



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 05:09 PM BST

PDB ID : 6RL0  
Title : Recombinant Pseudomonas stutzeri nitrous oxide reductase, form I  
Authors : Zhang, L.; Wuest, A.; Prasser, B.; Mueller, C.; Einsle, O.  
Deposited on : 2019-04-30  
Resolution : 1.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1  
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) : 2.13.1

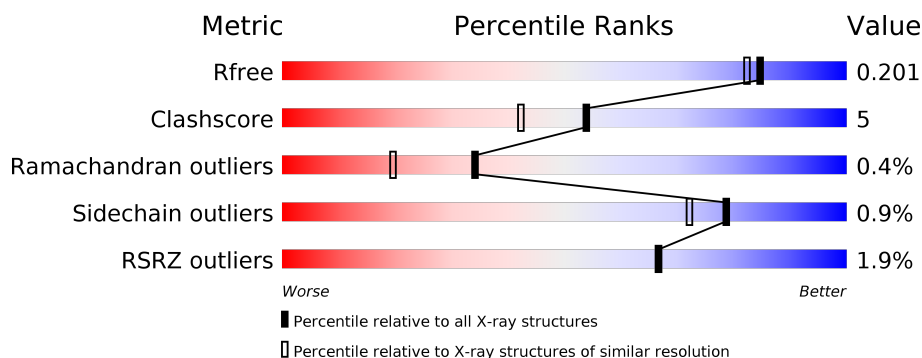
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	638	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	638	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	638	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>9%</div> </div> </div>
1	D	638	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	702	-	-	X	-
3	CL	C	702	-	-	X	-
7	FMT	D	706	-	-	X	-

## 2 Entry composition [i](#)

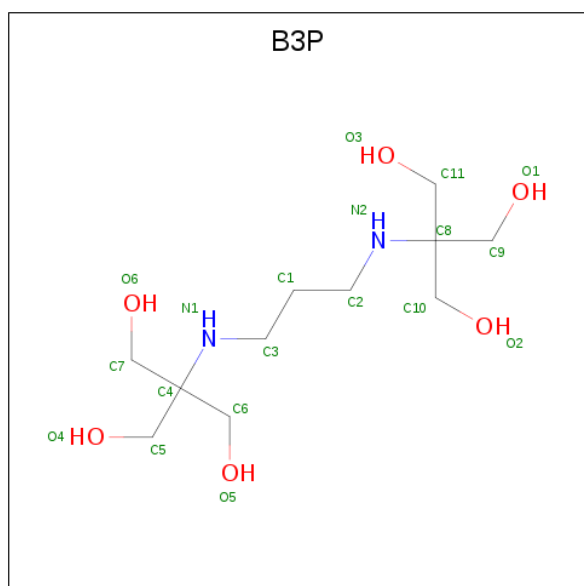
There are 10 unique types of molecules in this entry. The entry contains 19996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	3	0
			4610	2914	794	870	32			
1	B	584	Total	C	N	O	S	0	4	0
			4615	2917	795	871	32			
1	C	582	Total	C	N	O	S	0	3	0
			4596	2907	791	866	32			
1	D	581	Total	C	N	O	S	0	2	0
			4581	2897	789	863	32			

- Molecule 2 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	11	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			19	11	2	6		
2	C	1	Total	C	N	O	0	0
			19	11	2	6		
2	D	1	Total	C	N	O	0	0
			19	11	2	6		

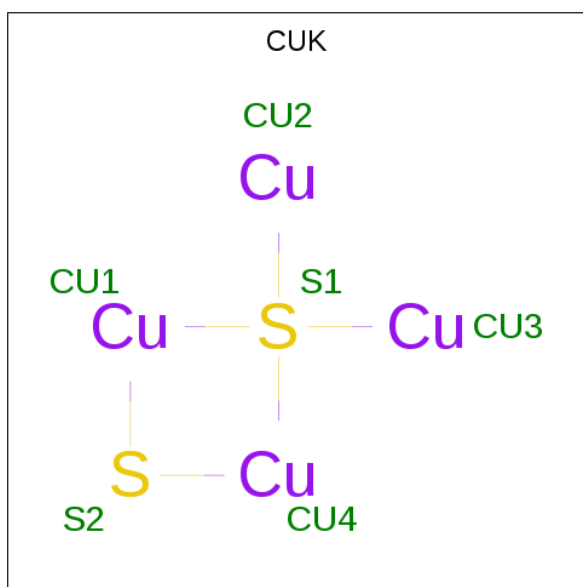
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

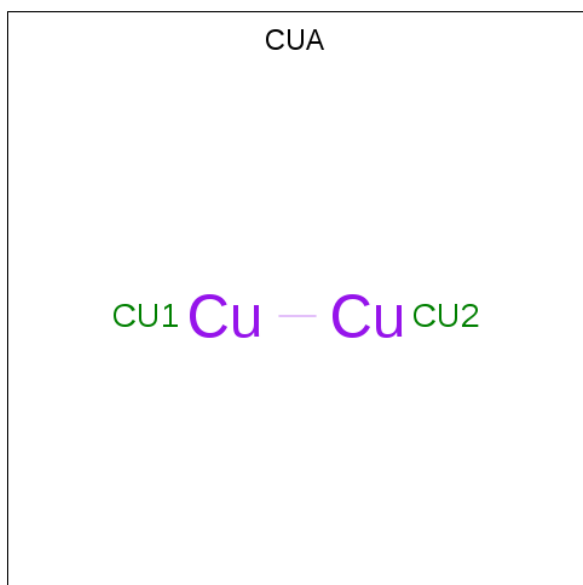
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is [4Cu:2S] cluster (three-letter code: CUK) (formula: Cu<sub>4</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by author).



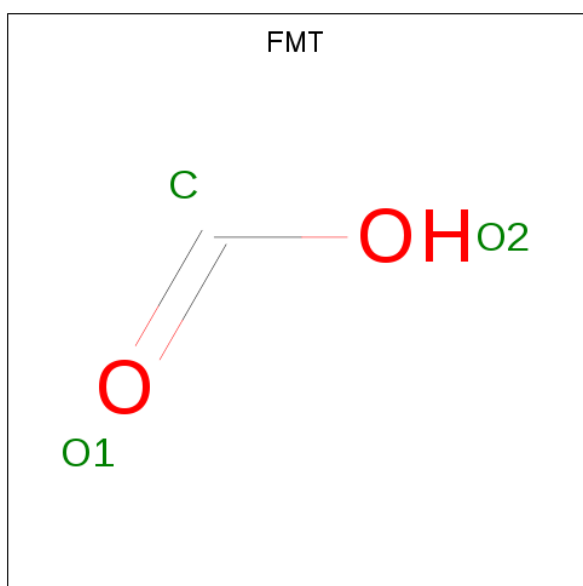
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Cu	S	0	0
			6	4	2		
5	B	1	Total	Cu	S	0	0
			6	4	2		
5	C	1	Total	Cu	S	0	0
			6	4	2		
5	D	1	Total	Cu	S	0	0
			6	4	2		

- Molecule 6 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cu 2 2	0	0
6	B	1	Total Cu 2 2	0	0
6	C	1	Total Cu 2 2	0	0
6	D	1	Total Cu 2 2	0	0

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 3 1 2	0	0
7	B	1	Total C O 3 1 2	0	0
7	C	1	Total C O 3 1 2	0	0
7	C	1	Total C O 3 1 2	0	0
7	D	1	Total C O 3 1 2	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	K 1	0	0
8	D	1	Total 1	K 1	0	0
8	C	1	Total 1	K 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Na 1	0	0
9	A	1	Total 1	Na 1	0	0
9	D	1	Total 1	Na 1	0	0
9	C	1	Total 1	Na 1	0	0

- Molecule 10 is water.

