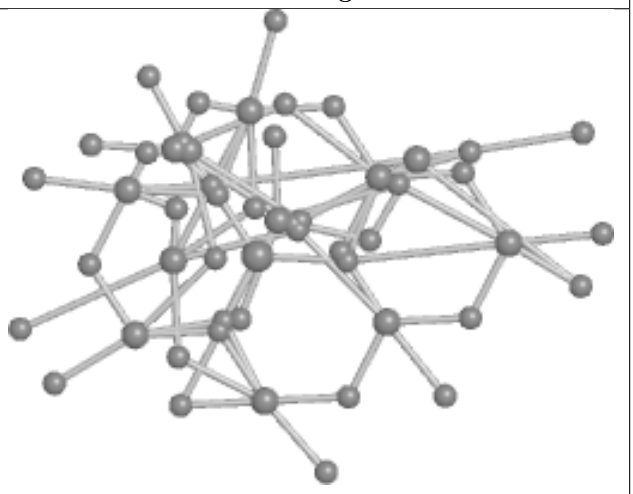
Bond lengths



Bond angles

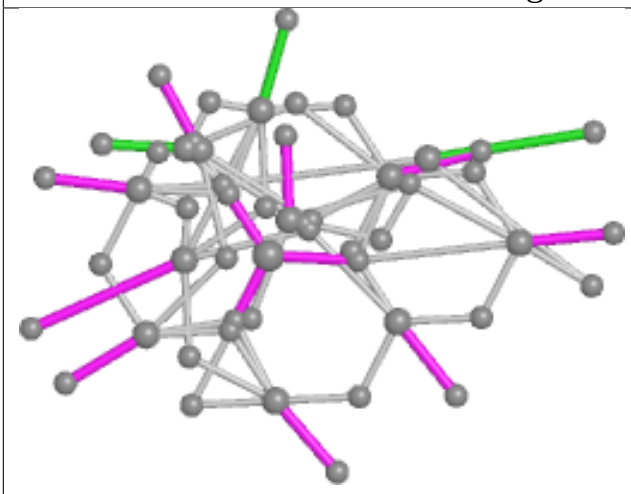


Torsions

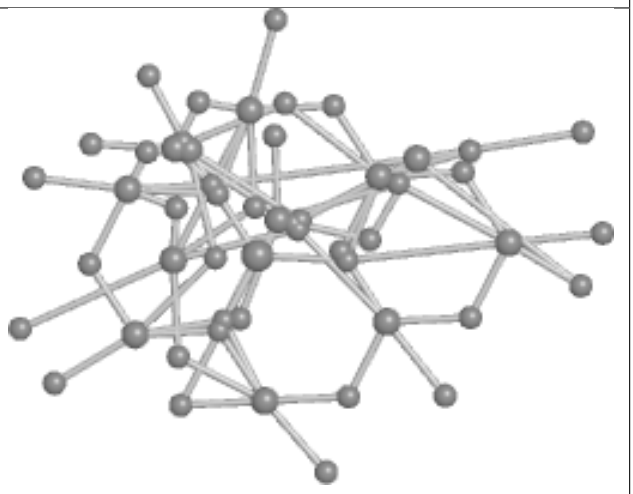


Rings

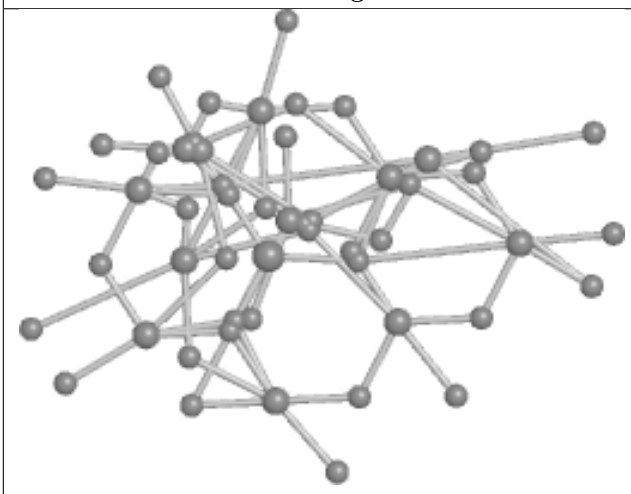
Ligand SIW A 406



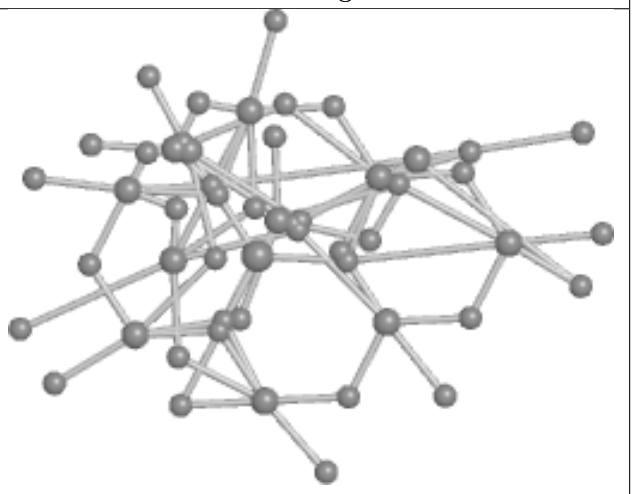
Bond lengths



Bond angles

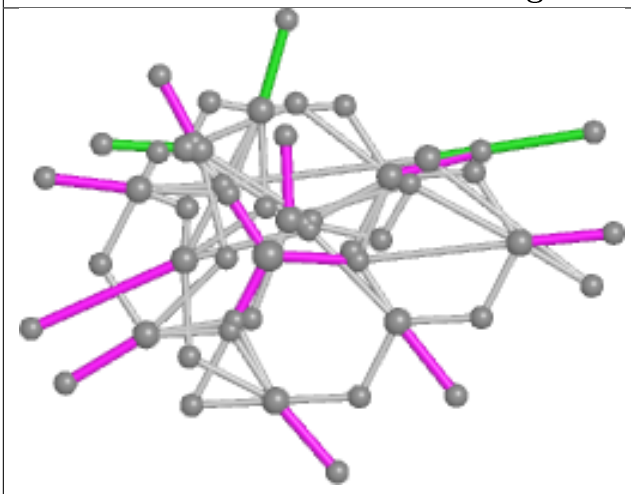


Torsions

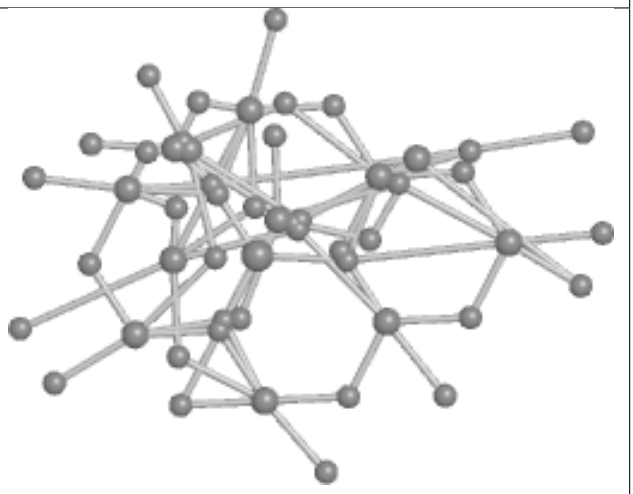


Rings

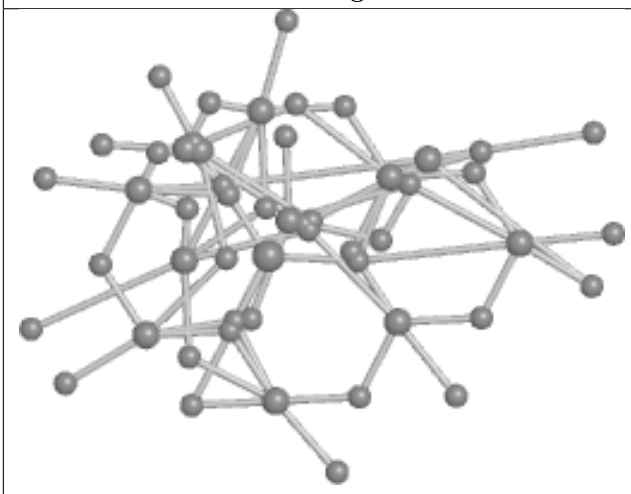
Ligand SIW B 402



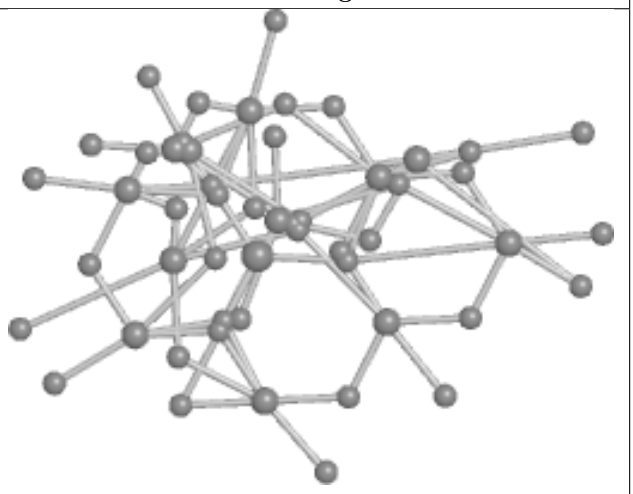
Bond lengths



Bond angles

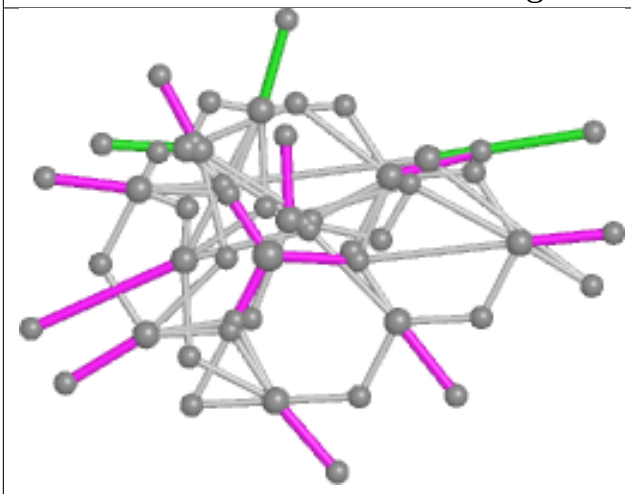


Torsions

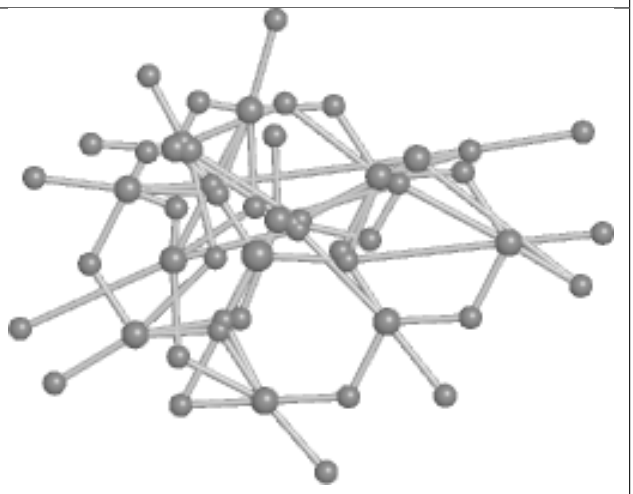


Rings

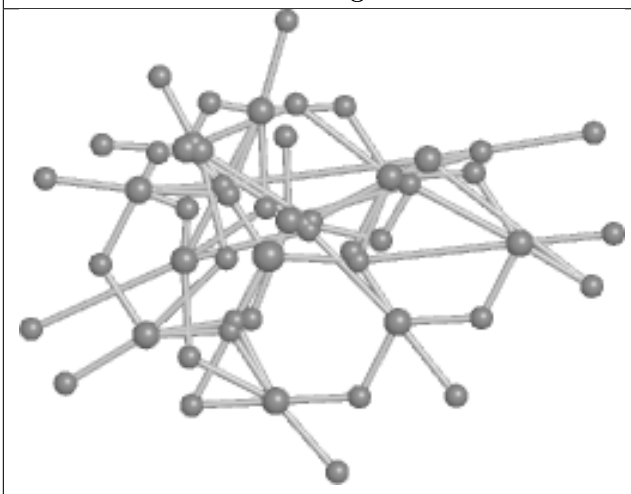
Ligand SIW A 407



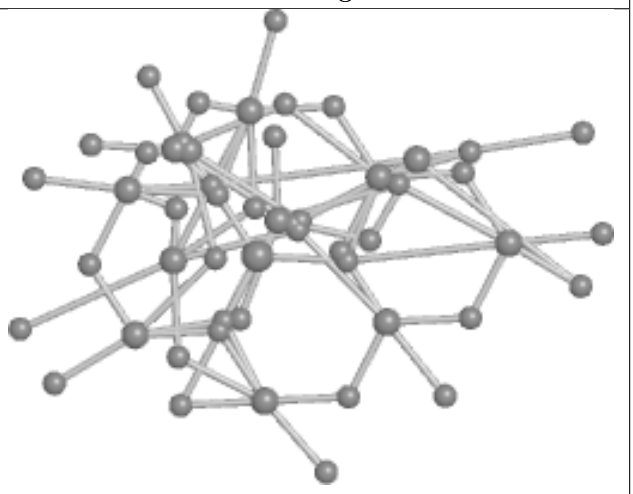
Bond lengths



Bond angles

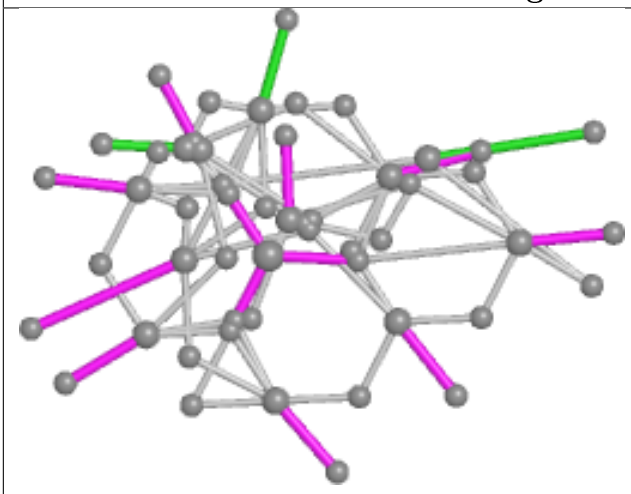


Torsions

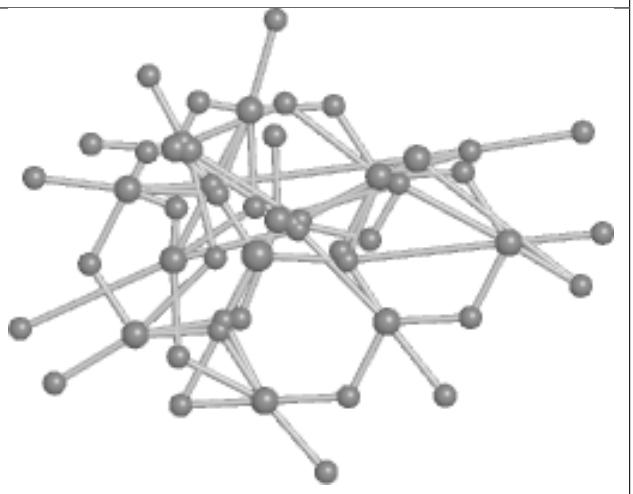


Rings

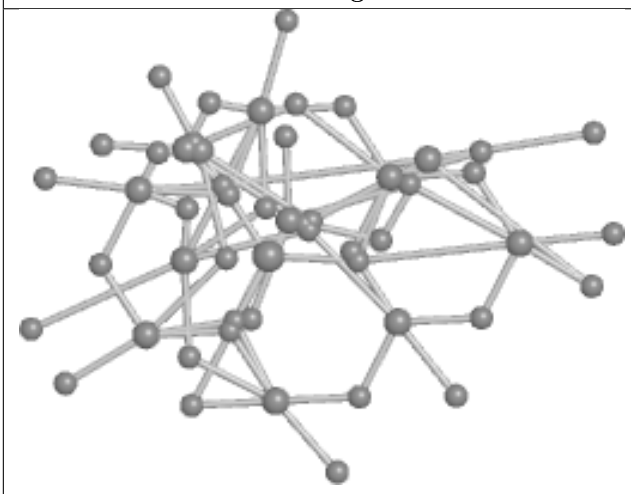
Ligand SIW C 404



