Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2026 – 01:36 am BST

PDB ID	:	6YU9 / pdb_00006yu9
Title	:	CO-dehydrogenase homodimer from Clostridium autoethanogenum at 1.90-A resolution
Authors	:	Wagner, T.; Lemaire, O.N.
Deposited on	:	2020-04-26
Resolution	:	1.90 Å(reported)

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

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

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

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

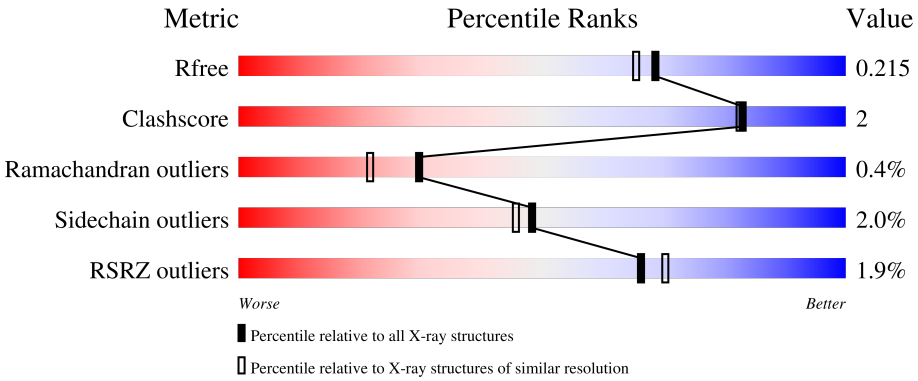
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	631	91% 8%
1	B	631	94% 5%
1	C	631	5% 90% 9%
1	D	631	94% 5%

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
4	XCC	B	703	-	-	X	-
4	XCC	D	703	-	-	X	-

2 Entry composition

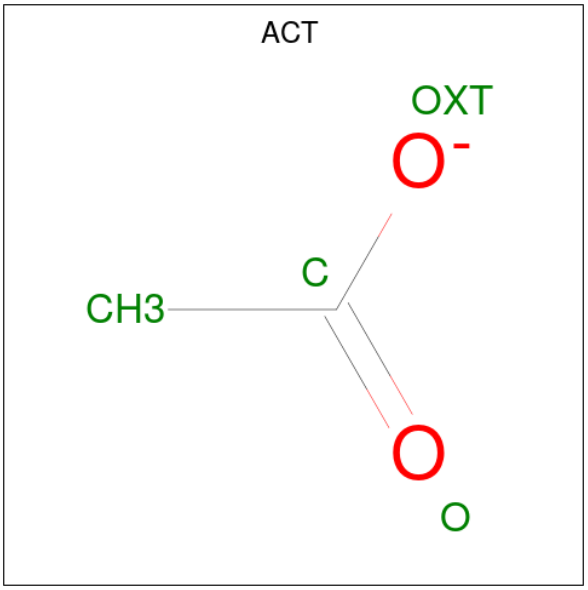
There are 7 unique types of molecules in this entry. The entry contains 20109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	2	0
			4743	2978	818	907	40			
1	B	628	Total	C	N	O	S	0	2	0
			4725	2969	816	900	40			
1	C	626	Total	C	N	O	S	0	1	0
			4700	2953	810	897	40			
1	D	628	Total	C	N	O	S	0	2	0
			4721	2966	815	900	40			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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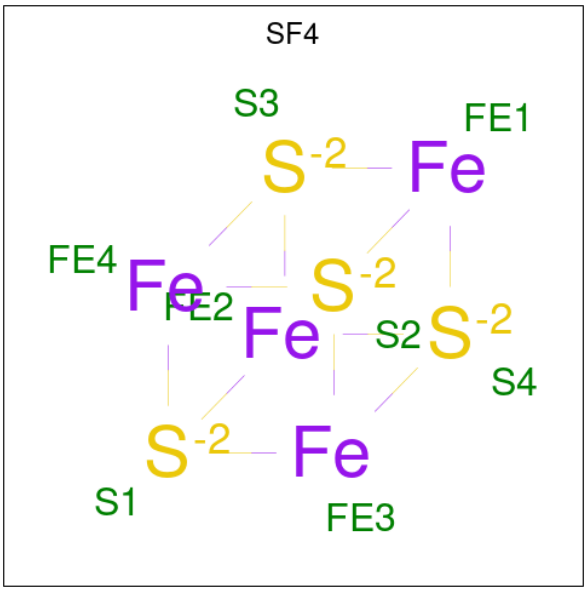
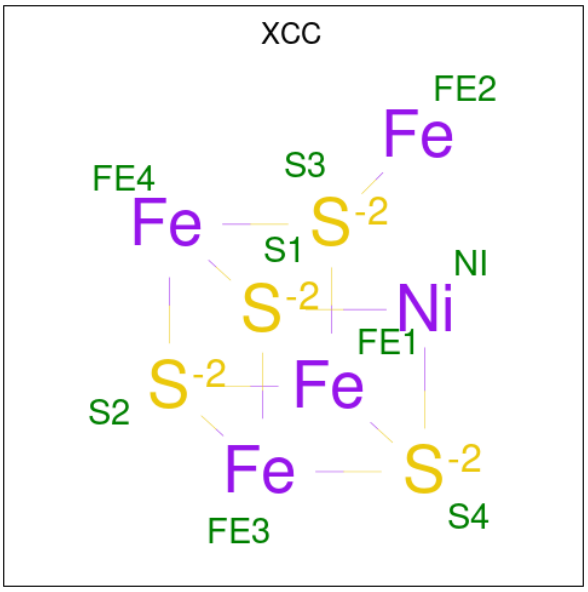
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



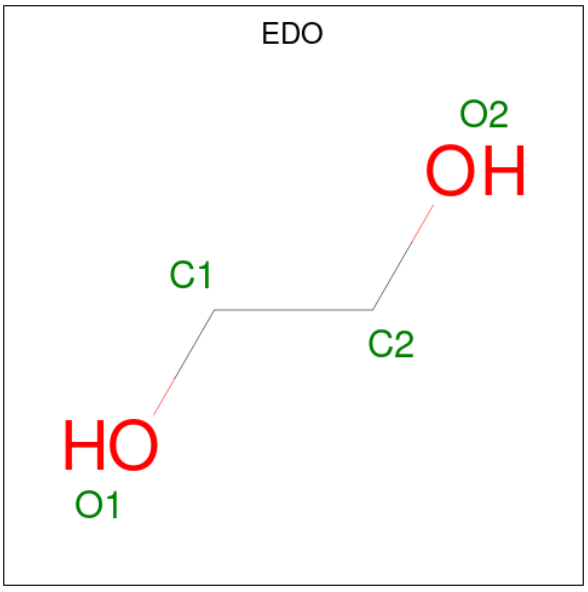
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

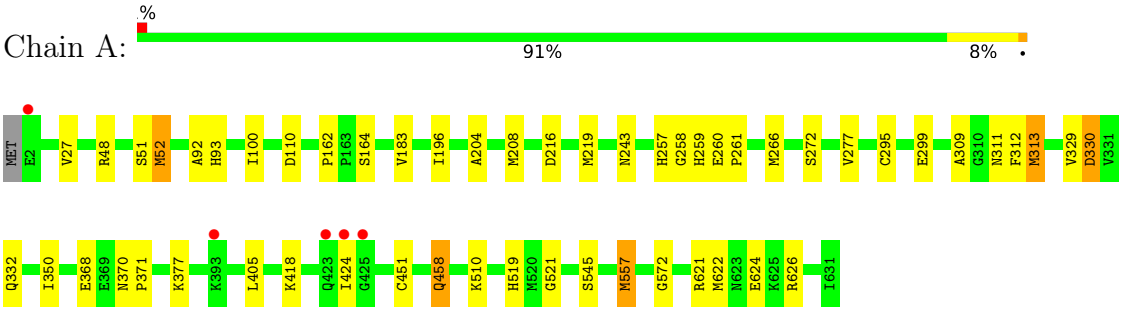
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	327	Total O 327 327	0	0
7	B	291	Total O 291 291	0	1
7	C	185	Total O 185 185	0	0
7	D	304	Total O 304 304	0	0

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.

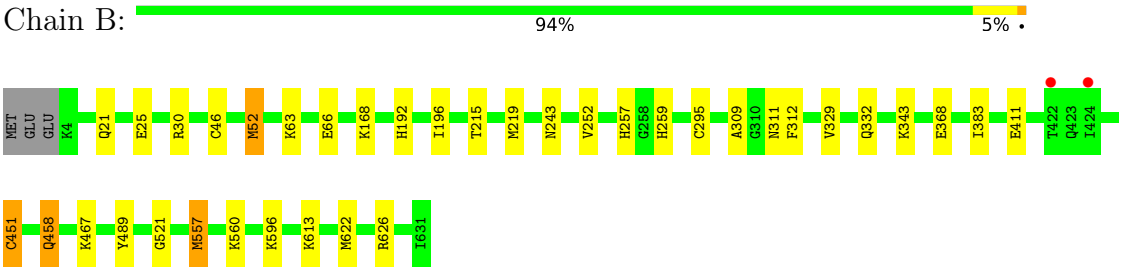
• Molecule 1: Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor)

Chain A:



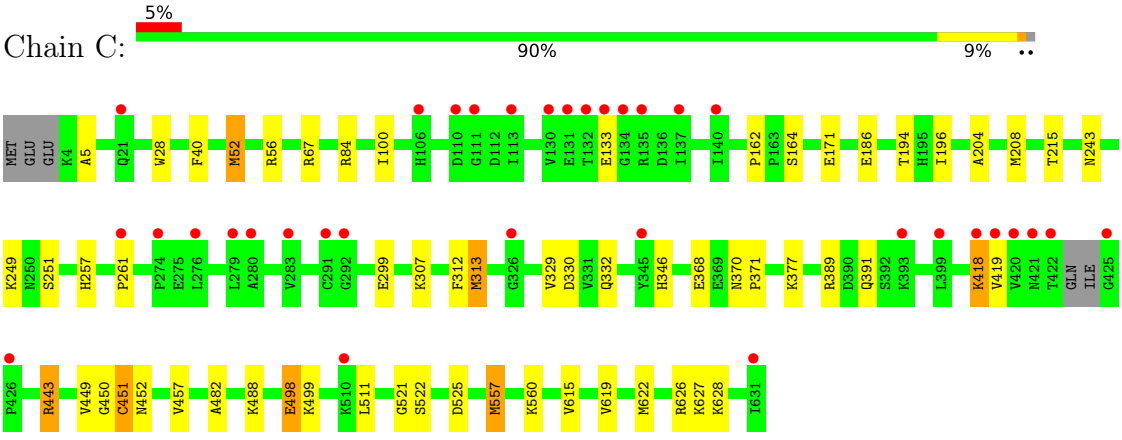
• Molecule 1: Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor)

Chain B:



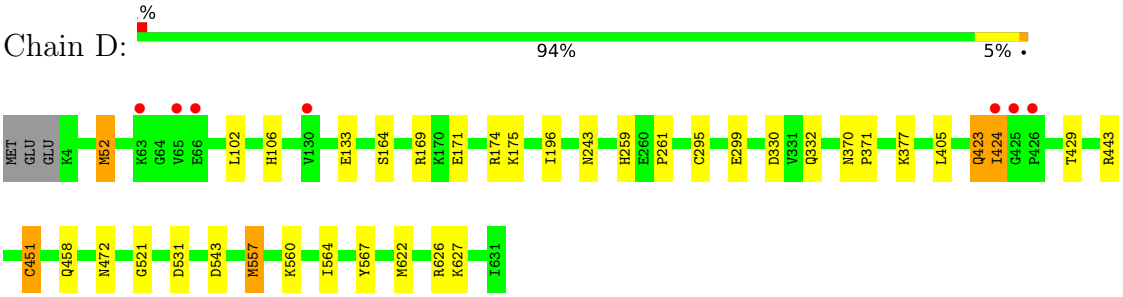
• Molecule 1: Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor)

Chain C:



• Molecule 1: Carbon-monoxide dehydrogenase (Acceptor),Carbon-monoxide dehydrogenase (Acceptor)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.53Å 109.45Å 129.28Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	49.75 – 1.90 49.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	48.0 (49.75-1.90) 48.0 (49.75-1.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.87Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.158 , 0.203 0.169 , 0.215	Depositor DCC
R_{free} test set	5295 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20109	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XCC, EDO, CL, ACT, SF4

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	0.95	2/4823 (0.0%)	1.06	6/6522 (0.1%)
1	B	0.96	1/4805 (0.0%)	1.02	3/6498 (0.0%)
1	C	0.92	3/4776 (0.1%)	1.04	7/6458 (0.1%)
1	D	0.95	1/4802 (0.0%)	1.04	3/6495 (0.0%)
All	All	0.94	7/19206 (0.0%)	1.04	19/25973 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	ASP	CA-C	5.97	1.55	1.52
1	B	309	ALA	CA-C	5.72	1.60	1.52
1	A	557	MET	SD-CE	-5.38	1.66	1.79
1	C	313	MET	SD-CE	-5.37	1.66	1.79
1	C	615	VAL	CA-C	5.18	1.59	1.52
1	D	531	ASP	CA-C	5.18	1.59	1.52
1	A	309	ALA	CA-C	5.01	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	521	GLY	N-CA-C	6.98	118.61	111.56
1	A	521	GLY	N-CA-C	6.83	118.46	111.56
1	B	521	GLY	N-CA-C	6.76	118.39	111.56
1	C	521	GLY	N-CA-C	6.29	117.91	111.56
1	D	52	MET	N-CA-C	-6.29	104.31	112.23
1	A	52	MET	N-CA-C	-6.06	104.79	111.82
1	D	330	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	52	MET	N-CA-C	-5.48	105.46	111.82
1	B	311	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	350	ILE	N-CA-C	5.37	115.59	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	ASN	CA-CB-CG	5.32	117.92	112.60
1	C	449	VAL	N-CA-CB	-5.24	106.58	112.45
1	C	162	PRO	N-CA-C	5.15	116.09	110.58
1	C	450	GLY	N-CA-C	5.12	119.33	112.17
1	A	162	PRO	N-CA-C	5.10	116.03	110.58
1	B	52	MET	N-CA-C	-5.06	105.95	111.82
1	A	330	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	482	ALA	CA-C-N	5.01	127.00	120.28
1	C	482	ALA	C-N-CA	5.01	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

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	4743	0	4819	33	0
1	B	4725	0	4815	21	0
1	C	4700	0	4782	30	0
1	D	4721	0	4800	20	0
2	A	16	0	12	0	0
2	D	4	0	3	0	0
3	A	8	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	2	0
4	C	9	0	0	1	0
4	D	9	0	0	3	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	C	1	0	0	0	0
7	A	327	0	0	5	0
7	B	291	0	0	2	0
7	C	185	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	304	0	0	1	0
All	All	20109	0	19243	93	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 2.

