



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 07:17 pm BST

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)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

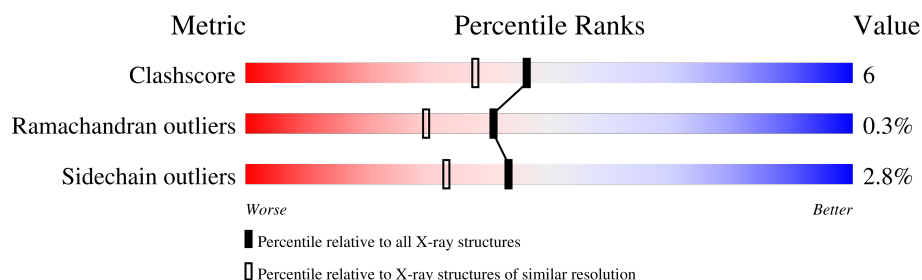
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	100	
2	BBB	122	
3	CCC	570	

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
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<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

Continued on next page...

Continued from previous page...

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

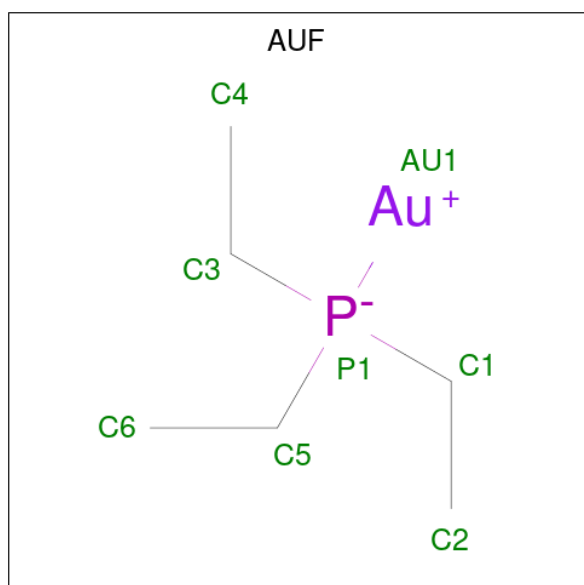
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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

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

- Molecule 8 is triethylphosphanuidylgold(1+) (three-letter code: AUF) (formula: C<sub>6</sub>H<sub>15</sub>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 [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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Urease subunit gamma

Chain AAA:  91% 8% .



- Molecule 2: Urease subunit beta

Chain BBB:  92% 7% .



- Molecule 3: Urease subunit alpha

Chain CCC:  87% 11% ..





## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.80Å 131.80Å 189.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.98 – 1.87	Depositor
% Data completeness (in resolution range)	100.0 (65.98-1.87)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.165 , 0.210	Depositor
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.659	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: O, NI, EDO, KCX, AUF, SO4, CXM

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(°)	Ideal(°)
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 [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	AAA	811	0	830	8	0
2	BBB	992	0	961	8	0
3	CCC	4458	0	4419	58	0

*Continued on next page...*

*Continued from previous page...*

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.