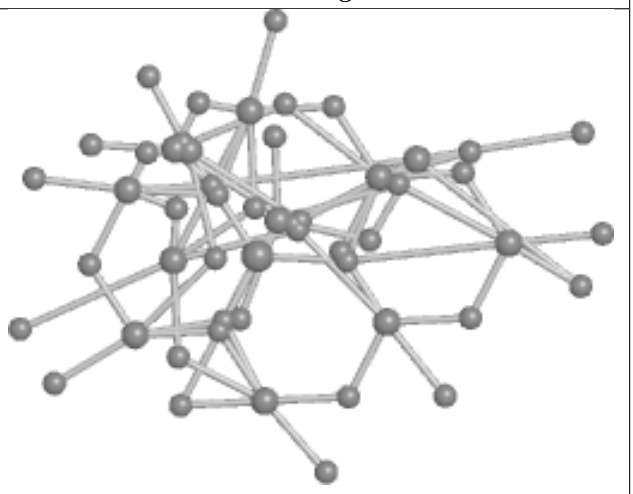
Bond lengths



Bond angles

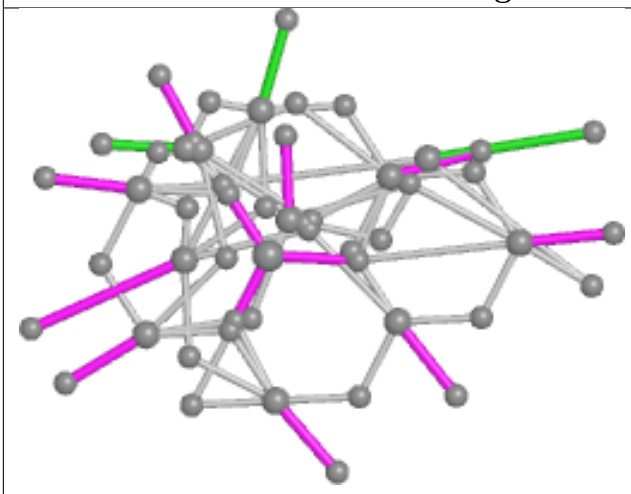


Torsions

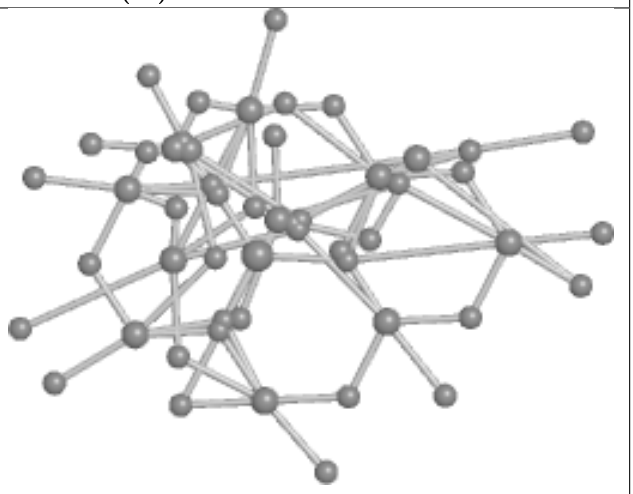


Rings

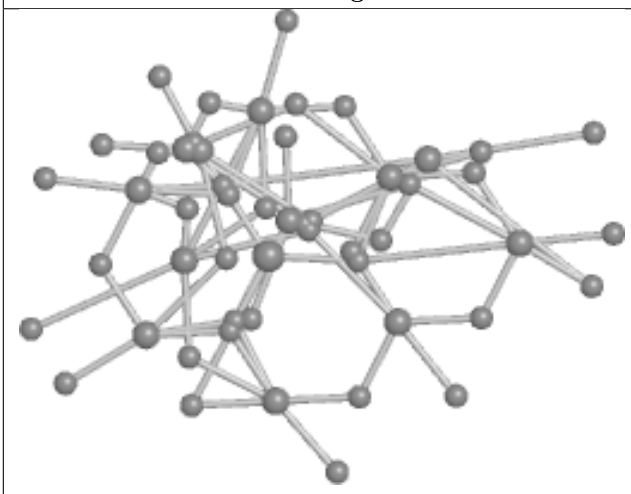
Ligand SIW C 403 (B)



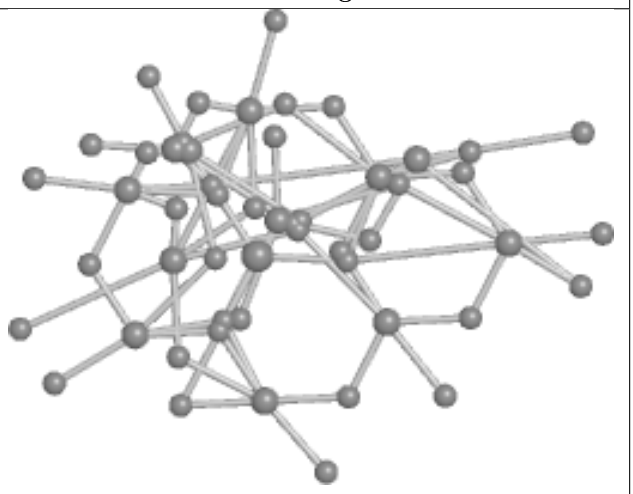
Bond lengths



Bond angles

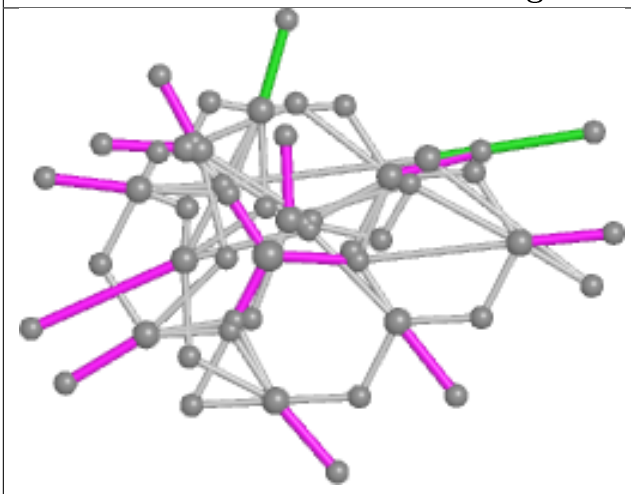


Torsions

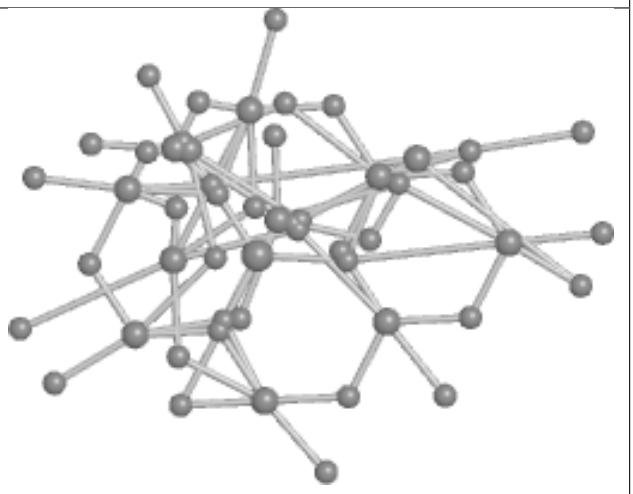


Rings

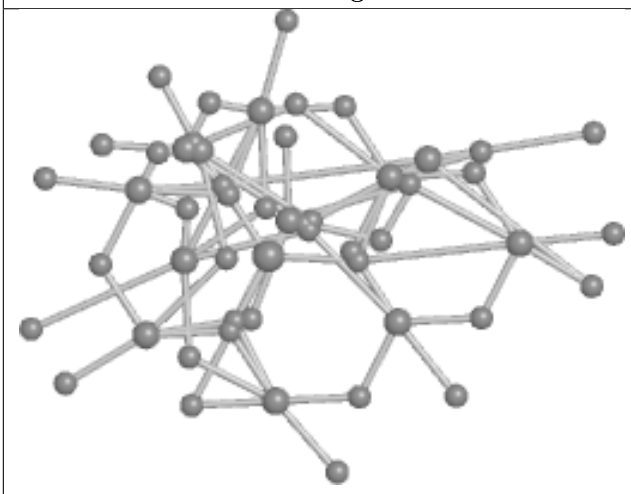
Ligand SIW A 403



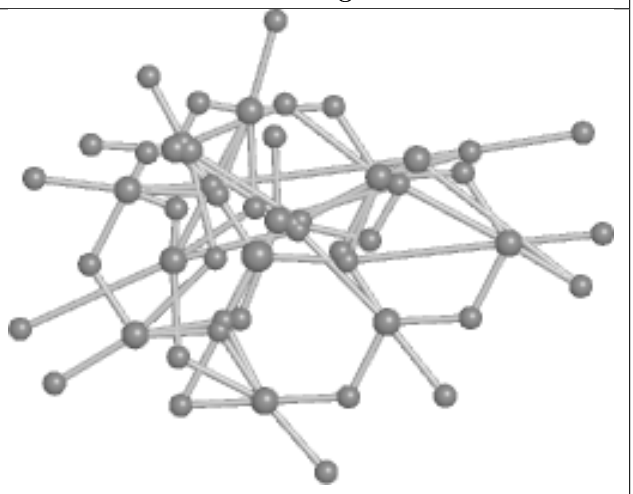
Bond lengths



Bond angles

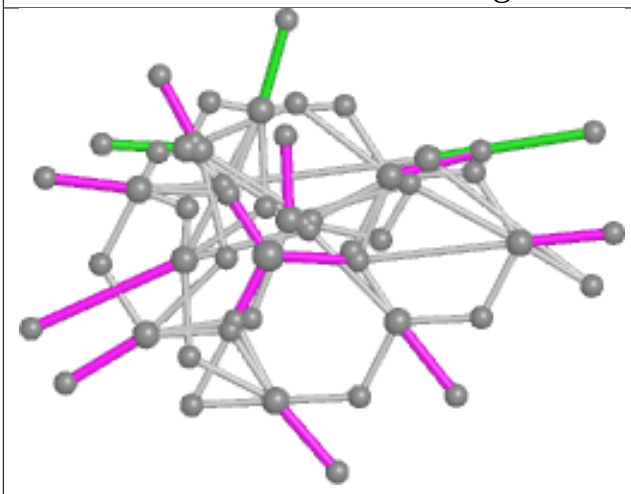


Torsions

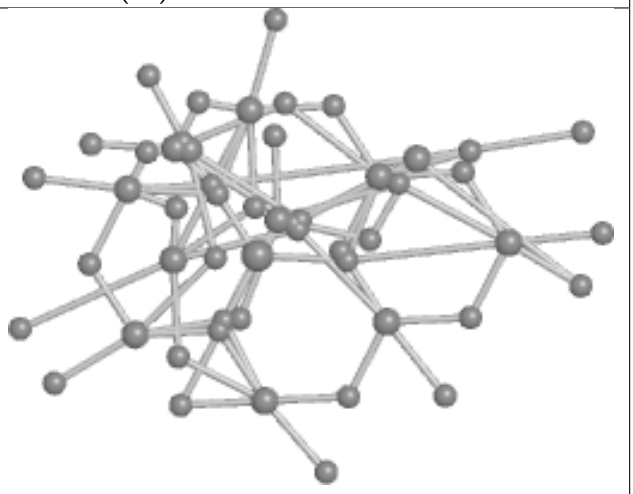


Rings

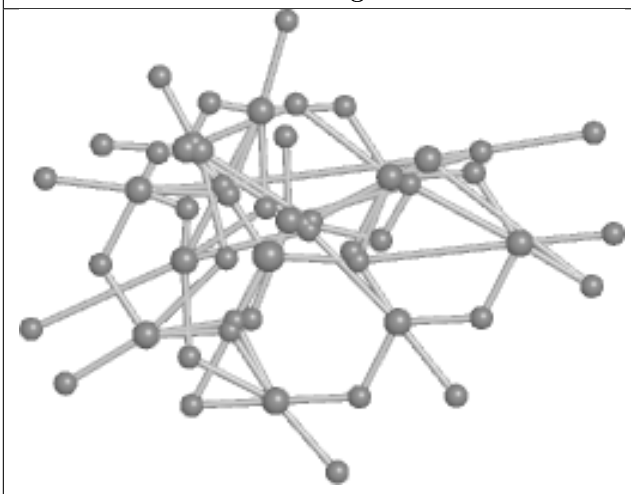
Ligand SIW C 403 (A)



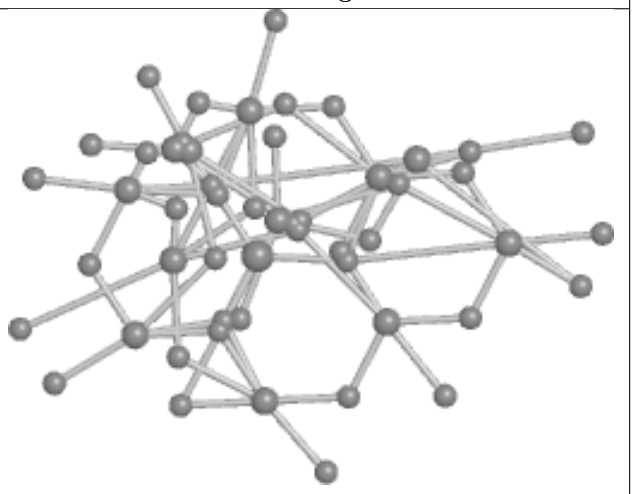
Bond lengths



Bond angles

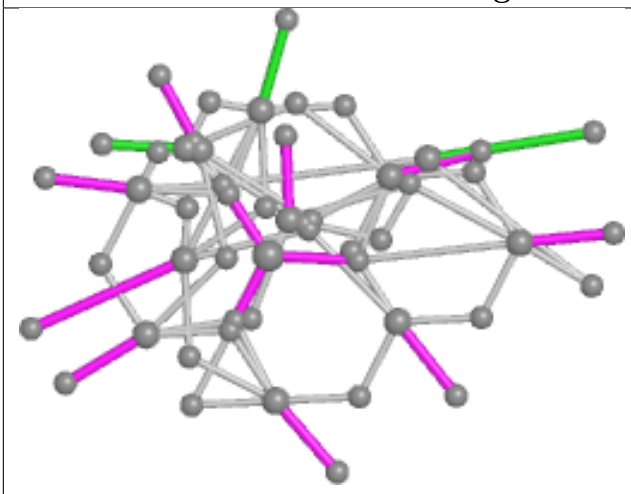


Torsions

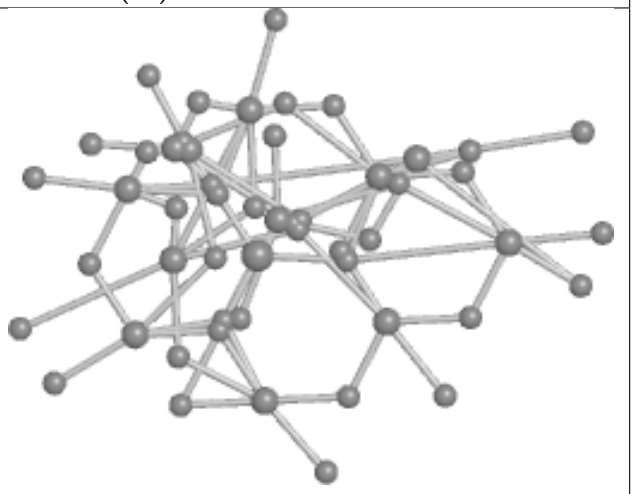


Rings

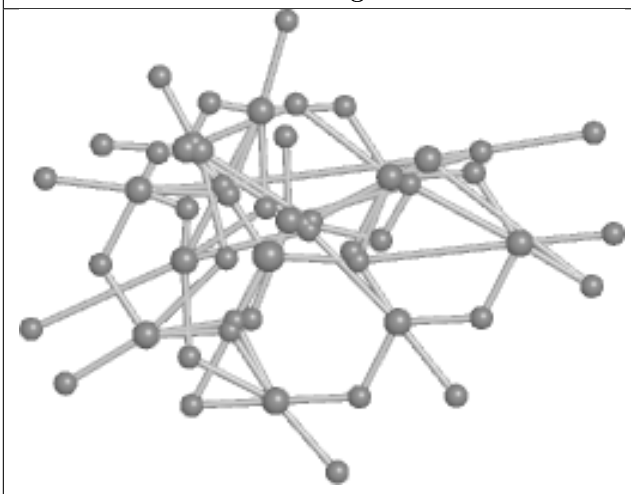
Ligand SIW B 401 (A)



