



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:57 AM UTC

PDB ID : 7Q06 / pdb_00007q06
Title : Crystal structure of TPADO in complex with 2-OH-TPA
Authors : Zahn, M.; Kincannon, W.M.; DuBois, J.L.; McGeehan, J.E.
Deposited on : 2021-10-14
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

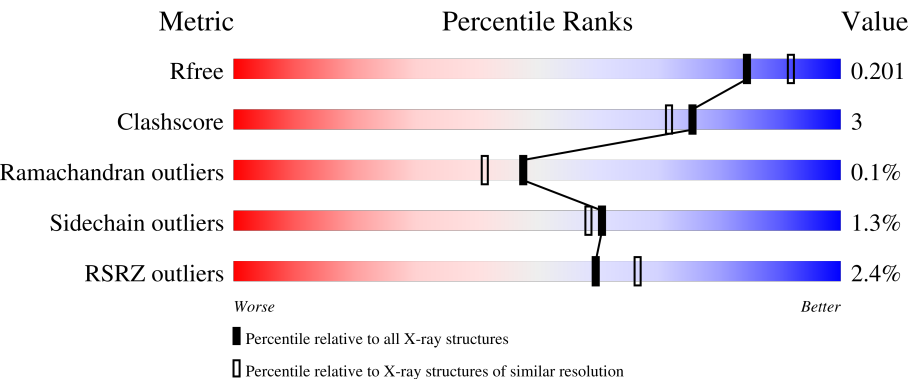
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	154	86%13%.
1	B	154	% 86%12%.
1	C	154	86%14%
2	D	428	3% 86%5%9%
2	E	428	4% 87%7%6%

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Mol	Chain	Length	Quality of chain
2	F	428	3% 83% 6% 11%
3	H	129	94% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28363 atoms, of which 13468 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 Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	40	0	0
			2390	757	1181	208	236	8			
1	B	154	Total	C	H	N	O	S	40	0	0
			2390	757	1181	208	236	8			
1	C	154	Total	C	H	N	O	S	40	0	0
			2390	757	1181	208	236	8			

- Molecule 2 is a protein called Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	389	Total	C	H	N	O	S	86	2	0
			6050	1944	2976	534	583	13			
2	E	403	Total	C	H	N	O	S	95	2	0
			6260	2013	3071	561	602	13			
2	F	381	Total	C	H	N	O	S	84	2	0
			5906	1895	2906	523	568	14			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	initiating methionine	UNP Q3C1D5
D	0	GLY	-	expression tag	UNP Q3C1D5
D	414	GLU	-	expression tag	UNP Q3C1D5
D	415	ASN	-	expression tag	UNP Q3C1D5
D	416	LEU	-	expression tag	UNP Q3C1D5
D	417	TYR	-	expression tag	UNP Q3C1D5
D	418	PHE	-	expression tag	UNP Q3C1D5
D	419	GLN	-	expression tag	UNP Q3C1D5
D	420	GLY	-	expression tag	UNP Q3C1D5
D	421	HIS	-	expression tag	UNP Q3C1D5
D	422	HIS	-	expression tag	UNP Q3C1D5

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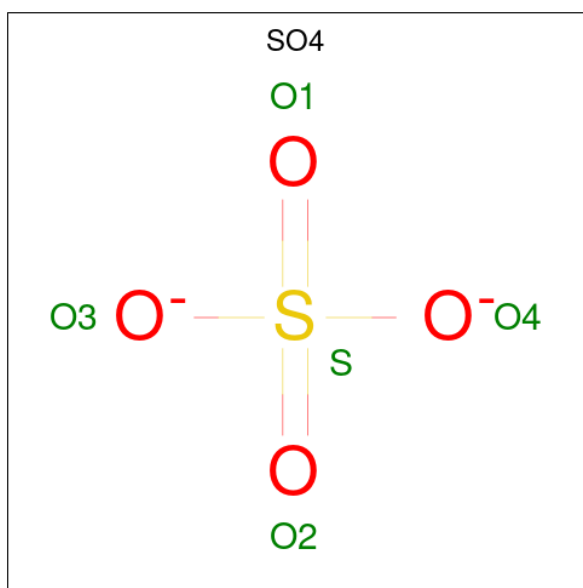
Chain	Residue	Modelled	Actual	Comment	Reference
D	423	HIS	-	expression tag	UNP Q3C1D5
D	424	HIS	-	expression tag	UNP Q3C1D5
D	425	HIS	-	expression tag	UNP Q3C1D5
D	426	HIS	-	expression tag	UNP Q3C1D5
E	-1	MET	-	initiating methionine	UNP Q3C1D5
E	0	GLY	-	expression tag	UNP Q3C1D5
E	414	GLU	-	expression tag	UNP Q3C1D5
E	415	ASN	-	expression tag	UNP Q3C1D5
E	416	LEU	-	expression tag	UNP Q3C1D5
E	417	TYR	-	expression tag	UNP Q3C1D5
E	418	PHE	-	expression tag	UNP Q3C1D5
E	419	GLN	-	expression tag	UNP Q3C1D5
E	420	GLY	-	expression tag	UNP Q3C1D5
E	421	HIS	-	expression tag	UNP Q3C1D5
E	422	HIS	-	expression tag	UNP Q3C1D5
E	423	HIS	-	expression tag	UNP Q3C1D5
E	424	HIS	-	expression tag	UNP Q3C1D5
E	425	HIS	-	expression tag	UNP Q3C1D5
E	426	HIS	-	expression tag	UNP Q3C1D5
F	-1	MET	-	initiating methionine	UNP Q3C1D5
F	0	GLY	-	expression tag	UNP Q3C1D5
F	414	GLU	-	expression tag	UNP Q3C1D5
F	415	ASN	-	expression tag	UNP Q3C1D5
F	416	LEU	-	expression tag	UNP Q3C1D5
F	417	TYR	-	expression tag	UNP Q3C1D5
F	418	PHE	-	expression tag	UNP Q3C1D5
F	419	GLN	-	expression tag	UNP Q3C1D5
F	420	GLY	-	expression tag	UNP Q3C1D5
F	421	HIS	-	expression tag	UNP Q3C1D5
F	422	HIS	-	expression tag	UNP Q3C1D5
F	423	HIS	-	expression tag	UNP Q3C1D5
F	424	HIS	-	expression tag	UNP Q3C1D5
F	425	HIS	-	expression tag	UNP Q3C1D5
F	426	HIS	-	expression tag	UNP Q3C1D5

- Molecule 3 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	129	Total	C	H	N	O	S	22	0	0
			1961	613	960	193	185	10			

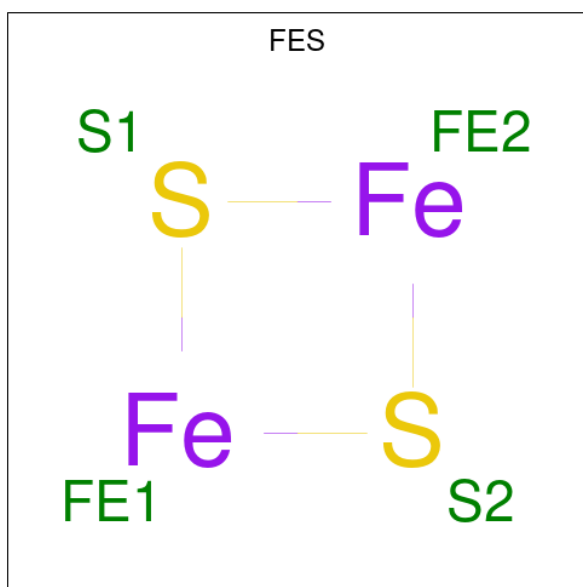
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest")

by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

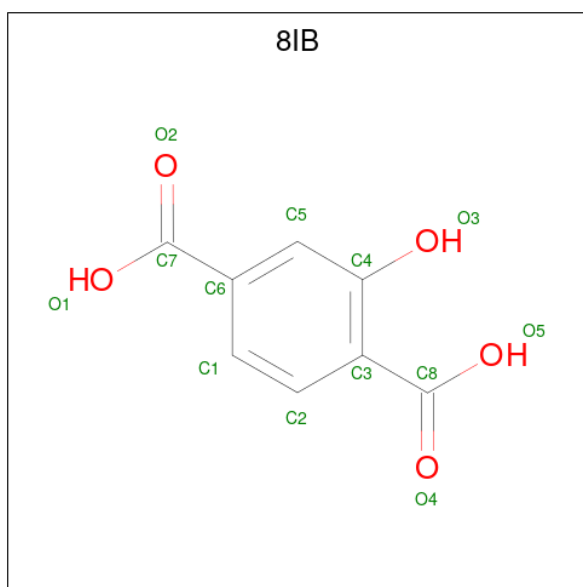


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		
5	E	1	Total	Fe	S	0	0
			4	2	2		
5	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Fe	0	0
			1	1		
6	F	1	Total	Fe	0	0
			1	1		

- Molecule 7 is 2-Hydroxyterephthalic acid (CCD ID: 8IB) (formula: C₈H₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	1	0
			17	8	4	5		
7	E	1	Total	C	H	O	1	0
			17	8	4	5		
7	F	1	Total	C	H	O	1	0
			17	8	4	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	115	Total	O	0	0
			115	115		
8	B	89	Total	O	0	0
			89	89		
8	C	95	Total	O	0	0
			95	95		
8	D	142	Total	O	0	0
			142	142		
8	E	255	Total	O	0	0
			255	255		
8	F	176	Total	O	0	0
			176	176		
8	H	49	Total	O	0	0
			49	49		

3 Residue-property plots

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: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain A: 



- Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain B: 



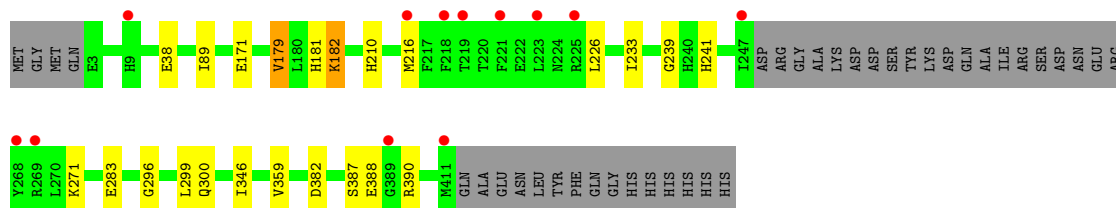
- Molecule 1: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit beta 1

Chain C: 



- Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2

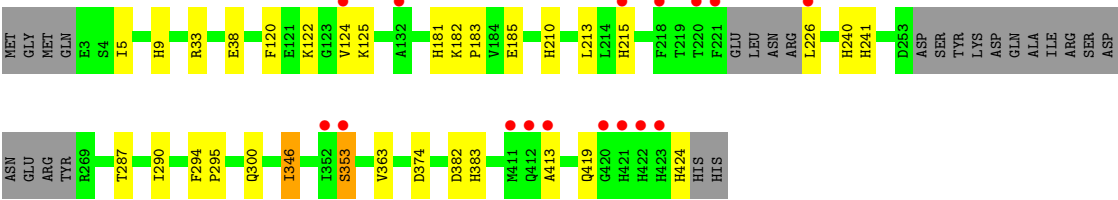
Chain D: 



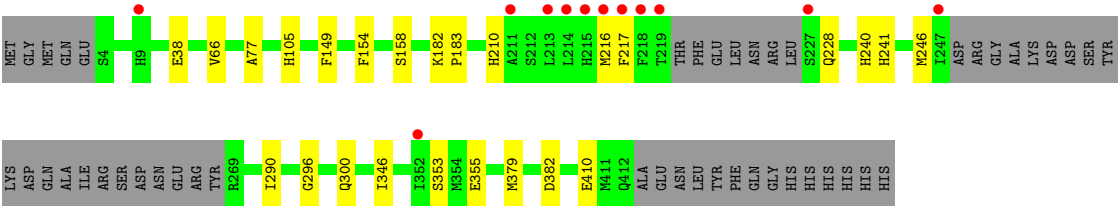
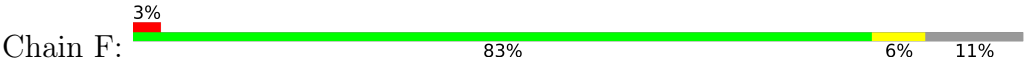
- Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2

Chain E: 





● Molecule 2: Terephthalate 1,2-dioxygenase, terminal oxygenase component subunit alpha 2



