Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 10:18 pm BST

PDB ID	:	7QBV / pdb_00007qbv
Title	:	B12-dependent radical SAM methyltransferase, Mmp10 with [4Fe-4S] cluster, cobalamin, and S-adenosyl-L-homocysteine bound.
Authors	:	Fyfe, C.D.; Chavas, L.M.G.; Legrand, P.; Benjdia, A.; Berteau, O.
Deposited on	:	2021-11-19
Resolution	:	2.70 Å(reported)

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

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

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

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

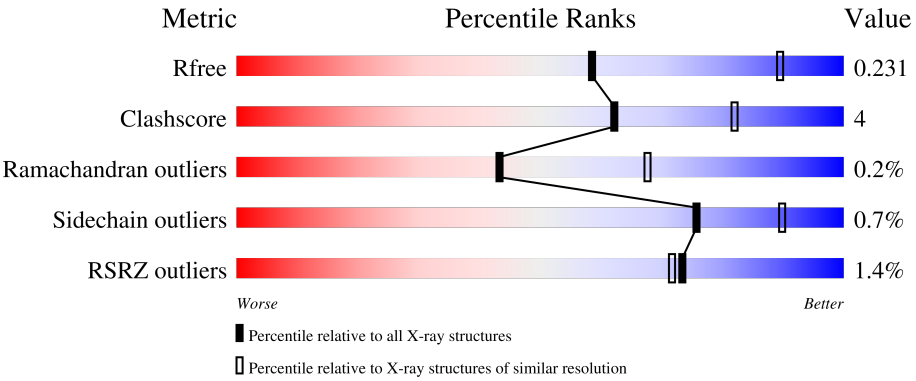
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	436	87% 6% 6%
1	B	436	87% 7% 6%
1	C	436	87% 7% 6%
1	D	436	3% 86% 7% 7%

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
5	COB	A	504	X	-	-	-
5	COB	B	504	X	-	-	-
5	COB	C	504	X	-	-	-
5	COB	D	504	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13237 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 Methyl coenzyme M reductase-arginine methyltransferase Mmp10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3172	2024	520	608	20			
1	B	411	Total	C	N	O	S	0	0	0
			3172	2024	520	608	20			
1	C	411	Total	C	N	O	S	0	0	0
			3172	2024	520	608	20			
1	D	407	Total	C	N	O	S	0	0	0
			3146	2010	516	600	20			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A832SFM5
A	-23	ALA	-	expression tag	UNP A0A832SFM5
A	-22	SER	-	expression tag	UNP A0A832SFM5
A	-21	TRP	-	expression tag	UNP A0A832SFM5
A	-20	SER	-	expression tag	UNP A0A832SFM5
A	-19	HIS	-	expression tag	UNP A0A832SFM5
A	-18	PRO	-	expression tag	UNP A0A832SFM5
A	-17	GLN	-	expression tag	UNP A0A832SFM5
A	-16	PHE	-	expression tag	UNP A0A832SFM5
A	-15	GLU	-	expression tag	UNP A0A832SFM5
A	-14	LYS	-	expression tag	UNP A0A832SFM5
A	-13	SER	-	expression tag	UNP A0A832SFM5
A	-12	GLY	-	expression tag	UNP A0A832SFM5
A	-11	GLY	-	expression tag	UNP A0A832SFM5
A	-10	GLY	-	expression tag	UNP A0A832SFM5
A	-9	GLY	-	expression tag	UNP A0A832SFM5
A	-8	GLY	-	expression tag	UNP A0A832SFM5
A	-7	GLU	-	expression tag	UNP A0A832SFM5
A	-6	ASN	-	expression tag	UNP A0A832SFM5
A	-5	LEU	-	expression tag	UNP A0A832SFM5

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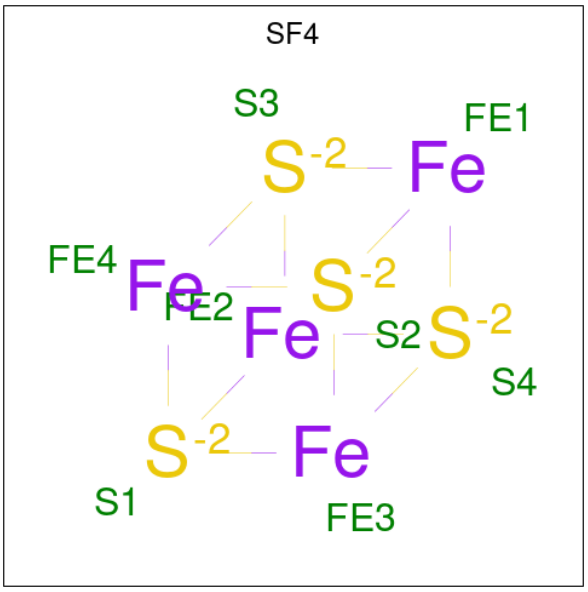
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	expression tag	UNP A0A832SFM5
A	-3	PHE	-	expression tag	UNP A0A832SFM5
A	-2	GLN	-	expression tag	UNP A0A832SFM5
A	-1	GLY	-	expression tag	UNP A0A832SFM5
A	0	HIS	-	expression tag	UNP A0A832SFM5
B	-24	MET	-	initiating methionine	UNP A0A832SFM5
B	-23	ALA	-	expression tag	UNP A0A832SFM5
B	-22	SER	-	expression tag	UNP A0A832SFM5
B	-21	TRP	-	expression tag	UNP A0A832SFM5
B	-20	SER	-	expression tag	UNP A0A832SFM5
B	-19	HIS	-	expression tag	UNP A0A832SFM5
B	-18	PRO	-	expression tag	UNP A0A832SFM5
B	-17	GLN	-	expression tag	UNP A0A832SFM5
B	-16	PHE	-	expression tag	UNP A0A832SFM5
B	-15	GLU	-	expression tag	UNP A0A832SFM5
B	-14	LYS	-	expression tag	UNP A0A832SFM5
B	-13	SER	-	expression tag	UNP A0A832SFM5
B	-12	GLY	-	expression tag	UNP A0A832SFM5
B	-11	GLY	-	expression tag	UNP A0A832SFM5
B	-10	GLY	-	expression tag	UNP A0A832SFM5
B	-9	GLY	-	expression tag	UNP A0A832SFM5
B	-8	GLY	-	expression tag	UNP A0A832SFM5
B	-7	GLU	-	expression tag	UNP A0A832SFM5
B	-6	ASN	-	expression tag	UNP A0A832SFM5
B	-5	LEU	-	expression tag	UNP A0A832SFM5
B	-4	TYR	-	expression tag	UNP A0A832SFM5
B	-3	PHE	-	expression tag	UNP A0A832SFM5
B	-2	GLN	-	expression tag	UNP A0A832SFM5
B	-1	GLY	-	expression tag	UNP A0A832SFM5
B	0	HIS	-	expression tag	UNP A0A832SFM5
C	-24	MET	-	initiating methionine	UNP A0A832SFM5
C	-23	ALA	-	expression tag	UNP A0A832SFM5
C	-22	SER	-	expression tag	UNP A0A832SFM5
C	-21	TRP	-	expression tag	UNP A0A832SFM5
C	-20	SER	-	expression tag	UNP A0A832SFM5
C	-19	HIS	-	expression tag	UNP A0A832SFM5
C	-18	PRO	-	expression tag	UNP A0A832SFM5
C	-17	GLN	-	expression tag	UNP A0A832SFM5
C	-16	PHE	-	expression tag	UNP A0A832SFM5
C	-15	GLU	-	expression tag	UNP A0A832SFM5
C	-14	LYS	-	expression tag	UNP A0A832SFM5
C	-13	SER	-	expression tag	UNP A0A832SFM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLY	-	expression tag	UNP A0A832SFM5
C	-11	GLY	-	expression tag	UNP A0A832SFM5
C	-10	GLY	-	expression tag	UNP A0A832SFM5
C	-9	GLY	-	expression tag	UNP A0A832SFM5
C	-8	GLY	-	expression tag	UNP A0A832SFM5
C	-7	GLU	-	expression tag	UNP A0A832SFM5
C	-6	ASN	-	expression tag	UNP A0A832SFM5
C	-5	LEU	-	expression tag	UNP A0A832SFM5
C	-4	TYR	-	expression tag	UNP A0A832SFM5
C	-3	PHE	-	expression tag	UNP A0A832SFM5
C	-2	GLN	-	expression tag	UNP A0A832SFM5
C	-1	GLY	-	expression tag	UNP A0A832SFM5
C	0	HIS	-	expression tag	UNP A0A832SFM5
D	-24	MET	-	initiating methionine	UNP A0A832SFM5
D	-23	ALA	-	expression tag	UNP A0A832SFM5
D	-22	SER	-	expression tag	UNP A0A832SFM5
D	-21	TRP	-	expression tag	UNP A0A832SFM5
D	-20	SER	-	expression tag	UNP A0A832SFM5
D	-19	HIS	-	expression tag	UNP A0A832SFM5
D	-18	PRO	-	expression tag	UNP A0A832SFM5
D	-17	GLN	-	expression tag	UNP A0A832SFM5
D	-16	PHE	-	expression tag	UNP A0A832SFM5
D	-15	GLU	-	expression tag	UNP A0A832SFM5
D	-14	LYS	-	expression tag	UNP A0A832SFM5
D	-13	SER	-	expression tag	UNP A0A832SFM5
D	-12	GLY	-	expression tag	UNP A0A832SFM5
D	-11	GLY	-	expression tag	UNP A0A832SFM5
D	-10	GLY	-	expression tag	UNP A0A832SFM5
D	-9	GLY	-	expression tag	UNP A0A832SFM5
D	-8	GLY	-	expression tag	UNP A0A832SFM5
D	-7	GLU	-	expression tag	UNP A0A832SFM5
D	-6	ASN	-	expression tag	UNP A0A832SFM5
D	-5	LEU	-	expression tag	UNP A0A832SFM5
D	-4	TYR	-	expression tag	UNP A0A832SFM5
D	-3	PHE	-	expression tag	UNP A0A832SFM5
D	-2	GLN	-	expression tag	UNP A0A832SFM5
D	-1	GLY	-	expression tag	UNP A0A832SFM5
D	0	HIS	-	expression tag	UNP A0A832SFM5

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

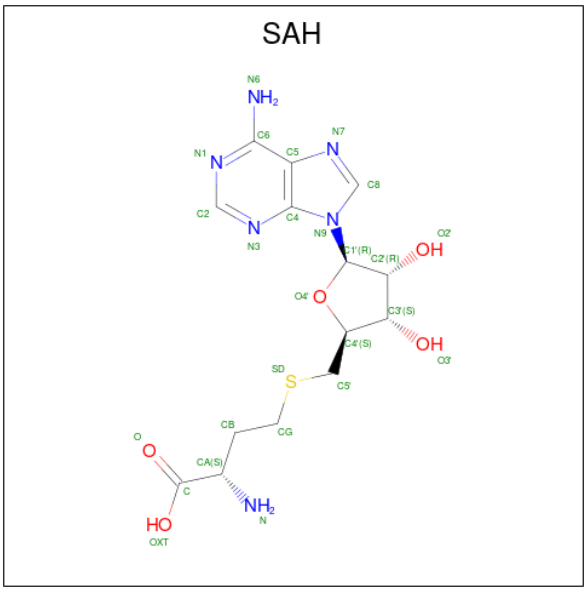


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

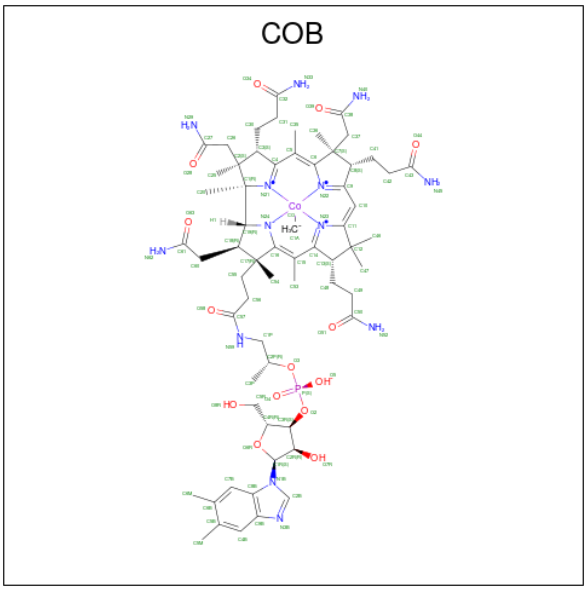
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is CO-METHYLCOBALAMIN (CCD ID: COB) (formula: $C_{63}H_{92}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
5	B	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
5	C	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
5	D	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

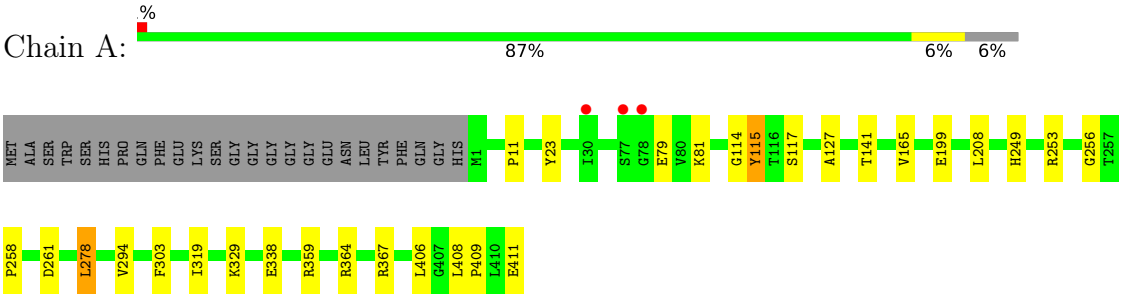
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	O	0	0
			14	14		
7	B	18	Total	O	0	0
			18	18		
7	C	16	Total	O	0	0
			16	16		
7	D	15	Total	O	0	0
			15	15		

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.