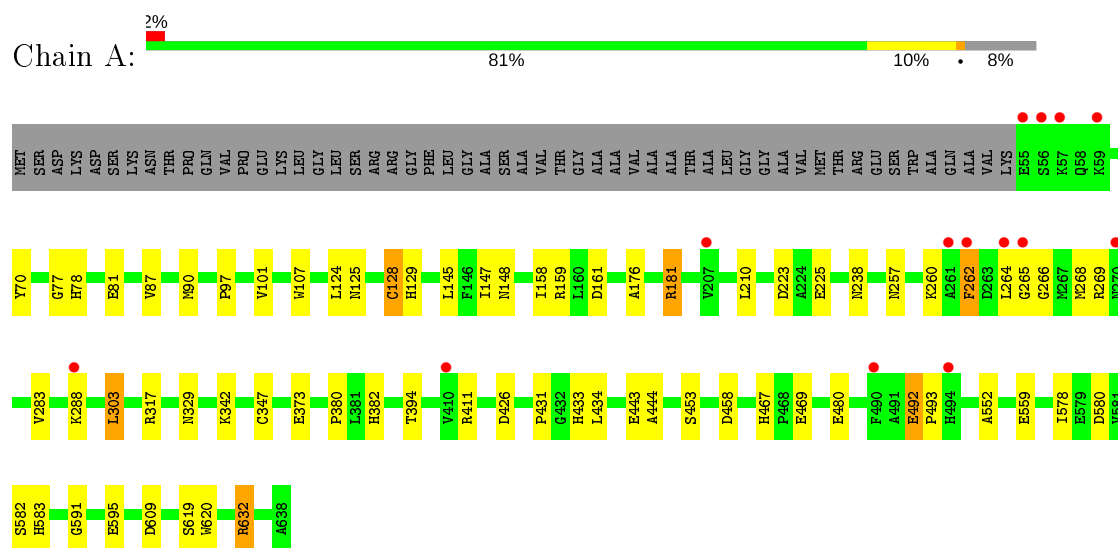
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	413	Total 413	O 413	0	0
10	B	392	Total 392	O 392	0	0
10	C	362	Total 362	O 362	0	0
10	D	288	Total 288	O 288	0	0



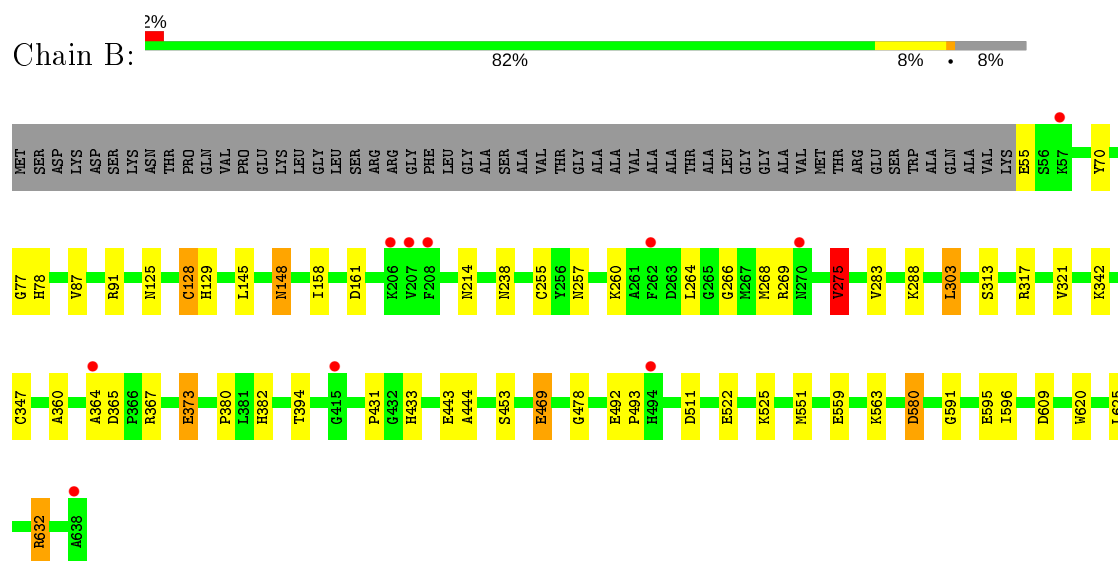
### 3 Residue-property plots [i](#)

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.

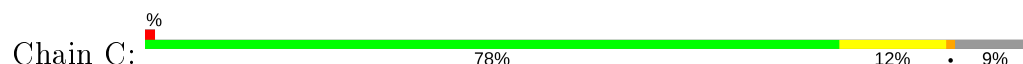
- Molecule 1: Nitrous-oxide reductase



- Molecule 1: Nitrous-oxide reductase



- Molecule 1: Nitrous-oxide reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.92Å 73.37Å 136.34Å 90.00° 95.07° 90.00°	Depositor
Resolution (Å)	48.91 – 1.78 48.91 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-1.78) 100.0 (48.91-1.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.157 , 0.192 0.167 , 0.201	Depositor DCC
$R_{free}$ test set	10244 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.8	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	0.97	EDS
Total number of atoms	19996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1041e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CL, NA, FMT, B3P, CUA, CUK, K, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.06	9/4732 (0.2%)	1.02	18/6406 (0.3%)
1	B	1.07	9/4740 (0.2%)	1.01	21/6417 (0.3%)
1	C	1.06	6/4718 (0.1%)	1.04	25/6387 (0.4%)
1	D	1.02	8/4700 (0.2%)	0.96	13/6364 (0.2%)
All	All	1.06	32/18890 (0.2%)	1.01	77/25574 (0.3%)

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	CYS	CB-SG	-10.44	1.64	1.82
1	A	81	GLU	CD-OE2	-7.59	1.17	1.25
1	D	567	GLU	CD-OE2	7.04	1.33	1.25
1	D	128	CYS	CB-SG	-6.91	1.70	1.82
1	A	595	GLU	CB-CG	6.90	1.65	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	609	ASP	CB-CG-OD2	-14.59	105.17	118.30
1	A	609	ASP	CB-CG-OD2	-12.12	107.40	118.30
1	C	634	MET	CG-SD-CE	-10.41	83.55	100.20
1	A	159	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	C	609	ASP	CB-CG-OD1	9.44	126.80	118.30

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	4610	0	4480	53	0
1	B	4615	0	4486	39	0
1	C	4596	0	4469	56	0
1	D	4581	0	4450	55	0
2	A	19	0	26	0	0
2	B	19	0	26	1	0
2	C	19	0	26	0	0
2	D	19	0	26	0	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	2	0
3	D	1	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	1	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	3	0	1	0	0
7	B	3	0	1	0	0
7	C	6	0	2	0	0
7	D	3	0	1	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	413	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	392	0	0	8	1
10	C	362	0	0	7	1
10	D	288	0	0	7	1
All	All	19996	0	17994	192	3

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 5.

The worst 5 of 192 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:C:271[B]:GLU:OE2	10:C:801:HOH:O	1.70	1.08
1:B:255:CYS:HB2	10:B:987:HOH:O	1.52	1.07
1:C:314:LYS:HD2	10:C:1131:HOH:O	1.58	1.02
1:B:288:LYS:HE2	10:B:1118:HOH:O	1.65	0.95
1:A:578:ILE:HG12	10:A:965:HOH:O	1.71	0.90

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1102:HOH:O	10:C:1136:HOH:O[1_565]	1.29	0.91
10:A:803:HOH:O	10:D:1060:HOH:O[1_565]	1.39	0.81
10:B:801:HOH:O	10:B:1080:HOH:O[2_555]	2.14	0.06

## 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	585/638 (92%)	560 (96%)	23 (4%)	2 (0%)	41 25
1	B	586/638 (92%)	561 (96%)	23 (4%)	2 (0%)	41 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	583/638 (91%)	560 (96%)	20 (3%)	3 (0%)	29	14
1	D	581/638 (91%)	558 (96%)	21 (4%)	2 (0%)	41	25
All	All	2335/2552 (92%)	2239 (96%)	87 (4%)	9 (0%)	34	19

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	623	HIS
1	A	342	LYS
1	B	342	LYS
1	B	365	ASP
1	C	342	LYS

### 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	502/537 (94%)	500 (100%)	2 (0%)	91	88
1	B	503/537 (94%)	498 (99%)	5 (1%)	76	68
1	C	500/537 (93%)	495 (99%)	5 (1%)	76	68
1	D	498/537 (93%)	493 (99%)	5 (1%)	76	68
All	All	2003/2148 (93%)	1986 (99%)	17 (1%)	78	76

