



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2020 – 02:20 pm GMT

PDB ID : 6ZO1
Title : 1.61 Å resolution 3,5-dimethylcatechol (3,5-dimethylbenzene-1,2-diol) inhibited *Sporosarcina pasteurii* urease
Authors : Mazzei, L.; Ciani, M.; Musiani, F.; Ciurli, S.
Deposited on : 2020-07-07
Resolution : 1.61 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.15.1
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) : 2.15.1

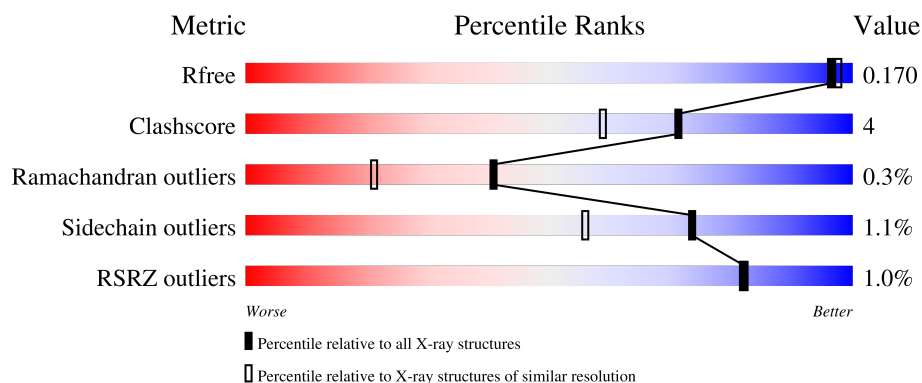
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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></div> </div>
2	BBB	122	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
3	CCC	570	<div> <div></div> <div>92%</div> <div>8%</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
4	EDO	CCC	621	-	-	X	-
5	SO4	CCC	627	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7069 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	8	0
			842	528	144	162	8			

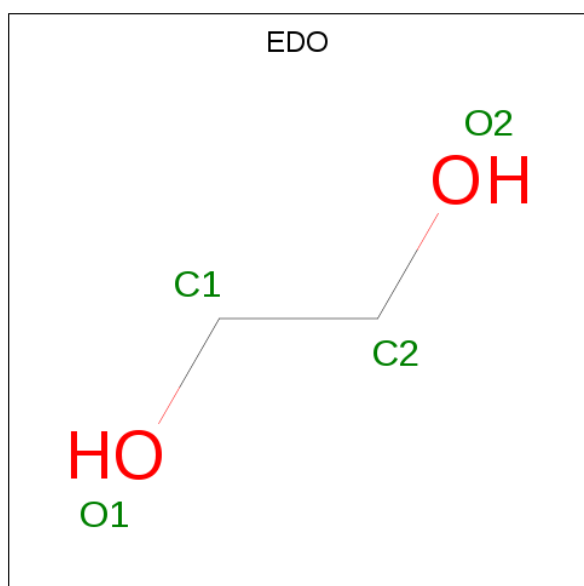
- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	122	Total	C	N	O	S	0	4	0
			984	607	177	199	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	22	0
			4482	2816	769	869	28			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	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	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	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

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		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

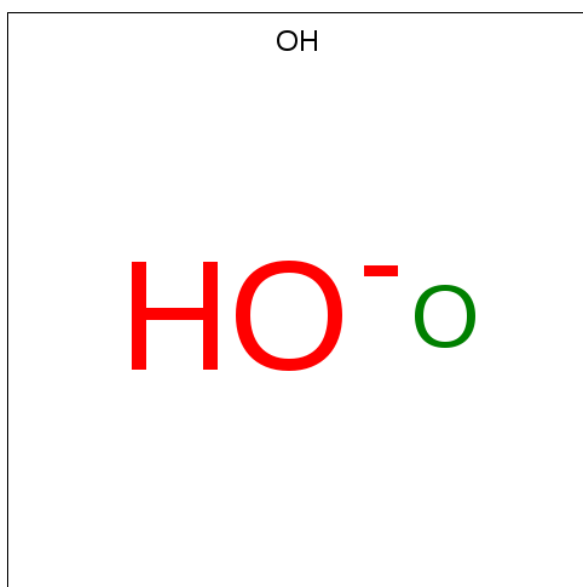
Continued from previous page...

