



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:06 am BST

PDB ID : 6N2O  
Title : 2-oxoglutarate:ferredoxin oxidoreductase from *Magnetococcus marinus* with  
2-oxoglutarate, coenzyme A and succinyl-CoA bound  
Authors : Chen, P.Y.-T.; Drennan, C.L.  
Deposited on : 2018-11-13  
Resolution : 2.82 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

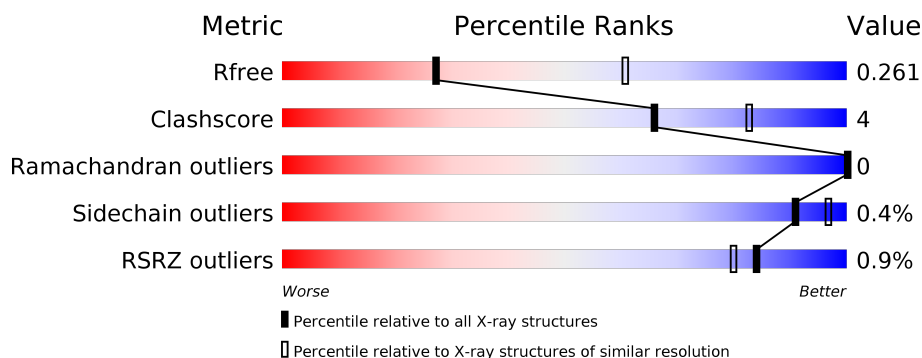
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 on 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	573	<div> <div></div> <div>89%11%</div> </div>
1	C	573	<div> <div>2%</div> <div>91%9%</div> </div>
2	B	292	<div> <div></div> <div>90%10%</div> </div>
2	D	292	<div> <div>%</div> <div>89%10%</div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13224 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.

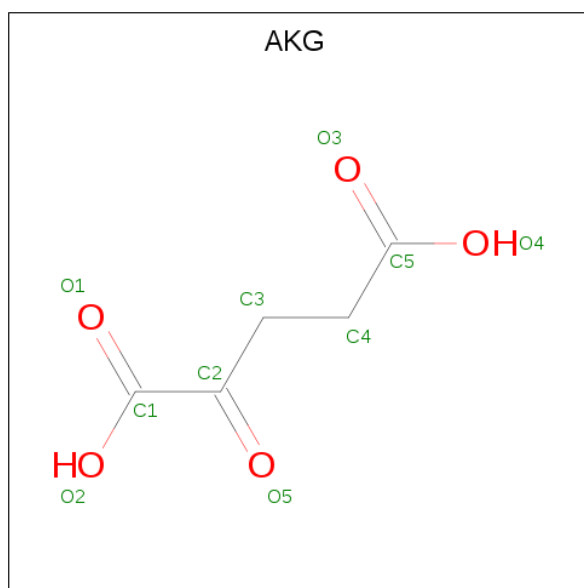
- Molecule 1 is a protein called Pyruvate flavodoxin/ferredoxin oxidoreductase domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4327	2754	716	831	26			
1	C	572	Total	C	N	O	S	0	0	0
			4288	2727	710	825	26			

- Molecule 2 is a protein called Pyruvate ferredoxin/flavodoxin oxidoreductase, beta subunit.

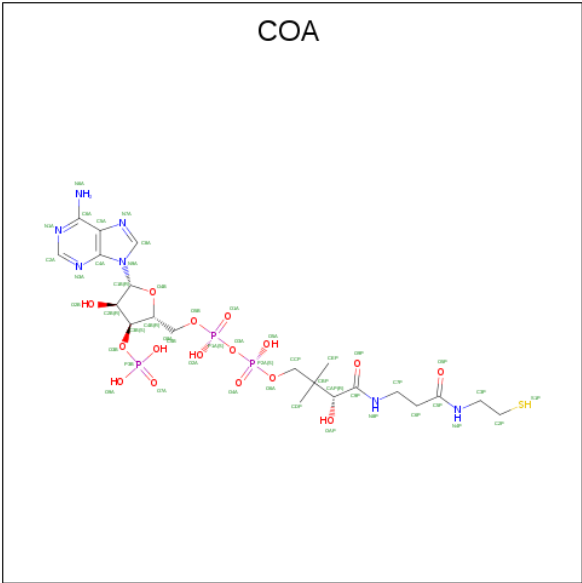
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2197	1391	376	410	20			
2	D	291	Total	C	N	O	S	0	0	0
			2207	1396	376	415	20			

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by author).



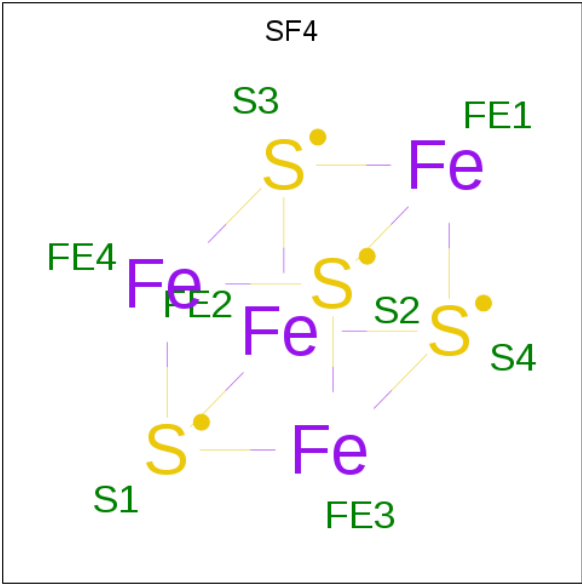
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by author).



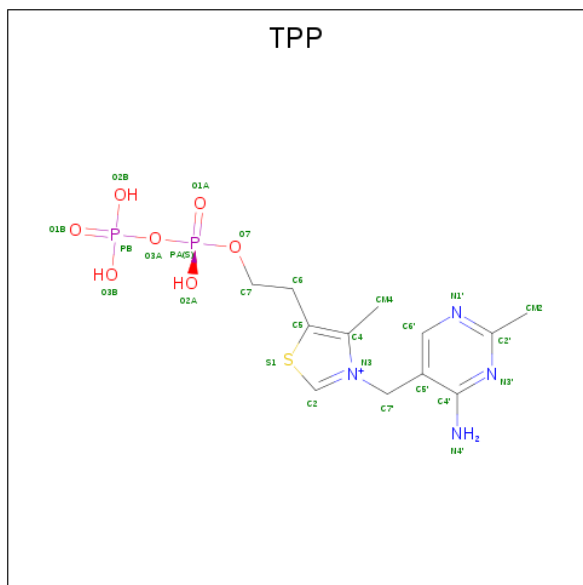
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 6 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ).

