



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2022 – 04:14 am BST

PDB ID : 7B58
Title : X-ray crystal structure of Sporosarcina pasteurii urease inhibited by Ag(PET3)Cl determined at 1.72 Angstroms
Authors : Mazzei, L.; Cianci, M.; Ciurli, S.
Deposited on : 2020-12-03
Resolution : 1.72 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 : 2.27
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

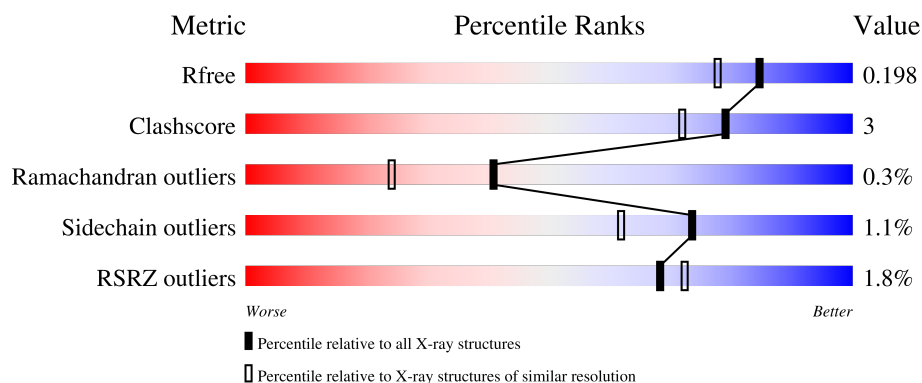
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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>95%</div> <div>5%</div> </div>
2	BBB	122	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>
3	CCC	570	<div> <div>2%</div> <div>92%</div> <div>7%</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 9 unique types of molecules in this entry. The entry contains 7000 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
			813	511	136	159	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	4	0
			987	609	179	198	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	16	0
			4429	2782	763	858	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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

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
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	79	Total O 79 79	0	0
9	BBB	122	Total O 122 122	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	CCC	420	Total 420	O 420	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:  95% 5%



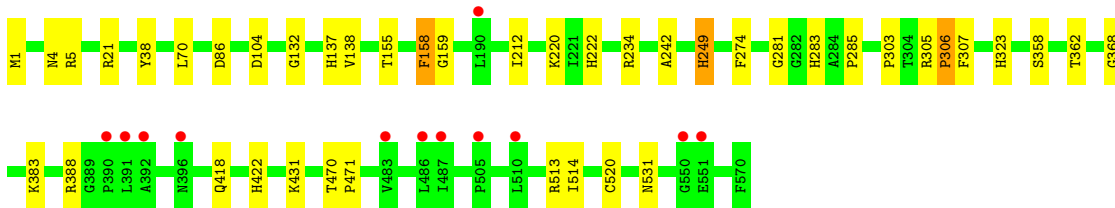
- Molecule 2: Urease subunit beta

Chain BBB:  91% 9% 2%



- Molecule 3: Urease subunit alpha

Chain CCC:  92% 7% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.44Å 131.44Å 189.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.99 – 1.72 72.88 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.99-1.72) 99.9 (72.88-1.72)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.155 , 0.185 0.168 , 0.198	Depositor DCC
R_{free} test set	5112 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7000	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: EDO, O, SO4, CXM, AG, KCX, 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	0.77	0/819	0.83	0/1102
2	BBB	0.81	0/999	0.87	0/1341
3	CCC	0.77	0/4522	0.88	3/6123 (0.0%)
All	All	0.77	0/6340	0.87	3/8566 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	520	CYS	CB-CA-C	-8.65	93.09	110.40
3	CCC	388	ARG	NE-CZ-NH1	6.40	123.50	120.30
3	CCC	234	ARG	CG-CD-NE	-5.16	100.95	111.80

