



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2022 – 04:14 am BST

PDB ID : 7B59  
Title : X-ray crystal structure of Sporosarcina pasteurii urease inhibited by Ag(PET3)Br determined at 1.63 Angstroms  
Authors : Mazzei, L.; Cianci, M.; Ciurli, S.  
Deposited on : 2020-12-03  
Resolution : 1.63 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
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) : 2.27

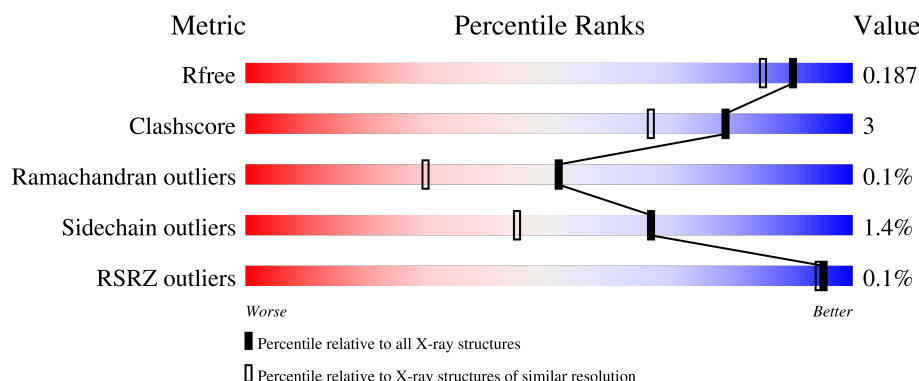
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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  $\leq 5\%$ . 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 style="width: 91%;"></div>91%<div style="width: 9%;"></div>9%</div>
2	BBB	122	<div><div style="width: 96%;"></div>96%<div style="width: 4%;"></div>..</div>
3	CCC	570	<div><div style="width: 93%;"></div>93%<div style="width: 6%;"></div>6%.</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
4	EDO	AAA	204	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7083 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	5	0
			814	513	137	157	7			

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	3	0
			976	603	175	197	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	570	Total	C	N	O	S	0	17	0
			4436	2784	765	860	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	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	BBB	1	Total	C	O	0	0
			4	2	2		
4	BBB	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		

- 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	BBB	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	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		

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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 SILVER ION (three-letter code: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	CCC	2	Total Ag 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	86	Total O 86 86	0	0
9	BBB	145	Total O 145 145	0	0
9	CCC	475	Total O 475 475	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: Urease subunit gamma

Chain AAA:  91% 9%



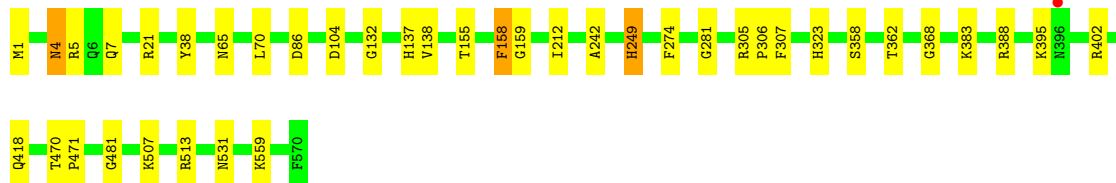
- Molecule 2: Urease subunit beta

Chain BBB:  96% . .



- Molecule 3: Urease subunit alpha

Chain CCC:  93% 6% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.41Å 131.41Å 189.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.80 – 1.63 113.80 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (113.80-1.63) 99.9 (113.80-1.63)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.149 , 0.177 0.162 , 0.187	Depositor DCC
$R_{free}$ test set	5954 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: EDO, SO4, KCX, O, CXM, AG, NI

