W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 01:40 pm GMT

PDB ID	:	7P7O
Title	:	X-RAY CRYSTAL STRUCTURE OF SPOROSARCINA PASTEURII UREASE INHIBITED BY THE GOLD(I)-DIPHOSPHINE COMPOUND Au(PEt3)2Cl DETERMINED AT 1.87 ANGSTROMS
Authors	:	Mazzei, L.; Ciurli, S.; Cianci, M.; Messori, L.; Massai, L.
Deposited on	:	2021-07-20
Resolution	:	1.87 Å(reported)

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

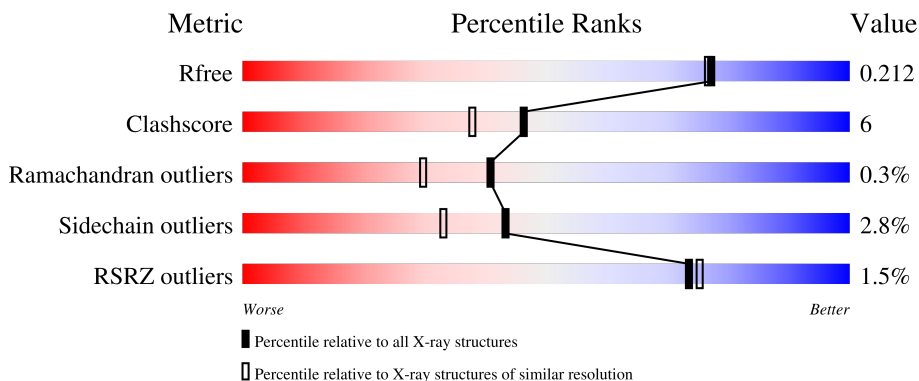|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	Percentile Ranks	Value
Rfree		0.212
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		2.8%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	AAA	100	91% 8% •
2	BBB	122	2% 92% 7% •
3	CCC	570	2% 87% 10% ••

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
4	EDO	BBB	201	-	-	-	X
5	SO4	AAA	203	-	-	-	X
5	SO4	CCC	622	-	-	X	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 6880 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	100	Total	C	N	O	S	0	4	0
			811	511	137	155	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	20	ALA	LEU	variant	UNP P41022
AAA	22	LYS	ARG	variant	UNP P41022

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	122	Total	C	N	O	S	0	5	0
			992	611	177	203	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	563	Total	C	N	O	S	0	23	0
			4458	2791	773	867	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	35	TYR	-	insertion	UNP P41020
CCC	?	-	VAL	deletion	UNP P41020

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total 4	C 2	O 2	0	0
4	AAA	1	Total 4	C 2	O 2	0	0
4	BBB	1	Total 4	C 2	O 2	0	0
4	CCC	1	Total 4	C 2	O 2	0	0
4	CCC	1	Total 4	C 2	O 2	0	0
4	CCC	1	Total 4	C 2	O 2	0	0
4	CCC	1	Total 4	C 2	O 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

W O R L D W I D E
PDB
PROTEIN DATA BANK

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total 5	O 4	S 1	0	0
5	AAA	1	Total 5	O 4	S 1	0	0
5	AAA	1	Total 5	O 4	S 1	0	0
5	AAA	1	Total 5	O 4	S 1	0	0
5	BBB	1	Total 5	O 4	S 1	0	0
5	BBB	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0
5	CCC	1	Total 5	O 4	S 1	0	0

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	CCC	2	Total 2	Ni 2	0	0

- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total 1	O 1	0	0

- Molecule 8 is triethylphosphanuidylgold(1+) (three-letter code: AUF) (formula: $C_6H_{15}AuP$).
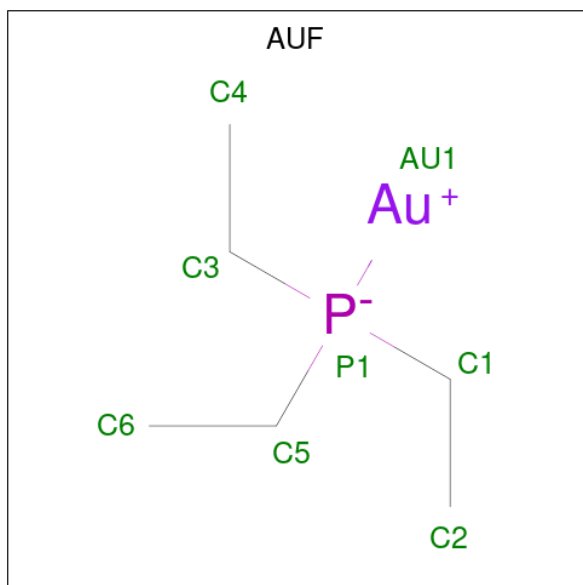
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	CCC	1	Total	Au	C	P	0	0
			8	1	6	1		
8	CCC	1	Total	Au	C	P	0	0
			8	1	6	1		
8	CCC	1	Total	Au	C	P	0	0
			8	1	6	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	64	Total	O	0	0
			64	64		
9	BBB	75	Total	O	0	0
			75	75		
9	CCC	330	Total	O	0	0
			330	330		

