Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 02:42 pm GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

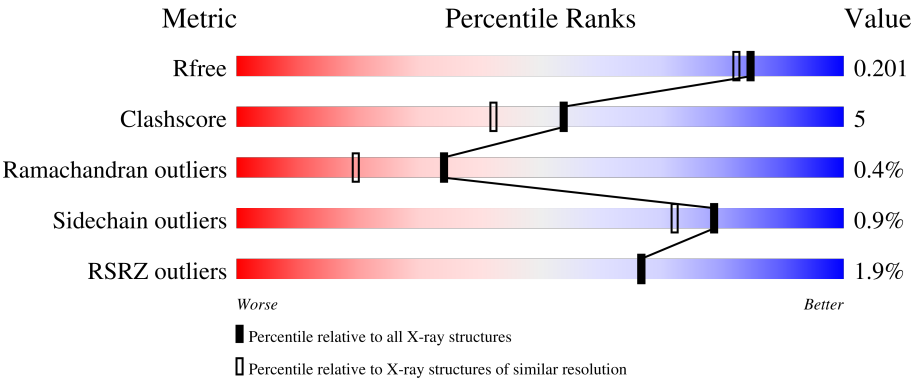
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 81% 10% • 8%
1	B	638	2% 82% 8% • 8%
1	C	638	% 78% 12% • 9%
1	D	638	2% 80% 10% • 9%

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 criteria:

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)

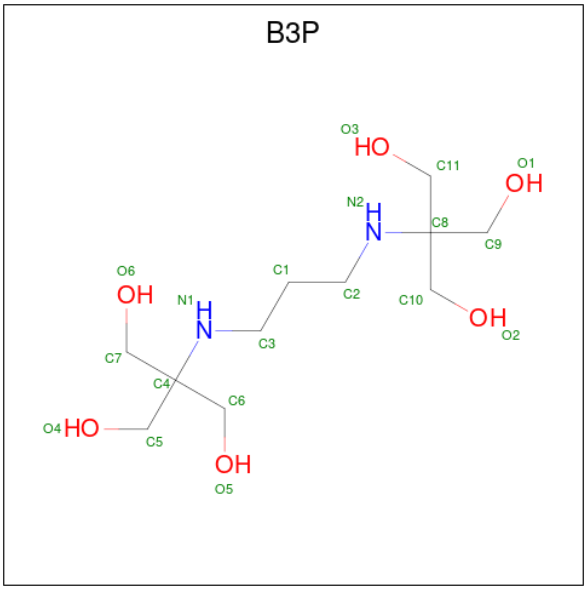
There are 10 unique types of molecules in this entry. The entry contains 19996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 19 11 2 6	0	0
2	C	1	Total C N O 19 11 2 6	0	0
2	D	1	Total C N O 19 11 2 6	0	0

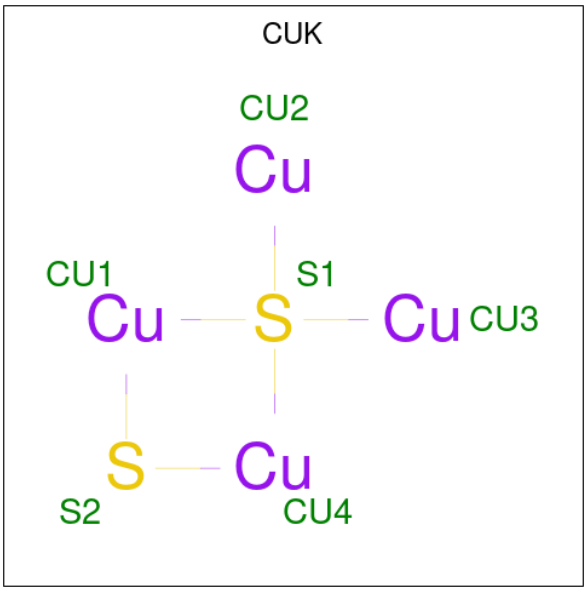
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

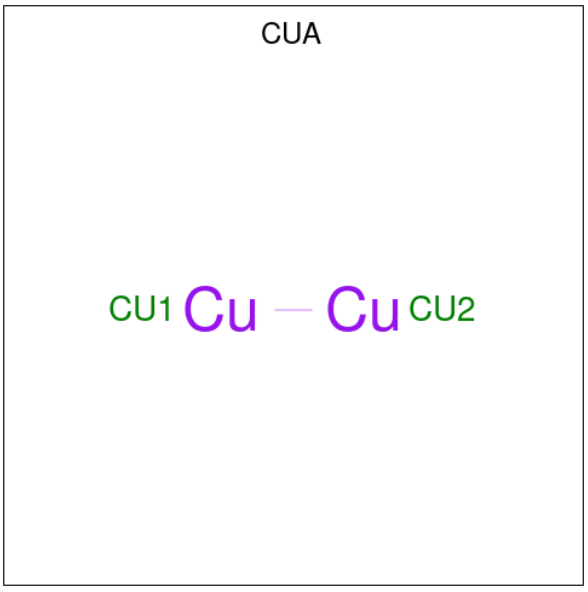
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is [4Cu:2S] cluster (three-letter code: CUK) (formula: Cu_4S_2) (labeled as "Ligand of Interest" by depositor).



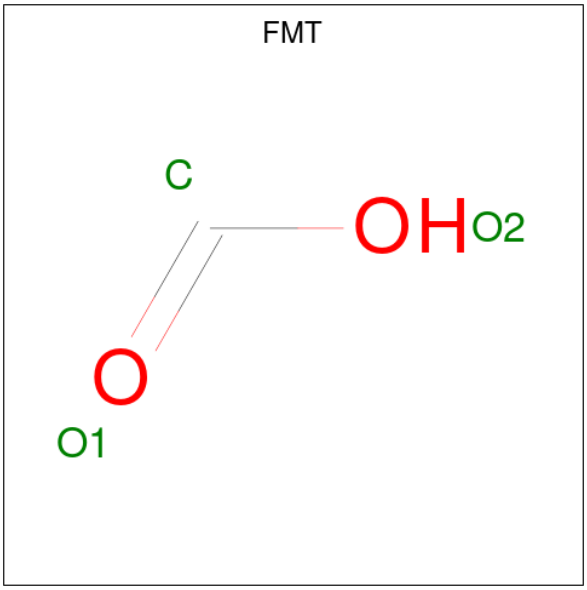
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cu S 6 4 2	0	0
5	B	1	Total Cu S 6 4 2	0	0
5	C	1	Total Cu S 6 4 2	0	0
5	D	1	Total Cu S 6 4 2	0	0

- Molecule 6 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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_2O_2).



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	A	1	Total K 1 1	0	0

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

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

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

- Molecule 10 is water.

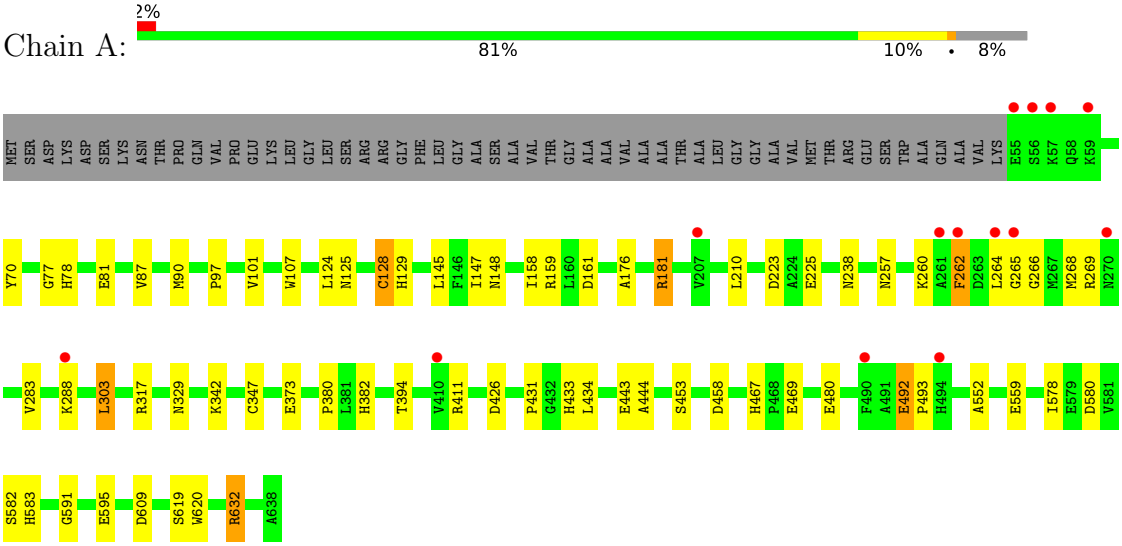
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	413	Total O 413 413	0	0
10	B	392	Total O 392 392	0	0
10	C	362	Total O 362 362	0	0
10	D	288	Total O 288 288	0	0

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.

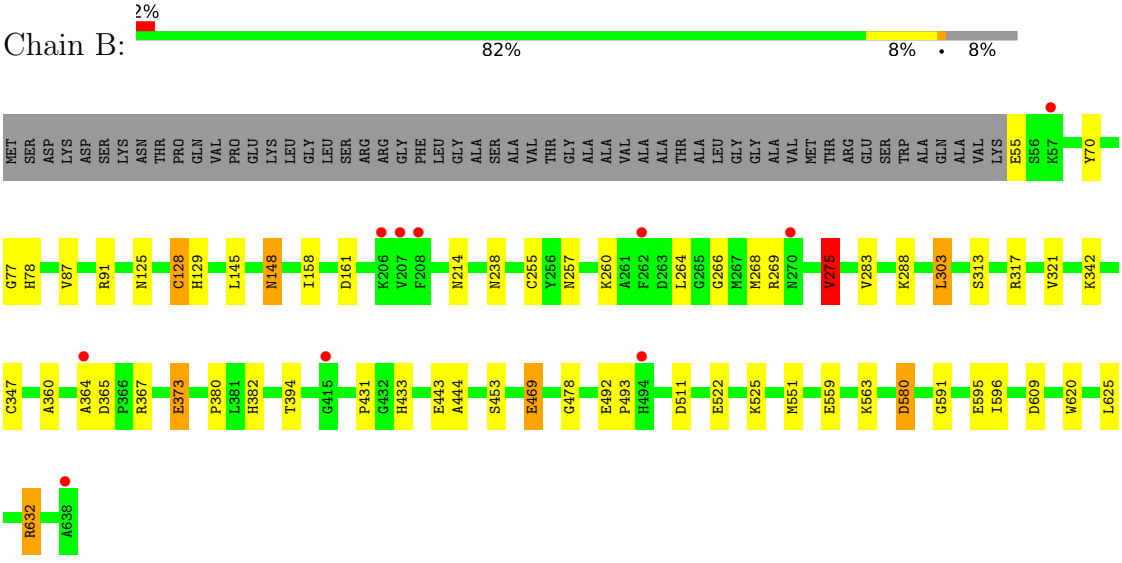
• Molecule 1: Nitrous-oxide reductase

Chain A:



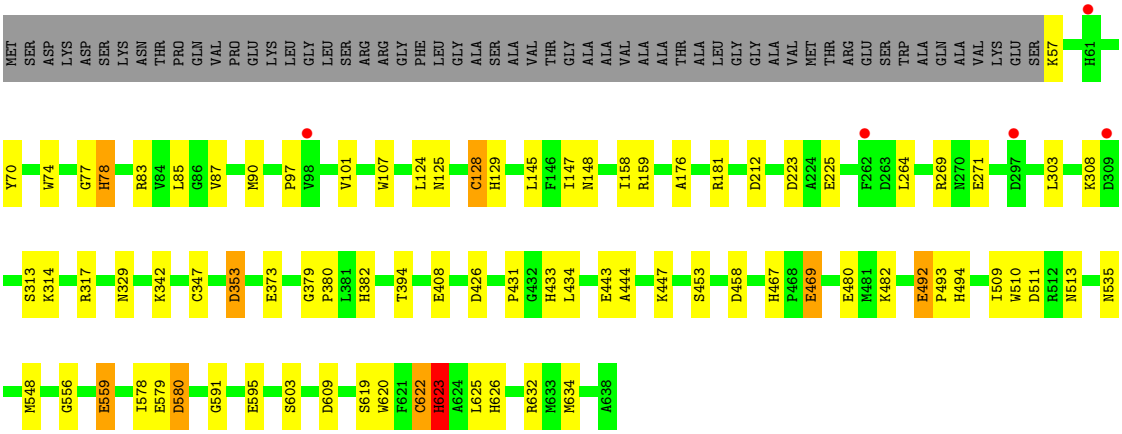
• Molecule 1: Nitrous-oxide reductase

Chain B:

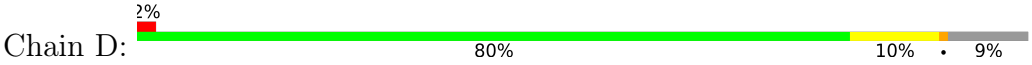


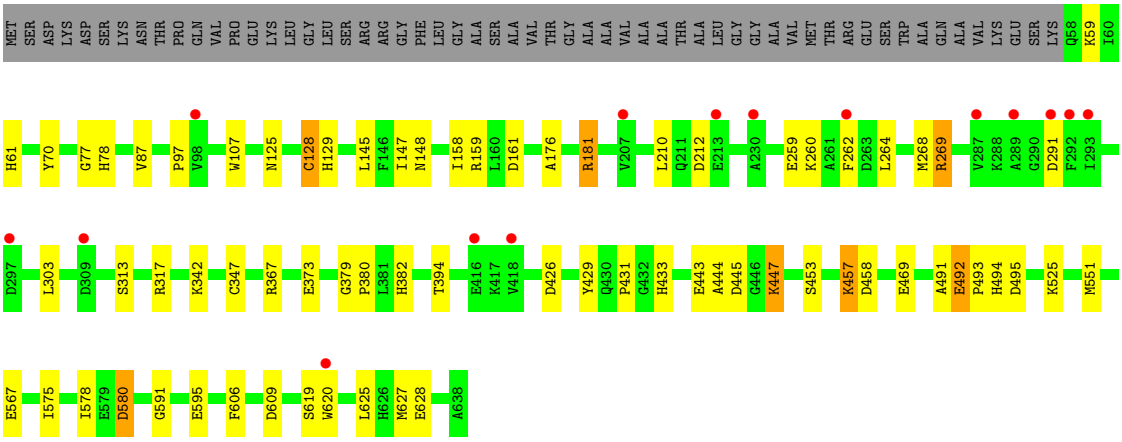
• Molecule 1: Nitrous-oxide reductase

Chain C:



• Molecule 1: Nitrous-oxide reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	23.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, FMT, NA, CL, CUK, CUA, B3P, K

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%)

All (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
1	B	373	GLU	CD-OE2	6.68	1.32	1.25
1	B	511	ASP	CB-CG	6.62	1.65	1.51
1	C	128	CYS	CB-SG	-6.54	1.71	1.82
1	A	128	CYS	CB-SG	-6.53	1.71	1.82
1	C	492	GLU	CD-OE1	6.46	1.32	1.25
1	B	469[A]	GLU	CD-OE2	-6.43	1.18	1.25
1	B	469[B]	GLU	CD-OE2	-6.43	1.18	1.25
1	D	367	ARG	CZ-NH1	6.23	1.41	1.33
1	D	595	GLU	CB-CG	6.18	1.63	1.52
1	C	603	SER	CB-OG	-6.07	1.34	1.42
1	D	181	ARG	CZ-NH2	5.91	1.40	1.33
1	C	559	GLU	CB-CG	-5.90	1.41	1.52
1	C	225	GLU	CD-OE1	5.88	1.32	1.25
1	D	628	GLU	CG-CD	5.68	1.60	1.51
1	B	469[A]	GLU	CG-CD	5.65	1.60	1.51
1	B	469[B]	GLU	CG-CD	5.65	1.60	1.51
1	D	595	GLU	CD-OE1	5.59	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	595	GLU	CB-CG	5.35	1.62	1.52
1	D	580	ASP	CB-CG	5.33	1.62	1.51
1	A	181	ARG	CZ-NH2	5.29	1.40	1.33
1	A	580	ASP	CB-CG	5.21	1.62	1.51
1	A	582	SER	CB-OG	5.14	1.49	1.42
1	C	492	GLU	CB-CG	-5.12	1.42	1.52
1	A	225	GLU	CG-CD	5.07	1.59	1.51
1	A	128	CYS	C-O	5.07	1.32	1.23
1	B	595	GLU	CD-OE2	5.07	1.31	1.25
1	A	492	GLU	CD-OE1	5.00	1.31	1.25

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	C	622	CYS	N-CA-C	-9.12	86.39	111.00
1	A	458	ASP	CB-CG-OD1	8.99	126.39	118.30
1	C	580	ASP	CB-CG-OD1	-8.94	110.26	118.30
1	A	609	ASP	CB-CG-OD1	8.58	126.02	118.30
1	A	161	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	B	563	LYS	CD-CE-NZ	8.38	130.97	111.70
1	C	492	GLU	OE1-CD-OE2	8.17	133.11	123.30
1	B	317	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	B	632	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	609	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	317	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	C	595	GLU	OE1-CD-OE2	-7.56	114.22	123.30
1	B	275	VAL	CG1-CB-CG2	7.54	122.97	110.90
1	C	458	ASP	CB-CG-OD1	7.32	124.89	118.30
1	D	493	PRO	C-N-CA	-7.19	103.72	121.70
1	D	595	GLU	OE1-CD-OE2	-7.19	114.67	123.30
1	B	469[A]	GLU	OE1-CD-OE2	-7.18	114.69	123.30
1	B	469[B]	GLU	OE1-CD-OE2	-7.18	114.69	123.30
1	B	493	PRO	C-N-CA	-7.09	103.96	121.70
1	A	632	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	623	HIS	N-CA-C	6.77	129.28	111.00
1	B	551	MET	CG-SD-CE	-6.65	89.57	100.20
1	B	303	LEU	CA-CB-CG	-6.63	100.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	353	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	C	317	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	128	CYS	CB-CA-C	-6.46	97.49	110.40
1	D	491	ALA	CB-CA-C	-6.44	100.44	110.10
1	A	303	LEU	CA-CB-CG	-6.38	100.64	115.30
1	D	426	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	580	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	D	161	ASP	CB-CG-OD1	6.30	123.97	118.30
1	D	458	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	580	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	C	493	PRO	C-N-CA	-6.21	106.17	121.70
1	A	493	PRO	C-N-CA	-6.20	106.19	121.70
1	B	632	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	426	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	493	PRO	O-C-N	-6.01	113.08	122.70
1	A	632	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	609	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	159	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	317	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	580	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	595	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	C	83	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	85	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	212	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	426	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	303	LEU	CB-CG-CD2	5.41	120.20	111.00
1	D	492	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	B	275	VAL	CA-CB-CG1	5.33	118.89	110.90
1	B	364	ALA	N-CA-C	-5.32	96.64	111.00
1	A	223	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	225	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	C	223	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	90	MET	CG-SD-CE	-5.28	91.76	100.20
1	D	495	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	469[A]	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	C	469[B]	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	B	161	ASP	CB-CG-OD1	5.24	123.01	118.30
1	B	493	PRO	O-C-N	-5.20	114.39	122.70
1	C	493	PRO	O-C-N	-5.19	114.40	122.70
1	D	212	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	91	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	408	GLU	OE1-CD-OE2	-5.14	117.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	269	ARG	CB-CA-C	-5.13	100.14	110.40
1	B	367	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	262	PHE	CB-CA-C	5.08	120.57	110.40
1	A	426	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	548	MET	CG-SD-CE	5.07	108.31	100.20
1	D	159	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	85	LEU	CB-CG-CD1	5.01	119.52	111.00