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	0.81	0/820	0.86	0/1102
2	BBB	0.80	0/988	0.87	0/1327
3	CCC	0.77	0/4529	0.88	2/6132 (0.0%)
All	All	0.78	0/6337	0.87	2/8561 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	388	ARG	NE-CZ-NH1	7.38	123.99	120.30
3	CCC	402	ARG	NE-CZ-NH1	5.02	122.81	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	814	0	834	7	0
2	BBB	976	0	959	4	0
3	CCC	4436	0	4423	23	0
4	AAA	16	0	24	5	0
4	BBB	16	0	24	0	0
4	CCC	24	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	5	0	0	0	0
5	BBB	20	0	0	0	0
5	CCC	65	0	0	3	0
6	CCC	2	0	0	0	0
7	CCC	1	0	0	0	0
8	CCC	2	0	0	0	0
9	AAA	86	0	0	2	0
9	BBB	145	0	0	1	0
9	CCC	475	0	0	2	0
All	All	7083	0	6300	33	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 3.

All (33) 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:AAA:79:ASP:O	4:AAA:204:EDO:H21	1.87	0.75
3:CCC:38:TYR:CE2	5:CCC:622:SO4:O4	2.44	0.70
3:CCC:513[A]:ARG:NE	4:CCC:611:EDO:O1	2.23	0.66
2:BBB:17:GLY:O	3:CCC:5[A]:ARG:HG2	1.98	0.63
4:AAA:204:EDO:O1	9:AAA:301:HOH:O	2.05	0.61
2:BBB:126:GLU:O	9:BBB:401:HOH:O	2.15	0.60
4:CCC:611:EDO:H21	5:CCC:621:SO4:O4	2.06	0.55
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.94	0.49
1:AAA:32:TYR:OH	4:AAA:204:EDO:H12	2.14	0.48
1:AAA:62:HIS:HD2	9:AAA:376:HOH:O	1.96	0.48
3:CCC:481:GLY:HA3	9:CCC:1057:HOH:O	2.13	0.47
3:CCC:358:SER:HA	3:CCC:531:ASN:HB3	1.97	0.47
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.50	0.46
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	3.04	0.45
1:AAA:81[A]:GLN:HG2	1:AAA:94:THR:OG1	2.17	0.45
3:CCC:307:PHE:O	3:CCC:383:LYS:HE3	2.17	0.45
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.17	0.45
3:CCC:4:ASN:ND2	3:CCC:7:GLN:H	2.15	0.44
3:CCC:362:THR:O	3:CCC:368:GLY:HA3	2.17	0.43
2:BBB:10:GLY:HA2	3:CCC:21:ARG:O	2.19	0.43
3:CCC:132:GLY:HA3	3:CCC:155:THR:OG1	2.19	0.42
3:CCC:470:THR:N	3:CCC:471:PRO:CD	2.83	0.42
3:CCC:65:ASN:OD1	5:CCC:624:SO4:O1	2.37	0.42
1:AAA:77:ILE:HG23	4:AAA:204:EDO:H11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:212:ILE:HG21	3:CCC:242:ALA:HB1	2.02	0.41
1:AAA:79:ASP:O	4:AAA:204:EDO:C2	2.64	0.41
1:AAA:30:LEU:HD13	1:AAA:38:ILE:HD12	2.03	0.41
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	3.03	0.41
3:CCC:513[A]:ARG:NH2	4:CCC:611:EDO:O1	2.53	0.41
3:CCC:507[A]:LYS:HD3	9:CCC:1072:HOH:O	2.20	0.41
3:CCC:138:VAL:O	3:CCC:159:GLY:HA3	2.21	0.41
3:CCC:513[B]:ARG:HH11	3:CCC:513[B]:ARG:HD3	1.69	0.41
3:CCC:305:ARG:HA	3:CCC:306:PRO:HA	1.87	0.40

There are no symmetry-related clashes.