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	813	0	825	3	0
2	BBB	987	0	971	8	0
3	CCC	4429	0	4422	26	0
4	AAA	20	0	30	1	0
4	BBB	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CCC	32	0	48	3	0
5	AAA	10	0	0	0	0
5	BBB	15	0	0	0	0
5	CCC	60	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	79	0	0	0	0
9	BBB	122	0	0	2	0
9	CCC	420	0	0	2	0
All	All	7000	0	6308	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)
3:CCC:38:TYR:CZ	5:CCC:614:SO4:O3	2.51	0.64
2:BBB:17:GLY:O	3:CCC:5[A]:ARG:HG2	1.97	0.64
3:CCC:513[A]:ARG:NE	4:CCC:612:EDO:O1	2.30	0.63
3:CCC:38:TYR:CE2	5:CCC:614:SO4:O3	2.56	0.58
3:CCC:422:HIS:O	5:CCC:617:SO4:O4	2.21	0.58
3:CCC:513[A]:ARG:NH2	4:CCC:612:EDO:O1	2.38	0.53
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	3.00	0.49
1:AAA:30:LEU:HD13	1:AAA:38:ILE:HD12	1.95	0.49
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	2.95	0.49
2:BBB:19:ILE:HG12	3:CCC:5[A]:ARG:HD2	1.95	0.48
3:CCC:514:ILE:O	4:CCC:612:EDO:H21	2.14	0.47
3:CCC:307:PHE:O	3:CCC:383:LYS:HE3	2.15	0.47
3:CCC:362:THR:O	3:CCC:368:GLY:HA3	2.14	0.47
1:AAA:73:VAL:N	1:AAA:74:PRO:CD	2.78	0.47
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.98	0.45
3:CCC:132:GLY:HA3	3:CCC:155:THR:OG1	2.17	0.45
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.17	0.45
3:CCC:212:ILE:HG21	3:CCC:242:ALA:HB1	1.99	0.45
3:CCC:470:THR:N	3:CCC:471:PRO:CD	2.81	0.44
3:CCC:513[B]:ARG:NH2	9:CCC:725:HOH:O	2.50	0.43
3:CCC:358:SER:HA	3:CCC:531:ASN:HB3	2.01	0.43
3:CCC:138:VAL:O	3:CCC:159:GLY:HA3	2.19	0.42
2:BBB:5:ASN:HB2	9:BBB:384:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:305:ARG:HA	3:CCC:306:PRO:HA	1.85	0.42
2:BBB:109:ASN:HB3	9:BBB:389:HOH:O	2.18	0.42
2:BBB:57:PHE:O	2:BBB:124:GLY:HA3	2.19	0.42
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.54	0.41
3:CCC:303:PRO:HG3	3:CCC:368:GLY:HA2	2.02	0.41
1:AAA:67[B]:ASP:OD1	4:AAA:204:EDO:H11	2.21	0.41
2:BBB:31[B]:ARG:HD3	2:BBB:82:GLU:OE2	2.21	0.40
3:CCC:431[A]:LYS:NZ	9:CCC:704:HOH:O	2.28	0.40
2:BBB:10:GLY:HA2	3:CCC:21:ARG:O	2.21	0.40
3:CCC:220:KCX:CX	3:CCC:222:HIS:HD2	2.34	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	103/100 (103%)	103 (100%)	0	0	100	100
2	BBB	124/122 (102%)	117 (94%)	6 (5%)	1 (1%)	19	6
3	CCC	583/570 (102%)	562 (96%)	20 (3%)	1 (0%)	47	30
All	All	810/792 (102%)	782 (96%)	26 (3%)	2 (0%)	41	30

All (2) Ramachandran outliers are listed below:

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

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%)	88 (100%)	0	100	100
2	BBB	105/101 (104%)	105 (100%)	0	100	100
3	CCC	473/458 (103%)	466 (98%)	7 (2%)	65	49
All	All	666/642 (104%)	659 (99%)	7 (1%)	73	62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CCC	1	MET
3	CCC	4	ASN
3	CCC	158	PHE
3	CCC	249	HIS
3	CCC	285	PRO
3	CCC	306	PRO
3	CCC	323	HIS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	0.60	0	4,12,14	0.37	0
1	CXM	AAA	1	1	6,10,11	0.59	0	5,11,13	1.12	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, 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	$\# Z > 2$
4	EDO	AAA	203	-	3,3,3	0.69	0	2,2,2	0.59	0
4	EDO	AAA	205	-	3,3,3	1.02	0	2,2,2	0.54	0
4	EDO	CCC	612	-	3,3,3	0.51	0	2,2,2	0.05	0
5	SO4	CCC	624	-	4,4,4	0.40	0	6,6,6	0.05	0
4	EDO	CCC	610	-	3,3,3	0.44	0	2,2,2	0.52	0
4	EDO	CCC	607	-	3,3,3	0.19	0	2,2,2	0.20	0
4	EDO	AAA	204	-	3,3,3	0.29	0	2,2,2	0.99	0
5	SO4	CCC	617	-	4,4,4	0.35	0	6,6,6	0.17	0
5	SO4	CCC	621	-	4,4,4	0.34	0	6,6,6	0.08	0
4	EDO	CCC	606	-	3,3,3	0.25	0	2,2,2	0.62	0
5	SO4	AAA	207	-	4,4,4	0.34	0	6,6,6	0.07	0
4	EDO	CCC	613	-	3,3,3	0.45	0	2,2,2	0.42	0
5	SO4	BBB	204	-	4,4,4	0.31	0	6,6,6	0.05	0
5	SO4	CCC	625	-	4,4,4	0.33	0	6,6,6	0.09	0
4	EDO	BBB	202	-	3,3,3	0.28	0	2,2,2	1.37	0
4	EDO	AAA	202	-	3,3,3	0.61	0	2,2,2	0.72	0
5	SO4	CCC	614	-	4,4,4	0.36	0	6,6,6	0.16	0
5	SO4	BBB	205	-	4,4,4	0.32	0	6,6,6	0.15	0
5	SO4	CCC	622	-	4,4,4	0.32	0	6,6,6	0.13	0
4	EDO	CCC	603	-	3,3,3	0.76	0	2,2,2	0.25	0
5	SO4	CCC	616	-	4,4,4	0.33	0	6,6,6	0.09	0
4	EDO	BBB	201	-	3,3,3	0.34	0	2,2,2	1.17	0
5	SO4	CCC	623	-	4,4,4	0.35	0	6,6,6	0.10	0
5	SO4	CCC	619	8	4,4,4	0.34	0	6,6,6	0.12	0
4	EDO	CCC	611	-	3,3,3	0.24	0	2,2,2	0.76	0
5	SO4	BBB	203	-	4,4,4	0.33	0	6,6,6	0.21	0
4	EDO	AAA	201	-	3,3,3	1.08	0	2,2,2	0.56	0
5	SO4	CCC	620	-	4,4,4	0.30	0	6,6,6	0.07	0
5	SO4	CCC	615	-	4,4,4	0.38	0	6,6,6	0.16	0
5	SO4	AAA	206	-	4,4,4	0.32	0	6,6,6	0.22	0
5	SO4	CCC	618	-	4,4,4	0.25	0	6,6,6	0.43	0
4	EDO	CCC	605	-	3,3,3	0.42	0	2,2,2	0.25	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	201	-	-	1/1/1/1	-
4	EDO	AAA	203	-	-	1/1/1/1	-
4	EDO	CCC	611	-	-	0/1/1/1	-
4	EDO	CCC	606	-	-	0/1/1/1	-
4	EDO	AAA	205	-	-	0/1/1/1	-
4	EDO	AAA	201	-	-	0/1/1/1	-
4	EDO	CCC	612	-	-	1/1/1/1	-
4	EDO	CCC	613	-	-	0/1/1/1	-
4	EDO	CCC	605	-	-	0/1/1/1	-
4	EDO	CCC	610	-	-	1/1/1/1	-
4	EDO	BBB	202	-	-	1/1/1/1	-
4	EDO	AAA	202	-	-	0/1/1/1	-
4	EDO	CCC	603	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	0/1/1/1	-
4	EDO	AAA	204	-	-	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	BBB	202	EDO	O1-C1-C2-O2
4	CCC	610	EDO	O1-C1-C2-O2
4	AAA	203	EDO	O1-C1-C2-O2
4	BBB	201	EDO	O1-C1-C2-O2
4	CCC	612	EDO	O1-C1-C2-O2
4	AAA	204	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	612	EDO	3	0
4	AAA	204	EDO	1	0
5	CCC	617	SO4	1	0
5	CCC	614	SO4	2	0