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:B:288:LYS:CE	10:B:1118:HOH:O	2.19	0.88
1:C:57:LYS:HG2	10:C:867:HOH:O	1.77	0.84
1:B:238[A]:ASN:OD1	1:B:257:ASN:HB3	1.80	0.82
1:A:238[B]:ASN:OD1	1:A:257:ASN:HB3	1.83	0.79
1:B:382[B]:HIS:CE1	1:B:433:HIS:HD1	2.00	0.78
1:A:469[A]:GLU:HG3	1:A:492:GLU:HA	1.66	0.78
1:B:382[A]:HIS:CE1	1:B:433:HIS:CE1	2.75	0.75
1:C:382[B]:HIS:CE1	1:C:433:HIS:CE1	2.74	0.74
1:D:382[A]:HIS:CE1	1:D:433:HIS:HD1	2.05	0.73
1:D:606:PHE:HA	7:D:706:FMT:H	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469[B]:GLU:HG3	1:B:492:GLU:HA	1.70	0.73
1:A:382[A]:HIS:CE1	1:A:433:HIS:CE1	2.77	0.73
1:B:360:ALA:O	10:B:801:HOH:O	2.06	0.72
1:C:129:HIS:H	1:C:148:ASN:HD21	1.37	0.72
1:C:509:ILE:O	1:C:509:ILE:HD12	1.91	0.71
1:A:619:SER:O	1:D:78:HIS:CE1	2.44	0.71
1:C:469[A]:GLU:HG3	1:C:492:GLU:HA	1.71	0.71
1:B:283:VAL:HG13	1:B:303:LEU:HD13	1.73	0.70
1:C:579:GLU:O	10:C:802:HOH:O	2.09	0.70
1:A:382[B]:HIS:CE1	3:A:702:CL:CL	2.81	0.70
1:A:480:GLU:CD	10:A:816:HOH:O	2.29	0.70
1:D:129:HIS:H	1:D:148:ASN:HD21	1.41	0.69
1:A:283:VAL:HG13	1:A:303:LEU:HD13	1.74	0.69
1:A:264:LEU:HD23	1:A:268:MET:HE2	1.73	0.69
1:A:129:HIS:H	1:A:148:ASN:HD21	1.40	0.68
1:D:469[A]:GLU:HG3	1:D:492:GLU:HA	1.75	0.68
1:B:129:HIS:H	1:B:148:ASN:HD21	1.44	0.66
1:C:453:SER:O	1:C:469[B]:GLU:HG3	1.96	0.65
1:C:509:ILE:HD12	1:C:509:ILE:C	2.17	0.64
1:C:622:CYS:O	1:C:626:HIS:HB2	1.97	0.64
1:D:128:CYS:HB3	1:D:148:ASN:O	1.97	0.64
1:A:266:GLY:HA2	1:A:269:ARG:CZ	2.27	0.64
1:B:288:LYS:HE3	10:B:1118:HOH:O	1.94	0.61
1:D:578:ILE:CD1	10:D:961:HOH:O	2.46	0.61
1:C:382[A]:HIS:CE1	1:C:433:HIS:HD1	2.18	0.61
1:D:578:ILE:HG13	10:D:961:HOH:O	2.01	0.61
5:A:704:CUK:S1	1:D:627:MET:HE3	2.40	0.60
1:A:382[B]:HIS:HE1	3:A:702:CL:CL	2.21	0.60
1:B:264:LEU:HG	1:B:268:MET:CE	2.32	0.60
1:A:260:LYS:O	1:A:262:PHE:CE1	2.55	0.60
1:C:129:HIS:CE1	1:C:494:HIS:CE1	2.90	0.59
1:A:210:LEU:HB2	1:A:262:PHE:CE1	2.37	0.59
1:D:129:HIS:CE1	1:D:494:HIS:CE1	2.90	0.59
1:A:559:GLU:OE1	1:A:632:ARG:NH2	2.36	0.58
1:C:382[A]:HIS:CE1	3:C:702:CL:CL	2.93	0.58
1:A:78:HIS:CE1	1:D:619:SER:O	2.57	0.58
1:A:264:LEU:HD23	1:A:268:MET:CE	2.33	0.58
1:D:210:LEU:HB2	1:D:262:PHE:CE2	2.37	0.58
1:A:382[B]:HIS:CE1	1:A:433:HIS:HD1	2.22	0.58
1:C:511:ASP:HB3	1:C:513:ASN:OD1	2.03	0.58
1:D:429:TYR:CE2	1:D:457:LYS:HE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ALA:HB2	1:A:583:HIS:HE1	1.68	0.56
1:B:522:GLU:OE1	1:B:525:LYS:NZ	2.33	0.56
1:B:78:HIS:CE1	1:C:619:SER:O	2.59	0.56
1:D:494:HIS:HE1	10:D:824:HOH:O	1.88	0.56
1:C:128:CYS:HB2	1:C:147:ILE:HG12	1.88	0.56
1:C:329:ASN:HD21	1:C:382[A]:HIS:CE1	2.24	0.56
1:C:382[A]:HIS:HD2	1:C:434:LEU:H	1.53	0.55
1:A:411:ARG:NH2	10:A:806:HOH:O	2.37	0.55
1:C:382[A]:HIS:CE1	1:C:433:HIS:ND1	2.76	0.54
1:C:509:ILE:HD13	1:C:510:TRP:O	2.07	0.54
1:C:453:SER:O	1:C:469[B]:GLU:CG	2.55	0.54
1:D:210:LEU:HB3	1:D:262:PHE:CZ	2.44	0.53
1:C:580:ASP:HB3	10:C:802:HOH:O	2.07	0.53
1:A:329:ASN:HD21	1:A:382[B]:HIS:CE1	2.27	0.53
1:D:382[B]:HIS:NE2	1:D:433:HIS:CE1	2.77	0.53
1:B:382[B]:HIS:CD2	3:B:702:CL:CL	2.99	0.52
1:A:77:GLY:HA2	1:A:128:CYS:O	2.10	0.52
1:A:181:ARG:HH22	1:A:382[B]:HIS:HE1	1.57	0.52
1:C:128:CYS:HB3	1:C:148:ASN:O	2.10	0.52
1:A:382[B]:HIS:HD2	1:A:434:LEU:H	1.58	0.51
1:D:494:HIS:CE1	10:D:824:HOH:O	2.64	0.51
1:D:578:ILE:HD12	10:D:961:HOH:O	2.07	0.50
1:B:266:GLY:HA2	1:B:269:ARG:CZ	2.41	0.50
1:A:145:LEU:HD22	1:A:158:ILE:HD12	1.94	0.50
1:D:259:GLU:HG2	1:D:269:ARG:HB2	1.93	0.49
1:A:380:PRO:HA	1:A:394:THR:O	2.13	0.49
1:C:509:ILE:C	1:C:509:ILE:CD1	2.81	0.49
1:A:210:LEU:HB3	1:A:262:PHE:CZ	2.48	0.49
1:D:210:LEU:CB	1:D:262:PHE:CE2	2.95	0.49
1:B:275:VAL:HG13	1:B:321:VAL:HG21	1.95	0.49
1:A:431:PRO:HA	1:A:453:SER:HA	1.95	0.49
1:D:129:HIS:H	1:D:148:ASN:ND2	2.10	0.49
1:A:467:HIS:HB2	1:D:580:ASP:OD1	2.12	0.48
1:D:145:LEU:HD22	1:D:158:ILE:HD12	1.93	0.48
1:A:382[B]:HIS:CE1	1:A:433:HIS:ND1	2.81	0.48
1:D:578:ILE:CG1	10:D:961:HOH:O	2.58	0.48
1:B:55:GLU:HA	1:B:55:GLU:OE1	2.13	0.48
1:D:380:PRO:HA	1:D:394:THR:O	2.13	0.48
1:D:382[B]:HIS:CE1	1:D:433:HIS:CE1	3.01	0.48
1:D:77:GLY:HA2	1:D:128:CYS:O	2.13	0.48
1:D:453:SER:O	1:D:469[B]:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:TYR:OH	1:C:447:LYS:HD3	2.13	0.48
1:C:480:GLU:OE1	1:C:482:LYS:NZ	2.47	0.48
1:B:431:PRO:HA	1:B:453:SER:HA	1.96	0.47
1:D:264:LEU:HG	1:D:268:MET:HE2	1.96	0.47
1:A:288:LYS:HD2	10:A:801:HOH:O	2.15	0.47
1:C:431:PRO:HA	1:C:453:SER:HA	1.97	0.47
1:D:347:CYS:O	1:D:373:GLU:HA	2.15	0.47
1:D:431:PRO:HA	1:D:453:SER:HA	1.96	0.47
1:B:380:PRO:HA	1:B:394:THR:O	2.15	0.47
1:B:625:LEU:HD13	1:C:264:LEU:HD11	1.96	0.47
1:A:480:GLU:HG3	10:A:816:HOH:O	2.15	0.47
2:B:701:B3P:O5	2:B:701:B3P:H32	2.15	0.46
1:D:525:LYS:HE2	10:D:1069:HOH:O	2.15	0.46
1:C:382[A]:HIS:HE1	3:C:702:CL:CL	2.35	0.46
1:C:129:HIS:H	1:C:148:ASN:ND2	2.09	0.46
1:D:382[B]:HIS:CE1	1:D:433:HIS:CG	3.03	0.46
1:B:77:GLY:HA2	1:B:128:CYS:O	2.15	0.46
1:C:77:GLY:HA2	1:C:128:CYS:O	2.16	0.46
1:B:70:TYR:HB2	1:B:87:VAL:HB	1.98	0.45
1:D:59:LYS:HG3	1:D:61:HIS:H	1.81	0.45
1:A:129:HIS:N	1:A:148:ASN:HD21	2.11	0.45
1:A:480:GLU:CG	10:A:816:HOH:O	2.65	0.45
1:C:380:PRO:HA	1:C:394:THR:O	2.15	0.45
1:D:382[B]:HIS:CE1	1:D:433:HIS:CD2	3.04	0.45
1:B:260:LYS:HE3	10:B:1125:HOH:O	2.15	0.45
1:C:578:ILE:H	1:C:578:ILE:HD12	1.82	0.45
1:A:347:CYS:O	1:A:373:GLU:HA	2.16	0.45
1:A:382[B]:HIS:CD2	1:A:433:HIS:HD1	2.34	0.45
1:B:129:HIS:H	1:B:148:ASN:ND2	2.13	0.45
1:D:260:LYS:O	1:D:262:PHE:CE2	2.70	0.45
1:B:145:LEU:HD22	1:B:158:ILE:HD12	1.99	0.45
1:B:264:LEU:CD1	1:B:268:MET:HE2	2.47	0.45
1:A:148:ASN:HD22	1:A:148:ASN:H	1.65	0.45
1:B:580:ASP:OD1	1:C:467:HIS:HB2	2.17	0.44
1:C:148:ASN:H	1:C:148:ASN:HD22	1.66	0.44
1:D:382[A]:HIS:CD2	3:D:702:CL:CL	3.07	0.44
1:B:125:ASN:OD1	1:C:591:GLY:HA2	2.17	0.44
1:A:210:LEU:HD13	1:A:262:PHE:CD2	2.52	0.44
1:B:55:GLU:HG3	1:B:478:GLY:HA3	1.98	0.44
1:C:101:VAL:HG21	1:C:124:LEU:HD22	2.00	0.44
1:C:353:ASP:HB2	10:C:893:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382[B]:HIS:ND1	1:D:433:HIS:HA	2.33	0.44
1:D:551:MET:HE2	1:D:575:ILE:HD11	1.99	0.44
1:A:181:ARG:HH22	1:A:382[B]:HIS:CE1	2.36	0.44
1:A:264:LEU:HD21	1:D:625:LEU:HD13	1.98	0.44
1:B:214:ASN:ND2	10:B:813:HOH:O	2.51	0.44
1:C:347:CYS:O	1:C:373:GLU:HA	2.17	0.44
1:D:148:ASN:HD22	1:D:148:ASN:H	1.66	0.43
1:C:97:PRO:HB2	1:C:107:TRP:CD1	2.53	0.43
1:A:125:ASN:OD1	1:D:591:GLY:HA2	2.18	0.43
1:A:443:GLU:O	1:A:444:ALA:C	2.57	0.43
1:D:70:TYR:HB2	1:D:87:VAL:HB	2.00	0.43
1:D:379:GLY:N	1:D:380:PRO:HD3	2.33	0.43
1:A:210:LEU:HD13	1:A:262:PHE:CE2	2.54	0.43
1:B:129:HIS:N	1:B:148:ASN:HD21	2.13	0.43
1:A:265:GLY:HA2	1:A:268:MET:CE	2.49	0.43
1:B:347:CYS:O	1:B:373:GLU:HA	2.19	0.43
1:D:606:PHE:HA	7:D:706:FMT:C	2.45	0.43
1:D:59:LYS:HE3	1:D:61:HIS:O	2.19	0.43
1:A:210:LEU:CB	1:A:262:PHE:CZ	3.02	0.42
1:C:181:ARG:HH22	1:C:382[A]:HIS:HE1	1.66	0.42
1:C:622:CYS:O	1:C:623:HIS:O	2.37	0.42
1:D:128:CYS:HB2	1:D:147:ILE:HG12	2.01	0.42
1:C:382[A]:HIS:CD2	1:C:433:HIS:HD1	2.36	0.42
1:A:70:TYR:HB2	1:A:87:VAL:HB	2.00	0.42
1:B:268:MET:HE1	1:C:625:LEU:HD13	2.02	0.42
1:B:443:GLU:O	1:B:444:ALA:C	2.57	0.42
1:C:559:GLU:HA	1:C:632:ARG:O	2.19	0.42
1:C:379:GLY:N	1:C:380:PRO:HD3	2.35	0.42
1:C:78:HIS:CE1	1:C:492:GLU:HB3	2.54	0.42
1:A:268:MET:HB2	1:A:268:MET:HE3	1.55	0.41
1:B:632:ARG:HD3	10:B:988:HOH:O	2.19	0.41
1:A:97:PRO:HB2	1:A:107:TRP:CD1	2.55	0.41
1:D:443:GLU:O	1:D:444:ALA:C	2.58	0.41
1:A:101:VAL:HG21	1:A:124:LEU:HD22	2.03	0.41
1:A:559:GLU:HA	1:A:632:ARG:O	2.21	0.41
1:A:264:LEU:O	1:A:268:MET:HE2	2.20	0.41
1:C:269:ARG:HD2	10:C:815:HOH:O	2.20	0.41
1:A:591:GLY:HA2	1:D:125:ASN:OD1	2.20	0.41
1:B:148:ASN:H	1:B:148:ASN:HD22	1.68	0.41
1:C:303:LEU:HD22	1:C:303:LEU:N	2.35	0.41
1:C:535:ASN:OD1	1:C:556:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382[A]:HIS:CE1	1:C:433:HIS:CE1	3.09	0.41
1:C:443:GLU:O	1:C:444:ALA:C	2.59	0.41
1:D:97:PRO:HB2	1:D:107:TRP:CD1	2.56	0.41
1:D:264:LEU:HG	1:D:268:MET:CE	2.51	0.41
1:A:90:MET:HG3	10:A:1067:HOH:O	2.21	0.41
1:B:559:GLU:HA	1:B:632:ARG:O	2.21	0.41
1:C:145:LEU:HD22	1:C:158:ILE:HD12	2.03	0.41
1:B:591:GLY:HA2	1:C:125:ASN:OD1	2.21	0.40
1:D:181:ARG:HH22	1:D:382[A]:HIS:HE2	1.70	0.40
1:D:303:LEU:HD22	1:D:303:LEU:N	2.37	0.40
1:D:453:SER:O	1:D:469[B]:GLU:CG	2.68	0.40
1:C:70:TYR:HB2	1:C:87:VAL:HB	2.04	0.40
1:D:445:ASP:O	1:D:447:LYS:HD2	2.21	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2335/2552 (92%)	2239 (96%)	87 (4%)	9 (0%)	34 19