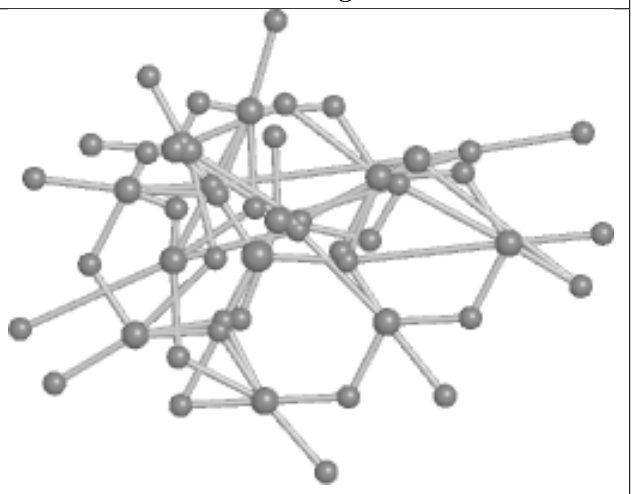
Bond lengths



Bond angles

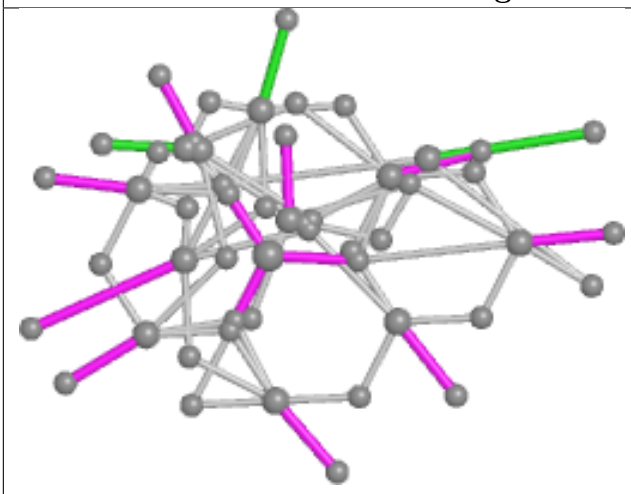


Torsions

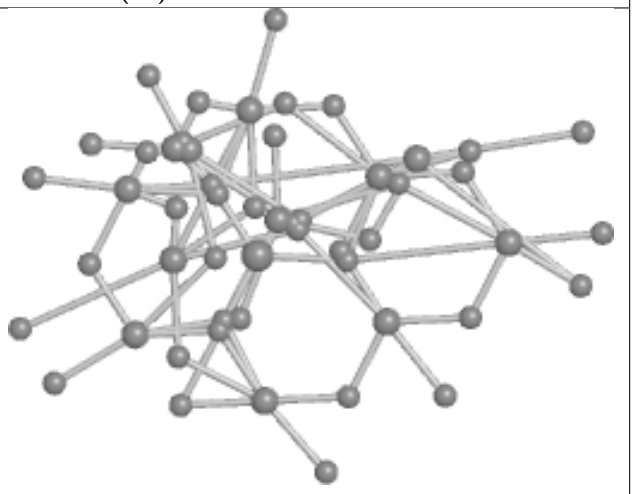


Rings

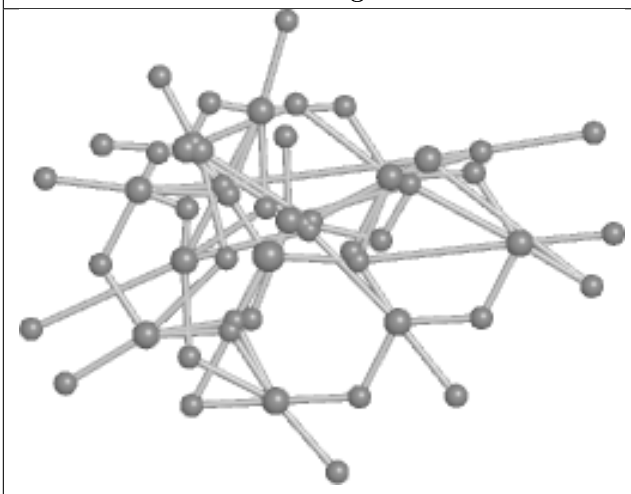
Ligand SIW B 401 (B)



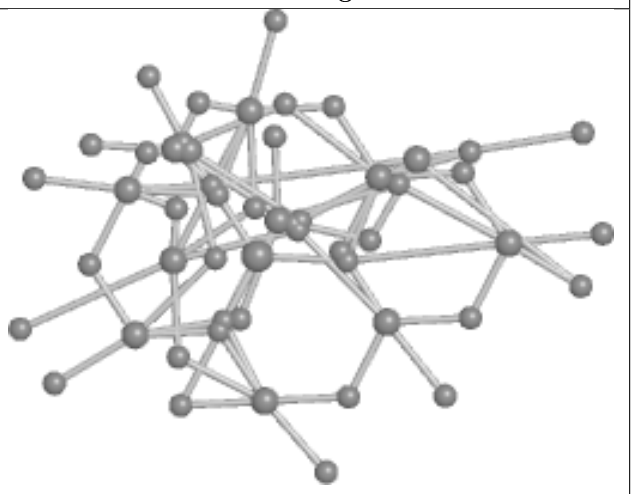
Bond lengths



Bond angles

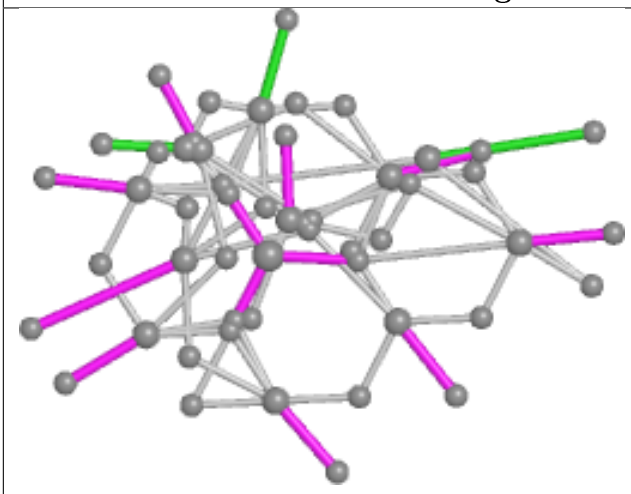


Torsions

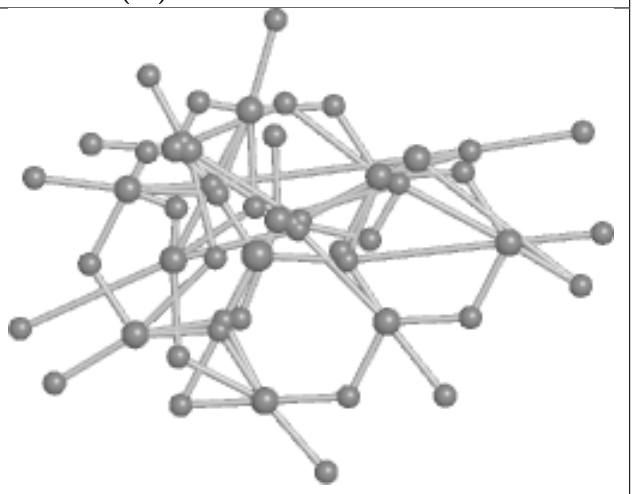


Rings

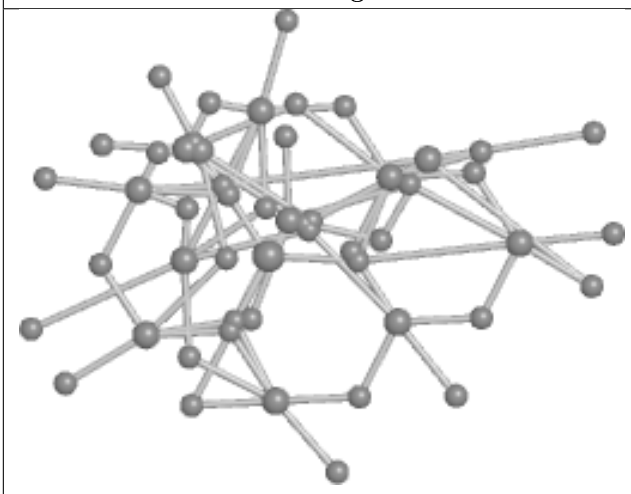
Ligand SIW C 402 (B)



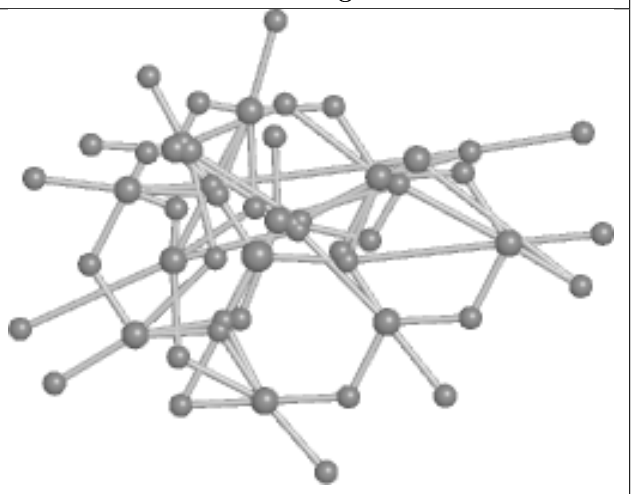
Bond lengths



Bond angles

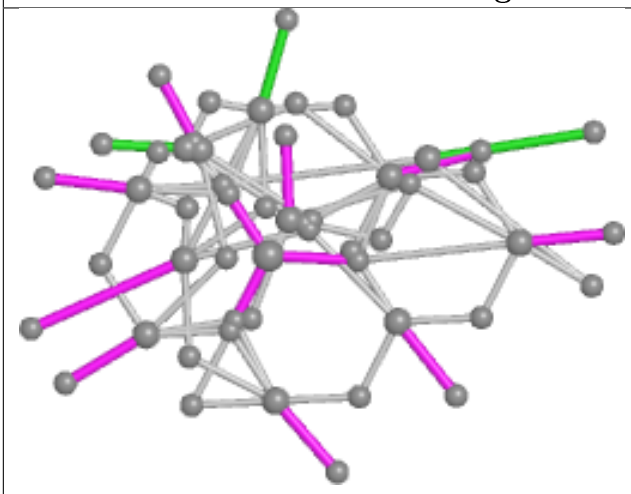


Torsions

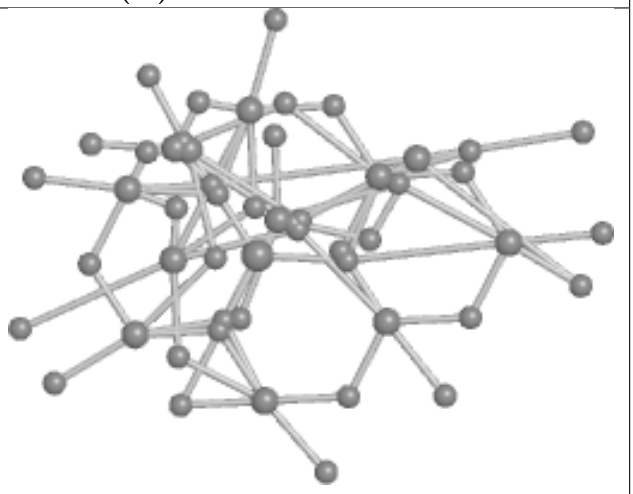


Rings

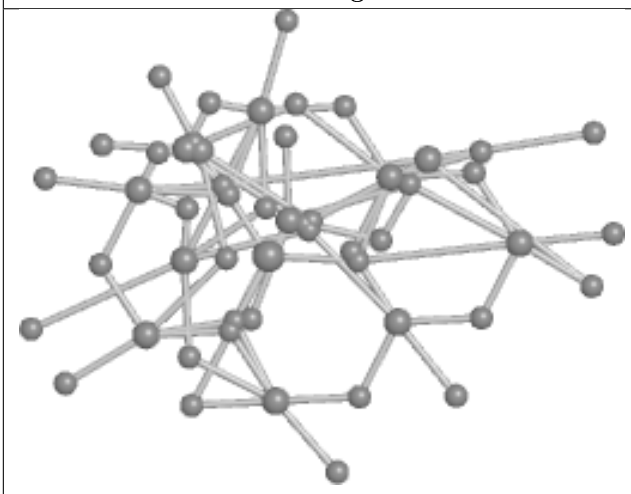
Ligand SIW C 401 (B)



