



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2025 – 04:16 PM EDT

PDB ID : 8V0J / pdb\_00008v0j  
Title : Structure of the complex between Human LIAS and H-protein in the presence of s-adenosyl-l-methionine  
Authors : Esakova, O.A.; Warui, D.M.; Neti, S.S.; Alumasa, J.N.; Booker, S.J.  
Deposited on : 2023-11-17  
Resolution : 2.58 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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

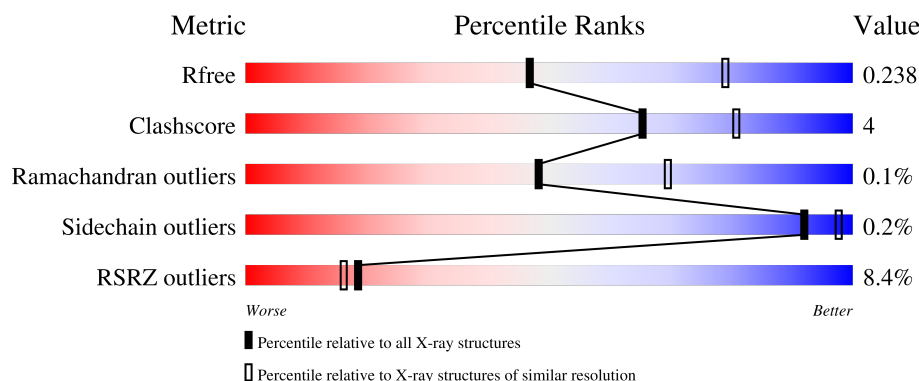
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	368	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>17%</div> </div> </div>
1	B	368	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>7%</div> <div>18%</div> </div> </div>
1	C	368	<div> <div>17%</div> <div> <div></div> <div>68%</div> <div>10%</div> <div>21%</div> </div> </div>
2	D	173	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>7%</div> <div>28%</div> </div> </div>
2	E	173	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>7%</div> <div>27%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	173	<div><div><div>8%</div><div>8%</div><div></div></div><div>90%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9413 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 Lipoyl synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	292	Total	C	N	O	S	0	0	0
			2300	1454	399	432	15			
1	A	305	Total	C	N	O	S	0	0	0
			2411	1520	427	449	15			
1	B	301	Total	C	N	O	S	0	0	0
			2378	1500	418	445	15			

- Molecule 2 is a protein called Glycine cleavage system H protein, mitochondrial.

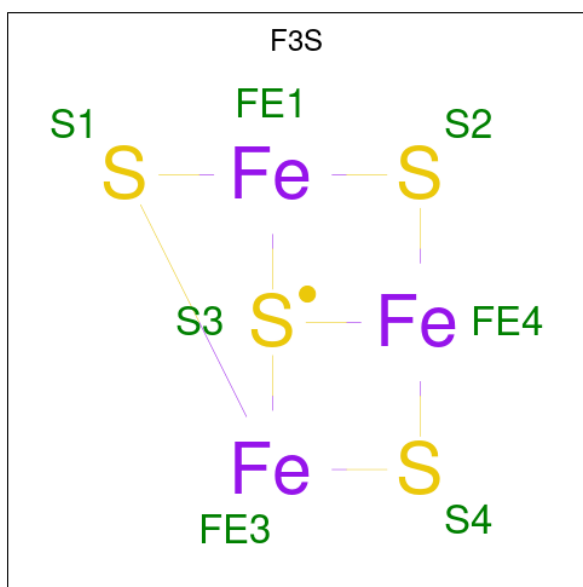
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	17	Total	C	N	O		0	0	0
			121	76	20	25				
2	D	124	Total	C	N	O	S	0	0	0
			959	605	149	201	4			
2	E	126	Total	C	N	O	S	0	0	0
			978	615	151	208	4			

- Molecule 3 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
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



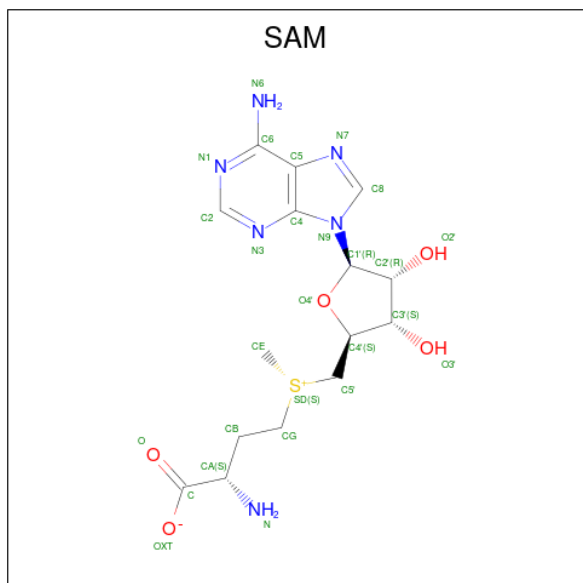
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	Fe	S	0	0
			6	3	3		

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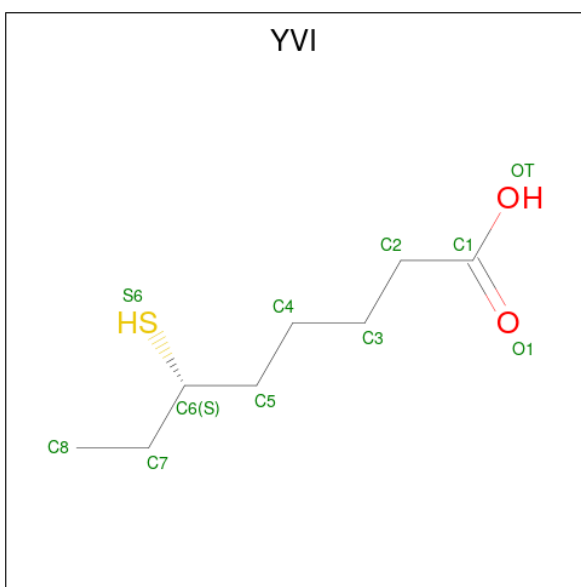
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			6	3	3		
4	B	1	Total	Fe	S	0	0
			6	3	3		

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ) (labeled as "Ligand of Interest" by depositor).



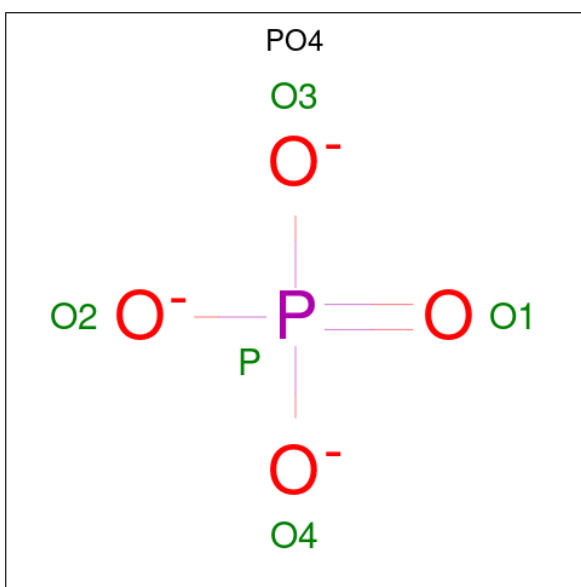
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
5	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
5	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 6 is 6-THIOOCTANOIC ACID (CCD ID: YVI) (formula:  $C_8H_{16}O_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	O	S	0	0
			10	8	1	1		
6	D	1	Total	C	O	S	0	0
			10	8	1	1		
6	E	1	Total	C	O	S	0	0
			10	8	1	1		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

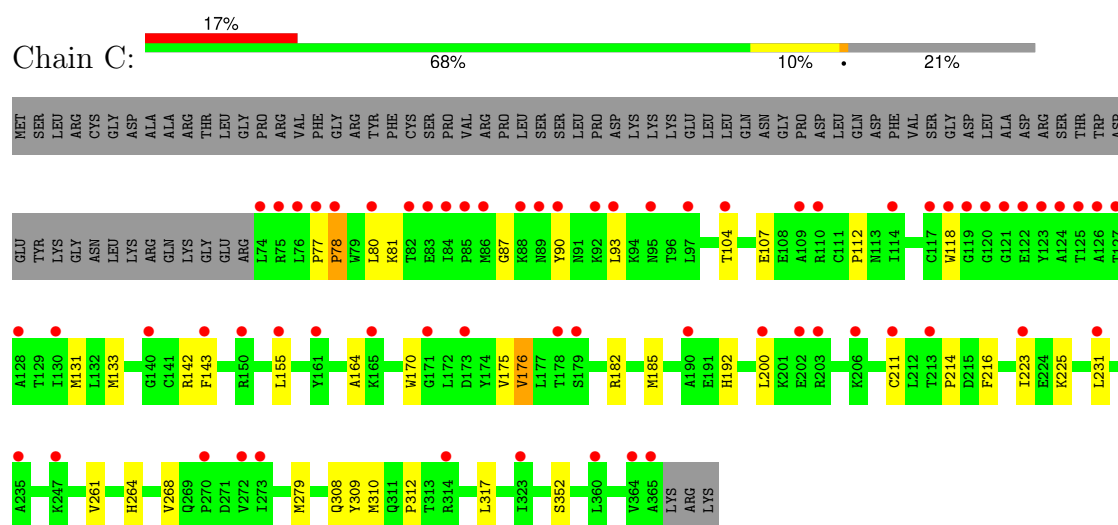
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	6	Total	O	0	0
			6	6		
8	A	64	Total	O	0	0
			64	64		
8	B	17	Total	O	0	0
			17	17		
8	F	1	Total	O	0	0
			1	1		
8	D	12	Total	O	0	0
			12	12		
8	E	3	Total	O	0	0
			3	3		



