



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2026 – 01:30 pm BST

PDB ID : 9R9Q / pdb\_00009r9q  
Title : [FeFe]-hydrogenase from Nitratidesulfovibrio vulgaris str. Hildenborough at pH 5.04  
Authors : Bikbaev, K.; Span, I.  
Deposited on : 2025-05-20  
Resolution : 1.62 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

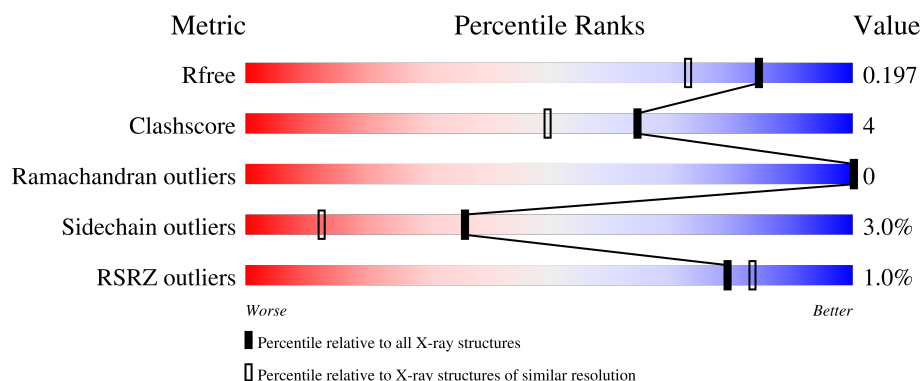
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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  $\geq 3$ , 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	405	<div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div>
2	B	88	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7821 atoms, of which 3795 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 Periplasmic [Fe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	400	Total	C	H	N	O	S	255	5	0
			6114	1951	3041	512	575	35			

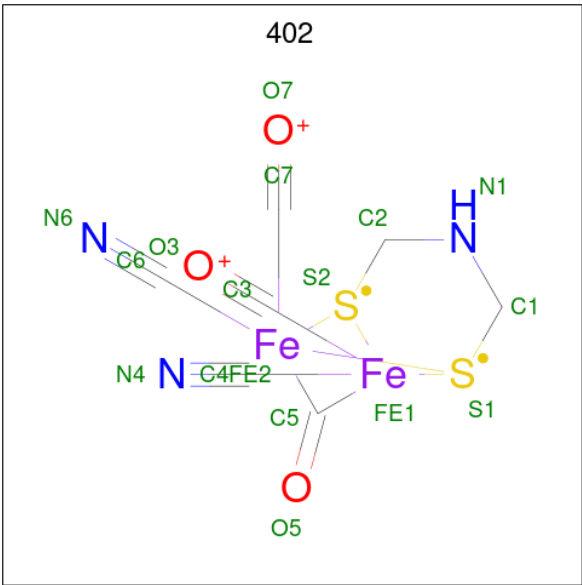
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	TRP	-	expression tag	UNP P07598
A	399	SER	-	expression tag	UNP P07598
A	400	HIS	-	expression tag	UNP P07598
A	401	PRO	-	expression tag	UNP P07598
A	402	GLN	-	expression tag	UNP P07598
A	403	PHE	-	expression tag	UNP P07598
A	404	GLU	-	expression tag	UNP P07598
A	405	LYS	-	expression tag	UNP P07598

- Molecule 2 is a protein called Periplasmic [Fe] hydrogenase small subunit.

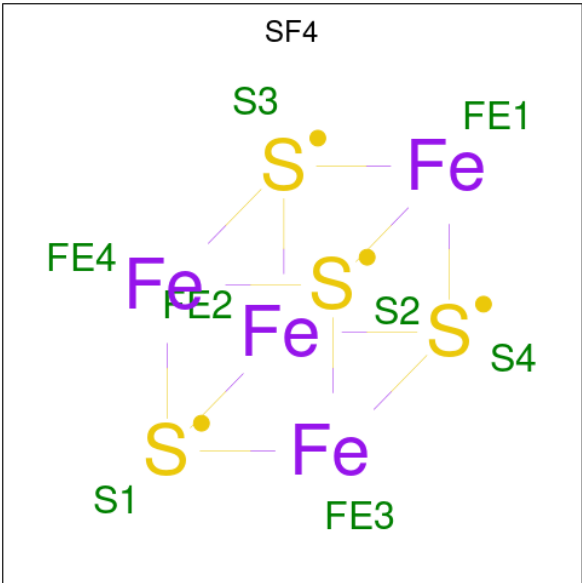
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	87	Total	C	H	N	O	S	50	4	0
			1452	466	729	124	132	1			

- Molecule 3 is dicarbonyl[bis(cyanide-kappaC)]-mu-(iminodimethanethiolatato-1kappaS:2kappaS)-mu-(oxomethylidene)diiron(2+) (CCD ID: 402) (formula: C<sub>7</sub>H<sub>5</sub>Fe<sub>2</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Fe	H	N	O	S		
3	A	1	24	7	2	7	3	3	2	1	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



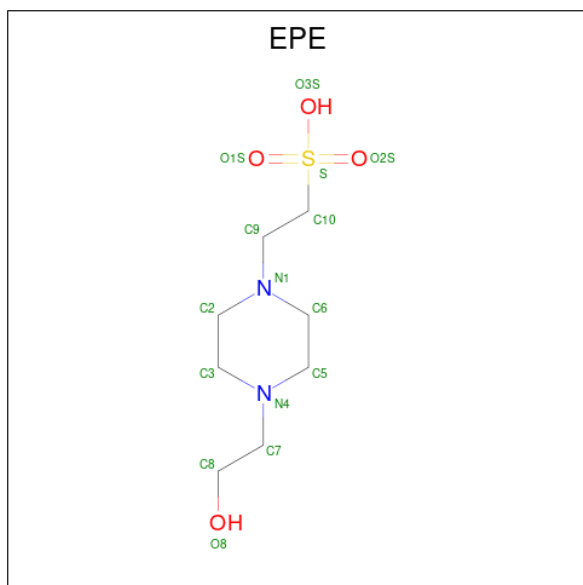
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
4	A	1	8	4	4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	2	0
			33	8	18	2	4	1		