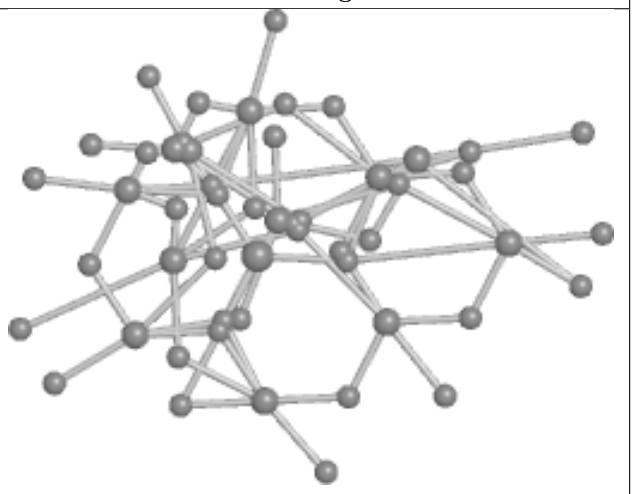
Bond lengths



Bond angles

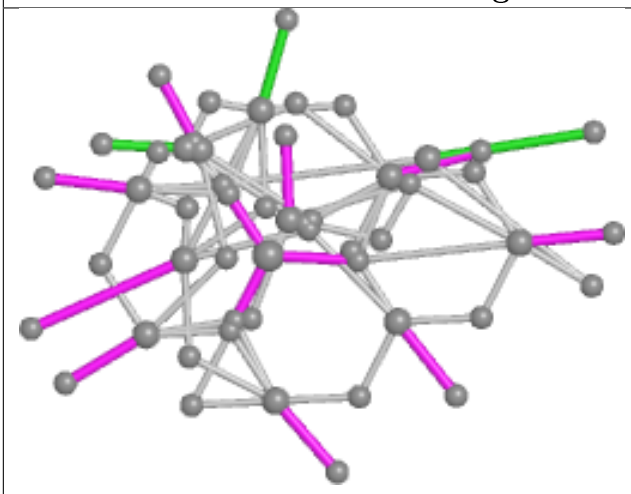


Torsions

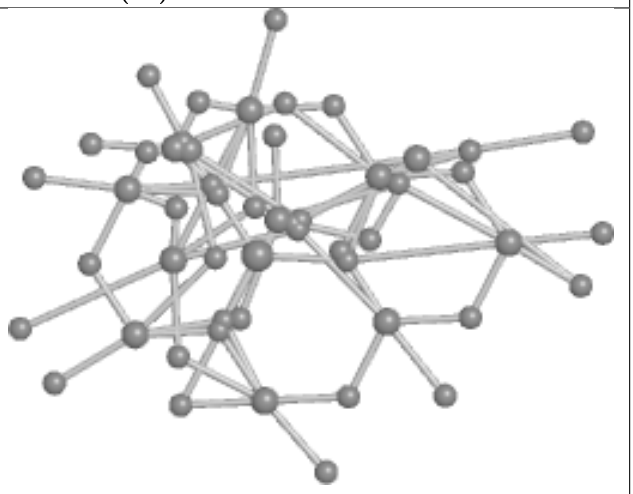


Rings

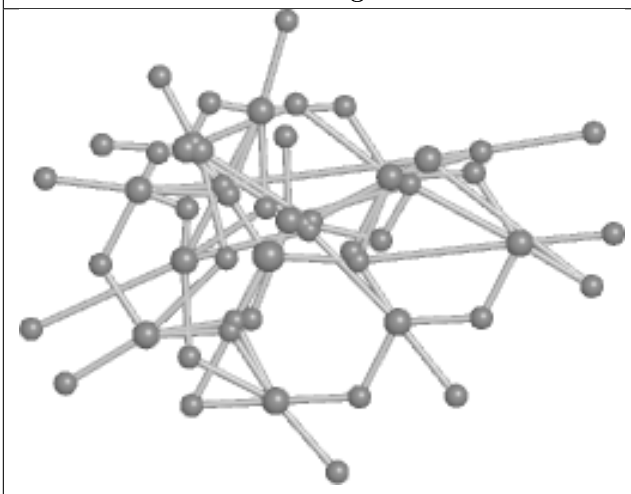
Ligand SIW A 402 (A)



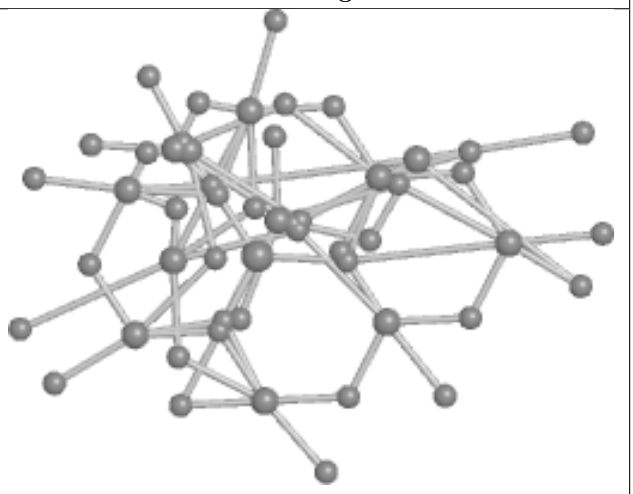
Bond lengths



Bond angles

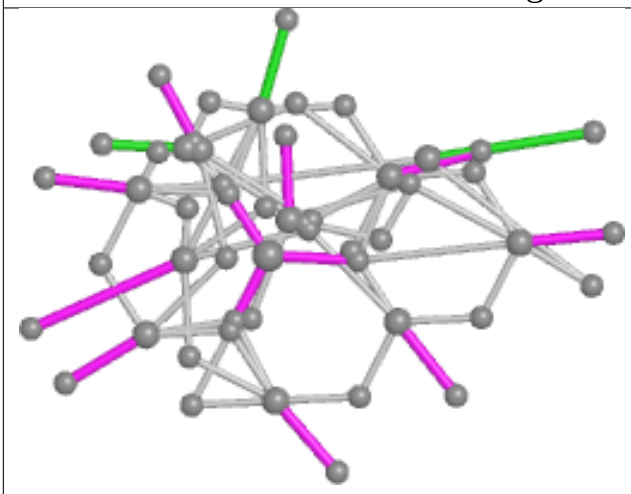


Torsions

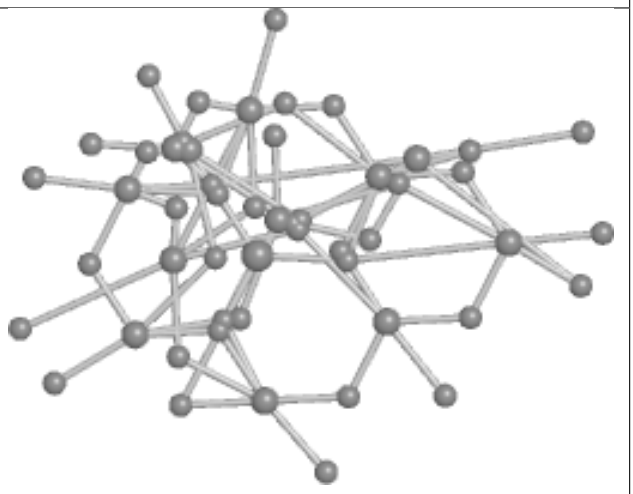


Rings

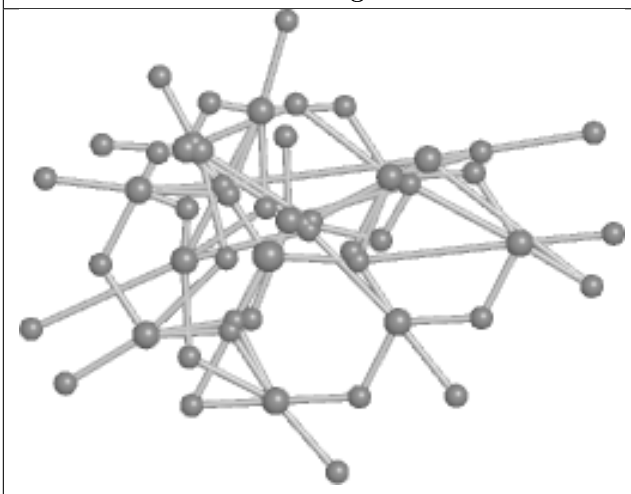
Ligand SIW B 403



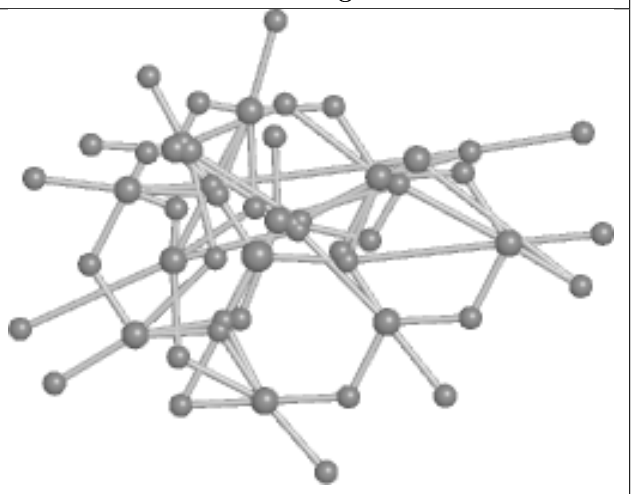
Bond lengths



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	318/324 (98%)	0.41	37 (11%) 4 6	26, 35, 54, 61	22 (6%)
1	B	318/324 (98%)	0.21	18 (5%) 23 30	26, 35, 55, 69	16 (5%)
1	C	313/324 (96%)	0.65	45 (14%) 2 3	26, 35, 55, 61	23 (7%)
All	All	949/972 (97%)	0.42	100 (10%) 6 8	26, 35, 55, 69	61 (6%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	7.6
1	B	261	ASP	7.3
1	C	280	THR	6.9
1	B	182	ASN	6.9
1	C	80	THR	6.1
1	C	200	THR	5.7
1	C	158	ILE	5.7
1	C	261	ASP	5.4
1	A	238	ILE	5.3
1	A	182	ASN	4.8
1	B	183	ILE	4.8
1	B	221	ASP	4.6
1	C	277	ASP	4.6
1	C	263	ILE	4.6
1	C	180	ASN	4.5
1	C	233	VAL	4.3
1	A	185	VAL	4.3
1	B	262	ASN	4.2
1	C	278	ILE	4.1
1	B	181	ASP	4.0
1	A	181	ASP	3.9
1	A	120	THR	3.8
1	C	282	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	262	ASN	3.8
1	B	222	ASN	3.7
1	C	141	ASP	3.7
1	A	79	LYS	3.7
1	C	198	ILE	3.5
1	C	313	VAL	3.5
1	A	197	ASP	3.4
1	B	318	ILE	3.4
1	A	222	ASN	3.3
1	B	263	ILE	3.2
1	A	285	ARG	3.2
1	C	61	ASP	3.2
1	A	319	LYS	3.2
1	B	302	ASN	3.1
1	C	238	ILE	3.1
1	C	197	ASP	3.0
1	B	223	ILE	3.0
1	C	83	SER	2.9
1	C	302	ASN	2.9
1	A	122	GLN	2.9
1	C	183	ILE	2.9
1	A	126	THR	2.8
1	C	41	GLY	2.8
1	C	193	VAL	2.8
1	C	30	ASP	2.7
1	C	157	ASP	2.7
1	C	38	ILE	2.7
1	C	118	ILE	2.6
1	A	142	ASN	2.6
1	A	237	ASP	2.6
1	C	181	ASP	2.6
1	A	23	ILE	2.6
1	B	23	ILE	2.6
1	A	193	VAL	2.5
1	A	123	SER	2.5
1	A	78	ILE	2.5
1	A	263	ILE	2.5
1	A	240	THR	2.4
1	C	204	LEU	2.4
1	B	103	ILE	2.4
1	A	124	LEU	2.4
1	A	153	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	62	ASN	2.4
1	C	116	TRP	2.3
1	C	103	ILE	2.3
1	A	159	LYS	2.3
1	A	125	ARG	2.3
1	A	61	ASP	2.3
1	C	247	LEU	2.3
1	A	205	ARG	2.2
1	A	119	LYS	2.2
1	A	43	SER	2.2
1	B	141	ASP	2.2
1	A	195	VAL	2.2
1	B	20	ASN	2.2
1	C	85	ARG	2.2
1	C	260	ASN	2.2
1	B	237	ASP	2.2
1	A	62	ASN	2.2
1	B	180	ASN	2.2
1	A	22	ASN	2.1
1	C	315	VAL	2.1
1	A	158	ILE	2.1
1	C	40	THR	2.1
1	A	276	TRP	2.1
1	B	320	THR	2.1
1	C	185	VAL	2.1
1	C	139	PHE	2.1
1	C	279	LYS	2.1
1	A	286	THR	2.1
1	C	16	SER	2.1
1	C	88	GLN	2.1
1	A	8	GLN	2.1
1	C	271	SER	2.1
1	A	241	GLY	2.0
1	C	303	ILE	2.0
1	C	82	GLN	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)

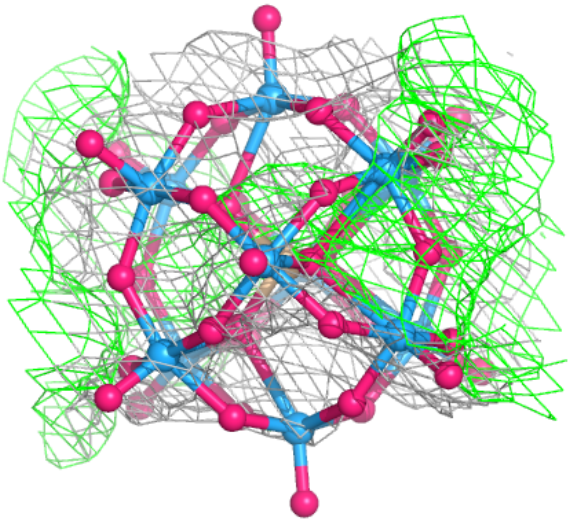
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

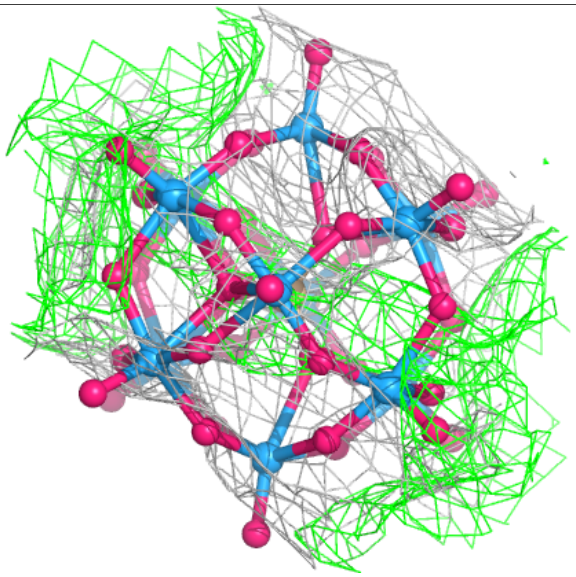
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SIW	A	406	53/53	0.70	0.27	75,75,75,75	53
2	SIW	A	404	53/53	0.74	0.23	65,65,65,65	53
2	SIW	A	407	53/53	0.74	0.30	65,65,65,65	53
2	SIW	B	403	53/53	0.81	0.22	65,65,65,65	53
2	SIW	A	405	53/53	0.82	0.25	65,65,65,65	53
2	SIW	A	403	53/53	0.83	0.23	65,65,65,65	53
2	SIW	C	404	53/53	0.87	0.24	65,65,65,65	53
2	SIW	B	402	53/53	0.95	0.19	23,36,41,51	53
2	SIW	B	401[B]	53/53	0.96	0.18	27,44,55,67	53
2	SIW	B	401[A]	53/53	0.96	0.18	34,45,53,62	53
2	SIW	A	401[B]	53/53	0.97	0.19	28,46,52,60	53
2	SIW	A	401[A]	53/53	0.97	0.19	31,46,52,55	53
2	SIW	C	401[B]	53/53	0.97	0.18	34,47,53,60	53
2	SIW	C	401[A]	53/53	0.97	0.18	35,47,55,61	53
2	SIW	C	402[B]	53/53	0.98	0.17	31,40,43,44	53
2	SIW	A	402[B]	53/53	0.98	0.17	27,36,38,39	53
2	SIW	A	402[A]	53/53	0.98	0.17	27,36,38,40	53
2	SIW	C	402[A]	53/53	0.98	0.17	35,40,43,46	53
2	SIW	C	403[B]	53/53	0.99	0.18	56,56,56,56	53
2	SIW	C	403[A]	53/53	0.99	0.18	56,56,56,56	53

