



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2026 – 01:22 pm BST

PDB ID : 9REY / pdb\_00009rey  
Title : Sporosarcina pasteurii urease in complex with a hydrophilic derivative of Ebsulfur at 1.96 Å  
Authors : Mazzei, L.; Ciurli, S.; Cianci, M.; Paul, A.  
Deposited on : 2025-06-04  
Resolution : 1.96 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

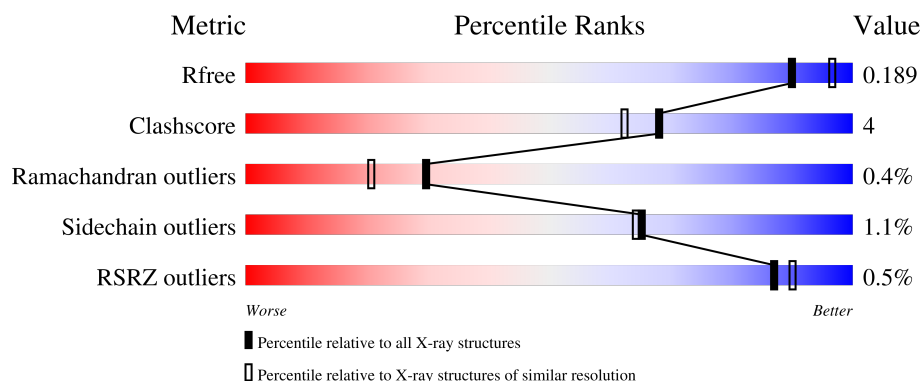
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

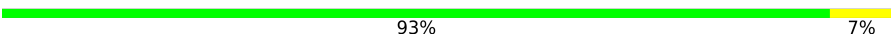
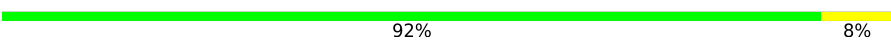

The reported resolution of this entry is 1.96 Å.

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))
$R_{free}$	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	A	100	 93% 7%
2	B	122	 92% 8%
3	C	570	 % 90% 9% .

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	SO4	C	611	-	-	X	-
4	SO4	C	621	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7041 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	A	100	Total	C	N	O	S	0	7	0
			828	521	140	159	8			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	4	0
			983	607	177	198	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	570	Total	C	N	O	S	0	19	0
			4453	2795	769	862	27			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



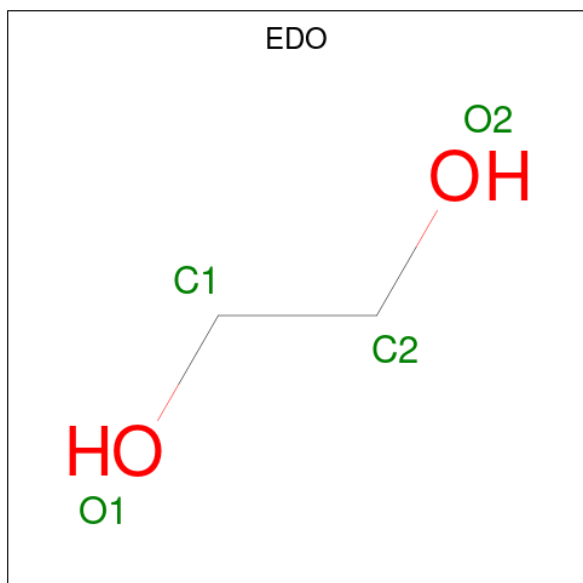
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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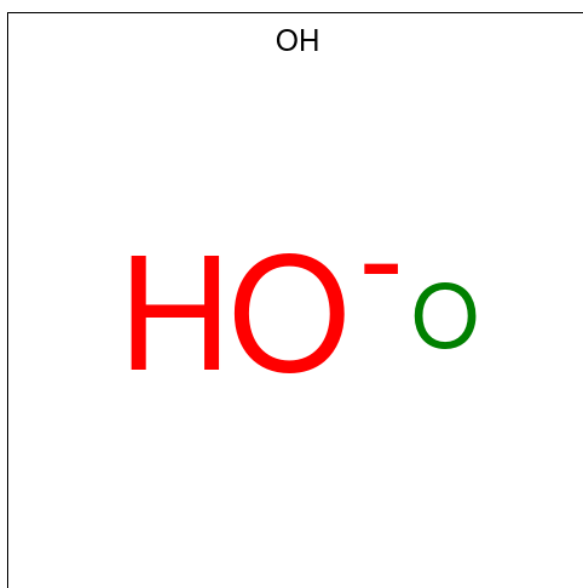
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