## 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	AAA	103/100 (103%)	103 (100%)	0	0	100	100
2	BBB	123/122 (101%)	116 (94%)	6 (5%)	1 (1%)	19	4
3	CCC	584/570 (102%)	563 (96%)	21 (4%)	0	100	100
All	All	810/792 (102%)	782 (96%)	27 (3%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	99	ILE

### 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	AAA	88/83 (106%)	87 (99%)	1 (1%)	73	55
2	BBB	104/101 (103%)	103 (99%)	1 (1%)	76	59
3	CCC	474/458 (104%)	467 (98%)	7 (2%)	65	42
All	All	666/642 (104%)	657 (99%)	9 (1%)	67	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	66	ARG
2	BBB	126	GLU
3	CCC	1	MET
3	CCC	4	ASN
3	CCC	158	PHE
3	CCC	249	HIS
3	CCC	323	HIS
3	CCC	395	LYS
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	$\# Z  > 2$
1	CXM	AAA	1	1	6,10,11	0.89	0	5,11,13	0.90	0
3	KCX	CCC	220	3,6	7,11,12	0.49	0	4,12,14	0.36	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	-	1/7/10/12	-
3	KCX	CCC	220	3,6	-	0/7/10/12	-

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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 5 are monoatomic - leaving 32 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	616	-	4,4,4	0.43	0	6,6,6	0.43	0
5	SO4	CCC	620	-	4,4,4	0.31	0	6,6,6	0.06	0
5	SO4	CCC	624	-	4,4,4	0.52	0	6,6,6	0.34	0
5	SO4	CCC	613	-	4,4,4	0.35	0	6,6,6	0.17	0
4	EDO	AAA	202	-	3,3,3	0.95	0	2,2,2	0.49	0
5	SO4	CCC	618	8	4,4,4	0.29	0	6,6,6	0.14	0
4	EDO	CCC	604	-	3,3,3	0.32	0	2,2,2	0.15	0
5	SO4	BBB	307	-	4,4,4	0.32	0	6,6,6	0.14	0
5	SO4	CCC	612	-	4,4,4	0.47	0	6,6,6	0.19	0
5	SO4	CCC	615	-	4,4,4	0.30	0	6,6,6	0.48	0
4	EDO	BBB	303	-	3,3,3	0.49	0	2,2,2	0.30	0
4	EDO	BBB	301	-	3,3,3	0.60	0	2,2,2	0.14	0
5	SO4	CCC	619	-	4,4,4	0.38	0	6,6,6	0.04	0
5	SO4	BBB	308	-	4,4,4	0.37	0	6,6,6	0.08	0
5	SO4	CCC	622	-	4,4,4	0.46	0	6,6,6	0.24	0
5	SO4	CCC	617	-	4,4,4	0.31	0	6,6,6	0.21	0
4	EDO	AAA	203	-	3,3,3	0.59	0	2,2,2	0.28	0
4	EDO	CCC	603	-	3,3,3	0.17	0	2,2,2	0.96	0
5	SO4	BBB	305	-	4,4,4	0.29	0	6,6,6	0.11	0
4	EDO	BBB	304	-	3,3,3	0.42	0	2,2,2	0.40	0
5	SO4	AAA	205	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	BBB	306	-	4,4,4	0.37	0	6,6,6	0.35	0
5	SO4	CCC	621	-	4,4,4	0.43	0	6,6,6	0.28	0
5	SO4	CCC	623	-	4,4,4	0.32	0	6,6,6	0.14	0
4	EDO	CCC	606	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	CCC	610	-	3,3,3	0.54	0	2,2,2	0.55	0
4	EDO	BBB	302	-	3,3,3	0.32	0	2,2,2	1.02	0
4	EDO	AAA	201	-	3,3,3	1.15	0	2,2,2	0.51	0
4	EDO	AAA	204	-	3,3,3	0.90	0	2,2,2	1.21	0
4	EDO	CCC	607	-	3,3,3	0.85	0	2,2,2	0.43	0
4	EDO	CCC	611	-	3,3,3	0.30	0	2,2,2	0.09	0
5	SO4	CCC	614	-	4,4,4	0.30	0	6,6,6	0.18	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	BBB	302	-	-	0/1/1/1	-
4	EDO	AAA	201	-	-	1/1/1/1	-
4	EDO	AAA	204	-	-	1/1/1/1	-
4	EDO	BBB	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	203	-	-	1/1/1/1	-
4	EDO	CCC	607	-	-	0/1/1/1	-
4	EDO	CCC	603	-	-	0/1/1/1	-
4	EDO	AAA	202	-	-	0/1/1/1	-
4	EDO	BBB	301	-	-	1/1/1/1	-
4	EDO	BBB	304	-	-	1/1/1/1	-
4	EDO	CCC	604	-	-	0/1/1/1	-
4	EDO	CCC	611	-	-	0/1/1/1	-
4	EDO	CCC	606	-	-	0/1/1/1	-
4	EDO	CCC	610	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	203	EDO	O1-C1-C2-O2
4	BBB	304	EDO	O1-C1-C2-O2
4	BBB	301	EDO	O1-C1-C2-O2
4	CCC	610	EDO	O1-C1-C2-O2
4	AAA	204	EDO	O1-C1-C2-O2
4	AAA	201	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	624	SO4	1	0
5	CCC	622	SO4	1	0
5	CCC	621	SO4	1	0
4	AAA	204	EDO	5	0
4	CCC	611	EDO	3	0

