



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:03 PM UTC

PDB ID : 8UGO / pdb_00008ugo
Title : Structure of the complex between Human LIAS and H-protein in the presence of 5'-deoxyadenosine
Authors : Esakova, O.A.; Warui, D.M.; Neti, S.S.; Alumasa, J.N.; Booker, S.J.
Deposited on : 2023-10-05
Resolution : 2.45 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

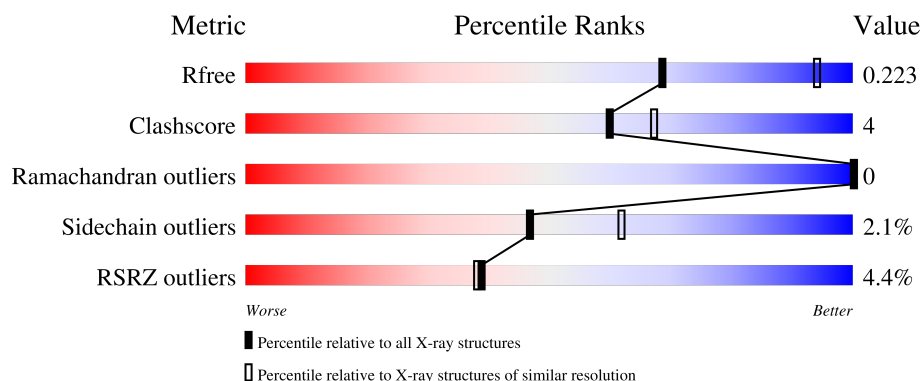
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	368	2% 73% 8% • 19%
1	B	368	75% 7% • 18%
1	D	368	2% 70% 11% 19%
2	C	173	2% 64% 8% • 28%
2	E	173	2% 62% 7% • 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	173	18% 54% 14% 32%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10316 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	A	299	Total	C	N	O	S	0	1	0
			2346	1479	416	436	15			
1	B	303	Total	C	N	O	S	0	1	0
			2397	1512	424	445	16			
1	D	299	Total	C	N	O	S	0	0	0
			2343	1478	414	436	15			

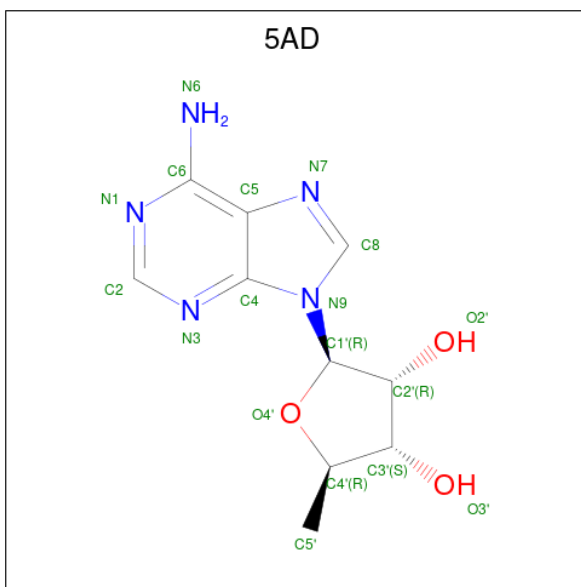
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	LYS	conflict	UNP O43766
B	368	ALA	LYS	conflict	UNP O43766
D	368	ALA	LYS	conflict	UNP O43766

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

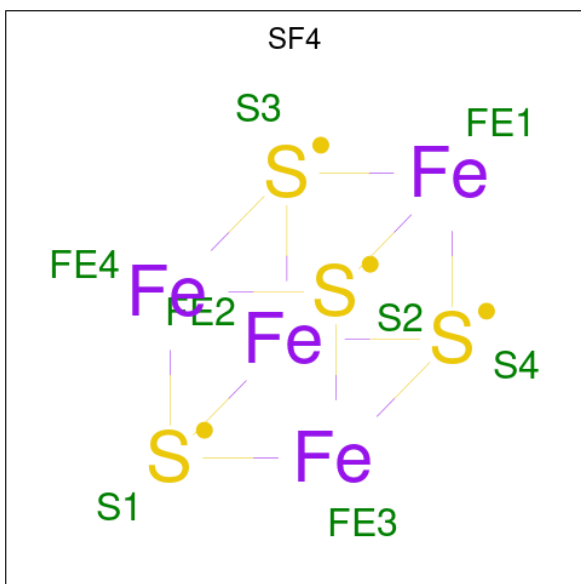
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	121	Total	C	N	O	S	0	0	0
			937	590	146	197	4			
2	C	125	Total	C	N	O	S	0	0	0
			967	611	150	202	4			
2	F	118	Total	C	N	O	S	0	0	0
			914	577	143	190	4			

- Molecule 3 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: C₁₀H₁₃N₅O₃) (labeled as "Ligand of Interest" by depositor).



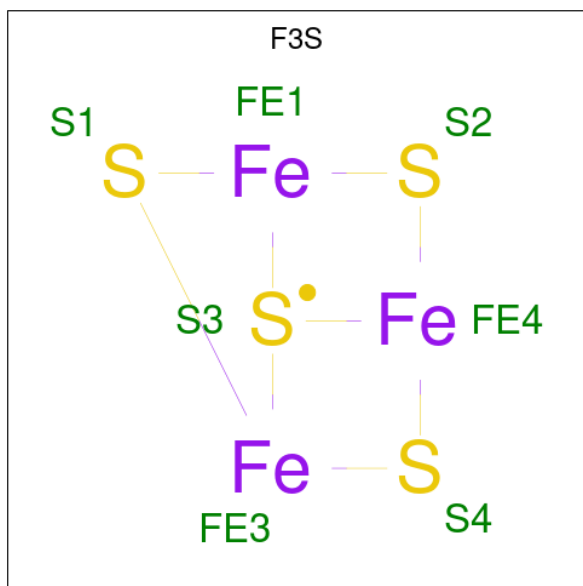
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		
3	B	1	Total	C	N	O	0	0
			18	10	5	3		
3	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



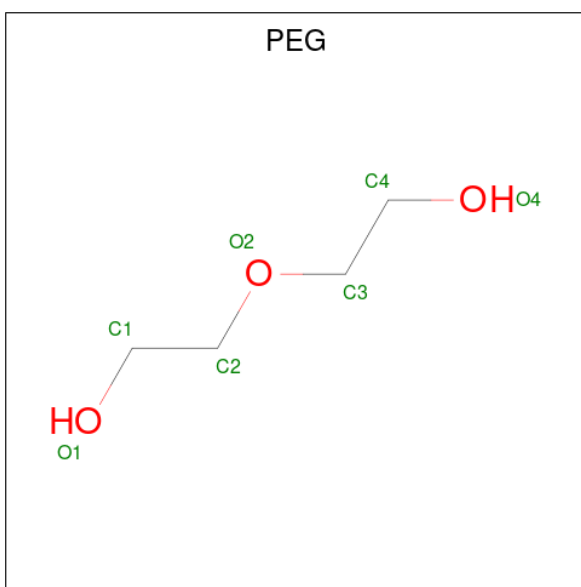
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



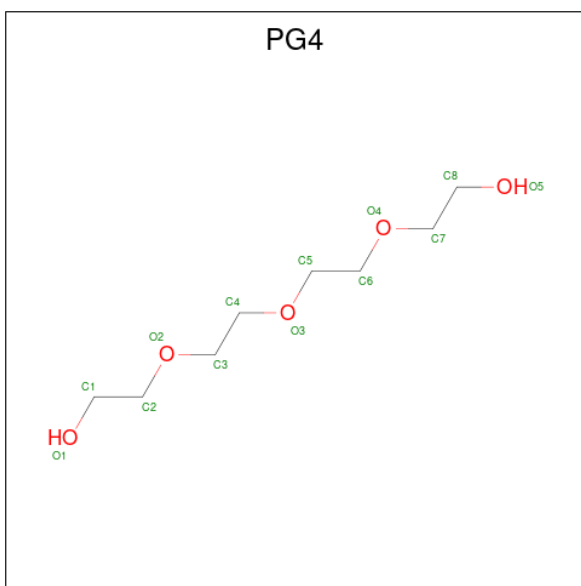
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			6	3	3		
5	B	1	Total	Fe	S	0	0
			6	3	3		
5	D	1	Total	Fe	S	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



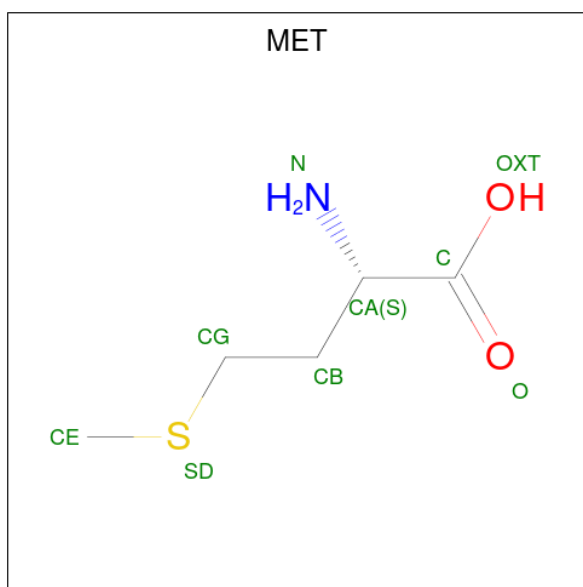
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



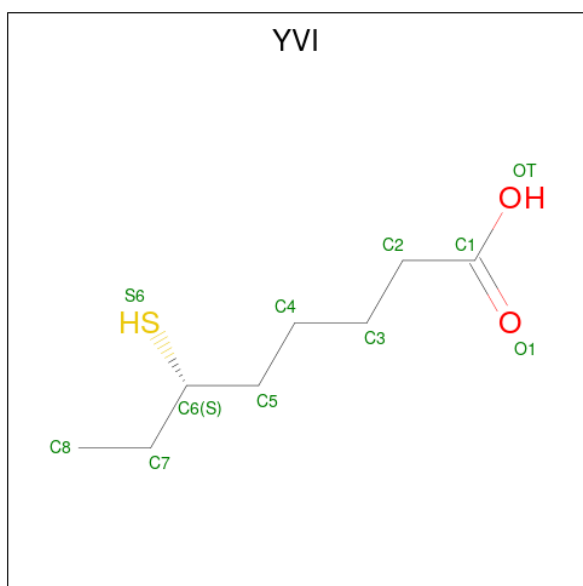
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



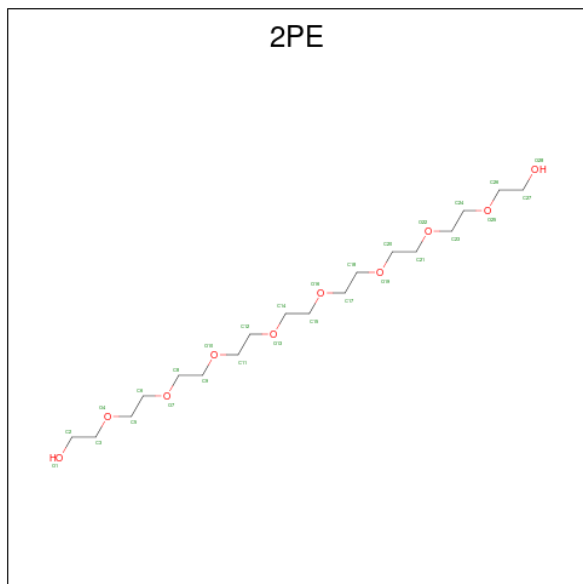
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
8	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
8	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 9 is 6-THIOOCTANOIC ACID (CCD ID: YVI) (formula: C₈H₁₆O₂S) (labeled as "Ligand of Interest" by depositor).