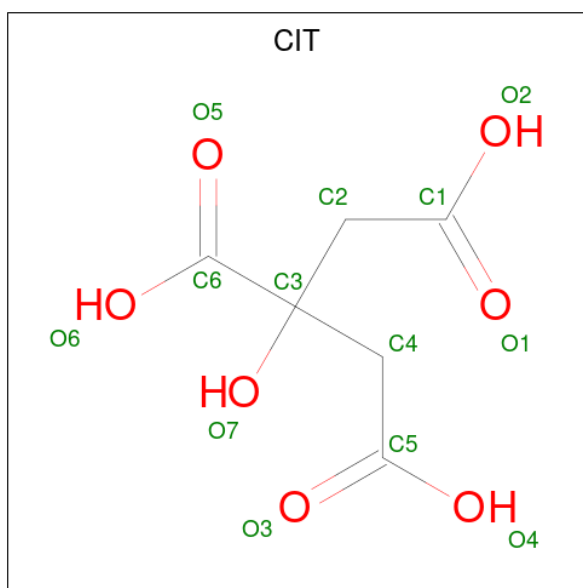
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	2	Total Ni 2 2	0	0

- Molecule 7 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

- Molecule 8 is CITRIC ACID (CCD ID: CIT) (formula:  $\text{C}_6\text{H}_8\text{O}_7$ ).

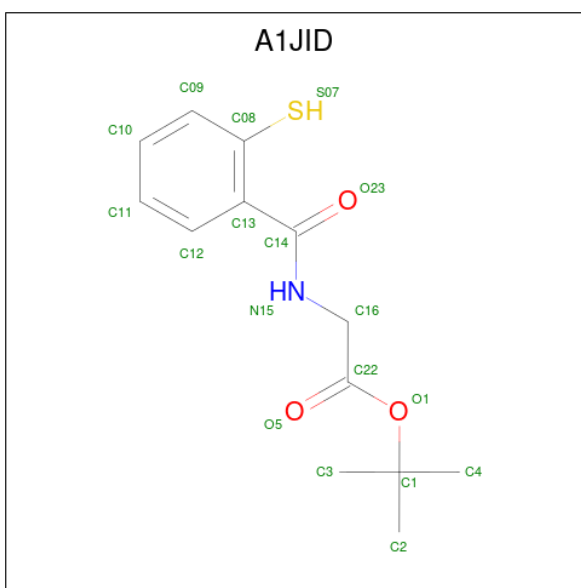


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is {tert}-butyl 2-[(2-sulfanylphenyl)carbonylamino]ethanoate (CCD ID: A1JID)

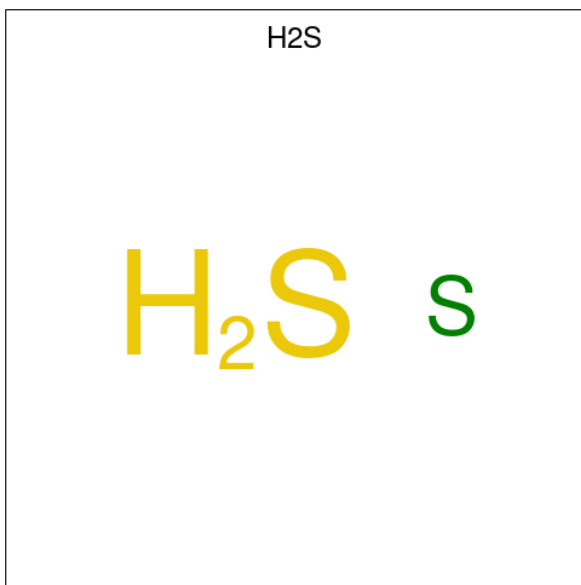


(formula:  $C_{13}H_{17}NO_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	S	0	0
			18	13	1	3	1		