● Molecule 3: Lysozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	220.31Å 220.31Å 83.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	190.80 – 1.95 190.80 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.5 (190.80-1.95) 83.8 (190.80-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.165 , 0.202 0.163 , 0.201	Depositor DCC
R_{free} test set	8122 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28363	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8IB, FES, FE, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.26	5/1232 (0.4%)	1.33	0/1671
1	B	1.25	4/1232 (0.3%)	1.32	2/1671 (0.1%)
1	C	1.21	3/1232 (0.2%)	1.32	1/1671 (0.1%)
2	D	1.19	3/3150 (0.1%)	1.33	4/4253 (0.1%)
2	E	1.22	5/3270 (0.2%)	1.30	7/4413 (0.2%)
2	F	1.20	3/3073 (0.1%)	1.28	6/4147 (0.1%)
3	H	1.16	0/1021	1.42	1/1379 (0.1%)
All	All	1.21	23/14210 (0.2%)	1.32	21/19205 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	210	HIS	CE1-NE2	7.19	1.39	1.32
1	B	81	HIS	CE1-NE2	6.97	1.39	1.32
2	E	346	ILE	C-O	6.96	1.32	1.23
1	B	77	HIS	CE1-NE2	6.73	1.39	1.32
1	B	114	GLU	CD-OE2	6.51	1.37	1.25
1	A	81	HIS	CE1-NE2	6.25	1.38	1.32
1	C	46	GLU	C-O	-5.94	1.16	1.24
2	F	210	HIS	CE1-NE2	5.90	1.38	1.32
2	F	149	PHE	C-O	5.74	1.31	1.23
1	A	35	HIS	CE1-NE2	5.73	1.38	1.32
2	F	240	HIS	CE1-NE2	5.72	1.38	1.32
2	E	210	HIS	CE1-NE2	5.58	1.38	1.32
2	E	363	VAL	C-O	5.49	1.30	1.24
1	A	46	GLU	C-O	-5.35	1.17	1.24
1	C	75	GLU	C-O	5.34	1.30	1.23
2	D	239	GLY	C-O	5.22	1.30	1.23
2	E	413	ALA	C-O	5.20	1.30	1.24
2	E	240	HIS	CE1-NE2	5.14	1.37	1.32
2	D	89	ILE	C-O	-5.12	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ARG	C-O	5.11	1.30	1.23
1	A	64	ARG	C-O	5.05	1.30	1.24
1	B	115	VAL	C-O	-5.04	1.19	1.23
1	C	115	VAL	C-O	-5.02	1.19	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	182	LYS	CB-CA-C	-8.47	98.76	110.37
2	F	217	PHE	CA-C-O	-7.33	113.35	120.90
2	E	382	ASP	CA-C-N	6.24	129.57	120.71
2	E	382	ASP	C-N-CA	6.24	129.57	120.71
2	F	382	ASP	CA-C-N	6.20	129.52	120.71
2	F	382	ASP	C-N-CA	6.20	129.52	120.71
2	D	382	ASP	CA-C-N	6.01	129.25	120.71
2	D	382	ASP	C-N-CA	6.01	129.25	120.71
2	E	424	HIS	CA-C-O	5.94	130.89	120.80
1	B	3	ASN	CA-C-N	5.65	127.85	120.28
1	B	3	ASN	C-N-CA	5.65	127.85	120.28
3	H	19	ASN	CA-CB-CG	-5.57	107.03	112.60
2	E	9	HIS	CB-CA-C	5.55	119.67	110.90
2	F	379	MET	CG-SD-CE	-5.53	88.72	100.90
2	E	374	ASP	CA-CB-CG	5.34	117.94	112.60
2	F	154	PHE	CA-C-N	5.29	125.69	121.61
2	F	154	PHE	C-N-CA	5.29	125.69	121.61
2	E	383	HIS	CA-CB-CG	5.17	118.97	113.80
1	C	94	THR	CA-CB-OG1	-5.11	101.94	109.60
2	E	419	GLN	CB-CA-C	5.05	118.81	110.88
2	D	359	VAL	N-CA-CB	5.02	117.37	110.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1209	1181	1176	18	0
1	B	1209	1181	1176	17	0
1	C	1209	1181	1176	17	0
2	D	3074	2976	2963	9	0
2	E	3189	3071	3052	16	0
2	F	3000	2906	2892	11	0
3	H	1001	960	959	3	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	1	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	D	13	4	0	0	0
7	E	13	4	0	2	0
7	F	13	4	0	2	0
8	A	115	0	0	4	0
8	B	89	0	0	4	0
8	C	95	0	0	0	0
8	D	142	0	0	1	0
8	E	255	0	0	3	0
8	F	176	0	0	0	0
8	H	49	0	0	0	0
All	All	14895	13468	13394	81	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 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:TRP:HE3	1:C:65:ILE:HD11	1.23	1.04
1:C:26:TRP:CE3	1:C:65:ILE:HD11	2.03	0.92
1:B:103:MET:HE1	1:C:103:MET:HE1	1.56	0.86
2:F:228:GLN:HB2	2:F:246:MET:O	1.77	0.85
1:B:46:GLU:OE2	8:B:301:HOH:O	2.04	0.74
1:A:62:THR:HG21	2:D:271:LYS:HE2	1.68	0.74
1:C:61:LEU:O	1:C:65:ILE:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:OE1	8:A:201:HOH:O	2.13	0.66
1:B:103:MET:HE1	1:C:103:MET:CE	2.25	0.65
2:E:185:GLU:OE2	8:E:601:HOH:O	2.14	0.65
1:A:33:ASP:HB3	8:A:300:HOH:O	1.97	0.64
2:D:226:LEU:HD12	2:E:120:PHE:CE2	2.34	0.62
1:A:46:GLU:OE2	8:A:202:HOH:O	2.16	0.61
1:C:21:ASP:HA	1:C:23:MET:CE	2.31	0.60
1:C:11:ASN:HB3	1:C:83:LEU:HD13	1.89	0.55
1:B:79:TYR:CE2	1:B:152:LEU:HB2	2.43	0.54
1:B:21:ASP:HA	1:B:23:MET:HE2	1.90	0.54
2:D:181:HIS:CD2	2:D:182:LYS:HG3	2.43	0.54
2:E:290:ILE:HG13	7:E:504:8IB:C5	2.38	0.53
1:B:23:MET:HE3	1:B:152:LEU:HD22	1.91	0.52
2:E:300:GLN:HE22	2:E:346:ILE:HG21	1.75	0.52
2:F:300:GLN:O	2:F:300:GLN:HG3	2.10	0.52
1:A:23:MET:CG	1:A:65:ILE:HD12	2.40	0.51
1:A:23:MET:HG2	1:A:65:ILE:HD12	1.93	0.51
1:C:21:ASP:HA	1:C:23:MET:HE1	1.93	0.51
1:B:68:LEU:HD21	1:B:152:LEU:HD23	1.93	0.50
2:D:300:GLN:HG3	2:D:300:GLN:O	2.10	0.50
2:F:300:GLN:HE22	2:F:346:ILE:HG21	1.76	0.50
1:A:103:MET:HE1	1:C:103:MET:HE1	1.93	0.50
1:C:21:ASP:HA	1:C:23:MET:HE2	1.93	0.49
1:A:79:TYR:CE2	1:A:152:LEU:HB2	2.48	0.49
1:C:79:TYR:CE2	1:C:152:LEU:HB2	2.48	0.49
2:E:287:THR:HA	4:E:503:SO4:O2	2.12	0.49
1:C:23:MET:HE3	1:C:152:LEU:HD22	1.93	0.49
2:E:300:GLN:O	2:E:300:GLN:HG3	2.12	0.49
2:D:38[A]:GLU:OE1	8:D:601:HOH:O	2.20	0.48
2:E:124:VAL:HG12	2:E:125:LYS:HD2	1.95	0.48
1:A:23:MET:HE3	1:A:152:LEU:HD22	1.95	0.48
1:B:114:GLU:OE1	8:B:302:HOH:O	2.19	0.48
1:C:19:ASP:OD1	1:C:81:HIS:ND1	2.45	0.47
1:B:11:ASN:HB3	1:B:83:LEU:HD13	1.96	0.47
1:A:33:ASP:CB	8:A:300:HOH:O	2.59	0.47
1:B:76:ARG:HG2	8:B:365:HOH:O	2.15	0.47
1:A:68:LEU:HD21	1:A:152:LEU:HD23	1.96	0.47
2:E:346:ILE:HA	2:E:353:SER:OG	2.15	0.47
2:F:38[B]:GLU:OE1	2:F:158:SER:OG	2.28	0.46
2:E:5:ILE:HD11	8:E:681:HOH:O	2.14	0.46
3:H:21:ARG:HH11	3:H:21:ARG:HG2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:290:ILE:HG13	7:E:504:8IB:C4	2.46	0.46
2:F:346:ILE:HA	2:F:353:SER:OG	2.15	0.46
2:E:213:LEU:HD23	2:F:105:HIS:HA	1.98	0.46
1:C:73:ILE:HB	2:F:355:GLU:HG2	1.98	0.45
1:A:20:SER:O	1:A:21:ASP:CB	2.63	0.45
2:D:171:GLU:HG2	2:D:233:ILE:HG21	1.98	0.45
3:H:111:TRP:CD1	3:H:115:CYS:HB2	2.51	0.45
2:D:226:LEU:HD12	2:E:120:PHE:CD2	2.52	0.45
1:A:103:MET:HE1	1:B:103:MET:HE1	1.99	0.44
2:F:290:ILE:HG13	7:F:504:8IB:C5	2.48	0.44
2:F:290:ILE:HG13	7:F:504:8IB:C4	2.48	0.44
1:C:149:LEU:C	1:C:149:LEU:HD12	2.43	0.43
2:E:181:HIS:NE2	2:E:182:LYS:HE2	2.33	0.43
1:B:76:ARG:HG3	8:B:379:HOH:O	2.18	0.42
1:B:18:VAL:O	1:B:23:MET:HE1	2.18	0.42
2:D:300:GLN:HE22	2:D:346:ILE:HG21	1.85	0.42
1:A:149:LEU:C	1:A:149:LEU:HD12	2.44	0.42
1:A:85:LEU:HD11	1:C:8:ALA:HB1	2.00	0.42
2:E:294:PHE:HA	2:E:295:PRO:HA	1.86	0.42
2:F:66:VAL:O	2:F:77:ALA:HA	2.20	0.42
1:C:35:HIS:O	1:C:136:GLU:HA	2.19	0.42
2:E:182:LYS:HB2	2:E:183:PRO:CD	2.49	0.42
1:A:20:SER:O	1:A:21:ASP:HB3	2.19	0.41
1:B:35:HIS:O	1:B:136:GLU:HA	2.20	0.41
1:B:132:LEU:HA	1:B:132:LEU:HD12	1.87	0.41
2:D:179:VAL:HG13	2:D:299:LEU:HD21	2.01	0.41
1:A:52:ILE:HD11	1:A:150:MET:SD	2.61	0.41
1:B:149:LEU:HD12	1:B:149:LEU:C	2.46	0.41
2:F:182:LYS:HB2	2:F:183:PRO:CD	2.50	0.41
1:A:35:HIS:O	1:A:136:GLU:HA	2.21	0.41
1:B:19:ASP:OD1	1:B:81:HIS:ND1	2.47	0.40
2:E:33:ARG:HD3	8:E:730:HOH:O	2.21	0.40
3:H:83:LEU:HD22	3:H:91:SER:HA	2.03	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	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
1	B	152/154 (99%)	147 (97%)	5 (3%)	0	100	100
1	C	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
2	D	387/428 (90%)	369 (95%)	17 (4%)	1 (0%)	36	28
2	E	399/428 (93%)	384 (96%)	15 (4%)	0	100	100
2	F	377/428 (88%)	364 (97%)	12 (3%)	1 (0%)	36	28
3	H	127/129 (98%)	127 (100%)	0	0	100	100
All	All	1746/1875 (93%)	1685 (96%)	59 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	296	GLY
2	F	296	GLY

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	129/129 (100%)	128 (99%)	1 (1%)	73	74
1	B	129/129 (100%)	129 (100%)	0	100	100
1	C	129/129 (100%)	129 (100%)	0	100	100
2	D	324/355 (91%)	317 (98%)	7 (2%)	45	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	334/355 (94%)	327 (98%)	7 (2%)	47	41
2	F	316/355 (89%)	313 (99%)	3 (1%)	70	70
3	H	105/105 (100%)	103 (98%)	2 (2%)	50	45
All	All	1466/1557 (94%)	1446 (99%)	20 (1%)	61	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
2	D	179	VAL
2	D	216	MET
2	D	241	HIS
2	D	283	GLU
2	D	387	SER
2	D	388	GLU
2	D	390	ARG
2	E	38	GLU
2	E	122	LYS
2	E	215[A]	HIS
2	E	215[B]	HIS
2	E	226	LEU
2	E	241	HIS
2	E	353	SER
2	F	216	MET
2	F	241	HIS
2	F	410	GLU
3	H	25	LEU
3	H	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	135	GLN
2	D	101	GLN
2	D	181	HIS
2	D	228	GLN
2	D	310	GLN
2	D	322	ASN
2	E	7	GLN

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Mol	Chain	Res	Type
2	E	303	GLN
2	E	310	GLN
2	E	322	ASN
2	E	424	HIS
2	F	204	ASN
2	F	303	GLN
2	F	310	GLN
2	F	322	ASN
3	H	44	ASN
3	H	46	ASN
3	H	57	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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FES	F	501	2	0,4,4	-	-	-		
5	FES	D	501	2	0,4,4	-	-	-		
4	SO4	E	503	-	4,4,4	0.31	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	8IB	F	504	-	13,13,13	1.19	2 (15%)	18,18,18	0.71	0
7	8IB	D	504	-	13,13,13	0.98	1 (7%)	18,18,18	0.83	0
5	FES	E	501	2	0,4,4	-	-	-	-	-
4	SO4	H	201	-	4,4,4	0.32	0	6,6,6	0.35	0
4	SO4	E	502	-	4,4,4	0.58	0	6,6,6	0.26	0
4	SO4	F	502	-	4,4,4	0.67	0	6,6,6	0.45	0
4	SO4	D	502	-	4,4,4	0.41	0	6,6,6	0.12	0
4	SO4	B	201	-	4,4,4	0.32	0	6,6,6	0.13	0
7	8IB	E	504	-	13,13,13	1.19	3 (23%)	18,18,18	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FES	F	501	2	-	-	0/1/1/1
5	FES	D	501	2	-	-	0/1/1/1
7	8IB	F	504	-	-	0/8/8/8	0/1/1/1
7	8IB	D	504	-	-	0/8/8/8	0/1/1/1
5	FES	E	501	2	-	-	0/1/1/1
7	8IB	E	504	-	-	0/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	504	8IB	O4-C8	2.40	1.29	1.22
7	D	504	8IB	C6-C7	2.32	1.54	1.49
7	E	504	8IB	C3-C8	2.30	1.54	1.49
7	E	504	8IB	O1-C7	-2.28	1.23	1.30
7	F	504	8IB	C6-C7	2.23	1.54	1.49
7	F	504	8IB	C3-C8	2.07	1.54	1.49

There are no bond angle outliers.

There are no chirality outliers.