## 5.7 Other polymers [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	99/100 (99%)	-0.82	0 <a href="#">100</a> <a href="#">100</a>	24, 28, 34, 47	0
2	BBB	122/122 (100%)	-0.80	0 <a href="#">100</a> <a href="#">100</a>	26, 30, 48, 72	0
3	CCC	569/570 (99%)	-0.83	1 (0%) <a href="#">95</a> <a href="#">94</a>	23, 27, 39, 74	0
All	All	790/792 (99%)	-0.82	1 (0%) <a href="#">95</a> <a href="#">94</a>	23, 28, 41, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CCC	396	ASN	2.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CXM	AAA	1	11/12	0.96	0.07	25,28,31,32	0
3	KCX	CCC	220	12/13	0.98	0.04	22,24,27,27	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

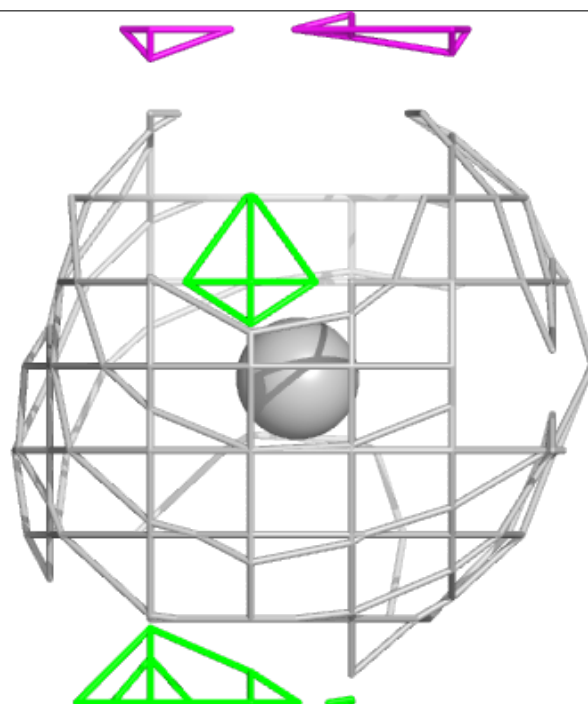
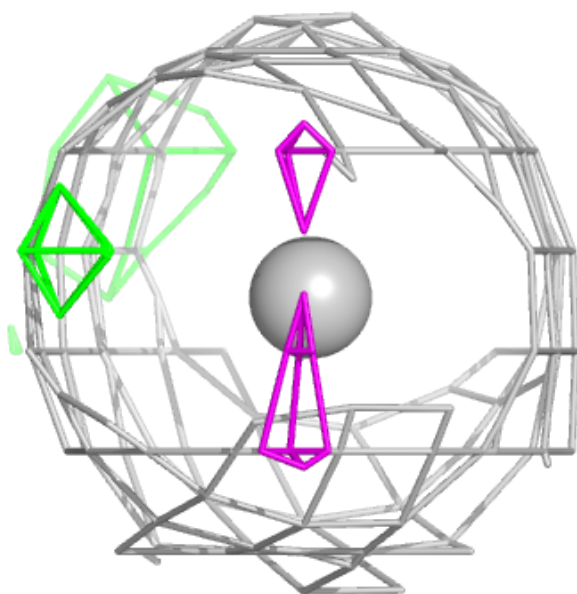
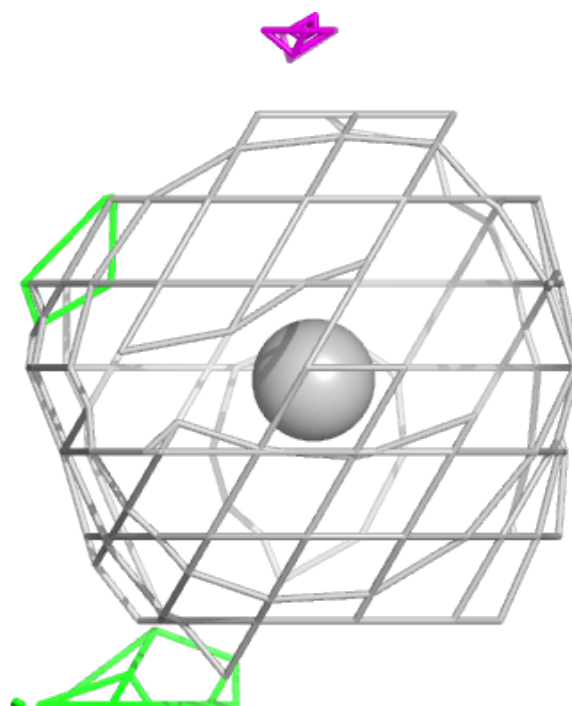
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	CCC	614	5/5	0.58	0.22	41,48,57,59	5
5	SO4	CCC	624	5/5	0.74	0.26	39,42,50,51	5
4	EDO	BBB	304	4/4	0.75	0.22	65,67,71,74	0
4	EDO	CCC	611	4/4	0.82	0.23	35,39,44,48	4
4	EDO	BBB	303	4/4	0.84	0.20	66,71,74,77	0
5	SO4	AAA	205	5/5	0.84	0.28	83,83,87,97	5
4	EDO	BBB	301	4/4	0.85	0.19	65,65,66,78	0
5	SO4	BBB	306	5/5	0.86	0.20	38,43,64,70	5
5	SO4	CCC	613	5/5	0.86	0.17	67,68,78,84	0
