Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2026 – 09:25 pm BST

PDB ID	:	8CM5 / pdb_00008cm5
Title	:	W-formate dehydrogenase C872A from Desulfovibrio vulgaris
Authors	:	Vilela-Alves, G.; Mota, C.; Klymanska, K.; Oliveira, A.R.; Manuel, R.R.; Pereira, I.C.; Romao, M.J.
Deposited on	:	2023-02-17
Resolution	:	2.15 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:

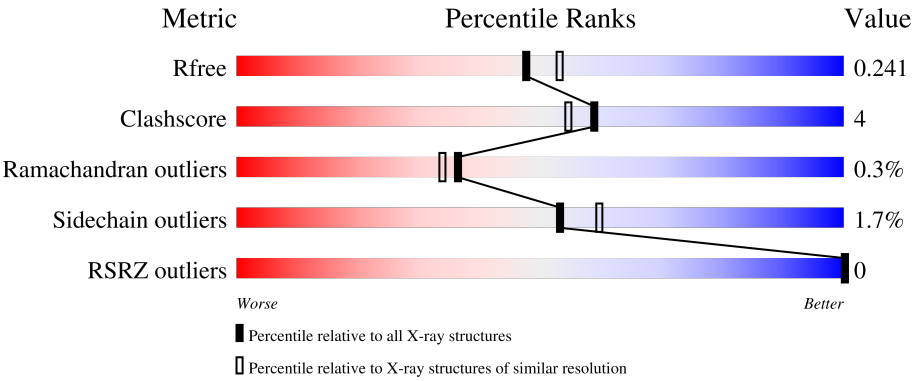
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	1013	84% 12%
1	C	1013	86% 10%
1	K	1013	84% 12%
1	R	1013	82% 13%
2	B	215	89% 10%

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Mol	Chain	Length	Quality of chain
2	D	215	93% 7%
2	L	215	89% 10%
2	S	215	89% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	C	1101	-	-	X	-
3	PEG	D	401	-	-	X	-
3	PEG	L	301	-	-	X	-
3	PEG	L	302	-	-	X	-
3	PEG	S	302	-	-	X	-
8	GOL	S	301	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 38677 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 Formate dehydrogenase, alpha subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	974	Total	C	N	O	S	Se	0	0	0
			7628	4863	1329	1395	40	1			
1	C	974	Total	C	N	O	S	Se	0	0	0
			7628	4863	1329	1395	40	1			
1	K	973	Total	C	N	O	S	Se	0	0	0
			7621	4858	1328	1394	40	1			
1	R	973	Total	C	N	O	S	Se	0	0	0
			7621	4858	1328	1394	40	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	872	ALA	CYS	engineered mutation	UNP Q72EJ1
A	1006	TRP	-	expression tag	UNP Q72EJ1
A	1007	SER	-	expression tag	UNP Q72EJ1
A	1008	HIS	-	expression tag	UNP Q72EJ1
A	1009	PRO	-	expression tag	UNP Q72EJ1
A	1010	GLN	-	expression tag	UNP Q72EJ1
A	1011	PHE	-	expression tag	UNP Q72EJ1
A	1012	GLU	-	expression tag	UNP Q72EJ1
A	1013	LYS	-	expression tag	UNP Q72EJ1
C	872	ALA	CYS	engineered mutation	UNP Q72EJ1
C	1006	TRP	-	expression tag	UNP Q72EJ1
C	1007	SER	-	expression tag	UNP Q72EJ1
C	1008	HIS	-	expression tag	UNP Q72EJ1
C	1009	PRO	-	expression tag	UNP Q72EJ1
C	1010	GLN	-	expression tag	UNP Q72EJ1
C	1011	PHE	-	expression tag	UNP Q72EJ1
C	1012	GLU	-	expression tag	UNP Q72EJ1
C	1013	LYS	-	expression tag	UNP Q72EJ1
K	872	ALA	CYS	engineered mutation	UNP Q72EJ1
K	1006	TRP	-	expression tag	UNP Q72EJ1

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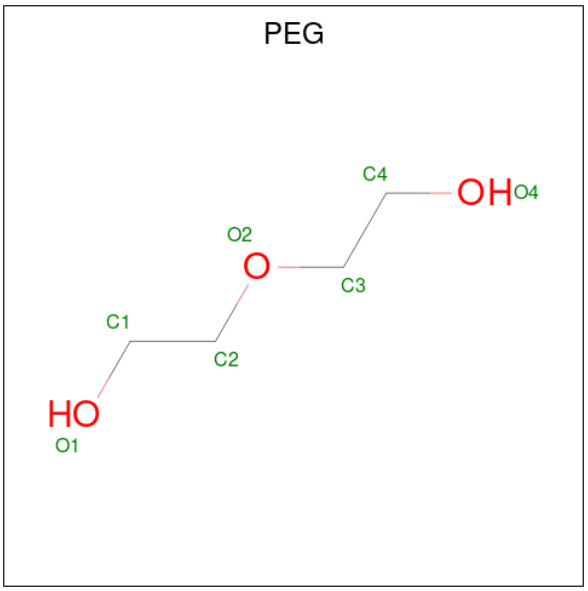
Chain	Residue	Modelled	Actual	Comment	Reference
K	1007	SER	-	expression tag	UNP Q72EJ1
K	1008	HIS	-	expression tag	UNP Q72EJ1
K	1009	PRO	-	expression tag	UNP Q72EJ1
K	1010	GLN	-	expression tag	UNP Q72EJ1
K	1011	PHE	-	expression tag	UNP Q72EJ1
K	1012	GLU	-	expression tag	UNP Q72EJ1
K	1013	LYS	-	expression tag	UNP Q72EJ1
R	872	ALA	CYS	engineered mutation	UNP Q72EJ1
R	1006	TRP	-	expression tag	UNP Q72EJ1
R	1007	SER	-	expression tag	UNP Q72EJ1
R	1008	HIS	-	expression tag	UNP Q72EJ1
R	1009	PRO	-	expression tag	UNP Q72EJ1
R	1010	GLN	-	expression tag	UNP Q72EJ1
R	1011	PHE	-	expression tag	UNP Q72EJ1
R	1012	GLU	-	expression tag	UNP Q72EJ1
R	1013	LYS	-	expression tag	UNP Q72EJ1

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit, putative.

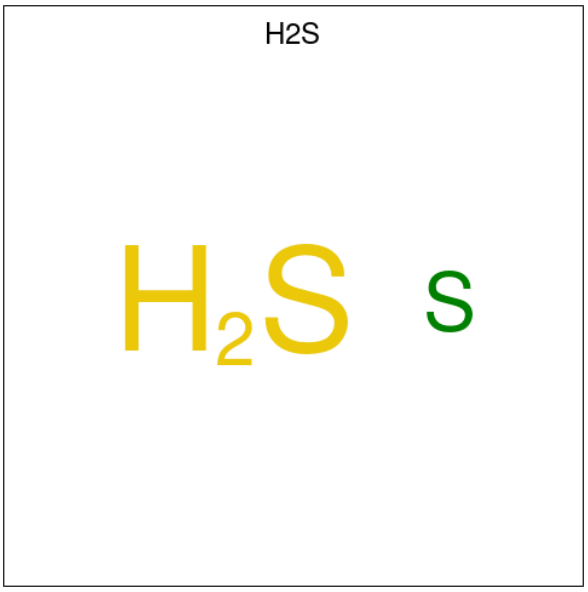
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			
2	D	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			
2	L	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			
2	S	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	L	1	Total	C	O	0	0
			7	4	3		
3	L	1	Total	C	O	0	0
			7	4	3		
3	S	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).

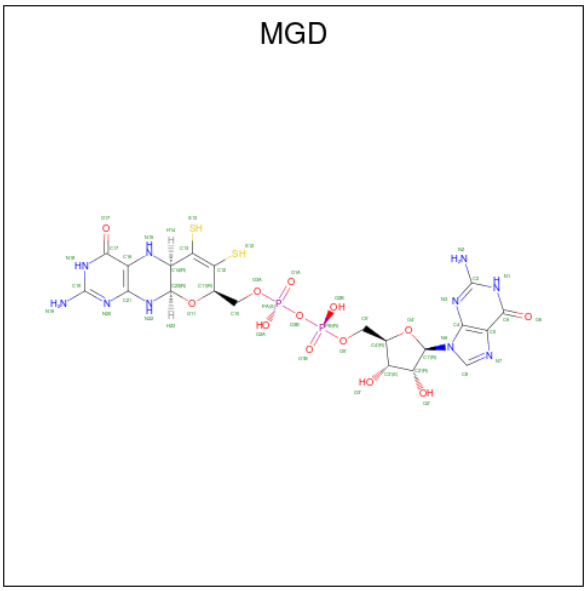


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total S 1 1	0	0
4	C	1	Total S 1 1	0	0
4	K	1	Total S 1 1	0	0
4	R	1	Total S 1 1	0	0

- Molecule 5 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

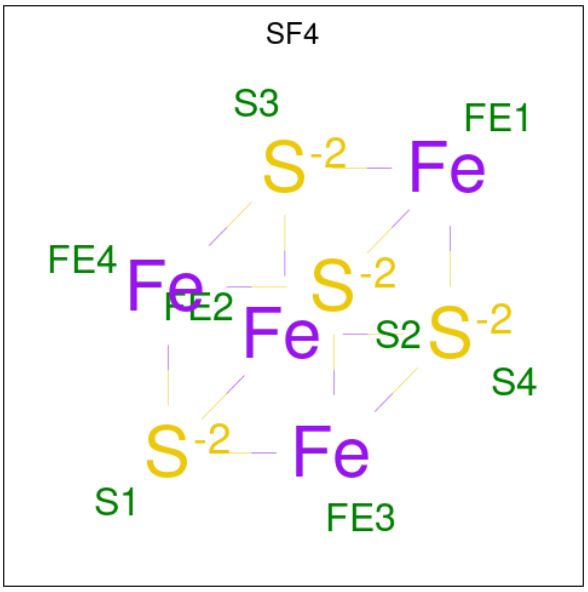
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total W 1 1	0	0
5	C	1	Total W 1 1	0	0
5	K	1	Total W 1 1	0	0
5	R	1	Total W 1 1	0	0

- Molecule 6 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	R	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	R	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	C	1	Total Fe S 8 4 4	0	0
7	D	1	Total Fe S 8 4 4	0	0
7	D	1	Total Fe S 8 4 4	0	0
7	D	1	Total Fe S 8 4 4	0	0
7	K	1	Total Fe S 8 4 4	0	0
7	L	1	Total Fe S 8 4 4	0	0
7	L	1	Total Fe S 8 4 4	0	0
7	L	1	Total Fe S 8 4 4	0	0
7	R	1	Total Fe S 8 4 4	0	0
7	S	1	Total Fe S 8 4 4	0	0

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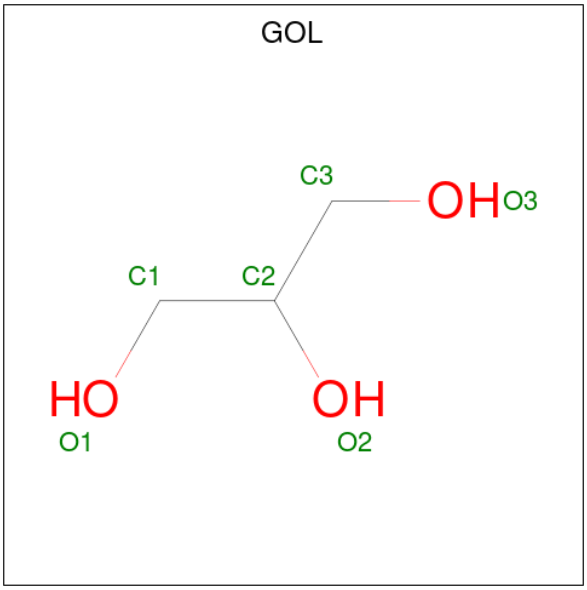
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	1	Total Fe S 8 4 4	0	0
7	S	1	Total Fe S 8 4 4	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	194	Total O 194 194	0	0
9	B	99	Total O 99 99	0	0
9	C	171	Total O 171 171	0	0
9	D	90	Total O 90 90	0	0
9	K	114	Total O 114 114	0	0
9	L	56	Total O 56 56	0	0

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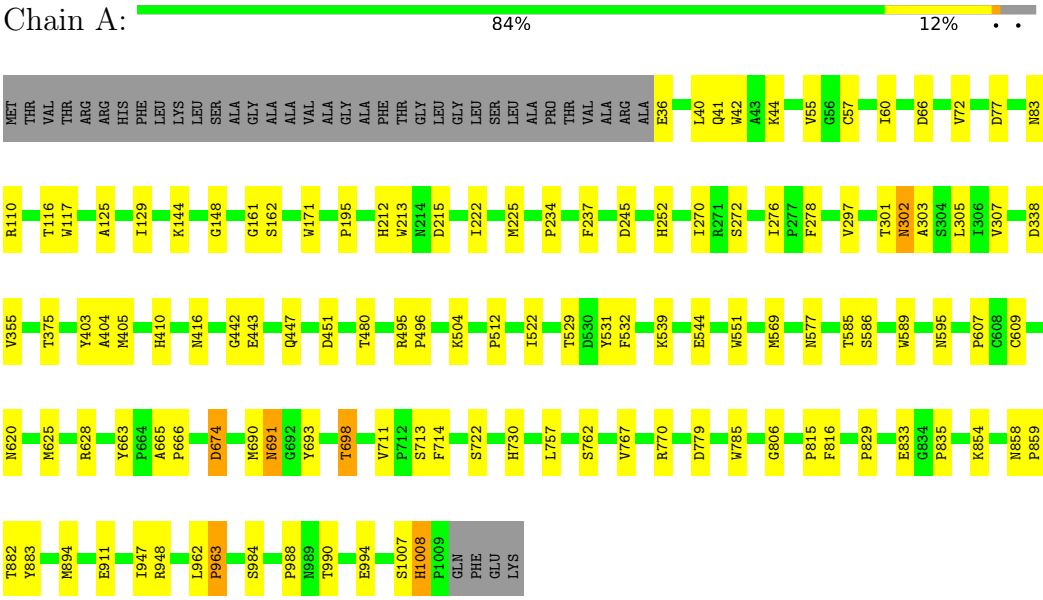
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	R	154	Total O 154 154	0	0
9	S	85	Total O 85 85	0	0

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.

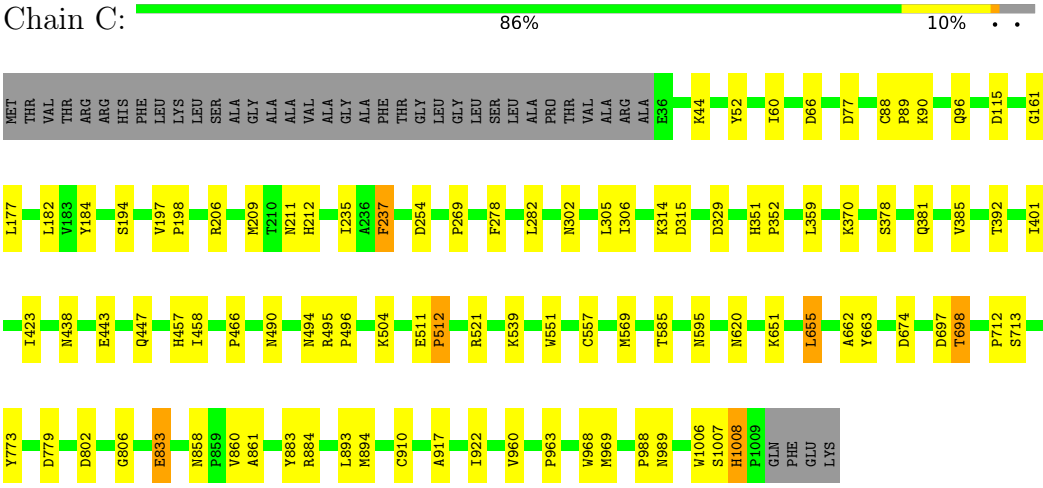
• Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain A:



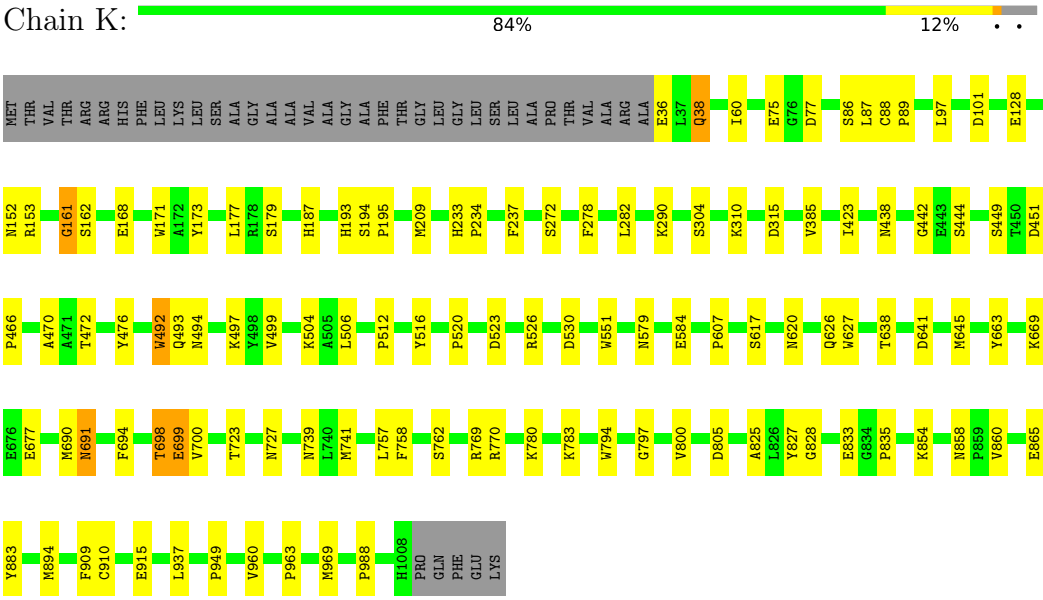
• Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain C:



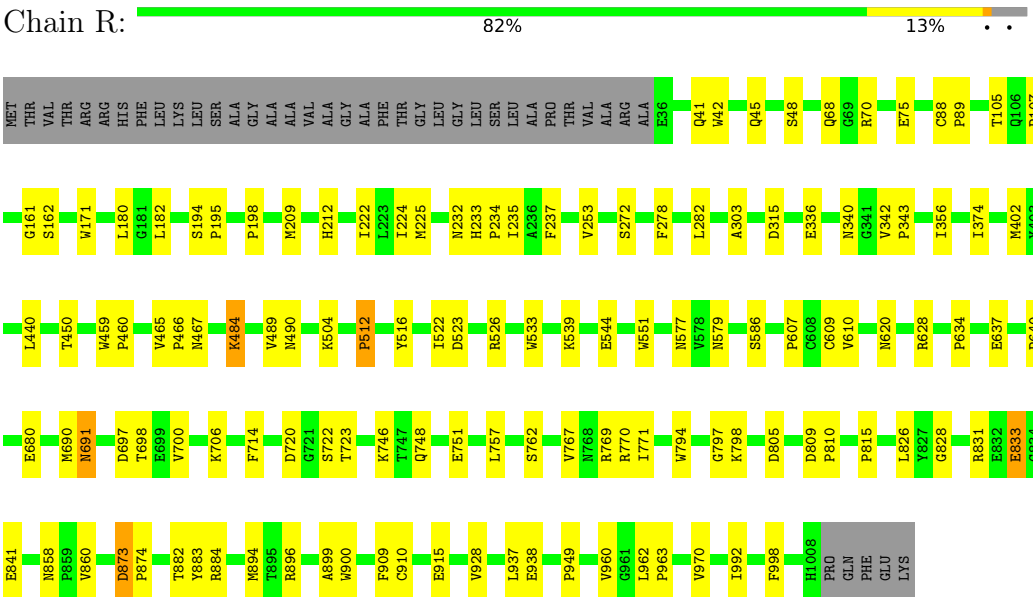
• Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain K:



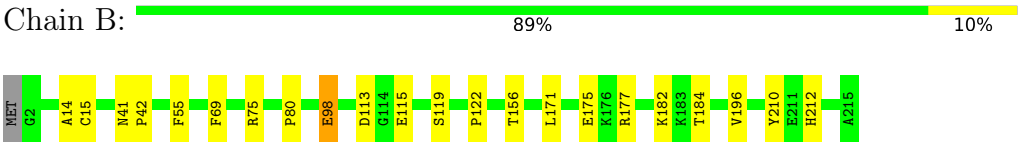
• Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain R:



• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain B:



• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain D:





• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain L:

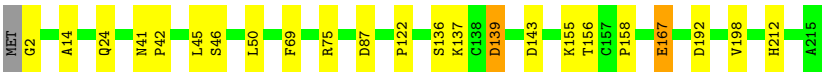




• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain S:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.44Å 261.06Å 126.21Å 90.00° 90.58° 90.00°	Depositor
Resolution (Å)	48.83 – 2.15 48.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.83-2.15) 96.8 (48.83-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.240 0.189 , 0.241	Depositor DCC
R_{free} test set	12240 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 16.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	38677	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, W, SEC, H2S, MGD, 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	1.10	2/7834 (0.0%)	1.41	17/10629 (0.2%)
1	C	1.11	1/7834 (0.0%)	1.42	18/10629 (0.2%)
1	K	1.11	1/7826 (0.0%)	1.43	10/10617 (0.1%)
1	R	1.10	1/7826 (0.0%)	1.42	12/10617 (0.1%)
2	B	1.14	1/1699 (0.1%)	1.39	4/2302 (0.2%)
2	D	1.13	2/1699 (0.1%)	1.44	8/2302 (0.3%)
2	L	1.13	1/1699 (0.1%)	1.48	7/2302 (0.3%)
2	S	1.16	1/1699 (0.1%)	1.46	5/2302 (0.2%)
All	All	1.11	10/38116 (0.0%)	1.42	81/51700 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	R	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	122	PRO	C-O	-6.47	1.15	1.24
1	A	607	PRO	C-O	-5.71	1.17	1.23
2	D	122	PRO	C-O	-5.67	1.16	1.24
1	R	107	PRO	C-O	-5.50	1.17	1.23
1	K	584	GLU	C-O	5.36	1.30	1.24
1	A	252	HIS	CE1-NE2	5.25	1.37	1.32
2	L	122	PRO	C-O	-5.19	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	359	LEU	C-O	5.14	1.30	1.24
2	D	158	PRO	C-O	-5.09	1.18	1.24
2	S	212	HIS	CE1-NE2	5.05	1.37	1.32

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	143	ASP	CA-CB-CG	13.04	125.64	112.60
2	S	143	ASP	CA-CB-CG	12.27	124.87	112.60
1	K	101	ASP	CA-CB-CG	8.50	121.10	112.60
2	D	143	ASP	CA-CB-CG	8.25	120.85	112.60
1	C	595	ASN	CB-CA-C	7.31	117.78	110.33
1	A	806	GLY	CA-C-N	6.79	126.55	120.10
1	A	806	GLY	C-N-CA	6.79	126.55	120.10
1	A	451	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	307	VAL	CA-C-N	6.30	126.33	120.34
1	A	307	VAL	C-N-CA	6.30	126.33	120.34
1	C	806	GLY	CA-C-N	6.19	125.98	120.10
1	C	806	GLY	C-N-CA	6.19	125.98	120.10
2	B	55	PHE	CA-CB-CG	6.17	119.97	113.80
2	L	47	TYR	CA-C-O	-6.11	114.03	120.63
2	S	139	ASP	CA-CB-CG	6.10	118.70	112.60
1	R	998	PHE	CA-C-O	-5.99	114.26	121.32
2	B	80	PRO	N-CA-C	5.94	117.95	110.70
1	C	802	ASP	CA-CB-CG	5.91	118.51	112.60
2	S	87	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	447	GLN	CA-C-N	5.83	126.41	120.00
1	A	447	GLN	C-N-CA	5.83	126.41	120.00
2	D	142	ASN	CA-C-N	5.79	128.83	120.79
2	D	142	ASN	C-N-CA	5.79	128.83	120.79
2	L	87	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	447	GLN	CA-C-N	5.77	126.34	119.94
1	C	447	GLN	C-N-CA	5.77	126.34	119.94
1	R	450	THR	CA-C-N	5.74	127.97	120.28
1	R	450	THR	C-N-CA	5.74	127.97	120.28
1	C	833	GLU	CB-CA-C	-5.73	98.86	109.29
1	C	443	GLU	CA-C-N	5.72	128.21	120.38
1	C	443	GLU	C-N-CA	5.72	128.21	120.38
1	K	97	LEU	CA-C-N	5.67	126.12	119.94
1	K	97	LEU	C-N-CA	5.67	126.12	119.94
2	D	105	PHE	CA-C-O	-5.64	114.62	121.05
1	R	833	GLU	CB-CA-C	-5.62	100.70	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	610	VAL	CA-C-N	5.59	127.77	120.28
1	R	610	VAL	C-N-CA	5.59	127.77	120.28
2	L	177	ARG	N-CA-C	-5.57	105.36	111.82
1	A	72	VAL	N-CA-C	-5.56	108.08	113.53
1	K	161	GLY	CA-C-O	-5.51	118.35	122.37
1	K	530	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	443	GLU	CA-C-N	5.49	129.05	120.82
1	A	443	GLU	C-N-CA	5.49	129.05	120.82
1	C	392	THR	CA-C-N	5.48	126.99	120.14
1	C	392	THR	C-N-CA	5.48	126.99	120.14
1	R	652	VAL	N-CA-C	-5.44	105.42	110.53
1	R	873	ASP	CB-CA-C	5.43	116.40	110.15
1	A	480	THR	CA-CB-OG1	-5.42	101.47	109.60
1	K	641	ASP	CA-C-N	5.33	125.85	119.94
1	K	641	ASP	C-N-CA	5.33	125.85	119.94
1	A	833	GLU	CB-CA-C	-5.32	100.39	109.65
1	R	899	ALA	CA-C-O	-5.28	114.95	120.55
1	K	520	PRO	N-CA-C	5.25	119.28	111.41
1	C	254	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	833	GLU	N-CA-CB	5.22	118.20	110.53
1	R	815	PRO	N-CA-C	5.20	121.29	114.27
2	D	82	CYS	CA-C-N	5.19	127.50	120.44
2	D	82	CYS	C-N-CA	5.19	127.50	120.44
1	A	948	ARG	CB-CA-C	5.18	117.10	109.22
1	A	302	ASN	CA-C-N	5.17	128.58	120.82
1	A	302	ASN	C-N-CA	5.17	128.58	120.82
1	C	96	GLN	N-CA-C	-5.14	106.52	112.89
2	L	106	THR	CA-C-N	5.14	127.88	120.38
2	L	106	THR	C-N-CA	5.14	127.88	120.38
2	D	166	ASP	CB-CA-C	5.11	118.86	109.46
2	D	115	GLU	CB-CG-CD	5.11	121.28	112.60
2	B	113	ASP	CA-C-N	5.10	125.76	119.99
2	B	113	ASP	C-N-CA	5.10	125.76	119.99
1	R	831	ARG	CA-C-N	5.10	127.11	120.28
1	R	831	ARG	C-N-CA	5.10	127.11	120.28
1	C	329	ASP	CA-CB-CG	5.09	117.69	112.60
1	K	310	LYS	CA-C-N	5.09	128.33	121.05
1	K	310	LYS	C-N-CA	5.09	128.33	121.05
1	C	168	GLU	CA-C-N	5.08	127.09	120.28
1	C	168	GLU	C-N-CA	5.08	127.09	120.28
1	A	595	ASN	CB-CA-C	5.06	115.79	110.17
2	S	122	PRO	CB-CA-C	-5.04	104.27	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	674	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	237	PHE	CA-CB-CG	-5.02	108.78	113.80
2	L	175	GLU	CB-CG-CD	5.01	121.12	112.60
2	S	192	ASP	CB-CA-C	5.00	115.41	110.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	SER	Peptide
1	A	40	LEU	Peptide
1	C	1007	SER	Peptide
1	R	723	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7628	0	7454	71	0
1	C	7628	0	7454	54	0
1	K	7621	0	7447	66	0
1	R	7621	0	7447	83	0
2	B	1664	0	1633	8	0
2	D	1664	0	1633	6	0
2	L	1664	0	1633	19	0
2	S	1664	0	1633	24	0
3	A	7	0	10	0	0
3	C	7	0	10	4	0
3	D	7	0	9	4	0
3	L	14	0	18	13	0
3	S	7	0	9	13	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	K	1	0	0	0	0
4	R	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	1	0	0	0	0
5	R	1	0	0	0	0
6	A	94	0	44	4	0
6	C	94	0	44	2	0
6	K	94	0	44	4	0
6	R	94	0	44	5	0
7	A	8	0	0	1	0
7	B	24	0	0	0	0
7	C	8	0	0	0	0
7	D	24	0	0	0	0
7	K	8	0	0	0	0
7	L	24	0	0	0	0
7	R	8	0	0	0	0
7	S	24	0	0	0	0
8	S	6	0	8	4	0
9	A	194	0	0	3	0
9	B	99	0	0	1	0
9	C	171	0	0	3	0
9	D	90	0	0	0	0
9	K	114	0	0	2	0
9	L	56	0	0	2	0
9	R	154	0	0	2	0
9	S	85	0	0	0	0
All	All	38677	0	36574	328	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 4.