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(Å ²)	Q<0.9
1	AAA	99/100 (99%)	-0.44	0 100 100	27, 30, 40, 53	0
2	BBB	122/122 (100%)	-0.38	2 (1%) 72 76	29, 34, 50, 72	0
3	CCC	569/570 (99%)	-0.36	12 (2%) 63 67	25, 30, 44, 83	0
All	All	790/792 (99%)	-0.37	14 (1%) 68 72	25, 31, 45, 83	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CCC	396	ASN	3.4
3	CCC	487	ILE	3.1
3	CCC	550	GLY	3.1
3	CCC	486	LEU	2.9
3	CCC	483	VAL	2.7
2	BBB	126	GLU	2.7
3	CCC	391	LEU	2.7
2	BBB	120	LEU	2.6
3	CCC	392	ALA	2.5
3	CCC	390	PRO	2.2
3	CCC	190	LEU	2.2
3	CCC	510	LEU	2.2
3	CCC	505	PRO	2.1
3	CCC	551	GLU	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	0.96	0.10	27,30,36,36	0
3	KCX	CCC	220	12/13	0.98	0.04	24,27,31,31	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
5	SO4	AAA	206	5/5	0.77	0.28	52,93,114,124	0
4	EDO	AAA	204	4/4	0.78	0.12	65,77,77,78	0
4	EDO	AAA	203	4/4	0.80	0.23	54,55,60,65	0
4	EDO	CCC	610	4/4	0.81	0.23	69,69,73,87	0
5	SO4	CCC	623	5/5	0.81	0.28	118,125,138,141	0
5	SO4	CCC	625	5/5	0.83	0.27	105,115,122,128	0
5	SO4	BBB	205	5/5	0.85	0.21	81,87,98,100	0
4	EDO	CCC	612	4/4	0.86	0.18	52,59,60,70	0
5	SO4	CCC	621	5/5	0.86	0.25	96,115,132,134	0
4	EDO	BBB	201	4/4	0.88	0.11	42,51,51,52	0
4	EDO	BBB	202	4/4	0.88	0.37	57,60,60,60	0
5	SO4	CCC	615	5/5	0.88	0.18	72,79,80,84	0
5	SO4	CCC	616	5/5	0.89	0.10	79,80,84,85	5
5	SO4	CCC	617	5/5	0.90	0.23	59,84,99,112	0
5	SO4	CCC	614	5/5	0.90	0.34	68,92,109,121	0
4	EDO	CCC	613	4/4	0.91	0.32	61,68,71,73	0
5	SO4	AAA	207	5/5	0.91	0.19	122,122,124,138	5
5	SO4	CCC	620	5/5	0.92	0.19	91,93,96,106	0
5	SO4	BBB	204	5/5	0.92	0.42	73,75,87,92	5
5	SO4	BBB	203	5/5	0.93	0.18	103,108,111,122	0
5	SO4	CCC	618	5/5	0.93	0.17	38,41,56,58	5
4	EDO	CCC	611	4/4	0.93	0.20	39,39,57,65	0
5	SO4	CCC	622	5/5	0.94	0.19	70,79,99,106	0
4	EDO	CCC	603	4/4	0.94	0.06	41,42,43,43	0
4	EDO	CCC	607	4/4	0.94	0.17	40,47,48,48	0
4	EDO	AAA	205	4/4	0.95	0.09	30,43,47,49	0
4	EDO	AAA	201	4/4	0.96	0.13	35,41,44,44	0

Continued on next page...