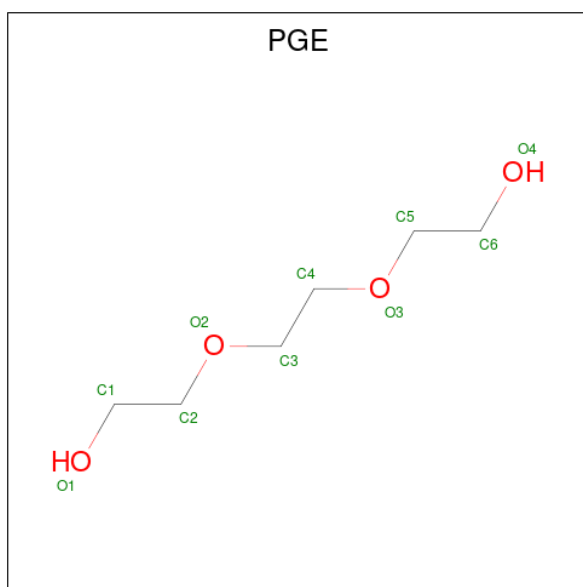
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	1	Total	C	O	S	0	0
			10	8	1	1		
9	C	1	Total	C	O	S	0	0
			10	8	1	1		
9	F	1	Total	C	O	S	0	0
			10	8	1	1		

- Molecule 10 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



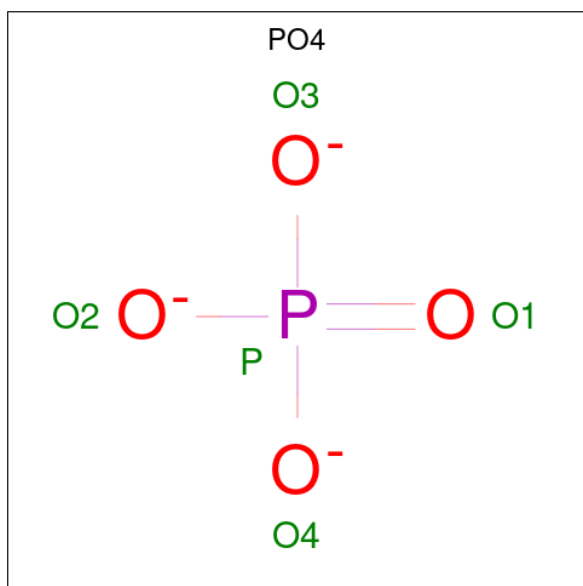
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			28	18	10		

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	O	P	0	0
			5	4	1		

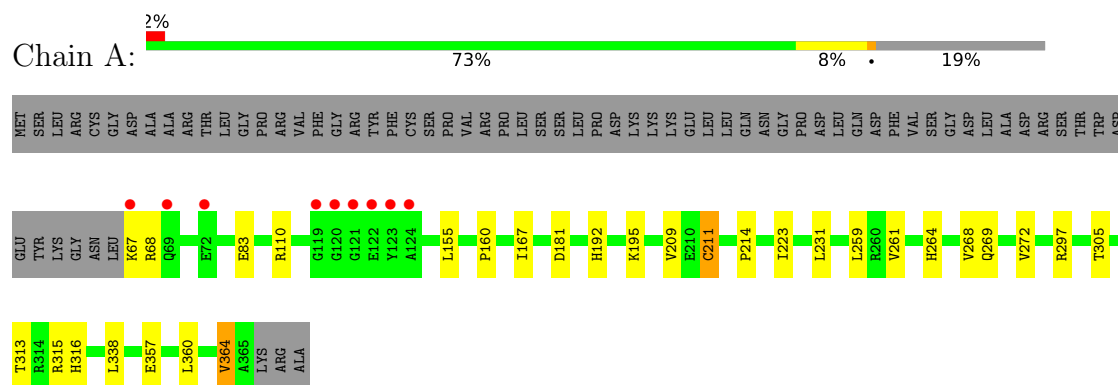
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	53	Total 53	O 53	0	0
13	E	11	Total 11	O 11	0	0
13	B	90	Total 90	O 90	0	0
13	C	21	Total 21	O 21	0	0
13	D	19	Total 19	O 19	0	0
13	F	2	Total 2	O 2	0	0

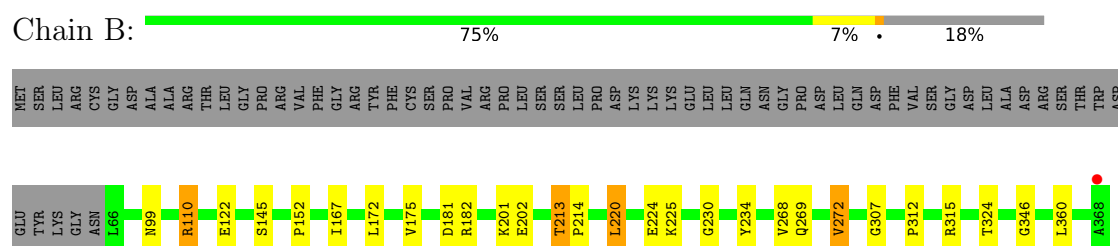
3 Residue-property plots [i](#)

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.

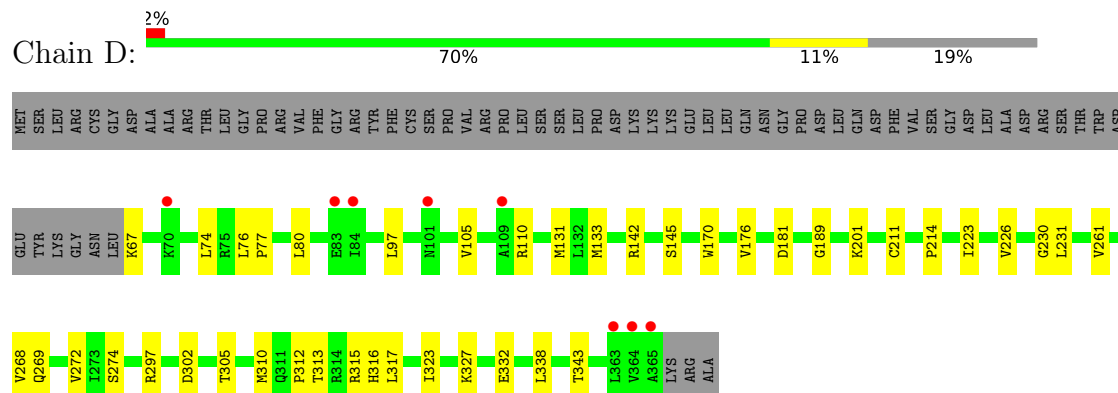
- Molecule 1: Lipoyl synthase, mitochondrial



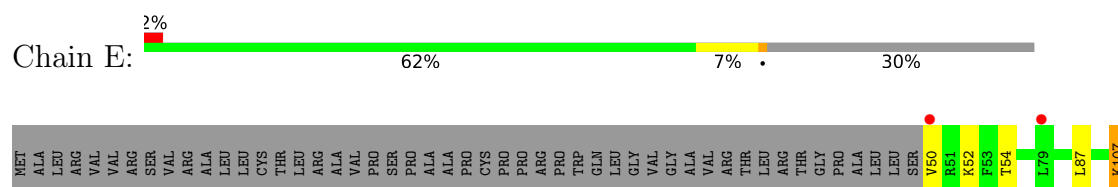
- Molecule 1: Lipoyl synthase, mitochondrial



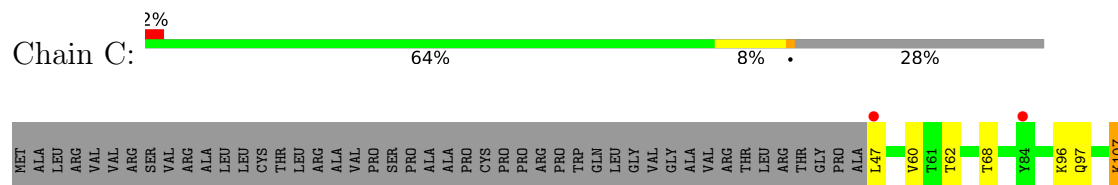
- Molecule 1: Lipoyl synthase, mitochondrial



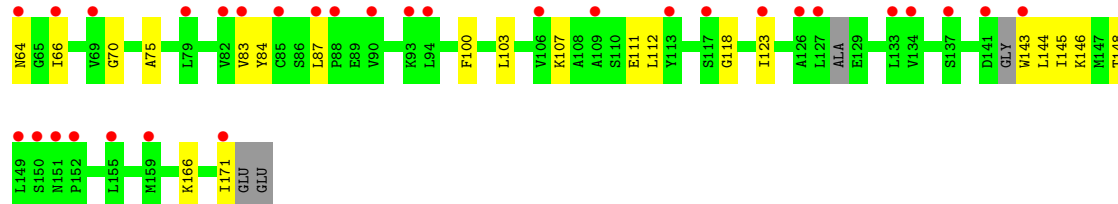
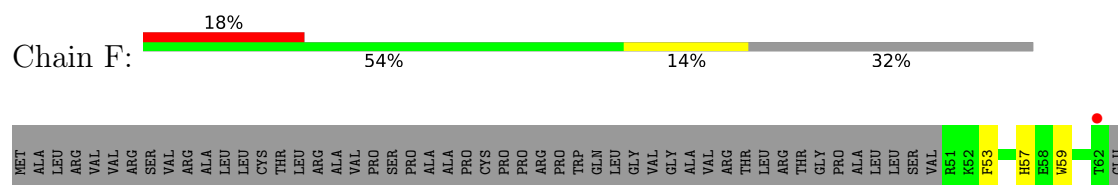
- Molecule 2: Glycine cleavage system H protein, mitochondrial



- Molecule 2: Glycine cleavage system H protein, mitochondrial



- Molecule 2: Glycine cleavage system H protein, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.68Å 169.21Å 183.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.06 – 2.45 38.06 – 2.45	Depositor EDS
% Data completeness (in resolution range)	71.4 (38.06-2.45) 84.4 (38.06-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.223 0.185 , 0.223	Depositor DCC
R_{free} test set	1973 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10316	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: PO4, SF4, 2PE, PGE, PG4, YVI, PEG, 5AD, F3S

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	0.12	0/2397	0.33	0/3244
1	B	0.15	0/2446	0.31	0/3308
1	D	0.10	0/2391	0.29	0/3236
2	C	0.17	0/983	0.33	0/1331
2	E	0.16	0/953	0.31	1/1290 (0.1%)
2	F	0.18	0/927	0.36	0/1250
All	All	0.14	0/10097	0.32	1/13659 (0.0%)

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
2	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	107	LYS	O-C-N	-5.83	114.27	122.26

