



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 07:19 pm BST

PDB ID : 7P7N
Title : X-RAY CRYSTAL STRUCTURE OF SPOROSARCINA PASTEURII UREASE INHIBITED BY THE GOLD(I)-PHOSPHINE COMPOUND Au(Pet3)I DETERMINED AT 1.80 ANGSTROMS
Authors : Mazzei, L.; Ciurli, S.
Deposited on : 2021-07-20
Resolution : 1.80 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 ⓘ 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	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

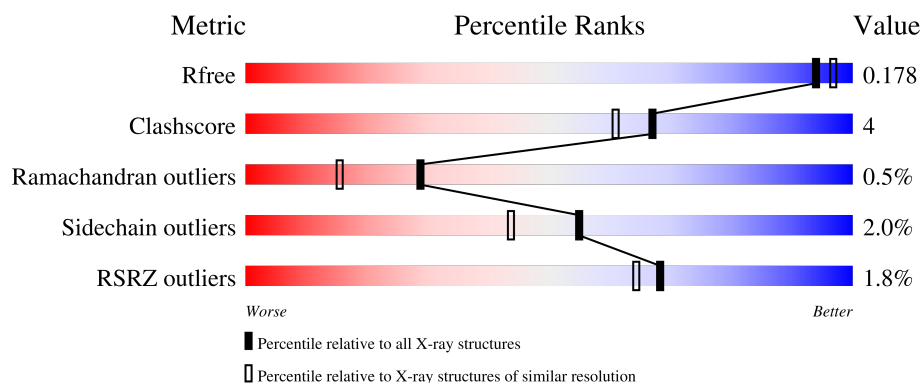
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	100	<div> <div></div> <div>97%</div> <div>.</div> </div>
2	BBB	122	<div> <div>%</div> <div>94%</div> <div>5% .</div> </div>
3	CCC	570	<div> <div>2%</div> <div>89%</div> <div>9% ..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	CCC	614	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6931 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	3	0
			802	505	135	154	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	6	0
			1003	617	181	204	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	564	Total	C	N	O	S	0	21	0
			4435	2776	761	872	26			

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: C₂H₆O₂).



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	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		
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: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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	0	0
			5	4	1		

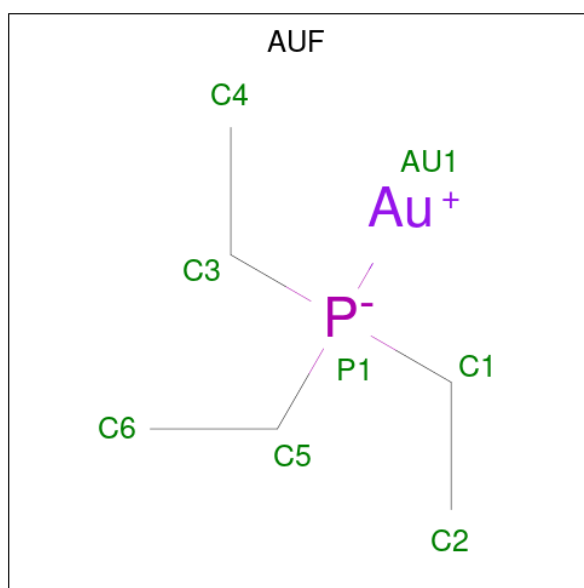
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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

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

- Molecule 8 is triethylphosphanuidylgold(1+) (three-letter code: AUF) (formula: C₆H₁₅AuP).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	CCC	1	Total	Au	C	P	0	0
			8	1	6	1		

- Molecule 9 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	CCC	5	Total	Au	0	0
			5	5		

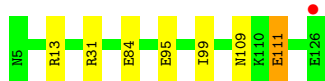
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	70	Total 70	O 70	0	0
10	BBB	103	Total 103	O 103	0	0
10	CCC	375	Total 375	O 375	0	0