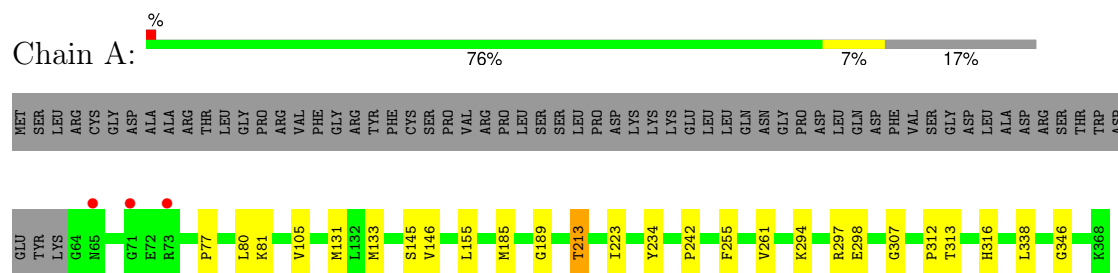
### 3 Residue-property plots [i](#)

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.

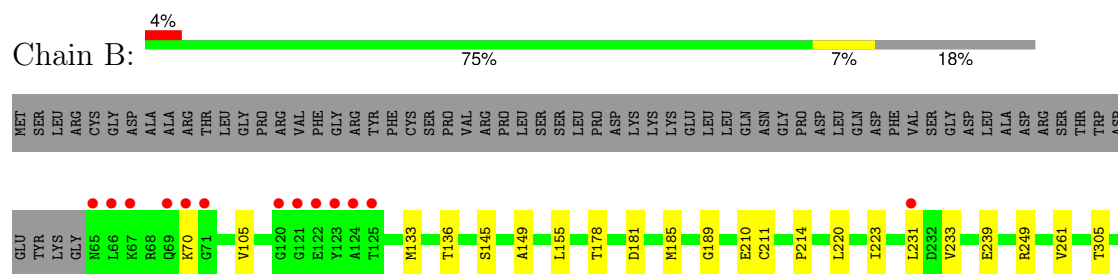
- Molecule 1: Lipoyl synthase, mitochondrial



- Molecule 1: Lipoyl synthase, mitochondrial



- Molecule 1: Lipoyl synthase, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.26Å 171.38Å 196.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.28 – 2.58 38.28 – 2.58	Depositor EDS
% Data completeness (in resolution range)	73.2 (38.28-2.58) 84.7 (38.28-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.198 , 0.236 0.198 , 0.238	Depositor DCC
$R_{free}$ test set	1960 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: PO4, F3S, YVI, SAM, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.10	0/2460	0.26	0/3325
1	B	0.09	0/2427	0.24	0/3284
1	C	0.10	0/2349	0.26	0/3183
2	D	0.14	0/975	0.24	0/1320
2	E	0.14	0/994	0.24	0/1344
2	F	0.27	0/120	0.32	0/159
All	All	0.11	0/9325	0.25	0/12615

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2411	0	2427	15	0
1	B	2378	0	2385	14	0
1	C	2300	0	2299	28	0
2	D	959	0	930	4	0
2	E	978	0	942	6	0
2	F	121	0	117	5	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	0	0	0
3	C	8	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
5	A	27	0	22	1	0
5	B	27	0	22	3	0
5	C	27	0	22	2	0
6	D	10	0	0	0	0
6	E	10	0	0	0	0
6	F	10	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
8	A	64	0	0	0	0
8	B	17	0	0	0	0
8	C	6	0	0	0	0
8	D	12	0	0	0	0
8	E	3	0	0	0	0
8	F	1	0	0	0	0
All	All	9413	0	9166	68	0

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

All (68) 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:B:155:LEU:HG	1:B:185:MET:HE3	1.77	0.67
1:C:143:PHE:HE2	5:C:403:SAM:H2'	1.63	0.62
1:B:105:VAL:HG21	5:B:403:SAM:HE1	1.82	0.61
1:B:239:GLU:HG3	1:B:249:ARG:HD3	1.81	0.61
1:C:112:PRO:HD3	2:F:107:LYS:HE2	1.83	0.60
1:C:155:LEU:HG	1:C:185:MET:HE3	1.85	0.59
1:C:312:PRO:HG3	5:C:403:SAM:HN61	1.69	0.57
1:C:78:PRO:HA	1:C:81:LYS:HE3	1.87	0.56
1:C:164:ALA:HA	1:C:200:LEU:HD13	1.88	0.55
1:A:313:THR:HG1	1:A:316:HIS:HD1	1.52	0.55
1:A:131:MET:HE1	1:A:146:VAL:HG21	1.90	0.54
2:E:54:THR:HG22	2:E:158:LEU:HD22	1.88	0.53
1:A:105:VAL:HG21	5:A:403:SAM:H5'1	1.88	0.53
2:E:123:ILE:HG22	2:E:145:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ARG:HB3	1:C:317:LEU:HG	1.90	0.53
1:C:77:PRO:HG2	1:C:80:LEU:HB2	1.90	0.52
1:C:310:MET:HB3	2:F:107:LYS:HB2	1.93	0.51
1:A:213:THR:HG21	1:A:234:TYR:OH	2.11	0.51
1:C:211:CYS:HB2	1:C:231:LEU:HD21	1.93	0.51
1:C:107:GLU:HG3	1:C:118:TRP:HH2	1.75	0.50
1:C:176:VAL:HG11	1:C:352:SER:HB2	1.93	0.50
1:C:223:ILE:HD13	1:C:261:VAL:HA	1.92	0.50
1:C:87:GLY:HA2	1:C:90:TYR:HB3	1.94	0.50
1:C:133:MET:HE2	1:C:192:HIS:HB3	1.93	0.49
1:C:310:MET:HB2	2:F:107:LYS:HE3	1.94	0.49
1:A:77:PRO:HD2	1:A:80:LEU:HD12	1.94	0.49
1:C:142:ARG:HA	1:C:142:ARG:HE	1.78	0.48
2:E:112:LEU:HD13	2:E:144:LEU:HD13	1.95	0.48
1:A:145:SER:HB3	1:A:312:PRO:HB2	1.94	0.48
2:D:51:ARG:HG2	2:D:59:TRP:HB2	1.95	0.48
2:E:159:MET:HB3	2:E:163:ALA:HB3	1.96	0.48
1:C:104:THR:HA	1:C:131:MET:H	1.79	0.47
1:B:211:CYS:HB2	1:B:231:LEU:HD21	1.97	0.47
1:B:223:ILE:HD13	1:B:261:VAL:HA	1.97	0.47
1:C:175:VAL:HG11	1:C:200:LEU:HD21	1.97	0.46
1:C:214:PRO:HG2	1:C:216:PHE:CE1	2.51	0.45
1:B:70:LYS:HA	1:B:70:LYS:HD2	1.78	0.45
1:B:178:THR:OG1	5:B:403:SAM:HE2	2.16	0.45
1:C:279:MET:HE2	1:C:309:TYR:HB2	2.00	0.44
1:A:223:ILE:HD13	1:A:261:VAL:HA	1.99	0.44
1:B:145:SER:HB3	1:B:312:PRO:HB2	1.98	0.44
1:C:80:LEU:HD11	1:C:308:GLN:HG2	2.00	0.44
1:A:294:LYS:NZ	1:A:298:GLU:OE2	2.43	0.44
2:D:123:ILE:HG22	2:D:145:ILE:HG22	2.00	0.44
1:C:310:MET:HE2	2:F:107:LYS:HB2	2.00	0.43
1:B:220:LEU:HD12	1:B:220:LEU:H	1.83	0.43
1:C:133:MET:HG2	1:C:155:LEU:HD21	2.00	0.43
1:B:305:THR:HG23	1:B:349:VAL:HG12	2.01	0.42
1:B:181:ASP:OD1	1:B:214:PRO:HB3	2.19	0.42
2:E:165:GLU:OE2	2:E:169:LYS:NZ	2.46	0.42
1:C:133:MET:HB3	1:C:182:ARG:HH11	1.85	0.42
1:A:297:ARG:HG3	1:A:338:LEU:HB3	2.01	0.42
1:A:133:MET:SD	1:A:189:GLY:HA3	2.60	0.41
1:A:307:GLY:HA2	1:A:346:GLY:O	2.21	0.41
1:A:81:LYS:HG2	2:D:109:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:HD22	1:C:170:TRP:CD2	2.56	0.41
1:A:313:THR:HG1	1:A:316:HIS:CE1	2.38	0.41
2:D:62:THR:HG21	2:D:155:LEU:HD11	2.03	0.41
2:F:75:ALA:O	2:F:79:LEU:HB2	2.20	0.41
2:E:137:SER:OG	2:E:140:GLU:HB2	2.21	0.41
1:B:133:MET:SD	1:B:189:GLY:HA3	2.61	0.41
1:B:136:THR:HG21	1:B:149:ALA:HB3	2.02	0.41
1:C:264:HIS:O	1:C:268:VAL:HG22	2.21	0.40
1:C:225:LYS:HA	1:C:225:LYS:HD2	1.90	0.40
1:A:155:LEU:HG	1:A:185:MET:HE3	2.03	0.40
1:A:242:PRO:HG3	1:A:255:PHE:CG	2.56	0.40
1:B:210:GLU:HB2	1:B:233:VAL:HB	2.03	0.40
5:B:403:SAM:HE3	5:B:403:SAM:H4'	1.59	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	303/368 (82%)	295 (97%)	8 (3%)	0	100	100
1	B	299/368 (81%)	289 (97%)	10 (3%)	0	100	100
1	C	290/368 (79%)	276 (95%)	13 (4%)	1 (0%)	37	57
2	D	122/173 (70%)	118 (97%)	4 (3%)	0	100	100
2	E	124/173 (72%)	117 (94%)	7 (6%)	0	100	100
2	F	13/173 (8%)	13 (100%)	0	0	100	100
All	All	1151/1623 (71%)	1108 (96%)	42 (4%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	78	PRO

