



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:23 pm GMT

PDB ID : 6ZNY  
Title : 1.89 Å resolution 4-methylcatechol (4-methylbenzene-1,2-diol) inhibited Sporosarcina pasteurii urease  
Authors : Mazzei, L.; Cianci, M.; Musiani, F.; Ciurli, S.  
Deposited on : 2020-07-07  
Resolution : 1.89 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

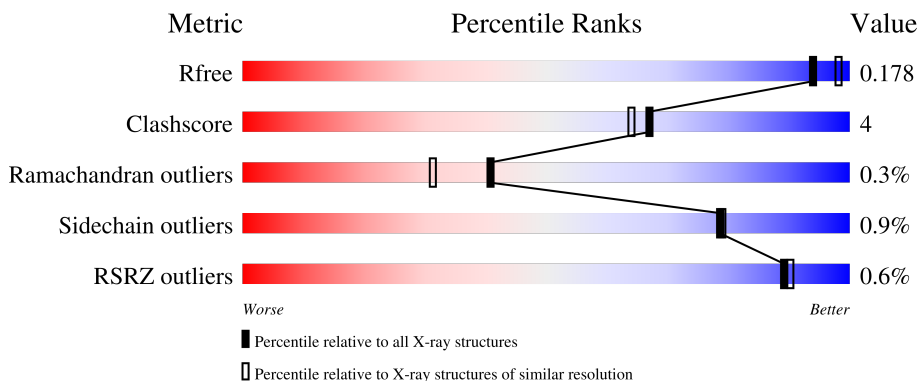
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	 92% 8%
2	BBB	122	 93% 7%
3	CCC	570	 91% 8% .

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	CCC	614	-	-	X	-
5	SO4	AAA	208	-	-	X	-
5	SO4	BBB	204	-	-	X	-
5	SO4	CCC	624	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7006 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
			Total	C	N	O	S			
1	AAA	100	834	523	143	161	7	0	7	0

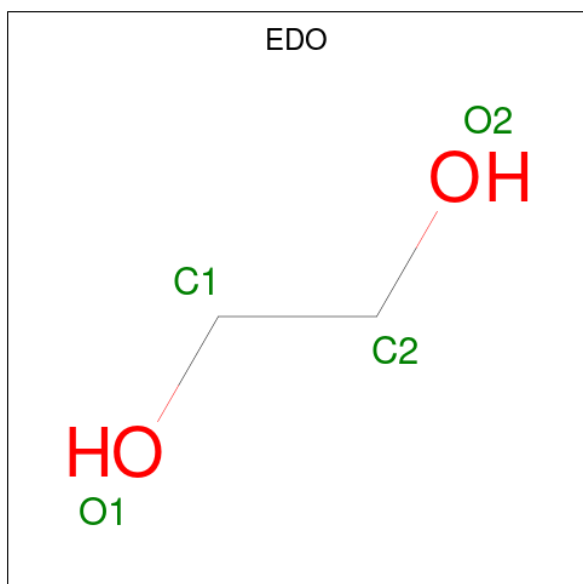
- Molecule 2 is a protein called Urease subunit beta.

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

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	CCC	570	4449	2793	765	864	27	0	17	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



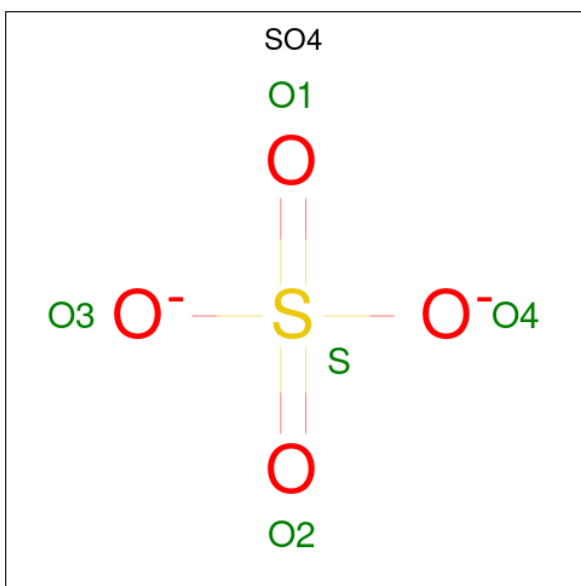
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1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