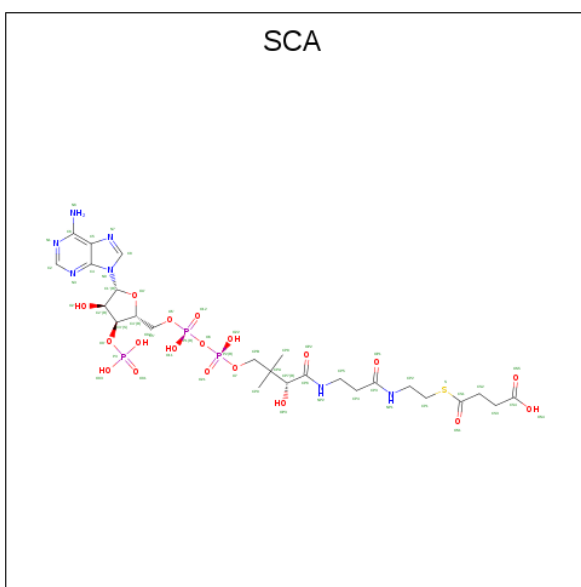


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
6	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SUCCINYL-COENZYME A (three-letter code: SCA) (formula:  $C_{25}H_{40}N_7O_{19}P_3S$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		

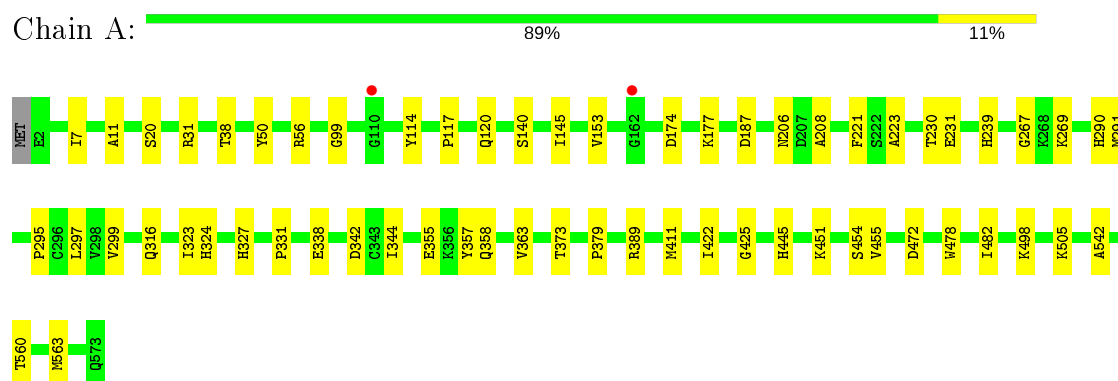
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total O 8 8	0	0
9	B	6	Total O 6 6	0	0
9	C	6	Total O 6 6	0	0
9	D	2	Total O 2 2	0	0

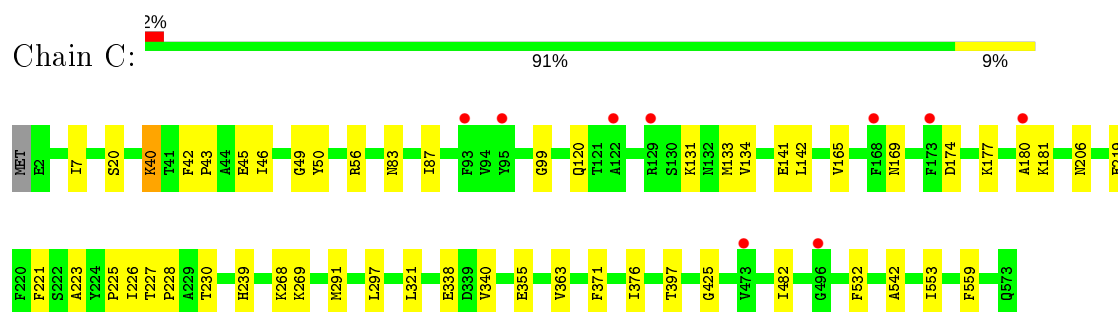
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

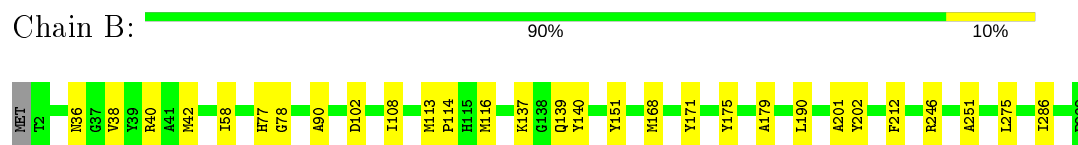
- Molecule 1: Pyruvate flavodoxin/ferredoxin oxidoreductase domain protein



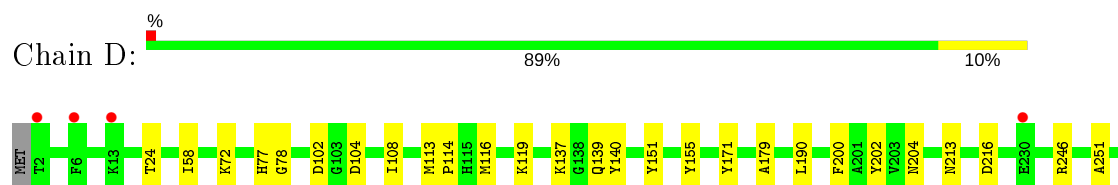
- Molecule 1: Pyruvate flavodoxin/ferredoxin oxidoreductase domain protein



- Molecule 2: Pyruvate ferredoxin/flavodoxin oxidoreductase, beta subunit



- Molecule 2: Pyruvate ferredoxin/flavodoxin oxidoreductase, beta subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.41Å 100.53Å 202.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.01 – 2.82 90.01 – 2.82	Depositor EDS
% Data completeness (in resolution range)	89.5 (90.01-2.82) 89.5 (90.01-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.212 , 0.261 0.212 , 0.261	Depositor DCC
$R_{free}$ test set	1929 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: MG, SF4, SCA, COA, TPP, AKG

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	0.26	0/4422	0.44	0/5990
1	C	0.26	0/4383	0.44	0/5944
2	B	0.26	0/2253	0.45	0/3052
2	D	0.26	0/2263	0.45	0/3065
All	All	0.26	0/13321	0.44	0/18051