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

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- 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	95	Total O 95 95	0	0
8	CCC	401	Total O 401 401	0	0

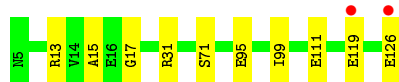
3 Residue-property plots

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.

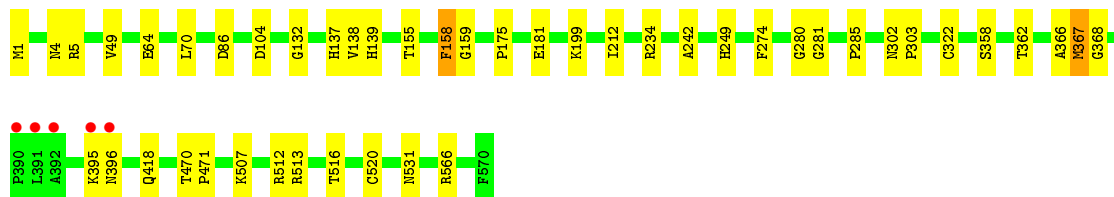
- Molecule 1: Urease subunit gamma



- 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, α , β , γ	131.57Å 131.57Å 188.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.49 – 1.61 45.49 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.49-1.61) 99.6 (45.49-1.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.136 , 0.159 0.150 , 0.170	Depositor DCC
R_{free} test set	6228 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7069	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: NI, QO5, OH, EDO, CXM, SO4, KCX