All (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
1	D	342	LYS
1	C	176	ALA
1	D	176	ALA
1	A	176	ALA

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	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

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ILE
1	A	620	TRP
1	B	148	ASN
1	B	275	VAL
1	B	313	SER
1	B	596	ILE

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Mol	Chain	Res	Type
1	B	620	TRP
1	C	74	TRP
1	C	78	HIS
1	C	308	LYS
1	C	313	SER
1	C	620	TRP
1	D	291	ASP
1	D	313	SER
1	D	447	LYS
1	D	457	LYS
1	D	620	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	148	ASN
1	A	214	ASN
1	A	583	HIS
1	B	148	ASN
1	B	214	ASN
1	C	61	HIS
1	C	129	HIS
1	C	148	ASN
1	C	494	HIS
1	D	129	HIS
1	D	148	ASN
1	D	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 (i)

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	$\#\|Z\| > 2$
6	CUA	C	705	1	0,1,1	-	-	-		
2	B3P	A	701	-	18,18,18	1.16	1 (5%)	21,23,23	1.80	6 (28%)
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%)
7	FMT	C	706	-	2,2,2	0.33	0	1,1,1	0.72	0
7	FMT	D	706	-	2,2,2	0.14	0	1,1,1	0.66	0
7	FMT	A	706	-	2,2,2	0.27	0	1,1,1	0.85	0
2	B3P	B	701	-	18,18,18	0.89	0	21,23,23	1.52	3 (14%)
5	CUK	B	704	1	0,6,6	-	-	-		
7	FMT	B	706	-	2,2,2	0.05	0	1,1,1	0.27	0
6	CUA	B	705	1	0,1,1	-	-	-		
5	CUK	A	704	1	0,6,6	-	-	-		
6	CUA	A	705	1	0,1,1	-	-	-		
5	CUK	D	704	1	0,6,6	-	-	-		
7	FMT	C	707	-	2,2,2	1.10	0	1,1,1	1.18	0
5	CUK	C	704	1	0,6,6	-	-	-		
6	CUA	D	705	1	0,1,1	-	-	-		

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CUK	D	704	1	-	-	0/1/1/1
5	CUK	C	704	1	-	-	0/1/1/1

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

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
2	D	701	B3P	C3-N1-C4	3.55	121.11	116.08
2	C	701	B3P	C3-N1-C4	3.13	120.52	116.08
2	A	701	B3P	C6-C4-N1	-2.78	100.68	109.03
2	B	701	B3P	O4-C5-C4	-2.67	106.23	111.63
2	D	701	B3P	O3-C11-C8	-2.19	107.19	111.63
2	B	701	B3P	C11-C8-C10	-2.18	105.43	110.04
2	A	701	B3P	O2-C10-C8	-2.12	107.34	111.63
2	A	701	B3P	C5-C4-N1	2.12	115.40	109.03
2	A	701	B3P	C7-C4-C6	-2.11	105.58	110.04
2	C	701	B3P	C6-C4-N1	2.01	115.08	109.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

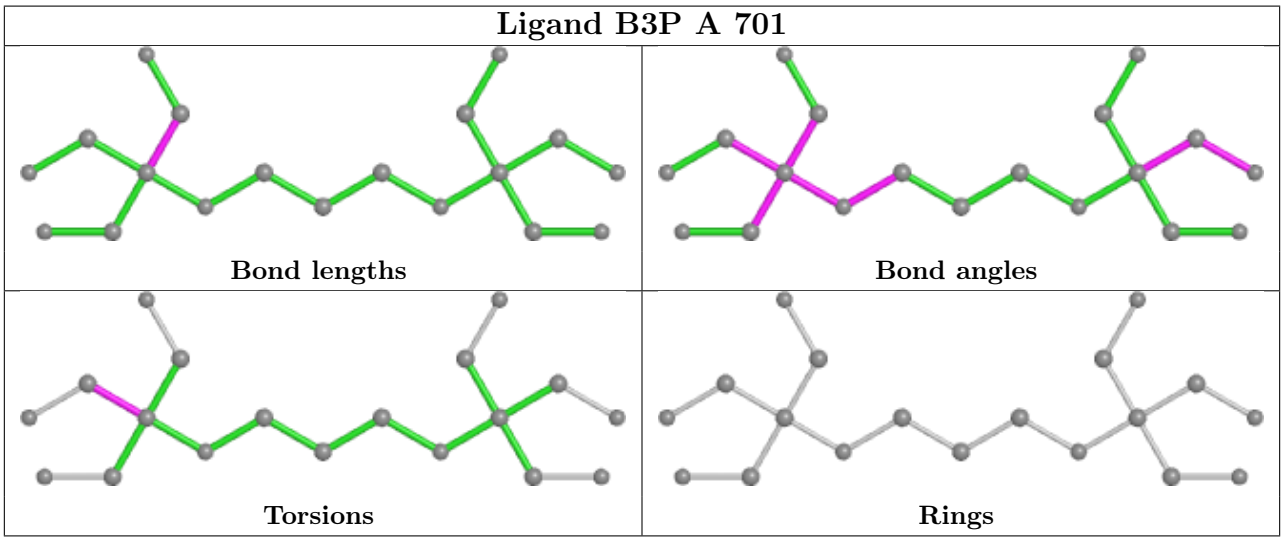
Mol	Chain	Res	Type	Atoms
2	D	701	B3P	O2-C10-C8-C9
2	C	701	B3P	N2-C8-C9-O1
2	A	701	B3P	C7-C4-C6-O5
2	B	701	B3P	C7-C4-C6-O5
2	A	701	B3P	N1-C4-C6-O5
2	D	701	B3P	O2-C10-C8-N2
2	D	701	B3P	C9-C8-N2-C2
2	C	701	B3P	C10-C8-C9-O1

There are no ring outliers.

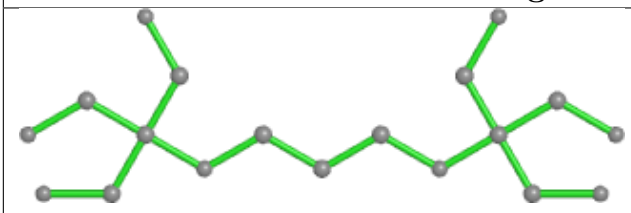
3 monomers are involved in 4 short contacts:

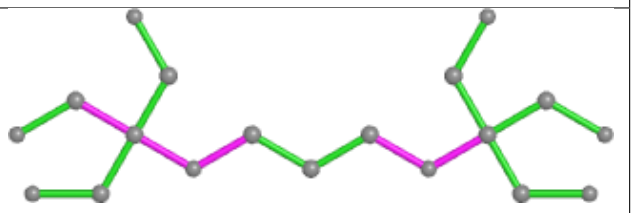
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	706	FMT	2	0
2	B	701	B3P	1	0
5	A	704	CUK	1	0

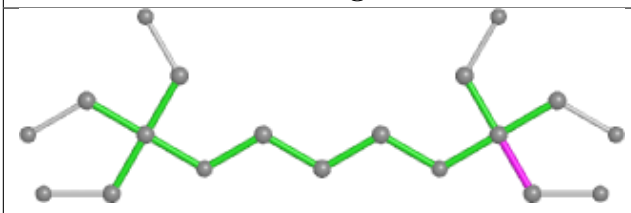
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

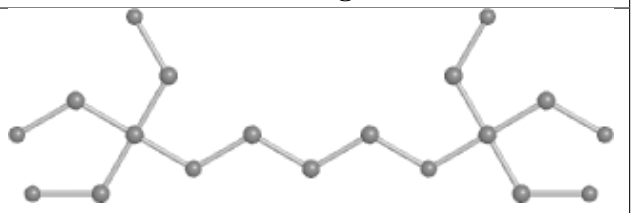


Ligand B3P C 701

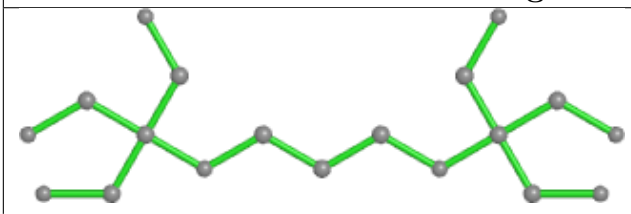

Bond lengths


Bond angles


Torsions


Rings

Ligand B3P D 701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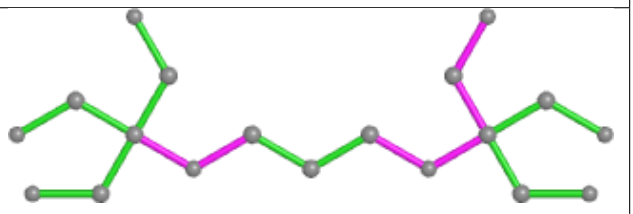
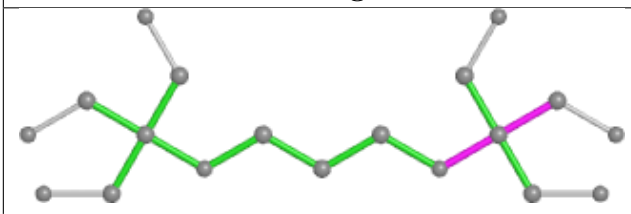
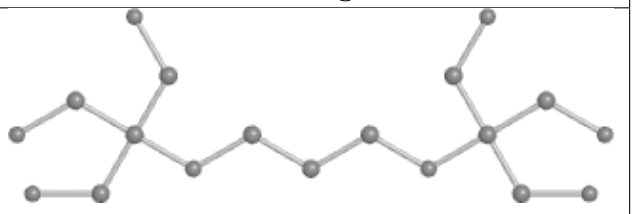
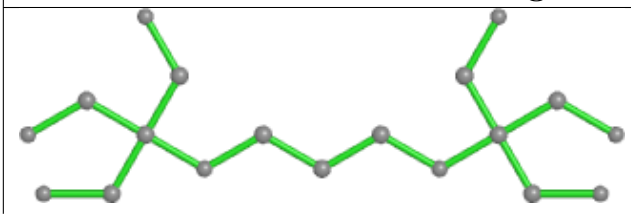
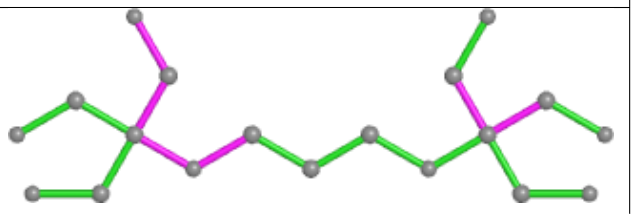