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	4327	0	4274	40	0
1	C	4288	0	4187	35	0
2	B	2197	0	2138	19	0
2	D	2207	0	2151	19	0
3	A	10	0	4	0	0
4	A	48	0	32	2	0
5	B	8	0	0	0	0
5	D	8	0	0	0	0
6	B	26	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	26	0	15	3	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	C	55	0	35	7	0
9	A	8	0	0	0	0
9	B	6	0	0	0	0
9	C	6	0	0	0	0
9	D	2	0	0	0	0
All	All	13224	0	12852	105	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 (105) 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:542:ALA:HB2	1:C:542:ALA:HB2	1.67	0.75
1:C:221:PHE:HE1	1:C:223:ALA:HB2	1.55	0.71
1:C:99:GLY:HA3	1:C:120:GLN:HG3	1.77	0.67
1:A:221:PHE:HE1	1:A:223:ALA:HB2	1.60	0.66
2:D:139:GLN:HG3	2:D:151:TYR:HB3	1.77	0.65
1:A:99:GLY:HA3	1:A:120:GLN:HG3	1.77	0.65
8:C:601:SCA:OS1	6:D:402:TPP:N4'	2.23	0.65
1:C:43:PRO:HG3	1:C:49:GLY:HA3	1.79	0.64
1:C:46:ILE:HD13	8:C:601:SCA:H52	1.81	0.63
1:A:38:THR:HG1	1:A:373:THR:HG1	1.50	0.60
1:A:379:PRO:HG2	2:D:287:ILE:HD13	1.84	0.59
2:B:246:ARG:HG2	2:B:251:ALA:HA	1.85	0.57
2:B:139:GLN:HG3	2:B:151:TYR:HB3	1.85	0.57
1:A:174:ASP:HA	1:A:177:LYS:HB3	1.85	0.57
1:C:142:LEU:HG	1:C:180:ALA:HB1	1.86	0.57
1:C:40:LYS:HE2	1:C:371:PHE:HB3	1.87	0.57
8:C:601:SCA:H8	8:C:601:SCA:H5'2	1.85	0.57
1:A:208:ALA:HB1	1:A:344:ILE:HG13	1.89	0.55
1:C:221:PHE:CE1	1:C:223:ALA:HB2	2.40	0.55
1:C:20:SER:OG	8:C:601:SCA:O12	2.18	0.54
1:C:338:GLU:HG3	1:C:482:ILE:HB	1.90	0.53
2:D:114:PRO:HG3	2:D:171:TYR:CZ	2.43	0.53
1:A:357:TYR:CE2	1:A:455:VAL:HG22	2.45	0.52
2:D:113:MET:HA	2:D:116:MET:HE3	1.91	0.52
1:C:206:ASN:ND2	1:C:228:PRO:O	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HH21	1:A:153:VAL:HG22	1.76	0.51
2:D:246:ARG:HG2	2:D:251:ALA:HA	1.92	0.51
2:B:179:ALA:HB2	2:B:190:LEU:HD12	1.92	0.51
1:A:323:ILE:HG22	1:A:324:HIS:CD2	2.46	0.51
1:C:141:GLU:HB3	1:C:181:LYS:HG3	1.93	0.50
1:A:338:GLU:HG3	1:A:482:ILE:HB	1.93	0.50
1:A:38:THR:OG1	1:A:373:THR:OG1	2.22	0.50
8:C:601:SCA:H91	2:D:137:LYS:NZ	2.27	0.50
1:A:221:PHE:CE1	1:A:223:ALA:HB2	2.42	0.50
1:C:269:LYS:HE2	1:C:355:GLU:HG3	1.93	0.50
2:D:179:ALA:HB2	2:D:190:LEU:HD12	1.92	0.50
2:B:77:HIS:CD2	2:B:108:ILE:HG21	2.47	0.49
2:B:175:TYR:HB3	2:B:201:ALA:HA	1.94	0.49
1:A:342:ASP:OD2	1:A:505:LYS:NZ	2.28	0.49
1:A:239:HIS:HB3	2:D:286:ILE:HD13	1.95	0.49
1:C:45:GLU:HG2	2:D:24:THR:HB	1.94	0.49
1:A:11:ALA:HB1	1:A:50:TYR:CE1	2.49	0.48
1:A:140:SER:HA	1:A:145:ILE:HB	1.94	0.48
2:B:102:ASP:N	2:B:102:ASP:OD1	2.46	0.48
1:A:299:VAL:HG22	1:A:363:VAL:HB	1.95	0.48
1:A:230:THR:HG21	2:B:139:GLN:NE2	2.29	0.47
1:C:227:THR:OG1	8:C:601:SCA:H21	2.15	0.47
1:A:290:HIS:CE1	1:A:331:PRO:HD2	2.49	0.47
1:A:327:HIS:HB3	1:C:321:LEU:HD22	1.97	0.47
2:B:114:PRO:HG3	2:B:171:TYR:CZ	2.50	0.47
1:C:340:VAL:HG12	1:C:376:ILE:HD13	1.96	0.47
1:C:226:ILE:HA	6:D:402:TPP:H7'1	1.97	0.47
1:C:46:ILE:O	8:C:601:SCA:H83	2.15	0.47
1:C:131:LYS:O	1:C:134:VAL:HG12	2.15	0.46
1:C:219:GLU:HB2	1:C:268:LYS:HB3	1.97	0.46
1:A:269:LYS:HE2	1:A:355:GLU:HG3	1.97	0.46
1:C:165:VAL:O	1:C:169:ASN:ND2	2.47	0.46
1:C:174:ASP:HA	1:C:177:LYS:HB3	1.97	0.46
1:C:43:PRO:HD3	1:C:50:TYR:O	2.16	0.46
1:C:553:ILE:HG12	1:C:559:PHE:CZ	2.51	0.46
2:B:90:ALA:HB1	1:C:268:LYS:HD2	1.97	0.46
2:B:168:MET:HG3	2:B:202:TYR:CG	2.51	0.46
1:A:297:LEU:HD11	1:A:363:VAL:HG23	1.98	0.45
2:D:119:LYS:HB3	2:D:264:LEU:HD13	1.98	0.45
2:B:58:ILE:HG21	6:B:402:TPP:N4'	2.31	0.45
1:C:83:ASN:O	1:C:87:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:GLY:HA3	2:D:108:ILE:HG23	1.99	0.45
1:A:117:PRO:HB2	1:A:120:GLN:HB2	1.99	0.45
2:B:286:ILE:HD13	1:C:239:HIS:HB3	1.99	0.45
1:A:11:ALA:HB1	1:A:50:TYR:HE1	1.80	0.44
1:C:174:ASP:N	1:C:174:ASP:OD1	2.50	0.44
2:D:202:TYR:CE2	2:D:204:ASN:HB2	2.53	0.44
1:C:133:MET:HG3	1:C:169:ASN:HB3	2.00	0.44
1:C:291:MET:HG2	1:C:425:GLY:O	2.18	0.43
1:C:225:PRO:HA	1:C:230:THR:HG22	1.99	0.43
1:A:472:ASP:N	1:A:498:LYS:O	2.48	0.43
1:A:267:GLY:HA2	1:A:389:ARG:NH1	2.33	0.43
2:B:36:ASN:O	2:B:40:ARG:HG3	2.18	0.43
1:A:7:ILE:HG12	1:A:56:ARG:HG3	2.01	0.43
1:A:206:ASN:HD22	1:A:231:GLU:HB2	1.83	0.43
1:A:295:PRO:HG3	1:A:358:GLN:HA	2.01	0.43
1:A:451:LYS:O	1:A:454:SER:OG	2.28	0.43
1:A:114:TYR:HH	1:A:187:ASP:H	1.67	0.43
2:B:78:GLY:HA3	2:B:108:ILE:HG23	2.01	0.42
2:B:275:LEU:HD11	2:D:155:TYR:CZ	2.54	0.42
2:B:137:LYS:HA	2:B:212:PHE:CZ	2.54	0.42
2:D:213:ASN:ND2	2:D:216:ASP:HB2	2.35	0.42
1:A:445:HIS:HB3	1:C:532:PHE:CE1	2.54	0.42
1:A:291:MET:HG2	1:A:425:GLY:O	2.19	0.42
4:A:602:COA:H8A	4:A:602:COA:H2B	1.75	0.42
1:A:560:THR:OG1	1:A:563:MET:HG3	2.20	0.42
1:C:297:LEU:HD11	1:C:363:VAL:HG23	2.01	0.42
1:A:358:GLN:NE2	1:A:411:MET:HG3	2.35	0.41
2:B:58:ILE:HG22	6:B:402:TPP:S1	2.60	0.41
1:A:174:ASP:OD1	1:A:174:ASP:N	2.54	0.41
2:D:58:ILE:HG22	6:D:402:TPP:S1	2.60	0.41
1:A:316:GLN:HB2	1:A:478:TRP:CH2	2.56	0.41
1:A:20:SER:HB3	4:A:602:COA:O1A	2.20	0.41
2:D:102:ASP:OD1	2:D:102:ASP:N	2.45	0.41
1:C:7:ILE:HG12	1:C:56:ARG:HG3	2.03	0.41
2:B:113:MET:HA	2:B:116:MET:HE3	2.02	0.40
2:B:38:VAL:O	2:B:42:MET:HG3	2.21	0.40
2:D:116:MET:HB3	2:D:200:PHE:CE1	2.56	0.40
1:A:422:ILE:HB	2:D:72:LYS:HG3	2.03	0.40
2:D:77:HIS:CE1	2:D:104:ASP:HA	2.57	0.40