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	0.74	0/849	0.87	0/1141
2	BBB	0.74	0/999	0.88	0/1342
3	CCC	0.76	1/4561 (0.0%)	0.89	3/6171 (0.0%)
All	All	0.75	1/6409 (0.0%)	0.89	3/8654 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	181	GLU	CD-OE1	5.10	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	520	CYS	CB-CA-C	-9.88	90.65	110.40
3	CCC	512	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	CCC	234	ARG	CG-CD-NE	-5.05	101.20	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	842	0	852	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	984	0	964	10	0
3	CCC	4482	0	4457	31	0
4	AAA	20	0	30	3	0
4	BBB	24	0	36	1	0
4	CCC	72	0	108	11	0
5	AAA	5	0	0	0	0
5	BBB	20	0	0	1	0
5	CCC	50	0	0	1	0
6	CCC	2	0	0	0	0
7	CCC	1	0	0	0	0
8	AAA	71	0	0	1	0
8	BBB	95	0	0	3	0
8	CCC	401	0	0	4	0
All	All	7069	0	6447	46	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 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)
3:CCC:64[B]:GLU:HG2	4:CCC:621:EDO:H22	1.48	0.95
3:CCC:64[B]:GLU:HG2	4:CCC:621:EDO:C2	2.01	0.89
1:AAA:66[B]:ARG:NH1	1:AAA:100:SER:OXT	2.09	0.85
1:AAA:32:TYR:OH	4:AAA:305:EDO:H22	1.89	0.73
2:BBB:111[A]:GLU:OE1	8:BBB:301:HOH:O	2.11	0.68
3:CCC:64[B]:GLU:HG2	4:CCC:621:EDO:H21	1.79	0.65
3:CCC:64[B]:GLU:CG	4:CCC:621:EDO:H22	2.25	0.64
4:CCC:613:EDO:O2	8:CCC:701:HOH:O	1.93	0.63
5:CCC:631:SO4:O2	8:CCC:702:HOH:O	2.16	0.59
2:BBB:17:GLY:O	3:CCC:5[A]:ARG:HG2	2.03	0.58
2:BBB:15:ALA:O	3:CCC:5[B]:ARG:HD2	2.03	0.58
1:AAA:79[A]:ASP:OD1	1:AAA:79[A]:ASP:O	2.23	0.56
2:BBB:111[A]:GLU:H	2:BBB:111[A]:GLU:CD	2.07	0.56
3:CCC:566:ARG:HH12	4:CCC:601:EDO:H21	1.70	0.56
1:AAA:77:ILE:HA	4:AAA:305:EDO:H21	1.90	0.54
3:CCC:280:GLY:HA2	3:CCC:367[B]:MET:SD	2.48	0.54
2:BBB:71:SER:OG	3:CCC:49:VAL:HG21	2.09	0.52
3:CCC:513[A]:ARG:NH2	4:CCC:615:EDO:O1	2.38	0.52
3:CCC:132:GLY:HA3	3:CCC:155:THR:OG1	2.10	0.51
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:126:GLU:O	8:BBB:302:HOH:O	2.19	0.50
3:CCC:362:THR:O	3:CCC:368:GLY:HA3	2.12	0.50
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.94	0.50
3:CCC:139:HIS:CD2	3:CCC:366[B]:ALA:HB3	2.46	0.50
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	2.96	0.49
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.13	0.49
3:CCC:64[B]:GLU:CG	4:CCC:621:EDO:C2	2.85	0.49
2:BBB:13:ARG:HD3	4:BBB:204:EDO:O2	2.14	0.48
2:BBB:119:GLU:HG3	8:BBB:337:HOH:O	2.13	0.47
1:AAA:79[A]:ASP:C	1:AAA:79[A]:ASP:OD1	2.53	0.47
3:CCC:507[A]:LYS:HD3	8:CCC:1032:HOH:O	2.14	0.46
3:CCC:470:THR:N	3:CCC:471:PRO:CD	2.79	0.46
3:CCC:302:ASN:N	3:CCC:303[A]:PRO:CD	2.79	0.46
1:AAA:32:TYR:HH	4:AAA:305:EDO:H22	1.79	0.46
3:CCC:64[B]:GLU:CD	8:CCC:709:HOH:O	2.54	0.45
1:AAA:100:SER:O	8:AAA:401:HOH:O	2.21	0.44
3:CCC:303[B]:PRO:HG3	3:CCC:368:GLY:HA2	2.00	0.44
3:CCC:516:THR:HG21	4:CCC:608:EDO:H21	2.00	0.44
3:CCC:138:VAL:O	3:CCC:159:GLY:HA3	2.18	0.43
3:CCC:358:SER:HA	3:CCC:531:ASN:HB3	2.01	0.43
3:CCC:175:PRO:HB3	3:CCC:199:LYS:HE3	2.01	0.42
3:CCC:212:ILE:HG21	3:CCC:242:ALA:HB1	2.02	0.41
3:CCC:566:ARG:HH12	4:CCC:601:EDO:C2	2.32	0.41
2:BBB:31[A]:ARG:NH2	5:BBB:207:SO4:O4	2.54	0.41
3:CCC:513[A]:ARG:NE	4:CCC:615:EDO:O1	2.49	0.41
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	3.08	0.41

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	106/100 (106%)	106 (100%)	0	0	100	100
2	BBB	124/122 (102%)	119 (96%)	4 (3%)	1 (1%)	19	5
3	CCC	587/570 (103%)	565 (96%)	20 (3%)	2 (0%)	41	21
All	All	817/792 (103%)	790 (97%)	24 (3%)	3 (0%)	41	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	CCC	367[A]	MET
3	CCC	367[B]	MET
2	BBB	99	ILE

5.3.2 Protein sidechains ⓘ

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	91/83 (110%)	90 (99%)	1 (1%)	73	56
2	BBB	105/101 (104%)	105 (100%)	0	100	100
3	CCC	478/457 (105%)	471 (98%)	7 (2%)	65	43
All	All	674/641 (105%)	666 (99%)	8 (1%)	73	52