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

- 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 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	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

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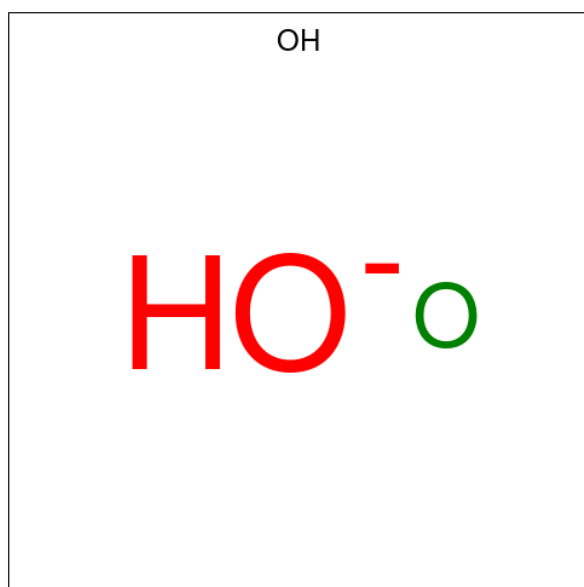
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total O S 5 4 1	0	0
5	CCC	1	Total O S 5 4 1	0	0
5	CCC	1	Total O S 5 4 1	0	0

- 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 HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	71	Total O 71 71	0	0
8	BBB	107	Total O 107 107	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	CCC	406	Total 406	O 406	0	0

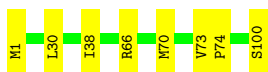


### 3 Residue-property plots [i](#)

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:  92% 8%



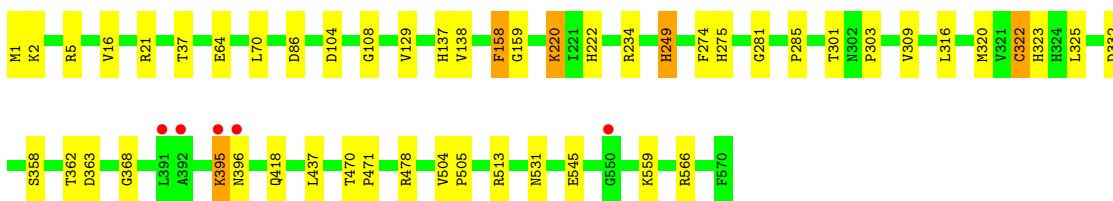
- Molecule 2: Urease subunit beta

Chain BBB:  93% 7%



- Molecule 3: Urease subunit alpha

Chain CCC:  91% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.02Å 131.02Å 188.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.27 – 1.89 97.27 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (97.27-1.89) 99.7 (97.27-1.89)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.159 , 0.178 0.159 , 0.178	Depositor DCC
$R_{free}$ test set	3779 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.837	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: QNQ, EDO, OH, CXM, SO4, 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	0.57	0/841	0.79	0/1131
2	BBB	0.57	0/998	0.85	0/1342
3	CCC	0.54	0/4526	0.80	1/6126 (0.0%)
All	All	0.55	0/6365	0.81	1/8599 (0.0%)

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	CCC	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	234	ARG	CG-CD-NE	-6.04	99.11	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	CCC	322	QNQ	Mainchain