### 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	262/317 (83%)	261 (100%)	1 (0%)	89	96
1	B	259/317 (82%)	259 (100%)	0	100	100
1	C	251/317 (79%)	250 (100%)	1 (0%)	89	96
2	D	107/146 (73%)	107 (100%)	0	100	100
2	E	109/146 (75%)	109 (100%)	0	100	100
2	F	13/146 (9%)	13 (100%)	0	100	100
All	All	1001/1389 (72%)	999 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	176	VAL
1	A	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	237	ASN
1	A	192	HIS
1	A	264	HIS
1	B	237	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

14 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	F3S	B	402	1,6	0,7,9	-	-	-		
4	F3S	C	402	1,6	0,7,9	-	-	-		
5	SAM	C	403	3	23,29,29	1.14	2 (8%)	20,42,42	2.52	7 (35%)
6	YVI	F	201	2,4	7,9,10	0.29	0	5,9,11	1.07	0
3	SF4	C	401	1,5	0,12,12	-	-	-		
7	PO4	E	202	-	4,4,4	0.96	0	6,6,6	0.45	0
6	YVI	D	201	2,4	7,9,10	0.27	0	5,9,11	1.01	0
5	SAM	A	403	3	23,29,29	1.19	1 (4%)	20,42,42	1.97	3 (15%)
5	SAM	B	403	3	23,29,29	1.26	3 (13%)	20,42,42	1.64	2 (10%)
3	SF4	B	401	1,5	0,12,12	-	-	-		
3	SF4	A	401	1,5	0,12,12	-	-	-		
7	PO4	D	202	-	4,4,4	0.96	0	6,6,6	0.44	0
4	F3S	A	402	1,6	0,7,9	-	-	-		
6	YVI	E	201	2,4	7,9,10	0.28	0	5,9,11	1.13	1 (20%)

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
6	YVI	F	201	2,4	-	0/7/8/9	-
5	SAM	C	403	3	-	6/13/33/33	0/3/3/3
4	F3S	C	402	1,6	-	-	0/2/2/3
4	F3S	B	402	1,6	-	-	0/2/2/3
4	F3S	A	402	1,6	-	-	0/2/2/3
6	YVI	D	201	2,4	-	0/7/8/9	-
5	SAM	A	403	3	-	9/13/33/33	0/3/3/3
5	SAM	B	403	3	-	6/13/33/33	0/3/3/3
3	SF4	B	401	1,5	-	-	0/6/5/5
3	SF4	A	401	1,5	-	-	0/6/5/5
3	SF4	C	401	1,5	-	-	0/6/5/5
6	YVI	E	201	2,4	-	2/7/8/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	SAM	C2-N3	4.03	1.38	1.32
5	A	403	SAM	C2-N3	3.83	1.38	1.32
5	C	403	SAM	C2-N3	3.72	1.37	1.32
5	B	403	SAM	C2-N1	2.41	1.38	1.33
5	B	403	SAM	OXT-C	-2.30	1.23	1.30
5	C	403	SAM	OXT-C	-2.10	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	SAM	N3-C2-N1	-6.58	119.74	128.67
5	A	403	SAM	N3-C2-N1	-6.22	120.23	128.67
5	B	403	SAM	N3-C2-N1	-6.20	120.25	128.67
5	C	403	SAM	O4'-C1'-N9	5.80	116.44	108.75
5	A	403	SAM	O4'-C1'-N9	4.24	114.37	108.75
5	C	403	SAM	C4'-O4'-C1'	-3.86	106.39	109.92
5	C	403	SAM	OXT-C-O	-3.35	116.48	124.08
5	A	403	SAM	OXT-C-O	-2.75	117.84	124.08
5	C	403	SAM	C1'-N9-C4	-2.71	121.89	126.64
5	B	403	SAM	OXT-C-O	-2.70	117.95	124.08
5	C	403	SAM	CG-SD-C5'	-2.25	97.93	103.43
6	E	201	YVI	C8-C7-C6	-2.05	111.61	114.67
5	C	403	SAM	O4'-C4'-C5'	2.01	113.95	108.88

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	SAM	N-CA-CB-CG
5	C	403	SAM	C-CA-CB-CG
5	C	403	SAM	CB-CG-SD-C5'
5	A	403	SAM	N-CA-CB-CG
5	A	403	SAM	CB-CG-SD-CE
5	A	403	SAM	CB-CG-SD-C5'
5	A	403	SAM	O4'-C4'-C5'-SD
5	A	403	SAM	C3'-C4'-C5'-SD
5	B	403	SAM	C4'-C5'-SD-CE
5	B	403	SAM	O4'-C4'-C5'-SD
5	B	403	SAM	C3'-C4'-C5'-SD
5	A	403	SAM	OXT-C-CA-N
5	B	403	SAM	O-C-CA-N
5	C	403	SAM	OXT-C-CA-N
5	A	403	SAM	C-CA-CB-CG
5	A	403	SAM	CA-CB-CG-SD
5	B	403	SAM	CA-CB-CG-SD
5	C	403	SAM	CB-CG-SD-CE
5	B	403	SAM	OXT-C-CA-N
5	C	403	SAM	CA-CB-CG-SD
6	E	201	YVI	C4-C5-C6-S6
6	E	201	YVI	C4-C5-C6-C7
5	A	403	SAM	O-C-CA-N

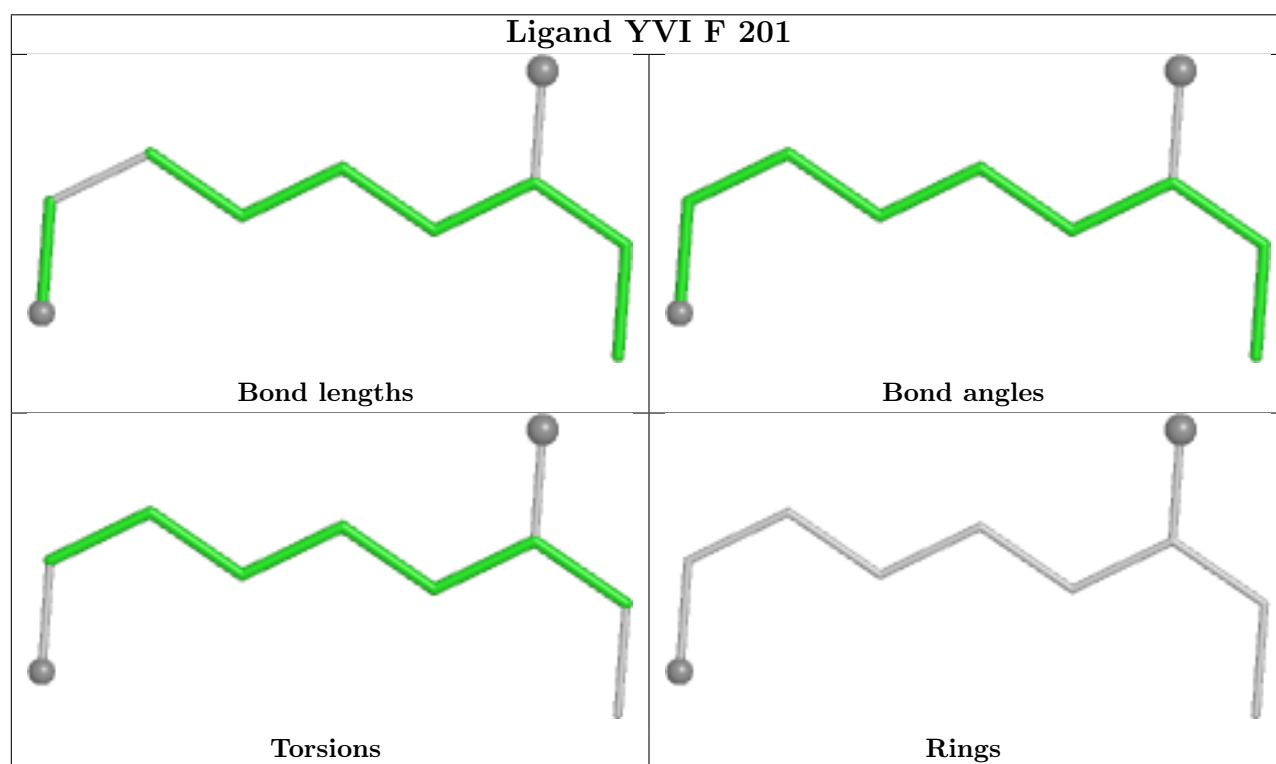
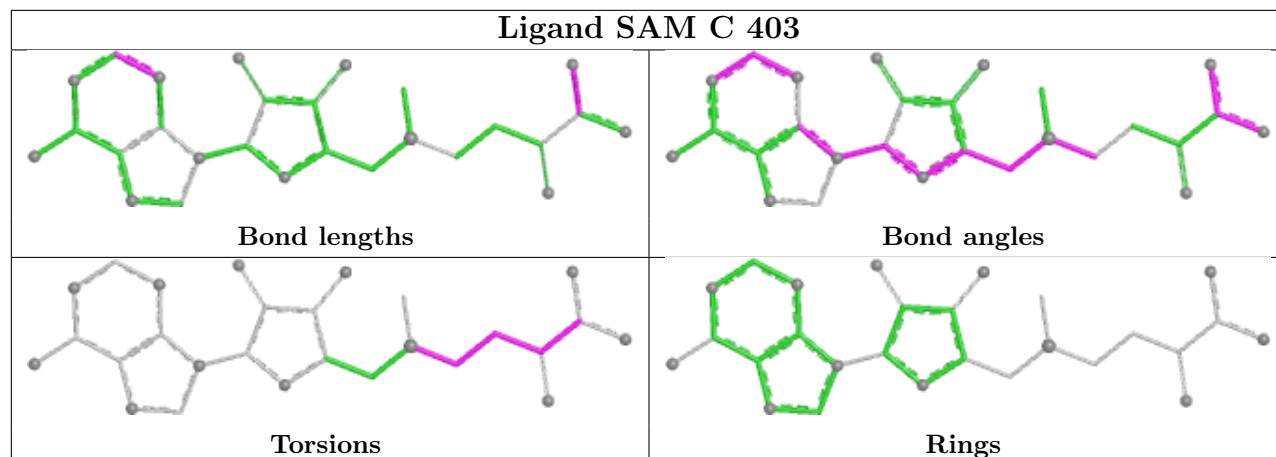
There are no ring outliers.