All (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
3:CCC:318[B]:MET:CE	3:CCC:367[B]:MET:HE3	2.08	0.84
3:CCC:318[B]:MET:O	3:CCC:318[B]:MET:CE	2.27	0.81
3:CCC:318[B]:MET:CE	3:CCC:367[B]:MET:CE	2.58	0.81
3:CCC:287[B]:ILE:O	3:CCC:287[B]:ILE:HD13	1.85	0.76
3:CCC:318[B]:MET:HE1	3:CCC:367[B]:MET:CE	2.15	0.76
3:CCC:318[B]:MET:HE1	8:CCC:608:AUF:C6	2.16	0.75
1:AAA:63:VAL:O	4:AAA:202:EDO:H11	1.88	0.73
5:CCC:620:SO4:O3	9:CCC:701:HOH:O	2.05	0.73
2:BBB:31:ARG:HG2	2:BBB:84[B]:GLU:HG2	1.70	0.72
3:CCC:318[B]:MET:HE1	3:CCC:367[B]:MET:HE3	1.73	0.71
3:CCC:63[B]:THR:HG22	9:CCC:844:HOH:O	1.92	0.69
3:CCC:4[A]:ASN:HD21	3:CCC:7:GLN:HE21	1.41	0.69
2:BBB:111:GLU:H	2:BBB:111:GLU:CD	1.97	0.68
5:CCC:622:SO4:O2	9:CCC:702:HOH:O	2.10	0.67
7:CCC:604:O:O	9:CCC:703:HOH:O	2.13	0.66
3:CCC:367[A]:MET:SD	8:CCC:609:AUF:C4	2.84	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CCC:610:AUF:AU1	8:CCC:610:AUF:P1	2.27	0.62
3:CCC:318[B]:MET:CE	3:CCC:367[B]:MET:HE1	2.30	0.61
2:BBB:31:ARG:N	5:BBB:202:SO4:O3	2.25	0.60
3:CCC:318[B]:MET:HE2	3:CCC:367[B]:MET:HE3	1.82	0.60
1:AAA:79:ASP:OD1	1:AAA:96:HIS:CD2	2.46	0.59
3:CCC:321:VAL:HG12	8:CCC:608:AUF:C6	2.33	0.59
8:CCC:608:AUF:C2	8:CCC:608:AUF:C4	2.82	0.57
8:CCC:608:AUF:P1	8:CCC:608:AUF:AU1	2.33	0.57
3:CCC:301:THR:CG2	3:CCC:363:ASP:HB2	2.36	0.56
3:CCC:318[B]:MET:CE	8:CCC:608:AUF:C6	2.83	0.55
1:AAA:29[A]:LYS:HE2	9:AAA:328:HOH:O	2.09	0.53
3:CCC:350:ILE:HD11	3:CCC:555:CYS:HB2	1.91	0.53
3:CCC:64[A]:GLU:O	3:CCC:65:ASN:HB2	2.10	0.52
3:CCC:294:PRO:HD2	4:CCC:607:EDO:C2	2.40	0.51
2:BBB:115:GLN:NE2	9:BBB:301:HOH:O	2.42	0.51
2:BBB:126:GLU:HA	2:BBB:126:GLU:OE1	2.11	0.51
3:CCC:312:ILE:HG22	3:CCC:316:LEU:HD22	1.93	0.51
3:CCC:294:PRO:HD2	4:CCC:607:EDO:H22	1.93	0.50
3:CCC:322:CYS:SG	3:CCC:327:GLN:HB2	2.51	0.50
3:CCC:538:ASP:HA	4:CCC:605:EDO:O1	2.10	0.50
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	2.99	0.49
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.93	0.49
3:CCC:325:LEU:HD21	5:CCC:622:SO4:O1	2.12	0.49
3:CCC:366:ALA:O	3:CCC:367[B]:MET:HG2	2.13	0.49
3:CCC:4[A]:ASN:ND2	3:CCC:7:GLN:HE21	2.11	0.48
2:BBB:125:VAL:O	2:BBB:126:GLU:C	2.52	0.47
3:CCC:323:HIS:HD2	3:CCC:329:ILE:O	1.97	0.47
3:CCC:318[B]:MET:HG3	3:CCC:367[B]:MET:CE	2.46	0.46
3:CCC:303:PRO:HG3	3:CCC:368:GLY:HA2	1.97	0.46
3:CCC:249:HIS:HE1	5:CCC:623:SO4:O4	1.98	0.46
3:CCC:326:LYS:CB	3:CCC:326:LYS:NZ	2.79	0.45
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	2.99	0.45
3:CCC:318[B]:MET:CE	3:CCC:318[B]:MET:C	2.83	0.45
3:CCC:318[B]:MET:O	3:CCC:318[B]:MET:HE2	2.14	0.45
3:CCC:220:KCX:CX	3:CCC:222:HIS:HD2	2.30	0.45
3:CCC:353:ASP:OD2	3:CCC:388[A]:ARG:HD3	2.17	0.44
1:AAA:30:LEU:HD13	1:AAA:38:ILE:HD12	1.98	0.44
3:CCC:301:THR:HG21	3:CCC:363:ASP:HB2	1.98	0.44
3:CCC:307:PHE:O	3:CCC:383:LYS:HE3	2.18	0.44
3:CCC:318[B]:MET:CG	3:CCC:367[B]:MET:HE1	2.47	0.44
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.52	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:318[B]:MET:CE	3:CCC:318[B]:MET:CA	2.95	0.44
3:CCC:201:HIS:CD2	3:CCC:225:TRP:HB2	2.54	0.43
3:CCC:274:PHE:O	3:CCC:275:HIS:C	2.57	0.43
3:CCC:314:GLU:O	3:CCC:317:ASP:HB3	2.19	0.43
2:BBB:126:GLU:OE1	2:BBB:126:GLU:CA	2.67	0.42
3:CCC:318[B]:MET:HG3	3:CCC:367[B]:MET:SD	2.59	0.42
3:CCC:488:HIS:CE1	3:CCC:511[B]:LYS:HD2	2.55	0.42
3:CCC:321:VAL:HG13	5:CCC:622:SO4:S	2.45	0.41
3:CCC:302:ASN:N	3:CCC:303:PRO:CD	2.84	0.41
1:AAA:1:CXM:ON1	9:AAA:301:HOH:O	2.22	0.41
1:AAA:96:HIS:O	1:AAA:97:ASN:C	2.60	0.41
3:CCC:302:ASN:N	3:CCC:303:PRO:HD3	2.36	0.41
3:CCC:305:ARG:HA	3:CCC:306:PRO:HA	1.79	0.41
3:CCC:99:LYS:C	3:CCC:99:LYS:HD3	2.41	0.40
3:CCC:299:SER:HB3	3:CCC:359:MET:HB2	2.02	0.40
1:AAA:10:LYS:NZ	5:AAA:204:SO4:O3	2.28	0.40
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BBB	18	GLU
2	BBB	54[A]	GLU
2	BBB	54[B]	GLU
2	BBB	111	GLU
2	BBB	126	GLU
3	CCC	1[A]	MET
3	CCC	1[B]	MET
3	CCC	4[A]	ASN
3	CCC	4[B]	ASN
3	CCC	7	GLN
3	CCC	158	PHE
3	CCC	249	HIS
3	CCC	285	PRO
3	CCC	316	LEU
3	CCC	326	LYS
3	CCC	395	LYS
3	CCC	396	ASN
3	CCC	446	LYS
3	CCC	549	ASP
3	CCC	553	LEU
3	CCC	554	THR