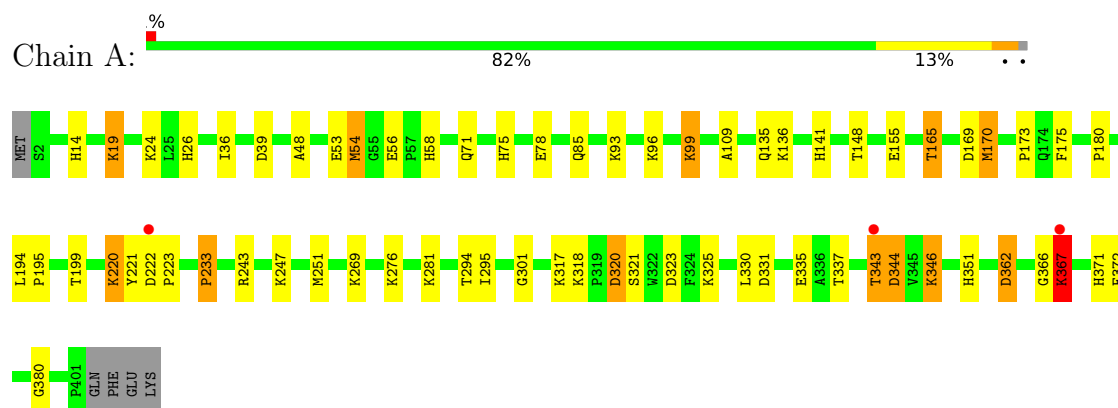
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	137	Total O 137 137	0	0
6	B	37	Total O 37 37	0	0

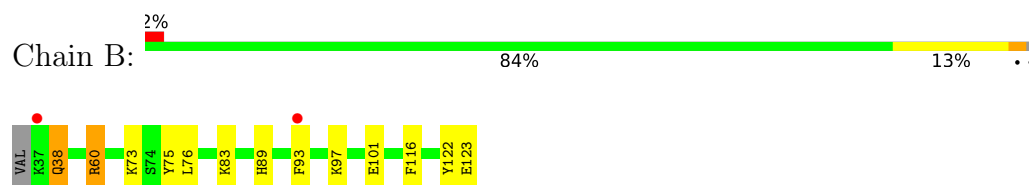
### 3 Residue-property plots [i](#)

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: Periplasmic [Fe] hydrogenase large subunit



- Molecule 2: Periplasmic [Fe] hydrogenase small subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.45Å 84.94Å 88.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 1.62 44.07 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.07-1.62) 99.0 (44.07-1.62)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.170 , 0.197 0.170 , 0.197	Depositor DCC
$R_{free}$ test set	2289 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 402, SF4, EPE

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	1.51	16/3171 (0.5%)	1.42	38/4292 (0.9%)
2	B	2.00	3/763 (0.4%)	1.97	11/1029 (1.1%)
All	All	1.62	19/3934 (0.5%)	1.54	49/5321 (0.9%)

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	6
2	B	0	2
All	All	0	8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	GLN	CD-OE1	45.25	2.09	1.23
1	A	367	LYS	N-CA	41.24	1.97	1.46
1	A	367	LYS	C-O	-27.92	0.88	1.24
1	A	367	LYS	CA-CB	-26.72	1.04	1.53
1	A	320[A]	ASP	CB-CG	25.80	2.16	1.52
1	A	320[B]	ASP	CB-CG	25.80	2.16	1.52
2	B	101	GLU	CD-OE1	20.55	1.64	1.25
1	A	367	LYS	CA-C	19.59	1.81	1.52
1	A	96	LYS	CD-CE	17.99	2.06	1.52
2	B	101	GLU	CD-OE2	-14.46	0.97	1.25
1	A	220	LYS	CE-NZ	12.39	1.86	1.49
1	A	93	LYS	CG-CD	11.16	1.85	1.52
1	A	346	LYS	CD-CE	10.36	1.83	1.52
1	A	247	LYS	CE-NZ	8.03	1.73	1.49

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	ASP	CB-CG	-7.71	1.32	1.52
1	A	136	LYS	CE-NZ	-7.53	1.26	1.49
1	A	276	LYS	CG-CD	-6.46	1.33	1.52
1	A	165	THR	C-O	6.32	1.32	1.24
1	A	135	GLN	CD-OE1	-5.04	1.14	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	GLN	OE1-CD-NE2	-44.74	77.86	122.60
2	B	38	GLN	CG-CD-NE2	-20.71	85.34	116.40
1	A	346	LYS	CD-CE-NZ	18.64	171.55	111.90
1	A	317	LYS	N-CA-CB	-15.48	84.61	111.08
1	A	165	THR	CA-C-O	15.42	137.53	119.18
1	A	367	LYS	O-C-N	14.82	140.58	122.21
1	A	320[A]	ASP	CB-CG-OD1	-14.37	85.34	118.40
1	A	320[B]	ASP	CB-CG-OD1	-14.37	85.34	118.40
1	A	19	LYS	CD-CE-NZ	12.78	152.80	111.90
1	A	346	LYS	CG-CD-CE	-11.49	84.86	111.30
1	A	165	THR	O-C-N	-11.49	106.09	122.41
1	A	54	MET	CG-SD-CE	-11.01	76.67	100.90
1	A	96	LYS	CG-CD-CE	-10.87	86.31	111.30
1	A	320[A]	ASP	CB-CG-OD2	-10.54	94.17	118.40
1	A	320[B]	ASP	CB-CG-OD2	-10.54	94.17	118.40
1	A	24	LYS	CD-CE-NZ	10.01	143.93	111.90
2	B	73	LYS	CD-CE-NZ	-9.65	81.03	111.90
1	A	344	ASP	OD1-CG-OD2	-9.51	100.07	122.90
1	A	367	LYS	CA-CB-CG	8.71	131.51	114.10
1	A	169	ASP	CA-CB-CG	8.50	121.10	112.60
1	A	343	THR	CA-CB-OG1	-8.50	96.86	109.60
2	B	101	GLU	CG-CD-OE2	8.50	137.94	118.40
1	A	317	LYS	CB-CA-C	8.36	125.79	109.33
2	B	97	LYS	CD-CE-NZ	8.32	138.54	111.90
1	A	269	LYS	CG-CD-CE	-8.32	92.16	111.30
2	B	76	LEU	N-CA-C	-8.11	102.27	112.90
1	A	247	LYS	CD-CE-NZ	-8.03	86.20	111.90
1	A	136	LYS	CD-CE-NZ	7.71	136.57	111.90
1	A	276	LYS	CB-CG-CD	7.21	127.88	111.30
1	A	317	LYS	CA-CB-CG	-7.00	100.10	114.10
1	A	366	GLY	CA-C-N	-6.61	108.98	121.81
1	A	366	GLY	C-N-CA	-6.61	108.98	121.81
1	A	318	LYS	CA-CB-CG	-6.50	101.11	114.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ASP	CB-CG-OD2	6.49	133.32	118.40
1	A	372	PHE	CA-CB-CG	6.46	120.26	113.80
1	A	318	LYS	CB-CG-CD	-6.23	96.97	111.30
1	A	54	MET	CB-CG-SD	6.11	131.03	112.70
2	B	93	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	175	PHE	CA-CB-CG	5.84	119.64	113.80
2	B	60	ARG	CD-NE-CZ	5.68	132.35	124.40
2	B	76	LEU	N-CA-CB	5.65	118.81	110.33
2	B	75	TYR	CB-CA-C	5.53	121.43	110.42
1	A	276	LYS	CG-CD-CE	5.35	123.61	111.30
2	B	75	TYR	O-C-N	-5.22	115.64	122.59
1	A	362	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	222	ASP	CB-CA-C	5.21	118.26	109.67
1	A	367	LYS	N-CA-C	5.07	118.51	111.71
1	A	19	LYS	CG-CD-CE	5.05	122.91	111.30
1	A	26	HIS	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	THR	Mainchain
1	A	233	PRO	Peptide
1	A	243	ARG	Sidechain
1	A	320[A]	ASP	Sidechain
1	A	320[B]	ASP	Sidechain
1	A	344	ASP	Sidechain
2	B	38	GLN	Sidechain
2	B	60	ARG	Sidechain

