



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 02:13 PM EST

PDB ID : 7KDX  
Title : Crystal structure of Streptomyces tokunonesis TokK with hydroxycobalamin, 5'-deoxyadenosine, and methionine  
Authors : Knox, H.L.; Booker, S.J.; Boal, A.K.  
Deposited on : 2020-10-09  
Resolution : 1.79 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.25  
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) : 2.25

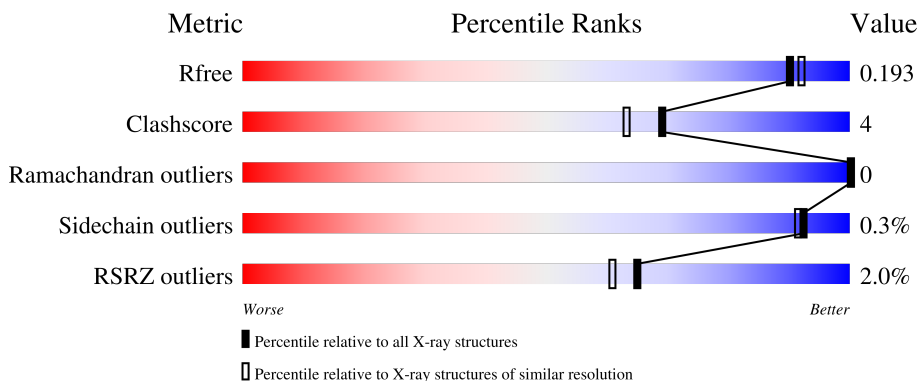
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	681	 2% 90% 6%
1	B	681	 2% 89% 9%

## 2 Entry composition [i](#)

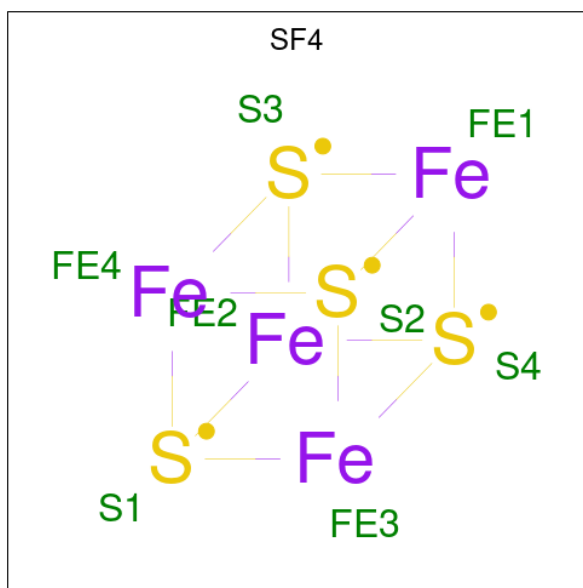
There are 9 unique types of molecules in this entry. The entry contains 11947 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methyltransferase TokK.

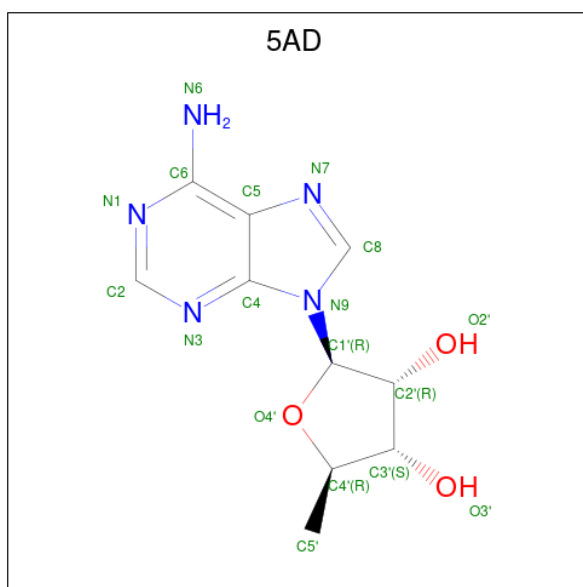
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	658	Total 5334	C 3395	N 930	O 979	S 30	0	11	0
1	B	664	Total 5386	C 3425	N 943	O 989	S 29	0	11	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



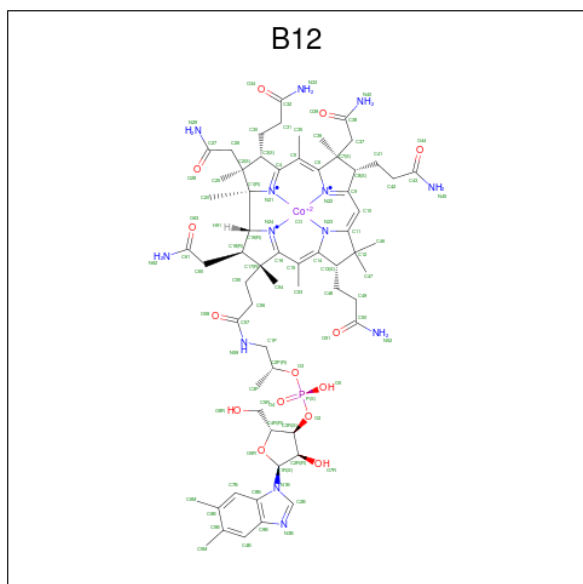
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ) (labeled as "Ligand of Interest" by depositor).



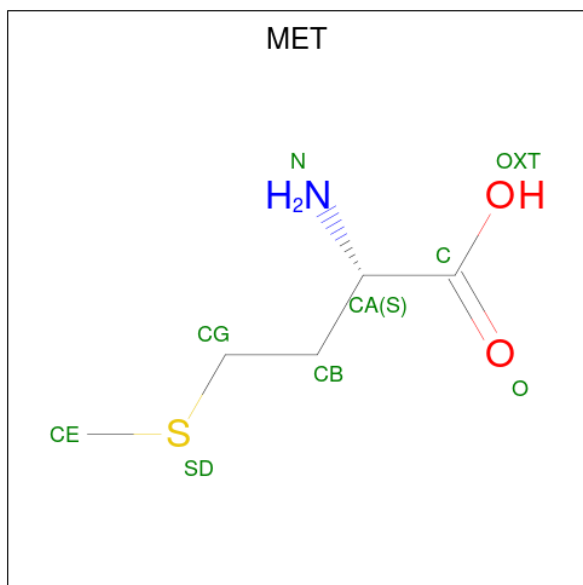
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
4	A	1	91	62	1	13	14	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
4	B	1	91	62	1	13	14	1	0	0

- Molecule 5 is METHIONINE (three-letter code: MET) (formula:  $C_5H_{11}NO_2S$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0
7	B	1	Total K 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total Cl 2 2	0	0

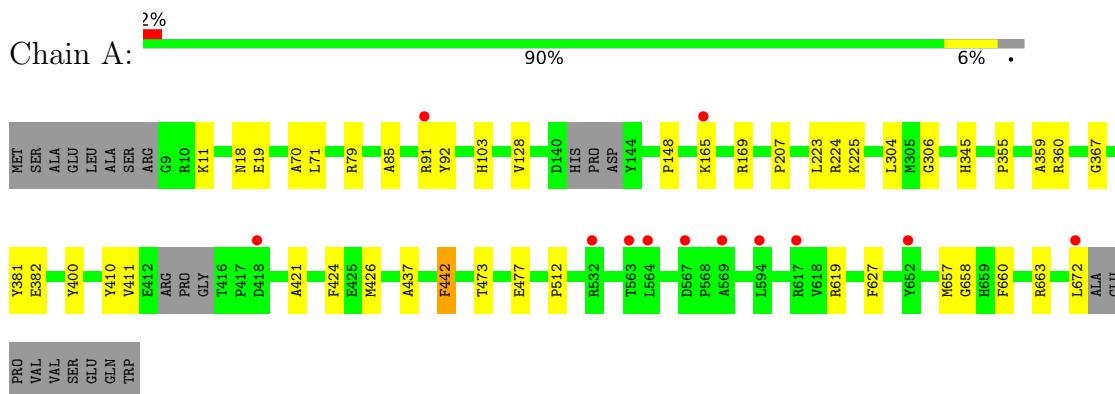
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	414	Total O 414 414	0	0
9	B	473	Total O 473 473	0	0

