Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2026 – 12:41 am BST

PDB ID	:	8RTM / pdb_00008rtm
Title	:	Af Aio C65F-C80G bound to Sb oxyanion
Authors	:	Engrola, F.; Romao, M.J.; Correia, M.; Santos-Silva, T.
Deposited on	:	2024-01-26
Resolution	:	1.87 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:

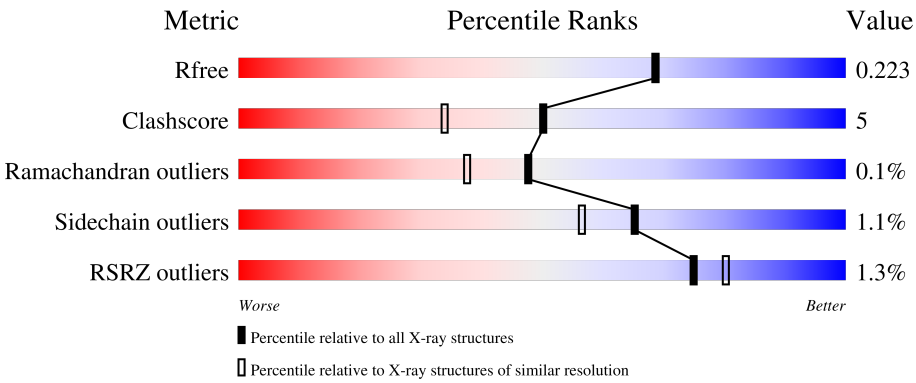
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	824	2% 89% 10% •
1	C	824	% 91% 8% •
1	E	824	2% 89% 10% •
1	G	824	% 90% 9% •
2	B	135	% 90% 10% •

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Mol	Chain	Length	Quality of chain
2	D	135	% 90% 9%
2	F	135	% 87% 13%
2	H	135	% 92% 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
10	PGE	A	918	-	-	X	-
10	PGE	G	913	-	-	X	-
16	P4G	C	911	-	-	X	-
17	1PE	C	912	-	-	X	-
17	1PE	G	910	-	-	X	-
7	PEG	A	909	-	-	X	-
7	PEG	A	914	-	-	X	-
7	PEG	A	915	-	-	X	-
7	PEG	A	917	-	-	X	-
7	PEG	B	2906	-	X	X	-
7	PEG	C	914	-	-	X	-
7	PEG	E	907	-	-	X	-
7	PEG	E	909	-	-	X	-
7	PEG	G	908	-	-	X	-
7	PEG	G	912	-	-	X	-
7	PEG	H	2201	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 33119 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 Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	824	6500	4091	1149	1219	41	0	3	0
1	C	824	6500	4091	1149	1219	41	0	3	0
1	E	824	6492	4085	1148	1218	41	0	2	0
1	G	824	6492	4085	1148	1218	41	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q7SIF4
A	77	ASP	ASN	conflict	UNP Q7SIF4
A	82	ASP	ASN	conflict	UNP Q7SIF4
C	2	ALA	-	expression tag	UNP Q7SIF4
C	77	ASP	ASN	conflict	UNP Q7SIF4
C	82	ASP	ASN	conflict	UNP Q7SIF4
E	2	ALA	-	expression tag	UNP Q7SIF4
E	77	ASP	ASN	conflict	UNP Q7SIF4
E	82	ASP	ASN	conflict	UNP Q7SIF4
G	2	ALA	-	expression tag	UNP Q7SIF4
G	77	ASP	ASN	conflict	UNP Q7SIF4
G	82	ASP	ASN	conflict	UNP Q7SIF4

- Molecule 2 is a protein called Arsenite oxidase subunit AioB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	135	1004	631	169	198	6	0	0	0
2	D	135	1004	631	169	198	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	135	1004	631	169	198	6	0	0	0
			Total	C	N	O	S			
2	H	135	1004	631	169	198	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

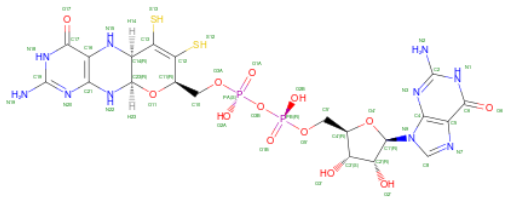
Chain	Residue	Modelled	Actual	Comment	Reference
B	65	PHE	CYS	conflict	UNP Q7SIF3
B	80	GLY	CYS	conflict	UNP Q7SIF3
D	65	PHE	CYS	conflict	UNP Q7SIF3
D	80	GLY	CYS	conflict	UNP Q7SIF3
F	65	PHE	CYS	conflict	UNP Q7SIF3
F	80	GLY	CYS	conflict	UNP Q7SIF3
H	65	PHE	CYS	conflict	UNP Q7SIF3
H	80	GLY	CYS	conflict	UNP Q7SIF3

- Molecule 3 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
3	A	1	1	1	0	0

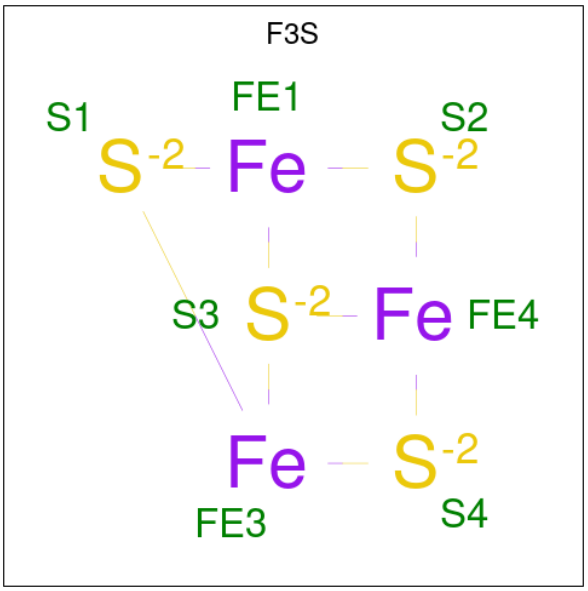
- Molecule 4 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).

MGD



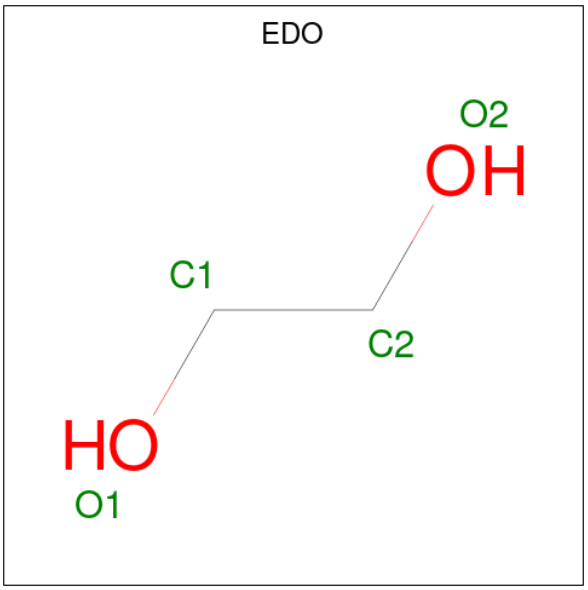
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	47	20	10	13	2	2	0	0
4	A	1	47	20	10	13	2	2	0	0
4	C	1	47	20	10	13	2	2	0	0
4	C	1	47	20	10	13	2	2	0	0
4	E	1	47	20	10	13	2	2	0	0
4	E	1	47	20	10	13	2	2	0	0
4	G	1	47	20	10	13	2	2	0	0
4	G	1	47	20	10	13	2	2	0	0

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



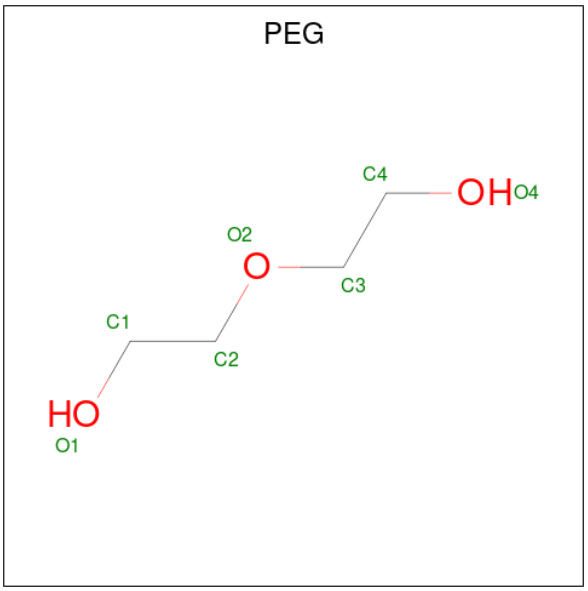
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	A	1	7	3	4	0	0
5	C	1	7	3	4	0	0
5	E	1	7	3	4	0	0
5	G	1	7	3	4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	C	1	7	4	3		0	0
			Total	C	O			
7	C	1	7	4	3		0	0

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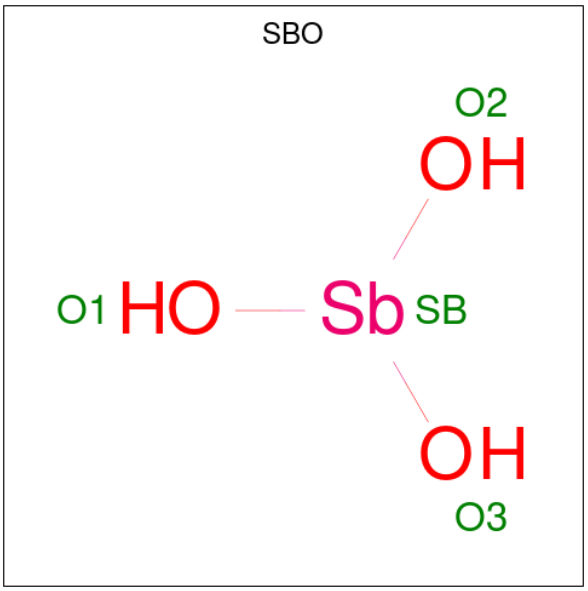
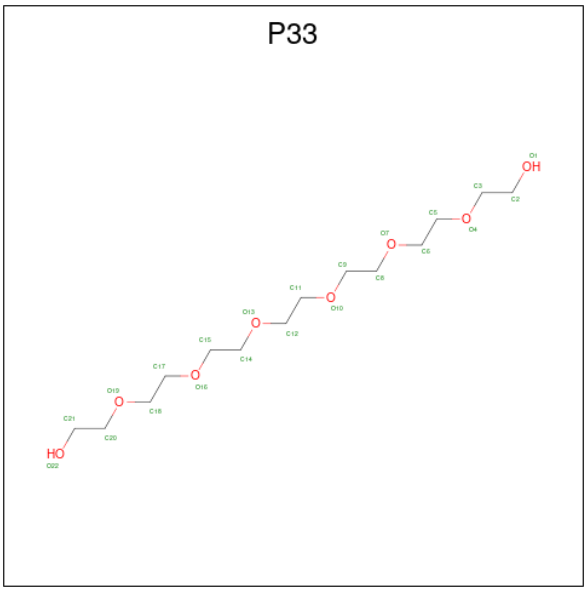
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	C	1	7	4	3		0	0
			Total	C	O			
7	C	1	7	4	3		0	0
			Total	C	O			
7	E	1	7	4	3		0	0
			Total	C	O			
7	E	1	7	4	3		0	0
			Total	C	O			
7	E	1	7	4	3		0	0
			Total	C	O			
7	E	1	7	4	3		0	0
			Total	C	O			
7	E	1	7	4	3		0	0
			Total	C	O			
7	E	1	7	4	3		0	0
			Total	C	O			
7	F	1	7	4	3		0	0
			Total	C	O			
7	G	1	7	4	3		0	0
			Total	C	O			
7	G	1	7	4	3		0	0
			Total	C	O			
7	G	1	7	4	3		0	0
			Total	C	O			
7	G	1	7	4	3		0	0
			Total	C	O			
7	H	1	7	4	3		0	0

- Molecule 8 is TRIHYDROXYANTIMONITE(III) (CCD ID: SBO) (formula: H_3O_3Sb) (labeled as "Ligand of Interest" by depositor).



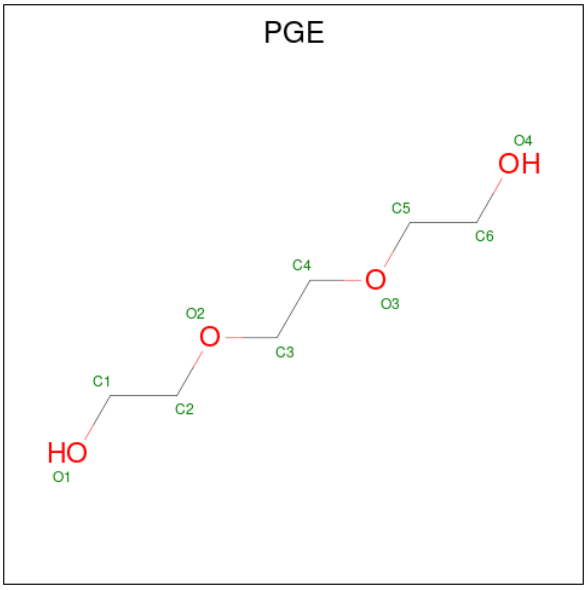
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	Sb		
8	A	1	3	2	1	0	0
			Total	O	Sb		
8	C	1	4	3	1	0	0
			Total	O	Sb		
8	E	1	4	3	1	0	0
			Total	O	Sb		
8	G	1	3	2	1	0	0

- Molecule 9 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	22	14	8	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	10	6	4	0	0
			Total	C	O		
10	A	1	10	6	4	0	0
			Total	C	O		
10	C	1	10	6	4	0	0
			Total	C	O		
10	E	1	10	6	4	0	0
			Total	C	O		
10	G	1	10	6	4	0	0

- Molecule 11 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	1	1	1	0	0
			Total	O		
11	C	1	1	1	0	0
			Total	O		
11	E	1	1	1	0	0

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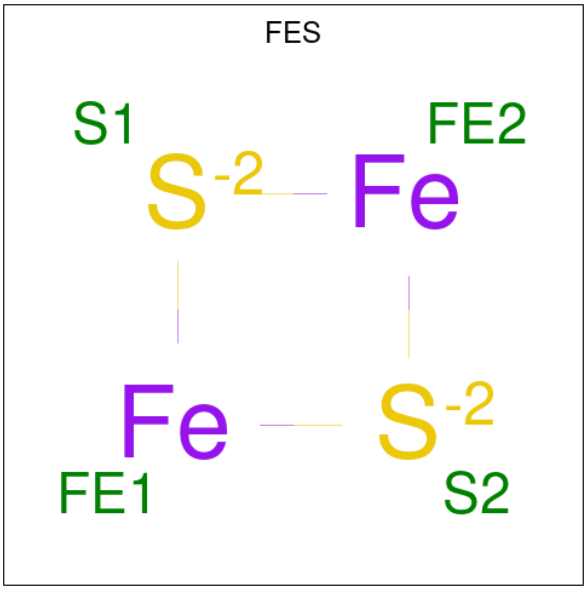
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	G	1	1	1	0	0

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

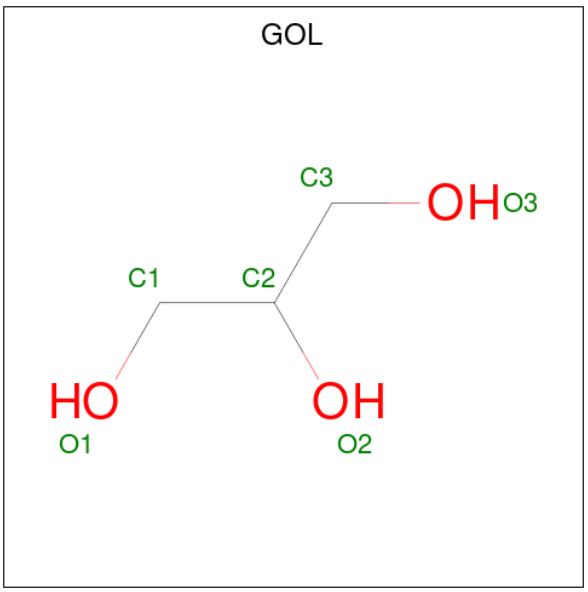
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
12	A	1	1	1	0	0
			Total	Na		
12	C	1	1	1	0	0
			Total	Na		
12	E	1	1	1	0	0
			Total	Na		
12	G	1	1	1	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
13	B	1	4	2	2	0	0
			Total	Fe	S		
13	D	1	4	2	2	0	0
			Total	Fe	S		
13	F	1	4	2	2	0	0
			Total	Fe	S		
13	H	1	4	2	2	0	0

- Molecule 14 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

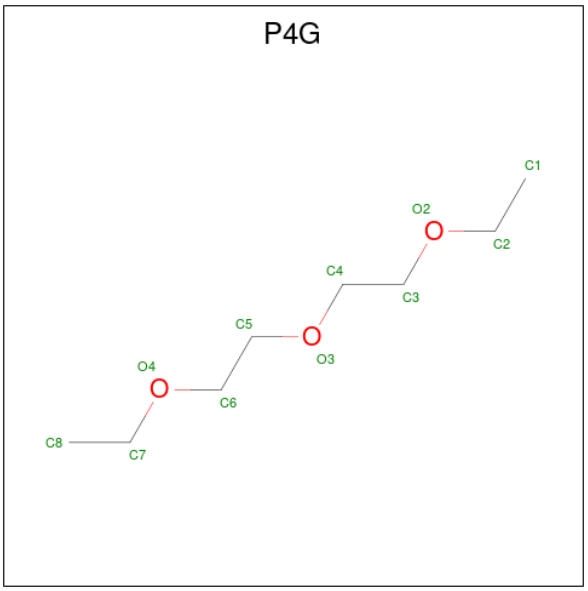


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	B	1	6	3	3	0	0
			Total	C	O		
14	B	1	6	3	3	0	0
			Total	C	O		
14	E	1	6	3	3	0	0

- Molecule 15 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

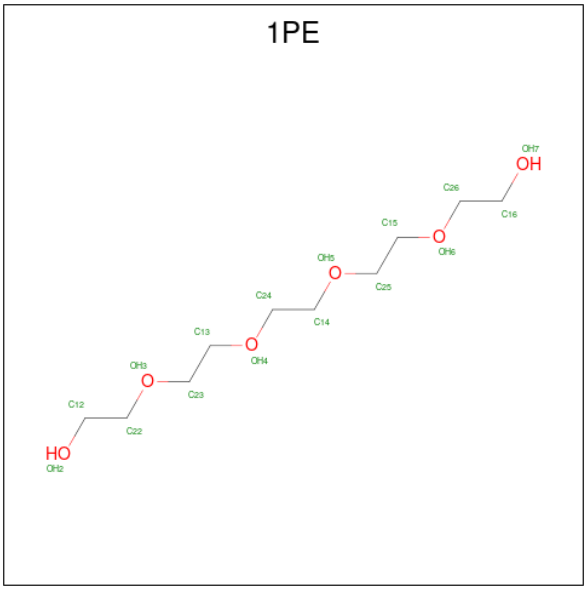
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
15	C	1	1	1	0	0
			Total	Mo		
15	E	1	1	1	0	0
			Total	Mo		
15	G	1	1	1	0	0

- Molecule 16 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula: $C_8H_{18}O_3$).



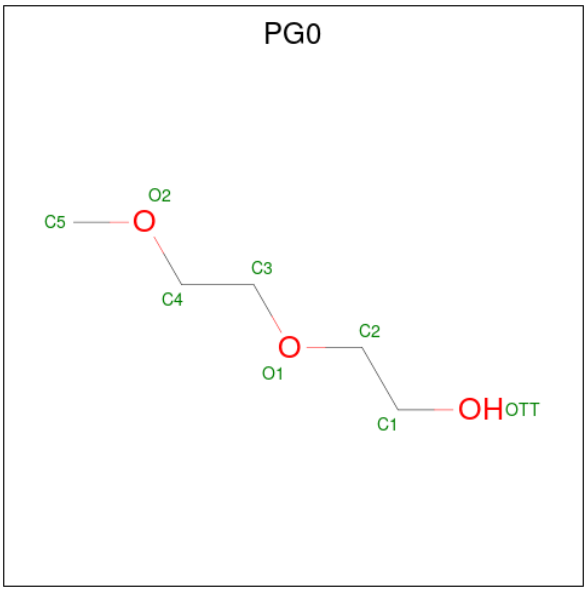
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
16	C	1	11	8	3	0	0

- Molecule 17 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
17	C	1	16	10	6	0	0
17	G	1	16	10	6	0	0

- Molecule 18 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	C	1	8	5	3	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	453	453	453	0	0
19	B	90	90	90	0	0
19	C	487	487	487	0	0
19	D	90	90	90	0	0
19	E	487	487	487	0	0
19	F	90	90	90	0	0
19	G	492	492	492	0	0
19	H	83	83	83	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: Arsenite oxidase subunit AioA

Chain A: 2% 89% 10%

A2 P3 N4 D5 C24 I25 Y33 K34 L38 R55 P59 P60 L65 T66 P67 H76 D77 I83 P87 D88 K89 V92 T100 D133 T134 K153 Q157 G158 V159 G170 R208 K258 N267 R295 T307 K333 R343 L344

S345 E348 M359 R362 A372 K385 D392 V410 G411 R412 G434 D441 N459 S463 L469 I473 Q482 A483 M484 Q485 K486 A487 M495 I499 S512 P517 M527 P533 L538 N542 M561 I566 R569 R575

D581 G582 K583 A584 F590 T597 N603 R607 R608 P612 G613 Q620 D669 K672 P677 W680 Q689 R695 F696 W697 L698 N699 R702 D713 L718 D734 T741 T770 T800 G808 F819 A825

• Molecule 1: Arsenite oxidase subunit AioA

Chain C: 9% 91% 8%

A2 P3 N4 I25 H31 T66 R80 S95 K121 W131 T134 A141 Q157 G170 R208 K258 R262 N267 R295 V296 L297 K333 K340 S345 E348 M359 R362 A372 K385 D392 V395 V404

V410 G411 R412 C417 K437 R450 N459 S463 M484 Q485 K486 A487 T492 I499 A521 M541 N542 R546 K580 D581 E598 N603 R607 G613 S619 V646 T662 E663 D670 W680 N681 R695 L698 N699 R702

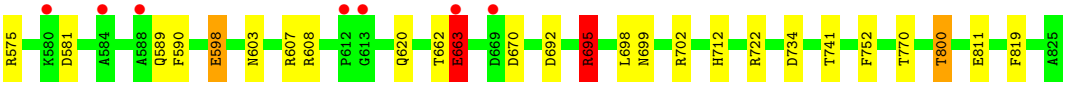
D713 R722 D734 T741 E764 T770 T800 E811 E812 F813 F819 A825

• Molecule 1: Arsenite oxidase subunit AioA

Chain E: 2% 89% 10%

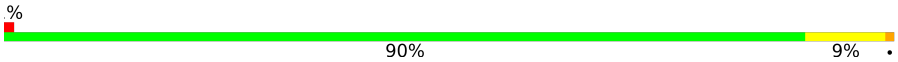
A2 P3 N4 D5 I25 H31 W32 Y33 P45 G51 V63 R80 I83 S95 T100 K121 D129 D133 T134 A141 K153 D154 Q157 G170 R208 Q223 K258 N267 R295 V296 L297 K333 S345 L346 D347 E348

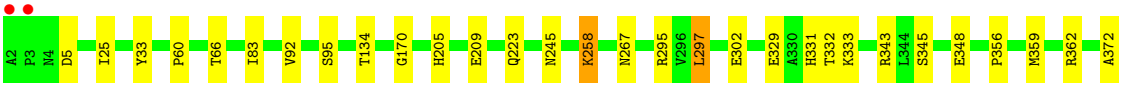
M359 R362 A372 H381 K385 D392 V404 V410 G411 R412 C417 K436 K448 G449 R450 N459 S463 Q467 Q475 Q485 K486 A487 T492 M495 Y500 E501 A502 T503 Q504 E522 P533 L538 M541 N542 R545 R546

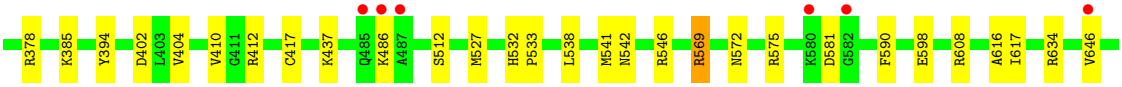


• Molecule 1: Arsenite oxidase subunit AioA

Chain G:

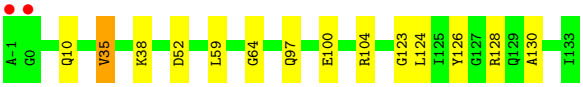






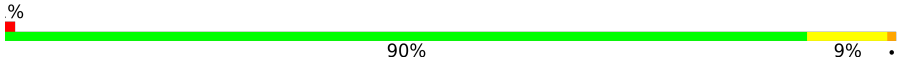
• Molecule 2: Arsenite oxidase subunit AioB

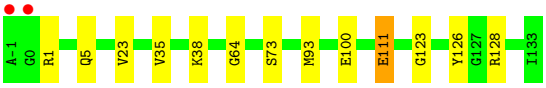
Chain B:



• Molecule 2: Arsenite oxidase subunit AioB

Chain D:



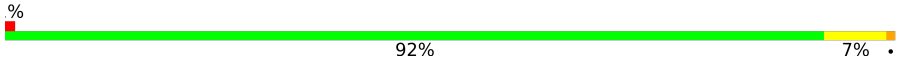


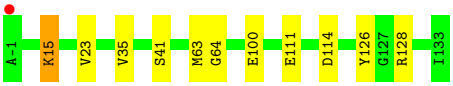
• Molecule 2: Arsenite oxidase subunit AioB

Chain F:

• Molecule 2: Arsenite oxidase subunit AioB

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.25Å 109.12Å 117.00Å 82.33° 89.68° 83.69°	Depositor
Resolution (Å)	48.94 – 1.87 48.94 – 1.87	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.94-1.87) 96.8 (48.94-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.179 , 0.214 0.191 , 0.223	Depositor DCC
R_{free} test set	17518 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33119	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.77% 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: EDO, PEG, FES, P33, MO, PGE, SBO, GOL, 1PE, P4G, PG0, MGD, O, F3S, 4MO, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.95	2/6661 (0.0%)	1.25	20/9029 (0.2%)
1	C	0.95	1/6661 (0.0%)	1.24	18/9029 (0.2%)
1	E	0.94	2/6653 (0.0%)	1.27	24/9018 (0.3%)
1	G	0.93	0/6653	1.25	22/9018 (0.2%)
2	B	1.00	2/1026 (0.2%)	1.27	0/1397
2	D	1.01	0/1026	1.31	4/1397 (0.3%)
2	F	0.98	0/1026	1.30	4/1397 (0.3%)
2	H	0.94	0/1026	1.27	2/1397 (0.1%)
All	All	0.95	7/30732 (0.0%)	1.26	94/41682 (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	5
1	C	0	7
1	E	0	6
1	G	0	5
2	B	0	1
2	D	0	1
2	F	0	2
2	H	0	2
All	All	0	29

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	HIS	CG-CD2	-5.97	1.29	1.35
2	B	52	ASP	N-CA	-5.87	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	PRO	CA-CB	5.50	1.61	1.53
2	B	130	ALA	CA-CB	-5.14	1.44	1.53
1	E	712	HIS	CG-CD2	-5.12	1.30	1.35
1	E	381	HIS	ND1-CE1	5.07	1.37	1.32
1	C	619	SER	CA-CB	-5.05	1.45	1.53