5	SO4	CCC	621	5/5	0.87	0.20	24,36,42,54	5
5	SO4	CCC	622	5/5	0.87	0.23	44,59,75,78	5
4	EDO	BBB	302	4/4	0.87	0.14	49,51,51,55	0
5	SO4	CCC	623	5/5	0.88	0.24	64,72,83,92	5
4	EDO	CCC	610	4/4	0.88	0.22	54,59,59,61	0
4	EDO	AAA	204	4/4	0.90	0.17	41,43,49,55	0
4	EDO	AAA	203	4/4	0.91	0.12	40,51,57,63	0
5	SO4	CCC	617	5/5	0.91	0.25	62,72,80,83	5
5	SO4	CCC	612	5/5	0.92	0.14	35,37,43,46	5
5	SO4	BBB	308	5/5	0.93	0.30	59,59,71,73	5
5	SO4	CCC	620	5/5	0.94	0.10	79,79,82,82	5
4	EDO	CCC	607	4/4	0.94	0.07	42,42,43,43	0
4	EDO	CCC	603	4/4	0.94	0.14	46,50,52,55	0
5	SO4	CCC	616	5/5	0.94	0.17	39,42,63,64	5
5	SO4	BBB	305	5/5	0.94	0.20	75,90,95,107	0
4	EDO	AAA	201	4/4	0.95	0.08	31,37,39,40	0
5	SO4	CCC	615	5/5	0.95	0.10	31,31,46,50	5
4	EDO	AAA	202	4/4	0.95	0.09	30,33,36,37	0
4	EDO	CCC	606	4/4	0.96	0.07	33,34,36,37	0
5	SO4	BBB	307	5/5	0.96	0.13	76,86,89,101	0
7	O	CCC	605	1/1	0.96	0.04	23,23,23,23	0
4	EDO	CCC	604	4/4	0.97	0.09	37,43,45,47	0
5	SO4	CCC	619	5/5	0.98	0.04	53,54,55,55	5
5	SO4	CCC	618	5/5	0.99	0.06	31,31,33,34	0
6	NI	CCC	602	1/1	1.00	0.06	26,26,26,26	0
6	NI	CCC	601	1/1	1.00	0.08	27,27,27,27	0
8	AG	CCC	608	1/1	1.00	0.06	31,31,31,31	1
8	AG	CCC	609	1/1	1.00	0.05	31,31,31,31	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.