### 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	834	0	844	4	0
2	BBB	983	0	964	7	1
3	CCC	4449	0	4419	40	0
4	AAA	28	0	42	0	0
4	BBB	12	0	18	1	0
4	CCC	68	0	102	13	0
5	AAA	5	0	0	2	0
5	BBB	15	0	0	2	0
5	CCC	25	0	0	2	0
6	CCC	2	0	0	0	0
7	CCC	1	0	0	0	0
8	AAA	71	0	0	0	0
8	BBB	107	0	0	1	0
8	CCC	406	0	0	0	0
All	All	7006	0	6389	50	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 (50) 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:37:THR:HA	4:CCC:612:EDO:H12	1.41	1.01
3:CCC:64[B]:GLU:HG2	4:CCC:614:EDO:H22	1.46	0.98
3:CCC:64[B]:GLU:HG2	4:CCC:614:EDO:C2	2.06	0.85
3:CCC:323:HIS:CE1	5:CCC:624:SO4:O3	2.49	0.65
3:CCC:64[B]:GLU:CG	4:CCC:614:EDO:H22	2.27	0.62
3:CCC:37:THR:HA	4:CCC:612:EDO:C1	2.24	0.60
2:BBB:111[A]:GLU:CD	2:BBB:111[A]:GLU:H	2.04	0.60
1:AAA:70[A]:MET:HB3	5:AAA:208:SO4:O1	2.04	0.57
3:CCC:108:GLY:H	4:CCC:607:EDO:C1	2.18	0.57
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.86	0.56
3:CCC:395:LYS:HD3	3:CCC:396:ASN:N	2.23	0.54
1:AAA:66[B]:ARG:HD2	1:AAA:100:SER:O	2.08	0.54
3:CCC:395:LYS:HD3	3:CCC:396:ASN:H	1.75	0.51
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.11	0.51
3:CCC:513[A]:ARG:NE	4:CCC:618:EDO:O1	2.44	0.51
3:CCC:325:LEU:HB3	3:CCC:332:ASP:HB3	1.92	0.50
3:CCC:478:ARG:HH12	4:CCC:620:EDO:H12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:513[A]:ARG:NH2	4:CCC:618:EDO:O1	2.43	0.49
3:CCC:64[B]:GLU:HG2	4:CCC:614:EDO:H21	1.92	0.49
3:CCC:108:GLY:H	4:CCC:607:EDO:H12	1.77	0.49
3:CCC:220:KCX:CX	3:CCC:222:HIS:HD2	2.25	0.49
3:CCC:64[B]:GLU:CG	4:CCC:614:EDO:C2	2.85	0.49
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	2.96	0.49
3:CCC:5[A]:ARG:NH2	3:CCC:16:VAL:O	2.45	0.48
3:CCC:303:PRO:HG3	3:CCC:368:GLY:HA2	1.96	0.47
3:CCC:323:HIS:HE1	5:CCC:624:SO4:O3	1.98	0.47
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	3.03	0.47
2:BBB:31[B]:ARG:HG2	2:BBB:31[B]:ARG:HH11	1.79	0.46
1:AAA:30:LEU:HD13	1:AAA:38:ILE:HD12	1.97	0.45
4:BBB:202:EDO:H21	8:BBB:364:HOH:O	2.16	0.45
5:AAA:208:SO4:O1	3:CCC:566:ARG:NH1	2.49	0.45
3:CCC:129:VAL:HG22	3:CCC:437:LEU:HG	1.98	0.45
3:CCC:362:THR:O	3:CCC:368:GLY:HA3	2.17	0.45
1:AAA:73:VAL:N	1:AAA:74:PRO:CD	2.81	0.44
3:CCC:108:GLY:H	4:CCC:607:EDO:H11	1.83	0.43
3:CCC:309:VAL:HG11	3:CCC:559:LYS:HG2	2.00	0.43
2:BBB:10:GLY:HA2	3:CCC:21:ARG:O	2.18	0.43
2:BBB:15:ALA:O	3:CCC:5[B]:ARG:HD2	2.19	0.43
3:CCC:470:THR:N	3:CCC:471:PRO:CD	2.82	0.43
3:CCC:1:MET:HG2	3:CCC:2:LYS:N	2.34	0.42
3:CCC:301:THR:CG2	3:CCC:363:ASP:HB2	2.49	0.42
2:BBB:31[A]:ARG:NH1	5:BBB:204:SO4:O4	2.52	0.42
2:BBB:31[B]:ARG:HG2	2:BBB:31[B]:ARG:NH1	2.35	0.42
3:CCC:137:HIS:CD2	3:CCC:363:ASP:HA	2.55	0.42
3:CCC:138:VAL:O	3:CCC:159:GLY:HA3	2.20	0.42
3:CCC:316:LEU:O	3:CCC:320:MET:HG2	2.20	0.42
3:CCC:504:VAL:N	3:CCC:505:PRO:CD	2.84	0.41
3:CCC:358:SER:HA	3:CCC:531:ASN:HB3	2.02	0.41
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.56	0.41

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)
2:BBB:5:ASN:N	2:BBB:16:GLU:OE1[8_676]	2.15	0.05