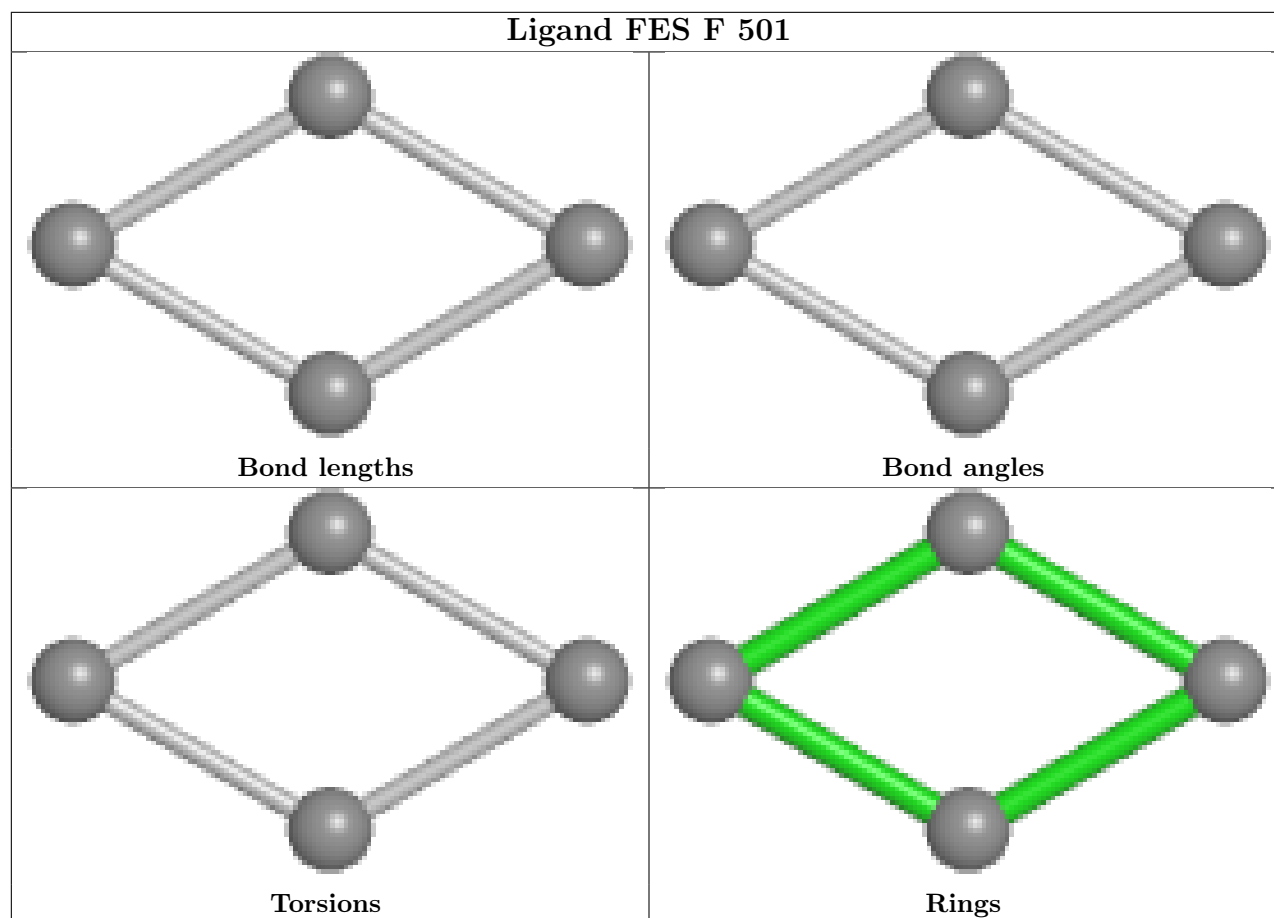
There are no torsion outliers.

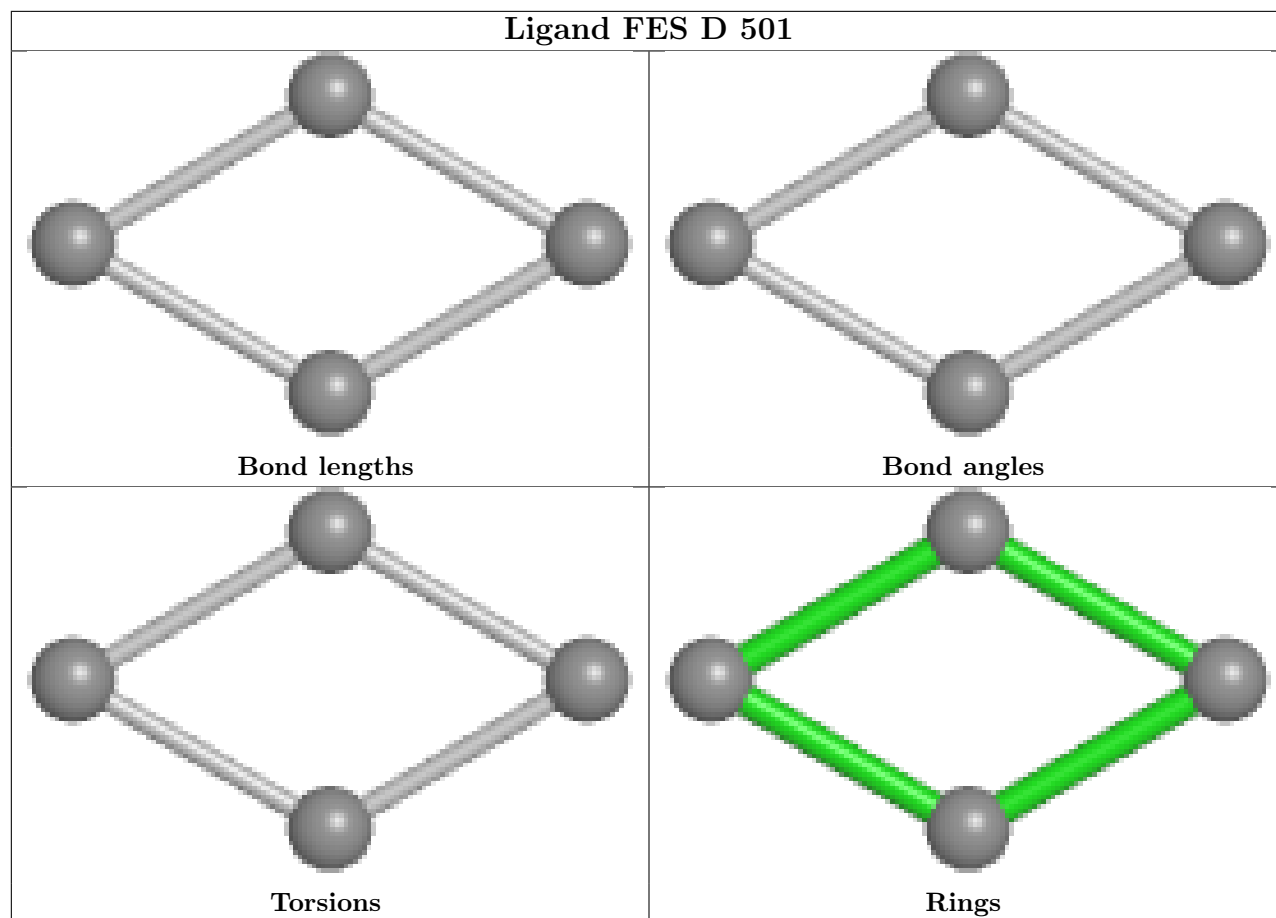
There are no ring outliers.

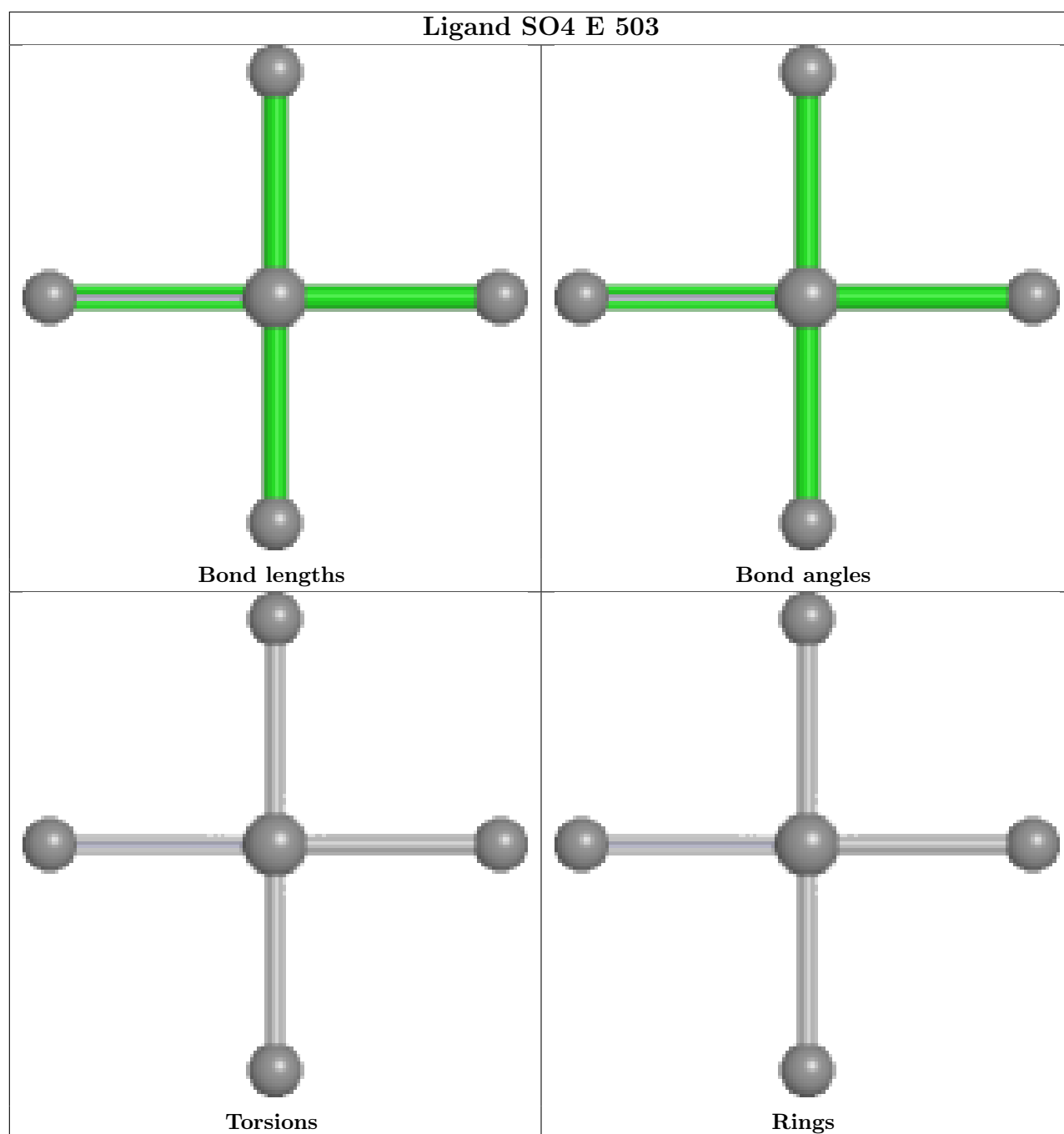
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	503	SO4	1	0
7	F	504	8IB	2	0
7	E	504	8IB	2	0

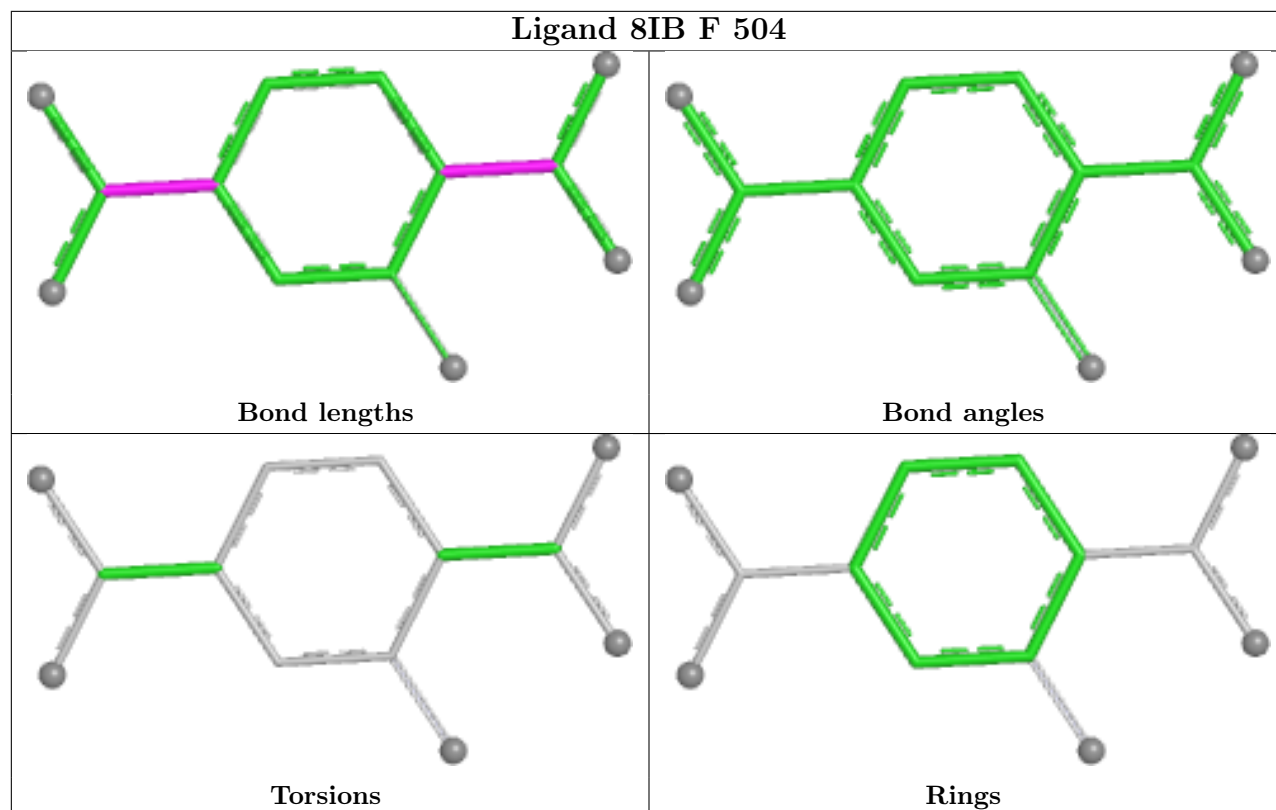
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