## 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	3073	3041	3005	28	7
2	B	723	729	713	5	0
3	A	17	7	5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	0	1	0
5	A	15	18	18	0	0
6	A	137	0	0	0	0
6	B	37	0	0	0	0
All	All	4026	3795	3741	29	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (29) 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:A:367:LYS:C	1:A:367:LYS:CB	2.49	0.85
1:A:346:LYS:H	1:A:371:HIS:HD2	1.25	0.84
1:A:367:LYS:CB	1:A:367:LYS:N	2.51	0.74
1:A:351:HIS:CD2	1:A:380:GLY:H	2.10	0.70
1:A:351:HIS:HD2	1:A:380:GLY:H	1.40	0.69
1:A:14:HIS:HD2	1:A:85:GLN:OE1	1.77	0.67
1:A:39:ASP:OD1	1:A:58:HIS:HE1	1.80	0.64
1:A:223:PRO:HB3	1:A:251:MET:HE1	1.80	0.62
1:A:367:LYS:C	1:A:367:LYS:HB2	2.25	0.61
1:A:141:HIS:HE1	1:A:221:TYR:OH	1.84	0.61
1:A:71:GLN:O	1:A:75:HIS:HD2	1.86	0.59
1:A:48:ALA:HA	2:B:116:PHE:CE2	2.39	0.58
1:A:199:THR:OG1	2:B:89:HIS:HD2	1.86	0.57
1:A:295:ILE:O	1:A:301:GLY:HA3	2.09	0.53
1:A:155:GLU:OE1	2:B:89:HIS:HE1	1.93	0.51
1:A:109:ALA:HB3	1:A:233:PRO:HG3	1.93	0.50
1:A:331:ASP:O	1:A:351:HIS:HE1	1.96	0.49
1:A:56:GLU:O	1:A:58:HIS:HD2	1.96	0.49
1:A:367:LYS:N	1:A:367:LYS:HG3	2.28	0.48
1:A:48:ALA:HA	2:B:116:PHE:CD2	2.52	0.45
1:A:170[B]:MET:HE3	1:A:195[B]:PRO:O	2.19	0.43
1:A:180:PRO:HD2	4:A:502:SF4:S3	2.59	0.43
1:A:367:LYS:N	1:A:367:LYS:CG	2.82	0.41
1:A:36:ILE:HG12	1:A:78:GLU:HG3	2.01	0.41
1:A:141:HIS:CE1	1:A:221:TYR:OH	2.69	0.41
1:A:194:LEU:N	1:A:195[B]:PRO:CD	2.84	0.41
2:B:122:TYR:CE1	2:B:123:GLU:HG2	2.56	0.41
1:A:330:LEU:O	1:A:331:ASP:C	2.62	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HD2	1:A:321:SER:OG[1_655]	1.07	0.53
1:A:99:LYS:HZ2	1:A:325:LYS:HE2[1_655]	1.20	0.40
1:A:19:LYS:HZ3	1:A:346:LYS:HZ1[1_655]	1.23	0.37
1:A:99:LYS:CD	1:A:321:SER:OG[1_655]	1.85	0.35
1:A:14:HIS:HE1	1:A:53:GLU:OE1[4_555]	1.48	0.12
1:A:19:LYS:HZ3	1:A:337:THR:OG1[1_655]	1.52	0.08
1:A:99:LYS:HD3	1:A:323:ASP:OD2[1_655]	1.53	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	403/405 (100%)	396 (98%)	7 (2%)	0	100	100
2	B	88/88 (100%)	86 (98%)	2 (2%)	0	100	100
All	All	491/493 (100%)	482 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	330/330 (100%)	318 (96%)	12 (4%)	31	9
2	B	79/76 (104%)	78 (99%)	1 (1%)	61	39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	409/406 (101%)	396 (97%)	13 (3%)	36	11

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	MET
1	A	99	LYS
1	A	148	THR
1	A	170[A]	MET
1	A	170[B]	MET
1	A	220	LYS
1	A	281	LYS
1	A	294	THR
1	A	335	GLU
1	A	343	THR
1	A	362	ASP
1	A	367	LYS
2	B	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	58	HIS
1	A	75	HIS
1	A	135	GLN
1	A	141	HIS
1	A	174	GLN
1	A	351	HIS
1	A	371	HIS
2	B	89	HIS
2	B	91	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	SF4	A	503	1	0,12,12	-	-	-		
4	SF4	A	502	1	0,12,12	-	-	-		
5	EPE	A	505	-	15,15,15	0.69	1 (6%)	18,20,20	0.43	0
4	SF4	A	504	1	0,12,12	-	-	-		
3	402	A	501	1	13,19,19	5.49	7 (53%)	2,36,36	2.66	2 (100%)