All (93) 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:D:451:CYS:HB3	4:D:703:XCC:S2	2.09	0.91
1:C:557:MET:HG3	1:D:52:MET:HG3	1.62	0.82
1:A:52:MET:HG3	1:B:557:MET:HG3	1.71	0.73
1:B:451:CYS:HB3	4:B:703:XCC:S2	2.28	0.72
1:C:52:MET:HG3	1:D:557:MET:HG3	1.72	0.71
1:B:312:PHE:CE2	1:B:557:MET:HE2	2.32	0.65
1:C:419:VAL:HG11	1:C:511:LEU:HG	1.78	0.64
1:C:261:PRO:HB3	1:C:299:GLU:HG2	1.82	0.61
1:A:100:ILE:HD11	1:A:261:PRO:CG	2.33	0.58
1:D:622:MET:O	1:D:626:ARG:HG3	2.03	0.58
1:A:100:ILE:HD11	1:A:261:PRO:HG2	1.87	0.57
1:D:560:LYS:HE3	4:D:703:XCC:S4	2.46	0.56
1:B:622:MET:O	1:B:626:ARG:HG3	2.06	0.56
1:D:261:PRO:HB3	1:D:299:GLU:HG2	1.89	0.55
1:C:560:LYS:HE3	4:C:703:XCC:S4	2.48	0.54
1:A:52:MET:HG3	1:B:557:MET:CG	2.39	0.53
1:A:557:MET:HG3	1:B:52:MET:HG3	1.91	0.53
1:C:488:LYS:NZ	7:C:806:HOH:O	2.41	0.52
1:A:277:VAL:HG13	7:A:833:HOH:O	2.09	0.51
1:A:622:MET:O	1:A:626[A]:ARG:HG3	2.11	0.51
1:A:312:PHE:CE2	1:A:557:MET:HE2	2.45	0.51
1:C:391:GLN:HA	1:C:391:GLN:OE1	2.11	0.51
1:A:261:PRO:HB3	1:A:299:GLU:HG2	1.92	0.50
1:C:346:HIS:CE1	1:C:389:ARG:HG3	2.47	0.49
1:A:418:LYS:NZ	7:A:803:HOH:O	2.45	0.48
1:B:252:VAL:HG11	1:B:383:ILE:HA	1.95	0.48
1:C:40:PHE:CE2	1:C:56:ARG:HD2	2.49	0.48
1:D:564:ILE:HA	1:D:567:TYR:CE2	2.49	0.48
1:A:545:SER:HA	1:A:572:GLY:O	2.14	0.47
1:C:418:LYS:N	1:C:418:LYS:HD2	2.29	0.47
1:D:458:GLN:OE1	7:D:801:HOH:O	2.20	0.47
1:A:48:ARG:NH1	1:B:46:CYS:SG	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HE3	7:B:884:HOH:O	2.13	0.47
1:B:467:LYS:NZ	1:B:489:TYR:OH	2.48	0.47
1:A:257:HIS:HB3	1:A:329:VAL:HG12	1.95	0.47
1:C:257:HIS:O	1:C:329:VAL:HA	2.15	0.46
1:B:215:THR:O	1:B:219:MET:HB2	2.14	0.46
1:C:204:ALA:O	1:C:208:MET:HG3	2.15	0.46
1:C:443:ARG:NE	1:C:619:VAL:HG13	2.30	0.46
1:A:312:PHE:CZ	1:A:557:MET:HE2	2.51	0.46
1:B:257:HIS:O	1:B:329:VAL:HA	2.16	0.46
1:A:93:HIS:ND1	1:A:216:ASP:OD2	2.41	0.45
1:A:27:VAL:HG11	1:A:313:MET:HG2	1.99	0.45
1:C:249:LYS:O	1:C:389:ARG:NH1	2.49	0.45
1:D:171:GLU:HG3	1:D:175:LYS:HE2	1.98	0.45
1:A:51:SER:OG	1:B:557:MET:HA	2.17	0.45
1:D:443:ARG:NH1	1:D:472:ASN:O	2.47	0.45
1:A:110:ASP:HB2	7:A:895:HOH:O	2.17	0.44
1:A:557:MET:CG	1:B:52:MET:HG3	2.47	0.44
1:C:313:MET:HG3	1:C:452:ASN:CB	2.47	0.44
1:C:418:LYS:N	1:C:418:LYS:CD	2.79	0.44
1:D:405:LEU:N	1:D:405:LEU:HD23	2.31	0.44
1:A:272:SER:HB3	7:A:1015:HOH:O	2.17	0.44
1:D:259:HIS:CD2	1:D:295:CYS:HB2	2.53	0.44
1:C:370:ASN:N	1:C:371:PRO:HD3	2.32	0.44
1:A:183:VAL:HG23	1:A:219:MET:HE2	1.99	0.44
1:B:411:GLU:HA	1:B:411:GLU:OE1	2.18	0.44
1:A:266:MET:HA	1:A:266:MET:HE2	2.00	0.43
1:C:498:GLU:HG2	1:C:499:LYS:N	2.33	0.43
1:C:84:ARG:NE	1:C:194:THR:OG1	2.43	0.43
1:C:622:MET:O	1:C:626:ARG:HG3	2.17	0.43
1:A:257:HIS:O	1:A:329:VAL:HA	2.19	0.43
1:C:312:PHE:CE2	1:C:557:MET:HE2	2.54	0.43
1:D:169:ARG:NH2	1:D:543:ASP:OD2	2.50	0.43
1:C:67:ARG:NH2	7:C:813:HOH:O	2.50	0.43
1:A:92:ALA:HA	1:B:192:HIS:CD2	2.54	0.42
1:A:260:GLU:HB2	7:A:814:HOH:O	2.18	0.42
1:A:621:ARG:O	1:A:624:GLU:HG3	2.20	0.42
1:C:5:ALA:O	1:C:457:VAL:HG22	2.18	0.42
1:D:557:MET:HE1	4:D:703:XCC:S2	2.59	0.42
1:D:370:ASN:N	1:D:371:PRO:HD3	2.34	0.42
1:C:557:MET:CG	1:D:52:MET:HG3	2.41	0.42
1:A:204:ALA:O	1:A:208:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:GLN:O	1:B:458:GLN:HG3	2.20	0.42
1:D:171:GLU:OE2	1:D:174:ARG:NH1	2.53	0.42
1:A:405:LEU:HB2	1:A:519:HIS:HB3	2.02	0.41
1:A:622:MET:O	1:A:626[B]:ARG:HG3	2.20	0.41
1:B:560:LYS:HE3	4:B:703:XCC:S4	2.60	0.41
1:A:370:ASN:N	1:A:371:PRO:HD3	2.35	0.41
1:B:259:HIS:CD2	1:B:295:CYS:HB2	2.55	0.41
1:D:423:GLN:O	1:D:424:ILE:C	2.63	0.41
1:C:451:CYS:CB	1:C:557:MET:HE3	2.51	0.41
1:C:186:GLU:HG3	1:C:215:THR:HG21	2.02	0.41
1:D:102:LEU:O	1:D:106[A]:HIS:ND1	2.54	0.41
1:B:343:LYS:HG2	7:B:1067:HOH:O	2.20	0.41
1:A:458:GLN:O	1:A:458:GLN:HG3	2.20	0.41
1:B:25:GLU:OE2	1:B:30:ARG:HD3	2.21	0.41
1:C:28:TRP:CZ2	1:C:313:MET:HE3	2.55	0.41
1:C:100:ILE:HD11	1:C:261:PRO:CG	2.51	0.41
1:C:52:MET:HG3	1:D:557:MET:CG	2.46	0.40
1:C:522:SER:O	1:C:525:ASP:HB2	2.21	0.40
1:A:259:HIS:CD2	1:A:295:CYS:HB2	2.56	0.40
1:A:258:GLY:HA3	1:A:330:ASP:OD1	2.21	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	630/631 (100%)	602 (96%)	25 (4%)	3 (0%)	24	16
1	B	628/631 (100%)	602 (96%)	24 (4%)	2 (0%)	36	29
1	C	623/631 (99%)	597 (96%)	24 (4%)	2 (0%)	36	29
1	D	628/631 (100%)	600 (96%)	25 (4%)	3 (0%)	24	16
All	All	2509/2524 (99%)	2401 (96%)	98 (4%)	10 (0%)	30	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	ASN
1	A	243	ASN
1	C	243	ASN
1	D	243	ASN
1	A	332	GLN
1	A	424	ILE
1	B	332	GLN
1	C	332	GLN
1	D	332	GLN
1	D	424	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	520/520 (100%)	512 (98%)	8 (2%)	57	56
1	B	519/520 (100%)	509 (98%)	10 (2%)	50	47
1	C	516/520 (99%)	501 (97%)	15 (3%)	37	31
1	D	518/520 (100%)	509 (98%)	9 (2%)	53	52
All	All	2073/2080 (100%)	2031 (98%)	42 (2%)	48	46

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	SER
1	A	196	ILE
1	A	313	MET
1	A	368	GLU
1	A	377	LYS
1	A	451	CYS
1	A	458	GLN
1	A	510	LYS
1	B	21	GLN
1	B	63	LYS

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Mol	Chain	Res	Type
1	B	66	GLU
1	B	196	ILE
1	B	368	GLU
1	B	451	CYS
1	B	458	GLN
1	B	557	MET
1	B	596	LYS
1	B	613	LYS
1	C	133	GLU
1	C	164	SER
1	C	171	GLU
1	C	196	ILE
1	C	251	SER
1	C	307	LYS
1	C	368	GLU
1	C	377	LYS
1	C	418	LYS
1	C	443	ARG
1	C	451	CYS
1	C	498	GLU
1	C	557	MET
1	C	627	LYS
1	C	628	LYS
1	D	133	GLU
1	D	164	SER
1	D	196	ILE
1	D	377	LYS
1	D	423	GLN
1	D	429	THR
1	D	451	CYS
1	D	557	MET
1	D	627	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	428	GLN
1	B	199	ASN
1	B	388	ASN
1	B	595	ASN
1	B	612	HIS

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Mol	Chain	Res	Type
1	C	428	GLN
1	D	370	ASN
1	D	388	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	D	701	-	3,3,3	0.84	0	3,3,3	0.39	0
4	XCC	A	706	7,1	0,12,12	-	-	-		
3	SF4	C	701	1	0,12,12	-	-	-		
2	ACT	A	703	-	3,3,3	0.79	0	3,3,3	0.66	0
3	SF4	A	705	1	0,12,12	-	-	-		
3	SF4	B	704	1	0,12,12	-	-	-		
3	SF4	C	702	1	0,12,12	-	-	-		
3	SF4	D	702	1	0,12,12	-	-	-		
5	EDO	B	701	-	3,3,3	0.49	0	2,2,2	0.43	0
4	XCC	C	703	1	0,12,12	-	-	-		
4	XCC	D	703	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACT	A	701	-	3,3,3	0.79	0	3,3,3	0.69	0
5	EDO	D	704	-	3,3,3	0.67	0	2,2,2	0.26	0
3	SF4	B	702	1	0,12,12	-	-	-		
4	XCC	B	703	1	0,12,12	-	-	-		
2	ACT	A	704	-	3,3,3	0.85	0	3,3,3	0.63	0
2	ACT	A	702	-	3,3,3	0.79	0	3,3,3	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XCC	A	706	7,1	-	-	0/4/4/4
3	SF4	C	701	1	-	-	0/6/5/5
3	SF4	A	705	1	-	-	0/6/5/5
3	SF4	C	702	1	-	-	0/6/5/5
3	SF4	D	702	1	-	-	0/6/5/5
5	EDO	B	701	-	-	0/1/1/1	-
4	XCC	C	703	1	-	-	0/4/4/4
5	EDO	D	704	-	-	1/1/1/1	-
4	XCC	D	703	1	-	-	0/4/4/4
3	SF4	B	702	1	-	-	0/6/5/5
4	XCC	B	703	1	-	-	0/4/4/4
3	SF4	B	704	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	704	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	703	XCC	1	0
4	D	703	XCC	3	0