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	74	TRP
1	C	78	HIS
1	D	313	SER
1	B	620	TRP
1	D	447	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	ASN
1	C	61	HIS
1	D	129	HIS
1	B	148	ASN
1	C	494	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 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	$\# Z  > 2$
2	B3P	C	701	-	18,18,18	0.87	0	21,23,23	1.77	3 (14%)
2	B3P	D	701	-	18,18,18	0.78	0	21,23,23	1.69	3 (14%)
5	CUK	C	704	1	0,6,6	0.00	-	-		
6	CUA	D	705	1	0,1,1	0.00	-	-		
7	FMT	C	707	-	0,2,2	0.00	-	0,1,1	0.00	-
6	CUA	B	705	1	0,1,1	0.00	-	-		
7	FMT	B	706	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	706	-	0,2,2	0.00	-	0,1,1	0.00	-
5	CUK	A	704	1	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CUK	B	704	1	0,6,6	0.00	-	-		
7	FMT	C	706	-	0,2,2	0.00	-	0,1,1	0.00	-
5	CUK	D	704	1	0,6,6	0.00	-	-		
2	B3P	B	701	-	18,18,18	0.89	0	21,23,23	1.52	3 (14%)
6	CUA	C	705	1	0,1,1	0.00	-	-		
7	FMT	A	706	-	0,2,2	0.00	-	0,1,1	0.00	-
6	CUA	A	705	1	0,1,1	0.00	-	-		
2	B3P	A	701	-	18,18,18	1.16	1 (5%)	21,23,23	1.80	6 (28%)

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
2	B3P	C	701	-	-	2/28/28/28	-
2	B3P	D	701	-	-	3/28/28/28	-
5	CUK	C	704	1	-	-	0/1/1/1
5	CUK	A	704	1	-	-	0/1/1/1
5	CUK	D	704	1	-	-	0/1/1/1
2	B3P	B	701	-	-	1/28/28/28	-
5	CUK	B	704	1	-	-	0/1/1/1
2	B3P	A	701	-	-	2/28/28/28	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	B3P	C5-C4	3.22	1.57	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	B3P	C2-N2-C8	5.15	123.39	116.08
2	C	701	B3P	C2-N2-C8	4.95	123.11	116.08
2	B	701	B3P	C3-N1-C4	4.71	122.77	116.08
2	A	701	B3P	C6-C4-C5	3.68	117.83	110.04
2	A	701	B3P	C3-N1-C4	3.61	121.20	116.08

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

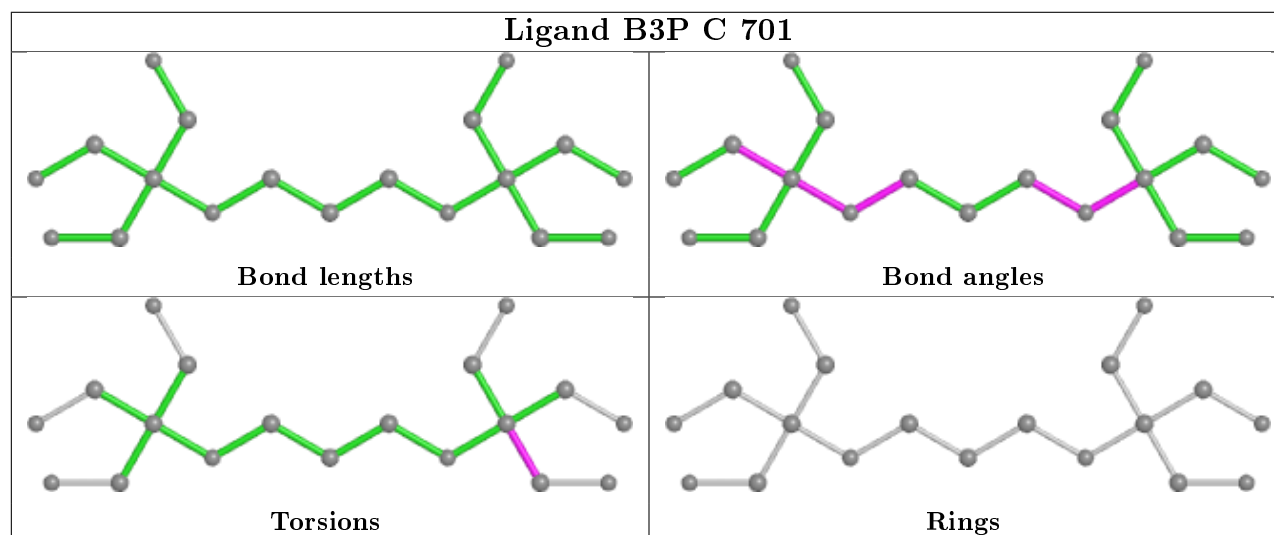
Mol	Chain	Res	Type	Atoms
2	D	701	B3P	O2-C10-C8-C9
2	C	701	B3P	N2-C8-C9-O1
2	A	701	B3P	C7-C4-C6-O5
2	B	701	B3P	C7-C4-C6-O5
2	A	701	B3P	N1-C4-C6-O5

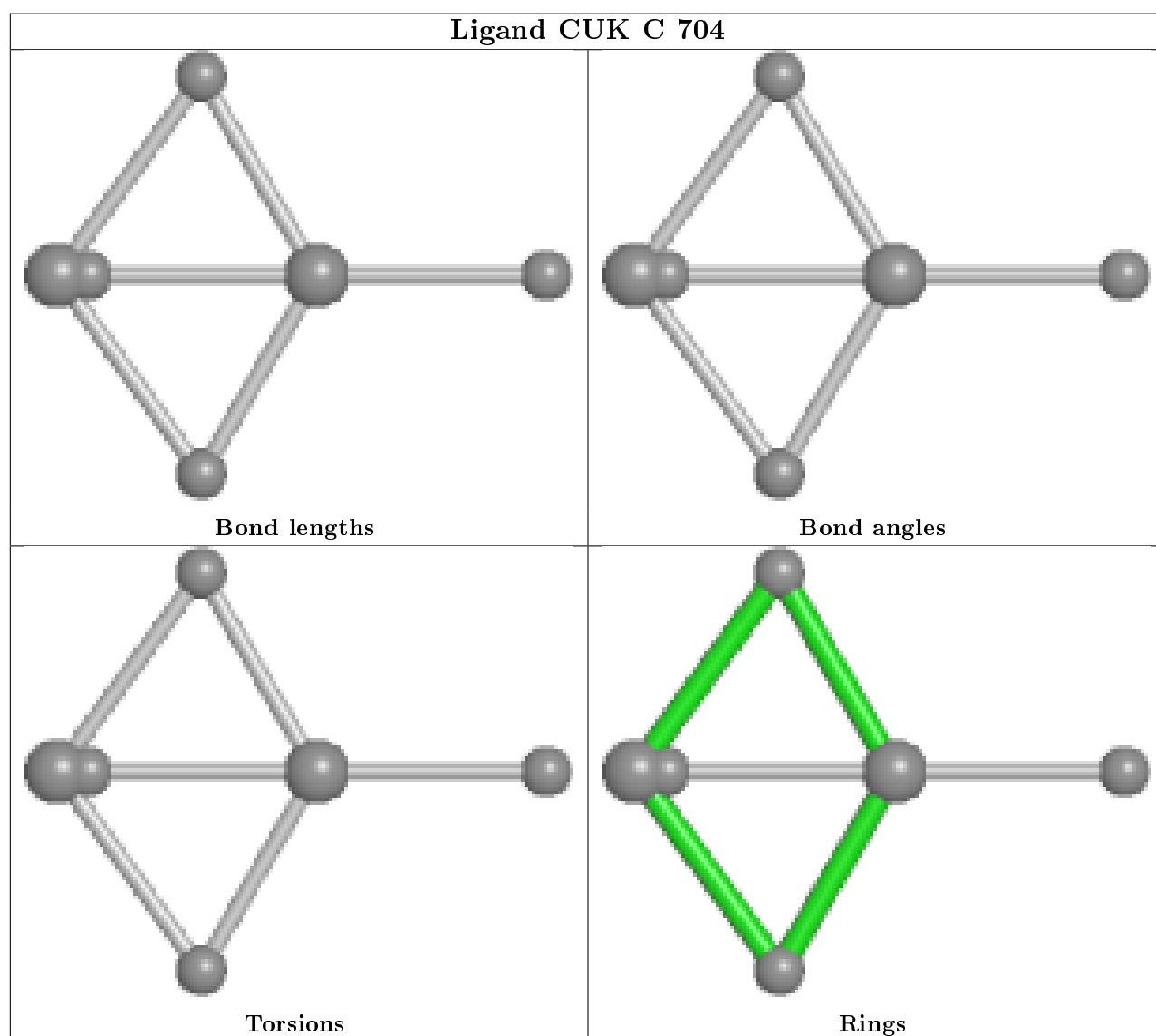
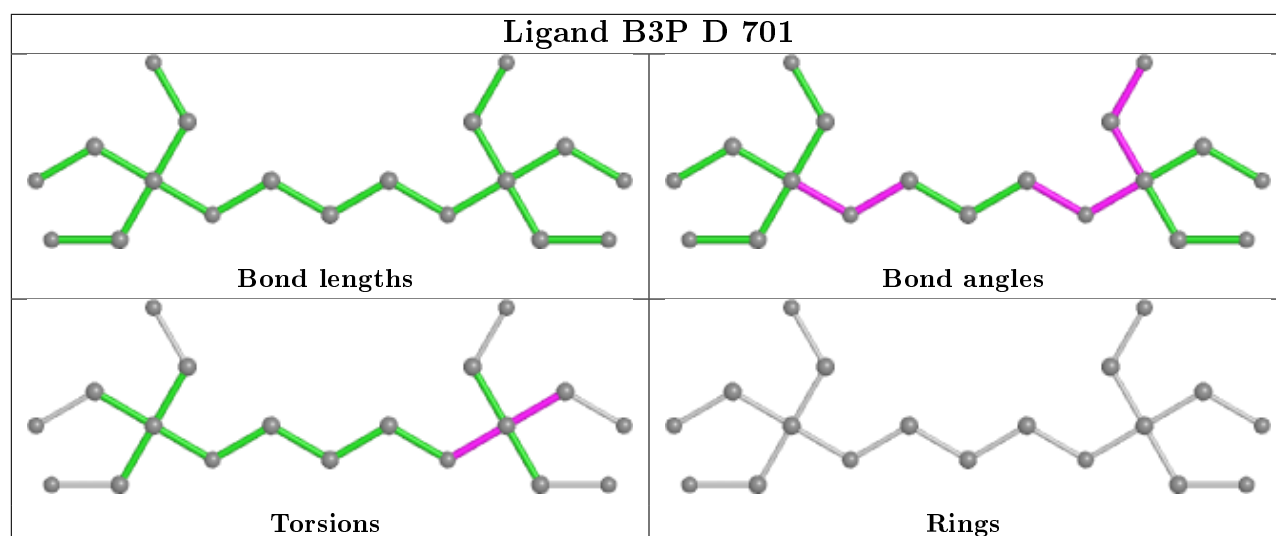
There are no ring outliers.