- Molecule 10 is HYDROSULFURIC ACID (CCD ID: H2S) (formula:  $H_2S$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	S	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	76	Total 76	O 76	0	0
11	B	103	Total 103	O 103	0	0
11	C	367	Total 367	O 367	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Urease subunit gamma

Chain A:  93% 7%




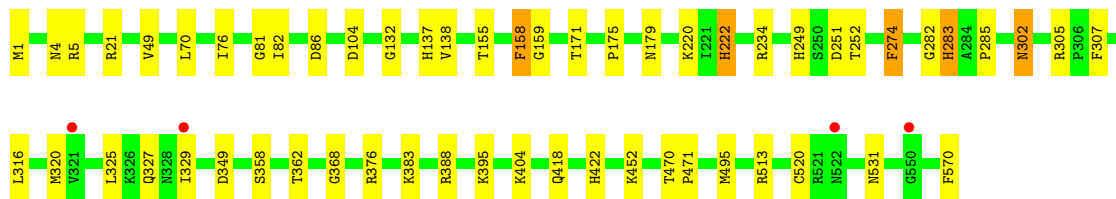
- Molecule 2: Urease subunit beta

Chain B:  92% 8%



- Molecule 3: Urease subunit alpha

Chain C:  90% 9% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.20Å 131.20Å 188.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.73 – 1.96 48.73 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.73-1.96) 99.9 (48.73-1.96)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.140 , 0.178 0.153 , 0.189	Depositor DCC
$R_{free}$ test set	3373 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.8	EDS
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
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7041	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 3.83% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2S, KCX, CSS, CIT, NI, A1JID, OH, EDO, 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	A	1.03	0/837	1.23	0/1126
2	B	1.01	0/998	1.25	1/1342 (0.1%)
3	C	1.08	3/4544 (0.1%)	1.28	10/6151 (0.2%)
All	All	1.07	3/6379 (0.0%)	1.27	11/8619 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	222	HIS	CE1-NE2	5.99	1.38	1.32
3	C	422	HIS	CE1-NE2	5.70	1.38	1.32
3	C	329	ILE	N-CA	5.51	1.50	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	520	CYS	CB-CA-C	-8.54	93.74	109.29
3	C	570	PHE	CA-C-O	-7.87	107.42	120.80
3	C	251	ASP	CA-CB-CG	7.56	120.16	112.60
2	B	126	GLU	CA-C-O	-6.66	109.47	120.80
3	C	234	ARG	CG-CD-NE	-5.89	99.03	112.00
3	C	104	ASP	CA-CB-CG	5.67	118.27	112.60
3	C	495	MET	CA-C-N	5.09	127.93	120.71
3	C	495	MET	C-N-CA	5.09	127.93	120.71
3	C	274	PHE	CA-CB-CG	5.08	118.88	113.80
3	C	4	ASN	CB-CA-C	5.05	118.83	109.54
3	C	302	ASN	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	828	0	847	9	0
2	B	983	0	964	6	0
3	C	4453	0	4443	28	0
4	A	5	0	0	0	0
4	B	30	0	0	0	0
4	C	85	0	0	4	1
5	A	12	0	18	2	0
5	B	16	0	24	0	0
5	C	48	0	72	0	0
6	C	2	0	0	0	0
7	C	1	0	0	0	0
8	C	13	0	5	0	0
9	C	18	0	0	1	0
10	C	1	0	0	0	0
11	A	76	0	0	2	0
11	B	103	0	0	1	0
11	C	367	0	0	5	1
All	All	7041	0	6373	46	1