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	SF4	A	503	1	-	-	0/6/5/5
4	SF4	A	502	1	-	-	0/6/5/5
5	EPE	A	505	-	-	1/9/19/19	0/1/1/1
4	SF4	A	504	1	-	-	0/6/5/5
3	402	A	501	1	-	-	0/5/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	402	C2-S2	-11.08	1.65	1.85
3	A	501	402	C1-S1	-10.26	1.66	1.85
3	A	501	402	S1-FE1	-8.36	2.14	2.26
3	A	501	402	S2-FE2	-5.55	2.18	2.26
3	A	501	402	S2-FE1	-5.30	2.18	2.26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	402	S1-FE2	-4.77	2.19	2.26
5	A	505	EPE	O3S-S	2.51	1.56	1.47
3	A	501	402	O5-C5	2.15	1.21	1.17

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	402	S2-C2-N1	-3.15	108.52	117.18
3	A	501	402	S1-C1-N1	-2.06	111.51	117.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

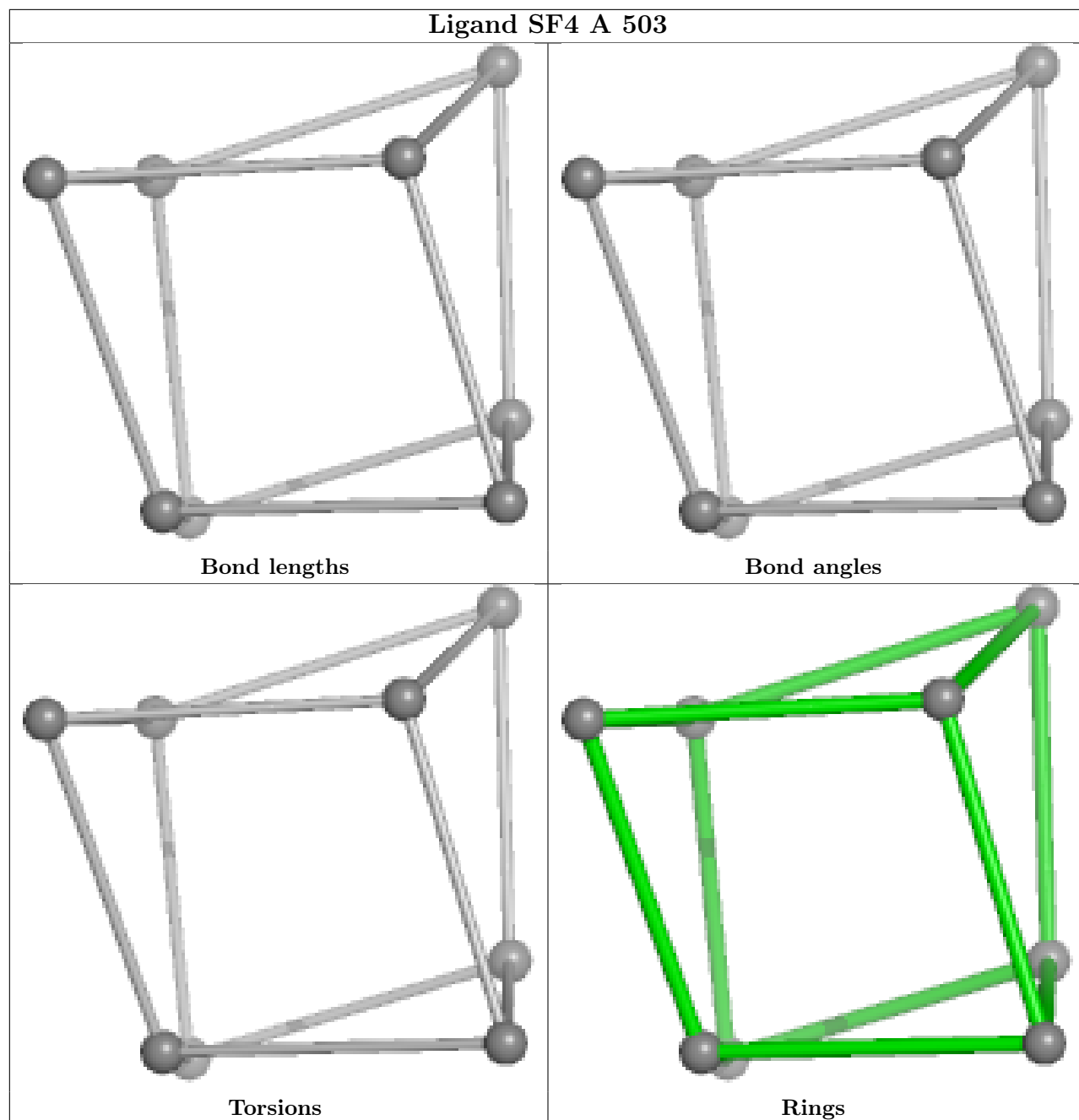
Mol	Chain	Res	Type	Atoms
5	A	505	EPE	C10-C9-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

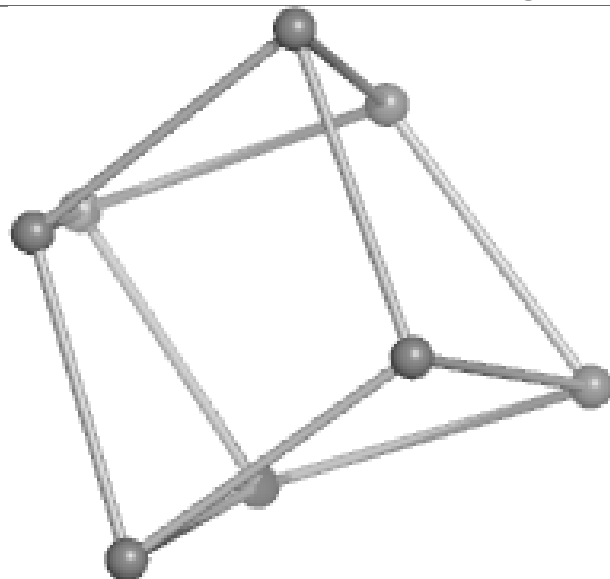
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	SF4	1	0