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	6,10,11	0.64	0	5,11,13	1.20	1 (20%)
3	KCX	CCC	220	3,6	7,11,12	0.73	0	4,12,14	0.51	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
1	CXM	AAA	1	1	-	2/7/10/12	-
3	KCX	CCC	220	3,6	-	0/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	1	CXM	C-CA-N	2.09	113.50	109.73

There are no chirality outliers.

All (2) 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

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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	BBB	202	-	4,4,4	0.34	0	6,6,6	0.10	0
4	EDO	CCC	607	-	3,3,3	0.44	0	2,2,2	0.58	0
5	SO4	CCC	623	-	4,4,4	0.32	0	6,6,6	0.15	0
5	SO4	AAA	203	-	4,4,4	0.31	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	613	-	4,4,4	0.30	0	6,6,6	0.17	0
5	SO4	AAA	206	-	4,4,4	0.30	0	6,6,6	0.17	0
5	SO4	CCC	617	-	4,4,4	0.34	0	6,6,6	0.11	0
5	SO4	CCC	614	-	4,4,4	0.26	0	6,6,6	0.07	0
5	SO4	AAA	205	-	4,4,4	0.25	0	6,6,6	0.23	0
4	EDO	BBB	201	-	3,3,3	0.31	0	2,2,2	1.01	0
5	SO4	CCC	620	-	4,4,4	0.33	0	6,6,6	0.14	0
4	EDO	AAA	202	-	3,3,3	1.20	0	2,2,2	0.76	0
8	AUF	CCC	610	3	6,7,7	0.34	0	6,9,9	0.84	0
5	SO4	CCC	615	-	4,4,4	0.35	0	6,6,6	0.27	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	AAA	204	-	4,4,4	0.48	0	6,6,6	0.27	0
4	EDO	CCC	603	-	3,3,3	0.63	0	2,2,2	0.93	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
5	SO4	CCC	618	-	4,4,4	0.29	0	6,6,6	0.12	0
4	EDO	CCC	606	-	3,3,3	0.32	0	2,2,2	0.93	0
5	SO4	CCC	622	-	4,4,4	0.31	0	6,6,6	0.25	0
5	SO4	CCC	619	-	4,4,4	0.35	0	6,6,6	0.12	0
5	SO4	CCC	612	-	4,4,4	0.34	0	6,6,6	0.32	0
5	SO4	CCC	611	-	4,4,4	0.32	0	6,6,6	0.11	0
8	AUF	CCC	608	3	6,7,7	0.26	0	6,9,9	0.64	0
5	SO4	CCC	616	-	4,4,4	0.39	0	6,6,6	0.29	0
4	EDO	AAA	201	-	3,3,3	0.47	0	2,2,2	0.56	0
8	AUF	CCC	609	3	6,7,7	0.78	0	6,9,9	0.61	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	603	-	-	0/1/1/1	-
4	EDO	CCC	605	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	0/1/1/1	-
8	AUF	CCC	610	3	-	4/6/9/9	-
4	EDO	BBB	201	-	-	1/1/1/1	-
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	-
8	AUF	CCC	609	3	-	4/6/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	CCC	608	AUF	C2-C1-P1-C3
8	CCC	610	AUF	C4-C3-P1-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	AAA	202	EDO	O1-C1-C2-O2
4	BBB	201	EDO	O1-C1-C2-O2
8	CCC	608	AUF	C6-C5-P1-C1
8	CCC	610	AUF	C4-C3-P1-C5
8	CCC	609	AUF	C6-C5-P1-C3
8	CCC	609	AUF	C6-C5-P1-C1
8	CCC	608	AUF	C6-C5-P1-C3
8	CCC	609	AUF	C2-C1-P1-C5
8	CCC	608	AUF	C2-C1-P1-C5
8	CCC	610	AUF	C2-C1-P1-C5
8	CCC	609	AUF	C2-C1-P1-C3
8	CCC	610	AUF	C6-C5-P1-C3
4	CCC	606	EDO	O1-C1-C2-O2