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	295	ARG	CD-NE-CZ	9.31	137.43	124.40
1	E	295	ARG	CD-NE-CZ	9.01	137.02	124.40
1	E	412	ARG	CD-NE-CZ	8.32	136.05	124.40
1	E	741	THR	CA-CB-OG1	-8.20	97.30	109.60
2	D	111	GLU	CB-CG-CD	7.65	125.60	112.60
1	G	295	ARG	CD-NE-CZ	7.59	135.03	124.40
1	E	295	ARG	NE-CZ-NH2	-7.50	112.45	119.20
1	C	741	THR	CA-CB-OG1	-7.44	98.44	109.60
2	F	111	GLU	CB-CG-CD	7.38	125.14	112.60
1	A	295	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	E	819	PHE	CA-CB-CG	-7.27	106.53	113.80
1	C	295	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	A	295	ARG	CD-NE-CZ	7.15	134.41	124.40
1	A	741	THR	CA-CB-OG1	-6.97	99.14	109.60
1	C	412	ARG	CD-NE-CZ	6.83	133.96	124.40
1	A	258	LYS	CB-CA-C	6.73	122.28	110.85
1	E	663	GLU	CB-CG-CD	6.71	124.01	112.60
1	G	718	LEU	N-CA-CB	6.63	119.87	110.12
1	A	412	ARG	CD-NE-CZ	6.62	133.67	124.40
1	G	741	THR	CA-CB-OG1	-6.55	99.77	109.60
2	F	123	GLY	N-CA-C	-6.53	105.49	112.08
2	H	111	GLU	CB-CG-CD	6.44	123.55	112.60
1	G	590	PHE	CA-CB-CG	-6.42	107.38	113.80
1	C	258	LYS	CB-CA-C	6.37	121.67	110.85
1	E	598	GLU	CB-CG-CD	6.35	123.39	112.60
1	E	258	LYS	CB-CA-C	6.30	121.56	110.85
1	A	569	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	C	581	ASP	CA-CB-CG	6.24	118.83	112.60
1	C	819	PHE	CA-CB-CG	-6.14	107.66	113.80
2	D	23	VAL	N-CA-CB	-6.14	103.63	110.99
1	G	5	ASP	CA-CB-CG	6.11	118.71	112.60
1	G	721	GLU	CG-CD-OE2	6.11	132.46	118.40
1	G	721	GLU	CG-CD-OE1	-6.09	104.40	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	5	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	734	ASP	CA-CB-CG	6.08	118.68	112.60
1	C	734	ASP	CA-CB-CG	6.05	118.65	112.60
1	E	348	GLU	CG-CD-OE2	-6.04	104.51	118.40
1	E	800	THR	CA-CB-OG1	-6.00	100.61	109.60
1	E	811	GLU	N-CA-CB	5.98	118.91	110.12
1	E	134	THR	CA-CB-OG1	-5.98	100.64	109.60
1	G	258	LYS	CB-CA-C	5.97	121.00	110.85
1	G	569	ARG	NH1-CZ-NH2	5.96	127.05	119.30
1	G	598	GLU	CB-CG-CD	5.94	122.70	112.60
1	G	412	ARG	CD-NE-CZ	5.94	132.71	124.40
1	G	819	PHE	CA-CB-CG	-5.91	107.89	113.80
1	C	811	GLU	N-CA-CB	5.90	118.80	110.12
1	E	734	ASP	CA-CB-CG	5.86	118.46	112.60
1	G	295	ARG	NE-CZ-NH2	-5.86	113.93	119.20
1	E	4	ASN	CB-CA-C	-5.83	100.35	110.09
1	A	486	LYS	N-CA-C	-5.83	106.00	113.23
1	C	134	THR	CA-CB-OG1	-5.83	100.86	109.60
1	G	134	THR	CA-CB-OG1	-5.77	100.94	109.60
1	A	819	PHE	CA-CB-CG	-5.75	108.05	113.80
2	D	111	GLU	CG-CD-OE1	5.65	131.39	118.40
1	E	581	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	5	ASP	CA-CB-CG	5.62	118.22	112.60
1	E	590	PHE	CA-CB-CG	-5.61	108.19	113.80
1	E	348	GLU	CG-CD-OE1	5.59	131.26	118.40
1	G	581	ASP	CA-CB-CG	5.59	118.19	112.60
2	F	99	THR	OG1-CB-CG2	5.58	120.47	109.30
1	C	713	ASP	CA-CB-CG	5.58	118.18	112.60
1	E	662	THR	CA-CB-OG1	-5.54	101.28	109.60
1	E	486	LYS	N-CA-C	-5.53	106.04	112.89
1	C	764	GLU	CG-CD-OE2	-5.52	105.70	118.40
1	C	662	THR	CA-CB-OG1	-5.50	101.35	109.60
1	G	356	PRO	N-CA-CB	5.45	108.09	103.35
1	G	800	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	581	ASP	CA-CB-CG	5.38	117.97	112.60
1	C	813	PHE	CA-CB-CG	5.37	119.17	113.80
1	C	340	LYS	CB-CA-C	-5.35	102.45	110.90
1	E	695	ARG	CB-CG-CD	5.30	123.50	111.30
1	G	734	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	77	ASP	CA-CB-CG	5.28	117.88	112.60
2	D	123	GLY	N-CA-C	-5.27	106.67	112.04
1	G	569	ARG	NE-CZ-NH2	-5.26	114.47	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	441	ASP	CA-CB-CG	5.23	117.83	112.60
1	G	402	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	689	GLN	CB-CA-C	-5.20	102.16	110.79
1	C	598	GLU	CB-CG-CD	5.20	121.43	112.60
2	H	23	VAL	N-CA-CB	-5.20	102.55	110.86
1	G	713	ASP	CA-CB-CG	5.17	117.78	112.60
1	A	134	THR	CA-CB-OG1	-5.15	101.87	109.60
1	E	133	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	484	MET	CG-SD-CE	5.12	112.16	100.90
1	C	348	GLU	CG-CD-OE2	-5.12	106.64	118.40
1	A	590	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	159	VAL	N-CA-CB	-5.11	105.02	111.46
1	E	752	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	133	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	713	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	295	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	E	692	ASP	CA-CB-CG	5.05	117.65	112.60
2	F	84	GLU	CB-CA-C	5.02	118.44	109.65
1	G	634	ARG	CG-CD-NE	-5.02	100.96	112.00

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	ARG	Sidechain
1	A	55	ARG	Sidechain
1	A	608	ARG	Sidechain
1	A	695	ARG	Sidechain
1	A	702	ARG	Sidechain
2	B	128	ARG	Sidechain
1	C	262	ARG	Sidechain
1	C	450	ARG	Sidechain
1	C	607	ARG	Sidechain
1	C	695	ARG	Sidechain
1	C	702	ARG	Sidechain
1	C	722	ARG	Sidechain
1	C	80	ARG	Sidechain
2	D	128	ARG	Sidechain
1	E	545	ARG	Sidechain
1	E	608	ARG	Sidechain
1	E	695	ARG	Sidechain
1	E	702	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	722	ARG	Sidechain
1	E	80	ARG	Sidechain
2	F	128	ARG	Sidechain
2	F	63	MET	Peptide
1	G	378	ARG	Sidechain
1	G	608	ARG	Sidechain
1	G	695	ARG	Sidechain
1	G	702	ARG	Sidechain
1	G	722	ARG	Sidechain
2	H	128	ARG	Sidechain
2	H	63	MET	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	6500	0	6283	79	0
1	C	6500	0	6283	43	0
1	E	6492	0	6273	65	0
1	G	6492	0	6273	58	0
2	B	1004	0	986	20	0
2	D	1004	0	986	7	0
2	F	1004	0	986	9	0
2	H	1004	0	986	4	0
3	A	1	0	0	0	0
4	A	94	0	44	2	0
4	C	94	0	44	2	0
4	E	94	0	44	2	0
4	G	94	0	44	2	0
5	A	7	0	0	0	0
5	C	7	0	0	0	0
5	E	7	0	0	0	0
5	G	7	0	0	0	0
6	A	12	0	18	1	0
6	C	24	0	36	0	0
6	E	16	0	24	3	0
6	G	12	0	18	1	0
7	A	63	0	87	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	21	0	30	17	0
7	C	28	0	40	12	0
7	E	42	0	60	13	0
7	F	7	0	10	0	0
7	G	28	0	40	12	0
7	H	7	0	10	4	0
8	A	3	0	0	0	0
8	C	4	0	0	1	0
8	E	4	0	0	1	0
8	G	3	0	0	1	0
9	A	22	0	30	6	0
10	A	20	0	28	7	0
10	C	10	0	14	1	0
10	E	10	0	14	3	0
10	G	10	0	14	9	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	0	0	1	0
11	G	1	0	0	0	0
12	A	1	0	0	0	0
12	C	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
13	B	4	0	0	0	0
13	D	4	0	0	0	0
13	F	4	0	0	0	0
13	H	4	0	0	0	0
14	B	12	0	16	4	0
14	E	6	0	8	0	0
15	C	1	0	0	0	0
15	E	1	0	0	1	0
15	G	1	0	0	0	0
16	C	11	0	18	21	0
17	C	16	0	22	8	0
17	G	16	0	22	12	0
18	C	8	0	12	5	0
19	A	453	0	0	9	0
19	B	90	0	0	3	0
19	C	487	0	0	11	0
19	D	90	0	0	3	0
19	E	487	0	0	12	0
19	F	90	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	G	492	0	0	7	0
19	H	83	0	0	2	0
All	All	33119	0	29803	320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (320) 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)
7:A:914:PEG:H11	7:A:914:PEG:H41	1.32	1.11
1:A:620:GLN:HE21	7:A:915:PEG:H42	1.10	1.08
1:A:208:ARG:HH12	10:A:918:PGE:H42	1.27	0.99
1:A:208:ARG:HH12	10:A:918:PGE:C4	1.76	0.98
1:C:157:GLN:HG2	19:C:1336:HOH:O	1.64	0.98
1:G:616:ALA:HA	7:G:912:PEG:H12	1.48	0.95
1:C:646:VAL:HG12	19:C:1401:HOH:O	1.66	0.95
2:B:100:GLU:CB	7:B:2906:PEG:H11	1.98	0.93
2:B:100:GLU:CG	7:B:2906:PEG:H11	2.00	0.92
1:E:157:GLN:HG2	19:E:1256:HOH:O	1.68	0.92
1:C:437:LYS:HG3	18:C:916:PG0:H51	1.51	0.91
2:B:100:GLU:HG3	7:B:2906:PEG:H11	1.52	0.91
1:A:620:GLN:NE2	7:A:915:PEG:H42	1.88	0.89
1:G:617:ILE:H	7:G:912:PEG:H11	1.37	0.88
1:G:92:VAL:HA	10:G:913:PGE:H52	1.56	0.86
10:G:913:PGE:H2	19:G:1419:HOH:O	1.74	0.86
1:C:121:LYS:HE3	19:C:1006:HOH:O	1.76	0.85
1:G:437:LYS:HZ1	17:G:910:1PE:H241	1.43	0.83
2:B:124:LEU:O	7:B:2906:PEG:H21	1.76	0.83
1:G:801:TRP:HE1	7:G:908:PEG:C1	1.90	0.83
7:A:917:PEG:H12	19:A:1348:HOH:O	1.77	0.83
1:E:359[B]:MET:SD	1:E:362:ARG:NH1	2.51	0.83
2:B:100:GLU:HG3	7:B:2906:PEG:C1	2.08	0.82
1:C:521:ALA:O	17:C:912:1PE:H231	1.79	0.82
1:G:769:GLN:OE1	7:G:908:PEG:H32	1.80	0.81
16:C:911:P4G:H52	16:C:911:P4G:O2	1.81	0.81
16:C:911:P4G:H11	1:E:504:GLN:HA	1.61	0.81
15:E:903:4MO:MO	11:E:918:O:O	1.51	0.80
1:E:95:SER:OG	10:E:916:PGE:H22	1.81	0.80
1:G:816:THR:HG22	19:G:1272:HOH:O	1.82	0.79
1:G:791:ARG:HD3	17:G:910:1PE:H261	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:GLU:OE1	7:G:908:PEG:H31	1.83	0.78
1:G:95:SER:OG	10:G:913:PGE:H5	1.82	0.78
2:B:124:LEU:CD2	7:B:2906:PEG:H42	2.15	0.77
16:C:911:P4G:H81	1:E:153:LYS:HE2	1.67	0.75
1:G:359[B]:MET:SD	1:G:362:ARG:NH1	2.59	0.75
1:E:663:GLU:CD	1:E:663:GLU:H	1.95	0.75
1:A:484:MET:HE2	1:A:499:ILE:HD11	1.68	0.75
1:A:2:ALA:HB2	1:E:2:ALA:HB2	1.68	0.74
1:C:681:ASN:HB2	7:C:914:PEG:H42	1.68	0.74
1:G:791:ARG:HH11	17:G:910:1PE:H162	1.52	0.73
1:G:617:ILE:N	7:G:912:PEG:H11	2.03	0.73
1:C:484:MET:HE2	1:C:499:ILE:HD11	1.70	0.72
2:B:59:LEU:HD22	7:B:2901:PEG:H42	1.71	0.72
1:C:131:TRP:HE1	17:C:912:1PE:H232	1.54	0.71
1:C:95:SER:OG	10:C:917:PGE:H22	1.90	0.71
1:A:89:LYS:HE3	7:A:917:PEG:H32	1.72	0.71
2:B:124:LEU:HD23	7:B:2906:PEG:H42	1.70	0.71
1:E:129:ASP:HB3	1:E:485:GLN:HE22	1.56	0.70
1:G:245:ASN:O	10:G:913:PGE:H22	1.91	0.70
1:A:680:TRP:CE3	7:A:914:PEG:H21	2.27	0.70
1:G:223:GLN:HE22	10:G:913:PGE:H3	1.57	0.70
1:A:2:ALA:CB	1:A:3:PRO:HD2	2.23	0.69
1:G:223:GLN:HE22	10:G:913:PGE:C3	2.05	0.69
1:A:343:ARG:NH1	19:A:1001:HOH:O	2.26	0.68
1:C:392:ASP:OD2	16:C:911:P4G:H51	1.93	0.68
17:C:912:1PE:C22	17:C:912:1PE:H261	2.23	0.68
1:A:208:ARG:HH12	10:A:918:PGE:H4	1.58	0.68
1:A:34:LYS:NZ	7:A:909:PEG:H12	2.09	0.68
16:C:911:P4G:H62	19:C:1080:HOH:O	1.93	0.68
1:A:34:LYS:NZ	7:A:909:PEG:C1	2.58	0.67
1:A:59:PRO:HA	7:B:2901:PEG:H22	1.77	0.67
1:G:617:ILE:H	7:G:912:PEG:C1	2.06	0.67
2:H:15:LYS:HE3	19:H:2368:HOH:O	1.93	0.67
2:F:38:LYS:HD2	19:F:345:HOH:O	1.94	0.67
8:C:918:SBO:O3	19:C:1001:HOH:O	2.11	0.66
1:A:484:MET:HE2	1:A:499:ILE:CD1	2.25	0.66
1:A:34:LYS:HZ3	7:A:909:PEG:C1	2.08	0.66
8:E:917:SBO:SB	19:E:1122:HOH:O	2.93	0.66
1:G:791:ARG:NH1	17:G:910:1PE:H162	2.11	0.65
17:C:912:1PE:H261	17:C:912:1PE:H221	1.78	0.65
7:H:2201:PEG:H32	19:H:2305:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:LYS:HD2	19:D:356:HOH:O	1.97	0.64
16:C:911:P4G:C8	1:E:153:LYS:HE2	2.28	0.64
1:A:2:ALA:CB	1:E:2:ALA:HB2	2.28	0.64
7:B:2906:PEG:H31	19:B:3031:HOH:O	1.98	0.63
2:B:124:LEU:O	7:B:2906:PEG:C2	2.45	0.63
2:B:123:GLY:HA2	14:B:2905:GOL:H11	1.81	0.63
2:B:100:GLU:HB3	7:B:2906:PEG:H11	1.78	0.63
1:G:343:ARG:NH1	19:G:1002:HOH:O	2.32	0.63
7:A:914:PEG:H31	19:A:1177:HOH:O	1.99	0.62
1:G:646:VAL:HG13	19:G:1482:HOH:O	1.98	0.62
1:G:801:TRP:HE1	7:G:908:PEG:H12	1.64	0.62
1:A:38[B]:LEU:C	1:A:38[B]:LEU:HD13	2.25	0.61
1:G:359[B]:MET:HE3	7:G:911:PEG:H12	1.82	0.61
1:A:2:ALA:CB	1:A:3:PRO:CD	2.79	0.60
1:A:385:LYS:HE2	4:A:903:MGD:S13	2.41	0.60
16:C:911:P4G:H13	1:E:450:ARG:HE	1.67	0.60
1:G:698:LEU:HB2	1:G:800:THR:HG23	1.83	0.60
1:A:38[B]:LEU:HD22	19:F:382:HOH:O	2.01	0.60
1:G:791:ARG:HH11	17:G:910:1PE:C16	2.15	0.59
1:G:801:TRP:HE1	7:G:908:PEG:H11	1.66	0.59
1:A:2:ALA:HB1	1:A:3:PRO:CD	2.31	0.59
1:E:450:ARG:NH1	1:E:500:TYR:CZ	2.70	0.59
1:A:38[B]:LEU:C	1:A:38[B]:LEU:CD1	2.76	0.59
17:C:912:1PE:C13	17:C:912:1PE:OH5	2.51	0.59
16:C:911:P4G:H13	1:E:450:ARG:NH2	2.18	0.58
1:E:698:LEU:HB2	1:E:800:THR:HG23	1.85	0.58
1:A:620:GLN:HE21	7:A:915:PEG:C4	2.01	0.58
18:C:916:PG0:C1	19:E:1193:HOH:O	2.50	0.58
1:A:698:LEU:HB2	1:A:800:THR:HG23	1.87	0.57
7:A:914:PEG:H11	7:A:914:PEG:C4	2.02	0.57
1:C:680:TRP:CE3	7:C:914:PEG:H22	2.40	0.57
1:C:484:MET:HE2	1:C:499:ILE:CD1	2.34	0.57
1:A:359[B]:MET:SD	1:A:362:ARG:NH1	2.78	0.57
1:C:613:GLY:N	19:C:1003:HOH:O	2.33	0.57
1:C:698:LEU:HB2	1:C:800:THR:HG23	1.87	0.56
16:C:911:P4G:H13	1:E:450:ARG:NE	2.19	0.56
1:A:208:ARG:NH1	10:A:918:PGE:C4	2.59	0.56
1:A:208:ARG:NH1	10:A:918:PGE:H42	2.09	0.56
7:C:919:PEG:H21	2:D:93:MET:HE2	1.88	0.56
1:C:395:VAL:HG21	16:C:911:P4G:H42	1.88	0.56
1:A:2:ALA:HB1	1:A:3:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:437:LYS:NZ	17:G:910:1PE:H241	2.20	0.56
1:A:34:LYS:HZ2	7:A:909:PEG:H12	1.70	0.56
1:G:333:LYS:HE2	1:G:333:LYS:HA	1.88	0.56
2:B:123:GLY:CA	14:B:2905:GOL:H11	2.36	0.55
6:E:906:EDO:H12	19:E:1022:HOH:O	2.06	0.55
1:C:680:TRP:CZ3	7:C:914:PEG:H22	2.40	0.55
1:A:392:ASP:OD2	7:A:914:PEG:O4	2.24	0.55
1:G:209:GLU:OE2	17:G:910:1PE:H141	2.06	0.55
1:E:2:ALA:HB3	1:E:3:PRO:HD3	1.88	0.55
1:A:170:GLY:HA2	4:A:903:MGD:C6	2.37	0.55
1:E:450:ARG:HG3	1:E:450:ARG:HH11	1.72	0.55
17:C:912:1PE:OH5	17:C:912:1PE:H131	2.07	0.54
7:E:913:PEG:C4	2:F:93:MET:HB3	2.38	0.54
1:C:267:ASN:ND2	1:C:372:ALA:HB3	2.23	0.54
1:E:208:ARG:HB3	7:E:909:PEG:H12	1.89	0.54
7:C:913:PEG:H42	19:C:1226:HOH:O	2.05	0.54
1:G:205:HIS:CE1	17:G:910:1PE:H131	2.43	0.54
16:C:911:P4G:O2	16:C:911:P4G:C5	2.54	0.53
16:C:911:P4G:C1	1:E:450:ARG:HE	2.20	0.53
16:C:911:P4G:H12	7:E:911:PEG:H21	1.90	0.53
1:A:680:TRP:CE3	7:A:914:PEG:C2	2.90	0.53
1:C:208:ARG:HH22	7:C:909:PEG:H41	1.73	0.53
1:E:450:ARG:HD2	1:E:503:THR:OG1	2.08	0.53
1:A:597:THR:OG1	7:A:908:PEG:H41	2.08	0.53
1:A:208:ARG:NH1	10:A:918:PGE:H4	2.22	0.52
7:C:913:PEG:C4	19:C:1226:HOH:O	2.57	0.52
1:A:133:ASP:OD1	9:A:912:P33:H201	2.10	0.52
2:B:38:LYS:HD2	19:B:3028:HOH:O	2.09	0.52
18:C:916:PG0:H42	1:E:501:GLU:OE2	2.10	0.52
1:A:561:MET:HE3	1:A:566:ILE:HG12	1.91	0.52
1:A:482:GLN:OE1	1:E:475:GLN:OE1	2.28	0.52
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.74	0.52
16:C:911:P4G:H13	1:E:450:ARG:HH21	1.74	0.52
1:G:267:ASN:OD1	1:G:372:ALA:HB3	2.09	0.52
7:E:913:PEG:H42	2:F:93:MET:HB3	1.93	0.51
1:C:131:TRP:HE1	17:C:912:1PE:C23	2.23	0.51
1:E:385:LYS:HE2	4:E:902:MGD:S13	2.51	0.51
1:C:31:HIS:HE1	19:C:1109:HOH:O	1.94	0.51
16:C:911:P4G:H12	7:E:911:PEG:C2	2.40	0.51
1:C:345:SER:OG	1:C:348:GLU:HG3	2.12	0.50
16:C:911:P4G:H13	1:E:450:ARG:CZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:GLY:HA2	4:G:902:MGD:C6	2.41	0.50
1:E:208:ARG:CB	7:E:909:PEG:H12	2.41	0.50
1:A:2:ALA:CB	1:E:2:ALA:CB	2.89	0.50
1:A:680:TRP:HE3	7:A:914:PEG:H21	1.75	0.50
6:G:905:EDO:O1	6:G:914:EDO:H22	2.12	0.50
1:E:663:GLU:CD	1:E:663:GLU:N	2.68	0.50
1:G:385:LYS:HE2	4:G:902:MGD:S13	2.52	0.50
1:A:87:PRO:O	7:A:917:PEG:H41	2.11	0.49
1:A:34:LYS:NZ	7:A:909:PEG:H11	2.26	0.49
2:B:104:ARG:HH12	14:B:2905:GOL:H2	1.77	0.49
1:C:695:ARG:HD3	19:C:1157:HOH:O	2.12	0.49
7:E:907:PEG:C3	19:E:1266:HOH:O	2.60	0.49
1:G:345:SER:OG	1:G:348:GLU:HG3	2.12	0.49
7:A:913:PEG:H12	19:A:1080:HOH:O	2.11	0.49
9:A:912:P33:H32	1:E:522:GLU:HB3	1.94	0.49
1:E:2:ALA:HB3	1:E:3:PRO:CD	2.43	0.49
1:C:4:ASN:HB2	19:D:364:HOH:O	2.13	0.49
1:A:38[B]:LEU:CD2	19:F:382:HOH:O	2.60	0.48
1:C:404:VAL:HG11	1:C:417:CYS:HB2	1.96	0.48
1:E:25:ILE:O	1:E:542:ASN:HB2	2.13	0.48
1:G:331:HIS:NE2	7:G:907:PEG:H31	2.28	0.48
1:A:718:LEU:HD12	1:A:718:LEU:N	2.27	0.48
1:G:95:SER:HG	10:G:913:PGE:H5	1.75	0.48
1:C:359[B]:MET:HE1	1:C:362:ARG:HE	1.79	0.48
1:G:60:PRO:HD3	7:H:2201:PEG:H42	1.94	0.48
1:E:267:ASN:OD1	1:E:372:ALA:HB3	2.13	0.48
1:C:437:LYS:HG3	18:C:916:PG0:C5	2.34	0.48
1:A:2:ALA:HB3	1:A:3:PRO:HD2	1.94	0.48
1:A:333:LYS:HE2	19:A:1431:HOH:O	2.13	0.47
2:H:64:GLY:HA3	2:H:126:TYR:CD2	2.49	0.47
1:C:267:ASN:HD21	1:C:372:ALA:HB3	1.79	0.47
1:E:297:LEU:CD2	1:E:359[A]:MET:HE3	2.44	0.47
1:G:652:LYS:CG	19:G:1302:HOH:O	2.62	0.47
17:C:912:1PE:H261	17:C:912:1PE:H222	1.97	0.47
1:A:808:GLY:HA3	19:E:1187:HOH:O	2.15	0.47
1:C:385:LYS:HE2	4:C:904:MGD:S13	2.54	0.47
1:A:60:PRO:HG3	7:B:2901:PEG:H41	1.97	0.47
1:A:333:LYS:NZ	1:A:333:LYS:HB3	2.30	0.47
2:F:1:ARG:CZ	2:F:5:GLN:HG2	2.45	0.47
16:C:911:P4G:H42	7:C:914:PEG:H41	1.98	0.46
2:D:1:ARG:CZ	2:D:5:GLN:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:SER:OG	1:E:348:GLU:HG3	2.15	0.46
1:E:404:VAL:HG11	1:E:417:CYS:HB2	1.98	0.46
1:A:517:PRO:HG3	9:A:912:P33:C14	2.46	0.46
2:B:100:GLU:HG3	7:B:2906:PEG:H12	1.92	0.46
1:C:25:ILE:O	1:C:542:ASN:HB2	2.15	0.46
1:E:154:ASP:OD2	1:E:450:ARG:NH1	2.48	0.46
2:B:64:GLY:HA3	2:B:126:TYR:CD2	2.51	0.46
1:E:533:PRO:HG3	1:E:538:LEU:HD13	1.98	0.46
1:G:297:LEU:CD2	1:G:359[A]:MET:HE3	2.45	0.46
1:A:267:ASN:OD1	1:A:372:ALA:HB3	2.15	0.46
7:A:917:PEG:H42	19:A:1093:HOH:O	2.15	0.46
1:E:589:GLN:NE2	19:E:1002:HOH:O	2.22	0.46
1:E:121:LYS:HE3	19:E:1059:HOH:O	2.16	0.46
17:G:910:1PE:H141	17:G:910:1PE:C23	2.46	0.46
1:E:129:ASP:HB3	1:E:485:GLN:NE2	2.27	0.45
1:E:170:GLY:HA2	4:E:902:MGD:C6	2.46	0.45
2:F:64:GLY:HA3	2:F:126:TYR:CD2	2.50	0.45
1:A:4:ASN:HB2	19:A:1088:HOH:O	2.16	0.45
1:E:95:SER:HG	10:E:916:PGE:H22	1.79	0.45
1:G:791:ARG:CD	17:G:910:1PE:H261	2.40	0.45
7:E:907:PEG:H31	7:E:909:PEG:H42	1.98	0.45
1:A:485:GLN:HA	1:A:485:GLN:NE2	2.32	0.45
16:C:911:P4G:C1	1:E:504:GLN:HA	2.39	0.45
1:C:141:ALA:HB1	1:C:492:THR:HG21	1.99	0.45
16:C:911:P4G:H81	1:E:153:LYS:CE	2.43	0.45
7:E:907:PEG:H32	19:E:1266:HOH:O	2.16	0.45
8:G:909:SBO:SB	19:G:1154:HOH:O	3.15	0.45
1:A:34:LYS:CE	7:A:909:PEG:H11	2.48	0.44
1:A:67:PRO:HD2	7:B:2906:PEG:H12	2.00	0.44
1:C:170:GLY:HA2	4:C:904:MGD:C6	2.47	0.44
1:C:699:ASN:HB3	1:C:770:THR:O	2.18	0.44
2:D:64:GLY:HA3	2:D:126:TYR:CD2	2.51	0.44
1:A:517:PRO:HG3	9:A:912:P33:H141	2.00	0.44
1:C:66:THR:HB	2:D:100:GLU:HG3	1.98	0.44
1:A:718:LEU:HD12	1:A:718:LEU:H	1.83	0.44
7:H:2201:PEG:C4	7:H:2201:PEG:C1	2.95	0.44
7:C:919:PEG:H11	7:C:919:PEG:H32	1.59	0.44
1:E:699:ASN:HB3	1:E:770:THR:O	2.18	0.44
6:A:919:EDO:C1	19:B:3010:HOH:O	2.66	0.44
1:E:333:LYS:HD2	1:E:670:ASP:OD2	2.17	0.44
1:E:487:ALA:HB3	1:E:495:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:2201:PEG:H42	7:H:2201:PEG:H12	1.98	0.44
1:G:404:VAL:HG11	1:G:417:CYS:HB2	1.99	0.44
1:C:437:LYS:CG	18:C:916:PG0:H51	2.36	0.44
1:E:100:THR:HB	2:F:97:GLN:HA	1.98	0.43
1:A:699:ASN:HB3	1:A:770:THR:O	2.18	0.43
6:E:906:EDO:C1	19:E:1022:HOH:O	2.62	0.43
1:A:680:TRP:CZ3	7:A:914:PEG:H22	2.53	0.43
1:G:33:TYR:O	1:G:83:ILE:HA	2.19	0.43
7:C:919:PEG:H22	19:D:319:HOH:O	2.18	0.43
1:C:392:ASP:OD2	16:C:911:P4G:C5	2.64	0.43
1:A:92:VAL:HA	10:A:916:PGE:H62	2.00	0.43
1:E:63:VAL:HG23	7:E:910:PEG:H12	2.01	0.43
9:A:912:P33:C9	19:E:1012:HOH:O	2.66	0.43
6:E:905:EDO:H22	6:E:914:EDO:O1	2.19	0.43
1:A:307:THR:HG21	7:A:914:PEG:H12	2.00	0.42
1:E:223:GLN:HE22	10:E:916:PGE:H4	1.83	0.42
1:G:359[B]:MET:CE	7:G:911:PEG:H12	2.49	0.42
1:G:533:PRO:HG3	1:G:538:LEU:HD13	2.01	0.42
1:G:575:ARG:HH11	1:G:575:ARG:HD3	1.66	0.42
9:A:912:P33:H182	9:A:912:P33:H152	1.70	0.42
1:E:603:ASN:OD1	1:E:607:ARG:HD3	2.19	0.42
2:B:100:GLU:CG	7:B:2906:PEG:C1	2.78	0.42
1:C:603:ASN:OD1	1:C:607:ARG:HD3	2.19	0.42
1:G:25:ILE:O	1:G:542:ASN:HB2	2.20	0.42
1:A:25:ILE:O	1:A:542:ASN:HB2	2.20	0.42
7:A:915:PEG:H31	7:A:915:PEG:H11	1.25	0.42
1:A:33:TYR:O	1:A:83:ILE:HA	2.20	0.42
1:A:434:GLY:HA3	19:A:1310:HOH:O	2.20	0.42
1:G:541:MET:HA	1:G:546:ARG:O	2.20	0.42
1:E:333:LYS:CD	1:E:670:ASP:OD2	2.67	0.42
1:E:459:ASN:HB3	1:E:463:SER:OG	2.20	0.42
1:G:737:GLN:OE1	1:G:767:ARG:NH2	2.52	0.42
1:A:672:LYS:NZ	19:A:1026:HOH:O	2.53	0.42
1:C:459:ASN:HB3	1:C:463:SER:OG	2.20	0.42
2:F:70:ASP:HB2	2:F:77:LYS:HE2	2.02	0.42
1:G:223:GLN:NE2	10:G:913:PGE:H3	2.29	0.42
1:G:695:ARG:HG2	1:G:696:PHE:CD2	2.55	0.42
1:C:395:VAL:HG21	16:C:911:P4G:C4	2.49	0.42
1:G:695:ARG:NH2	19:G:1020:HOH:O	2.51	0.42
1:A:34:LYS:HZ3	7:A:909:PEG:H11	1.83	0.41
1:A:65:LEU:O	7:B:2906:PEG:H41	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:PRO:HG3	1:A:538:LEU:HD13	2.02	0.41
17:G:910:1PE:H251	17:G:910:1PE:H242	1.89	0.41
1:E:575:ARG:HH11	1:E:575:ARG:HD3	1.61	0.41
1:A:66:THR:HB	2:B:100:GLU:HG3	2.01	0.41
1:E:45:PRO:O	1:E:51:GLY:HA2	2.21	0.41
1:A:345:SER:OG	1:A:348:GLU:HG3	2.21	0.41
7:C:909:PEG:H21	19:C:1023:HOH:O	2.21	0.41
1:E:620:GLN:HG2	7:E:907:PEG:H21	2.03	0.41
1:C:541:MET:HA	1:C:546:ARG:O	2.20	0.41
1:E:448:LYS:HD3	7:E:911:PEG:H11	2.02	0.41
2:F:111:GLU:HB3	19:F:389:HOH:O	2.21	0.41
1:G:223:GLN:NE2	10:G:913:PGE:C3	2.78	0.41
1:G:332:THR:O	1:G:333:LYS:HE2	2.20	0.41
1:C:141:ALA:CB	1:C:492:THR:HG21	2.51	0.41
1:E:208:ARG:CA	7:E:909:PEG:H12	2.50	0.41
2:F:1:ARG:NH1	2:F:5:GLN:HG2	2.36	0.41
1:A:575:ARG:HH11	1:A:575:ARG:HD3	1.62	0.41
1:E:31:HIS:HE1	19:E:1177:HOH:O	2.03	0.41
1:E:141:ALA:CB	1:E:492:THR:HG21	2.50	0.41
1:A:459:ASN:HB3	1:A:463:SER:OG	2.21	0.41
1:A:469:LEU:O	1:A:473:ILE:HG12	2.21	0.41
1:A:487:ALA:HB3	1:A:495:MET:HE1	2.03	0.41
1:A:603:ASN:OD1	1:A:607:ARG:HD3	2.20	0.41
1:C:333:LYS:CD	1:C:670:ASP:OD2	2.69	0.41
2:D:64:GLY:HA3	2:D:126:TYR:CE2	2.56	0.41
1:E:346:LEU:HD23	1:E:346:LEU:HA	1.92	0.41
1:G:66:THR:HB	2:H:100:GLU:HG3	2.03	0.41
1:A:485:GLN:NE2	1:E:467:GLN:NE2	2.69	0.41
1:A:695:ARG:HG2	1:A:696:PHE:CD2	2.56	0.41
1:E:541:MET:HA	1:E:546:ARG:O	2.20	0.41
1:G:394:TYR:CZ	17:G:910:1PE:H161	2.55	0.41
1:G:532:HIS:HB2	1:G:533:PRO:CD	2.51	0.41
1:E:33:TYR:O	1:E:83:ILE:HA	2.20	0.40
1:A:512:SER:O	1:A:527:MET:HA	2.21	0.40
2:B:35:VAL:HG21	14:B:2903:GOL:H12	2.03	0.40
2:H:15:LYS:HG3	2:H:114:ASP:OD2	2.22	0.40
1:A:100:THR:HB	2:B:97:GLN:HA	2.03	0.40
1:C:2:ALA:N	1:C:3:PRO:CD	2.83	0.40
1:E:500:TYR:HE1	1:E:504:GLN:NE2	2.19	0.40
1:G:512:SER:O	1:G:527:MET:HA	2.21	0.40
7:C:913:PEG:H41	2:D:73:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:572:ASN:HD22	1:G:572:ASN:HA	1.76	0.40
1:G:699:ASN:HB3	1:G:770:THR:O	2.22	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	824/824 (100%)	796 (97%)	27 (3%)	1 (0%)	48	37
1	C	824/824 (100%)	793 (96%)	30 (4%)	1 (0%)	48	37
1	E	823/824 (100%)	792 (96%)	30 (4%)	1 (0%)	48	37
1	G	823/824 (100%)	793 (96%)	30 (4%)	0	100	100
2	B	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
2	D	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
2	F	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
2	H	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
All	All	3826/3836 (100%)	3689 (96%)	134 (4%)	3 (0%)	48	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	392	ASP
1	A	392	ASP
1	C	392	ASP