3 Residue-property plots ⓘ

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: Urease subunit gamma

Chain AAA:
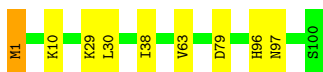
• Molecule 2: Urease subunit beta

Chain BBB:
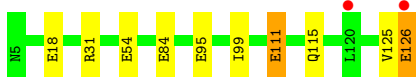
• Molecule 3: Urease subunit alpha

Chain CCC:
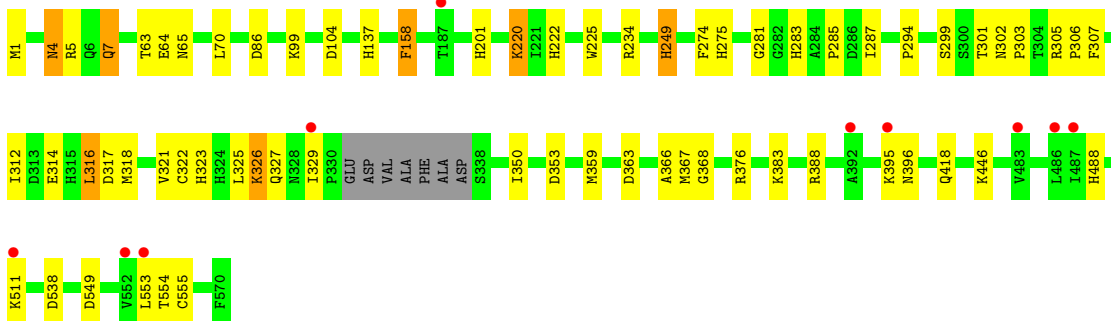
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.80Å 131.80Å 189.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.98 – 1.87 65.90 – 1.87	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.98-1.87) 100.0 (65.90-1.87)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.165 , 0.210 0.167 , 0.212	Depositor DCC
R_{free} test set	4006 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6880	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CXM, AUF, O, SO4, NI, EDO, KCX

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	AAA	0.64	0/811	0.88	0/1089
2	BBB	0.62	0/1004	0.88	0/1351
3	CCC	0.61	0/4525	0.91	5/6124 (0.1%)
All	All	0.61	0/6340	0.90	5/8564 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	5	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	CCC	234	ARG	CG-CD-NE	-6.89	97.32	111.80
3	CCC	5	ARG	CG-CD-NE	-5.98	99.24	111.80
3	CCC	5	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	CCC	376	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	AAA	811	0	830	8	0
2	BBB	992	0	961	8	0
3	CCC	4458	0	4419	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	8	0	12	1	0
4	BBB	4	0	6	0	0
4	CCC	16	0	24	3	0
5	AAA	20	0	0	1	0
5	BBB	10	0	0	1	0
5	CCC	65	0	0	7	0
6	CCC	2	0	0	0	0
7	CCC	1	0	0	1	0
8	CCC	24	0	0	7	0
9	AAA	64	0	0	2	0
9	BBB	75	0	0	1	0
9	CCC	330	0	0	4	0
All	All	6880	0	6252	79	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 6.

The worst 5 of 79 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)
3:CCC:321:VAL:HG13	5:CCC:622:SO4:O3	1.25	1.35
3:CCC:321:VAL:CG1	5:CCC:622:SO4:O3	1.98	1.12
3:CCC:318[B]:MET:HE3	3:CCC:318[B]:MET:O	1.66	0.94
1:AAA:79:ASP:OD1	1:AAA:96:HIS:HD2	1.53	0.90
3:CCC:318[B]:MET:SD	3:CCC:367[B]:MET:HE1	2.13	0.87

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	102/100 (102%)	102 (100%)	0	0	100	100
2	BBB	125/122 (102%)	122 (98%)	2 (2%)	1 (1%)	19	9
3	CCC	580/570 (102%)	552 (95%)	27 (5%)	1 (0%)	47	37
All	All	807/792 (102%)	776 (96%)	29 (4%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	99	ILE
3	CCC	283	HIS