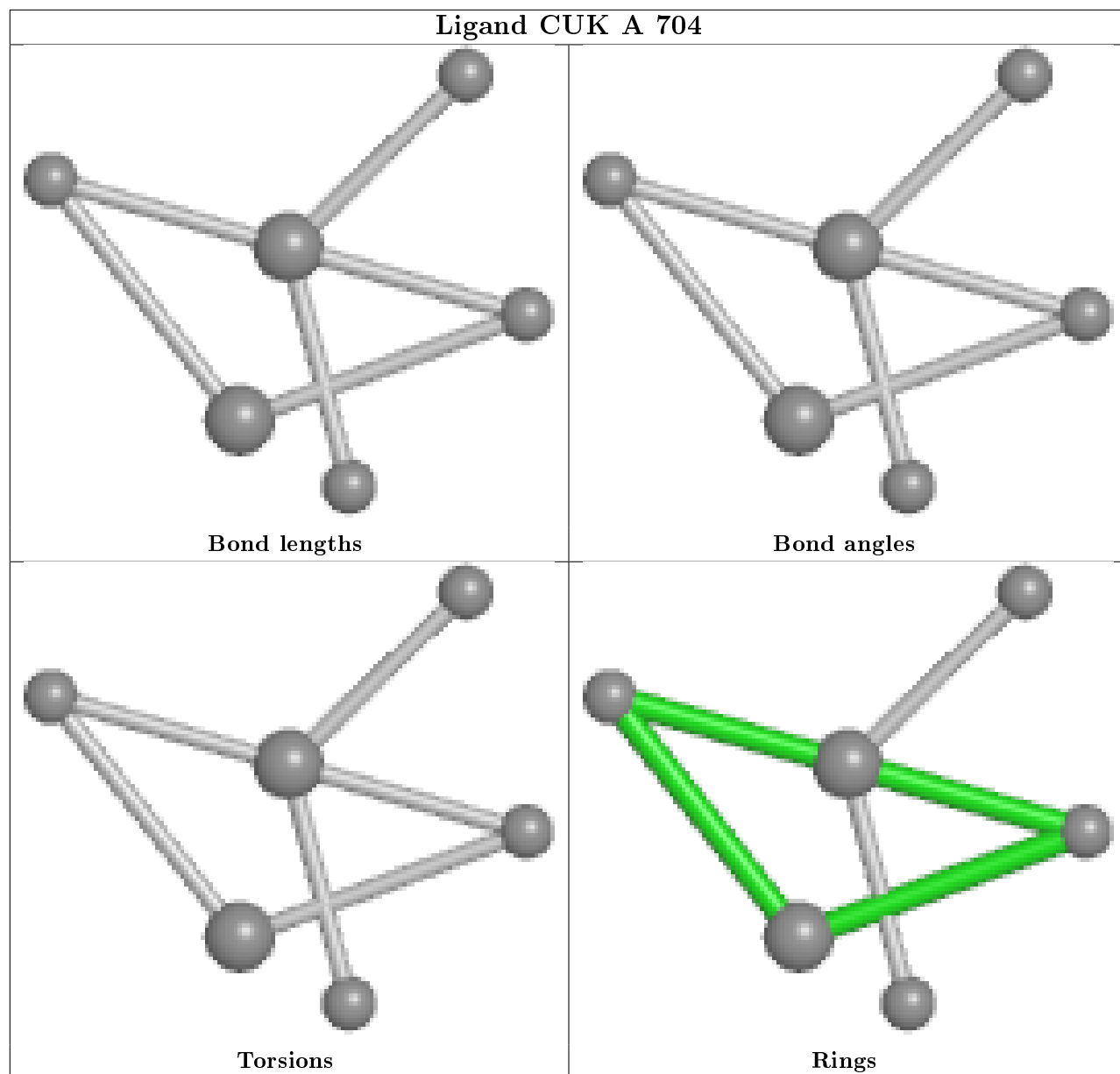
3 monomers are involved in 4 short contacts:

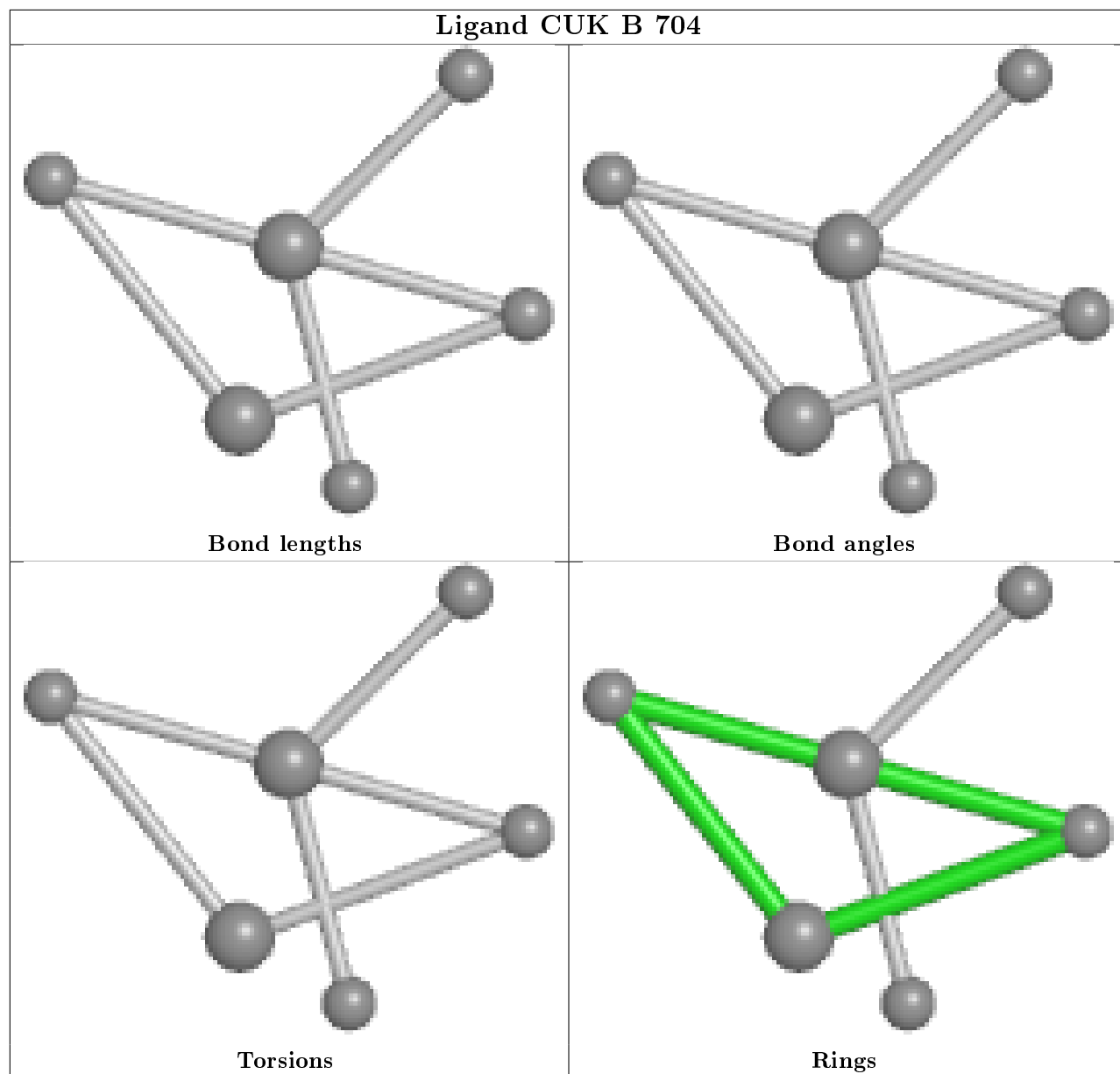
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	706	FMT	2	0
5	A	704	CUK	1	0
2	B	701	B3P	1	0

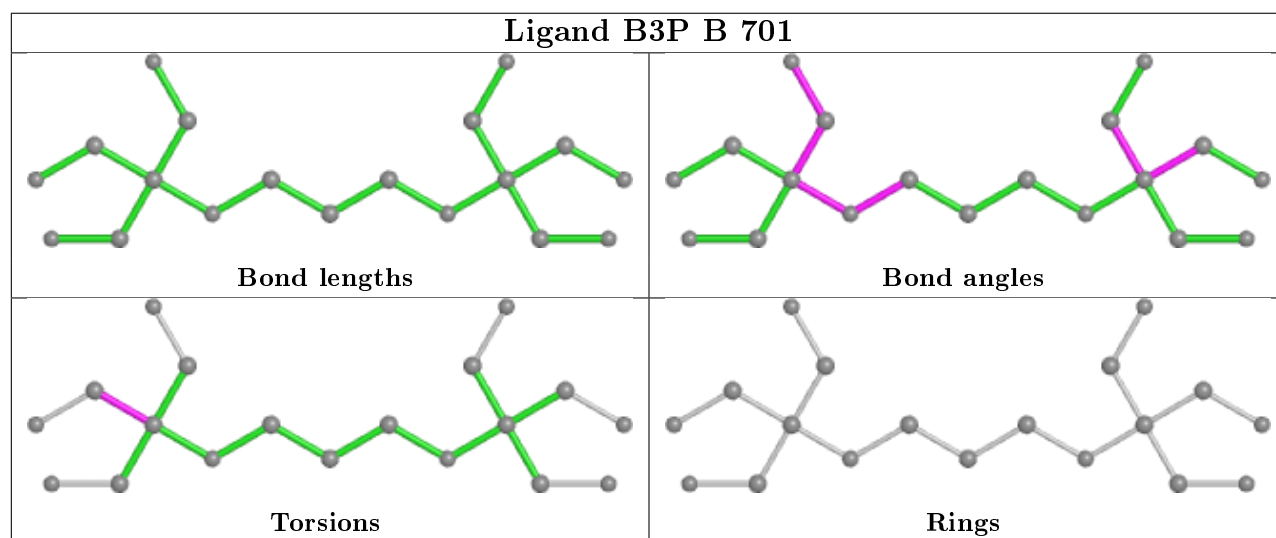
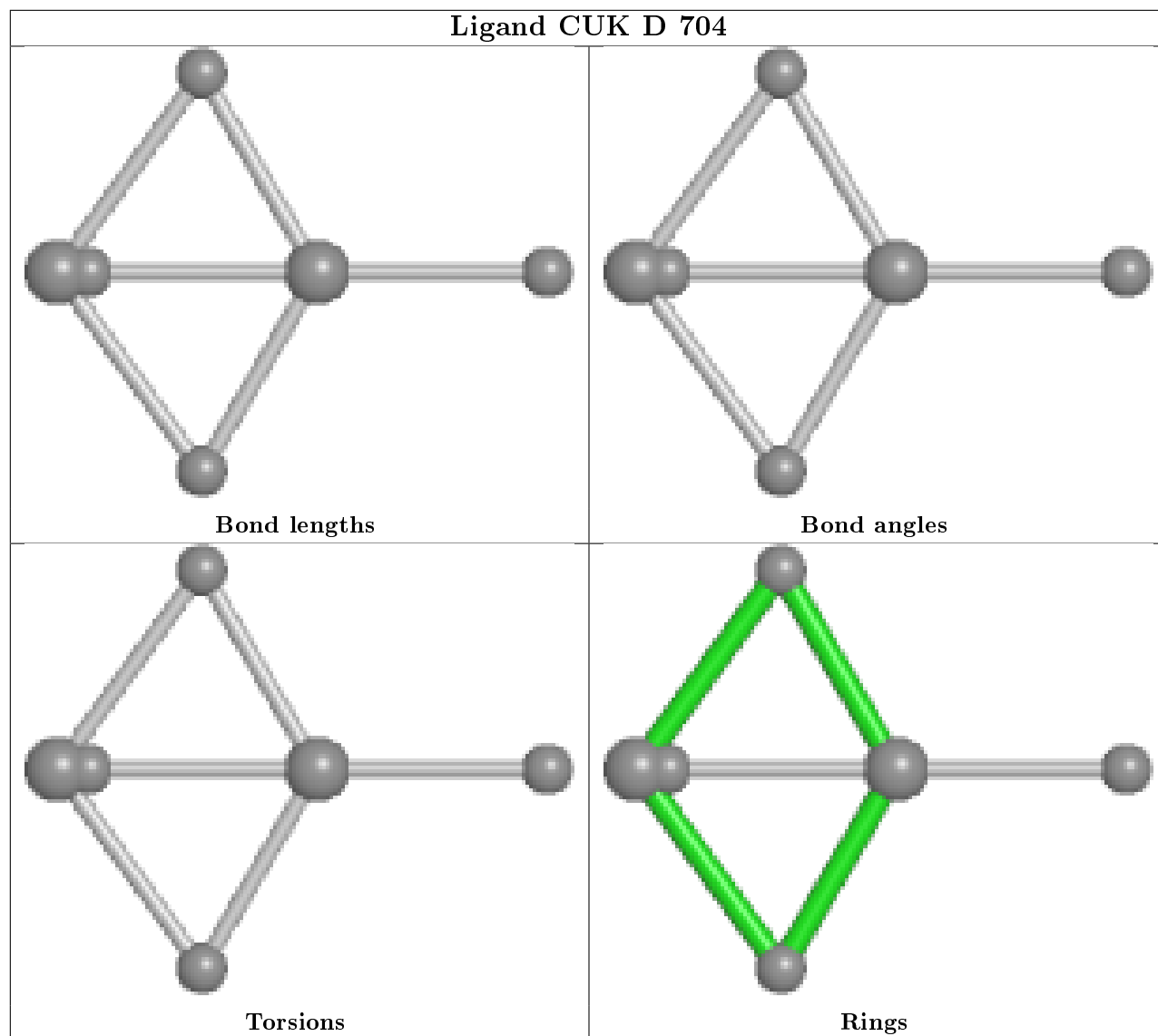
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