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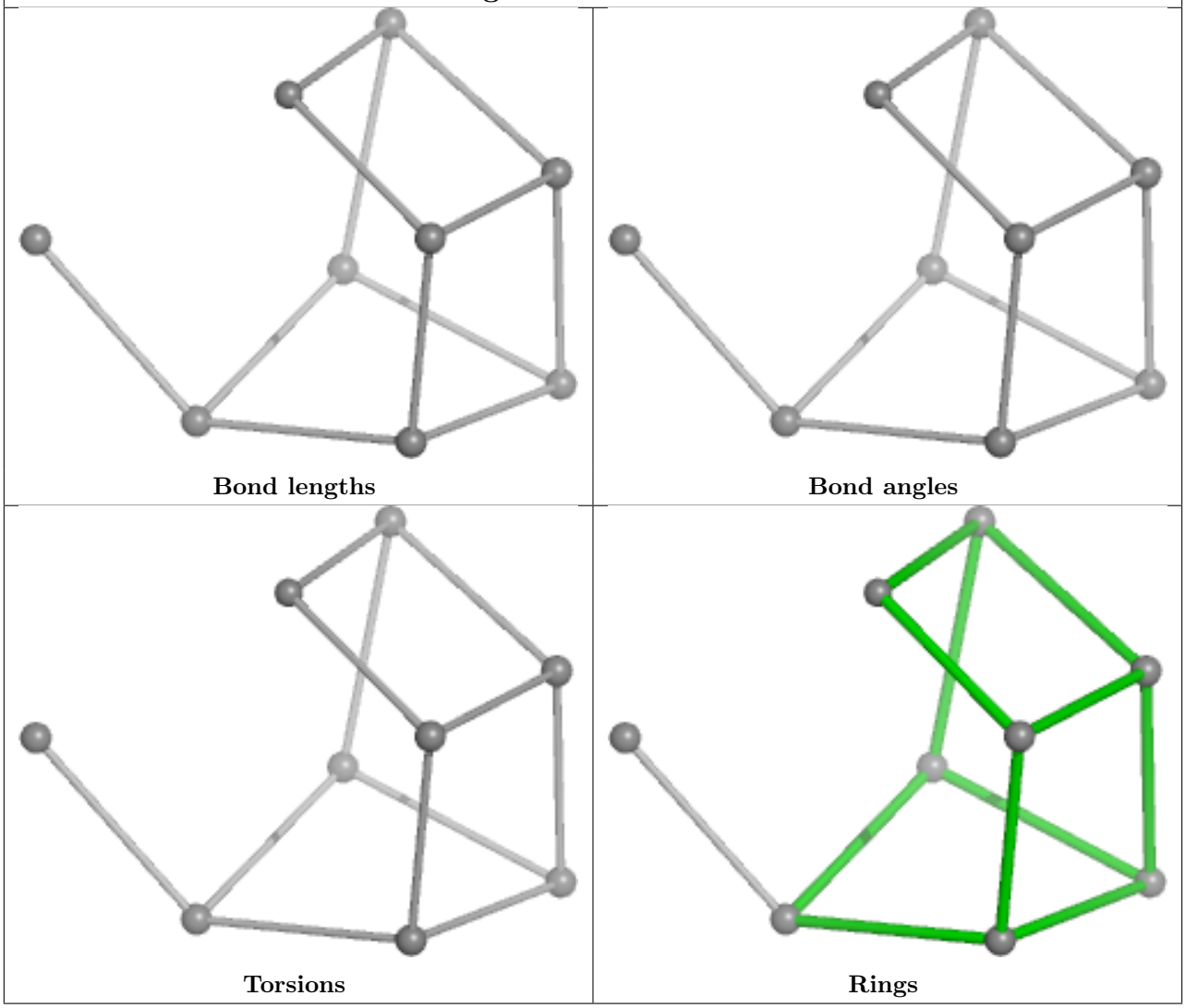
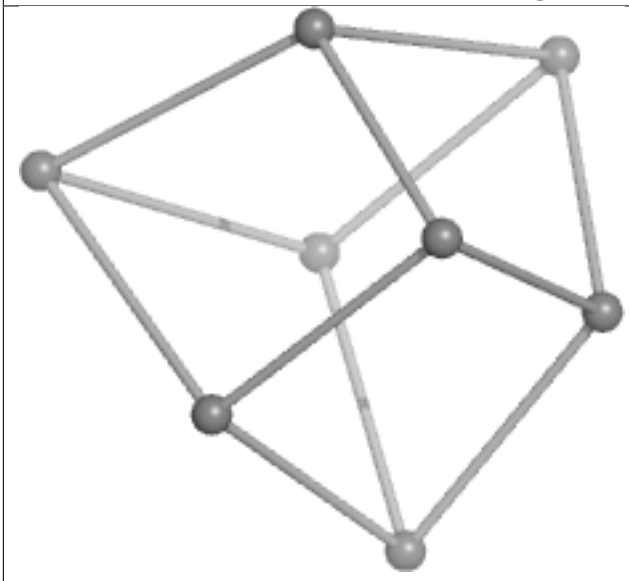
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	XCC	2	0

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.

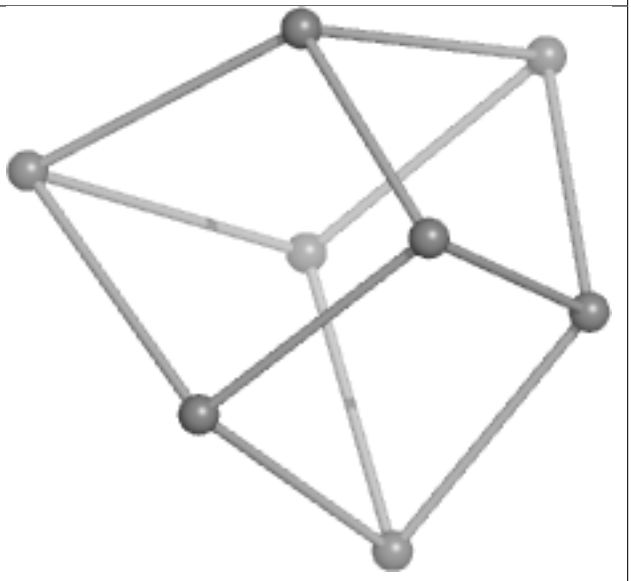
Ligand XCC A 706



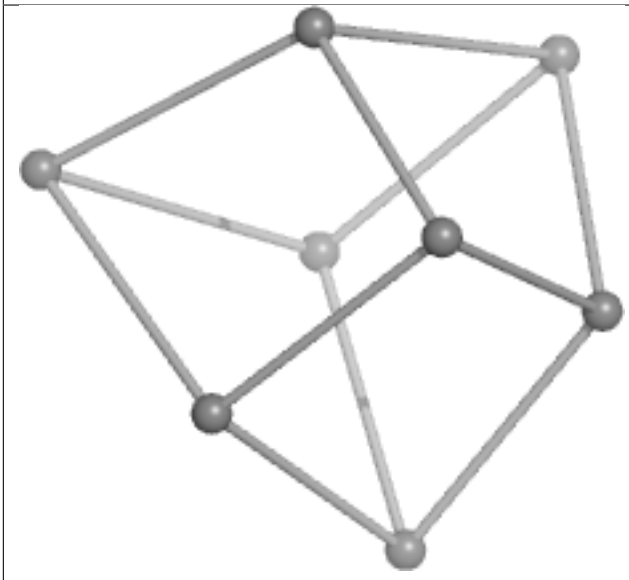
Ligand SF4 C 701



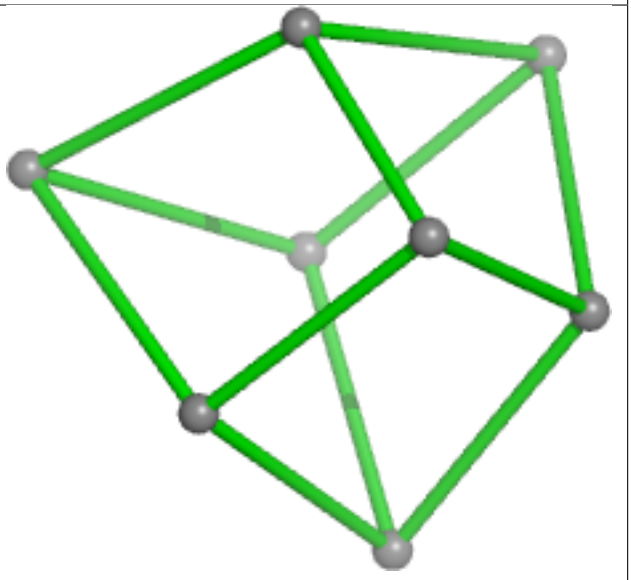
Bond lengths



Bond angles

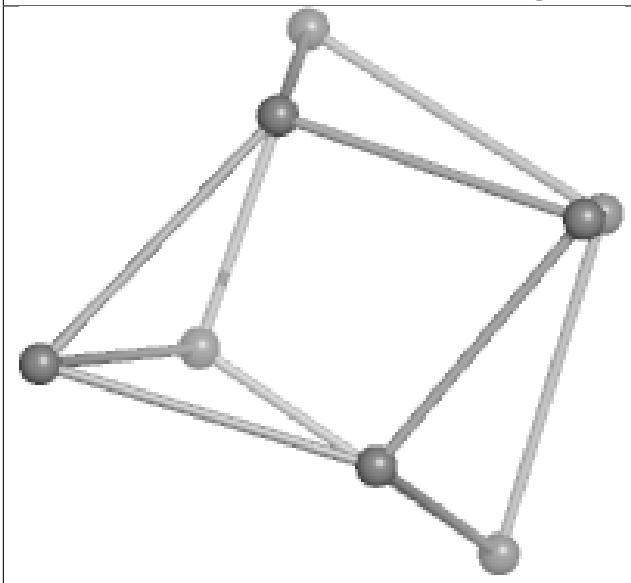


Torsions



Rings

Ligand SF4 A 705



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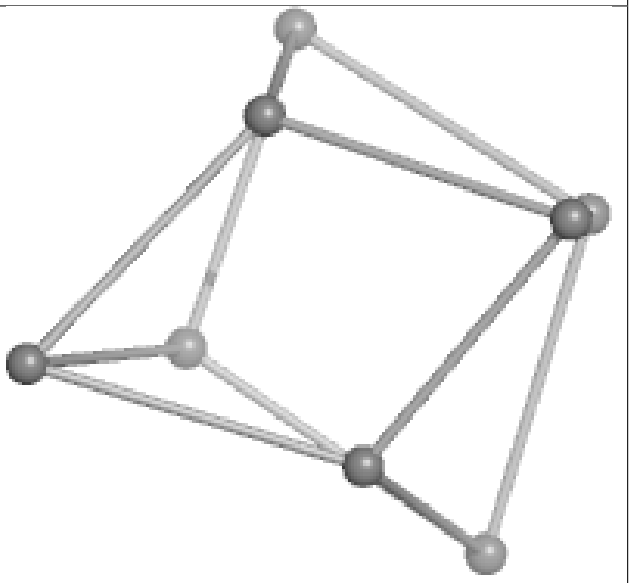

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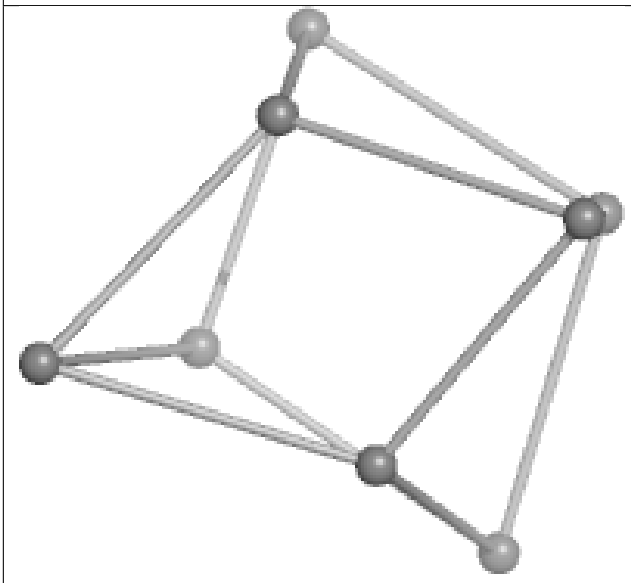
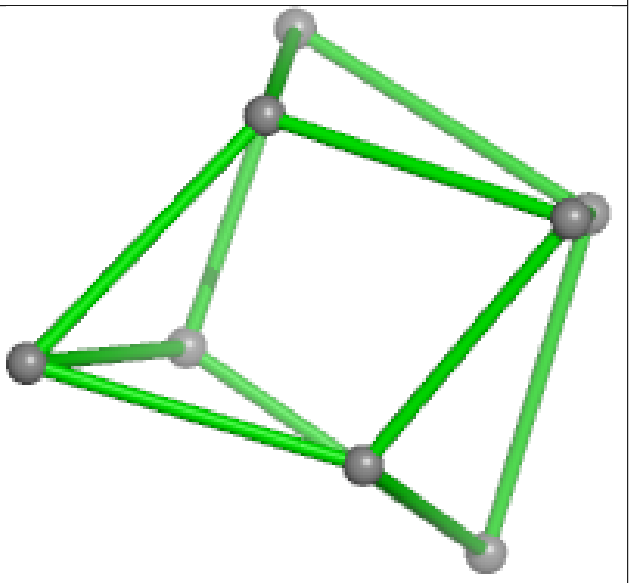
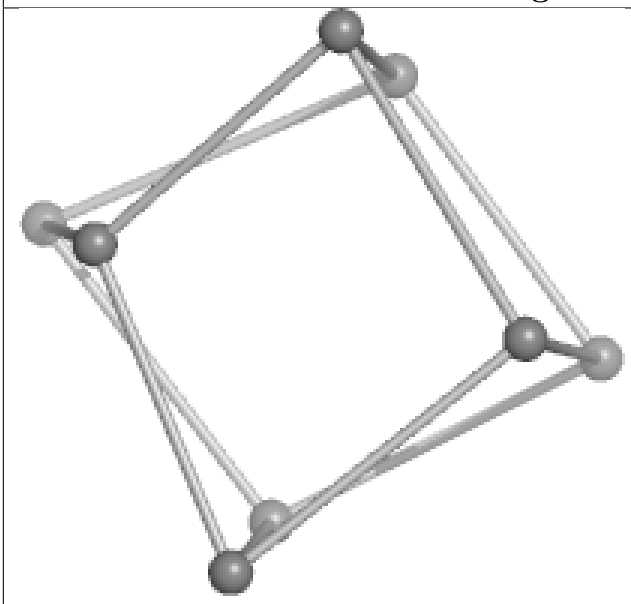