There are no symmetry-related clashes.

## 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	570/573 (100%)	550 (96%)	20 (4%)	0	100	100
1	C	570/573 (100%)	547 (96%)	23 (4%)	0	100	100
2	B	289/292 (99%)	280 (97%)	9 (3%)	0	100	100
2	D	289/292 (99%)	278 (96%)	11 (4%)	0	100	100
All	All	1718/1730 (99%)	1655 (96%)	63 (4%)	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	455/463 (98%)	455 (100%)	0	100	100
1	C	444/463 (96%)	441 (99%)	3 (1%)	84	95
2	B	227/232 (98%)	226 (100%)	1 (0%)	91	97
2	D	230/232 (99%)	229 (100%)	1 (0%)	91	97
All	All	1356/1390 (98%)	1351 (100%)	5 (0%)	91	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	140	TYR
1	C	40	LYS

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Mol	Chain	Res	Type
1	C	42	PHE
1	C	397	THR
2	D	140	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	TPP	D	402	8,7	22,27,27	2.16	7 (31%)	29,40,40	2.31	8 (27%)
4	COA	A	602	-	41,50,50	0.84	1 (2%)	52,75,75	1.40	6 (11%)
8	SCA	C	601	6	46,57,57	2.29	2 (4%)	58,84,84	2.76	9 (15%)
5	SF4	D	401	2	0,12,12	0.00	-	-	-	-
6	TPP	B	402	7	22,27,27	1.98	6 (27%)	29,40,40	1.82	6 (20%)
5	SF4	B	401	2	0,12,12	0.00	-	-	-	-
3	AKG	A	601	-	3,9,9	0.28	0	4,11,11	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	D	401	2	-	-	0/6/5/5
4	COA	A	602	-	-	12/44/64/64	0/3/3/3
8	SCA	C	601	6	-	12/50/72/72	0/3/3/3
6	TPP	D	402	8,7	-	1/16/17/17	0/2/2/2
6	TPP	B	402	7	-	1/16/17/17	0/2/2/2
5	SF4	B	401	2	-	-	0/6/5/5
3	AKG	A	601	-	-	0/3/9/9	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	601	SCA	OS1-CS1	14.57	1.44	1.21
6	D	402	TPP	C6-C5	5.33	1.53	1.50
6	B	402	TPP	C4-N3	-4.77	1.35	1.39
6	D	402	TPP	C4-N3	-3.94	1.36	1.39
6	D	402	TPP	C4'-N4'	3.81	1.43	1.34
6	B	402	TPP	C4'-N4'	3.63	1.43	1.34
6	B	402	TPP	C7'-N3	-3.29	1.42	1.48
6	D	402	TPP	C7'-N3	-3.19	1.42	1.48
6	D	402	TPP	C7'-C5'	3.15	1.57	1.51
6	B	402	TPP	C7'-C5'	3.09	1.57	1.51
4	A	602	COA	P2A-O6A	2.76	1.70	1.59
8	C	601	SCA	P2-O7	2.65	1.70	1.59
6	B	402	TPP	C6-C5	2.64	1.52	1.50
6	B	402	TPP	C6'-C5'	2.46	1.42	1.37
6	D	402	TPP	C6'-C5'	2.34	1.42	1.37
6	D	402	TPP	C2-N3	2.19	1.40	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	601	SCA	OS1-CS1-CS2	-13.39	108.18	123.99
8	C	601	SCA	OS1-CS1-S	-11.46	107.73	122.61
6	D	402	TPP	C6-C5-C4	-8.87	120.31	127.43
6	B	402	TPP	C6-C5-C4	-5.29	123.19	127.43
8	C	601	SCA	N3-C2-N1	-4.63	121.44	128.68
4	A	602	COA	N3A-C2A-N1A	-4.49	121.66	128.68
8	C	601	SCA	CS2-CS1-S	-4.49	108.23	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	601	SCA	CP8-CPA-CP9	-4.30	100.41	109.17
4	A	602	COA	CEP-CBP-CDP	-3.76	101.50	109.17
4	A	602	COA	C7P-N8P-C9P	3.43	128.71	122.59
6	D	402	TPP	CM4-C4-N3	3.31	126.76	122.53
6	D	402	TPP	C6'-N1'-C2'	3.11	121.26	115.96
6	B	402	TPP	N4'-C4'-N3'	3.02	121.30	117.03
4	A	602	COA	C3P-N4P-C5P	2.92	128.26	122.84
6	B	402	TPP	C6'-N1'-C2'	2.88	120.87	115.96
6	B	402	TPP	C5'-C6'-N1'	-2.87	119.04	123.82
8	C	601	SCA	CP1-S-CS1	2.81	110.61	101.87
6	D	402	TPP	C5'-C6'-N1'	-2.73	119.27	123.82
6	D	402	TPP	CM4-C4-C5	-2.57	121.98	127.60
6	D	402	TPP	PA-O3A-PB	-2.56	124.04	132.83
6	B	402	TPP	PA-O3A-PB	-2.54	124.10	132.83
6	D	402	TPP	N4'-C4'-N3'	2.45	120.50	117.03
4	A	602	COA	C3B-C2B-C1B	2.45	105.31	99.89
8	C	601	SCA	CP8-CPA-CPB	2.31	112.00	108.23
8	C	601	SCA	CP5-CP4-CP3	-2.29	108.54	112.36
6	B	402	TPP	CM4-C4-N3	2.26	125.41	122.53
8	C	601	SCA	CP2-NP1-CP3	2.08	126.70	122.84
6	D	402	TPP	N1'-C2'-N3'	-2.08	121.97	125.54
4	A	602	COA	C1B-N9A-C4A	2.01	130.17	126.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	COA	C3B-O3B-P3B-O7A
4	A	602	COA	C5B-O5B-P1A-O1A
4	A	602	COA	C5B-O5B-P1A-O2A
4	A	602	COA	C5P-C6P-C7P-N8P
8	C	601	SCA	C5'-O5'-P1-O12
8	C	601	SCA	P2-O6-P1-O5'
8	C	601	SCA	CPB-O7-P2-O6
8	C	601	SCA	CP2-CP1-S-CS1
8	C	601	SCA	OS1-CS1-S-CP1
8	C	601	SCA	CS2-CS1-S-CP1
4	A	602	COA	O5P-C5P-C6P-C7P
4	A	602	COA	N4P-C5P-C6P-C7P
4	A	602	COA	P2A-O3A-P1A-O5B
4	A	602	COA	C4B-C5B-O5B-P1A
8	C	601	SCA	C5'-O5'-P1-O6