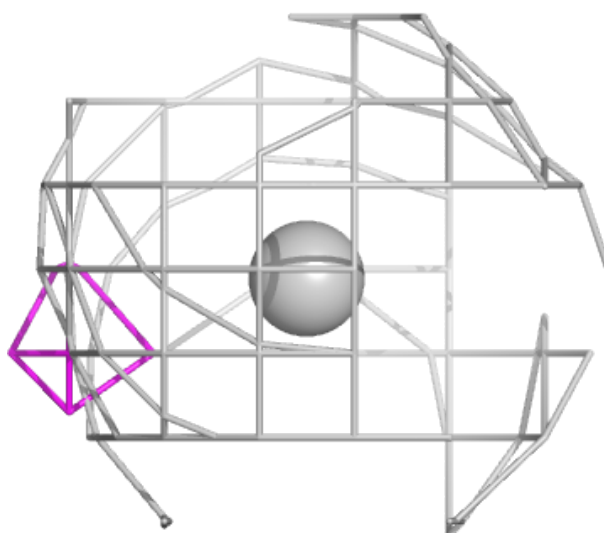
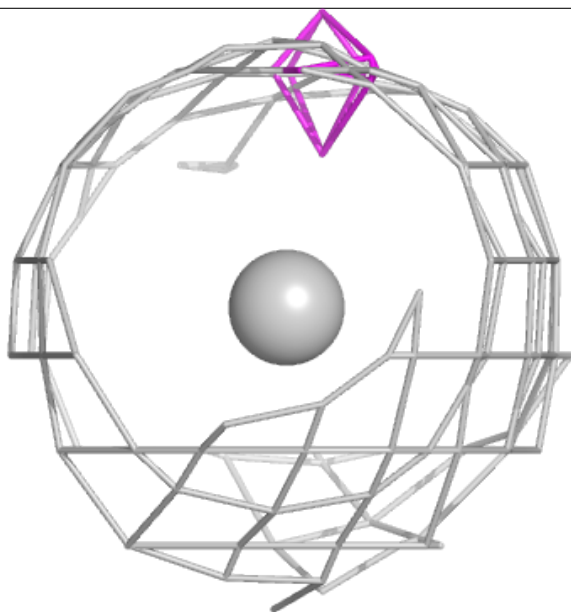
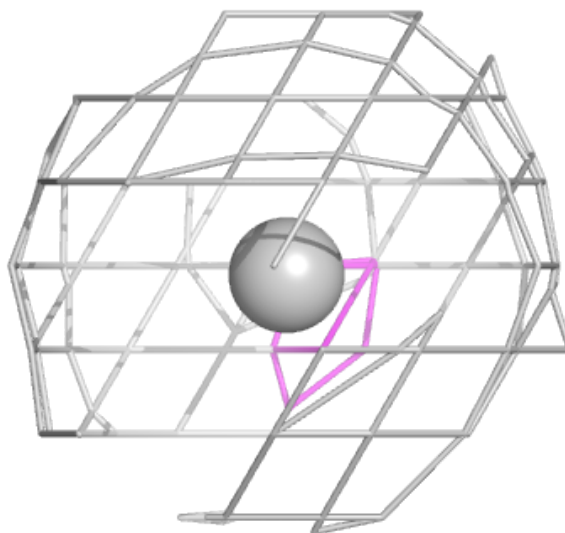
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	CCC	606	4/4	0.96	0.10	51,55,56,59	0
4	EDO	CCC	605	4/4	0.97	0.08	34,35,36,36	0
4	EDO	AAA	202	4/4	0.97	0.10	34,40,40,42	0
7	O	CCC	604	1/1	0.97	0.06	26,26,26,26	0
5	SO4	CCC	624	5/5	0.98	0.12	68,71,77,77	5
5	SO4	CCC	619	5/5	0.99	0.04	33,33,35,36	0
6	NI	CCC	602	1/1	1.00	0.04	29,29,29,29	0
6	NI	CCC	601	1/1	1.00	0.04	29,29,29,29	0
8	AG	CCC	608	1/1	1.00	0.03	33,33,33,33	0
8	AG	CCC	609	1/1	1.00	0.03	32,32,32,32	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.