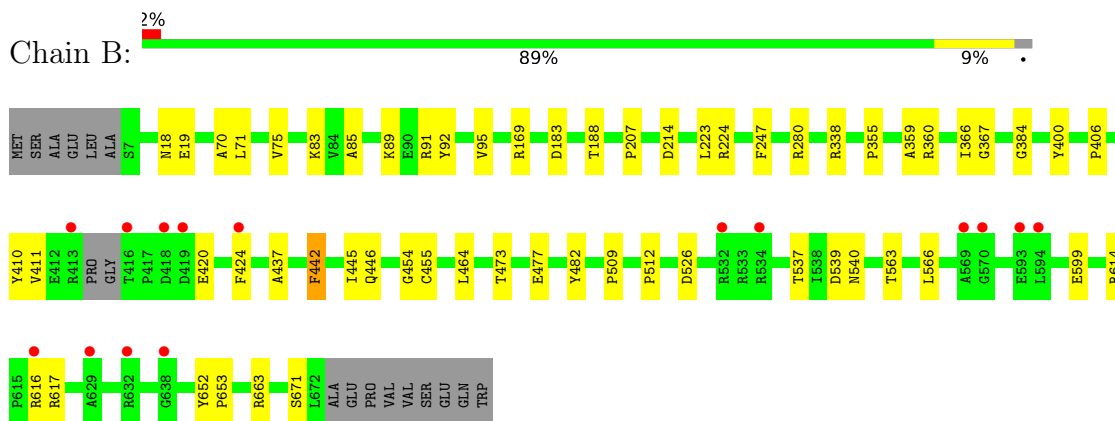
### 3 Residue-property plots [i](#)

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: Methyltransferase TokK



- Molecule 1: Methyltransferase TokK





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.64Å 137.74Å 77.91Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	41.35 – 1.79 41.35 – 1.79	Depositor EDS
% Data completeness (in resolution range)	69.1 (41.35-1.79) 92.9 (41.35-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.165 , 0.193 0.165 , 0.193	Depositor DCC
$R_{free}$ test set	2644 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CL, SF4, B12, 5AD, EDO

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	0.27	0/5502	0.45	0/7462
1	B	0.27	0/5558	0.46	0/7541
All	All	0.27	0/11060	0.46	0/15003

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

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	5334	0	5200	29	0
1	B	5386	0	5240	41	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	18	0	13	0	0
3	B	18	0	13	0	0
4	A	91	0	88	6	0
4	B	91	0	88	11	0
5	A	9	0	8	0	0
5	B	9	0	8	0	0
6	A	28	0	42	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	56	0	84	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	2	0	0	0	0
9	A	414	0	0	2	0
9	B	473	0	0	8	0
All	All	11947	0	10784	81	0

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1902:B12:H552	4:B:1902:B12:H531	1.63	0.80
4:A:703:B12:H531	4:A:703:B12:H552	1.65	0.78
4:B:1902:B12:N45	9:B:2003:HOH:O	2.19	0.75
4:B:1902:B12:H351	4:B:1902:B12:H371	1.68	0.74
1:B:616:ARG:NH2	1:B:671:SER:OG	2.21	0.73
1:B:526:ASP:OD1	9:B:2001:HOH:O	2.07	0.72
1:B:663:ARG:NH2	9:B:2004:HOH:O	2.23	0.71
1:B:614:ARG:HH22	1:B:616:ARG:HH11	1.39	0.70
1:A:360:ARG:NH1	1:A:477:GLU:OE2	2.24	0.70
4:A:703:B12:H371	4:A:703:B12:H351	1.73	0.70
1:A:627:PHE:HA	1:A:663[A]:ARG:HH22	1.58	0.69
1:B:537:THR:OG1	1:B:539[A]:ASP:OD1	2.08	0.69
4:A:703:B12:H203	4:A:703:B12:H301	1.75	0.68
1:A:18:ASN:HB3	4:A:703:B12:H522	1.59	0.66
1:B:360:ARG:NH2	1:B:477:GLU:OE2	2.28	0.66
4:B:1902:B12:H301	4:B:1902:B12:H203	1.76	0.65
1:A:411:VAL:HG13	1:A:512:PRO:HG3	1.80	0.63
1:B:19:GLU:HG3	1:B:410:TYR:CZ	2.34	0.63
1:B:616:ARG:HH21	1:B:671:SER:HG	1.46	0.62
1:B:247:PHE:HE1	6:B:1910:EDO:H21	1.63	0.62
1:B:18:ASN:HB3	4:B:1902:B12:H522	1.64	0.62
1:B:214:ASP:H	4:B:1902:B12:H292	1.48	0.60
1:A:381:TYR:HB3	6:A:708:EDO:H21	1.82	0.60
1:B:207:PRO:HD3	1:B:223:LEU:HD21	1.85	0.59
1:B:75:VAL:H	4:B:1902:B12:H332	1.54	0.56
1:B:188:THR:HG21	6:B:1914:EDO:H12	1.87	0.56
1:B:411:VAL:HG13	1:B:512:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HA	1:B:224:ARG:HG2	1.90	0.53
1:A:658:GLY:O	1:A:663[A]:ARG:NH2	2.41	0.53
1:B:75:VAL:HG21	1:B:424[A]:PHE:HD1	1.73	0.52
1:B:71:LEU:HD11	1:B:85:ALA:HB2	1.90	0.52
1:A:207:PRO:HD3	1:A:223:LEU:HD21	1.92	0.51
1:A:148:PRO:HG3	1:A:165:LYS:HE2	1.93	0.51
1:A:71:LEU:HD11	1:A:85:ALA:HB2	1.92	0.51
1:B:183:ASP:OD2	9:B:2002:HOH:O	2.19	0.51
1:B:384:GLY:HA3	1:B:424[A]:PHE:CZ	2.45	0.50
1:A:382:GLU:HG3	1:A:442:PHE:CE2	2.47	0.50
1:A:355:PRO:HB3	1:A:400:TYR:CG	2.47	0.50
4:B:1902:B12:H401	4:B:1902:B12:C6	2.25	0.50
1:A:79[A]:ARG:HD2	1:A:421:ALA:O	2.13	0.49
1:A:19:GLU:HG3	1:A:410:TYR:CZ	2.48	0.49
1:B:280:ARG:HE	6:B:1910:EDO:H12	1.78	0.49
1:B:406:PRO:O	1:B:509:PRO:HB3	2.13	0.48
1:B:614:ARG:NH2	1:B:616:ARG:HH11	2.10	0.48
1:A:345:HIS:CG	1:A:657:MET:HG2	2.50	0.47
1:B:89:LYS:NZ	1:B:95:VAL:O	2.44	0.47
1:B:540:ASN:ND2	9:B:2006:HOH:O	2.27	0.46
1:A:619:ARG:HB2	1:A:672:LEU:HD21	1.98	0.46
1:A:11:LYS:NZ	9:A:808:HOH:O	2.39	0.46
1:B:91:ARG:NH2	9:B:2021:HOH:O	2.48	0.46
1:B:70:ALA:HB1	4:B:1902:B12:HM52	1.98	0.46
4:B:1902:B12:H251	4:B:1902:B12:H291	1.81	0.46
1:A:91:ARG:HE	1:A:92:TYR:HE2	1.63	0.45
1:A:367:GLY:HA3	1:A:473:THR:OG1	2.16	0.45
1:A:359:ALA:HB2	1:A:437:ALA:HB1	1.99	0.45
1:A:660:PHE:CE1	6:A:709:EDO:H12	2.52	0.44
1:B:355:PRO:HB3	1:B:400:TYR:CG	2.52	0.44
1:B:338:ARG:NH1	9:B:2019:HOH:O	2.46	0.44
1:B:83:LYS:NZ	1:B:420:GLU:OE2	2.37	0.44
1:B:366:ILE:HD13	1:B:445:ILE:HD13	1.99	0.44
4:A:703:B12:H401	4:A:703:B12:C6	2.31	0.44
1:A:627:PHE:HA	1:A:663[A]:ARG:NH2	2.30	0.43
1:A:225:LYS:HE3	6:B:1901:EDO:H22	2.00	0.43
1:A:18:ASN:HB2	9:A:1051:HOH:O	2.19	0.42
1:A:304:LEU:HG	1:A:306:GLY:H	1.84	0.42
1:B:442:PHE:O	1:B:446:GLN:HG2	2.19	0.42
1:B:92:TYR:O	1:B:95:VAL:HG12	2.20	0.42
1:B:18:ASN:HB2	9:B:2286:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLY:O	1:B:455[A]:CYS:HB2	2.20	0.42
1:A:169:ARG:HA	1:A:224:ARG:HG2	2.01	0.42
1:B:652:TYR:CD1	1:B:653:PRO:HA	2.55	0.41
1:B:464:LEU:HD22	1:B:566:LEU:HD13	2.01	0.41
1:B:367:GLY:HA3	1:B:473:THR:OG1	2.20	0.41
1:A:424:PHE:CE1	1:A:426:MET:HB2	2.56	0.41
1:B:599:GLU:OE1	1:B:617:ARG:NH1	2.48	0.41
1:A:424:PHE:CD1	6:A:707:EDO:H12	2.56	0.41
1:B:482:TYR:CE1	1:B:563:THR:HG21	2.56	0.41
1:A:70:ALA:HB1	4:A:703:B12:HM52	2.03	0.41
4:B:1902:B12:H562	4:B:1902:B12:H18	1.89	0.41
1:A:128:VAL:HG11	1:A:165:LYS:HE3	2.04	0.40
1:B:359:ALA:HB2	1:B:437:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/681 (97%)	646 (97%)	17 (3%)	0	100	100
1	B	671/681 (98%)	652 (97%)	19 (3%)	0	100	100
All	All	1334/1362 (98%)	1298 (97%)	36 (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	561/569 (99%)	559 (100%)	2 (0%)	91	89
1	B	567/569 (100%)	566 (100%)	1 (0%)	93	92
All	All	1128/1138 (99%)	1125 (100%)	3 (0%)	92	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	442	PHE
1	B	442	PHE