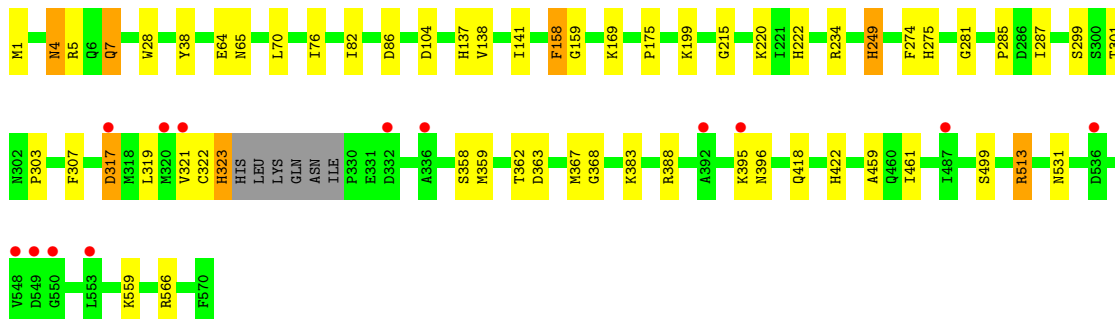
- Molecule 1: Urease subunit gamma



- Chain BBB:  %



- Chain CCC:  89% 9% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.65Å 131.65Å 189.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.91 – 1.80 72.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.91-1.80) 100.0 (72.80-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.155 , 0.176 0.157 , 0.178	Depositor DCC
R_{free} test set	4419 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6931	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: AUF, EDO, CXM, KCX, O, NI, SO4, AU

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	0/802	0.86	0/1078
2	BBB	0.58	0/1015	0.84	0/1365
3	CCC	0.62	0/4502	0.84	6/6097 (0.1%)
All	All	0.62	0/6319	0.84	6/8540 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	566	ARG	NE-CZ-NH2	-7.13	116.73	120.30
3	CCC	5	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	CCC	513	ARG	CG-CD-NE	-6.03	99.13	111.80
3	CCC	5	ARG	CB-CG-CD	-5.90	96.25	111.60
3	CCC	234	ARG	CG-CD-NE	-5.51	100.22	111.80
3	CCC	388	ARG	NE-CZ-NH1	5.08	122.84	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	802	0	818	2	0
2	BBB	1003	0	973	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	4435	0	4372	30	0
4	AAA	16	0	24	0	0
4	BBB	4	0	6	0	0
4	CCC	32	0	48	7	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	0	0
8	CCC	8	0	0	0	0
9	CCC	5	0	0	0	0
10	AAA	70	0	0	1	0
10	BBB	103	0	0	1	0
10	CCC	375	0	0	5	0
All	All	6931	0	6241	49	0