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	678/676 (100%)	669 (99%)	9 (1%)	61	50
1	C	678/676 (100%)	674 (99%)	4 (1%)	78	72
1	E	677/676 (100%)	671 (99%)	6 (1%)	70	63
1	G	677/676 (100%)	669 (99%)	8 (1%)	63	53
2	B	110/110 (100%)	108 (98%)	2 (2%)	51	38
2	D	110/110 (100%)	108 (98%)	2 (2%)	51	38
2	F	110/110 (100%)	107 (97%)	3 (3%)	39	23
2	H	110/110 (100%)	107 (97%)	3 (3%)	39	23
All	All	3150/3144 (100%)	3113 (99%)	37 (1%)	65	53

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	38[A]	LEU
1	A	38[B]	LEU
1	A	153	LYS
1	A	258	LYS
1	A	333	LYS
1	A	410	VAL
1	A	486	LYS
1	A	695	ARG
2	B	10	GLN
2	B	35	VAL
1	C	258	LYS
1	C	297	LEU
1	C	410	VAL
1	C	485	GLN
2	D	35	VAL
2	D	111	GLU
1	E	258	LYS
1	E	297	LEU

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Mol	Chain	Res	Type
1	E	410	VAL
1	E	598	GLU
1	E	663	GLU
1	E	695	ARG
2	F	10	GLN
2	F	35	VAL
2	F	41	SER
1	G	258	LYS
1	G	297	LEU
1	G	329	GLU
1	G	410	VAL
1	G	486	LYS
1	G	569	ARG
1	G	652	LYS
1	G	695	ARG
2	H	15	LYS
2	H	35	VAL
2	H	41	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	320	GLN
1	A	461	GLN
1	A	475	GLN
1	A	485	GLN
2	B	51	ASN
1	C	31	HIS
1	C	216	ASN
1	C	267	ASN
1	C	270	GLN
1	C	442	GLN
1	C	461	GLN
1	C	611	GLN
1	C	688	GLN
1	C	720	GLN
2	D	5	GLN
2	D	10	GLN
1	E	31	HIS
1	E	216	ASN
1	E	270	GLN

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Mol	Chain	Res	Type
1	E	461	GLN
1	E	475	GLN
1	E	485	GLN
1	E	611	GLN
1	E	688	GLN
2	F	51	ASN
1	G	216	ASN
1	G	223	GLN
1	G	270	GLN
1	G	461	GLN
1	G	572	ASN
1	G	611	GLN
1	G	688	GLN
1	G	720	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 89 ligands modelled in this entry, 12 are monoatomic - leaving 77 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	MGD	G	901	15	45,52,52	1.13	3 (6%)	54,81,81	1.18	4 (7%)
7	PEG	C	909	-	6,6,6	0.25	0	5,5,5	0.39	0
6	EDO	G	906	-	3,3,3	0.39	0	2,2,2	1.00	0
7	PEG	E	912	-	6,6,6	0.47	0	5,5,5	0.21	0
7	PEG	A	907	-	6,6,6	0.72	0	5,5,5	0.43	0
7	PEG	A	921	-	6,6,6	0.45	0	5,5,5	0.36	0
18	PG0	C	916	-	7,7,7	1.19	0	6,6,6	0.90	0
10	PGE	G	913	-	9,9,9	0.92	0	8,8,8	1.18	2 (25%)
4	MGD	E	902	15	45,52,52	1.21	3 (6%)	54,81,81	1.24	7 (12%)
6	EDO	C	910	-	3,3,3	0.38	0	2,2,2	0.32	0
6	EDO	A	905	-	3,3,3	0.31	0	2,2,2	0.28	0
7	PEG	A	917	-	6,6,6	0.64	0	5,5,5	0.55	0
5	F3S	E	904	1	0,9,9	-	-	-		
7	PEG	A	910	-	6,6,6	0.74	0	5,5,5	0.63	0
7	PEG	F	202	-	6,6,6	0.47	0	5,5,5	0.48	0
14	GOL	B	2903	-	5,5,5	0.33	0	5,5,5	0.60	0
7	PEG	A	914	-	6,6,6	0.79	0	5,5,5	0.84	0
6	EDO	E	914	-	3,3,3	0.23	0	2,2,2	0.28	0
8	SBO	G	909	11	0,2,3	-	-	-		
6	EDO	E	915	-	3,3,3	1.17	0	2,2,2	0.90	0
6	EDO	E	905	-	3,3,3	0.21	0	2,2,2	0.31	0
7	PEG	E	910	-	6,6,6	0.50	0	5,5,5	0.51	0
7	PEG	G	911	-	6,6,6	0.58	0	5,5,5	0.36	0
7	PEG	G	907	-	6,6,6	0.70	0	5,5,5	0.50	0
7	PEG	E	907	-	6,6,6	0.37	0	5,5,5	0.13	0
4	MGD	A	902	3	45,52,52	0.83	0	54,81,81	1.10	4 (7%)
10	PGE	C	917	-	9,9,9	1.38	1 (11%)	8,8,8	0.93	0
7	PEG	C	919	-	6,6,6	1.10	0	5,5,5	0.61	0
16	P4G	C	911	-	10,10,10	0.45	0	9,9,9	0.69	0
4	MGD	C	904	15	45,52,52	1.05	3 (6%)	54,81,81	1.07	3 (5%)
9	P33	A	912	-	21,21,21	1.19	3 (14%)	20,20,20	1.01	1 (5%)
7	PEG	A	908	-	6,6,6	0.96	0	5,5,5	0.64	0
6	EDO	C	907	-	3,3,3	0.90	0	2,2,2	0.51	0
4	MGD	A	903	3	45,52,52	0.89	1 (2%)	54,81,81	1.15	4 (7%)
7	PEG	B	2904	-	6,6,6	0.38	0	5,5,5	0.45	0
8	SBO	A	911	19,11	0,2,3	-	-	-		
13	FES	H	2202	2	0,4,4	-	-	-		
7	PEG	E	911	-	6,6,6	0.37	0	5,5,5	0.42	0
7	PEG	H	2201	-	6,6,6	0.74	0	5,5,5	0.51	0
7	PEG	E	909	-	6,6,6	0.44	0	5,5,5	0.58	0
17	1PE	G	910	-	15,15,15	0.80	0	14,14,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SBO	C	918	19,11	0,3,3	-	-	-		
10	PGE	A	918	-	9,9,9	0.93	0	8,8,8	0.84	0
6	EDO	C	906	-	3,3,3	0.18	0	2,2,2	0.32	0
7	PEG	A	909	-	6,6,6	0.37	0	5,5,5	0.53	0
4	MGD	G	902	15	45,52,52	1.06	4 (8%)	54,81,81	1.34	3 (5%)
6	EDO	C	905	-	3,3,3	0.46	0	2,2,2	0.14	0
14	GOL	E	908	-	5,5,5	0.23	0	5,5,5	0.53	0
6	EDO	C	908	-	3,3,3	0.56	0	2,2,2	0.69	0
7	PEG	C	913	-	6,6,6	1.09	1 (16%)	5,5,5	0.56	0
7	PEG	C	914	-	6,6,6	0.44	0	5,5,5	0.92	0
7	PEG	G	908	-	6,6,6	0.46	0	5,5,5	0.55	0
14	GOL	B	2905	-	5,5,5	0.23	0	5,5,5	0.82	0
6	EDO	G	905	-	3,3,3	0.46	0	2,2,2	0.47	0
7	PEG	B	2901	-	6,6,6	0.69	0	5,5,5	0.53	0
13	FES	D	201	2	0,4,4	-	-	-		
17	1PE	C	912	-	15,15,15	1.11	2 (13%)	14,14,14	1.04	0
7	PEG	G	912	-	6,6,6	0.75	0	5,5,5	0.91	0
5	F3S	C	901	1	0,9,9	-	-	-		
7	PEG	A	913	-	6,6,6	0.46	0	5,5,5	0.30	0
4	MGD	E	901	15	45,52,52	0.77	1 (2%)	54,81,81	1.13	5 (9%)
5	F3S	A	904	1	0,9,9	-	-	-		
13	FES	B	2902	2	0,4,4	-	-	-		
5	F3S	G	903	1	0,9,9	-	-	-		
6	EDO	E	906	-	3,3,3	0.52	0	2,2,2	0.58	0
8	SBO	E	917	11	0,3,3	-	-	-		
7	PEG	A	915	-	6,6,6	1.00	0	5,5,5	0.86	0
7	PEG	B	2906	-	6,6,6	2.04	3 (50%)	5,5,5	1.74	1 (20%)
7	PEG	E	913	-	6,6,6	1.15	1 (16%)	5,5,5	0.83	0
10	PGE	E	916	-	9,9,9	1.30	1 (11%)	8,8,8	1.14	1 (12%)
4	MGD	C	902	15	45,52,52	0.87	1 (2%)	54,81,81	1.11	4 (7%)
6	EDO	A	919	-	3,3,3	0.41	0	2,2,2	0.39	0
6	EDO	G	914	-	3,3,3	0.62	0	2,2,2	0.58	0
6	EDO	C	915	-	3,3,3	0.33	0	2,2,2	0.88	0
13	FES	F	201	2	0,4,4	-	-	-		
6	EDO	A	906	-	3,3,3	0.56	0	2,2,2	0.63	0
10	PGE	A	916	-	9,9,9	0.98	1 (11%)	8,8,8	1.23	1 (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	MGD	G	901	15	-	4/22/66/66	0/6/6/6
7	PEG	B	2901	-	-	2/4/4/4	-
7	PEG	C	909	-	-	3/4/4/4	-
7	PEG	E	910	-	-	4/4/4/4	-
4	MGD	A	903	3	-	5/22/66/66	0/6/6/6
7	PEG	B	2904	-	-	4/4/4/4	-
7	PEG	G	911	-	-	3/4/4/4	-
13	FES	D	201	2	-	-	0/1/1/1
17	1PE	C	912	-	-	8/13/13/13	-
6	EDO	G	906	-	-	1/1/1/1	-
13	FES	H	2202	2	-	-	0/1/1/1
7	PEG	G	912	-	-	0/4/4/4	-
5	F3S	C	901	1	-	-	0/3/3/3
7	PEG	A	913	-	-	0/4/4/4	-
4	MGD	E	901	15	-	4/22/66/66	0/6/6/6
7	PEG	G	907	-	-	3/4/4/4	-
7	PEG	E	911	-	-	4/4/4/4	-
7	PEG	E	907	-	-	3/4/4/4	-
4	MGD	A	902	3	-	4/22/66/66	0/6/6/6
7	PEG	H	2201	-	-	2/4/4/4	-
5	F3S	A	904	1	-	-	0/3/3/3
13	FES	B	2902	2	-	-	0/1/1/1
7	PEG	E	909	-	-	1/4/4/4	-
17	1PE	G	910	-	-	7/13/13/13	-
5	F3S	G	903	1	-	-	0/3/3/3
7	PEG	E	912	-	-	3/4/4/4	-
7	PEG	A	907	-	-	1/4/4/4	-
10	PGE	A	918	-	-	4/7/7/7	-
10	PGE	C	917	-	-	5/7/7/7	-
6	EDO	E	906	-	-	1/1/1/1	-
6	EDO	C	906	-	-	1/1/1/1	-
7	PEG	A	909	-	-	3/4/4/4	-
7	PEG	A	915	-	-	1/4/4/4	-
7	PEG	A	921	-	-	2/4/4/4	-
7	PEG	B	2906	-	-	3/4/4/4	-
7	PEG	E	913	-	-	3/4/4/4	-
18	PG0	C	916	-	-	2/5/5/5	-
4	MGD	G	902	15	-	3/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PGE	G	913	-	-	3/7/7/7	-
4	MGD	E	902	15	-	4/22/66/66	0/6/6/6
6	EDO	C	910	-	-	1/1/1/1	-
6	EDO	A	905	-	-	1/1/1/1	-
7	PEG	C	919	-	-	2/4/4/4	-
7	PEG	A	917	-	-	2/4/4/4	-
6	EDO	C	905	-	-	0/1/1/1	-
7	PEG	A	910	-	-	2/4/4/4	-
5	F3S	E	904	1	-	-	0/3/3/3
10	PGE	E	916	-	-	5/7/7/7	-
7	PEG	F	202	-	-	2/4/4/4	-
14	GOL	B	2903	-	-	0/4/4/4	-
14	GOL	E	908	-	-	0/4/4/4	-
16	P4G	C	911	-	-	6/8/8/8	-
7	PEG	A	914	-	-	2/4/4/4	-
6	EDO	C	908	-	-	0/1/1/1	-
6	EDO	E	914	-	-	0/1/1/1	-
7	PEG	C	913	-	-	3/4/4/4	-
7	PEG	C	914	-	-	1/4/4/4	-
4	MGD	C	902	15	-	5/22/66/66	0/6/6/6
4	MGD	C	904	15	-	4/22/66/66	0/6/6/6
6	EDO	A	919	-	-	1/1/1/1	-
9	P33	A	912	-	-	8/19/19/19	-
7	PEG	G	908	-	-	3/4/4/4	-
14	GOL	B	2905	-	-	4/4/4/4	-
6	EDO	G	914	-	-	1/1/1/1	-
7	PEG	A	908	-	-	3/4/4/4	-
6	EDO	E	915	-	-	1/1/1/1	-
6	EDO	C	915	-	-	1/1/1/1	-
13	FES	F	201	2	-	-	0/1/1/1
6	EDO	A	906	-	-	1/1/1/1	-
6	EDO	G	905	-	-	0/1/1/1	-
6	EDO	C	907	-	-	1/1/1/1	-
6	EDO	E	905	-	-	1/1/1/1	-
10	PGE	A	916	-	-	4/7/7/7	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	902	MGD	C10-C11	-4.98	1.45	1.52
4	G	901	MGD	C23-C14	-4.25	1.50	1.53
10	C	917	PGE	C4-C3	3.71	1.68	1.49
4	E	902	MGD	C23-C14	3.52	1.56	1.53
4	C	904	MGD	C10-C11	-3.31	1.47	1.52
4	G	902	MGD	C23-N22	-3.13	1.39	1.45
7	B	2906	PEG	O4-C4	3.05	1.57	1.42
4	C	902	MGD	C23-C14	-2.96	1.51	1.53
4	G	902	MGD	C23-C14	2.82	1.55	1.53
4	E	901	MGD	C23-C14	-2.78	1.51	1.53
10	E	916	PGE	C4-C3	2.66	1.62	1.49
4	A	903	MGD	C23-C14	-2.54	1.51	1.53
4	C	904	MGD	C23-N22	-2.47	1.41	1.45
4	G	901	MGD	C21-N22	-2.46	1.32	1.35
7	B	2906	PEG	C2-C1	2.43	1.62	1.49
7	E	913	PEG	O4-C4	2.40	1.54	1.42
9	A	912	P33	C17-C18	2.30	1.60	1.49
4	C	904	MGD	C23-C14	-2.29	1.51	1.53
9	A	912	P33	C8-C9	2.28	1.60	1.49
4	G	901	MGD	PA-O2A	-2.26	1.44	1.55
10	A	916	PGE	C4-C3	2.25	1.60	1.49
17	C	912	1PE	C23-C13	2.23	1.60	1.49
4	E	902	MGD	C16-C17	-2.22	1.36	1.42
4	G	902	MGD	C16-C17	-2.21	1.36	1.42
17	C	912	1PE	C25-C15	2.16	1.60	1.49
7	B	2906	PEG	C3-C4	2.14	1.60	1.49
4	G	902	MGD	PB-O2B	-2.11	1.45	1.55
9	A	912	P33	C5-C6	2.10	1.59	1.49
7	C	913	PEG	O4-C4	2.04	1.52	1.42

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	902	MGD	O11-C23-C14	5.82	112.85	108.96
4	G	901	MGD	O11-C23-N22	-3.67	104.79	108.57
4	A	903	MGD	O11-C23-C14	3.52	111.31	108.96
4	G	902	MGD	C19-N20-C21	3.43	119.62	113.43
4	G	901	MGD	C4'-O4'-C1'	-3.42	101.92	109.47
4	E	902	MGD	O11-C23-C14	3.37	111.21	108.96
4	C	902	MGD	O11-C23-N22	-3.35	105.13	108.57
4	A	902	MGD	C19-N20-C21	3.21	119.23	113.43
4	C	904	MGD	O2'-C2'-C3'	2.91	121.22	111.82
4	E	901	MGD	C4'-O4'-C1'	-2.89	103.08	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	904	MGD	O11-C23-C14	2.87	110.88	108.96
4	A	902	MGD	C4'-O4'-C1'	-2.79	103.31	109.47
4	A	903	MGD	C19-N20-C21	2.79	118.46	113.43
4	C	902	MGD	PA-O3B-PB	2.76	142.28	132.83
4	G	901	MGD	O2A-PA-O1A	2.72	125.68	112.24
4	G	901	MGD	C19-N20-C21	2.70	118.31	113.43
4	E	902	MGD	O17-C17-C16	-2.61	121.26	127.24
4	E	902	MGD	O2A-PA-O3A	-2.52	96.03	107.75
10	A	916	PGE	C5-O3-C4	2.51	124.16	113.29
4	E	901	MGD	O2A-PA-O1A	2.48	124.50	112.24
4	A	902	MGD	O2'-C2'-C3'	2.41	119.63	111.82
4	E	902	MGD	C19-N20-C21	2.41	117.79	113.43
10	E	916	PGE	O2-C2-C1	2.41	120.67	110.07
4	A	902	MGD	O11-C23-N22	-2.39	106.11	108.57
10	G	913	PGE	O3-C4-C3	2.37	121.08	110.39
4	E	901	MGD	O11-C23-C14	2.34	110.52	108.96
7	B	2906	PEG	O1-C1-C2	2.29	125.12	111.81
10	G	913	PGE	O3-C5-C6	2.27	120.04	110.07
4	E	901	MGD	C19-N20-C21	2.20	117.41	113.43
4	G	902	MGD	O17-C17-C16	-2.18	122.24	127.24
4	E	902	MGD	C17-C16-N15	2.16	122.55	116.76
4	A	903	MGD	C17-C16-N15	2.15	122.52	116.76
4	C	902	MGD	O3'-C3'-C2'	2.15	118.77	111.82
4	E	902	MGD	O2'-C2'-C3'	2.14	118.74	111.82
4	C	904	MGD	C19-N20-C21	2.13	117.27	113.43
4	E	901	MGD	C19-N18-C17	-2.11	121.24	125.10
4	E	902	MGD	O2B-PB-O1B	2.09	122.56	112.24
4	C	902	MGD	O2A-PA-O1A	2.07	122.45	112.24
9	A	912	P33	O16-C15-C14	2.05	119.63	110.39
4	A	903	MGD	C4-C5-N7	-2.04	107.48	110.72

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	MGD	PA-O3B-PB-O5'
4	A	902	MGD	C5'-O5'-PB-O1B
4	A	902	MGD	C5'-O5'-PB-O3B
4	A	903	MGD	C5'-O5'-PB-O1B
4	A	903	MGD	O4'-C4'-C5'-O5'
4	C	902	MGD	PA-O3B-PB-O5'
4	C	902	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	C	902	MGD	C5'-O5'-PB-O3B
4	C	904	MGD	PA-O3B-PB-O5'
4	C	904	MGD	C5'-O5'-PB-O1B
4	E	901	MGD	C5'-O5'-PB-O1B
4	E	901	MGD	C5'-O5'-PB-O3B
4	E	902	MGD	C5'-O5'-PB-O1B
4	G	901	MGD	C5'-O5'-PB-O1B
4	G	901	MGD	C5'-O5'-PB-O3B
4	G	902	MGD	C5'-O5'-PB-O1B
14	B	2905	GOL	O1-C1-C2-C3
7	A	915	PEG	C1-C2-O2-C3
7	A	921	PEG	C4-C3-O2-C2
9	A	912	P33	C18-C17-O16-C15
7	A	914	PEG	C1-C2-O2-C3
10	E	916	PGE	C4-C3-O2-C2
16	C	911	P4G	C3-C4-O3-C5
17	G	910	1PE	C14-C24-OH4-C13
17	G	910	1PE	C16-C26-OH6-C15
7	E	911	PEG	C1-C2-O2-C3
17	C	912	1PE	C13-C23-OH3-C22
7	A	917	PEG	O1-C1-C2-O2
7	F	202	PEG	O1-C1-C2-O2
7	F	202	PEG	C4-C3-O2-C2
7	B	2904	PEG	C1-C2-O2-C3
7	E	913	PEG	C1-C2-O2-C3
7	H	2201	PEG	C4-C3-O2-C2
4	A	903	MGD	C3'-C4'-C5'-O5'
4	E	902	MGD	O4'-C4'-C5'-O5'
4	G	902	MGD	O4'-C4'-C5'-O5'
17	G	910	1PE	OH4-C13-C23-OH3
7	C	919	PEG	C1-C2-O2-C3
17	G	910	1PE	OH5-C14-C24-OH4
17	G	910	1PE	C24-C14-OH5-C25
10	C	917	PGE	O2-C3-C4-O3
10	E	916	PGE	O2-C3-C4-O3
16	C	911	P4G	O3-C5-C6-O4
7	A	910	PEG	C1-C2-O2-C3
10	G	913	PGE	C6-C5-O3-C4
18	C	916	PG0	O1-C3-C4-O2
9	A	912	P33	O7-C8-C9-O10
9	A	912	P33	O4-C5-C6-O7
7	A	908	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	908	PEG	O2-C3-C4-O4
7	A	909	PEG	O1-C1-C2-O2
7	A	914	PEG	O1-C1-C2-O2
7	A	921	PEG	O1-C1-C2-O2
7	B	2901	PEG	O1-C1-C2-O2
7	B	2904	PEG	O1-C1-C2-O2
7	E	907	PEG	O1-C1-C2-O2
7	E	911	PEG	O2-C3-C4-O4
7	E	913	PEG	O1-C1-C2-O2
7	G	908	PEG	O1-C1-C2-O2
7	H	2201	PEG	O1-C1-C2-O2
10	A	916	PGE	O3-C5-C6-O4
10	E	916	PGE	O1-C1-C2-O2
7	A	907	PEG	O2-C3-C4-O4
7	A	910	PEG	O1-C1-C2-O2
7	C	913	PEG	O2-C3-C4-O4
7	C	919	PEG	O1-C1-C2-O2
7	E	909	PEG	O1-C1-C2-O2
7	G	908	PEG	O2-C3-C4-O4
7	G	911	PEG	O1-C1-C2-O2
10	C	917	PGE	O1-C1-C2-O2
14	B	2905	GOL	C1-C2-C3-O3
7	B	2904	PEG	O2-C3-C4-O4
7	E	910	PEG	O1-C1-C2-O2
10	C	917	PGE	O3-C5-C6-O4
14	B	2905	GOL	O1-C1-C2-O2
4	G	902	MGD	C3'-C4'-C5'-O5'
7	G	907	PEG	O2-C3-C4-O4
6	A	905	EDO	O1-C1-C2-O2
6	E	905	EDO	O1-C1-C2-O2
6	G	906	EDO	O1-C1-C2-O2
6	G	914	EDO	O1-C1-C2-O2
9	A	912	P33	O10-C11-C12-O13
7	C	909	PEG	O1-C1-C2-O2
4	E	902	MGD	C3'-C4'-C5'-O5'
17	C	912	1PE	C14-C24-OH4-C13
17	C	912	1PE	OH6-C15-C25-OH5
7	C	909	PEG	O2-C3-C4-O4
7	E	911	PEG	O1-C1-C2-O2
10	G	913	PGE	O3-C5-C6-O4
16	C	911	P4G	O2-C3-C4-O3
17	C	912	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
7	C	914	PEG	O1-C1-C2-O2
6	C	915	EDO	O1-C1-C2-O2
9	A	912	P33	O16-C17-C18-O19
10	G	913	PGE	O1-C1-C2-O2
16	C	911	P4G	C1-C2-O2-C3
7	B	2906	PEG	O2-C3-C4-O4
6	A	919	EDO	O1-C1-C2-O2
6	C	906	EDO	O1-C1-C2-O2
6	C	910	EDO	O1-C1-C2-O2
10	A	916	PGE	O2-C3-C4-O3
4	A	903	MGD	PA-O3B-PB-O5'
4	E	901	MGD	PA-O3B-PB-O5'
4	E	902	MGD	PA-O3B-PB-O5'
4	G	901	MGD	PA-O3B-PB-O5'
7	G	908	PEG	C4-C3-O2-C2
7	E	912	PEG	C4-C3-O2-C2
7	E	910	PEG	C4-C3-O2-C2
10	E	916	PGE	C6-C5-O3-C4
17	C	912	1PE	C25-C15-OH6-C26
10	C	917	PGE	C3-C4-O3-C5
7	E	907	PEG	C1-C2-O2-C3
7	C	909	PEG	C1-C2-O2-C3
7	E	910	PEG	C1-C2-O2-C3
7	E	913	PEG	C4-C3-O2-C2
7	G	911	PEG	C1-C2-O2-C3
7	B	2904	PEG	C4-C3-O2-C2
10	A	918	PGE	C6-C5-O3-C4
4	A	902	MGD	C5'-O5'-PB-O2B
4	C	902	MGD	C5'-O5'-PB-O2B
4	G	901	MGD	C5'-O5'-PB-O2B
7	B	2901	PEG	O2-C3-C4-O4
7	E	912	PEG	O1-C1-C2-O2
7	G	907	PEG	C1-C2-O2-C3
10	A	918	PGE	C3-C4-O3-C5
7	B	2906	PEG	C1-C2-O2-C3
9	A	912	P33	C5-C6-O7-C8
10	A	916	PGE	C3-C4-O3-C5
17	G	910	1PE	C13-C23-OH3-C22
17	C	912	1PE	C16-C26-OH6-C15
10	A	916	PGE	O1-C1-C2-O2
7	G	911	PEG	C4-C3-O2-C2
10	A	918	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	C	907	EDO	O1-C1-C2-O2
6	E	906	EDO	O1-C1-C2-O2
6	E	915	EDO	O1-C1-C2-O2
17	C	912	1PE	C23-C13-OH4-C24
7	E	912	PEG	C1-C2-O2-C3
10	E	916	PGE	C3-C4-O3-C5
14	B	2905	GOL	O2-C2-C3-O3
10	A	918	PGE	O2-C3-C4-O3
10	C	917	PGE	C4-C3-O2-C2
7	A	909	PEG	C1-C2-O2-C3
4	C	904	MGD	O4'-C4'-C5'-O5'
18	C	916	PG0	C4-C3-O1-C2
7	A	909	PEG	O2-C3-C4-O4
6	A	906	EDO	O1-C1-C2-O2
7	C	913	PEG	C4-C3-O2-C2
7	E	911	PEG	C4-C3-O2-C2
16	C	911	P4G	C5-C6-O4-C7
4	C	902	MGD	PB-O3B-PA-O1A
7	B	2906	PEG	O1-C1-C2-O2
7	A	917	PEG	O2-C3-C4-O4
17	C	912	1PE	OH5-C14-C24-OH4
16	C	911	P4G	C6-C5-O3-C4
4	C	904	MGD	C5'-O5'-PB-O3B
9	A	912	P33	C12-C11-O10-C9
9	A	912	P33	O13-C14-C15-O16
4	A	903	MGD	PB-O3B-PA-O2A
7	E	907	PEG	O2-C3-C4-O4
17	G	910	1PE	C12-C22-OH3-C23
4	E	901	MGD	C5'-O5'-PB-O2B
7	C	913	PEG	O1-C1-C2-O2
7	G	907	PEG	O1-C1-C2-O2
7	A	908	PEG	C4-C3-O2-C2
7	E	910	PEG	O2-C3-C4-O4

There are no ring outliers.