3 monomers are involved in 6 short contacts:

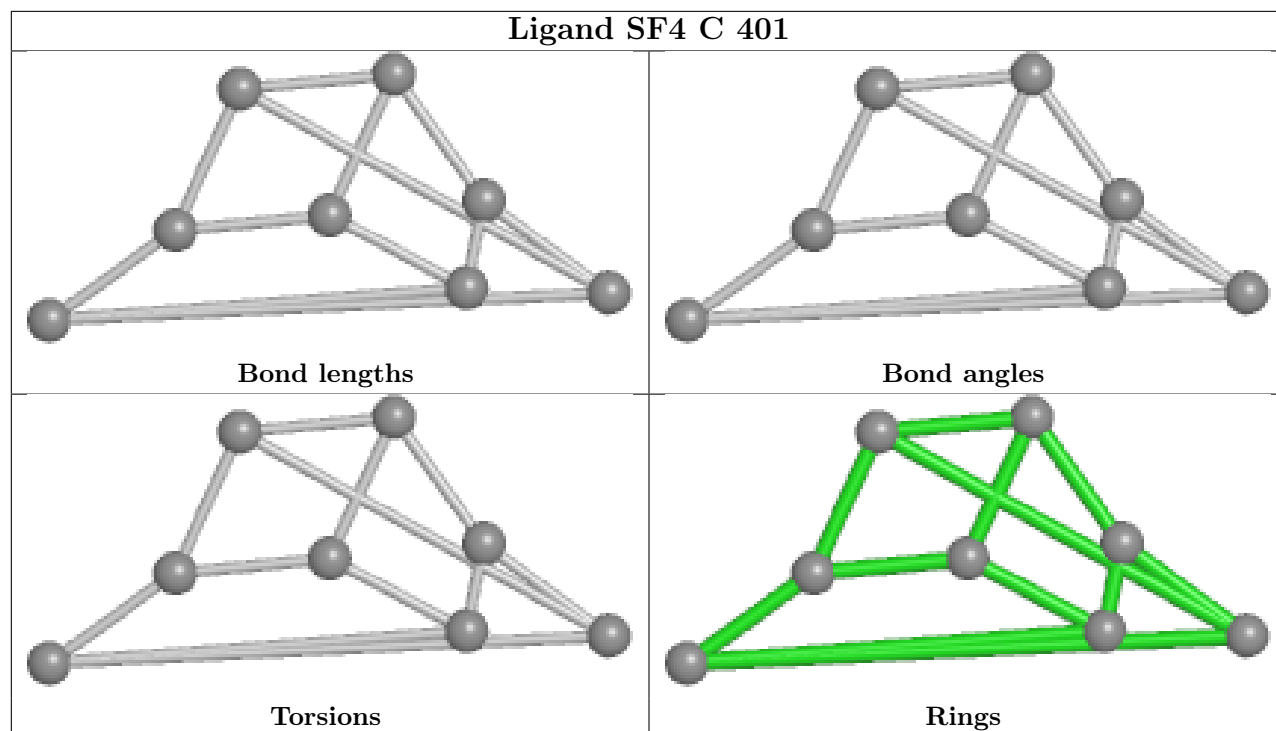
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	SAM	2	0
5	A	403	SAM	1	0
5	B	403	SAM	3	0

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

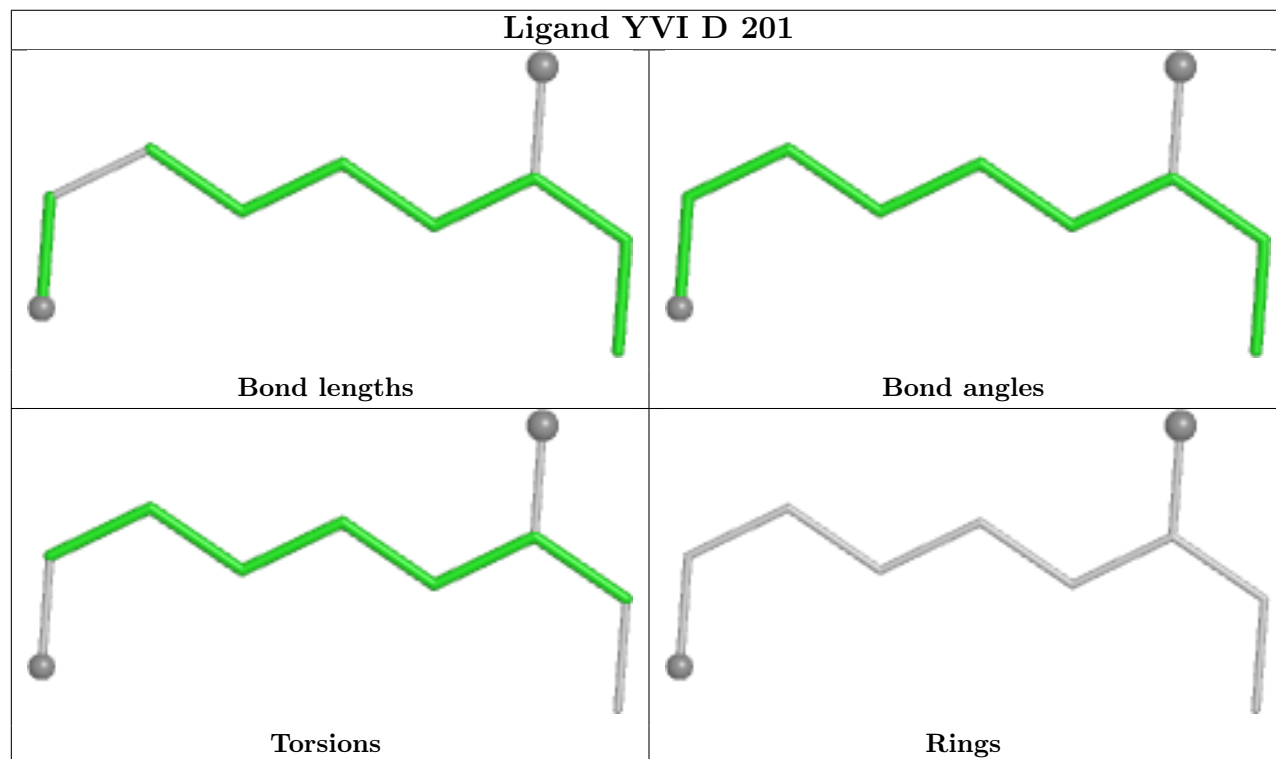
equivalents in the CSD to analyse the geometry.