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

All (49) 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)
5:CCC:616:SO4:O3	10:CCC:701:HOH:O	1.90	0.88
5:CCC:626:SO4:O4	4:CCC:630:EDO:H12	1.85	0.77
4:CCC:628:EDO:H11	4:CCC:629:EDO:H21	1.69	0.73
2:BBB:13[B]:ARG:CG	2:BBB:13[B]:ARG:HH11	2.03	0.72
2:BBB:111:GLU:H	2:BBB:111:GLU:CD	1.95	0.69
5:CCC:617:SO4:O1	10:CCC:702:HOH:O	2.14	0.66
2:BBB:13[A]:ARG:HG3	3:CCC:28:TRP:CZ3	2.36	0.60
2:BBB:109[B]:ASN:OD1	2:BBB:111:GLU:OE1	2.21	0.58
3:CCC:422:HIS:O	5:CCC:620:SO4:O4	2.22	0.56
2:BBB:13[B]:ARG:HH11	2:BBB:13[B]:ARG:HG3	1.72	0.54
3:CCC:64[A]:GLU:O	3:CCC:65:ASN:HB2	2.10	0.51
4:CCC:603:EDO:C1	10:CCC:808:HOH:O	2.58	0.50
3:CCC:362:THR:O	3:CCC:368:GLY:HA3	2.12	0.50
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.46	0.50
3:CCC:4[A]:ASN:HD21	3:CCC:7:GLN:NE2	2.10	0.50
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.94	0.49
3:CCC:323:HIS:ND1	3:CCC:323:HIS:C	2.65	0.49
4:CCC:603:EDO:H21	10:CCC:1007:HOH:O	2.11	0.49
3:CCC:175:PRO:HB3	3:CCC:199:LYS:HE3	1.94	0.49
4:CCC:628:EDO:H11	4:CCC:629:EDO:C2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:459:ALA:HB1	3:CCC:461[B]:ILE:HD12	1.94	0.49
2:BBB:109[A]:ASN:ND2	10:BBB:303:HOH:O	2.46	0.48
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	3.02	0.47
3:CCC:301:THR:CG2	3:CCC:363:ASP:HB2	2.44	0.47
2:BBB:31:ARG:HG2	2:BBB:84[B]:GLU:HG2	1.97	0.47
2:BBB:13[B]:ARG:CG	2:BBB:13[B]:ARG:NH1	2.73	0.46
3:CCC:358:SER:HA	3:CCC:531:ASN:HB3	1.97	0.46
3:CCC:215:GLY:HA2	3:CCC:499:SER:CB	2.46	0.46
3:CCC:303:PRO:HG3	3:CCC:368:GLY:HA2	1.98	0.46
1:AAA:30:LEU:HD13	1:AAA:38:ILE:HD12	1.98	0.45
3:CCC:64[B]:GLU:HG2	5:CCC:624:SO4:O3	2.16	0.45
3:CCC:38:TYR:CE2	5:CCC:614:SO4:O4	2.69	0.45
3:CCC:141:ILE:HD11	3:CCC:169:LYS:HA	1.98	0.45
1:AAA:62:HIS:HD2	10:AAA:365:HOH:O	2.00	0.45
3:CCC:38:TYR:CZ	5:CCC:614:SO4:O4	2.70	0.45
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	3.01	0.44
3:CCC:317[B]:ASP:O	3:CCC:317[B]:ASP:OD1	2.35	0.44
3:CCC:287[B]:ILE:O	3:CCC:287[B]:ILE:HD13	2.17	0.44
3:CCC:299:SER:HB3	3:CCC:359:MET:HB2	1.99	0.43
3:CCC:513:ARG:NE	4:CCC:630:EDO:O2	2.48	0.43
2:BBB:31:ARG:N	5:BBB:202:SO4:O3	2.40	0.42
4:CCC:603:EDO:H12	10:CCC:808:HOH:O	2.19	0.42
3:CCC:76:ILE:O	3:CCC:82:ILE:HA	2.20	0.41
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.20	0.41
3:CCC:220:KCX:CX	3:CCC:222:HIS:HD2	2.34	0.41
2:BBB:13[B]:ARG:HG3	2:BBB:13[B]:ARG:NH1	2.36	0.41
3:CCC:307:PHE:O	3:CCC:383:LYS:HE3	2.21	0.41
3:CCC:138:VAL:O	3:CCC:159:GLY:HA3	2.22	0.40
3:CCC:303:PRO:HG2	3:CCC:367:MET:O	2.22	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	101/100 (101%)	101 (100%)	0	0	100	100
2	BBB	126/122 (103%)	121 (96%)	4 (3%)	1 (1%)	19	7
3	CCC	579/570 (102%)	549 (95%)	27 (5%)	3 (0%)	29	15
All	All	806/792 (102%)	771 (96%)	31 (4%)	4 (0%)	29	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	99	ILE
3	CCC	321	VAL
3	CCC	322	CYS
3	CCC	275	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	86/83 (104%)	86 (100%)	0	100	100
2	BBB	107/101 (106%)	106 (99%)	1 (1%)	78	75
3	CCC	473/458 (103%)	458 (97%)	15 (3%)	39	25
All	All	666/642 (104%)	650 (98%)	16 (2%)	55	36

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BBB	111	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	CCC	317[A]	ASP
3	CCC	317[B]	ASP
3	CCC	319	LEU
3	CCC	323	HIS
3	CCC	395	LYS
3	CCC	396	ASN
3	CCC	559	LYS