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 4 are monoatomic - leaving 29 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	EDO	B	1913	-	3,3,3	0.48	0	2,2,2	0.33	0
6	EDO	A	705	-	3,3,3	0.44	0	2,2,2	0.46	0
4	B12	A	703	9	90,101,101	0.89	3 (3%)	137,166,166	1.04	9 (6%)
6	EDO	B	1909	-	3,3,3	0.46	0	2,2,2	0.22	0
6	EDO	B	1912	-	3,3,3	0.42	0	2,2,2	0.43	0
3	5AD	B	1904	-	17,20,20	0.68	0	15,30,30	0.62	0
6	EDO	A	711	-	3,3,3	0.47	0	2,2,2	0.27	0
6	EDO	B	1911	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	B	1907	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	B	1914	-	3,3,3	0.41	0	2,2,2	0.37	0
6	EDO	A	710	-	3,3,3	0.46	0	2,2,2	0.24	0
6	EDO	B	1908	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	A	709	-	3,3,3	0.46	0	2,2,2	0.28	0
6	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.39	0
4	B12	B	1902	9	90,101,101	0.93	3 (3%)	137,166,166	1.02	9 (6%)
6	EDO	A	708	-	3,3,3	0.45	0	2,2,2	0.25	0
6	EDO	B	1906	-	3,3,3	0.50	0	2,2,2	0.26	0
6	EDO	B	1901	-	3,3,3	0.45	0	2,2,2	0.36	0
5	MET	B	1905	2	4,8,8	0.42	0	2,9,9	0.21	0
6	EDO	B	1917	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	B	1918	-	3,3,3	0.48	0	2,2,2	0.25	0
2	SF4	A	701	1,5	0,12,12	-	-	-	-	-
3	5AD	A	702	-	17,20,20	0.69	0	15,30,30	0.61	0
5	MET	A	704	2	4,8,8	0.28	0	2,9,9	0.21	0
6	EDO	A	707	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	B	1916	-	3,3,3	0.45	0	2,2,2	0.42	0
2	SF4	B	1903	1,5	0,12,12	-	-	-	-	-
6	EDO	B	1915	-	3,3,3	0.44	0	2,2,2	0.31	0
6	EDO	B	1910	-	3,3,3	0.45	0	2,2,2	0.29	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
6	EDO	B	1913	-	-	0/1/1/1	-
6	EDO	A	705	-	-	0/1/1/1	-
4	B12	A	703	9	-	9/52/223/223	0/3/11/11
6	EDO	B	1909	-	-	1/1/1/1	-
6	EDO	B	1912	-	-	0/1/1/1	-
3	5AD	B	1904	-	-	0/0/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	711	-	-	0/1/1/1	-
6	EDO	B	1911	-	-	0/1/1/1	-
6	EDO	B	1907	-	-	0/1/1/1	-
6	EDO	B	1914	-	-	0/1/1/1	-
6	EDO	A	710	-	-	0/1/1/1	-
6	EDO	B	1908	-	-	0/1/1/1	-
6	EDO	A	709	-	-	0/1/1/1	-
6	EDO	A	706	-	-	1/1/1/1	-
4	B12	B	1902	9	-	20/52/223/223	0/3/11/11
6	EDO	A	708	-	-	1/1/1/1	-
6	EDO	B	1906	-	-	0/1/1/1	-
6	EDO	B	1901	-	-	0/1/1/1	-
5	MET	B	1905	2	-	1/4/8/8	-
6	EDO	B	1917	-	-	1/1/1/1	-
6	EDO	B	1918	-	-	0/1/1/1	-
2	SF4	A	701	1,5	-	-	0/6/5/5
3	5AD	A	702	-	-	0/0/20/20	0/3/3/3
5	MET	A	704	2	-	1/4/8/8	-
6	EDO	A	707	-	-	0/1/1/1	-
6	EDO	B	1916	-	-	0/1/1/1	-
2	SF4	B	1903	1,5	-	-	0/6/5/5
6	EDO	B	1915	-	-	0/1/1/1	-
6	EDO	B	1910	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1902	B12	C14-N23	6.88	1.43	1.35
4	A	703	B12	C14-N23	6.34	1.43	1.35
4	B	1902	B12	C9-N22	2.44	1.36	1.30
4	A	703	B12	C9-N22	2.44	1.36	1.30
4	A	703	B12	O3-C2P	-2.30	1.39	1.45
4	B	1902	B12	O3-C2P	-2.13	1.40	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	B12	C13-C14-C15	4.02	130.48	124.32
4	B	1902	B12	C13-C14-C15	3.97	130.40	124.32
4	B	1902	B12	C15-C16-N24	-3.03	118.06	122.42
4	B	1902	B12	C35-C5-C4	-3.02	110.65	116.79
4	A	703	B12	C1-C19-C18	-2.91	117.11	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	B12	C15-C16-N24	-2.89	118.25	122.42
4	A	703	B12	C35-C5-C4	-2.88	110.93	116.79
4	B	1902	B12	C13-C14-N23	-2.83	105.25	109.10
4	A	703	B12	C13-C14-N23	-2.82	105.27	109.10
4	A	703	B12	C17-C16-C15	2.75	130.59	126.26
4	B	1902	B12	C17-C16-C15	2.45	130.13	126.26
4	A	703	B12	C8-C7-C6	2.39	105.02	100.92
4	B	1902	B12	C1-C19-C18	-2.34	118.05	121.88
4	B	1902	B12	C8-C7-C6	2.28	104.83	100.92
4	B	1902	B12	C35-C5-C6	2.25	126.01	122.43
4	A	703	B12	C35-C5-C6	2.24	126.00	122.43
4	B	1902	B12	C16-C15-C14	2.11	124.45	121.25
4	A	703	B12	C16-C15-C14	2.08	124.40	121.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	B12	C7-C37-C38-O39
4	A	703	B12	C7-C37-C38-N40
4	A	703	B12	C3R-O2-P-O5
4	B	1902	B12	C2-C26-C27-O28
4	B	1902	B12	C7-C37-C38-O39
4	B	1902	B12	C3R-O2-P-O5
4	B	1902	B12	C2-C26-C27-N29
4	B	1902	B12	C7-C37-C38-N40
6	B	1917	EDO	O1-C1-C2-O2
4	B	1902	B12	C30-C31-C32-N33
4	B	1902	B12	C41-C42-C43-O44
4	A	703	B12	C3R-O2-P-O4
4	B	1902	B12	C3R-O2-P-O4
4	B	1902	B12	C18-C17-C55-C56
6	A	708	EDO	O1-C1-C2-O2
4	B	1902	B12	C30-C31-C32-O34
4	B	1902	B12	C41-C42-C43-N45
4	B	1902	B12	C38-C37-C7-C36
5	A	704	MET	C-CA-CB-CG
5	B	1905	MET	C-CA-CB-CG
4	B	1902	B12	C16-C17-C55-C56
6	B	1910	EDO	O1-C1-C2-O2
4	A	703	B12	C3R-O2-P-O3
4	B	1902	B12	C3R-O2-P-O3

