



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 08:32 PM EDT

PDB ID : 5FSD  
Title : 1.75 Å resolution 2,5-dihydroxybenzenesulfonate inhibited *Sporosarcina pasteurii* urease  
Authors : Mazzei, L.; Ciani, M.; Musiani, F.; Ciurli, S.  
Deposited on : 2016-01-04  
Resolution : 1.75 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

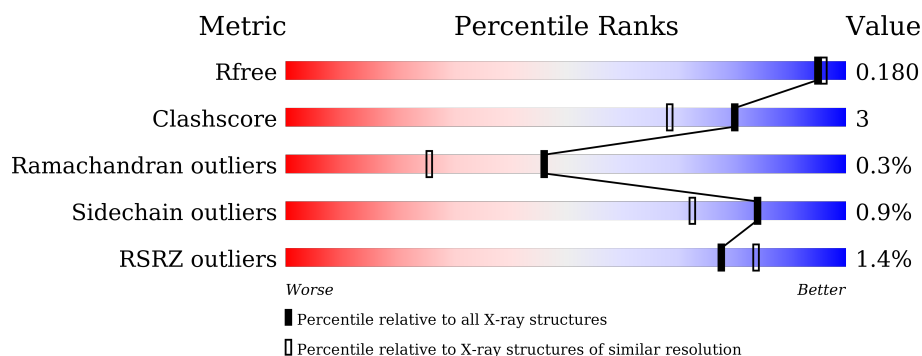
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 style="width: 97%;"></div> <div>97%</div> </div>
2	B	126	<div> <div style="width: 90%;"></div> <div>90%</div> <div style="width: 6%;"></div> <div>6%</div> </div>
3	C	570	<div> <div style="width: 2%;"></div> <div>2%</div> <div style="width: 92%;"></div> <div>92%</div> <div style="width: 8%;"></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	B	1127	-	-	-	X
4	EDO	B	1128	-	-	-	X
4	EDO	C	1572	-	-	-	X
4	EDO	C	1573	-	-	X	X
4	EDO	C	1574	-	-	-	X
4	EDO	C	1575	-	-	-	X
4	EDO	C	1577	-	-	-	X
4	EDO	C	1578	-	-	-	X
4	EDO	C	1579	-	-	-	X
5	SO4	A	1105	-	-	-	X
5	SO4	C	1583	-	-	-	X
5	SO4	C	1585	-	-	-	X
8	DBX	C	1587	-	-	-	X
8	DBX	C	1588	-	-	X	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7016 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	6	0
			823	518	139	158	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	LEU	CONFLICT	UNP P41022
A	22	LYS	ARG	CONFLICT	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	3	0
			979	605	179	194	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	2796	765	864	28			

There are 10 discrepancies between the modelled and reference sequences:

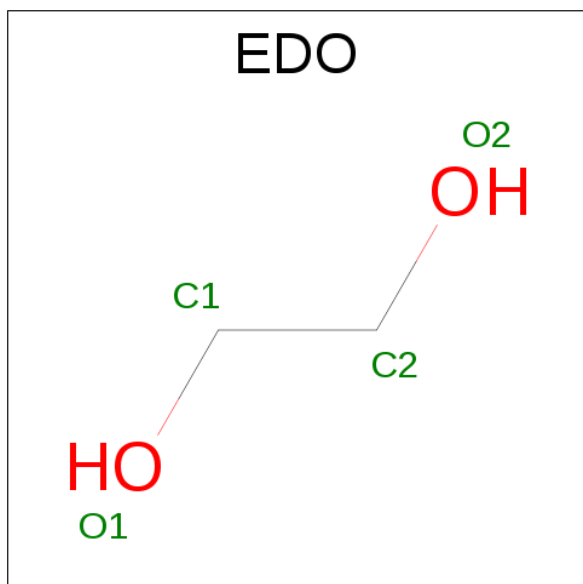
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	GLN	ARG	CONFLICT	UNP P41020
C	28	TRP	GLY	CONFLICT	UNP P41020
C	29	ILE	-	INSERTION	UNP P41020
C	36	THR	TYR	CONFLICT	UNP P41020
C	37	THR	TYR	CONFLICT	UNP P41020
C	38	TYR	LEU	CONFLICT	UNP P41020
C	42	ALA	VAL	CONFLICT	UNP P41020
C	263	LEU	VAL	CONFLICT	UNP P41020