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	107	LYS	Mainchain

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	2346	0	2348	14	0
1	B	2397	0	2410	17	0
1	D	2343	0	2347	23	0
2	C	967	0	941	11	0
2	E	937	0	903	6	0
2	F	914	0	877	18	0
3	A	18	0	13	0	0
3	B	18	0	13	2	0
3	D	18	0	13	0	0
4	A	8	0	0	0	0
4	B	8	0	0	1	0
4	D	8	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	D	6	0	0	0	0
6	A	7	0	10	0	0
7	A	13	0	18	0	0
8	A	9	0	8	1	0
8	B	9	0	8	2	0
8	D	9	0	8	0	0
9	C	10	0	0	1	0
9	E	10	0	0	0	0
9	F	10	0	0	0	0
10	B	28	0	38	1	0
11	B	10	0	14	2	0
12	B	5	0	0	0	0
13	A	53	0	0	0	0
13	B	90	0	0	0	0
13	C	21	0	0	0	0
13	D	19	0	0	0	0
13	E	11	0	0	1	0
13	F	2	0	0	0	0
All	All	10316	0	9969	87	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 (87) 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:357:GLU:HG2	1:B:360:LEU:HD21	1.74	0.70
1:A:313:THR:HG22	1:A:315:ARG:H	1.60	0.66
2:E:123:ILE:HG22	2:E:145:ILE:HG22	1.78	0.66
1:B:224:GLU:HG2	1:B:268:VAL:HG21	1.78	0.65
1:D:313:THR:HG22	1:D:315:ARG:H	1.61	0.65
2:F:123:ILE:HG22	2:F:145:ILE:HG22	1.79	0.64
1:A:313:THR:HB	1:A:316:HIS:ND1	2.14	0.63
2:C:62:THR:HG21	2:C:155:LEU:HD11	1.82	0.62
1:D:269:GLN:HG2	1:D:272:VAL:HG13	1.79	0.62
1:D:110:ARG:O	2:F:107:LYS:HD2	2.00	0.61
1:B:269:GLN:HG3	1:B:272:VAL:HB	1.81	0.61
1:A:67:LYS:HE3	1:A:68:ARG:HG3	1.83	0.59
1:B:145:SER:HB3	1:B:312:PRO:HB2	1.87	0.57
1:B:213:THR:HG21	1:B:234:TYR:OH	2.04	0.57
2:F:103:LEU:HD21	2:F:144:LEU:HD21	1.87	0.57
1:D:142:ARG:HB3	1:D:317:LEU:HG	1.88	0.55
1:B:99:ASN:HB3	10:B:404:2PE:H92	1.88	0.55
1:A:181:ASP:OD1	1:A:214:PRO:HB3	2.08	0.54
1:A:211:CYS:HB2	1:A:231:LEU:HD22	1.91	0.53
1:D:313:THR:HB	1:D:316:HIS:ND1	2.23	0.53
1:D:67:LYS:HB2	1:D:74:LEU:HD11	1.90	0.52
1:D:76:LEU:HD12	1:D:77:PRO:HD2	1.91	0.52
1:D:201:LYS:HE3	1:D:230:GLY:O	2.09	0.52
1:D:181:ASP:OD1	1:D:214:PRO:HB3	2.09	0.52
2:C:116:LEU:HD13	2:C:149:LEU:HG	1.91	0.52
1:D:211:CYS:HB2	1:D:231:LEU:HD22	1.92	0.52
2:F:166:LYS:HG2	2:F:171:ILE:HA	1.92	0.52
1:A:360:LEU:HA	1:A:364:VAL:HG13	1.92	0.51
2:E:116:LEU:HD13	2:E:149:LEU:HG	1.92	0.51
2:F:166:LYS:HE3	2:F:171:ILE:HG23	1.93	0.51
1:D:77:PRO:HG2	1:D:80:LEU:HB2	1.92	0.51
1:B:225:LYS:HA	11:B:405:PGE:H52	1.92	0.50
1:B:181:ASP:OD1	1:B:214:PRO:HB3	2.12	0.50
1:D:312:PRO:HA	2:F:107:LYS:HG2	1.94	0.50
1:A:83:GLU:HG3	1:B:122:GLU:HG2	1.94	0.49
2:F:100:PHE:CZ	2:F:112:LEU:HB3	2.48	0.49
2:C:116:LEU:HD21	2:C:155:LEU:HD23	1.94	0.49
2:E:54:THR:HG22	2:E:158:LEU:HD22	1.94	0.49
1:D:274:SER:HB2	1:D:302:ASP:H	1.78	0.49
1:B:110:ARG:O	2:C:107:LYS:HE3	2.14	0.48
1:D:310:MET:HE2	2:F:107:LYS:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:PRO:HG2	1:B:182:ARG:CZ	2.44	0.47
2:F:83:VAL:HG13	2:F:84:TYR:HD2	1.79	0.47
2:C:159:MET:HE1	2:C:167:TYR:CD1	2.49	0.47
1:A:160:PRO:HD3	1:A:192:HIS:CE1	2.50	0.47
2:F:143:TRP:CZ3	2:F:146:LYS:HG3	2.50	0.47
1:D:297:ARG:HG3	1:D:338:LEU:HB3	1.97	0.47
1:A:269:GLN:O	1:A:272:VAL:HG22	2.15	0.47
2:C:162:GLU:H	2:C:162:GLU:CD	2.23	0.46
2:F:87:LEU:HD21	2:F:144:LEU:HD23	1.97	0.46
1:B:307:GLY:HA2	1:B:346:GLY:O	2.15	0.46
2:E:52:LYS:NZ	13:E:302:HOH:O	2.49	0.46
1:B:167:ILE:HG13	1:B:172:LEU:HD12	1.98	0.45
2:C:47:LEU:HD23	2:C:47:LEU:HA	1.72	0.45
3:B:401:5AD:H5'3	8:B:406:MET:SD	2.56	0.45
4:B:402:SF4:S1	8:B:406:MET:HE3	2.57	0.45
1:D:145:SER:HB3	1:D:312:PRO:HB2	1.99	0.44
1:D:323:ILE:HG23	1:D:327:LYS:HB3	1.99	0.44
1:A:223:ILE:HD11	1:A:261:VAL:HG22	1.99	0.44
1:B:201:LYS:HE3	1:B:230:GLY:O	2.18	0.43
1:B:220:LEU:O	1:B:224:GLU:HG3	2.19	0.43
1:B:225:LYS:HZ2	11:B:405:PGE:H22	1.83	0.43
1:A:264:HIS:O	1:A:268:VAL:HG23	2.19	0.43
2:E:87:LEU:HD11	2:E:127:LEU:HD12	2.00	0.42
2:F:57:HIS:HB3	2:F:75:ALA:HB2	2.01	0.42
1:B:315:ARG:HE	1:B:315:ARG:HB2	1.71	0.42
1:D:297:ARG:HD2	1:D:297:ARG:HA	1.83	0.42
1:D:332:GLU:HG3	1:D:343:THR:O	2.19	0.42
2:F:70:GLY:HA2	2:F:144:LEU:HD12	2.00	0.42
8:A:406:MET:SD	8:A:406:MET:N	2.92	0.42
2:C:60:VAL:HA	2:C:68:THR:O	2.19	0.42
1:A:259:LEU:HA	1:A:259:LEU:HD12	1.86	0.42
1:D:223:ILE:HD13	1:D:261:VAL:HA	2.01	0.42
2:E:123:ILE:HD12	2:E:125:GLU:HG2	2.01	0.42
2:C:96:LYS:HE2	2:C:96:LYS:HB3	1.87	0.42
2:F:66:ILE:HG22	2:F:148:THR:HA	2.01	0.42
2:C:96:LYS:HG2	2:C:97:GLN:HG3	2.02	0.41
3:B:401:5AD:H5'1	9:C:201:YVI:C8	2.51	0.41
2:F:111:GLU:H	2:F:111:GLU:HG2	1.68	0.41
2:F:53:PHE:CE1	2:F:59:TRP:HB3	2.55	0.41
2:C:122:GLU:HB3	2:C:146:LYS:HB2	2.02	0.41
1:D:133:MET:SD	1:D:189:GLY:HA3	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HG3	1:A:338:LEU:HB3	2.01	0.41
2:F:118:GLY:HA3	2:F:148:THR:O	2.21	0.40
1:D:105:VAL:N	1:D:131:MET:HB2	2.36	0.40
1:D:97:LEU:HD21	1:D:170:TRP:HH2	1.87	0.40
2:F:59:TRP:CE2	2:F:70:GLY:HA3	2.56	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	298/368 (81%)	290 (97%)	8 (3%)	0	100	100
1	B	302/368 (82%)	293 (97%)	9 (3%)	0	100	100
1	D	297/368 (81%)	286 (96%)	11 (4%)	0	100	100
2	C	123/173 (71%)	118 (96%)	5 (4%)	0	100	100
2	E	119/173 (69%)	114 (96%)	5 (4%)	0	100	100
2	F	110/173 (64%)	107 (97%)	3 (3%)	0	100	100
All	All	1249/1623 (77%)	1208 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	253/316 (80%)	245 (97%)	8 (3%)	34	49
1	B	260/316 (82%)	253 (97%)	7 (3%)	39	54
1	D	253/316 (80%)	249 (98%)	4 (2%)	55	69
2	C	108/146 (74%)	107 (99%)	1 (1%)	70	81
2	E	104/146 (71%)	102 (98%)	2 (2%)	50	64
2	F	101/146 (69%)	100 (99%)	1 (1%)	68	77
All	All	1079/1386 (78%)	1056 (98%)	23 (2%)	47	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	155	LEU
1	A	167	ILE
1	A	195	LYS
1	A	209	VAL
1	A	211	CYS
1	A	305	THR
1	A	364	VAL
2	E	50	VAL
2	E	134	VAL
1	B	110	ARG
1	B	175	VAL
1	B	202	GLU
1	B	213	THR
1	B	220	LEU
1	B	272	VAL
1	B	324	THR
2	C	107	LYS
1	D	176	VAL
1	D	226	VAL
1	D	268	VAL
1	D	305	THR
2	F	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	269	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	237	ASN
1	D	101	ASN
1	D	103	HIS
1	D	362	ASN

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](#)

20 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	$\# Z > 2$
9	YVI	E	201	2,5	7,9,10	0.30	0	5,9,11	1.01	0
12	PO4	B	407	-	4,4,4	0.95	0	6,6,6	0.43	0
5	F3S	D	403	9,1	0,7,9	-	-	-	-	-
10	2PE	B	404	-	27,27,27	0.12	0	26,26,26	0.08	0
8	MET	D	404	-	7,8,8	0.96	1 (14%)	5,9,9	1.89	1 (20%)
4	SF4	A	402	8,1	0,12,12	-	-	-	-	-
9	YVI	C	201	2,5	7,9,10	0.27	0	5,9,11	0.70	0
8	MET	B	406	4	7,8,8	0.87	1 (14%)	5,9,9	1.83	1 (20%)
4	SF4	B	402	8,1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5AD	D	402	-	20,20,20	3.66	10 (50%)	28,30,30	2.71	15 (53%)
6	PEG	A	404	-	6,6,6	0.10	0	5,5,5	0.13	0
8	MET	A	406	4	7,8,8	0.87	1 (14%)	5,9,9	1.50	1 (20%)
5	F3S	A	403	9,1	0,7,9	-	-	-	-	-
7	PG4	A	405	-	12,12,12	0.13	0	11,11,11	0.59	0
9	YVI	F	201	2,5	7,9,10	0.38	0	5,9,11	0.76	0
4	SF4	D	401	1	0,12,12	-	-	-	-	-
11	PGE	B	405	-	9,9,9	0.31	0	8,8,8	0.33	0
5	F3S	B	403	9,1	0,7,9	-	-	-	-	-
3	5AD	B	401	-	20,20,20	3.65	9 (45%)	28,30,30	2.52	12 (42%)
3	5AD	A	401	-	20,20,20	3.65	10 (50%)	28,30,30	2.74	15 (53%)