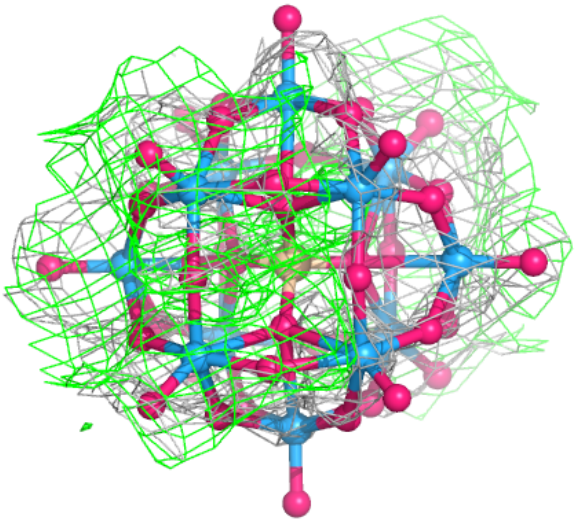
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SIW A 406:

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

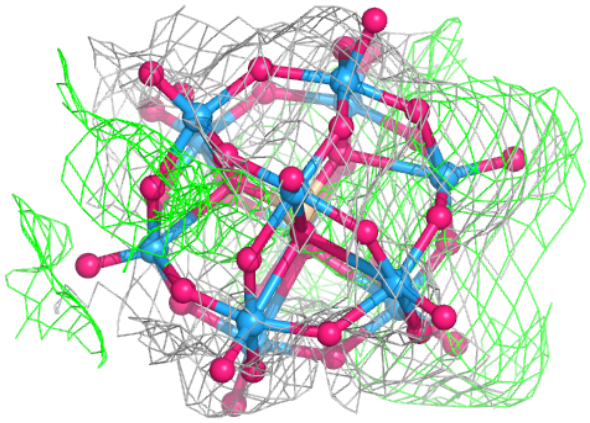


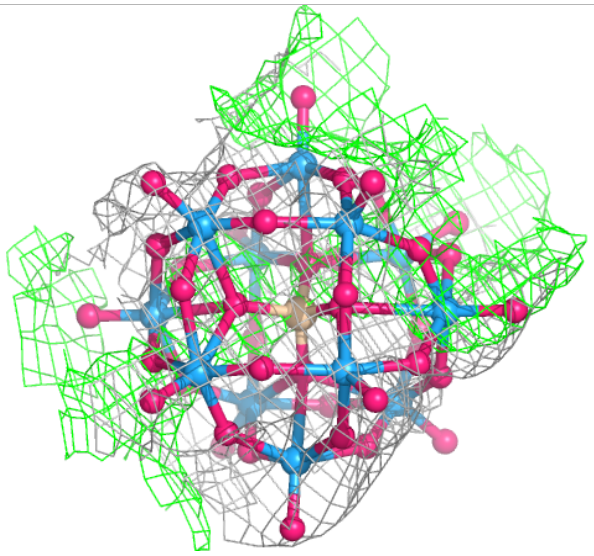


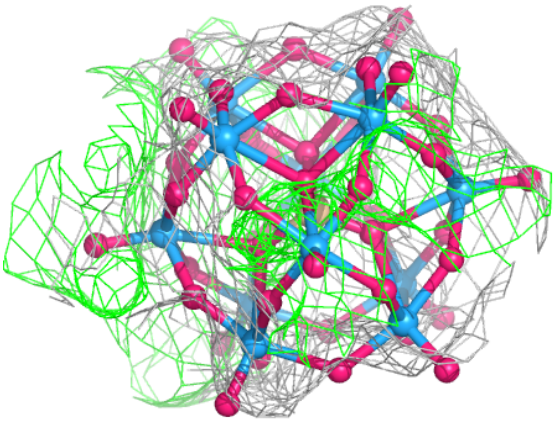


Electron density around SIW A 404:

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

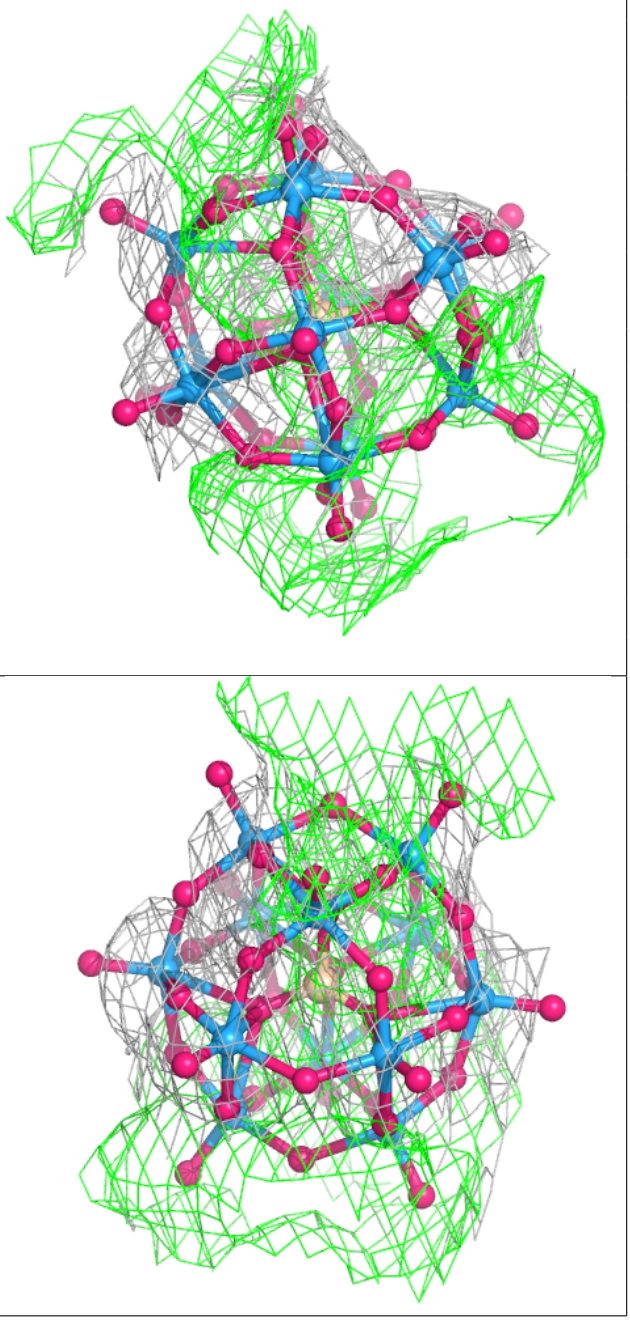






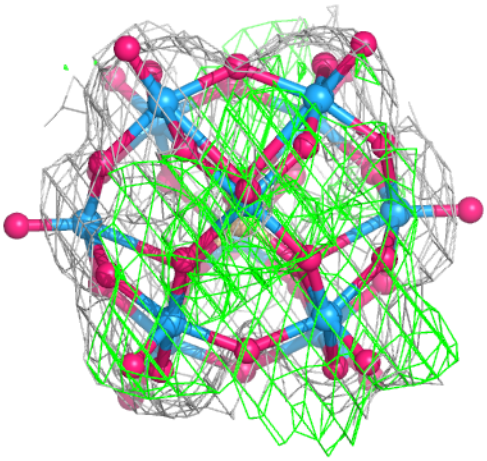
Electron density around SIW A 407:

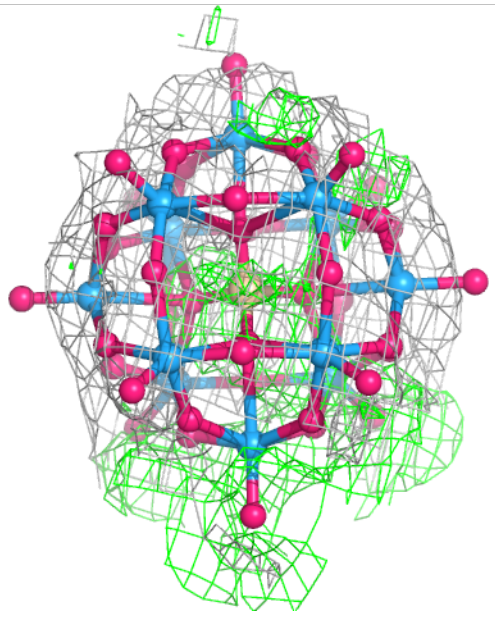
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

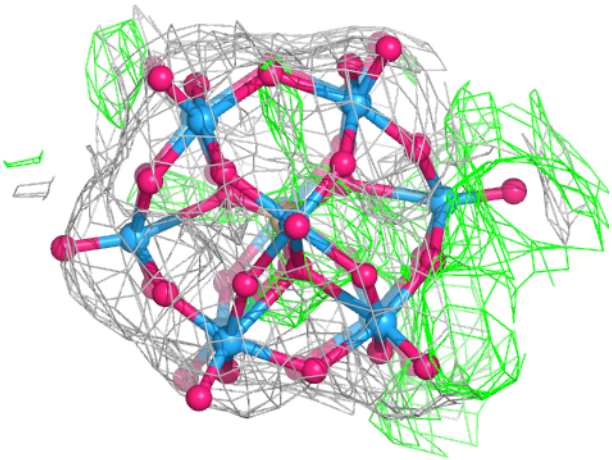


Electron density around SIW B 403:

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

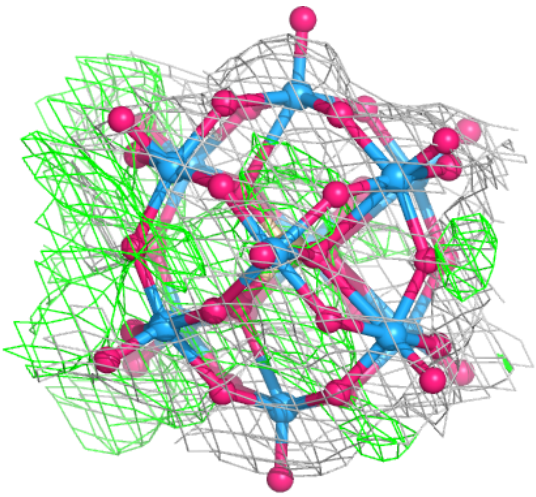


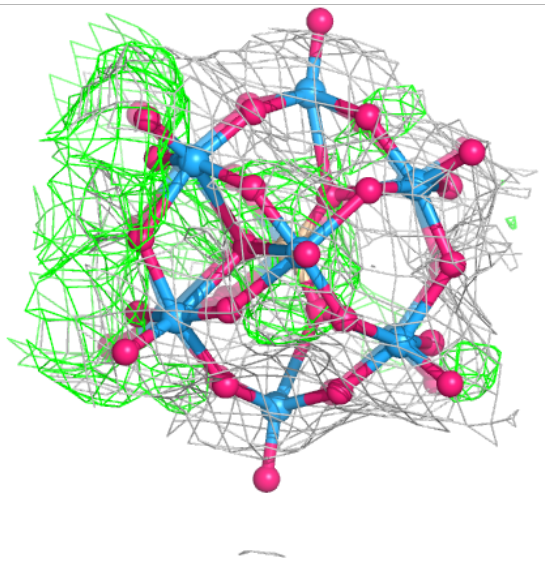


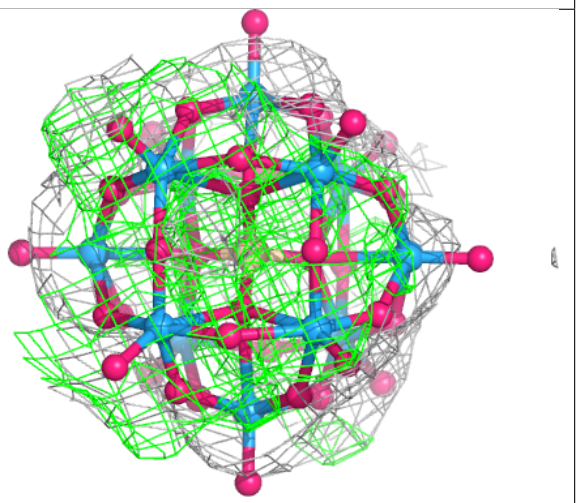


Electron density around SIW A 405:

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

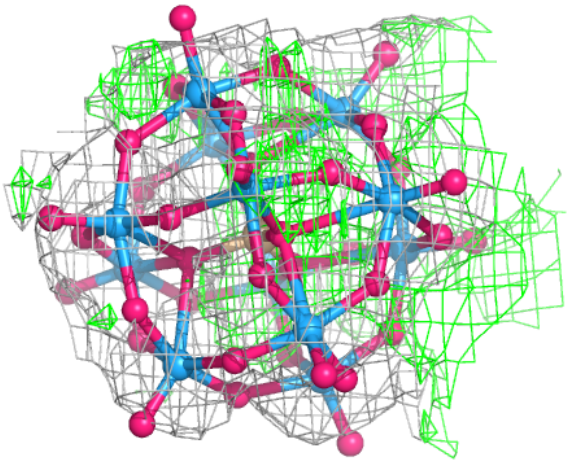


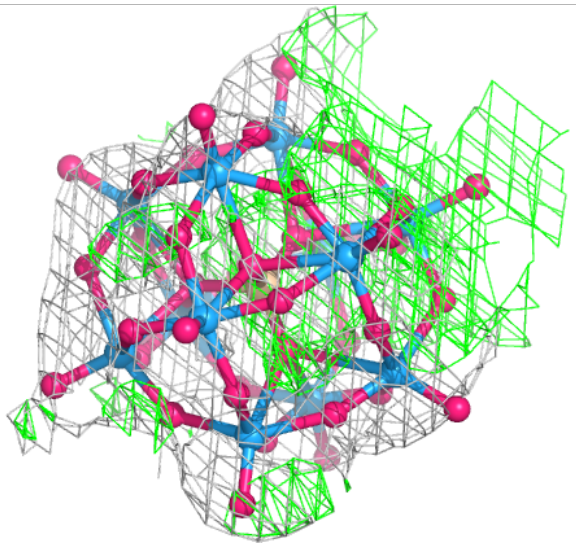


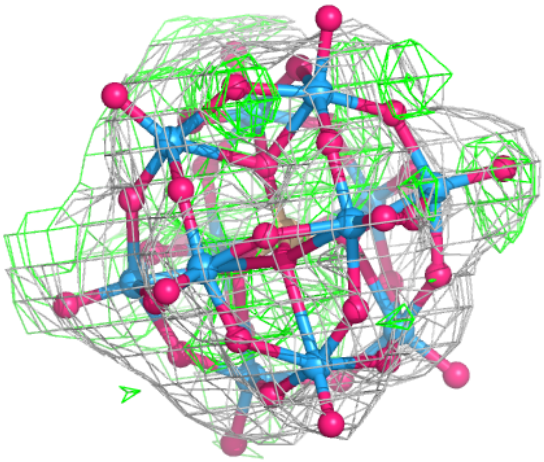


Electron density around SIW A 403:

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

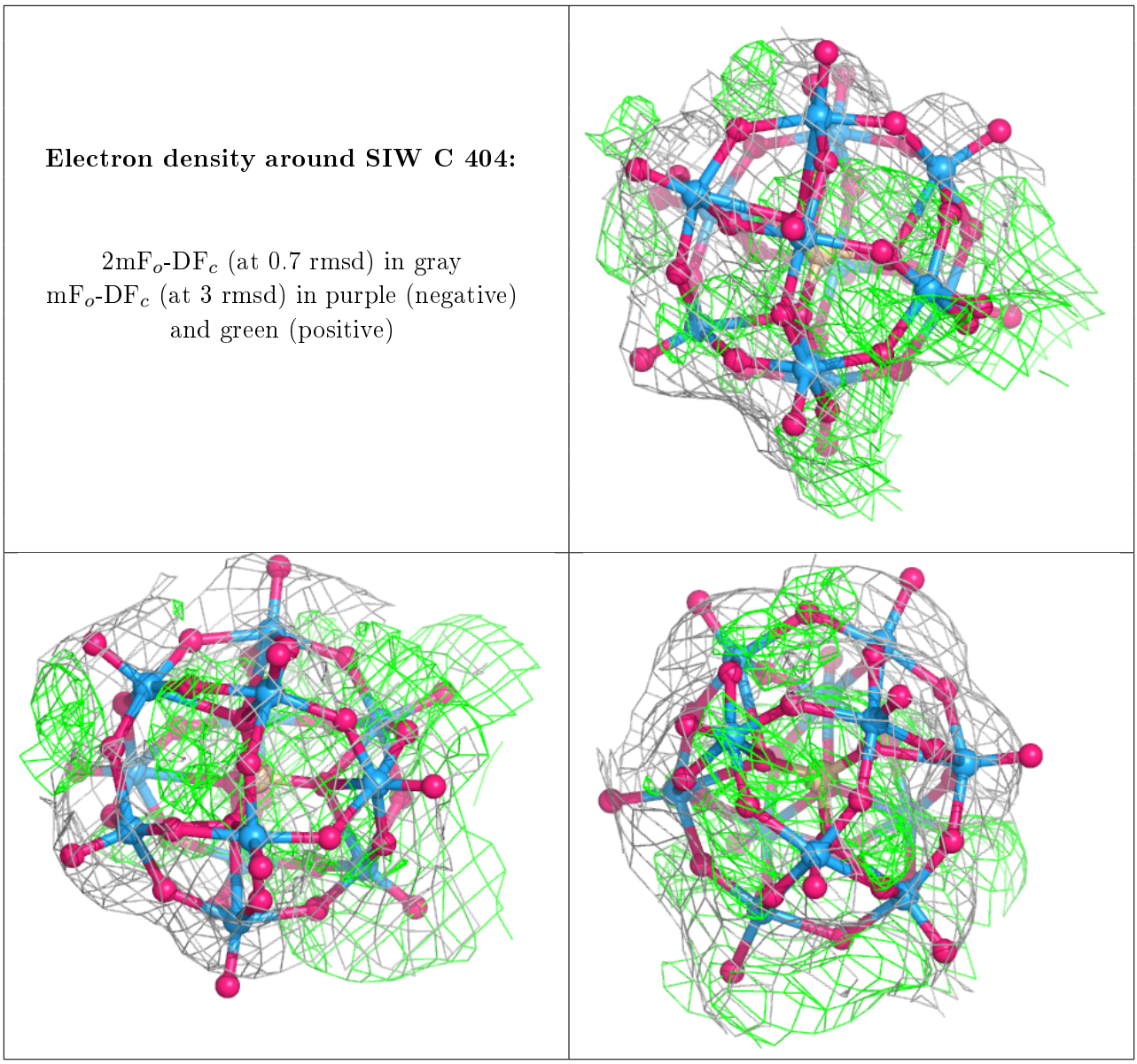






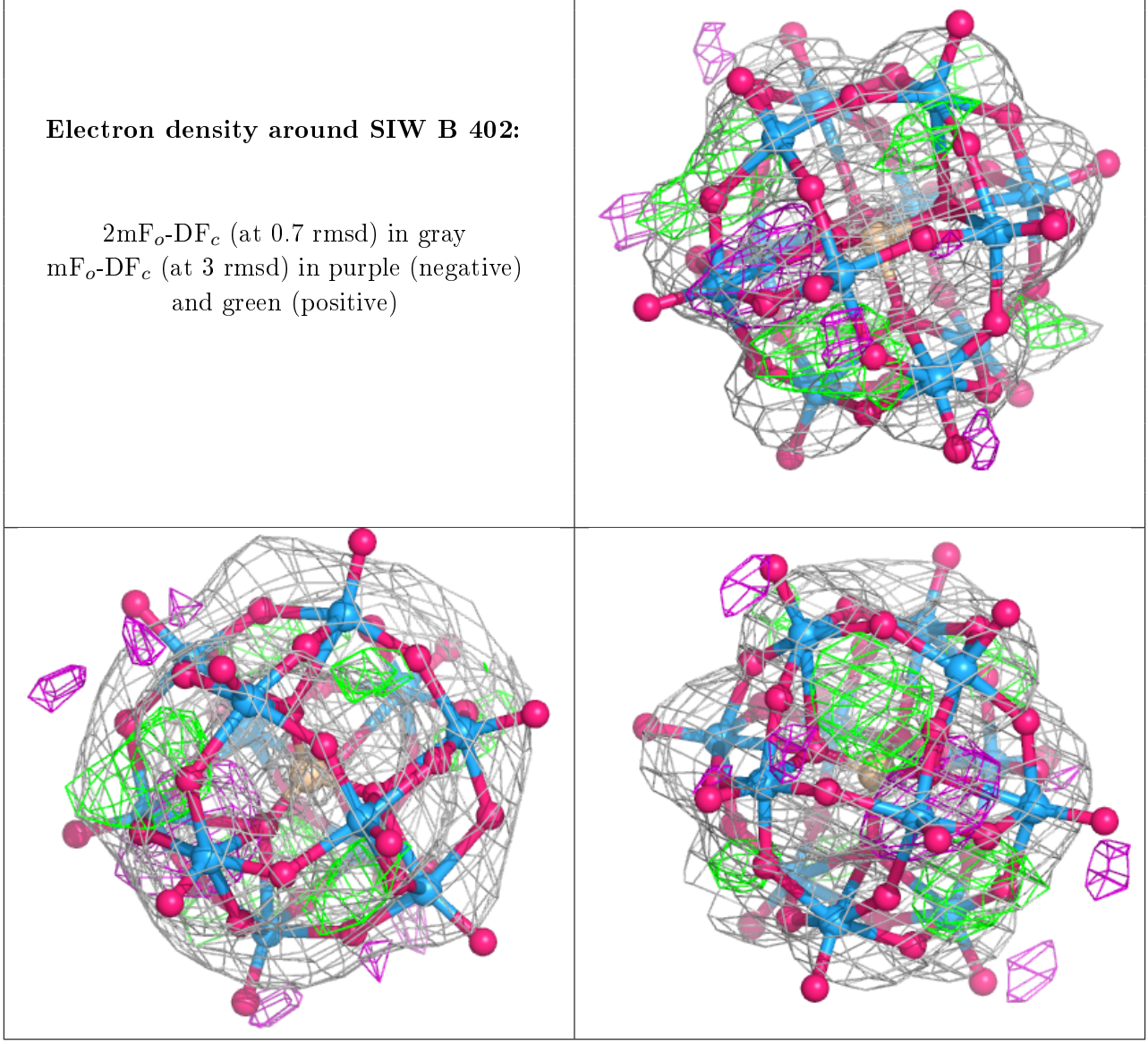
Electron density around SIW C 404:

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



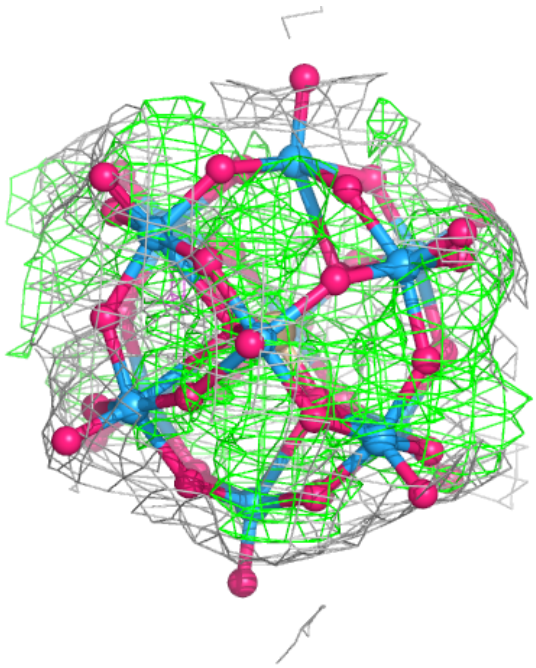
Electron density around SIW B 402:

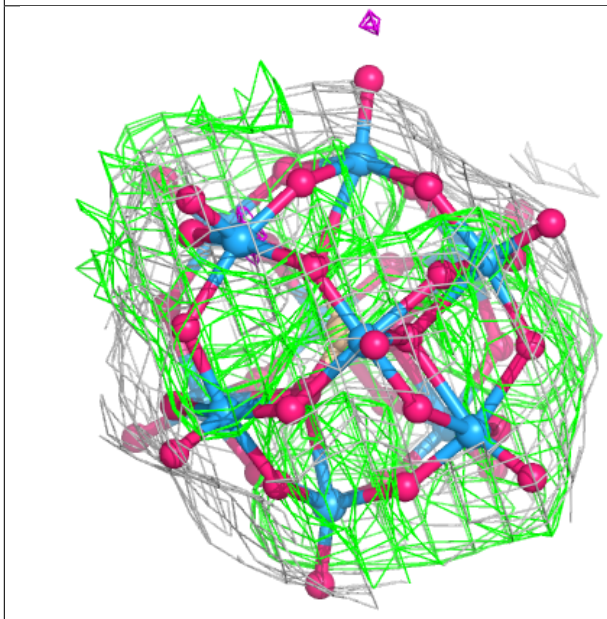
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

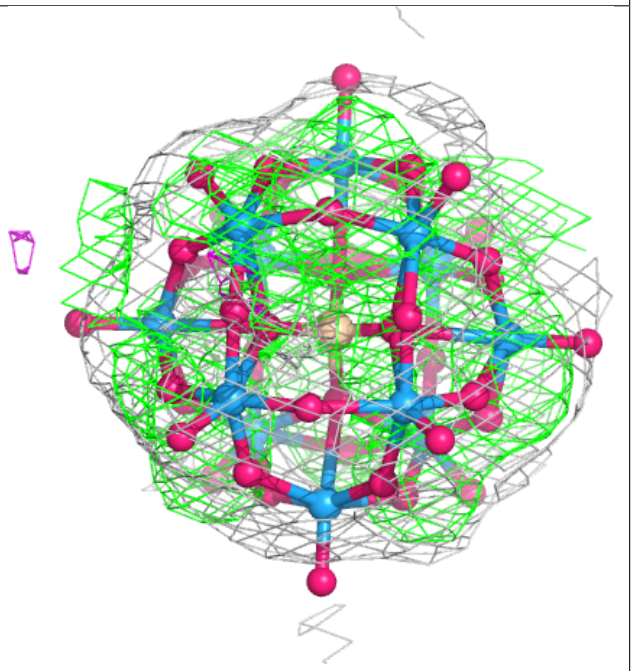


Electron density around SIW B 401 (B):

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

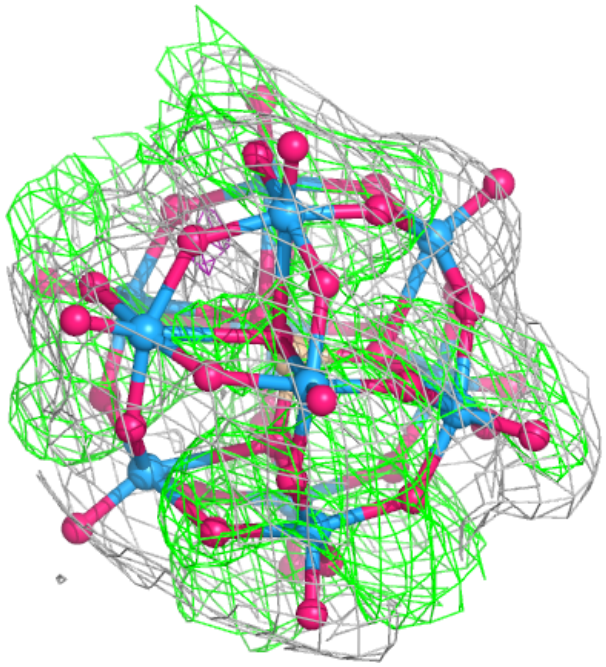


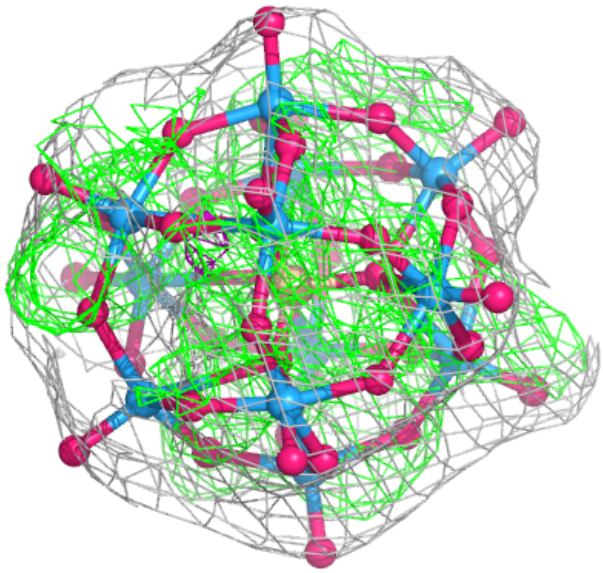


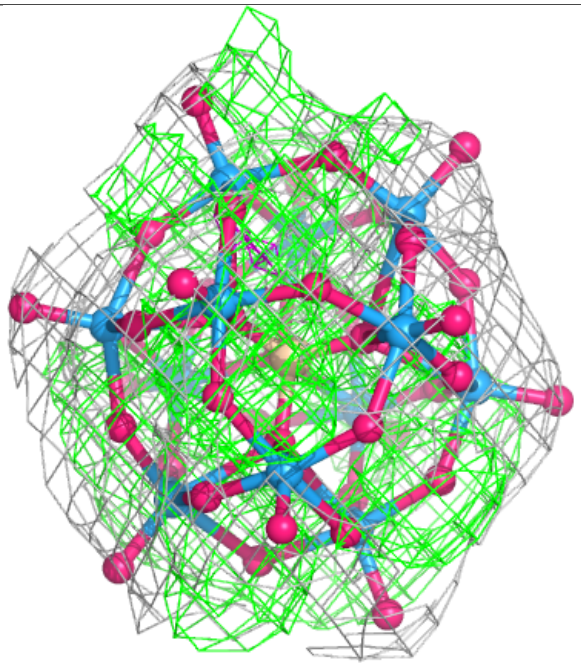


Electron density around SIW B 401 (A):