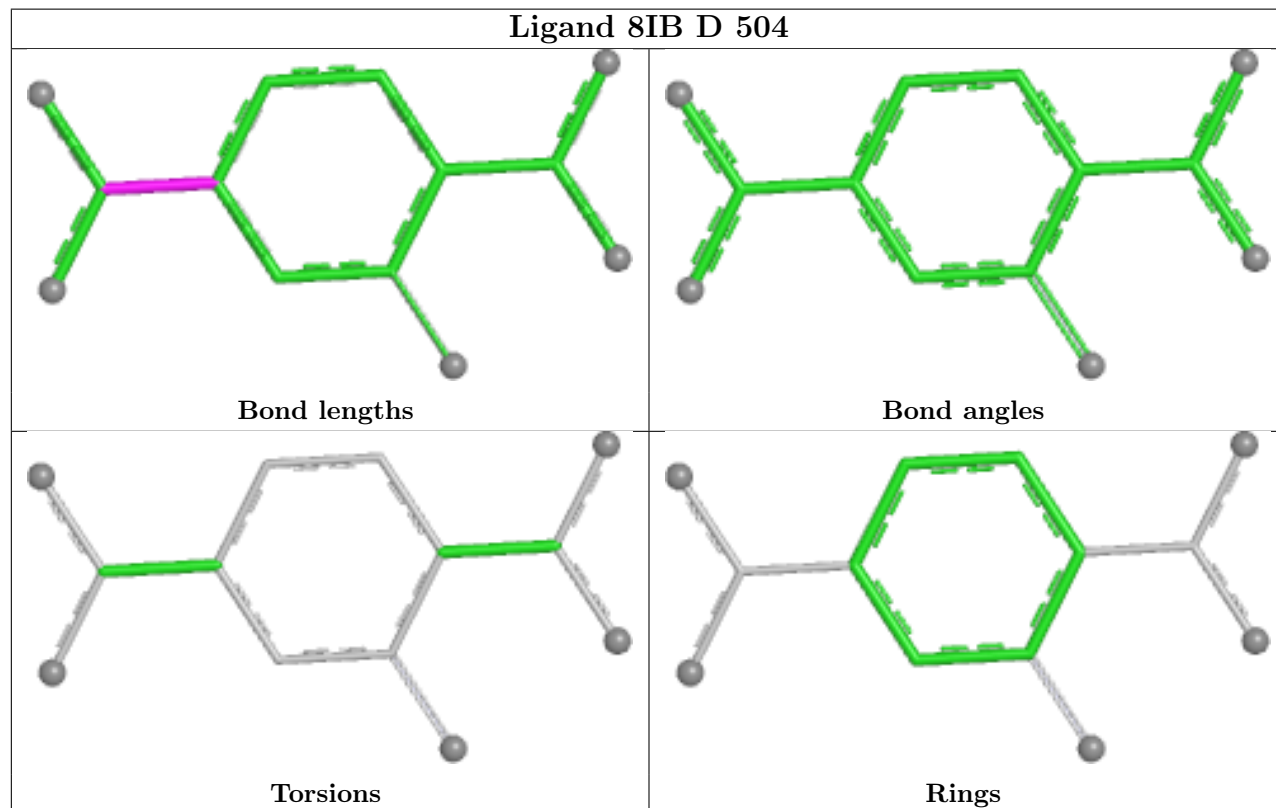


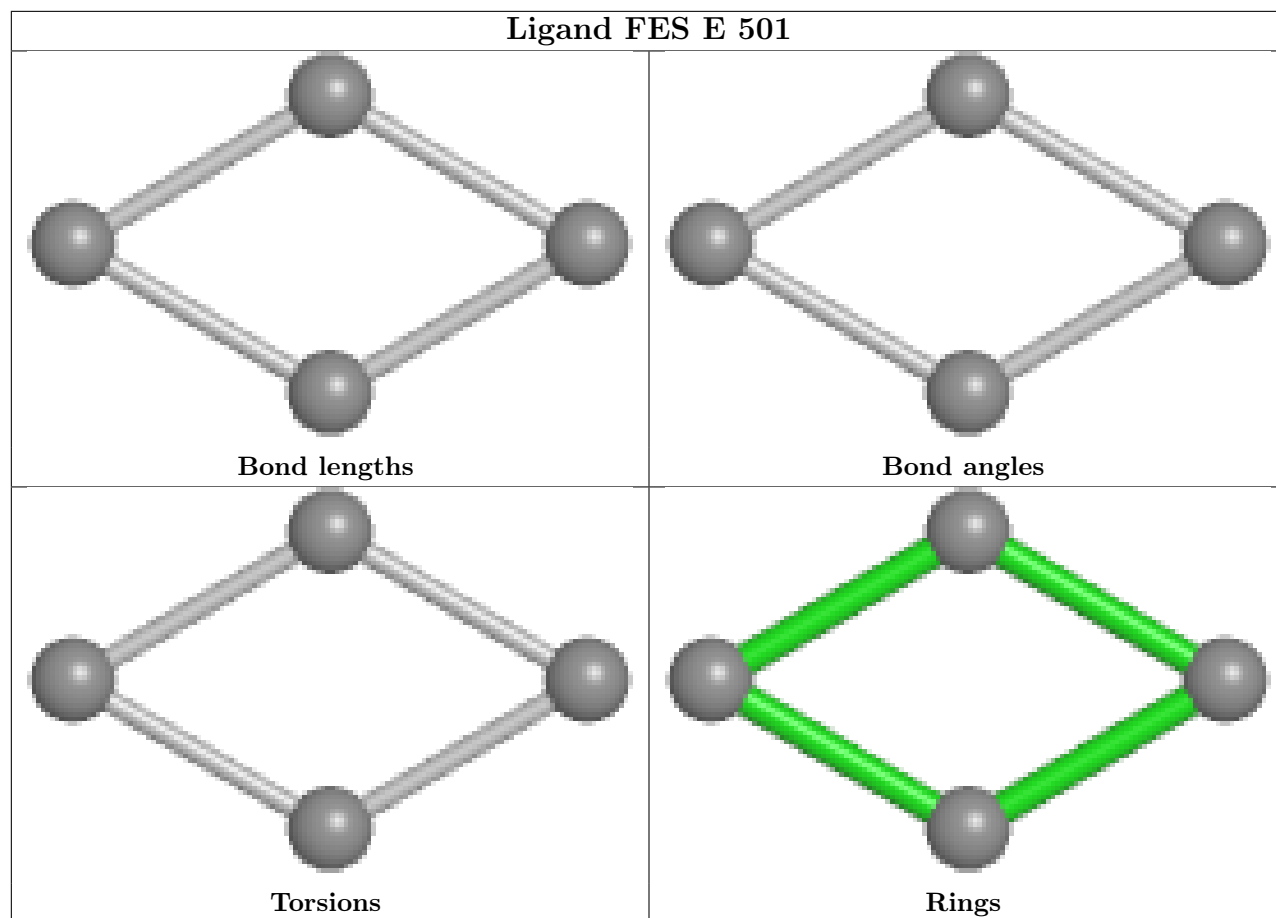


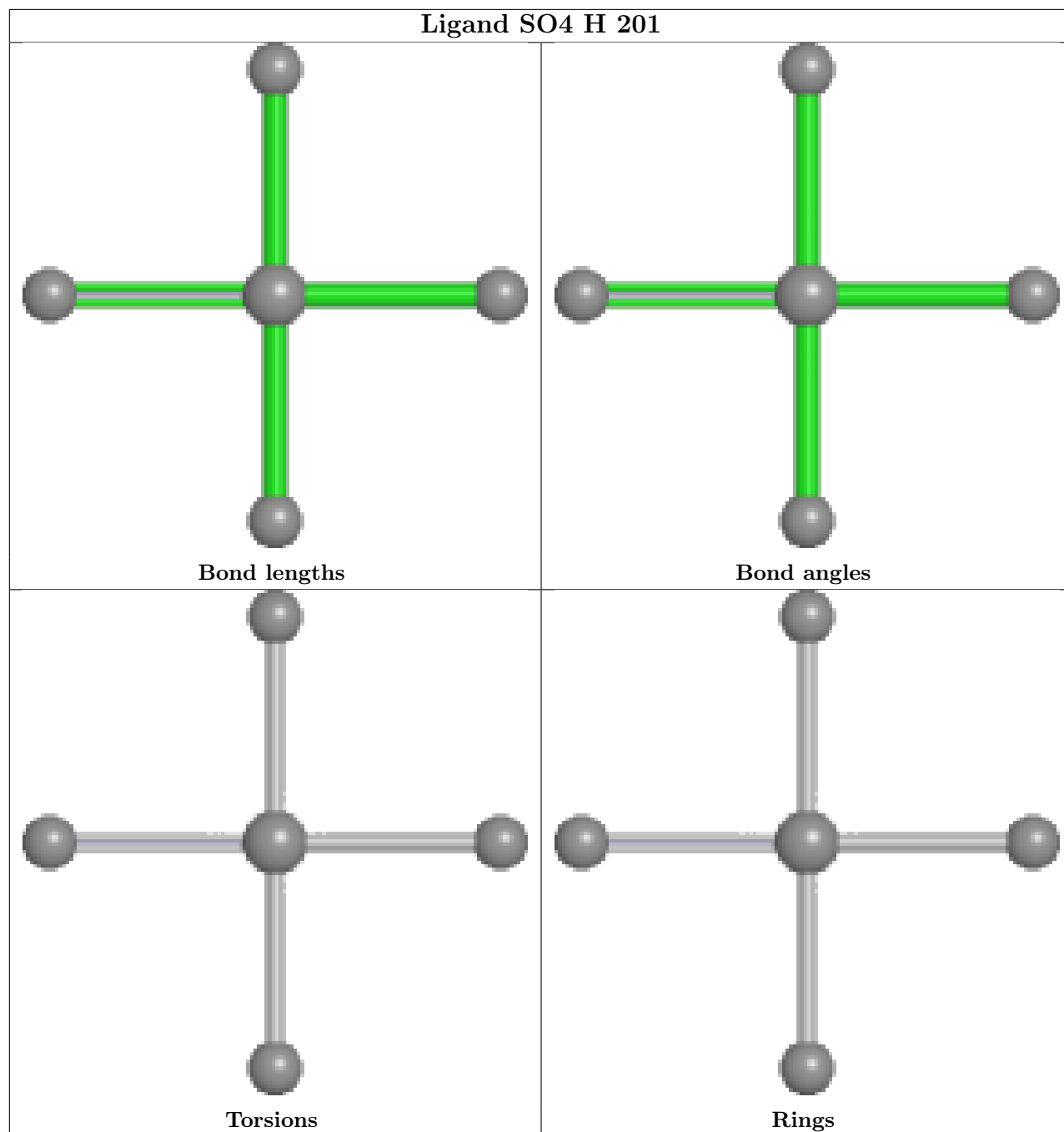
Ligand 8IB F 504

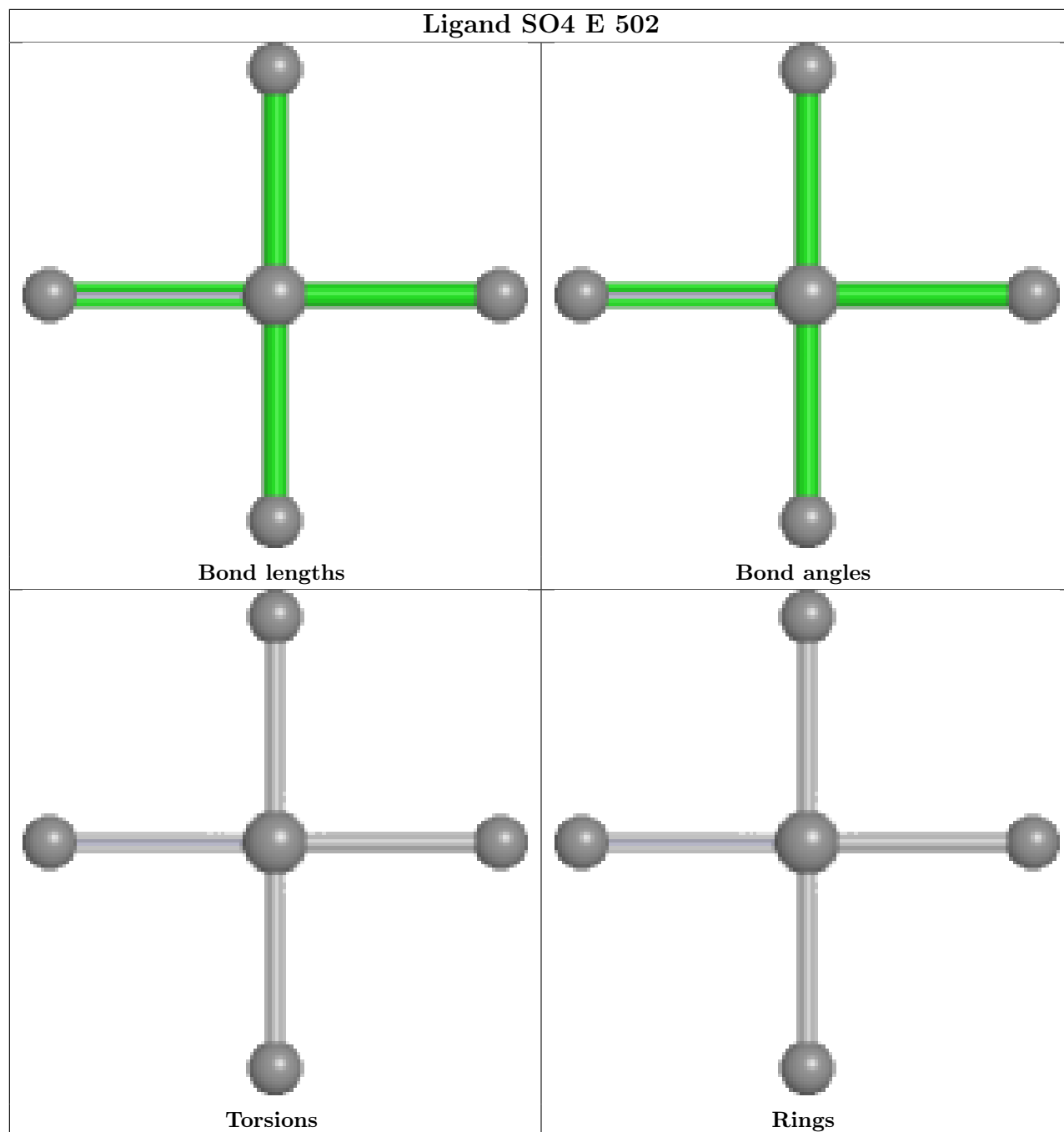


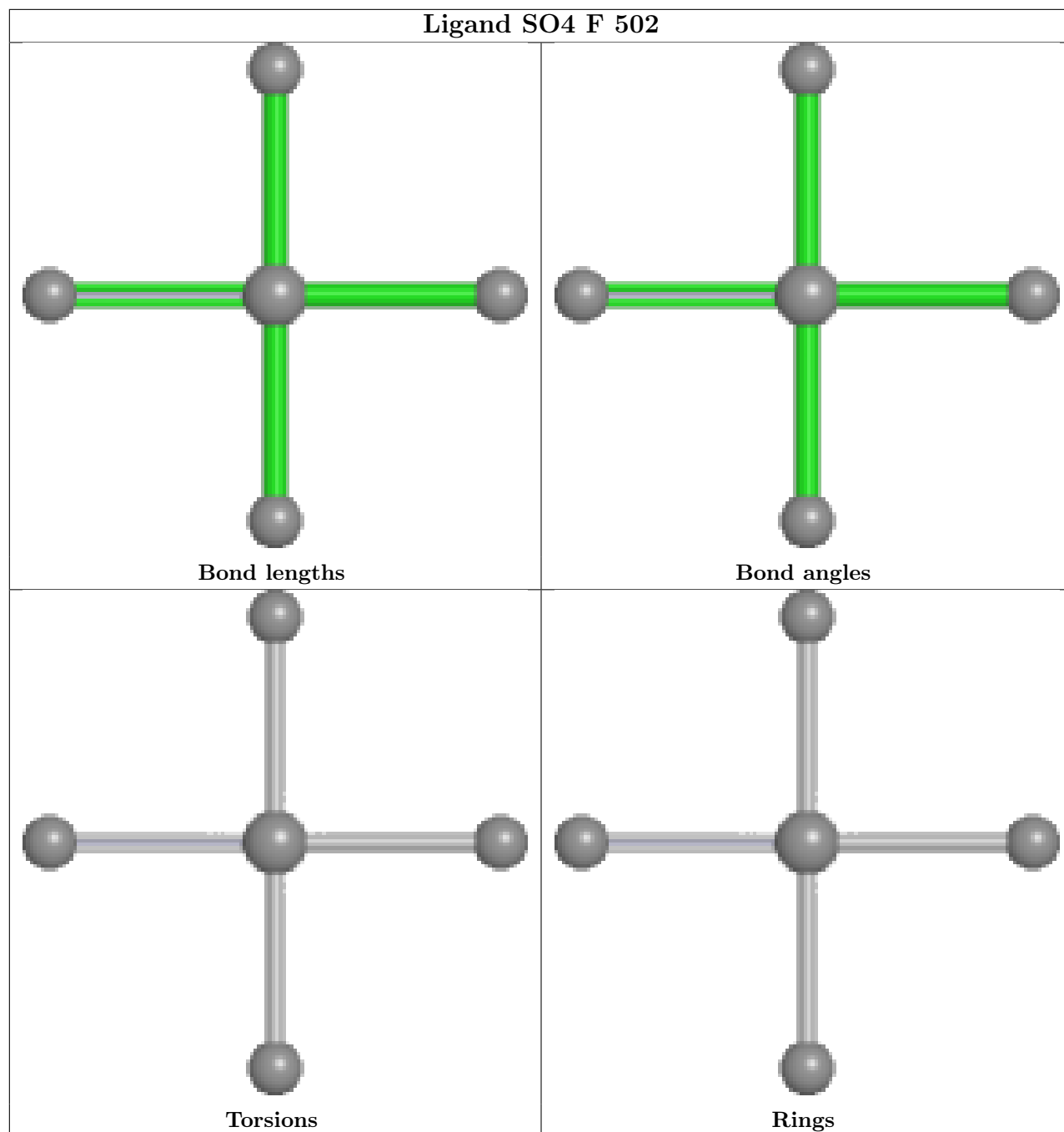
Ligand 8IB D 504

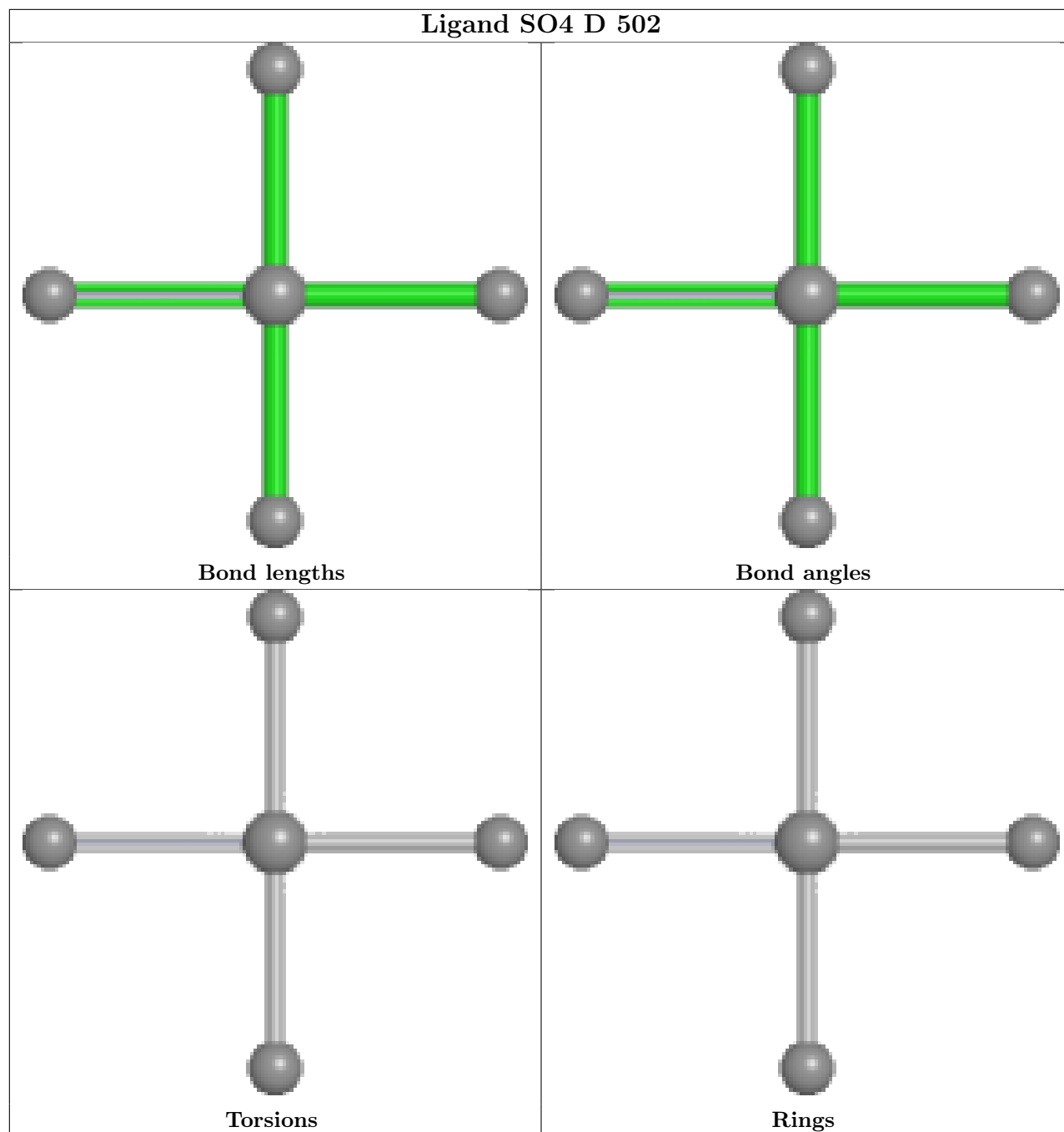


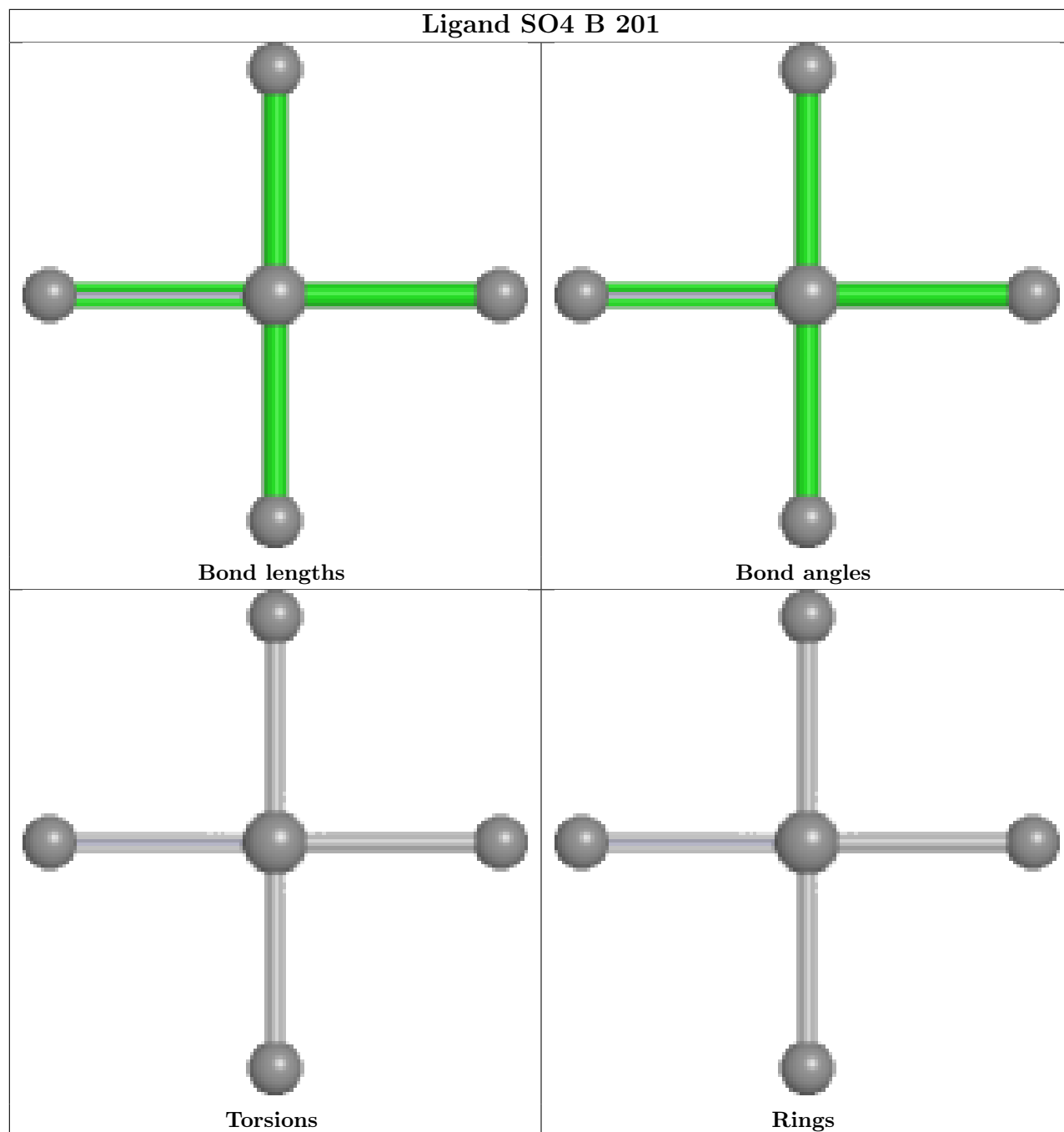


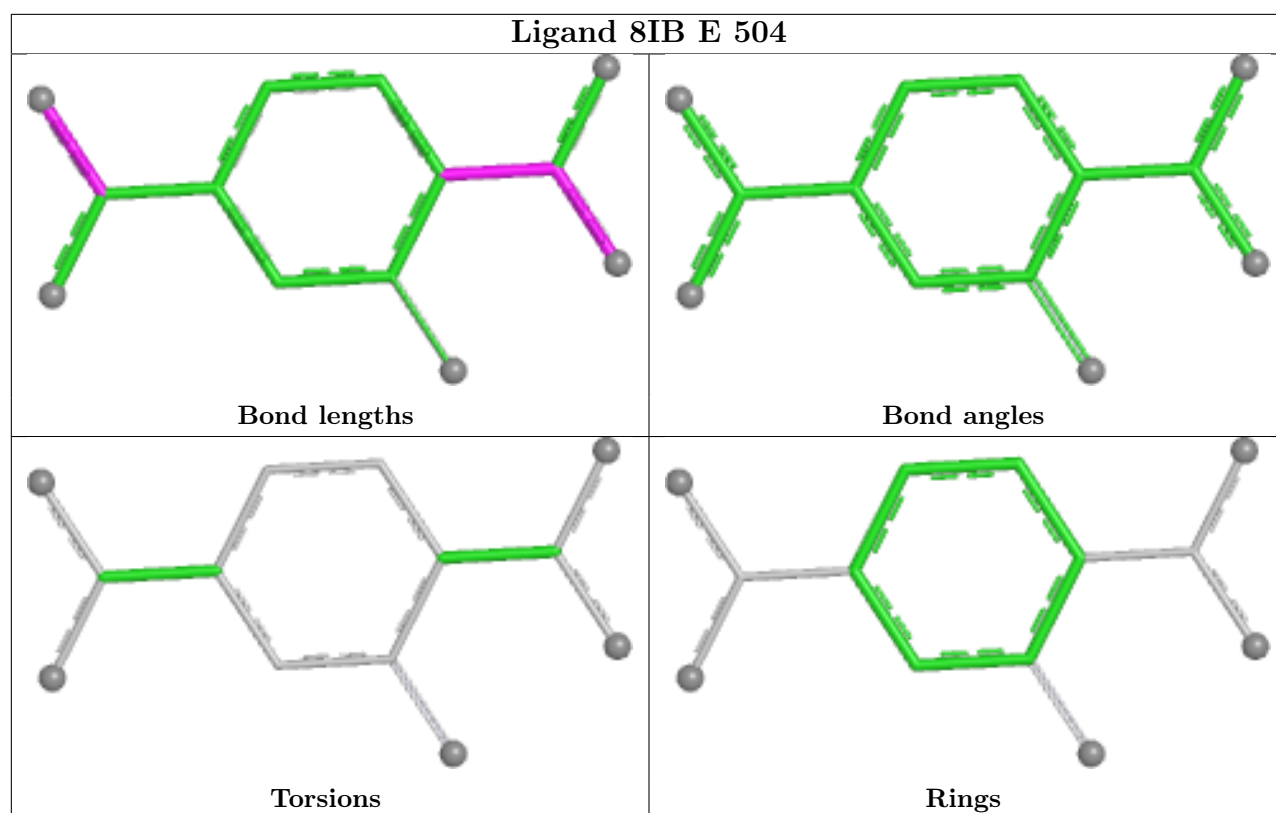












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	154/154 (100%)	-0.38	0 100 100	27, 37, 55, 77	0
1	B	154/154 (100%)	-0.16	2 (1%) 75 81	27, 39, 65, 92	0
1	C	154/154 (100%)	-0.32	0 100 100	28, 40, 60, 77	0
2	D	389/428 (90%)	0.06	12 (3%) 51 58	20, 47, 78, 110	2 (0%)
2	E	403/428 (94%)	-0.18	16 (3%) 42 49	24, 39, 69, 117	2 (0%)
2	F	381/428 (89%)	-0.13	12 (3%) 51 58	27, 41, 70, 116	2 (0%)
3	H	129/129 (100%)	-0.18	0 100 100	29, 43, 70, 83	0
All	All	1764/1875 (94%)	-0.15	42 (2%) 59 66	20, 41, 71, 117	6 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	247	ILE	6.4