## 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	105/100 (105%)	105 (100%)	0	0	100	100
2	BBB	124/122 (102%)	120 (97%)	3 (2%)	1 (1%)	19	9
3	CCC	583/570 (102%)	555 (95%)	27 (5%)	1 (0%)	47	38
All	All	812/792 (102%)	780 (96%)	30 (4%)	2 (0%)	41	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	99	ILE
3	CCC	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	AAA	90/83 (108%)	90 (100%)	0	100	100
2	BBB	105/101 (104%)	104 (99%)	1 (1%)	76	76
3	CCC	474/457 (104%)	468 (99%)	6 (1%)	69	68
All	All	669/641 (104%)	662 (99%)	7 (1%)	78	76

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

Mol	Chain	Res	Type
2	BBB	119	GLU

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Mol	Chain	Res	Type
3	CCC	158	PHE
3	CCC	249	HIS
3	CCC	285	PRO
3	CCC	395	LYS
3	CCC	545[A]	GLU
3	CCC	545[B]	GLU

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](#)

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
3	KCX	CCC	220	6,3	9,11,12	2.09	1 (11%)	5,12,14	2.64	1 (20%)
1	CXM	AAA	1	1	8,10,11	2.48	1 (12%)	7,11,13	2.01	1 (14%)
3	QNQ	CCC	322	3	14,15,16	1.50	1 (7%)	12,20,22	1.33	1 (8%)