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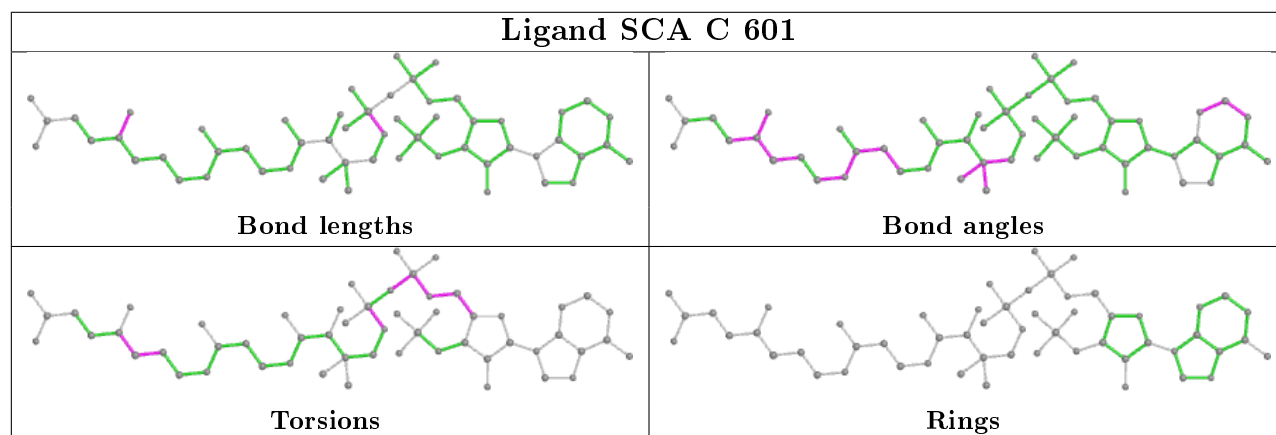
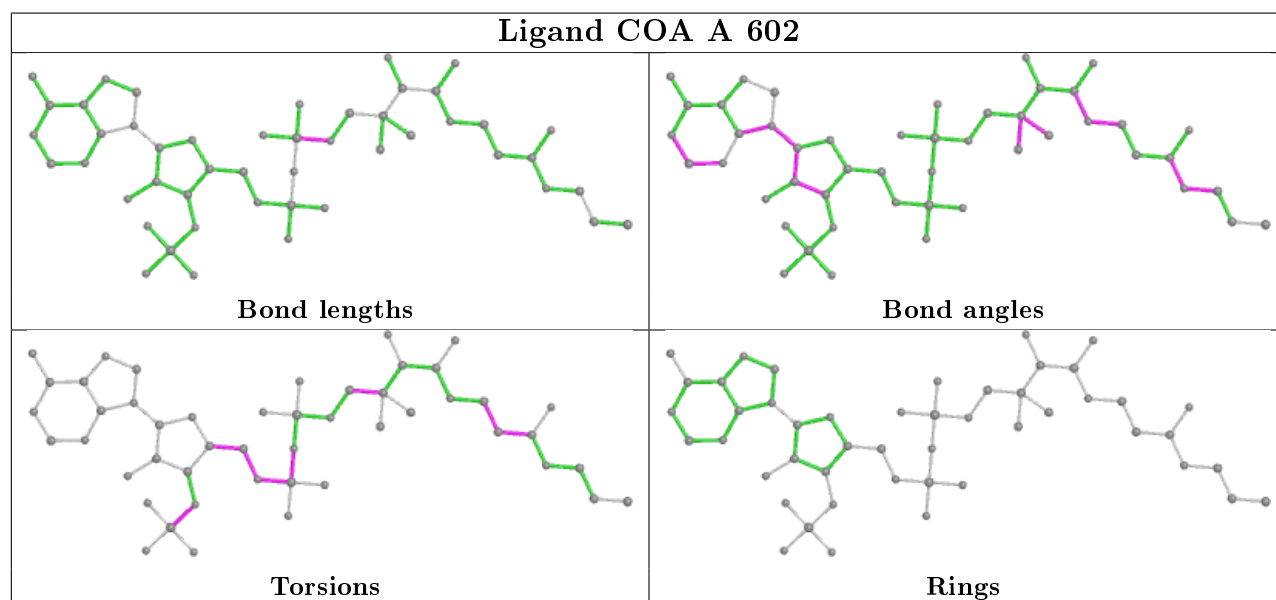
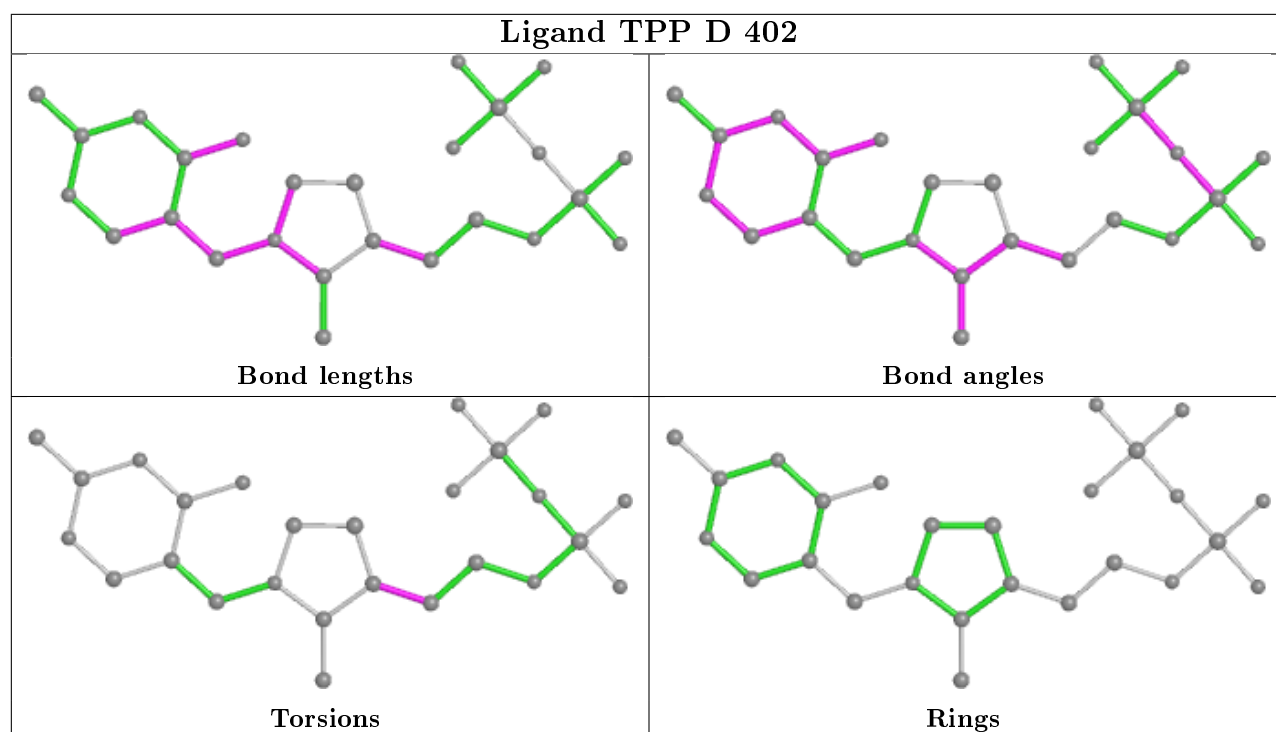
Mol	Chain	Res	Type	Atoms
8	C	601	SCA	C5'-O5'-P1-O11
8	C	601	SCA	CPB-O7-P2-O21
6	B	402	TPP	C4-C5-C6-C7
8	C	601	SCA	C4'-C5'-O5'-P1
4	A	602	COA	CEP-CBP-CCP-O6A
4	A	602	COA	C3B-O3B-P3B-O9A
4	A	602	COA	C5B-O5B-P1A-O3A
8	C	601	SCA	P2-O6-P1-O12
4	A	602	COA	O4B-C4B-C5B-O5B
8	C	601	SCA	O4'-C4'-C5'-O5'
6	D	402	TPP	C4-C5-C6-C7