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

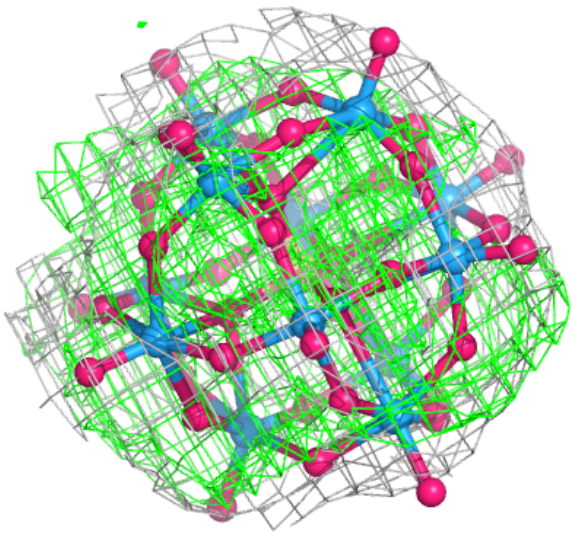


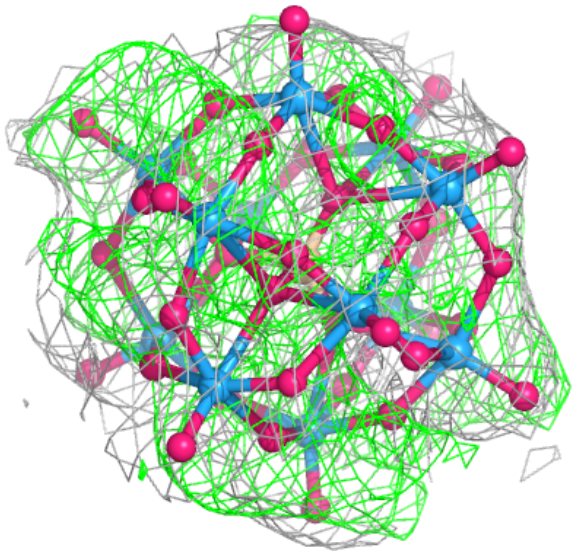


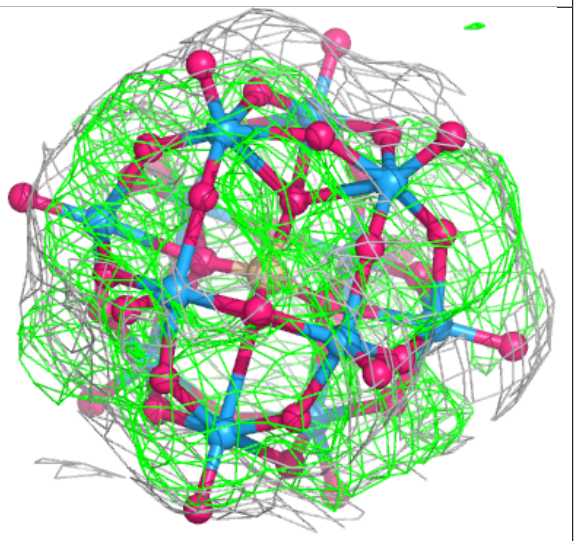


Electron density around SIW A 401 (B):

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

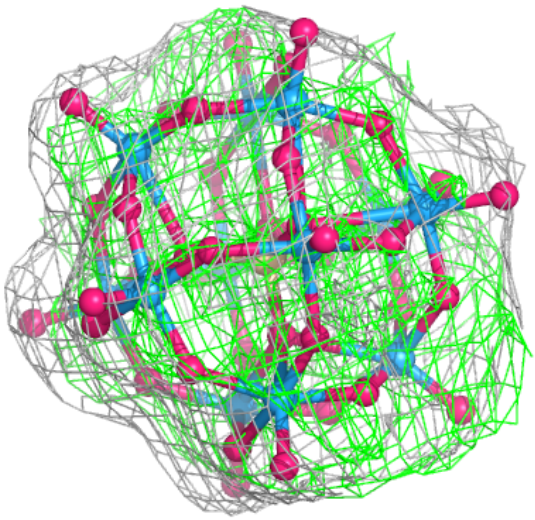


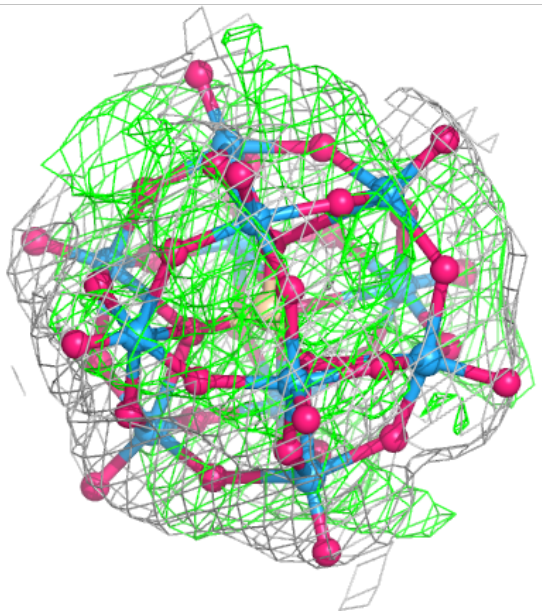


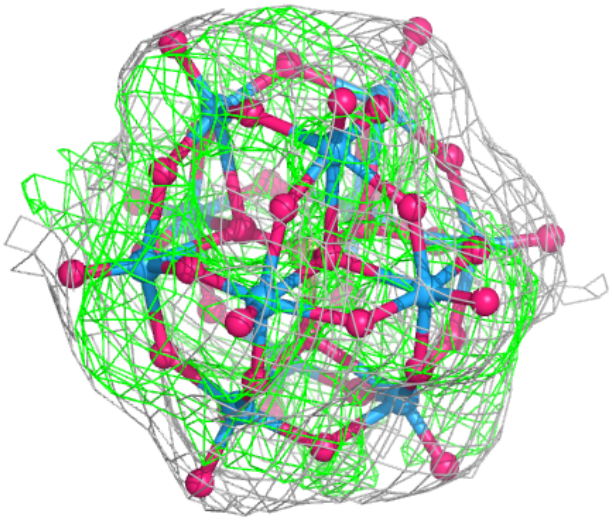


Electron density around SIW A 401 (A):

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

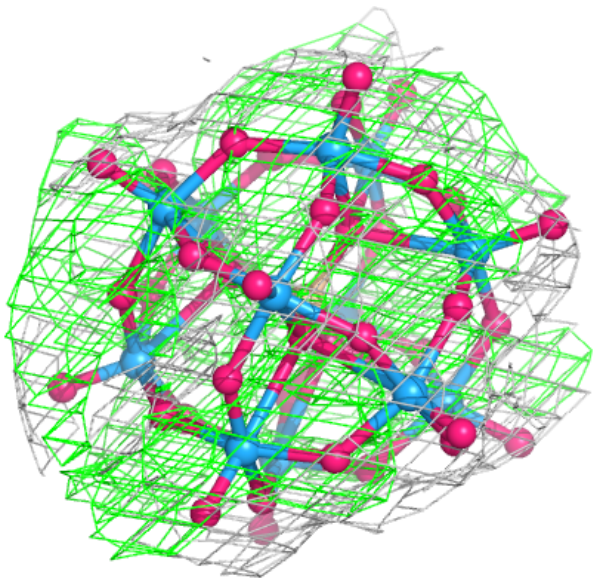


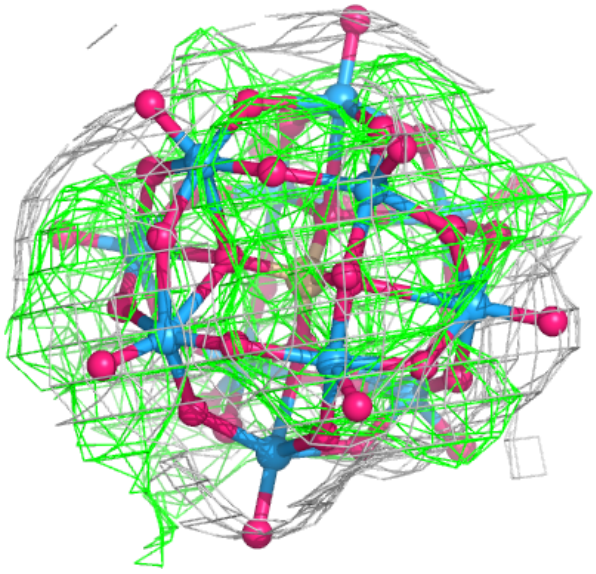


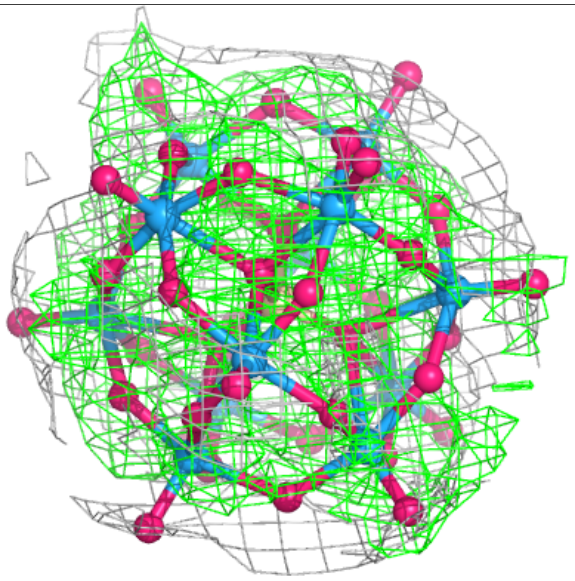


Electron density around SIW C 401 (B):

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

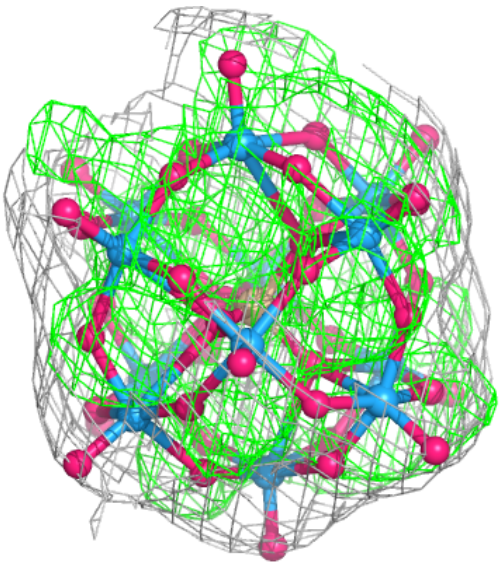


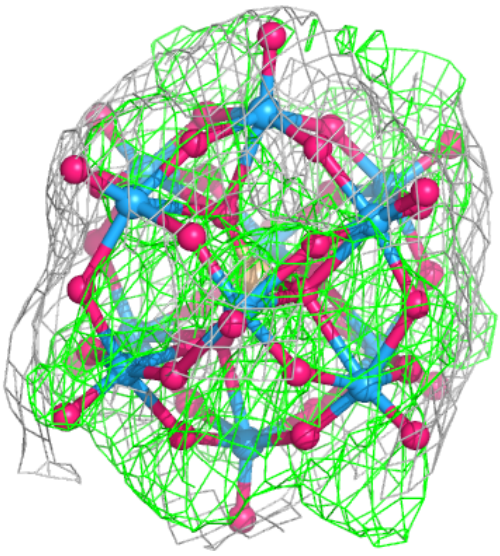


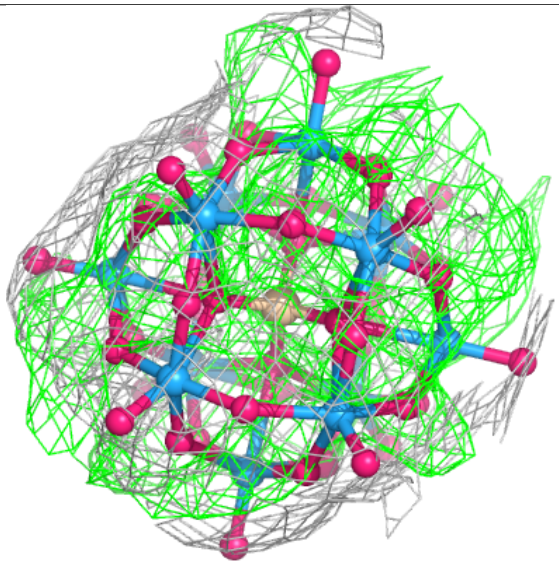


Electron density around SIW C 401 (A):

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

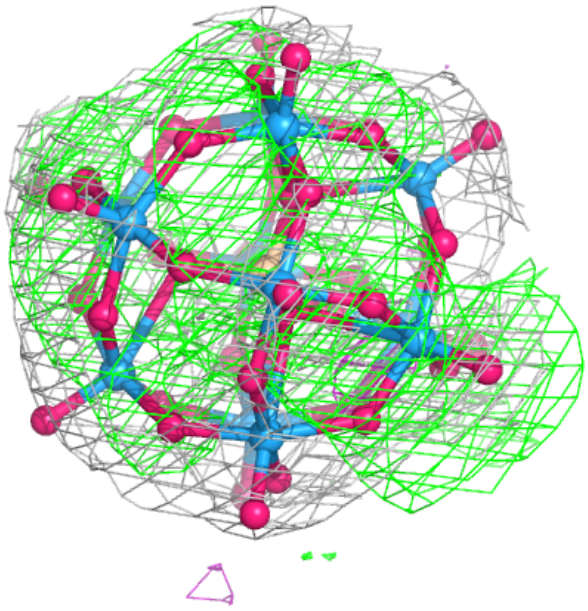


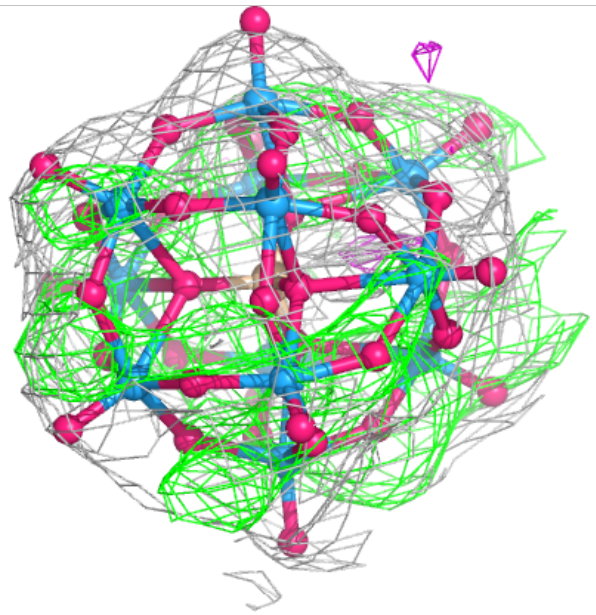


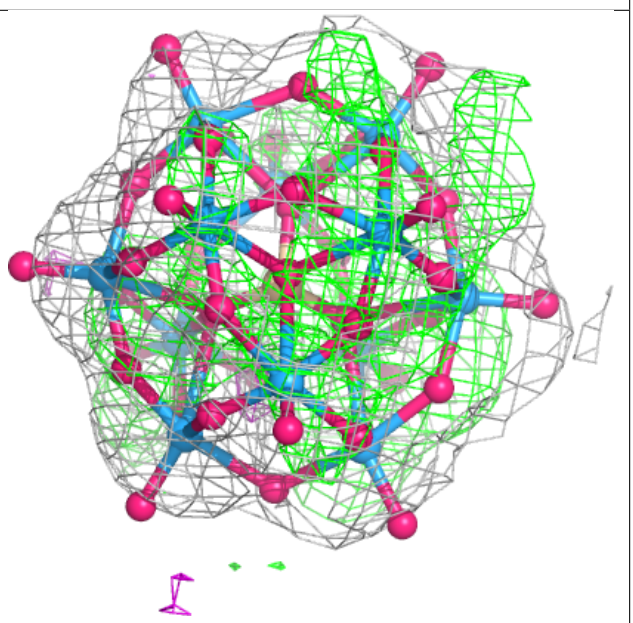


Electron density around SIW C 402 (B):