Torsions



Rings

Ligand SF4 B 704



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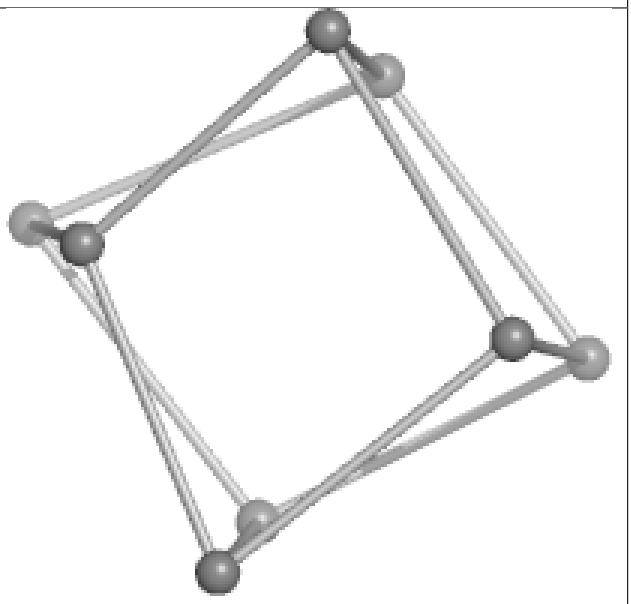

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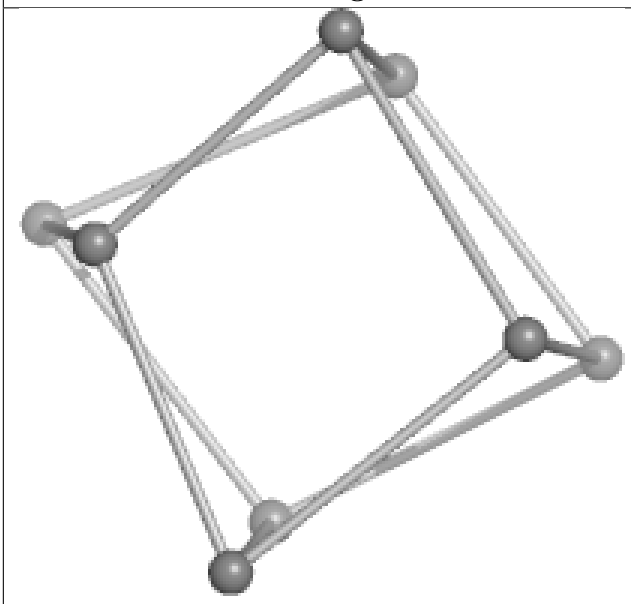

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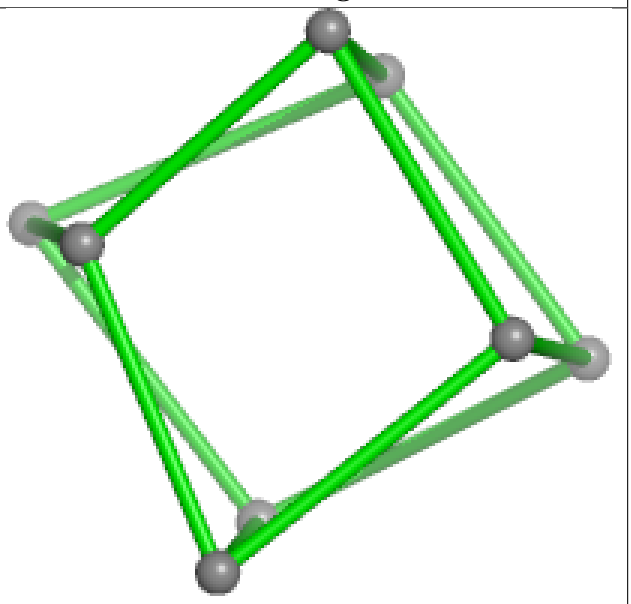
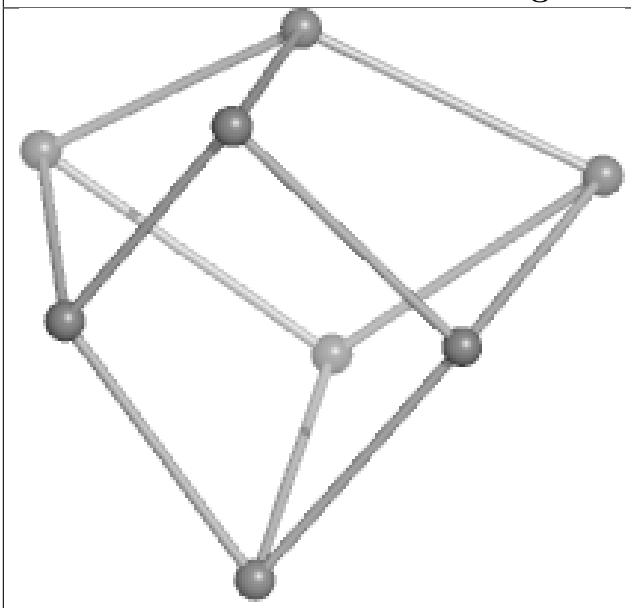


Rings

Ligand SF4 C 702



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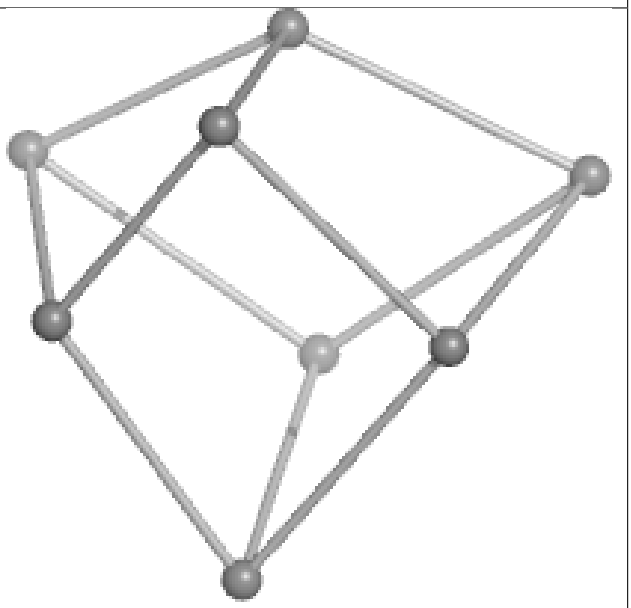

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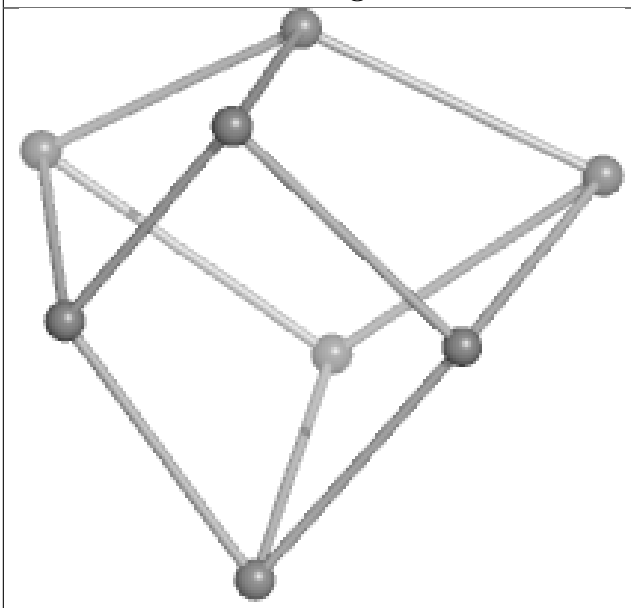

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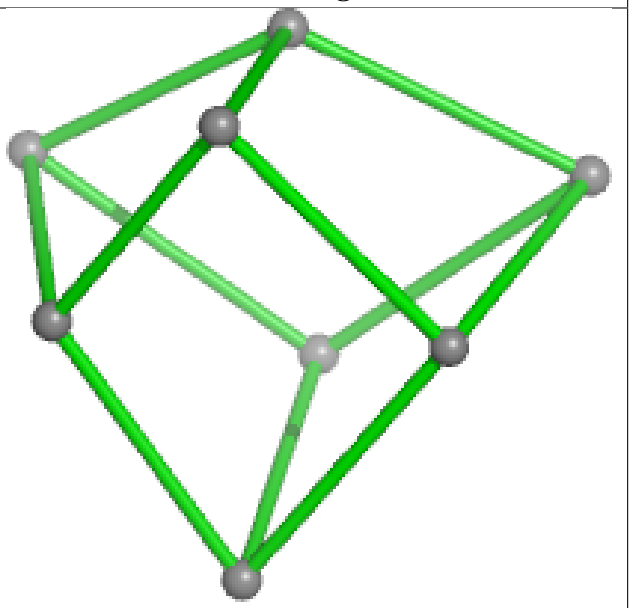
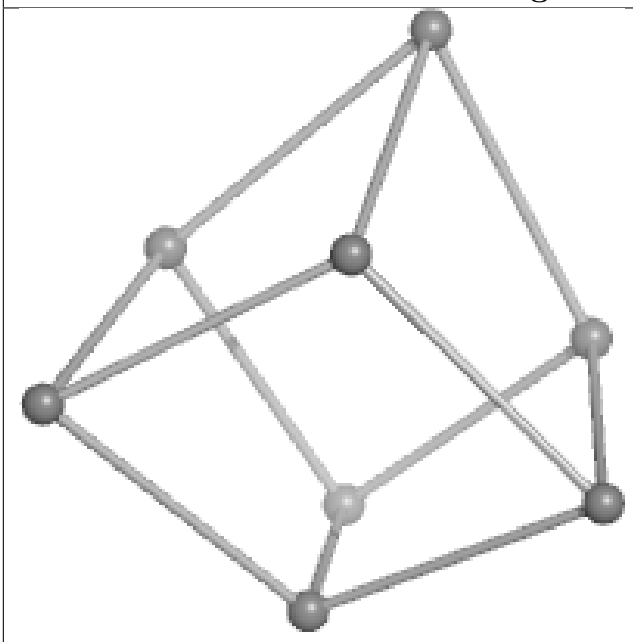


Rings

Ligand SF4 D 702



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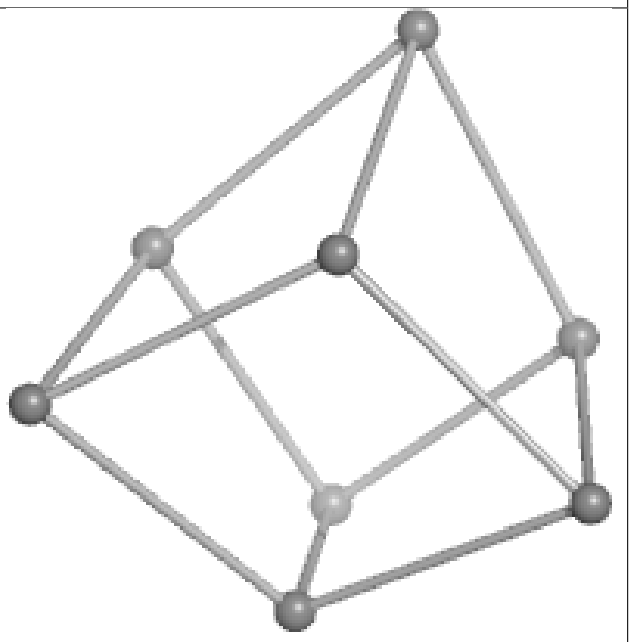

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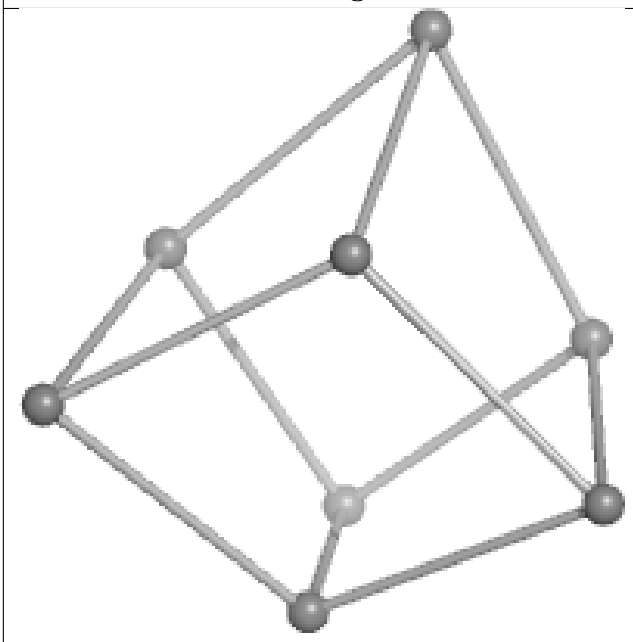

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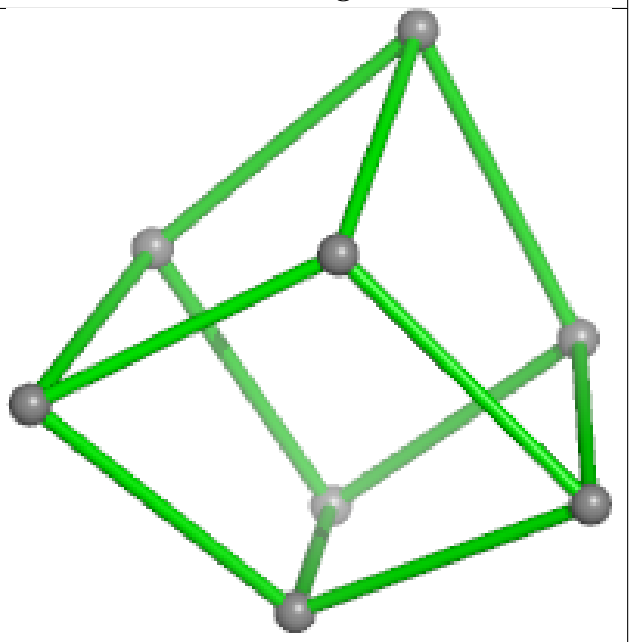
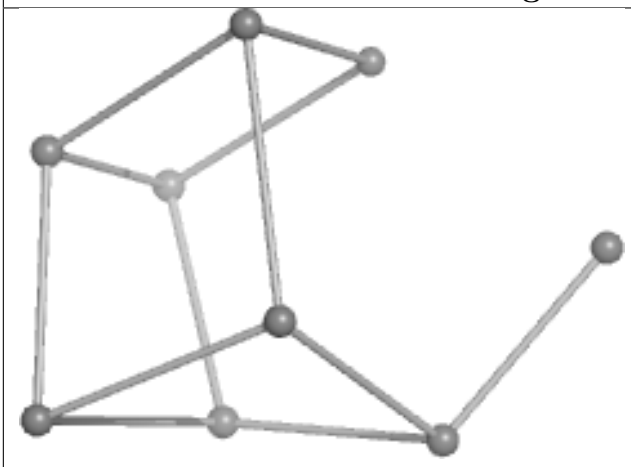
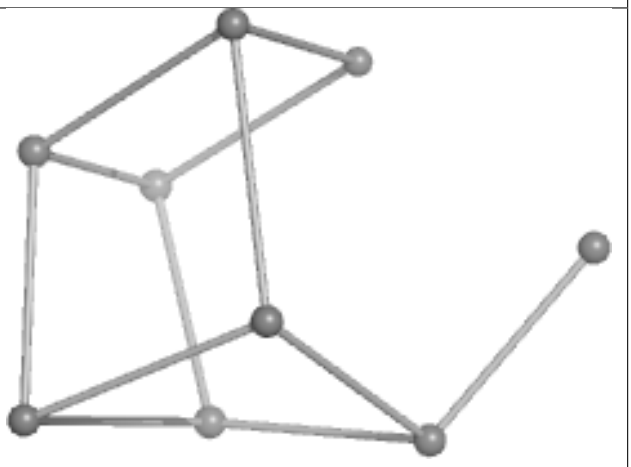