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 (46) 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)
4:C:621:SO4:O2	11:C:701:HOH:O	1.86	0.94
4:C:611:SO4:O1	11:C:702:HOH:O	1.90	0.89
1:A:44[B]:MET:HA	1:A:44[B]:MET:HE2	1.60	0.83
4:C:623:SO4:O1	11:C:703:HOH:O	1.99	0.80
1:A:44[B]:MET:HE3	1:A:82:ALA:HB1	1.81	0.63
1:A:44[B]:MET:CE	1:A:84:ALA:HB2	2.31	0.59
2:B:13:ARG:HD3	11:B:390:HOH:O	2.06	0.56
3:C:70:LEU:HD11	3:C:86:ASP:HB3	1.87	0.55
9:C:606:A1JID:S07	9:C:606:A1JID:O23	2.67	0.52
2:B:19:ILE:HG12	3:C:5[A]:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44[B]:MET:CE	1:A:82:ALA:HB1	2.41	0.51
2:B:71:SER:OG	3:C:49:VAL:HG21	2.11	0.51
3:C:513[B]:ARG:NH2	11:C:710:HOH:O	2.43	0.50
1:A:44[B]:MET:HE2	1:A:44[B]:MET:CA	2.37	0.50
3:C:388[B]:ARG:HB2	3:C:388[B]:ARG:HH11	1.76	0.50
3:C:171:THR:HG22	3:C:222:HIS:CG	2.48	0.48
1:A:44[B]:MET:HE2	1:A:84:ALA:HB2	1.94	0.48
3:C:220:KCX:CX	3:C:222:HIS:HD2	2.26	0.48
5:A:202:EDO:H22	11:A:349:HOH:O	2.13	0.48
3:C:358:SER:HA	3:C:531:ASN:HB3	1.96	0.47
2:B:15:ALA:O	3:C:5[B]:ARG:HG3	2.14	0.47
3:C:302:ASN:O	3:C:376:ARG:HD3	2.15	0.46
3:C:137:HIS:CE1	3:C:274:PHE:CD2	3.03	0.46
1:A:44[B]:MET:HE3	1:A:82:ALA:CB	2.44	0.46
3:C:362:THR:O	3:C:368:GLY:HA3	2.16	0.46
3:C:316:LEU:HD23	3:C:316:LEU:HA	1.85	0.46
3:C:138:VAL:O	3:C:159:GLY:HA3	2.16	0.46
3:C:175:PRO:O	3:C:179:ASN:HB2	2.16	0.45
5:A:202:EDO:C2	11:A:349:HOH:O	2.64	0.45
1:A:30:LEU:HD13	1:A:38:ILE:HD12	1.99	0.44
3:C:132:GLY:HA3	3:C:155:THR:OG1	2.18	0.44
4:C:621:SO4:O4	11:C:704:HOH:O	2.20	0.44
3:C:305:ARG:NH1	3:C:349:ASP:OD1	2.47	0.43
3:C:307:PHE:O	3:C:383:LYS:HE3	2.19	0.43
3:C:320:MET:HA	3:C:325:LEU:HB2	1.99	0.43
2:B:57:PHE:O	2:B:124:GLY:HA3	2.18	0.43
2:B:10:GLY:HA2	3:C:21:ARG:O	2.19	0.42
3:C:158:PHE:CE2	3:C:418[A]:GLN:CG	3.02	0.42
3:C:76:ILE:O	3:C:82:ILE:HA	2.20	0.41
1:A:73:VAL:N	1:A:74:PRO:CD	2.84	0.41
3:C:252:THR:HA	3:C:282:GLY:C	2.46	0.41
3:C:316:LEU:O	3:C:320:MET:HG2	2.20	0.41
3:C:81:GLY:HA2	3:C:404:LYS:HE2	2.04	0.40
3:C:320:MET:O	3:C:325:LEU:N	2.51	0.40
3:C:282:GLY:O	3:C:283:HIS:C	2.64	0.40
3:C:470:THR:N	3:C:471:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:611:SO4:O4	11:C:702:HOH:O[12_565]	1.91	0.29

## 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	A	105/100 (105%)	105 (100%)	0	0	100	100
2	B	124/122 (102%)	118 (95%)	4 (3%)	2 (2%)	7	2
3	C	585/570 (103%)	561 (96%)	23 (4%)	1 (0%)	43	36
All	All	814/792 (103%)	784 (96%)	27 (3%)	3 (0%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ILE
3	C	283	HIS
2	B	52	ASN

### 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	A	90/83 (108%)	90 (100%)	0	100	100
2	B	105/101 (104%)	105 (100%)	0	100	100
3	C	475/457 (104%)	468 (98%)	7 (2%)	57	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	670/641 (104%)	663 (99%)	7 (1%)	65	67