All (328) 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)
2:L:125:ILE:HG23	3:L:301:PEG:H21	1.42	0.97
2:L:137:LYS:HA	3:L:301:PEG:H32	1.47	0.96
1:R:224:ILE:HG12	1:R:402:MET:HE3	1.47	0.92
2:S:137:LYS:HA	3:S:302:PEG:H31	1.50	0.91
1:R:224:ILE:HG12	1:R:402:MET:CE	2.00	0.90
1:A:569:MET:HE1	1:A:585:THR:HG23	1.59	0.82
2:L:125:ILE:HG23	3:L:301:PEG:C2	2.09	0.82
1:C:569:MET:HE1	1:C:585:THR:HG23	1.63	0.81
3:C:1101:PEG:H12	9:C:1300:HOH:O	1.85	0.77
2:S:137:LYS:HB2	3:S:302:PEG:H32	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:137:LYS:CA	3:L:301:PEG:H32	2.16	0.76
1:K:828:GLY:O	1:K:835:PRO:HA	1.88	0.74
1:K:173:TYR:CE2	1:K:177:LEU:HD11	2.25	0.72
2:L:137:LYS:HA	3:L:301:PEG:C3	2.20	0.70
2:S:137:LYS:CB	3:S:302:PEG:H32	2.22	0.70
1:R:698:THR:HG21	1:R:722:SER:HB3	1.73	0.70
1:R:839:HIS:ND1	9:R:1202:HOH:O	2.25	0.69
2:S:137:LYS:HA	3:S:302:PEG:H12	1.75	0.68
1:A:860:VAL:O	1:A:988:PRO:HB3	1.94	0.67
2:B:98:GLU:H	2:B:98:GLU:CD	2.02	0.67
1:A:245:ASP:OD2	9:A:1201:HOH:O	2.12	0.67
2:S:137:LYS:HA	3:S:302:PEG:C3	2.25	0.66
1:C:351:HIS:ND1	1:C:352:PRO:HD2	2.10	0.65
1:C:378:SER:OG	1:C:381:GLN:HG3	1.99	0.63
1:C:466:PRO:HB2	1:C:521:ARG:HG2	1.80	0.63
1:R:282:LEU:HD23	1:R:423:ILE:HD13	1.80	0.63
1:K:910:CYS:SG	1:K:960:VAL:HG13	2.39	0.62
1:A:41:GLN:HB3	1:A:42:TRP:CE3	2.35	0.62
1:R:757:LEU:HD22	1:R:770:ARG:HB2	1.80	0.61
1:K:470:ALA:O	1:K:516:TYR:OH	2.15	0.61
1:C:177:LEU:HD22	1:C:182:LEU:HD22	1.80	0.61
2:D:105:PHE:HB2	3:D:401:PEG:H21	1.82	0.61
1:R:828:GLY:O	1:R:835:PRO:HA	2.01	0.61
1:C:860:VAL:O	1:C:988:PRO:HB3	2.00	0.61
1:K:620:ASN:OD1	1:K:620:ASN:C	2.43	0.60
2:S:45:LEU:HB3	3:S:302:PEG:H21	1.84	0.60
1:K:494:ASN:OD1	1:K:497:LYS:NZ	2.35	0.59
1:R:224:ILE:CG1	1:R:402:MET:CE	2.76	0.59
1:A:302:ASN:O	1:A:355:VAL:HG21	2.02	0.59
1:R:162:SER:HB2	1:R:551:TRP:O	2.02	0.59
1:C:282:LEU:HD23	1:C:423:ILE:HD13	1.84	0.59
2:S:46:SER:O	3:S:302:PEG:O1	2.17	0.59
1:C:894:MET:SD	6:C:1105:MGD:H2'	2.43	0.59
1:K:171:TRP:HB2	1:K:690:MET:HE3	1.85	0.59
1:R:884:ARG:HH22	6:R:1104:MGD:H15	1.50	0.59
1:C:457:HIS:CD2	1:C:458:ILE:HG23	2.38	0.59
1:C:161:GLY:HA3	1:C:551:TRP:O	2.02	0.58
1:C:209:MET:HE2	1:C:212:HIS:HA	1.86	0.58
2:S:137:LYS:HA	3:S:302:PEG:C1	2.33	0.58
1:C:278:PHE:HZ	1:C:385:VAL:HG11	1.68	0.58
1:K:476:TYR:HE2	1:K:499:VAL:HG21	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:45:LEU:HB3	3:S:302:PEG:C2	2.33	0.58
2:L:139:ASP:HB3	3:L:302:PEG:H11	1.86	0.58
2:S:41:ASN:HA	2:S:42:PRO:C	2.28	0.58
1:A:125:ALA:O	1:A:129:ILE:HG13	2.03	0.57
2:L:137:LYS:H	3:L:302:PEG:H21	1.68	0.57
1:A:234:PRO:HD2	7:A:1106:SF4:S3	2.45	0.57
1:A:410:HIS:HA	1:A:994:GLU:HG3	1.87	0.57
1:R:794:TRP:CH2	1:R:797:GLY:O	2.57	0.57
2:S:137:LYS:CA	3:S:302:PEG:H31	2.31	0.57
1:K:75:GLU:OE2	2:L:155:LYS:NZ	2.31	0.56
1:C:211:ASN:HB2	1:C:438:ASN:HD21	1.69	0.56
1:R:222:ILE:CG2	1:R:402:MET:HE2	2.35	0.56
1:A:883:TYR:O	1:A:963:PRO:HA	2.06	0.56
1:R:225:MET:HE1	1:R:278:PHE:CD1	2.40	0.56
1:R:839:HIS:NE2	1:R:841:GLU:OE2	2.36	0.55
1:K:698:THR:OG1	1:K:699:GLU:N	2.39	0.55
2:L:105:PHE:HB2	3:L:302:PEG:H22	1.89	0.55
1:A:44:LYS:HB2	1:A:66:ASP:HA	1.89	0.55
1:A:302:ASN:O	1:A:355:VAL:CG2	2.55	0.55
2:L:41:ASN:HA	2:L:42:PRO:C	2.32	0.55
1:K:794:TRP:CH2	1:K:797:GLY:O	2.60	0.55
1:R:224:ILE:HG12	1:R:402:MET:HE2	1.87	0.54
1:A:303:ALA:HA	1:A:355:VAL:CG2	2.38	0.54
1:K:523:ASP:HB2	1:K:526:ARG:HD3	1.89	0.54
2:S:2:GLY:O	2:S:167:GLU:HG2	2.08	0.54
1:A:615:GLU:O	9:A:1202:HOH:O	2.18	0.54
1:A:303:ALA:HA	1:A:355:VAL:HG23	1.90	0.54
2:S:136:SER:HA	8:S:301:GOL:O2	2.08	0.54
1:K:194:SER:N	1:K:195:PRO:CD	2.72	0.53
1:K:758:PHE:O	1:K:770:ARG:NH1	2.41	0.53
1:C:162:SER:HB2	1:C:551:TRP:O	2.08	0.53
1:R:171:TRP:HB2	1:R:690:MET:HE3	1.90	0.53
1:R:577:ASN:OD1	1:R:586:SER:HB3	2.08	0.53
1:A:894:MET:SD	6:A:1105:MGD:H2'	2.48	0.53
1:C:511:GLU:O	1:C:512:PRO:C	2.51	0.53
1:R:697:ASP:O	1:R:698:THR:CG2	2.56	0.53
1:C:88:CYS:HB2	1:C:89:PRO:HD2	1.90	0.53
1:C:1006:TRP:HZ2	3:C:1101:PEG:H32	1.73	0.53
1:R:698:THR:HG21	1:R:722:SER:CB	2.38	0.53
1:R:910:CYS:SG	1:R:960:VAL:HG13	2.49	0.53
2:L:50:LEU:O	3:L:301:PEG:C1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.44	0.52
2:L:60:ARG:O	9:L:401:HOH:O	2.19	0.52
1:A:882:THR:HA	1:A:962:LEU:O	2.10	0.52
1:R:894:MET:SD	6:R:1104:MGD:H2'	2.49	0.52
1:R:224:ILE:CG1	1:R:402:MET:HE3	2.30	0.52
1:A:272:SER:HA	6:A:1104:MGD:O6	2.09	0.52
1:C:858:ASN:HB3	1:C:861:ALA:HB2	1.93	0.51
1:R:157:ILE:HG22	1:R:182:LEU:HD21	1.92	0.51
1:K:173:TYR:HB2	1:K:645:MET:HE1	1.93	0.51
1:R:194:SER:OG	1:R:195:PRO:HD3	2.10	0.51
1:K:769:ARG:HD3	1:K:805:ASP:HA	1.92	0.50
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.92	0.50
1:C:495:ARG:N	1:C:496:PRO:CD	2.74	0.50
1:C:833:GLU:CG	1:C:858:ASN:HD21	2.24	0.50
1:K:168:GLU:H	1:K:168:GLU:CD	2.19	0.50
2:L:137:LYS:HB2	3:L:301:PEG:H22	1.93	0.50
1:C:184:TYR:CZ	1:C:539:LYS:HE2	2.47	0.50
1:C:698:THR:HG21	1:C:722:SER:OG	2.12	0.50
2:L:137:LYS:N	3:L:302:PEG:H21	2.26	0.50
1:A:88:CYS:HB2	1:A:89:PRO:CD	2.42	0.50
1:A:162:SER:HB2	1:A:551:TRP:O	2.11	0.50
1:R:794:TRP:CE3	1:R:810:PRO:HD3	2.46	0.50
1:K:60:ILE:HG12	1:K:77:ASP:HA	1.93	0.49
1:R:48:SER:HA	1:R:628:ARG:HB2	1.94	0.49
1:R:697:ASP:O	1:R:698:THR:HG23	2.11	0.49
1:A:539:LYS:NZ	1:A:544:GLU:OE1	2.41	0.49
1:C:206:ARG:HB2	1:C:773:TYR:OH	2.13	0.49
1:R:609:CYS:SG	1:R:634:PRO:HB3	2.52	0.49
2:S:137:LYS:CG	8:S:301:GOL:H31	2.41	0.49
1:K:150:LEU:HD11	1:K:152:ASN:HD21	1.77	0.49
1:R:224:ILE:CD1	1:R:402:MET:CE	2.89	0.49
1:K:282:LEU:HD23	1:K:423:ILE:HD13	1.93	0.49
1:A:504:LYS:HD3	1:A:512:PRO:HD3	1.95	0.49
2:B:41:ASN:HA	2:B:42:PRO:C	2.38	0.49
1:K:272:SER:HA	6:K:1103:MGD:O6	2.13	0.49
1:K:451:ASP:O	1:K:727:ASN:ND2	2.46	0.49
1:K:894:MET:SD	6:K:1104:MGD:H2'	2.52	0.48
2:L:137:LYS:CB	3:L:301:PEG:H22	2.43	0.48
1:C:44:LYS:HB2	1:C:66:ASP:HA	1.95	0.48
1:R:928:VAL:O	1:R:938:GLU:HA	2.12	0.48
1:K:442:GLY:HA3	6:K:1103:MGD:C13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:523:ASP:HB2	1:R:526:ARG:HD3	1.94	0.48
2:D:137:LYS:HG3	3:D:401:PEG:H11	1.95	0.48
1:K:691:ASN:C	1:K:691:ASN:HD22	2.22	0.48
1:R:937:LEU:O	1:R:937:LEU:HD12	2.13	0.48
1:K:162:SER:HB2	1:K:551:TRP:O	2.14	0.48
2:S:137:LYS:CB	3:S:302:PEG:C3	2.92	0.48
1:K:459:TRP:CZ2	1:K:466:PRO:CD	2.97	0.47
2:L:143:ASP:HB3	9:L:456:HOH:O	2.14	0.47
1:A:911:GLU:HB3	1:A:947:ILE:CD1	2.44	0.47
1:R:467:ASN:HA	1:R:522:ILE:O	2.14	0.47
1:K:173:TYR:HB2	1:K:645:MET:CE	2.45	0.47
1:A:302:ASN:HB2	1:A:305:LEU:HD22	1.97	0.47
1:R:88:CYS:HB2	1:R:89:PRO:HD2	1.97	0.47
1:R:896:ARG:HD2	1:R:970:VAL:O	2.15	0.47
1:R:883:TYR:O	1:R:963:PRO:HA	2.14	0.47
1:A:495:ARG:N	1:A:496:PRO:CD	2.77	0.47
1:K:86:SER:O	1:K:87:LEU:HD23	2.14	0.47
1:R:459:TRP:CZ2	1:R:466:PRO:CD	2.98	0.47
1:R:937:LEU:HD12	1:R:937:LEU:C	2.40	0.47
1:A:116:THR:HG22	1:A:117:TRP:O	2.15	0.46
1:R:620:ASN:C	1:R:620:ASN:OD1	2.57	0.46
1:R:720:ASP:C	1:R:720:ASP:OD1	2.58	0.46
1:K:883:TYR:O	1:K:963:PRO:HA	2.16	0.46
1:K:909:PHE:CE2	1:K:963:PRO:HG3	2.49	0.46
2:S:137:LYS:HG3	8:S:301:GOL:H31	1.97	0.46
1:A:779:ASP:HB2	9:A:1360:HOH:O	2.14	0.46
1:K:452:GLN:HA	1:K:452:GLN:OE1	2.15	0.46
1:R:161:GLY:HA3	1:R:551:TRP:O	2.16	0.46
2:S:139:ASP:HB3	8:S:301:GOL:H11	1.97	0.46
2:B:171:LEU:O	2:B:175:GLU:HG2	2.15	0.46
1:R:833:GLU:HG2	1:R:858:ASN:HD21	1.80	0.46
1:A:88:CYS:CB	1:A:89:PRO:CD	2.94	0.46
2:D:137:LYS:CG	3:D:401:PEG:H11	2.45	0.46
1:R:714:PHE:CE2	1:R:767:VAL:HG13	2.51	0.46
1:A:212:HIS:CE1	1:A:215:ASP:HB2	2.51	0.46
1:C:1006:TRP:CZ2	3:C:1101:PEG:H32	2.51	0.46
1:K:694:PHE:CD1	1:K:723:THR:HG22	2.51	0.46
1:K:739:ASN:OD1	1:K:741:MET:HB2	2.16	0.46
1:K:833:GLU:CG	1:K:858:ASN:HD21	2.29	0.46
1:K:161:GLY:HA3	1:K:551:TRP:O	2.15	0.46
1:K:669:LYS:O	1:K:670:LEU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:HA3	1:A:551:TRP:O	2.16	0.46
1:A:195:PRO:HA	1:A:990:THR:HG21	1.98	0.46
1:R:404:ALA:HB3	6:R:1103:MGD:O2A	2.16	0.46
1:A:522:ILE:HB	1:A:531:TYR:CE2	2.51	0.45
1:R:225:MET:HE3	1:R:253:VAL:HG11	1.98	0.45
1:C:52:TYR:CD2	1:C:90:LYS:HB3	2.51	0.45
2:L:14:ALA:HB2	2:L:69:PHE:CG	2.51	0.45
1:K:153:ARG:NH1	1:K:523:ASP:OD1	2.44	0.45
1:C:968:TRP:CZ3	1:C:969:MET:HE3	2.51	0.45
1:R:303:ALA:HB1	1:R:356:ILE:HB	1.97	0.45
1:C:910:CYS:SG	1:C:960:VAL:HG13	2.57	0.45
1:R:484:LYS:HE3	1:R:484:LYS:HA	1.99	0.45
1:K:193:HIS:HB2	9:K:1271:HOH:O	2.17	0.45
1:A:297:VAL:HA	1:A:301:THR:HG23	1.98	0.45
1:A:911:GLU:HB3	1:A:947:ILE:HD11	1.99	0.45
1:C:968:TRP:CH2	1:C:969:MET:HE3	2.52	0.45
1:K:579:ASN:O	1:K:607:PRO:HA	2.18	0.45
1:R:640:PRO:O	1:R:644:ILE:HG13	2.17	0.45
2:B:210:TYR:CE2	2:B:212:HIS:HB2	2.51	0.44
1:C:884:ARG:HH22	6:C:1105:MGD:H15	1.64	0.44
1:K:607:PRO:HB2	1:K:638:THR:HG22	1.99	0.44
1:R:691:ASN:C	1:R:691:ASN:ND2	2.74	0.44
1:A:36:GLU:HG3	1:A:41:GLN:HG3	1.99	0.44
1:A:351:HIS:ND1	1:A:352:PRO:HD2	2.33	0.44
3:C:1101:PEG:C1	9:C:1300:HOH:O	2.54	0.44
1:R:915:GLU:OE1	1:R:949:PRO:HD3	2.18	0.44
1:A:625:MET:HE3	1:A:730:HIS:CE1	2.52	0.44
1:C:883:TYR:O	1:C:963:PRO:HA	2.17	0.44
1:A:60:ILE:HG12	1:A:77:ASP:HA	2.00	0.44
1:R:233:HIS:N	1:R:234:PRO:HD3	2.33	0.44
1:A:88:CYS:CB	1:A:89:PRO:HD2	2.48	0.44
1:A:711:VAL:HG12	1:A:713:SER:O	2.18	0.44
1:K:442:GLY:HA3	6:K:1103:MGD:S13	2.57	0.44
1:A:577:ASN:OD1	1:A:586:SER:HB3	2.18	0.44
1:C:306:ILE:HD12	1:C:351:HIS:CD2	2.53	0.44
1:A:625:MET:CE	1:A:730:HIS:CE1	3.01	0.44
1:C:197:VAL:HB	1:C:198:PRO:CD	2.48	0.44
1:R:489:VAL:O	1:R:490:ASN:C	2.60	0.44
2:S:50:LEU:O	3:S:302:PEG:H42	2.18	0.44
1:A:144:LYS:HD3	1:A:148:GLY:O	2.18	0.44
1:C:893:LEU:C	1:C:893:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:873:ASP:HA	1:R:874:PRO:HD3	1.91	0.44
1:A:663:TYR:O	1:A:666:PRO:HD2	2.18	0.43
1:C:351:HIS:ND1	1:C:352:PRO:CD	2.79	0.43
1:C:651:LYS:O	1:C:655:LEU:HD23	2.17	0.43
2:D:41:ASN:HA	2:D:42:PRO:C	2.42	0.43
1:K:304:SER:N	9:K:1207:HOH:O	2.41	0.43
1:C:401:ILE:HG12	1:C:420:MET:HG2	2.00	0.43
1:A:714:PHE:CE2	1:A:767:VAL:HG13	2.53	0.43
1:C:60:ILE:HG12	1:C:77:ASP:HA	2.00	0.43
1:R:41:GLN:HB3	1:R:42:TRP:CD1	2.53	0.43
1:R:195:PRO:HG3	1:R:992:ILE:HG21	2.00	0.43
1:R:342:VAL:O	1:R:343:PRO:C	2.59	0.43
1:R:516:TYR:O	1:R:516:TYR:CD2	2.71	0.43
1:A:55:VAL:HA	1:A:213:TRP:NE1	2.33	0.43
1:A:698:THR:HG21	1:A:722:SER:OG	2.18	0.43
1:A:301:THR:OG1	1:A:303:ALA:HB2	2.19	0.43
1:A:276:ILE:HG13	1:A:416:ASN:OD1	2.18	0.43
1:A:303:ALA:O	1:A:355:VAL:HG22	2.18	0.43
1:C:494:ASN:C	1:C:496:PRO:HD2	2.44	0.43
1:R:697:ASP:C	1:R:698:THR:HG23	2.43	0.43
1:K:209:MET:HG3	1:K:438:ASN:HA	2.01	0.43
1:R:579:ASN:O	1:R:607:PRO:HA	2.19	0.43
1:K:937:LEU:HD12	1:K:937:LEU:O	2.18	0.43
1:R:504:LYS:HD3	1:R:512:PRO:HD3	2.00	0.43
1:C:88:CYS:CB	1:C:89:PRO:HD2	2.48	0.43
1:K:233:HIS:N	1:K:234:PRO:HD3	2.33	0.43
1:R:68:GLN:HG2	1:R:70:ARG:HG2	2.01	0.43
1:R:194:SER:O	1:R:198:PRO:HD2	2.19	0.43
2:B:75:ARG:HB3	2:B:196:VAL:HB	2.01	0.42
2:D:105:PHE:HB2	3:D:401:PEG:C2	2.47	0.42
1:R:88:CYS:CB	1:R:89:PRO:HD2	2.49	0.42
1:R:212:HIS:HD2	9:R:1207:HOH:O	2.02	0.42
1:R:882:THR:HA	1:R:962:LEU:O	2.19	0.42
1:A:529:THR:HA	1:A:532:PHE:CD2	2.54	0.42
1:C:115:ASP:OD1	1:C:115:ASP:C	2.61	0.42
1:C:504:LYS:HD3	1:C:512:PRO:HD3	2.01	0.42
1:A:405:MET:HG2	6:A:1104:MGD:H101	2.00	0.42
1:C:302:ASN:HA	1:C:305:LEU:HD13	2.01	0.42
1:K:868:LYS:O	1:K:869:LYS:HD3	2.19	0.42
1:R:75:GLU:OE2	2:S:155:LYS:NZ	2.40	0.42
1:R:105:THR:O	1:R:637:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:PRO:HD2	1:C:381:GLN:HE22	1.85	0.42
1:A:89:PRO:HG3	2:B:15:CYS:O	2.19	0.42
2:D:14:ALA:HB2	2:D:69:PHE:CG	2.55	0.42
1:R:232:ASN:HA	6:R:1103:MGD:N20	2.35	0.42
1:K:88:CYS:CB	1:K:89:PRO:HD2	2.50	0.42
1:K:757:LEU:O	1:K:758:PHE:C	2.62	0.42
1:K:492:TRP:CE3	1:K:492:TRP:HA	2.55	0.42
1:R:180:LEU:HD21	1:R:652:VAL:HG11	2.02	0.42
1:A:225:MET:HE1	1:A:278:PHE:CD1	2.55	0.42
1:K:860:VAL:O	1:K:988:PRO:HB3	2.18	0.42
1:A:171:TRP:HB2	1:A:690:MET:HE3	2.02	0.42
1:C:209:MET:HG3	1:C:438:ASN:HA	2.02	0.42
1:C:712:PRO:HG2	1:C:716:PHE:CD2	2.55	0.42
1:C:194:SER:O	1:C:198:PRO:HD2	2.19	0.41
1:C:779:ASP:C	1:C:779:ASP:OD1	2.63	0.41
1:K:910:CYS:SG	1:K:960:VAL:CG1	3.08	0.41
1:R:459:TRP:HB3	1:R:460:PRO:HD2	2.02	0.41
1:R:539:LYS:NZ	1:R:544:GLU:OE1	2.52	0.41
1:R:900:TRP:CH2	2:S:24:GLN:HA	2.55	0.41
1:R:706:LYS:HD3	1:R:706:LYS:N	2.35	0.41
1:A:815:PRO:HG2	1:A:816:PHE:CD1	2.55	0.41
1:R:272:SER:HA	6:R:1103:MGD:O6	2.21	0.41
1:R:769:ARG:HD3	1:R:805:ASP:HA	2.02	0.41
1:A:57:CYS:SG	1:A:83:ASN:HB3	2.61	0.41
1:K:504:LYS:NZ	1:K:512:PRO:HD3	2.36	0.41
2:S:75:ARG:HA	2:S:198:VAL:HB	2.02	0.41
1:A:270:ILE:HG13	1:A:375:THR:HB	2.02	0.41
2:B:177:ARG:HD2	9:B:497:HOH:O	2.20	0.41
1:K:452:GLN:OE1	1:K:727:ASN:ND2	2.53	0.41
1:K:617:SER:HA	1:K:626:GLN:O	2.20	0.41
1:A:757:LEU:HD22	1:A:770:ARG:HB2	2.03	0.41
1:A:338:ASP:OD1	1:A:338:ASP:C	2.63	0.41
1:A:609:CYS:HB2	1:A:613:GLU:OE1	2.21	0.41
1:K:459:TRP:CZ2	1:K:466:PRO:HD3	2.56	0.41
1:K:915:GLU:OE1	1:K:949:PRO:HD3	2.20	0.41
2:L:201:LEU:C	2:L:201:LEU:HD23	2.45	0.41
1:A:615:GLU:HA	1:A:628:ARG:O	2.20	0.41
1:A:829:PRO:HA	1:A:835:PRO:HB3	2.02	0.41
1:C:833:GLU:OE2	1:C:989:ASN:ND2	2.53	0.41
1:K:88:CYS:HB2	1:K:89:PRO:HD2	2.03	0.41
1:K:617:SER:HB3	1:K:627:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:675:TRP:N	1:K:675:TRP:CD1	2.89	0.41
1:K:825:ALA:HB1	1:K:827:TYR:O	2.20	0.41
1:R:909:PHE:CE2	1:R:963:PRO:HG3	2.56	0.41
2:S:137:LYS:CA	3:S:302:PEG:C3	2.95	0.41
1:A:442:GLY:HA3	6:A:1104:MGD:S13	2.61	0.41
1:C:917:ALA:HB1	1:C:922:ILE:O	2.21	0.41
1:K:128:GLU:O	1:K:132:ARG:HG2	2.21	0.41
1:K:278:PHE:HZ	1:K:385:VAL:HG11	1.85	0.41
1:R:746:LYS:O	1:R:748:GLN:HG3	2.21	0.41
1:K:38:GLN:CD	1:K:38:GLN:H	2.29	0.40
2:L:137:LYS:HA	3:L:301:PEG:C4	2.51	0.40
1:A:858:ASN:HA	1:A:859:PRO:HD3	1.93	0.40
1:R:422:MET:HG2	1:R:826:LEU:HA	2.03	0.40
1:R:833:GLU:HG2	1:R:858:ASN:ND2	2.35	0.40
1:A:674:ASP:OD2	1:A:693:TYR:OH	2.39	0.40
1:C:314:LYS:O	1:C:315:ASP:C	2.64	0.40
1:C:557:CYS:HB3	9:C:1244:HOH:O	2.21	0.40
1:R:235:ILE:HD12	2:S:158:PRO:HB3	2.04	0.40
1:R:809:ASP:O	1:R:810:PRO:C	2.64	0.40
2:S:14:ALA:HB2	2:S:69:PHE:CG	2.56	0.40
1:A:665:ALA:HB3	1:A:666:PRO:HD3	2.03	0.40
1:C:833:GLU:HG2	1:C:858:ASN:HD21	1.86	0.40
1:K:187:HIS:CD2	1:K:449:SER:HG	2.35	0.40
1:K:506:LEU:O	1:K:671:ASN:HB3	2.21	0.40
1:R:225:MET:HE1	1:R:278:PHE:CG	2.55	0.40
1:A:110:ARG:HG3	1:A:589:TRP:CZ2	2.57	0.40
1:A:403:TYR:CD1	1:A:403:TYR:C	2.99	0.40
1:A:691:ASN:ND2	1:A:691:ASN:C	2.79	0.40
1:A:779:ASP:HB3	1:A:785:TRP:CH2	2.57	0.40
1:C:662:ALA:O	1:C:663:TYR:C	2.65	0.40
1:R:209:MET:CE	1:R:440:LEU:HD23	2.51	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	971/1013 (96%)	922 (95%)	45 (5%)	4 (0%)	30	26
1	C	971/1013 (96%)	934 (96%)	34 (4%)	3 (0%)	36	34
1	K	970/1013 (96%)	906 (93%)	58 (6%)	6 (1%)	21	15
1	R	970/1013 (96%)	926 (96%)	41 (4%)	3 (0%)	36	34
2	B	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	D	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
2	L	212/215 (99%)	199 (94%)	13 (6%)	0	100	100
2	S	212/215 (99%)	200 (94%)	12 (6%)	0	100	100
All	All	4730/4912 (96%)	4493 (95%)	221 (5%)	16 (0%)	36	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	HIS
1	C	1008	HIS
1	A	404	ALA
1	C	404	ALA
1	C	490	ASN
1	K	493	GLN
1	K	670	LEU
1	K	762	SER
1	R	533	TRP
1	R	762	SER
1	K	677	GLU
1	A	762	SER
1	A	870	ALA
1	K	444	SER
1	K	663	TYR
1	R	404	ALA

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	791/818 (97%)	782 (99%)	9 (1%)	65	72
1	C	791/818 (97%)	780 (99%)	11 (1%)	59	66
1	K	790/818 (97%)	772 (98%)	18 (2%)	44	49
1	R	790/818 (97%)	773 (98%)	17 (2%)	45	51
2	B	185/186 (100%)	179 (97%)	6 (3%)	34	36
2	D	185/186 (100%)	183 (99%)	2 (1%)	65	72
2	L	185/186 (100%)	182 (98%)	3 (2%)	55	61
2	S	185/186 (100%)	183 (99%)	2 (1%)	65	72
All	All	3902/4016 (97%)	3834 (98%)	68 (2%)	53	60

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	ILE
1	A	237	PHE
1	A	620	ASN
1	A	691	ASN
1	A	698	THR
1	A	854	LYS
1	A	963	PRO
1	A	984	SER
1	A	1008	HIS
2	B	98	GLU
2	B	115	GLU
2	B	119	SER
2	B	156	THR
2	B	182	LYS
2	B	184	THR
1	C	235	ILE
1	C	237	PHE
1	C	370	LYS
1	C	512	PRO
1	C	620	ASN
1	C	655	LEU
1	C	674	ASP
1	C	697	ASP
1	C	698	THR
1	C	713	SER
1	C	1008	HIS
2	D	20	ILE

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Mol	Chain	Res	Type
2	D	156	THR
1	K	36	GLU
1	K	38	GLN
1	K	179	SER
1	K	237	PHE
1	K	290	LYS
1	K	315	ASP
1	K	472	THR
1	K	492	TRP
1	K	691	ASN
1	K	698	THR
1	K	699	GLU
1	K	700	VAL
1	K	780	LYS
1	K	783	LYS
1	K	800	VAL
1	K	854	LYS
1	K	865	GLU
1	K	969	MET
2	L	20	ILE
2	L	115	GLU
2	L	156	THR
1	R	45	GLN
1	R	128	GLU
1	R	237	PHE
1	R	315	ASP
1	R	336	GLU
1	R	340	ASN
1	R	374	ILE
1	R	465	VAL
1	R	484	LYS
1	R	512	PRO
1	R	680	GLU
1	R	691	ASN
1	R	700	VAL
1	R	751	GLU
1	R	771	ILE
1	R	798	LYS
1	R	860	VAL
2	S	156	THR
2	S	167	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	760	ASN
1	C	106	GLN
1	C	289	ASN
1	C	357	ASN
1	C	383	GLN
1	C	493	GLN
1	C	563	ASN
1	C	709	GLN
1	K	106	GLN
1	K	214	ASN
1	K	289	ASN
1	K	710	GLN
1	R	102	GLN
1	R	152	ASN
1	R	289	ASN
1	R	325	ASN
1	R	727	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 4 are modelled with single atom and 4 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
3	PEG	D	401	-	6,6,6	0.75	0	5,5,5	0.73	0
7	SF4	L	304	2	0,12,12	-	-	-		
3	PEG	S	302	-	6,6,6	0.81	0	5,5,5	0.46	0
7	SF4	C	1106	1	0,12,12	-	-	-		
7	SF4	S	304	2	0,12,12	-	-	-		
7	SF4	L	305	2	0,12,12	-	-	-		
7	SF4	B	301	2	0,12,12	-	-	-		
7	SF4	B	302	2	0,12,12	-	-	-		
6	MGD	C	1105	5	45,52,52	1.50	1 (2%)	54,81,81	1.27	3 (5%)
7	SF4	L	303	2	0,12,12	-	-	-		
7	SF4	B	303	2	0,12,12	-	-	-		
7	SF4	D	404	2	0,12,12	-	-	-		
8	GOL	S	301	-	5,5,5	0.54	0	5,5,5	1.13	0
7	SF4	S	305	2	0,12,12	-	-	-		
6	MGD	K	1104	5	45,52,52	0.82	1 (2%)	54,81,81	1.01	1 (1%)
7	SF4	K	1105	1	0,12,12	-	-	-		
6	MGD	A	1104	5	45,52,52	0.74	2 (4%)	54,81,81	1.20	4 (7%)
6	MGD	C	1104	5	45,52,52	0.63	0	54,81,81	1.00	2 (3%)
7	SF4	A	1106	1	0,12,12	-	-	-		
7	SF4	D	402	2	0,12,12	-	-	-		
3	PEG	L	301	-	6,6,6	0.74	0	5,5,5	0.30	0
3	PEG	L	302	-	6,6,6	1.16	1 (16%)	5,5,5	0.33	0
7	SF4	D	403	2	0,12,12	-	-	-		
7	SF4	S	303	2	0,12,12	-	-	-		
6	MGD	R	1104	5	45,52,52	0.71	1 (2%)	54,81,81	1.15	5 (9%)
6	MGD	A	1105	5	45,52,52	0.75	1 (2%)	54,81,81	1.09	4 (7%)
3	PEG	C	1101	-	6,6,6	0.40	0	5,5,5	0.26	0
6	MGD	R	1103	5	45,52,52	0.53	0	54,81,81	0.95	2 (3%)
7	SF4	R	1105	1	0,12,12	-	-	-		
3	PEG	A	1101	-	6,6,6	0.21	0	5,5,5	0.14	0
6	MGD	K	1103	5	45,52,52	1.07	1 (2%)	54,81,81	1.11	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	401	-	-	2/4/4/4	-
7	SF4	L	304	2	-	-	0/6/5/5
3	PEG	S	302	-	-	2/4/4/4	-
7	SF4	C	1106	1	-	-	0/6/5/5
7	SF4	S	304	2	-	-	0/6/5/5
7	SF4	L	305	2	-	-	0/6/5/5
7	SF4	B	301	2	-	-	0/6/5/5
7	SF4	B	302	2	-	-	0/6/5/5
6	MGD	C	1105	5	-	6/22/66/66	0/6/6/6
7	SF4	L	303	2	-	-	0/6/5/5
7	SF4	B	303	2	-	-	0/6/5/5
7	SF4	D	404	2	-	-	0/6/5/5
8	GOL	S	301	-	-	4/4/4/4	-
7	SF4	S	305	2	-	-	0/6/5/5
6	MGD	K	1104	5	-	6/22/66/66	0/6/6/6
7	SF4	K	1105	1	-	-	0/6/5/5
6	MGD	A	1104	5	-	3/22/66/66	0/6/6/6
6	MGD	C	1104	5	-	2/22/66/66	0/6/6/6
7	SF4	A	1106	1	-	-	0/6/5/5
7	SF4	D	402	2	-	-	0/6/5/5
3	PEG	L	301	-	-	4/4/4/4	-
3	PEG	L	302	-	-	3/4/4/4	-
7	SF4	D	403	2	-	-	0/6/5/5
7	SF4	S	303	2	-	-	0/6/5/5
6	MGD	R	1104	5	-	6/22/66/66	0/6/6/6
6	MGD	A	1105	5	-	5/22/66/66	0/6/6/6
3	PEG	C	1101	-	-	2/4/4/4	-
6	MGD	R	1103	5	-	1/22/66/66	0/6/6/6
7	SF4	R	1105	1	-	-	0/6/5/5
3	PEG	A	1101	-	-	4/4/4/4	-
6	MGD	K	1103	5	-	2/22/66/66	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1105	MGD	C23-C14	9.12	1.60	1.53
6	K	1103	MGD	C23-C14	6.13	1.58	1.53
6	K	1104	MGD	C23-C14	3.62	1.56	1.53
6	A	1105	MGD	C23-C14	3.40	1.56	1.53
6	R	1104	MGD	C23-C14	2.81	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1104	MGD	C23-N22	-2.56	1.40	1.45
3	L	302	PEG	O1-C1	-2.18	1.30	1.42
6	A	1104	MGD	C10-C11	-2.00	1.49	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1105	MGD	O11-C23-C14	5.56	112.67	108.96
6	A	1104	MGD	O11-C23-C14	4.45	111.93	108.96
6	R	1104	MGD	O11-C23-C14	3.83	111.52	108.96
6	C	1105	MGD	O11-C23-N22	-3.76	104.70	108.57
6	A	1105	MGD	O11-C23-C14	3.60	111.37	108.96
6	A	1104	MGD	C19-N20-C21	3.39	119.56	113.43
6	K	1103	MGD	O11-C23-N22	-3.20	105.27	108.57
6	C	1104	MGD	C19-N20-C21	2.97	118.79	113.43
6	R	1104	MGD	C17-C16-N15	2.92	124.61	116.76
6	R	1104	MGD	C19-N20-C21	2.91	118.68	113.43
6	K	1103	MGD	C19-N20-C21	2.88	118.62	113.43
6	K	1104	MGD	O4'-C1'-C2'	-2.87	100.38	106.64
6	A	1105	MGD	C19-N20-C21	2.67	118.25	113.43
6	R	1103	MGD	PA-O3B-PB	2.57	141.64	132.83
6	C	1104	MGD	O11-C23-N22	2.53	111.16	108.57
6	R	1104	MGD	O4'-C1'-C2'	-2.52	101.14	106.64
6	R	1103	MGD	C19-N20-C21	2.52	117.97	113.43
6	C	1105	MGD	C19-N20-C21	2.42	117.80	113.43
6	A	1105	MGD	PA-O3B-PB	-2.26	125.08	132.83
6	K	1103	MGD	PA-O3B-PB	2.22	140.45	132.83
6	K	1103	MGD	O11-C23-C14	2.19	110.43	108.96
6	A	1104	MGD	PA-O3B-PB	2.14	140.16	132.83
6	R	1104	MGD	O2A-PA-O1A	2.08	122.50	112.24
6	K	1103	MGD	O2A-PA-O3A	2.07	117.34	107.75
6	A	1105	MGD	O5'-C5'-C4'	2.03	115.99	108.99
6	A	1104	MGD	C17-C16-N15	2.03	122.21	116.76

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1105	MGD	C5'-O5'-PB-O1B
6	A	1105	MGD	C5'-O5'-PB-O2B
6	A	1105	MGD	C4'-C5'-O5'-PB
6	C	1105	MGD	C5'-O5'-PB-O2B

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Mol	Chain	Res	Type	Atoms
6	C	1105	MGD	C4'-C5'-O5'-PB
6	C	1105	MGD	O4'-C4'-C5'-O5'
6	K	1103	MGD	PA-O3B-PB-O5'
6	K	1104	MGD	C5'-O5'-PB-O2B
6	K	1104	MGD	C4'-C5'-O5'-PB
6	R	1104	MGD	C5'-O5'-PB-O2B
6	R	1104	MGD	C4'-C5'-O5'-PB
6	R	1104	MGD	O4'-C4'-C5'-O5'
8	S	301	GOL	C1-C2-C3-O3
6	K	1104	MGD	O4'-C4'-C5'-O5'
3	L	302	PEG	O2-C3-C4-O4
3	L	302	PEG	O1-C1-C2-O2
8	S	301	GOL	O1-C1-C2-C3
3	S	302	PEG	O1-C1-C2-O2
8	S	301	GOL	O2-C2-C3-O3
3	D	401	PEG	O1-C1-C2-O2
3	C	1101	PEG	O2-C3-C4-O4
3	L	301	PEG	O2-C3-C4-O4
3	A	1101	PEG	O2-C3-C4-O4
6	K	1104	MGD	C3'-C4'-C5'-O5'
6	C	1104	MGD	O3A-C10-C11-O11
6	A	1104	MGD	PA-O3B-PB-O5'
6	R	1103	MGD	PA-O3B-PB-O5'
3	S	302	PEG	C1-C2-O2-C3
3	A	1101	PEG	C1-C2-O2-C3
6	C	1105	MGD	C5'-O5'-PB-O3B
6	R	1104	MGD	C5'-O5'-PB-O3B
8	S	301	GOL	O1-C1-C2-O2
3	L	301	PEG	C4-C3-O2-C2
6	C	1105	MGD	C5'-O5'-PB-O1B
6	R	1104	MGD	C5'-O5'-PB-O1B
3	C	1101	PEG	C1-C2-O2-C3
3	A	1101	PEG	O1-C1-C2-O2
3	A	1101	PEG	C4-C3-O2-C2
3	D	401	PEG	O2-C3-C4-O4
6	C	1105	MGD	C3'-C4'-C5'-O5'
6	R	1104	MGD	C3'-C4'-C5'-O5'
3	L	302	PEG	C1-C2-O2-C3
6	A	1104	MGD	O3A-C10-C11-O11
3	L	301	PEG	O1-C1-C2-O2
6	C	1104	MGD	PA-O3B-PB-O5'
6	A	1105	MGD	C5'-O5'-PB-O3B

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Mol	Chain	Res	Type	Atoms
6	K	1104	MGD	C5'-O5'-PB-O3B
6	A	1105	MGD	O4'-C4'-C5'-O5'
6	A	1104	MGD	PA-O3B-PB-O1B
6	K	1103	MGD	PA-O3B-PB-O1B
3	L	301	PEG	C1-C2-O2-C3
6	K	1104	MGD	C5'-O5'-PB-O1B

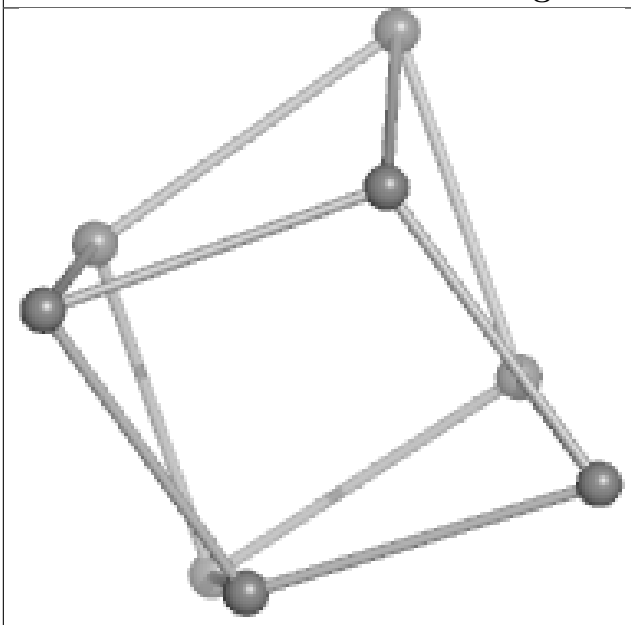
There are no ring outliers.