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	$\# Z > 2$
3	KCX	CCC	220	3,6	7,11,12	0.85	0	4,12,14	0.43	0
1	CXM	AAA	1	1	6,10,11	0.81	0	5,11,13	1.20	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
3	KCX	CCC	220	3,6	-	0/7/10/12	-
1	CXM	AAA	1	1	-	1/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 8 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	620	-	4,4,4	0.32	0	6,6,6	0.13	0
4	EDO	BBB	201	-	3,3,3	0.35	0	2,2,2	0.94	0
4	EDO	CCC	604	-	3,3,3	0.68	0	2,2,2	0.23	0
5	SO4	CCC	617	-	4,4,4	0.20	0	6,6,6	0.10	0
4	EDO	CCC	603	-	3,3,3	0.87	0	2,2,2	0.85	0
4	EDO	CCC	629	-	3,3,3	0.50	0	2,2,2	1.04	0
4	EDO	CCC	606	-	3,3,3	0.90	0	2,2,2	0.41	0
5	SO4	CCC	622	-	4,4,4	0.34	0	6,6,6	0.13	0
4	EDO	AAA	202	-	3,3,3	0.26	0	2,2,2	1.46	1 (50%)
4	EDO	AAA	203	-	3,3,3	1.11	0	2,2,2	0.28	0
5	SO4	CCC	619	-	4,4,4	0.34	0	6,6,6	0.14	0
5	SO4	BBB	202	-	4,4,4	0.31	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	CCC	621	-	4,4,4	0.38	0	6,6,6	0.15	0
5	SO4	CCC	626	-	4,4,4	0.35	0	6,6,6	0.14	0
5	SO4	CCC	624	-	4,4,4	0.33	0	6,6,6	0.27	0
4	EDO	AAA	204	-	3,3,3	0.94	0	2,2,2	0.46	0
4	EDO	CCC	607	-	3,3,3	0.62	0	2,2,2	0.52	0
5	SO4	CCC	623	-	4,4,4	0.31	0	6,6,6	0.12	0
5	SO4	CCC	614	-	4,4,4	0.33	0	6,6,6	0.25	0
8	AUF	CCC	608	3	6,7,7	0.90	0	6,9,9	0.47	0
5	SO4	CCC	625	-	4,4,4	0.38	0	6,6,6	0.07	0
4	EDO	AAA	201	-	3,3,3	0.78	0	2,2,2	0.91	0
4	EDO	CCC	628	-	3,3,3	0.49	0	2,2,2	0.41	0
4	EDO	CCC	630	-	3,3,3	0.42	0	2,2,2	0.22	0
5	SO4	BBB	203	-	4,4,4	0.26	0	6,6,6	0.12	0
5	SO4	CCC	615	-	4,4,4	0.21	0	6,6,6	0.13	0
4	EDO	CCC	627	-	3,3,3	0.88	0	2,2,2	0.41	0
5	SO4	CCC	616	-	4,4,4	0.34	0	6,6,6	0.13	0
5	SO4	CCC	618	-	4,4,4	0.21	0	6,6,6	0.09	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	627	-	-	1/1/1/1	-
4	EDO	CCC	630	-	-	0/1/1/1	-
4	EDO	AAA	202	-	-	1/1/1/1	-
4	EDO	AAA	203	-	-	1/1/1/1	-
4	EDO	BBB	201	-	-	0/1/1/1	-
4	EDO	CCC	604	-	-	1/1/1/1	-
8	AUF	CCC	608	3	-	1/6/9/9	-
4	EDO	CCC	603	-	-	1/1/1/1	-
4	EDO	AAA	201	-	-	0/1/1/1	-
4	EDO	CCC	629	-	-	1/1/1/1	-
4	EDO	CCC	606	-	-	1/1/1/1	-
4	EDO	AAA	204	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	0/1/1/1	-
4	EDO	CCC	628	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	202	EDO	O1-C1-C2	-2.06	97.11	111.91

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	202	EDO	O1-C1-C2-O2
4	AAA	203	EDO	O1-C1-C2-O2
4	CCC	603	EDO	O1-C1-C2-O2
4	CCC	606	EDO	O1-C1-C2-O2
8	CCC	608	AUF	C6-C5-P1-C3
4	CCC	604	EDO	O1-C1-C2-O2
4	CCC	629	EDO	O1-C1-C2-O2
4	CCC	627	EDO	O1-C1-C2-O2
4	CCC	628	EDO	O1-C1-C2-O2