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	AAA	87/83 (105%)	87 (100%)	0	100	100
2	BBB	106/101 (105%)	101 (95%)	5 (5%)	26	14
3	CCC	476/458 (104%)	460 (97%)	16 (3%)	37	25
All	All	669/642 (104%)	648 (97%)	21 (3%)	43	29

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CCC	326	LYS
3	CCC	446	LYS
3	CCC	554	THR
3	CCC	549	ASP
3	CCC	396	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	CXM	AAA	1	1	8,10,11	0.76	0	7,11,13	1.02	1 (14%)
3	KCX	CCC	220	6,3	9,11,12	2.20	1 (11%)	5,12,14	3.25	1 (20%)

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
1	CXM	AAA	1	1	-	4/9/10/12	-
3	KCX	CCC	220	6,3	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	220	KCX	OQ1-CX	6.05	1.32	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	220	KCX	OQ1-CX-NZ	-7.17	113.84	124.96
1	AAA	1	CXM	C-CA-N	2.09	113.50	109.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	CXM	O-C-CA-CB
1	AAA	1	CXM	C-CA-N-CN
1	AAA	1	CXM	CB-CA-N-CN
1	AAA	1	CXM	ON1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	1	CXM	1	0
3	CCC	220	KCX	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 3 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	$\#|Z| > 2$
5	SO4	CCC	611	-	4,4,4	0.32	0	6,6,6	0.11	0
5	SO4	CCC	619	-	4,4,4	0.35	0	6,6,6	0.12	0
5	SO4	CCC	623	-	4,4,4	0.32	0	6,6,6	0.15	0
5	SO4	CCC	618	-	4,4,4	0.29	0	6,6,6	0.12	0
5	SO4	CCC	614	-	4,4,4	0.26	0	6,6,6	0.07	0
8	AUF	CCC	610	3	6,7,7	0.34	0	6,9,9	0.84	0
5	SO4	CCC	612	-	4,4,4	0.34	0	6,6,6	0.32	0
4	EDO	BBB	201	-	3,3,3	0.31	0	2,2,2	1.01	0
5	SO4	CCC	617	-	4,4,4	0.34	0	6,6,6	0.11	0
5	SO4	CCC	621	-	4,4,4	0.42	0	6,6,6	0.05	0
5	SO4	CCC	620	-	4,4,4	0.33	0	6,6,6	0.14	0
4	EDO	CCC	606	-	3,3,3	0.32	0	2,2,2	0.93	0
4	EDO	AAA	202	-	3,3,3	1.20	0	2,2,2	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	CCC	622	-	4,4,4	0.31	0	6,6,6	0.25	0
4	EDO	CCC	603	-	3,3,3	0.63	0	2,2,2	0.93	0
5	SO4	AAA	203	-	4,4,4	0.31	0	6,6,6	0.11	0
5	SO4	CCC	616	-	4,4,4	0.39	0	6,6,6	0.29	0
5	SO4	AAA	205	-	4,4,4	0.25	0	6,6,6	0.23	0
8	AUF	CCC	609	3	6,7,7	0.78	0	6,9,9	0.61	0
4	EDO	AAA	201	-	3,3,3	0.47	0	2,2,2	0.56	0
4	EDO	CCC	605	-	3,3,3	0.71	0	2,2,2	1.39	0
5	SO4	BBB	203	-	4,4,4	0.32	0	6,6,6	0.20	0
8	AUF	CCC	608	3	6,7,7	0.26	0	6,9,9	0.64	0
5	SO4	AAA	206	-	4,4,4	0.30	0	6,6,6	0.17	0
4	EDO	CCC	607	-	3,3,3	0.44	0	2,2,2	0.58	0
5	SO4	AAA	204	-	4,4,4	0.48	0	6,6,6	0.27	0
5	SO4	CCC	615	-	4,4,4	0.35	0	6,6,6	0.27	0
5	SO4	BBB	202	-	4,4,4	0.34	0	6,6,6	0.10	0
5	SO4	CCC	613	-	4,4,4	0.30	0	6,6,6	0.17	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
4	EDO	CCC	606	-	-	1/1/1/1	-
4	EDO	AAA	202	-	-	1/1/1/1	-
8	AUF	CCC	608	3	-	4/6/9/9	-
4	EDO	AAA	201	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	0/1/1/1	-
8	AUF	CCC	609	3	-	4/6/9/9	-
4	EDO	CCC	603	-	-	0/1/1/1	-
4	EDO	CCC	605	-	-	0/1/1/1	-
8	AUF	CCC	610	3	-	4/6/9/9	-
4	EDO	BBB	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	CCC	608	AUF	C2-C1-P1-C3