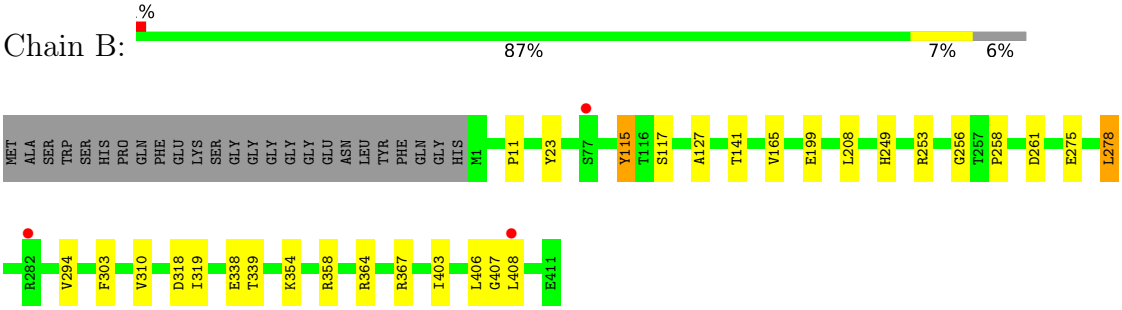
• Molecule 1: Methyl coenzyme M reductase-arginine methyltransferase Mmp10

Chain A:



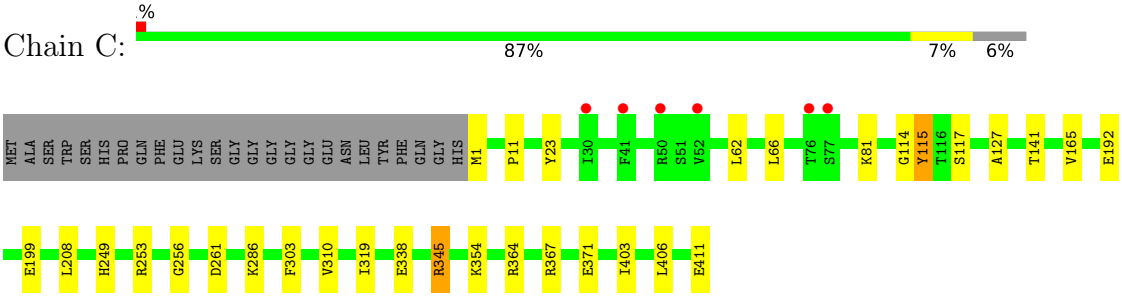
• Molecule 1: Methyl coenzyme M reductase-arginine methyltransferase Mmp10

Chain B:



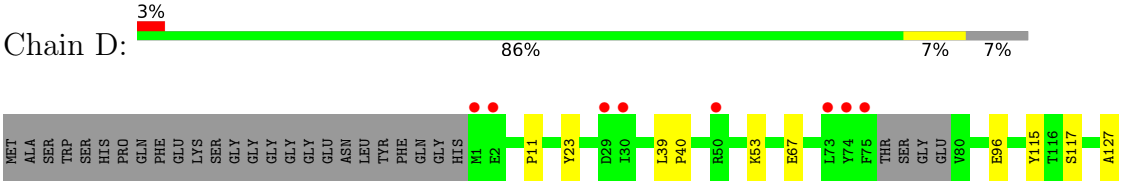
• Molecule 1: Methyl coenzyme M reductase-arginine methyltransferase Mmp10

Chain C:



• Molecule 1: Methyl coenzyme M reductase-arginine methyltransferase Mmp10

Chain D:




T141
D146
V165
K193
E199
L208
H249
R253
G256
D261
K286
F303
I319
D326
K329
A330
E338
R345
R364
R367
E371
L406
G407
L408
P409
L410
E411

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	155.50Å 163.00Å 77.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.70 49.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	76.7 (49.40-2.70) 76.8 (49.40-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-APR-2021)	Depositor
R, R_{free}	0.214 , 0.235 0.210 , 0.231	Depositor DCC
R_{free} test set	2680 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13237	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, SF4, NA, SAH, COB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.57	0/3232	0.93	1/4373 (0.0%)
1	B	0.57	0/3232	0.93	4/4373 (0.1%)
1	C	0.56	0/3232	0.94	1/4373 (0.0%)
1	D	0.55	0/3205	0.92	1/4335 (0.0%)
All	All	0.57	0/12901	0.93	7/17454 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	303	PHE	CA-CB-CG	-5.88	107.92	113.80
1	D	303	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	303	PHE	CA-CB-CG	-5.68	108.12	113.80
1	B	303	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	318	ASP	N-CA-C	5.57	117.03	111.07
1	B	358	ARG	CA-C-N	5.04	127.03	120.28
1	B	358	ARG	C-N-CA	5.04	127.03	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3172	0	3198	21	0
1	B	3172	0	3197	18	0
1	C	3172	0	3197	18	0
1	D	3146	0	3175	19	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
2	C	8	0	0	1	0
2	D	8	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	19	1	0
4	B	26	0	19	1	0
4	C	26	0	19	1	0
4	D	26	0	19	0	0
5	A	92	0	87	10	0
5	B	92	0	87	11	0
5	C	92	0	87	9	0
5	D	92	0	87	10	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	14	0	0	0	0
7	B	18	0	0	1	0
7	C	16	0	0	0	0
7	D	15	0	0	0	0
All	All	13237	0	13191	107	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 (107) 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)
5:C:504:COB:H601	5:C:504:COB:H262	1.58	0.85
5:A:504:COB:H601	5:A:504:COB:H262	1.59	0.85
5:B:504:COB:H601	5:B:504:COB:H262	1.59	0.84
5:D:504:COB:H601	5:D:504:COB:H262	1.58	0.84
1:B:338:GLU:HA	1:B:364:ARG:HG2	1.64	0.77
5:D:504:COB:H552	5:D:504:COB:H531	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:504:COB:H531	5:C:504:COB:H552	1.69	0.74
5:B:504:COB:H552	5:B:504:COB:H531	1.70	0.74
5:A:504:COB:H552	5:A:504:COB:H531	1.70	0.73
1:A:411:GLU:HB3	1:D:53:LYS:HE2	1.75	0.67
1:A:79:GLU:HG2	1:A:81:LYS:NZ	2.16	0.59
5:D:504:COB:H351	5:D:504:COB:H371	1.85	0.59
5:C:504:COB:H351	5:C:504:COB:H371	1.84	0.59
1:B:115:TYR:HB3	7:B:610:HOH:O	2.03	0.59
5:B:504:COB:H351	5:B:504:COB:H371	1.84	0.59
1:A:79:GLU:HG2	1:A:81:LYS:HZ2	1.68	0.59
5:A:504:COB:H351	5:A:504:COB:H371	1.85	0.58
1:A:338:GLU:HB2	1:A:408:LEU:HD21	1.85	0.58
1:D:11:PRO:HB3	2:D:501:SF4:S2	2.44	0.58
1:C:319:ILE:HG23	5:C:504:COB:O4	2.05	0.56
1:A:11:PRO:HB3	2:A:501:SF4:S2	2.47	0.55
5:B:504:COB:H351	5:B:504:COB:C37	2.37	0.55
5:C:504:COB:H351	5:C:504:COB:C37	2.36	0.55
5:A:504:COB:H351	5:A:504:COB:C37	2.37	0.54
5:B:504:COB:H531	5:B:504:COB:C55	2.37	0.54
5:D:504:COB:H351	5:D:504:COB:C37	2.38	0.54
1:C:286:LYS:NZ	1:C:411:GLU:H	2.06	0.54
5:C:504:COB:H531	5:C:504:COB:C55	2.36	0.54
1:D:319:ILE:HG23	5:D:504:COB:O4	2.07	0.54
5:D:504:COB:H531	5:D:504:COB:C55	2.36	0.54
5:A:504:COB:H531	5:A:504:COB:C55	2.37	0.52
1:C:117:SER:HA	1:C:141:THR:HB	1.93	0.51
1:C:127:ALA:HB2	1:C:165:VAL:HG13	1.92	0.51
1:D:127:ALA:HB2	1:D:165:VAL:HG13	1.91	0.51
1:A:409:PRO:HB2	1:A:411:GLU:HG2	1.93	0.51
1:C:11:PRO:HB3	2:C:501:SF4:S2	2.51	0.51
1:B:127:ALA:HB2	1:B:165:VAL:HG13	1.92	0.51
1:D:117:SER:HA	1:D:141:THR:HB	1.93	0.51
1:B:11:PRO:HB3	2:B:501:SF4:S2	2.51	0.50
1:B:339:THR:HG21	1:B:407:GLY:HA2	1.93	0.50
1:D:345:ARG:HD2	1:D:371:GLU:HB3	1.94	0.50
1:A:117:SER:HA	1:A:141:THR:HB	1.94	0.49
1:B:338:GLU:HB2	1:B:408:LEU:HD11	1.94	0.49
1:C:345:ARG:HD2	1:C:371:GLU:HB3	1.95	0.49
1:D:338:GLU:HA	1:D:364:ARG:HG2	1.94	0.49
1:A:127:ALA:HB2	1:A:165:VAL:HG13	1.94	0.49
1:B:117:SER:HA	1:B:141:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CE1	4:A:503:SAH:H3'	2.48	0.49
1:C:338:GLU:HA	1:C:364:ARG:HG2	1.95	0.49
1:A:253:ARG:NH2	1:A:261:ASP:OD1	2.46	0.48
1:D:326:ASP:HA	1:D:329:LYS:NZ	2.28	0.48
5:C:504:COB:H2B	5:C:504:COB:O2	2.13	0.48
1:D:253:ARG:NH2	1:D:261:ASP:OD1	2.46	0.48
1:B:253:ARG:NH2	1:B:261:ASP:OD1	2.45	0.48
1:B:275:GLU:HA	1:B:278:LEU:HD22	1.95	0.48
1:C:253:ARG:NH2	1:C:261:ASP:OD1	2.46	0.48
5:D:504:COB:H2B	5:D:504:COB:O2	2.13	0.47
5:B:504:COB:C61	5:B:504:COB:H252	2.44	0.47
5:C:504:COB:H621	5:C:504:COB:H18	1.64	0.47
5:A:504:COB:C61	5:A:504:COB:H252	2.44	0.47
5:B:504:COB:H2B	5:B:504:COB:O2	2.14	0.47
5:C:504:COB:C61	5:C:504:COB:H252	2.45	0.47
1:D:146:ASP:HB2	1:D:193:LYS:HZ2	1.80	0.47
1:A:338:GLU:HA	1:A:364:ARG:HG2	1.96	0.47
1:A:79:GLU:CG	1:A:81:LYS:NZ	2.78	0.47
1:C:286:LYS:HZ3	1:C:411:GLU:H	1.63	0.47
5:A:504:COB:H2B	5:A:504:COB:O2	2.14	0.46
5:D:504:COB:H252	5:D:504:COB:C61	2.45	0.46
5:D:504:COB:H621	5:D:504:COB:H18	1.62	0.46
1:C:367:ARG:HG3	1:C:406:LEU:HD13	1.98	0.46
1:A:199:GLU:OE1	1:A:249:HIS:HD2	1.99	0.46
1:C:199:GLU:OE1	1:C:249:HIS:HD2	1.99	0.46
1:A:278:LEU:HG	1:D:96:GLU:OE2	2.16	0.46
1:D:367:ARG:HG3	1:D:406:LEU:HD13	1.98	0.45
1:A:79:GLU:CG	1:A:81:LYS:HZ1	2.29	0.45
1:D:39:LEU:HD23	1:D:40:PRO:HD2	1.99	0.45
1:A:23:TYR:CD1	5:A:504:COB:H421	2.52	0.45
1:D:286:LYS:HG3	1:D:410:LEU:HD23	1.98	0.45
5:B:504:COB:H621	5:B:504:COB:H18	1.63	0.44
1:D:199:GLU:OE1	1:D:249:HIS:HD2	1.99	0.44
1:B:310:VAL:HG21	1:B:403:ILE:HD13	2.00	0.44
1:B:258:PRO:HB2	1:B:294:VAL:HG11	2.00	0.43
1:B:23:TYR:CD1	5:B:504:COB:H421	2.54	0.43
1:B:199:GLU:OE1	1:B:249:HIS:HD2	2.00	0.43
1:D:193:LYS:HB3	1:D:193:LYS:HE2	1.86	0.43
1:C:62:LEU:O	1:C:66:LEU:HG	2.19	0.42
1:A:367:ARG:HG3	1:A:406:LEU:HD13	2.01	0.42
1:B:208:LEU:O	1:B:256:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:TYR:CE1	4:B:503:SAH:H3'	2.55	0.42
1:C:208:LEU:O	1:C:256:GLY:HA2	2.20	0.42
1:B:367:ARG:HG3	1:B:406:LEU:HD13	2.02	0.41
1:D:23:TYR:CD1	5:D:504:COB:H421	2.55	0.41
5:B:504:COB:H422	5:B:504:COB:H372	2.02	0.41
1:C:1:MET:HB3	1:C:81:LYS:HG3	2.03	0.41
1:C:23:TYR:OH	4:C:503:SAH:H5'2	2.20	0.41
1:A:319:ILE:HG23	5:A:504:COB:O4	2.21	0.41
1:A:208:LEU:O	1:A:256:GLY:HA2	2.21	0.41
1:A:258:PRO:HB2	1:A:294:VAL:HG11	2.02	0.41
1:B:253:ARG:HH22	1:B:261:ASP:CG	2.29	0.41
1:C:253:ARG:HH22	1:C:261:ASP:CG	2.29	0.41
1:C:310:VAL:HG21	1:C:403:ILE:HD13	2.03	0.41
1:D:338:GLU:HB2	1:D:408:LEU:HD21	2.03	0.41
1:B:319:ILE:HG23	5:B:504:COB:O4	2.20	0.40
1:D:208:LEU:O	1:D:256:GLY:HA2	2.20	0.40
1:A:114:GLY:O	1:A:115:TYR:C	2.64	0.40
5:A:504:COB:H372	5:A:504:COB:H422	2.03	0.40
1:C:114:GLY:O	1:C:115:TYR:C	2.65	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	409/436 (94%)	405 (99%)	3 (1%)	1 (0%)	43	68
1	B	409/436 (94%)	404 (99%)	4 (1%)	1 (0%)	43	68
1	C	409/436 (94%)	405 (99%)	3 (1%)	1 (0%)	43	68
1	D	403/436 (92%)	398 (99%)	4 (1%)	1 (0%)	43	68
All	All	1630/1744 (94%)	1612 (99%)	14 (1%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	TYR
1	B	115	TYR
1	C	115	TYR
1	D	115	TYR

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	356/374 (95%)	353 (99%)	3 (1%)	73	88
1	B	356/374 (95%)	354 (99%)	2 (1%)	78	91
1	C	356/374 (95%)	353 (99%)	3 (1%)	73	88
1	D	353/374 (94%)	351 (99%)	2 (1%)	78	91
All	All	1421/1496 (95%)	1411 (99%)	10 (1%)	76	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	LEU
1	A	329	LYS
1	A	359	ARG
1	B	278	LEU
1	B	354	LYS
1	C	192	GLU
1	C	345	ARG
1	C	354	LYS
1	D	67	GLU
1	D	345	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN

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Mol	Chain	Res	Type
1	A	272	ASN
1	B	108	ASN
1	C	108	ASN
1	D	108	ASN
1	D	249	HIS
1	D	272	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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SAH	B	503	-	27,28,28	0.40	0	38,40,40	0.78	2 (5%)
5	COB	A	504	-	92,102,102	1.52	7 (7%)	148,170,170	1.61	19 (12%)
4	SAH	D	503	-	27,28,28	0.30	0	38,40,40	0.85	2 (5%)
2	SF4	B	501	1	0,12,12	-	-	-		
4	SAH	A	503	-	27,28,28	0.42	1 (3%)	38,40,40	0.70	2 (5%)
2	SF4	D	501	1	0,12,12	-	-	-		
2	SF4	C	501	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	COB	B	504	-	92,102,102	1.55	7 (7%)	148,170,170	1.62	20 (13%)
5	COB	C	504	-	92,102,102	1.52	7 (7%)	148,170,170	1.61	20 (13%)
5	COB	D	504	-	92,102,102	1.54	7 (7%)	148,170,170	1.63	18 (12%)
4	SAH	C	503	-	27,28,28	0.44	1 (3%)	38,40,40	0.96	2 (5%)
2	SF4	A	501	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAH	B	503	-	-	4/15/31/31	0/3/3/3
5	COB	A	504	-	1/1/36/38	14/56/231/231	0/3/11/11
4	SAH	D	503	-	-	9/15/31/31	0/3/3/3
2	SF4	B	501	1	-	-	0/6/5/5
4	SAH	A	503	-	-	5/15/31/31	0/3/3/3
5	COB	B	504	-	1/1/36/38	14/56/231/231	0/3/11/11
2	SF4	C	501	1	-	-	0/6/5/5
2	SF4	D	501	1	-	-	0/6/5/5
5	COB	C	504	-	1/1/36/38	14/56/231/231	0/3/11/11
5	COB	D	504	-	1/1/36/38	14/56/231/231	0/3/11/11
4	SAH	C	503	-	-	6/15/31/31	0/3/3/3
2	SF4	A	501	1	-	-	0/6/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	504	COB	C19-N24	-10.73	1.26	1.49
5	B	504	COB	C19-N24	-10.68	1.26	1.49
5	C	504	COB	C19-N24	-10.66	1.26	1.49
5	A	504	COB	C19-N24	-10.54	1.27	1.49
5	D	504	COB	C8B-C9B	5.45	1.49	1.40
5	B	504	COB	C8B-C9B	5.39	1.49	1.40
5	A	504	COB	C8B-C9B	5.18	1.49	1.40
5	C	504	COB	C8B-C9B	5.15	1.49	1.40
5	D	504	COB	C6B-C5B	3.71	1.50	1.40
5	B	504	COB	C6B-C5B	3.56	1.49	1.40
5	A	504	COB	C6B-C5B	3.40	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	504	COB	C6B-C5B	3.35	1.49	1.40
5	B	504	COB	C9B-N3B	-2.75	1.34	1.39
5	D	504	COB	C9B-N3B	-2.66	1.34	1.39
5	C	504	COB	C9B-N3B	-2.62	1.35	1.39
5	A	504	COB	C9B-N3B	-2.49	1.35	1.39
5	B	504	COB	C8B-N1B	-2.41	1.34	1.39
5	A	504	COB	C8B-N1B	-2.34	1.34	1.39
5	C	504	COB	C8B-N1B	-2.31	1.34	1.39
5	D	504	COB	C8B-N1B	-2.28	1.34	1.39
5	D	504	COB	C2B-N3B	2.28	1.35	1.31
5	A	504	COB	C2B-N3B	2.23	1.35	1.31
5	A	504	COB	C10-C9	2.22	1.45	1.39
5	C	504	COB	C10-C9	2.21	1.45	1.39
5	B	504	COB	C2B-N3B	2.19	1.35	1.31
5	C	504	COB	C2B-N3B	2.19	1.35	1.31
5	D	504	COB	C10-C9	2.10	1.45	1.39
5	B	504	COB	C10-C9	2.10	1.45	1.39
4	A	503	SAH	CB-CA	2.09	1.57	1.53
4	C	503	SAH	CB-CA	2.07	1.57	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	504	COB	C18-C19-N24	8.42	115.24	101.88
5	C	504	COB	C18-C19-N24	8.23	114.95	101.88
5	A	504	COB	C18-C19-N24	8.23	114.95	101.88
5	D	504	COB	C18-C19-N24	8.08	114.71	101.88
5	D	504	COB	C1-C19-C18	6.14	130.88	121.81
5	C	504	COB	C1-C19-C18	6.08	130.80	121.81
5	B	504	COB	C12-C11-C10	-5.79	118.25	123.54
5	A	504	COB	C1-C19-C18	5.79	130.37	121.81
5	B	504	COB	C1-C19-C18	5.78	130.36	121.81
5	A	504	COB	C12-C11-C10	-5.71	118.33	123.54
5	D	504	COB	C12-C11-C10	-5.68	118.35	123.54
5	C	504	COB	C12-C11-C10	-5.51	118.51	123.54
5	A	504	COB	C1-C19-N24	4.46	113.39	106.33
5	D	504	COB	C1-C19-N24	4.34	113.20	106.33
5	B	504	COB	C1-C19-N24	4.24	113.05	106.33
5	C	504	COB	C1-C19-N24	4.20	112.97	106.33
4	C	503	SAH	CB-CG-SD	-4.00	104.34	113.31
5	D	504	COB	C12-C11-N23	3.93	115.73	111.48
5	B	504	COB	C12-C11-N23	3.89	115.69	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	504	COB	C12-C11-N23	3.88	115.68	111.48
5	C	504	COB	C12-C11-N23	3.79	115.58	111.48
5	B	504	COB	C48-C13-C14	3.76	118.37	109.63
5	A	504	COB	C48-C13-C14	3.71	118.25	109.63
5	C	504	COB	C48-C13-C14	3.70	118.24	109.63
5	D	504	COB	C48-C13-C14	3.65	118.13	109.63
4	D	503	SAH	CB-CG-SD	-3.64	105.14	113.31
5	D	504	COB	C8B-C9B-N3B	-3.48	106.13	109.97
5	C	504	COB	C8B-C9B-N3B	-3.30	106.33	109.97
5	D	504	COB	C26-C2-C3	-3.25	101.67	107.41
4	B	503	SAH	CB-CA-N	3.17	118.49	110.17
5	B	504	COB	C8B-C9B-N3B	-3.17	106.47	109.97
5	D	504	COB	C3R-C2R-C1R	3.09	106.74	99.89
5	B	504	COB	C3R-C2R-C1R	3.08	106.72	99.89
5	A	504	COB	C8B-C9B-N3B	-3.04	106.61	109.97
5	A	504	COB	C26-C2-C3	-3.03	102.06	107.41
5	A	504	COB	C3R-C2R-C1R	2.96	106.45	99.89
5	D	504	COB	C37-C7-C6	2.91	116.27	107.12
5	B	504	COB	C20-C1-C19	-2.90	104.42	110.23
5	C	504	COB	C20-C1-C19	-2.88	104.46	110.23
5	C	504	COB	C26-C2-C3	-2.88	102.32	107.41
5	C	504	COB	C37-C7-C6	2.85	116.08	107.12
5	C	504	COB	C3R-C2R-C1R	2.84	106.17	99.89
5	D	504	COB	C20-C1-C19	-2.83	104.56	110.23
5	B	504	COB	C37-C7-C6	2.81	115.95	107.12
5	A	504	COB	C20-C1-C19	-2.81	104.60	110.23
5	B	504	COB	C26-C2-C3	-2.80	102.47	107.41
5	A	504	COB	C37-C7-C6	2.79	115.88	107.12
5	D	504	COB	C7B-C8B-C9B	-2.72	119.30	122.52
5	D	504	COB	C9B-N3B-C2B	2.66	107.61	104.44
5	C	504	COB	C9B-C8B-N1B	2.64	106.46	105.35
5	C	504	COB	C7B-C8B-C9B	-2.63	119.40	122.52
5	A	504	COB	O6R-C1R-N1B	2.60	113.19	108.06
5	B	504	COB	O6R-C1R-N1B	2.58	113.14	108.06
5	D	504	COB	C9B-C8B-N1B	2.57	106.43	105.35
4	B	503	SAH	CB-CG-SD	-2.50	107.69	113.31
5	C	504	COB	O6R-C1R-N1B	2.49	112.96	108.06
5	D	504	COB	O6R-C1R-N1B	2.46	112.91	108.06
5	B	504	COB	C9B-C8B-N1B	2.45	106.39	105.35
5	A	504	COB	C7B-C8B-C9B	-2.44	119.62	122.52
5	C	504	COB	C9B-N3B-C2B	2.44	107.34	104.44
5	B	504	COB	C7B-C8B-C9B	-2.37	119.71	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	SAH	CB-CA-N	2.33	116.27	110.17
5	A	504	COB	C9B-N3B-C2B	2.32	107.20	104.44
5	B	504	COB	C9B-N3B-C2B	2.31	107.19	104.44
5	C	504	COB	C41-C8-C7	2.26	120.36	114.14
5	A	504	COB	C30-C3-C4	2.25	114.87	109.63
5	B	504	COB	C42-C41-C8	-2.24	108.26	114.73
5	D	504	COB	C41-C8-C7	2.23	120.29	114.14
4	D	503	SAH	CB-CA-N	2.23	116.00	110.17
4	A	503	SAH	CB-CG-SD	-2.22	108.33	113.31
5	A	504	COB	C2P-C1P-N59	-2.22	109.66	112.93
5	D	504	COB	C30-C3-C4	2.15	114.62	109.63
5	B	504	COB	C41-C8-C7	2.14	120.02	114.14
5	C	504	COB	C30-C3-C4	2.11	114.54	109.63
5	A	504	COB	C41-C8-C7	2.11	119.94	114.14
5	C	504	COB	C9-C10-C11	-2.11	122.78	125.88
4	A	503	SAH	CB-CA-N	2.10	115.67	110.17
5	A	504	COB	C60-C18-C19	2.09	119.07	114.09
5	B	504	COB	C30-C3-C4	2.09	114.48	109.63
5	D	504	COB	C60-C18-C19	2.08	119.05	114.09
5	C	504	COB	C60-C18-C19	2.07	119.03	114.09
5	B	504	COB	C7-C6-N22	2.04	111.66	107.94
5	B	504	COB	O6R-C1R-C2R	-2.02	102.23	106.64
5	C	504	COB	C26-C2-C1	2.02	113.16	110.01
5	A	504	COB	C26-C2-C1	2.02	113.15	110.01

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	504	COB	C19
5	B	504	COB	C19
5	C	504	COB	C19
5	D	504	COB	C19

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	SAH	O4'-C4'-C5'-SD
4	A	503	SAH	C3'-C4'-C5'-SD
4	B	503	SAH	O-C-CA-N
4	B	503	SAH	O4'-C4'-C5'-SD
4	B	503	SAH	C3'-C4'-C5'-SD
4	C	503	SAH	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	D	503	SAH	O-C-CA-N
4	D	503	SAH	O4'-C4'-C5'-SD
4	D	503	SAH	C3'-C4'-C5'-SD
5	A	504	COB	C18-C60-C61-O63
5	A	504	COB	C18-C60-C61-N62
5	A	504	COB	C1P-C2P-O3-P
5	A	504	COB	C3P-C2P-O3-P
5	B	504	COB	C18-C60-C61-O63
5	B	504	COB	C18-C60-C61-N62
5	B	504	COB	C1P-C2P-O3-P
5	B	504	COB	C3P-C2P-O3-P
5	C	504	COB	C18-C60-C61-O63
5	C	504	COB	C18-C60-C61-N62
5	C	504	COB	C1P-C2P-O3-P
5	C	504	COB	C3P-C2P-O3-P
5	D	504	COB	C18-C60-C61-O63
5	D	504	COB	C18-C60-C61-N62
5	D	504	COB	C1P-C2P-O3-P
5	D	504	COB	C3P-C2P-O3-P
4	C	503	SAH	OXT-C-CA-N
4	A	503	SAH	OXT-C-CA-N
4	B	503	SAH	OXT-C-CA-N
4	D	503	SAH	OXT-C-CA-N
5	A	504	COB	C2R-C1R-N1B-C8B
5	A	504	COB	O6R-C1R-N1B-C8B
5	B	504	COB	C2R-C1R-N1B-C8B
5	B	504	COB	O6R-C1R-N1B-C8B
5	C	504	COB	C2R-C1R-N1B-C8B
5	C	504	COB	O6R-C1R-N1B-C8B
5	D	504	COB	C2R-C1R-N1B-C8B
5	D	504	COB	O6R-C1R-N1B-C8B
5	A	504	COB	C4-C3-C30-C31
5	B	504	COB	C4-C3-C30-C31
5	C	504	COB	C4-C3-C30-C31
5	D	504	COB	C4-C3-C30-C31
5	B	504	COB	C38-C37-C7-C6
5	A	504	COB	C2-C3-C30-C31
5	A	504	COB	C48-C49-C50-O51
5	A	504	COB	C48-C49-C50-N52
5	B	504	COB	C48-C49-C50-O51
5	B	504	COB	C48-C49-C50-N52
5	C	504	COB	C48-C49-C50-O51

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Mol	Chain	Res	Type	Atoms
5	C	504	COB	C48-C49-C50-N52
5	D	504	COB	C48-C49-C50-N52
4	A	503	SAH	O-C-CA-N
5	D	504	COB	C48-C49-C50-O51
5	B	504	COB	C2-C3-C30-C31
5	C	504	COB	C2-C3-C30-C31
5	D	504	COB	C2-C3-C30-C31
4	C	503	SAH	C2'-C1'-N9-C8
4	A	503	SAH	C-CA-CB-CG
4	D	503	SAH	C-CA-CB-CG
4	C	503	SAH	O-C-CA-CB
5	C	504	COB	C30-C31-C32-O34
5	C	504	COB	C30-C31-C32-N33
4	C	503	SAH	OXT-C-CA-CB
5	A	504	COB	C38-C37-C7-C6
5	A	504	COB	C30-C31-C32-O34
5	D	504	COB	C30-C31-C32-O34
5	D	504	COB	C30-C31-C32-N33
5	A	504	COB	C30-C31-C32-N33
4	D	503	SAH	O-C-CA-CB
5	C	504	COB	C38-C37-C7-C6
5	D	504	COB	C38-C37-C7-C6
4	D	503	SAH	CB-CG-SD-C5'
4	D	503	SAH	OXT-C-CA-CB
4	C	503	SAH	O4'-C1'-N9-C8
5	B	504	COB	C30-C31-C32-N33
4	D	503	SAH	N-CA-CB-CG
5	A	504	COB	C38-C37-C7-C36
5	B	504	COB	C38-C37-C7-C36
5	C	504	COB	C38-C37-C7-C36
5	D	504	COB	C38-C37-C7-C36
5	B	504	COB	C30-C31-C32-O34

There are no ring outliers.

11 monomers are involved in 47 short contacts:

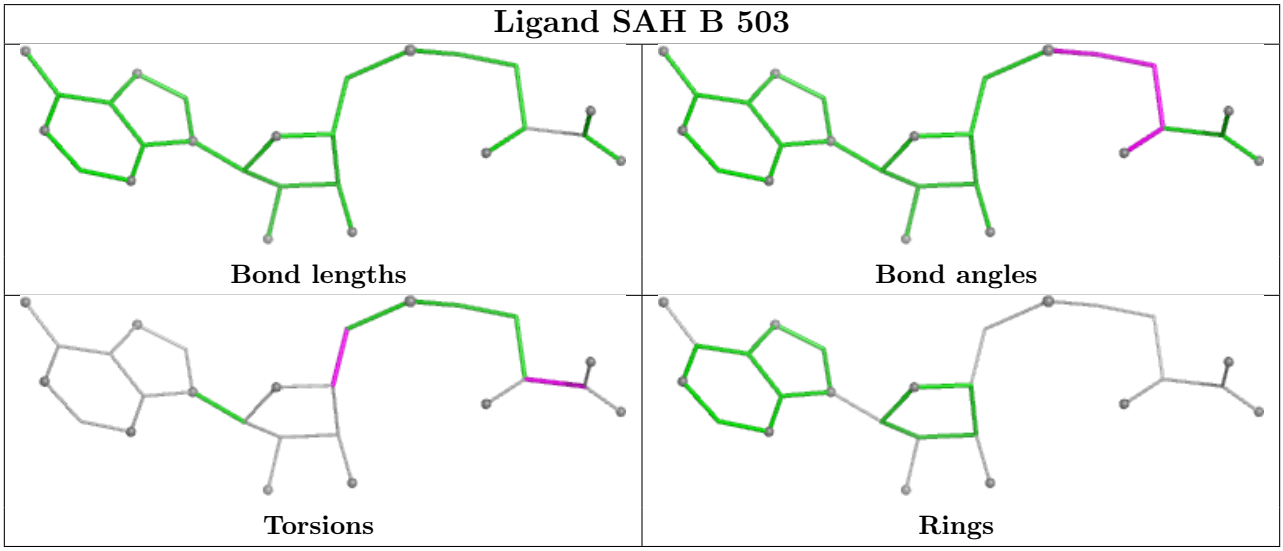
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	SAH	1	0
5	A	504	COB	10	0
2	B	501	SF4	1	0
4	A	503	SAH	1	0
2	D	501	SF4	1	0

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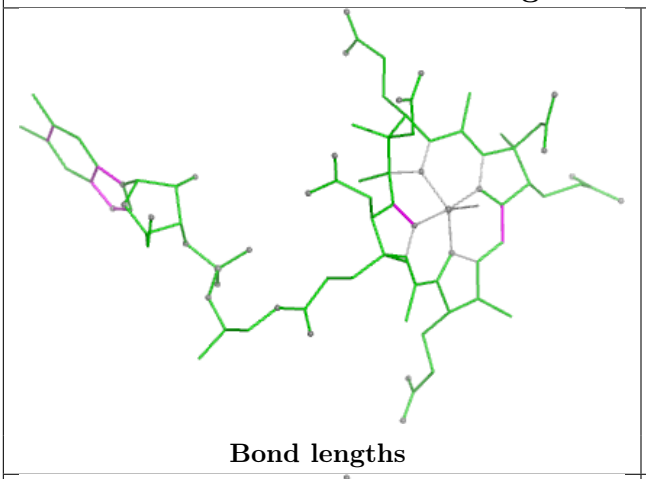
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	SF4	1	0
5	B	504	COB	11	0
5	C	504	COB	9	0
5	D	504	COB	10	0
4	C	503	SAH	1	0
2	A	501	SF4	1	0

