



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2026 – 01:15 pm BST

PDB ID : 9REX / pdb\_00009rex  
Title : Sporosarcina pasteurii urease in complex with an Ebsulfur derivative at 1.95 Å  
Authors : Mazzei, L.; Ciurli, S.; Paul, A.; Cianci, M.  
Deposited on : 2025-06-04  
Resolution : 1.95 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
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

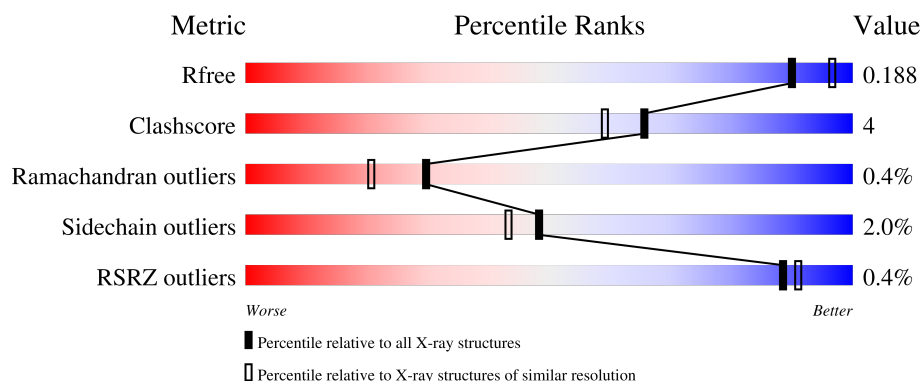
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	<div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div>
2	B	122	<div> <div>93%</div> <div>7%</div> </div>
3	C	570	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6898 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	8	0
			843	529	145	162	7			

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
			984	607	177	199	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	17	0
			4439	2786	765	862	26			

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 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
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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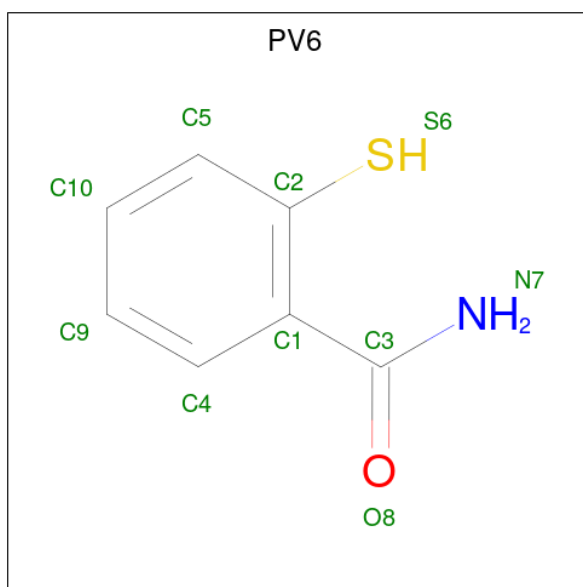
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	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 2-sulfanylbenezamide (CCD ID: PV6) (formula: C<sub>7</sub>H<sub>7</sub>NOS).

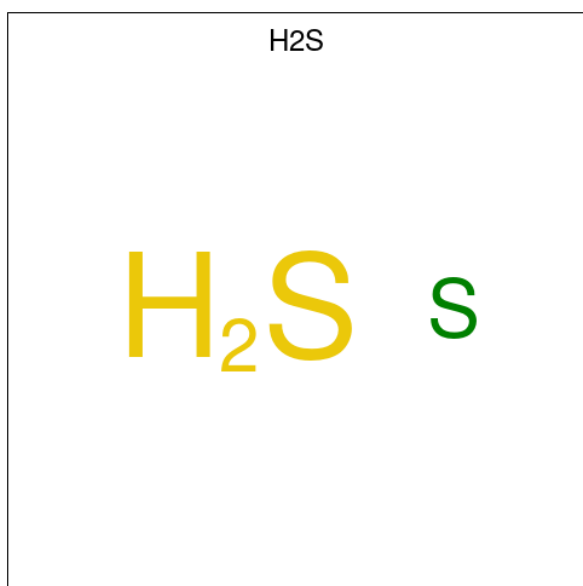


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

- Molecule 8 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 9 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H<sub>2</sub>S).



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

- Molecule 10 is water.