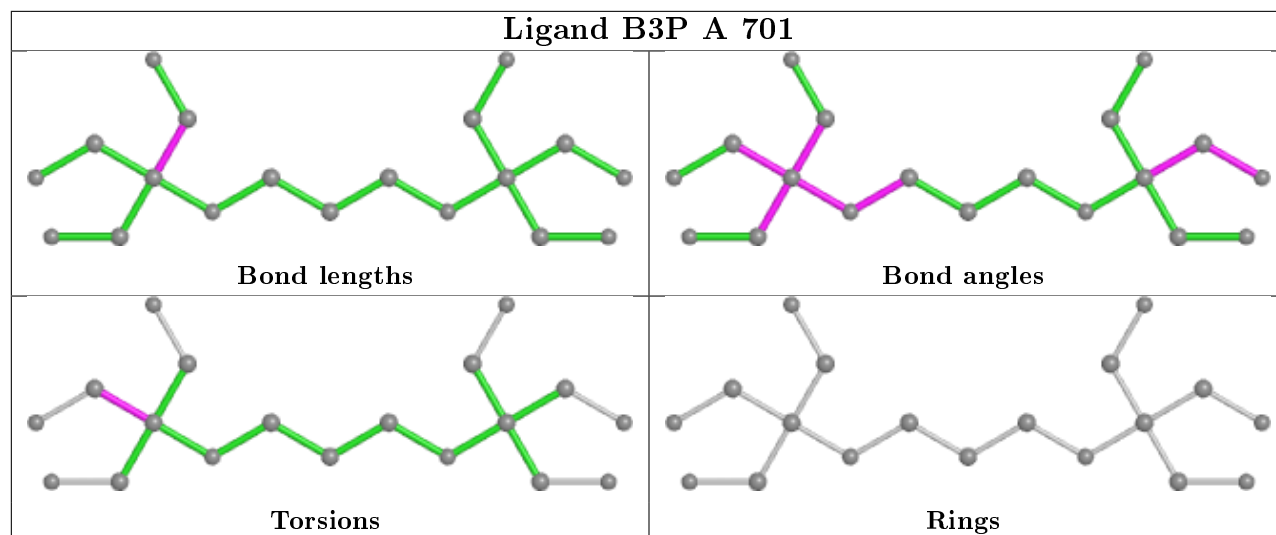












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	584/638 (91%)	-0.10	14 (2%) 59 58	15, 24, 46, 75	0
1	B	584/638 (91%)	-0.13	10 (1%) 70 70	16, 25, 47, 83	0
1	C	582/638 (91%)	-0.11	5 (0%) 84 84	16, 25, 46, 67	0
1	D	581/638 (91%)	0.04	15 (2%) 56 55	18, 28, 54, 81	0
All	All	2331/2552 (91%)	-0.08	44 (1%) 66 67	15, 26, 49, 83	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	PHE	7.0
1	B	262	PHE	5.9
1	B	364	ALA	5.3
1	D	262	PHE	3.5
1	D	292	PHE	3.4

### 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.

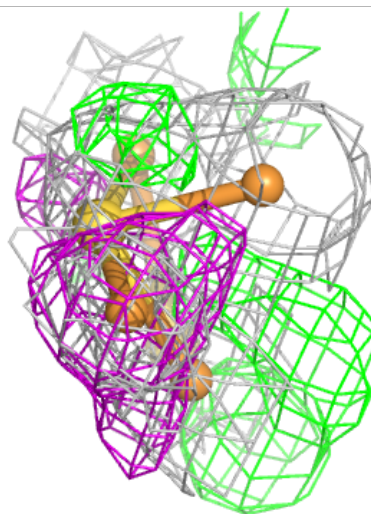
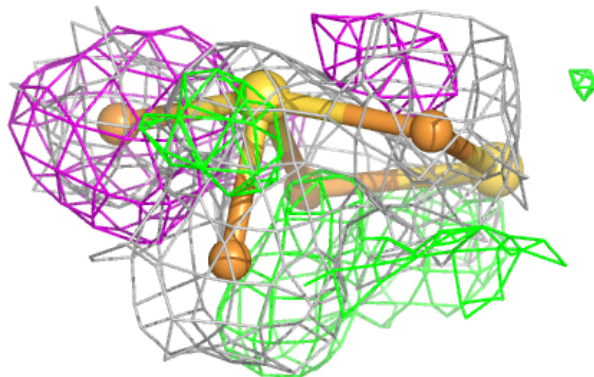
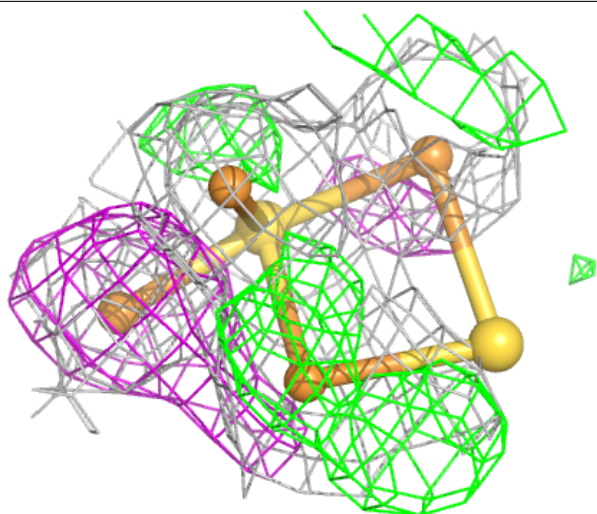


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CUK	A	704	6/6	0.89	0.16	26,39,46,50	6
5	CUK	B	704	6/6	0.89	0.15	28,43,46,48	6
7	FMT	C	707	3/3	0.91	0.23	35,35,39,41	0
9	NA	D	708	1/1	0.92	0.09	34,34,34,34	1
5	CUK	D	704	6/6	0.93	0.11	25,32,35,36	6
2	B3P	C	701	19/19	0.94	0.09	22,23,30,42	0
9	NA	C	709	1/1	0.94	0.09	30,30,30,30	0
2	B3P	D	701	19/19	0.95	0.09	22,24,29,30	0
5	CUK	C	704	6/6	0.95	0.09	23,29,31,38	6
7	FMT	B	706	3/3	0.95	0.21	22,22,28,37	0
2	B3P	A	701	19/19	0.95	0.09	21,24,31,45	0
2	B3P	B	701	19/19	0.95	0.08	21,23,29,32	0
9	NA	B	708	1/1	0.96	0.05	26,26,26,26	0
7	FMT	D	706	3/3	0.96	0.15	26,26,28,42	0
8	K	B	707	1/1	0.96	0.07	35,35,35,35	1
7	FMT	A	706	3/3	0.97	0.18	26,26,27,39	0
8	K	C	708	1/1	0.97	0.07	30,30,30,30	1
3	CL	B	702	1/1	0.98	0.08	28,28,28,28	1
4	CA	B	703	1/1	0.98	0.06	27,27,27,27	1
6	CUA	D	705	2/2	0.98	0.06	28,28,28,34	0
7	FMT	C	706	3/3	0.98	0.11	30,30,31,36	0
9	NA	A	708	1/1	0.99	0.04	27,27,27,27	0
8	K	D	707	1/1	0.99	0.04	30,30,30,30	1
8	K	A	707	1/1	0.99	0.06	34,34,34,34	1
4	CA	C	703	1/1	0.99	0.04	22,22,22,22	0
4	CA	A	703	1/1	0.99	0.05	27,27,27,27	1
3	CL	A	702	1/1	0.99	0.09	22,22,22,22	1
3	CL	D	702	1/1	0.99	0.07	26,26,26,26	1
6	CUA	C	705	2/2	0.99	0.06	26,26,26,33	0
6	CUA	B	705	2/2	0.99	0.04	24,24,24,29	0
6	CUA	A	705	2/2	0.99	0.05	25,25,25,29	0
4	CA	D	703	1/1	1.00	0.03	26,26,26,26	0
3	CL	C	702	1/1	1.00	0.08	26,26,26,26	1

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.