2	D	268	TYR	5.8
2	E	221	PHE	5.6
2	F	218	PHE	5.1
2	F	219	THR	4.6
2	F	214	LEU	4.3
2	D	247	ILE	3.9
2	F	215	HIS	3.8
2	D	221	PHE	3.8
2	D	389	GLY	3.7
2	D	225	ARG	3.5
2	D	223	LEU	3.4
2	D	411	MET	3.3
2	E	132	ALA	3.2
2	F	217	PHE	3.1
2	D	9	HIS	3.0
2	E	413	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	211	ALA	3.0
2	E	226	LEU	2.9
2	E	215[A]	HIS	2.9
2	F	213	LEU	2.9
2	F	216	MET	2.9
1	B	1	MET	2.8
2	F	9	HIS	2.8
2	E	421	HIS	2.8
2	E	422	HIS	2.8
2	D	218	PHE	2.7
1	B	93	ALA	2.6
2	F	352	ILE	2.6
2	E	420	GLY	2.6
2	E	423	HIS	2.5
2	E	412	GLN	2.5
2	D	219	THR	2.3
2	E	352	ILE	2.3
2	D	216	MET	2.3
2	E	220	THR	2.3
2	E	124	VAL	2.3
2	E	353	SER	2.2
2	F	227	SER	2.2
2	E	411	MET	2.1
2	E	218	PHE	2.1
2	D	269	ARG	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

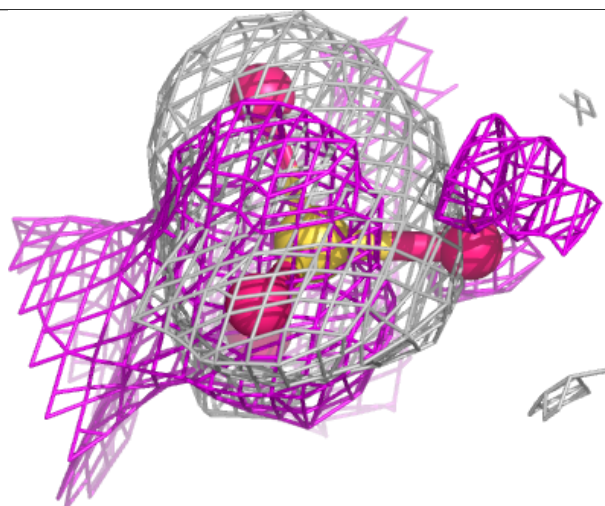
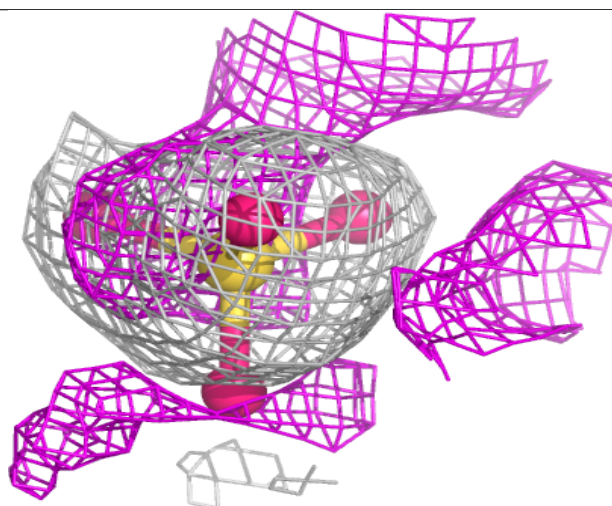
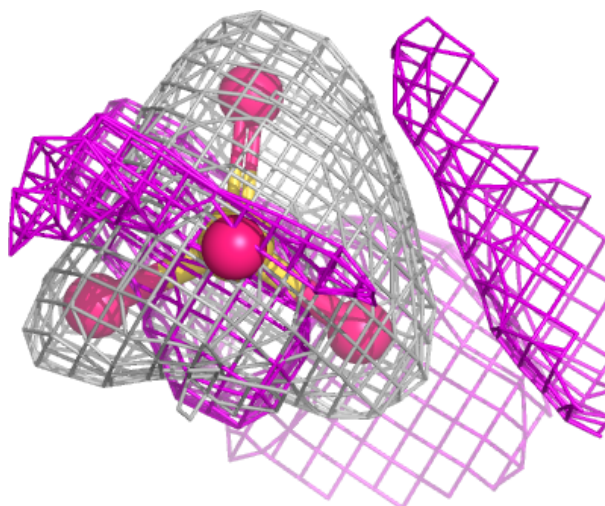
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	502	5/5	0.84	0.14	63,64,85,88	0