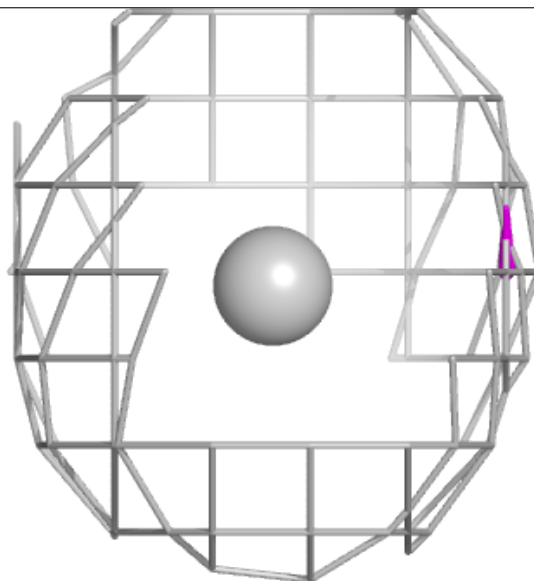
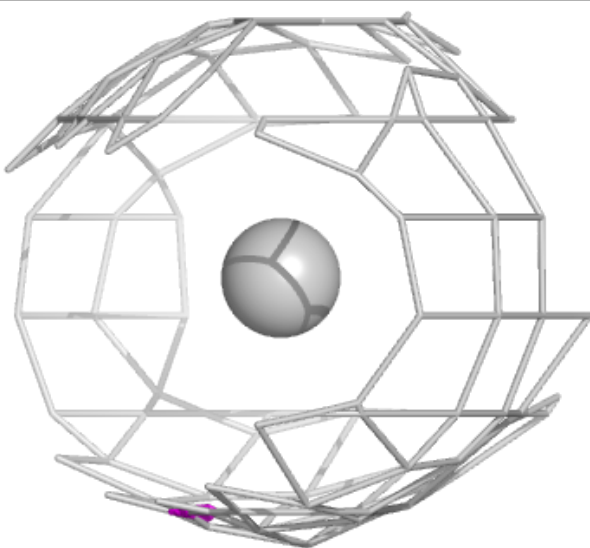
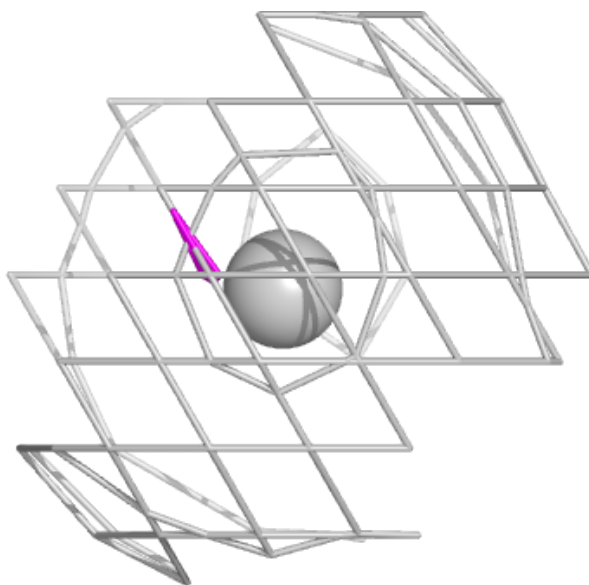
Electron density around AG CCC 608:

$2mF_o-DF_c$ (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.