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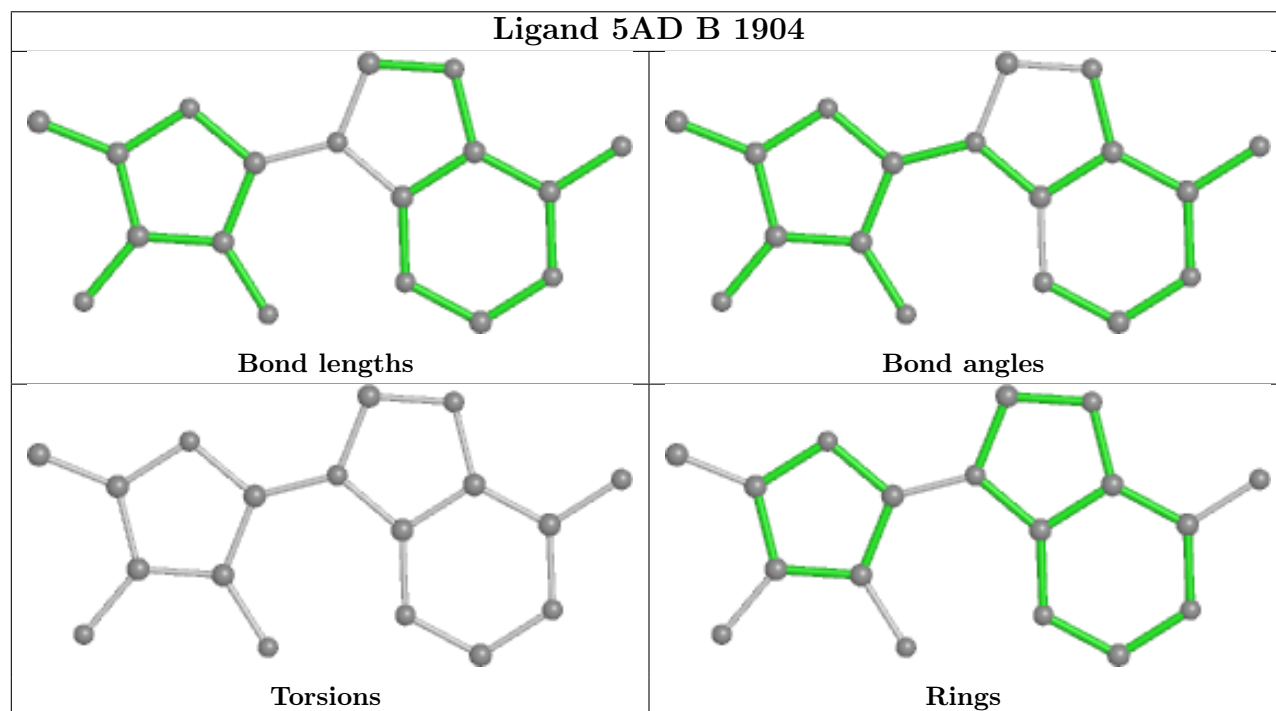
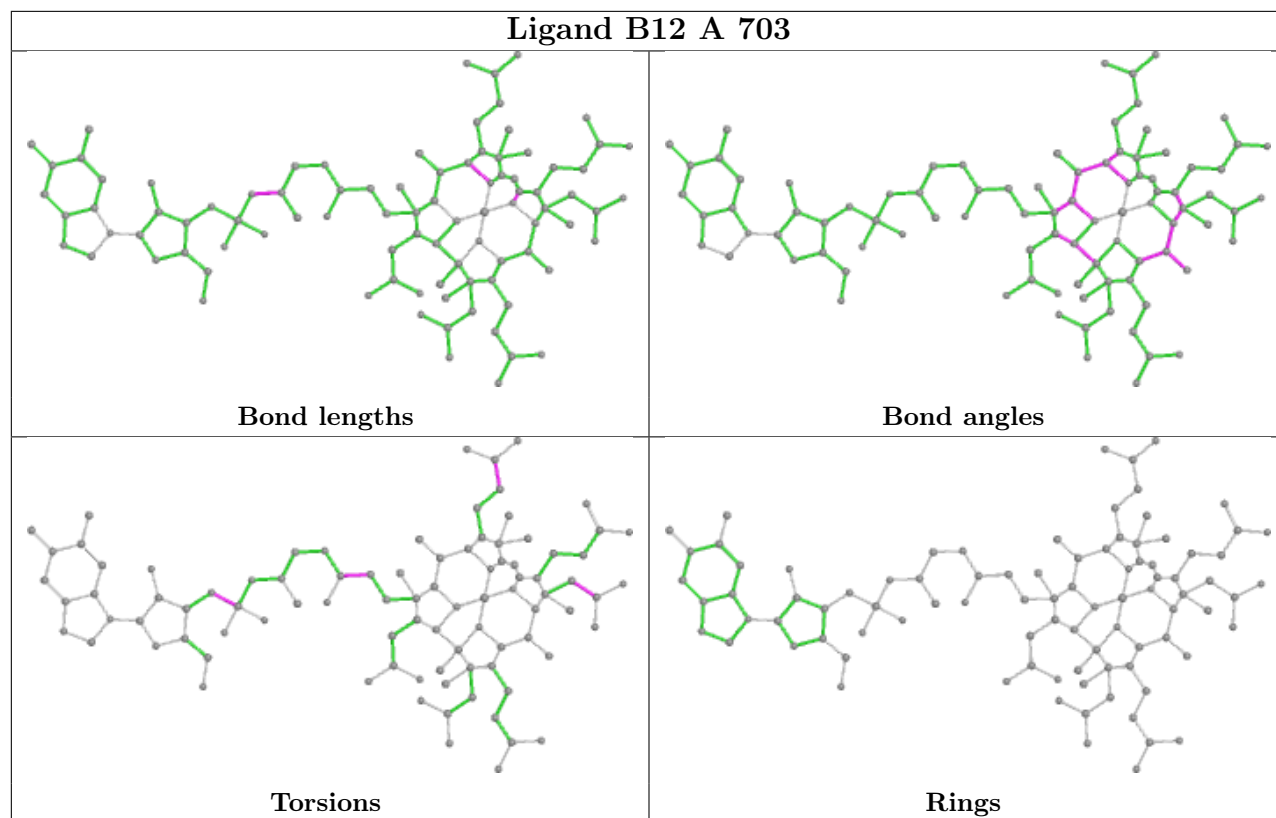
Mol	Chain	Res	Type	Atoms
4	B	1902	B12	C1-C2-C26-C27
4	B	1902	B12	C55-C56-C57-O58
6	B	1909	EDO	O1-C1-C2-O2
4	B	1902	B12	C48-C49-C50-N52
4	A	703	B12	C55-C56-C57-O58
4	B	1902	B12	C25-C2-C26-C27
4	B	1902	B12	C55-C56-C57-N59
4	A	703	B12	C55-C56-C57-N59
4	A	703	B12	C48-C49-C50-N52
4	B	1902	B12	C48-C49-C50-O51
6	A	706	EDO	O1-C1-C2-O2
4	A	703	B12	C48-C49-C50-O51