Bond angles

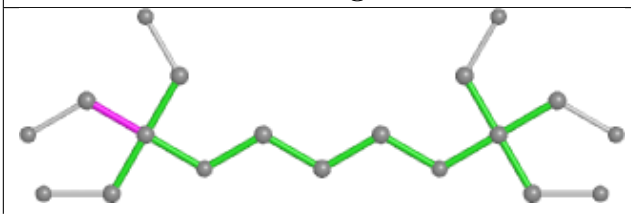

Torsions

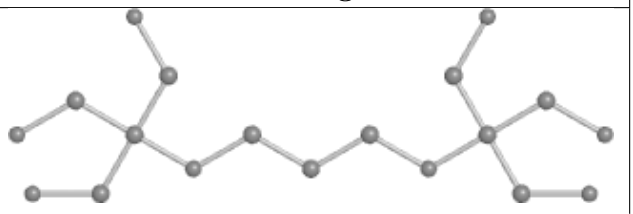

Rings

Ligand B3P B 701

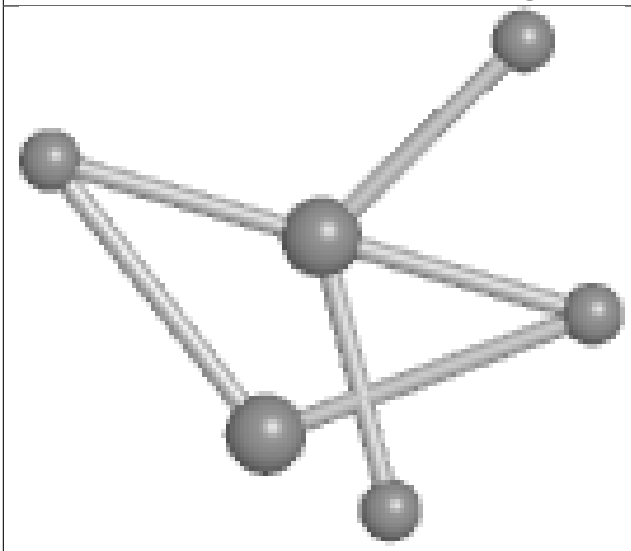

Bond lengths


Bond angles

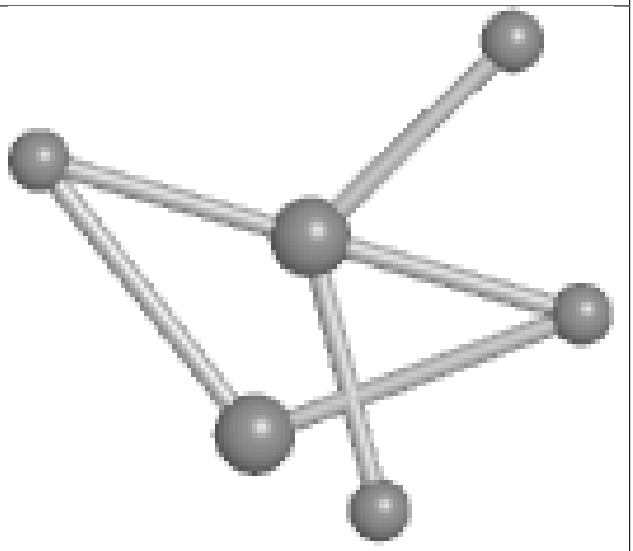

Torsions


Rings

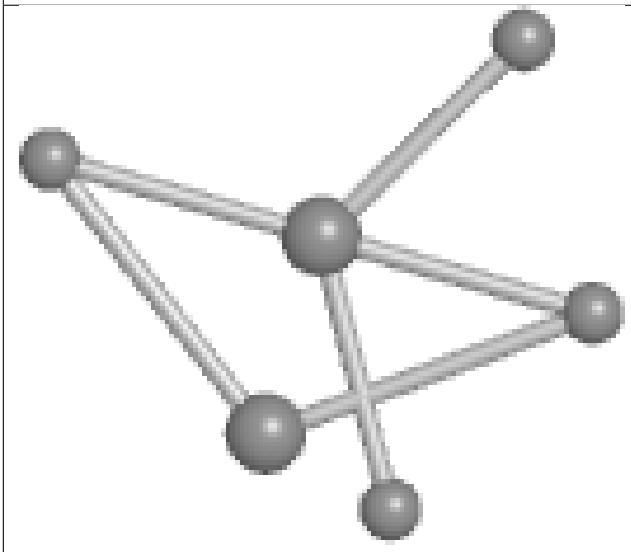
Ligand CUK B 704



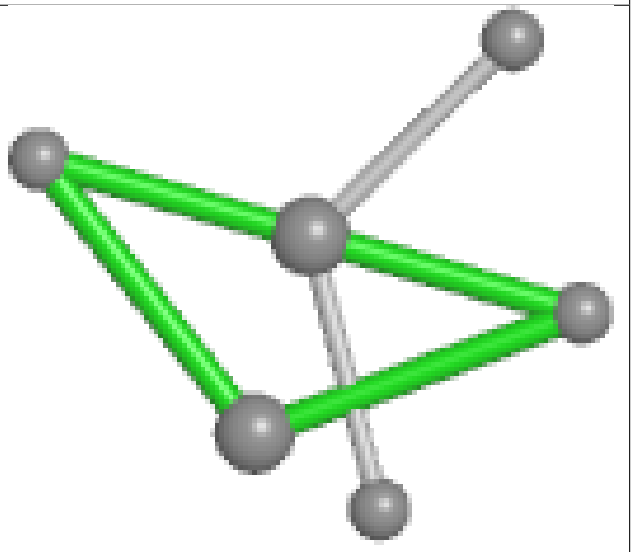
Bond lengths



Bond angles

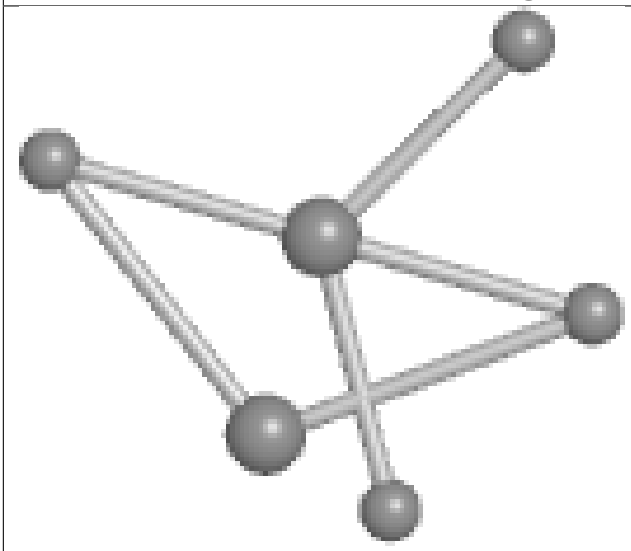


Torsions

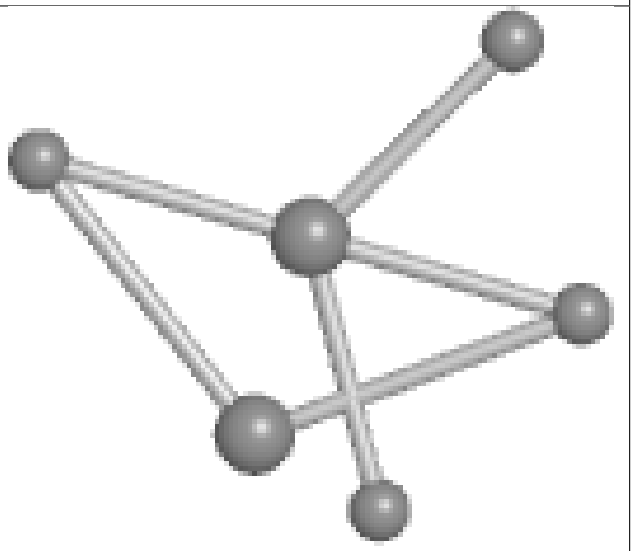


Rings

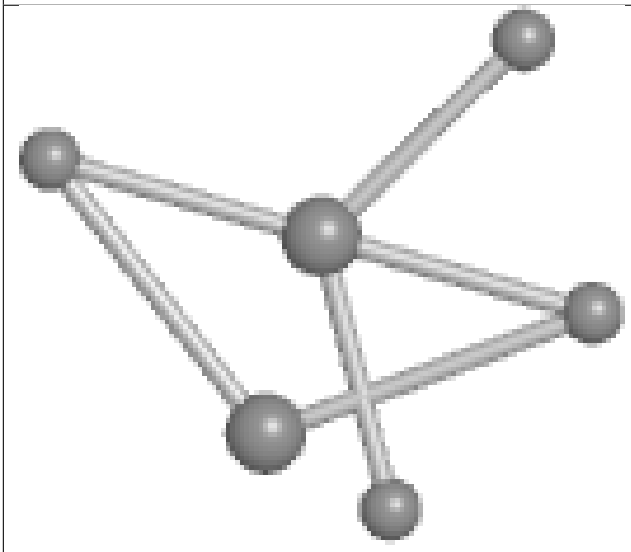
Ligand CUK A 704



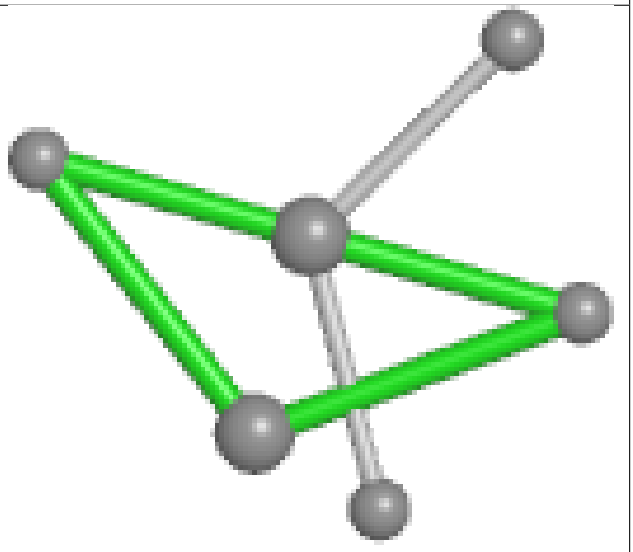
Bond lengths



Bond angles

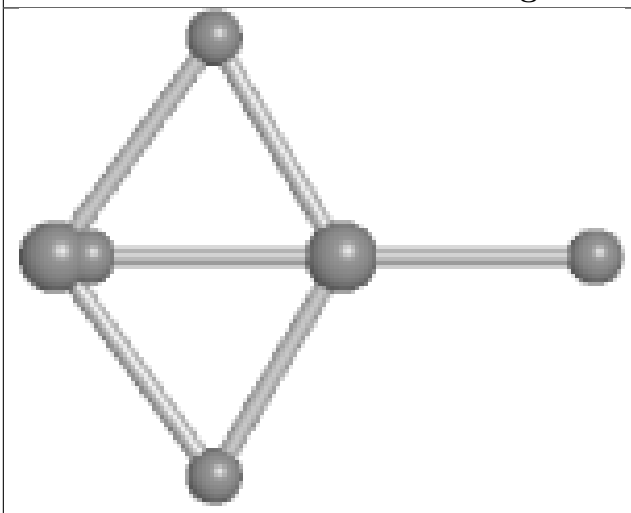


Torsions

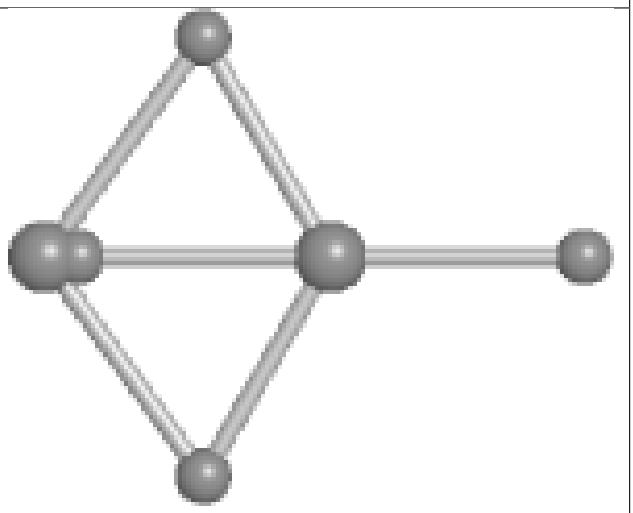


Rings

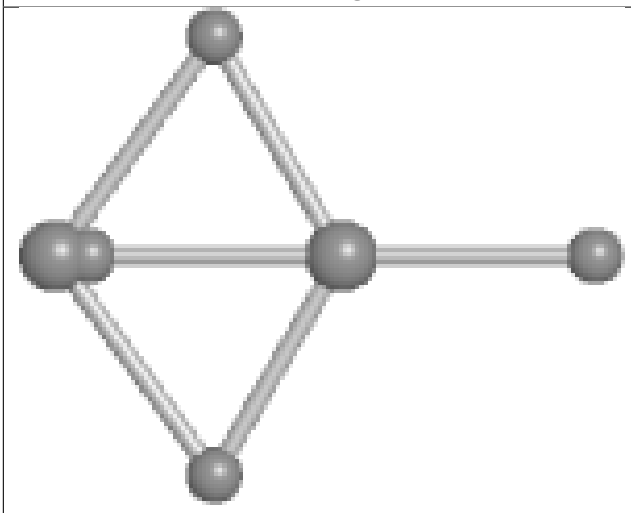
Ligand CUK D 704



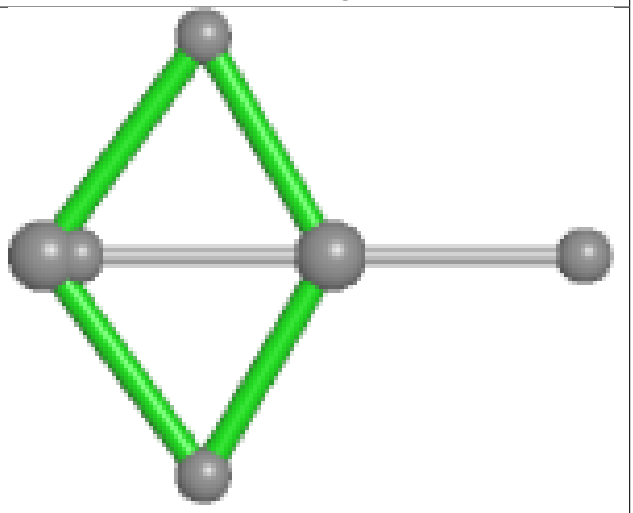
Bond lengths



Bond angles

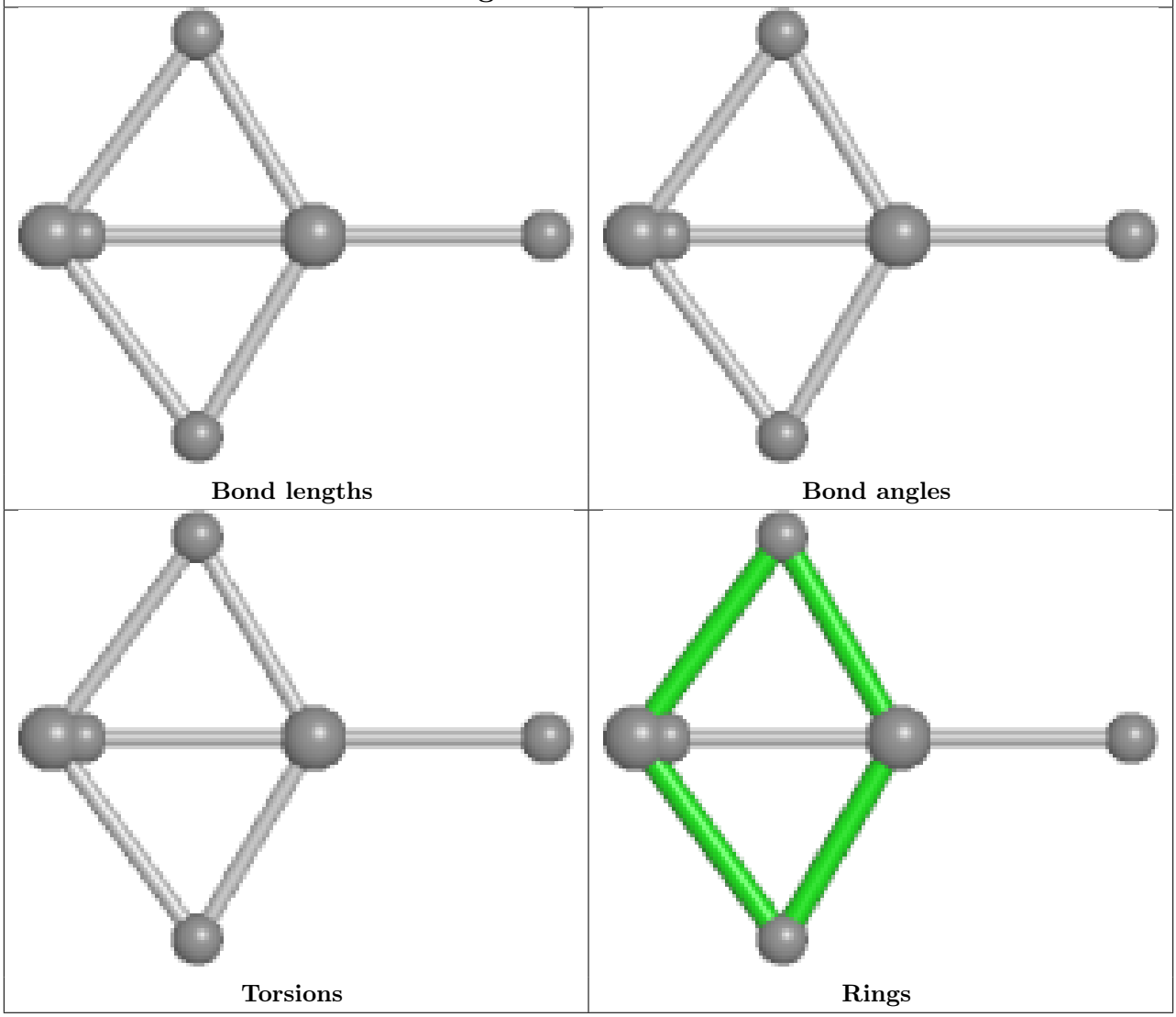


Torsions



Rings

Ligand CUK C 704



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	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

All (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
1	C	297	ASP	3.3
1	D	289	ALA	3.3
1	C	309	ASP	3.2