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

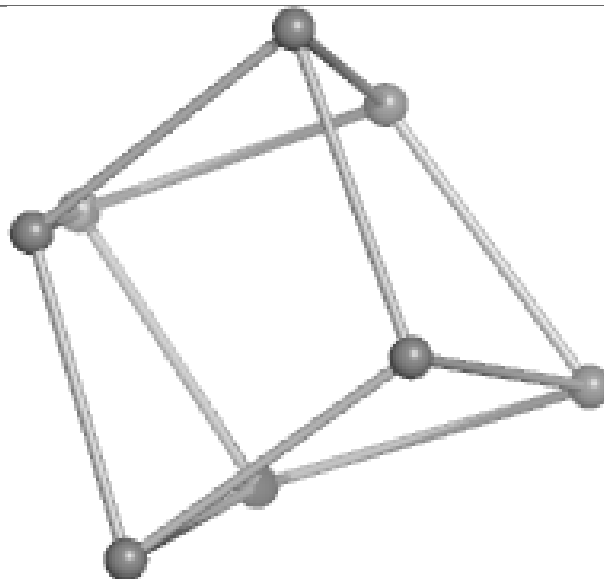




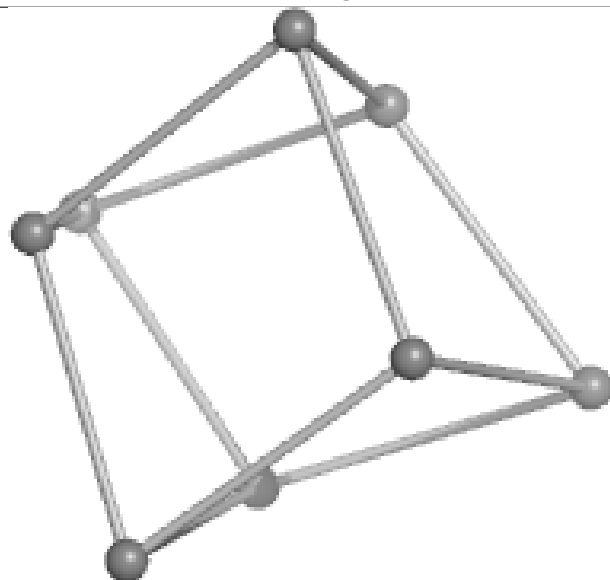
## Ligand SF4 A 502



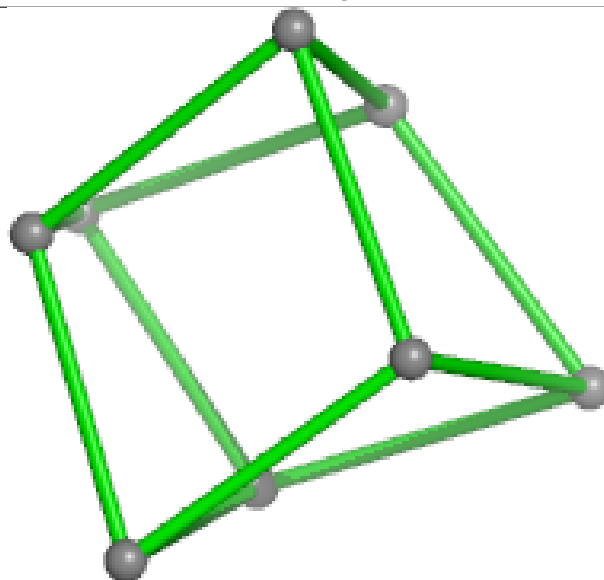
Bond lengths



Bond angles

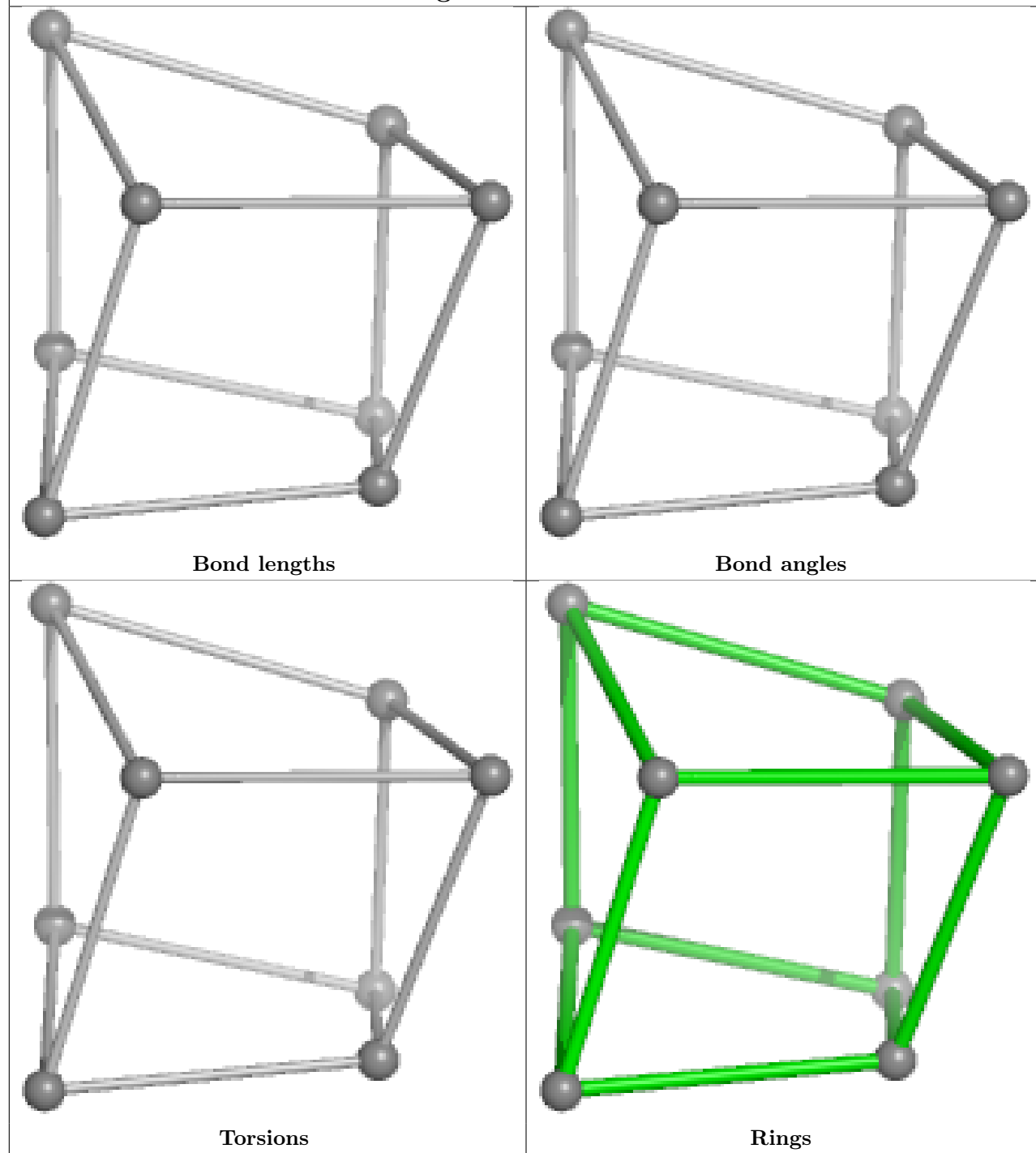


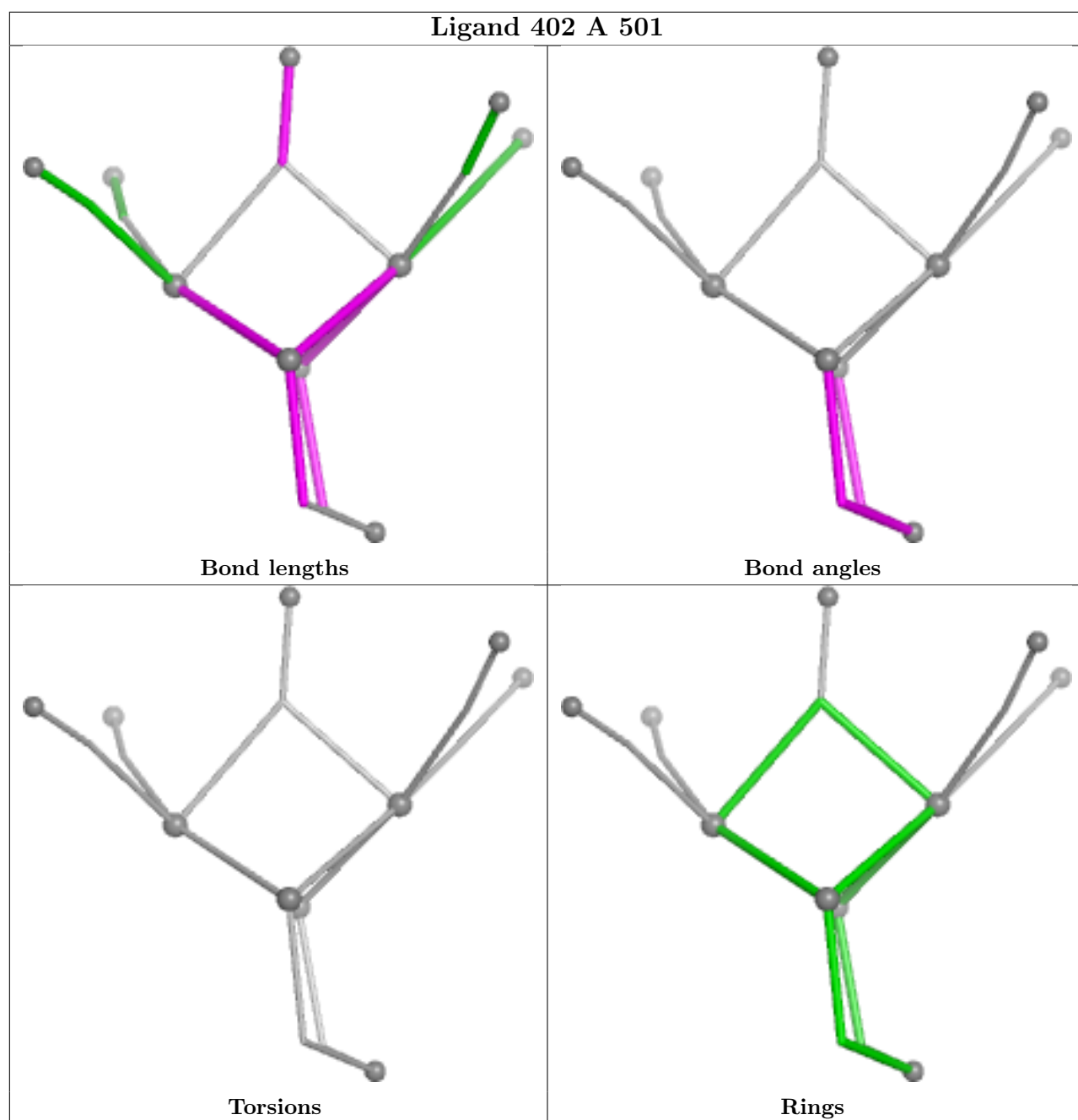
Torsions



Rings

## Ligand SF4 A 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/405 (98%)	-0.18	3 (0%) 82 86	7, 17, 31, 61	29 (7%)
2	B	87/88 (98%)	-0.11	2 (2%) 61 65	9, 19, 29, 33	8 (9%)
All	All	487/493 (98%)	-0.17	5 (1%) 79 83	7, 17, 31, 61	37 (7%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	LYS	3.3
1	A	343	THR	2.8
2	B	93	PHE	2.4
1	A	222	ASP	2.2
2	B	37[A]	LYS	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