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	6,3	-	0/9/10/12	-
1	CXM	AAA	1	1	-	3/9/10/12	-
3	QNQ	CCC	322	3	-	0/5/7/9	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	1	CXM	ON1-CN	6.76	1.34	1.21
3	CCC	220	KCX	OQ1-CX	6.03	1.32	1.21
3	CCC	322	QNQ	C6-SG	-4.92	1.72	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	220	KCX	OQ1-CX-NZ	-5.84	115.91	124.96
1	AAA	1	CXM	ON1-CN-N	-4.53	117.41	124.85
3	CCC	322	QNQ	C5-C6-SG	2.61	122.97	119.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	CXM	CB-CA-N-CN
1	AAA	1	CXM	ON1-CN-N-CA
1	AAA	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	CCC	220	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 36 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	BBB	203	-	3,3,3	0.29	0	2,2,2	0.70	0
4	EDO	CCC	608	-	3,3,3	0.51	0	2,2,2	0.91	0
4	EDO	CCC	617	-	3,3,3	0.40	0	2,2,2	0.75	0
4	EDO	AAA	202	-	3,3,3	0.64	0	2,2,2	1.26	0
4	EDO	CCC	613	-	3,3,3	0.44	0	2,2,2	0.67	0
4	EDO	CCC	611	-	3,3,3	0.36	0	2,2,2	1.11	0
5	SO4	BBB	206	-	4,4,4	0.28	0	6,6,6	0.19	0
4	EDO	CCC	620	-	3,3,3	0.61	0	2,2,2	1.45	1 (50%)
4	EDO	CCC	605	-	3,3,3	0.27	0	2,2,2	0.94	0
4	EDO	CCC	619	-	3,3,3	0.96	0	2,2,2	0.56	0
5	SO4	CCC	625	-	4,4,4	0.67	0	6,6,6	0.53	0
4	EDO	CCC	615	-	3,3,3	0.35	0	2,2,2	0.35	0
5	SO4	CCC	622	-	4,4,4	0.17	0	6,6,6	0.23	0
4	EDO	BBB	201	-	3,3,3	0.63	0	2,2,2	0.73	0
4	EDO	AAA	205	-	3,3,3	1.07	0	2,2,2	0.54	0
5	SO4	BBB	205	-	4,4,4	0.30	0	6,6,6	0.09	0
4	EDO	CCC	606	-	3,3,3	0.35	0	2,2,2	0.89	0
4	EDO	CCC	604	-	3,3,3	0.51	0	2,2,2	0.49	0
5	SO4	CCC	624	-	4,4,4	0.23	0	6,6,6	0.17	0
4	EDO	AAA	203	-	3,3,3	0.70	0	2,2,2	0.75	0
4	EDO	BBB	202	-	3,3,3	0.35	0	2,2,2	0.36	0
5	SO4	BBB	204	-	4,4,4	0.33	0	6,6,6	0.11	0
4	EDO	CCC	618	-	3,3,3	0.64	0	2,2,2	0.50	0
5	SO4	AAA	208	-	4,4,4	0.26	0	6,6,6	0.16	0
4	EDO	CCC	609	-	3,3,3	0.39	0	2,2,2	0.82	0
5	SO4	CCC	623	-	4,4,4	0.33	0	6,6,6	0.17	0
4	EDO	AAA	201	-	3,3,3	0.38	0	2,2,2	0.80	0
4	EDO	CCC	616	-	3,3,3	0.54	0	2,2,2	0.73	0
4	EDO	AAA	207	-	3,3,3	0.63	0	2,2,2	0.53	0
4	EDO	CCC	614	-	3,3,3	0.42	0	2,2,2	0.82	0
4	EDO	CCC	607	-	3,3,3	0.25	0	2,2,2	1.32	0
4	EDO	AAA	206	-	3,3,3	0.84	0	2,2,2	0.45	0
4	EDO	CCC	612	-	3,3,3	0.61	0	2,2,2	1.01	0
5	SO4	CCC	621	-	4,4,4	0.40	0	6,6,6	0.07	0
4	EDO	AAA	204	-	3,3,3	1.07	0	2,2,2	0.89	0
4	EDO	CCC	610	-	3,3,3	0.53	0	2,2,2	0.49	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	203	-	-	1/1/1/1	-
4	EDO	CCC	608	-	-	0/1/1/1	-
4	EDO	CCC	617	-	-	1/1/1/1	-
4	EDO	AAA	202	-	-	1/1/1/1	-
4	EDO	CCC	613	-	-	0/1/1/1	-
4	EDO	CCC	611	-	-	1/1/1/1	-
4	EDO	CCC	620	-	-	1/1/1/1	-
4	EDO	CCC	605	-	-	0/1/1/1	-
4	EDO	CCC	619	-	-	0/1/1/1	-
4	EDO	CCC	615	-	-	0/1/1/1	-
4	EDO	BBB	201	-	-	1/1/1/1	-
4	EDO	AAA	205	-	-	0/1/1/1	-
4	EDO	CCC	606	-	-	1/1/1/1	-
4	EDO	CCC	604	-	-	0/1/1/1	-
4	EDO	AAA	203	-	-	1/1/1/1	-
4	EDO	BBB	202	-	-	0/1/1/1	-
4	EDO	CCC	618	-	-	0/1/1/1	-
4	EDO	CCC	609	-	-	1/1/1/1	-
4	EDO	AAA	201	-	-	1/1/1/1	-
4	EDO	CCC	616	-	-	1/1/1/1	-
4	EDO	AAA	207	-	-	0/1/1/1	-
4	EDO	CCC	614	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	1/1/1/1	-
4	EDO	AAA	206	-	-	1/1/1/1	-
4	EDO	CCC	612	-	-	1/1/1/1	-
4	EDO	AAA	204	-	-	1/1/1/1	-
4	EDO	CCC	610	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	CCC	620	EDO	O1-C1-C2	-2.02	97.39	111.91