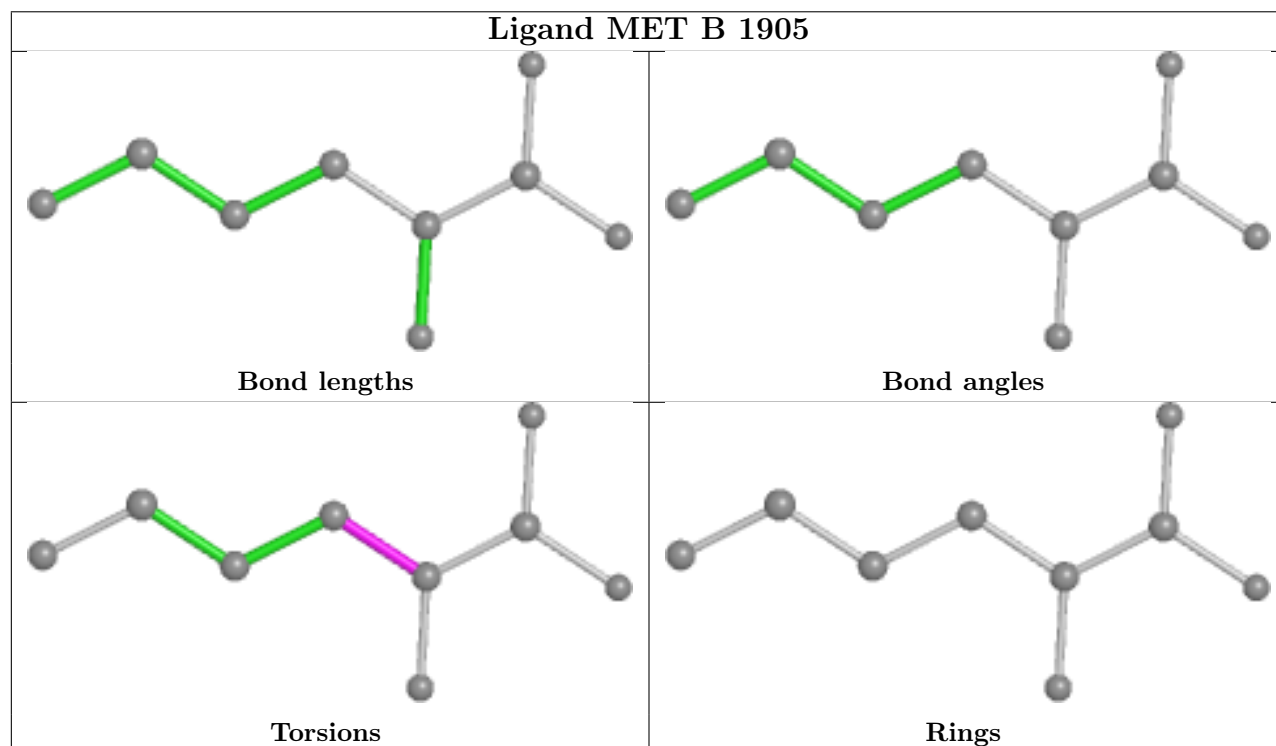
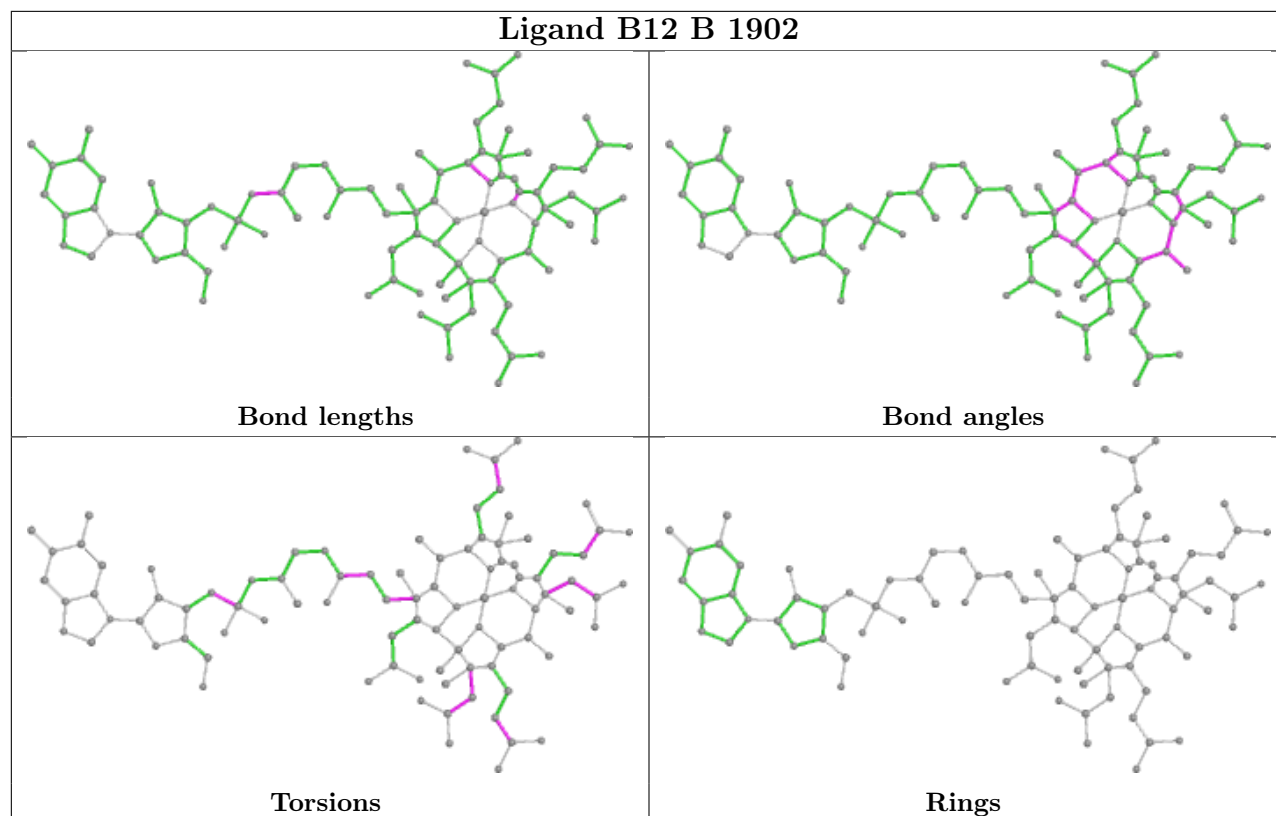
There are no ring outliers.

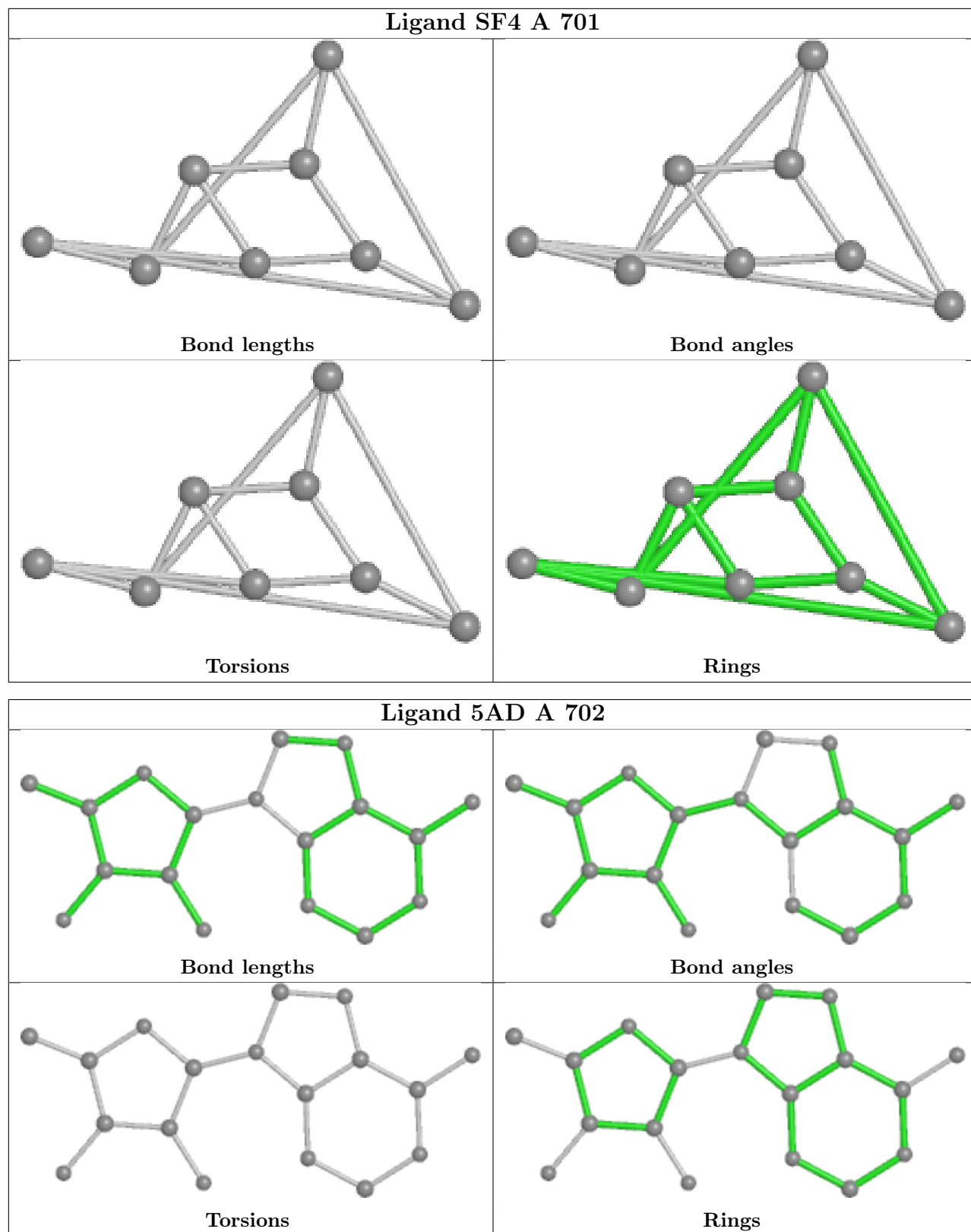
8 monomers are involved in 24 short contacts:

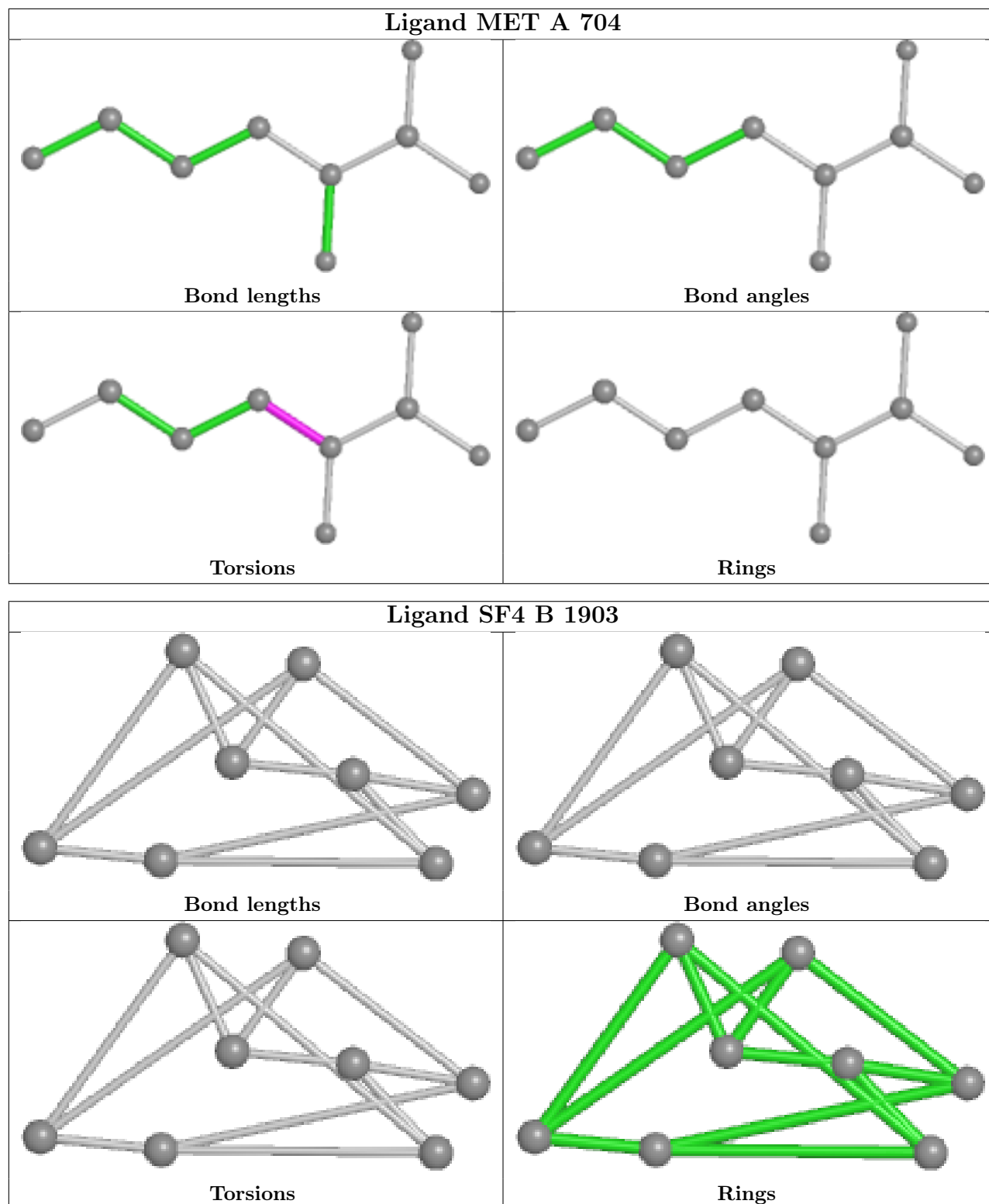
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	B12	6	0
6	B	1914	EDO	1	0
6	A	709	EDO	1	0
4	B	1902	B12	11	0
6	A	708	EDO	1	0
6	B	1901	EDO	1	0
6	A	707	EDO	1	0
6	B	1910	EDO	2	0

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 [i](#)

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	658/681 (96%)	0.13	12 (1%) 68 64	11, 25, 47, 78	0
1	B	664/681 (97%)	0.01	15 (2%) 60 56	10, 22, 43, 67	0
All	All	1322/1362 (97%)	0.07	27 (2%) 65 61	10, 23, 45, 78	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424[A]	PHE	4.7
1	B	569	ALA	4.1
1	A	532	ARG	3.9
1	A	652	TYR	3.7
1	B	570	GLY	3.6
1	A	563	THR	3.4
1	A	569	ALA	3.2
1	B	594	LEU	3.1
1	A	617	ARG	2.8
1	A	418	ASP	2.7
1	B	418	ASP	2.6
1	B	416	THR	2.5
1	B	638	GLY	2.5
1	B	419[A]	ASP	2.5
1	B	413	ARG	2.4
1	A	567	ASP	2.4
1	B	629	ALA	2.3
1	B	616	ARG	2.3
1	A	165	LYS	2.3
1	B	593	GLU	2.2
1	A	672	LEU	2.2
1	B	632	ARG	2.2
1	A	564	LEU	2.2
1	B	532	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	ARG	2.1
1	B	534	ARG	2.1
1	A	594	LEU	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 [i](#)

There are no monosaccharides 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.

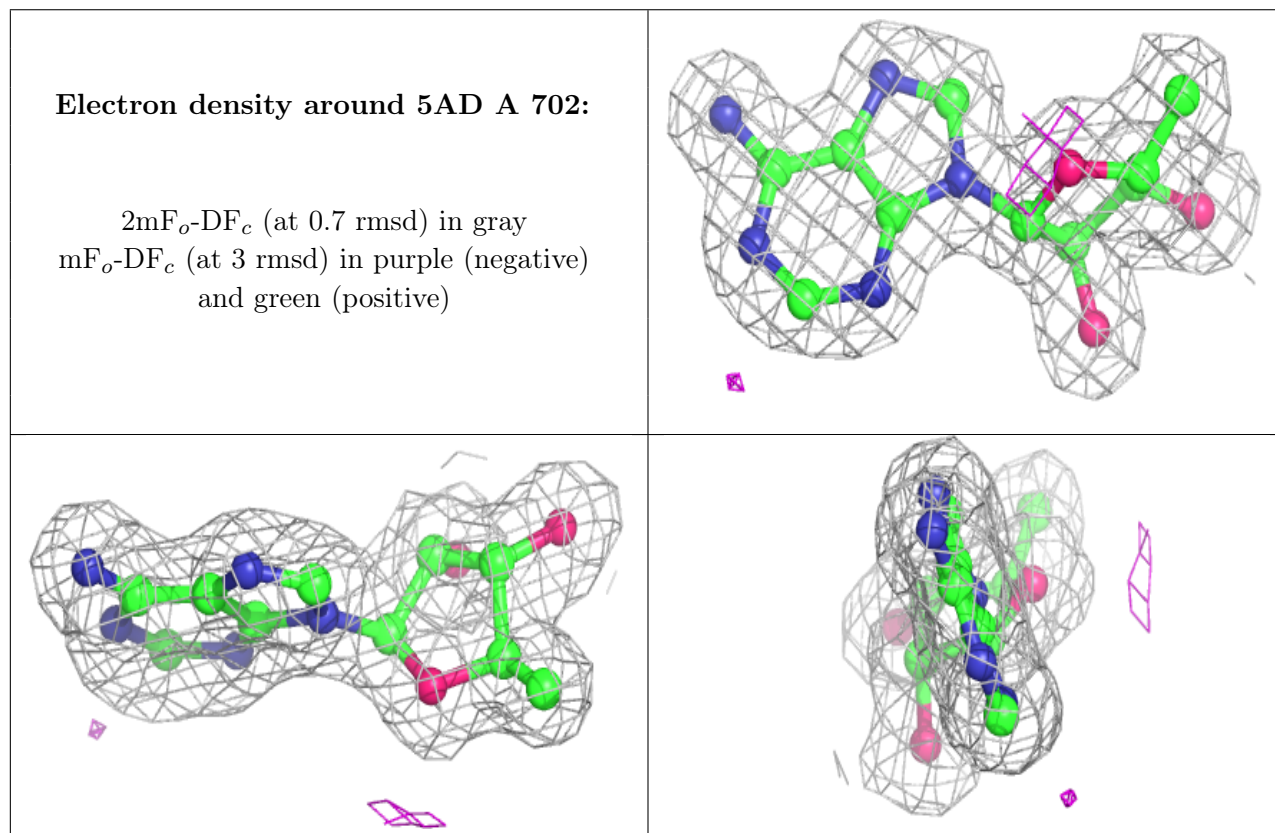
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	B	1919	1/1	0.78	0.09	66,66,66,66	0
6	EDO	B	1906	4/4	0.80	0.20	29,35,39,41	0
6	EDO	B	1907	4/4	0.83	0.20	42,42,44,44	0
6	EDO	A	706	4/4	0.84	0.17	45,46,46,46	0
6	EDO	B	1909	4/4	0.85	0.14	31,38,39,39	0
6	EDO	A	708	4/4	0.86	0.17	41,42,43,47	0
6	EDO	B	1918	4/4	0.87	0.15	41,41,41,42	0
6	EDO	B	1916	4/4	0.88	0.18	38,43,44,47	0
6	EDO	A	707	4/4	0.89	0.21	45,45,47,48	0
6	EDO	B	1917	4/4	0.89	0.21	35,37,38,40	0
6	EDO	B	1913	4/4	0.90	0.13	30,30,39,40	0
6	EDO	B	1910	4/4	0.91	0.17	31,35,38,42	0
6	EDO	B	1901	4/4	0.92	0.14	33,34,36,43	0
6	EDO	B	1912	4/4	0.93	0.15	37,38,40,44	0
6	EDO	B	1908	4/4	0.94	0.14	41,42,42,45	0
6	EDO	A	711	4/4	0.95	0.10	30,35,38,40	0
6	EDO	B	1911	4/4	0.95	0.17	30,35,38,41	0
6	EDO	A	710	4/4	0.96	0.10	20,21,24,27	0
6	EDO	B	1915	4/4	0.96	0.13	23,24,26,26	0
6	EDO	A	705	4/4	0.96	0.07	25,28,34,38	0