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

Mol	Chain	Res	Type
3	C	1	MET
3	C	158	PHE
3	C	249	HIS
3	C	285	PRO
3	C	327	GLN
3	C	395	LYS
3	C	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
2	B	109	ASN
3	C	4	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	A	1	1	8,10,11	0.57	0	7,11,13	1.01	0
3	CSS	C	322	3	4,6,7	0.46	0	1,6,8	0.76	0
3	KCX	C	220	6,3	9,11,12	0.49	0	5,12,14	0.59	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	A	1	1	-	3/9/10/12	-
3	CSS	C	322	3	-	0/1/5/7	-
3	KCX	C	220	6,3	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 45 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	SO4	C	612	-	4,4,4	0.37	0	6,6,6	0.19	0
4	SO4	C	623	-	4,4,4	0.41	0	6,6,6	0.13	0
5	EDO	B	209	-	3,3,3	0.59	0	2,2,2	0.30	0
5	EDO	A	204	-	3,3,3	0.67	0	2,2,2	0.28	0
5	EDO	C	627	-	3,3,3	0.44	0	2,2,2	0.57	0
5	EDO	C	604	-	3,3,3	0.54	0	2,2,2	0.30	0
4	SO4	B	202	-	4,4,4	0.33	0	6,6,6	0.06	0
8	CIT	C	605	6	12,12,12	1.55	2 (16%)	17,17,17	1.49	3 (17%)
5	EDO	C	629	-	3,3,3	0.84	0	2,2,2	0.56	0
4	SO4	B	203	-	4,4,4	0.33	0	6,6,6	0.23	0
4	SO4	C	613	-	4,4,4	0.37	0	6,6,6	0.06	0
4	SO4	B	201	-	4,4,4	0.42	0	6,6,6	0.20	0
5	EDO	C	624	-	3,3,3	0.62	0	2,2,2	0.50	0
4	SO4	C	611	-	4,4,4	0.29	0	6,6,6	0.11	0
4	SO4	C	614	-	4,4,4	0.29	0	6,6,6	0.31	0
4	SO4	C	619	-	4,4,4	0.29	0	6,6,6	0.16	0
4	SO4	C	607	-	4,4,4	0.41	0	6,6,6	0.16	0
5	EDO	A	202	-	3,3,3	0.31	0	2,2,2	0.74	0
5	EDO	C	632	-	3,3,3	0.35	0	2,2,2	0.44	0
5	EDO	C	634	-	3,3,3	0.47	0	2,2,2	0.44	0
4	SO4	C	618	-	4,4,4	0.31	0	6,6,6	0.18	0
9	A1JID	C	606	3	18,18,18	1.24	2 (11%)	24,25,25	1.43	4 (16%)
5	EDO	B	210	-	3,3,3	0.55	0	2,2,2	0.44	0
4	SO4	C	609	-	4,4,4	0.35	0	6,6,6	0.13	0
4	SO4	C	608	-	4,4,4	0.36	0	6,6,6	0.16	0
4	SO4	B	205	-	4,4,4	0.37	0	6,6,6	0.09	0
5	EDO	A	203	-	3,3,3	0.87	0	2,2,2	0.77	0
5	EDO	C	631	-	3,3,3	0.57	0	2,2,2	0.16	0
5	EDO	C	630	-	3,3,3	0.80	0	2,2,2	0.49	0