Rings

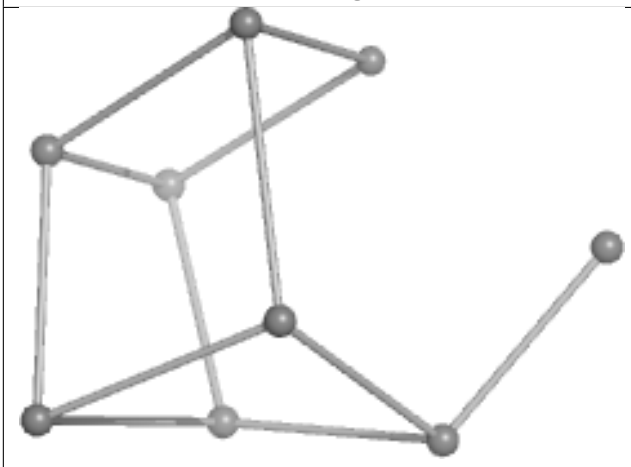
Ligand XCC C 703



Bond lengths



Bond angles



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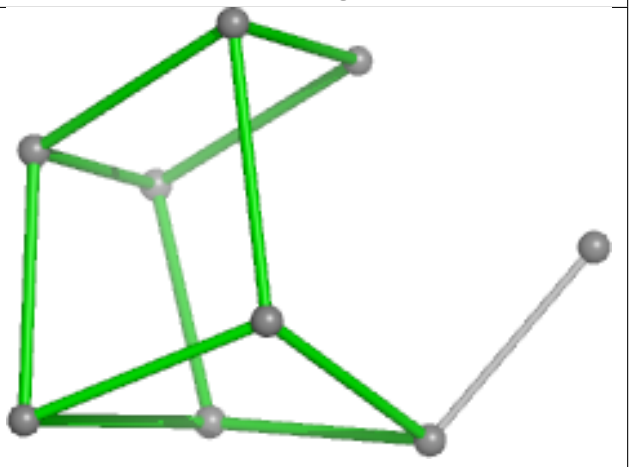

Rings

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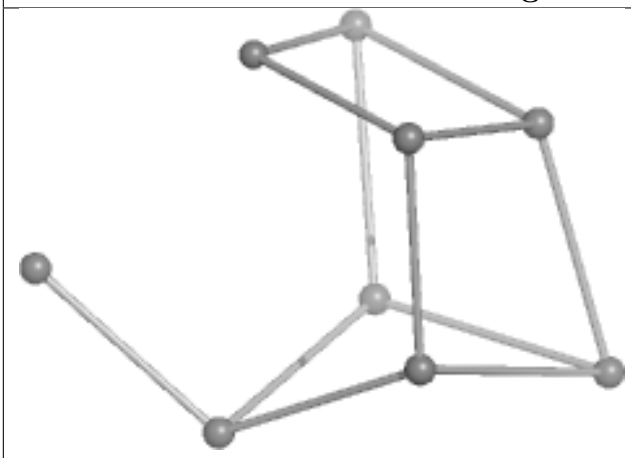
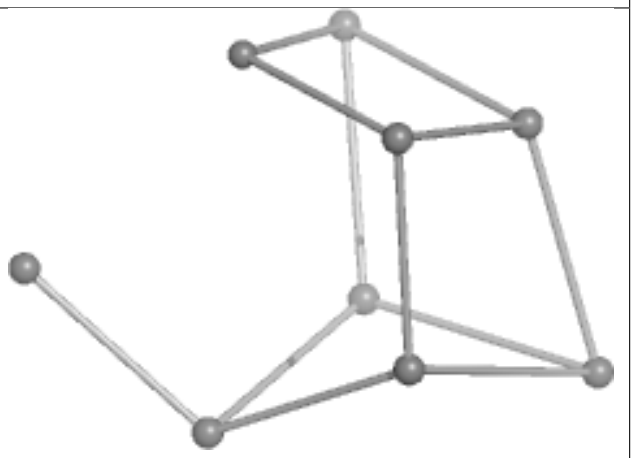
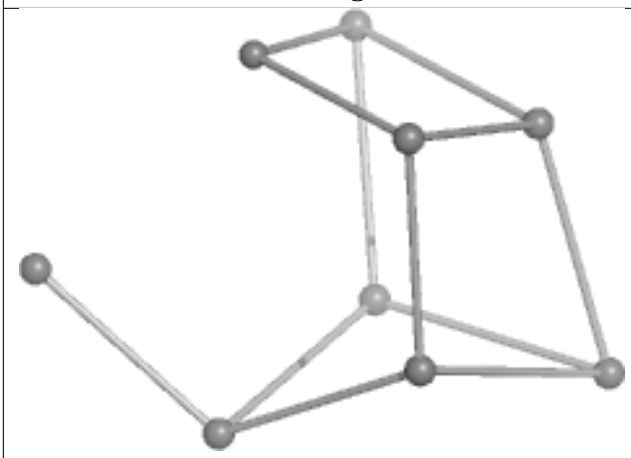


Bond lengths



Bond angles



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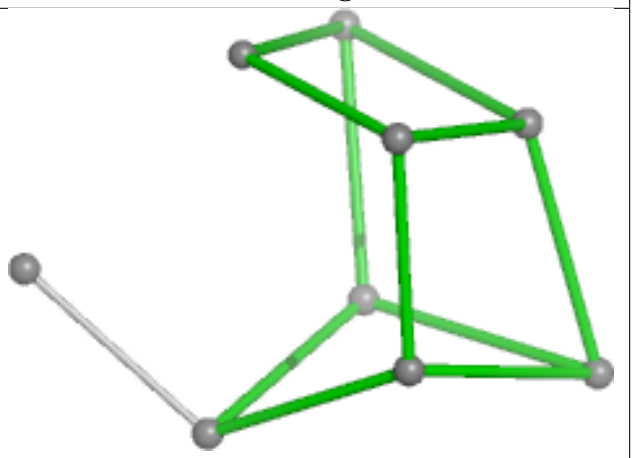
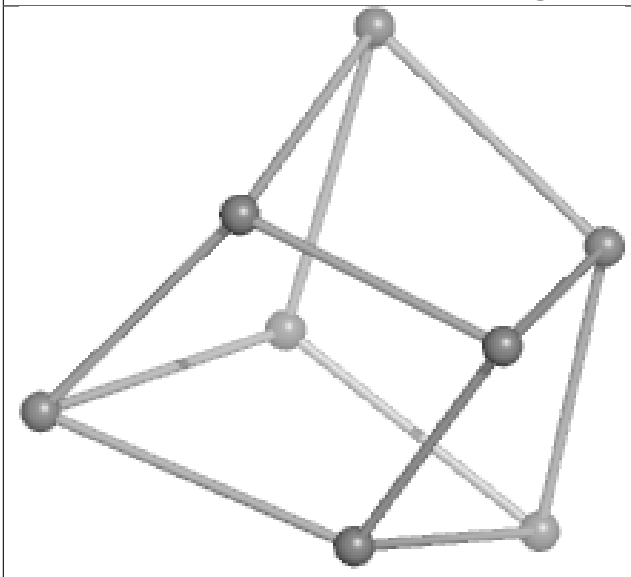
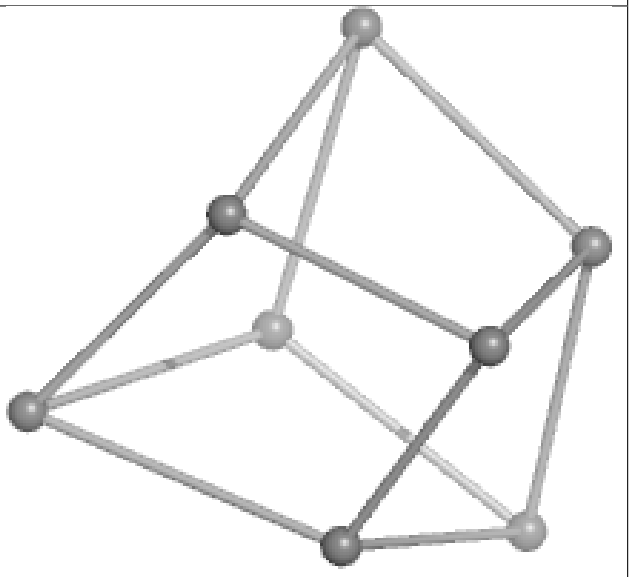