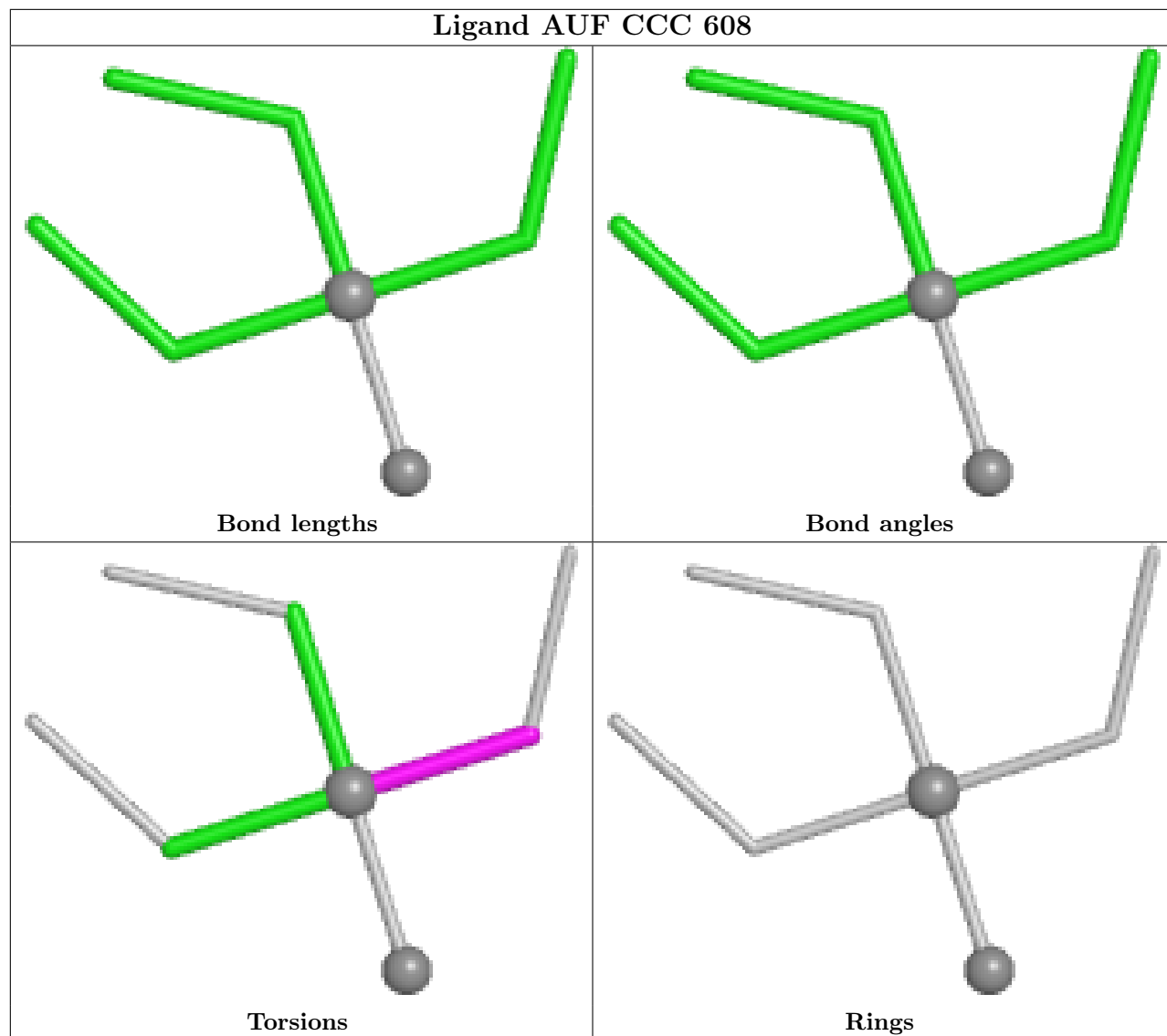
There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	620	SO4	1	0
5	CCC	617	SO4	1	0
4	CCC	603	EDO	3	0
4	CCC	629	EDO	2	0
5	BBB	202	SO4	1	0
5	CCC	626	SO4	1	0
5	CCC	624	SO4	1	0
5	CCC	614	SO4	2	0
4	CCC	628	EDO	2	0
4	CCC	630	EDO	2	0
5	CCC	616	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å ²)	Q<0.9
1	AAA	99/100 (99%)	-0.73	0 100 100	21, 26, 37, 46	0
2	BBB	122/122 (100%)	-0.60	1 (0%) 86 84	23, 29, 47, 71	0
3	CCC	563/570 (98%)	-0.34	13 (2%) 60 56	20, 26, 50, 117	0
All	All	784/792 (98%)	-0.43	14 (1%) 68 64	20, 26, 47, 117	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CCC	320	MET	3.7
3	CCC	549	ASP	3.6
3	CCC	332	ASP	3.6
3	CCC	395	LYS	3.6
3	CCC	321	VAL	3.3
3	CCC	548	VAL	3.0
3	CCC	336	ALA	2.8
3	CCC	550	GLY	2.7
3	CCC	536[A]	ASP	2.5
2	BBB	126	GLU	2.4
3	CCC	553	LEU	2.3
3	CCC	487	ILE	2.2
3	CCC	392	ALA	2.1
3	CCC	317[A]	ASP	2.0