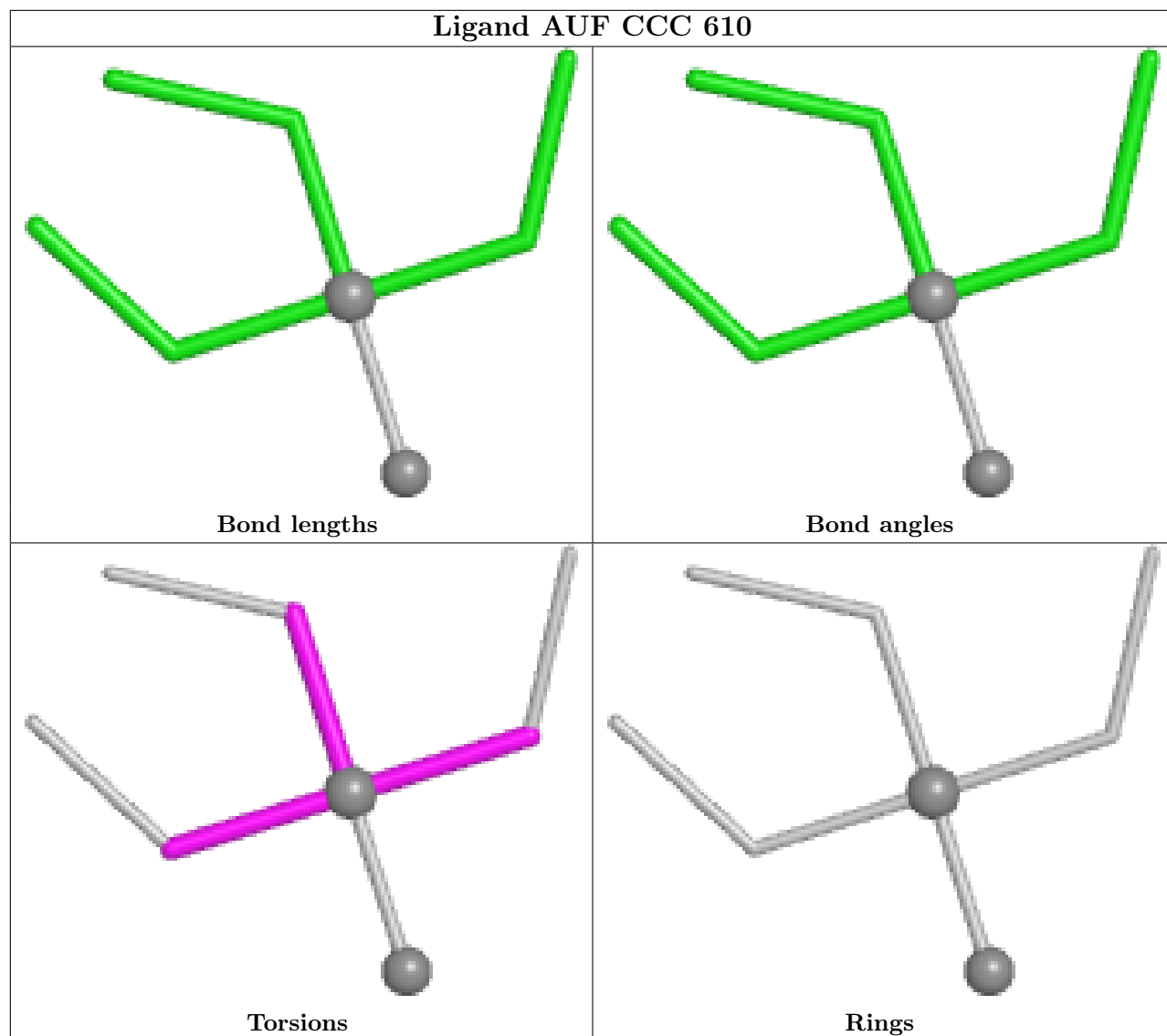
There are no ring outliers.