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	100	SER
3	CCC	1[A]	MET
3	CCC	1[B]	MET
3	CCC	4	ASN
3	CCC	158	PHE
3	CCC	285	PRO
3	CCC	395	LYS
3	CCC	396	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	QO5	CCC	322	3	15,16,17	1.41	1 (6%)	14,22,24	1.64	3 (21%)
1	CXM	AAA	1	1	6,10,11	0.54	0	5,11,13	0.95	0
3	KCX	CCC	220	3,6	7,11,12	0.58	0	4,12,14	0.90	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	QO5	CCC	322	3	-	0/5/7/9	0/1/1/1
1	CXM	AAA	1	1	-	1/7/10/12	-
3	KCX	CCC	220	3,6	-	0/7/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	322	QO5	C2-SG	-4.64	1.72	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	322	QO5	C3-C4-C5	-3.22	119.25	121.33
3	CCC	322	QO5	C1-C2-SG	2.74	123.14	119.48
3	CCC	322	QO5	C6-C5-C4	2.41	120.05	118.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	CXM	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 44 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	CCC	618	-	3,3,3	0.58	0	2,2,2	0.59	0
5	SO4	CCC	623	-	4,4,4	0.23	0	6,6,6	0.19	0
4	EDO	AAA	304	-	3,3,3	0.68	0	2,2,2	0.51	0
4	EDO	BBB	206	-	3,3,3	0.29	0	2,2,2	0.76	0
5	SO4	BBB	208	-	4,4,4	0.43	0	6,6,6	0.12	0
4	EDO	CCC	605	-	3,3,3	0.52	0	2,2,2	0.25	0
4	EDO	CCC	601	-	3,3,3	0.45	0	2,2,2	0.17	0
5	SO4	CCC	630	-	4,4,4	0.30	0	6,6,6	0.33	0
4	EDO	AAA	301	-	3,3,3	0.45	0	2,2,2	0.49	0
5	SO4	CCC	627	-	4,4,4	0.35	0	6,6,6	0.09	0
4	EDO	AAA	305	-	3,3,3	1.16	0	2,2,2	0.73	0
4	EDO	BBB	204	-	3,3,3	0.52	0	2,2,2	0.26	0
4	EDO	BBB	202	-	3,3,3	0.38	0	2,2,2	0.74	0
4	EDO	CCC	617	-	3,3,3	0.45	0	2,2,2	0.68	0
4	EDO	CCC	616	-	3,3,3	0.55	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	AAA	303	-	3,3,3	0.78	0	2,2,2	0.40	0
4	EDO	AAA	302	-	3,3,3	0.78	0	2,2,2	1.01	0
4	EDO	BBB	201	-	3,3,3	0.46	0	2,2,2	0.61	0
5	SO4	CCC	622	-	4,4,4	0.34	0	6,6,6	0.11	0
5	SO4	CCC	626	-	4,4,4	0.37	0	6,6,6	0.11	0
4	EDO	CCC	619	-	3,3,3	0.46	0	2,2,2	0.15	0
4	EDO	CCC	610	-	3,3,3	0.38	0	2,2,2	0.64	0
5	SO4	BBB	210	-	4,4,4	0.45	0	6,6,6	0.20	0
4	EDO	CCC	614	-	3,3,3	0.39	0	2,2,2	0.55	0
4	EDO	BBB	203	-	3,3,3	0.39	0	2,2,2	0.43	0
4	EDO	CCC	621	-	3,3,3	0.23	0	2,2,2	0.60	0
5	SO4	CCC	624	-	4,4,4	0.31	0	6,6,6	0.09	0
4	EDO	CCC	612	-	3,3,3	0.51	0	2,2,2	0.19	0
4	EDO	CCC	620	-	3,3,3	0.48	0	2,2,2	1.52	1 (50%)
5	SO4	CCC	628	-	4,4,4	0.36	0	6,6,6	0.06	0
4	EDO	CCC	611	-	3,3,3	0.64	0	2,2,2	0.48	0
4	EDO	CCC	607	-	3,3,3	0.60	0	2,2,2	0.97	0
4	EDO	BBB	205	-	3,3,3	0.80	0	2,2,2	0.23	0
4	EDO	CCC	613	-	3,3,3	0.76	0	2,2,2	0.72	0
4	EDO	CCC	608	-	3,3,3	0.79	0	2,2,2	0.95	0
4	EDO	CCC	609	-	3,3,3	0.68	0	2,2,2	0.70	0
5	SO4	CCC	625	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	CCC	631	-	4,4,4	0.42	0	6,6,6	0.69	0
5	SO4	CCC	629	-	4,4,4	0.20	0	6,6,6	0.51	0
4	EDO	CCC	615	-	3,3,3	0.87	0	2,2,2	0.49	0
4	EDO	CCC	606	-	3,3,3	0.44	0	2,2,2	1.10	0
5	SO4	AAA	306	-	4,4,4	0.28	0	6,6,6	0.08	0
5	SO4	BBB	207	-	4,4,4	0.36	0	6,6,6	0.11	0
5	SO4	BBB	209	-	4,4,4	0.39	0	6,6,6	0.09	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	CCC	618	-	-	0/1/1/1	-
4	EDO	AAA	304	-	-	0/1/1/1	-
4	EDO	BBB	206	-	-	0/1/1/1	-
4	EDO	CCC	605	-	-	1/1/1/1	-
4	EDO	CCC	601	-	-	1/1/1/1	-
4	EDO	AAA	301	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	305	-	-	1/1/1/1	-
4	EDO	BBB	204	-	-	1/1/1/1	-
4	EDO	BBB	202	-	-	1/1/1/1	-
4	EDO	CCC	617	-	-	0/1/1/1	-
4	EDO	CCC	616	-	-	0/1/1/1	-
4	EDO	AAA	303	-	-	0/1/1/1	-
4	EDO	AAA	302	-	-	0/1/1/1	-
4	EDO	BBB	201	-	-	0/1/1/1	-
4	EDO	CCC	619	-	-	0/1/1/1	-
4	EDO	CCC	610	-	-	1/1/1/1	-
4	EDO	CCC	614	-	-	0/1/1/1	-
4	EDO	BBB	203	-	-	0/1/1/1	-
4	EDO	CCC	621	-	-	0/1/1/1	-
4	EDO	CCC	612	-	-	0/1/1/1	-
4	EDO	CCC	620	-	-	0/1/1/1	-
4	EDO	CCC	611	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	0/1/1/1	-
4	EDO	BBB	205	-	-	1/1/1/1	-
4	EDO	CCC	613	-	-	1/1/1/1	-
4	EDO	CCC	608	-	-	1/1/1/1	-
4	EDO	CCC	609	-	-	0/1/1/1	-
4	EDO	CCC	615	-	-	0/1/1/1	-
4	EDO	CCC	606	-	-	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	-2.10	96.77	111.91