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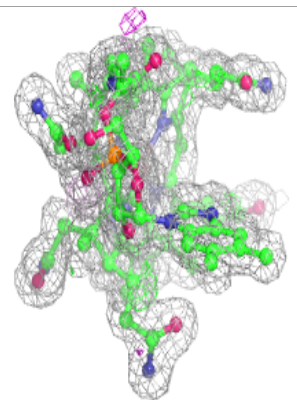
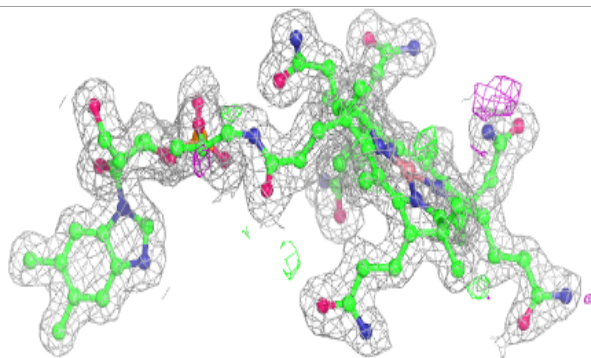
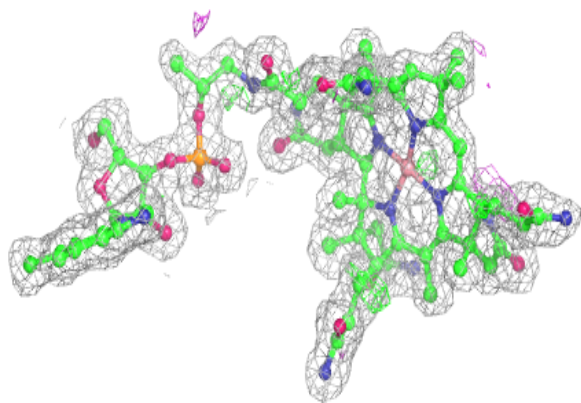
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	5AD	A	702	18/18	0.97	0.10	11,13,15,15	0
6	EDO	B	1914	4/4	0.98	0.09	20,22,29,33	0
4	B12	A	703	91/91	0.98	0.10	8,15,24,35	0
4	B12	B	1902	91/91	0.98	0.12	6,14,25,38	0
5	MET	A	704	9/9	0.98	0.11	8,11,14,14	0
6	EDO	A	709	4/4	0.98	0.07	21,21,21,22	0
7	K	A	712	1/1	0.98	0.09	21,21,21,21	0
3	5AD	B	1904	18/18	0.98	0.11	8,12,14,14	0
5	MET	B	1905	9/9	0.99	0.08	9,10,11,13	0
2	SF4	B	1903	8/8	0.99	0.08	11,12,13,13	0
2	SF4	A	701	8/8	0.99	0.08	11,12,13,14	0
8	CL	B	1920	1/1	0.99	0.04	28,28,28,28	0
7	K	B	1921	1/1	1.00	0.07	22,22,22,22	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.

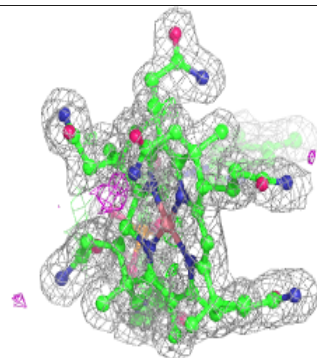
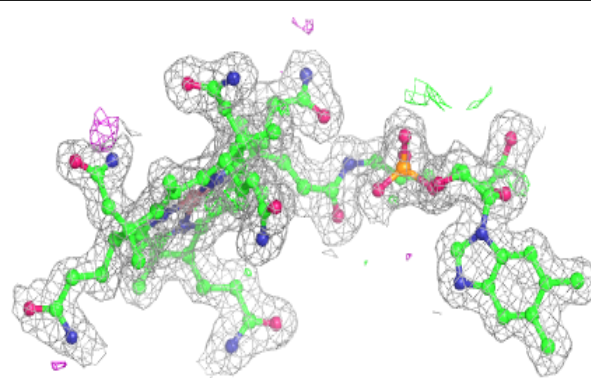
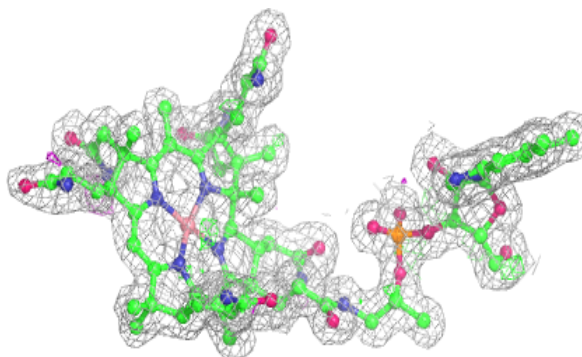


**Electron density around B12 A 703:**

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

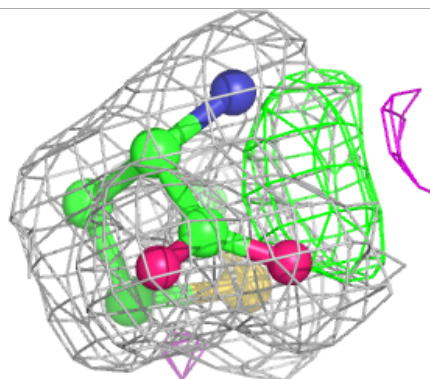
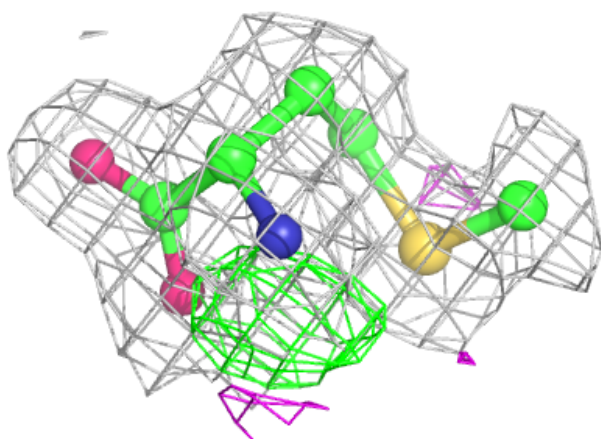
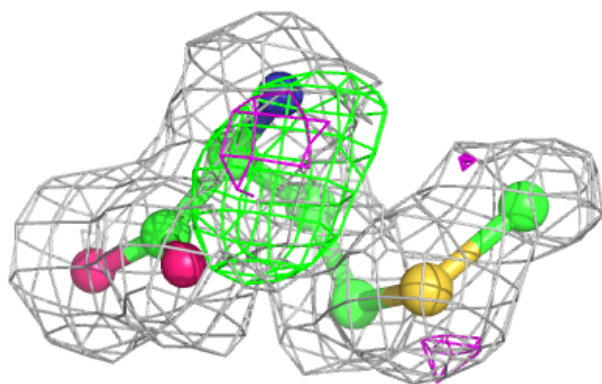
**Electron density around B12 B 1902:**

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



**Electron density around MET A 704:**

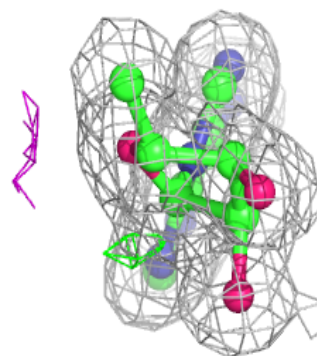
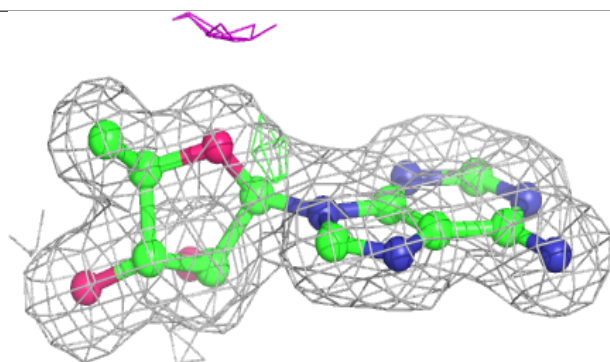
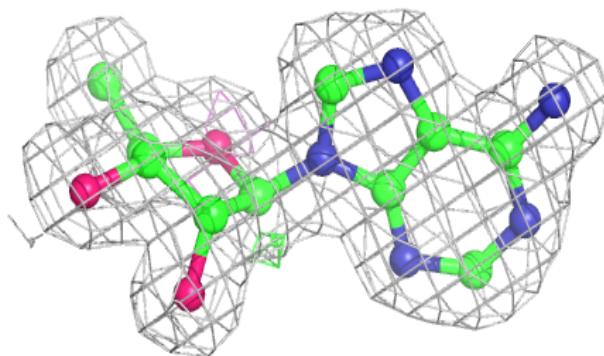
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