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Chain	Residue	Modelled	Actual	Comment	Reference
C	403	ALA	LEU	CONFLICT	UNP P41020
C	420	ILE	MET	CONFLICT	UNP P41020

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



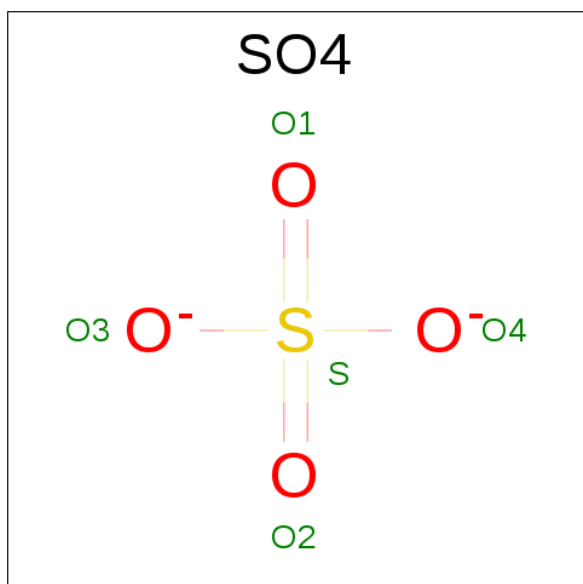
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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

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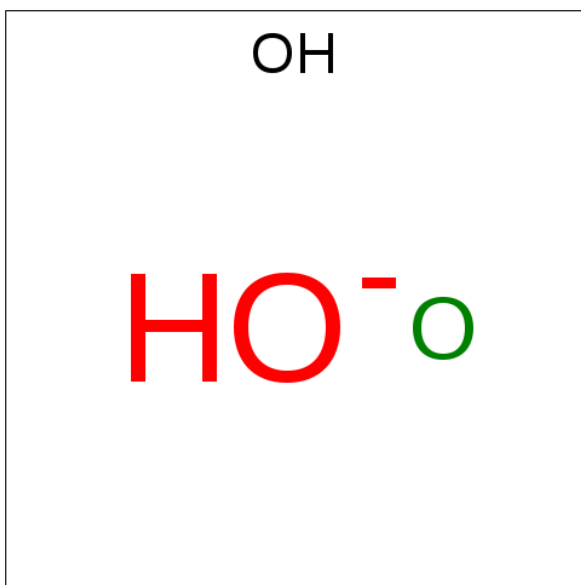
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

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

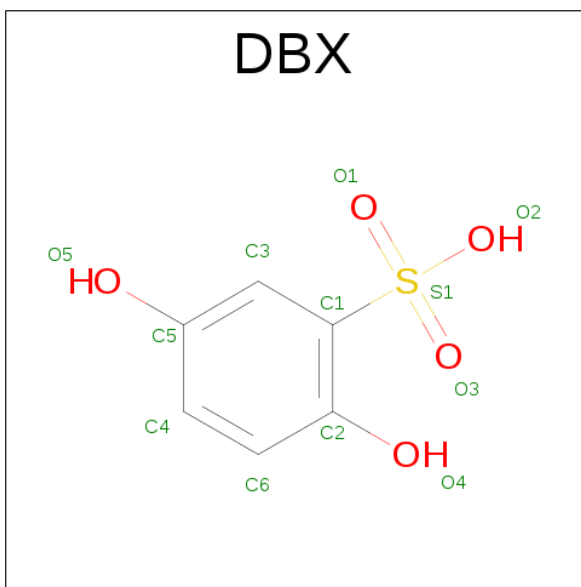
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Ni	0	0
			2	2		

- Molecule 7 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 8 is 2,5-DIHYDROXYBENZENESULFONIC ACID (three-letter code: DBX) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	O	S	0	0
			12	6	5	1		
8	C	1	Total	C	O	S	0	0
			12	6	5	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	83	Total	O	0	0
			83	83		
9	B	143	Total	O	0	0
			143	143		
9	C	414	Total	O	0	0
			414	414		



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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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:  97% .