14 monomers are involved in 54 short contacts:

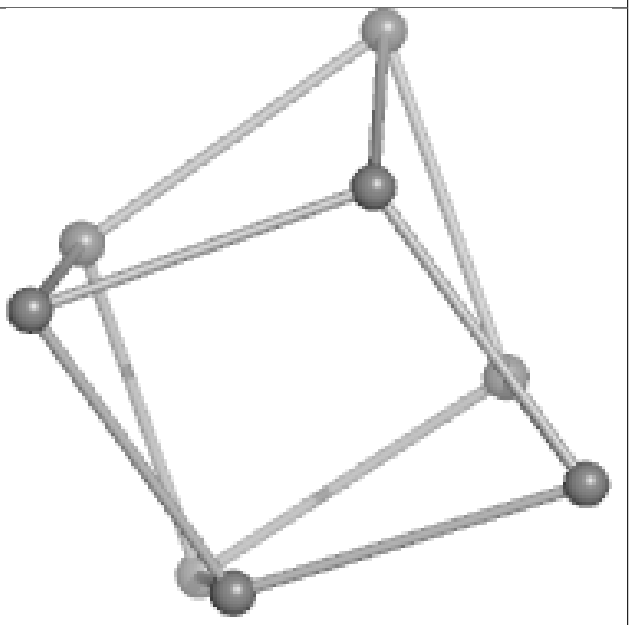
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	PEG	4	0
3	S	302	PEG	13	0
6	C	1105	MGD	2	0
8	S	301	GOL	4	0
6	K	1104	MGD	1	0
6	A	1104	MGD	3	0
7	A	1106	SF4	1	0
3	L	301	PEG	9	0
3	L	302	PEG	4	0
6	R	1104	MGD	2	0
6	A	1105	MGD	1	0
3	C	1101	PEG	4	0
6	R	1103	MGD	3	0
6	K	1103	MGD	3	0

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.

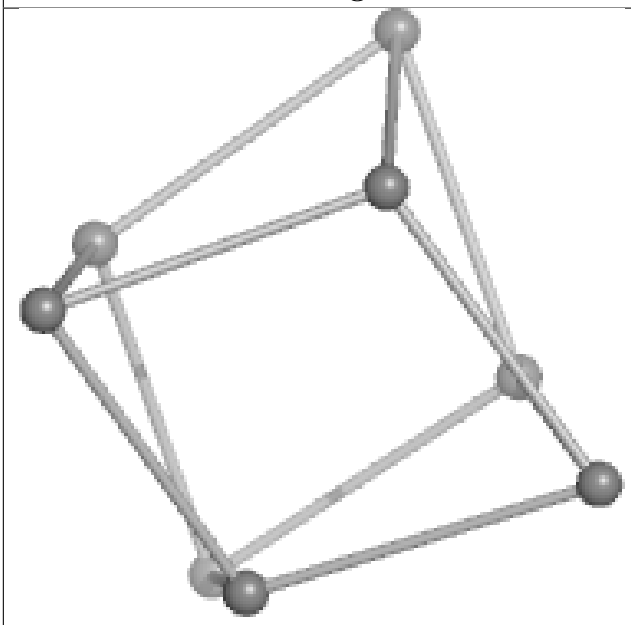
Ligand SF4 L 304



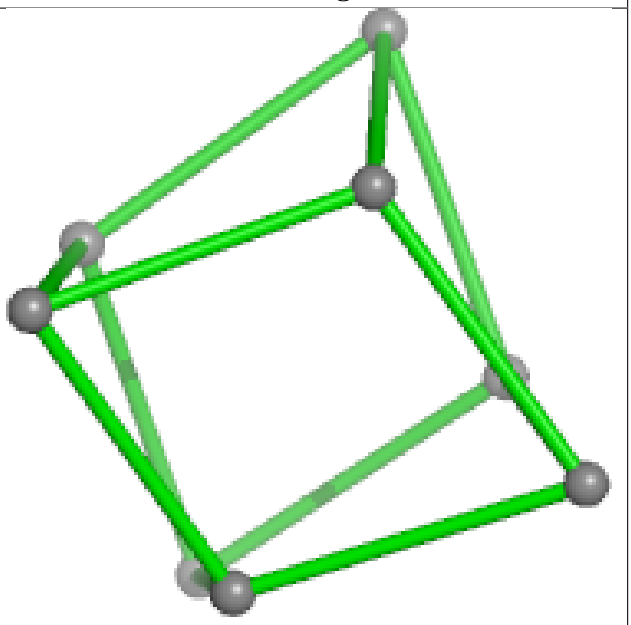
Bond lengths



Bond angles

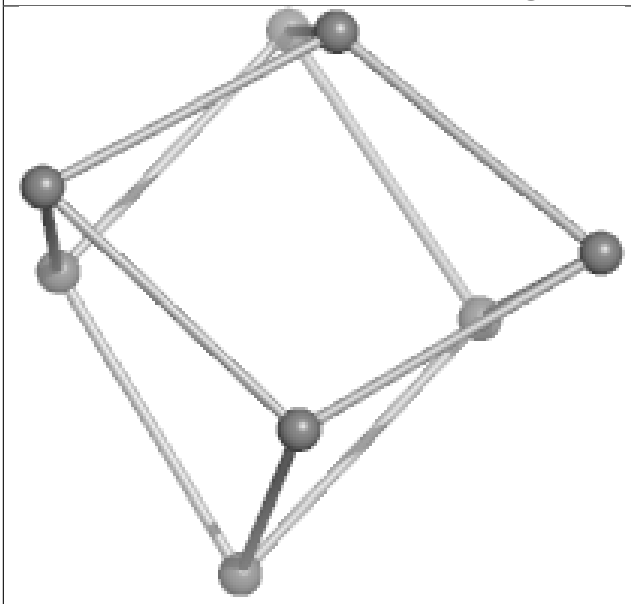


Torsions

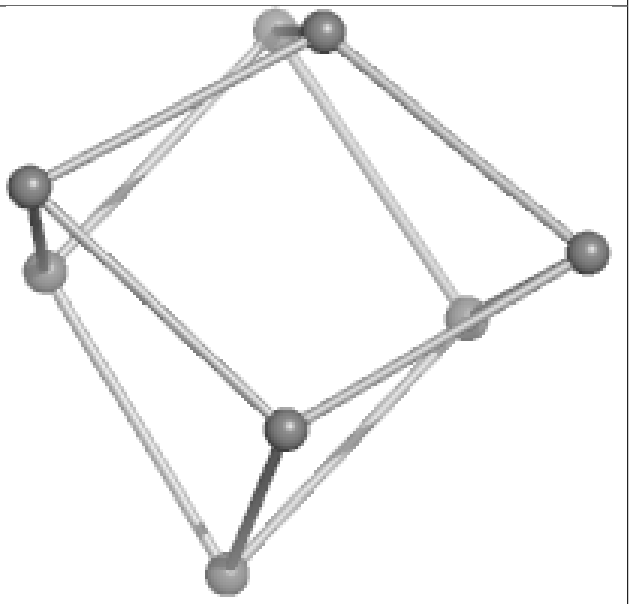


Rings

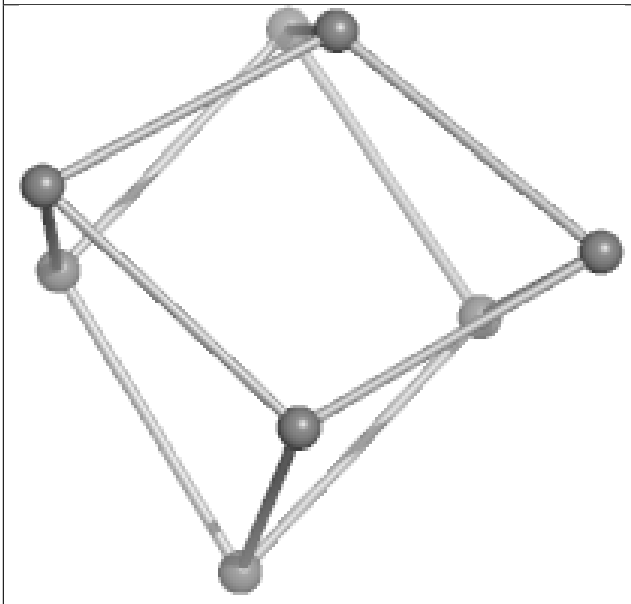
Ligand SF4 C 1106



Bond lengths



Bond angles



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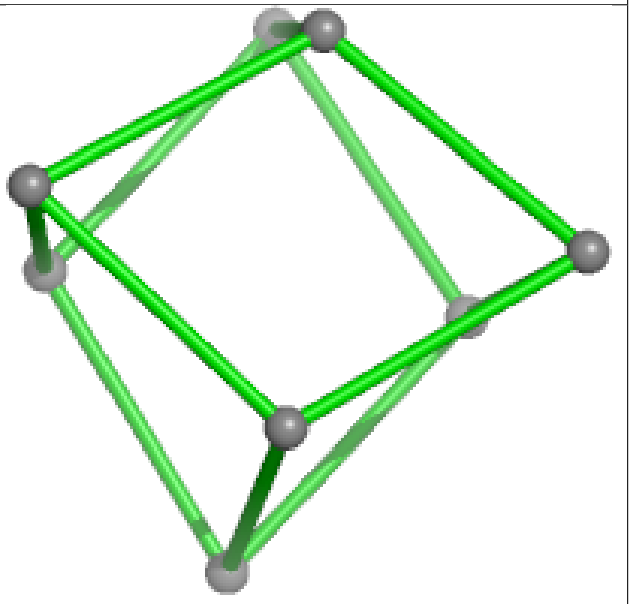
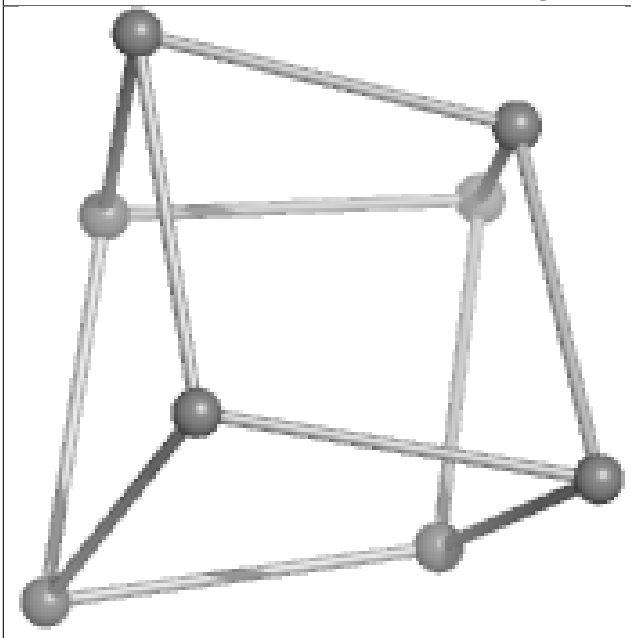


Rings

Ligand SF4 S 304



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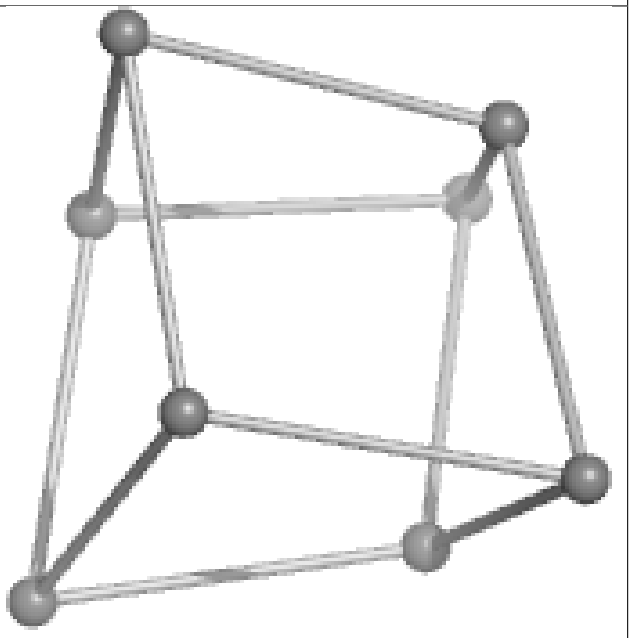
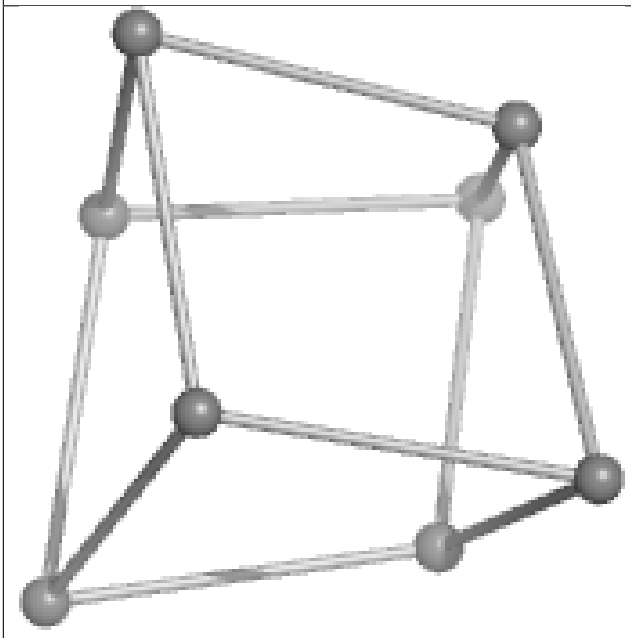
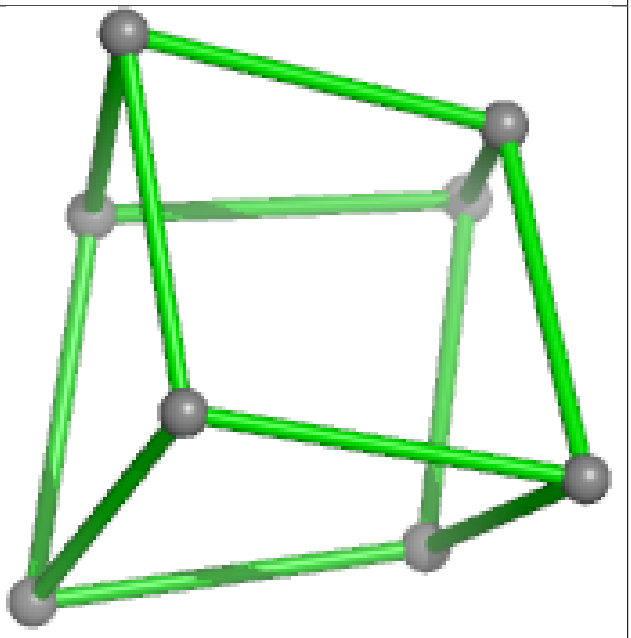


Bond angles

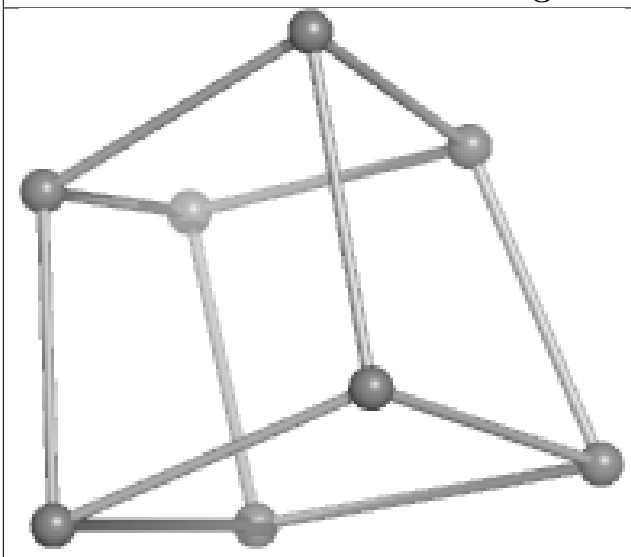


Torsions

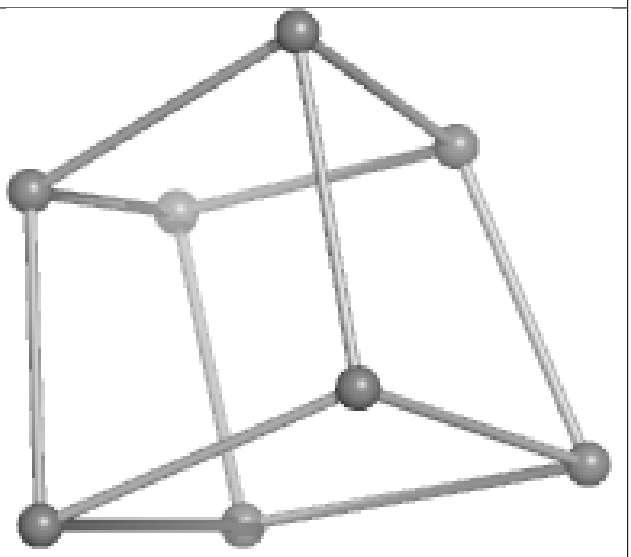


Rings

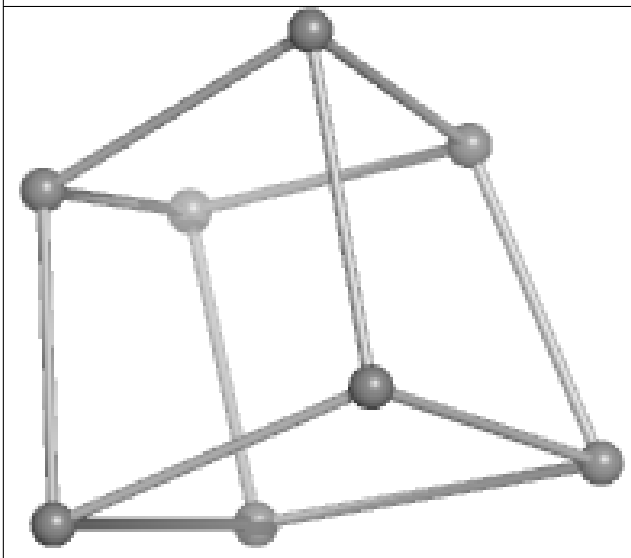
Ligand SF4 L 305



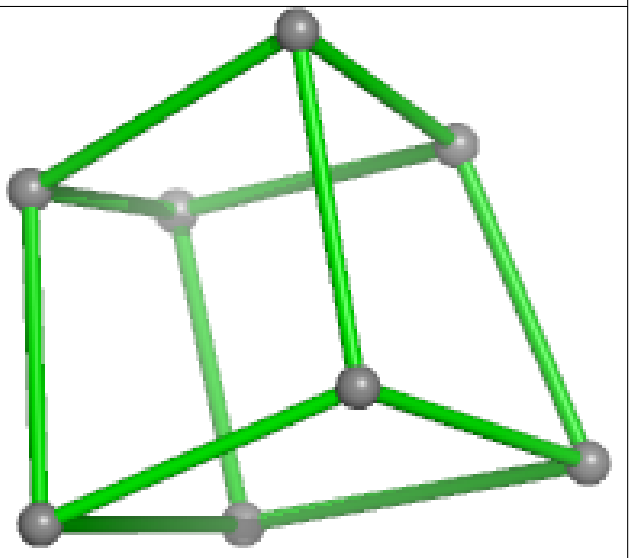
Bond lengths



Bond angles

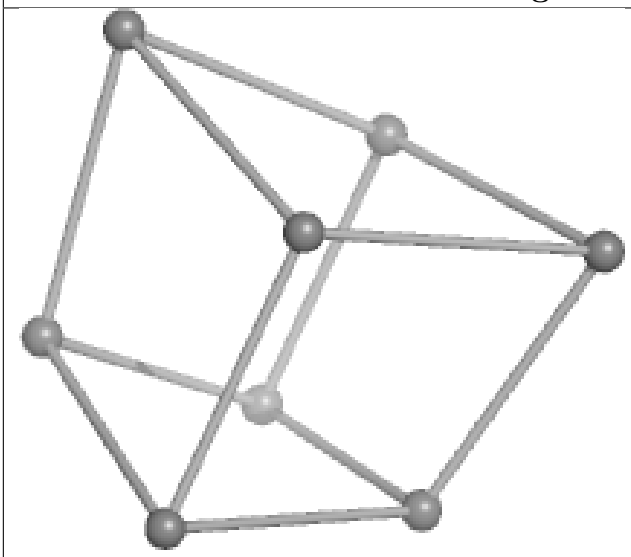


Torsions

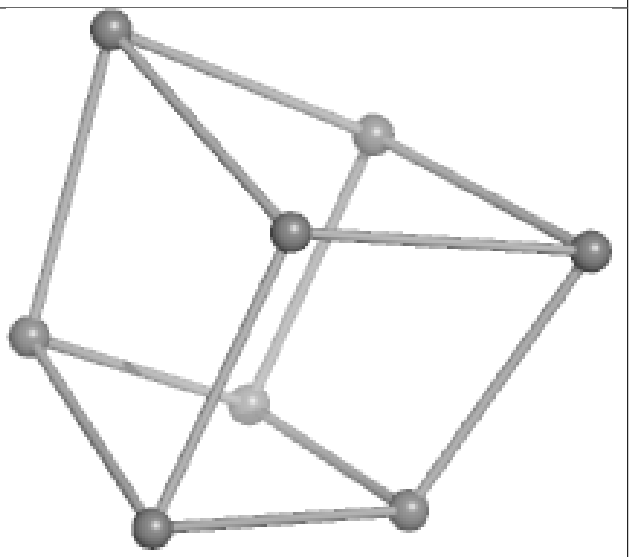


Rings

Ligand SF4 B 301



Bond lengths



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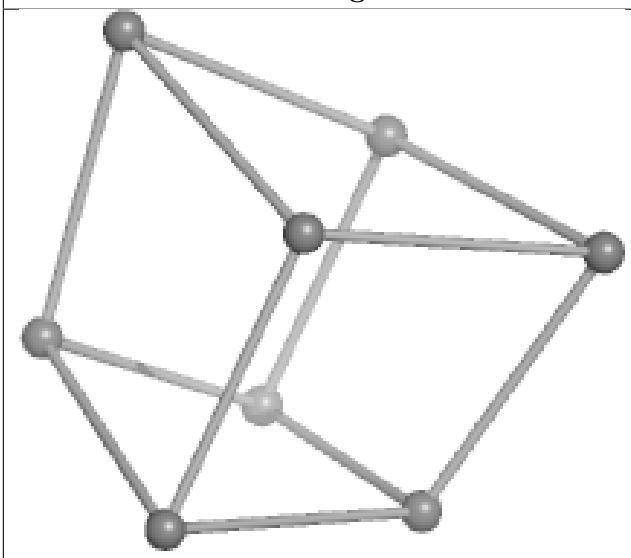

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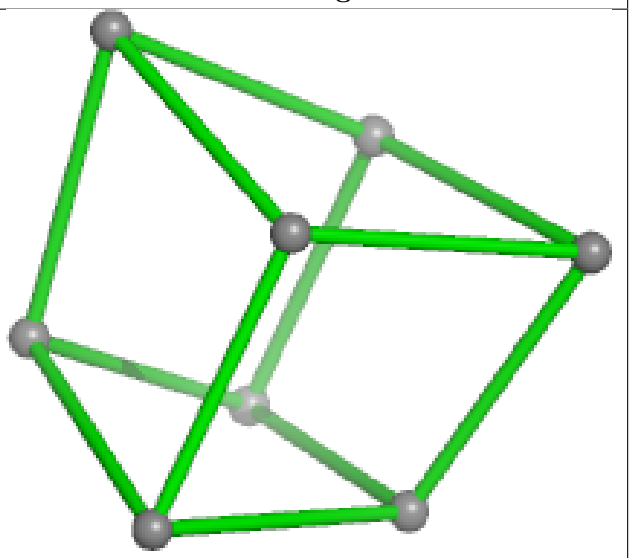

Rings

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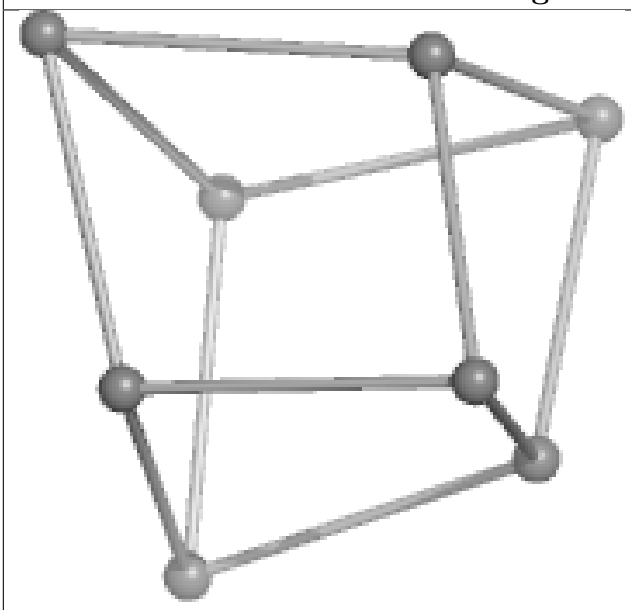

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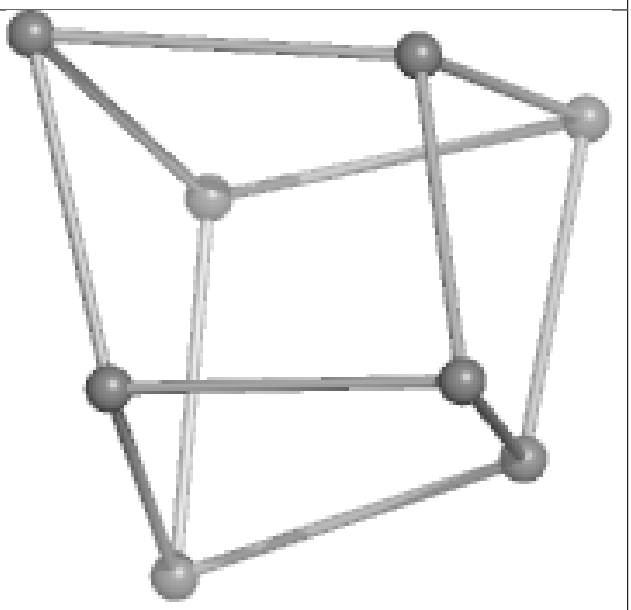

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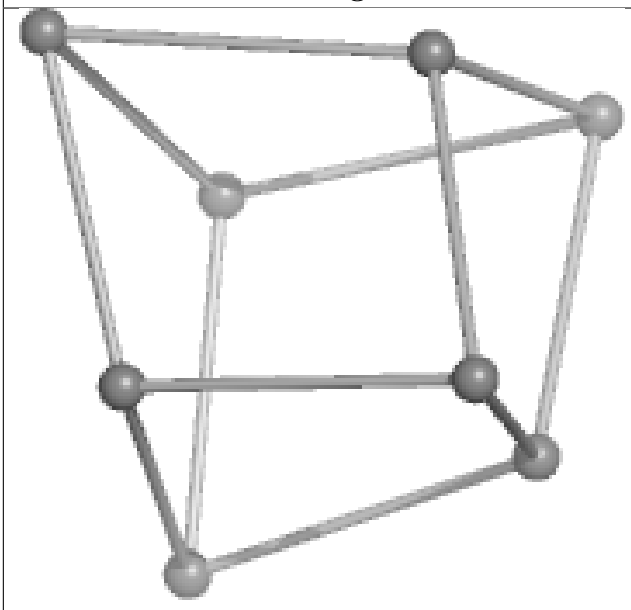

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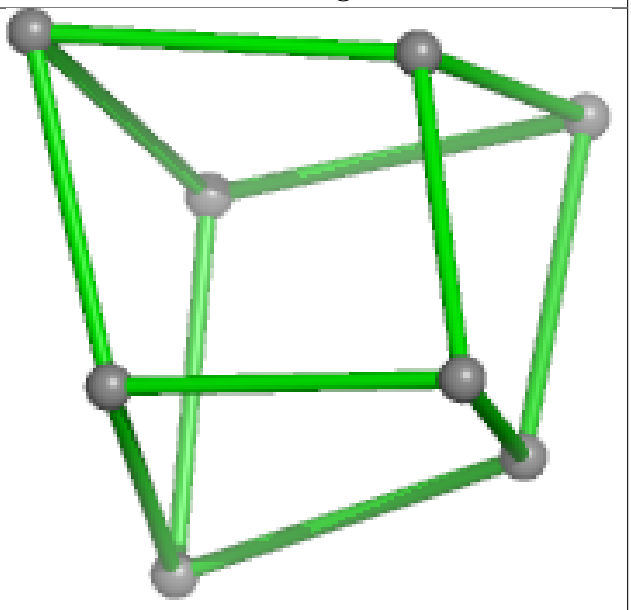
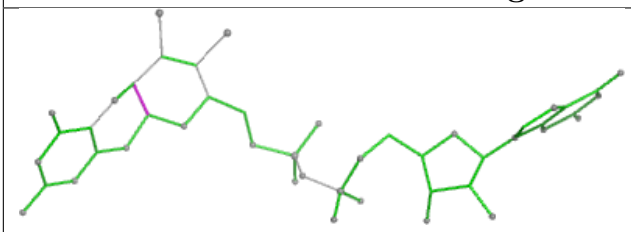
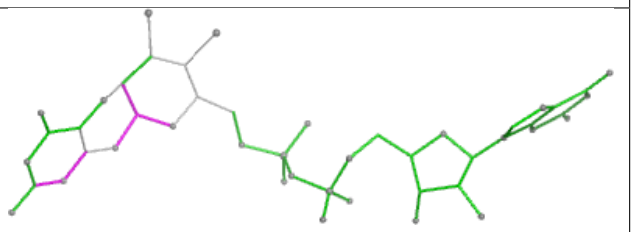


Rings

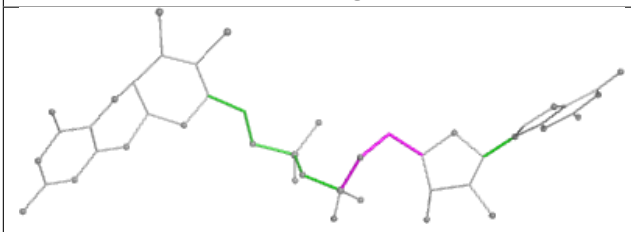
Ligand MGD C 1105



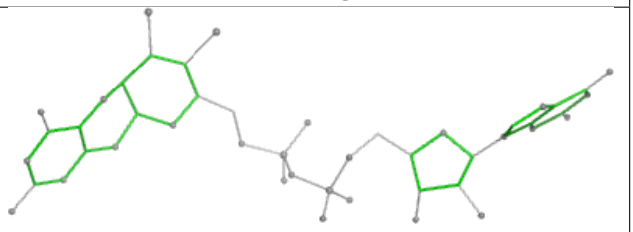
Bond lengths



Bond angles

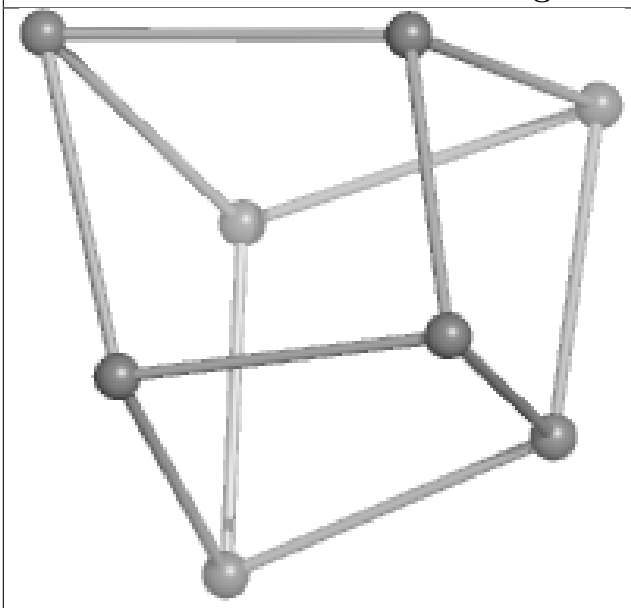


Torsions



Rings

Ligand SF4 L 303



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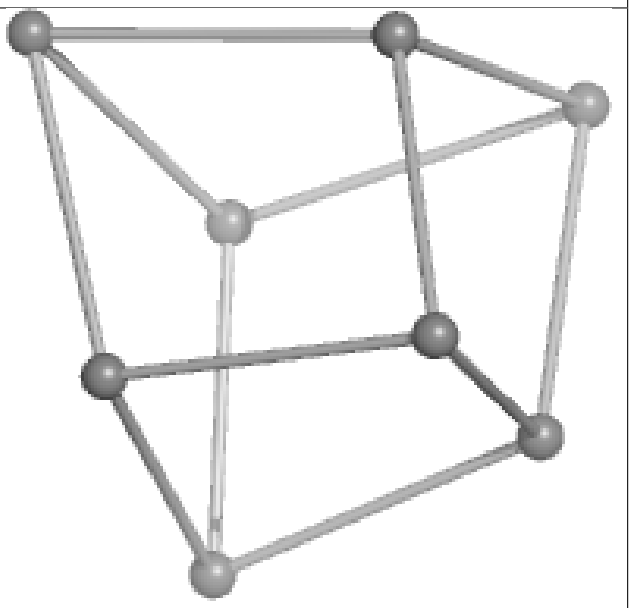