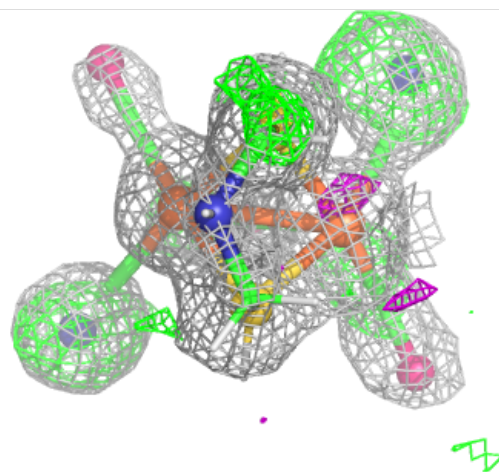
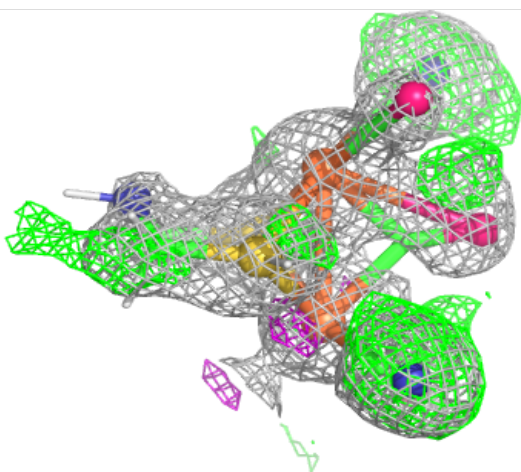
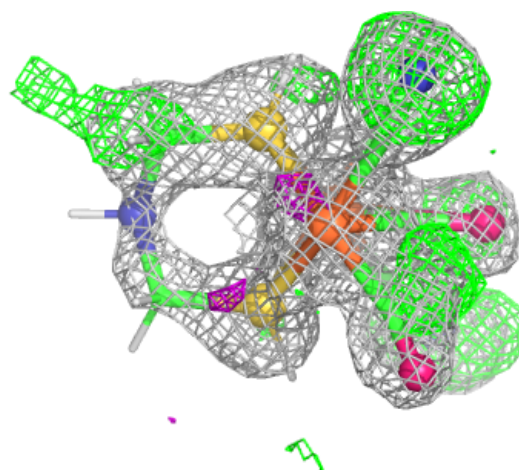
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
3	402	A	501	17/17	0.86	0.18	8,18,19,21	24
5	EPE	A	505	15/15	0.87	0.11	35,41,51,54	2
4	SF4	A	503	8/8	0.99	0.04	11,12,12,13	0
4	SF4	A	504	8/8	0.99	0.04	13,14,16,16	0
4	SF4	A	502	8/8	0.99	0.04	11,12,13,14	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.

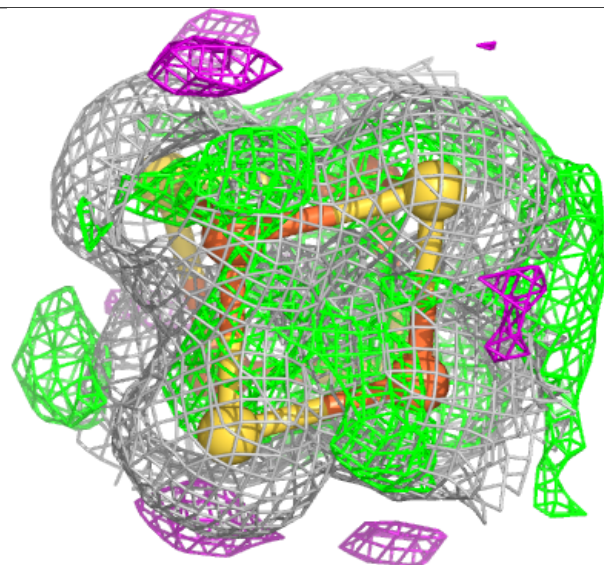
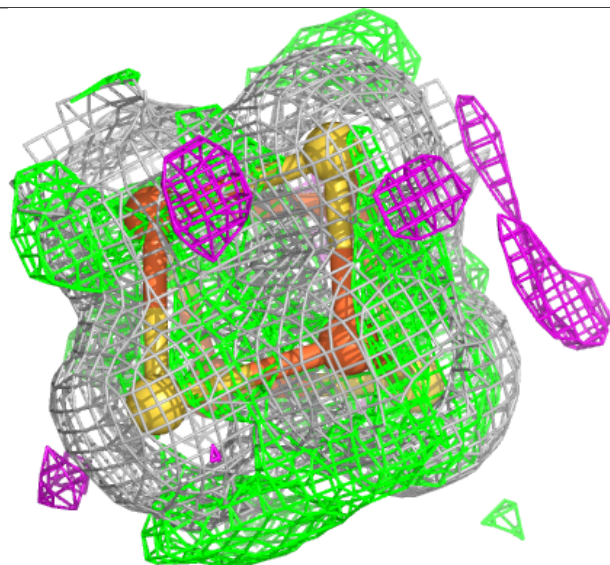
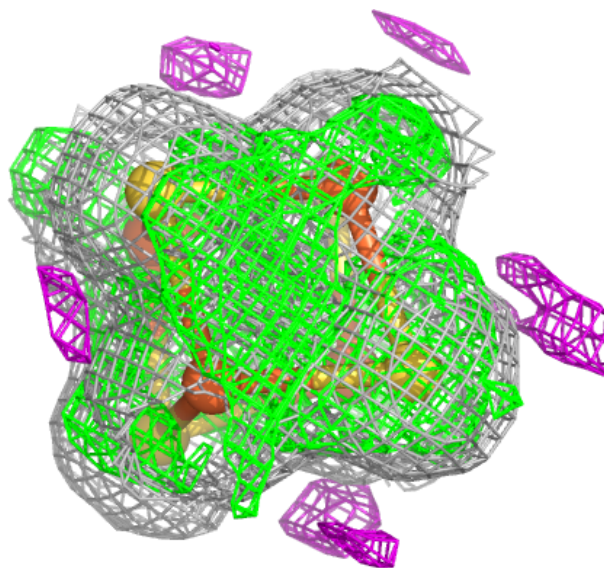
**Electron density around 402 A 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SF4 A 503:**