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
9	YVI	E	201	2,5	-	0/7/8/9	-
5	F3S	D	403	9,1	-	-	0/2/2/3
10	2PE	B	404	-	-	11/25/25/25	-
8	MET	D	404	-	-	4/8/8/8	-
4	SF4	A	402	8,1	-	-	0/6/5/5
9	YVI	C	201	2,5	-	1/7/8/9	-
8	MET	B	406	4	-	3/8/8/8	-
4	SF4	B	402	8,1	-	-	0/6/5/5
3	5AD	D	402	-	-	0/4/20/20	0/3/3/3
6	PEG	A	404	-	-	4/4/4/4	-
8	MET	A	406	4	-	1/8/8/8	-
5	F3S	A	403	9,1	-	-	0/2/2/3
7	PG4	A	405	-	-	4/10/10/10	-
9	YVI	F	201	2,5	-	1/7/8/9	-
4	SF4	D	401	1	-	-	0/6/5/5
11	PGE	B	405	-	-	3/7/7/7	-
5	F3S	B	403	9,1	-	-	0/2/2/3
3	5AD	B	401	-	-	0/4/20/20	0/3/3/3
3	5AD	A	401	-	-	0/4/20/20	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	5AD	C3'-C4'	8.18	1.64	1.52
3	D	402	5AD	C3'-C4'	8.15	1.64	1.52
3	A	401	5AD	C3'-C4'	8.00	1.64	1.52
3	A	401	5AD	O4'-C1'	7.34	1.59	1.42
3	B	401	5AD	C3'-C2'	-7.23	1.33	1.53
3	D	402	5AD	C3'-C2'	-7.20	1.33	1.53
3	A	401	5AD	C3'-C2'	-7.20	1.33	1.53
3	B	401	5AD	O4'-C1'	7.04	1.58	1.42
3	D	402	5AD	O4'-C1'	6.93	1.58	1.42
3	D	402	5AD	C1'-N9	-5.15	1.32	1.46
3	B	401	5AD	C1'-N9	-5.02	1.32	1.46
3	A	401	5AD	C1'-N9	-4.97	1.32	1.46
3	D	402	5AD	O4'-C4'	-4.78	1.30	1.44
3	B	401	5AD	O4'-C4'	-4.69	1.30	1.44
3	A	401	5AD	O4'-C4'	-4.57	1.31	1.44
3	A	401	5AD	C6-N6	4.57	1.45	1.34
3	D	402	5AD	C6-N6	4.52	1.45	1.34
3	B	401	5AD	C6-N6	4.43	1.45	1.34
3	D	402	5AD	C5-C4	-2.87	1.34	1.39
3	B	401	5AD	C5-C4	-2.71	1.34	1.39
3	A	401	5AD	C5-C4	-2.70	1.34	1.39
3	B	401	5AD	C5-N7	-2.47	1.34	1.39
3	A	401	5AD	C5-N7	-2.44	1.34	1.39
3	D	402	5AD	C5-N7	-2.44	1.34	1.39
3	D	402	5AD	O2'-C2'	2.23	1.48	1.43
3	B	401	5AD	O2'-C2'	2.20	1.48	1.43
8	A	406	MET	OXT-C	-2.20	1.23	1.30
8	D	404	MET	OXT-C	-2.20	1.23	1.30
3	A	401	5AD	O2'-C2'	2.20	1.48	1.43
8	B	406	MET	OXT-C	-2.17	1.23	1.30
3	A	401	5AD	C8-N9	-2.09	1.34	1.37
3	D	402	5AD	C8-N9	-2.08	1.34	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	5AD	C5'-C4'-C3'	-5.97	109.43	115.70
3	D	402	5AD	N3-C2-N1	-5.65	120.03	128.58
3	B	401	5AD	N3-C2-N1	-5.53	120.21	128.58
3	A	401	5AD	N3-C2-N1	-5.52	120.23	128.58
3	A	401	5AD	C5-C4-N3	-4.95	119.90	126.72
3	B	401	5AD	C5-C4-N3	-4.88	120.00	126.72
3	D	402	5AD	C5-C4-N3	-4.71	120.23	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	5AD	N9-C8-N7	-4.45	107.63	113.94
3	D	402	5AD	C5'-C4'-C3'	-4.27	111.22	115.70
3	D	402	5AD	N6-C6-N1	-4.20	109.03	118.38
3	B	401	5AD	N6-C6-N1	-4.19	109.04	118.38
3	A	401	5AD	N6-C6-N1	-4.15	109.13	118.38
3	A	401	5AD	N9-C8-N7	-4.15	108.05	113.94
3	B	401	5AD	N9-C8-N7	-4.00	108.25	113.94
8	D	404	MET	OXT-C-O	-3.81	115.44	124.08
8	B	406	MET	OXT-C-O	-3.80	115.45	124.08
3	D	402	5AD	C4-N9-C1'	-3.48	118.48	126.63
3	B	401	5AD	C4-N9-C1'	-3.46	118.53	126.63
8	A	406	MET	OXT-C-O	-3.32	116.55	124.08
3	B	401	5AD	C2-N3-C4	3.32	119.94	111.83
3	A	401	5AD	C2-N3-C4	3.31	119.91	111.83
3	D	402	5AD	C2-N3-C4	3.31	119.91	111.83
3	A	401	5AD	C5-C6-N6	3.17	131.14	123.29
3	A	401	5AD	N3-C4-N9	3.17	132.56	127.17
3	D	402	5AD	C2'-C3'-C4'	3.12	106.97	102.36
3	D	402	5AD	C5-C6-N6	3.10	130.96	123.29
3	B	401	5AD	N3-C4-N9	3.08	132.41	127.17
3	B	401	5AD	C5-C6-N6	3.05	130.84	123.29
3	A	401	5AD	C4-N9-C1'	-3.04	119.52	126.63
3	D	402	5AD	N3-C4-N9	2.96	132.21	127.17
3	B	401	5AD	C5'-C4'-C3'	-2.96	112.59	115.70
3	D	402	5AD	C5-N7-C8	2.93	108.05	103.45
3	A	401	5AD	C5-N7-C8	2.87	107.97	103.45
3	B	401	5AD	C1'-N9-C8	2.83	133.37	127.09
3	D	402	5AD	C4-N9-C8	2.75	108.62	105.74
3	B	401	5AD	C5-N7-C8	2.67	107.65	103.45
3	D	402	5AD	C3'-C2'-C1'	2.64	106.45	101.46
3	D	402	5AD	C1'-N9-C8	2.61	132.89	127.09
3	A	401	5AD	C2'-C3'-C4'	2.44	105.97	102.36
3	A	401	5AD	C4-N9-C8	2.42	108.28	105.74
3	A	401	5AD	C1'-N9-C8	2.30	132.20	127.09
3	B	401	5AD	C4-N9-C8	2.25	108.10	105.74
3	A	401	5AD	C6-C5-C4	2.15	120.11	117.18
3	D	402	5AD	C4-C5-N7	-2.13	108.14	110.58
3	A	401	5AD	C4-C5-N7	-2.11	108.17	110.58

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	406	MET	O-C-CA-N
8	D	404	MET	O-C-CA-N
10	B	404	2PE	O16-C17-C18-O19
6	A	404	PEG	O1-C1-C2-O2
8	D	404	MET	OXT-C-CA-N
8	B	406	MET	OXT-C-CA-N
10	B	404	2PE	O19-C20-C21-O22
6	A	404	PEG	O2-C3-C4-O4
11	B	405	PGE	O2-C3-C4-O3
10	B	404	2PE	O1-C2-C3-O4
10	B	404	2PE	C8-C9-O10-C11
10	B	404	2PE	C14-C15-O16-C17
10	B	404	2PE	C5-C6-O7-C8
7	A	405	PG4	C5-C6-O4-C7
9	C	201	YVI	C1-C2-C3-C4
10	B	404	2PE	C15-C14-O13-C12
10	B	404	2PE	O13-C14-C15-O16
6	A	404	PEG	C4-C3-O2-C2
7	A	405	PG4	C8-C7-O4-C6
7	A	405	PG4	O3-C5-C6-O4
7	A	405	PG4	C6-C5-O3-C4
11	B	405	PGE	C3-C4-O3-C5
10	B	404	2PE	C6-C5-O4-C3
8	B	406	MET	CA-CB-CG-SD
9	F	201	YVI	C4-C5-C6-S6
8	D	404	MET	O-C-CA-CB
8	D	404	MET	OXT-C-CA-CB
11	B	405	PGE	O3-C5-C6-O4
10	B	404	2PE	O22-C23-C24-O25
6	A	404	PEG	C1-C2-O2-C3
10	B	404	2PE	C11-C12-O13-C14
8	A	406	MET	OXT-C-CA-N

There are no ring outliers.

7 monomers are involved in 7 short contacts:

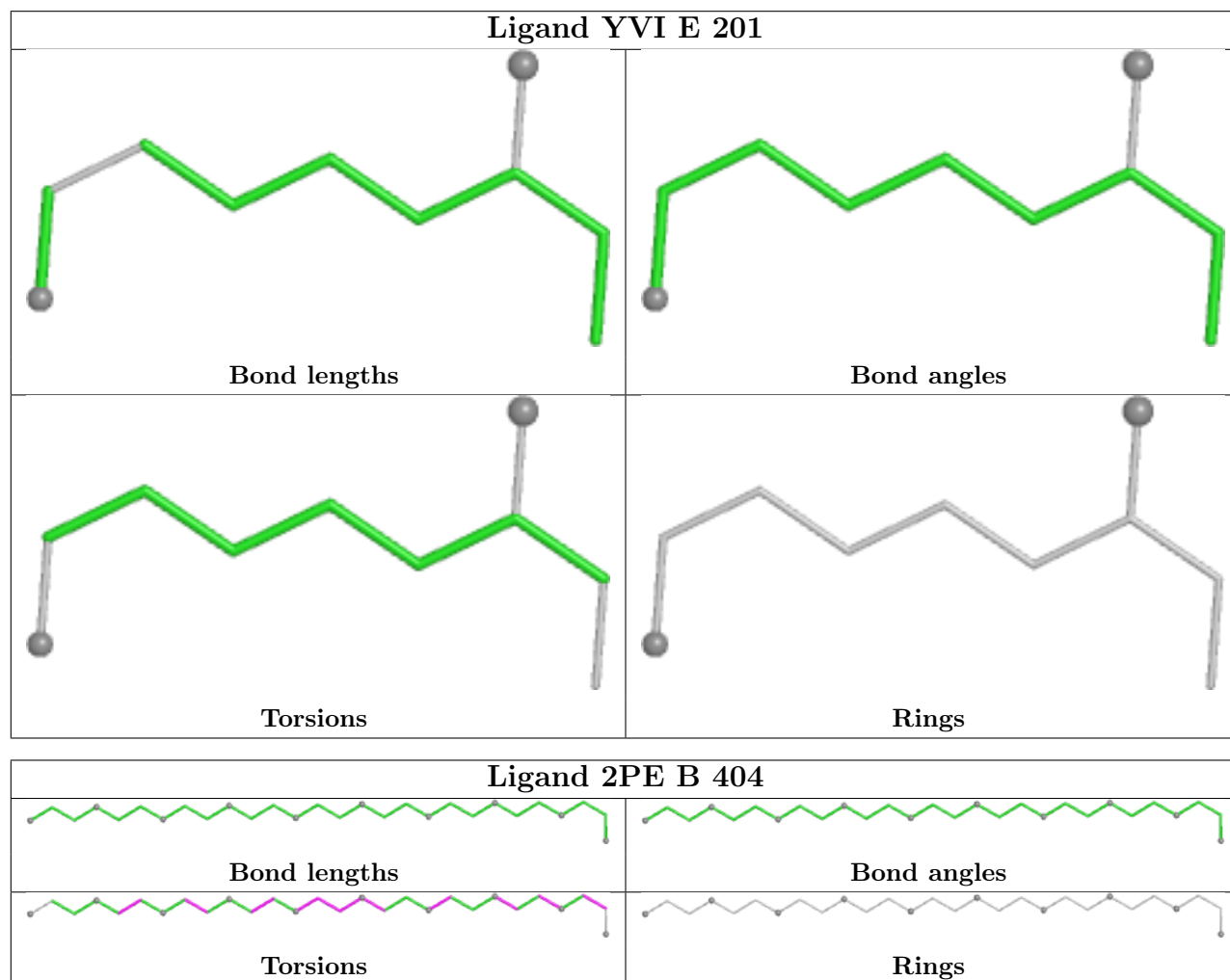
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	404	2PE	1	0
9	C	201	YVI	1	0
8	B	406	MET	2	0
4	B	402	SF4	1	0
8	A	406	MET	1	0
11	B	405	PGE	2	0