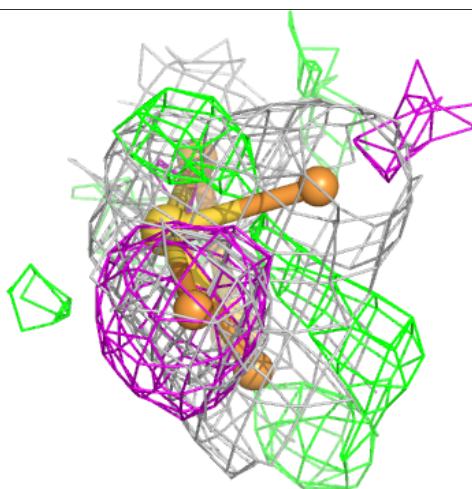
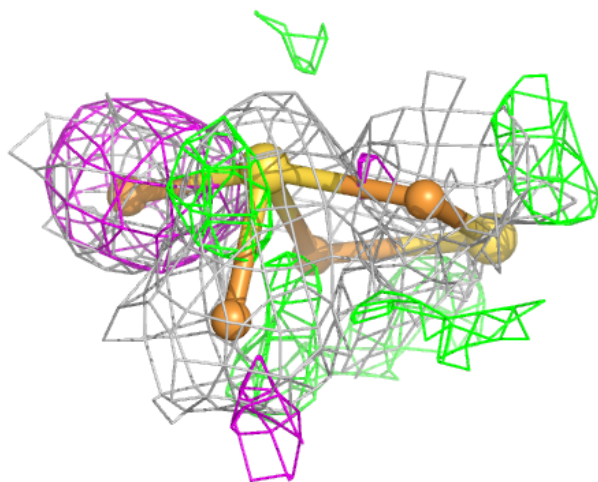
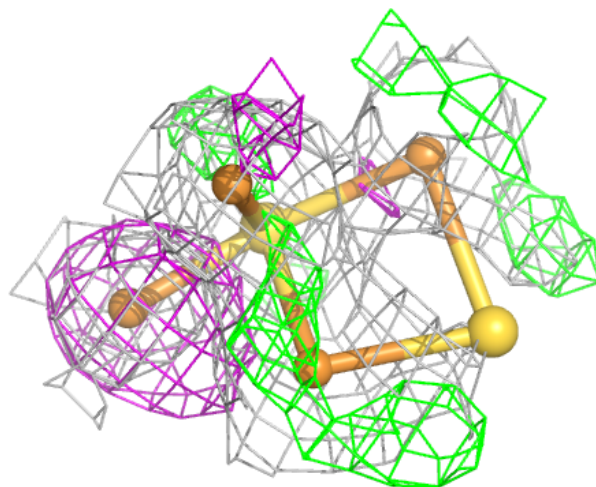
**Electron density around CUK A 704:**

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



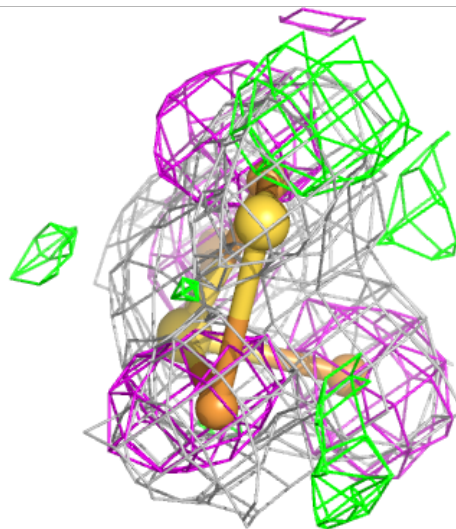
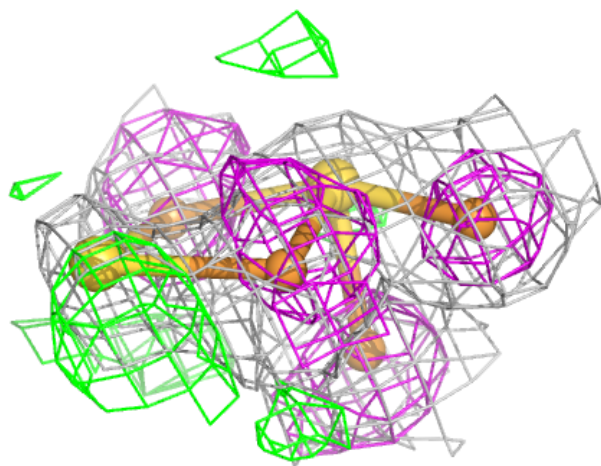
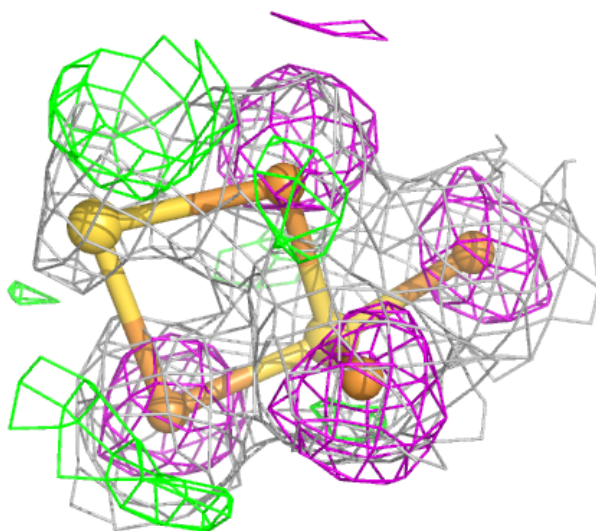
**Electron density around CUK B 704:**

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



**Electron density around CUK D 704:**

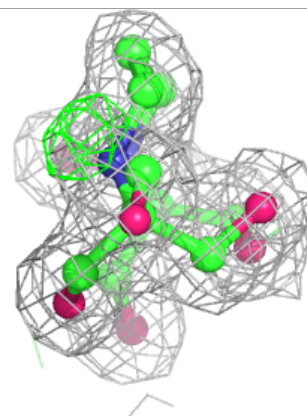
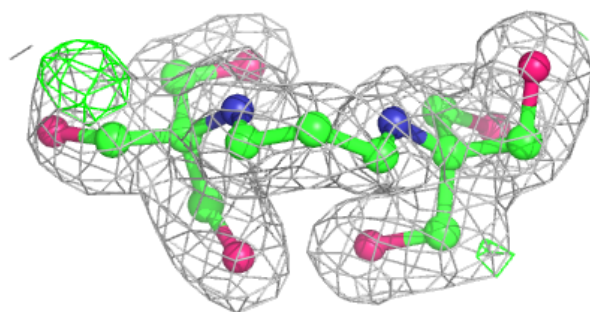
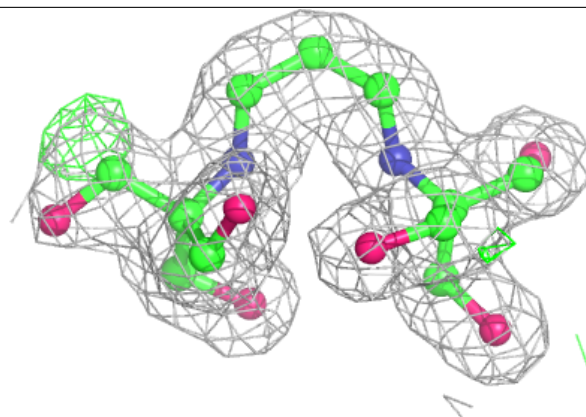
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