4	SO4	C	617	-	4,4,4	0.42	0	6,6,6	0.16	0
4	SO4	A	201	-	4,4,4	0.35	0	6,6,6	0.14	0
5	EDO	C	633	-	3,3,3	0.68	0	2,2,2	0.39	0
5	EDO	B	208	-	3,3,3	0.39	0	2,2,2	0.84	0
5	EDO	C	625	-	3,3,3	0.63	0	2,2,2	0.36	0
4	SO4	B	204	-	4,4,4	0.36	0	6,6,6	0.15	0
4	SO4	C	621	-	4,4,4	0.46	0	6,6,6	0.10	0
4	SO4	C	610	-	4,4,4	0.47	0	6,6,6	0.29	0
5	EDO	C	626	-	3,3,3	0.29	0	2,2,2	0.63	0
5	EDO	C	628	-	3,3,3	0.57	0	2,2,2	0.24	0
5	EDO	B	207	-	3,3,3	0.51	0	2,2,2	0.32	0
4	SO4	B	206	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	C	616	-	4,4,4	0.49	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	615	-	4,4,4	0.42	0	6,6,6	0.13	0
4	SO4	C	620	-	4,4,4	0.40	0	6,6,6	0.18	0
4	SO4	C	622	-	4,4,4	0.38	0	6,6,6	0.08	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
5	EDO	B	209	-	-	1/1/1/1	-
5	EDO	A	204	-	-	0/1/1/1	-
5	EDO	C	627	-	-	1/1/1/1	-
5	EDO	C	604	-	-	1/1/1/1	-
8	CIT	C	605	6	-	6/16/16/16	-
5	EDO	C	629	-	-	1/1/1/1	-
5	EDO	C	624	-	-	1/1/1/1	-
5	EDO	A	202	-	-	0/1/1/1	-
5	EDO	C	632	-	-	0/1/1/1	-
5	EDO	C	634	-	-	1/1/1/1	-
9	A1JID	C	606	3	-	0/14/14/14	0/1/1/1
5	EDO	A	203	-	-	1/1/1/1	-
5	EDO	C	631	-	-	1/1/1/1	-
5	EDO	C	630	-	-	1/1/1/1	-
5	EDO	C	633	-	-	1/1/1/1	-
5	EDO	B	208	-	-	1/1/1/1	-
5	EDO	C	625	-	-	0/1/1/1	-
5	EDO	C	628	-	-	0/1/1/1	-
5	EDO	C	626	-	-	0/1/1/1	-
5	EDO	B	207	-	-	0/1/1/1	-
5	EDO	B	210	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	606	A1JID	O1-C22	3.59	1.44	1.33
8	C	605	CIT	C3-C6	3.05	1.56	1.53
8	C	605	CIT	O1-C1	2.68	1.31	1.22
9	C	606	A1JID	O1-C1	-2.66	1.43	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	606	A1JID	O1-C22-C16	4.00	119.56	109.65
8	C	605	CIT	O6-C6-C3	3.33	118.84	113.05
8	C	605	CIT	O5-C6-C3	-3.18	117.75	122.25
9	C	606	A1JID	C22-C16-N15	-2.86	106.52	112.86
9	C	606	A1JID	C13-C14-N15	2.37	122.02	117.36
8	C	605	CIT	C4-C3-C6	-2.28	105.21	110.11
9	C	606	A1JID	O1-C22-O5	-2.16	119.65	124.97