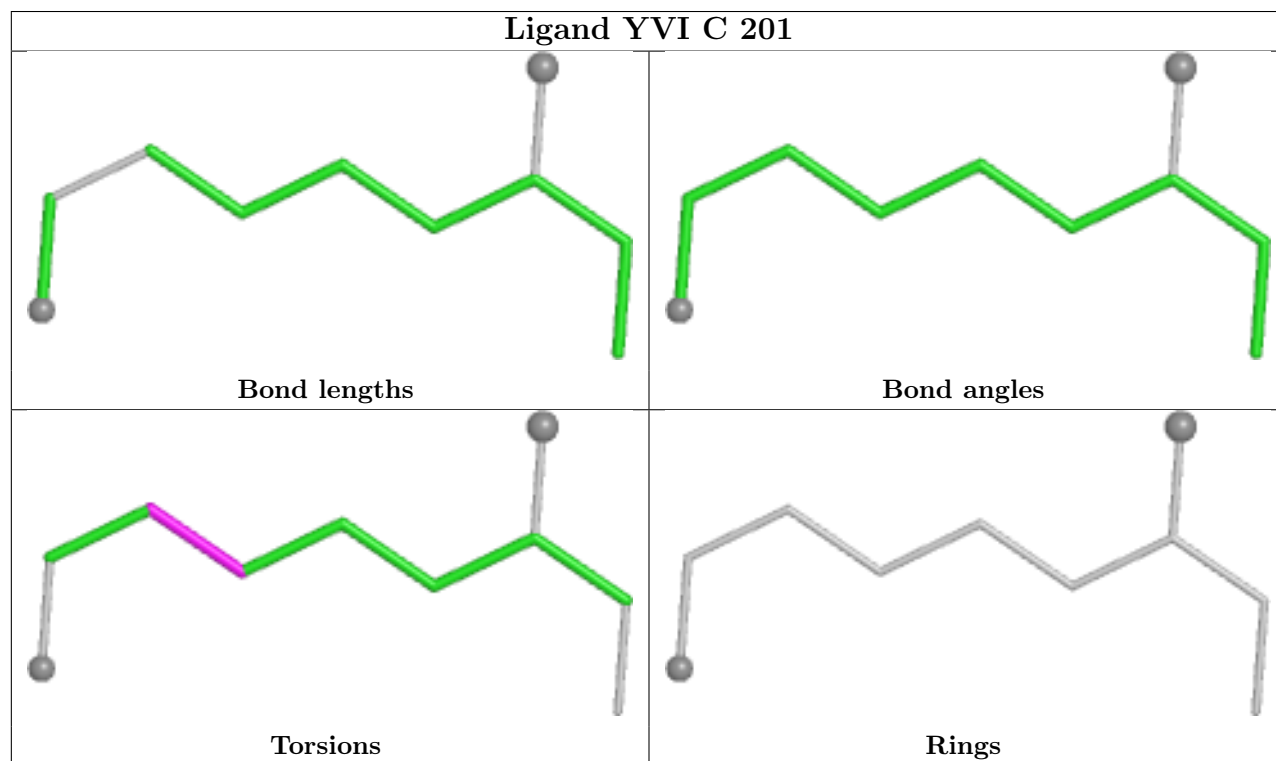
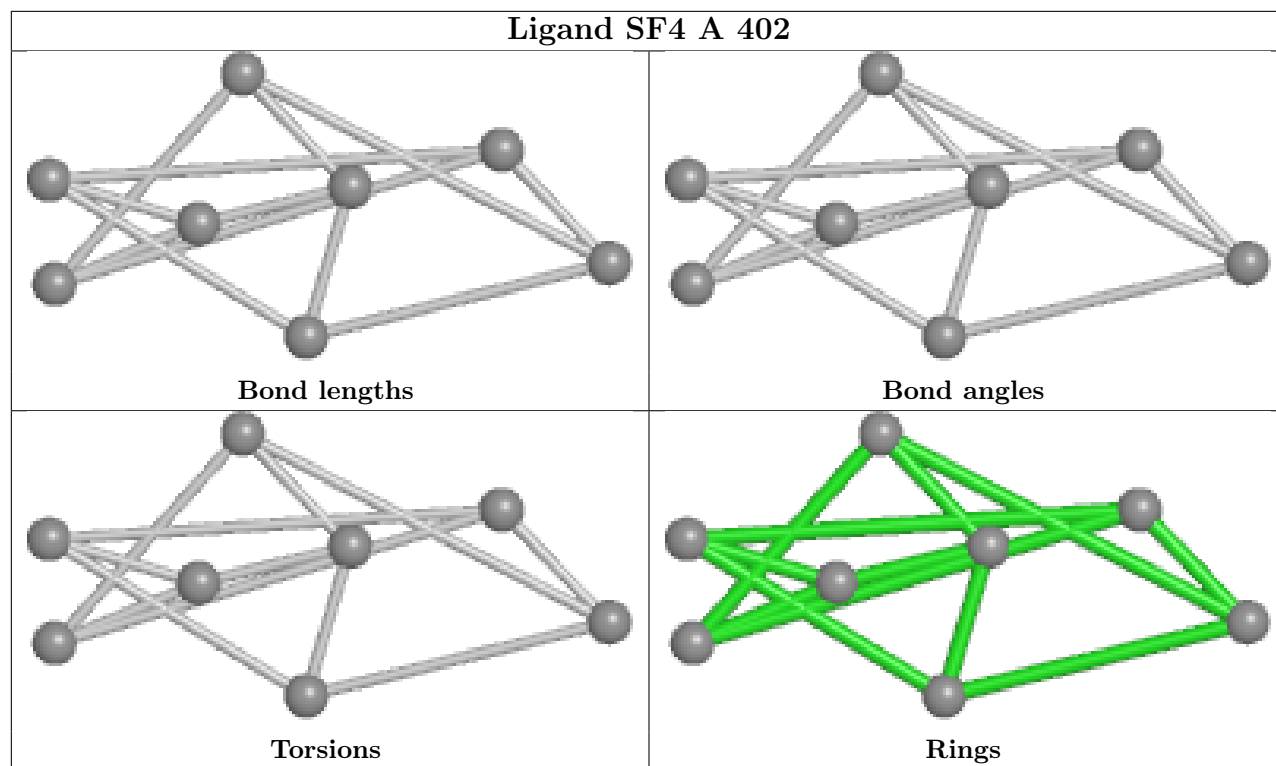
Continued on next page...

Continued from previous page...

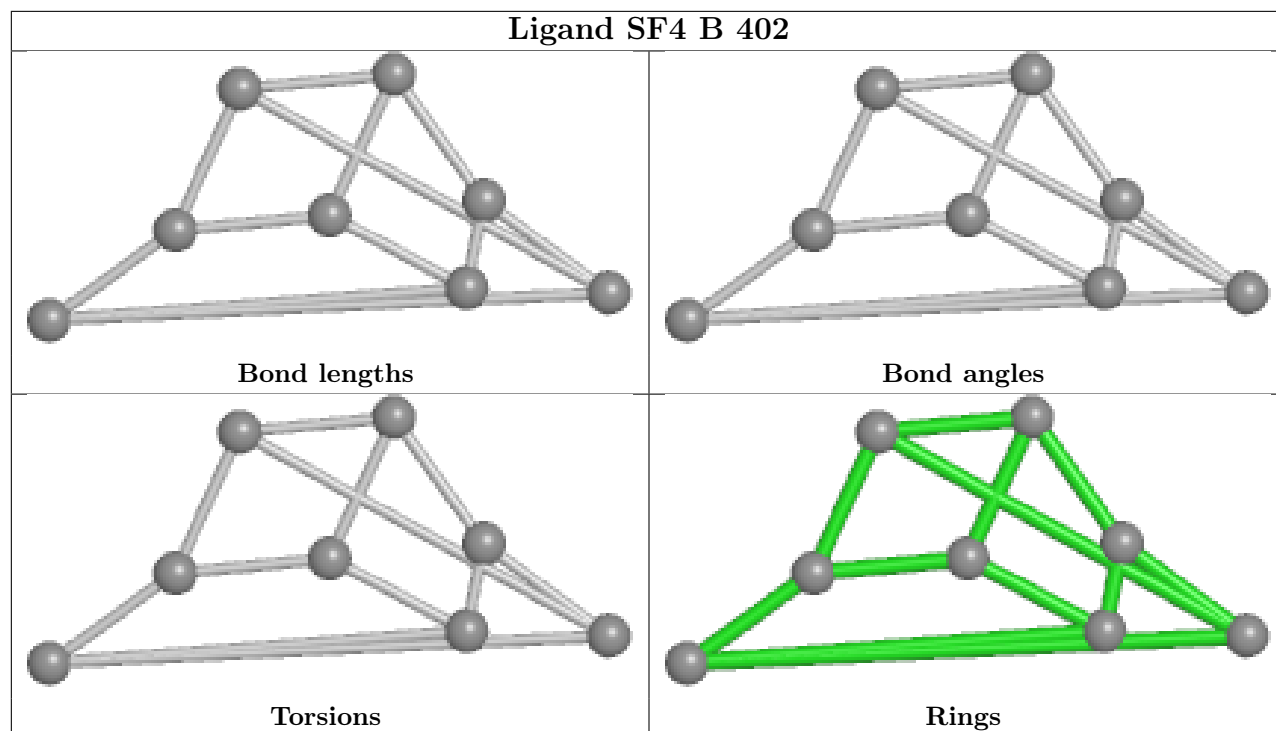
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	5AD	2	0

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.