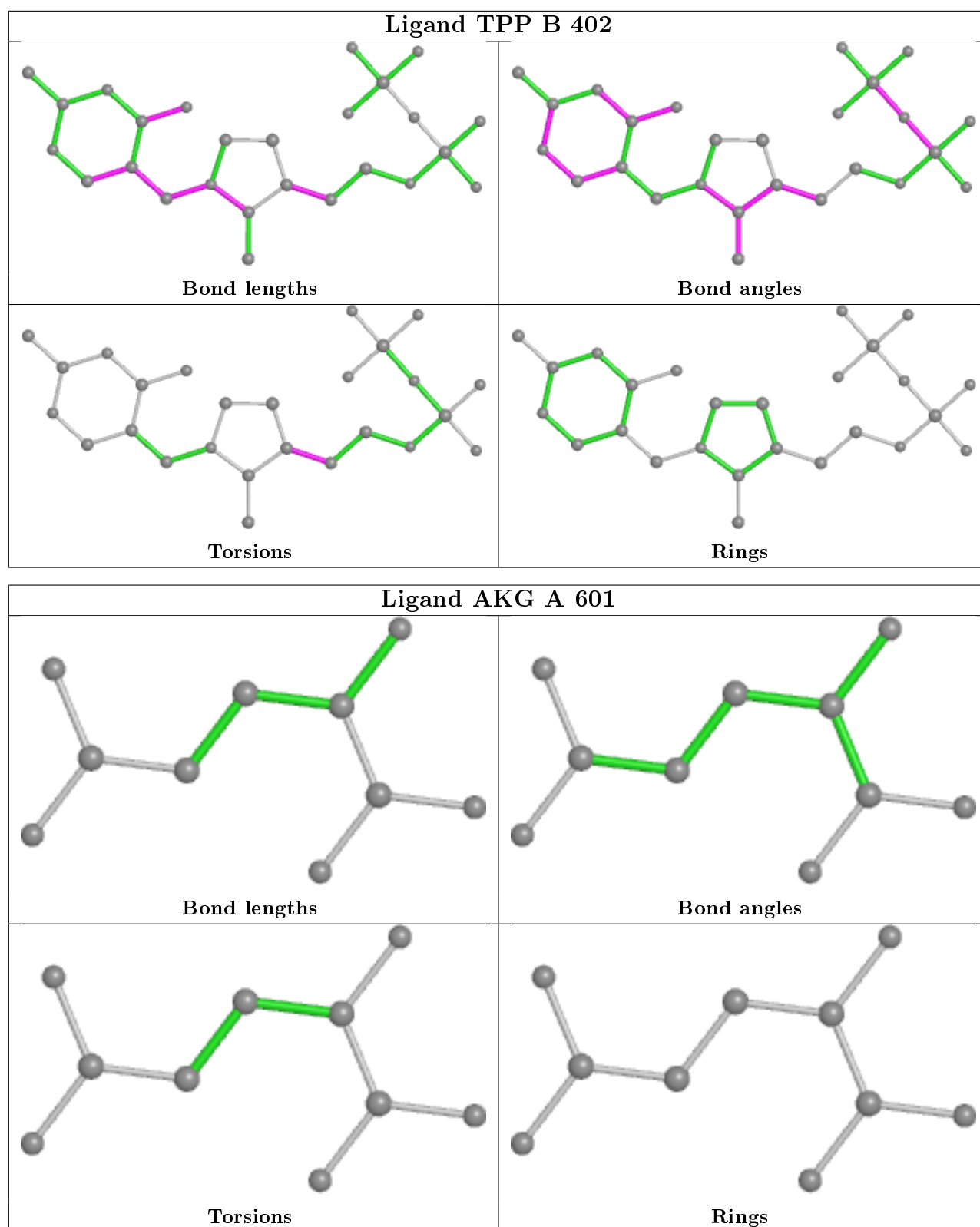
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	402	TPP	3	0
4	A	602	COA	2	0
8	C	601	SCA	7	0
6	B	402	TPP	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.