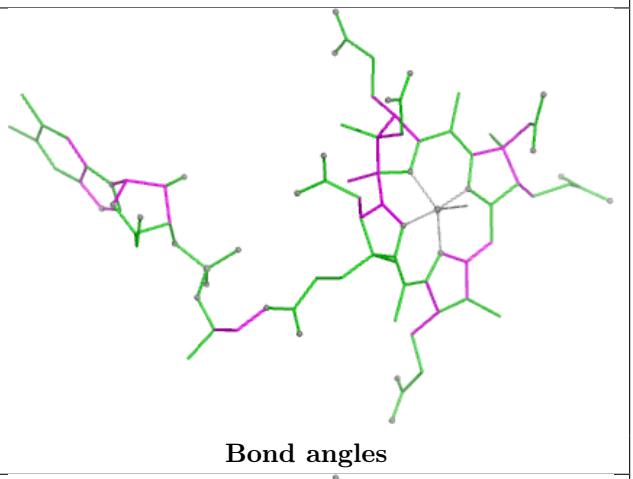
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



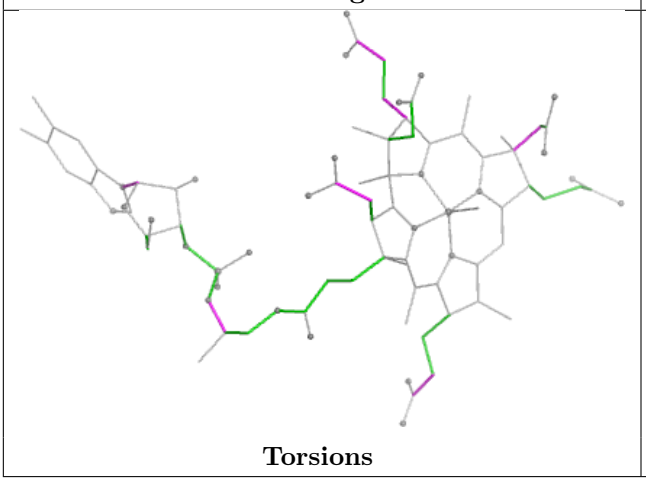
Ligand COB A 504



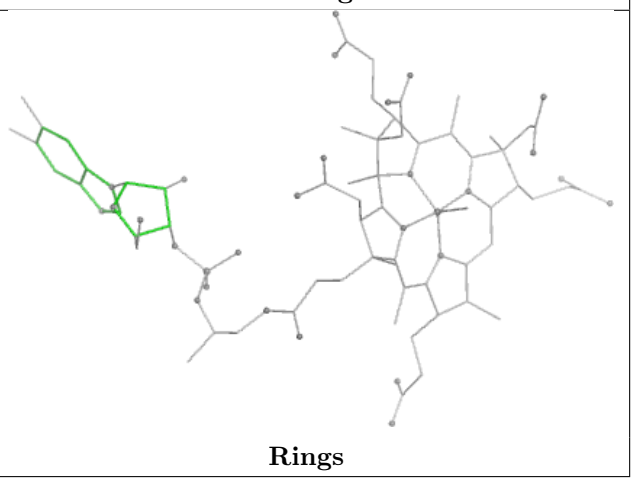
Bond lengths



Bond angles

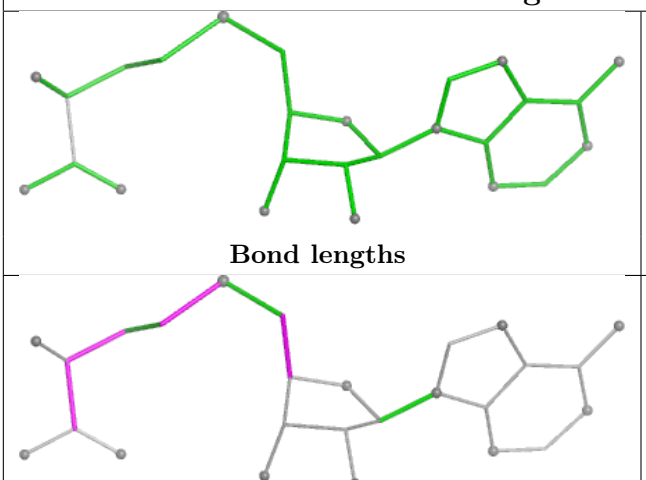


Torsions

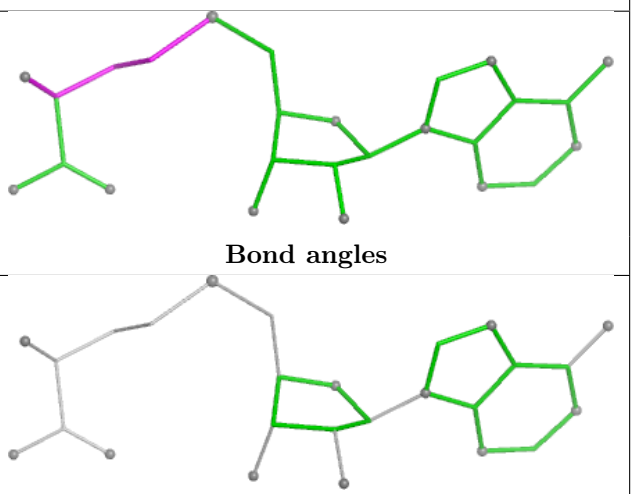


Rings

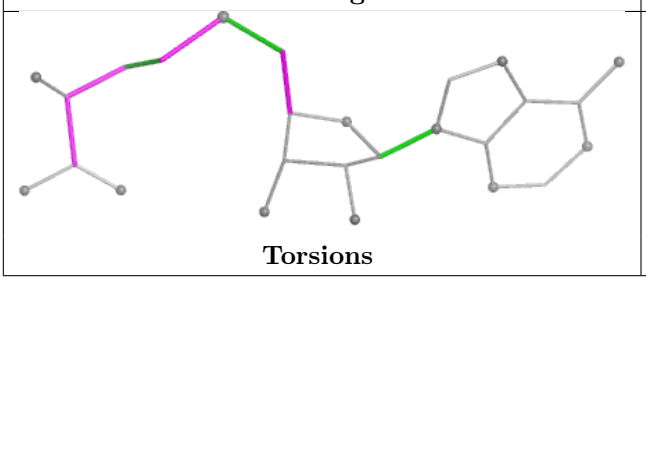
Ligand SAH D 503



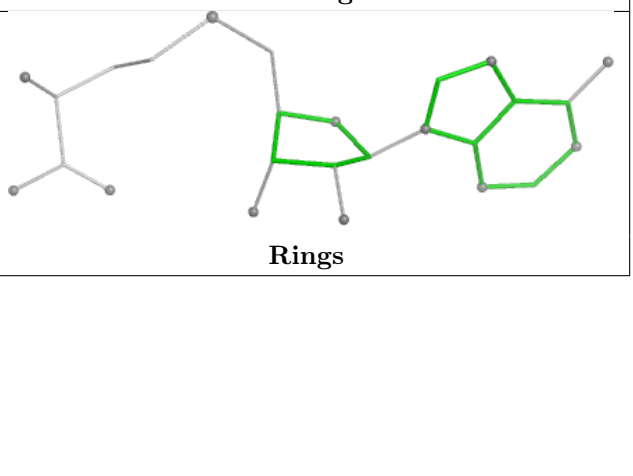
Bond lengths



Bond angles

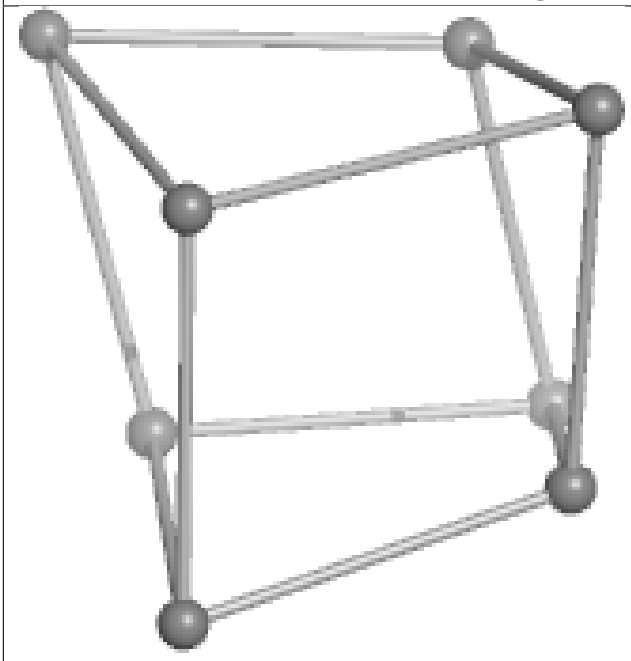


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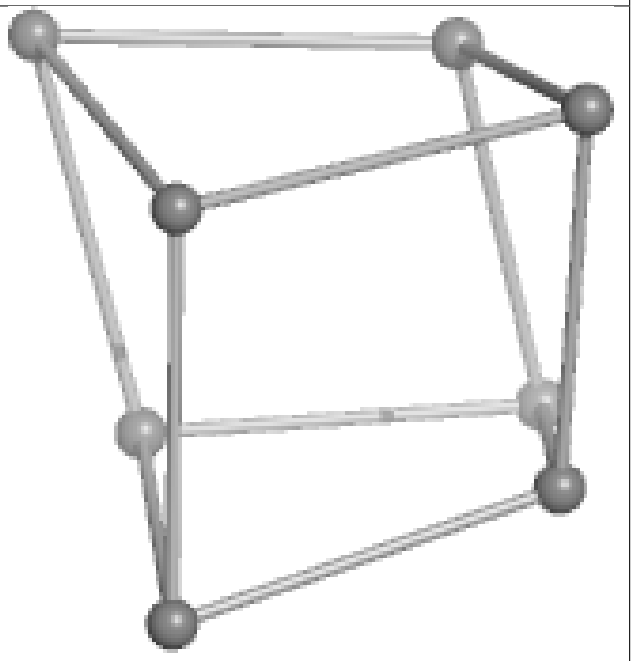


Rings

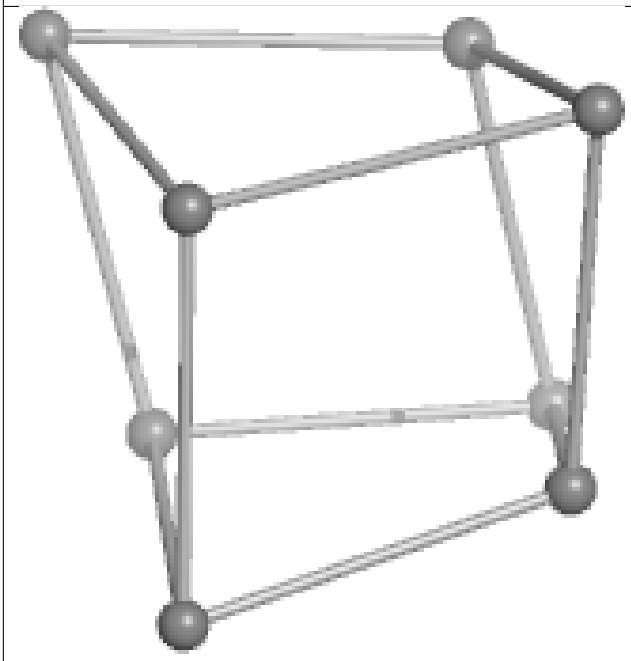
Ligand SF4 B 501



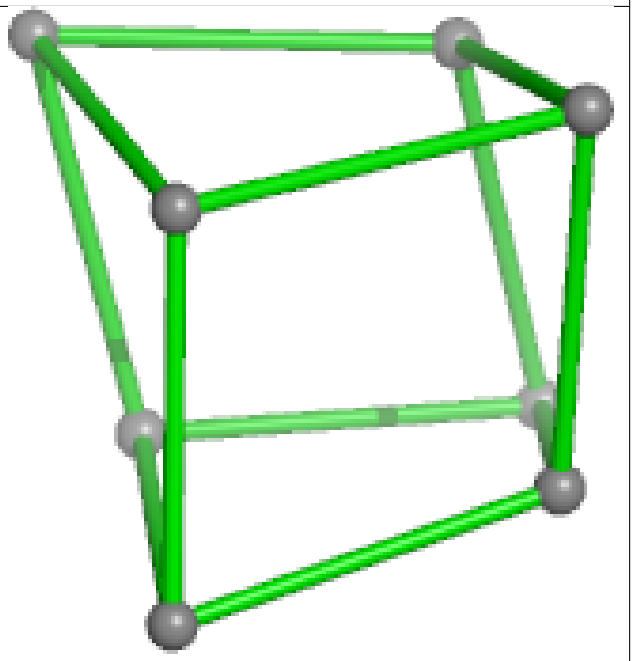
Bond lengths



Bond angles

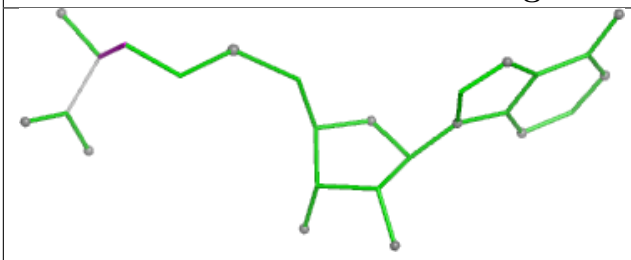


Torsions

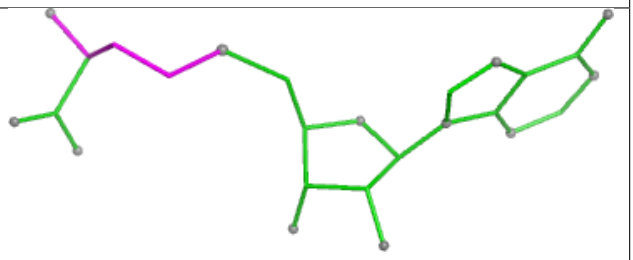


Rings

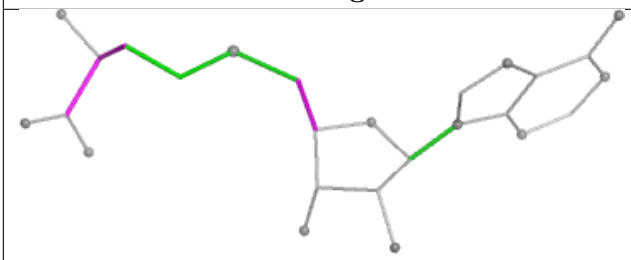
Ligand SAH A 503



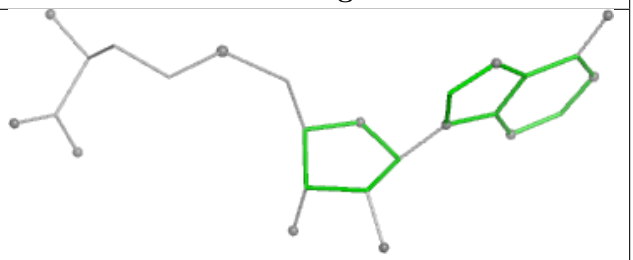
Bond lengths



Bond angles

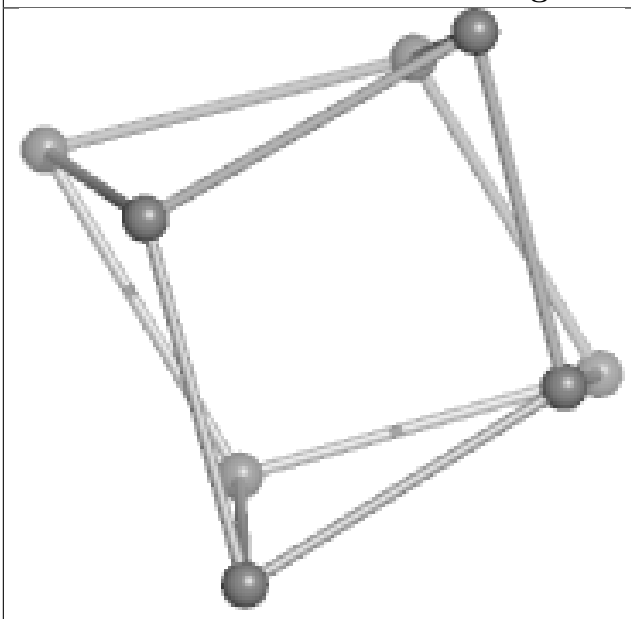


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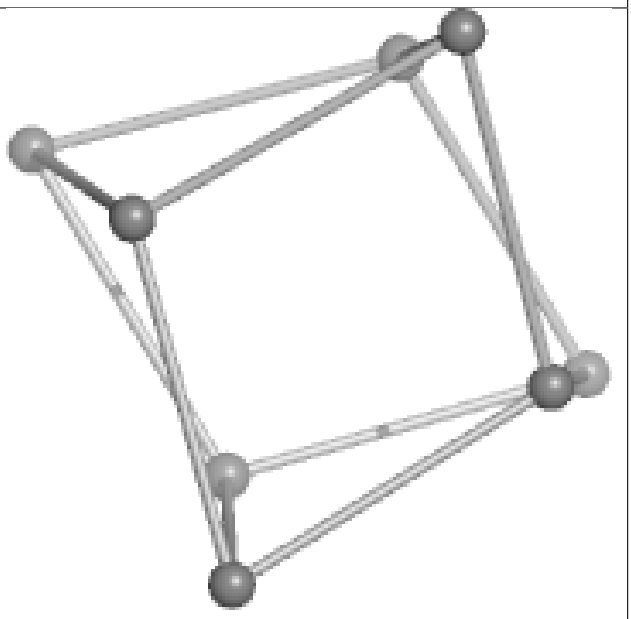