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	305	EDO	O1-C1-C2-O2
4	AAA	301	EDO	O1-C1-C2-O2
4	BBB	204	EDO	O1-C1-C2-O2
4	BBB	205	EDO	O1-C1-C2-O2
4	CCC	605	EDO	O1-C1-C2-O2
4	CCC	601	EDO	O1-C1-C2-O2
4	CCC	610	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	BBB	202	EDO	O1-C1-C2-O2
4	CCC	608	EDO	O1-C1-C2-O2
4	CCC	613	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	601	EDO	2	0
4	AAA	305	EDO	3	0
4	BBB	204	EDO	1	0
4	CCC	621	EDO	5	0
4	CCC	613	EDO	1	0
4	CCC	608	EDO	1	0
5	CCC	631	SO4	1	0
4	CCC	615	EDO	2	0
5	BBB	207	SO4	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, 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%)	-0.89	1 (1%) 82 82	18, 23, 30, 54	0
2	BBB	122/122 (100%)	-0.49	2 (1%) 72 71	20, 25, 42, 74	0
3	CCC	568/570 (99%)	-0.55	5 (0%) 84 84	18, 22, 37, 78	0
All	All	789/792 (99%)	-0.58	8 (1%) 82 82	18, 23, 37, 78	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	126	GLU	4.5
3	CCC	395	LYS	3.7
3	CCC	396	ASN	3.6
1	AAA	100	SER	3.2
3	CCC	391	LEU	2.9
3	CCC	392	ALA	2.6
2	BBB	119	GLU	2.6
3	CCC	390	PRO	2.4