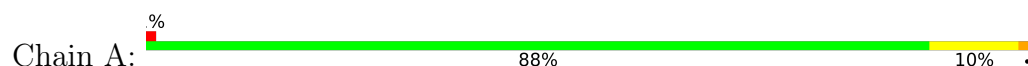
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	50	Total O 50 50	0	0
10	B	84	Total O 84 84	0	0
10	C	318	Total O 318 318	0	0



### 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.

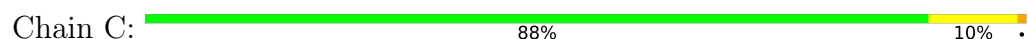
- Molecule 1: Urease subunit gamma



- Molecule 2: Urease subunit beta



- Molecule 3: Urease subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.37Å 131.37Å 188.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.73 – 1.95 48.73 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.73-1.95) 99.9 (48.73-1.95)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.149 , 0.187 0.150 , 0.188	Depositor DCC
$R_{free}$ test set	3532 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6898	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 3.80% 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: EDO, CXM, NI, SO4, H2S, KCX, O, PV6

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	0.61	0/850	0.97	1/1142 (0.1%)
2	B	0.59	0/999	1.10	1/1342 (0.1%)
3	C	0.65	0/4532	1.05	6/6136 (0.1%)
All	All	0.63	0/6381	1.05	8/8620 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	520	CYS	CB-CA-C	-8.57	94.75	109.65
3	C	251	ASP	CA-CB-CG	6.72	119.32	112.60
3	C	516	THR	CA-CB-OG1	-6.09	100.46	109.60
2	B	110	LYS	CB-CA-C	5.97	121.01	110.85
3	C	463	ASP	CA-CB-CG	5.94	118.54	112.60
3	C	274	PHE	CA-CB-CG	5.65	119.45	113.80
3	C	285	PRO	N-CA-CB	-5.28	96.80	102.60
1	A	44	MET	CA-CB-CG	-5.10	103.89	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	219	LEU	Mainchain
3	C	234	ARG	Sidechain
3	C	402	ARG	Sidechain

## 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	A	843	0	856	8	0
2	B	984	0	964	5	0
3	C	4439	0	4422	38	0
4	A	16	0	24	2	0
4	B	8	0	12	0	0
4	C	36	0	54	1	0
5	A	25	0	0	0	0
5	B	10	0	0	1	0
5	C	70	0	0	3	0
6	C	2	0	0	0	0
7	C	10	0	0	2	0
8	C	1	0	0	0	0
9	C	2	0	0	0	0
10	A	50	0	0	0	1
10	B	84	0	0	1	1
10	C	318	0	0	1	0
All	All	6898	0	6332	49	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 (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)
1:A:32:TYR:OH	4:A:204:EDO:H22	1.78	0.82
3:C:559:LYS:H	4:C:611:EDO:H11	1.46	0.80
3:C:326:LYS:HB2	3:C:329:ILE:HD12	1.69	0.74
2:B:33[B]:SER:HB3	2:B:82:GLU:HB2	1.80	0.62
2:B:21:ILE:HD11	3:C:1:MET:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:203:SO4:O2	10:B:301:HOH:O	2.14	0.61
2:B:15:ALA:O	3:C:5[B]:ARG:HG3	2.00	0.60
3:C:360[A]:MET:HE3	3:C:377:THR:HA	1.84	0.59
3:C:350:ILE:HG13	3:C:555:CYS:SG	2.47	0.55
3:C:81:GLY:HA2	3:C:404:LYS:HE2	1.90	0.54
3:C:323:HIS:NE2	5:C:617:SO4:O3	2.40	0.54
1:A:66[B]:ARG:HD2	1:A:100:SER:OXT	2.08	0.53
3:C:64[B]:GLU:HG2	5:C:615:SO4:O3	2.10	0.51
3:C:175:PRO:HB3	3:C:199:LYS:HE3	1.94	0.50
4:A:203:EDO:H11	3:C:566:ARG:HH12	1.76	0.50
3:C:70:LEU:HD11	3:C:86:ASP:HB3	1.94	0.49
3:C:259:LEU:HD11	3:C:290[B]:MET:HG3	1.95	0.49
3:C:303:PRO:HG3	3:C:368:GLY:HA2	1.94	0.49
3:C:301:THR:CG2	3:C:363:ASP:HB2	2.43	0.48
1:A:79[B]:ASP:CG	1:A:96[B]:HIS:HD1	2.22	0.47
3:C:350:ILE:CG1	3:C:555:CYS:SG	3.02	0.47
2:B:21:ILE:CD1	3:C:1:MET:HG2	2.45	0.47
3:C:554:THR:C	7:C:612:PV6:N7	2.72	0.46
1:A:81[B]:GLN:HG2	1:A:94:THR:OG1	2.16	0.46
3:C:384:MET:HA	3:C:384:MET:HE2	1.98	0.46
1:A:44:MET:HE3	1:A:82:ALA:HB1	1.97	0.45
3:C:274:PHE:O	3:C:275:HIS:C	2.60	0.45
1:A:30:LEU:HD13	1:A:38:ILE:HD12	1.99	0.45
1:A:79[A]:ASP:OD1	1:A:79[A]:ASP:C	2.60	0.45
3:C:249:HIS:CE1	3:C:281:GLY:HA3	2.52	0.45
3:C:327:GLN:H	3:C:327:GLN:HG2	1.55	0.45
3:C:303:PRO:HG2	3:C:367:MET:O	2.16	0.45
2:B:57:PHE:O	2:B:124:GLY:HA3	2.17	0.44
3:C:220:KCX:CX	3:C:222:HIS:HD2	2.30	0.44
3:C:158:PHE:CE2	3:C:418[A]:GLN:CG	3.01	0.44
3:C:152:ASN:OD1	10:C:701:HOH:O	2.21	0.44
3:C:138:VAL:O	3:C:159:GLY:HA3	2.18	0.44
3:C:169:LYS:NZ	5:C:624:SO4:O1	2.33	0.44
3:C:316:LEU:O	3:C:320:MET:HG2	2.18	0.43
3:C:329:ILE:HA	3:C:330:PRO:HD3	1.92	0.42
3:C:362:THR:O	3:C:368:GLY:HA3	2.20	0.42
3:C:470:THR:N	3:C:471:PRO:CD	2.83	0.41
3:C:325:LEU:HB3	3:C:332:ASP:HB3	2.02	0.41
3:C:554:THR:O	7:C:612:PV6:N7	2.53	0.41
3:C:175:PRO:O	3:C:179:ASN:HB2	2.21	0.40
3:C:461:ILE:HD11	3:C:469:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96[A]:HIS:CD2	1:A:96[A]:HIS:N	2.88	0.40
3:C:316:LEU:HD23	3:C:316:LEU:HA	1.88	0.40
3:C:129:VAL:HG22	3:C:437:LEU:HG	2.02	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)
10:A:335:HOH:O	10:B:320:HOH:O[8_676]	2.18	0.02