Rings

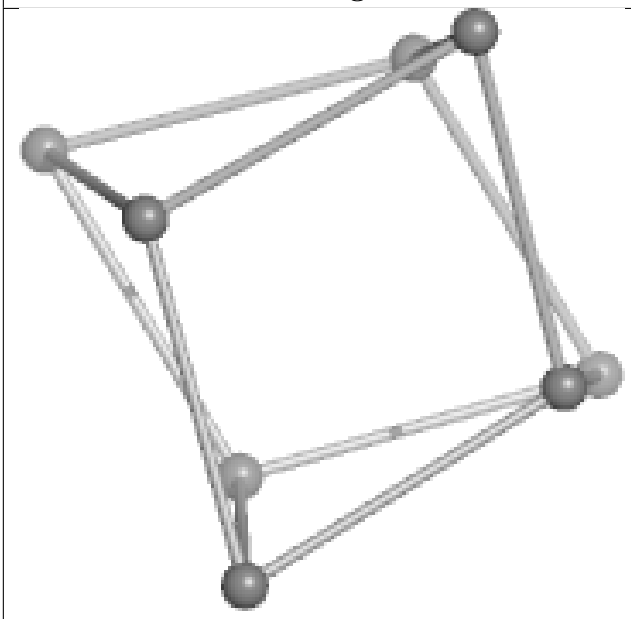
Ligand SF4 D 501



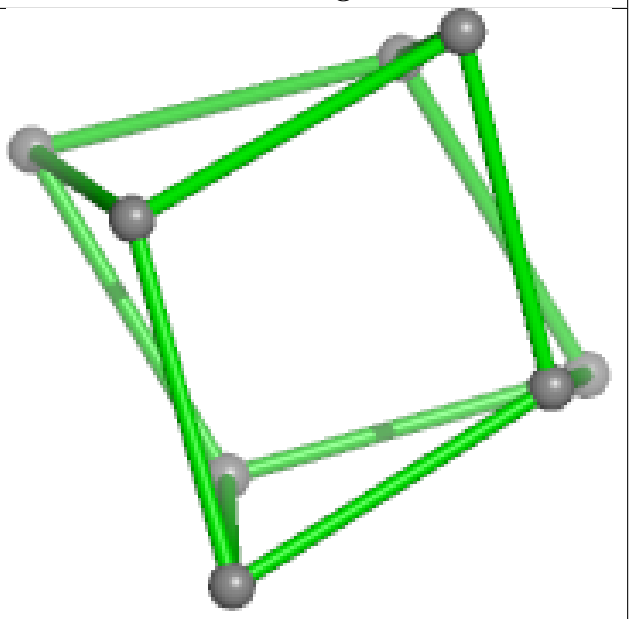
Bond lengths



Bond angles

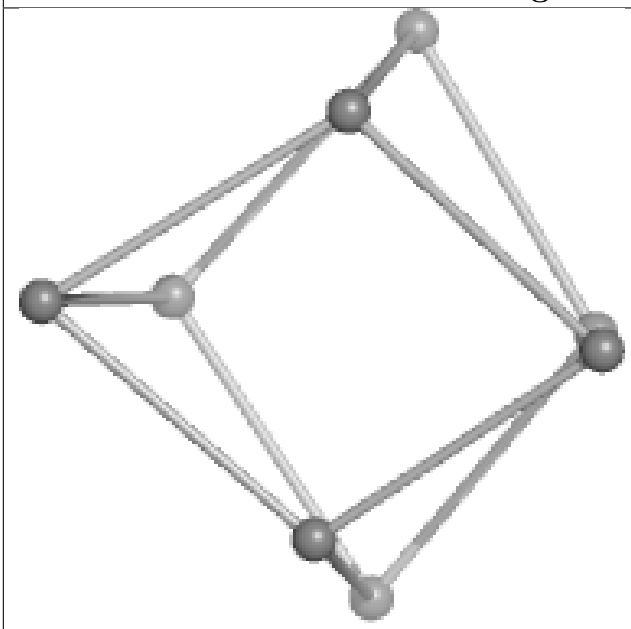


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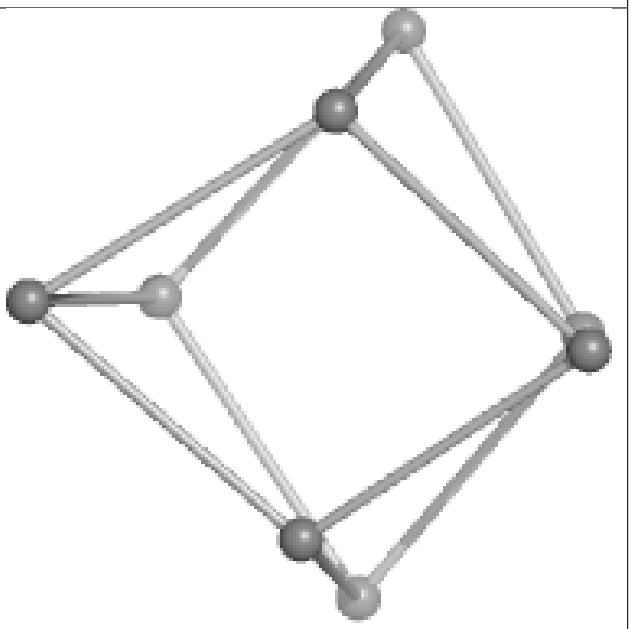


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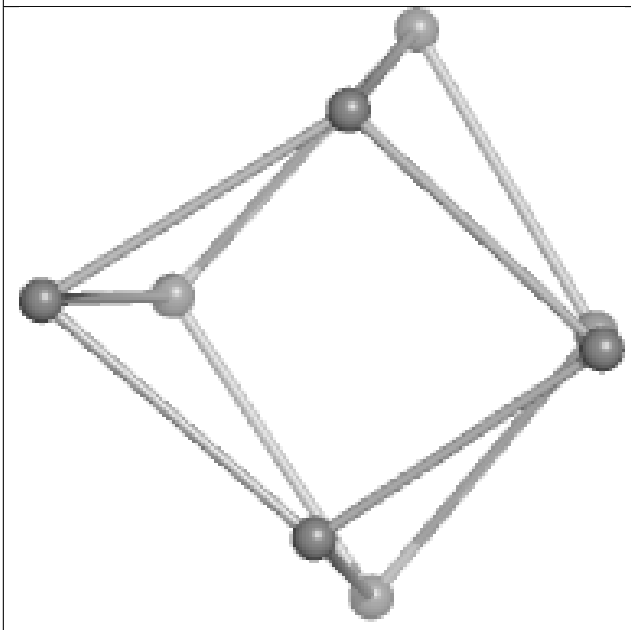
Ligand SF4 C 501



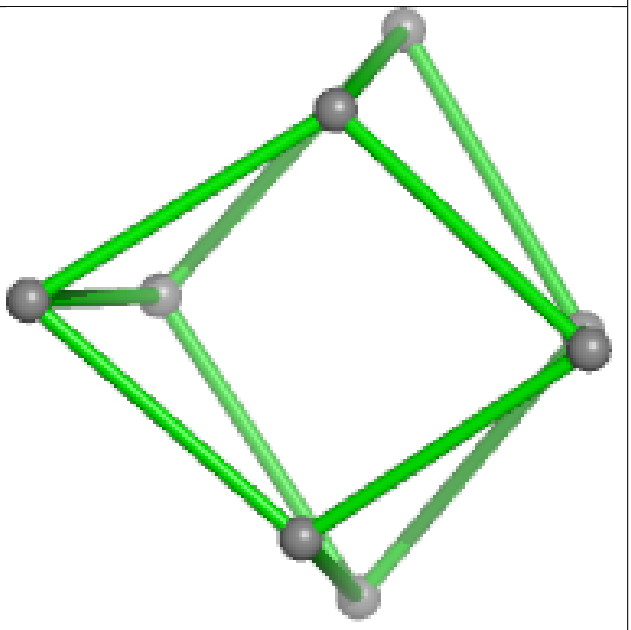
Bond lengths



Bond angles

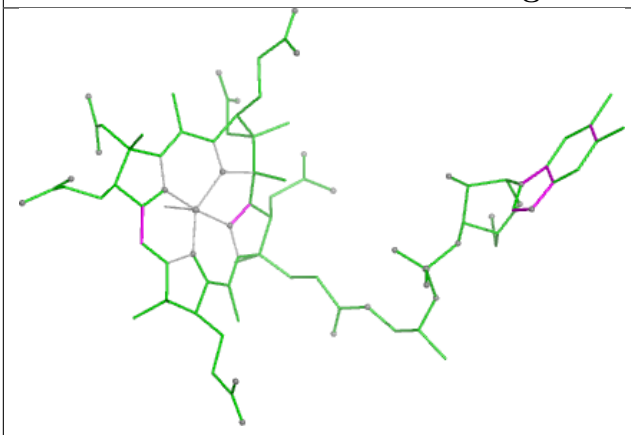


Torsions



Rings

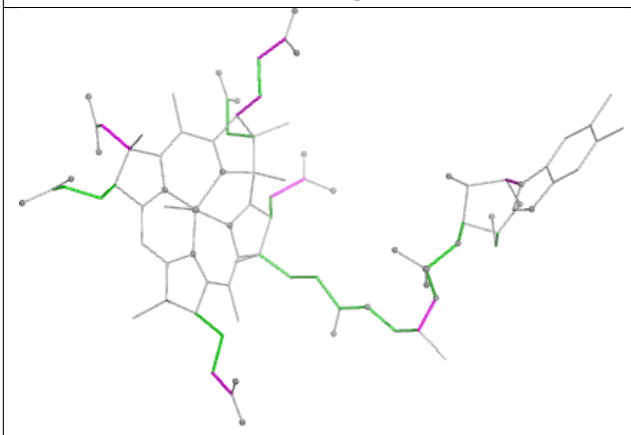
Ligand COB B 504



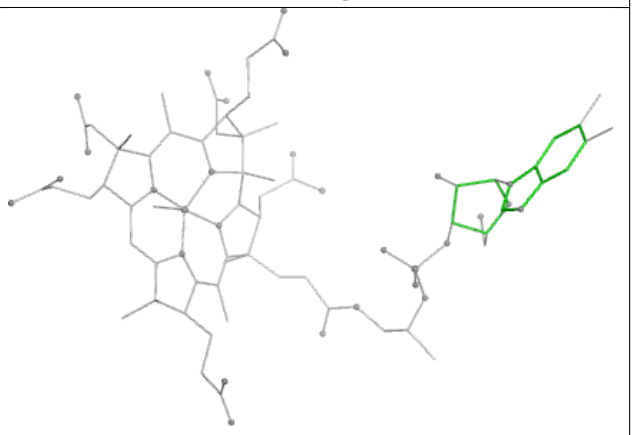
Bond lengths



Bond angles

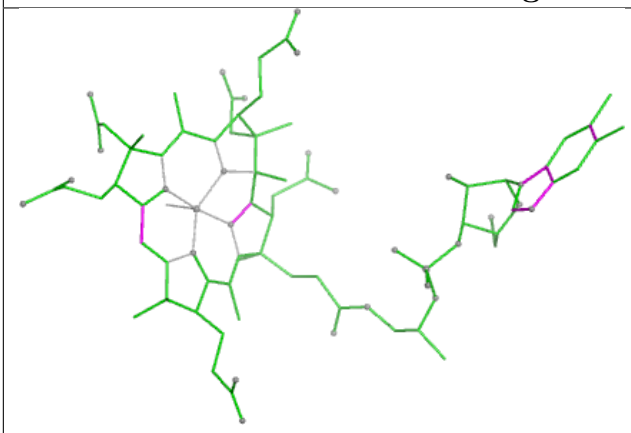


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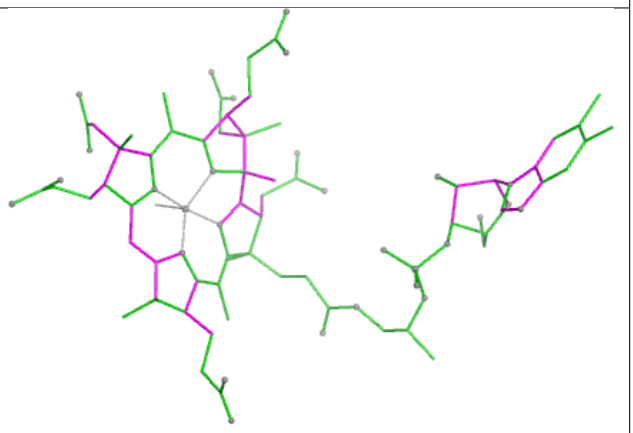


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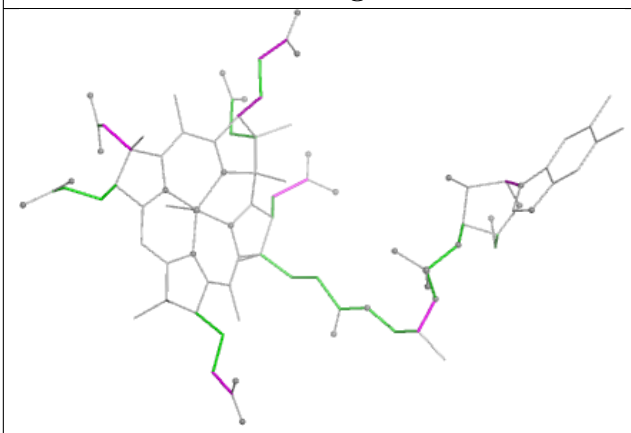
Ligand COB C 504