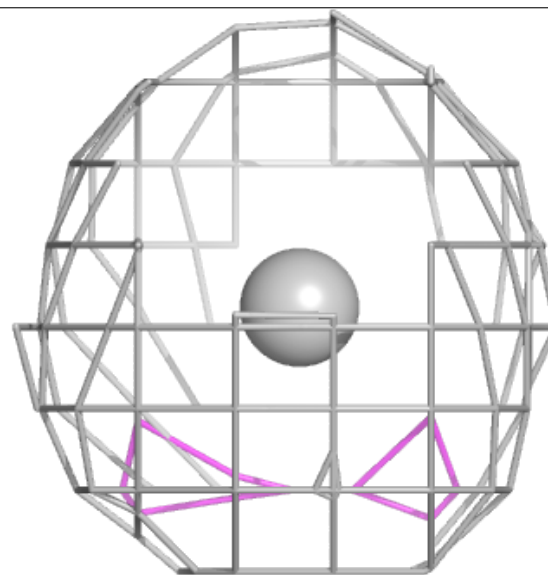
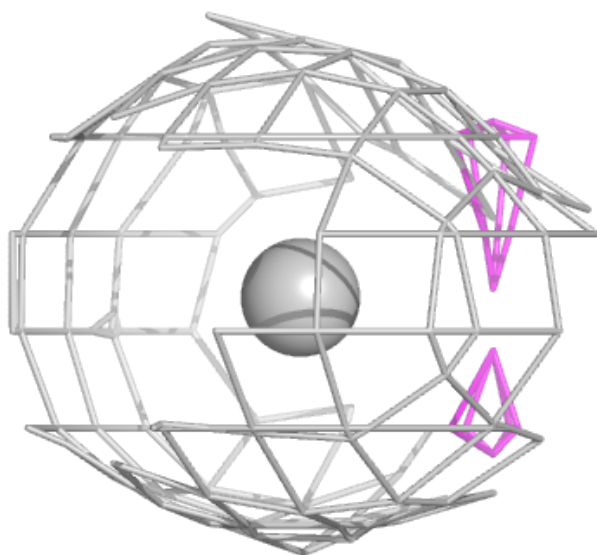
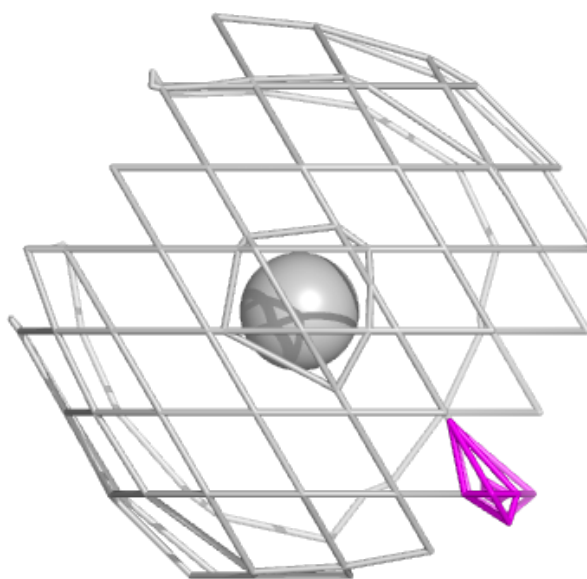
**Electron density around AG CCC 608:**

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



**Electron density around AG 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.