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Mol	Chain	Res	Type	Atoms
8	CCC	610	AUF	C4-C3-P1-C1
4	AAA	202	EDO	O1-C1-C2-O2
4	BBB	201	EDO	O1-C1-C2-O2
8	CCC	608	AUF	C6-C5-P1-C1

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	623	SO4	1	0
8	CCC	610	AUF	1	0
5	CCC	620	SO4	1	0
4	AAA	202	EDO	1	0
5	CCC	622	SO4	5	0
8	CCC	609	AUF	1	0
4	CCC	605	EDO	1	0
8	CCC	608	AUF	5	0
4	CCC	607	EDO	2	0
5	AAA	204	SO4	1	0
5	BBB	202	SO4	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 AUF CCC 610

Bond lengths

Bond angles

Torsions

Rings

Ligand AUF CCC 609

Bond lengths

Bond angles

Torsions

Rings

Ligand AUF CCC 608

Bond lengths

Bond angles

Torsions

Rings
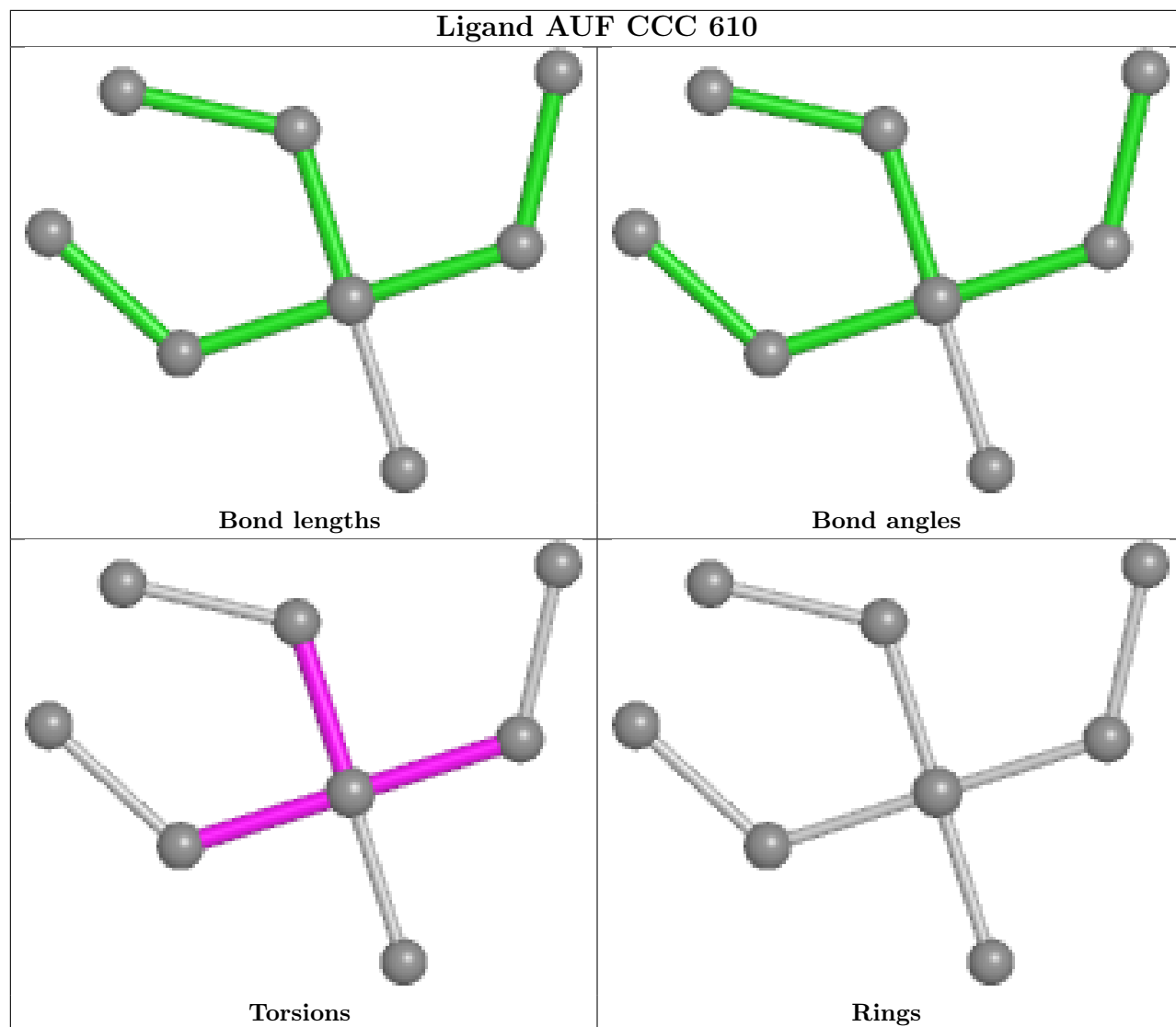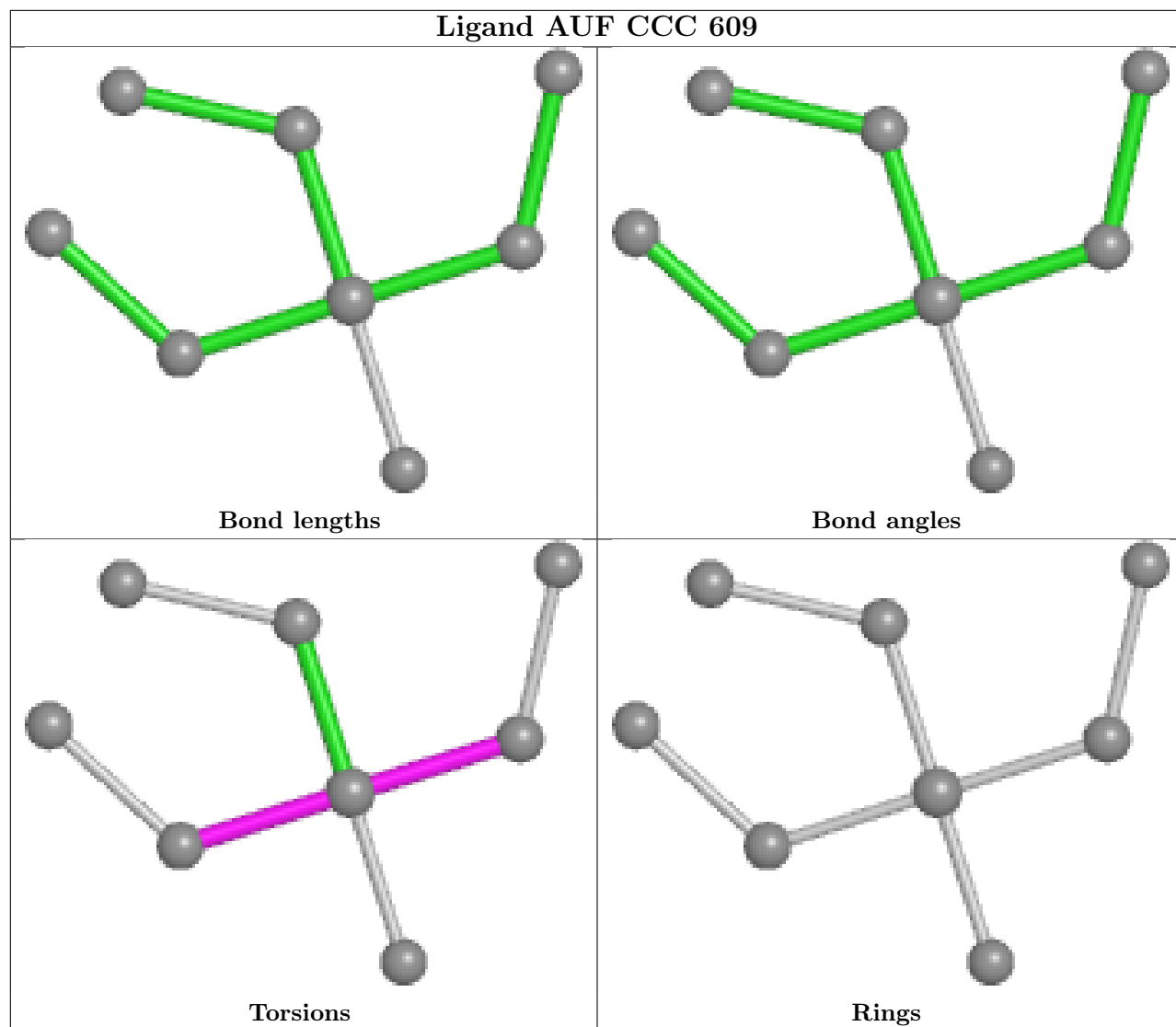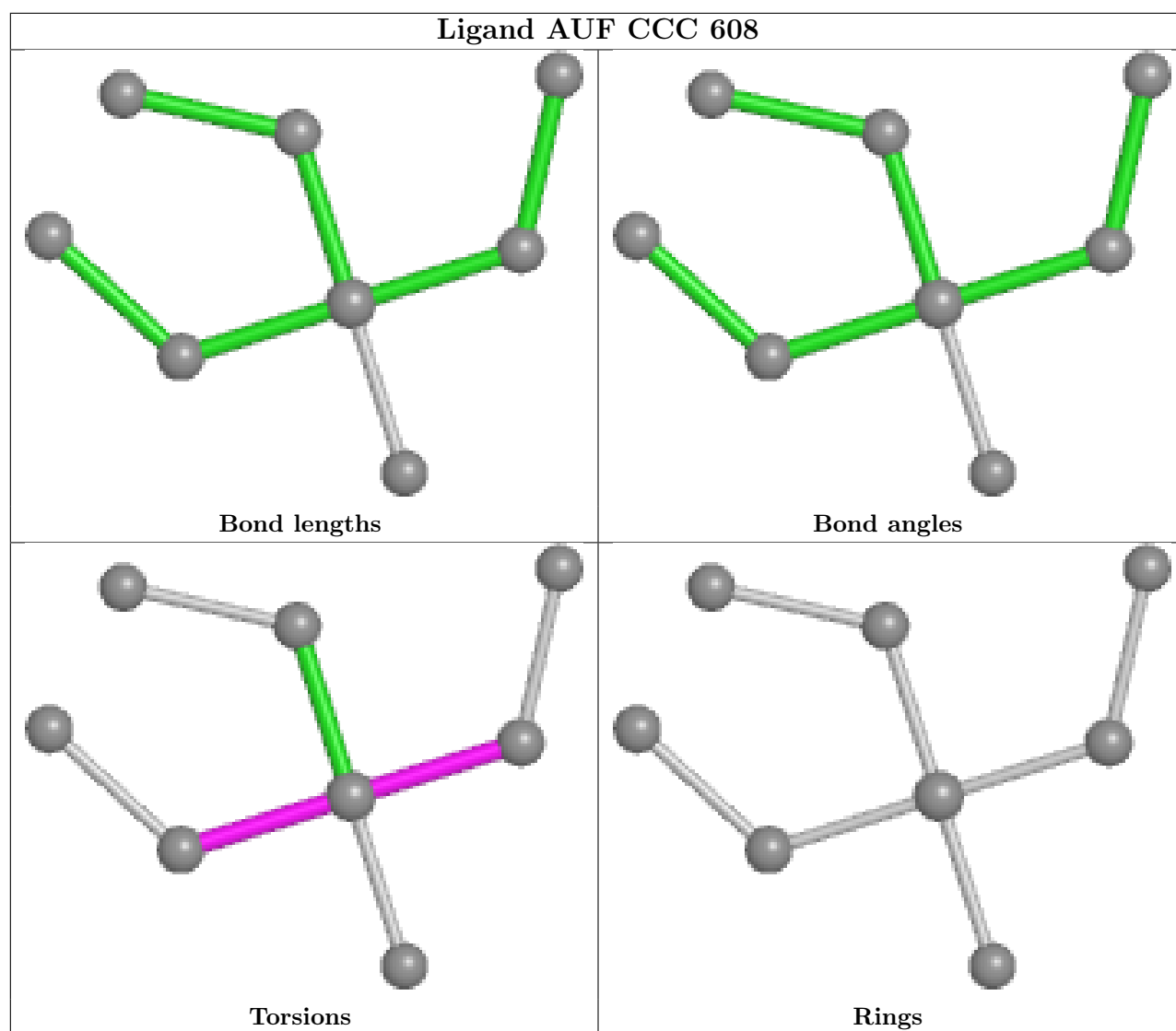
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	AAA	99/100 (99%)	-0.50	0	100	100	29, 33, 44, 60	0
2	BBB	122/122 (100%)	-0.36	2 (1%)	72	74	30, 36, 54, 92	0
3	CCC	562/570 (98%)	-0.23	10 (1%)	68	70	27, 33, 57, 95	0
All	All	783/792 (98%)	-0.28	12 (1%)	73	75	27, 33, 55, 95	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	126	GLU	3.6
3	CCC	553	LEU	3.3
3	CCC	395	LYS	3.2
2	BBB	120	LEU	2.5
3	CCC	487	ILE	2.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	CXM	AAA	1	11/12	0.97	0.11	30,32,41,41	0
3	KCX	CCC	220	12/13	0.98	0.06	26,28,35,35	0