1	A	56	SER	3.2
1	D	291	ASP	3.0
1	D	297	ASP	3.0
1	D	418	VAL	2.9
1	A	261	ALA	2.9
1	A	57	LYS	2.9
1	D	287	VAL	2.8
1	B	57	LYS	2.8
1	A	207	VAL	2.8
1	A	55	GLU	2.8
1	C	61	HIS	2.8
1	B	415	GLY	2.6
1	A	265	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	262	PHE	2.6
1	D	213	GLU	2.5
1	B	208	PHE	2.5
1	A	410	VAL	2.5
1	D	207	VAL	2.5
1	A	59	LYS	2.5
1	A	264	LEU	2.4
1	B	638	ALA	2.3
1	D	293	ILE	2.3
1	D	230	ALA	2.3
1	B	270	ASN	2.2
1	D	416	GLU	2.2
1	B	207	VAL	2.2
1	D	620	TRP	2.2
1	C	98	VAL	2.2
1	A	494	HIS	2.1
1	D	98	VAL	2.1
1	A	270	ASN	2.1
1	A	288	LYS	2.1
1	B	206	LYS	2.1
1	A	490	PHE	2.0
1	B	494	HIS	2.0
1	D	309	ASP	2.0

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^{th} 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.

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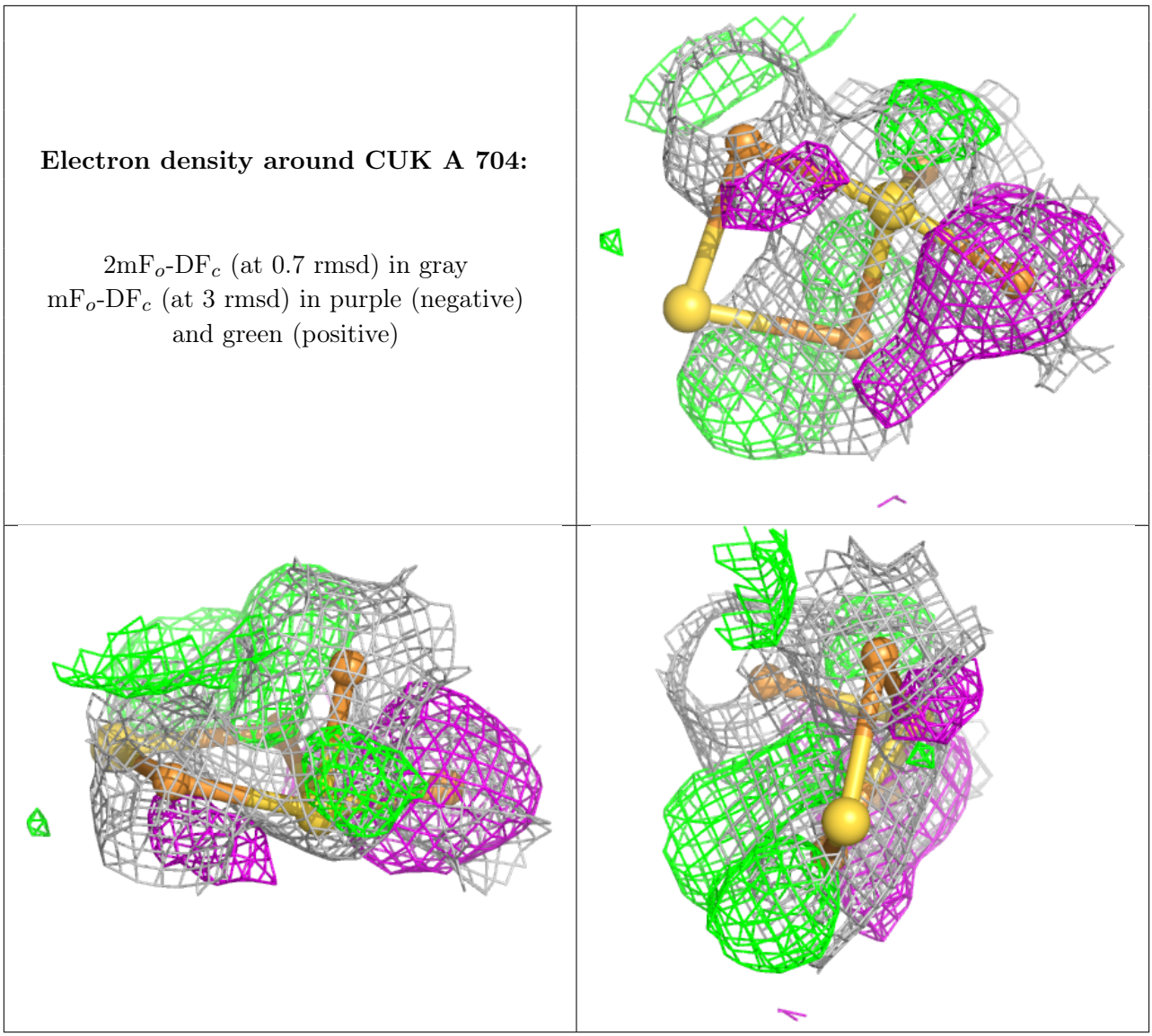
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CUK	A	704	6/6	0.89	0.16	26,39,46,50	6
5	CUK	B	704	6/6	0.89	0.15	28,43,46,48	6
7	FMT	C	707	3/3	0.91	0.23	35,35,39,41	0
9	NA	D	708	1/1	0.92	0.09	34,34,34,34	1
5	CUK	D	704	6/6	0.93	0.11	25,32,35,36	6
9	NA	C	709	1/1	0.94	0.09	30,30,30,30	0
2	B3P	C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