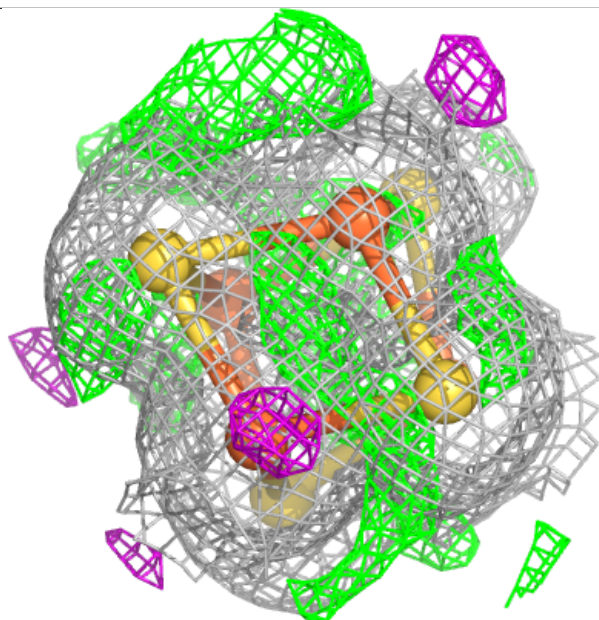
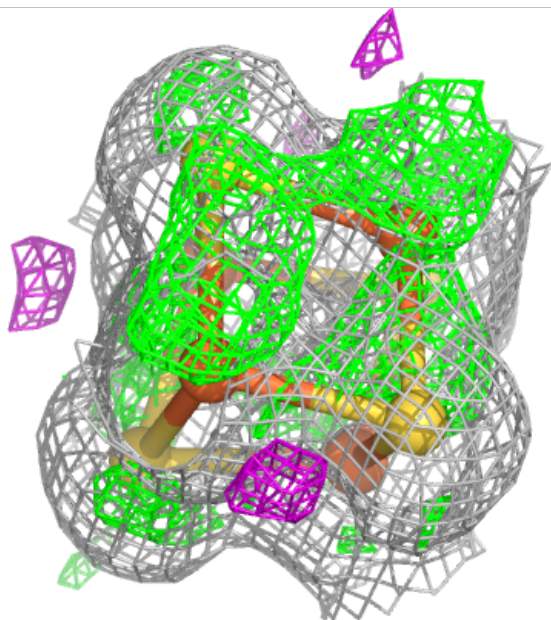
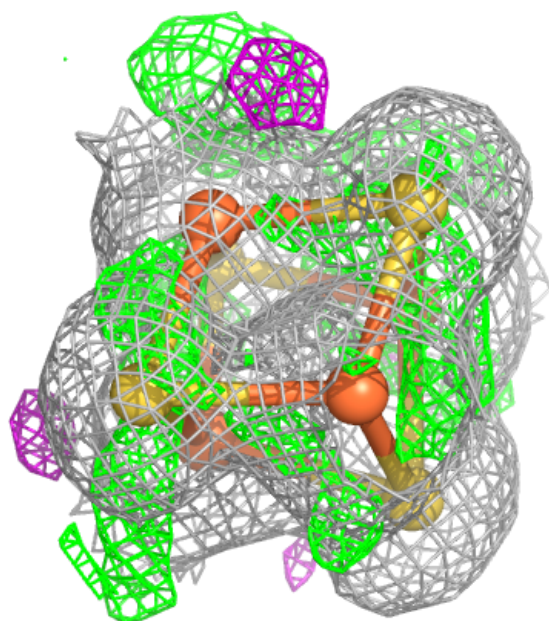
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





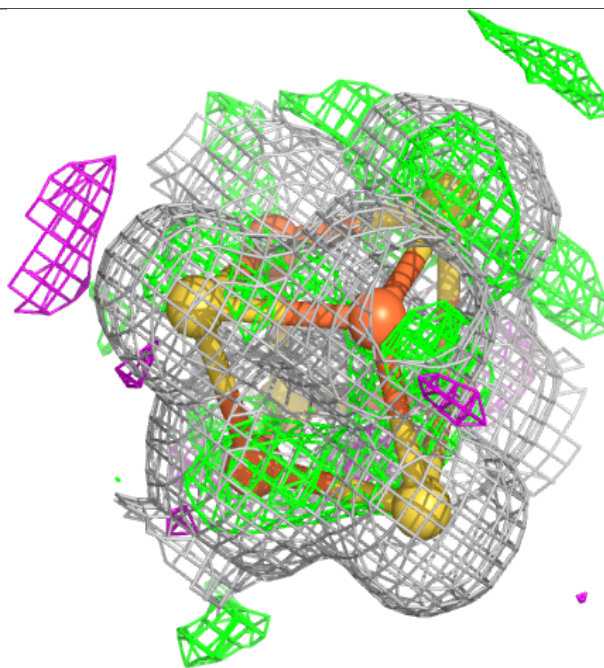
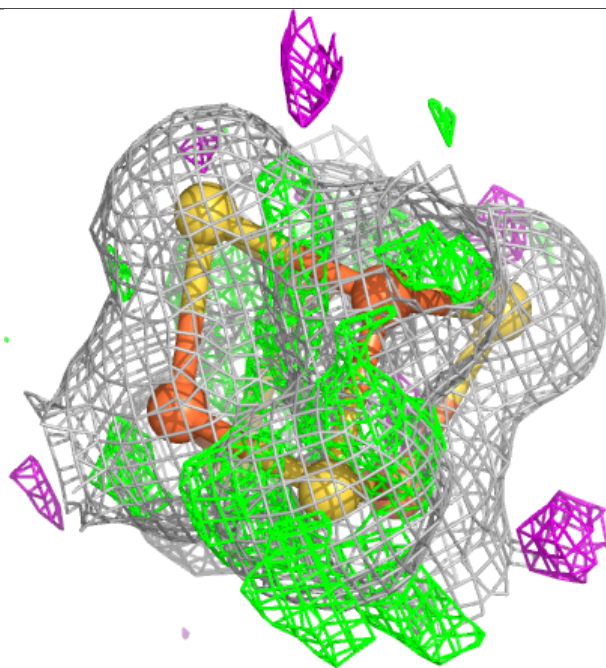
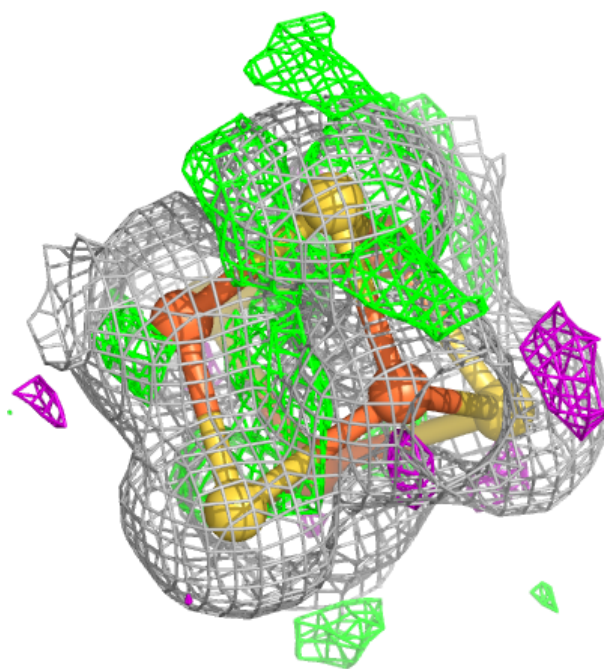
**Electron density around SF4 A 504:**

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



**Electron density around SF4 A 502:**

$2mF_o-DF_c$  (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.