11 monomers are involved in 20 short contacts:

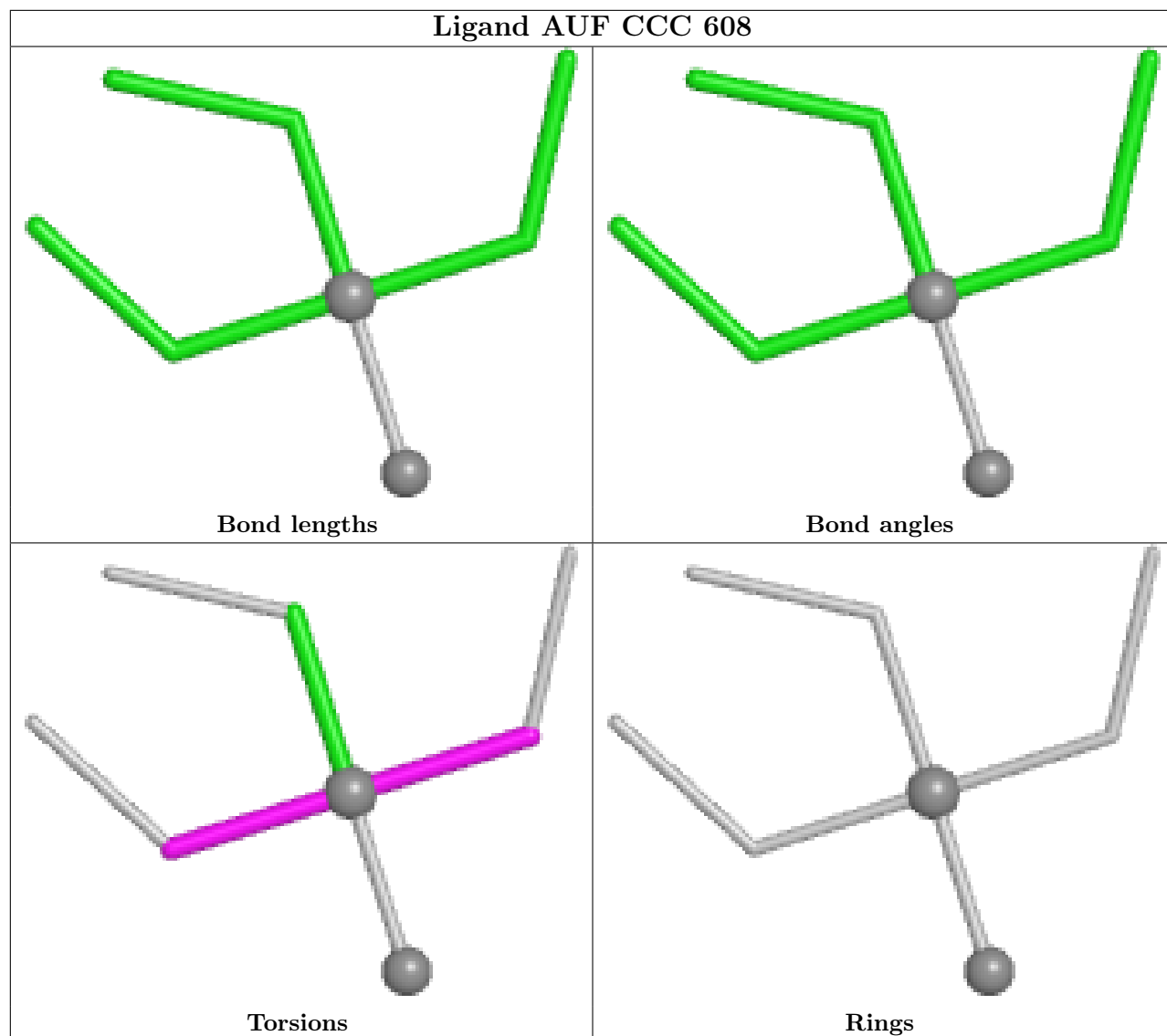
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	202	SO4	1	0
4	CCC	607	EDO	2	0
5	CCC	623	SO4	1	0
5	CCC	620	SO4	1	0
4	AAA	202	EDO	1	0
8	CCC	610	AUF	1	0
5	AAA	204	SO4	1	0
4	CCC	605	EDO	1	0
5	CCC	622	SO4	5	0
8	CCC	608	AUF	5	0
8	CCC	609	AUF	1	0