Rings

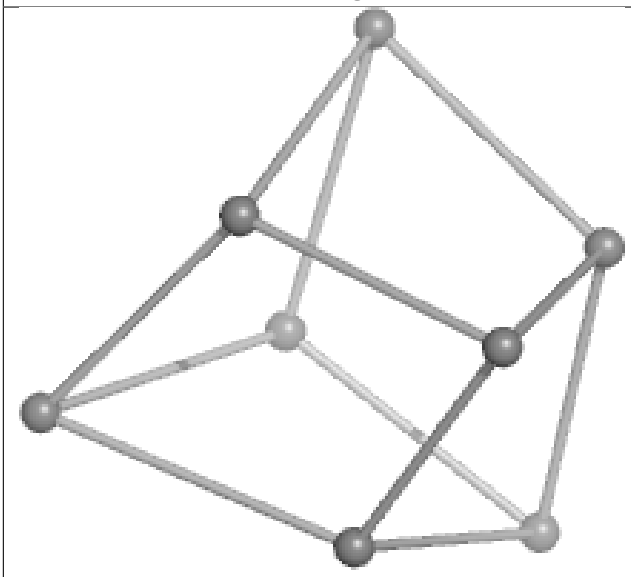
Ligand SF4 B 702



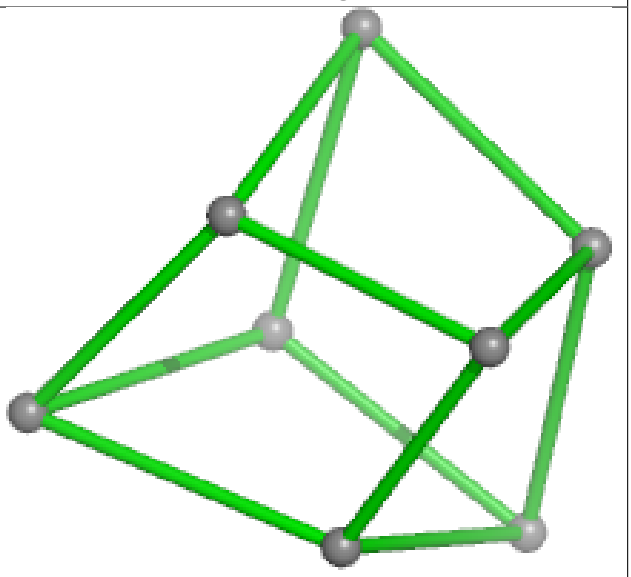
Bond lengths



Bond angles

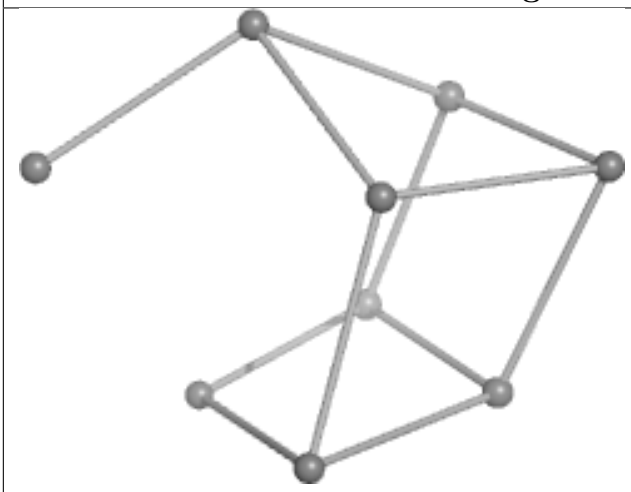


Torsions

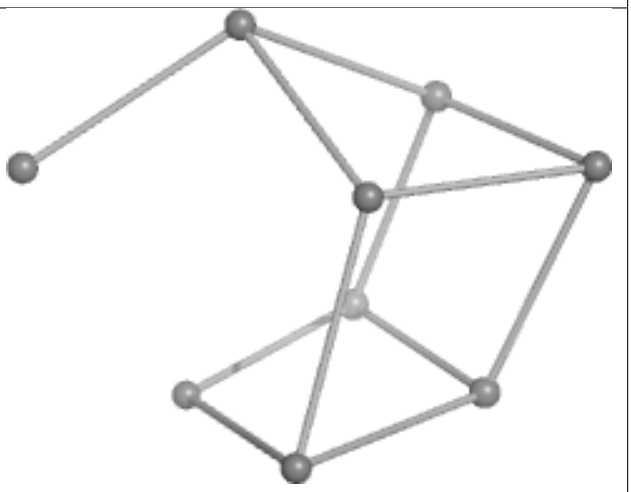


Rings

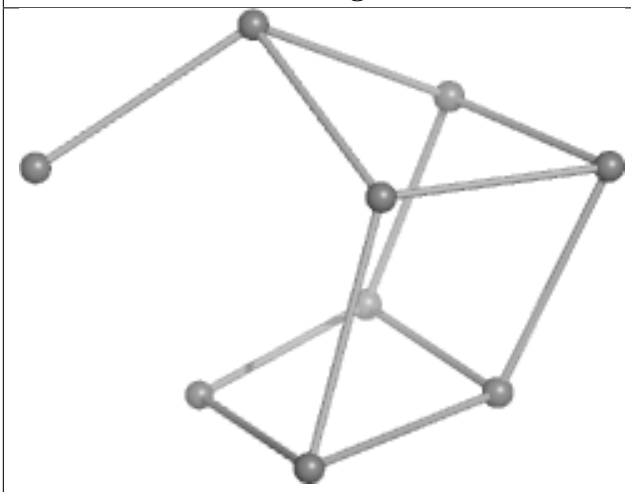
Ligand XCC B 703



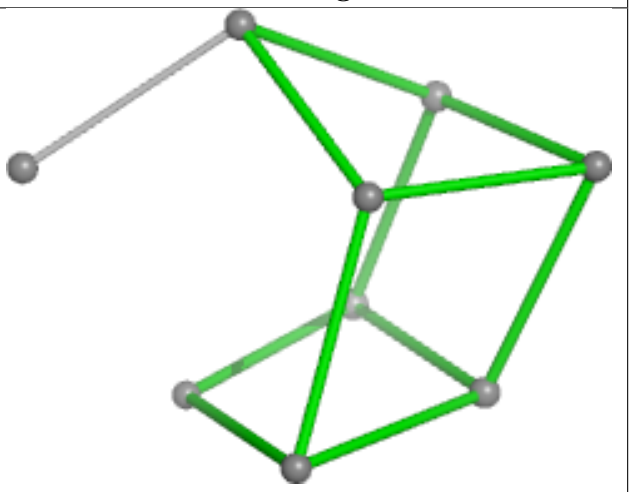
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	630/631 (99%)	-0.43	5 (0%) 82 85	8, 22, 46, 86	2 (0%)
1	B	628/631 (99%)	-0.31	2 (0%) 90 91	9, 25, 47, 85	2 (0%)
1	C	626/631 (99%)	0.35	34 (5%) 31 33	11, 37, 75, 123	1 (0%)
1	D	628/631 (99%)	-0.31	7 (1%) 78 80	10, 25, 52, 89	2 (0%)
All	All	2512/2524 (99%)	-0.18	48 (1%) 66 70	8, 26, 59, 123	7 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	422	THR	4.0
1	C	137	ILE	3.8
1	A	424	ILE	3.4
1	C	276	LEU	3.3
1	B	424	ILE	3.3
1	C	425	GLY	3.3
1	C	419	VAL	3.2
1	C	420	VAL	3.2
1	C	261	PRO	3.2
1	C	131	GLU	3.0
1	A	423	GLN	3.0
1	B	422	THR	3.0
1	C	132	THR	2.9
1	A	425	GLY	2.8
1	D	65	VAL	2.8
1	C	113	ILE	2.7
1	A	393	LYS	2.7
1	C	134	GLY	2.6
1	D	425	GLY	2.6
1	D	424	ILE	2.6
1	C	130	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	426	PRO	2.5
1	C	326	GLY	2.5
1	D	426	PRO	2.5
1	C	21	GLN	2.4
1	C	279	LEU	2.4
1	C	111	GLY	2.4
1	C	135	ARG	2.3
1	C	133	GLU	2.3
1	C	291	CYS	2.3
1	C	399	LEU	2.3
1	C	421	ASN	2.3
1	C	280	ALA	2.3
1	C	106	HIS	2.3
1	D	130	VAL	2.2
1	C	274	PRO	2.2
1	C	292	GLY	2.2
1	D	63	LYS	2.2
1	A	2	GLU	2.2
1	C	110	ASP	2.2
1	C	418	LYS	2.2
1	C	510	LYS	2.2
1	C	393	LYS	2.1
1	C	345	TYR	2.1
1	D	66	GLU	2.1
1	C	631	ILE	2.1
1	C	283	VAL	2.1
1	C	140	ILE	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 oligosaccharides 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,

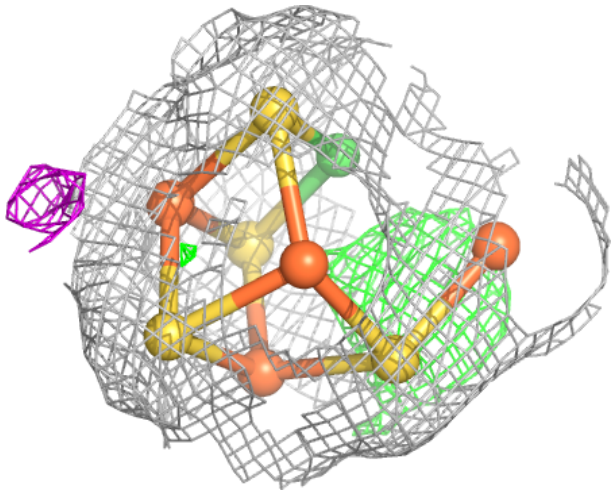
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

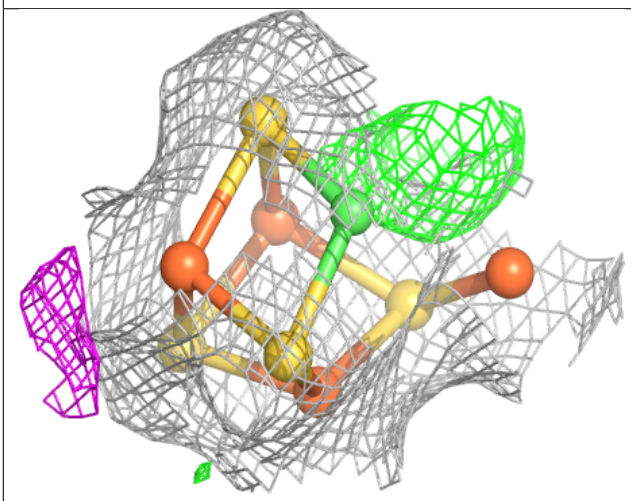
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	D	701	4/4	0.66	0.18	63,63,63,64	0
2	ACT	A	704	4/4	0.76	0.18	65,66,66,67	0
2	ACT	A	703	4/4	0.80	0.14	58,58,58,58	0
2	ACT	A	701	4/4	0.83	0.16	57,57,58,59	0
2	ACT	A	702	4/4	0.84	0.13	64,64,64,65	0
5	EDO	D	704	4/4	0.89	0.11	43,43,45,46	0
5	EDO	B	701	4/4	0.93	0.08	32,32,32,33	0
6	CL	C	704	1/1	0.94	0.07	63,63,63,63	0
4	XCC	A	706	9/9	0.98	0.03	22,24,28,40	0
4	XCC	B	703	9/9	0.98	0.03	18,22,30,39	0
4	XCC	C	703	9/9	0.98	0.04	26,30,35,45	0
3	SF4	A	705	8/8	0.99	0.03	13,15,17,18	0
3	SF4	B	702	8/8	0.99	0.04	19,21,24,24	0
3	SF4	B	704	8/8	0.99	0.04	16,17,19,19	0
4	XCC	D	703	9/9	0.99	0.03	17,20,29,33	0
3	SF4	C	701	8/8	0.99	0.04	28,29,30,31	0
3	SF4	C	702	8/8	0.99	0.03	19,20,22,24	0
3	SF4	D	702	8/8	0.99	0.03	24,25,27,28	0

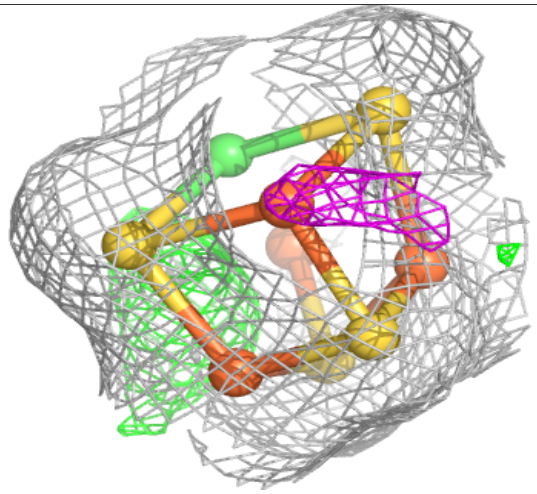
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XCC A 706:

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

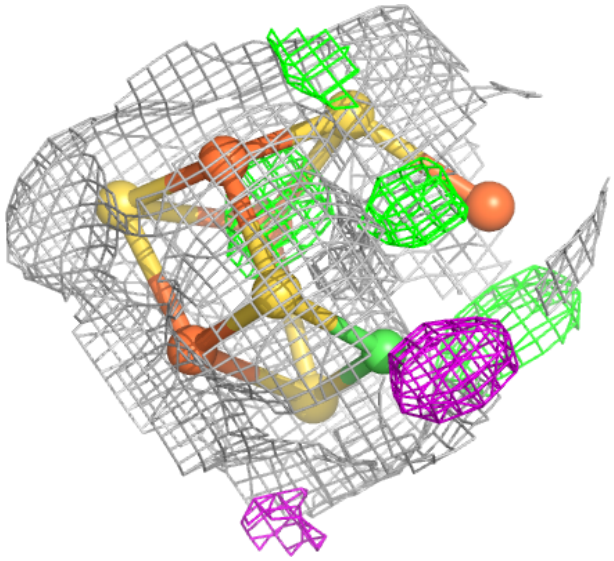


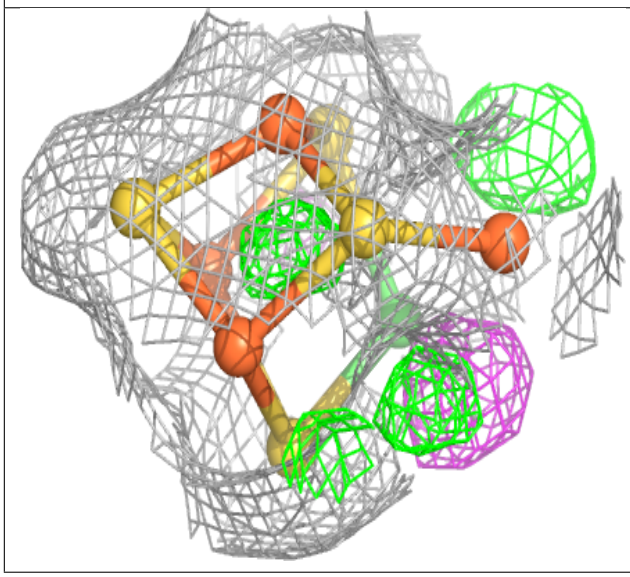


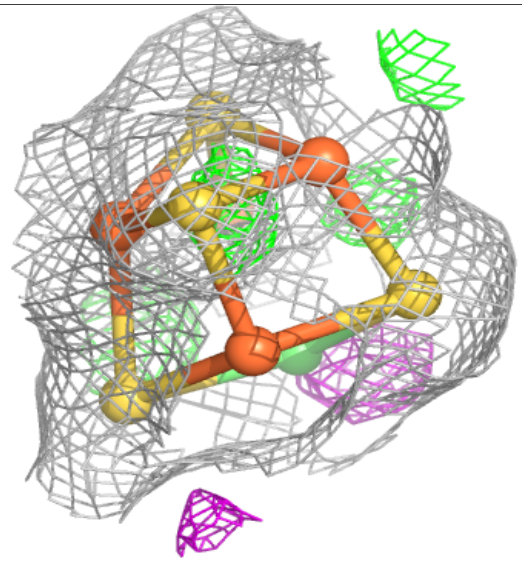


Electron density around XCC B 703:

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

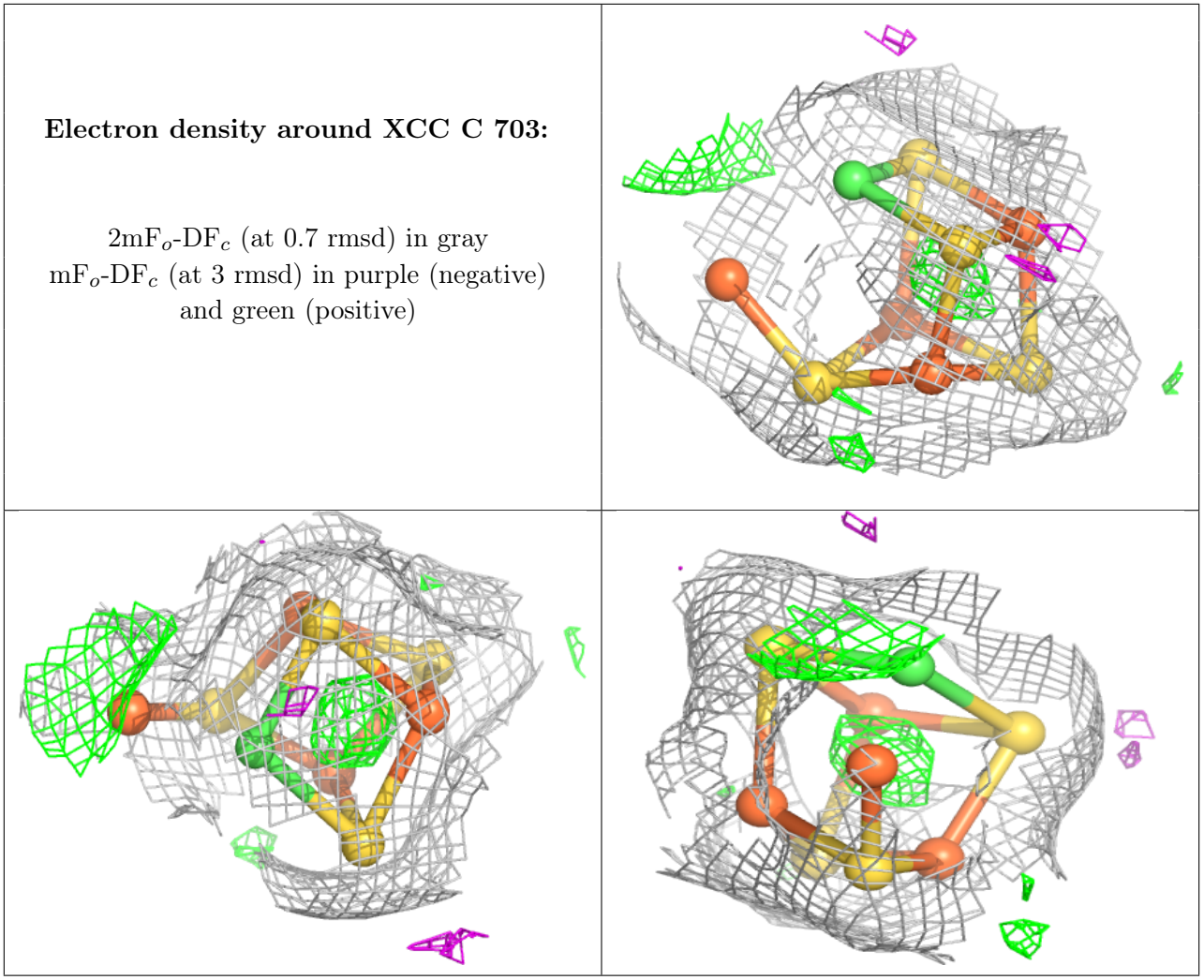






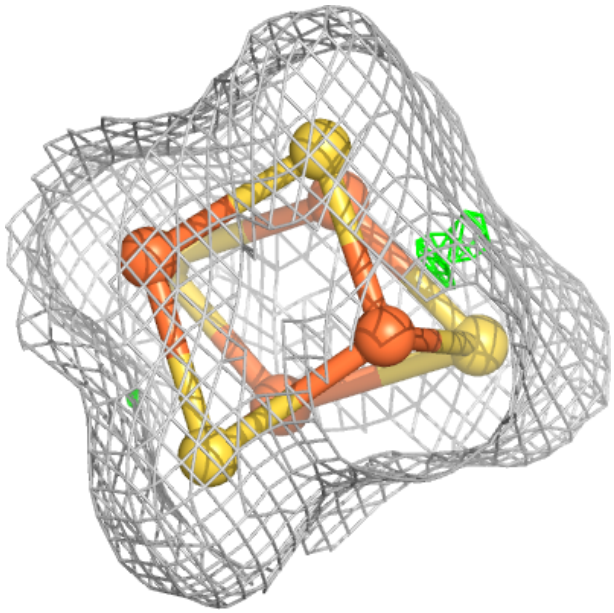
Electron density around XCC C 703:

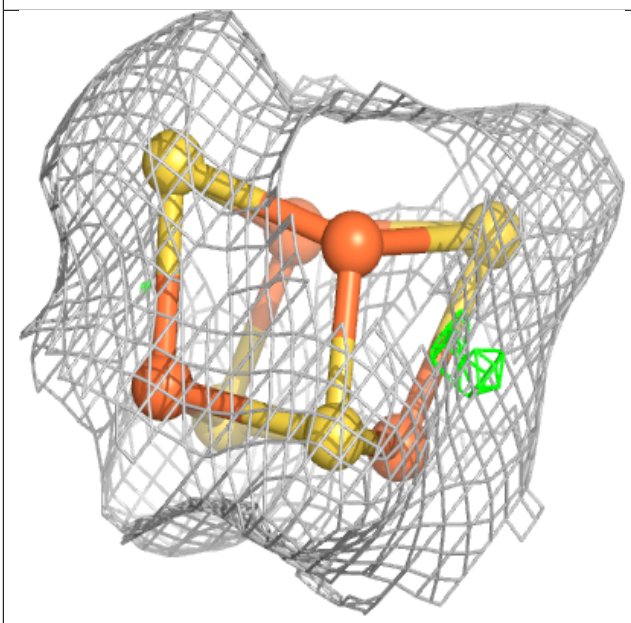
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

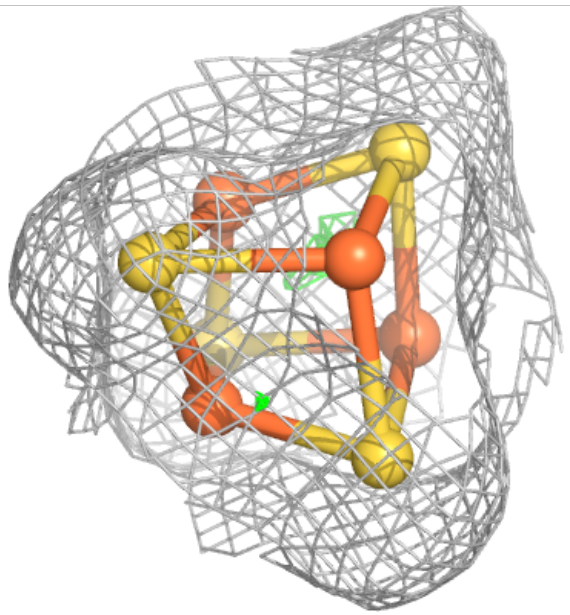


Electron density around SF4 A 705:

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

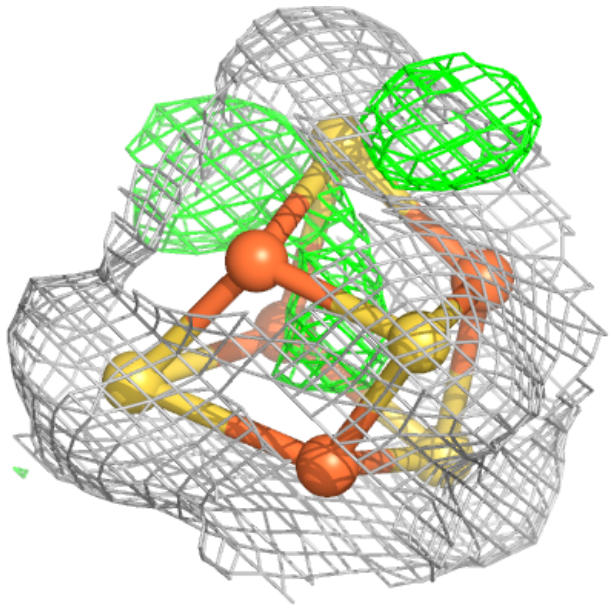


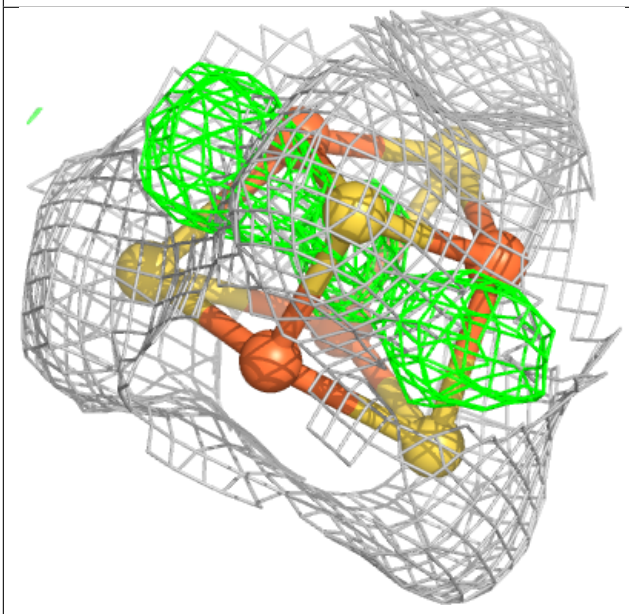


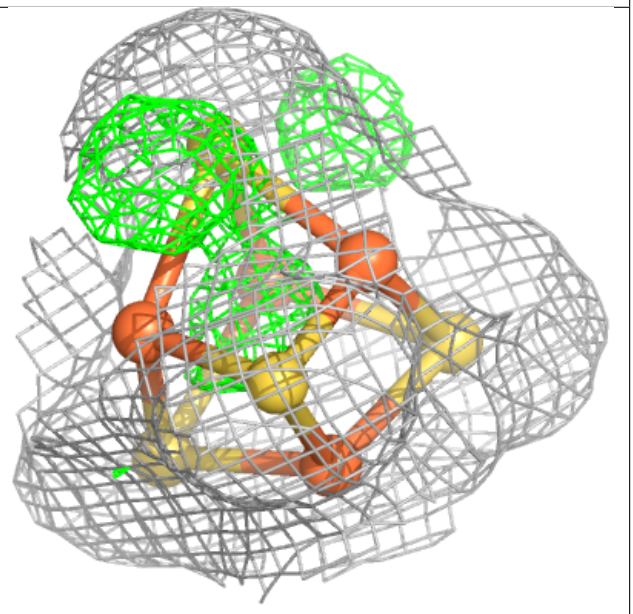


Electron density around SF4 B 702:

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

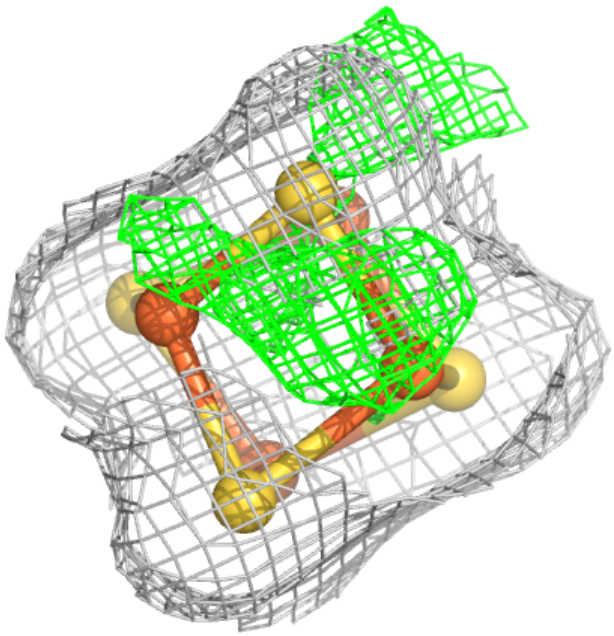


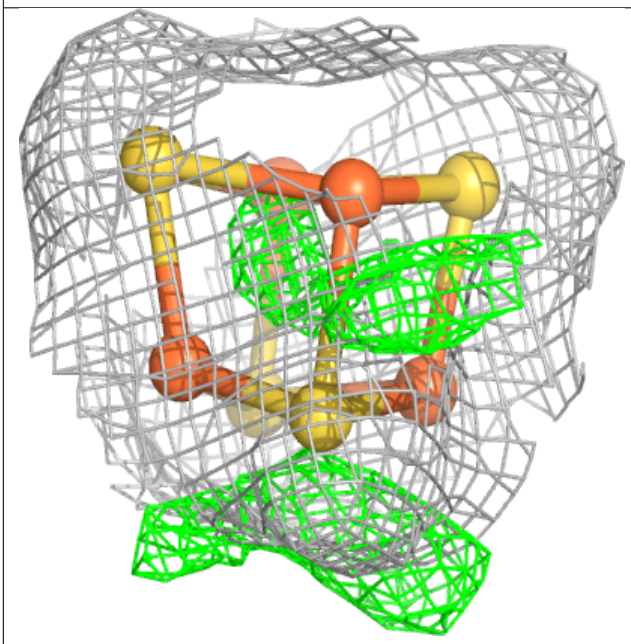


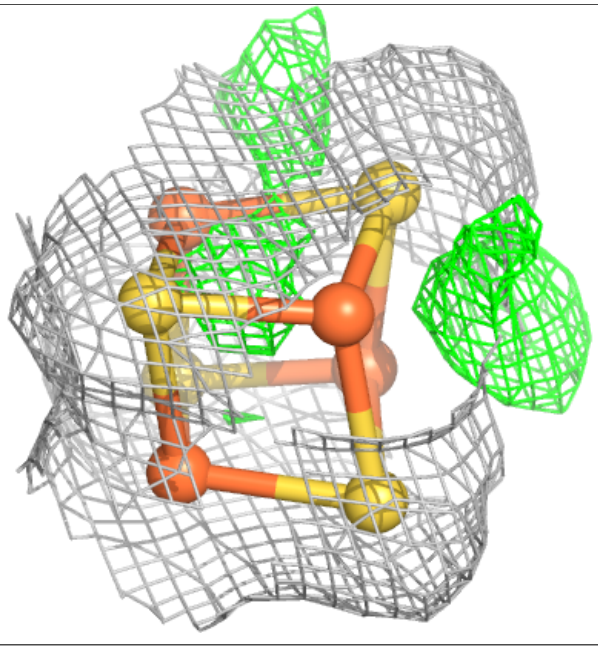


Electron density around SF4 B 704:

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

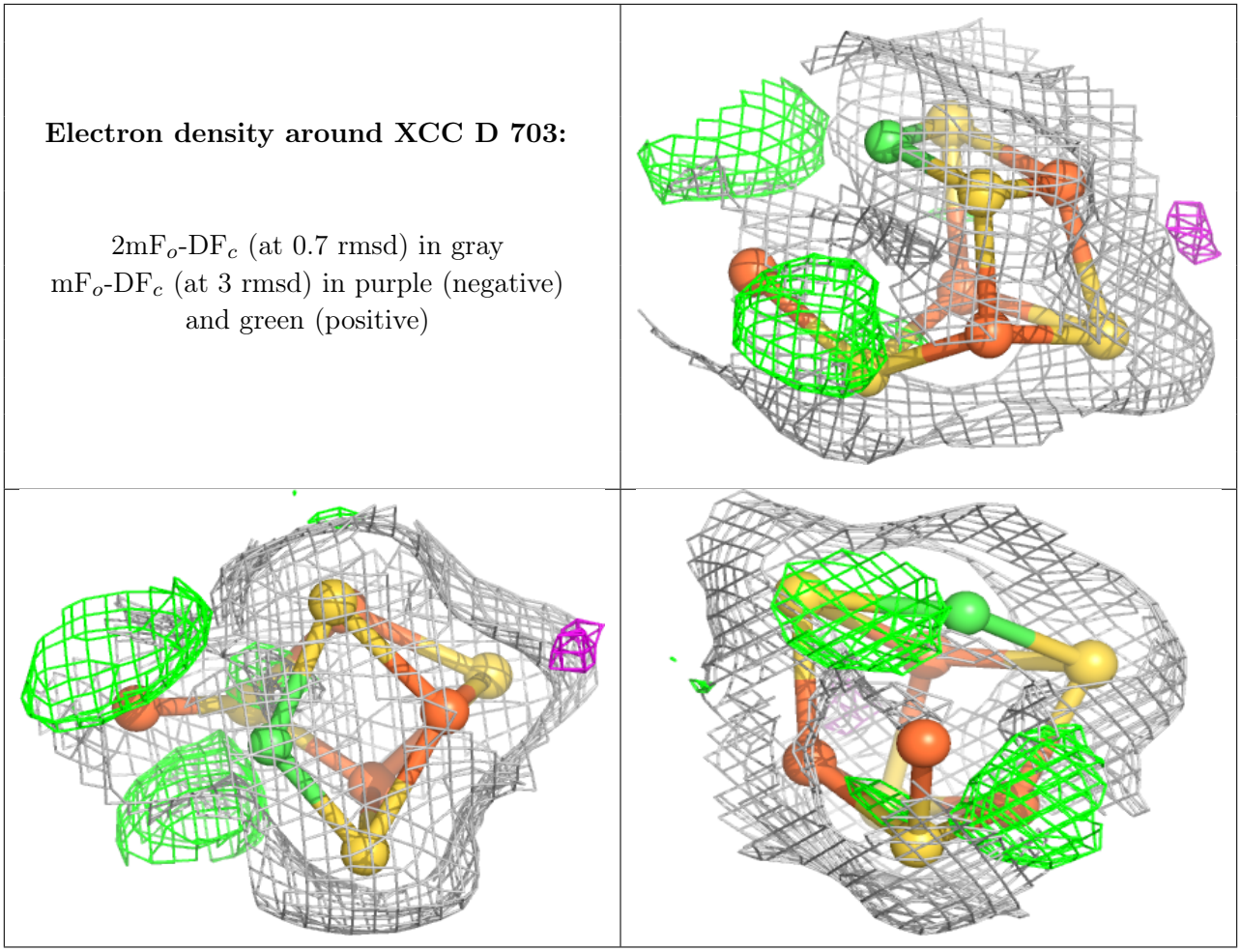






Electron density around XCC D 703:

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



Electron density around SF4 C 701:

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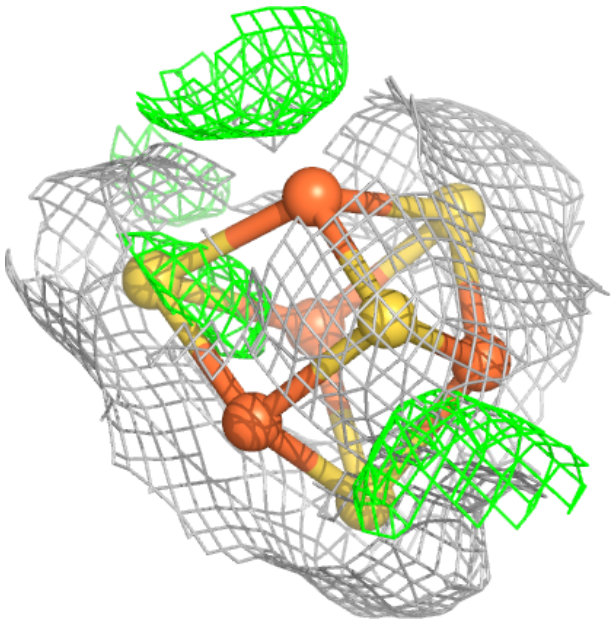
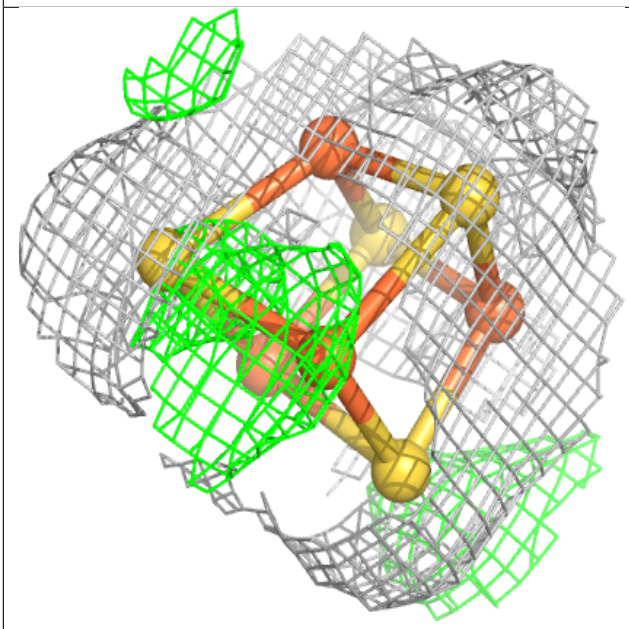
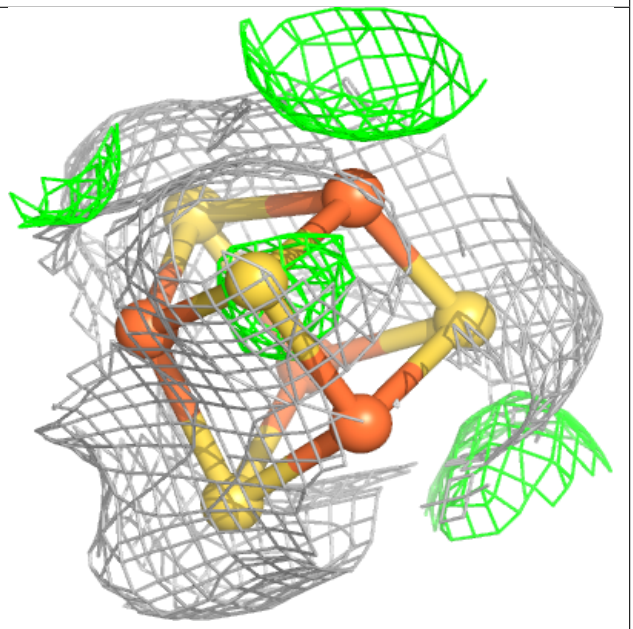
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

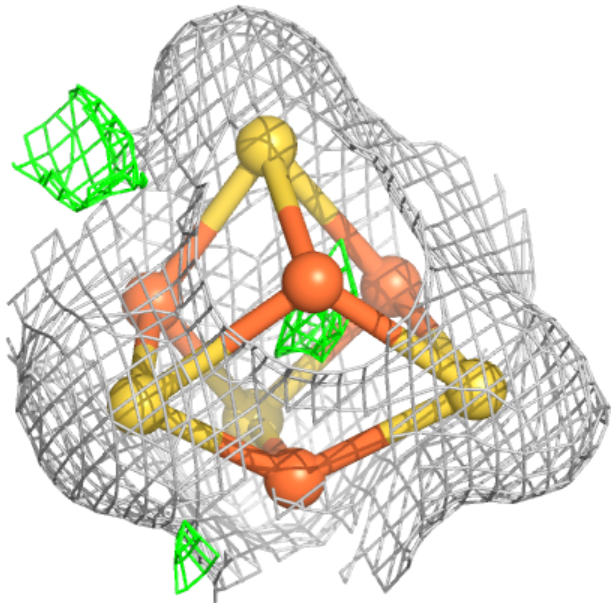


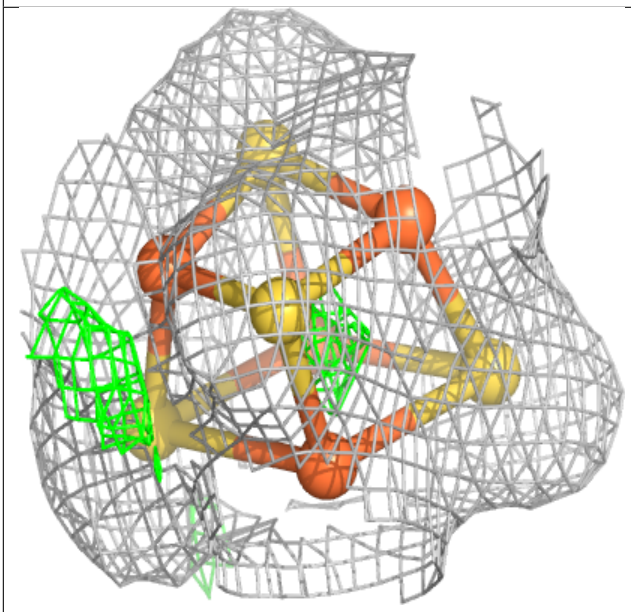


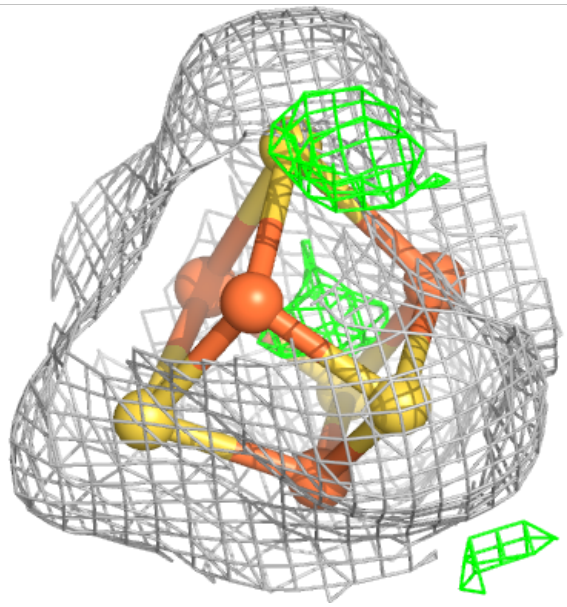


Electron density around SF4 C 702:

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







Electron density around SF4 D 702:

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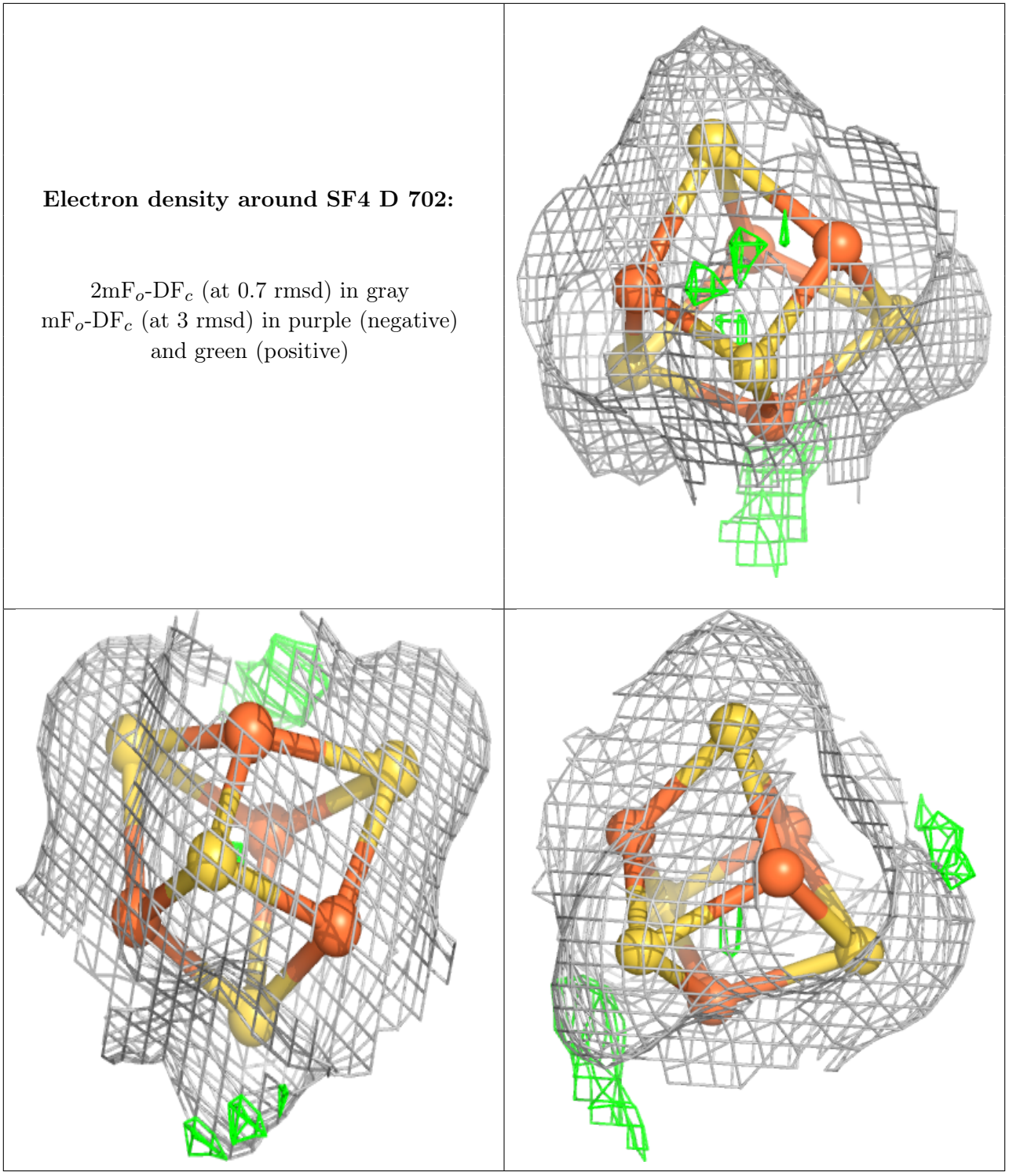
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.