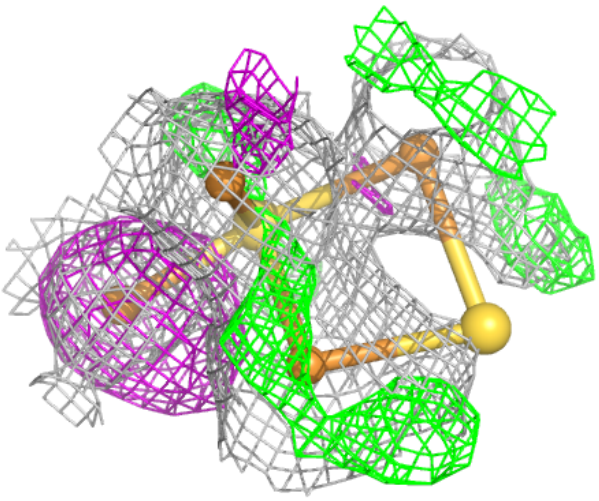
Electron density around CUK A 704:

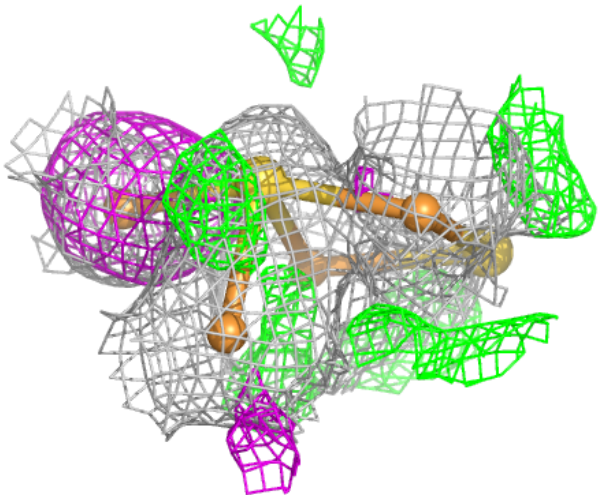
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

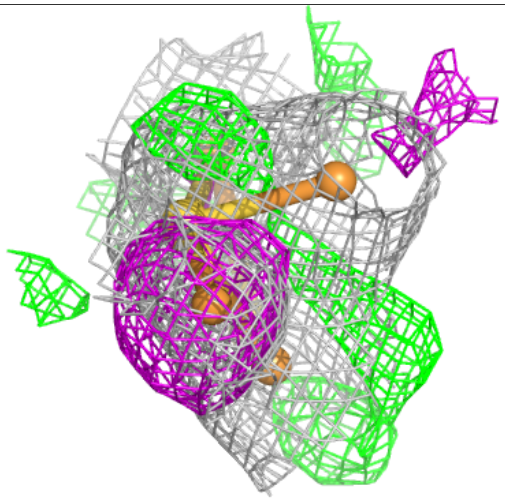


Electron density around CUK B 704:

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

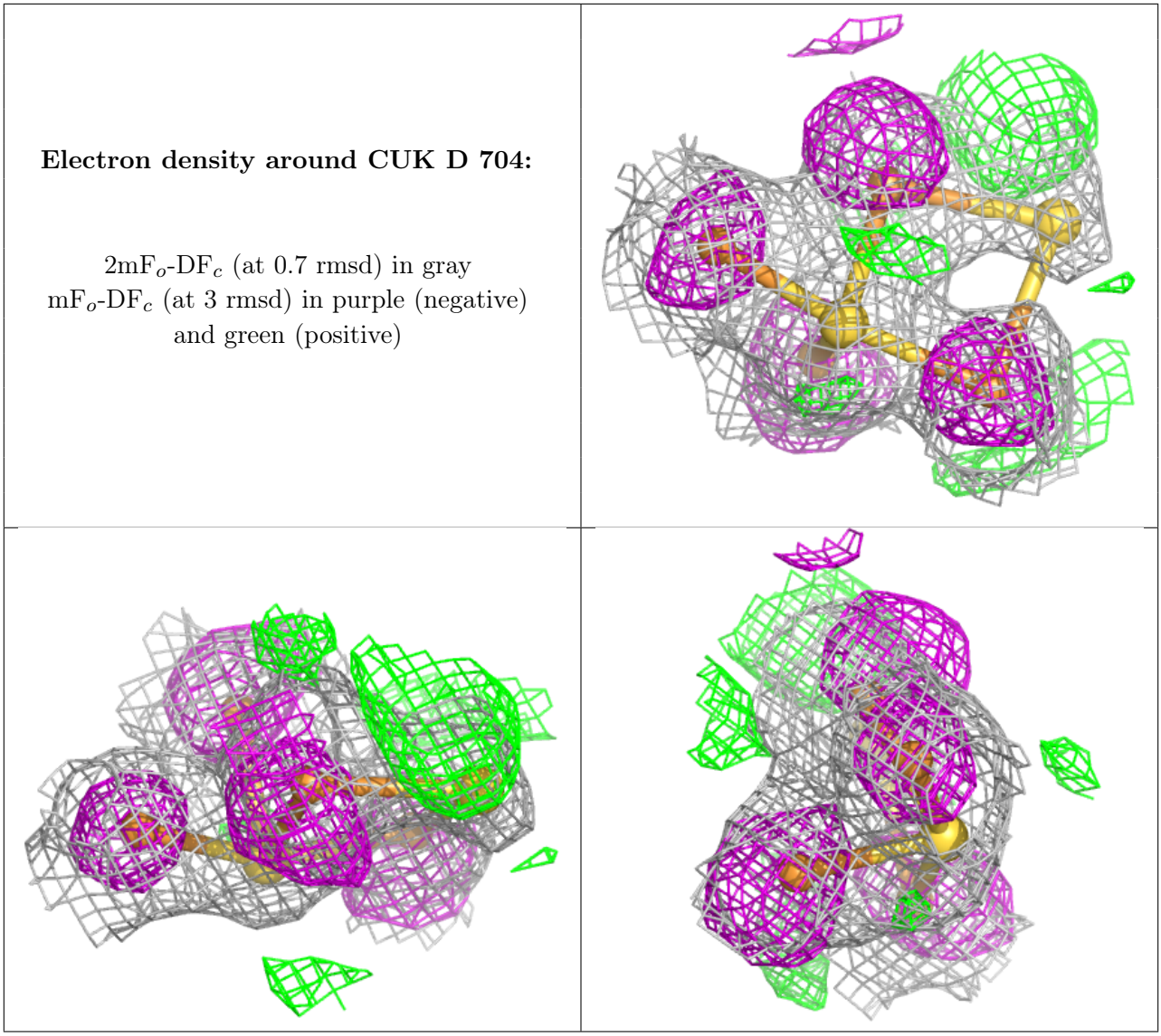






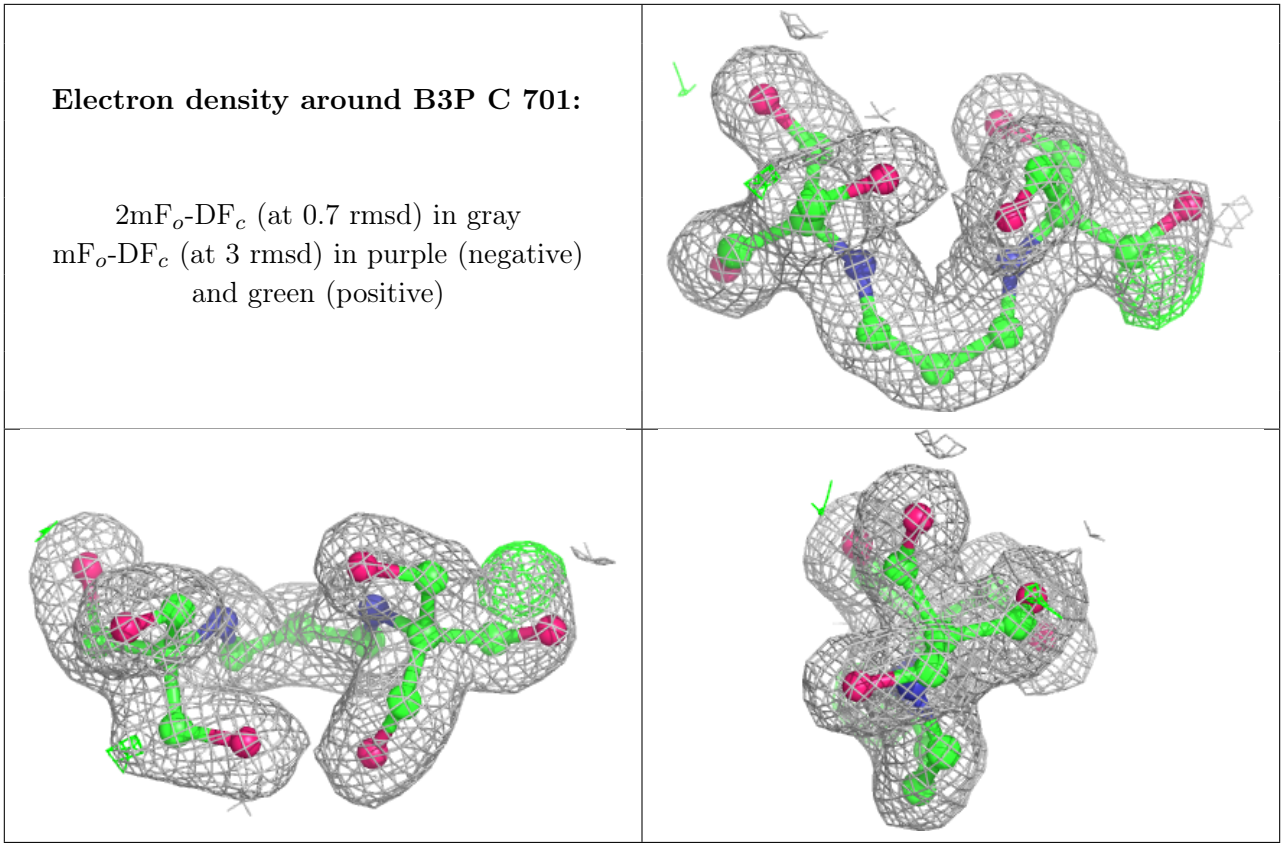
Electron density around CUK D 704:

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



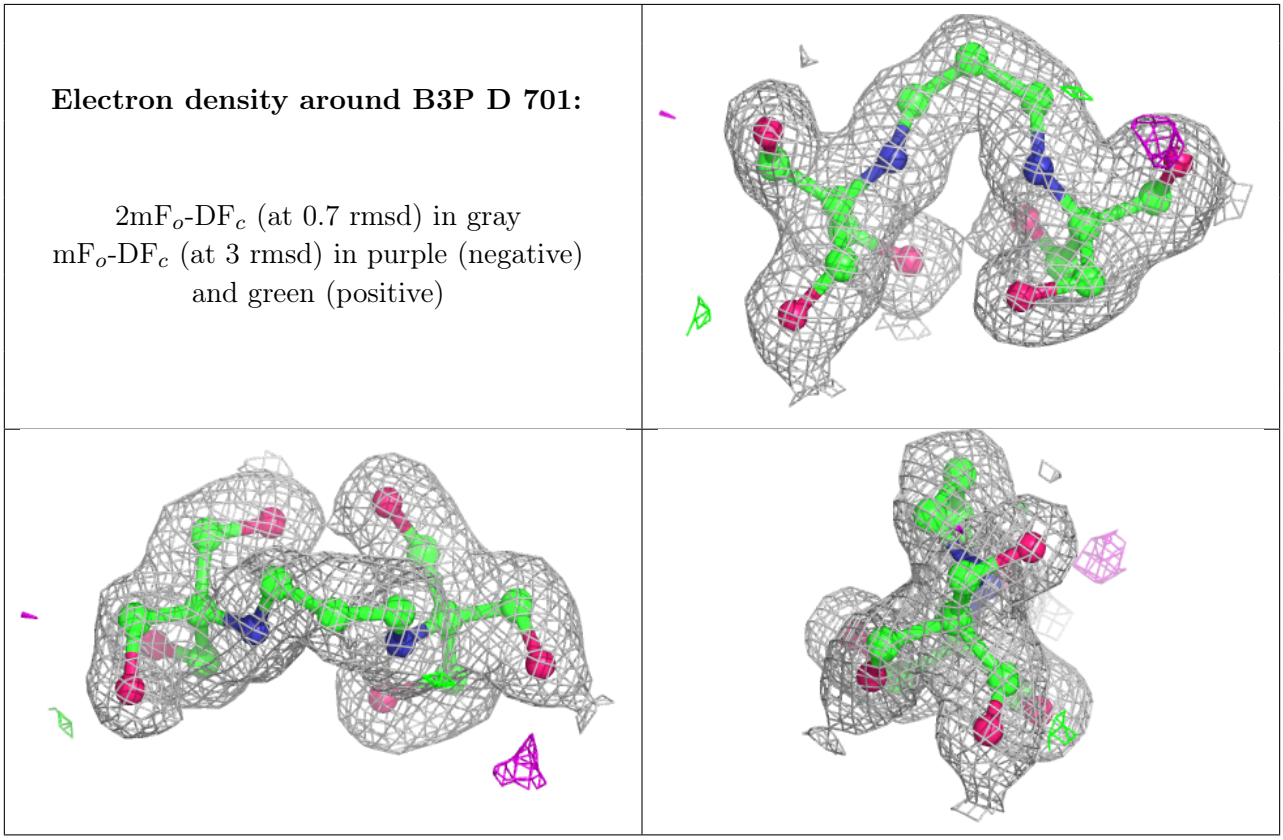
Electron density around B3P C 701:

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



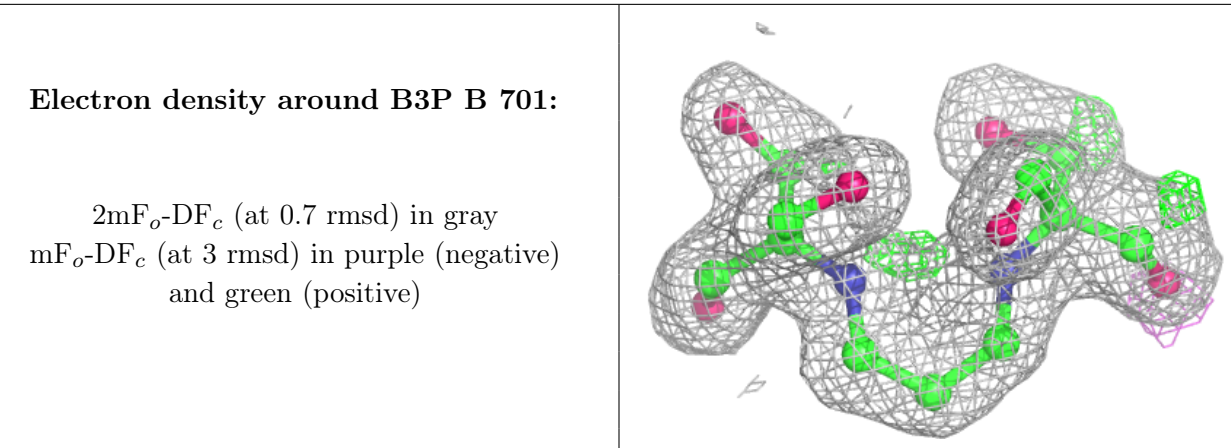
Electron density around B3P D 701:

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



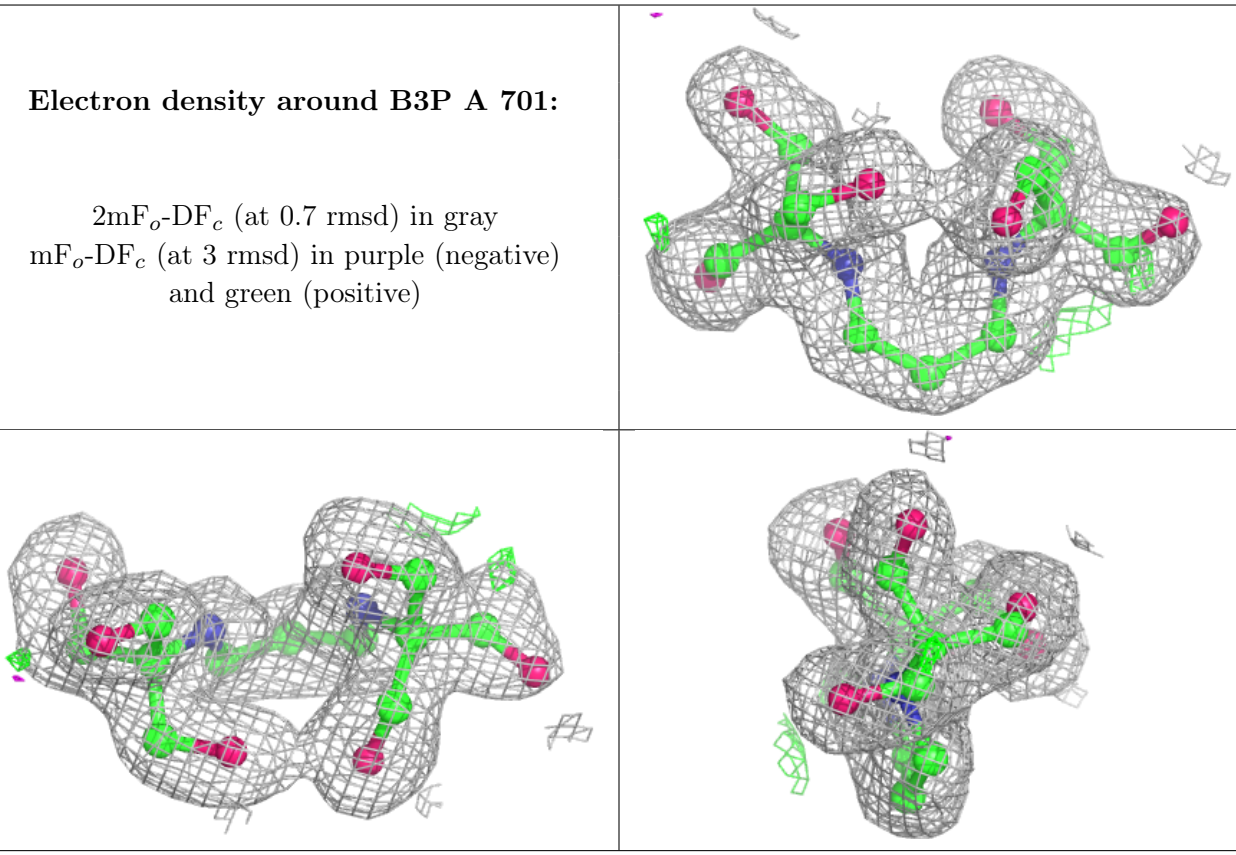
Electron density around B3P B 701:

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



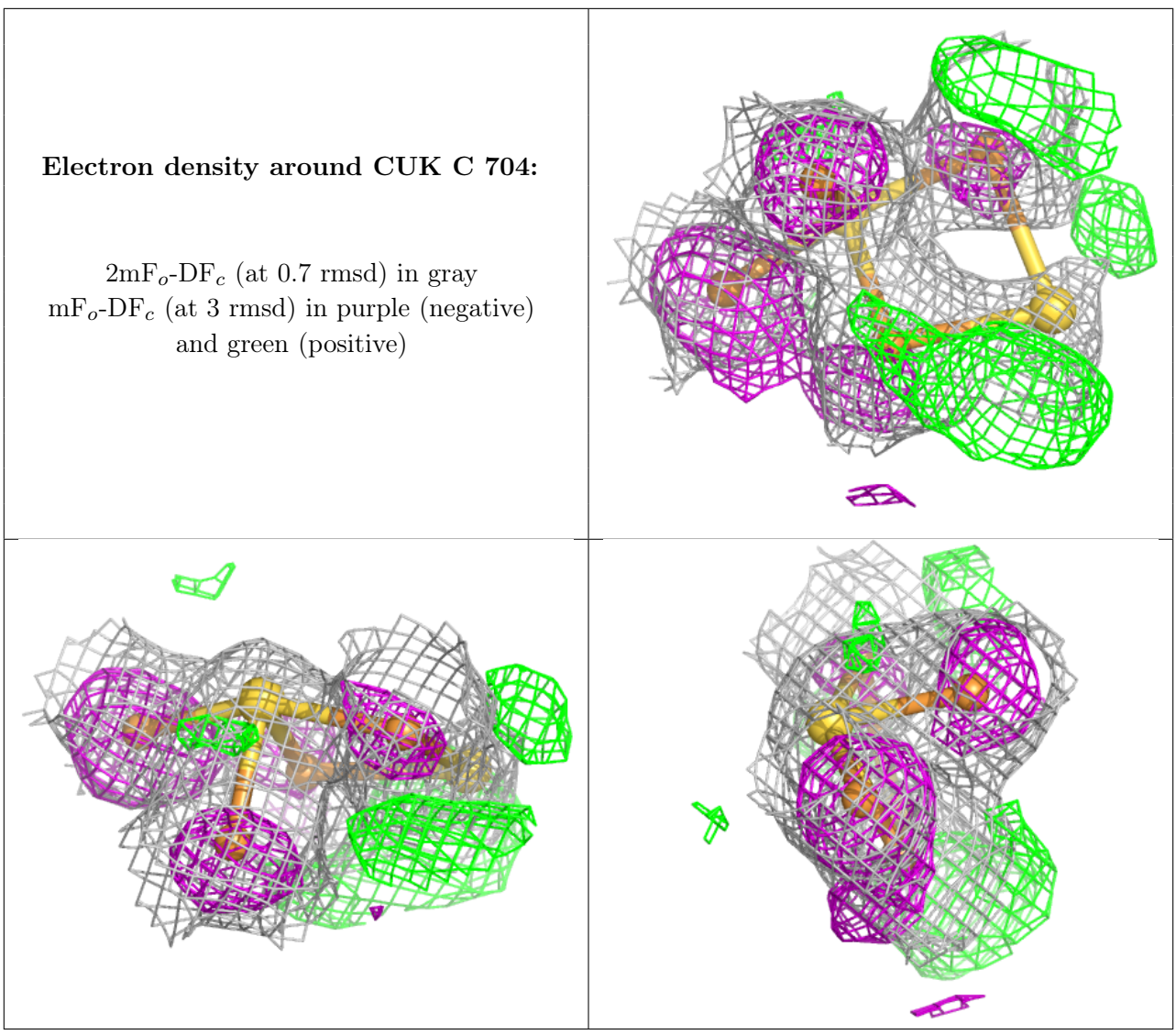
Electron density around B3P A 701:

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



Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.