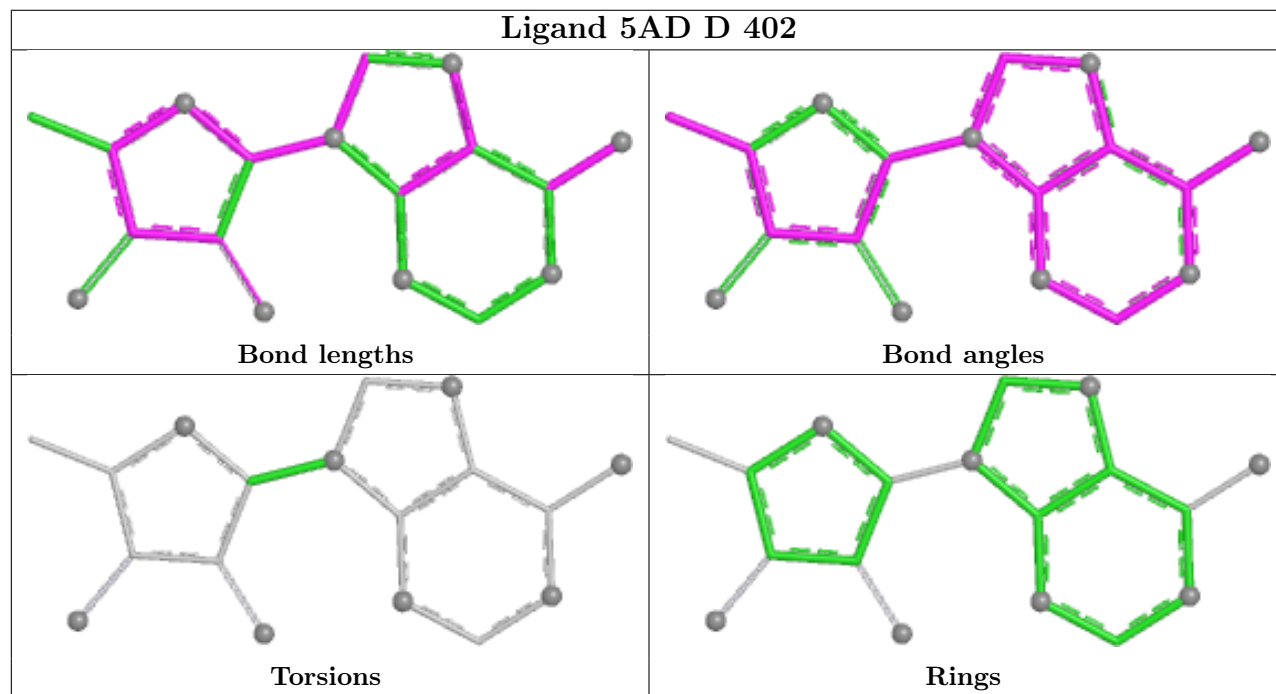


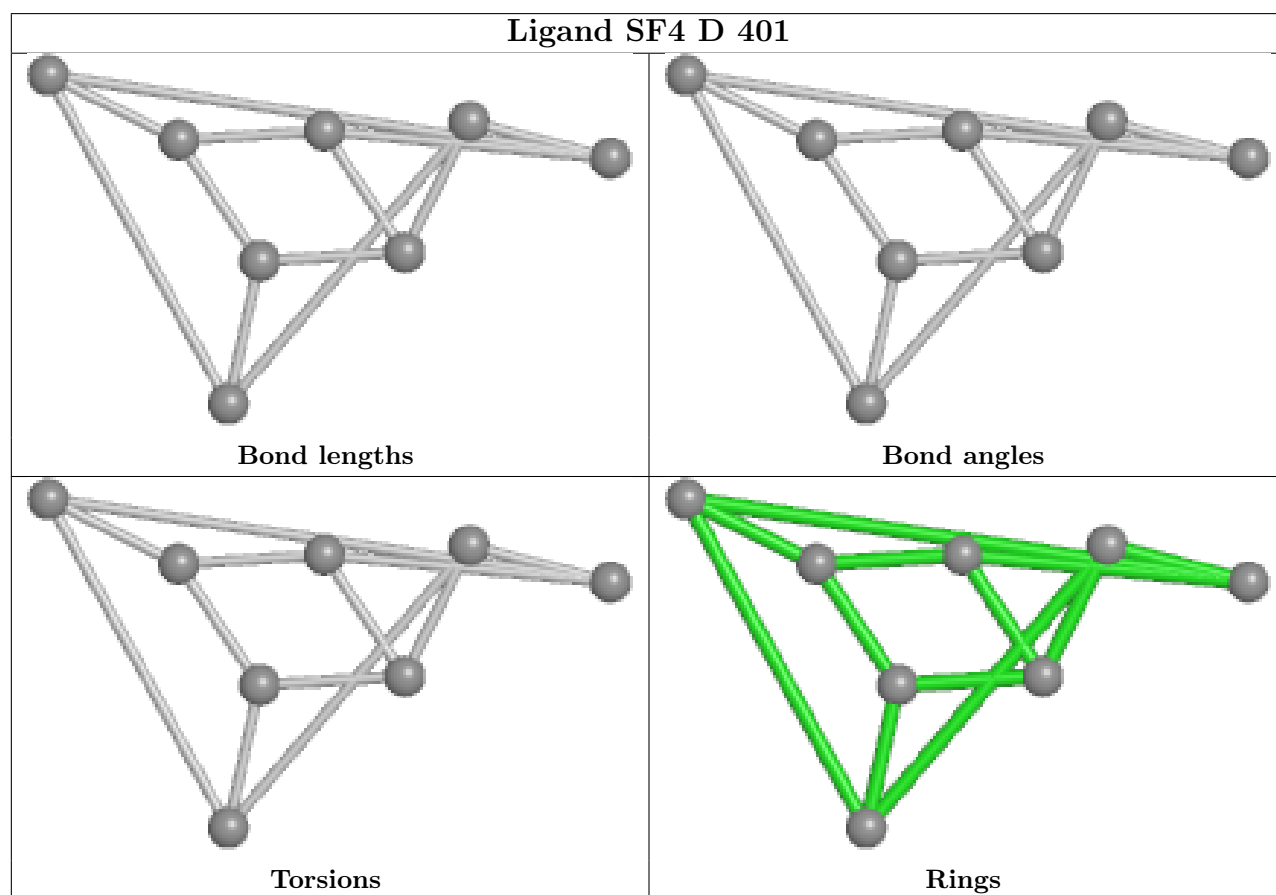
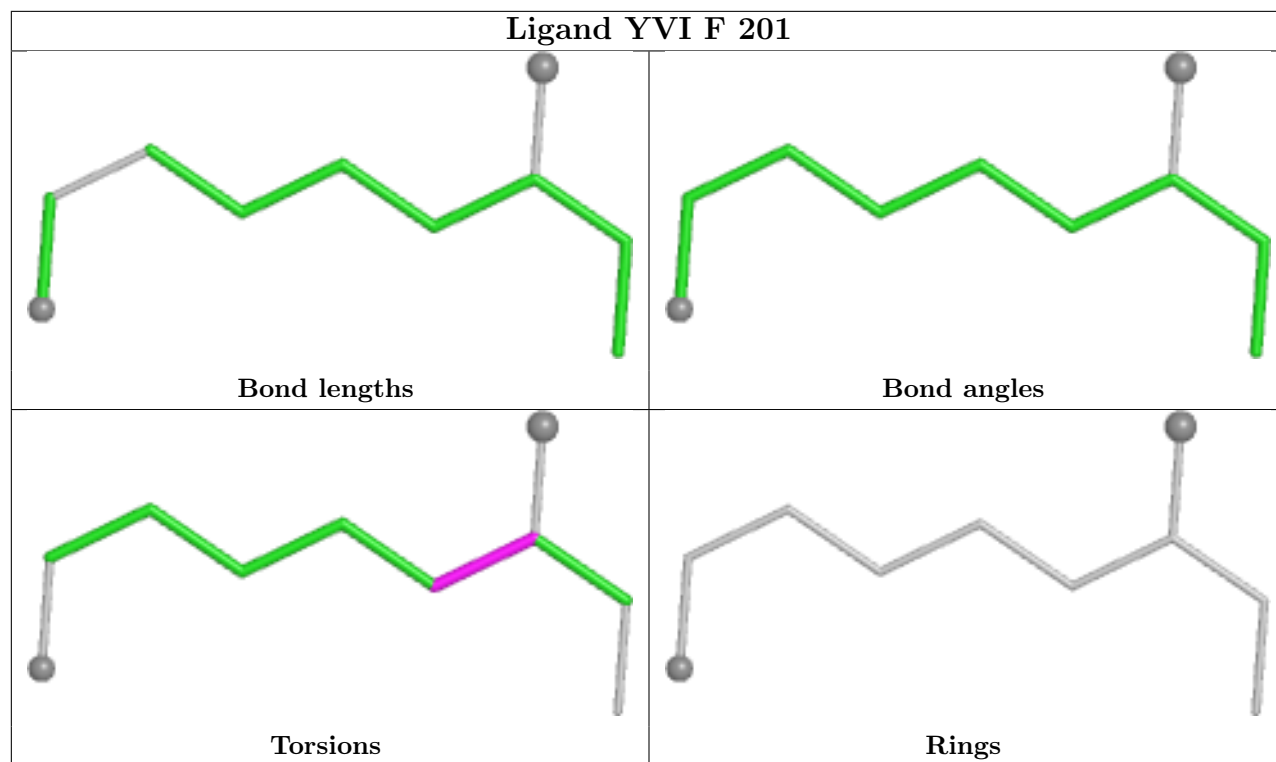


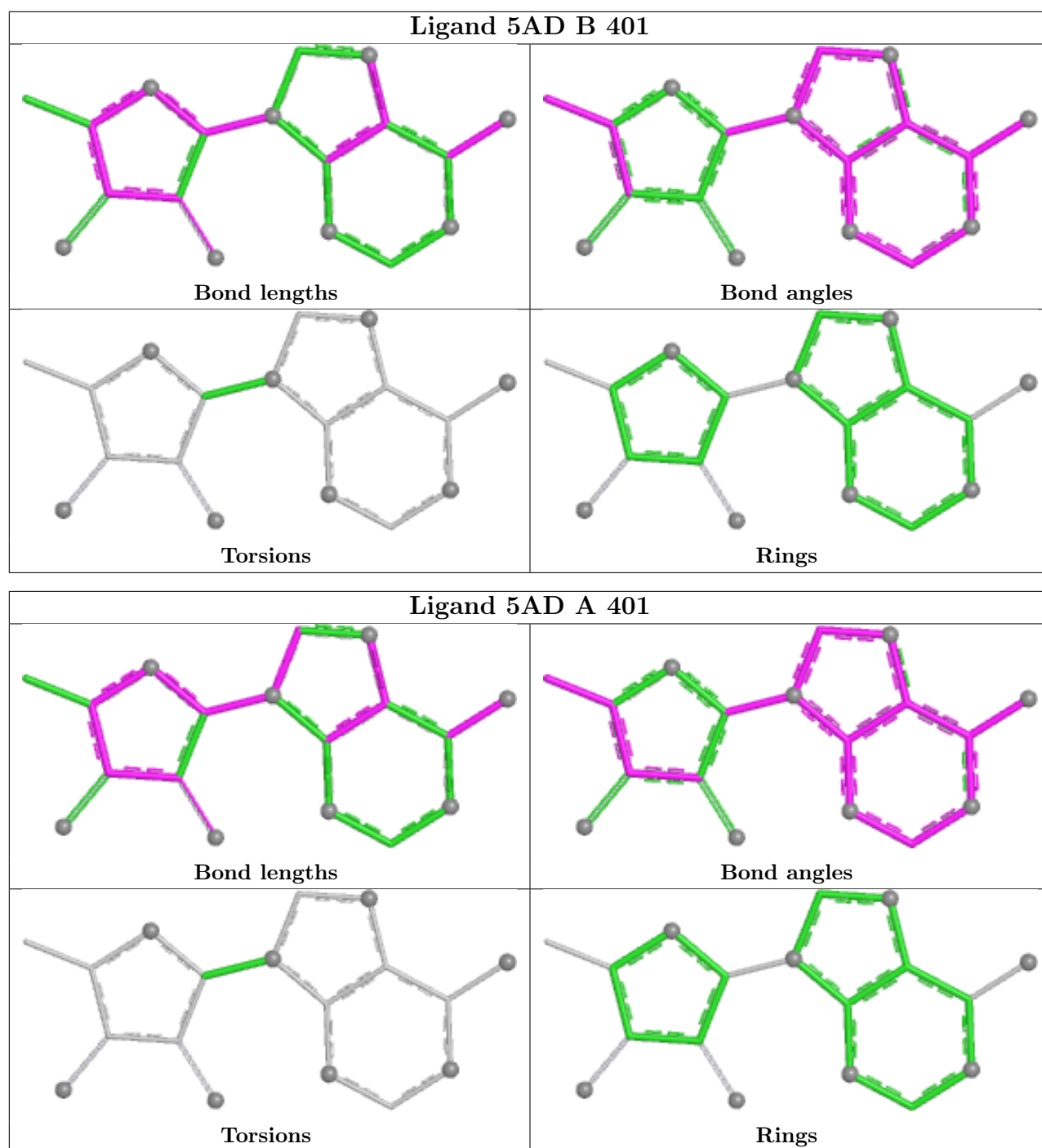
Ligand SF4 B 402



Ligand 5AD D 402







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, 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	299/368 (81%)	-0.13	9 (3%)	52	53	22, 36, 62, 104	1 (0%)
1	B	303/368 (82%)	-0.45	1 (0%)	90	91	12, 29, 50, 80	1 (0%)
1	D	299/368 (81%)	0.40	8 (2%)	56	57	38, 56, 81, 110	0
2	C	125/173 (72%)	-0.21	3 (2%)	59	62	28, 40, 56, 78	0
2	E	121/173 (69%)	0.05	3 (2%)	58	61	33, 50, 66, 77	0
2	F	118/173 (68%)	1.58	32 (27%)	1	1	66, 99, 121, 128	0
All	All	1265/1623 (77%)	0.09	56 (4%)	39	38	12, 44, 99, 128	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	123	ILE	4.4
2	F	126	ALA	4.4
1	A	123	TYR	4.0
2	F	90	VAL	3.9
1	D	84	ILE	3.8
2	F	171	ILE	3.5
2	E	50	VAL	3.4
2	F	141	ASP	3.4
2	F	93	LYS	3.4
1	A	67	LYS	3.3
1	A	120	GLY	3.3
1	D	365	ALA	3.1
1	B	368	ALA	3.0
2	F	85	CYS	3.0
2	F	66	ILE	2.9
2	F	149	LEU	2.9
2	F	62	THR	2.9
2	F	155	LEU	2.9
2	F	113	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	363	LEU	2.8
2	C	84	TYR	2.8
1	A	69	GLN	2.8
2	F	106	VAL	2.6
2	F	151	ASN	2.6
1	A	122	GLU	2.6
2	F	87	LEU	2.5
1	A	121	GLY	2.4
2	C	140	GLU	2.4
2	F	134	VAL	2.4
2	F	127	LEU	2.4
2	F	79	LEU	2.4
2	F	64	ASN	2.4
1	D	70	LYS	2.4
2	C	47	LEU	2.4
2	F	143	TRP	2.4
1	A	119	GLY	2.3
2	F	83	VAL	2.3
2	F	152	PRO	2.3
2	F	159	MET	2.3
2	F	88	PRO	2.3
1	A	124	ALA	2.2
2	F	137	SER	2.2
2	F	117	SER	2.2
1	A	72	GLU	2.2
1	D	109	ALA	2.2
1	D	101	ASN	2.1
2	E	79	LEU	2.1
2	F	150	SER	2.1
2	F	69	VAL	2.1
2	F	82	VAL	2.1
2	F	133	LEU	2.1
2	F	109	ALA	2.1
2	F	94	LEU	2.1
2	E	162	GLU	2.1
1	D	364	VAL	2.0
1	D	83	GLU	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