## 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	106/100 (106%)	106 (100%)	0	0	100	100
2	B	124/122 (102%)	120 (97%)	3 (2%)	1 (1%)	16	8
3	C	584/570 (102%)	560 (96%)	22 (4%)	2 (0%)	36	28
All	All	814/792 (103%)	786 (97%)	25 (3%)	3 (0%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ILE
3	C	283	HIS
3	C	275	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	A	91/83 (110%)	90 (99%)	1 (1%)	65	64
2	B	105/101 (104%)	104 (99%)	1 (1%)	68	67
3	C	474/458 (104%)	463 (98%)	11 (2%)	44	38
All	All	670/642 (104%)	657 (98%)	13 (2%)	48	45

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	SER
2	B	126	GLU
3	C	1	MET
3	C	7	GLN
3	C	158	PHE
3	C	249	HIS
3	C	285	PRO
3	C	305	ARG
3	C	327	GLN
3	C	395	LYS
3	C	396	ASN
3	C	452	LYS
3	C	559	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
2	B	109	ASN
3	C	7	GLN
3	C	179	ASN
3	C	254	ASN

### 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	C	220	6,3	9,11,12	0.51	0	5,12,14	0.31	0
1	CXM	A	1	1	8,10,11	0.64	0	7,11,13	1.04	1 (14%)