6.3 Carbohydrates ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	SO4	AAA	203	5/5	0.37	1.44	54,55,56,65	5
4	EDO	BBB	201	4/4	0.63	0.49	70,71,74,74	0
4	EDO	CCC	607	4/4	0.74	0.27	59,68,81,85	0
5	SO4	CCC	622	5/5	0.80	0.26	33,58,63,66	5
5	SO4	CCC	623	5/5	0.80	0.32	69,80,103,106	5
4	EDO	AAA	202	4/4	0.81	0.16	41,46,62,65	0
4	EDO	CCC	606	4/4	0.84	0.20	59,62,64,66	0
5	SO4	CCC	611	5/5	0.85	0.29	105,115,137,146	0
5	SO4	CCC	618	5/5	0.85	0.33	71,103,123,150	0
5	SO4	AAA	206	5/5	0.87	0.27	51,123,127,147	0
5	SO4	CCC	619	5/5	0.87	0.43	111,122,132,140	0
5	SO4	CCC	612	5/5	0.89	0.24	69,92,99,126	0
5	SO4	CCC	614	5/5	0.89	0.12	77,77,80,81	5
5	SO4	AAA	204	5/5	0.89	0.21	49,53,56,75	5
5	SO4	BBB	202	5/5	0.90	0.24	104,112,131,138	0
4	EDO	CCC	603	4/4	0.90	0.14	52,52,54,59	0
5	SO4	CCC	620	5/5	0.91	0.24	86,105,109,128	0
5	SO4	BBB	203	5/5	0.91	0.21	89,91,103,103	0
4	EDO	CCC	605	4/4	0.91	0.18	45,45,47,67	0
5	SO4	CCC	616	5/5	0.92	0.19	37,48,52,66	5
5	SO4	AAA	205	5/5	0.93	0.16	55,93,102,123	0
5	SO4	CCC	617	5/5	0.94	0.15	115,119,130,135	0
5	SO4	CCC	615	5/5	0.94	0.17	63,91,104,129	0
5	SO4	CCC	613	5/5	0.94	0.22	69,84,86,98	0
4	EDO	AAA	201	4/4	0.98	0.13	40,43,43,45	0
5	SO4	CCC	621	5/5	0.98	0.83	46,47,48,48	5
7	O	CCC	604	1/1	0.98	0.06	32,32,32,32	0
6	NI	CCC	602	1/1	1.00	0.07	36,36,36,36	0
6	NI	CCC	601	1/1	1.00	0.06	35,35,35,35	0
8	AUF	CCC	608	8/8	1.00	0.08	49,61,78,83	8
8	AUF	CCC	609	8/8	1.00	0.07	53,73,86,91	8
8	AUF	CCC	610	8/8	1.00	0.05	42,53,60,63	8