## 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 [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	572/573 (99%)	-0.01	2 (0%) 94 93	39, 62, 87, 117	0
1	C	572/573 (99%)	0.05	9 (1%) 72 65	37, 68, 98, 106	0
2	B	291/292 (99%)	-0.24	0 100 100	37, 48, 66, 83	0
2	D	291/292 (99%)	0.02	4 (1%) 75 69	44, 59, 77, 98	0
All	All	1726/1730 (99%)	-0.02	15 (0%) 84 80	37, 59, 93, 117	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	THR	4.8
1	A	110	GLY	4.6
1	A	162	GLY	3.5
1	C	180	ALA	3.4
1	C	122	ALA	3.4
2	D	6	PHE	3.0
1	C	95	TYR	2.6
1	C	93	PHE	2.6
1	C	168	PHE	2.6
2	D	13	LYS	2.5
1	C	173	PHE	2.4
1	C	473	VAL	2.3
1	C	129	ARG	2.2
1	C	496	GLY	2.2
2	D	230	GLU	2.1

### 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

There are no carbohydrates in this entry.

### 6.4 Ligands

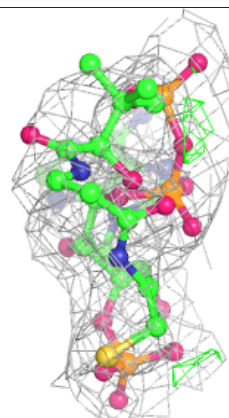
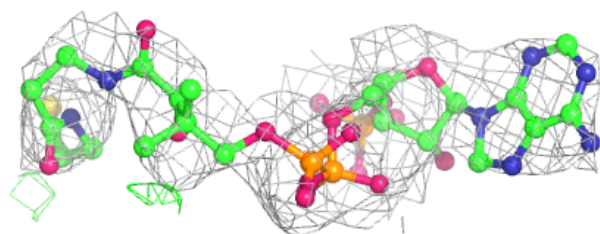
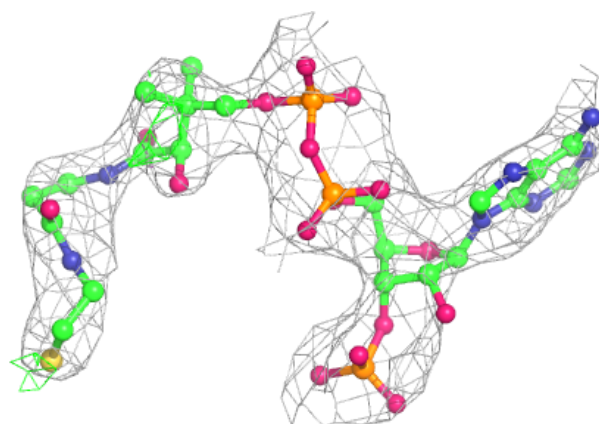
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	COA	A	602	48/48	0.84	0.21	71,93,107,113	0
8	SCA	C	601	55/55	0.90	0.25	56,81,90,92	0
3	AKG	A	601	10/10	0.91	0.29	47,48,53,54	0
6	TPP	D	402	26/26	0.95	0.20	47,53,57,60	0
7	MG	B	403	1/1	0.96	0.13	42,42,42,42	0
7	MG	D	403	1/1	0.96	0.11	46,46,46,46	0
6	TPP	B	402	26/26	0.97	0.17	39,44,46,48	0
5	SF4	B	401	8/8	0.99	0.16	38,40,43,43	0
5	SF4	D	401	8/8	0.99	0.11	50,52,54,61	0

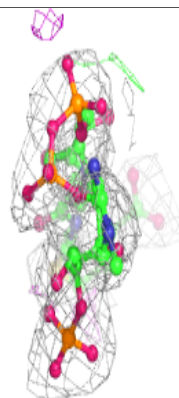
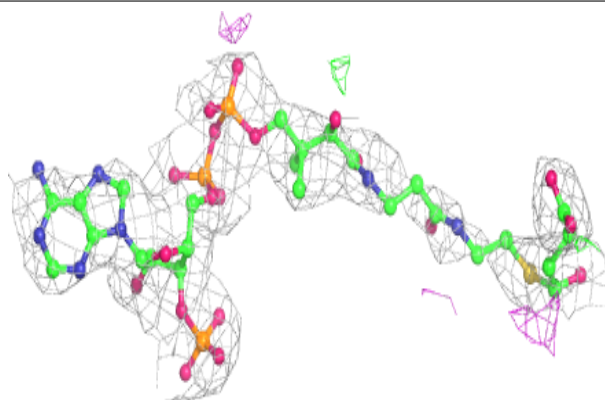
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around COA A 602:**