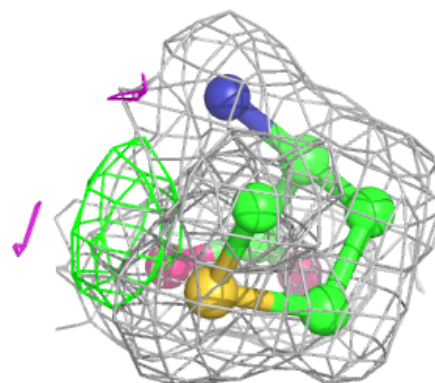
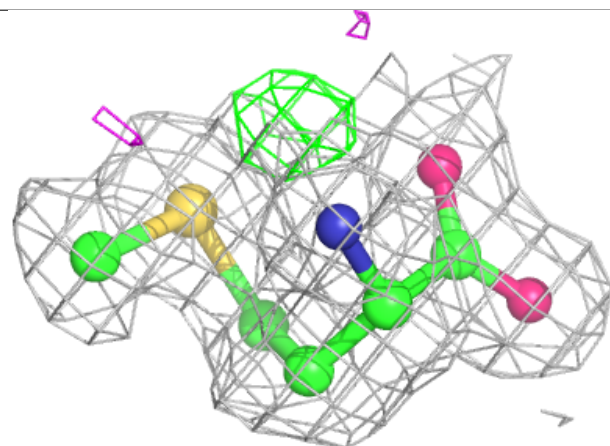
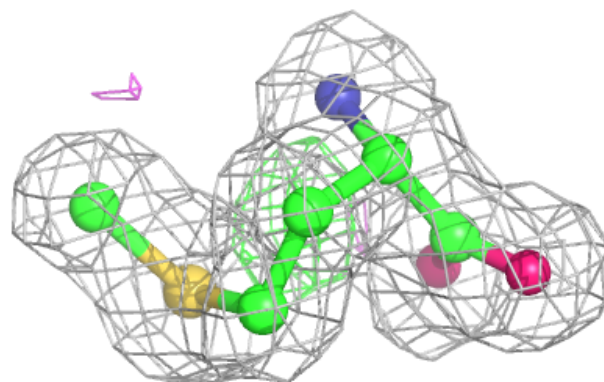


**Electron density around 5AD B 1904:**

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

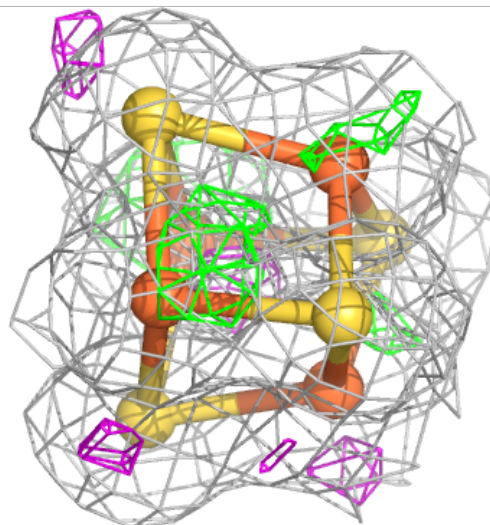
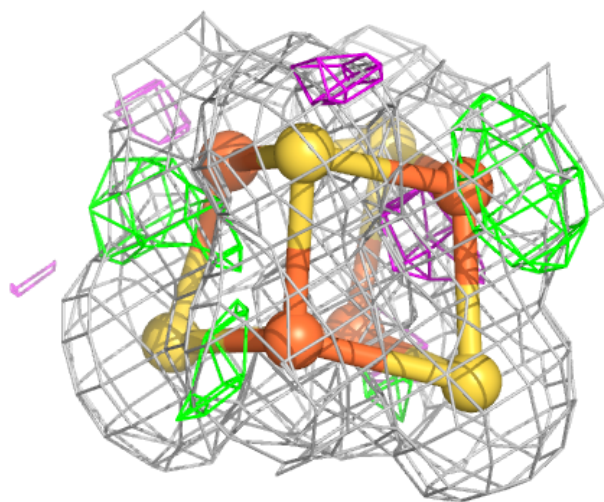
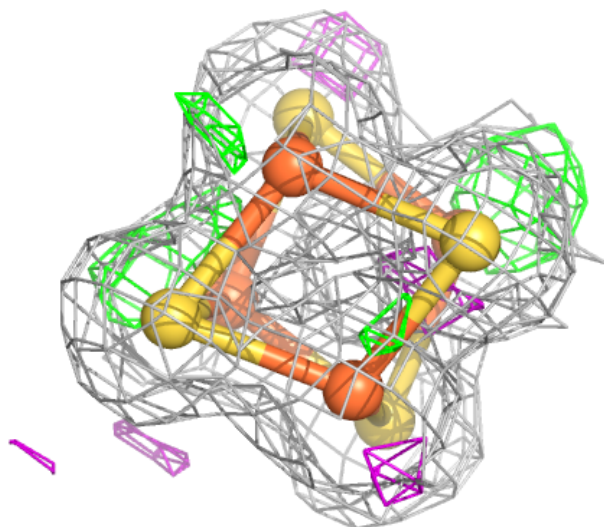
**Electron density around MET B 1905:**

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



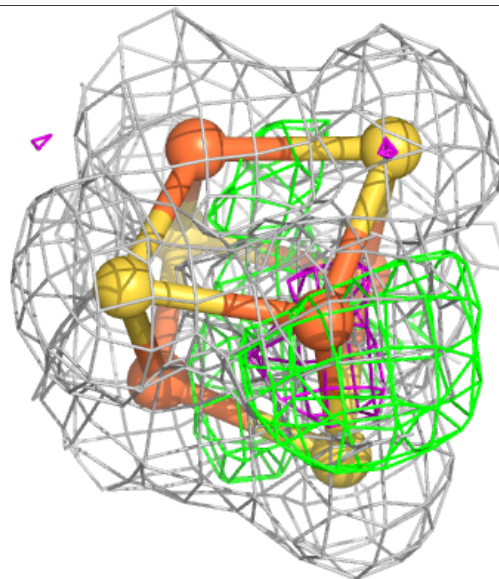
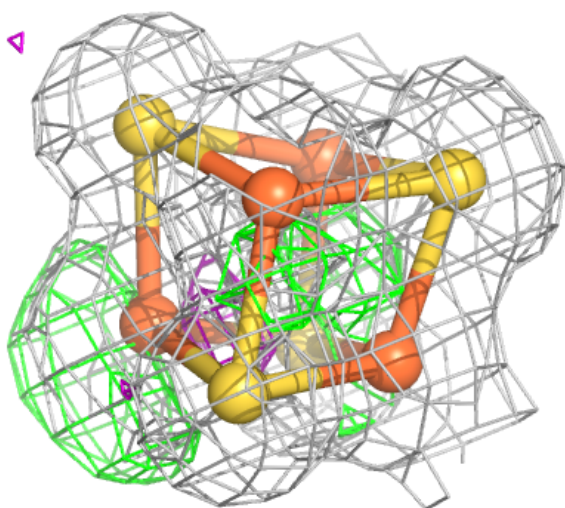
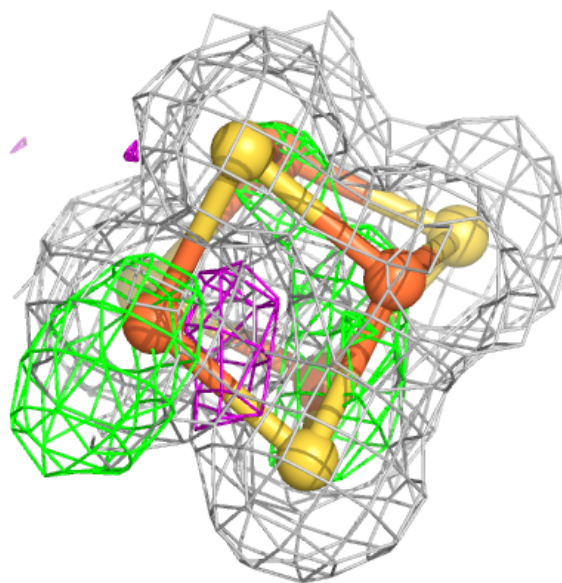
**Electron density around SF4 B 1903:**

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



**Electron density around SF4 A 701:**

$2mF_o-DF_c$  (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.