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

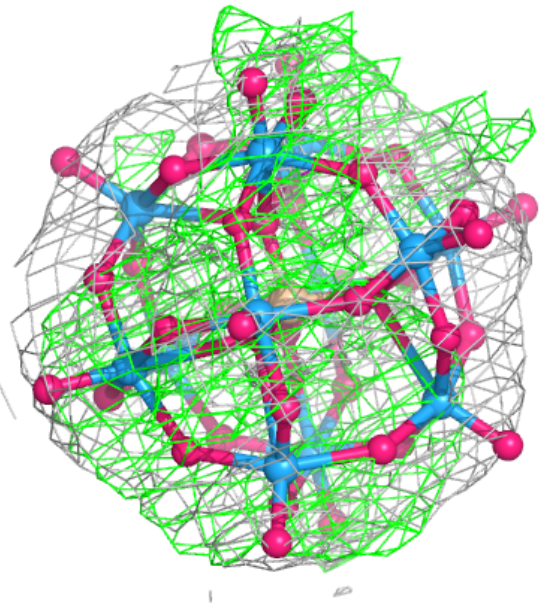


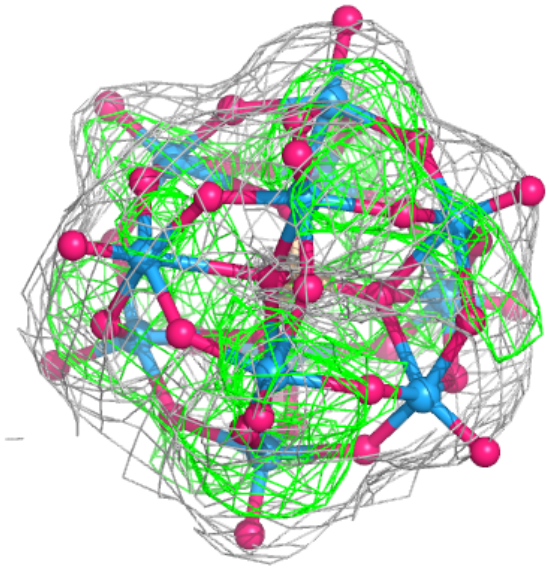


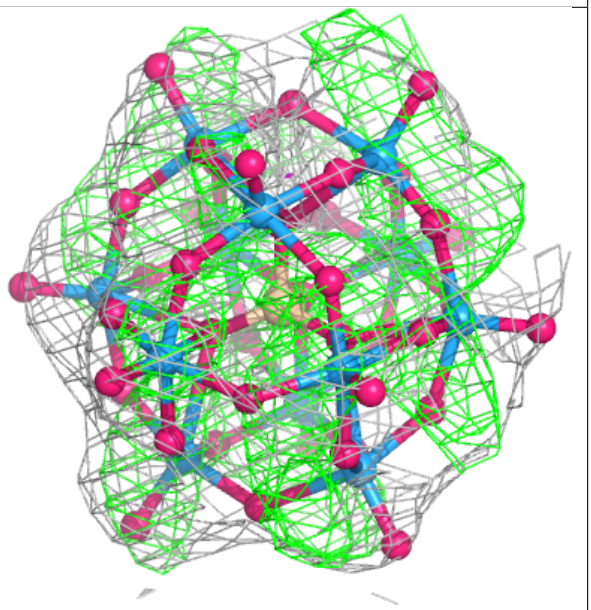


Electron density around SIW A 402 (B):

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

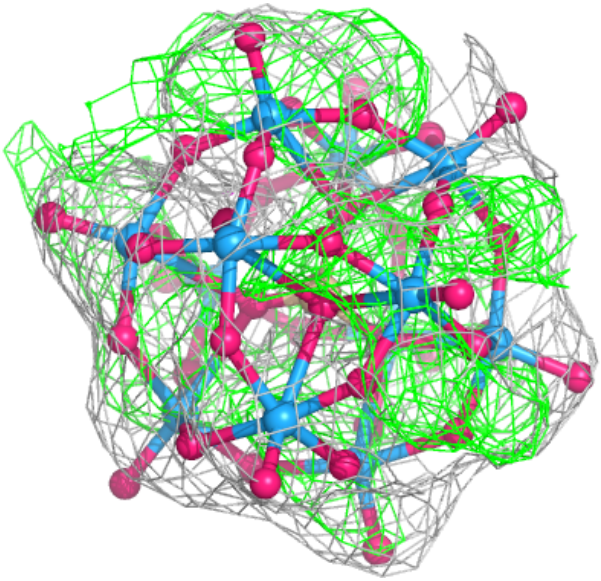


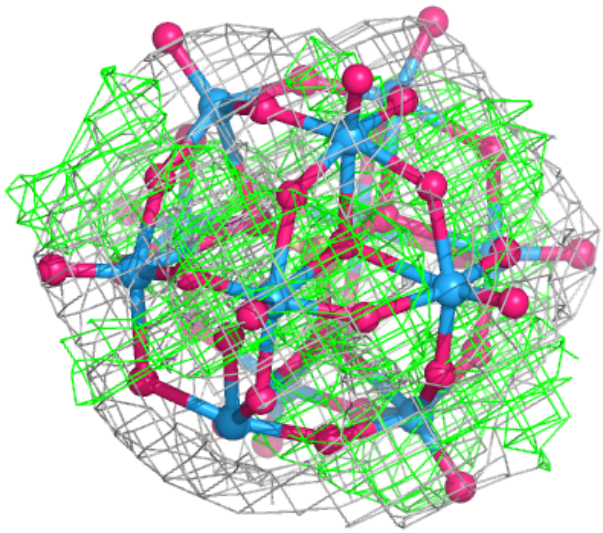


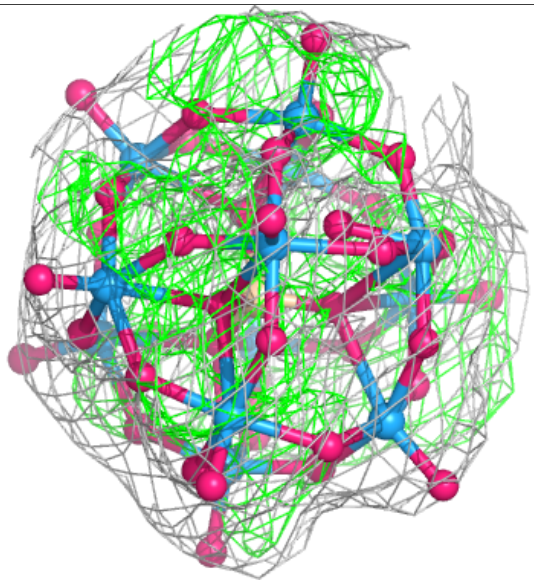


Electron density around SIW A 402 (A):

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

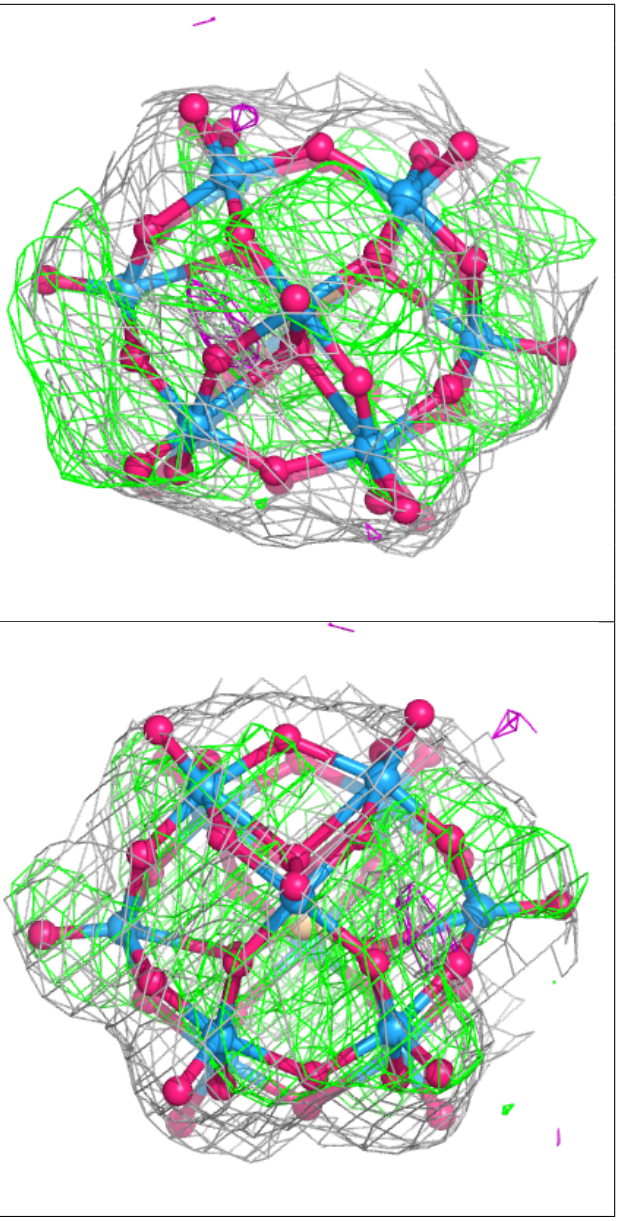






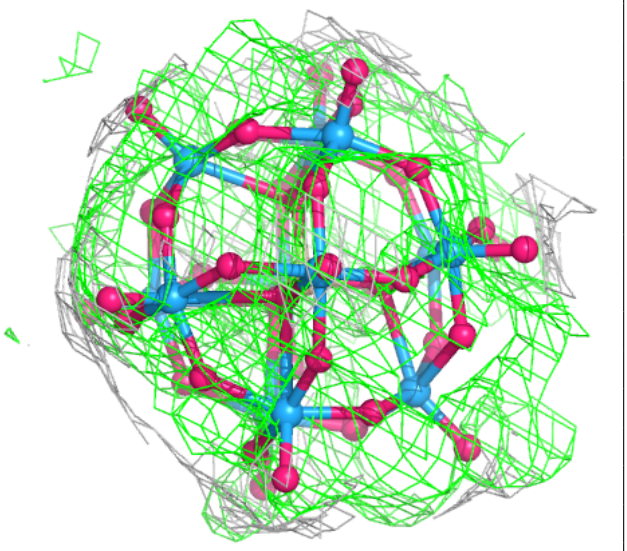
Electron density around SIW C 402 (A):

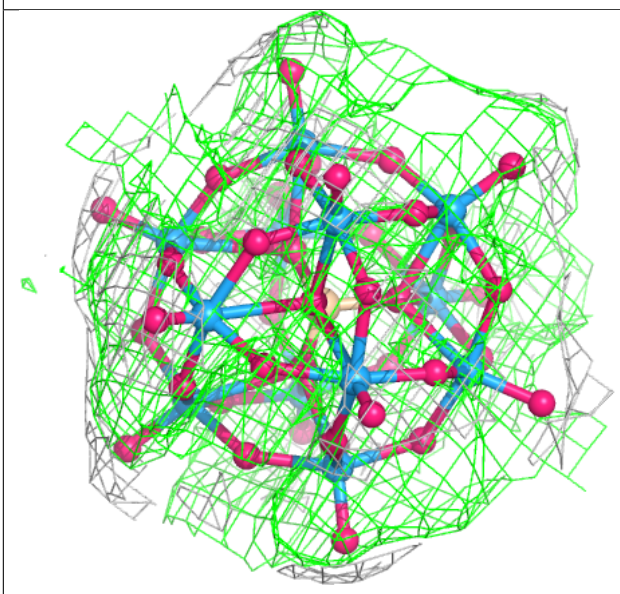
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

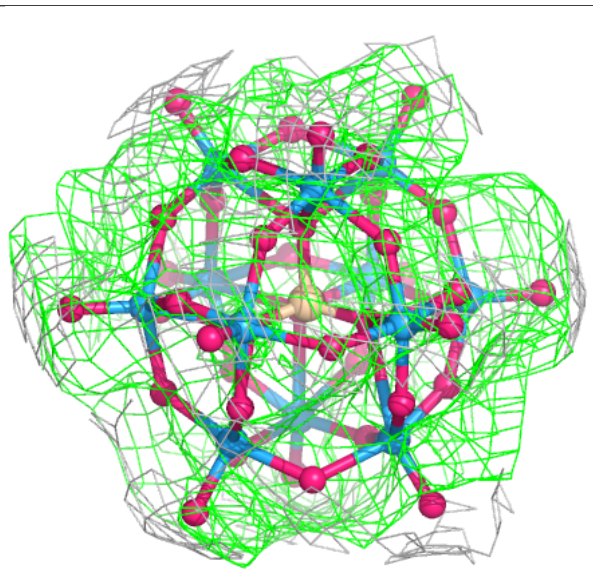


Electron density around SIW C 403 (B):

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

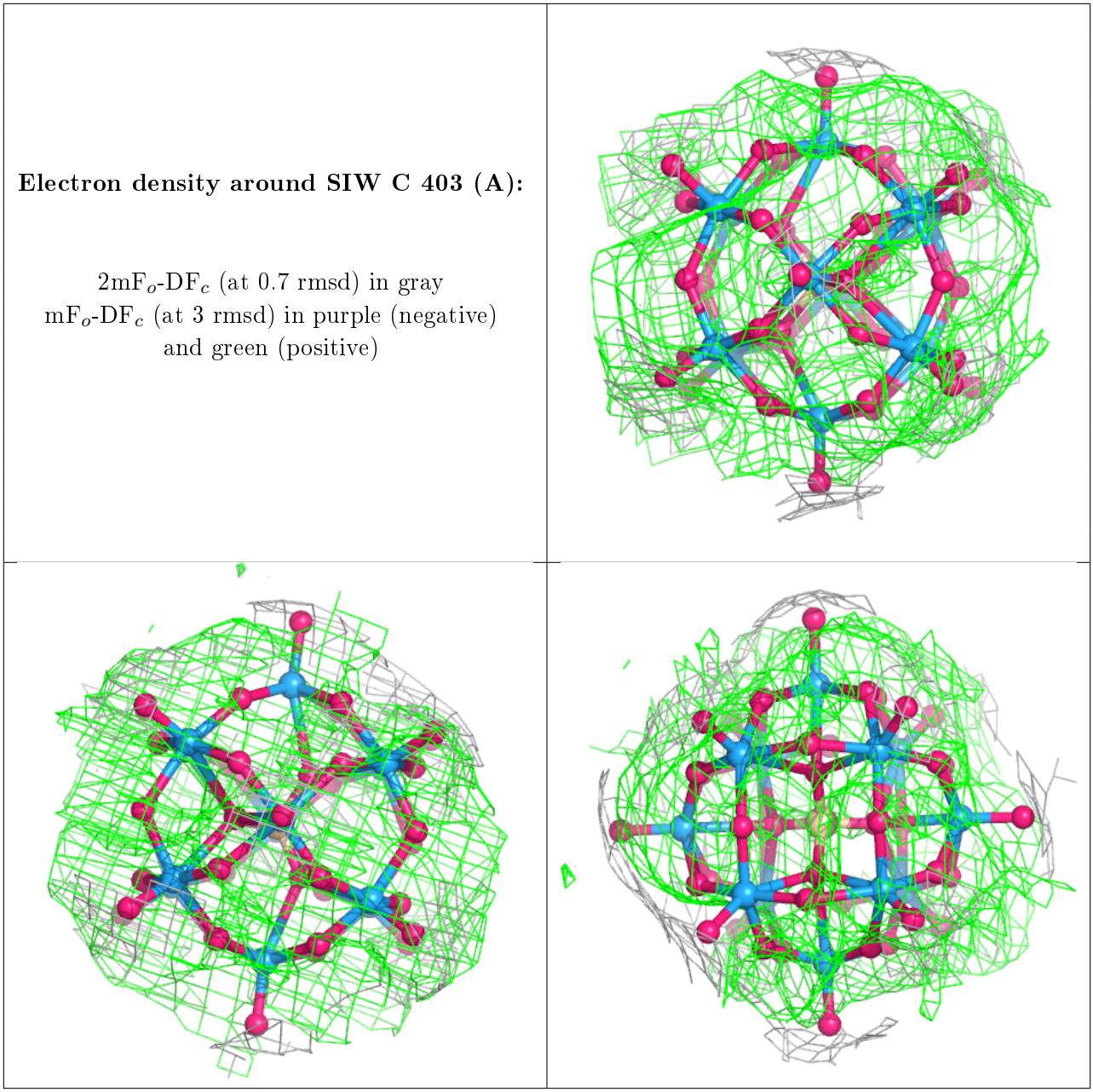






Electron density around SIW C 403 (A):

$2mF_o$-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

There are no such residues in this entry.