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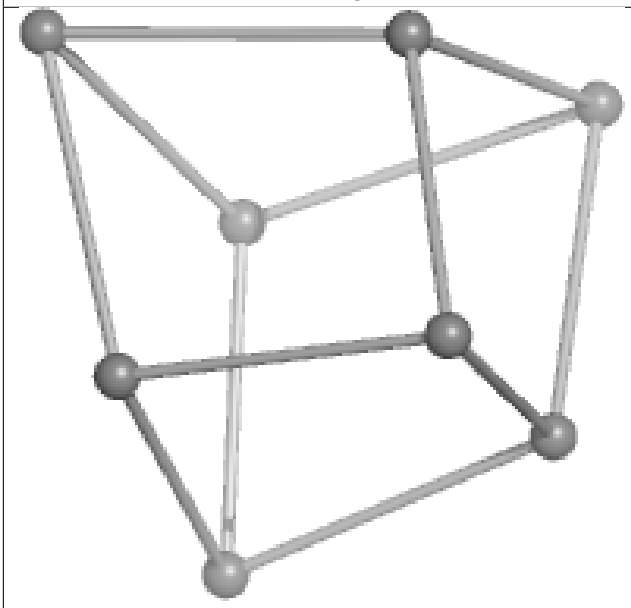
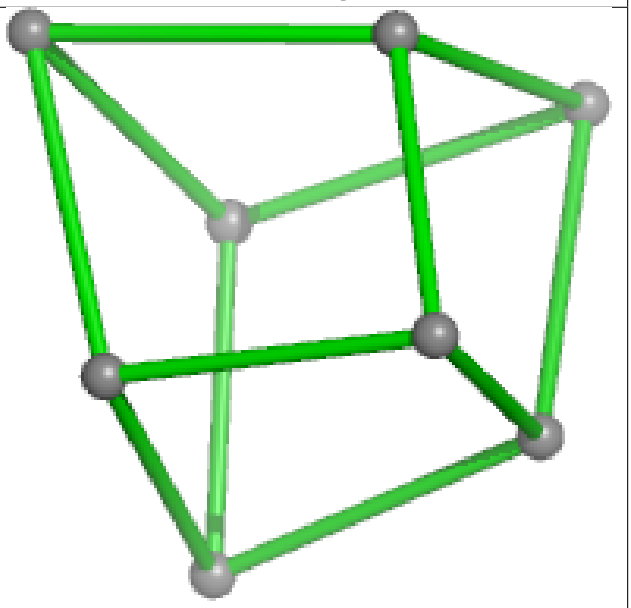
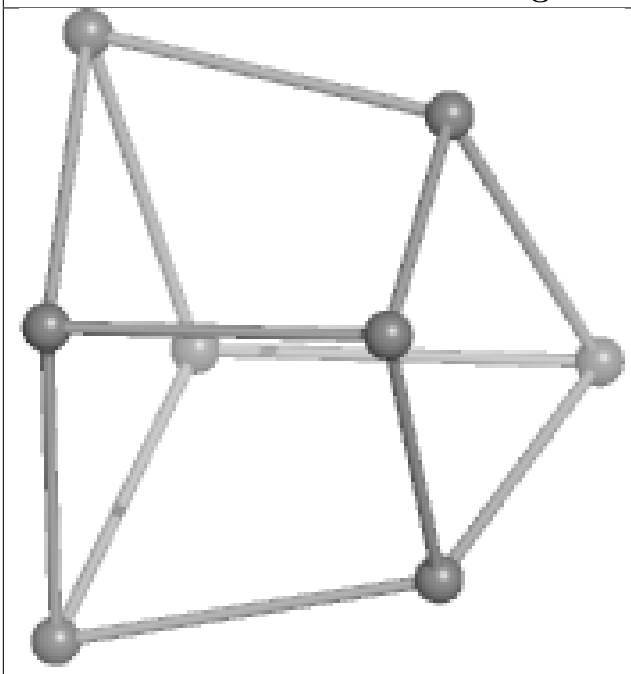


Torsions



Rings

Ligand SF4 B 303



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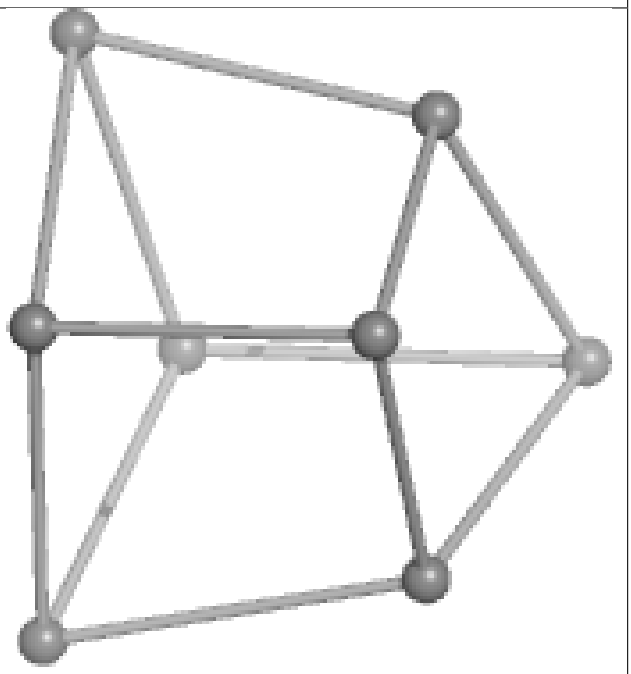

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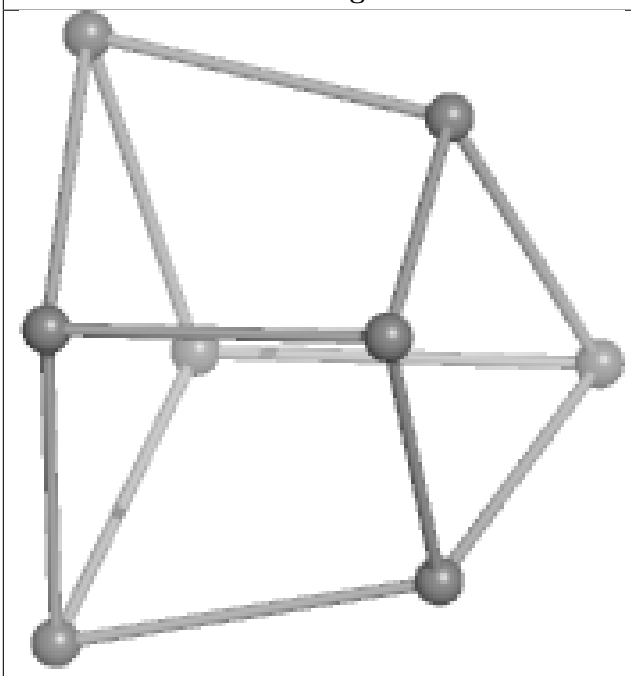

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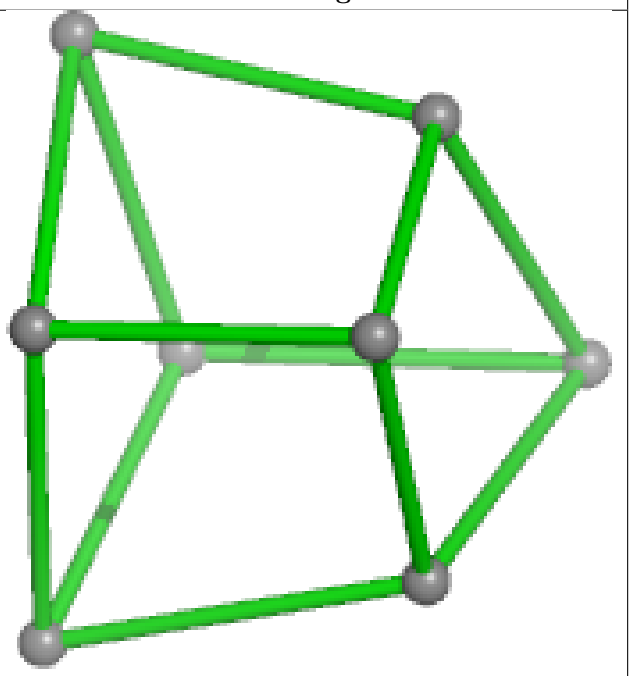
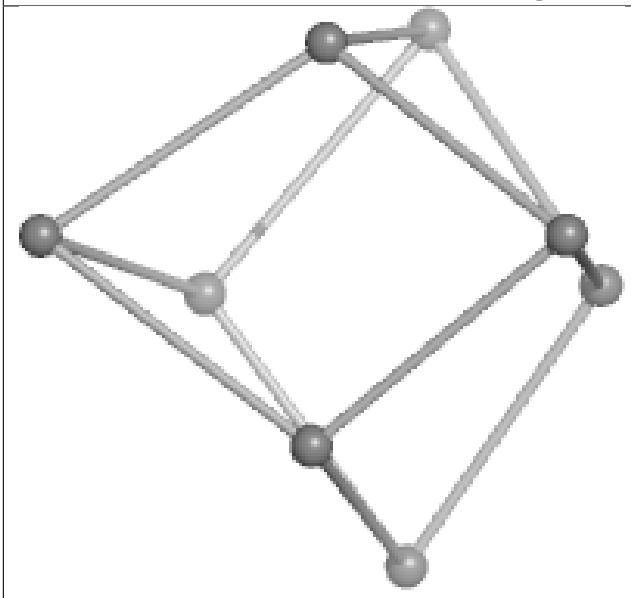


Rings

Ligand SF4 D 404



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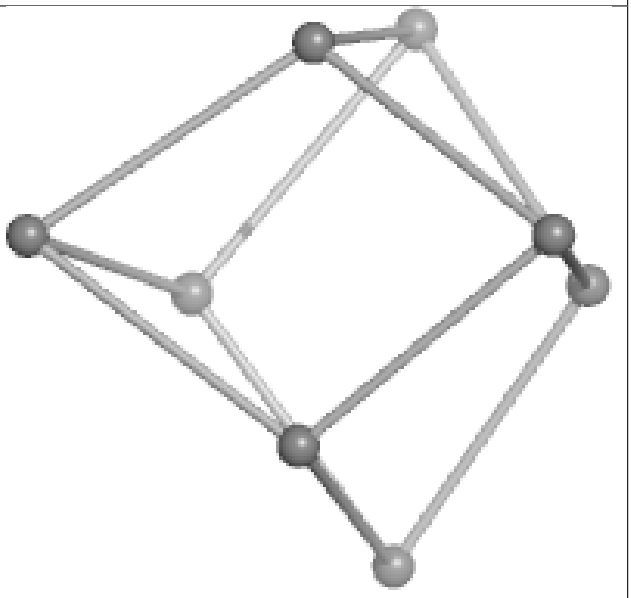
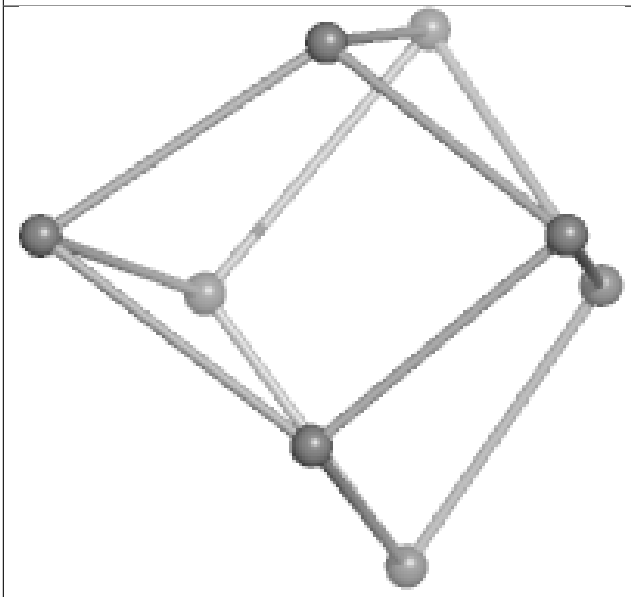


Bond angles



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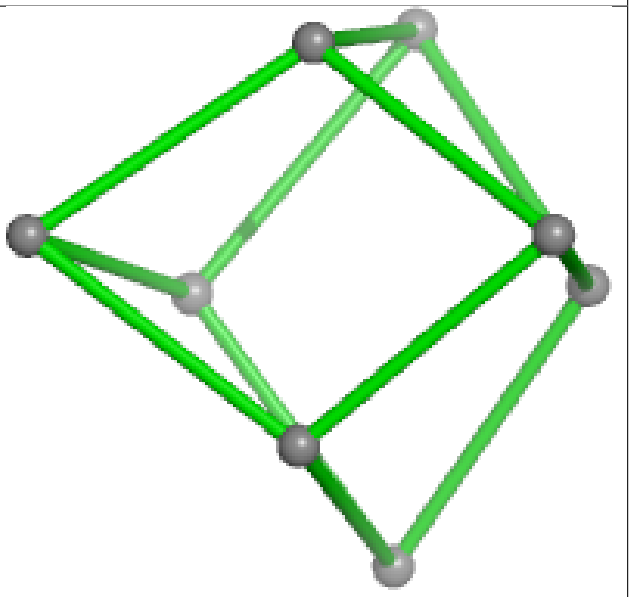
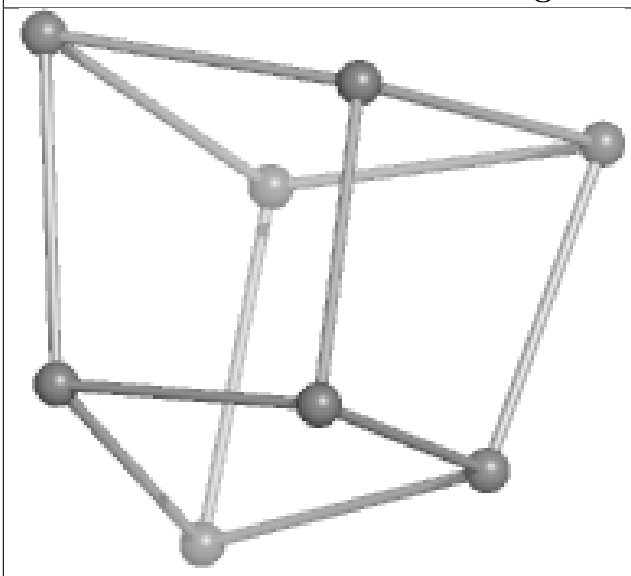


Rings

Ligand SF4 S 305



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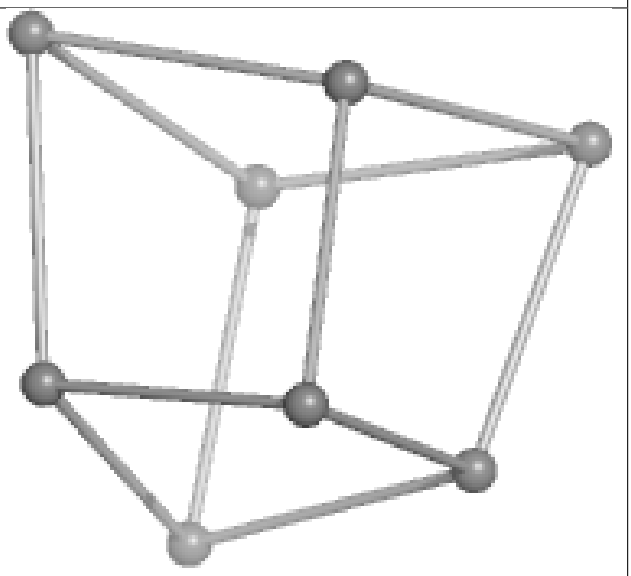

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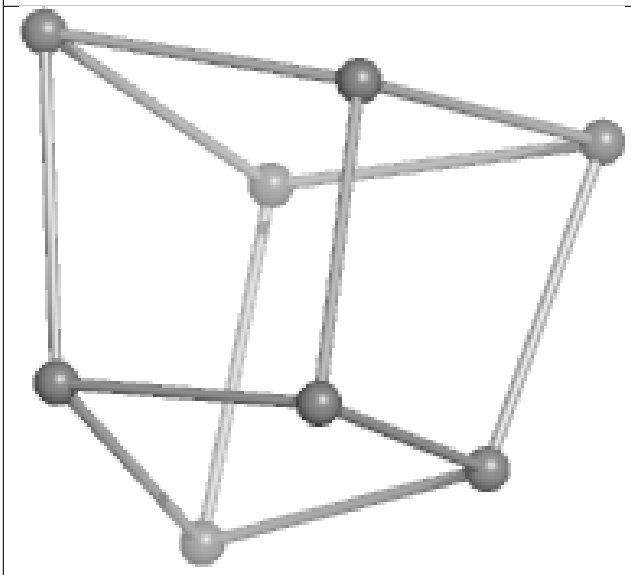

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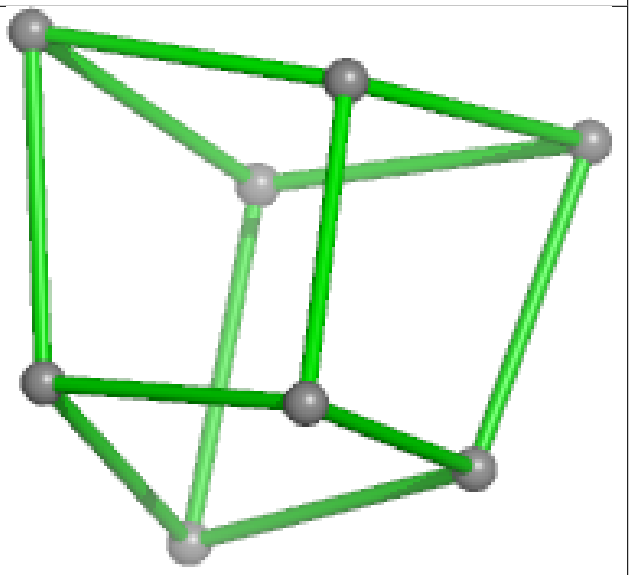
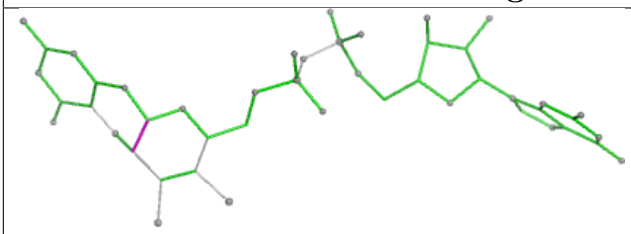


Rings

Ligand MGD K 1104



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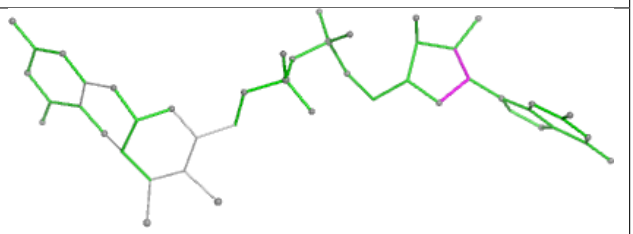

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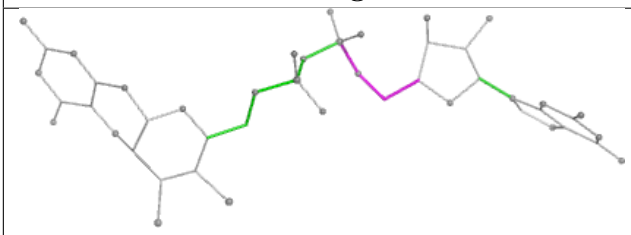

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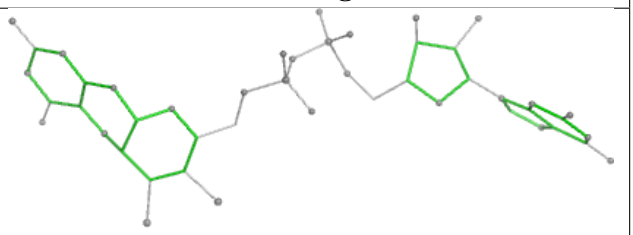
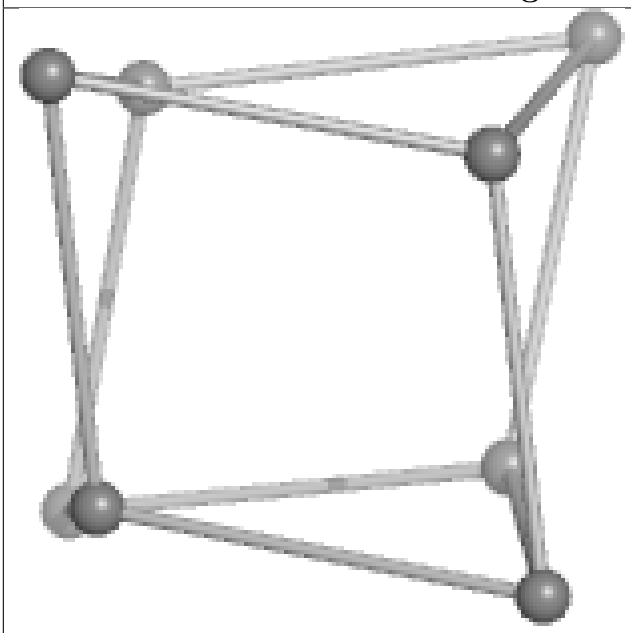


Rings

Ligand SF4 K 1105



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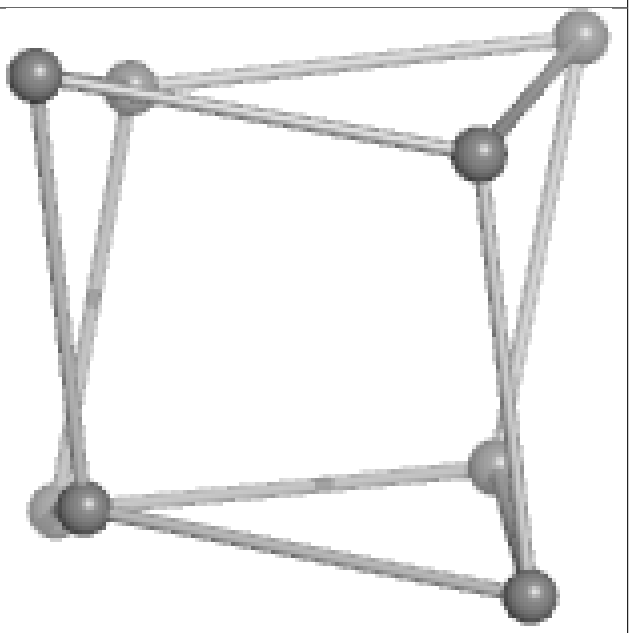

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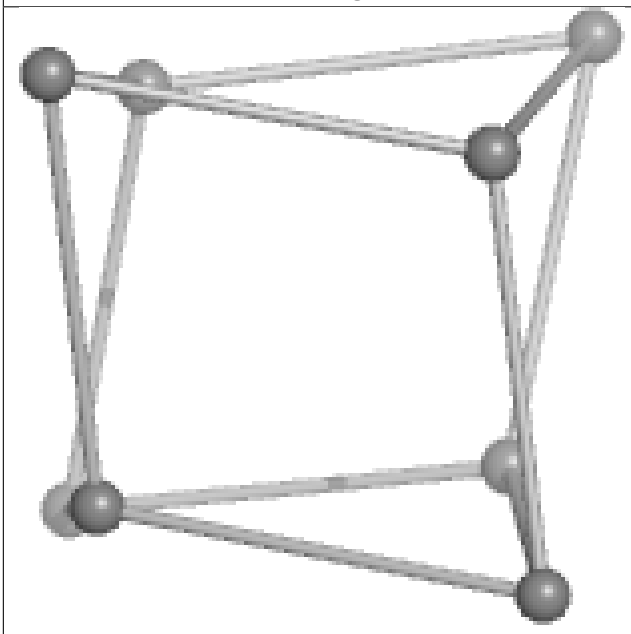

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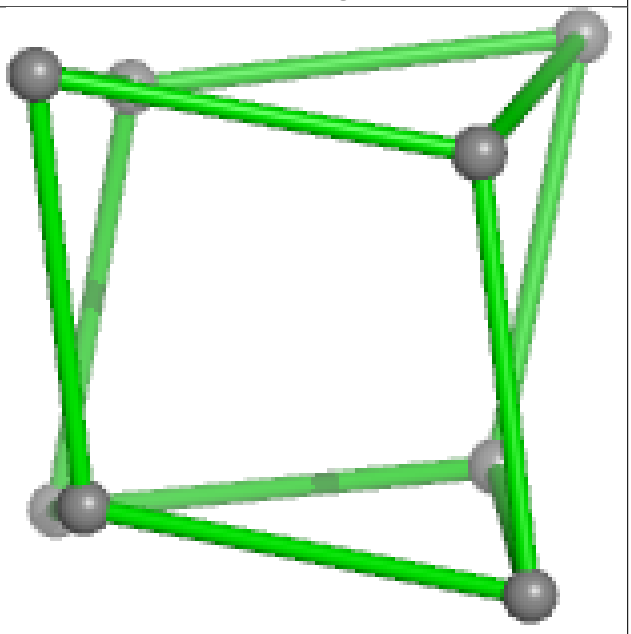
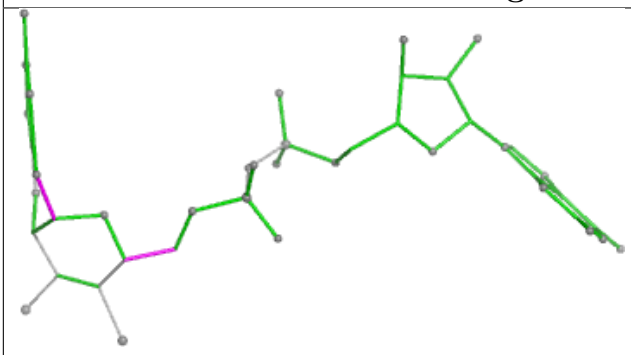


Rings

Ligand MGD A 1104



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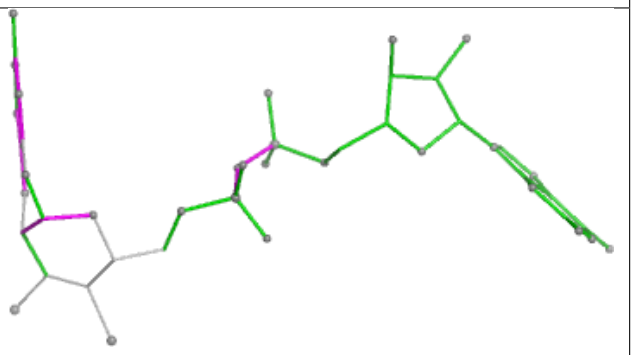

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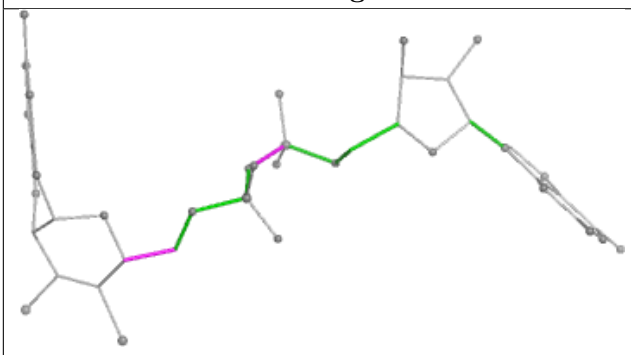

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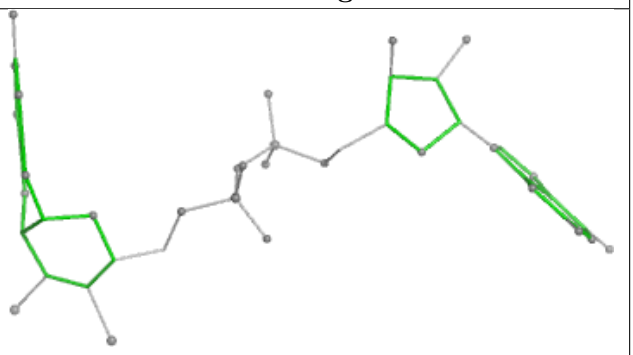
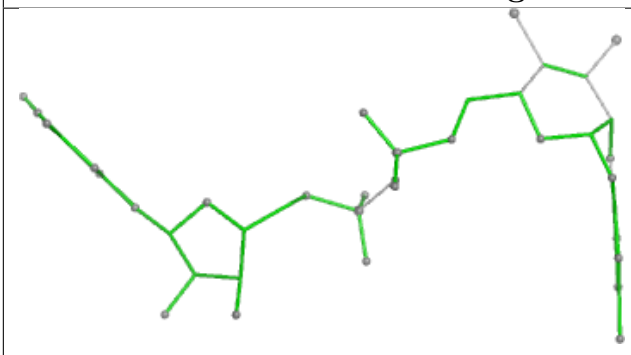


Rings

Ligand MGD C 1104



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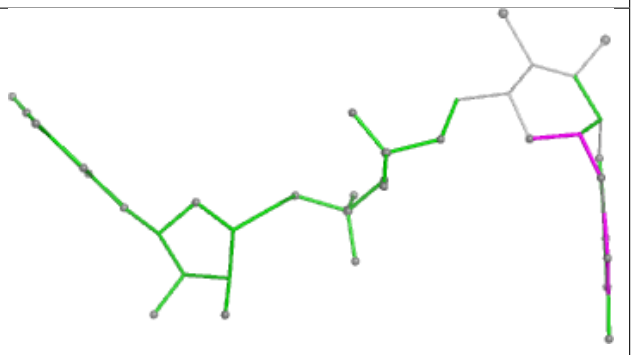

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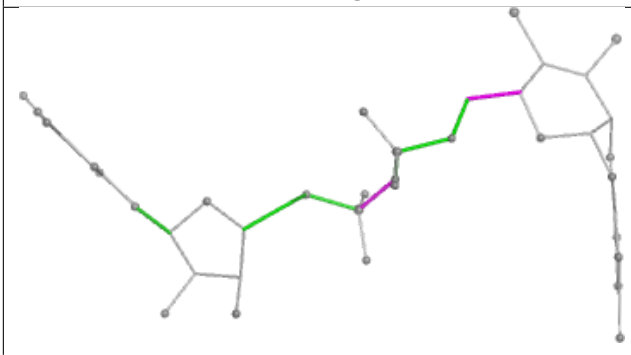

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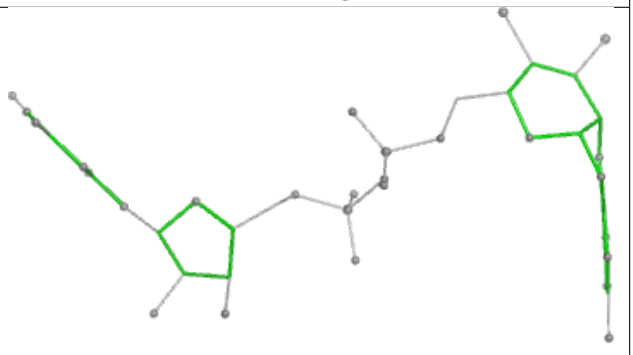
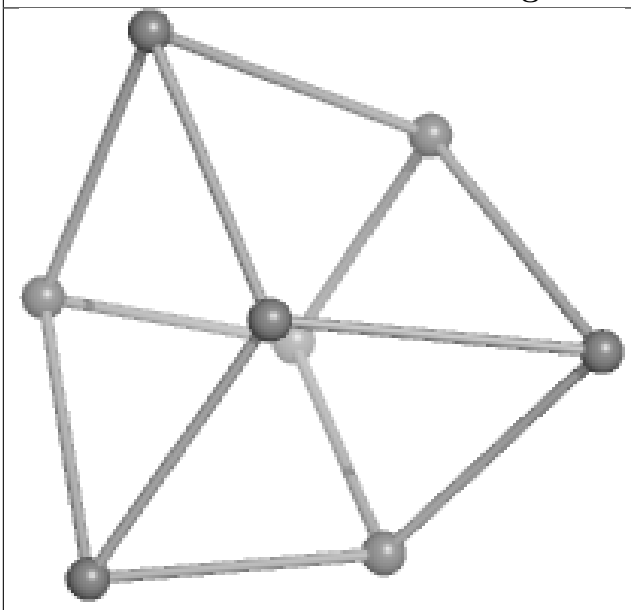


Rings

Ligand SF4 A 1106



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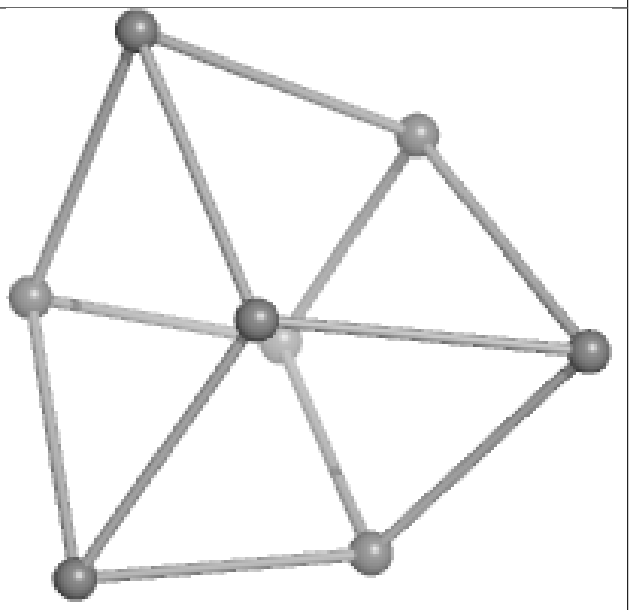

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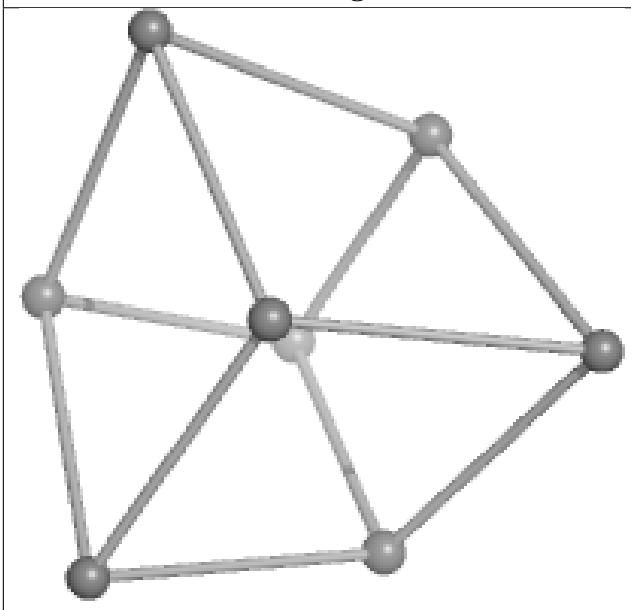