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, 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(Å ²)	Q<0.9
3	QO5	CCC	322	16/17	0.96	0.08	27,34,36,41	0
3	KCX	CCC	220	12/13	0.97	0.07	17,18,21,24	0
1	CXM	AAA	1	11/12	0.98	0.05	20,24,29,33	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 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(Å ²)	Q<0.9
4	EDO	AAA	301	4/4	0.71	0.17	74,80,82,84	0
5	SO4	CCC	627	5/5	0.72	0.41	96,103,107,111	0
5	SO4	CCC	625	5/5	0.74	0.30	81,108,111,124	0
4	EDO	AAA	302	4/4	0.76	0.14	46,47,53,53	0
4	EDO	CCC	608	4/4	0.78	0.25	50,51,58,61	0
4	EDO	BBB	204	4/4	0.78	0.35	67,68,72,73	0
5	SO4	CCC	631	5/5	0.78	0.25	37,38,82,86	0
4	EDO	CCC	616	4/4	0.80	0.22	47,48,51,52	0
5	SO4	CCC	623	5/5	0.81	0.32	61,69,91,93	0
4	EDO	CCC	618	4/4	0.84	0.17	43,47,48,51	0
4	EDO	CCC	620	4/4	0.85	0.13	41,42,44,46	0
4	EDO	BBB	202	4/4	0.85	0.12	59,62,66,75	0
4	EDO	CCC	606	4/4	0.85	0.14	40,43,46,49	0
4	EDO	CCC	605	4/4	0.86	0.13	52,55,59,67	0
4	EDO	CCC	611	4/4	0.86	0.27	42,56,58,58	0
4	EDO	CCC	612	4/4	0.87	0.28	59,61,63,70	0
4	EDO	CCC	601	4/4	0.87	0.11	38,47,49,60	0
5	SO4	CCC	628	5/5	0.87	0.29	103,104,107,123	0
4	EDO	AAA	305	4/4	0.87	0.09	29,30,37,39	0
4	EDO	CCC	615	4/4	0.88	0.14	35,35,40,41	0
5	SO4	CCC	624	5/5	0.88	0.19	77,77,84,84	5
4	EDO	CCC	613	4/4	0.89	0.15	36,41,44,56	0
4	EDO	CCC	610	4/4	0.89	0.16	50,51,60,60	0
5	SO4	BBB	210	5/5	0.90	0.24	39,52,62,65	5
4	EDO	CCC	621	4/4	0.90	0.14	40,44,46,48	0
4	EDO	BBB	206	4/4	0.90	0.20	40,40,40,51	0
4	EDO	CCC	609	4/4	0.91	0.19	51,53,55,56	0
4	EDO	CCC	619	4/4	0.91	0.16	36,46,47,55	0
4	EDO	BBB	205	4/4	0.91	0.14	40,47,48,61	0
4	EDO	BBB	203	4/4	0.91	0.11	63,64,65,67	0
4	EDO	BBB	201	4/4	0.91	0.10	45,60,63,63	0
5	SO4	AAA	306	5/5	0.91	0.29	75,85,94,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	CCC	622	5/5	0.92	0.18	56,89,94,101	0
4	EDO	AAA	303	4/4	0.93	0.21	36,43,46,49	0
4	EDO	CCC	607	4/4	0.94	0.16	34,36,45,45	0
5	SO4	BBB	209	5/5	0.94	0.20	60,64,72,77	0
5	SO4	BBB	208	5/5	0.95	0.13	48,52,55,56	5
5	SO4	CCC	626	5/5	0.95	0.45	87,92,101,116	0
5	SO4	BBB	207	5/5	0.96	0.27	49,66,75,76	0
4	EDO	CCC	617	4/4	0.96	0.17	34,39,39,43	0
4	EDO	AAA	304	4/4	0.97	0.09	26,28,29,30	0
7	OH	CCC	604	1/1	0.97	0.09	22,22,22,22	0
5	SO4	CCC	630	5/5	0.97	0.15	31,32,42,42	5
5	SO4	CCC	629	5/5	0.98	0.07	40,41,47,52	0
4	EDO	CCC	614	4/4	0.98	0.16	37,38,38,40	0
6	NI	CCC	603	1/1	1.00	0.02	21,21,21,21	0
6	NI	CCC	602	1/1	1.00	0.01	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.