4	SO4	F	502	5/5	0.87	0.14	52,59,77,88	0
4	SO4	E	503	5/5	0.88	0.14	96,97,101,104	0
4	SO4	B	201	5/5	0.88	0.12	107,108,116,119	0
4	SO4	E	502	5/5	0.89	0.13	64,66,76,93	0
7	8IB	E	504	13/13	0.89	0.16	50,66,74,80	1
6	FE	F	503	1/1	0.90	0.20	113,113,113,113	0
6	FE	D	503	1/1	0.90	0.15	111,111,111,111	0
7	8IB	F	504	13/13	0.92	0.10	50,59,65,70	1
7	8IB	D	504	13/13	0.94	0.09	45,57,63,65	1
4	SO4	H	201	5/5	0.95	0.11	52,54,70,80	0
5	FES	F	501	4/4	1.00	0.02	32,34,34,34	0
5	FES	D	501	4/4	1.00	0.02	40,41,42,45	0
5	FES	E	501	4/4	1.00	0.02	36,37,37,39	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.

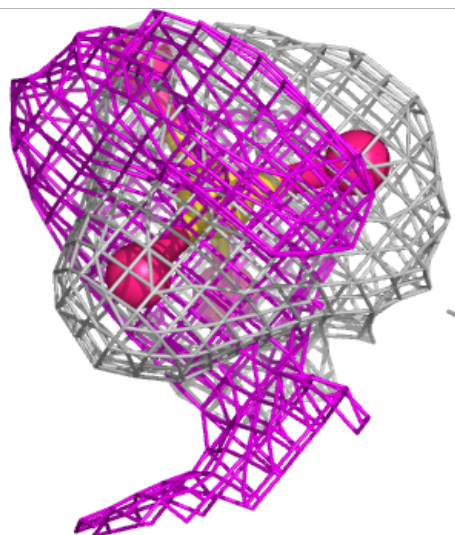
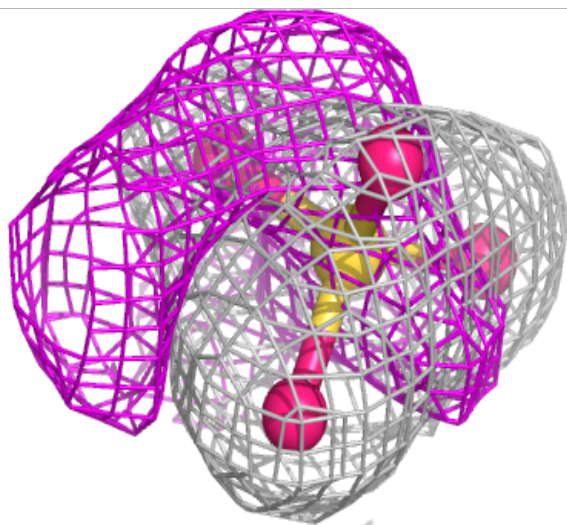
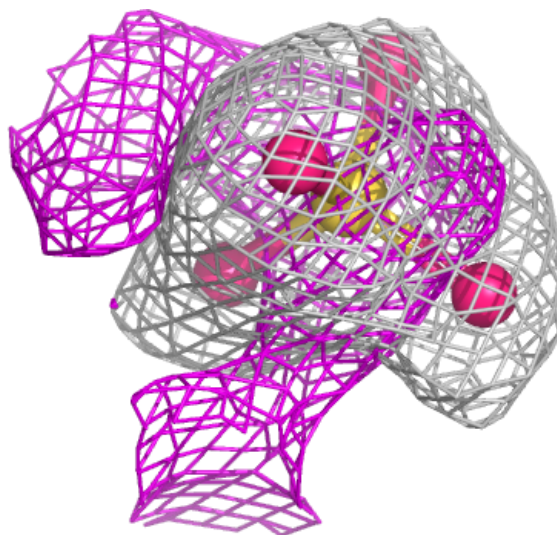
Electron density around SO4 D 502:

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



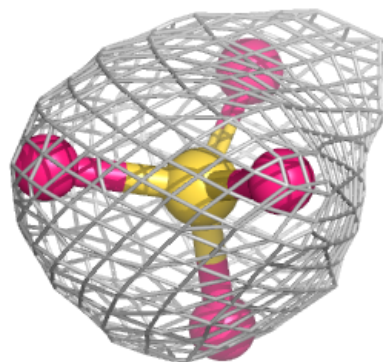
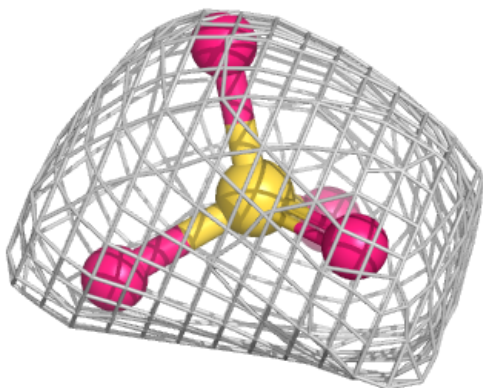
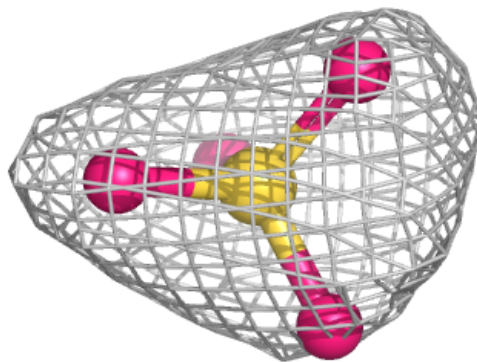
Electron density around SO4 F 502:

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

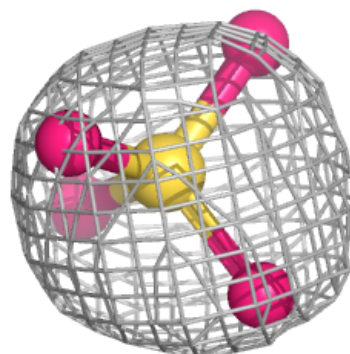
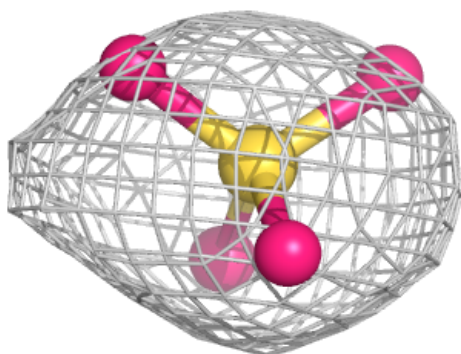
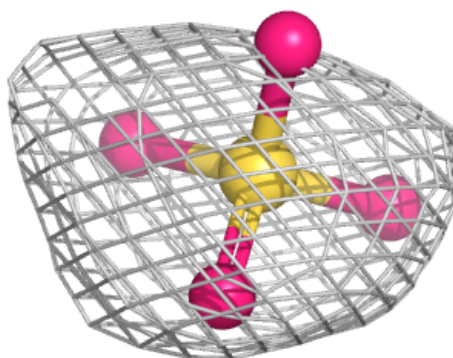


Electron density around SO4 E 503:

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

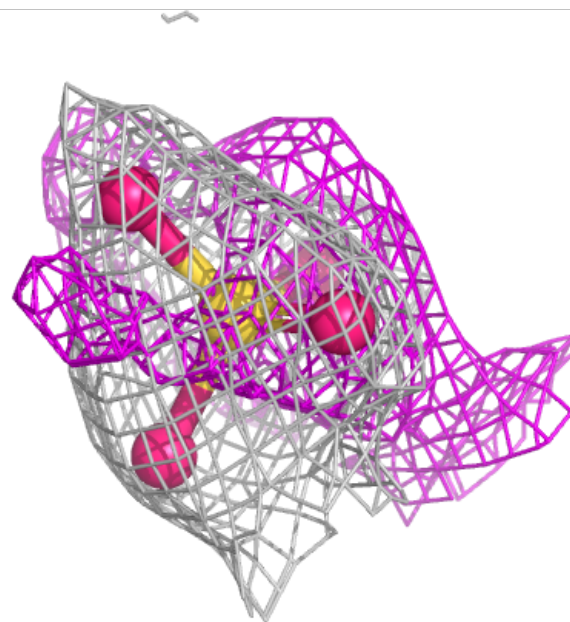
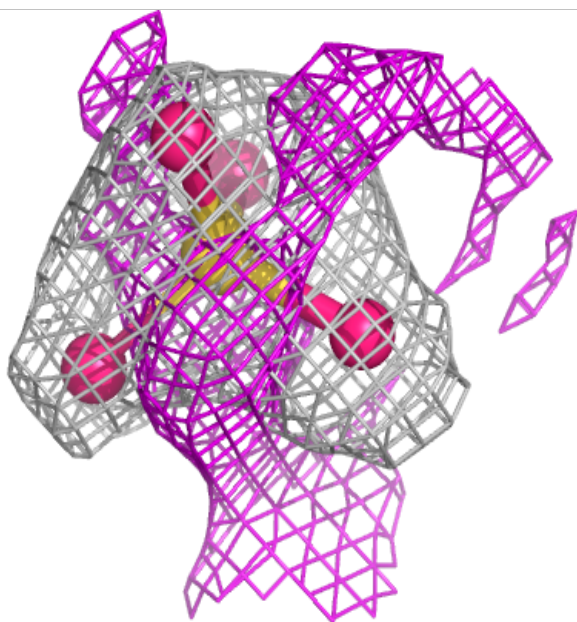
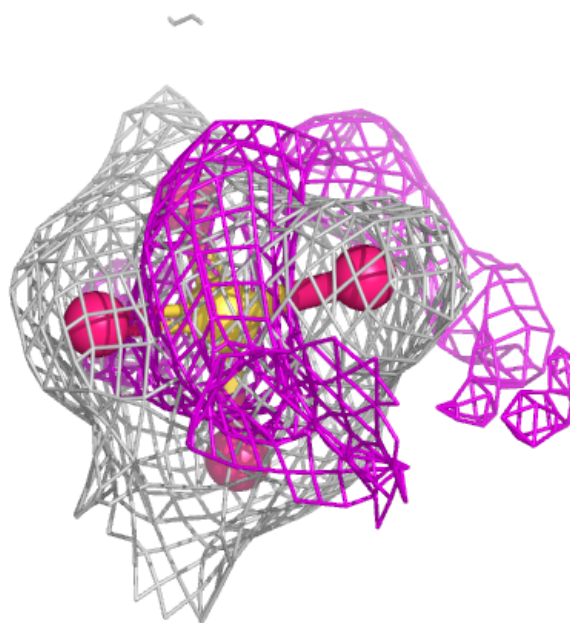
**Electron density around SO4 B 201:**

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



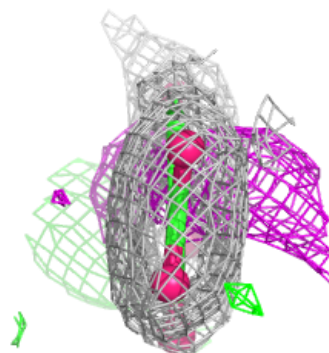
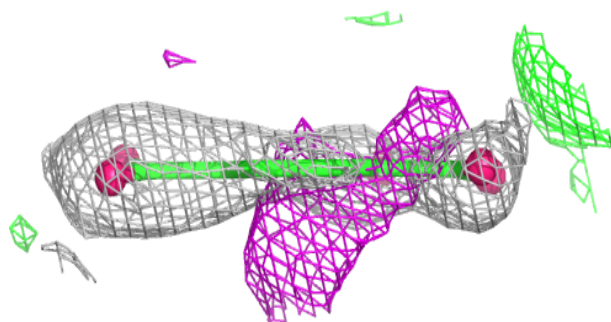
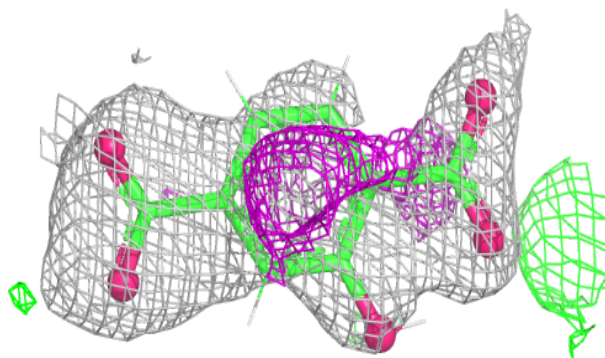
Electron density around SO4 E 502:

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



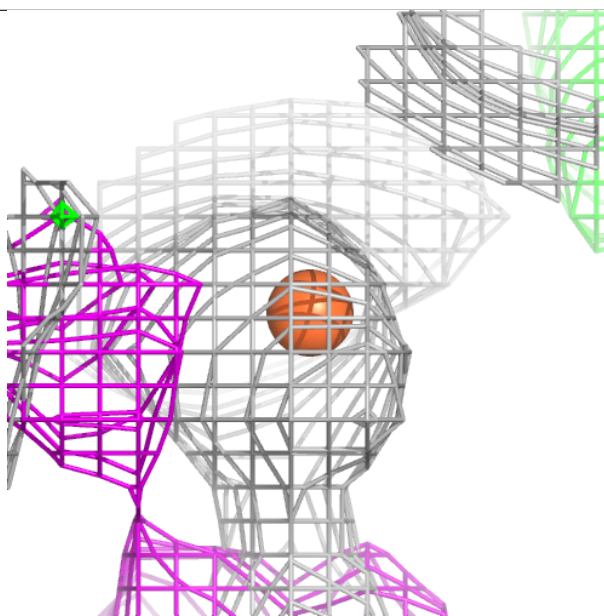
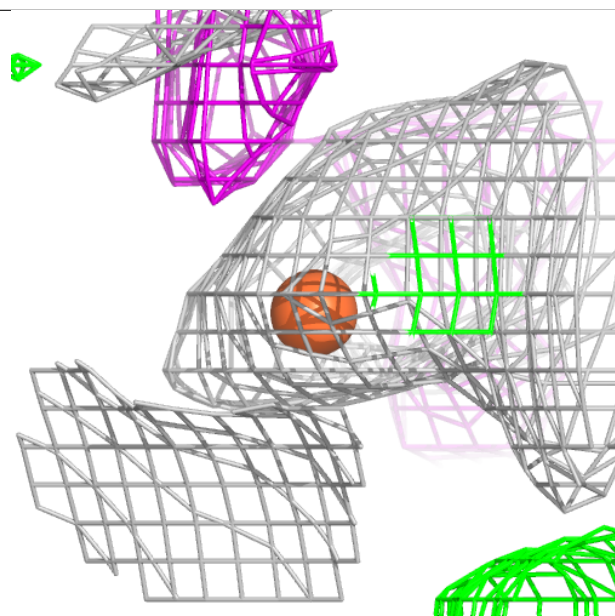
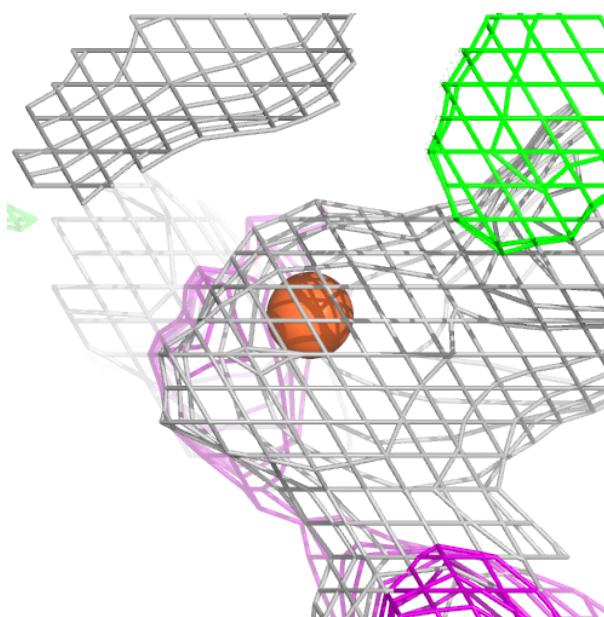
Electron density around 8IB E 504:

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



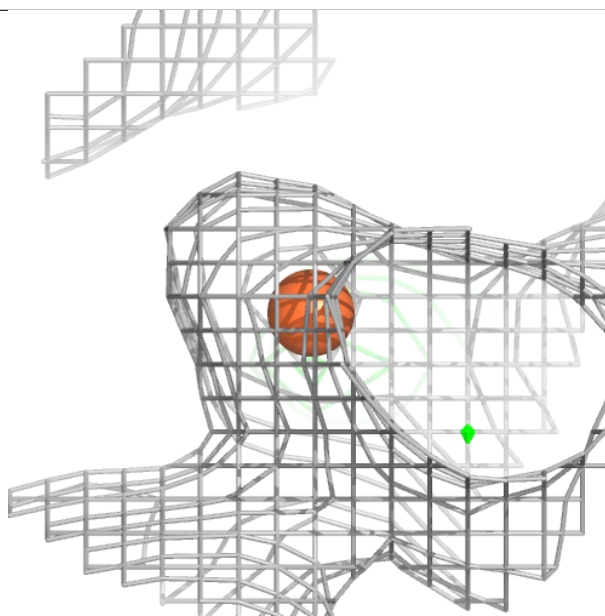
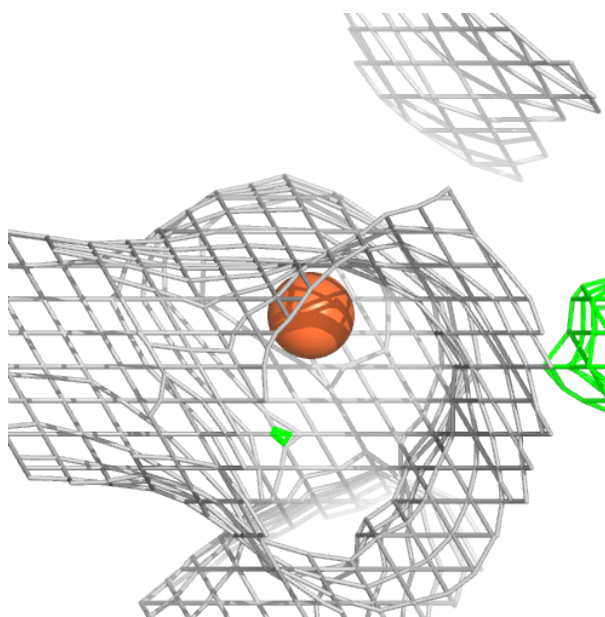
Electron density around FE F 503:

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



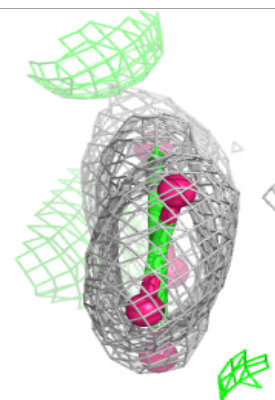
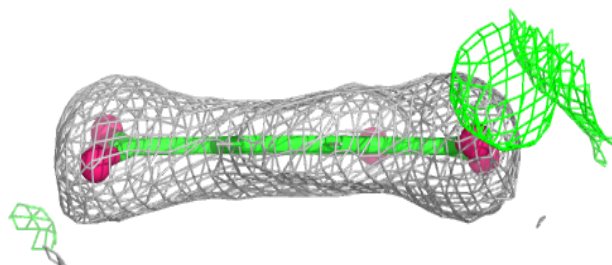
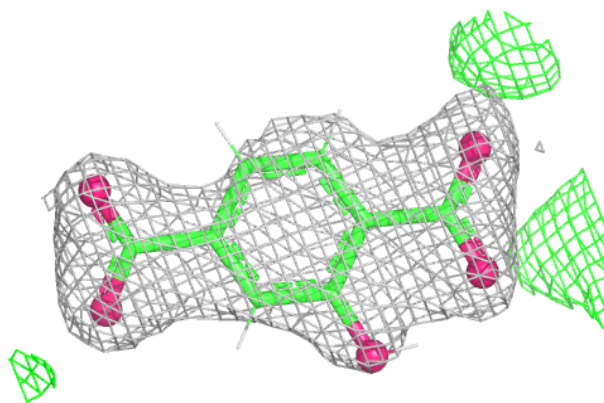
Electron density around FE D 503:

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

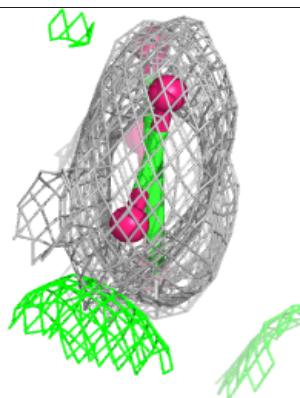
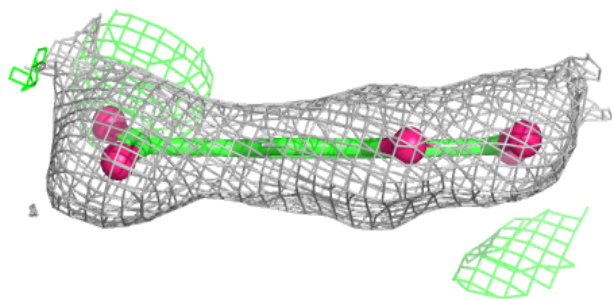
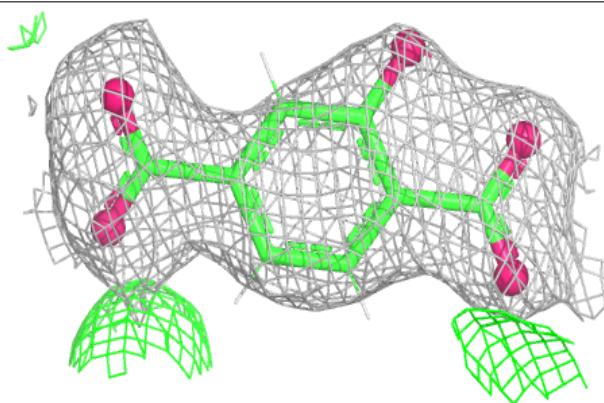


Electron density around 8IB F 504:

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

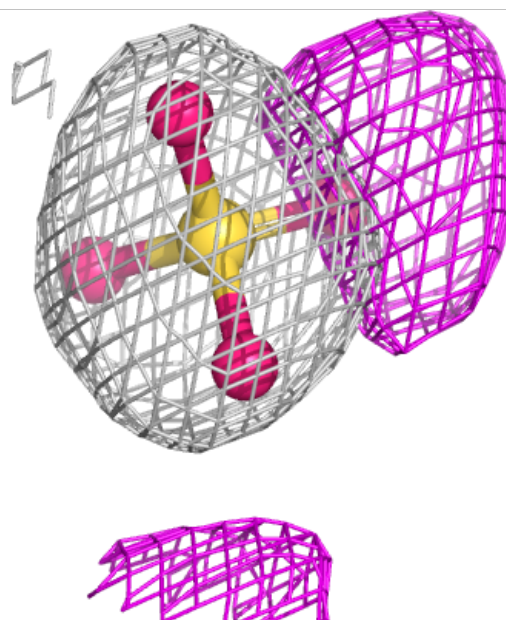
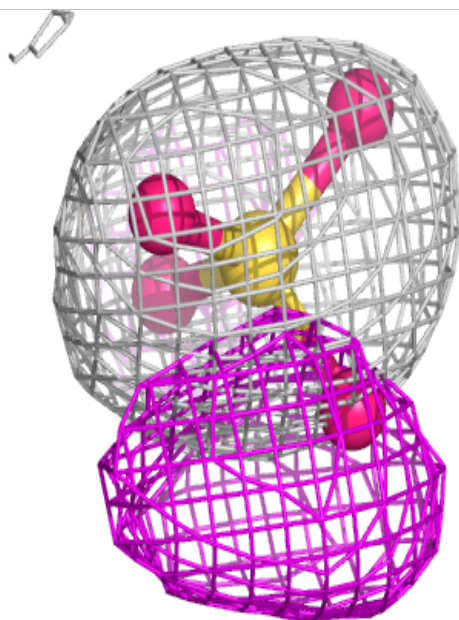
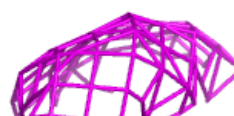
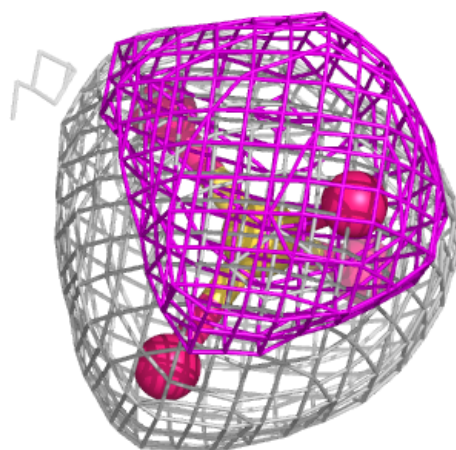
**Electron density around 8IB D 504:**

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



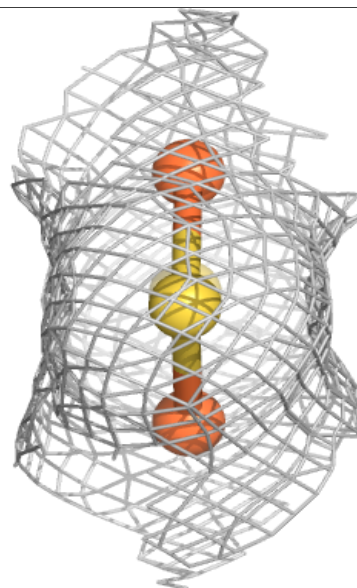
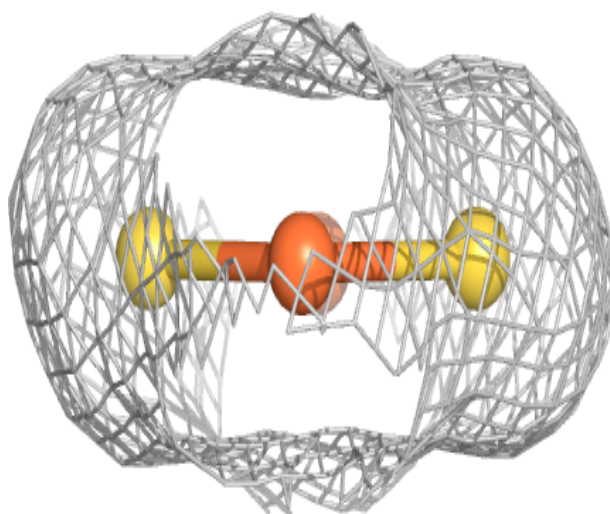
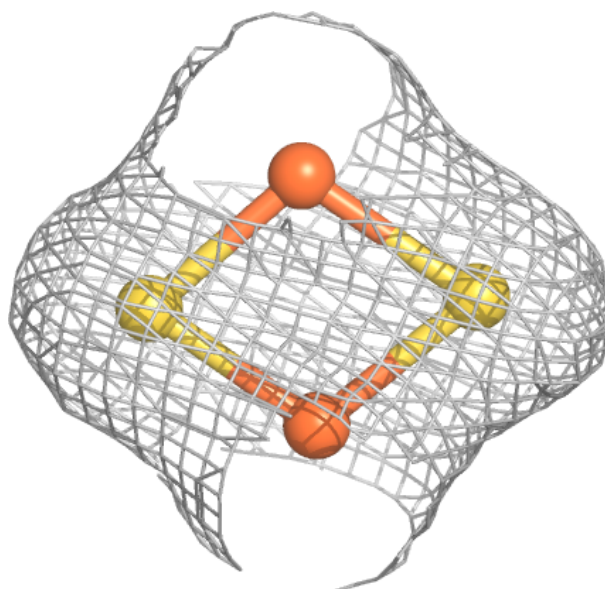
Electron density around SO4 H 201:

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



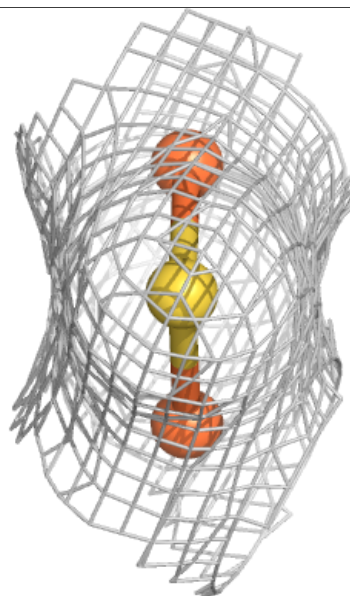
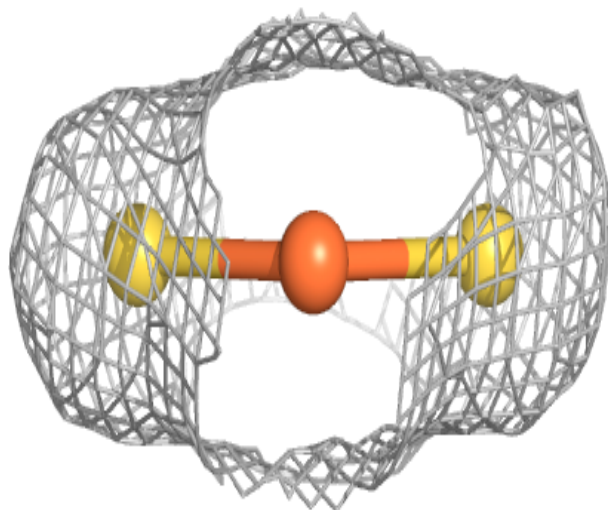
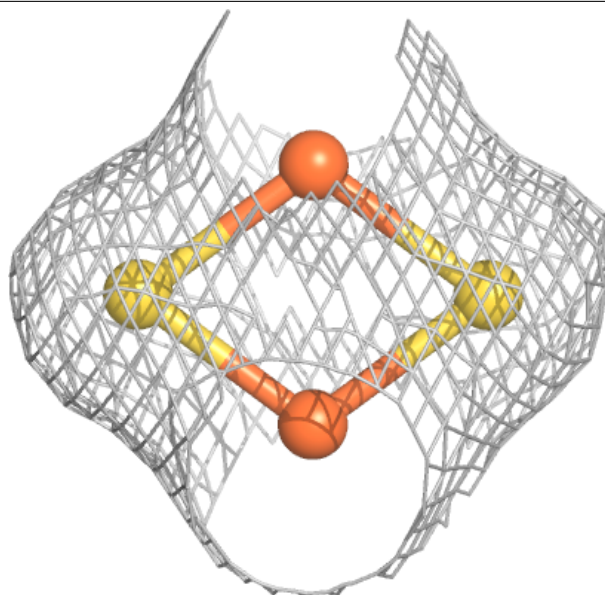
Electron density around FES F 501:

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



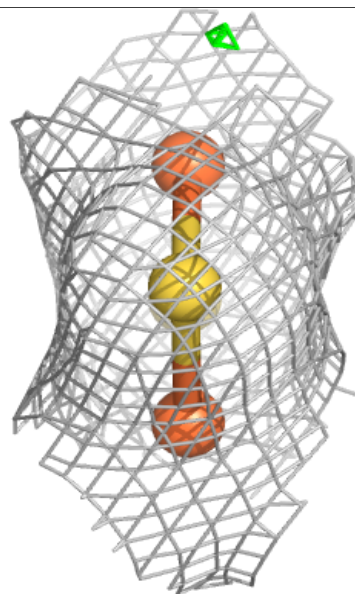
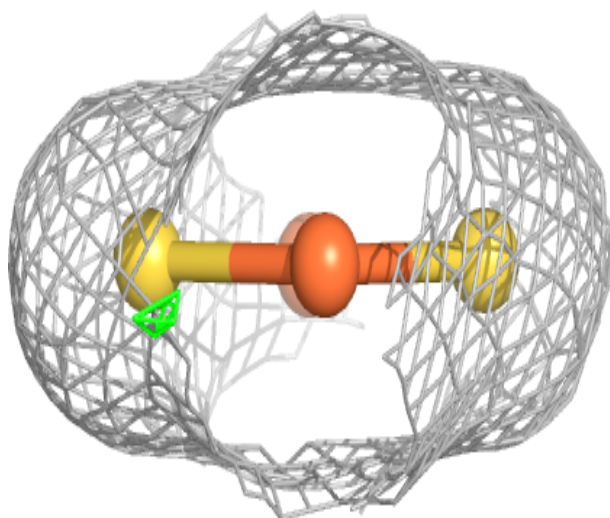
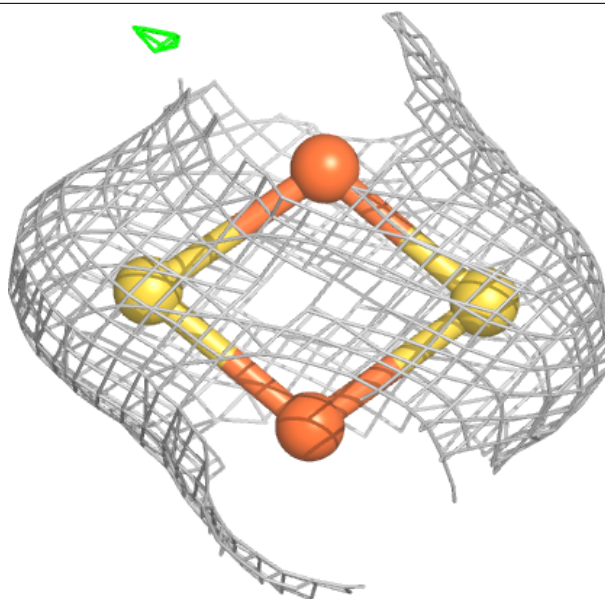
Electron density around FES D 501:

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



Electron density around FES E 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.