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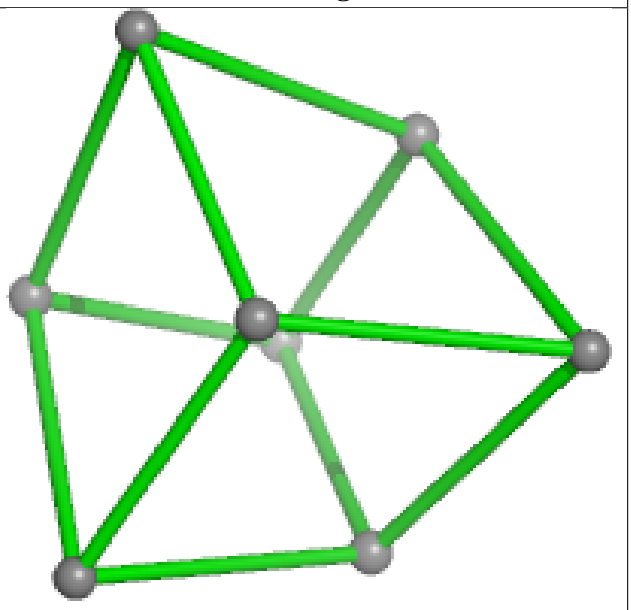
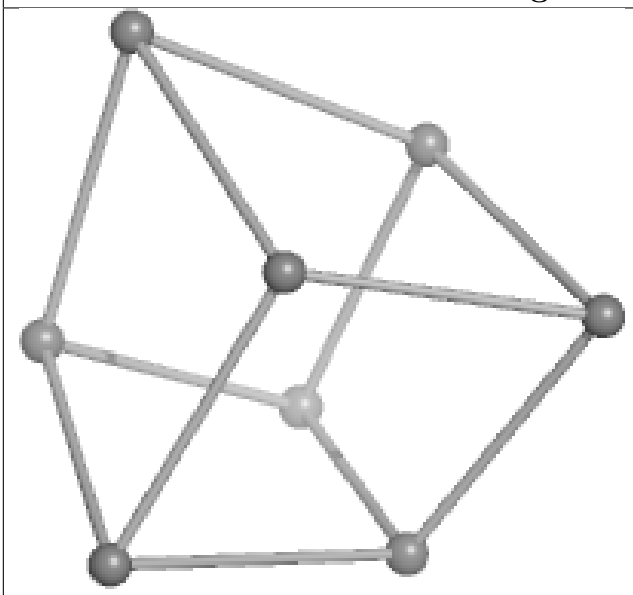


Rings

Ligand SF4 D 402



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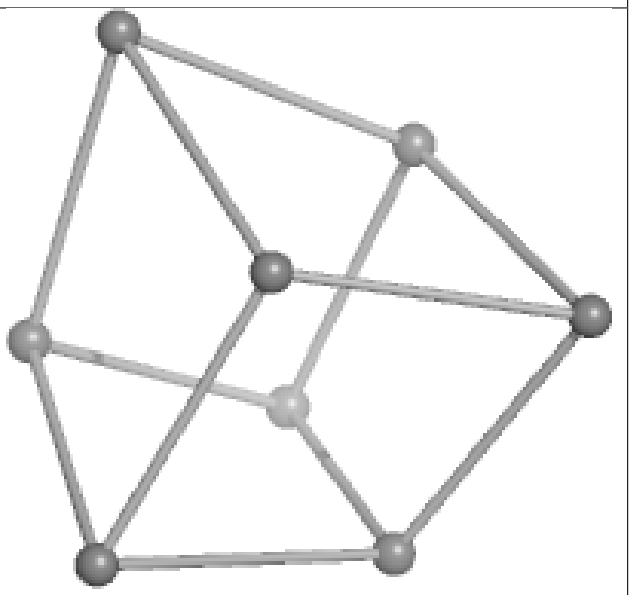

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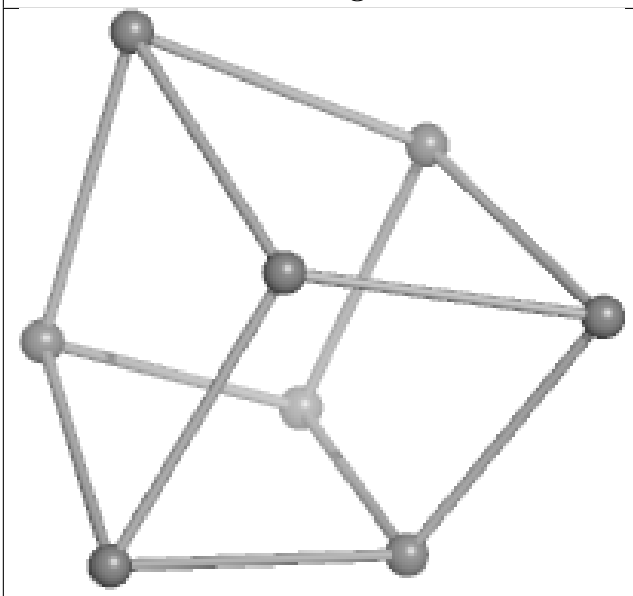

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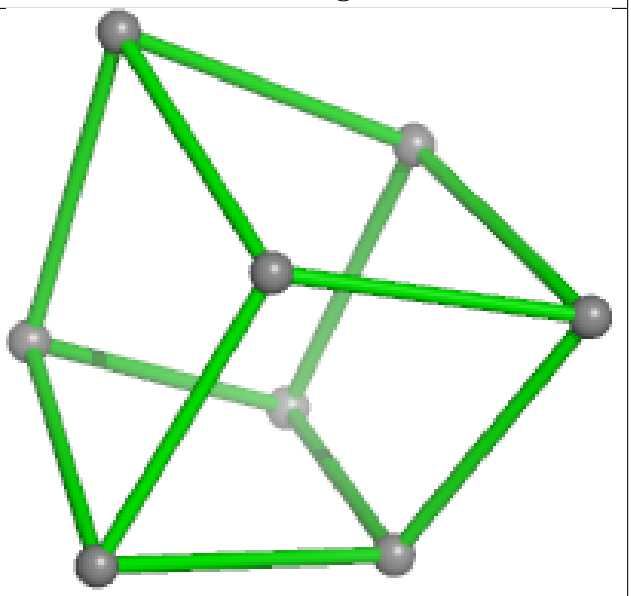
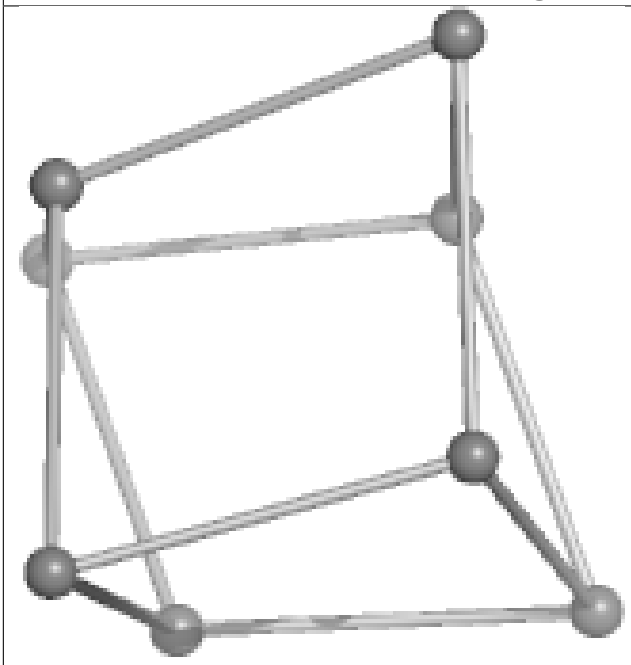


Rings

Ligand SF4 D 403



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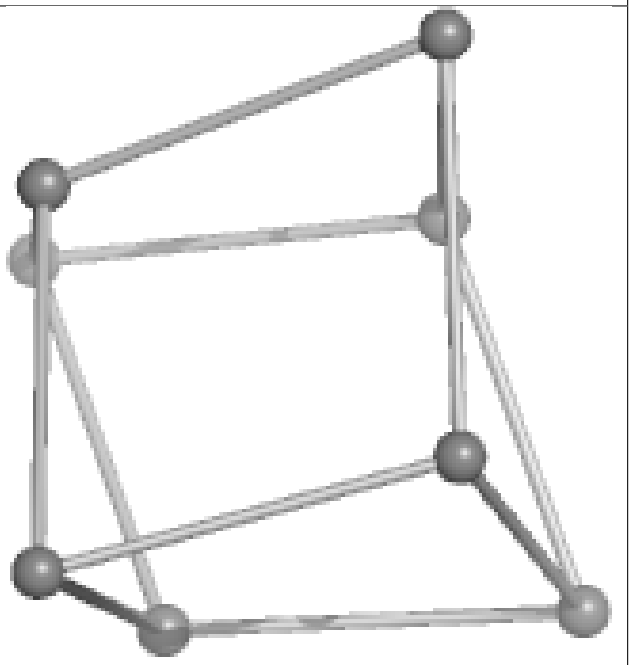

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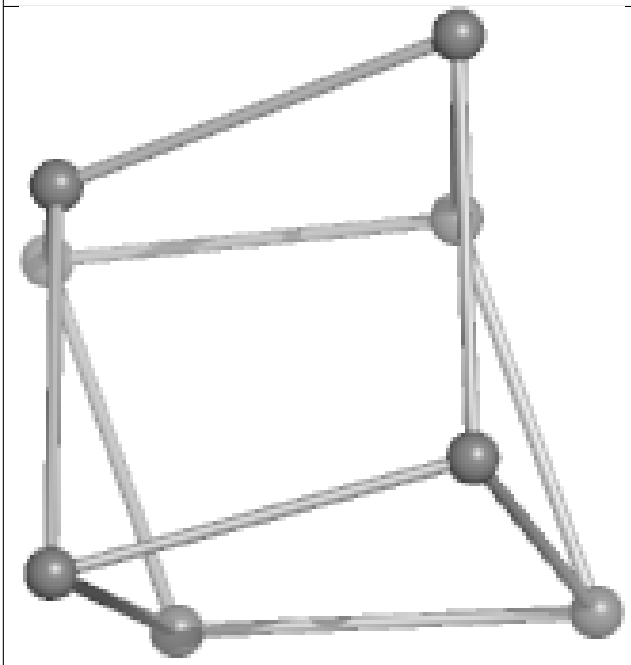

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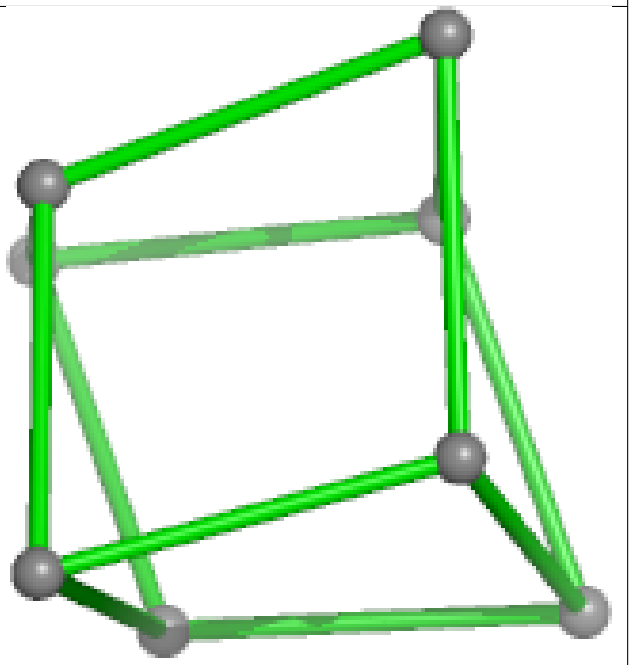
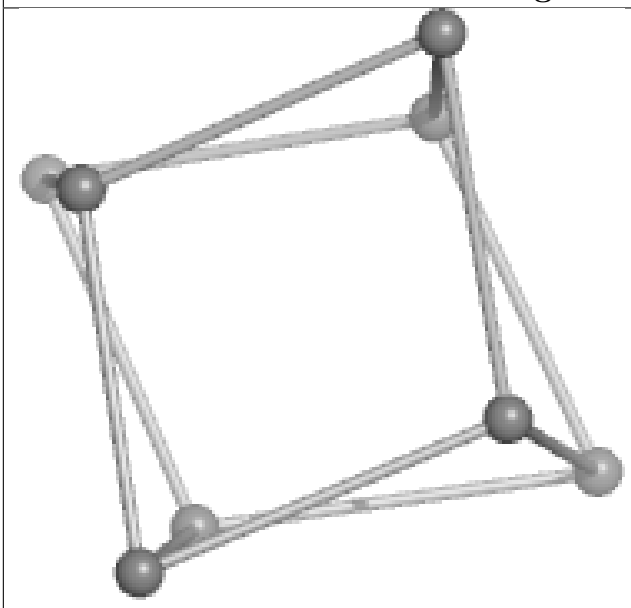


Rings

Ligand SF4 S 303



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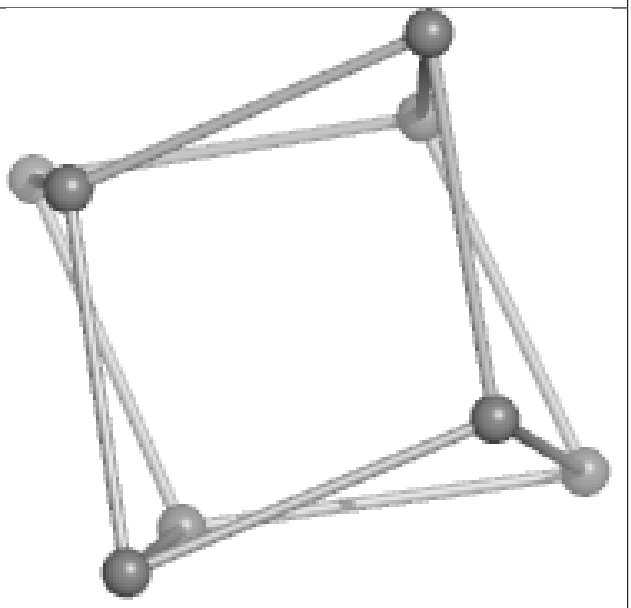

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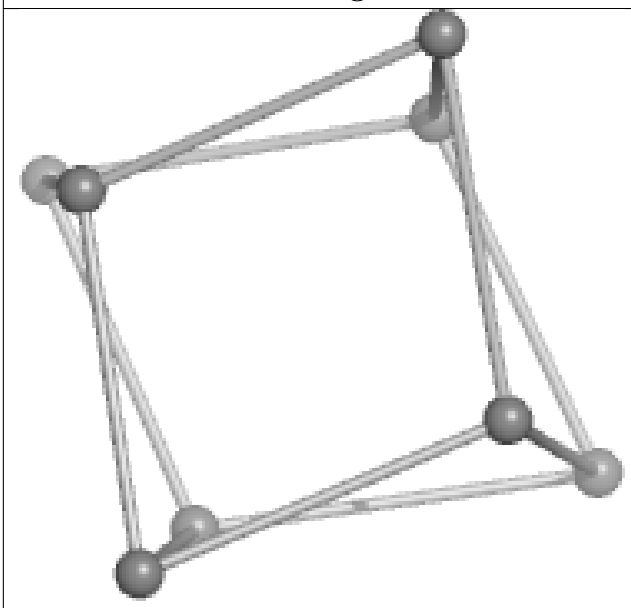

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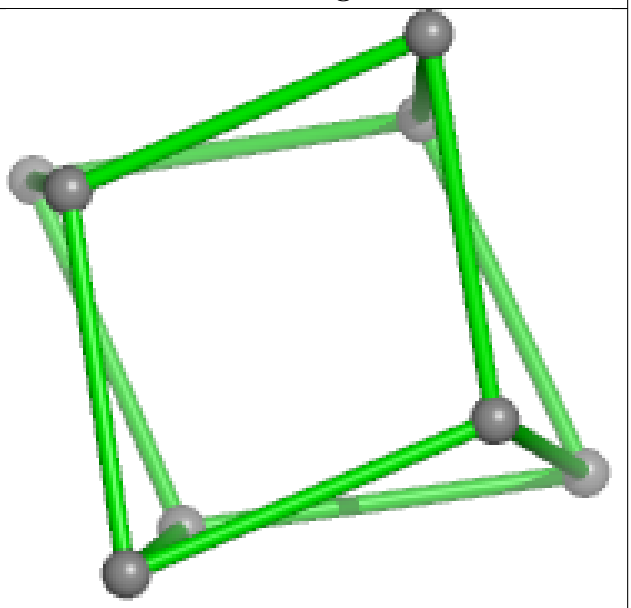
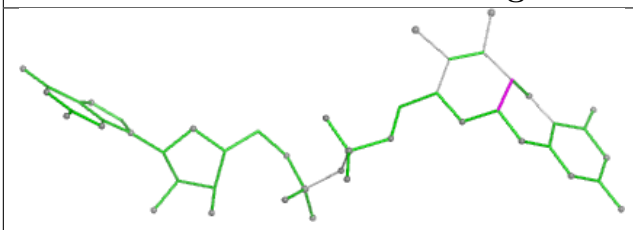


Rings

Ligand MGD R 1104



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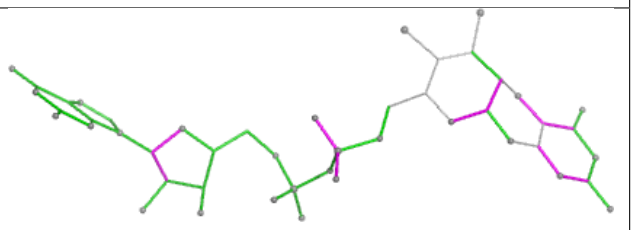
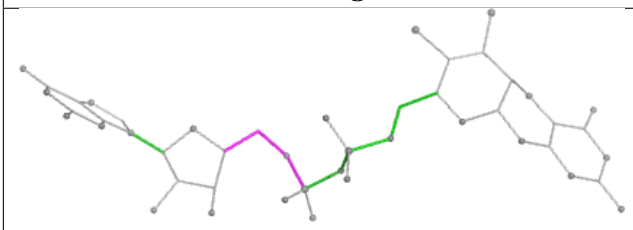


Bond angles



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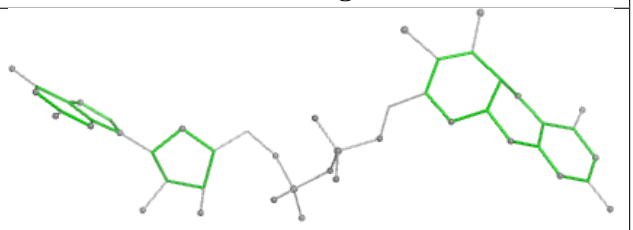
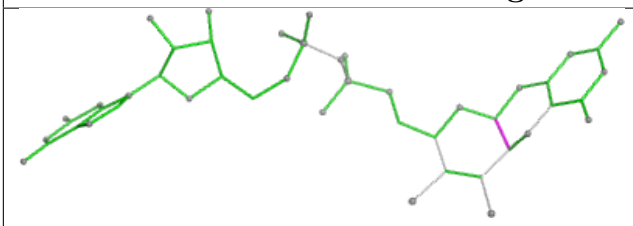


Rings

Ligand MGD A 1105



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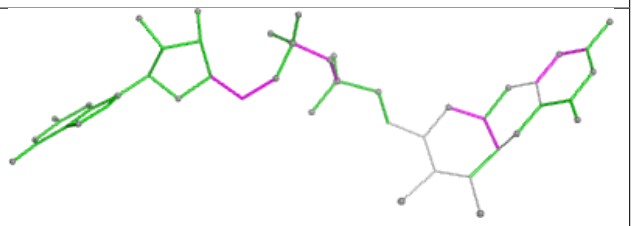
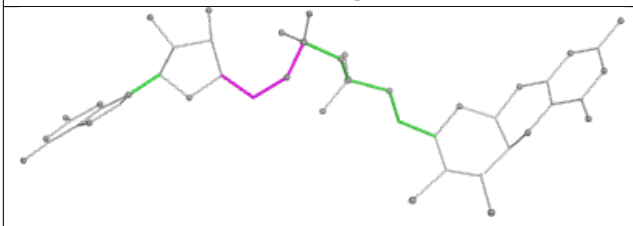


Bond angles



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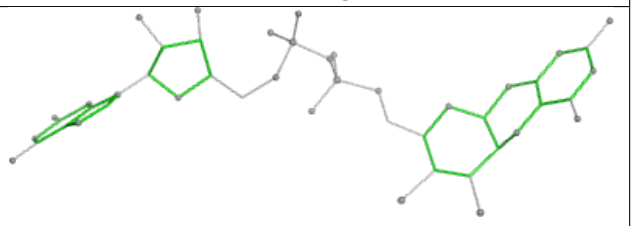
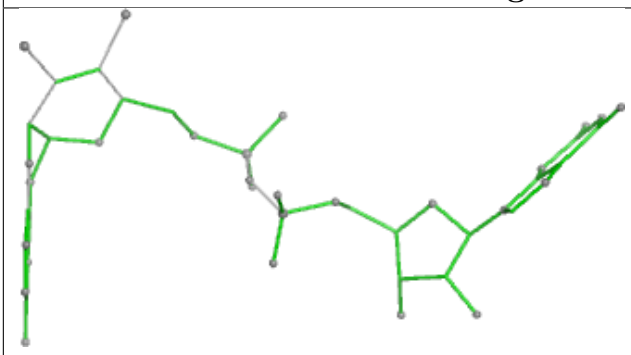
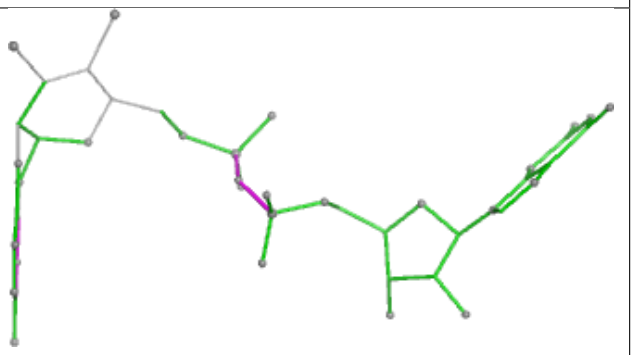


Rings

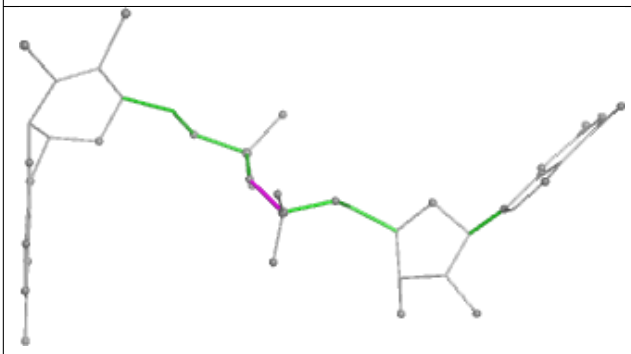
Ligand MGD R 1103



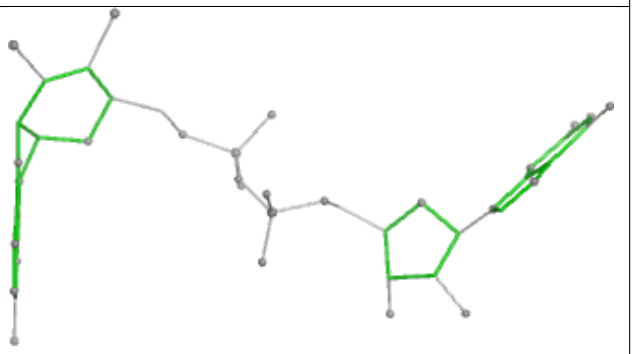
Bond lengths



Bond angles

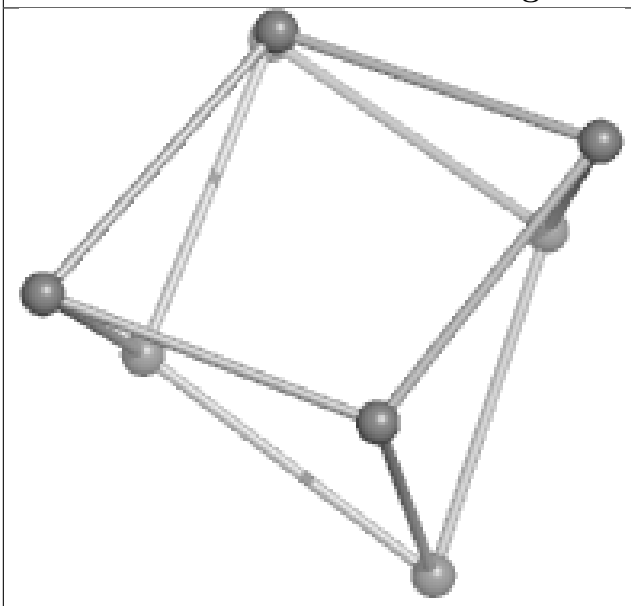


Torsions

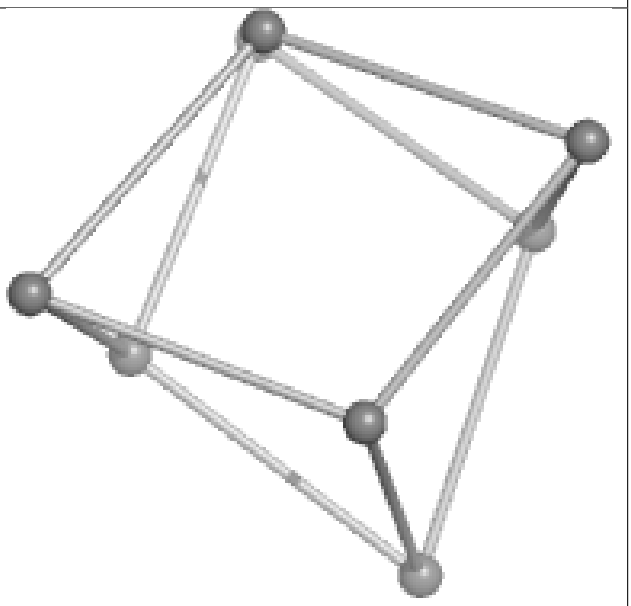


Rings

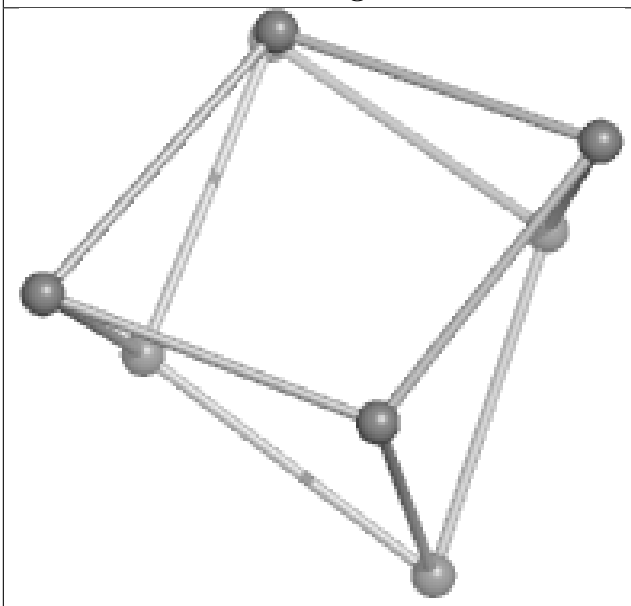
Ligand SF4 R 1105



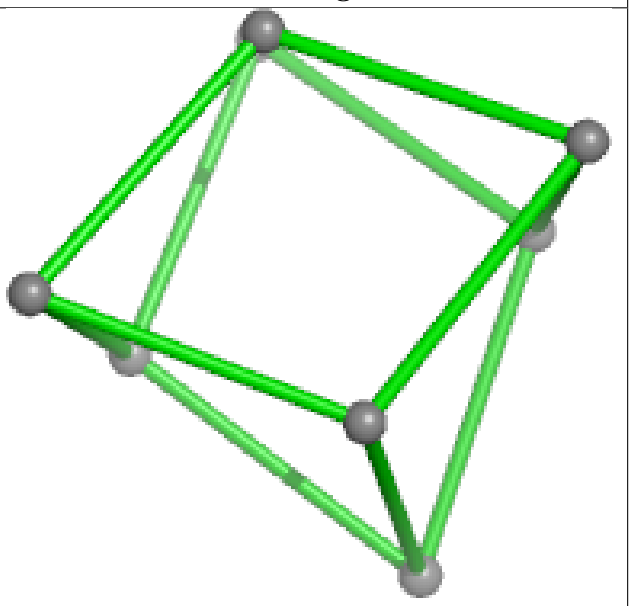
Bond lengths



Bond angles

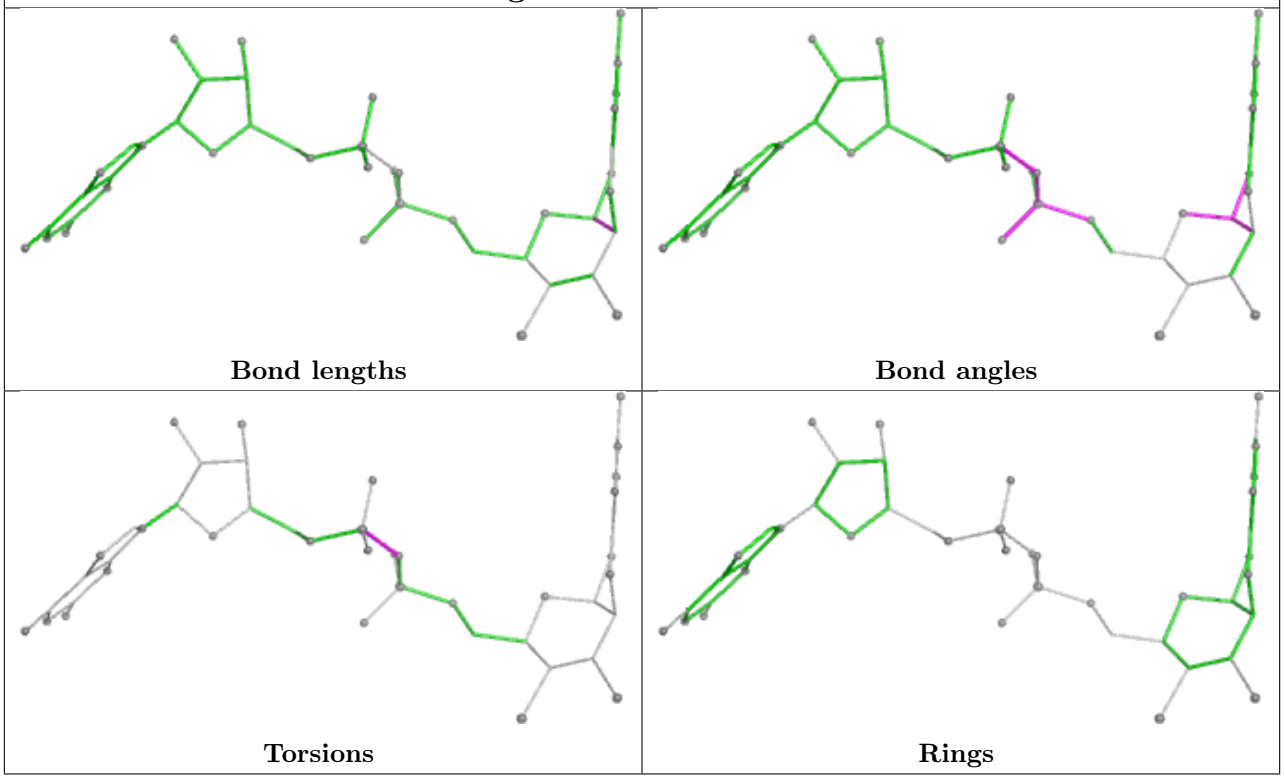


Torsions



Rings

Ligand MGD K 1103



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	973/1013 (96%)	-1.44	0	100	100	15, 33, 64, 94	0
1	C	973/1013 (96%)	-1.42	0	100	100	17, 36, 65, 97	0
1	K	972/1013 (95%)	-1.32	0	100	100	17, 41, 71, 102	0
1	R	972/1013 (95%)	-1.40	0	100	100	17, 38, 69, 100	0
2	B	214/215 (99%)	-1.61	0	100	100	14, 23, 42, 51	0
2	D	214/215 (99%)	-1.59	0	100	100	17, 25, 43, 57	0
2	L	214/215 (99%)	-1.62	0	100	100	15, 23, 43, 68	0
2	S	214/215 (99%)	-1.60	0	100	100	15, 24, 40, 66	0
All	All	4746/4912 (96%)	-1.43	0	100	100	14, 34, 65, 102	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

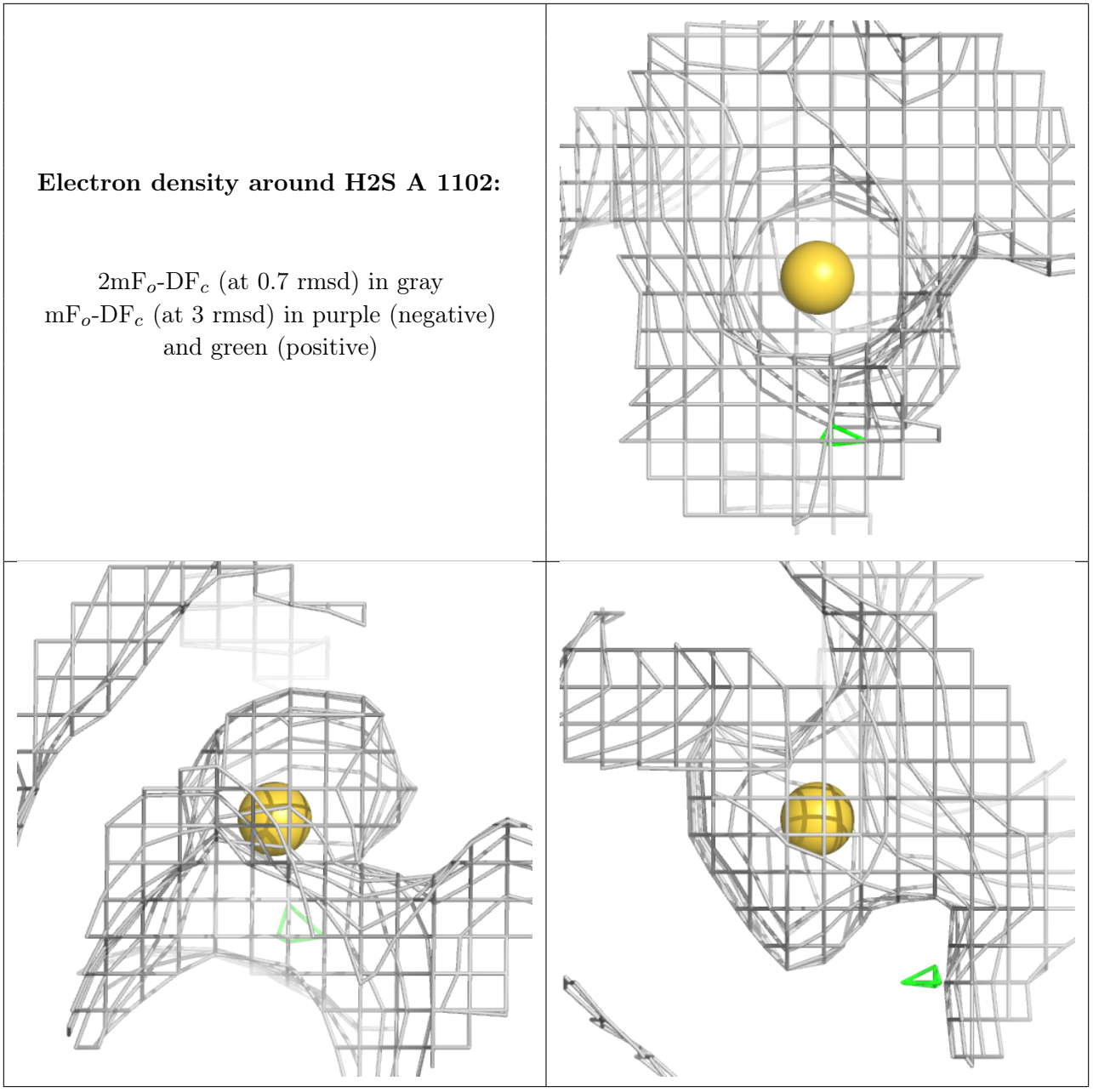
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	1101	7/7	0.99	0.04	46,53,62,65	0
3	PEG	C	1101	7/7	0.99	0.05	32,34,40,41	0
3	PEG	L	301	7/7	0.99	0.12	19,26,34,35	0
3	PEG	L	302	7/7	0.99	0.04	11,27,38,40	0
3	PEG	S	302	7/7	0.99	0.13	21,24,35,39	0
3	PEG	D	401	7/7	1.00	0.03	14,27,37,38	0
4	H2S	A	1102	1/1	1.00	0.03	38,38,38,38	0
4	H2S	C	1102	1/1	1.00	0.01	23,23,23,23	0
4	H2S	K	1101	1/1	1.00	0.02	20,20,20,20	0
4	H2S	R	1101	1/1	1.00	0.03	31,31,31,31	0
5	W	A	1103	1/1	1.00	0.00	20,20,20,20	0
5	W	C	1103	1/1	1.00	0.01	22,22,22,22	0
5	W	K	1102	1/1	1.00	0.01	24,24,24,24	0
5	W	R	1102	1/1	1.00	0.01	22,22,22,22	0
6	MGD	A	1104	47/47	1.00	0.02	14,18,22,29	0
6	MGD	A	1105	47/47	1.00	0.02	15,20,29,31	0
6	MGD	C	1104	47/47	1.00	0.02	16,22,25,26	0
6	MGD	C	1105	47/47	1.00	0.02	17,24,31,33	0
6	MGD	K	1103	47/47	1.00	0.02	19,23,31,35	0
6	MGD	K	1104	47/47	1.00	0.02	16,26,34,40	0
6	MGD	R	1103	47/47	1.00	0.02	18,21,25,27	0
6	MGD	R	1104	47/47	1.00	0.02	16,21,30,33	0
7	SF4	A	1106	8/8	1.00	0.01	16,17,18,20	0
7	SF4	B	301	8/8	1.00	0.01	13,15,16,16	0
7	SF4	B	302	8/8	1.00	0.01	16,17,20,21	0
7	SF4	B	303	8/8	1.00	0.01	15,17,19,19	0
7	SF4	C	1106	8/8	1.00	0.01	20,21,22,23	0
7	SF4	D	402	8/8	1.00	0.02	18,19,21,22	0
7	SF4	D	403	8/8	1.00	0.01	19,19,20,21	0
7	SF4	D	404	8/8	1.00	0.01	19,21,21,22	0
7	SF4	K	1105	8/8	1.00	0.01	18,19,20,21	0
7	SF4	L	303	8/8	1.00	0.01	16,17,18,18	0
7	SF4	L	304	8/8	1.00	0.01	16,17,17,17	0
7	SF4	L	305	8/8	1.00	0.01	17,17,18,19	0
7	SF4	R	1105	8/8	1.00	0.01	19,22,23,24	0
7	SF4	S	303	8/8	1.00	0.01	14,16,18,18	0
7	SF4	S	304	8/8	1.00	0.01	17,17,20,21	0
7	SF4	S	305	8/8	1.00	0.01	17,18,19,20	0
8	GOL	S	301	6/6	1.00	0.03	12,23,25,28	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.