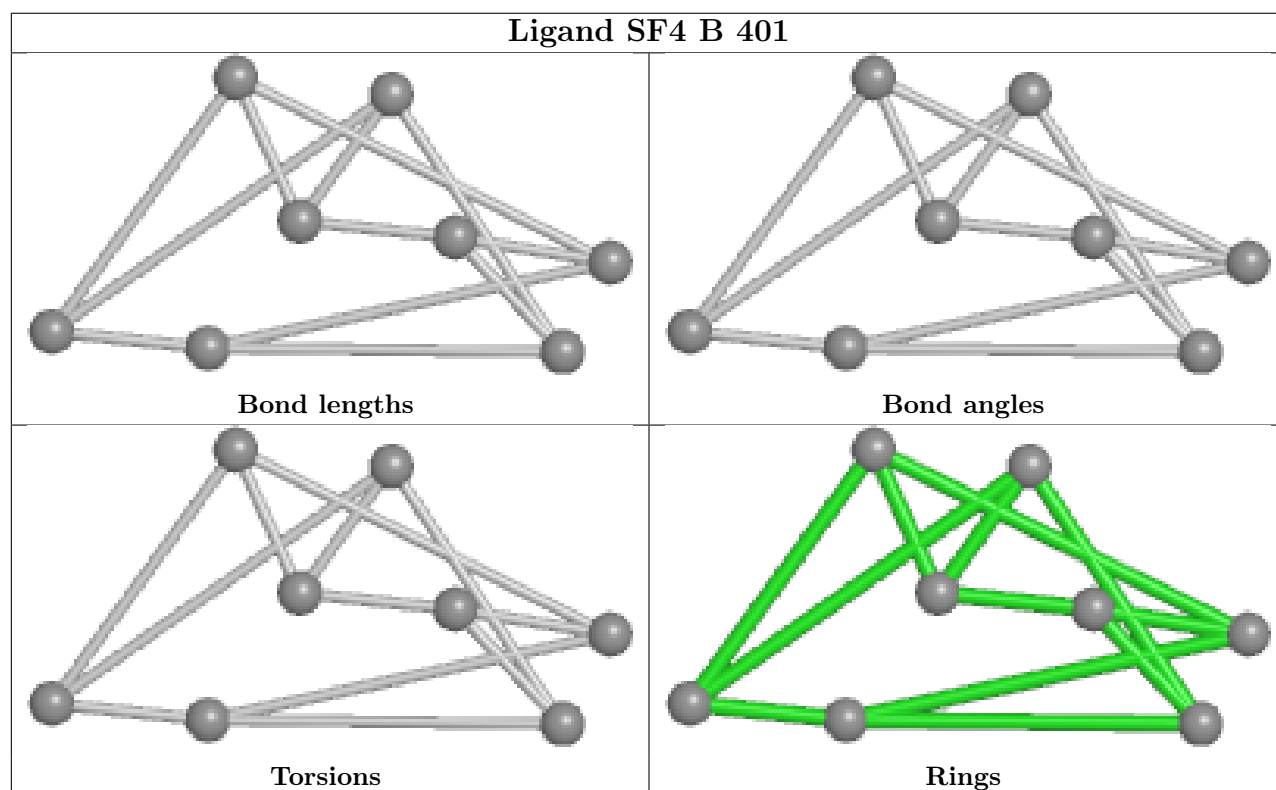
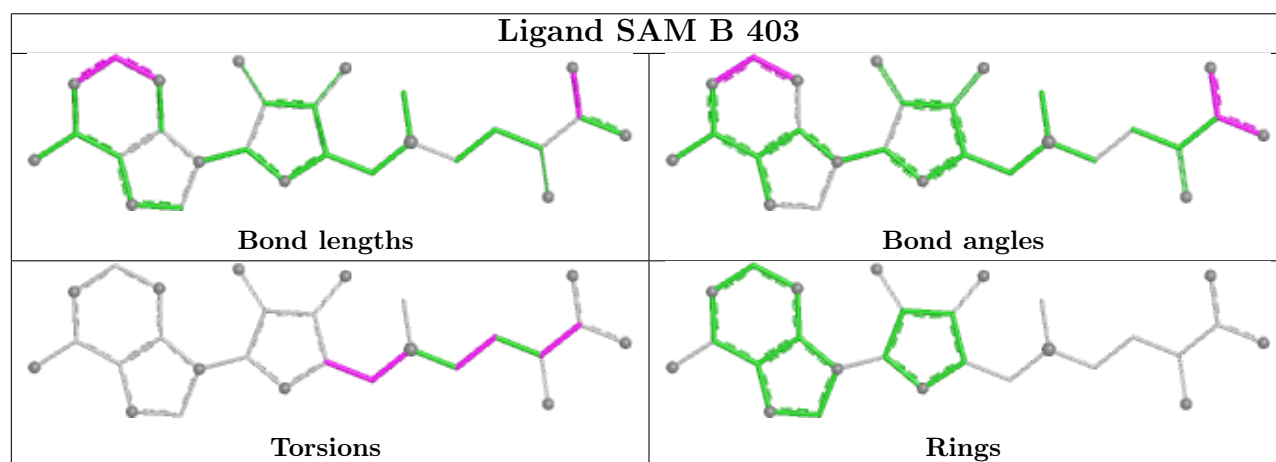
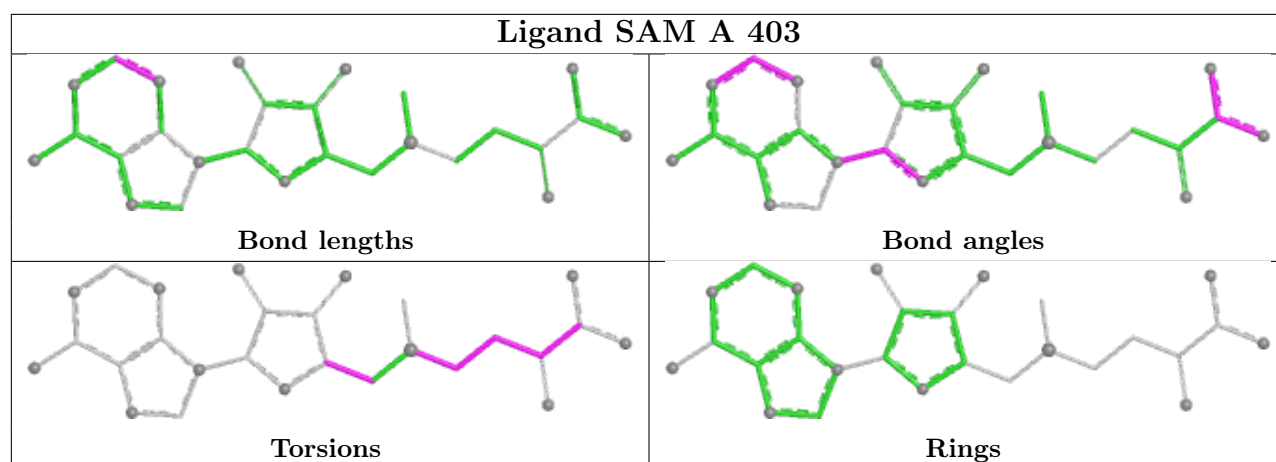