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	630	EDO	O1-C1-C2-O2
5	A	203	EDO	O1-C1-C2-O2
5	B	210	EDO	O1-C1-C2-O2
5	C	627	EDO	O1-C1-C2-O2
5	C	629	EDO	O1-C1-C2-O2
5	C	633	EDO	O1-C1-C2-O2
8	C	605	CIT	O7-C3-C4-C5
5	C	624	EDO	O1-C1-C2-O2
5	C	631	EDO	O1-C1-C2-O2
5	C	634	EDO	O1-C1-C2-O2
8	C	605	CIT	C2-C3-C4-C5
5	B	208	EDO	O1-C1-C2-O2
5	B	209	EDO	O1-C1-C2-O2
5	C	604	EDO	O1-C1-C2-O2
8	C	605	CIT	O2-C1-C2-C3
8	C	605	CIT	O1-C1-C2-C3
8	C	605	CIT	C2-C3-C6-O6
8	C	605	CIT	C4-C3-C6-O6

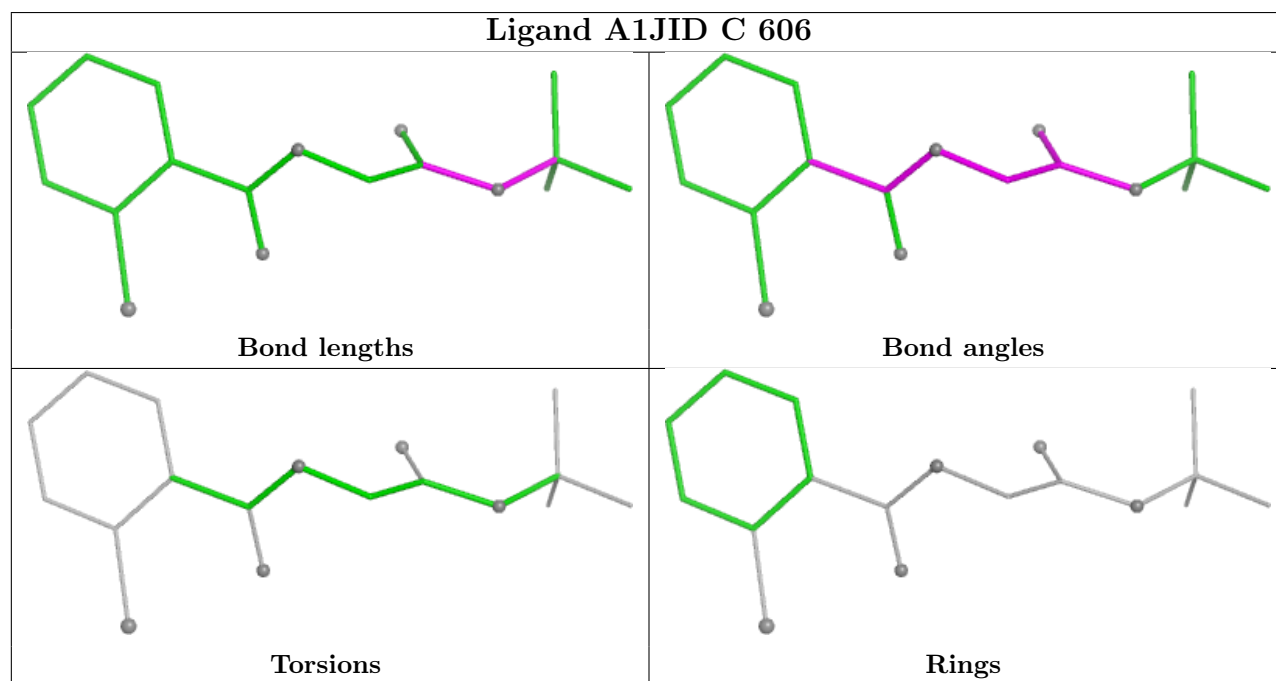
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	623	SO4	1	0
4	C	611	SO4	1	1
5	A	202	EDO	2	0
9	C	606	A1JID	1	0
4	C	621	SO4	2	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 [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	A	99/100 (99%)	-0.47	0 <a href="#">100</a> <a href="#">100</a>	18, 33, 42, 57	7 (7%)
2	B	122/122 (100%)	-0.23	0 <a href="#">100</a> <a href="#">100</a>	19, 36, 53, 83	4 (3%)
3	C	568/570 (99%)	-0.30	4 (0%) <a href="#">84</a> <a href="#">88</a>	15, 33, 58, 102	19 (3%)
All	All	789/792 (99%)	-0.31	4 (0%) <a href="#">87</a> <a href="#">90</a>	15, 33, 55, 102	30 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	329	ILE	3.7
3	C	550	GLY	2.5
3	C	522[A]	ASN	2.3
3	C	321	VAL	2.1