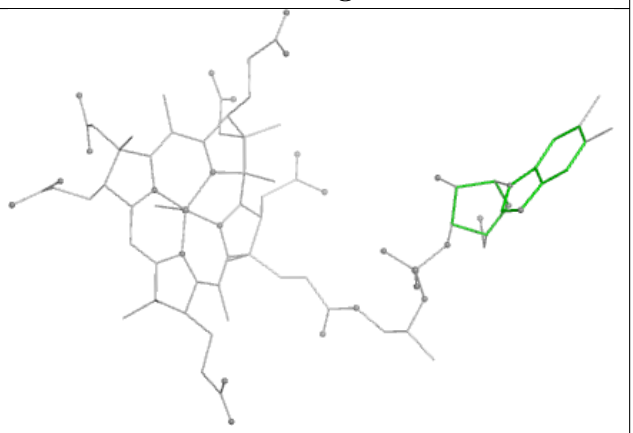
Bond lengths



Bond angles

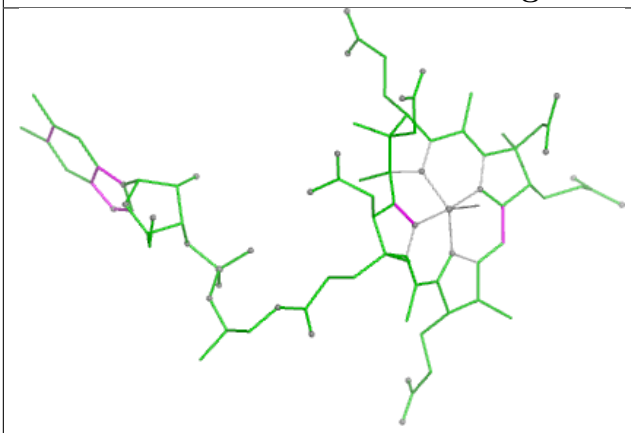


Torsions

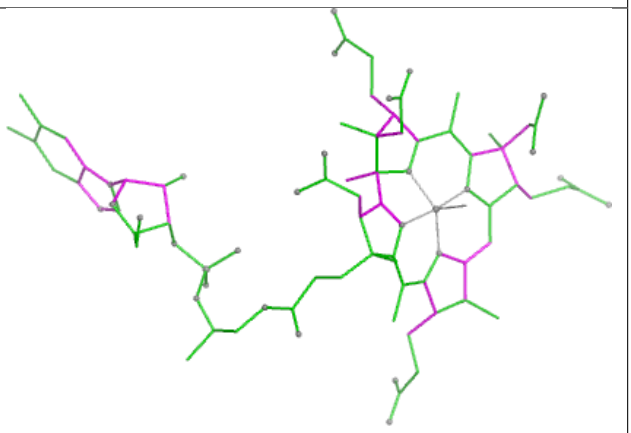


Rings

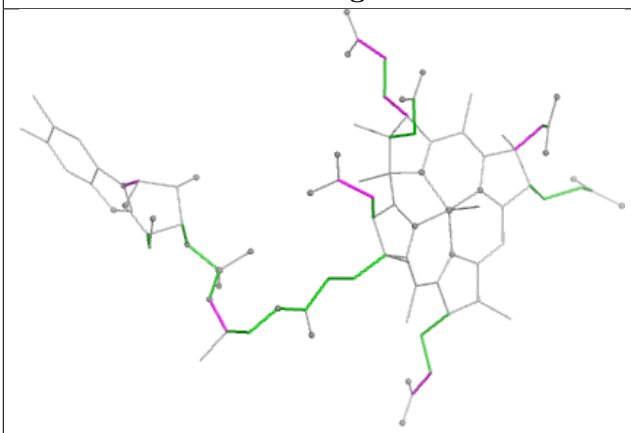
Ligand COB D 504



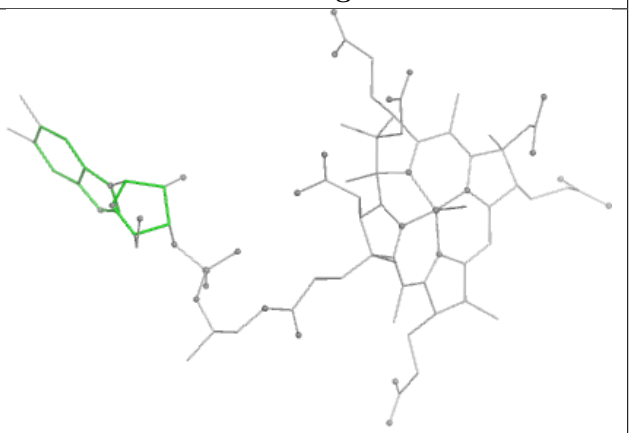
Bond lengths



Bond angles



Torsions



Rings

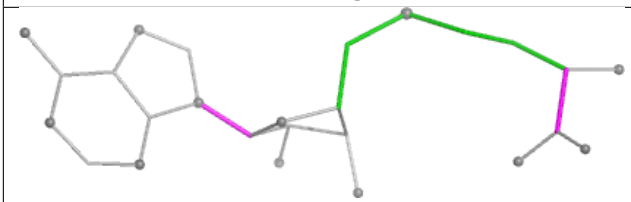
Ligand SAH C 503



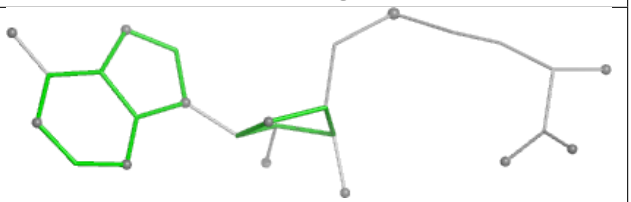
Bond lengths



Bond angles

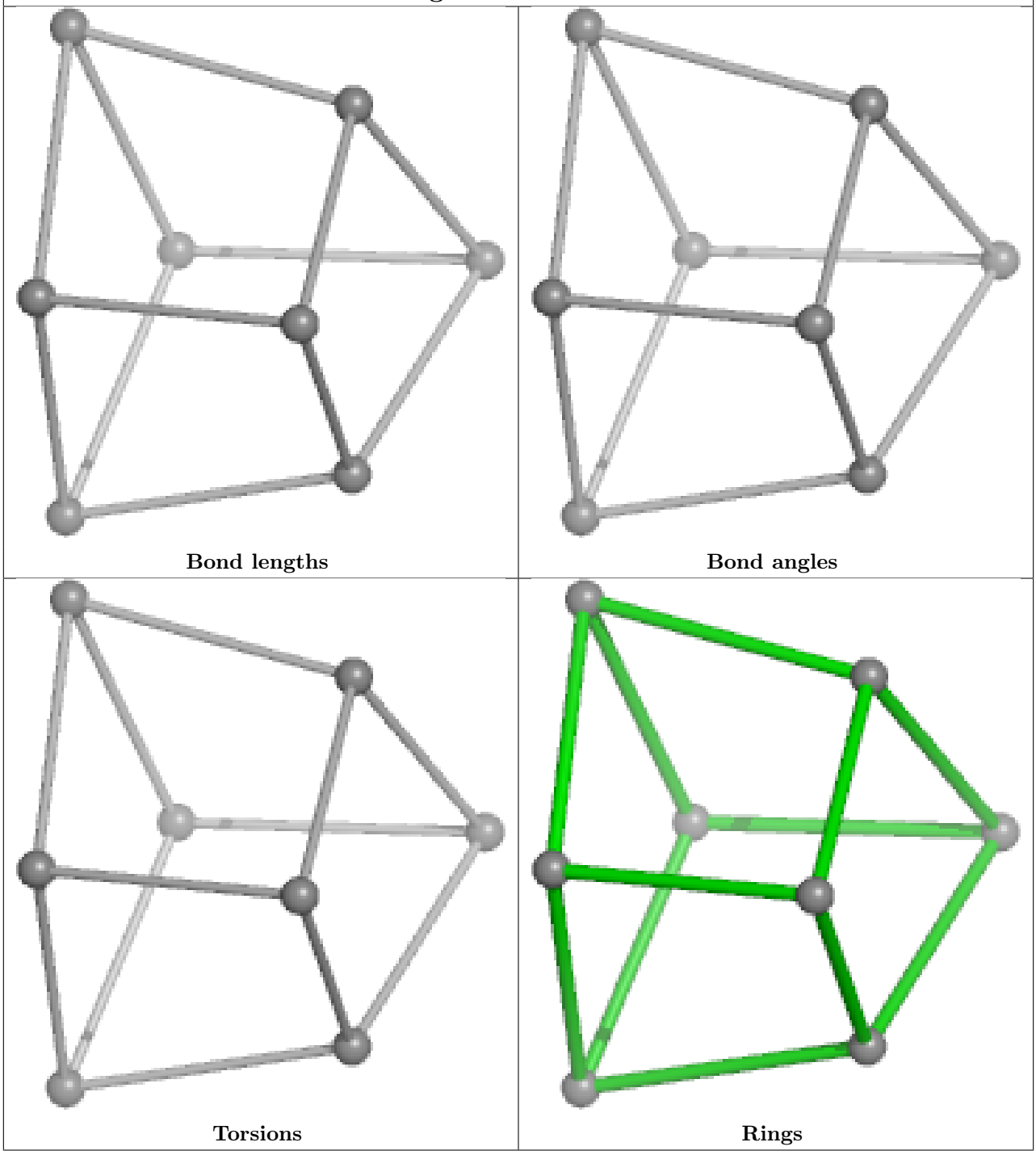


Torsions



Rings

Ligand SF4 A 501



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/436 (94%)	-0.05	3 (0%)	84	83	38, 53, 75, 91	0
1	B	411/436 (94%)	-0.01	3 (0%)	84	83	38, 55, 82, 108	0
1	C	411/436 (94%)	0.05	6 (1%)	72	70	40, 56, 89, 112	0
1	D	407/436 (93%)	0.36	11 (2%)	56	53	45, 67, 101, 148	0
All	All	1640/1744 (94%)	0.08	23 (1%)	73	72	38, 57, 92, 148	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	PHE	3.9
1	A	77	SER	3.7
1	D	75	PHE	3.4
1	D	73	LEU	3.2
1	D	2	GLU	3.0
1	D	1	MET	3.0
1	A	30	ILE	3.0
1	C	30	ILE	2.9
1	D	74	TYR	2.9
1	B	77	SER	2.8
1	C	77	SER	2.8
1	C	52	VAL	2.7
1	D	330	ALA	2.6
1	C	50	ARG	2.4
1	D	50	ARG	2.3
1	D	411	GLU	2.3
1	D	29	ASP	2.3
1	C	76	THR	2.3
1	A	78	GLY	2.3
1	D	30	ILE	2.2
1	B	408	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	410	LEU	2.0
1	B	282	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

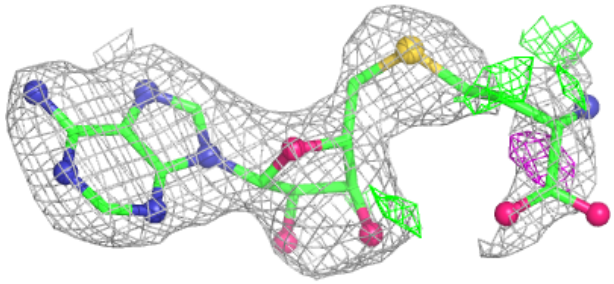
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

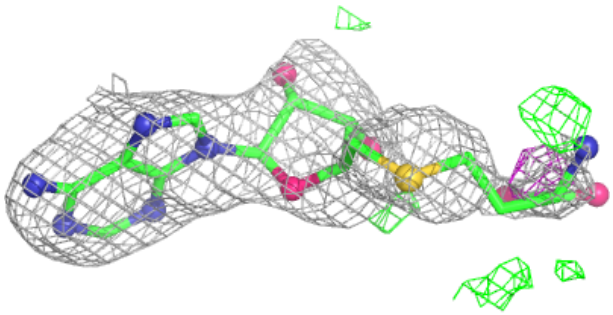
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SAH	D	503	26/26	0.86	0.14	56,60,67,67	0
4	SAH	C	503	26/26	0.89	0.13	50,54,61,62	0
4	SAH	A	503	26/26	0.90	0.11	44,48,55,56	0
6	NA	A	505	1/1	0.90	0.07	42,42,42,42	0
4	SAH	B	503	26/26	0.93	0.10	44,48,52,52	0
5	COB	D	504	92/92	0.94	0.11	46,48,49,50	0
5	COB	C	504	92/92	0.94	0.10	41,42,44,45	0
6	NA	B	505	1/1	0.94	0.08	39,39,39,39	0
6	NA	C	505	1/1	0.95	0.04	42,42,42,42	0
5	COB	B	504	92/92	0.96	0.09	38,40,48,48	0
5	COB	A	504	92/92	0.96	0.08	37,40,43,44	0
6	NA	D	505	1/1	0.98	0.04	36,36,36,36	0
2	SF4	A	501	8/8	0.99	0.05	42,42,42,43	0
2	SF4	B	501	8/8	0.99	0.04	40,40,40,40	0
2	SF4	C	501	8/8	0.99	0.05	49,49,49,49	0
2	SF4	D	501	8/8	0.99	0.05	57,58,58,58	0
3	FE	B	502	1/1	0.99	0.03	47,47,47,47	0
3	FE	C	502	1/1	0.99	0.02	67,67,67,67	0
3	FE	A	502	1/1	1.00	0.02	42,42,42,42	0
3	FE	D	502	1/1	1.00	0.01	74,74,74,74	0

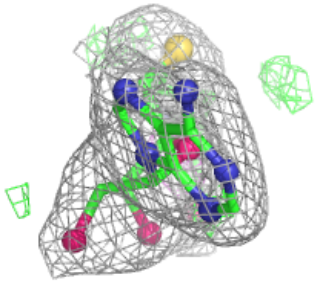
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH D 503:

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

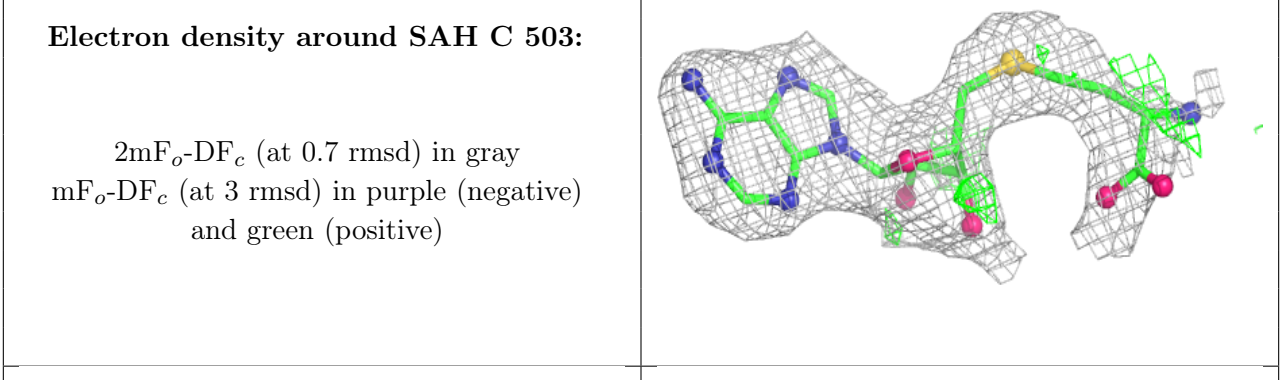






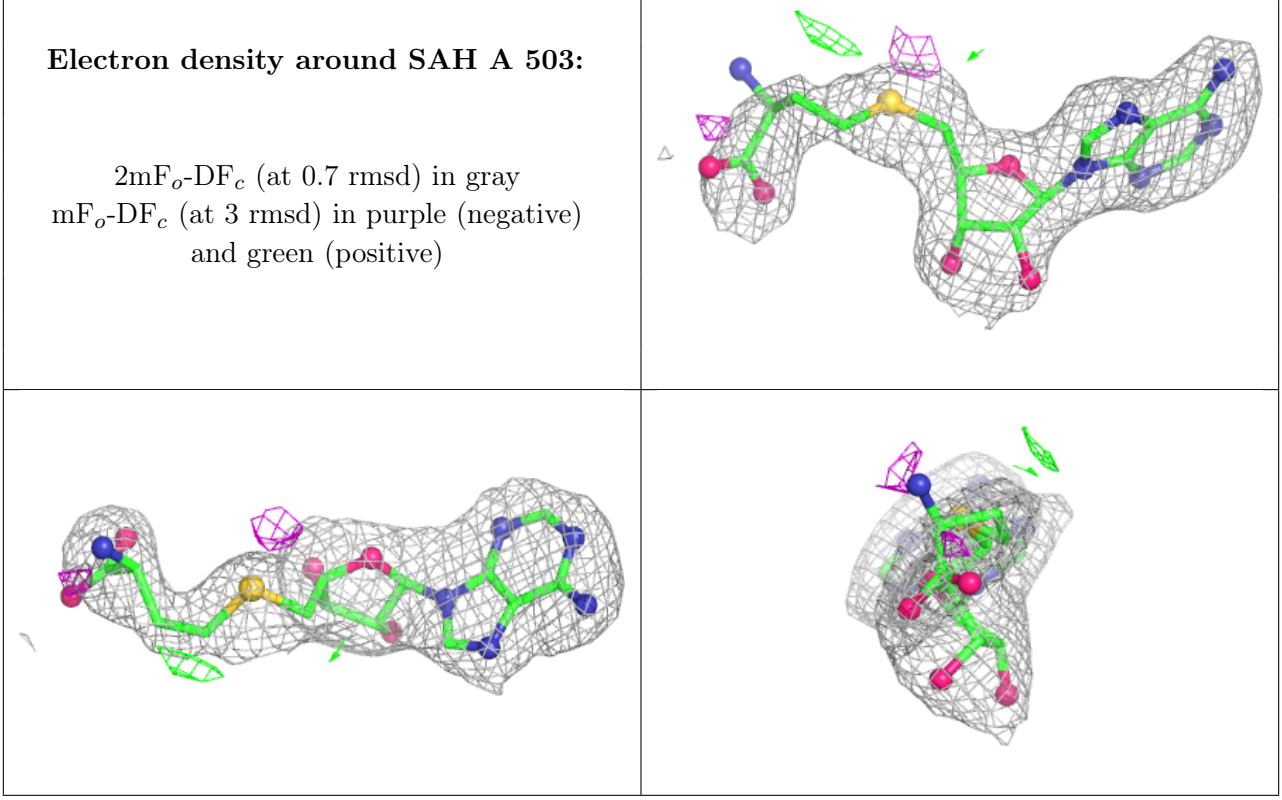
Electron density around SAH C 503:

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



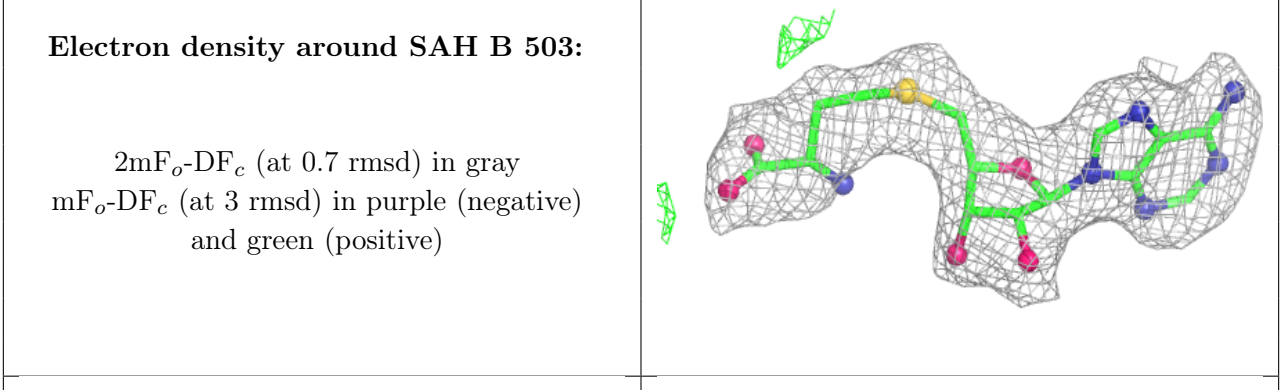
Electron density around SAH A 503:

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



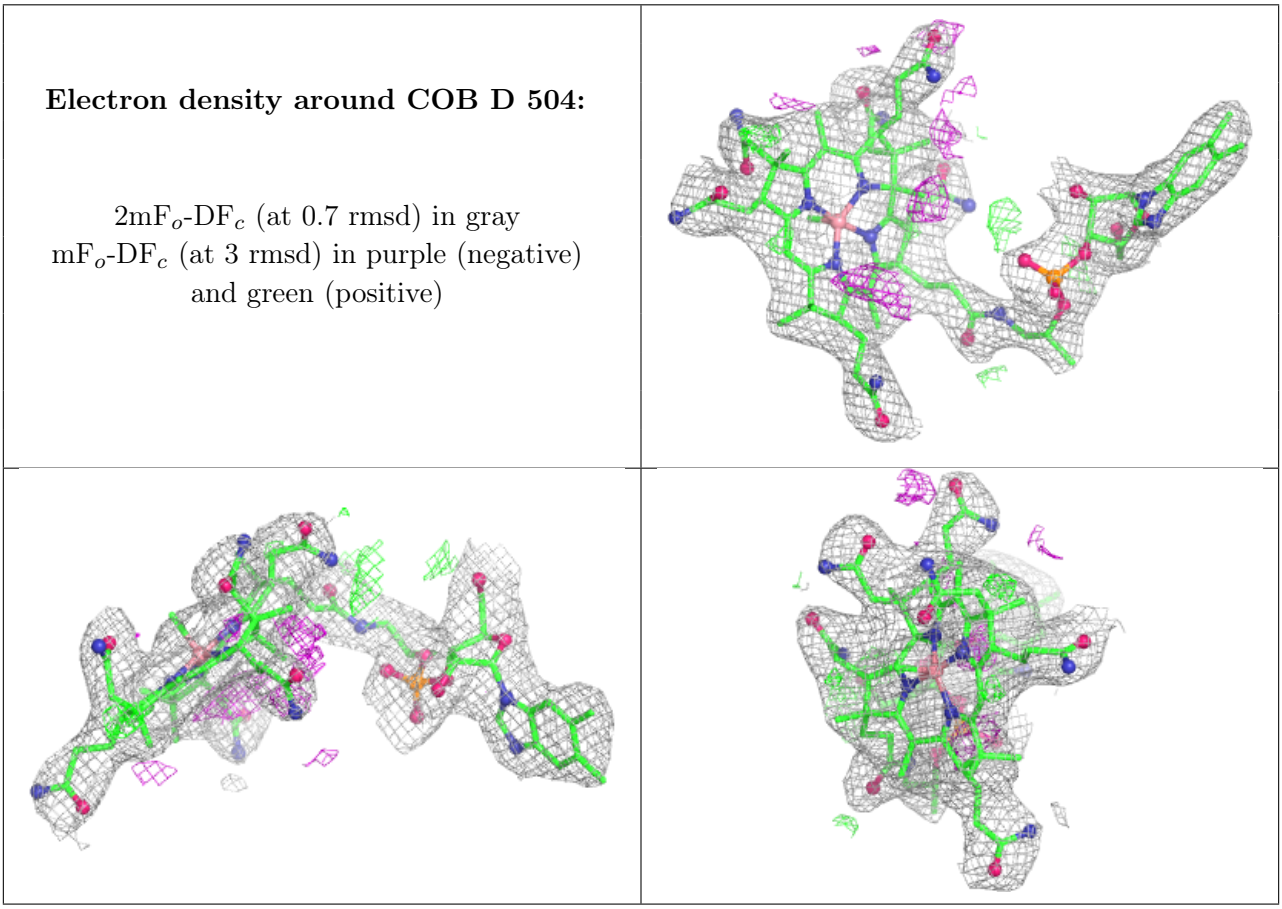
Electron density around SAH B 503:

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



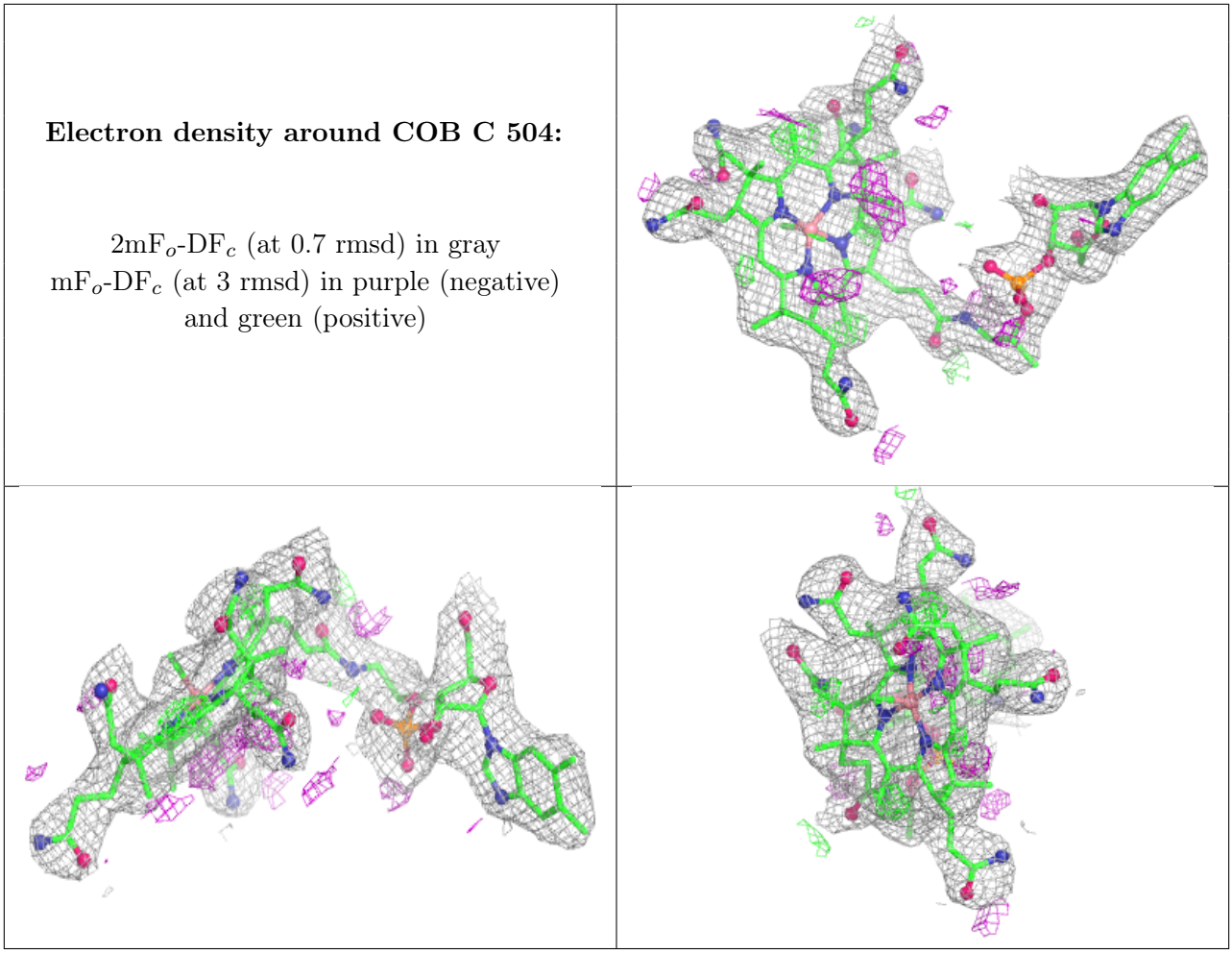
Electron density around COB D 504:

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



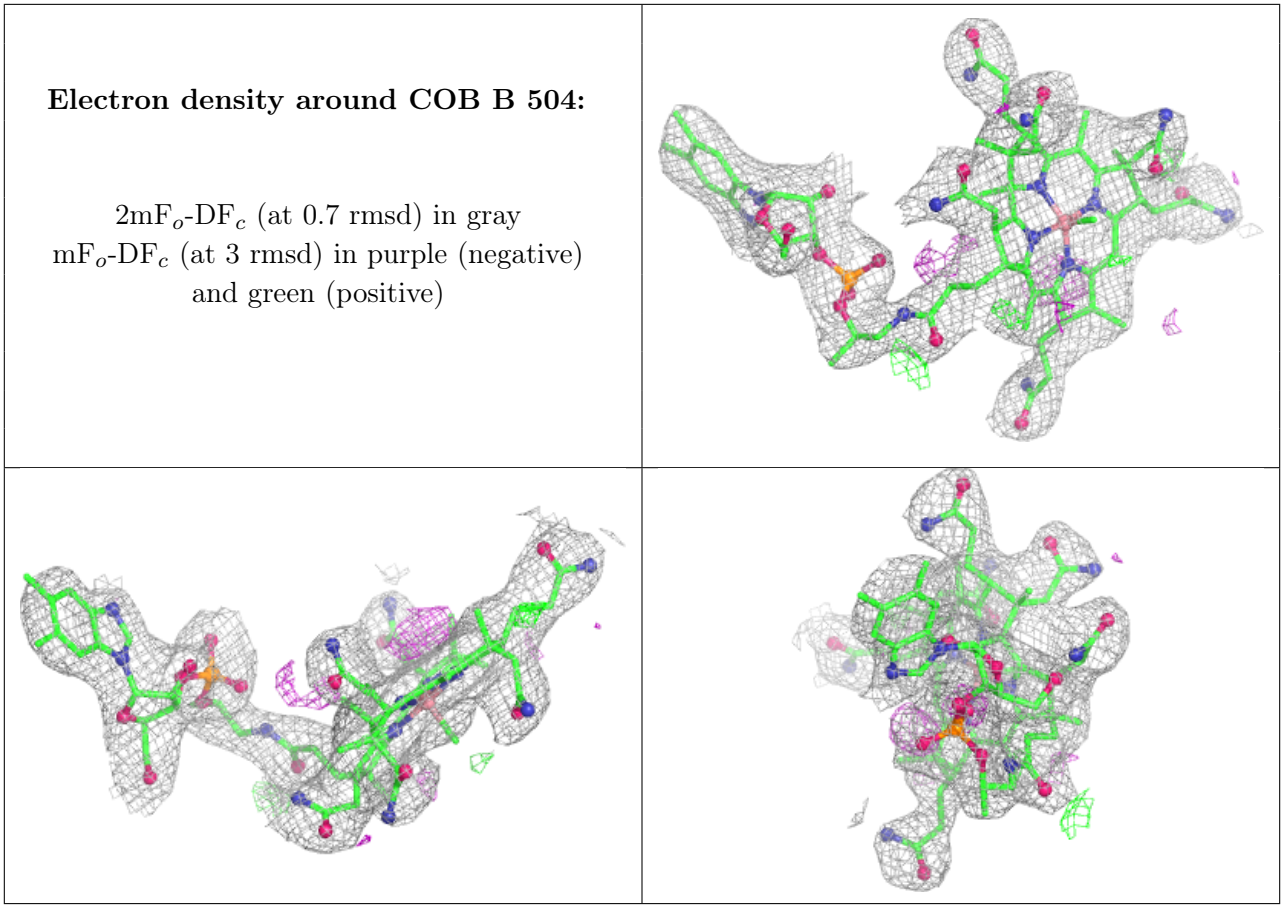
Electron density around COB C 504:

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



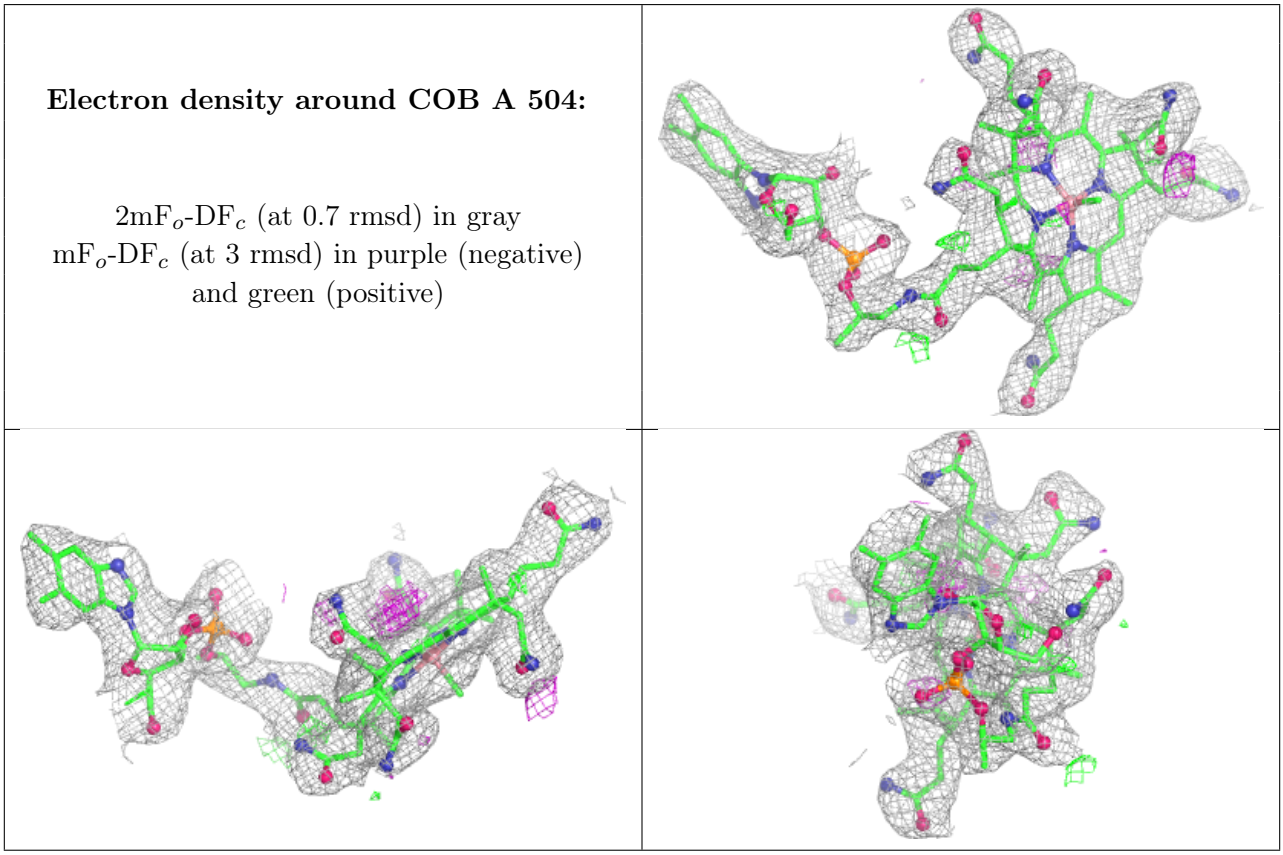
Electron density around COB B 504:

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



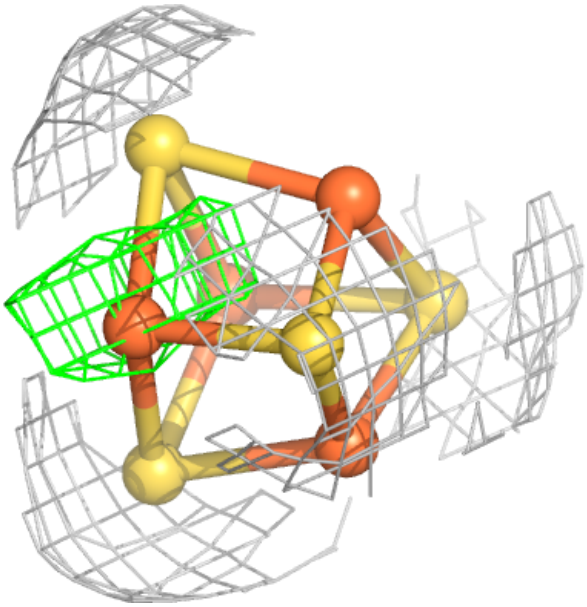
Electron density around COB A 504:

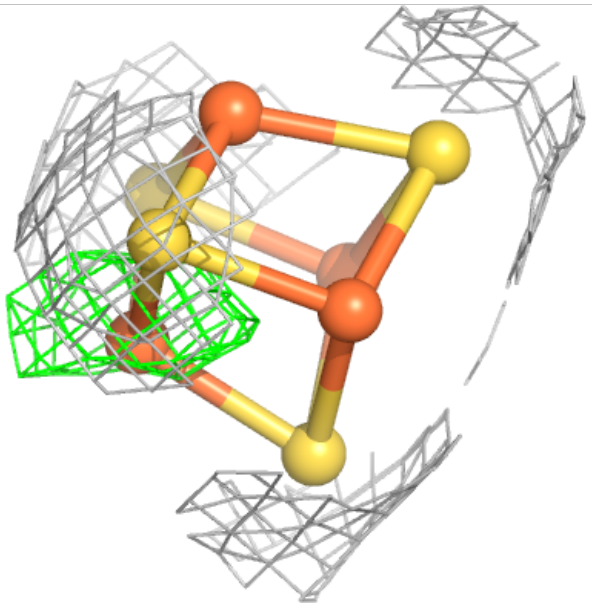
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

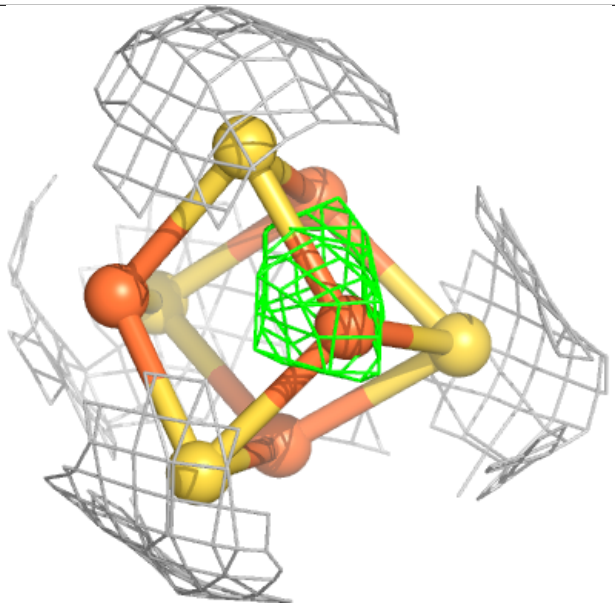


Electron density around SF4 A 501:

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

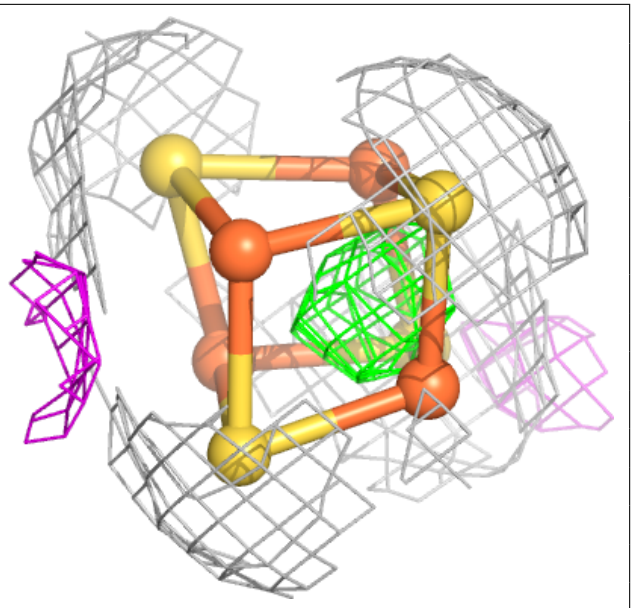


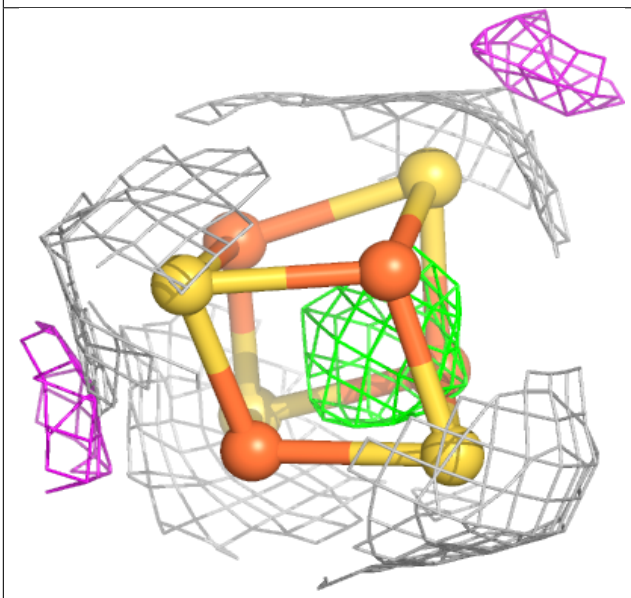


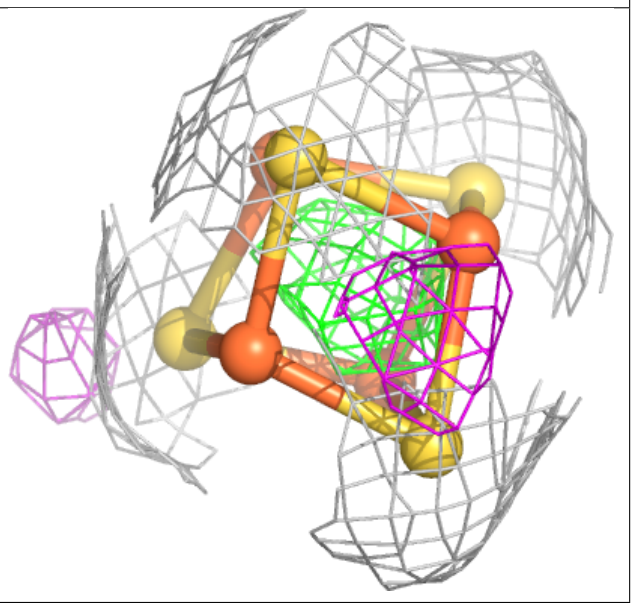


Electron density around SF4 B 501:

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

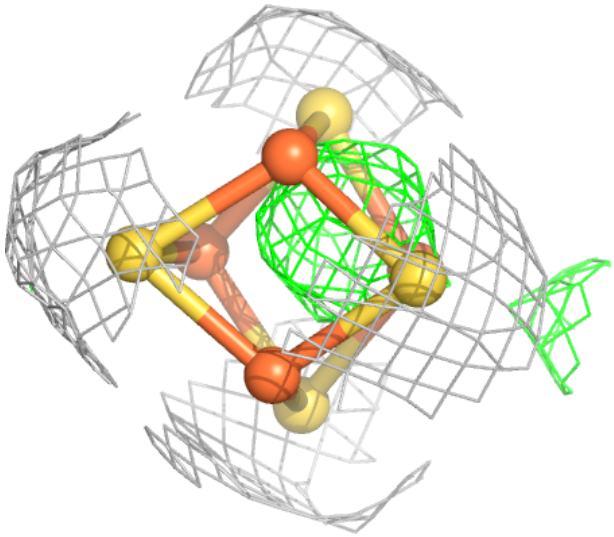


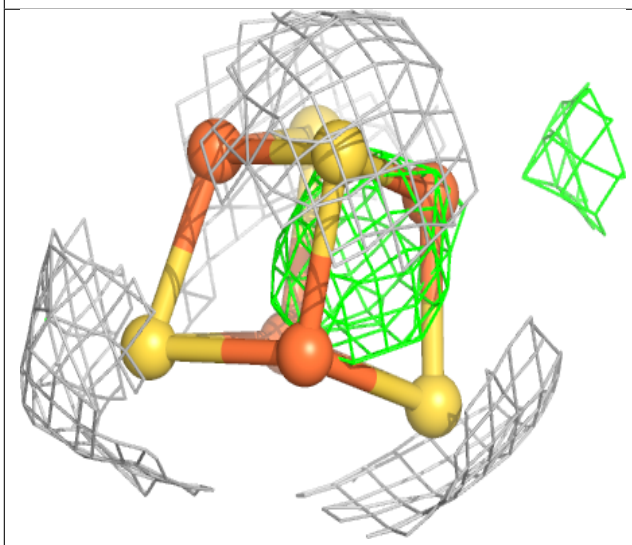


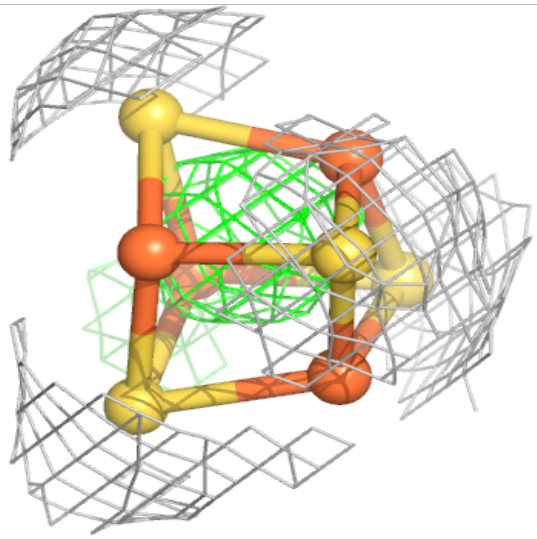


Electron density around SF4 C 501:

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

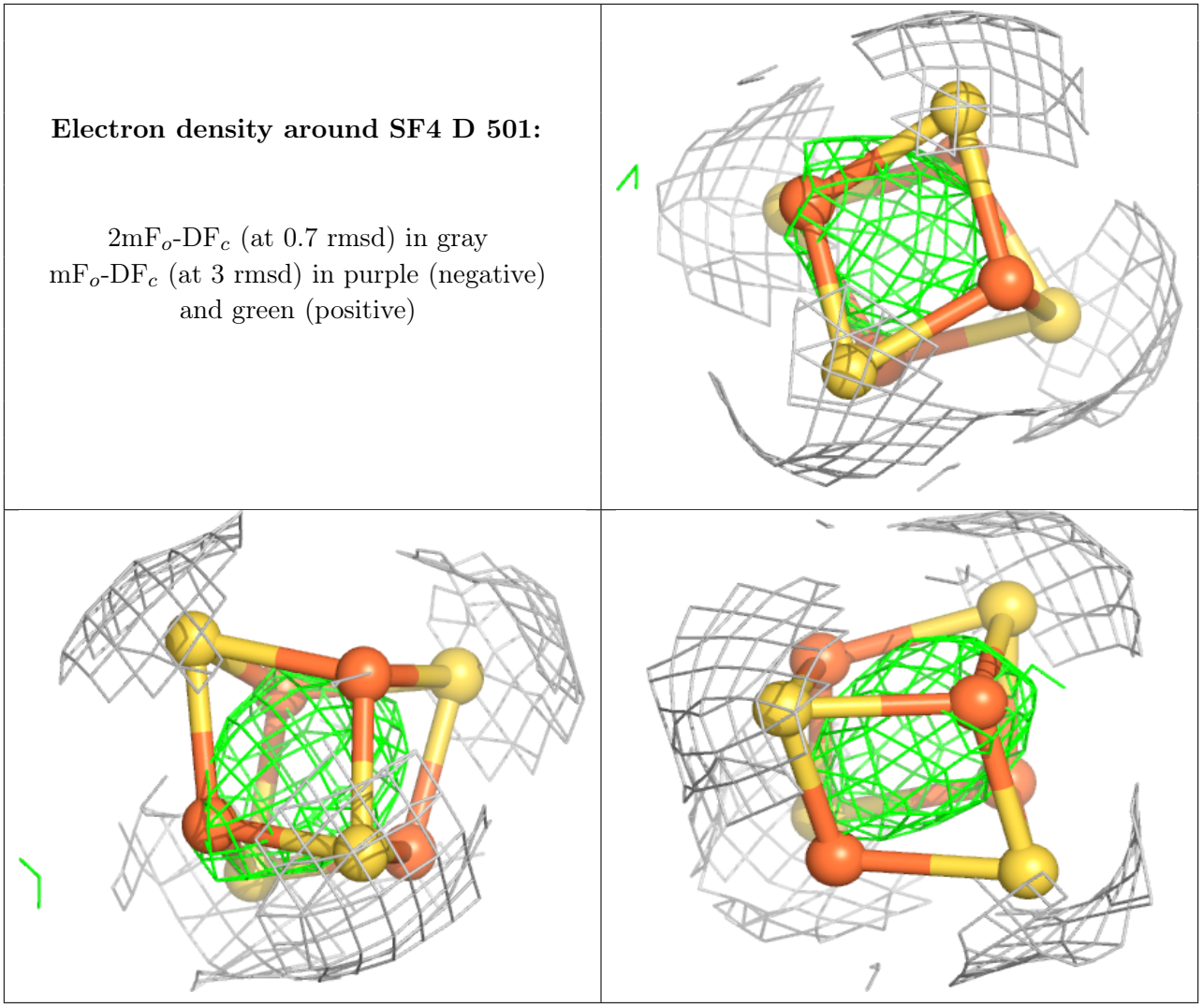






Electron density around SF4 D 501:

$2mF_o$-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.