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(\AA^2)	Q<0.9
1	CXM	AAA	1	11/12	0.97	0.10	22,25,30,31	0
3	KCX	CCC	220	12/13	0.98	0.06	20,22,31,33	0

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, 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.

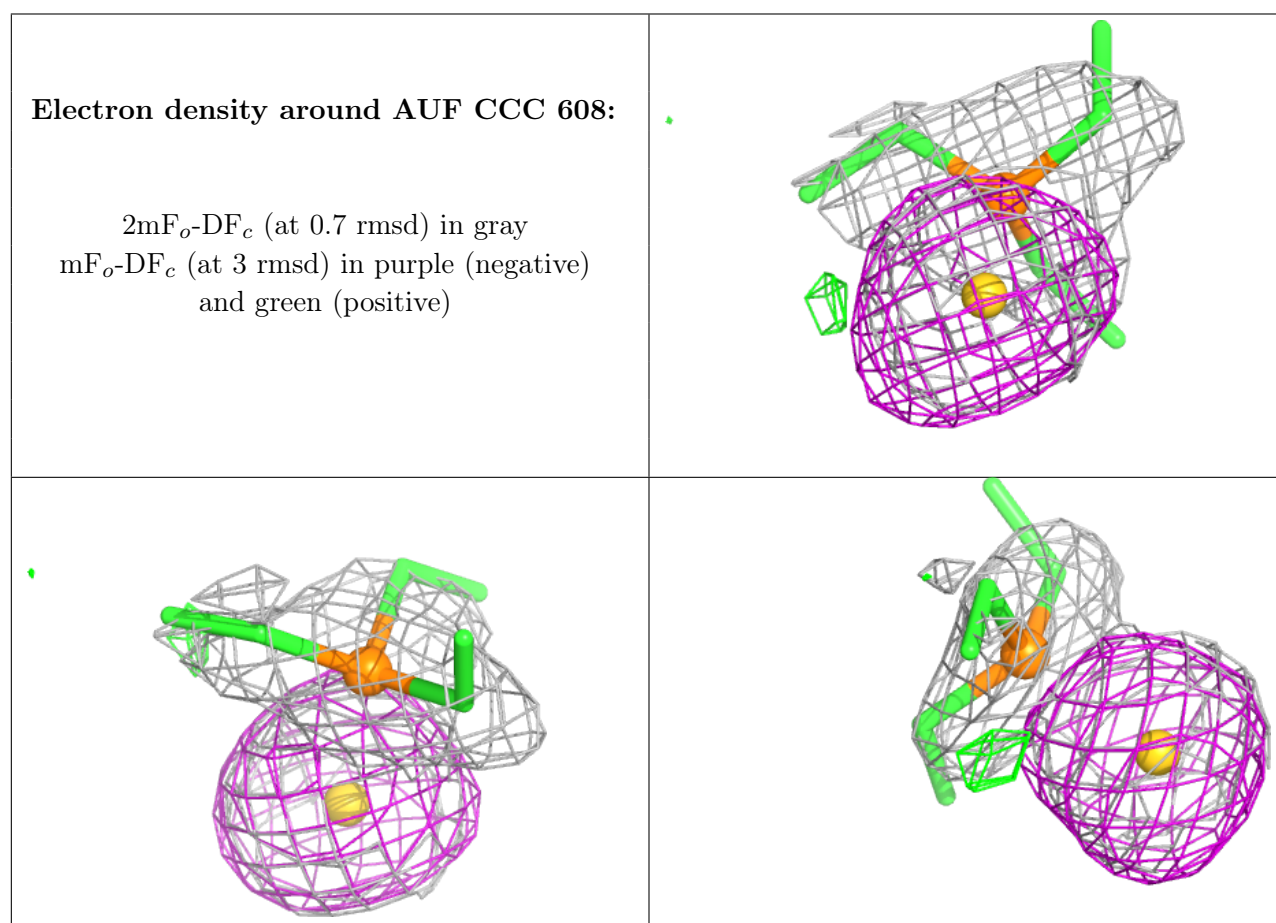
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	CCC	604	4/4	0.83	0.18	56,62,63,64	0
5	SO4	CCC	616	5/5	0.86	0.24	68,73,78,81	0
4	EDO	CCC	629	4/4	0.87	0.19	58,59,64,66	0
5	SO4	CCC	619	5/5	0.87	0.16	48,54,68,73	5
5	SO4	CCC	624	5/5	0.87	0.36	67,79,99,124	0
4	EDO	CCC	627	4/4	0.88	0.17	48,52,55,63	0
5	SO4	CCC	620	5/5	0.89	0.31	58,89,109,127	0
5	SO4	CCC	617	5/5	0.89	0.16	51,55,57,64	5
4	EDO	CCC	603	4/4	0.90	0.22	34,55,57,61	0
4	EDO	CCC	628	4/4	0.90	0.13	51,54,57,59	0
9	AU	CCC	613	1/1	0.90	0.13	96,96,96,96	1
5	SO4	CCC	623	5/5	0.91	0.31	90,101,113,118	0
5	SO4	CCC	618	5/5	0.91	0.27	62,74,91,95	0
5	SO4	CCC	622	5/5	0.91	0.30	97,111,128,137	0
5	SO4	CCC	621	5/5	0.92	0.20	48,59,68,72	5