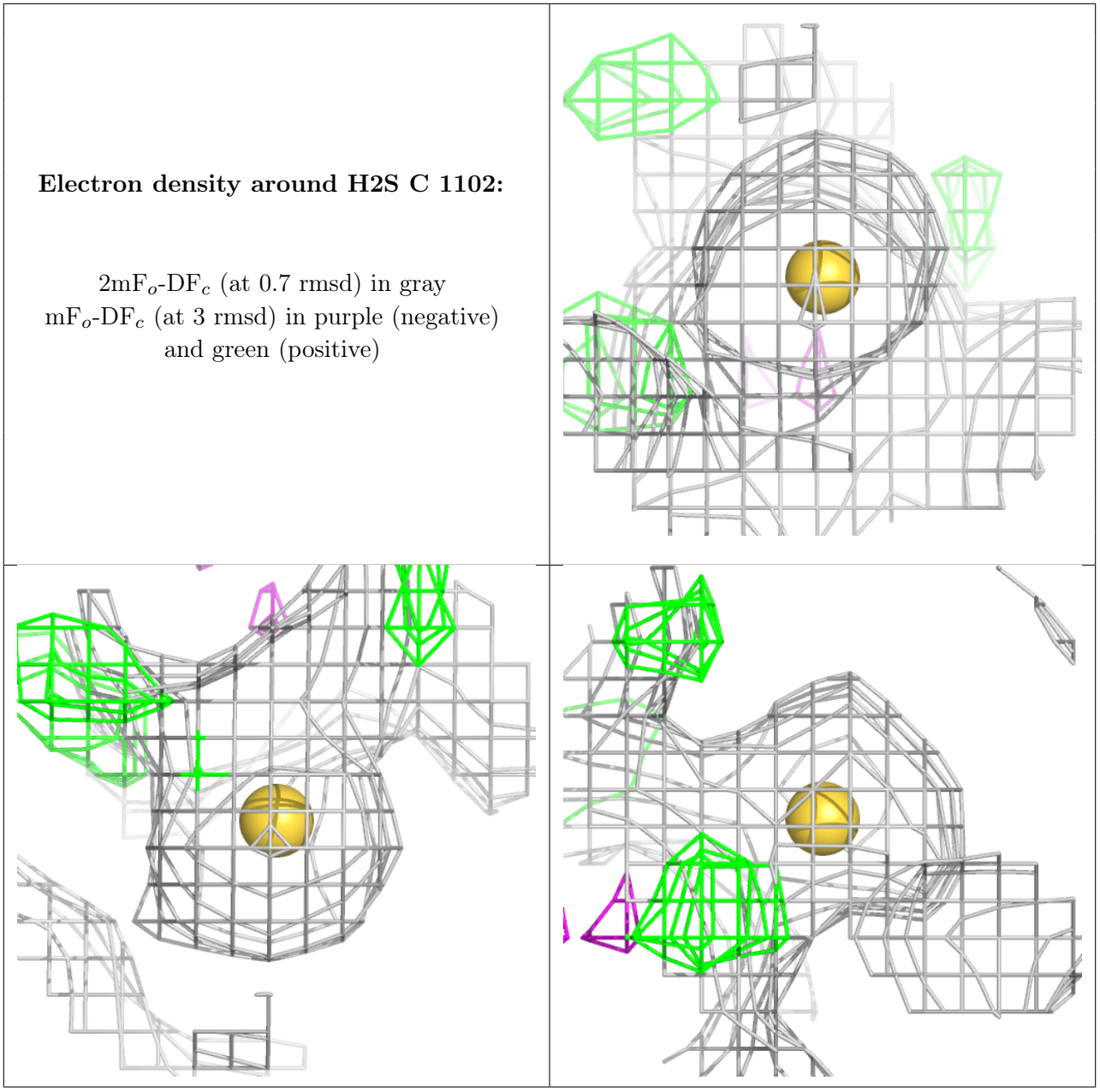
Electron density around H2S A 1102:

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



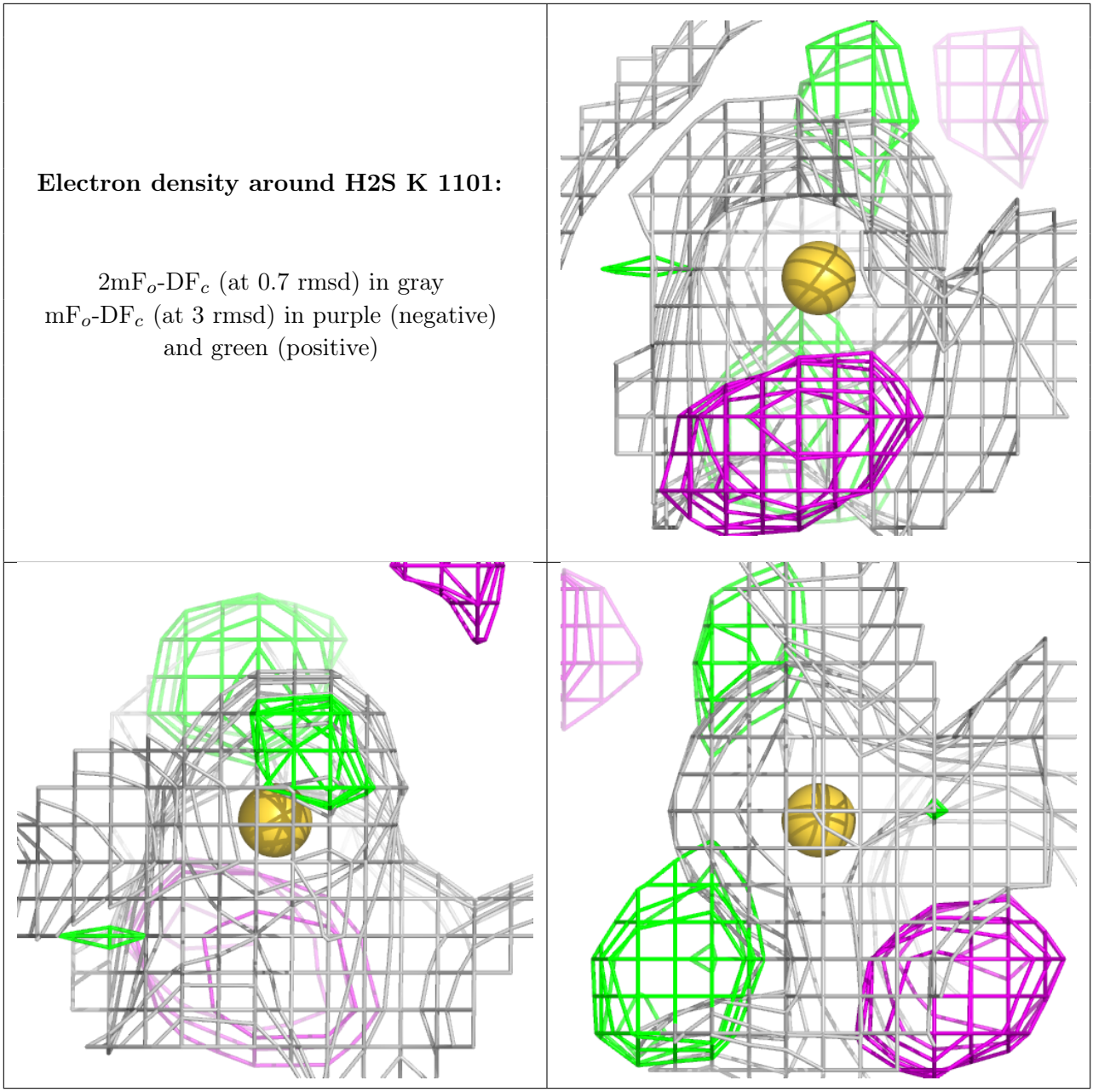
Electron density around H2S C 1102:

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



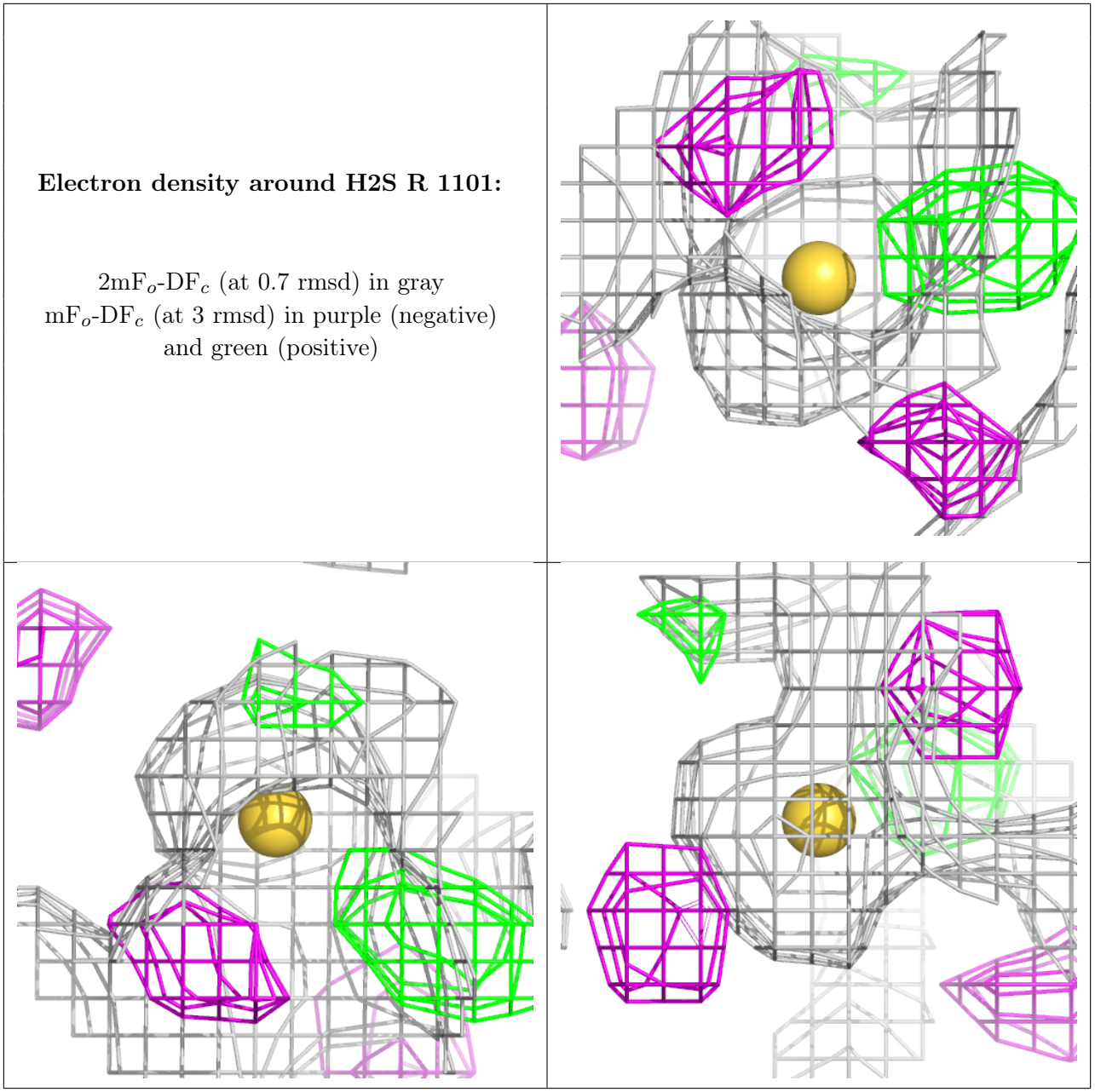
Electron density around H2S K 1101:

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



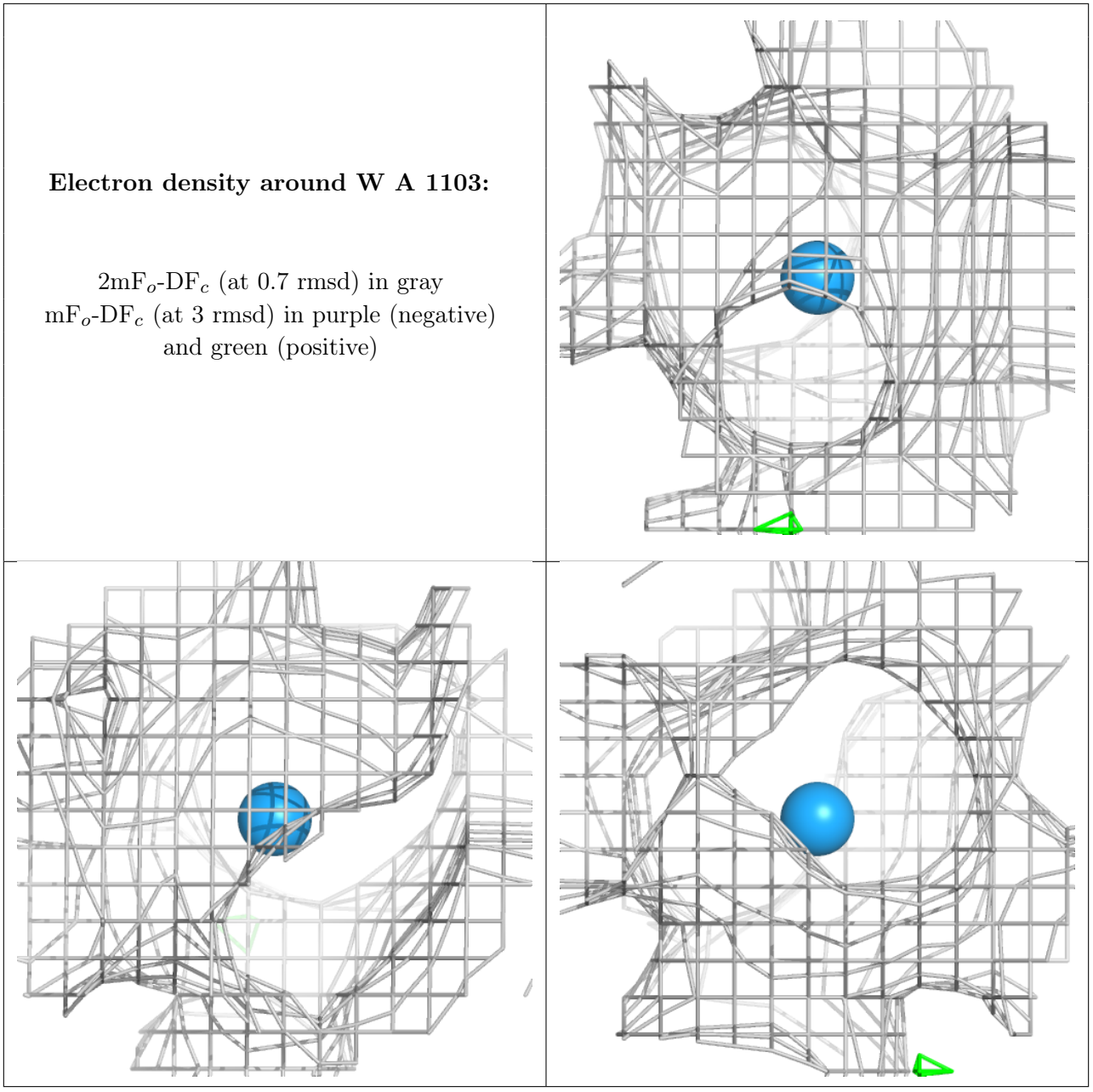
Electron density around H2S R 1101:

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



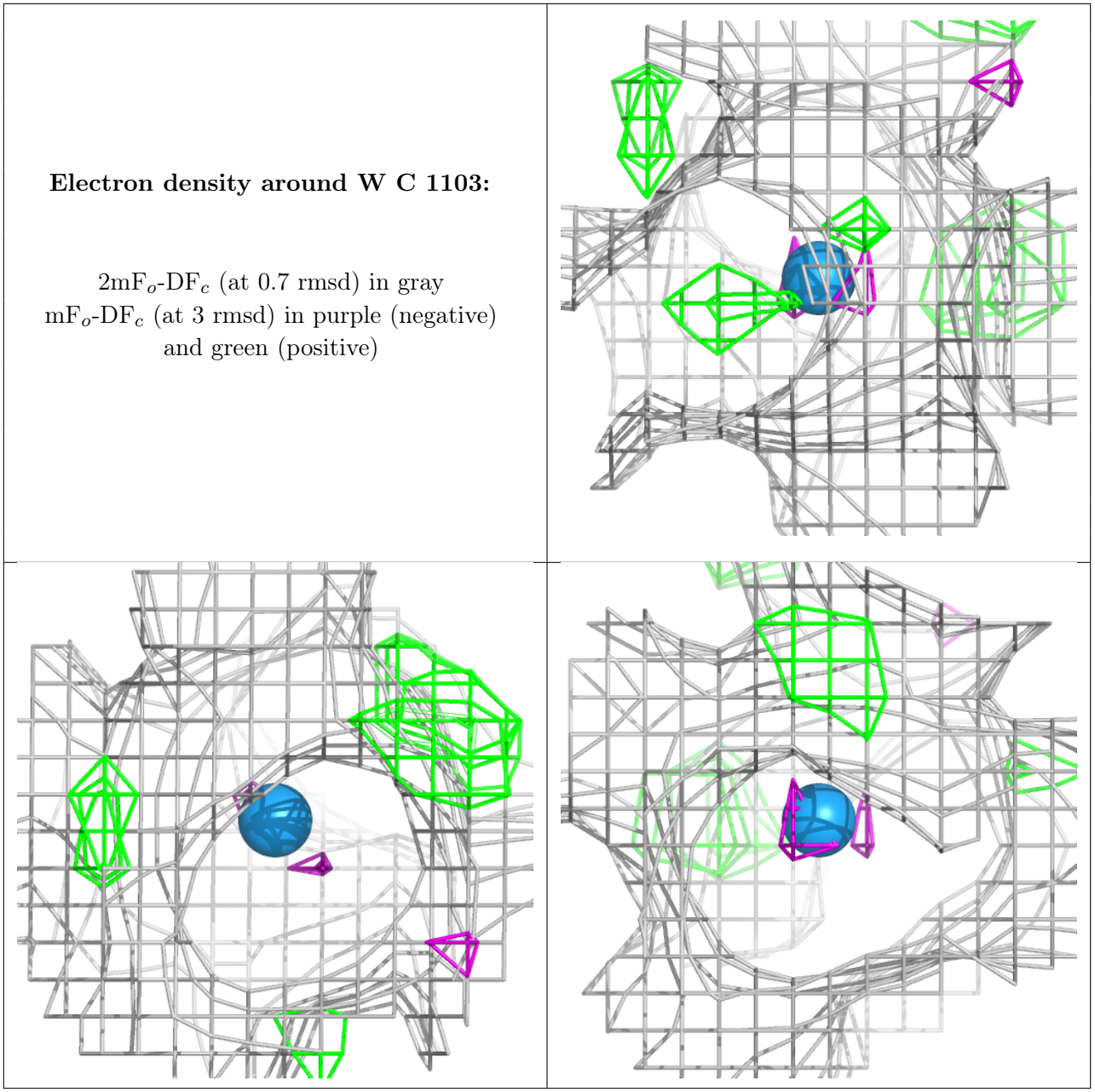
Electron density around W A 1103:

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



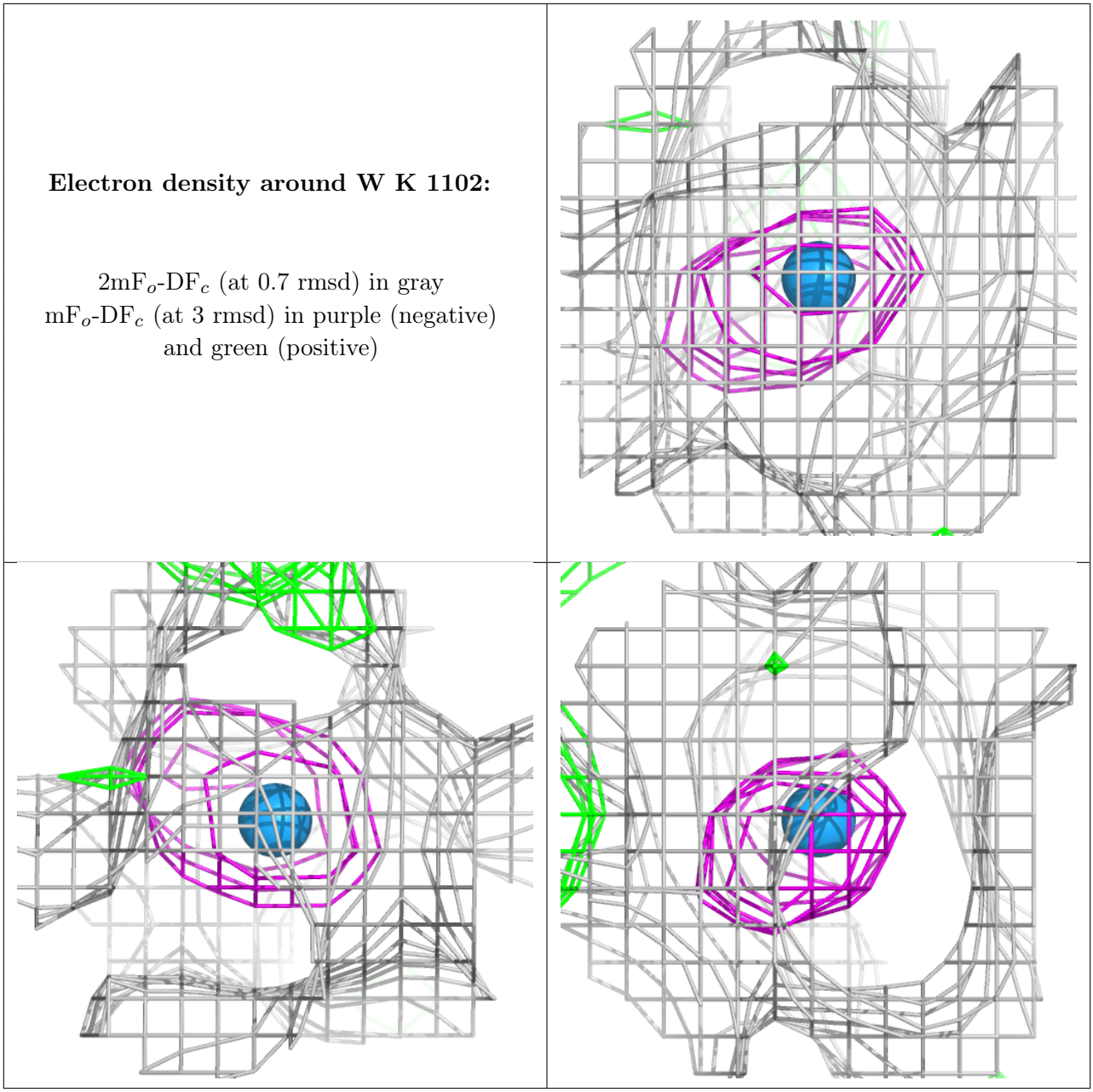
Electron density around W C 1103:

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



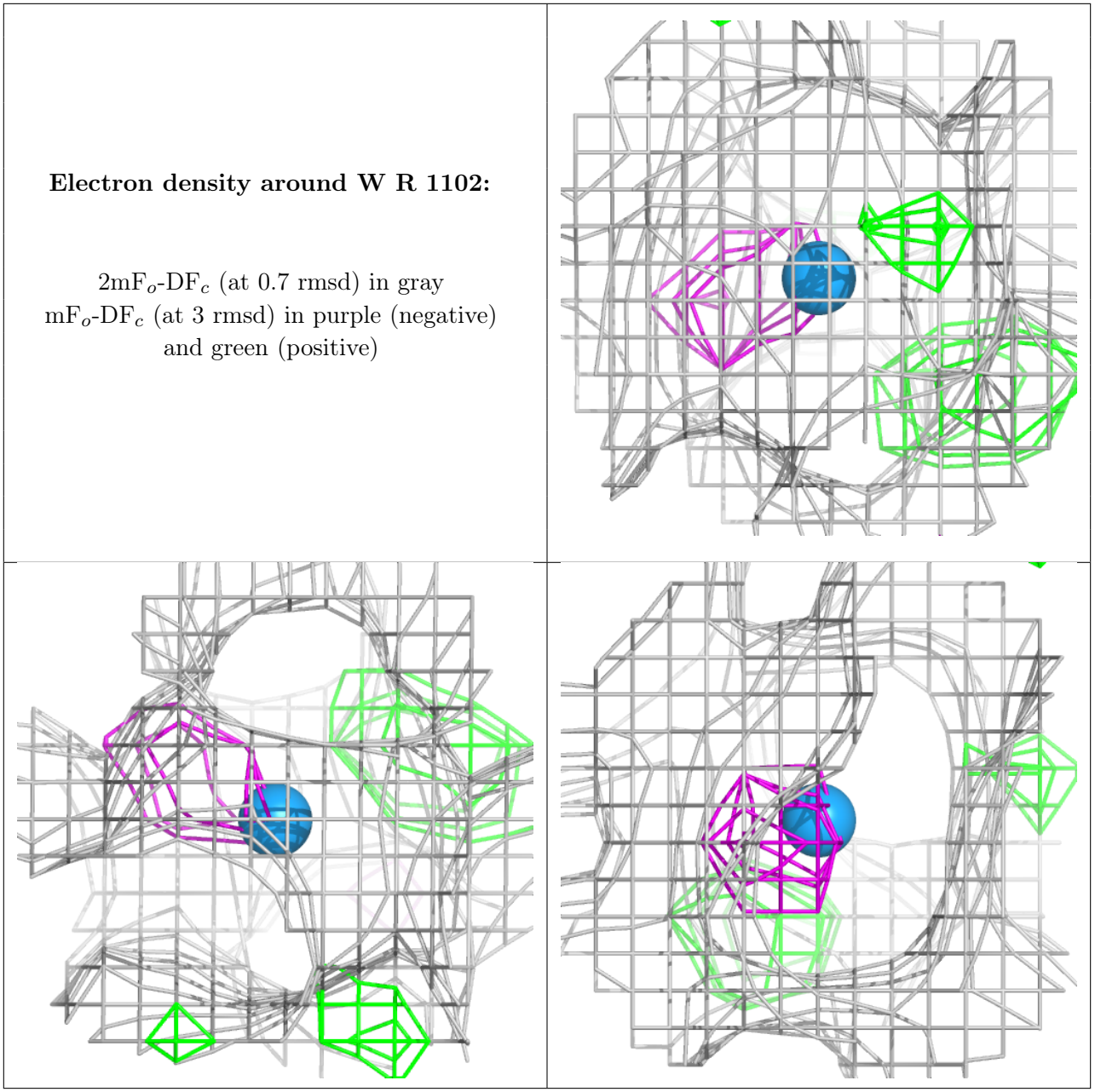
Electron density around W K 1102:

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



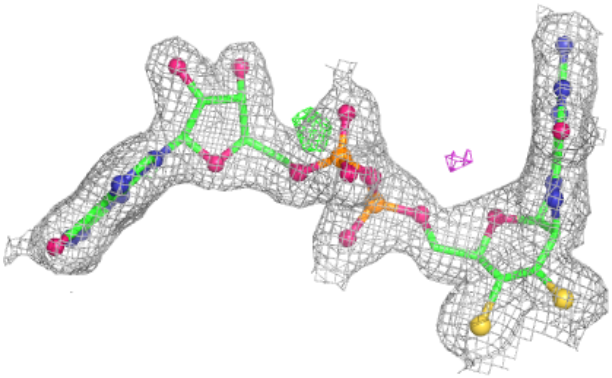
Electron density around W R 1102:

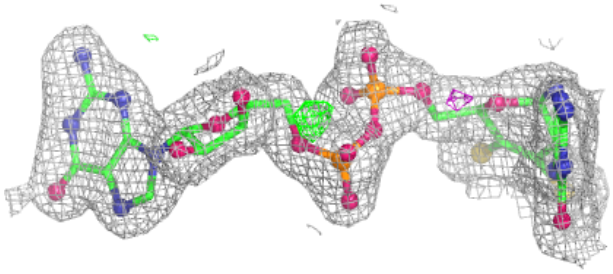
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

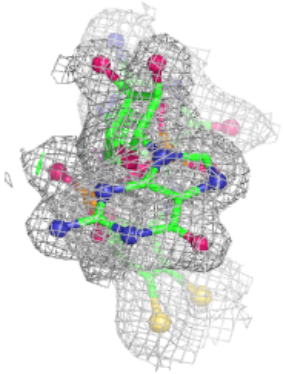


Electron density around MGD A 1104:

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

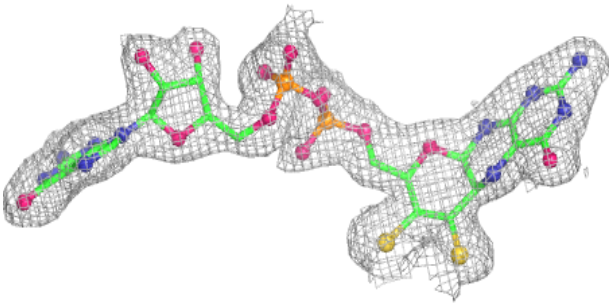


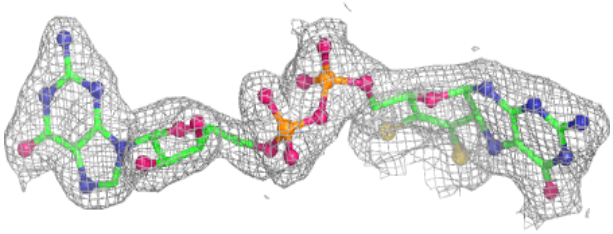


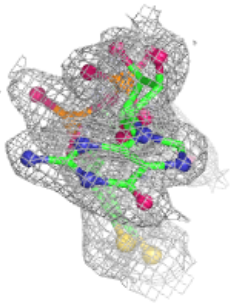


Electron density around MGD A 1105:

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

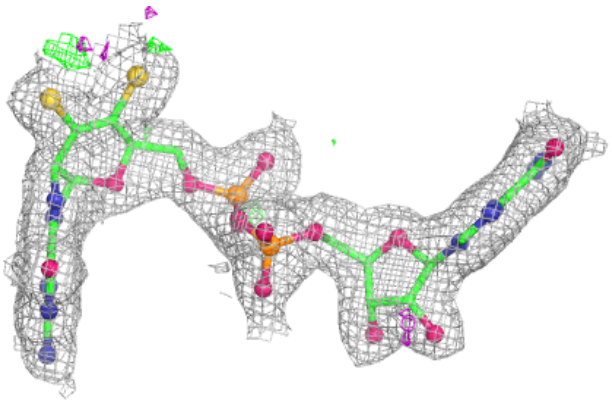


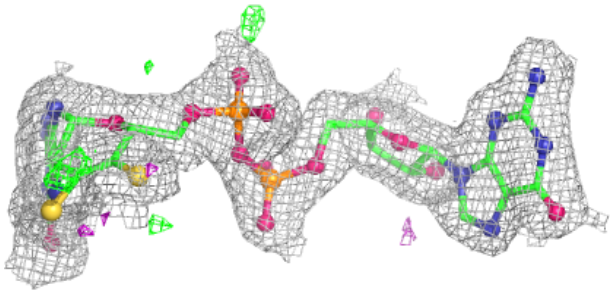


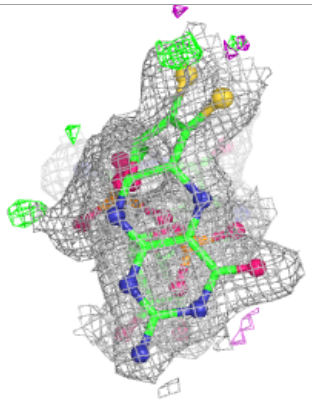


Electron density around MGD C 1104:

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

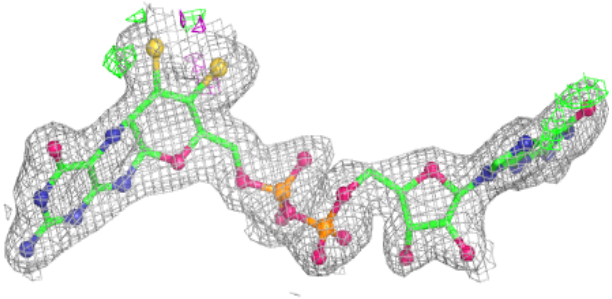


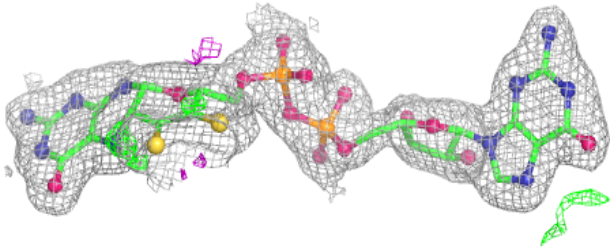


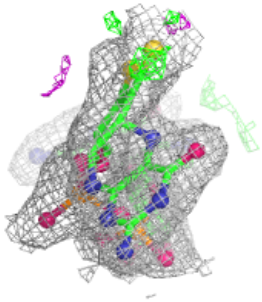


Electron density around MGD C 1105:

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

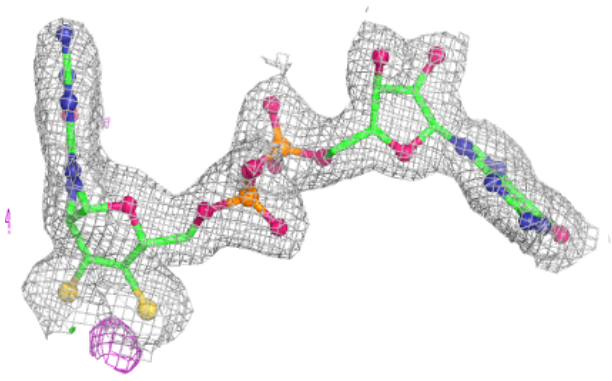


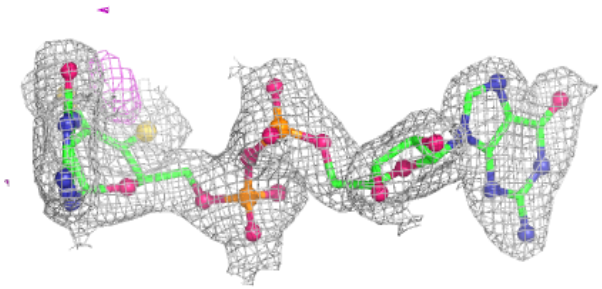


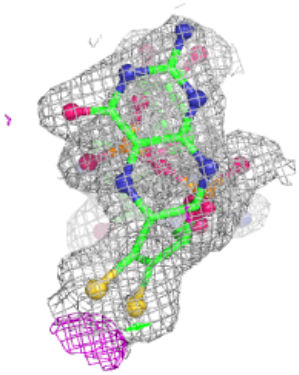


Electron density around MGD K 1103:

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

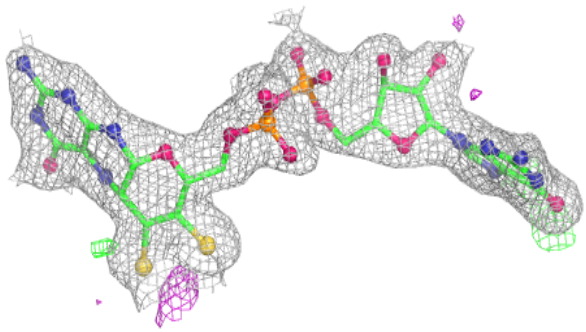


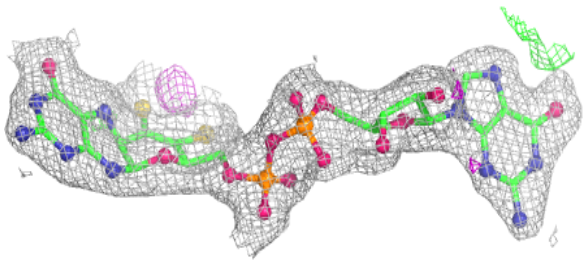


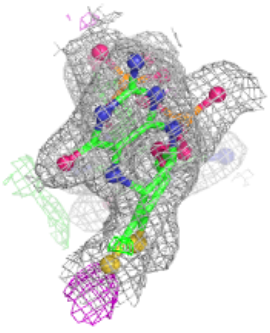


Electron density around MGD K 1104:

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

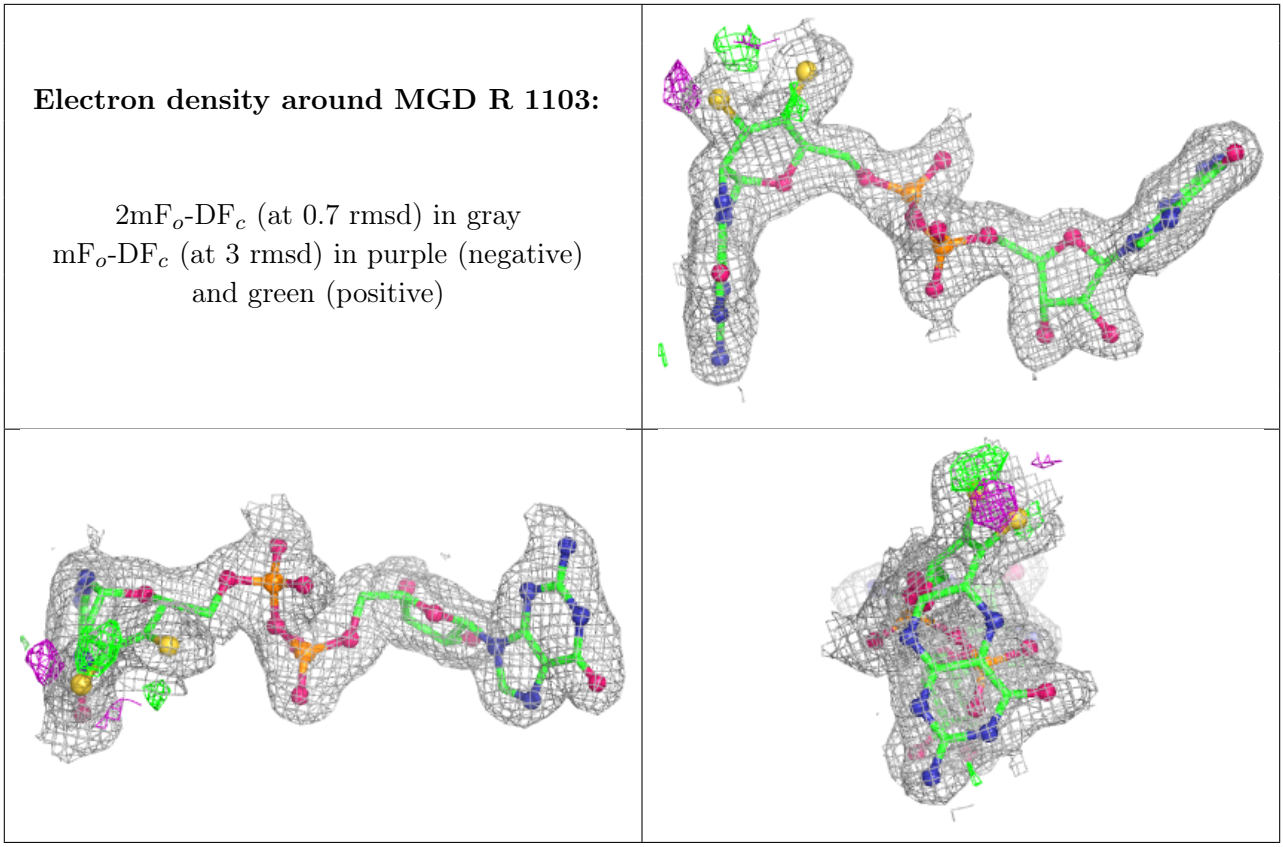






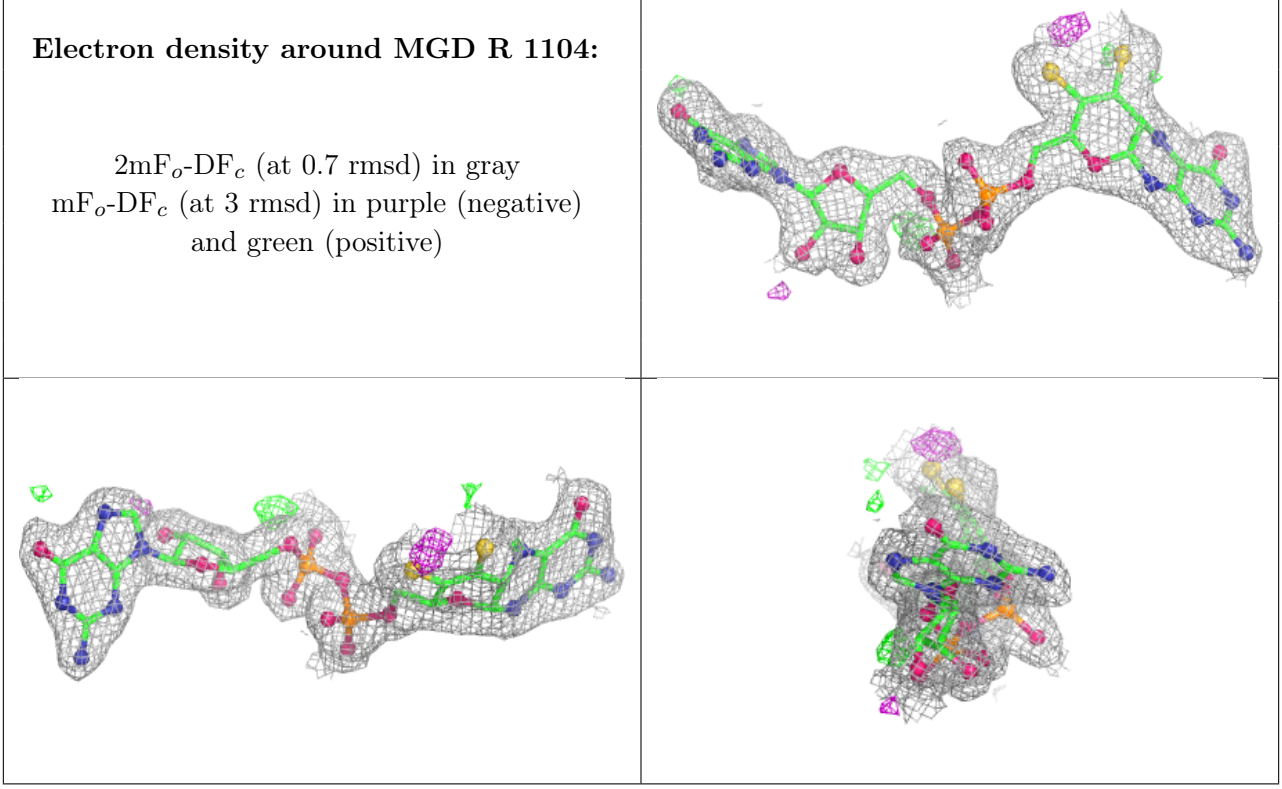
Electron density around MGD R 1103:

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



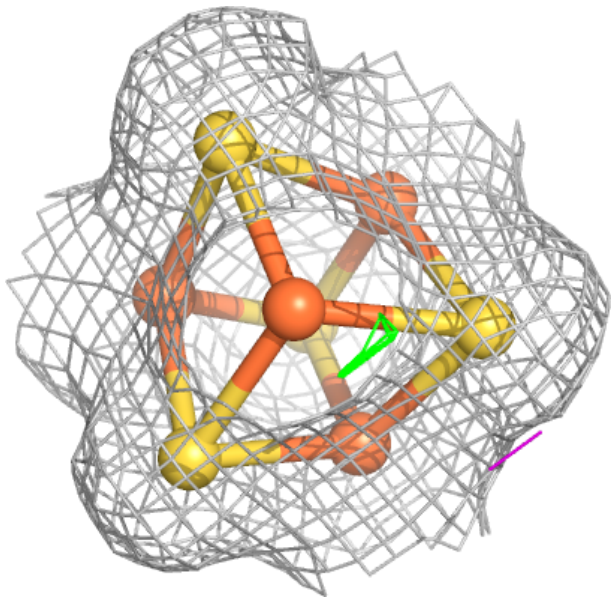
Electron density around MGD R 1104:

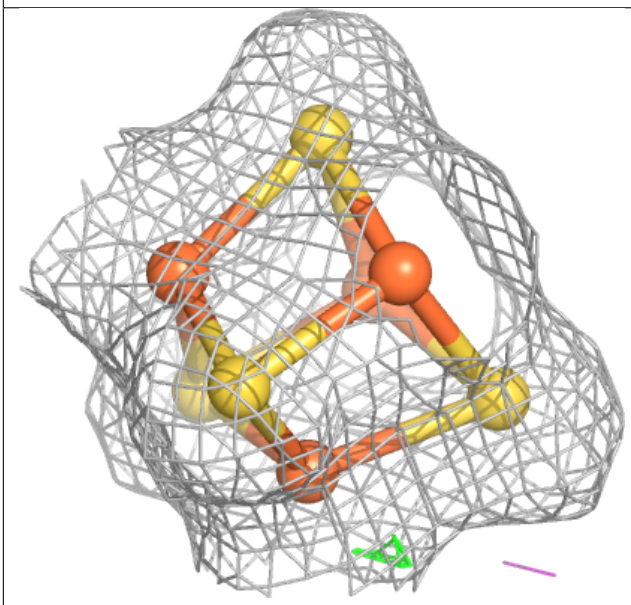
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

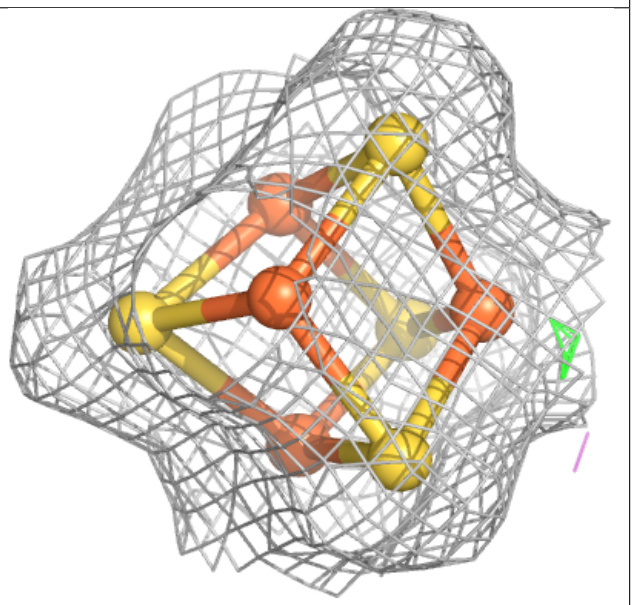


Electron density around SF4 A 1106:

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

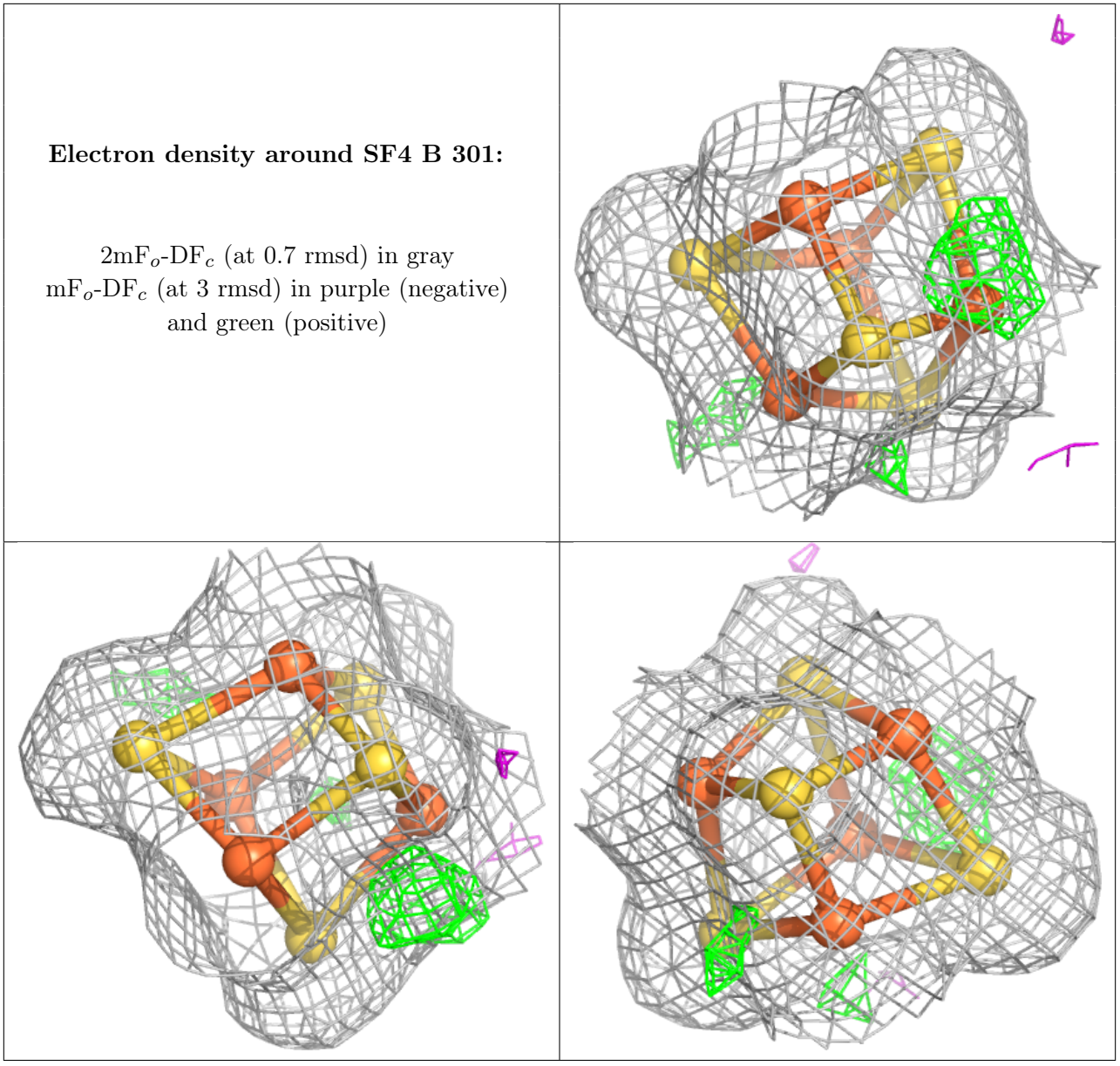






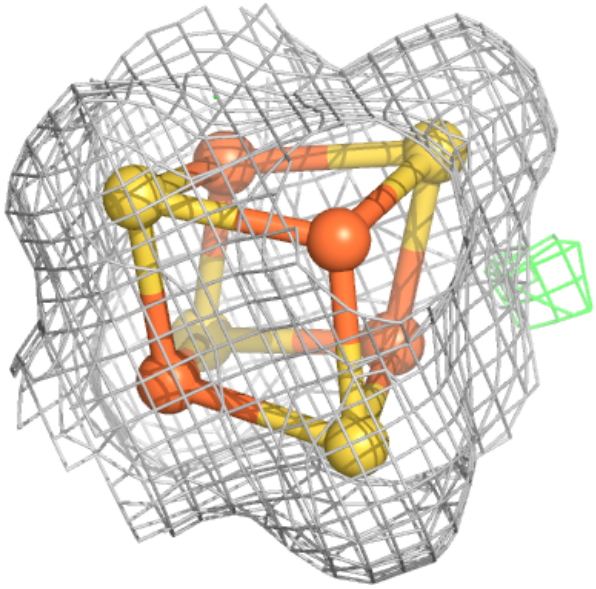
Electron density around SF4 B 301:

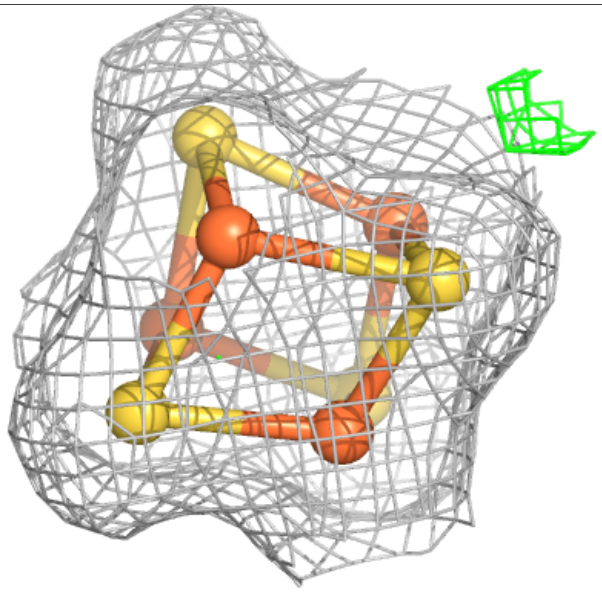
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

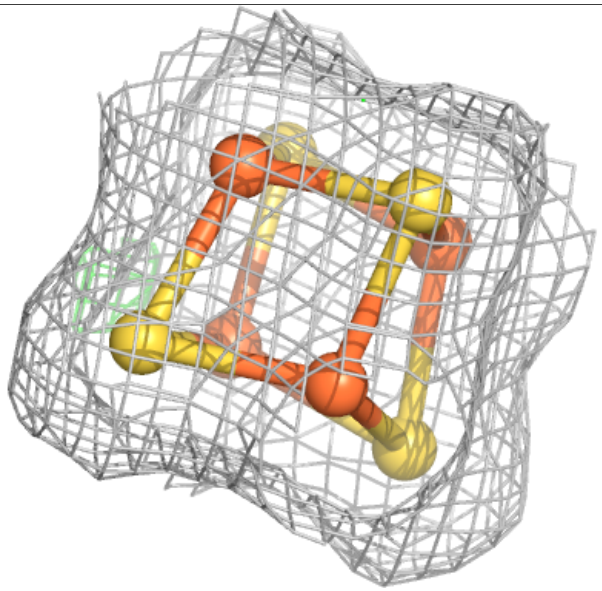


Electron density around SF4 B 302:

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

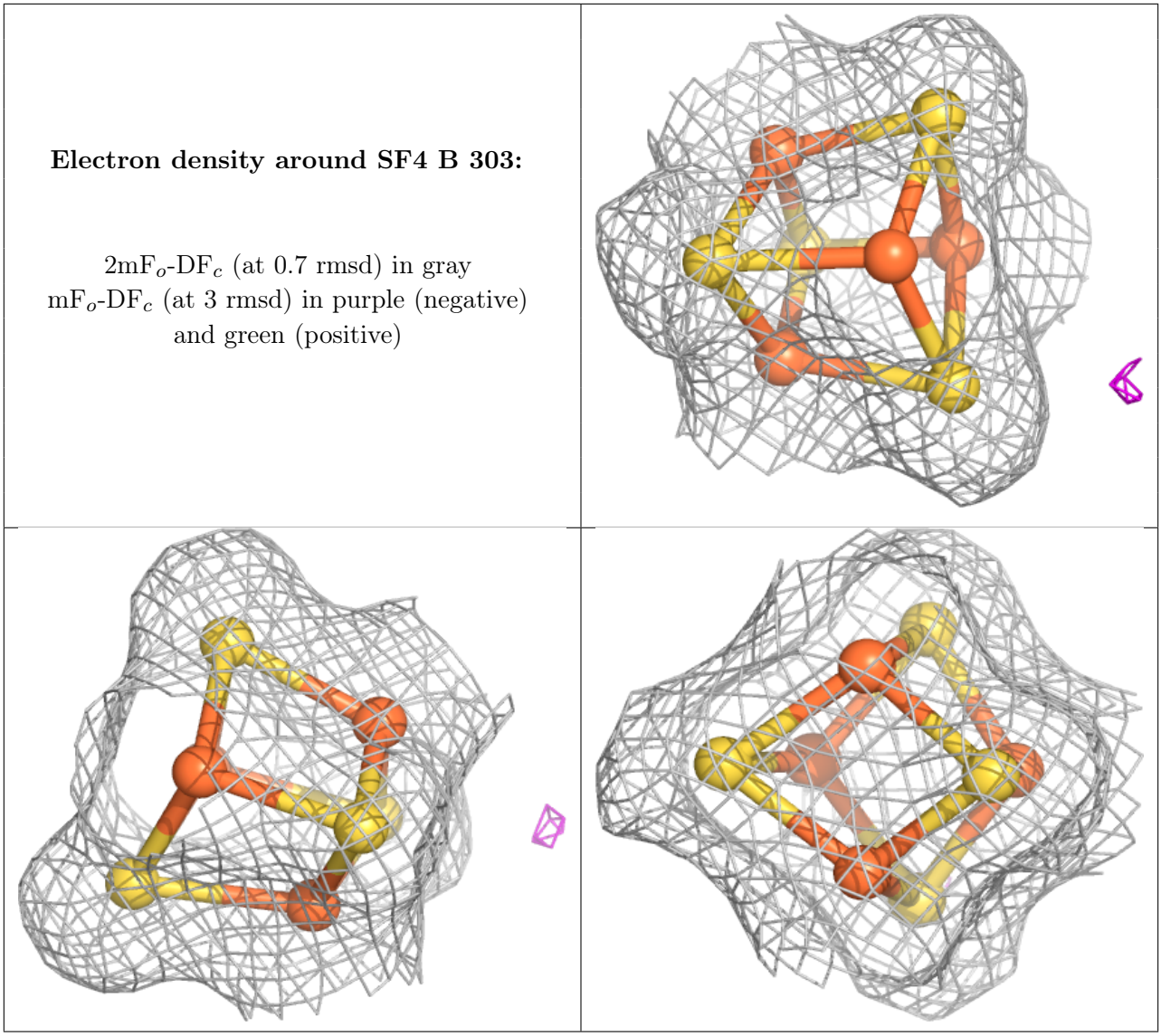






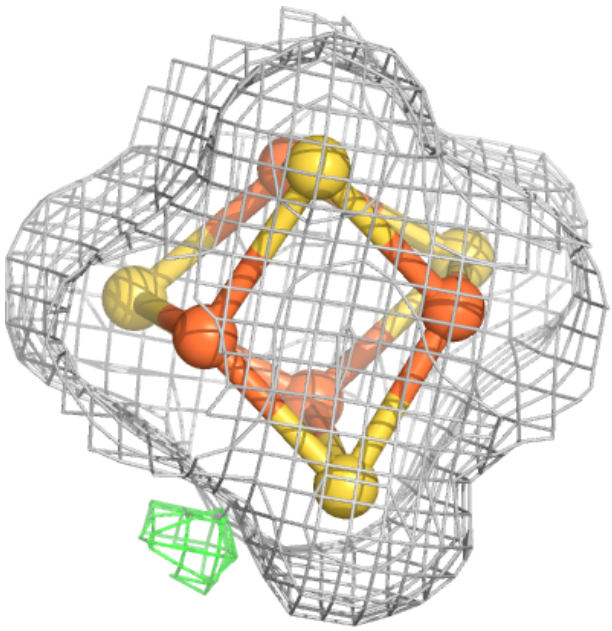
Electron density around SF4 B 303:

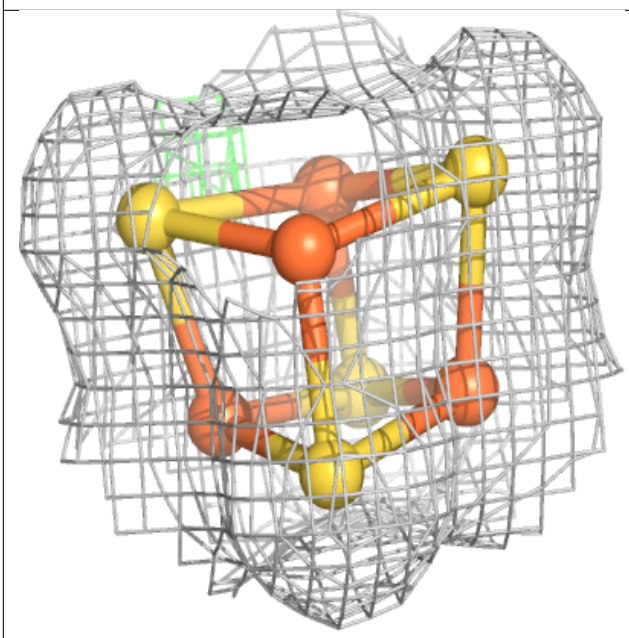
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

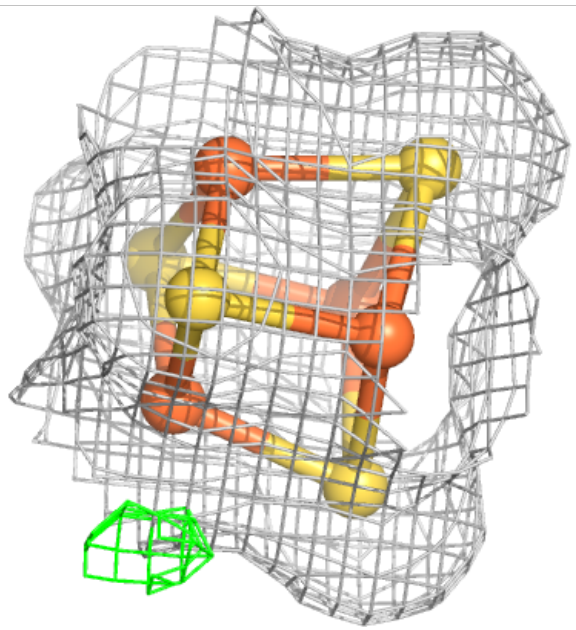


Electron density around SF4 C 1106:

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

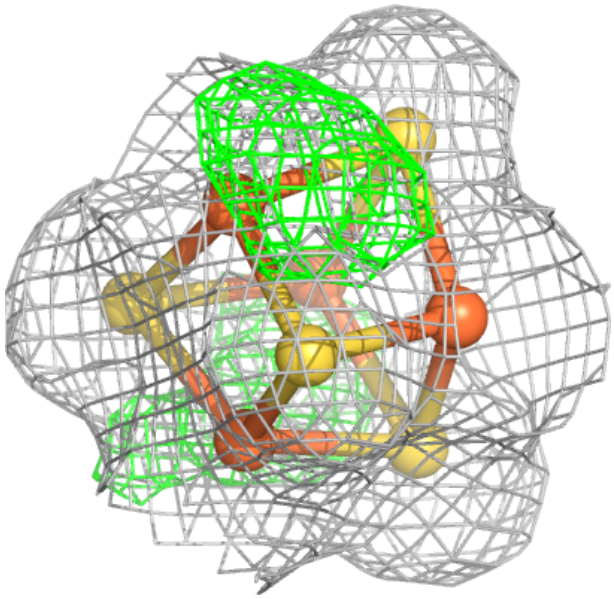


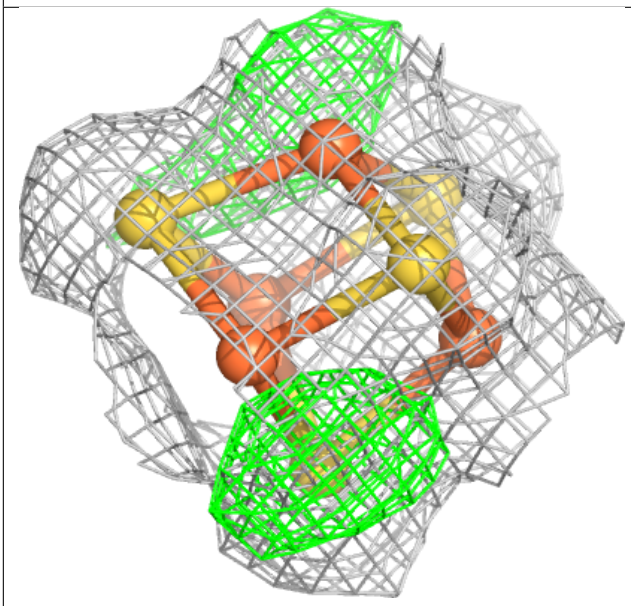


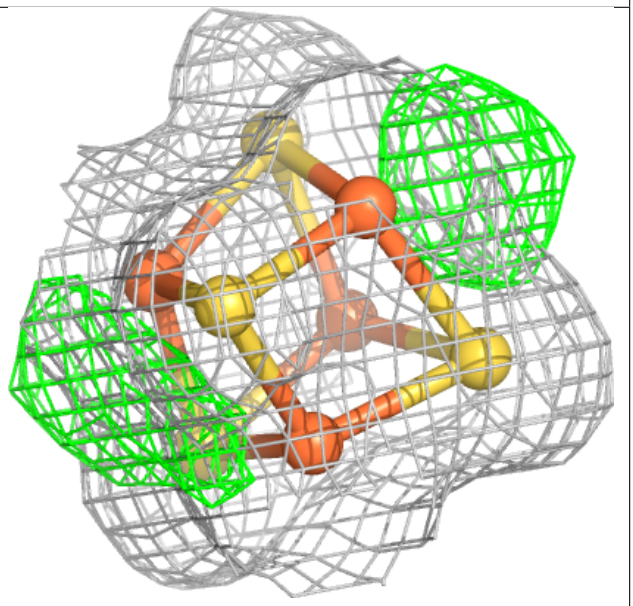


Electron density around SF4 D 402:

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

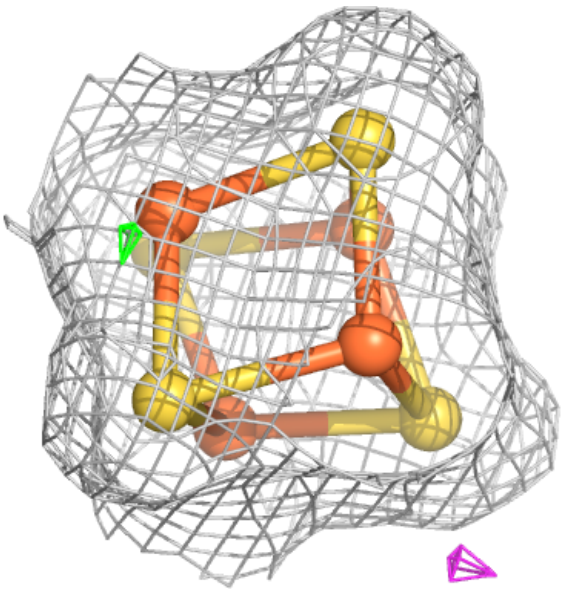


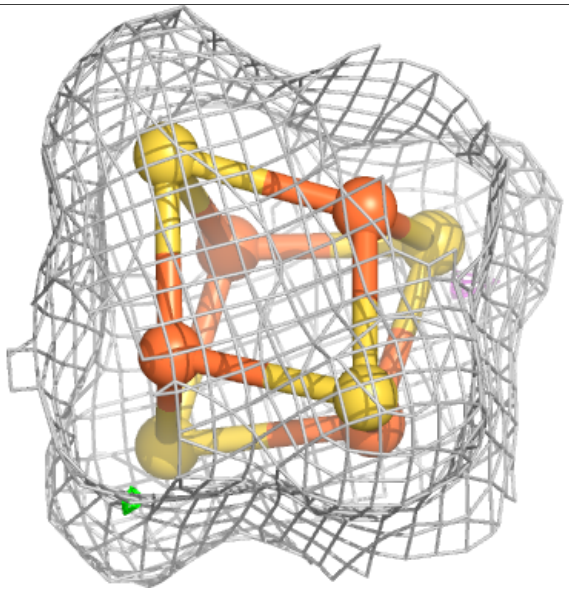


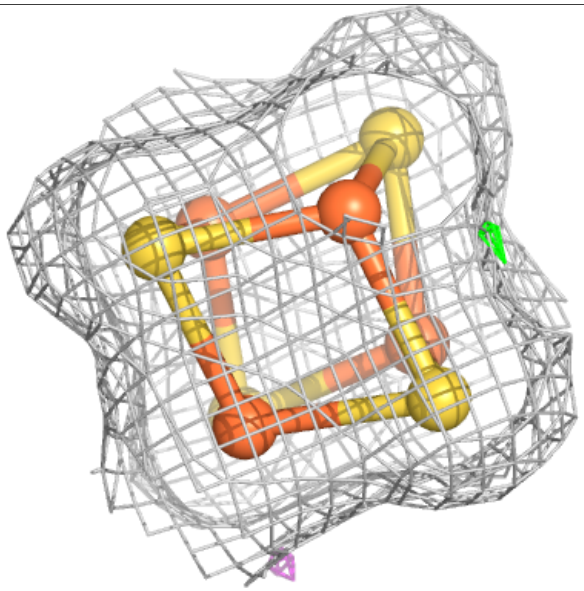


Electron density around SF4 D 403:

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

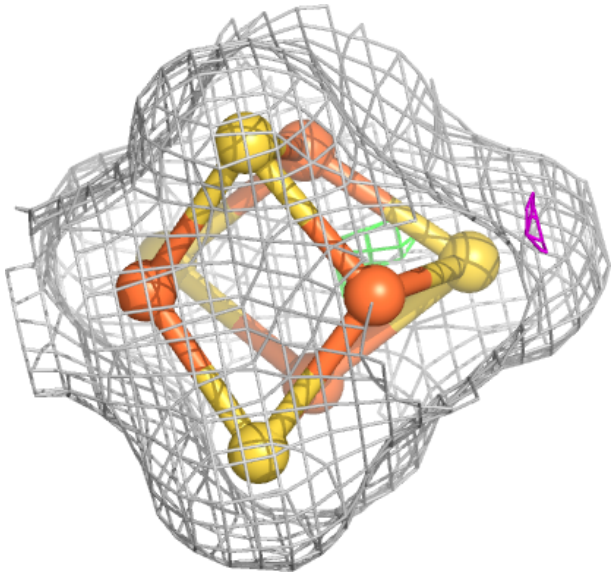


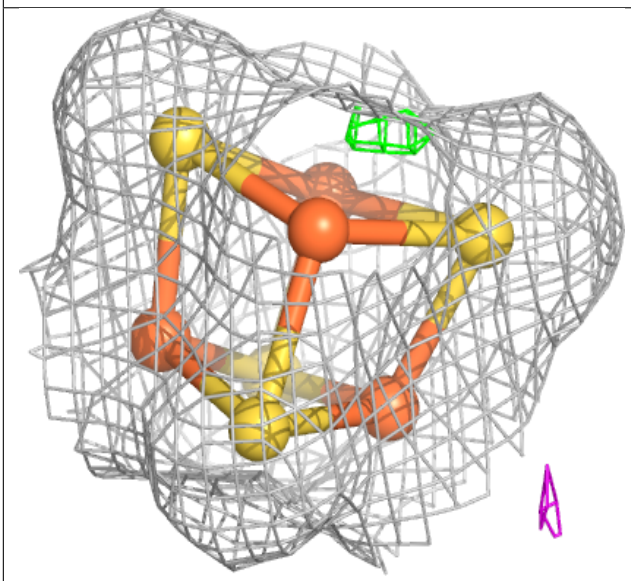


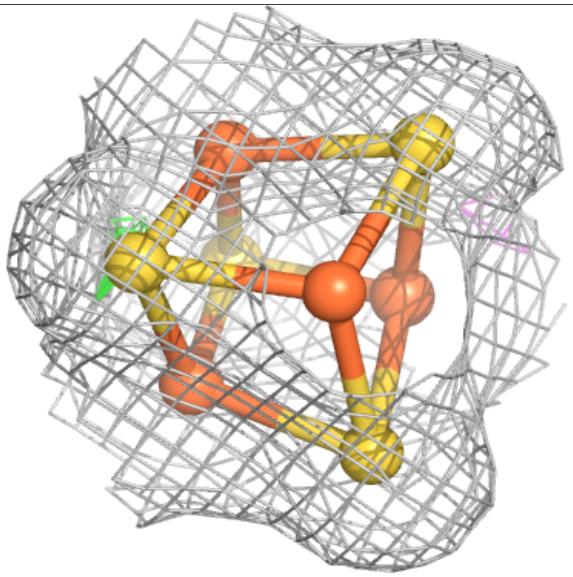


Electron density around SF4 D 404:

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

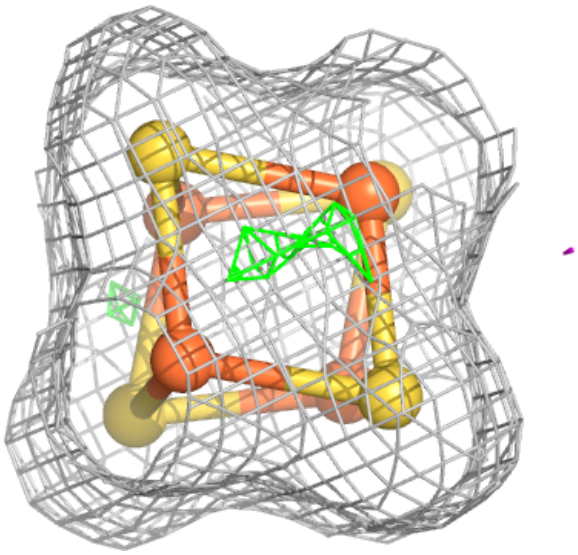


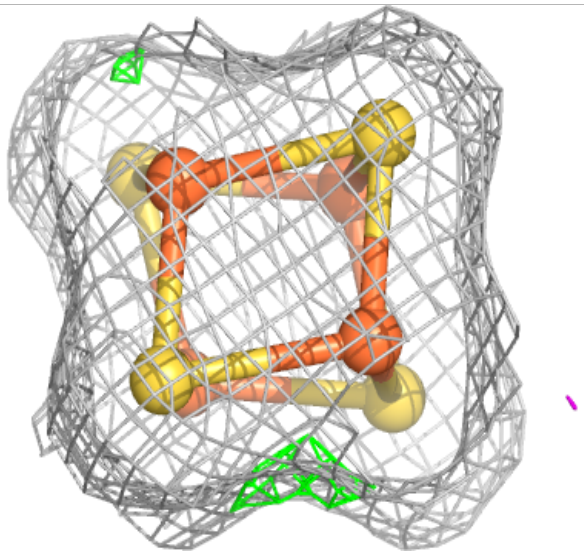


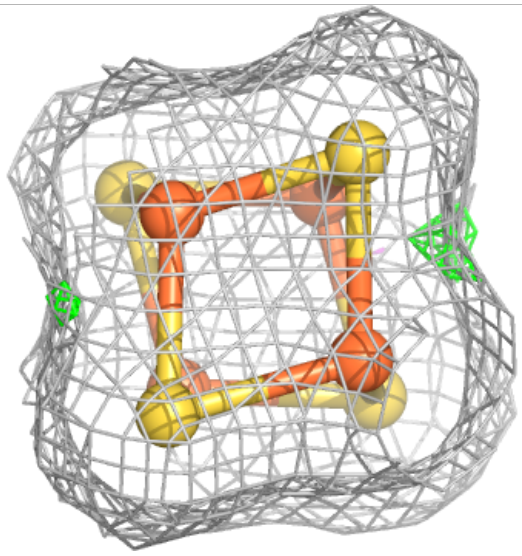


Electron density around SF4 K 1105:

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

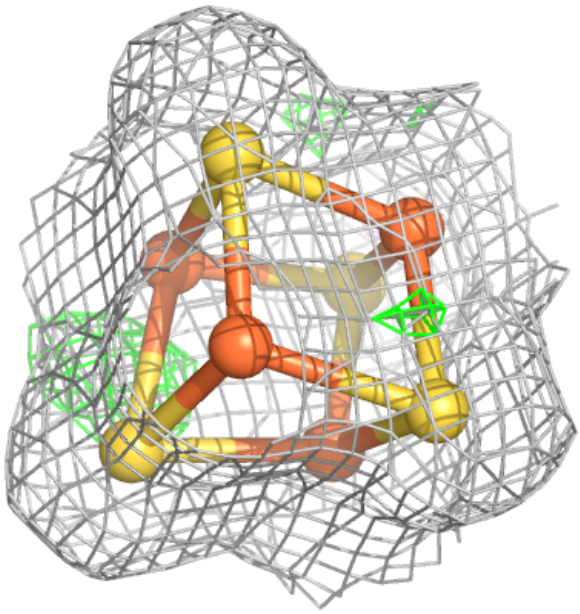


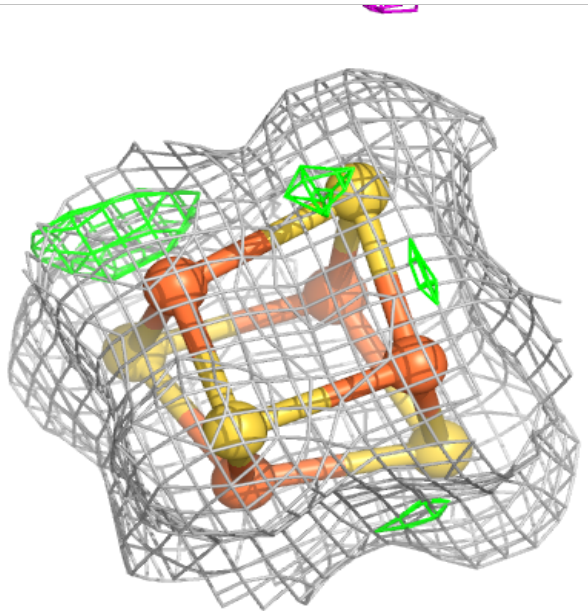


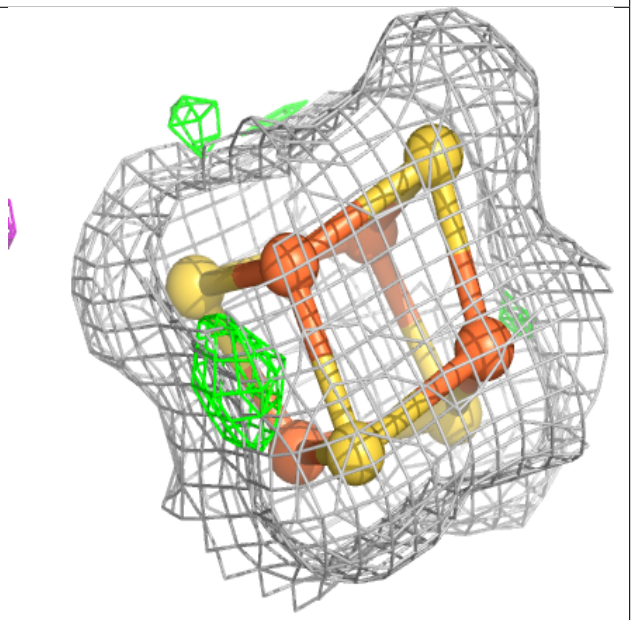


Electron density around SF4 L 303:

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

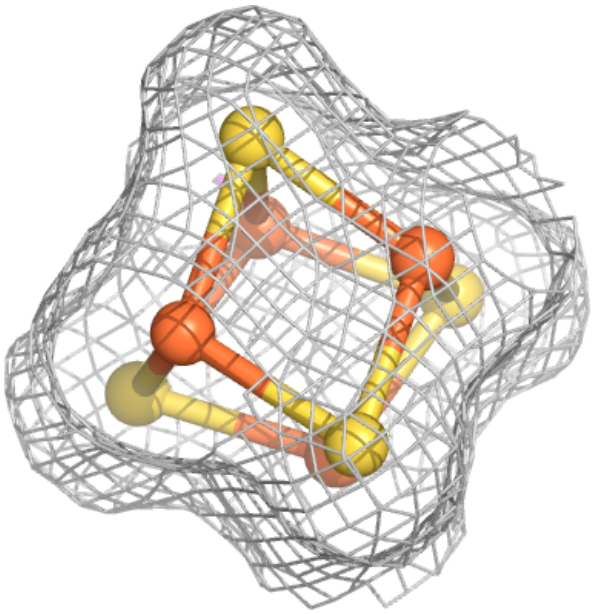


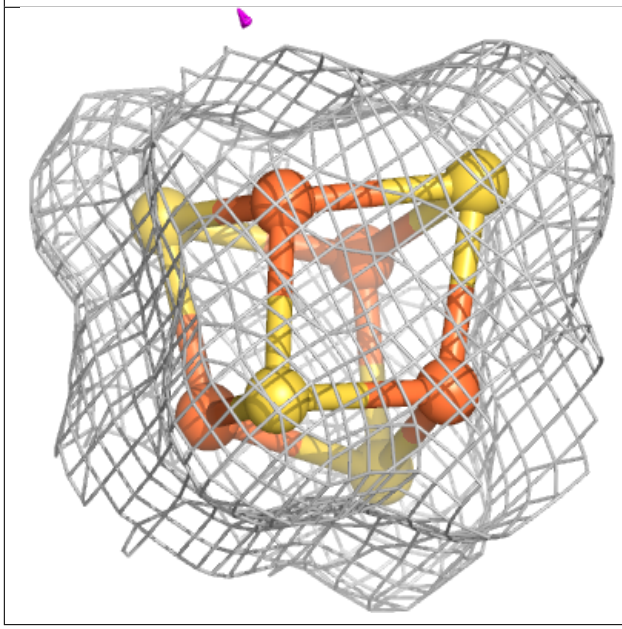


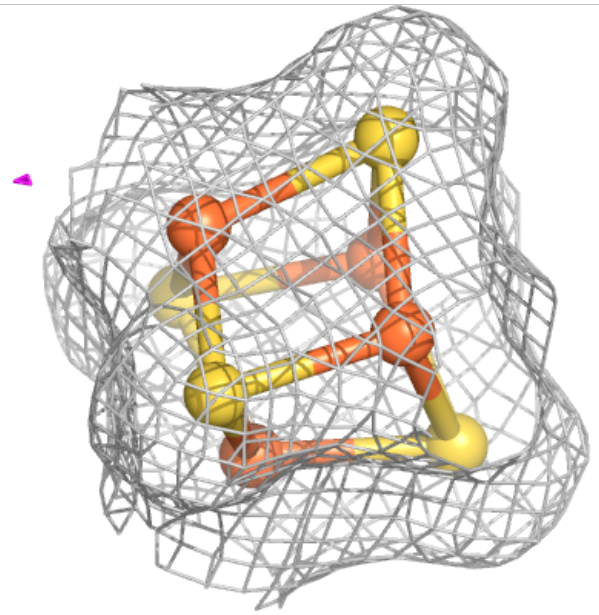


Electron density around SF4 L 304:

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

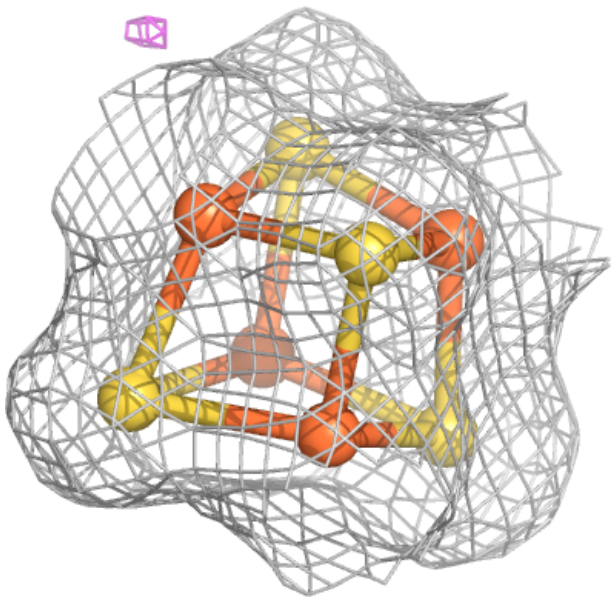


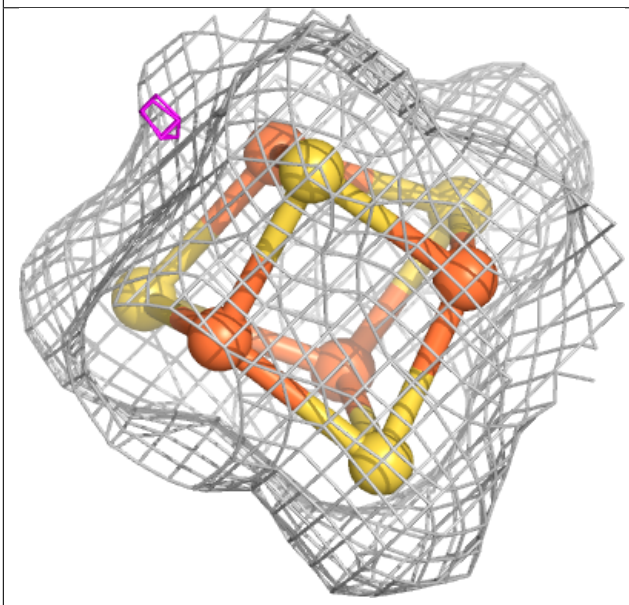


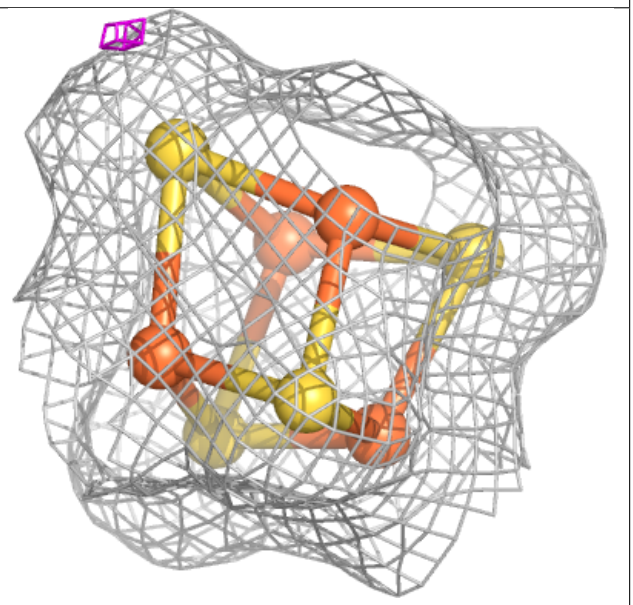


Electron density around SF4 L 305:

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

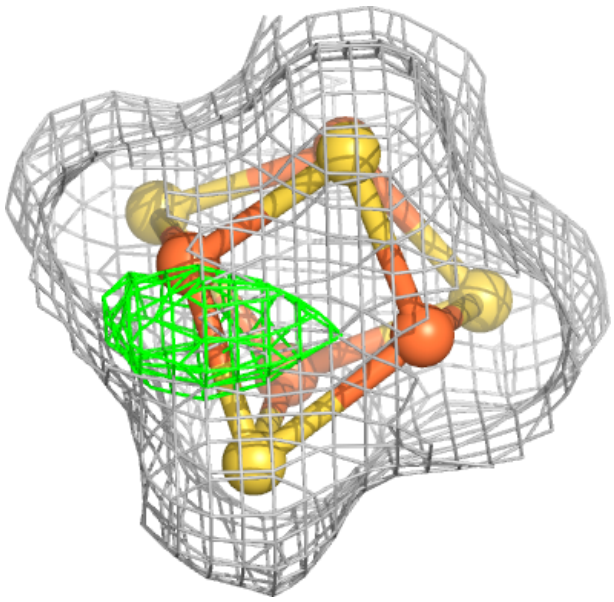


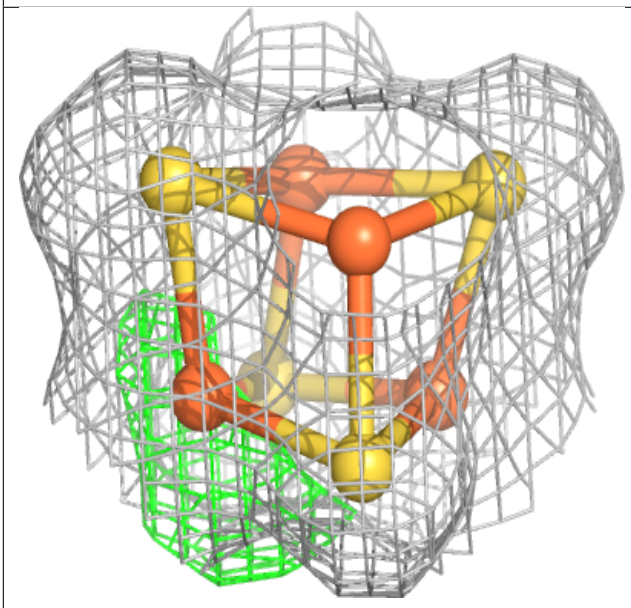


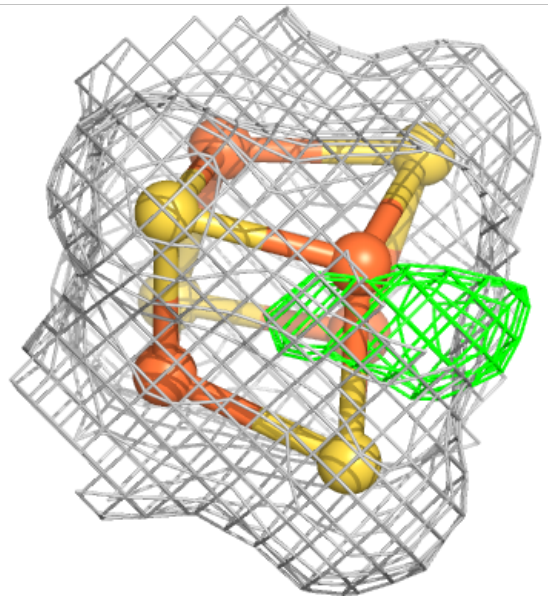


Electron density around SF4 R 1105:

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

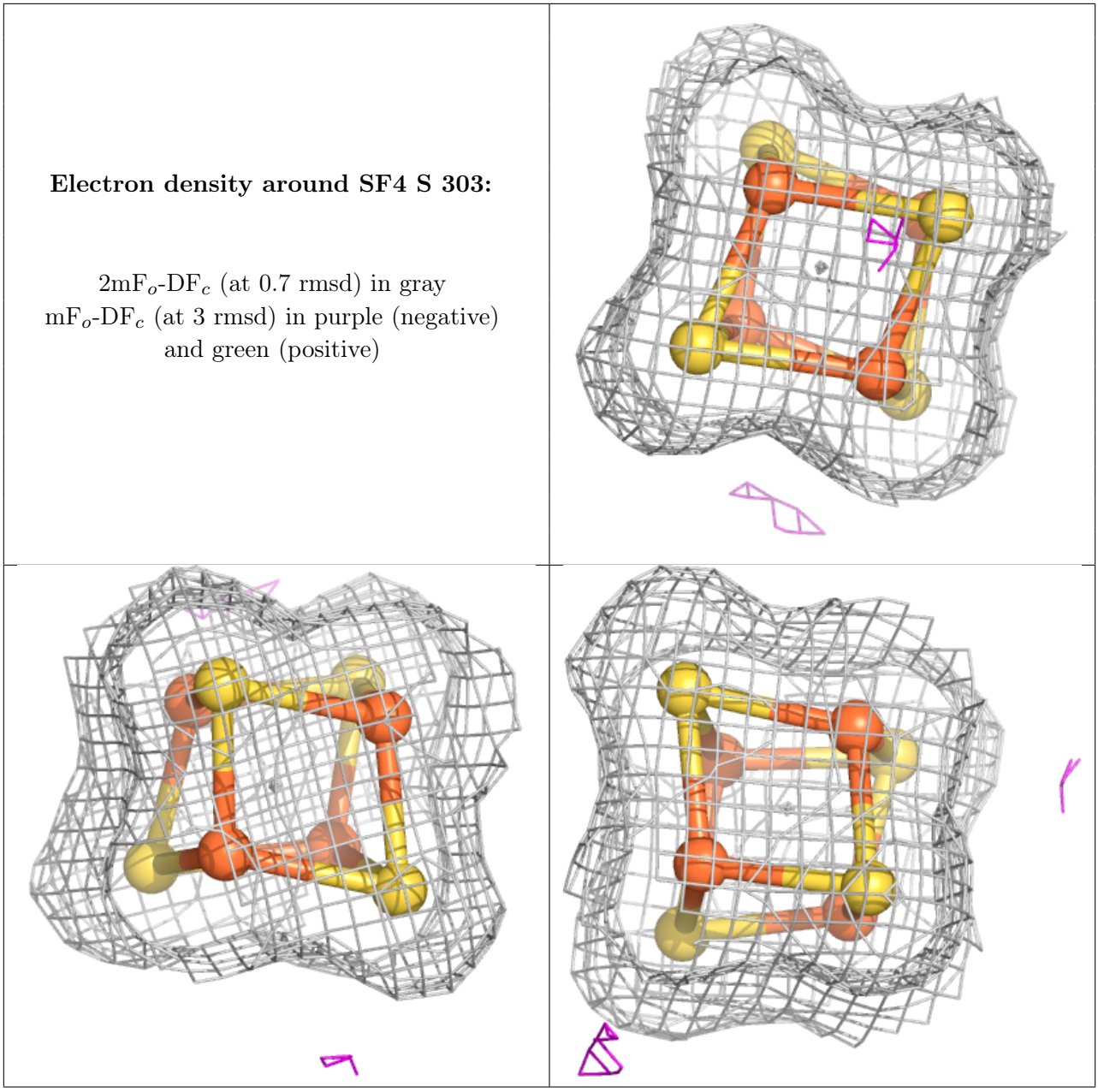






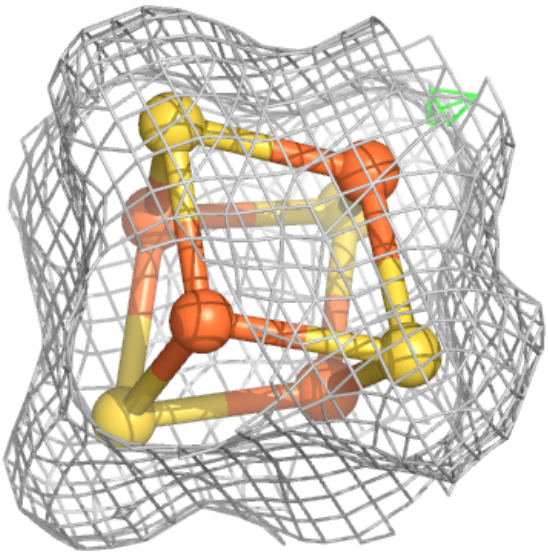
Electron density around SF4 S 303:

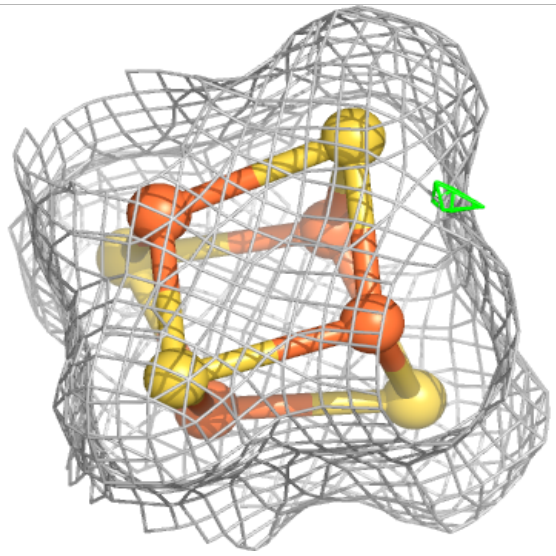
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

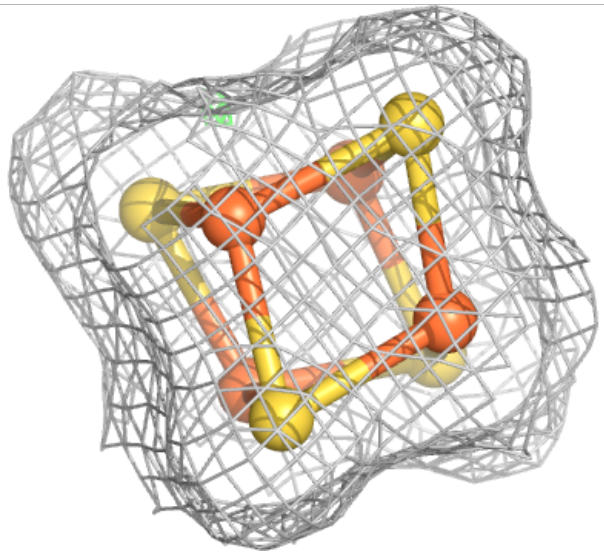


Electron density around SF4 S 304:

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

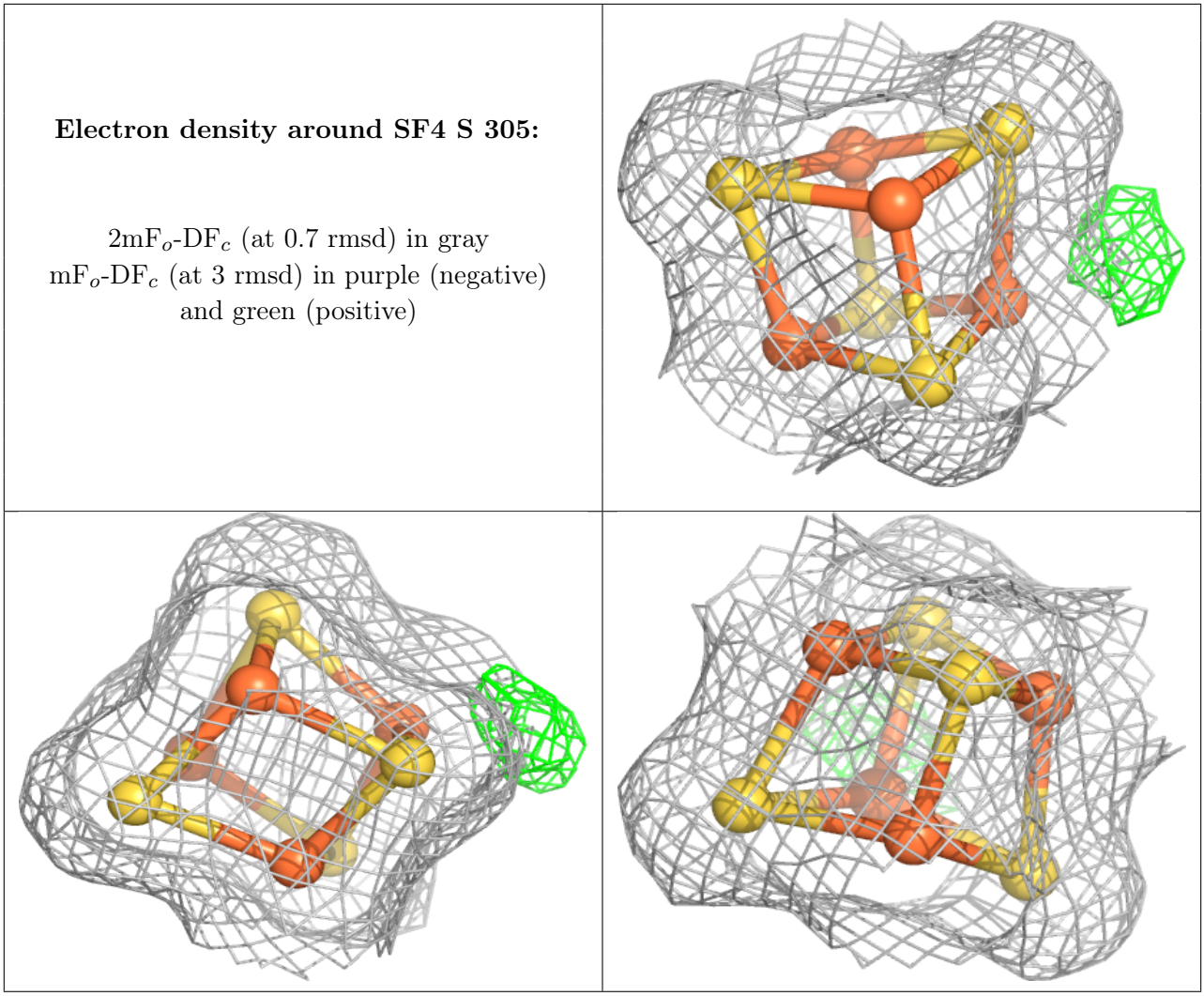






Electron density around SF4 S 305:

$2mF_o$-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.