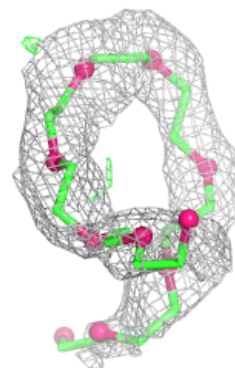
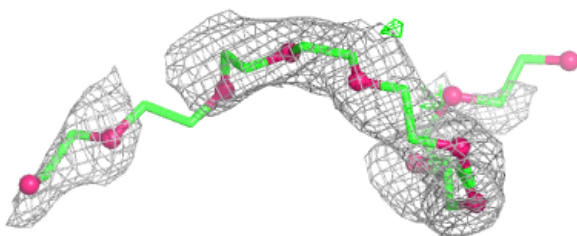
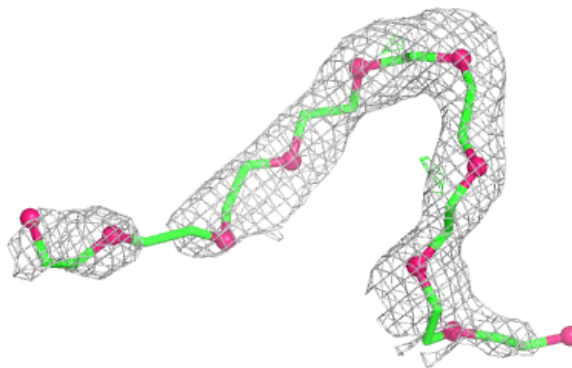
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
12	PO4	B	407	5/5	0.71	0.13	71,74,84,86	0
7	PG4	A	405	13/13	0.78	0.14	42,52,64,65	0
10	2PE	B	404	28/28	0.79	0.14	40,58,78,80	0
8	MET	B	406	9/9	0.81	0.18	31,33,37,47	0
8	MET	D	404	9/9	0.84	0.21	52,53,58,64	0
11	PGE	B	405	10/10	0.89	0.13	39,41,46,46	0
6	PEG	A	404	7/7	0.89	0.10	52,52,56,56	0
3	5AD	D	402	18/18	0.90	0.10	47,53,56,58	0
8	MET	A	406	9/9	0.91	0.11	24,30,36,36	0
3	5AD	A	401	18/18	0.92	0.09	27,32,36,36	0
9	YVI	F	201	10/11	0.93	0.12	49,52,54,56	0
3	5AD	B	401	18/18	0.95	0.07	21,23,27,28	0
9	YVI	E	201	10/11	0.97	0.07	28,30,31,33	0
9	YVI	C	201	10/11	0.97	0.08	20,23,27,32	0
4	SF4	D	401	8/8	0.97	0.05	35,41,49,53	0
5	F3S	D	403	6/7	0.98	0.04	47,51,52,54	0
4	SF4	B	402	8/8	0.98	0.04	15,19,22,26	0
4	SF4	A	402	8/8	0.98	0.04	23,26,31,33	0
5	F3S	B	403	6/7	0.98	0.05	20,22,23,26	0
5	F3S	A	403	6/7	0.99	0.03	27,27,31,34	0

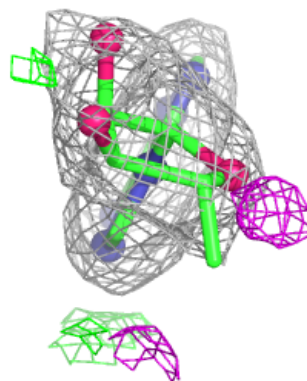
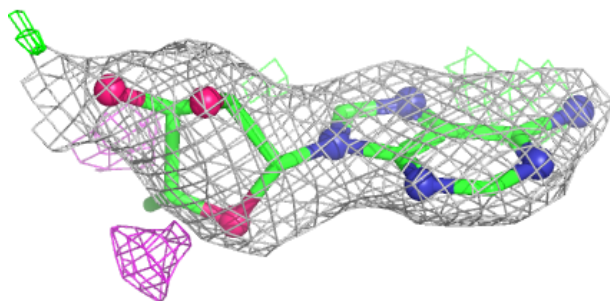
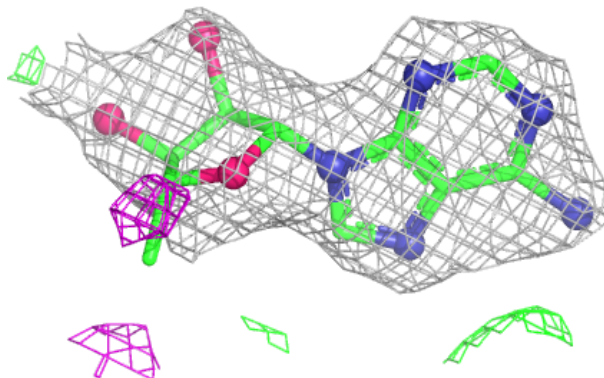
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PE B 404:

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

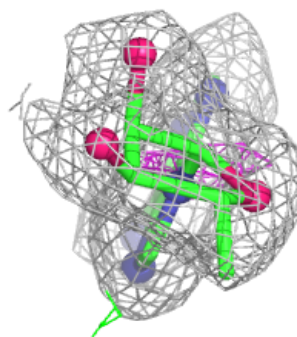
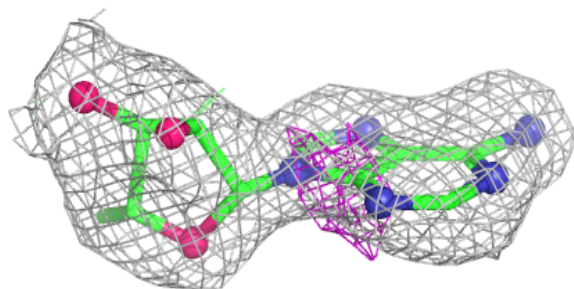
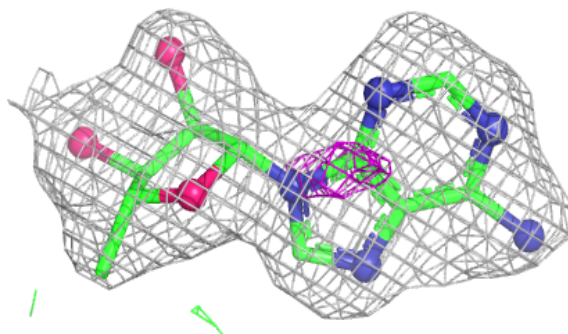
**Electron density around 5AD D 402:**

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

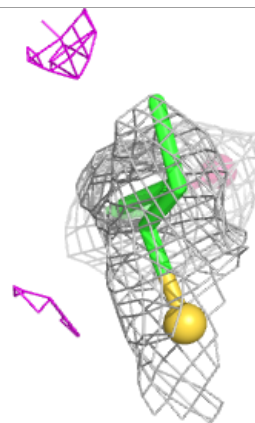
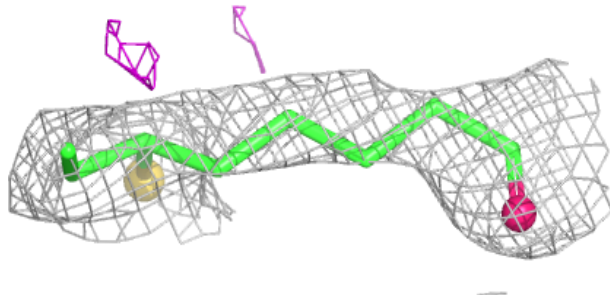
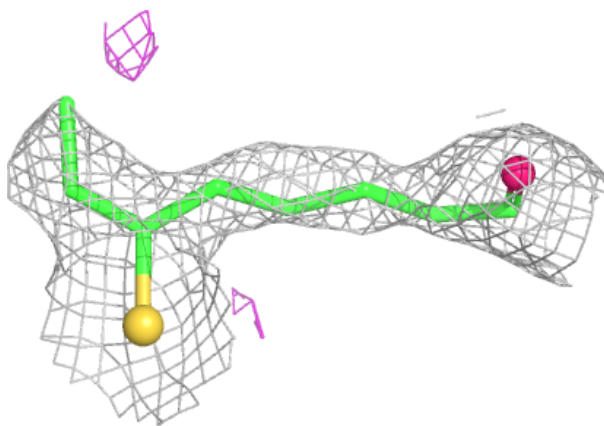


Electron density around 5AD A 401:

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

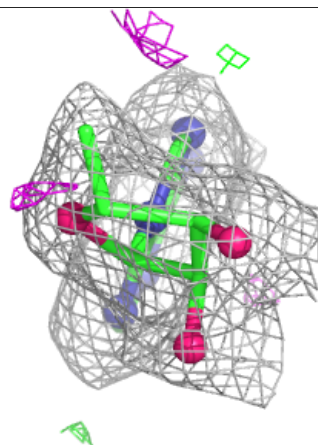
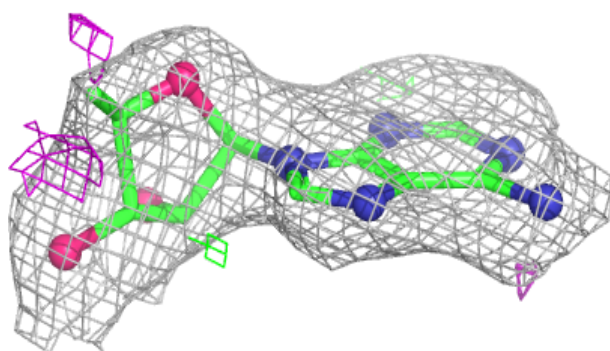
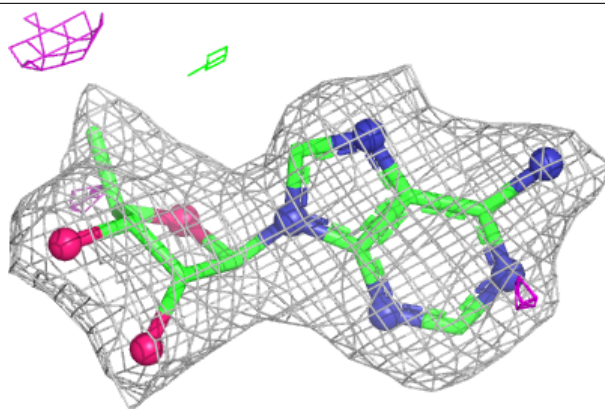
**Electron density around YVI F 201:**

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

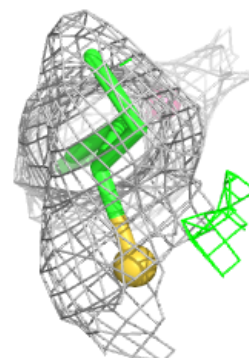
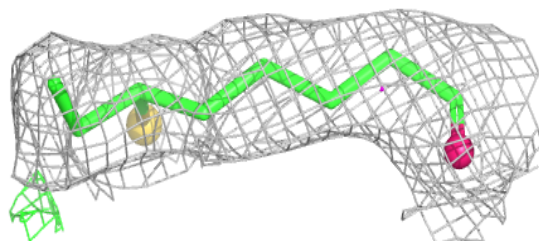
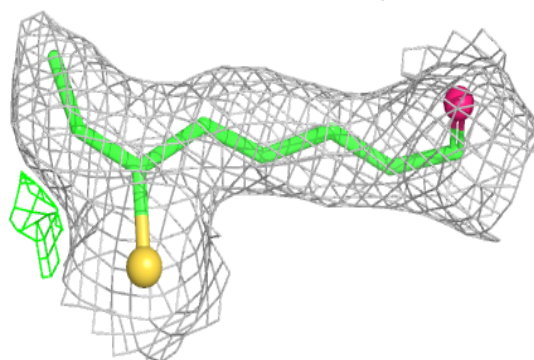


Electron density around 5AD B 401:

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

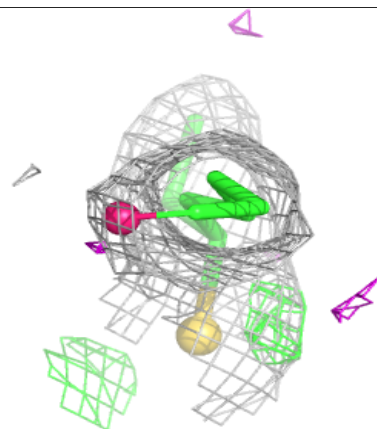
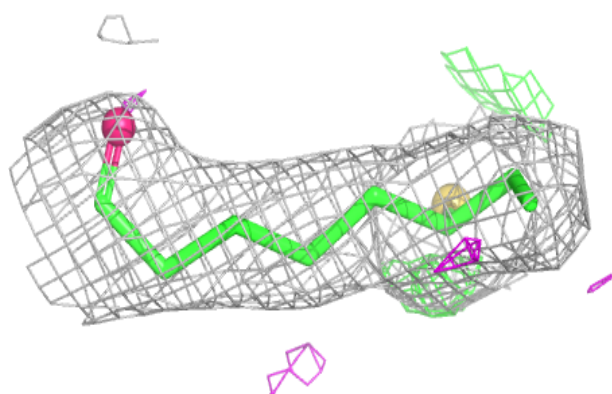
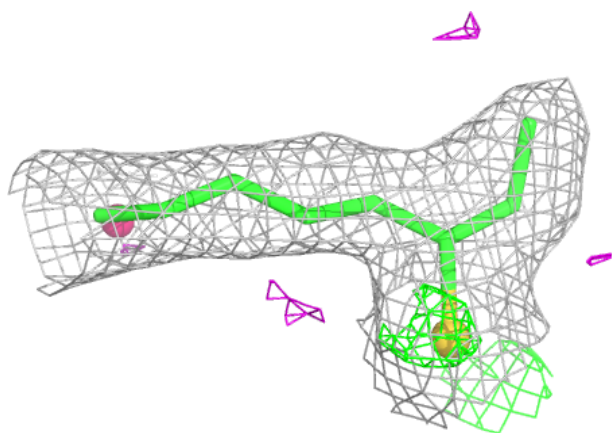
**Electron density around YVI E 201:**

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



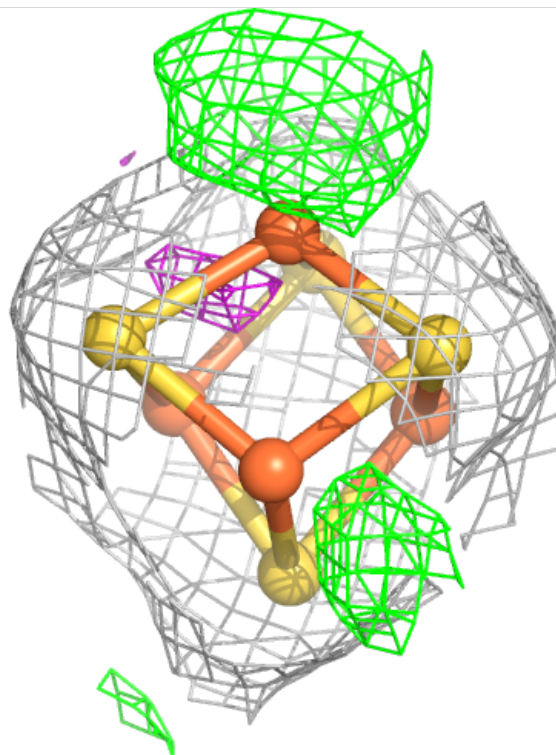
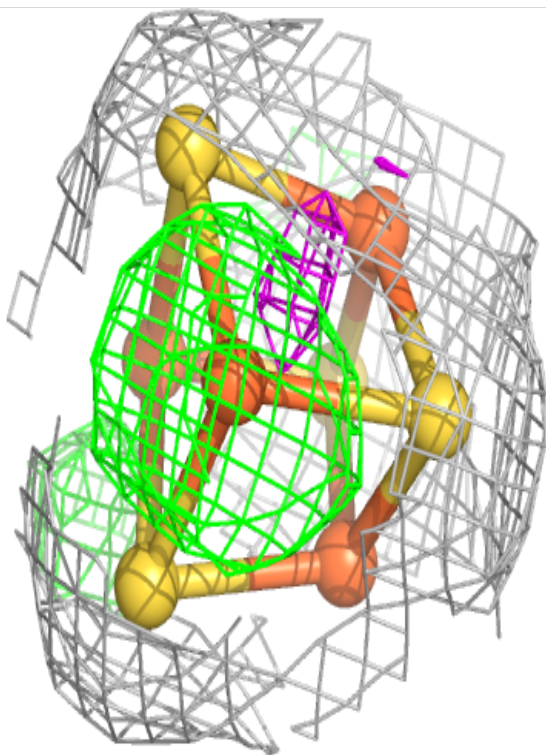
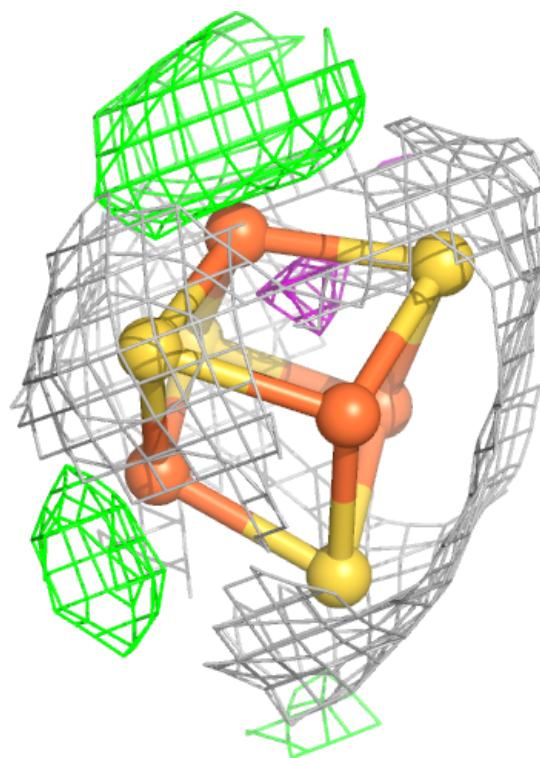
Electron density around YVI C 201:

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



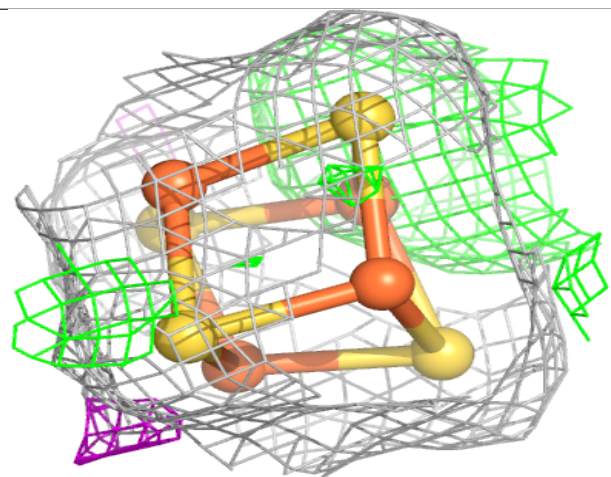
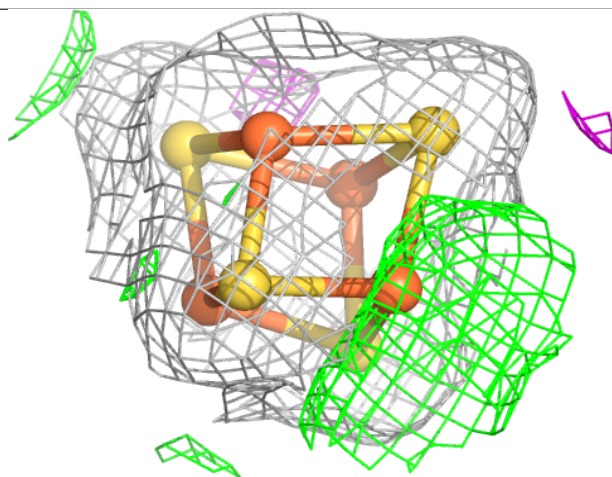
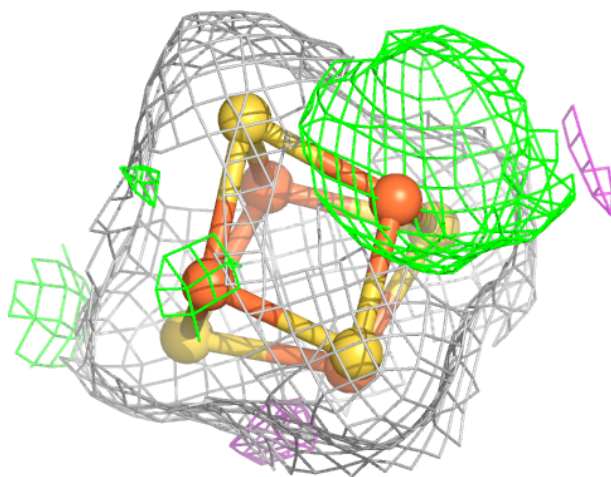
Electron density around SF4 D 401:

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



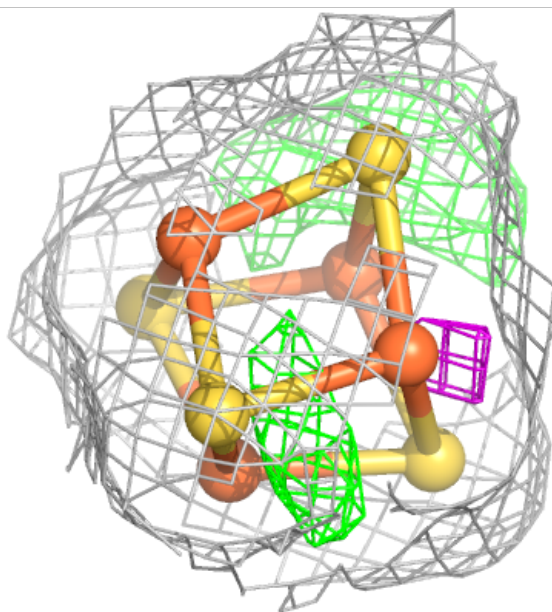
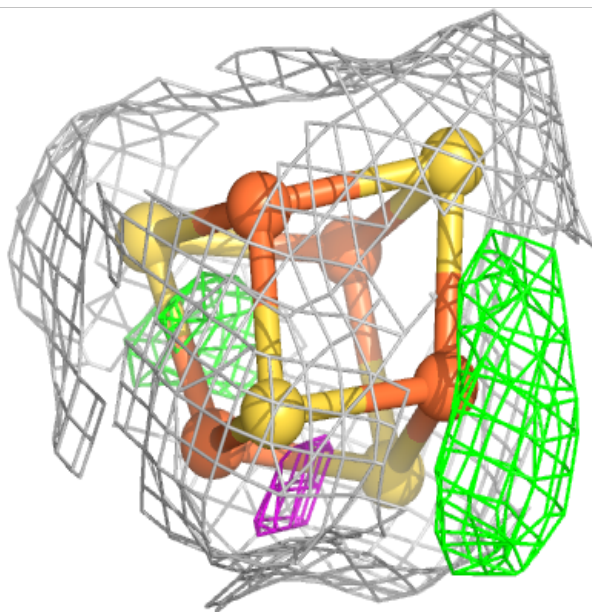
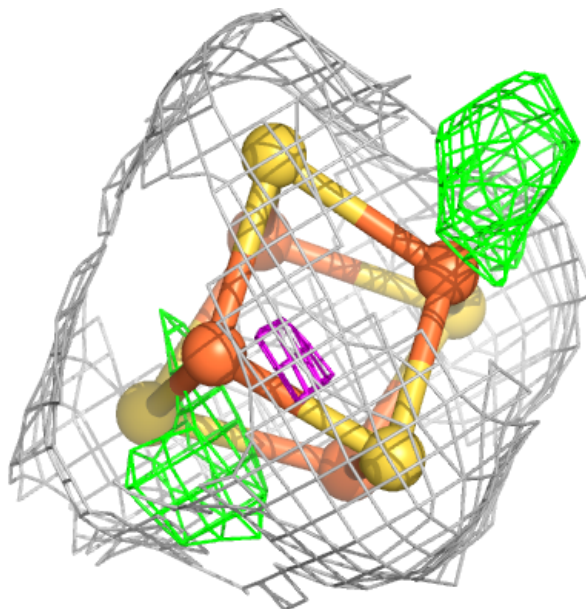
Electron density around SF4 B 402:

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



Electron density around SF4 A 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.