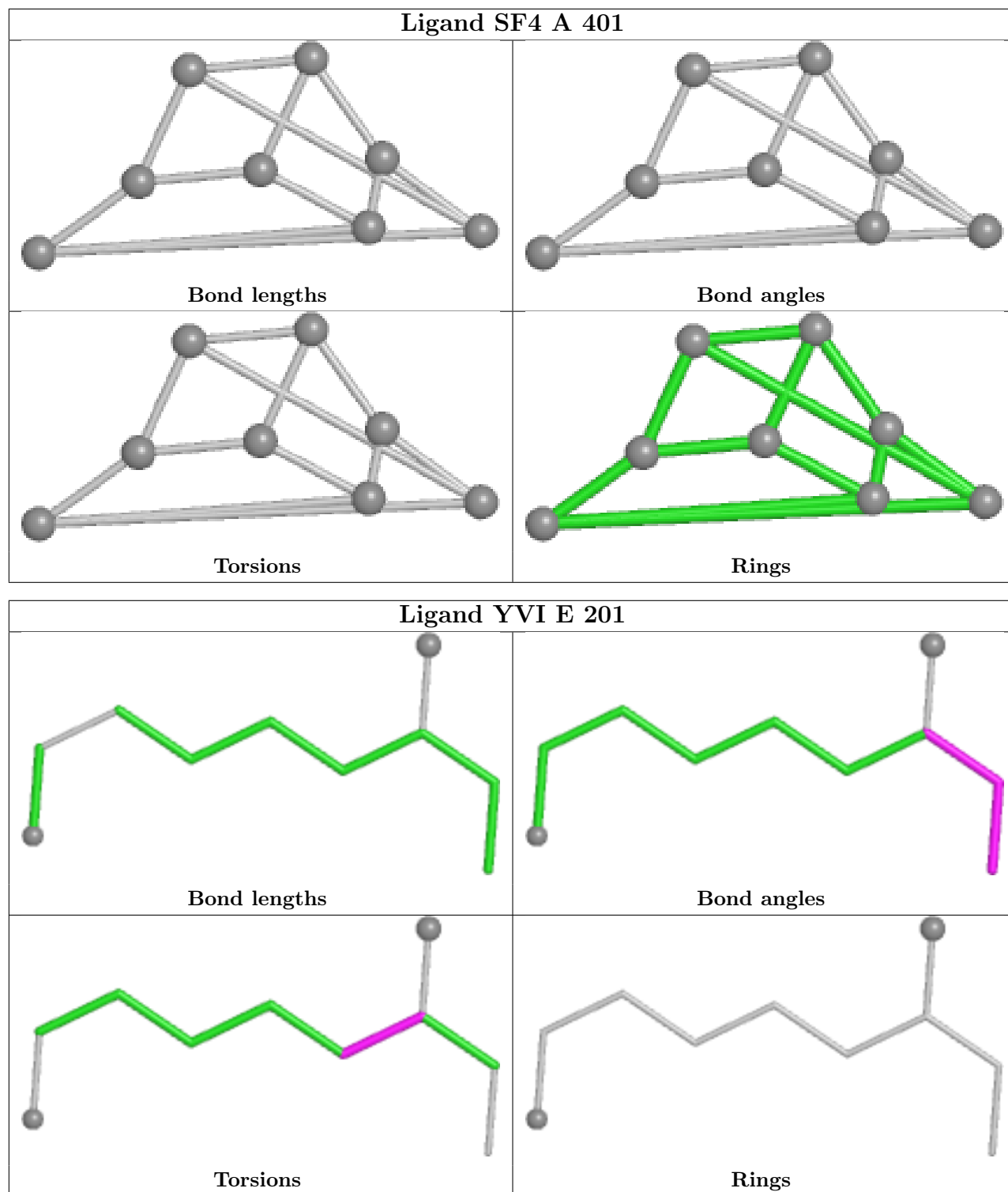
## Ligand SF4 C 401



## Ligand YVI D 201







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	305/368 (82%)	-0.41	3 (0%) 79 76	23, 34, 65, 128	0
1	B	301/368 (81%)	0.06	15 (4%) 35 31	29, 47, 75, 151	0
1	C	292/368 (79%)	1.37	64 (21%) 3 3	63, 94, 130, 146	0
2	D	124/173 (71%)	-0.08	1 (0%) 82 80	29, 52, 69, 80	0
2	E	126/173 (72%)	0.59	2 (1%) 70 66	43, 72, 95, 141	0
2	F	17/173 (9%)	2.63	13 (76%) 0 0	106, 124, 147, 160	0
All	All	1165/1623 (71%)	0.35	98 (8%) 18 16	23, 55, 120, 160	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	364	VAL	5.8
1	B	124	ALA	5.5
1	C	84	ILE	5.5
1	C	123	TYR	5.4
2	F	83	VAL	5.2
1	C	85	PRO	5.1
1	C	365	ALA	4.7
1	C	125	THR	4.6
1	C	76	LEU	4.4
1	B	365	ALA	4.3
1	C	118	TRP	4.2
1	C	140	GLY	4.0
1	C	86	MET	4.0
1	C	360	LEU	3.9
2	F	74	PHE	3.8
1	B	66	LEU	3.7
2	F	70	GLY	3.6
1	C	93	LEU	3.5
1	B	123	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	74	LEU	3.4
1	C	119	GLY	3.4
1	A	71	GLY	3.3
1	C	114	ILE	3.3
1	A	73	ARG	3.3
1	C	88	LYS	3.1
1	C	95	ASN	3.0
1	B	70	LYS	3.0
1	C	90	TYR	3.0
2	F	105	SER	3.0
1	B	125	THR	3.0
2	E	48	LEU	2.9
2	F	71	ILE	2.9
1	C	143	PHE	2.9
2	F	78	ALA	2.9
1	C	124	ALA	2.9
1	C	200	LEU	2.9
1	C	110	ARG	2.8
1	B	120	GLY	2.8
1	C	203	ARG	2.8
1	C	206	LYS	2.8
2	F	79	LEU	2.8
1	C	109	ALA	2.8
1	C	127	THR	2.7
2	F	82	VAL	2.7
1	C	97	LEU	2.7
1	C	130	ILE	2.7
1	C	122	GLU	2.7
1	B	121	GLY	2.7
1	C	126	ALA	2.6
1	C	89	ASN	2.6
1	C	121	GLY	2.6
1	B	67	LYS	2.5
1	C	120	GLY	2.5
1	C	128	ALA	2.5
1	B	122	GLU	2.5
1	C	155	LEU	2.5
1	C	83	GLU	2.5
1	C	272	VAL	2.5
1	C	77	PRO	2.5
1	C	150	ARG	2.5
2	D	48	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	75	ALA	2.4
2	F	73	ASN	2.4
2	F	107	LYS	2.4
1	C	273	ILE	2.4
1	C	104	THR	2.4
1	C	80	LEU	2.3
1	C	92	LYS	2.3
1	C	190	ALA	2.3
1	C	173	ASP	2.3
1	C	213	THR	2.3
1	B	69	GLN	2.3
1	C	235	ALA	2.3
1	C	211	CYS	2.3
1	C	270	PRO	2.2
1	B	231	LEU	2.2
1	C	82	THR	2.2
1	C	179	SER	2.2
2	F	72	SER	2.2
1	C	314	ARG	2.2
2	F	106	VAL	2.2
1	C	231	LEU	2.2
1	C	75	ARG	2.2
1	C	117	CYS	2.2
1	C	323	ILE	2.2
1	B	364	VAL	2.2
1	B	71	GLY	2.1
1	C	178	THR	2.1
1	C	171	GLY	2.1
1	C	202	GLU	2.1
1	C	165	LYS	2.1
2	E	171	ILE	2.1
1	C	161	TYR	2.1
1	C	78	PRO	2.1
1	C	247	LYS	2.1
1	C	223	ILE	2.0
1	A	65	ASN	2.0
1	B	65	ASN	2.0

## 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 [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

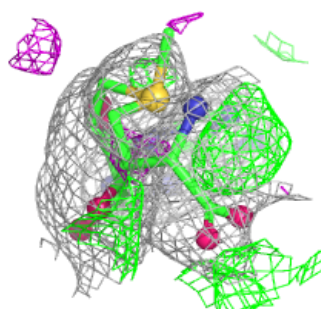
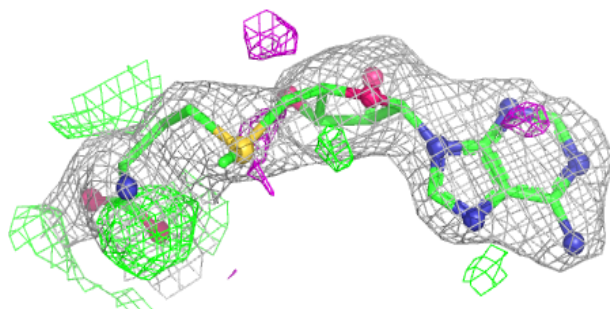
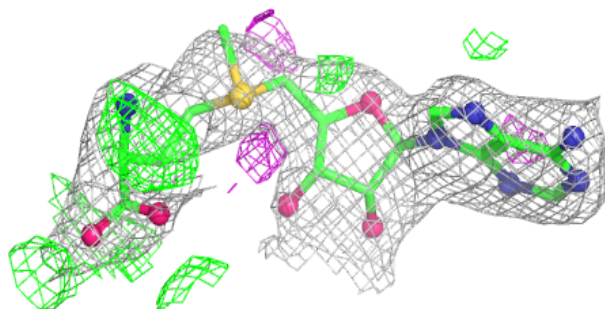
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	SAM	A	403	27/27	0.89	0.14	29,43,61,70	0
5	SAM	C	403	27/27	0.90	0.14	54,66,80,106	0
7	PO4	E	202	5/5	0.90	0.13	75,93,95,99	0
6	YVI	F	201	10/11	0.91	0.15	64,69,90,103	0
7	PO4	D	202	5/5	0.93	0.10	58,60,62,62	0
5	SAM	B	403	27/27	0.93	0.11	30,41,55,72	0
3	SF4	C	401	8/8	0.96	0.08	66,74,81,83	0
4	F3S	C	402	6/7	0.97	0.05	61,76,92,99	0
6	YVI	D	201	10/11	0.98	0.07	23,31,42,43	0
6	YVI	E	201	10/11	0.98	0.07	27,34,46,46	0
3	SF4	B	401	8/8	0.98	0.06	43,46,51,54	0
4	F3S	B	402	6/7	0.98	0.04	25,31,33,33	0
4	F3S	A	402	6/7	0.99	0.04	21,27,30,31	0
3	SF4	A	401	8/8	0.99	0.04	27,32,36,40	0