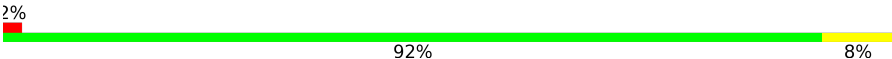


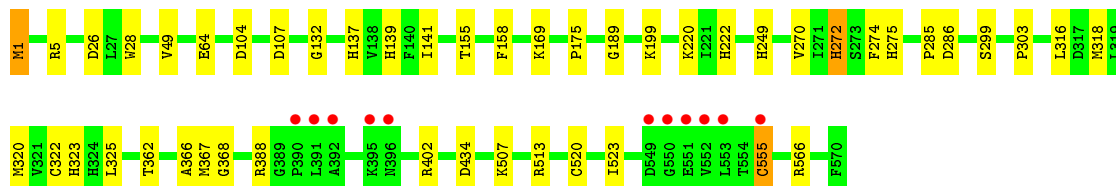
#### • Molecule 2: UREASE SUBUNIT BETA

Chain B:  90% 6% . .



#### • Molecule 3: UREASE SUBUNIT ALPHA

Chain C:  2% 92% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.31Å 131.31Å 188.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.72 – 1.75 97.43 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (113.72-1.75) 100.0 (97.43-1.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.134 , 0.170 0.149 , 0.180	Depositor DCC
$R_{free}$ test set	4763 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 96821 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NI, OH, EDO, CXM, DBX, 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	A	0.99	0/830	0.99	2/1116 (0.2%)
2	B	1.03	0/991	1.02	4/1332 (0.3%)
3	C	0.97	3/4540 (0.1%)	1.00	17/6147 (0.3%)
All	All	0.98	3/6361 (0.0%)	1.00	23/8595 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	520	CYS	CB-SG	-10.52	1.64	1.82
3	C	555[A]	CYS	CB-SG	-5.07	1.73	1.81
3	C	555[B]	CYS	CB-SG	-5.07	1.73	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	ARG	NE-CZ-NH2	-10.88	114.86	120.30
3	C	388	ARG	NE-CZ-NH1	10.09	125.35	120.30
3	C	520	CYS	CB-CA-C	-9.47	91.45	110.40
3	C	566	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	66	ARG	NE-CZ-NH2	-7.53	116.53	120.30
3	C	318	MET	CG-SD-CE	7.48	112.17	100.20
2	B	54	GLU	OE1-CD-OE2	7.22	131.97	123.30
3	C	388	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	66	ARG	NE-CZ-NH1	6.52	123.56	120.30
3	C	566	ARG	NE-CZ-NH1	6.28	123.44	120.30
3	C	402	ARG	NE-CZ-NH1	6.07	123.33	120.30
3	C	555[A]	CYS	CA-CB-SG	-5.64	103.84	114.00
3	C	555[B]	CYS	CA-CB-SG	-5.64	103.84	114.00
3	C	5	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	B	13[A]	ARG	NE-CZ-NH1	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13[B]	ARG	NE-CZ-NH1	5.47	123.04	120.30
3	C	26[A]	ASP	CB-CG-OD1	5.45	123.21	118.30
3	C	26[B]	ASP	CB-CG-OD1	5.45	123.21	118.30
2	B	37	ASP	CB-CG-OD1	5.37	123.13	118.30
3	C	107	ASP	CB-CG-OD1	5.19	122.97	118.30
3	C	434	ASP	CB-CG-OD1	5.18	122.96	118.30
3	C	286	ASP	CB-CG-OD1	5.17	122.95	118.30
3	C	322	CYS	CA-CB-SG	-5.11	104.80	114.00

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	823	0	836	2	0
2	B	979	0	965	7	0
3	C	4453	0	4436	38	0
4	A	12	0	18	2	0
4	B	8	0	12	1	0
4	C	44	0	66	9	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	15	0	0	1	0
6	C	2	0	0	0	0
7	C	1	0	0	0	0
8	C	24	0	7	5	0
9	A	83	0	0	1	0
9	B	143	0	0	1	0
9	C	414	0	0	4	1
All	All	7016	0	6340	43	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 3.