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	201	EDO	O1-C1-C2-O2
4	CCC	607	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	CCC	609	EDO	O1-C1-C2-O2
4	CCC	612	EDO	O1-C1-C2-O2
4	AAA	202	EDO	O1-C1-C2-O2
4	AAA	203	EDO	O1-C1-C2-O2
4	BBB	201	EDO	O1-C1-C2-O2
4	CCC	616	EDO	O1-C1-C2-O2
4	CCC	617	EDO	O1-C1-C2-O2
4	BBB	203	EDO	O1-C1-C2-O2
4	CCC	606	EDO	O1-C1-C2-O2
4	AAA	206	EDO	O1-C1-C2-O2
4	AAA	204	EDO	O1-C1-C2-O2
4	CCC	611	EDO	O1-C1-C2-O2
4	CCC	620	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	620	EDO	1	0
5	CCC	624	SO4	2	0
4	BBB	202	EDO	1	0
5	BBB	204	SO4	2	0
4	CCC	618	EDO	2	0
5	AAA	208	SO4	2	0
4	CCC	614	EDO	5	0
4	CCC	607	EDO	3	0
4	CCC	612	EDO	2	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	AAA	99/100 (99%)	-0.82	0 100 100	20, 24, 32, 47	0
2	BBB	122/122 (100%)	-0.83	0 100 100	21, 26, 45, 71	0
3	CCC	568/570 (99%)	-0.79	5 (0%) 84 85	19, 23, 38, 79	0
All	All	789/792 (99%)	-0.80	5 (0%) 89 90	19, 24, 39, 79	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CCC	396	ASN	3.6
3	CCC	392	ALA	3.3
3	CCC	391	LEU	2.5
3	CCC	395	LYS	2.4
3	CCC	550	GLY	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	QNQ	CCC	322	15/16	0.91	0.11	34,47,59,59	0
3	KCX	CCC	220	12/13	0.98	0.06	18,21,27,28	0
1	CXM	AAA	1	11/12	0.98	0.07	22,24,32,33	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	EDO	CCC	619	4/4	0.74	0.21	48,55,58,58	0
4	EDO	AAA	201	4/4	0.77	0.22	70,72,73,75	0
5	SO4	AAA	208	5/5	0.78	0.26	49,106,111,128	0
4	EDO	CCC	606	4/4	0.80	0.14	63,64,68,69	0
4	EDO	AAA	204	4/4	0.81	0.13	36,40,40,44	0
5	SO4	CCC	621	5/5	0.82	0.17	87,97,104,104	5
4	EDO	AAA	203	4/4	0.83	0.20	49,56,57,69	0
4	EDO	CCC	604	4/4	0.83	0.13	53,57,60,62	0
4	EDO	AAA	202	4/4	0.84	0.16	45,51,51,56	0
4	EDO	CCC	608	4/4	0.86	0.17	51,57,59,62	0
4	EDO	CCC	616	4/4	0.89	0.16	53,53,55,63	0
5	SO4	BBB	204	5/5	0.90	0.16	103,107,119,129	0
4	EDO	CCC	611	4/4	0.91	0.11	52,52,55,63	0
5	SO4	CCC	623	5/5	0.91	0.15	62,76,86,90	0
4	EDO	CCC	609	4/4	0.92	0.21	57,58,63,66	0
4	EDO	CCC	620	4/4	0.92	0.11	36,36,38,42	0
4	EDO	CCC	610	4/4	0.92	0.12	46,49,50,54	0
4	EDO	CCC	612	4/4	0.93	0.27	31,47,51,52	0
4	EDO	CCC	607	4/4	0.93	0.09	50,51,58,65	0
4	EDO	CCC	617	4/4	0.93	0.15	36,43,46,53	0
4	EDO	CCC	614	4/4	0.94	0.14	38,39,40,44	0
4	EDO	BBB	203	4/4	0.94	0.12	41,43,43,55	0
4	EDO	BBB	201	4/4	0.94	0.10	43,46,52,58	0
5	SO4	BBB	205	5/5	0.94	0.19	59,79,89,90	0
4	EDO	CCC	618	4/4	0.94	0.14	37,38,41,45	0
4	EDO	BBB	202	4/4	0.94	0.13	49,55,58,63	0
4	EDO	AAA	206	4/4	0.95	0.08	35,36,38,42	0
5	SO4	BBB	206	5/5	0.95	0.08	64,67,76,81	0
5	SO4	CCC	625	5/5	0.95	0.09	71,71,73,77	5
5	SO4	CCC	622	5/5	0.96	0.19	45,49,63,64	0
4	EDO	CCC	613	4/4	0.97	0.11	34,34,35,36	0
4	EDO	CCC	605	4/4	0.97	0.10	39,45,46,50	0
5	SO4	CCC	624	5/5	0.97	0.10	55,61,69,81	0
4	EDO	AAA	207	4/4	0.97	0.10	29,29,29,30	0
4	EDO	AAA	205	4/4	0.98	0.05	30,31,34,35	0
4	EDO	CCC	615	4/4	0.98	0.14	34,36,37,44	0
7	OH	CCC	603	1/1	0.99	0.04	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NI	CCC	602	1/1	1.00	0.06	26,26,26,26	0
6	NI	CCC	601	1/1	1.00	0.04	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.