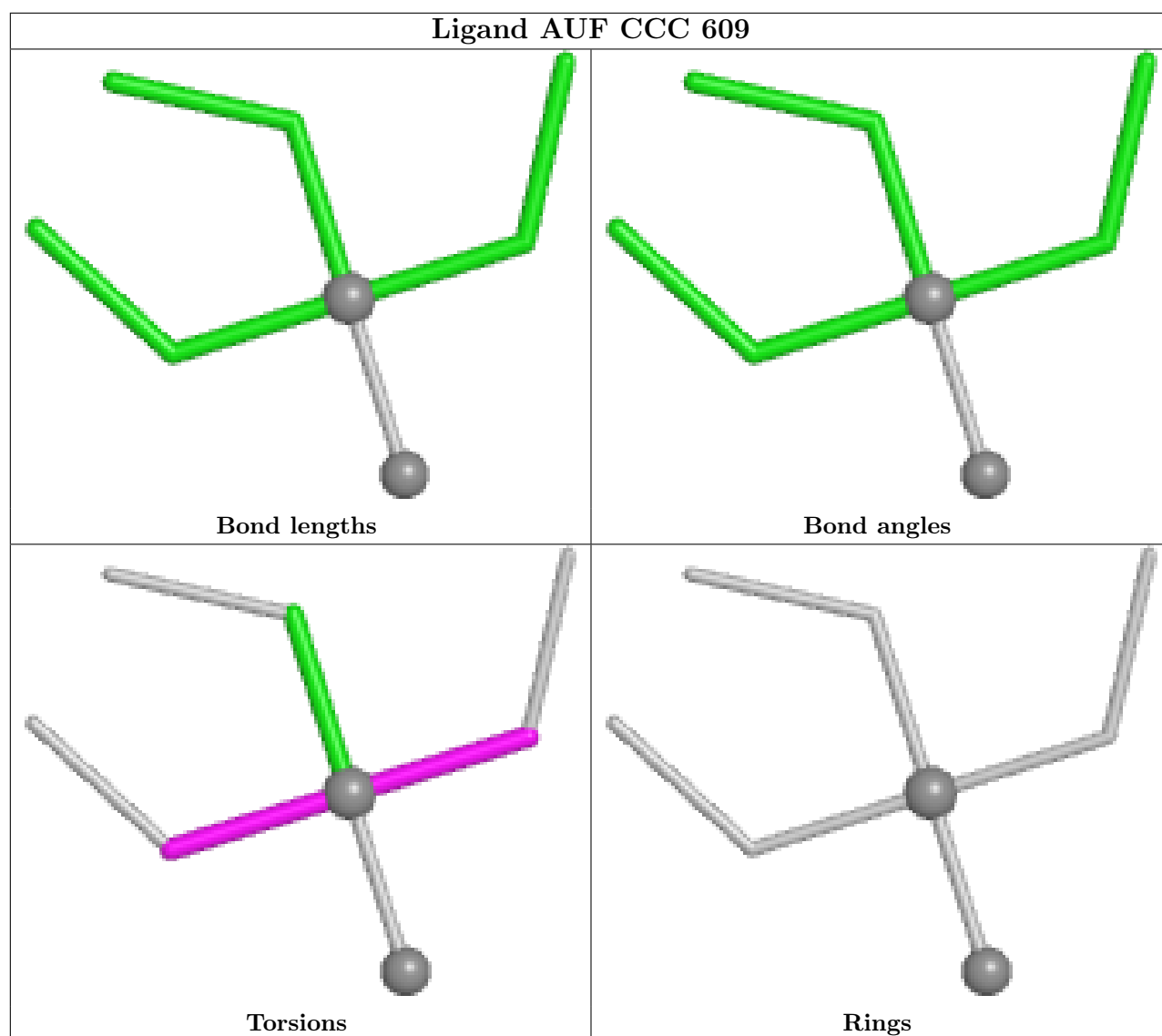
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand AUF CCC 610



## Ligand AUF CCC 608





## 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](#)

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.