### 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
3	CSS	C	322	7/8	0.86	0.14	65,67,79,85	0
1	CXM	A	1	11/12	0.96	0.08	29,34,41,43	0
3	KCX	C	220	12/13	0.97	0.08	27,33,40,42	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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
4	SO4	C	619	5/5	0.72	0.17	64,67,80,81	5
5	EDO	B	210	4/4	0.74	0.20	49,60,63,73	0
5	EDO	C	604	4/4	0.74	0.16	52,66,69,69	0
4	SO4	B	206	5/5	0.75	0.10	116,116,123,133	0
10	H2S	C	635	1/1	0.76	0.16	93,93,93,93	0
5	EDO	C	634	4/4	0.79	0.22	67,76,77,81	0
5	EDO	B	208	4/4	0.80	0.15	63,66,67,72	0
4	SO4	B	201	5/5	0.81	0.12	44,57,70,74	5
4	SO4	C	613	5/5	0.82	0.07	77,84,85,85	5
4	SO4	C	618	5/5	0.82	0.10	49,57,70,73	5
4	SO4	B	203	5/5	0.83	0.09	62,63,68,70	5
4	SO4	B	202	5/5	0.83	0.14	87,88,96,97	5
5	EDO	C	627	4/4	0.84	0.21	61,61,64,74	0
5	EDO	C	629	4/4	0.84	0.17	43,57,58,66	0
4	SO4	B	205	5/5	0.84	0.10	79,80,89,90	5
4	SO4	A	201	5/5	0.84	0.11	78,92,95,113	0
5	EDO	A	204	4/4	0.85	0.13	76,76,77,82	0
4	SO4	C	614	5/5	0.85	0.12	55,70,88,99	0
5	EDO	C	624	4/4	0.86	0.15	49,57,59,62	0
5	EDO	C	626	4/4	0.86	0.14	60,60,65,71	0
4	SO4	C	617	5/5	0.87	0.15	65,65,73,81	5
5	EDO	B	207	4/4	0.87	0.12	58,68,72,75	0
4	SO4	C	622	5/5	0.87	0.11	79,79,83,83	5
5	EDO	B	209	4/4	0.87	0.17	62,65,67,68	0
5	EDO	C	631	4/4	0.88	0.15	67,73,78,82	0
4	SO4	B	204	5/5	0.88	0.09	62,68,73,78	5
4	SO4	C	616	5/5	0.88	0.14	47,48,60,60	5
4	SO4	C	608	5/5	0.89	0.11	64,68,77,79	5
5	EDO	C	633	4/4	0.89	0.16	59,64,68,74	0
5	EDO	A	203	4/4	0.89	0.12	33,34,34,38	4
5	EDO	C	630	4/4	0.89	0.12	50,60,61,67	0
4	SO4	C	610	5/5	0.90	0.12	45,52,63,69	5
4	SO4	C	607	5/5	0.90	0.13	49,61,69,77	5
4	SO4	C	623	5/5	0.91	0.11	70,74,79,79	5
5	EDO	C	625	4/4	0.91	0.11	49,65,67,73	0
4	SO4	C	621	5/5	0.92	0.09	62,63,68,71	5
4	SO4	C	609	5/5	0.92	0.08	44,45,54,60	5

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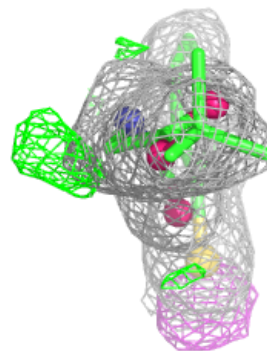
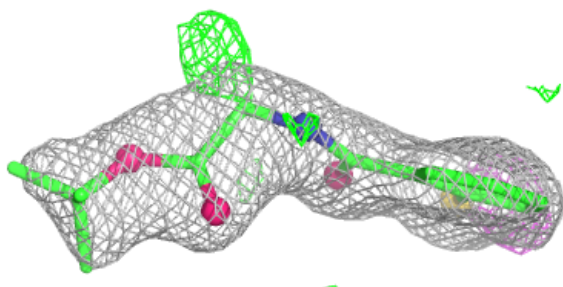
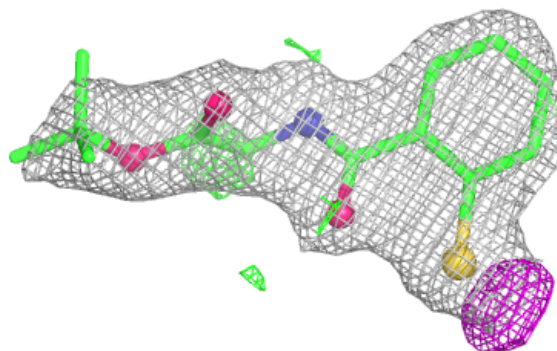
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	C	611	5/5	0.92	0.07	57,58,61,70	5
9	A1JID	C	606	18/18	0.92	0.12	47,52,59,59	18
4	SO4	C	620	5/5	0.92	0.10	56,61,67,68	5
5	EDO	A	202	4/4	0.93	0.12	50,59,65,65	0
8	CIT	C	605	13/13	0.93	0.09	38,45,54,56	13
4	SO4	C	612	5/5	0.95	0.13	36,46,50,57	5
5	EDO	C	632	4/4	0.96	0.08	48,48,49,52	0
5	EDO	C	628	4/4	0.96	0.11	41,41,42,43	0
4	SO4	C	615	5/5	0.96	0.11	48,51,55,57	5
7	OH	C	603	1/1	0.98	0.06	41,41,41,41	0
6	NI	C	601	1/1	1.00	0.05	42,42,42,42	0
6	NI	C	602	1/1	1.00	0.05	38,38,38,38	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 A1JID C 606:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.