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	C	220	6,3	-	0/9/10/12	-
1	CXM	A	1	1	-	2/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	O-C-CA	-2.19	119.05	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	C-CA-N-CN
1	A	1	CXM	CB-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 42 ligands modelled in this entry, 3 are monoatomic and 2 are modelled with single atom - leaving 37 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	C	615	-	4,4,4	0.42	0	6,6,6	0.12	0
5	SO4	A	209	-	4,4,4	0.34	0	6,6,6	0.05	0
5	SO4	C	617	-	4,4,4	0.35	0	6,6,6	0.18	0
5	SO4	C	621	-	4,4,4	0.33	0	6,6,6	0.07	0
4	EDO	A	203	-	3,3,3	0.29	0	2,2,2	0.39	0
5	SO4	C	623	-	4,4,4	0.34	0	6,6,6	0.07	0
5	SO4	C	626	-	4,4,4	0.35	0	6,6,6	0.06	0
5	SO4	A	208	-	4,4,4	0.39	0	6,6,6	0.06	0
4	EDO	C	607	-	3,3,3	0.25	0	2,2,2	0.83	0
4	EDO	C	610	-	3,3,3	0.11	0	2,2,2	0.40	0
5	SO4	B	204	-	4,4,4	0.35	0	6,6,6	0.17	0
4	EDO	C	605	-	3,3,3	0.25	0	2,2,2	0.33	0
4	EDO	A	202	-	3,3,3	0.10	0	2,2,2	0.07	0
4	EDO	C	603	-	3,3,3	0.09	0	2,2,2	0.33	0
5	SO4	C	620	-	4,4,4	0.41	0	6,6,6	0.04	0
7	PV6	C	612	3	10,10,10	2.00	2 (20%)	12,13,13	1.83	3 (25%)
4	EDO	B	201	-	3,3,3	0.37	0	2,2,2	0.55	0
5	SO4	C	614	-	4,4,4	0.35	0	6,6,6	0.13	0
4	EDO	C	609	-	3,3,3	0.21	0	2,2,2	0.48	0
5	SO4	A	206	-	4,4,4	0.40	0	6,6,6	0.05	0
4	EDO	C	608	-	3,3,3	0.17	0	2,2,2	0.50	0
5	SO4	A	205	-	4,4,4	0.34	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	C	624	-	4,4,4	0.33	0	6,6,6	0.41	0
5	SO4	A	207	-	4,4,4	0.42	0	6,6,6	0.27	0
5	SO4	C	622	-	4,4,4	0.35	0	6,6,6	0.25	0
4	EDO	B	202	-	3,3,3	0.09	0	2,2,2	0.06	0
4	EDO	C	606	-	3,3,3	0.15	0	2,2,2	0.64	0
5	SO4	B	203	-	4,4,4	0.46	0	6,6,6	0.06	0
5	SO4	C	616	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	C	613	-	4,4,4	0.43	0	6,6,6	0.06	0
4	EDO	A	201	-	3,3,3	0.43	0	2,2,2	1.02	0
4	EDO	C	604	-	3,3,3	0.24	0	2,2,2	0.69	0
4	EDO	C	611	-	3,3,3	0.13	0	2,2,2	0.60	0
4	EDO	A	204	-	3,3,3	0.72	0	2,2,2	0.81	0
5	SO4	C	625	-	4,4,4	0.36	0	6,6,6	0.10	0
5	SO4	C	618	-	4,4,4	0.35	0	6,6,6	0.30	0
5	SO4	C	619	-	4,4,4	0.33	0	6,6,6	0.17	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	A	201	-	-	1/1/1/1	-
4	EDO	C	607	-	-	1/1/1/1	-
4	EDO	C	609	-	-	0/1/1/1	-
4	EDO	C	608	-	-	1/1/1/1	-
4	EDO	C	610	-	-	1/1/1/1	-
4	EDO	C	604	-	-	0/1/1/1	-
4	EDO	C	611	-	-	1/1/1/1	-
4	EDO	A	204	-	-	1/1/1/1	-
4	EDO	A	202	-	-	1/1/1/1	-
4	EDO	C	603	-	-	0/1/1/1	-
4	EDO	C	605	-	-	1/1/1/1	-
4	EDO	A	203	-	-	1/1/1/1	-
4	EDO	C	606	-	-	1/1/1/1	-
7	PV6	C	612	3	-	4/4/4/4	0/1/1/1
4	EDO	B	202	-	-	0/1/1/1	-
4	EDO	B	201	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	612	PV6	C3-N7	5.37	1.43	1.33
7	C	612	PV6	C1-C3	3.00	1.54	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	612	PV6	O8-C3-N7	-4.28	116.50	122.58
7	C	612	PV6	O8-C3-C1	2.63	123.34	120.24
7	C	612	PV6	C1-C2-S6	2.03	126.06	120.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	605	EDO	O1-C1-C2-O2
4	C	610	EDO	O1-C1-C2-O2
4	C	611	EDO	O1-C1-C2-O2
4	A	203	EDO	O1-C1-C2-O2
4	A	204	EDO	O1-C1-C2-O2
7	C	612	PV6	C2-C1-C3-N7
7	C	612	PV6	C2-C1-C3-O8
4	C	606	EDO	O1-C1-C2-O2
4	C	608	EDO	O1-C1-C2-O2
4	A	202	EDO	O1-C1-C2-O2
4	A	201	EDO	O1-C1-C2-O2
4	C	607	EDO	O1-C1-C2-O2
7	C	612	PV6	C4-C1-C3-N7
7	C	612	PV6	C4-C1-C3-O8