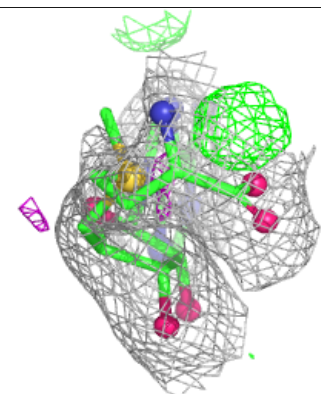
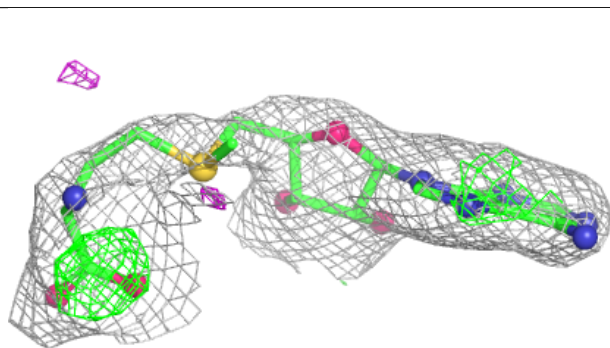
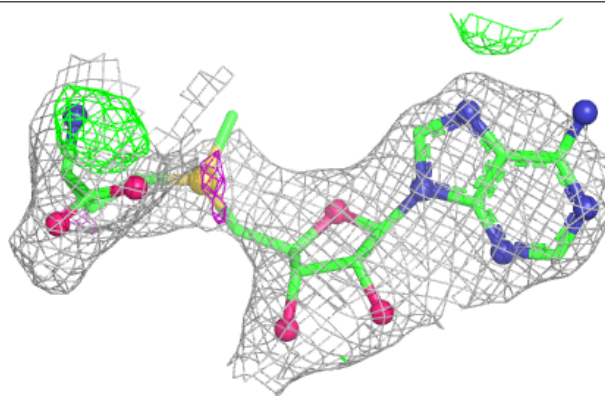
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAM A 403:**

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

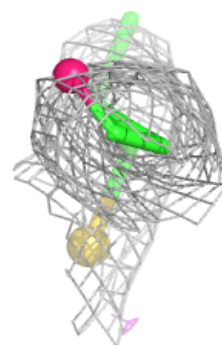
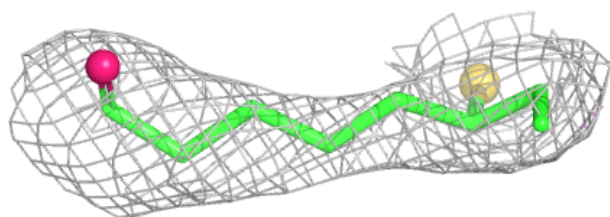
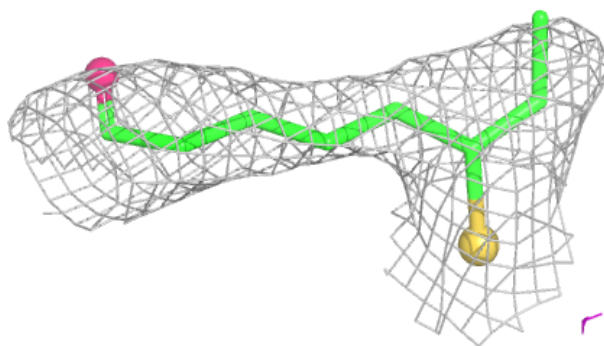
**Electron density around SAM C 403:**

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

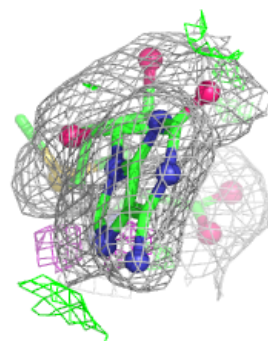
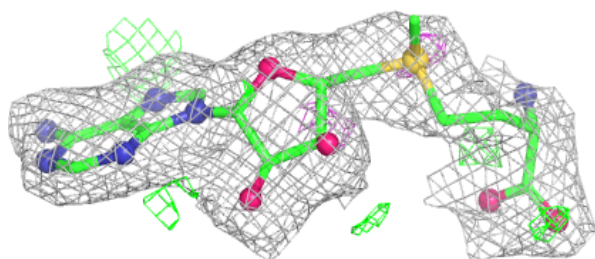
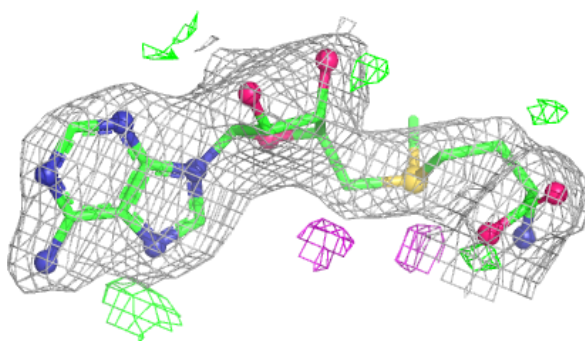


**Electron density around YVI F 201:**

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

**Electron density around SAM B 403:**

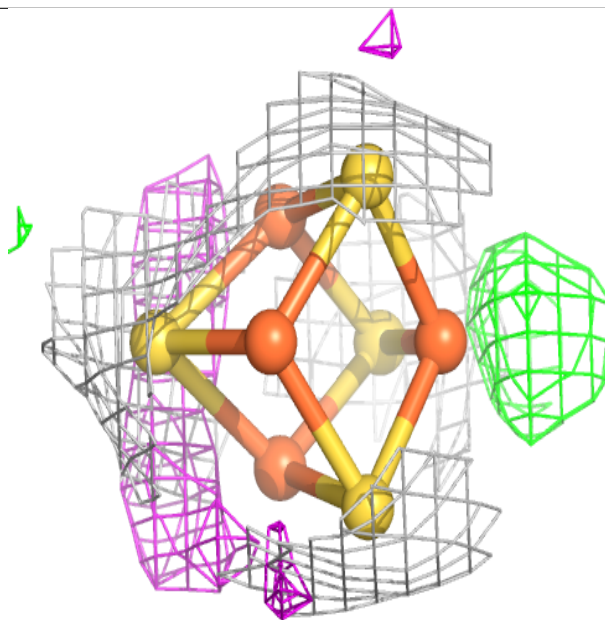
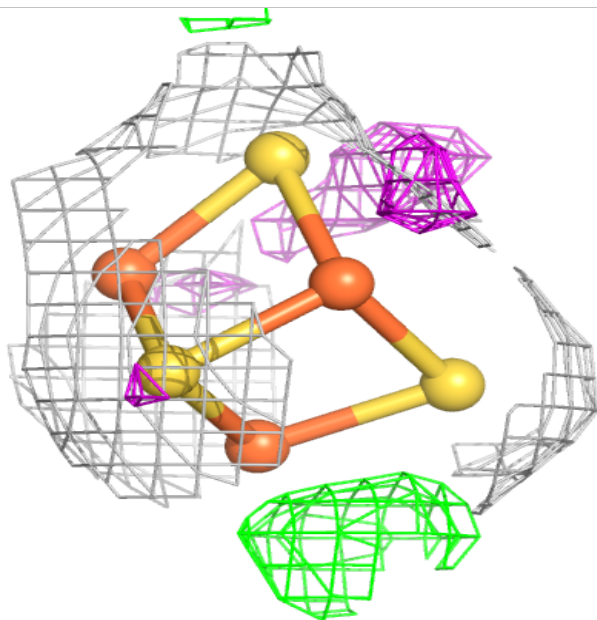
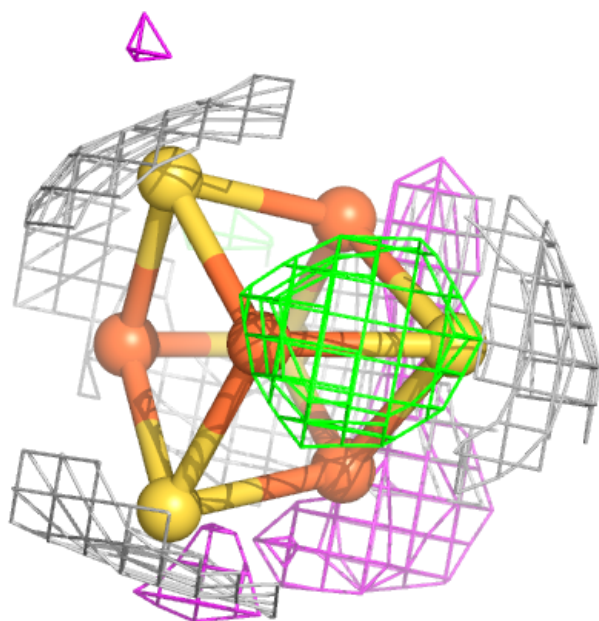
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





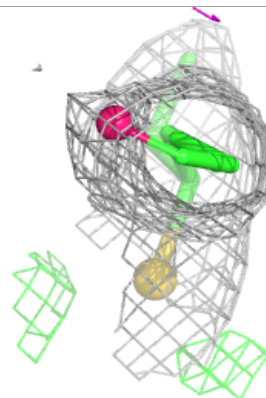
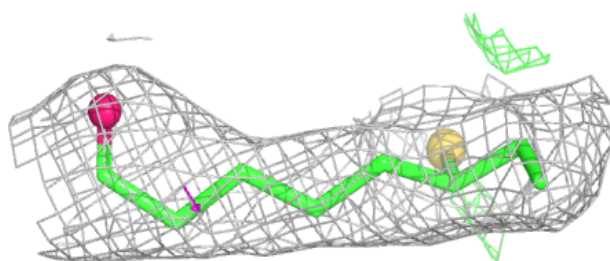
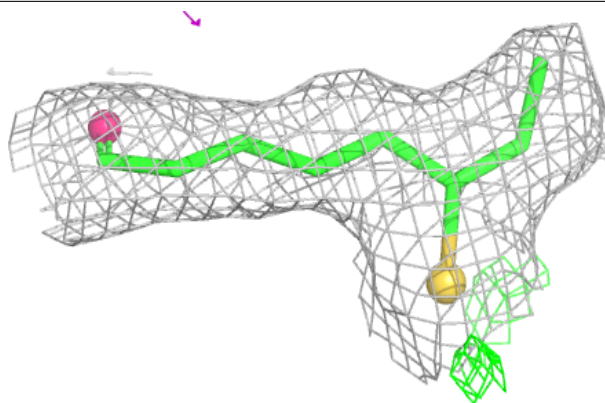
**Electron density around SF4 C 401:**