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

**Electron density around SCA C 601:**

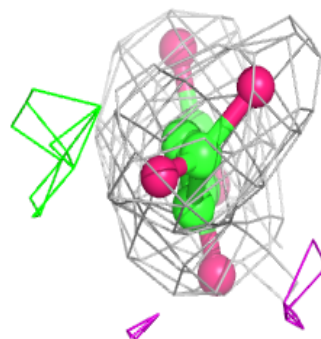
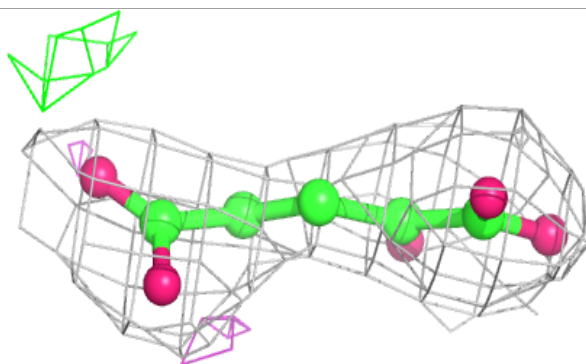
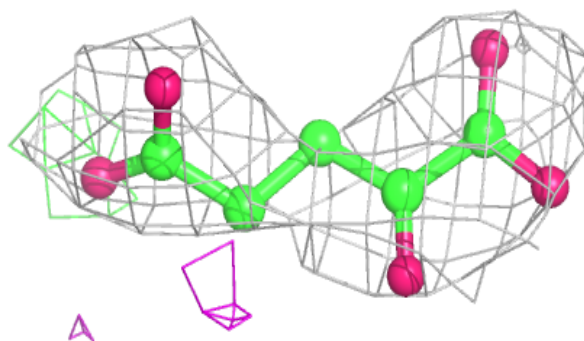
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



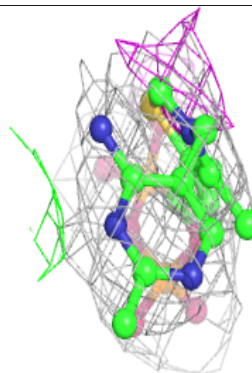
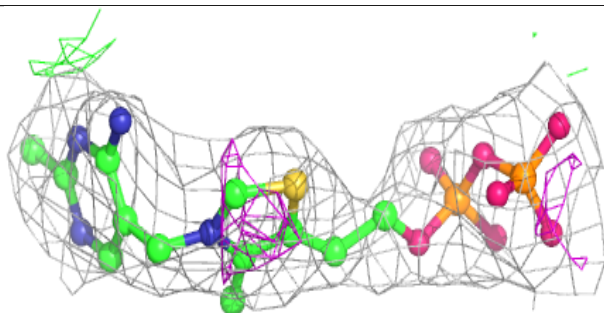
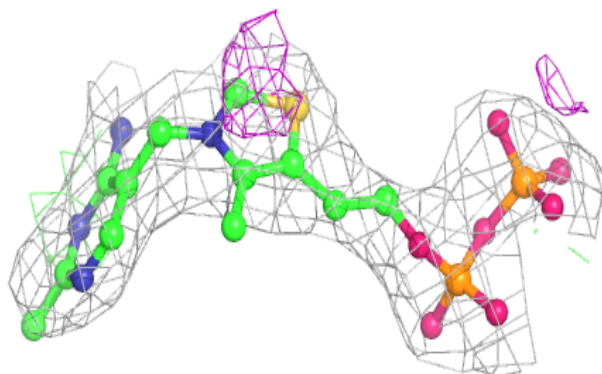


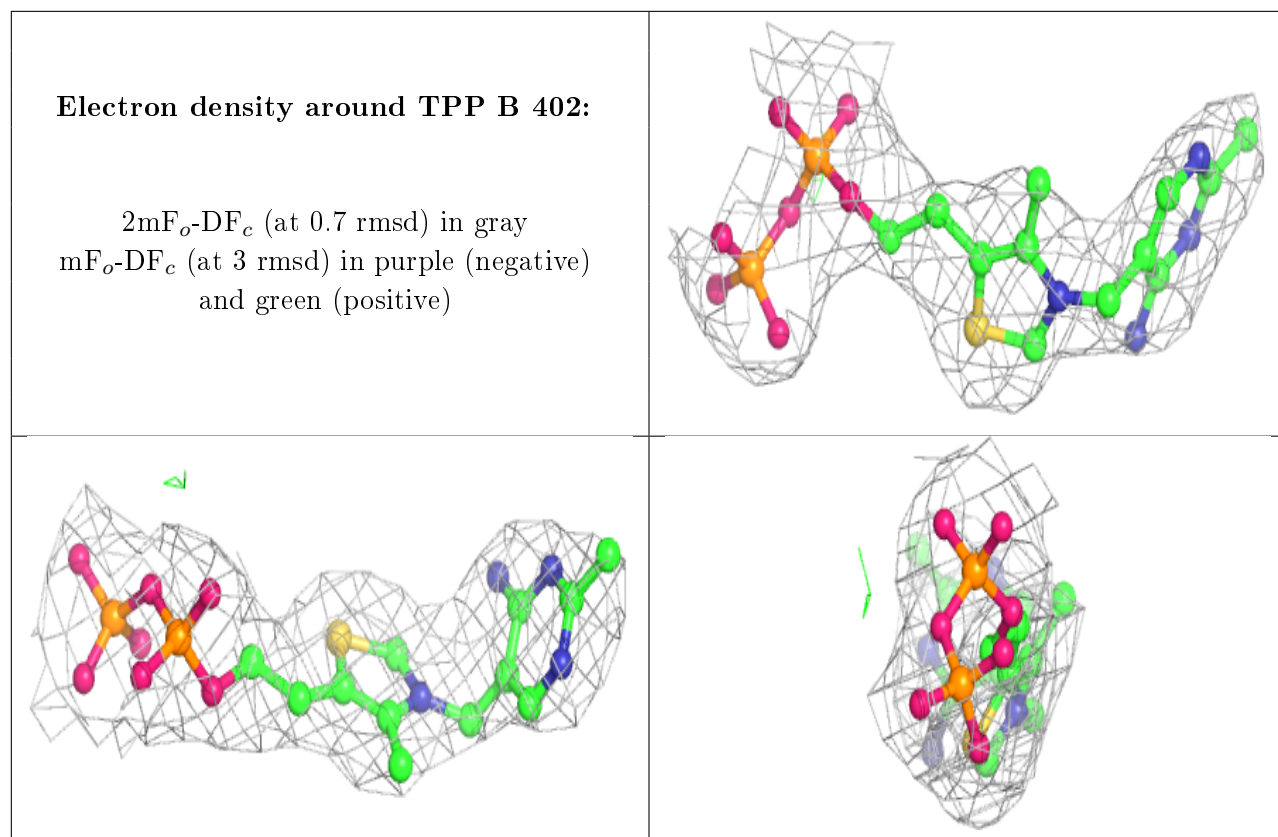
**Electron density around AKG A 601:**

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

**Electron density around TPP 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.