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	615	SO4	1	0
5	C	617	SO4	1	0
4	A	203	EDO	1	0
7	C	612	PV6	2	0
5	C	624	SO4	1	0
5	B	203	SO4	1	0
4	C	611	EDO	1	0
4	A	204	EDO	1	0

## 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%)	-0.72	1 (1%) 79 84	15, 27, 35, 59	8 (8%)
2	B	122/122 (100%)	-0.50	0 100 100	16, 30, 50, 86	4 (3%)
3	C	569/570 (99%)	-0.61	2 (0%) 88 91	12, 27, 47, 85	17 (2%)
All	All	790/792 (99%)	-0.61	3 (0%) 88 91	12, 27, 46, 86	29 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	554	THR	2.5
3	C	322	CYS	2.4
1	A	100	SER	2.0

### 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	A	1	11/12	0.98	0.06	26,30,38,39	0
3	KCX	C	220	12/13	0.98	0.05	21,26,33,33	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
5	SO4	C	626	5/5	0.67	0.15	117,135,158,159	0
9	H2S	C	628	1/1	0.69	0.22	89,89,89,89	0
5	SO4	C	624	5/5	0.74	0.20	47,59,74,89	5
9	H2S	C	629	1/1	0.75	0.19	93,93,93,93	0
5	SO4	A	209	5/5	0.76	0.13	111,114,126,145	0
4	EDO	C	605	4/4	0.78	0.20	57,59,67,69	0
4	EDO	A	203	4/4	0.78	0.19	38,54,58,65	0
5	SO4	C	621	5/5	0.79	0.22	103,115,126,135	0
5	SO4	C	616	5/5	0.80	0.11	78,78,79,79	5
5	SO4	B	204	5/5	0.82	0.11	62,62,71,71	5
5	SO4	C	620	5/5	0.82	0.08	68,71,77,77	5
5	SO4	C	625	5/5	0.82	0.12	70,87,93,95	5
5	SO4	C	623	5/5	0.83	0.14	101,110,135,145	0
4	EDO	C	608	4/4	0.83	0.19	54,68,69,75	0
4	EDO	A	204	4/4	0.84	0.13	38,42,42,46	0
5	SO4	C	622	5/5	0.84	0.15	50,64,70,82	5
5	SO4	C	613	5/5	0.85	0.13	48,52,53,57	5
4	EDO	C	610	4/4	0.87	0.13	55,55,56,67	0
4	EDO	C	611	4/4	0.88	0.10	37,44,45,52	0
5	SO4	A	207	5/5	0.88	0.14	31,37,42,46	5
5	SO4	C	618	5/5	0.88	0.14	49,62,70,73	5
5	SO4	A	208	5/5	0.89	0.18	89,89,96,105	5
7	PV6	C	612	10/10	0.89	0.15	54,81,87,90	0
5	SO4	A	205	5/5	0.90	0.14	43,45,54,61	5
4	EDO	C	606	4/4	0.90	0.13	40,47,48,48	0
4	EDO	A	201	4/4	0.91	0.12	46,50,52,55	0
4	EDO	B	201	4/4	0.92	0.15	46,46,49,53	0
4	EDO	B	202	4/4	0.92	0.11	43,66,70,70	0
4	EDO	C	607	4/4	0.92	0.12	57,58,59,61	0
4	EDO	C	604	4/4	0.92	0.10	42,49,50,51	0
4	EDO	C	609	4/4	0.92	0.10	43,47,48,49	0
5	SO4	A	206	5/5	0.94	0.11	50,50,51,52	5
4	EDO	C	603	4/4	0.94	0.10	47,55,55,62	0
5	SO4	C	614	5/5	0.94	0.08	43,45,56,56	5
5	SO4	C	615	5/5	0.94	0.10	52,59,63,64	5
5	SO4	C	617	5/5	0.95	0.08	49,53,59,69	0
5	SO4	B	203	5/5	0.96	0.10	41,44,46,49	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	C	619	5/5	0.96	0.16	32,45,48,59	5
4	EDO	A	202	4/4	0.98	0.05	32,33,34,34	0
8	O	C	627	1/1	0.99	0.03	28,28,28,28	0
6	NI	C	601	1/1	1.00	0.03	30,30,30,30	0
6	NI	C	602	1/1	1.00	0.03	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.