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

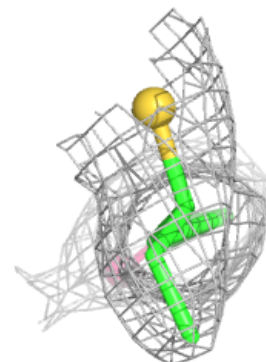
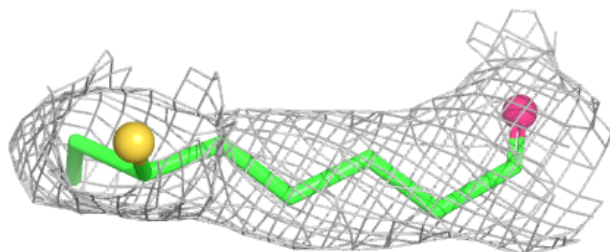
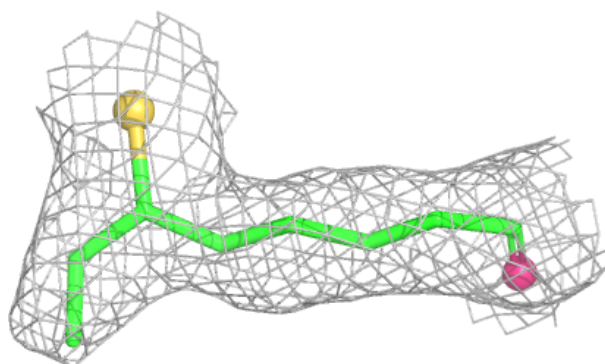


**Electron density around YVI D 201:**

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

**Electron density around YVI E 201:**

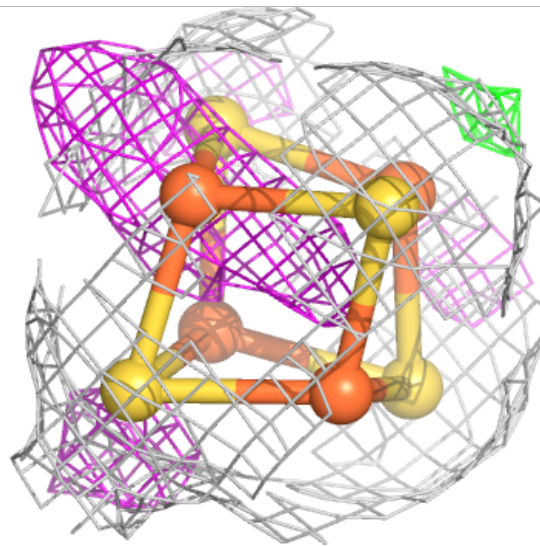
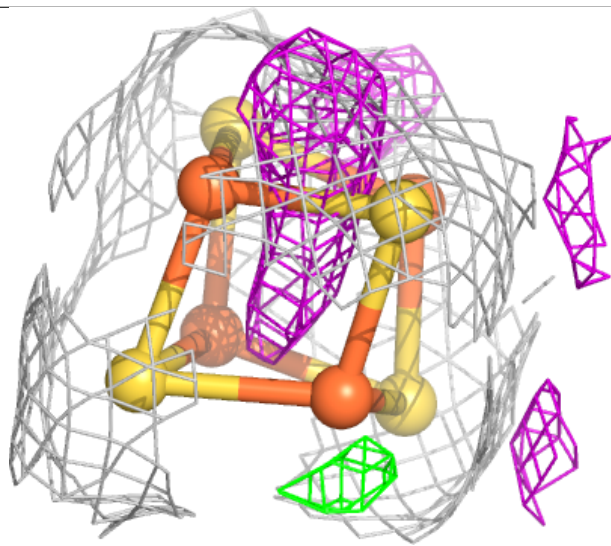
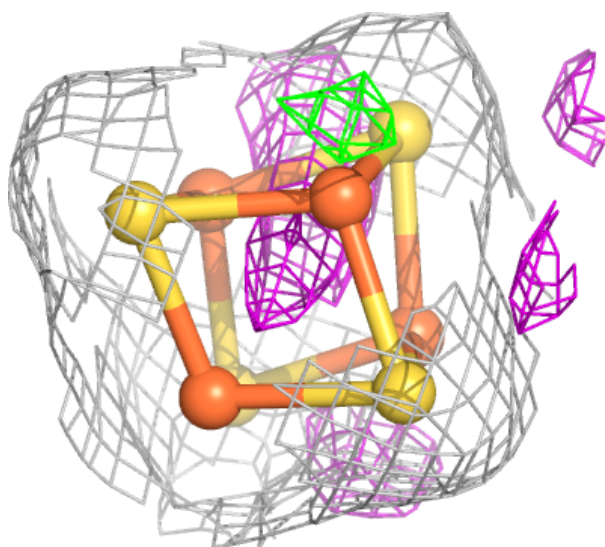
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





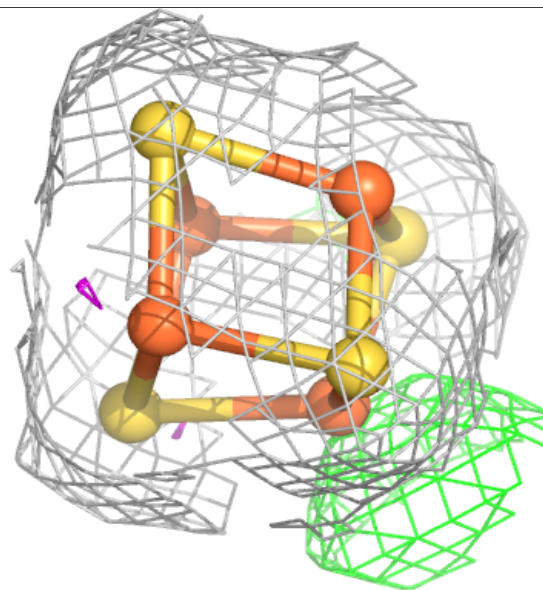
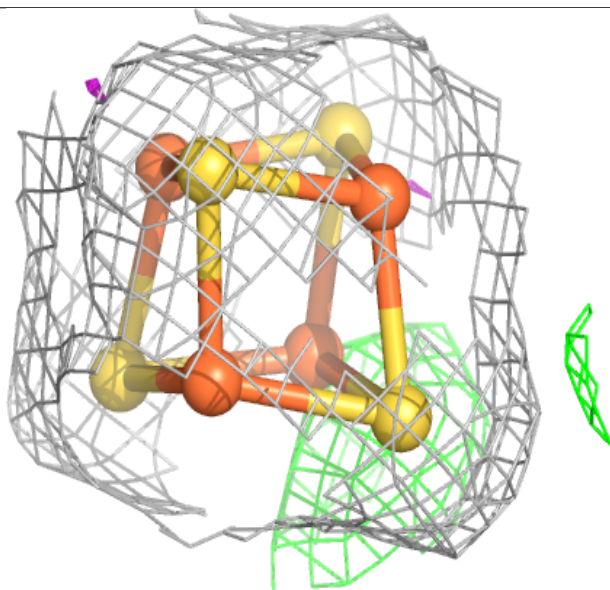
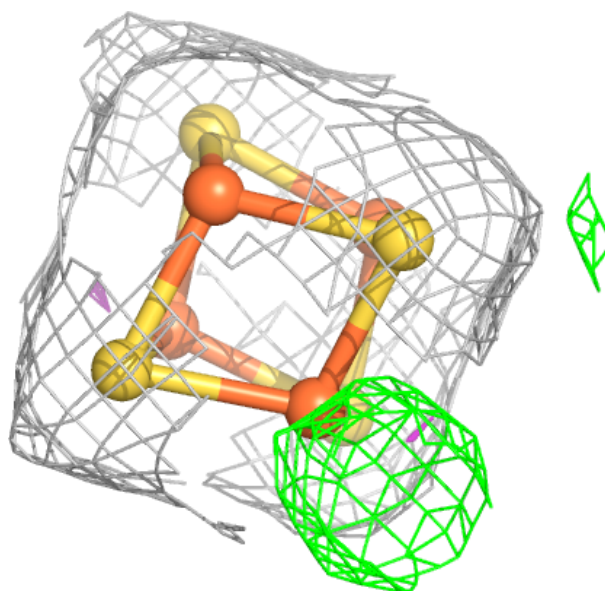
**Electron density around SF4 B 401:**

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



**Electron density around SF4 A 401:**

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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.