47 monomers are involved in 173 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	909	PEG	2	0
18	C	916	PG0	5	0
10	G	913	PGE	9	0
4	E	902	MGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	917	PEG	4	0
14	B	2903	GOL	1	0
7	A	914	PEG	9	0
6	E	914	EDO	1	0
8	G	909	SBO	1	0
6	E	905	EDO	1	0
7	E	910	PEG	1	0
7	G	911	PEG	2	0
7	G	907	PEG	1	0
7	E	907	PEG	4	0
10	C	917	PGE	1	0
7	C	919	PEG	3	0
16	C	911	P4G	21	0
4	C	904	MGD	2	0
9	A	912	P33	6	0
7	A	908	PEG	1	0
4	A	903	MGD	2	0
7	E	911	PEG	3	0
7	H	2201	PEG	4	0
7	E	909	PEG	4	0
17	G	910	1PE	12	0
8	C	918	SBO	1	0
10	A	918	PGE	6	0
7	A	909	PEG	7	0
4	G	902	MGD	2	0
7	C	913	PEG	3	0
7	C	914	PEG	4	0
7	G	908	PEG	5	0
14	B	2905	GOL	3	0
6	G	905	EDO	1	0
7	B	2901	PEG	3	0
17	C	912	1PE	8	0
7	G	912	PEG	4	0
7	A	913	PEG	1	0
6	E	906	EDO	2	0
8	E	917	SBO	1	0
7	A	915	PEG	4	0
7	B	2906	PEG	14	0
7	E	913	PEG	2	0
10	E	916	PGE	3	0
6	A	919	EDO	1	0
6	G	914	EDO	1	0

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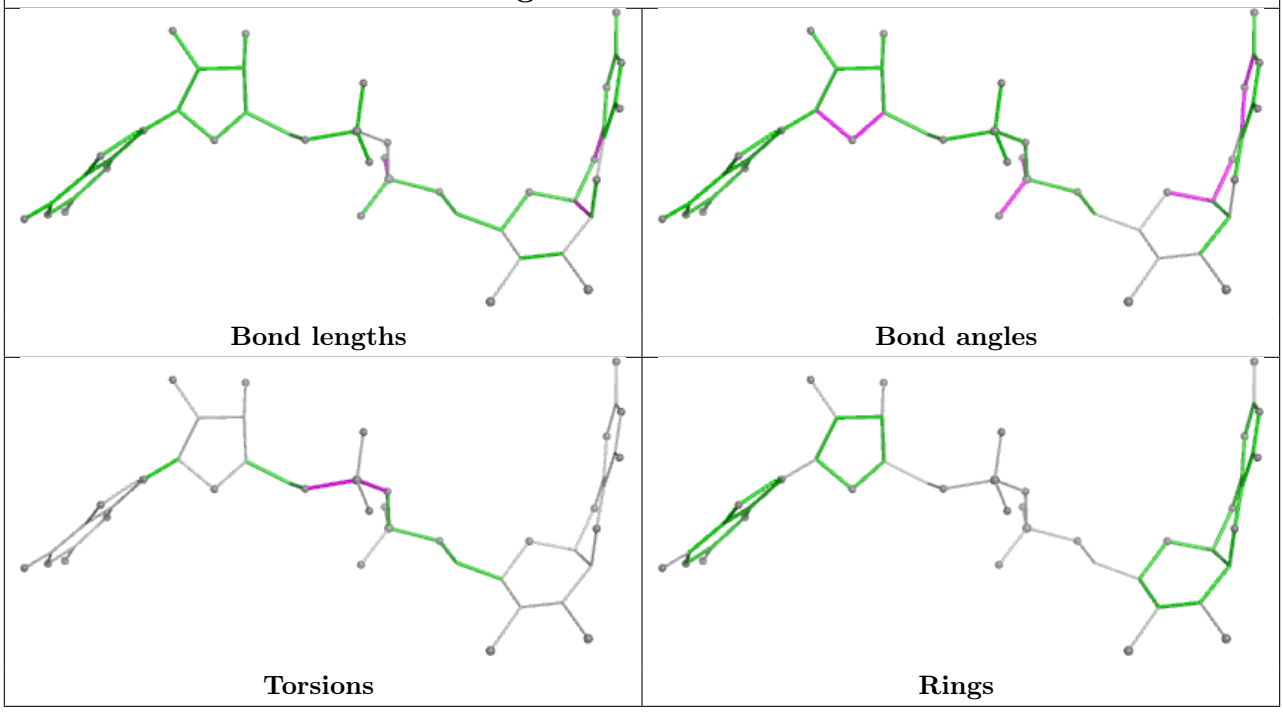
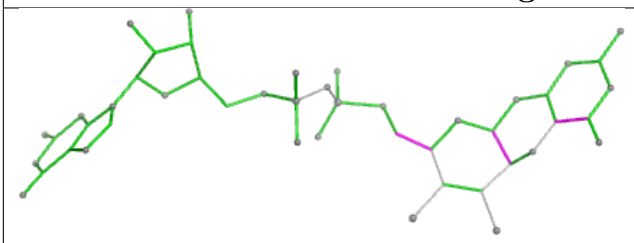
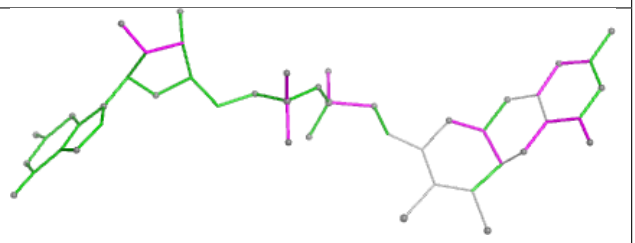
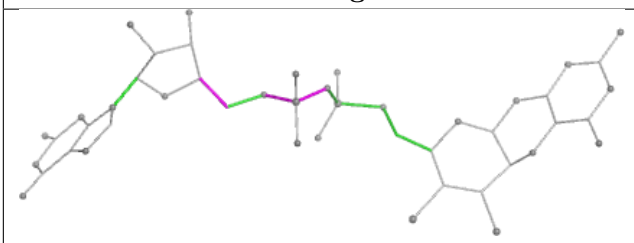
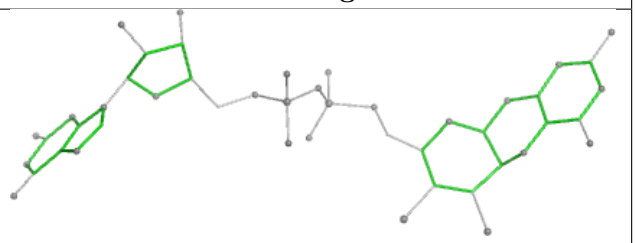
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	916	PGE	1	0

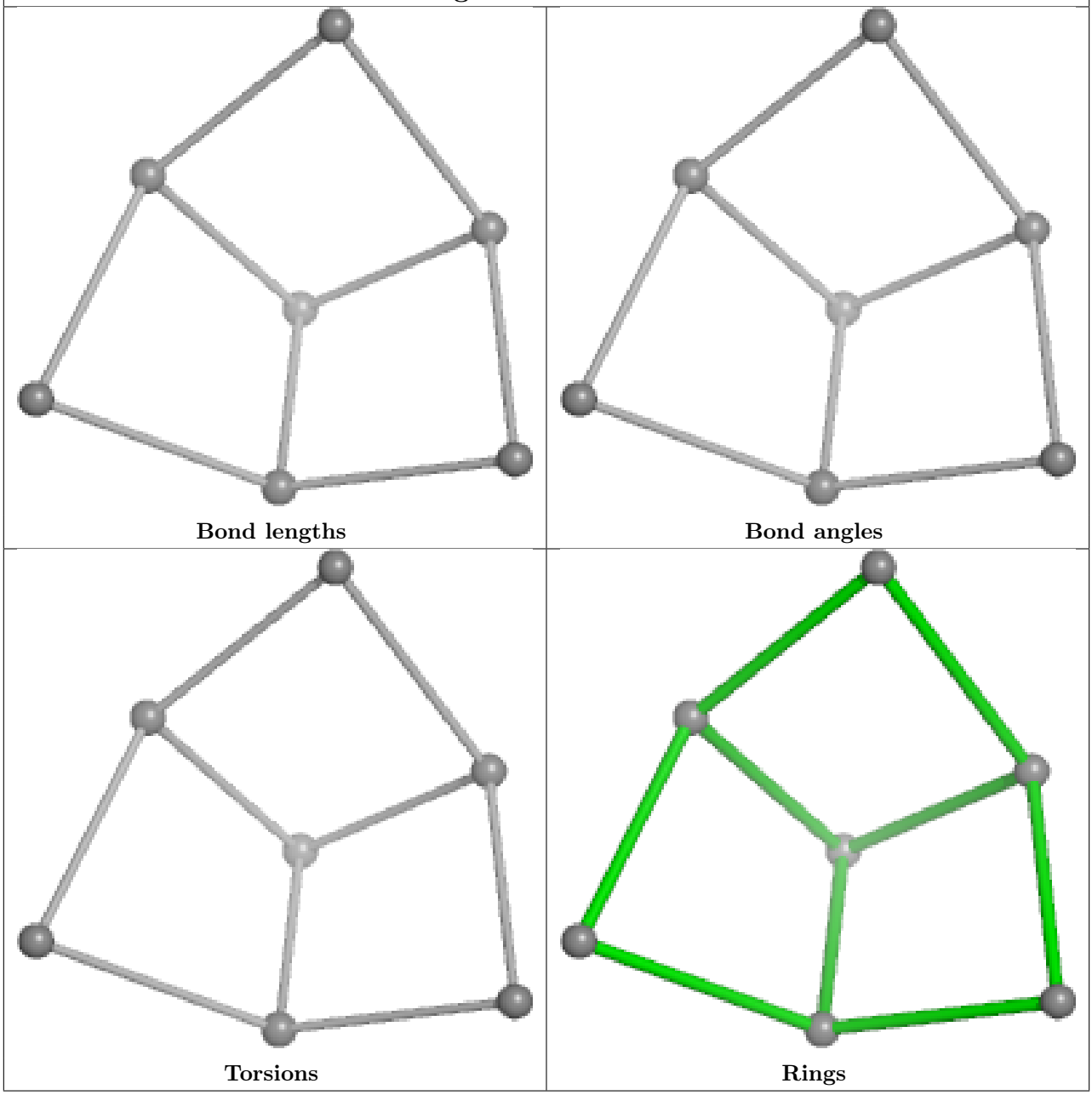
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 MGD G 901

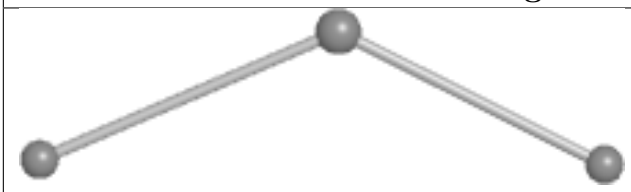


Ligand MGD E 902	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

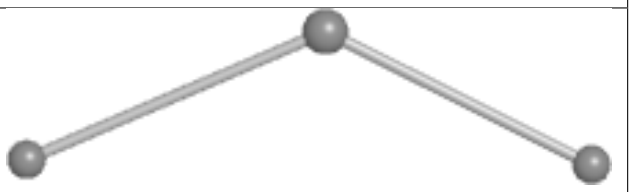
Ligand F3S E 904



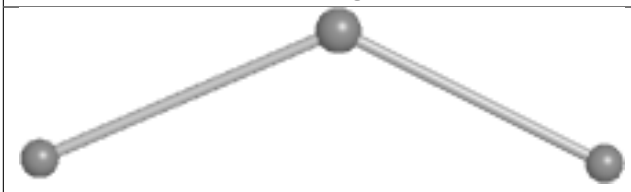
Ligand SBO G 909



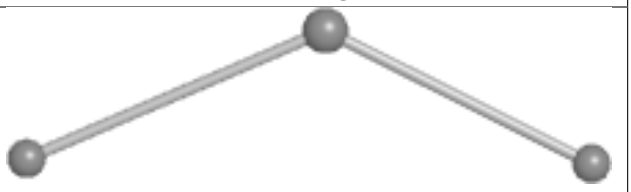
Bond lengths



Bond angles

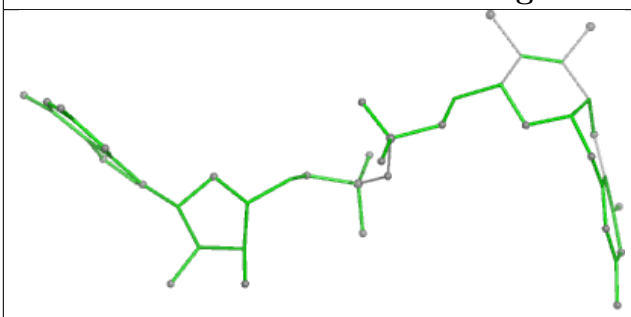


Torsions



Rings

Ligand MGD A 902



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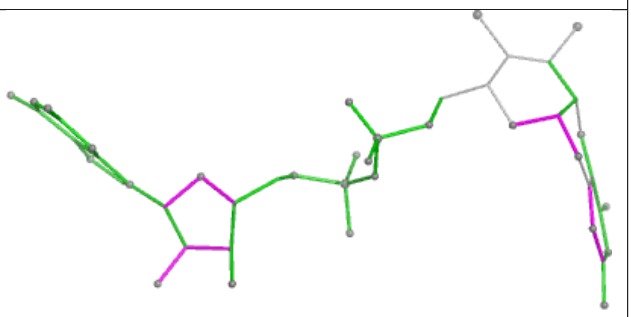

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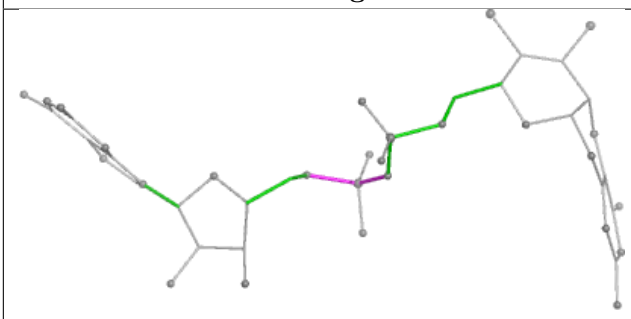

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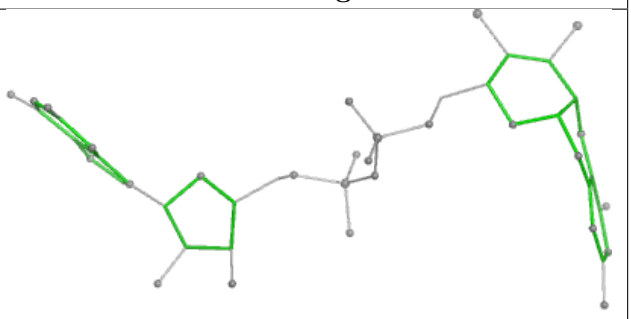
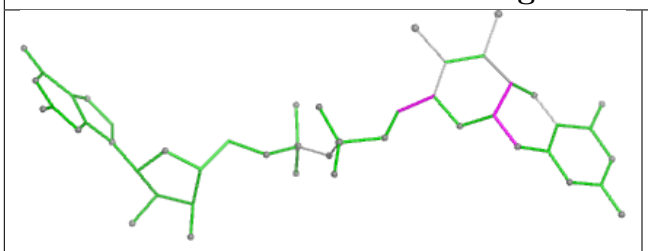


Rings

Ligand MGD C 904



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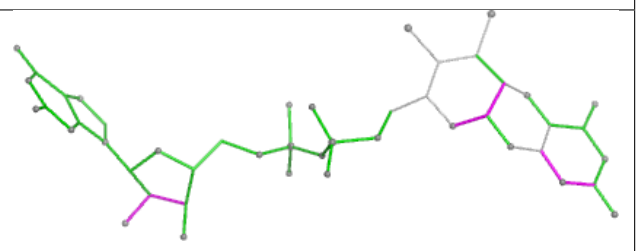
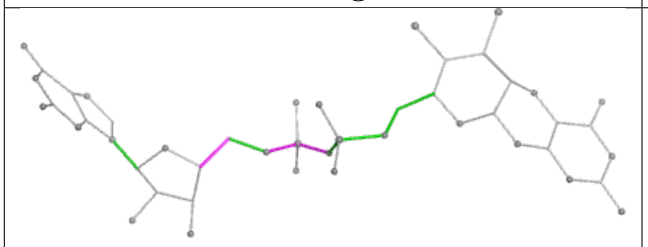


Bond angles



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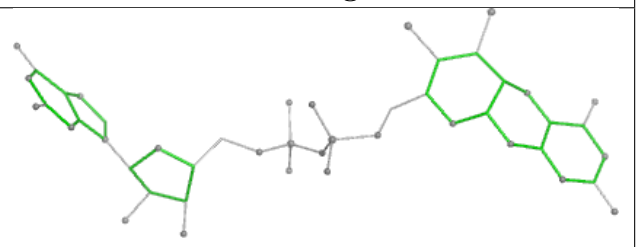
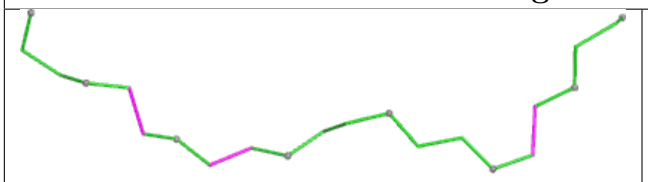


Rings

Ligand P33 A 912



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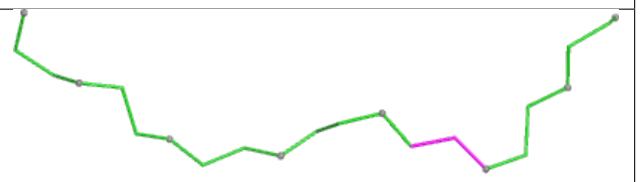

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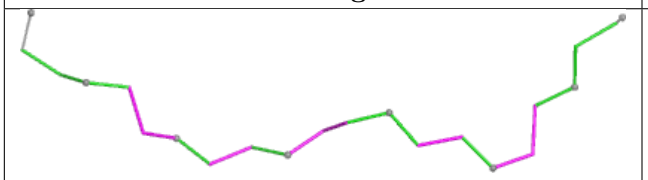

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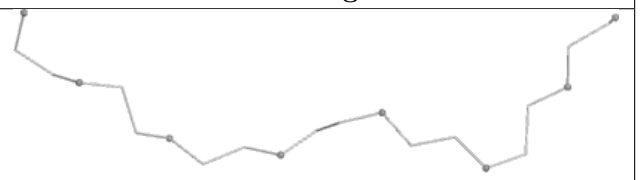
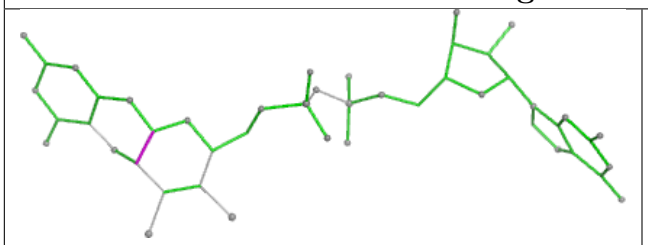


Rings

Ligand MGD A 903



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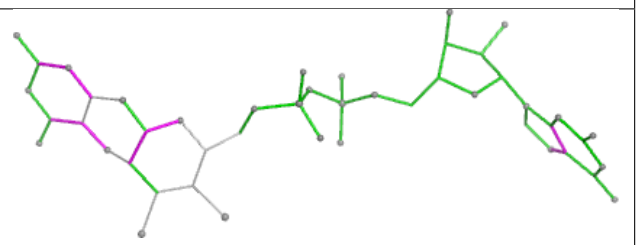

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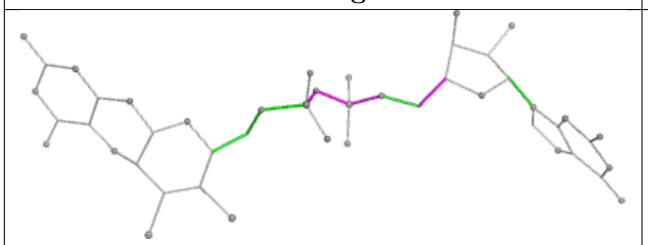

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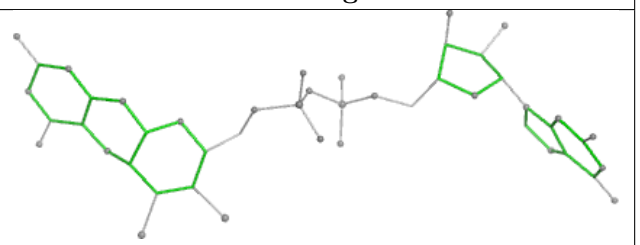
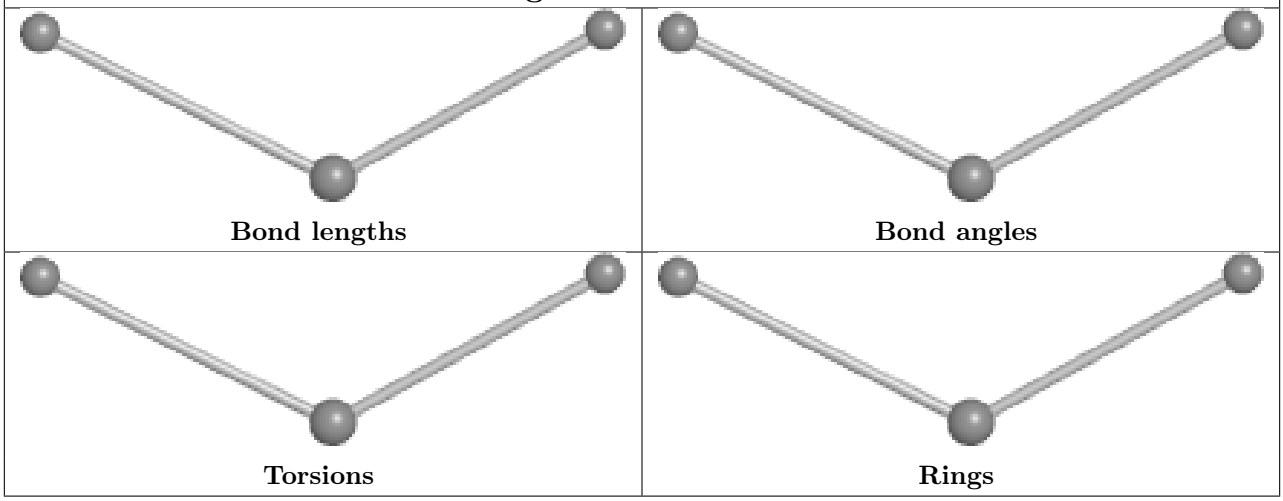
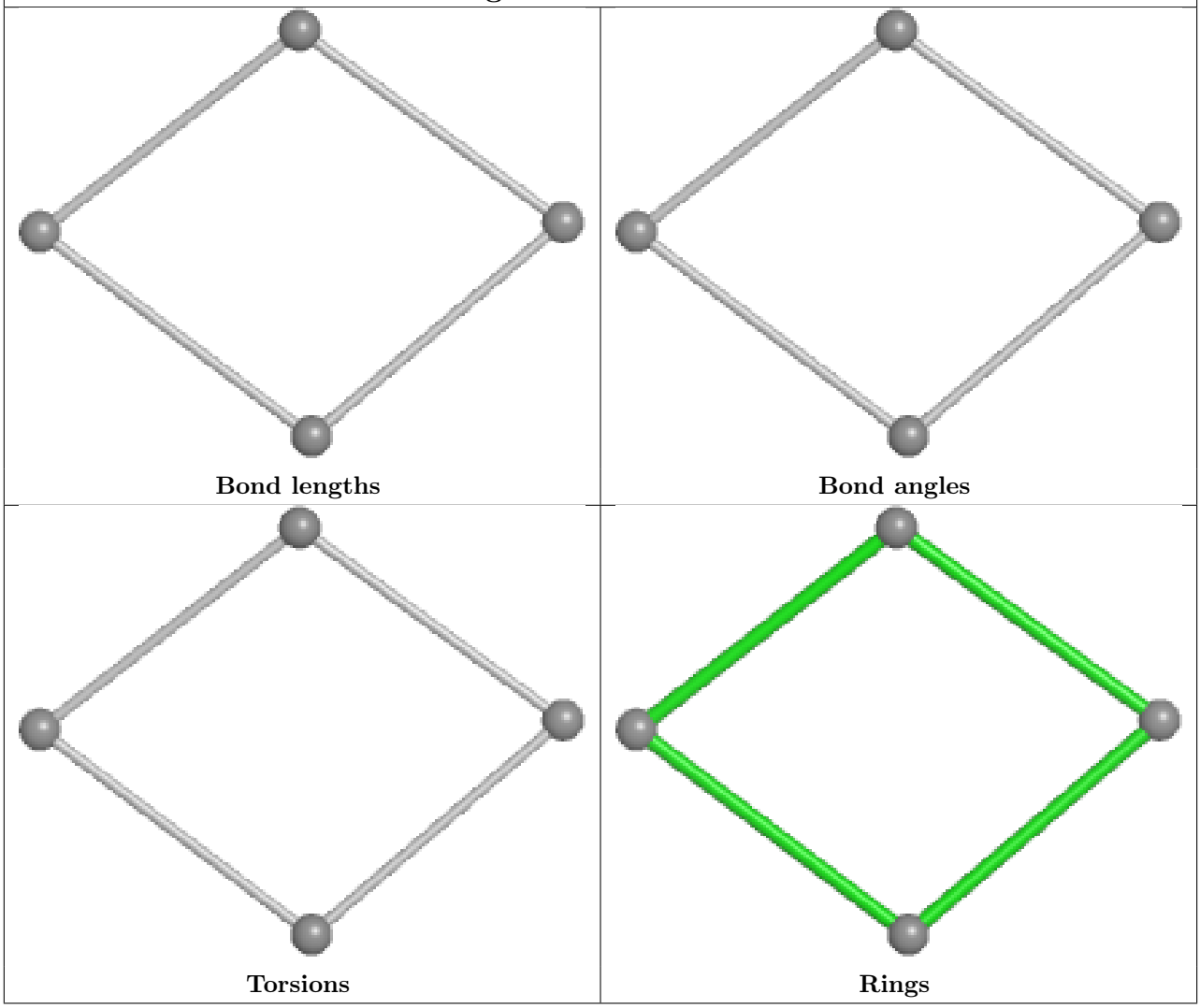


Rings

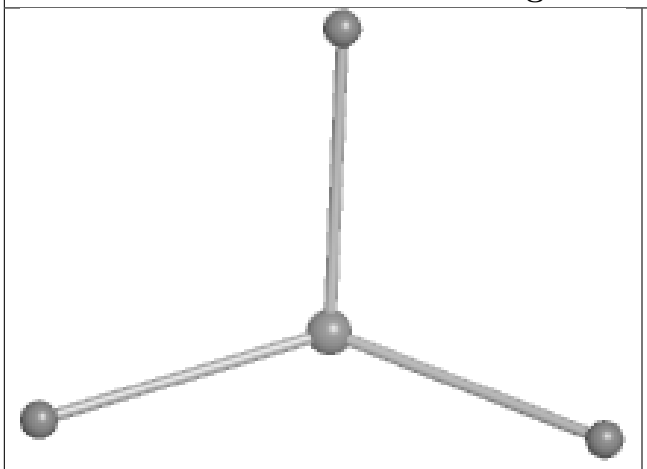
Ligand SBO A 911



Ligand FES H 2202



Ligand SBO C 918



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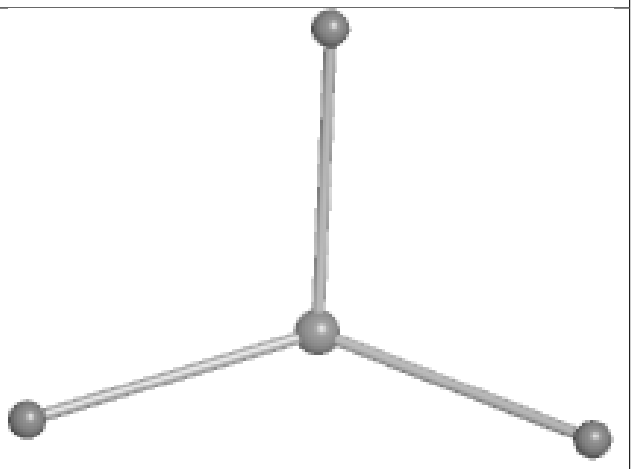
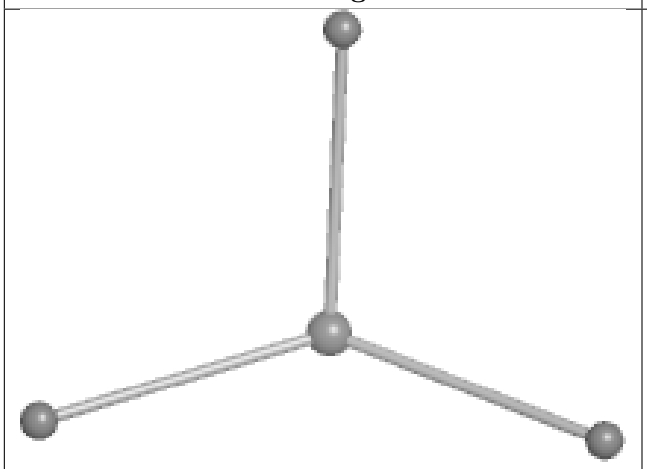