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.
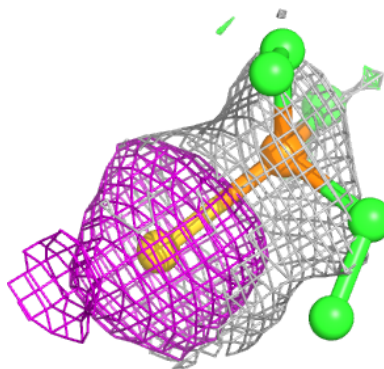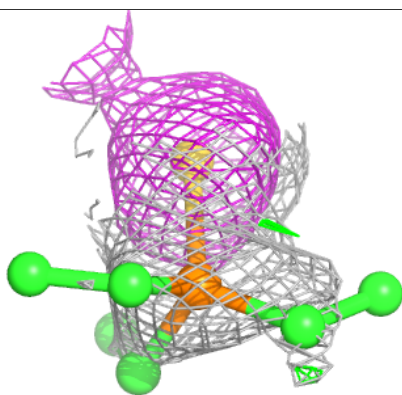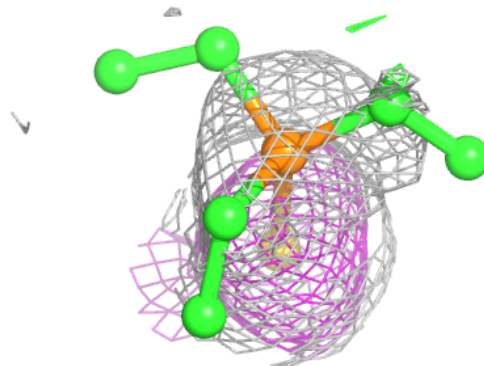
Electron density around AUF CCC 608:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
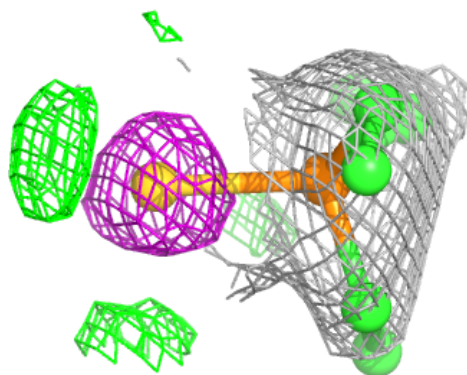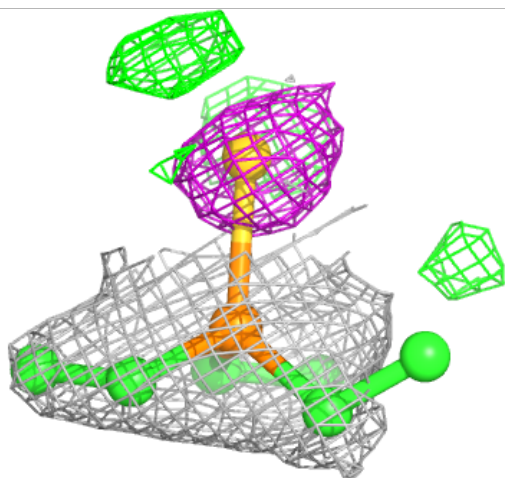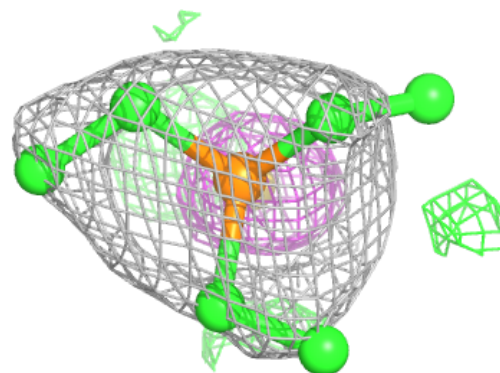and green (positive)
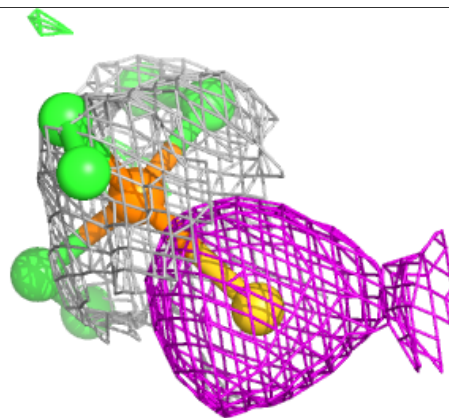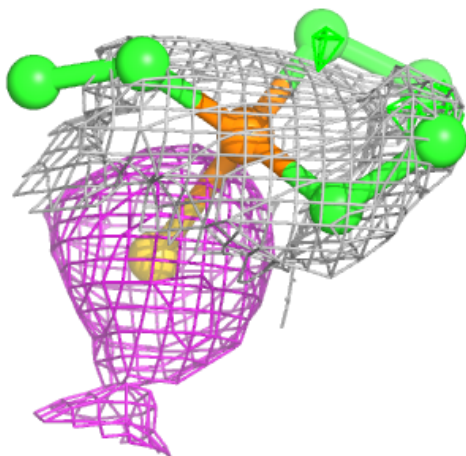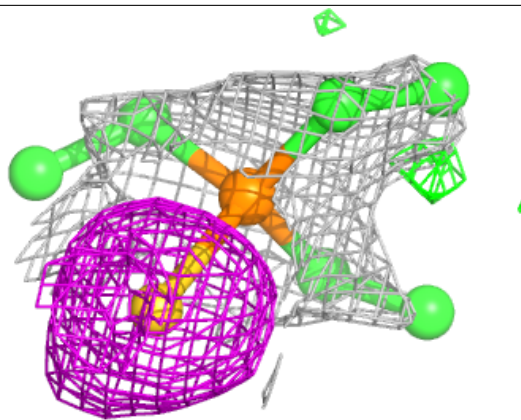
Electron density around AUF CCC 609:

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

Electron density around AUF CCC 610:

$2mF_o$-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.