4	EDO	AAA	203	4/4	0.92	0.09	32,34,41,42	0
4	EDO	CCC	606	4/4	0.92	0.17	37,44,45,47	0
5	SO4	CCC	614	5/5	0.92	0.29	56,74,94,113	0
5	SO4	CCC	626	5/5	0.92	0.18	32,50,57,64	5
4	EDO	AAA	202	4/4	0.92	0.12	42,43,45,48	0
4	EDO	AAA	201	4/4	0.93	0.14	42,51,53,55	0
4	EDO	CCC	630	4/4	0.94	0.16	42,53,55,57	0
5	SO4	CCC	625	5/5	0.94	0.24	85,90,90,91	5
5	SO4	BBB	202	5/5	0.94	0.29	89,91,100,112	0
7	O	CCC	605	1/1	0.94	0.06	30,30,30,30	0
5	SO4	BBB	203	5/5	0.94	0.23	71,78,83,84	0
5	SO4	CCC	615	5/5	0.95	0.24	55,64,81,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	BBB	201	4/4	0.96	0.06	45,45,46,54	0
4	EDO	AAA	204	4/4	0.96	0.10	31,39,39,43	0
4	EDO	CCC	607	4/4	0.96	0.17	36,42,44,44	0
9	AU	CCC	610	1/1	0.98	0.09	60,60,60,60	1
9	AU	CCC	611	1/1	0.99	0.06	55,55,55,55	1
9	AU	CCC	612	1/1	0.99	0.13	82,82,82,82	1
9	AU	CCC	609	1/1	0.99	0.11	69,69,69,69	1
8	AUF	CCC	608	8/8	1.00	0.12	41,64,70,80	0
6	NI	CCC	602	1/1	1.00	0.03	29,29,29,29	0
6	NI	CCC	601	1/1	1.00	0.03	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.