Bond angles



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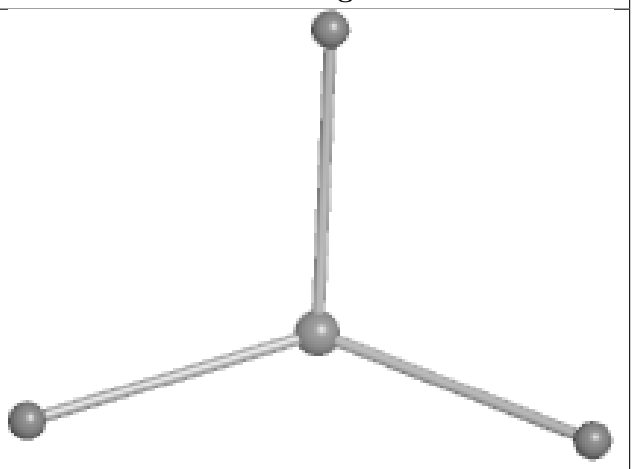
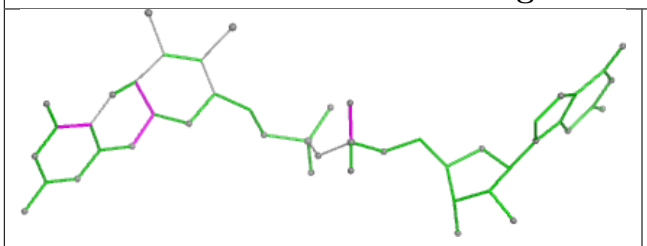


Rings

Ligand MGD G 902



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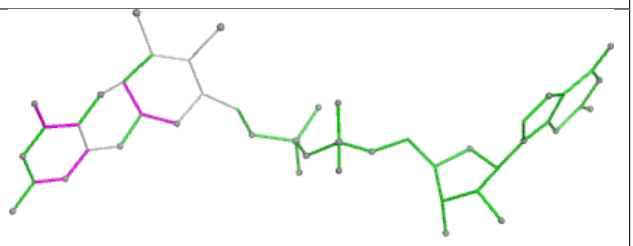

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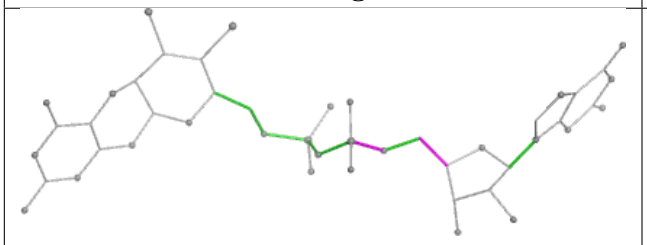

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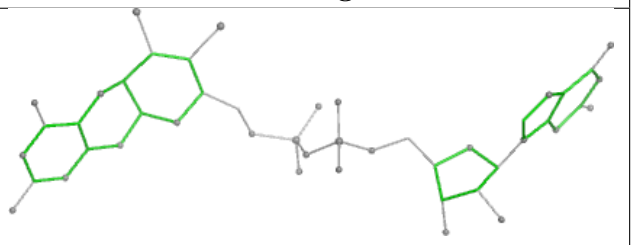
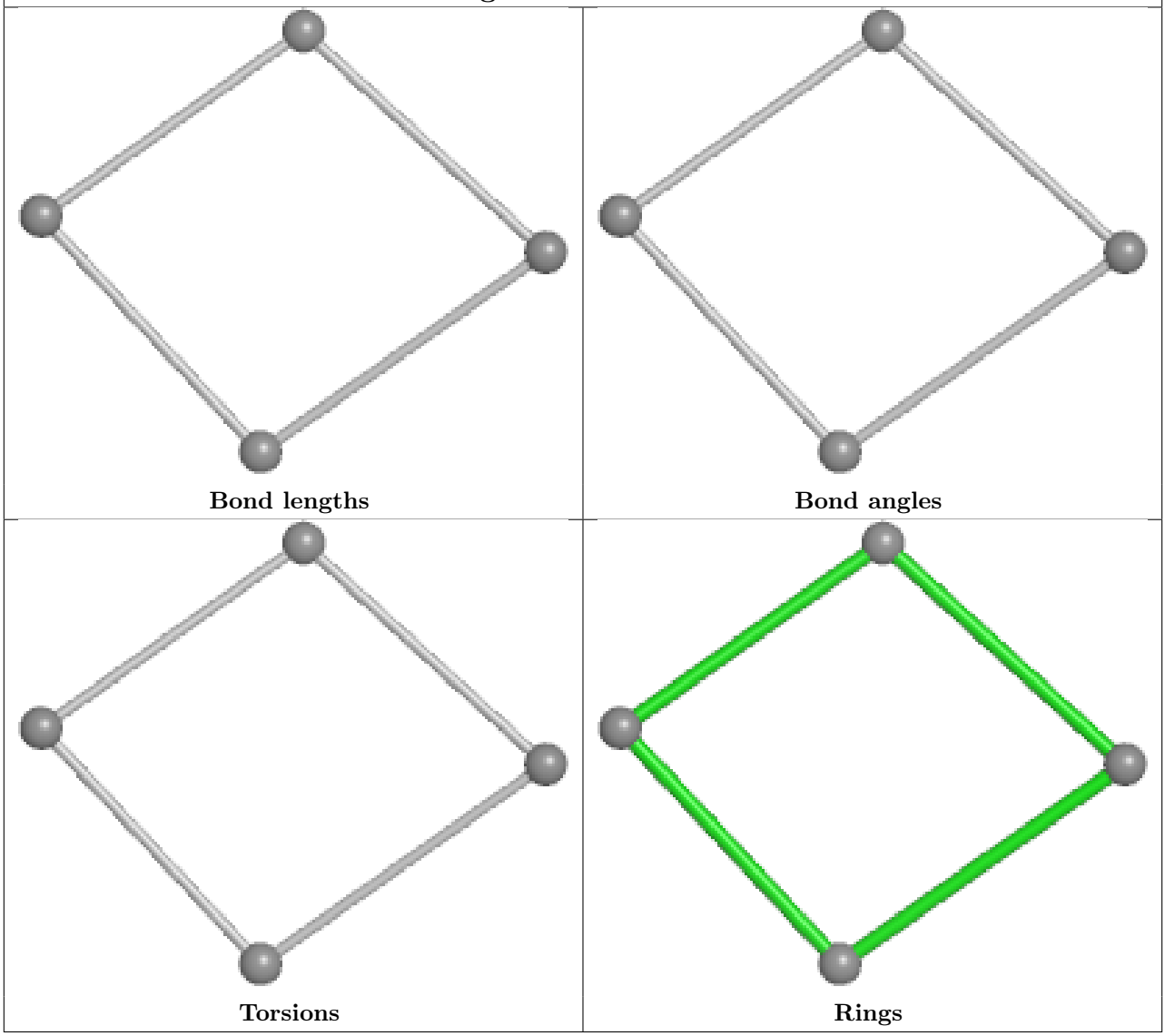


Rings

Ligand FES D 201



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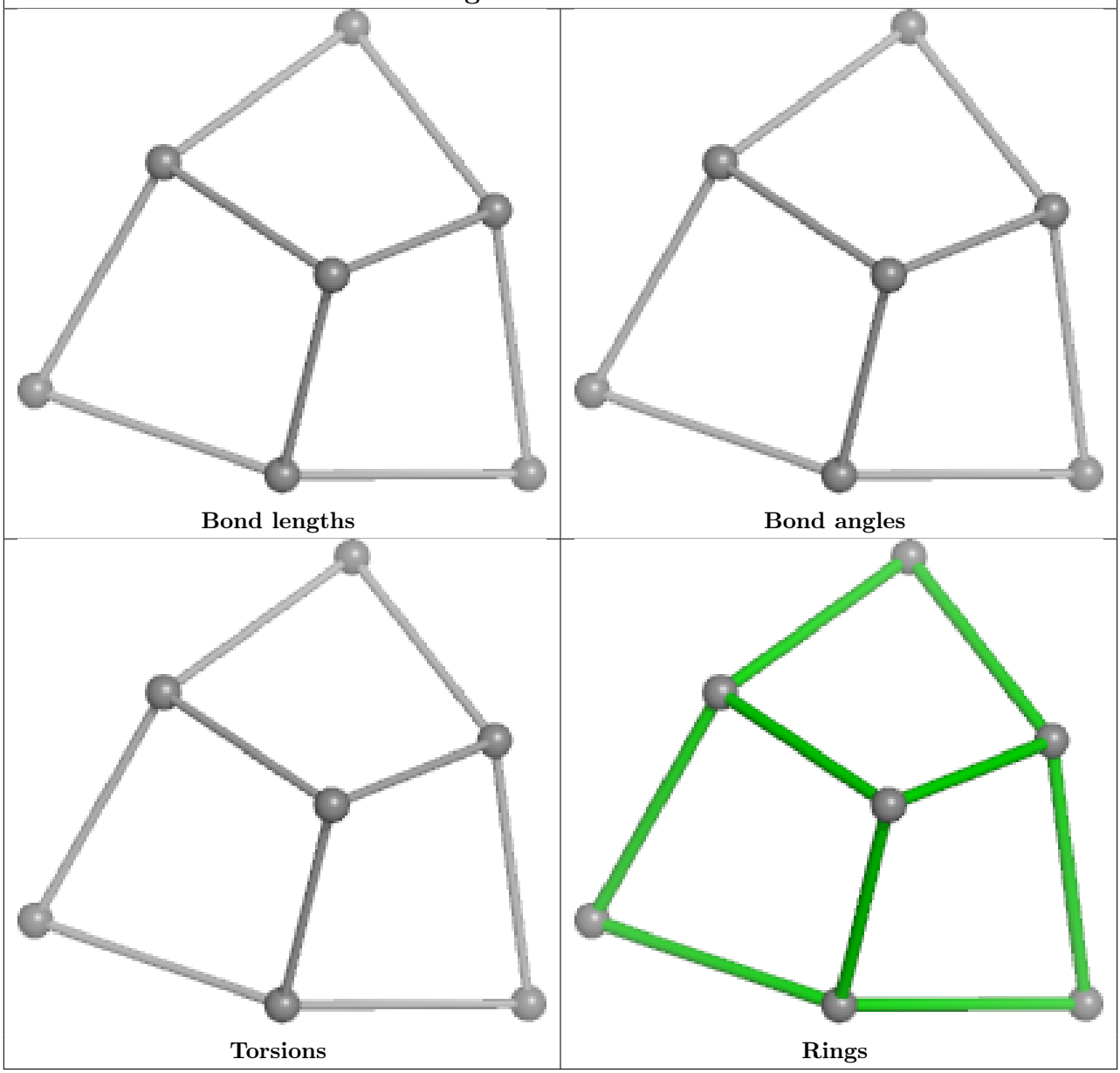

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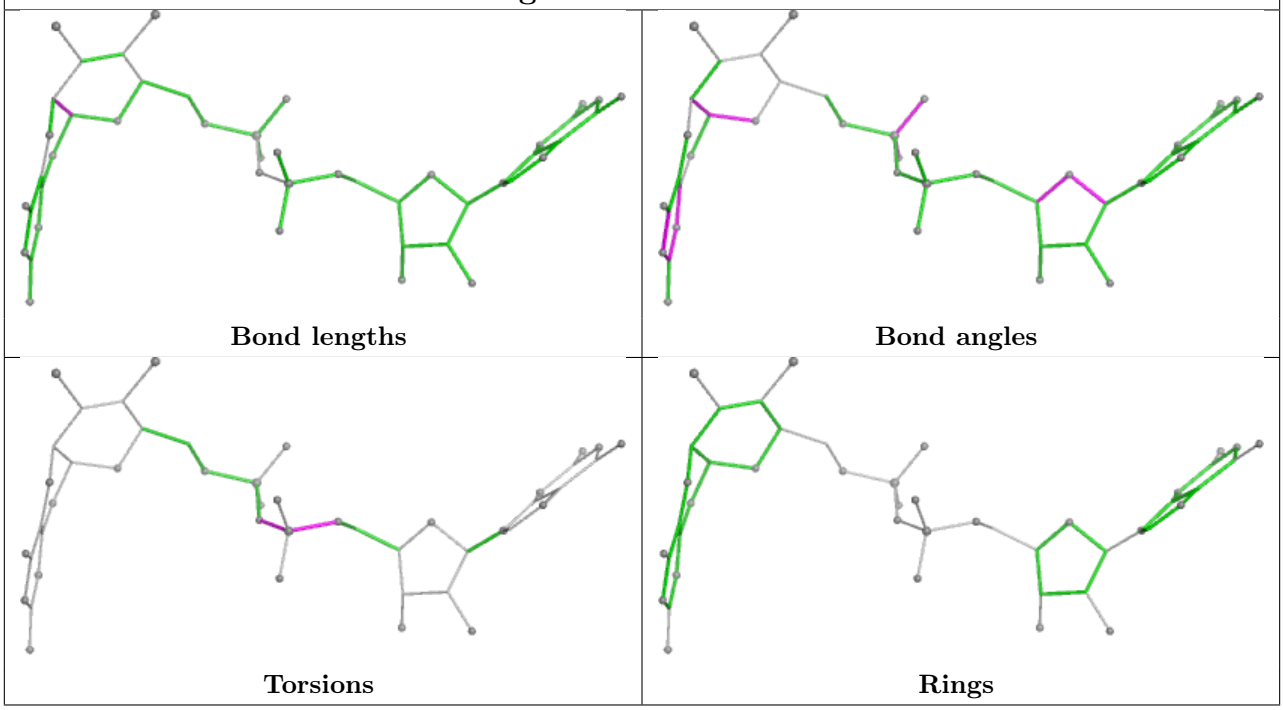
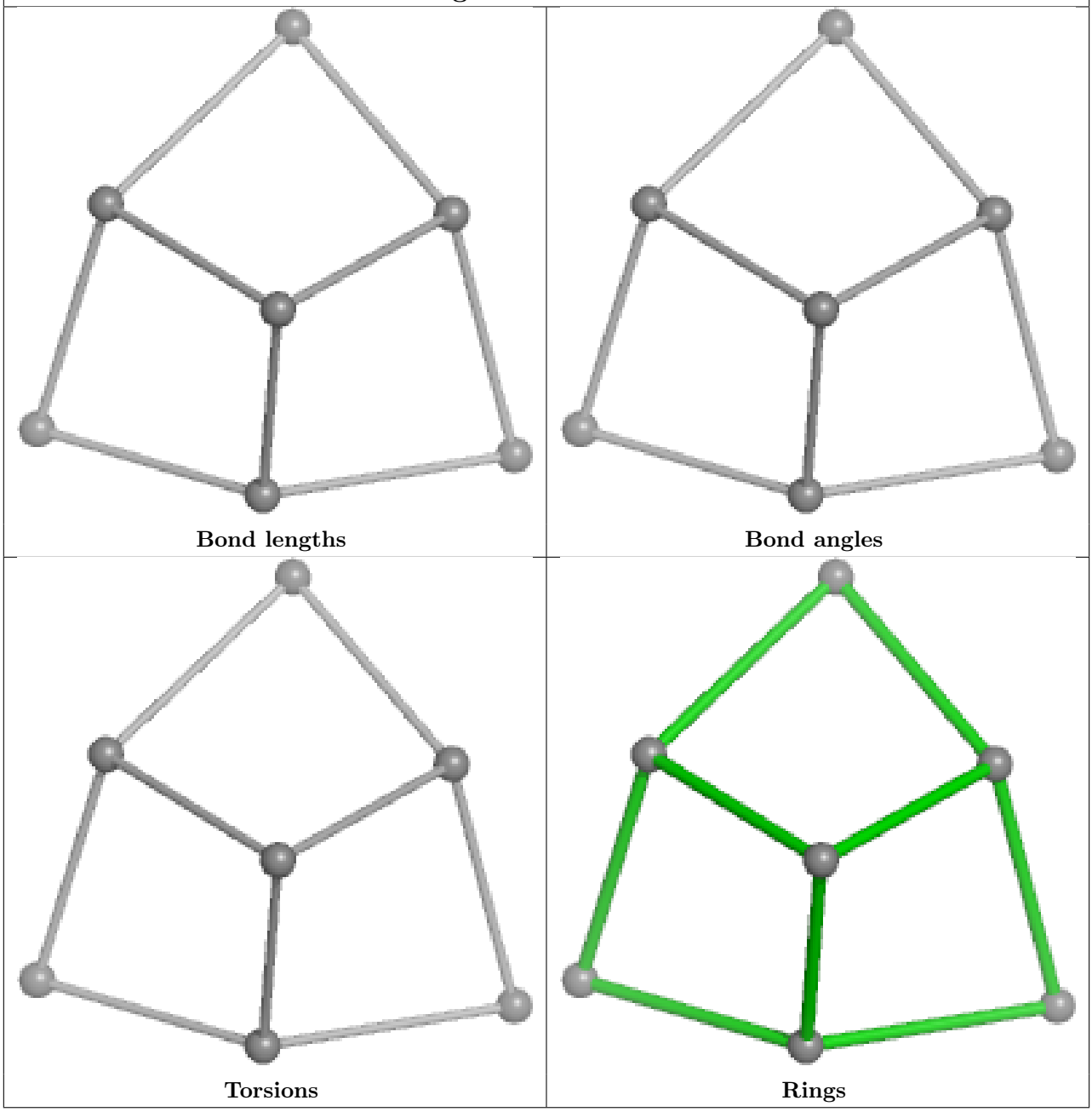
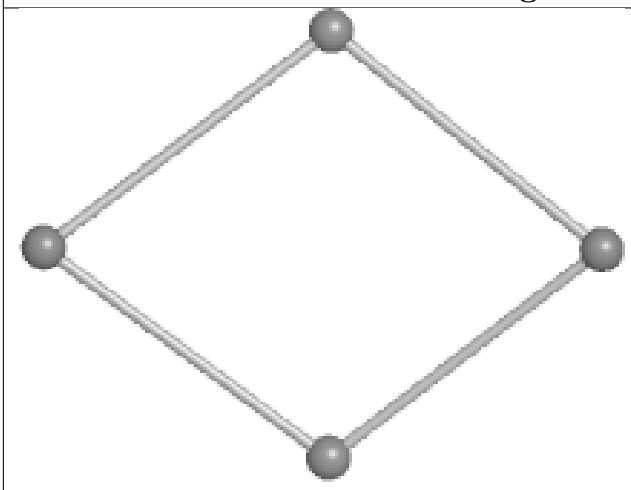


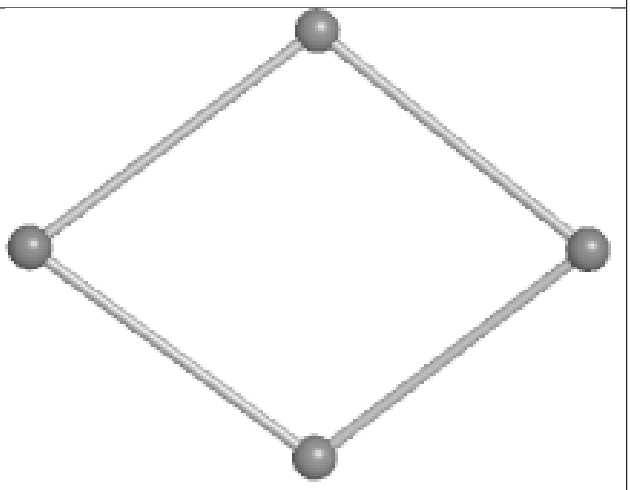
Ligand F3S A 904



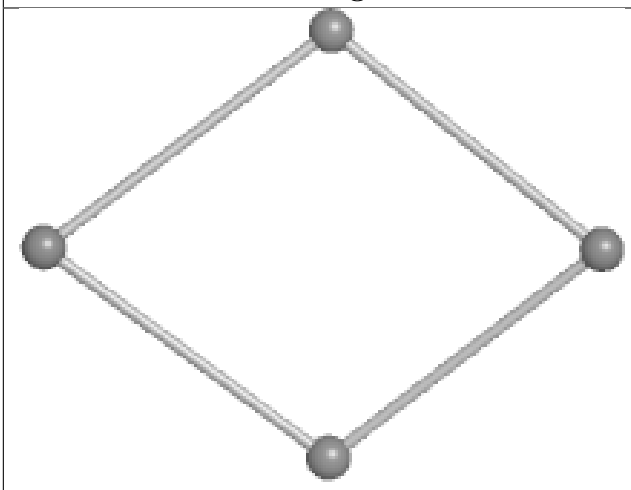
Ligand FES B 2902



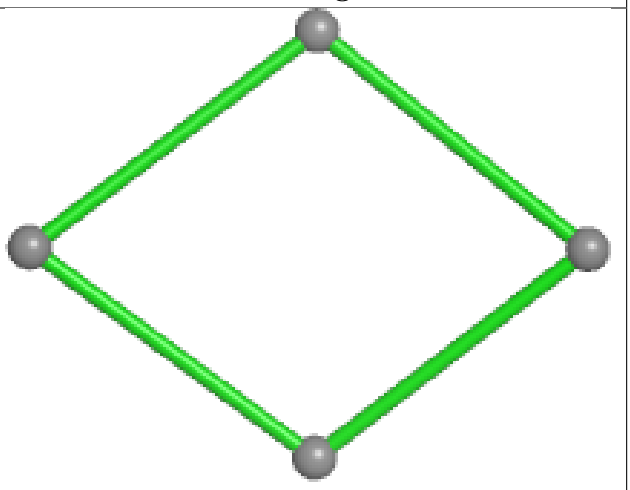
Bond lengths



Bond angles

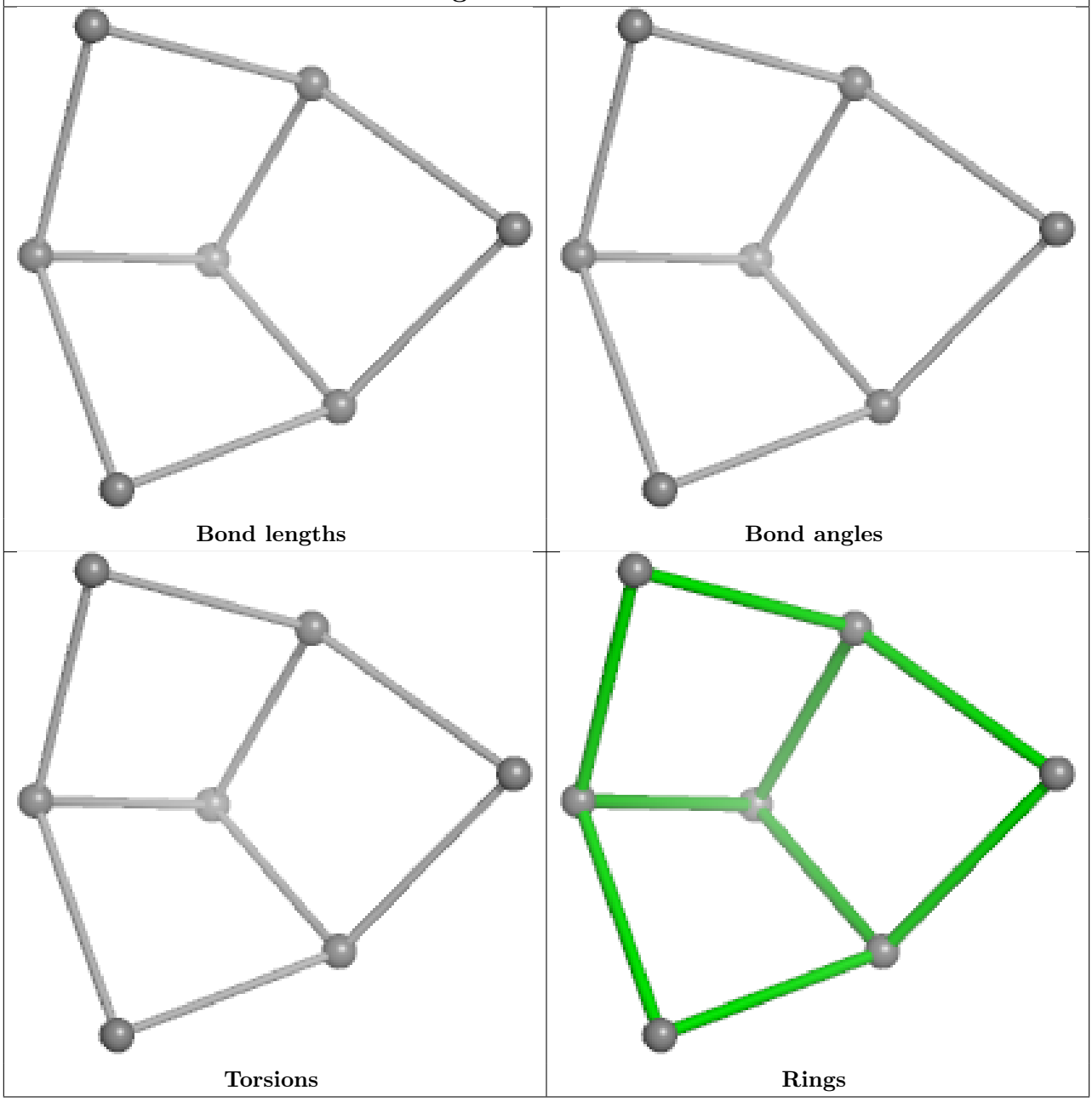


Torsions

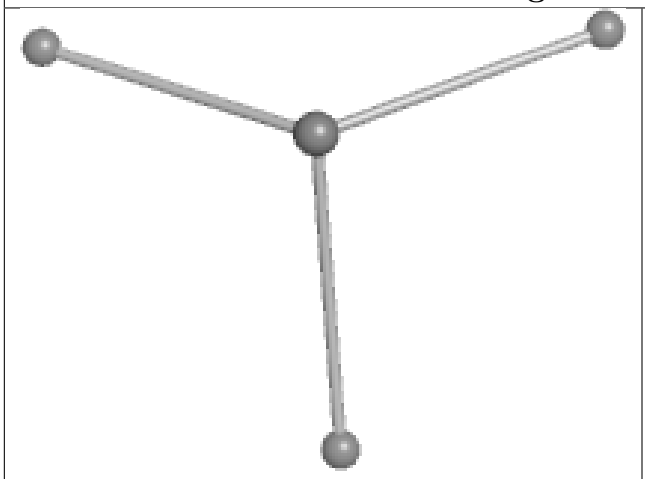


Rings

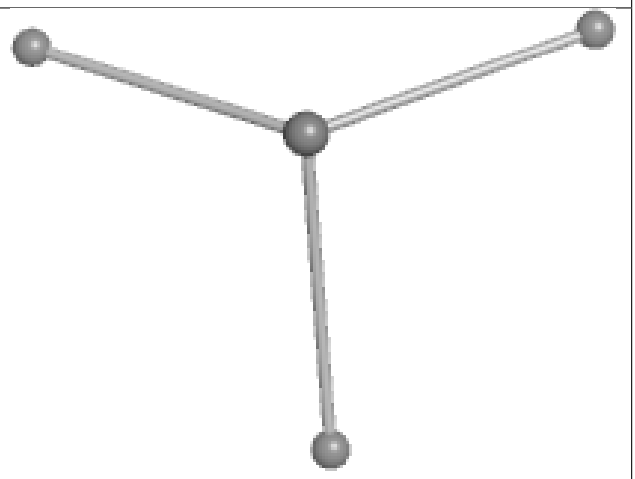
Ligand F3S G 903



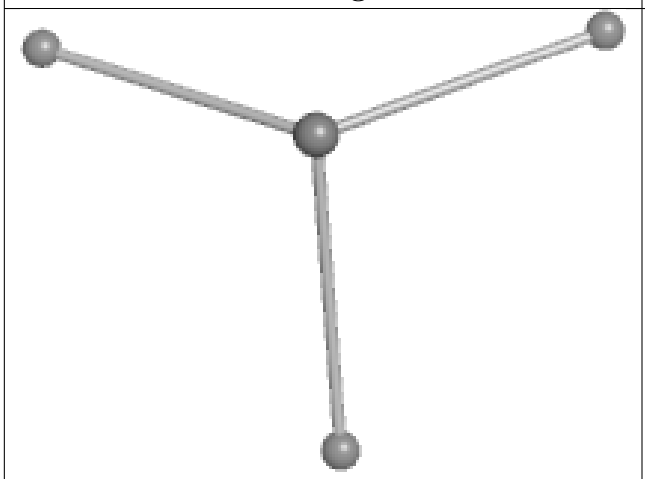
Ligand SBO E 917



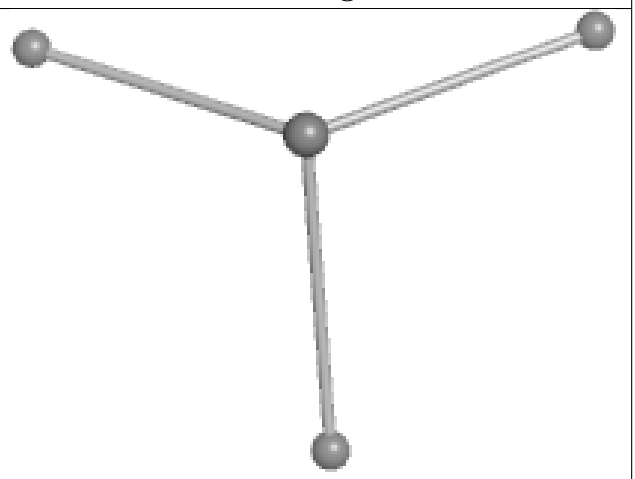
Bond lengths



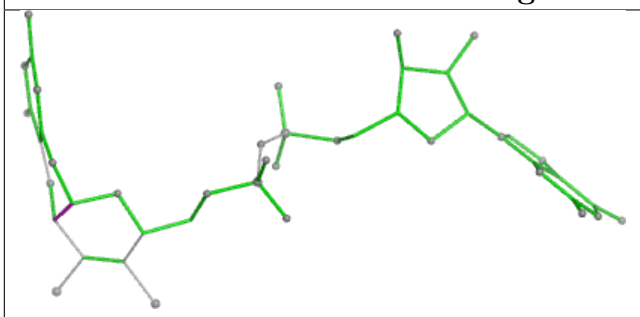
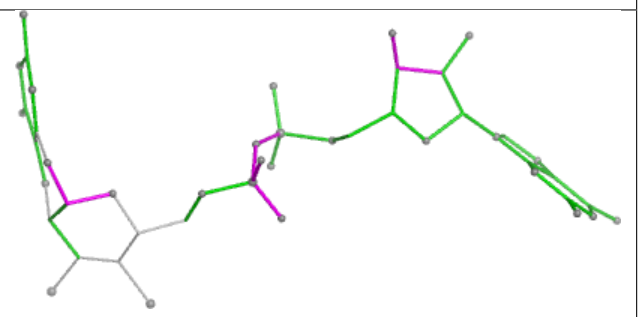
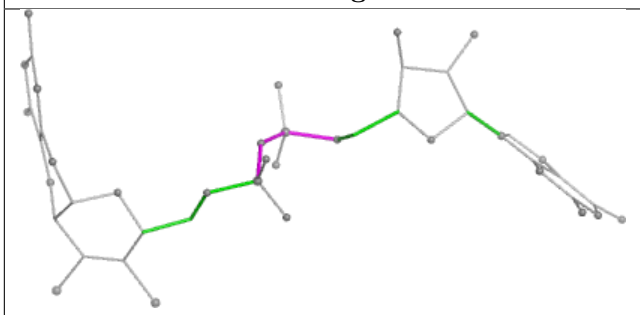
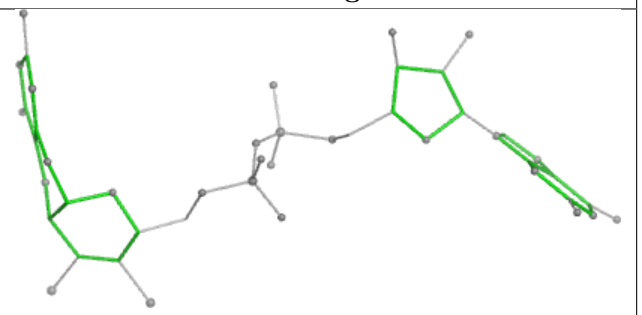
Bond angles