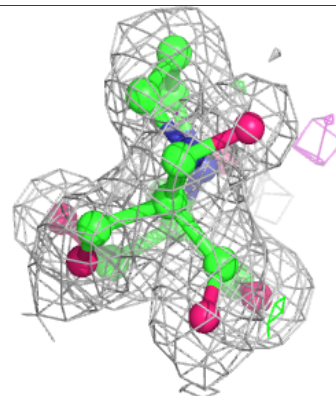
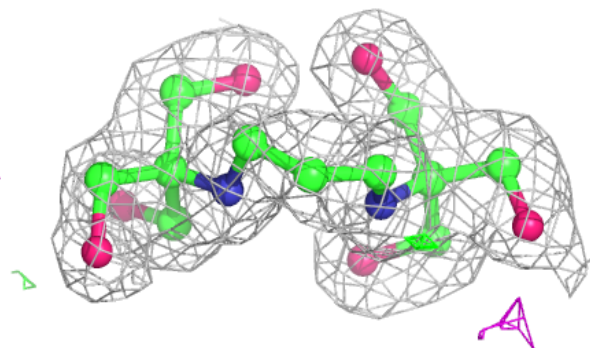
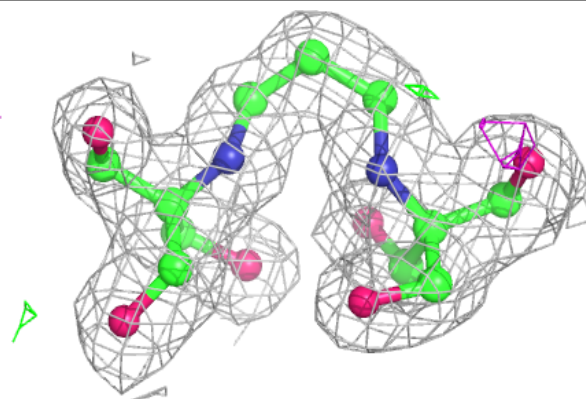


**Electron density around B3P C 701:**

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

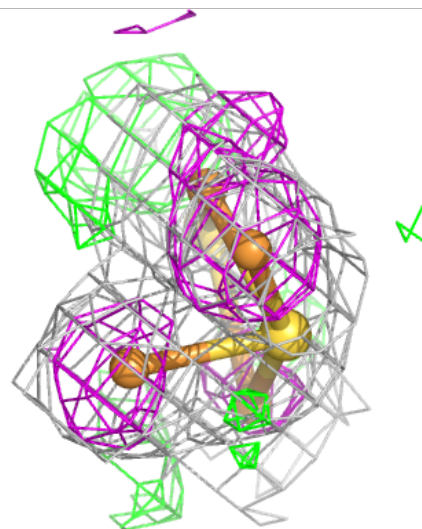
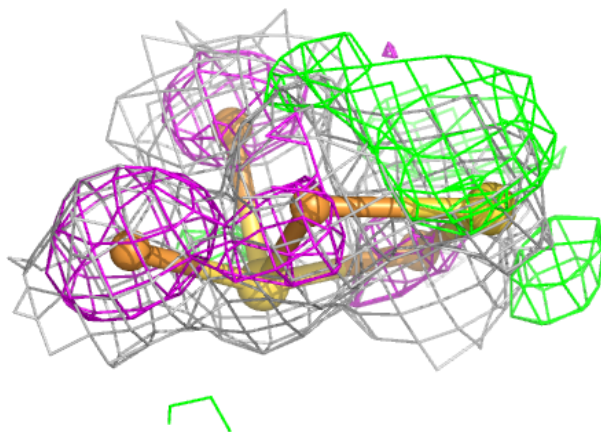
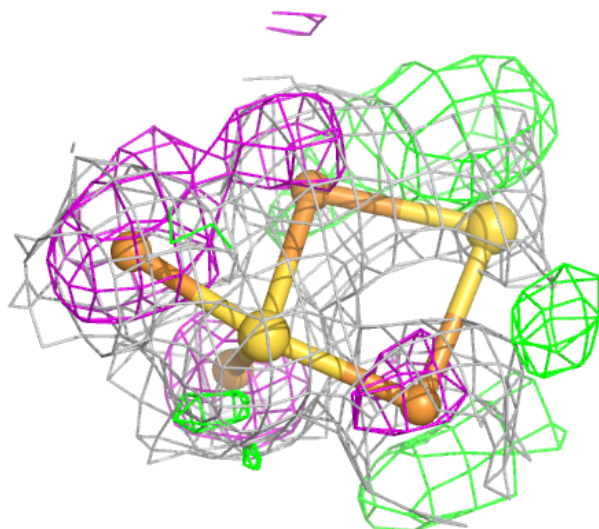
**Electron density around B3P D 701:**

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



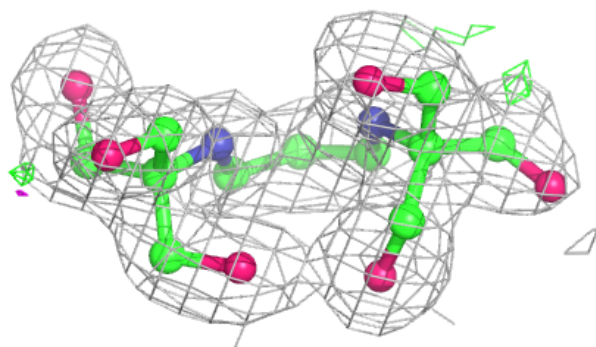
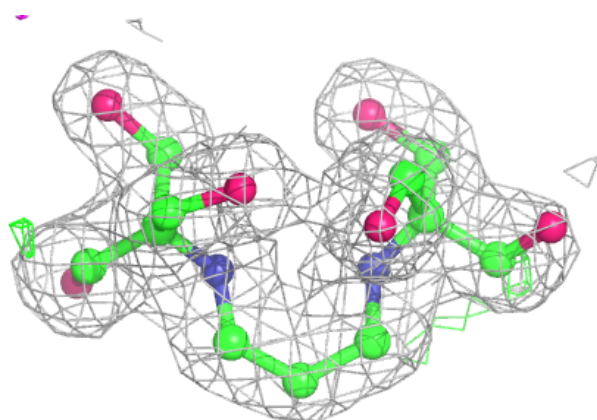
**Electron density around CUK C 704:**

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

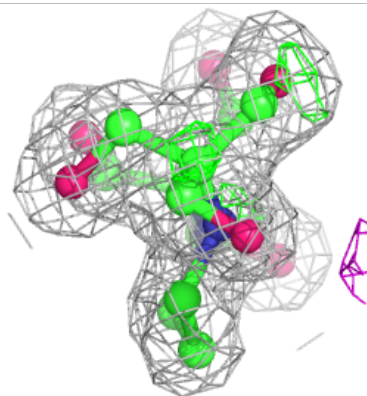
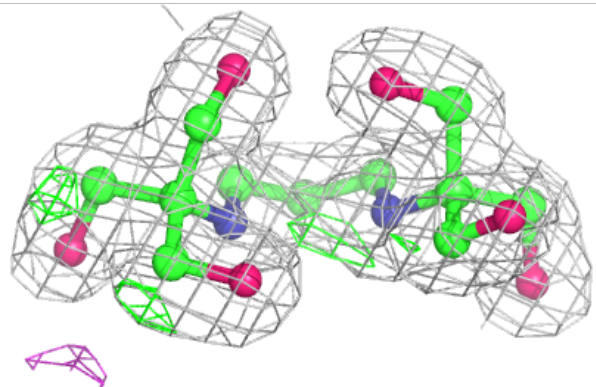
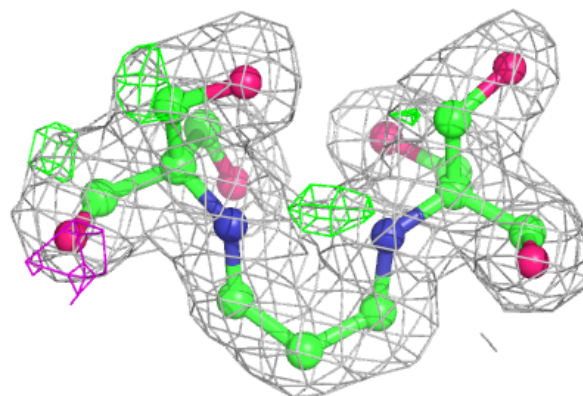


**Electron density around B3P A 701:**

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

**Electron density around B3P B 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.