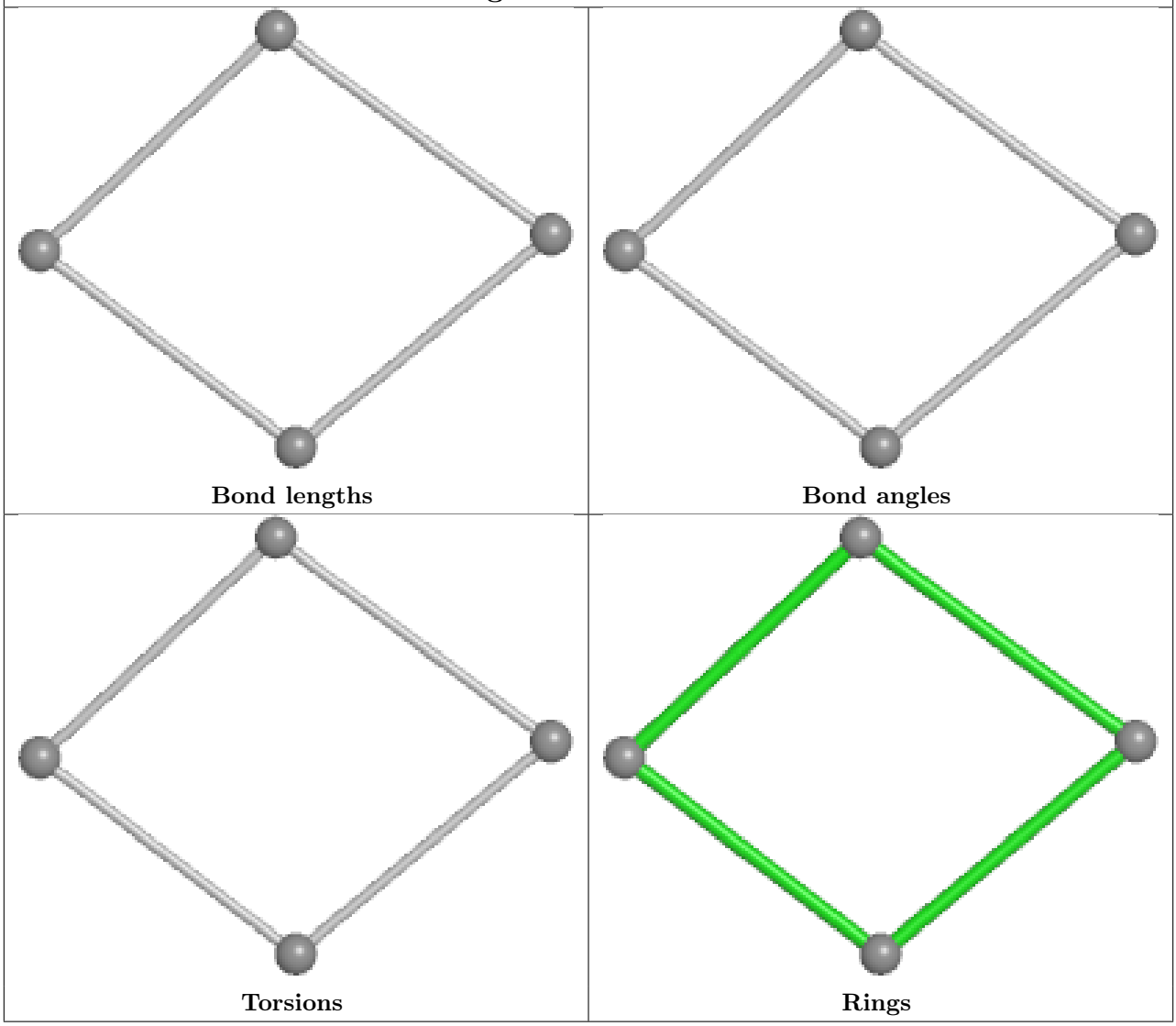
Torsions



Rings

Ligand MGD C 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES F 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	824/824 (100%)	-0.09	14 (1%)	69	74	11, 19, 34, 70	3 (0%)
1	C	824/824 (100%)	-0.15	6 (0%)	84	88	10, 18, 33, 57	3 (0%)
1	E	824/824 (100%)	-0.05	13 (1%)	70	75	10, 19, 34, 62	2 (0%)
1	G	824/824 (100%)	-0.13	8 (0%)	79	83	10, 18, 33, 62	2 (0%)
2	B	135/135 (100%)	-0.01	2 (1%)	72	77	12, 19, 30, 52	0
2	D	135/135 (100%)	0.01	2 (1%)	72	77	12, 19, 31, 56	0
2	F	135/135 (100%)	0.07	2 (1%)	72	77	13, 19, 33, 68	0
2	H	135/135 (100%)	-0.01	1 (0%)	84	88	12, 19, 32, 55	0
All	All	3836/3836 (100%)	-0.09	48 (1%)	75	80	10, 18, 34, 70	10 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	-1	ALA	6.0
1	G	2	ALA	5.7
1	E	2	ALA	5.6
1	C	2	ALA	5.6
1	A	2	ALA	5.5
2	F	0	GLY	4.8
2	B	-1	ALA	4.7
2	D	0	GLY	4.6
1	A	487	ALA	4.5
1	G	487	ALA	4.4
2	D	-1	ALA	4.3
1	A	38[A]	LEU	4.0
1	G	3	PRO	3.7
1	A	613	GLY	3.6
1	C	3	PRO	3.6
1	E	487	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	486	LYS	3.4
2	H	-1	ALA	3.2
1	E	580	LYS	3.1
1	G	485	GLN	3.1
1	A	3	PRO	3.1
1	G	646	VAL	3.0
1	E	613	GLY	2.9
1	A	612	PRO	2.9
1	E	3	PRO	2.8
1	C	485	GLN	2.6
1	E	486	LYS	2.6
1	G	580	LYS	2.6
1	A	157	GLN	2.5
1	A	486	LYS	2.5
1	G	582	GLY	2.5
1	E	588	ALA	2.5
1	C	487	ALA	2.5
1	A	582	GLY	2.4
1	E	436	LYS	2.4
1	A	669	ASP	2.4
1	A	485	GLN	2.4
1	E	669	ASP	2.3
1	A	584	ALA	2.3
1	E	485	GLN	2.3
1	C	663	GLU	2.2
1	A	482	GLN	2.2
2	B	0	GLY	2.2
1	C	580	LYS	2.2
1	A	4	ASN	2.1
1	E	612	PRO	2.1
1	E	663	GLU	2.1
1	E	584	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	PGE	C	917	10/10	0.66	0.29	22,38,42,45	0
10	PGE	E	916	10/10	0.67	0.25	24,37,42,44	0
7	PEG	G	907	7/7	0.72	0.23	37,45,54,59	0
7	PEG	E	907	7/7	0.73	0.26	45,55,63,67	0
7	PEG	A	907	7/7	0.75	0.20	32,37,42,43	0
7	PEG	H	2201	7/7	0.75	0.18	33,38,42,44	0
6	EDO	C	915	4/4	0.76	0.15	26,34,34,38	0
6	EDO	E	915	4/4	0.76	0.19	34,34,40,41	0
17	1PE	C	912	16/16	0.76	0.19	31,38,44,46	0
7	PEG	A	915	7/7	0.77	0.21	32,39,41,51	0
9	P33	A	912	22/22	0.78	0.20	29,41,50,74	0
7	PEG	C	909	7/7	0.78	0.18	37,40,49,53	0
10	PGE	A	918	10/10	0.79	0.21	27,44,51,52	0
6	EDO	A	919	4/4	0.79	0.18	31,36,37,43	0
10	PGE	A	916	10/10	0.80	0.22	27,35,47,65	0
7	PEG	E	913	7/7	0.80	0.17	23,33,38,42	0
7	PEG	A	917	7/7	0.80	0.17	31,37,51,52	0
7	PEG	A	921	7/7	0.80	0.18	16,24,41,42	0
7	PEG	E	909	7/7	0.80	0.19	43,51,56,62	0
7	PEG	G	912	7/7	0.81	0.19	29,38,46,52	0
10	PGE	G	913	10/10	0.82	0.20	21,33,41,45	0
17	1PE	G	910	16/16	0.82	0.20	31,44,56,69	0
7	PEG	F	202	7/7	0.83	0.19	41,44,50,52	0
6	EDO	G	914	4/4	0.83	0.17	33,41,44,48	0
7	PEG	G	908	7/7	0.83	0.15	39,45,48,49	0
7	PEG	G	911	7/7	0.83	0.19	37,46,60,62	0
6	EDO	C	910	4/4	0.83	0.16	42,45,48,50	0
16	P4G	C	911	11/11	0.83	0.15	30,36,41,44	0
7	PEG	E	910	7/7	0.83	0.15	26,36,45,45	0
7	PEG	C	913	7/7	0.83	0.18	24,41,47,50	0
18	PG0	C	916	8/8	0.83	0.18	26,39,46,51	0
7	PEG	A	909	7/7	0.84	0.14	36,41,48,50	0
6	EDO	E	905	4/4	0.84	0.23	41,42,48,49	0
14	GOL	B	2903	6/6	0.84	0.14	31,41,41,51	0
14	GOL	E	908	6/6	0.84	0.13	36,41,44,46	0
7	PEG	A	910	7/7	0.85	0.17	24,31,45,47	0
7	PEG	E	912	7/7	0.85	0.17	35,44,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	B	2904	7/7	0.85	0.16	31,50,59,66	0
7	PEG	B	2901	7/7	0.86	0.15	20,36,39,42	0
6	EDO	A	905	4/4	0.86	0.14	30,36,37,40	0
6	EDO	G	905	4/4	0.86	0.13	27,29,31,33	0
6	EDO	C	905	4/4	0.86	0.14	27,35,41,44	0
7	PEG	C	914	7/7	0.86	0.17	25,32,40,62	0
6	EDO	C	908	4/4	0.86	0.16	19,33,34,38	0
7	PEG	A	908	7/7	0.86	0.13	23,27,41,44	0
7	PEG	E	911	7/7	0.87	0.17	40,52,56,58	0
7	PEG	A	913	7/7	0.87	0.14	29,40,46,47	0
6	EDO	E	914	4/4	0.87	0.15	38,40,41,43	0
7	PEG	B	2906	7/7	0.88	0.17	18,27,40,46	0
7	PEG	C	919	7/7	0.89	0.13	21,26,34,35	0
6	EDO	E	906	4/4	0.89	0.12	20,23,25,29	0
6	EDO	C	906	4/4	0.89	0.12	30,37,41,51	0
7	PEG	A	914	7/7	0.89	0.15	29,35,44,51	0
14	GOL	B	2905	6/6	0.89	0.13	21,33,46,46	0
6	EDO	C	907	4/4	0.91	0.12	19,24,26,27	0
6	EDO	A	906	4/4	0.93	0.11	19,21,24,24	0
8	SBO	C	918	4/4	0.94	0.11	26,29,36,41	1
8	SBO	E	917	4/4	0.94	0.10	21,28,33,33	2
6	EDO	G	906	4/4	0.94	0.09	21,22,27,29	0
8	SBO	G	909	3/4	0.95	0.07	20,20,25,32	1
8	SBO	A	911	3/4	0.96	0.08	27,27,33,37	1
11	O	C	920	1/1	0.97	0.08	17,17,17,17	0
4	MGD	G	901	47/47	0.98	0.05	10,13,17,20	0
11	O	G	915	1/1	0.98	0.07	19,19,19,19	0
4	MGD	G	902	47/47	0.98	0.04	8,14,16,17	0
4	MGD	A	902	47/47	0.98	0.05	10,13,17,18	0
4	MGD	A	903	47/47	0.98	0.05	11,14,17,18	0
4	MGD	C	902	47/47	0.98	0.04	10,13,15,17	0
4	MGD	C	904	47/47	0.98	0.05	9,14,17,18	0
4	MGD	E	901	47/47	0.98	0.05	11,15,17,18	0
4	MGD	E	902	47/47	0.98	0.05	12,15,17,19	0
13	FES	H	2202	4/4	0.99	0.03	16,18,18,19	0
12	NA	A	922	1/1	0.99	0.05	9,9,9,9	0
12	NA	C	921	1/1	0.99	0.05	12,12,12,12	0
12	NA	E	919	1/1	0.99	0.05	12,12,12,12	0
12	NA	G	916	1/1	0.99	0.07	11,11,11,11	0
13	FES	B	2902	4/4	0.99	0.03	16,16,17,18	0
13	FES	D	201	4/4	0.99	0.03	14,15,16,16	0
13	FES	F	201	4/4	0.99	0.02	11,13,15,15	0

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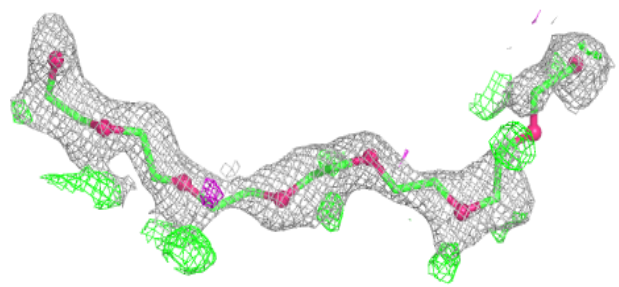
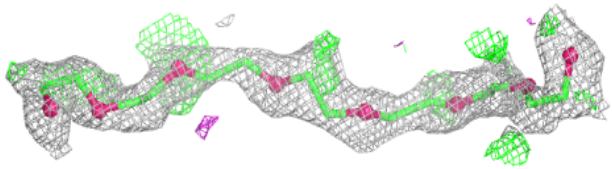
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	F3S	C	901	7/7	1.00	0.02	13,14,15,15	0
5	F3S	E	904	7/7	1.00	0.02	13,13,14,14	0
11	O	A	920	1/1	1.00	0.04	19,19,19,19	0
15	4MO	C	903	1/1	1.00	0.02	15,15,15,15	0
15	4MO	E	903	1/1	1.00	0.01	16,16,16,16	0
15	4MO	G	904	1/1	1.00	0.02	16,16,16,16	0
5	F3S	G	903	7/7	1.00	0.02	11,13,13,14	0
11	O	E	918	1/1	1.00	0.03	16,16,16,16	0
3	MO	A	901	1/1	1.00	0.02	15,15,15,15	0
5	F3S	A	904	7/7	1.00	0.02	12,14,15,15	0

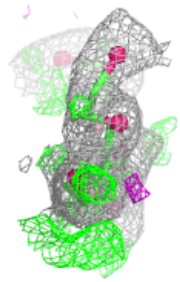
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P33 A 912:

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

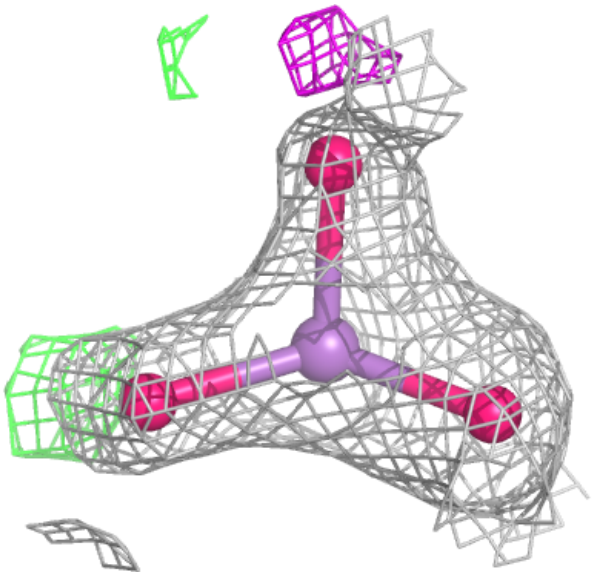


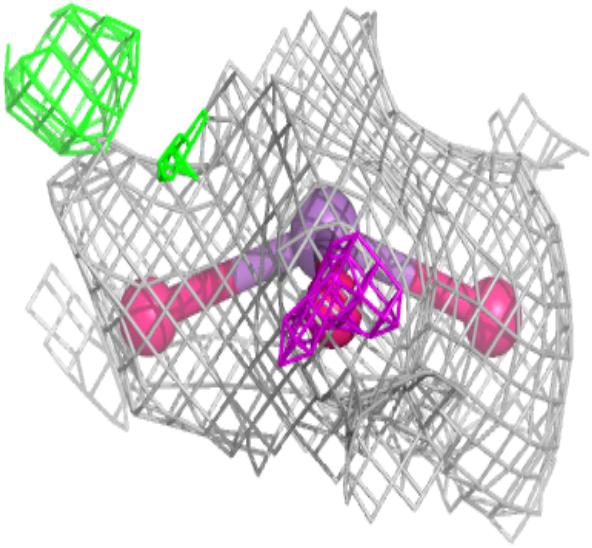


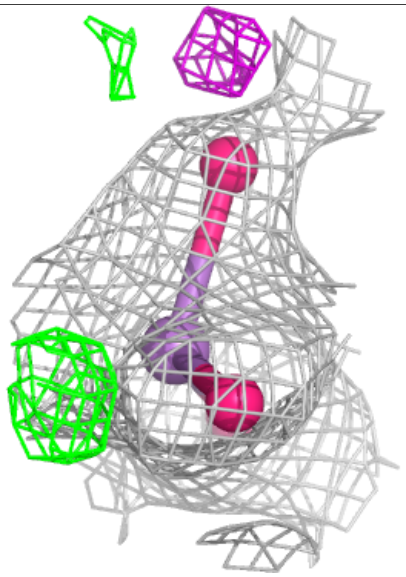


Electron density around SBO C 918:

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

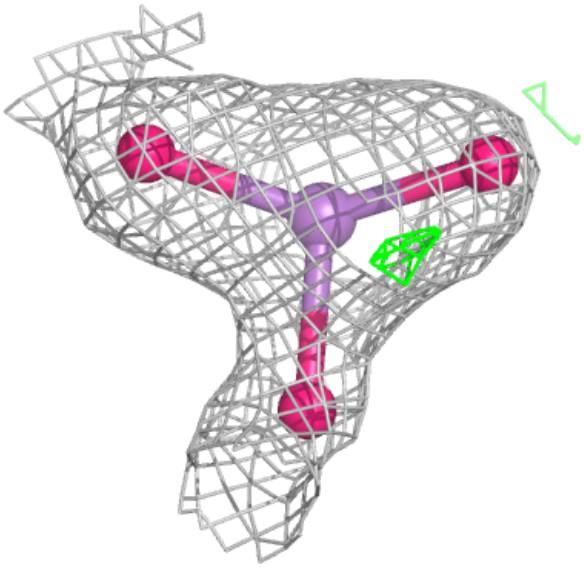


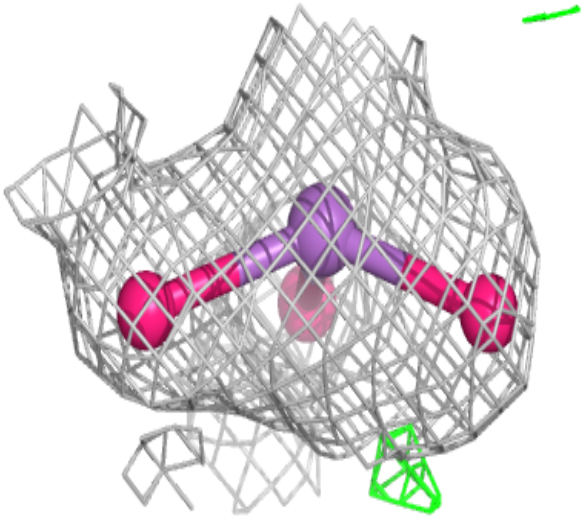


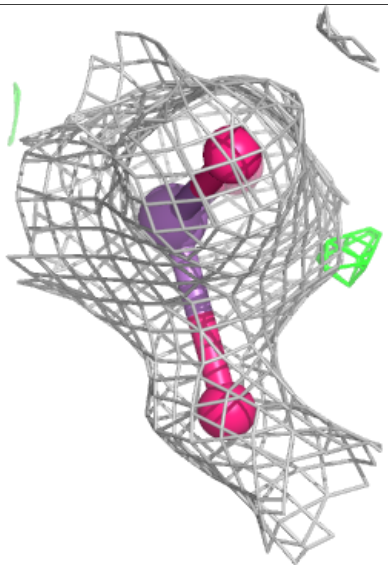


Electron density around SBO E 917:

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

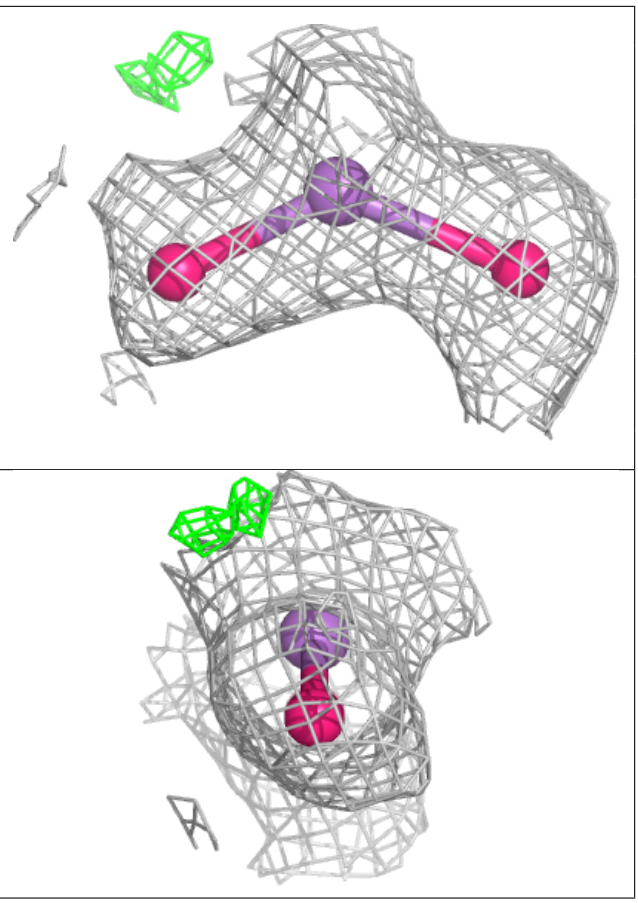






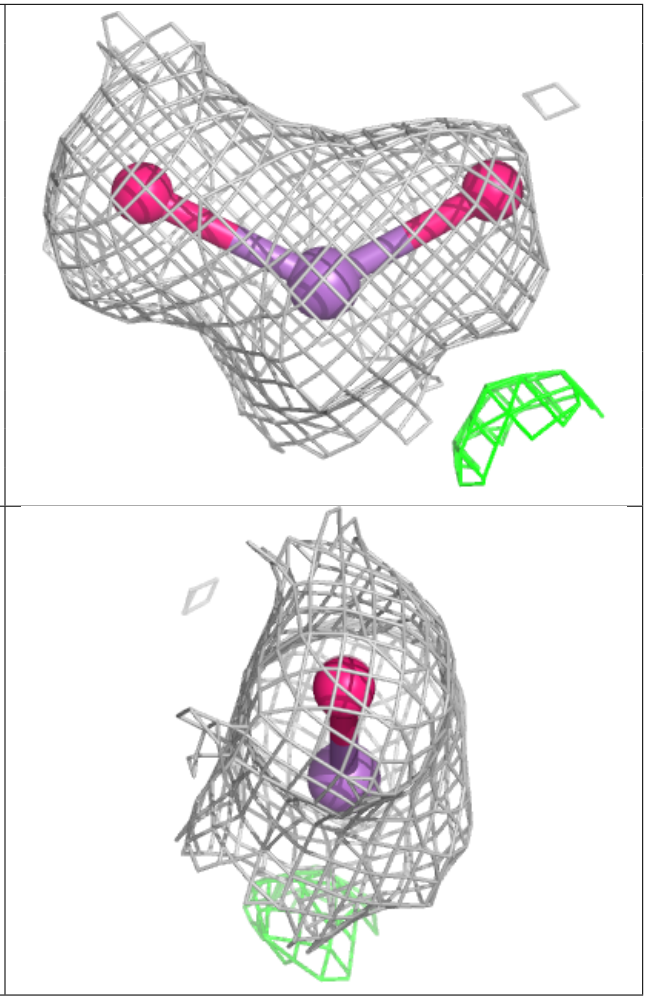
Electron density around SBO G 909:

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



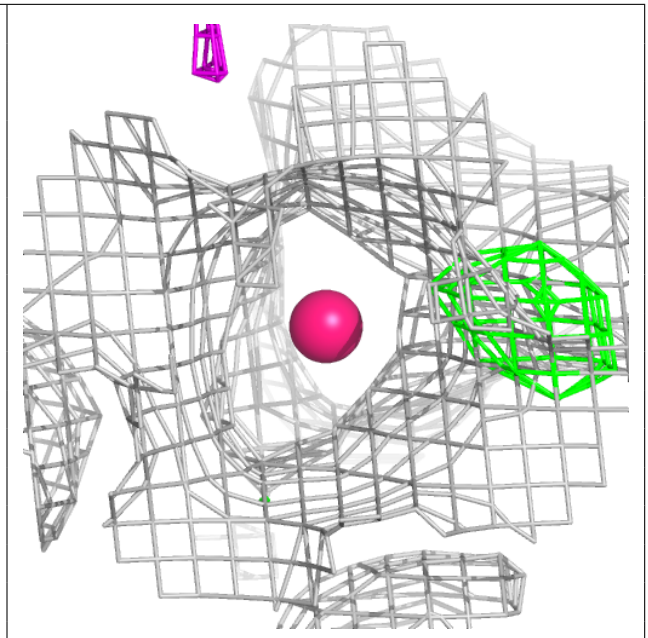
Electron density around SBO A 911:

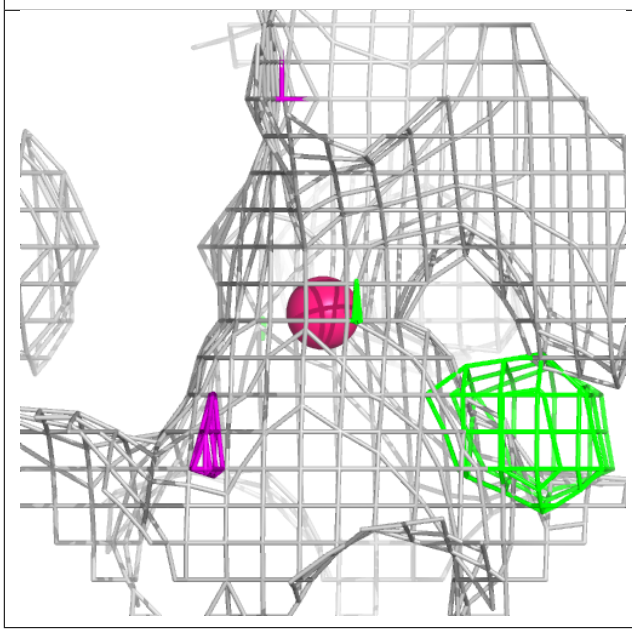
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

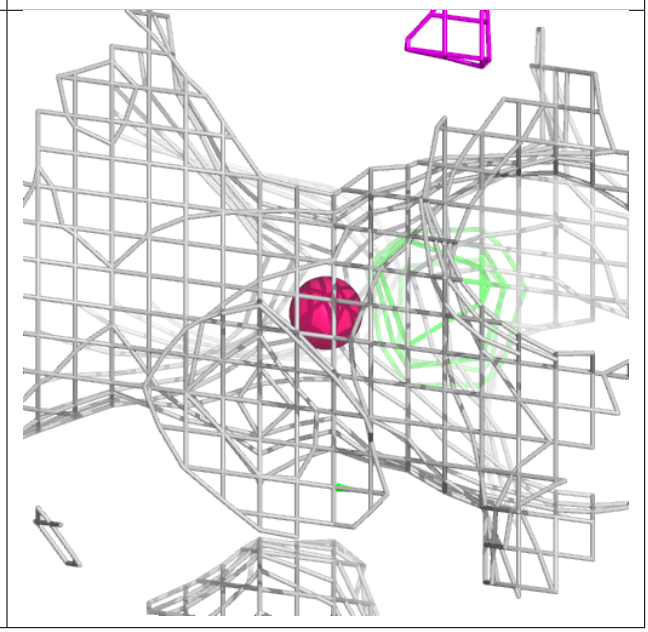


Electron density around O C 920:

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

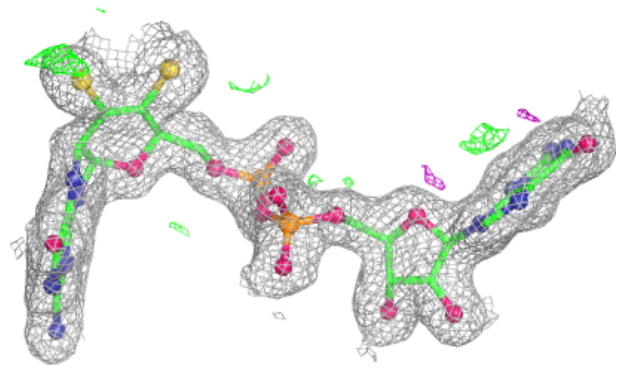


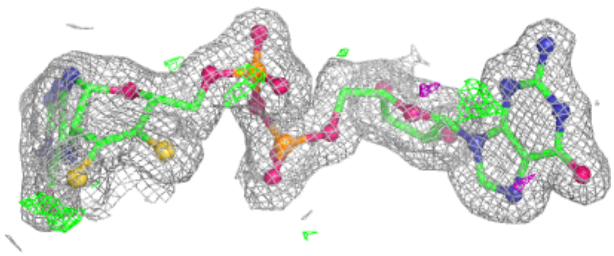




Electron density around MGD G 901:

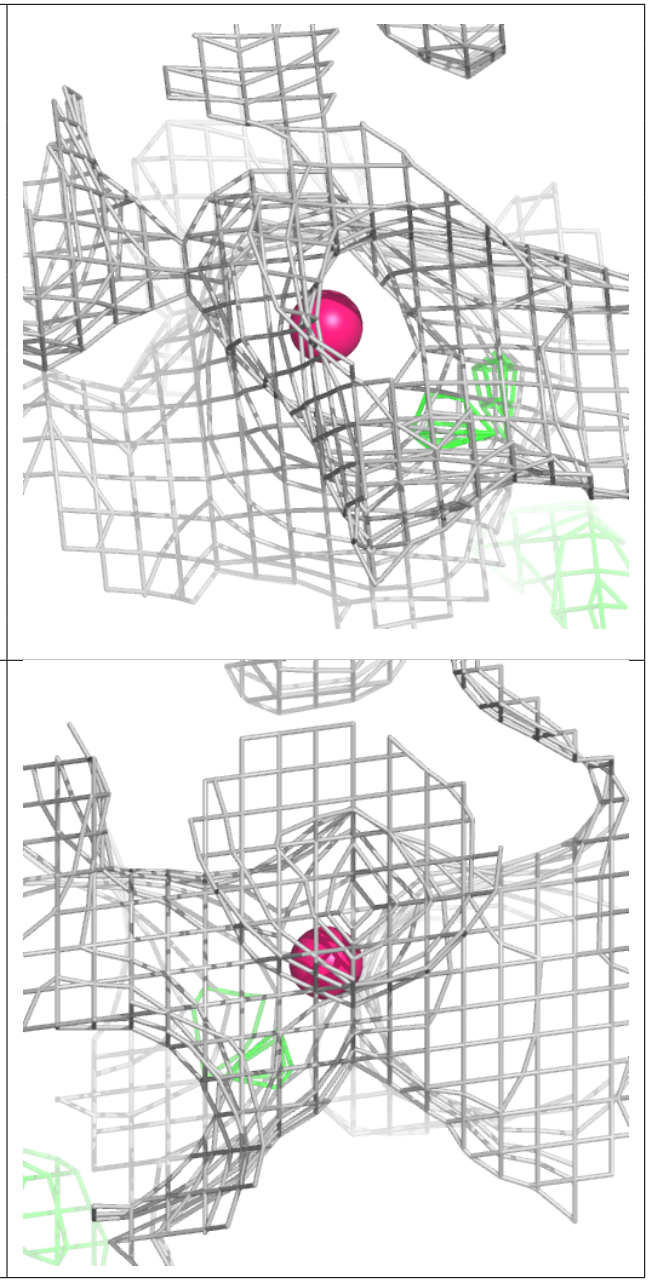
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





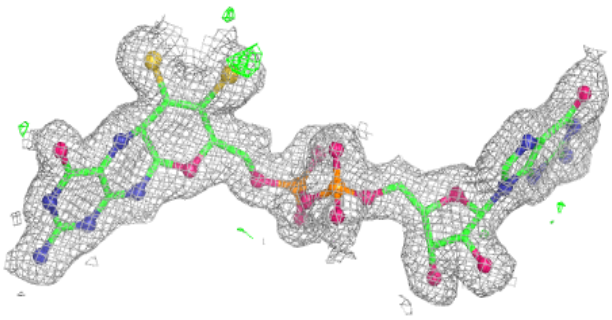
Electron density around O G 915:

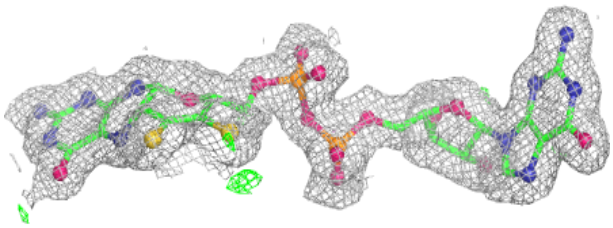
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

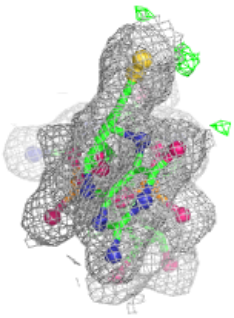


Electron density around MGD G 902:

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

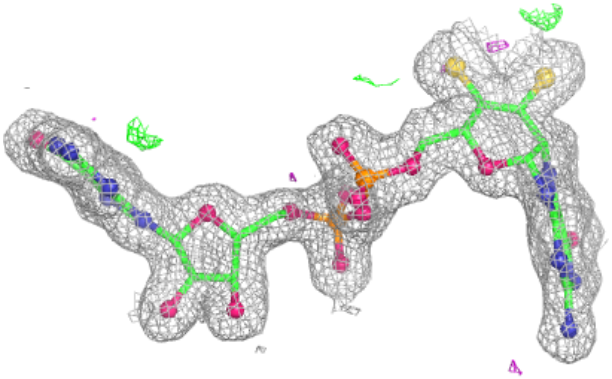


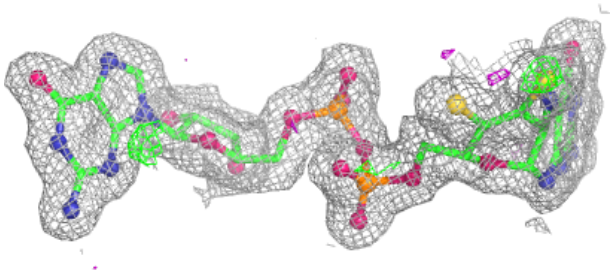


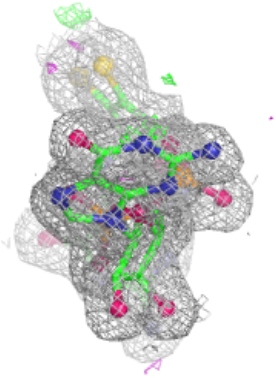


Electron density around MGD A 902:

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

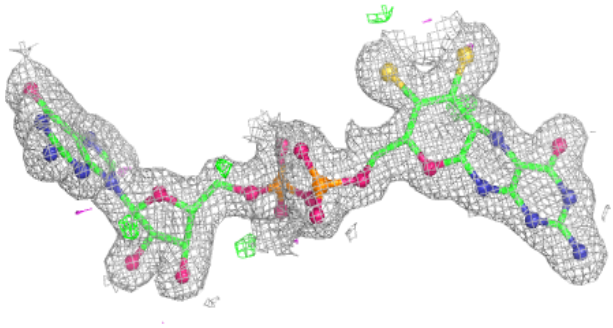


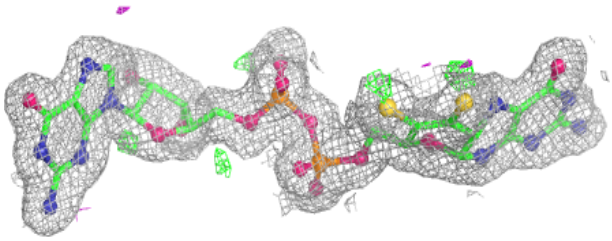


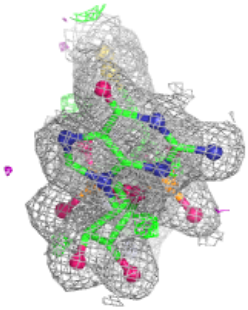


Electron density around MGD A 903:

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

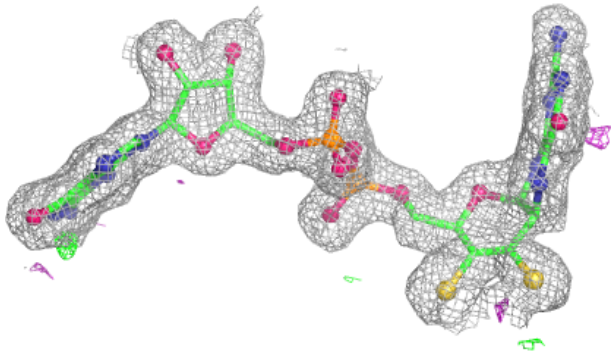


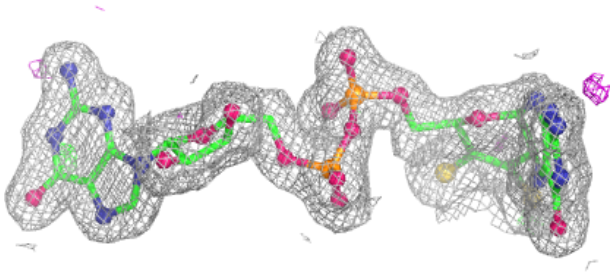


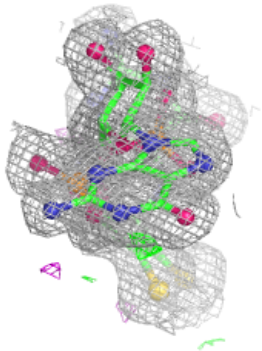


Electron density around MGD C 902:

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

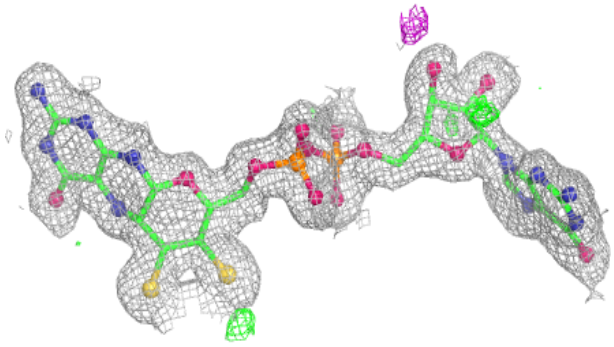


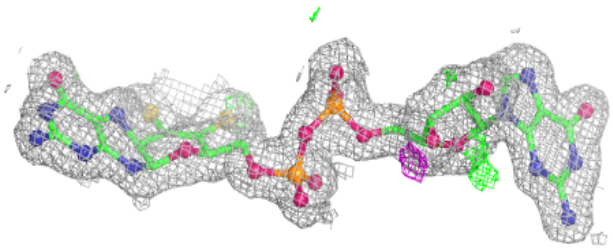


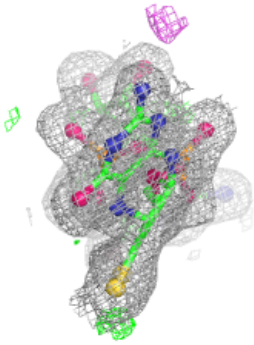


Electron density around MGD C 904:

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

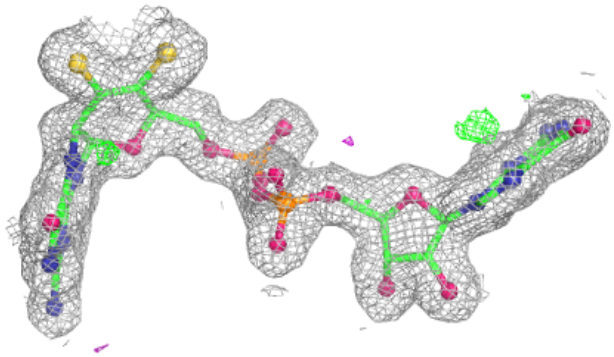


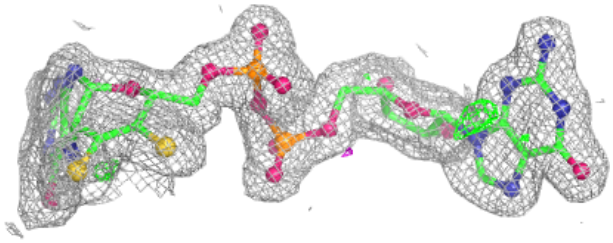


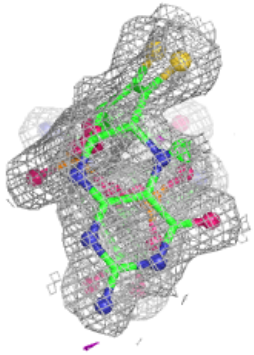


Electron density around MGD E 901:

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

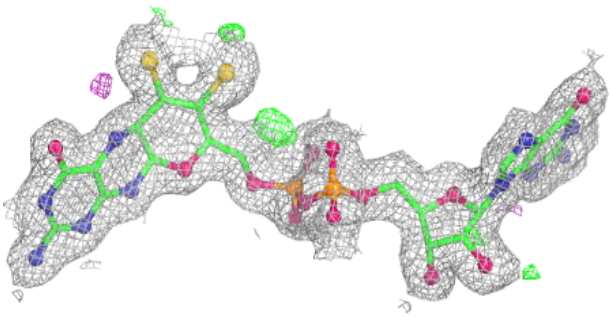


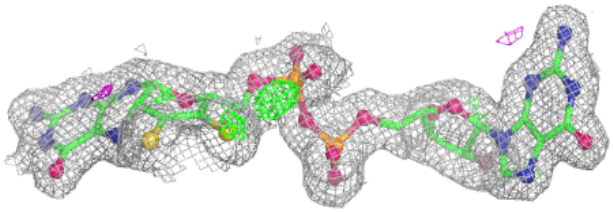


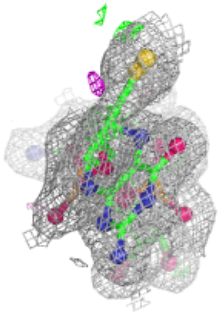


Electron density around MGD E 902:

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

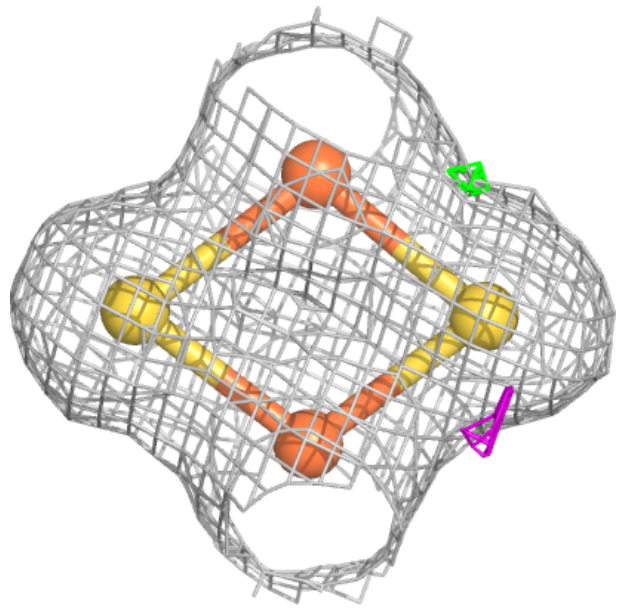


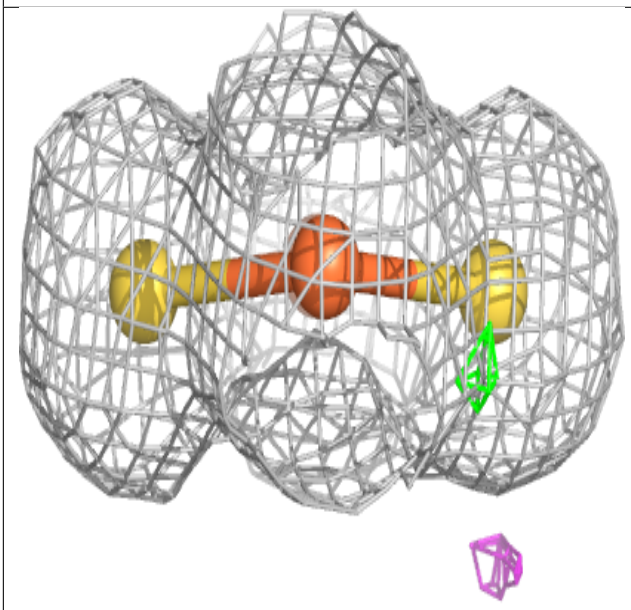


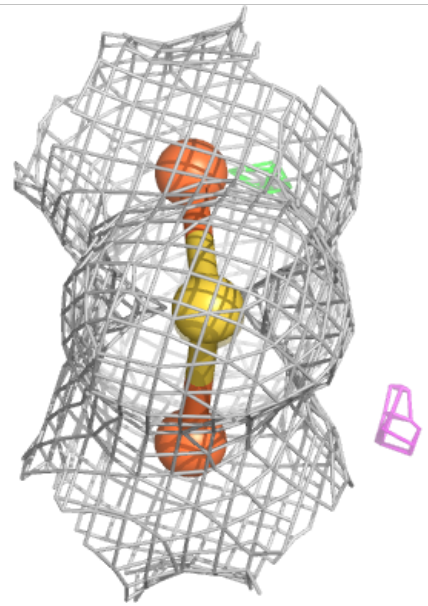


Electron density around FES H 2202:

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

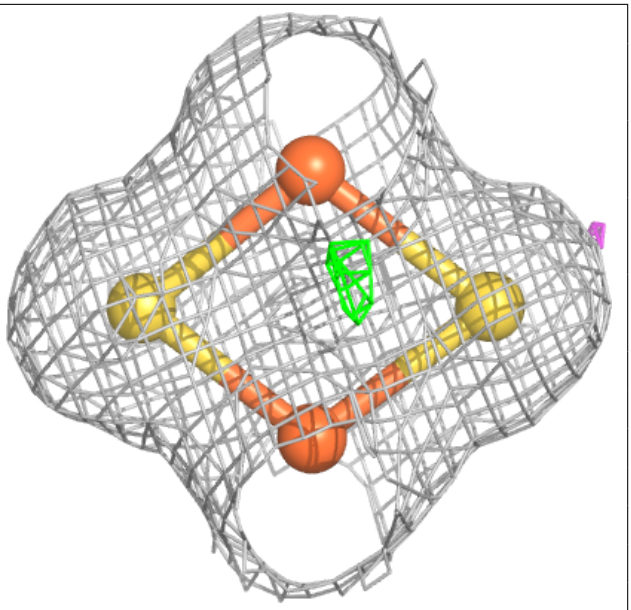


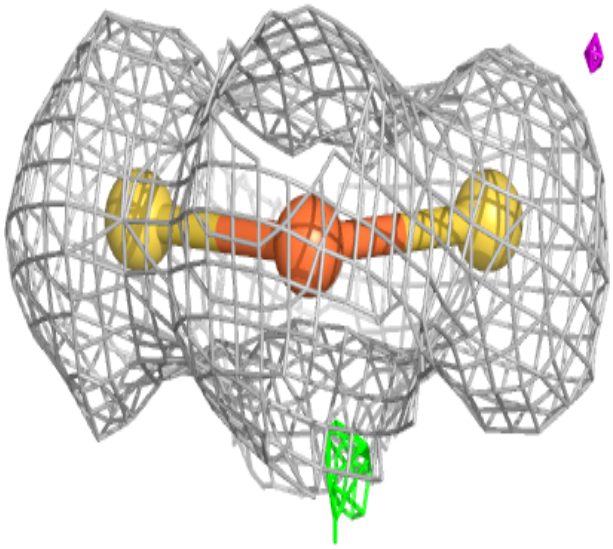


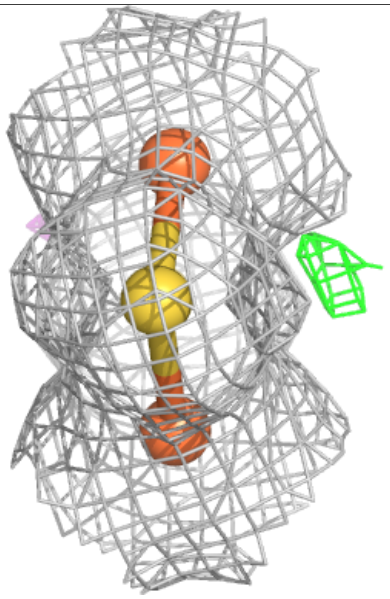


Electron density around FES B 2902:

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

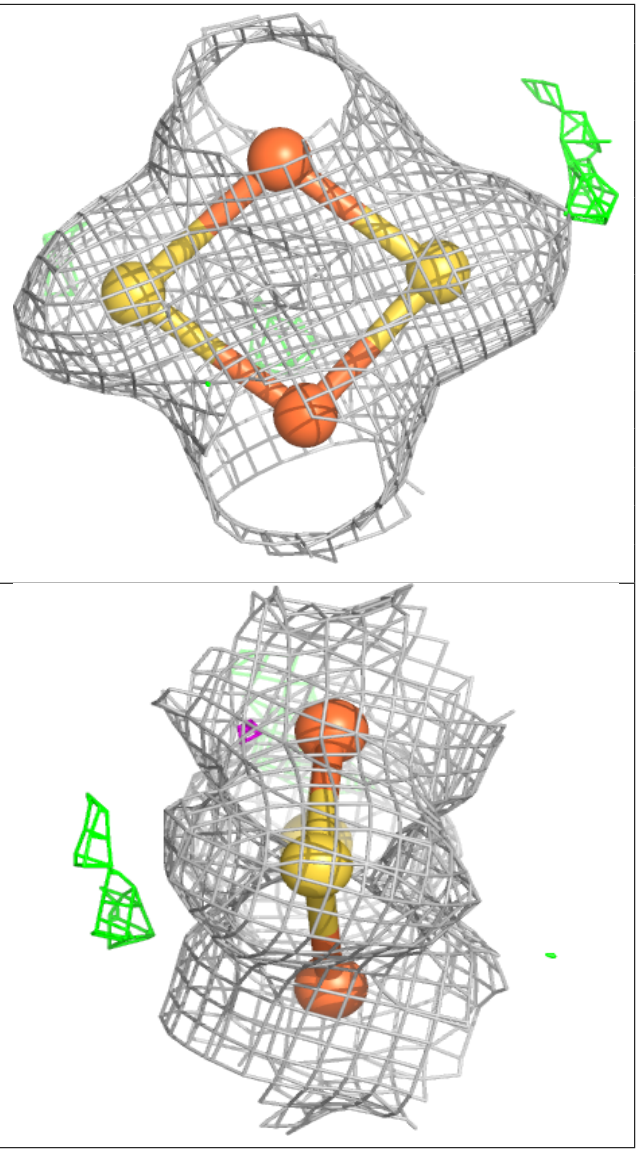






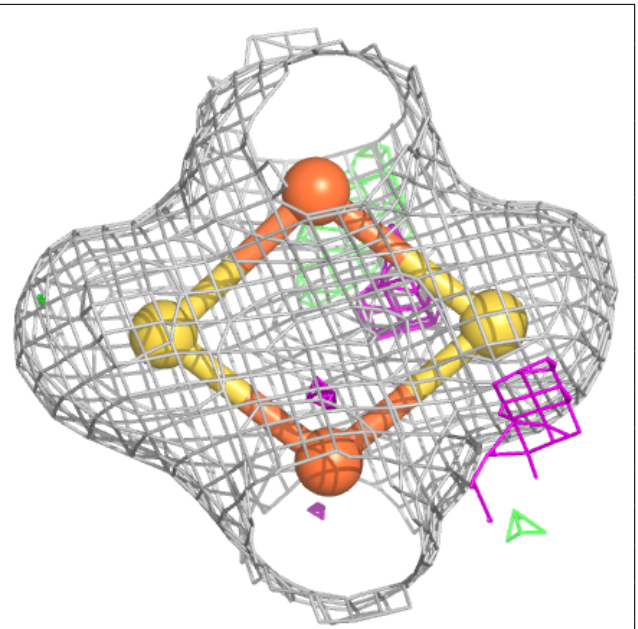
Electron density around FES D 201:

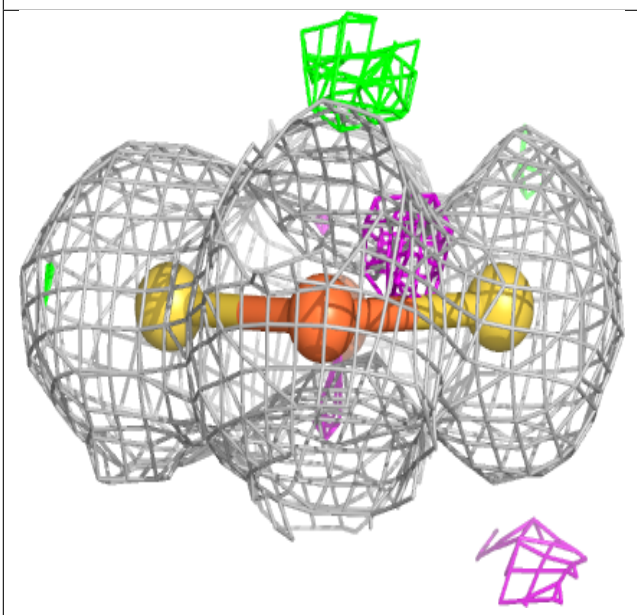
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

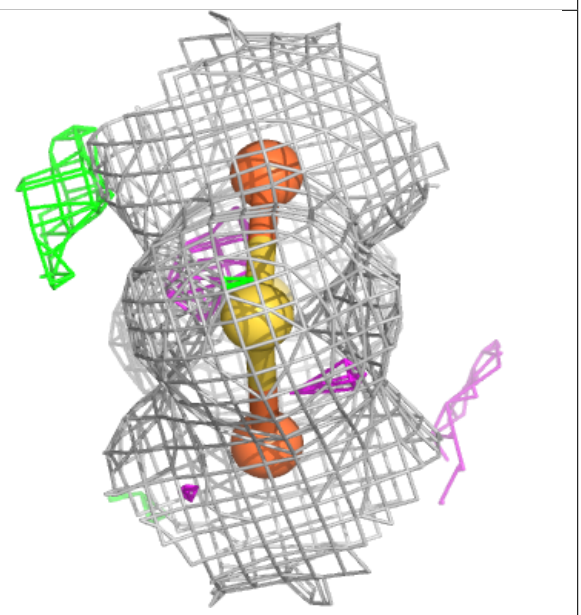


Electron density around FES F 201:

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

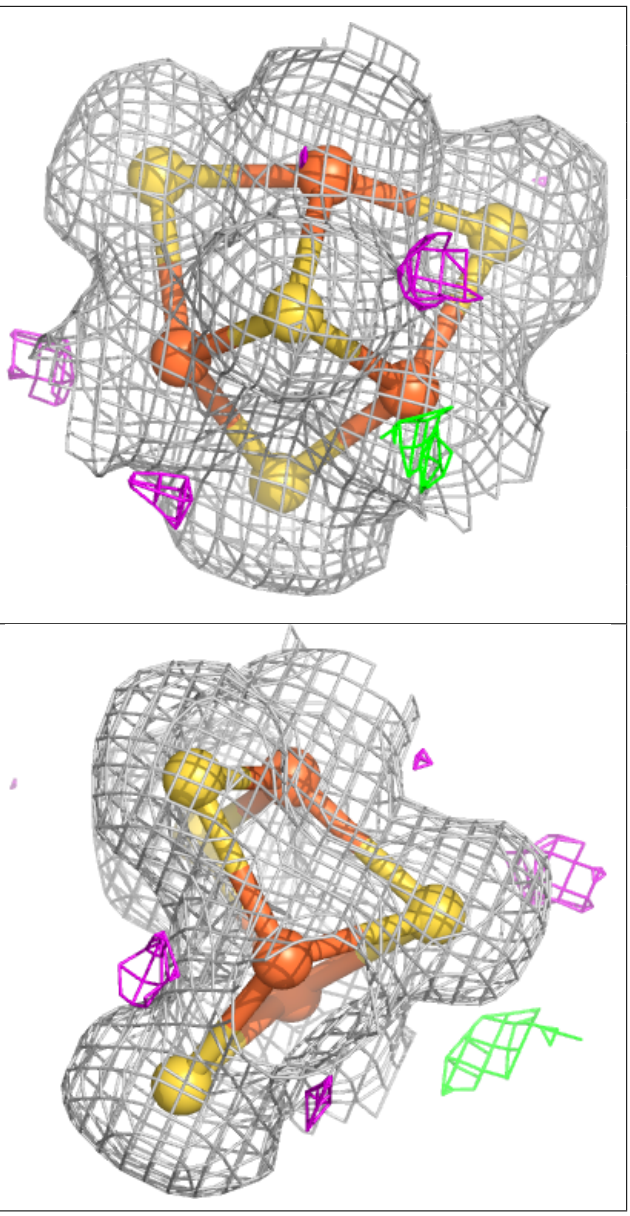






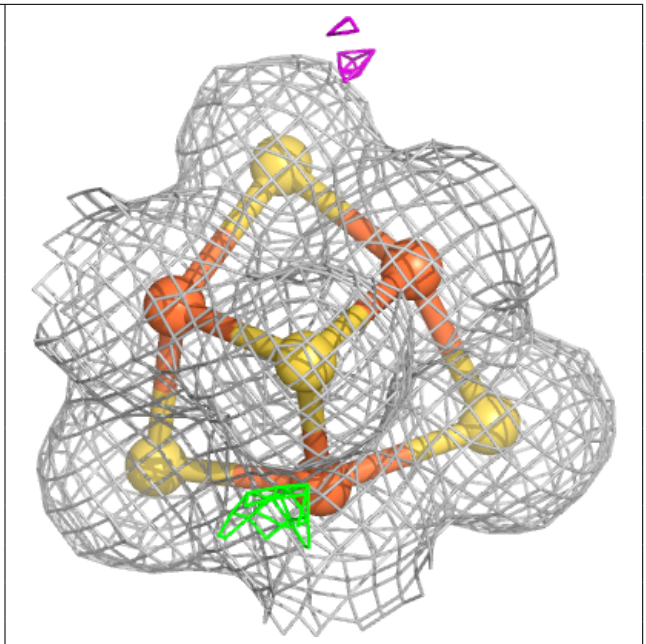
Electron density around F3S C 901:

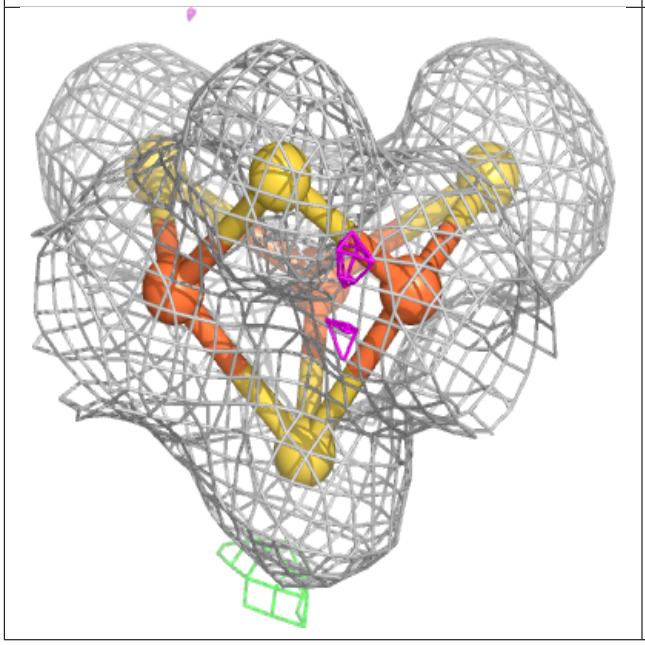
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

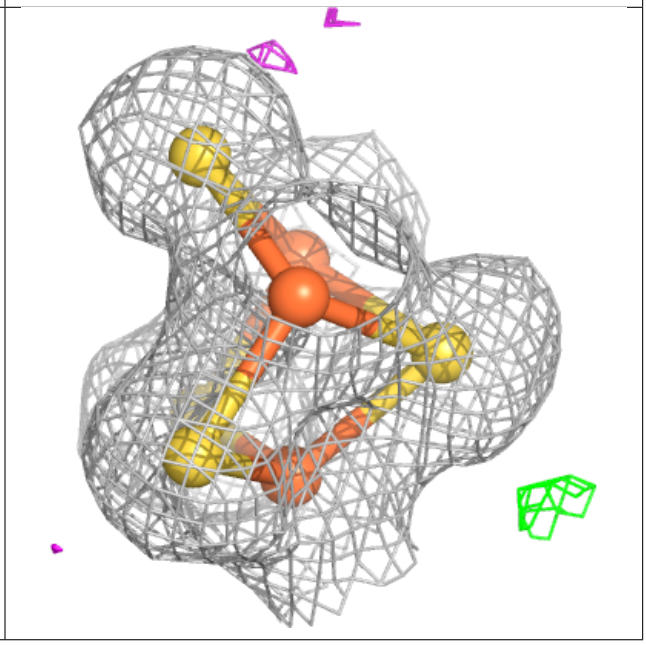


Electron density around F3S E 904:

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

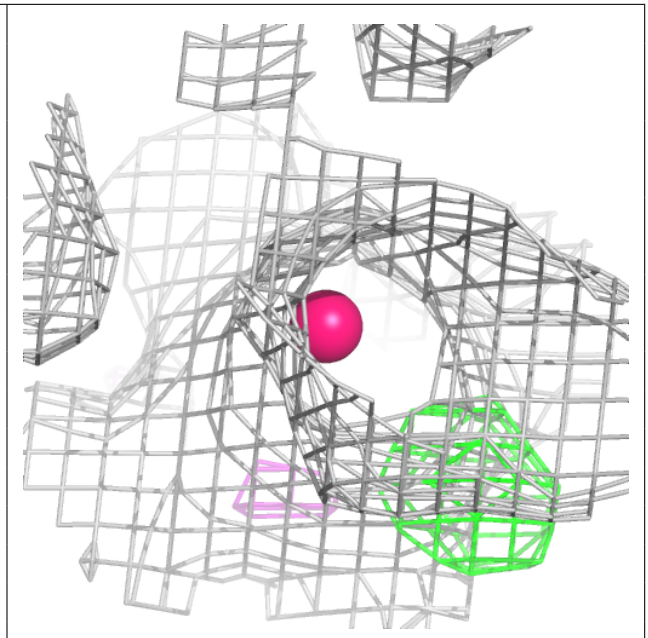


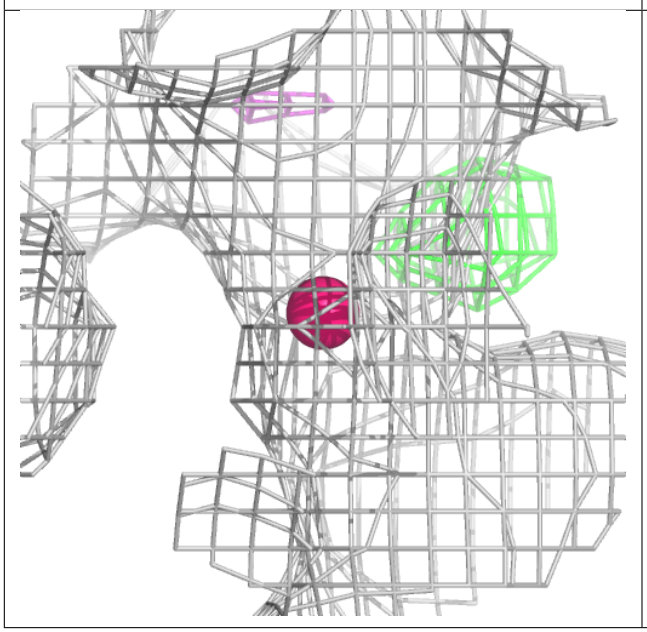


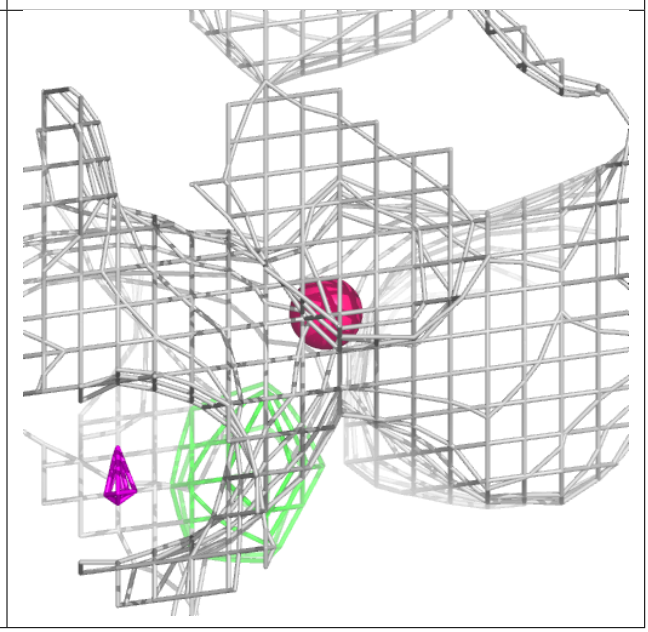


Electron density around O A 920:

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

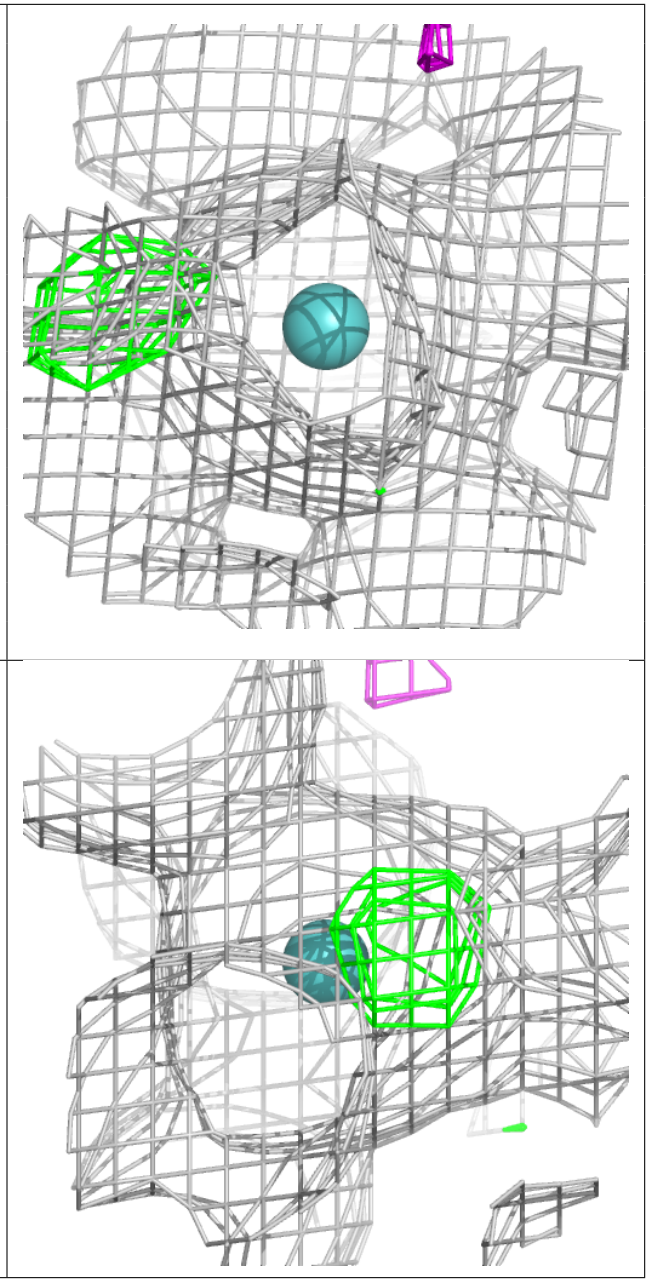






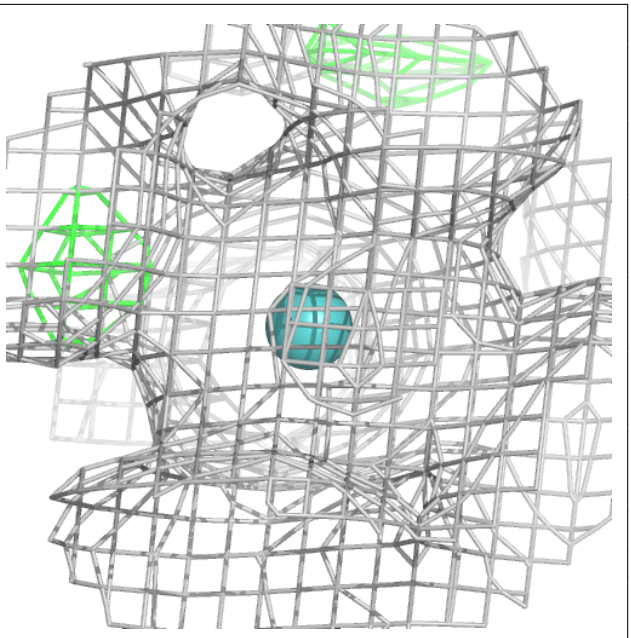
Electron density around 4MO C 903:

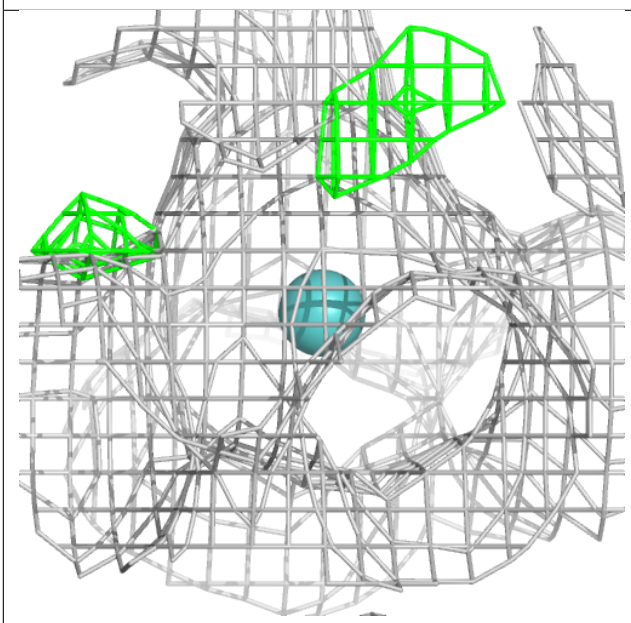
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

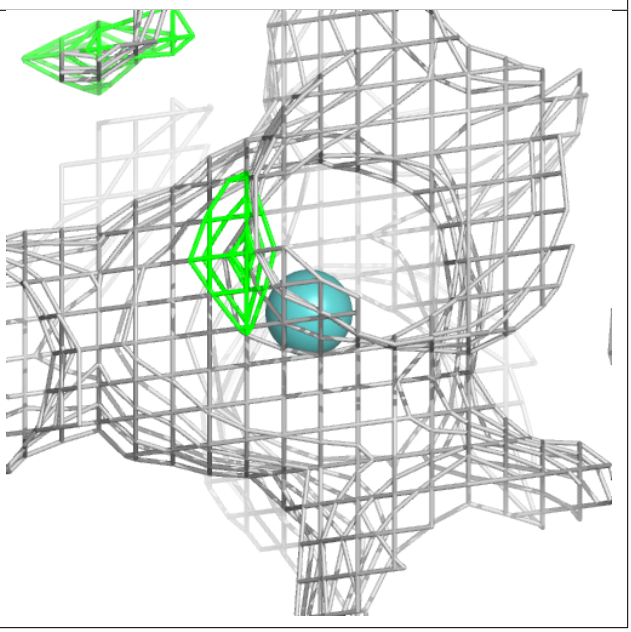


Electron density around 4MO E 903:

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

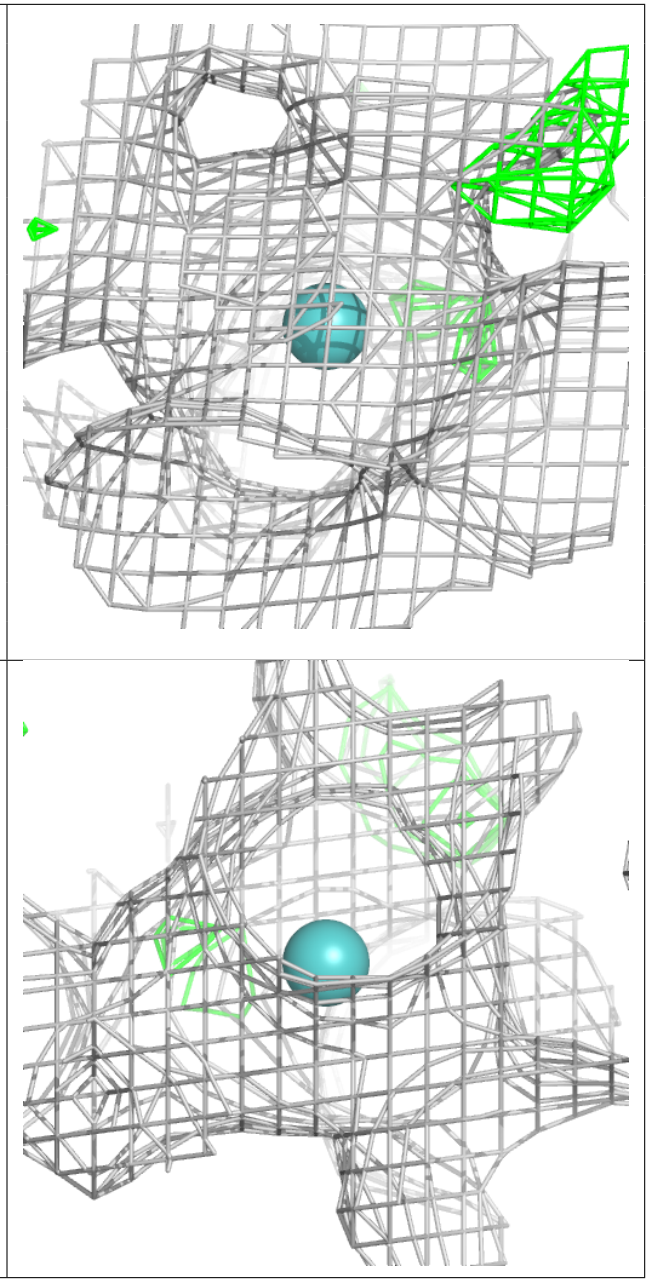






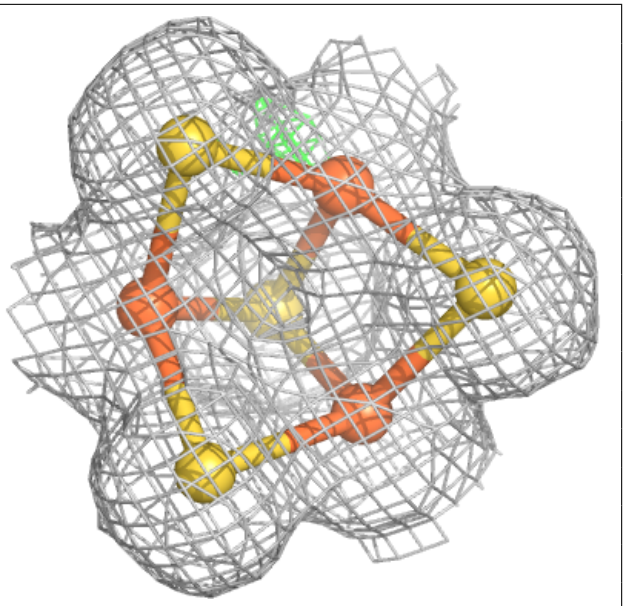
Electron density around 4MO G 904:

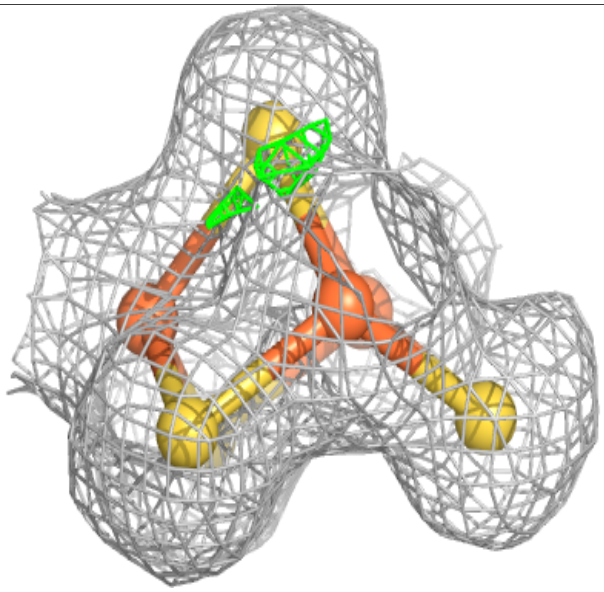
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

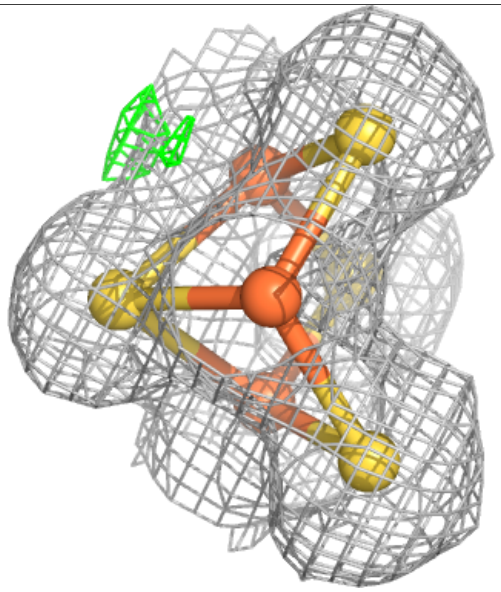


Electron density around F3S G 903:

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

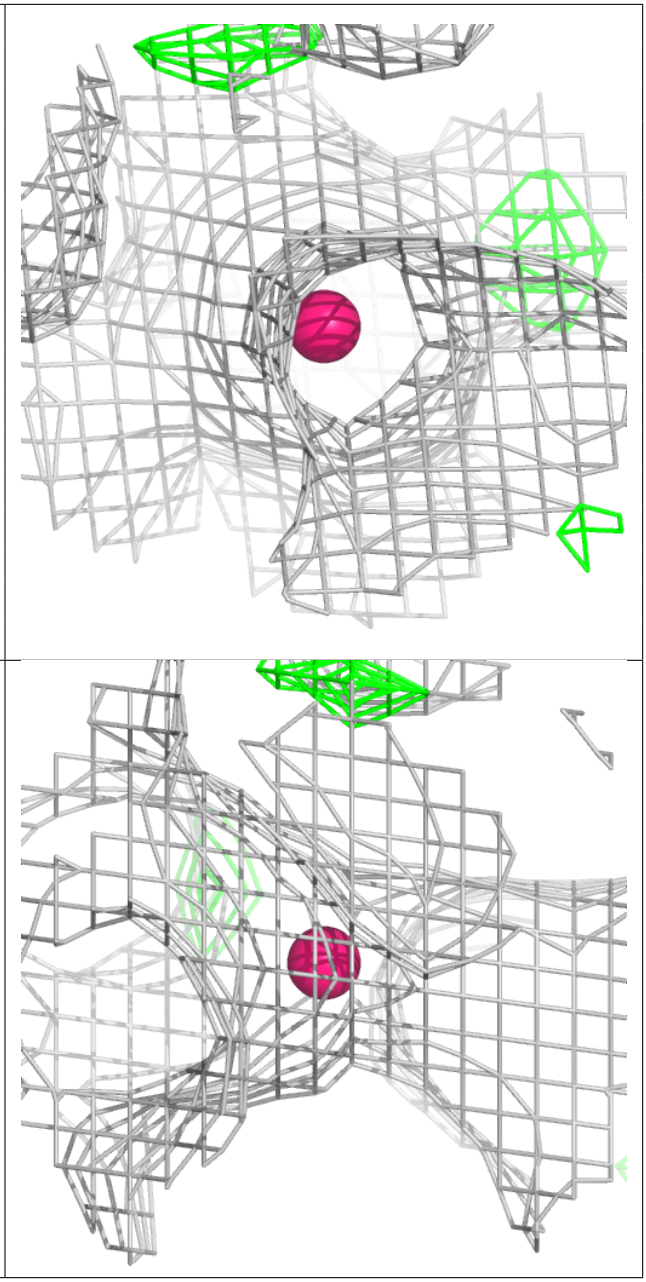






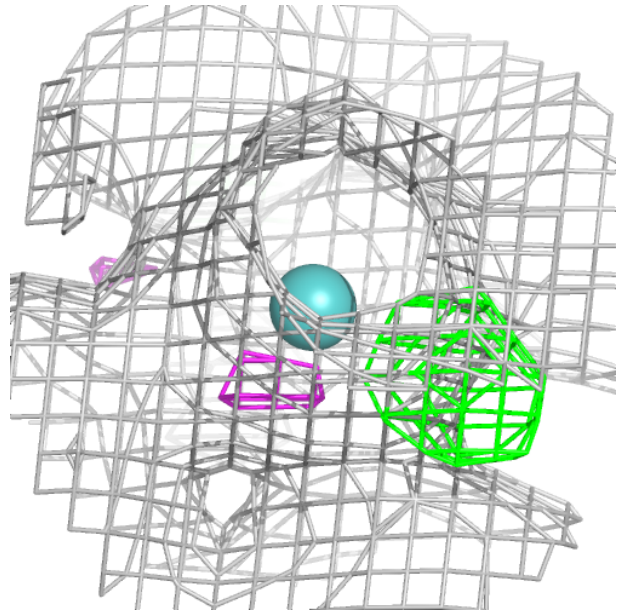
Electron density around O E 918:

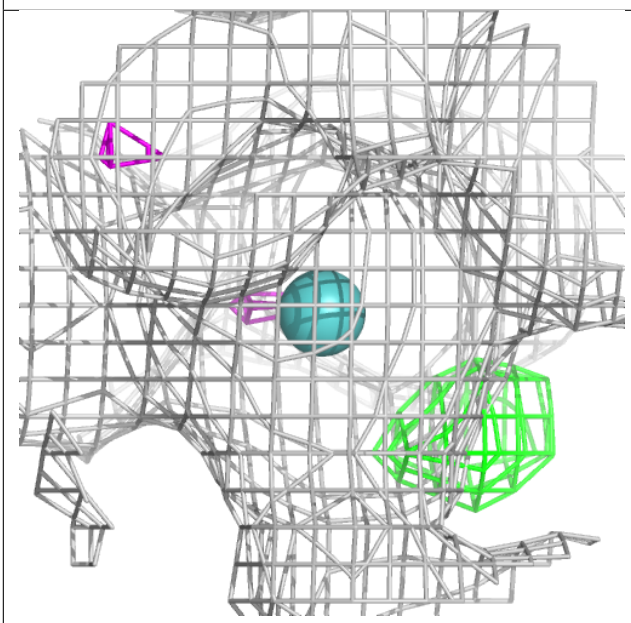
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

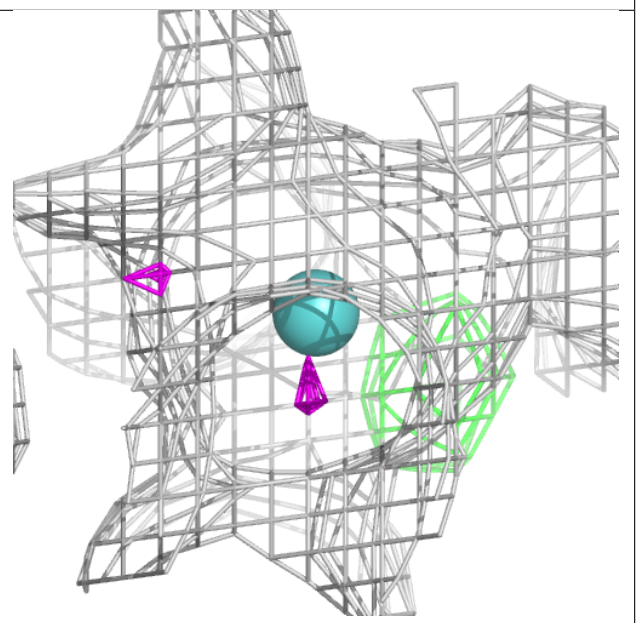


Electron density around MO A 901:

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

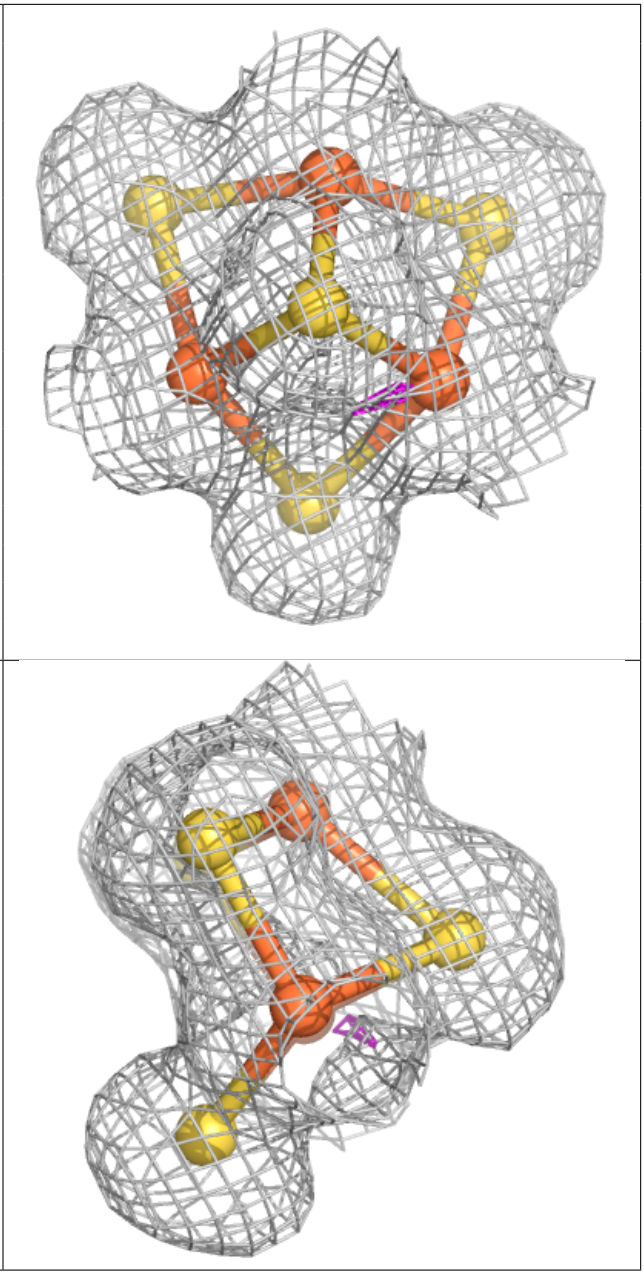






Electron density around F3S A 904:

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



6.5 Other polymers (i)

There are no such residues in this entry.