All (43) 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:C:555[B]:CYS:CB	8:C:1588:DBX:C4	1.82	1.52
3:C:555[B]:CYS:HB2	8:C:1588:DBX:C4	1.43	1.44
3:C:555[B]:CYS:HB3	8:C:1588:DBX:C4	1.53	1.22
3:C:555[B]:CYS:HB3	8:C:1588:DBX:C6	1.89	1.02
3:C:64[B]:GLU:HG2	4:C:1573:EDO:C1	2.07	0.84
3:C:64[B]:GLU:HG2	4:C:1573:EDO:H11	1.65	0.77
3:C:270[B]:VAL:HG11	3:C:523:ILE:O	1.88	0.74
2:B:83:MET:HB2	4:B:1128:EDO:H22	1.74	0.70
3:C:64[B]:GLU:HG2	4:C:1573:EDO:H12	1.74	0.69
1:A:32:TYR:OH	4:A:1103:EDO:H11	1.93	0.68
3:C:272:HIS:HE1	3:C:299:SER:OG	1.78	0.67
9:B:2086:HOH:O	3:C:1[B]:MET:HE3	1.96	0.64
3:C:270[B]:VAL:HG12	9:C:2373:HOH:O	1.96	0.64
3:C:323:HIS:NE2	5:C:1583:SO4:O4	2.30	0.60
9:A:2070:HOH:O	2:B:5[B]:ASN:O	2.15	0.60
3:C:270[B]:VAL:CG1	9:C:2373:HOH:O	2.55	0.55
3:C:555[B]:CYS:HB2	8:C:1588:DBX:C5	2.28	0.53
1:A:77:ILE:HA	4:A:1103:EDO:H12	1.91	0.53
3:C:513[B]:ARG:NH2	4:C:1575:EDO:O2	2.36	0.52
2:B:95:GLU:O	3:C:104:ASP:HB3	2.10	0.52
3:C:507[A]:LYS:HD3	9:C:2352:HOH:O	2.11	0.50
3:C:362:THR:O	3:C:368:GLY:HA3	2.12	0.50
3:C:64[B]:GLU:CG	4:C:1573:EDO:C1	2.86	0.49
3:C:316:LEU:O	3:C:320:MET:HG2	2.13	0.49
3:C:220:KCX:CX	3:C:222:HIS:HD2	2.27	0.48
3:C:64[B]:GLU:CG	4:C:1573:EDO:H11	2.39	0.47
3:C:323:HIS:HB2	3:C:325:LEU:HG	1.97	0.47
3:C:189:GLY:O	4:C:1576:EDO:H21	2.15	0.46
3:C:137:HIS:CE1	3:C:274:PHE:CD2	3.04	0.46
2:B:13[B]:ARG:HD3	3:C:28:TRP:CZ3	2.51	0.46
3:C:141:ILE:HD11	3:C:169:LYS:HA	1.99	0.45
3:C:139:HIS:CD2	3:C:366[B]:ALA:HB3	2.51	0.45
2:B:111:GLU:H	2:B:111:GLU:CD	2.18	0.45
3:C:132:GLY:HA3	3:C:155:THR:OG1	2.17	0.44
3:C:64[B]:GLU:CG	4:C:1573:EDO:H12	2.44	0.44
3:C:272:HIS:CE1	3:C:299:SER:OG	2.67	0.44
3:C:175:PRO:HB3	3:C:199:LYS:HE3	2.02	0.42
2:B:13[B]:ARG:HD3	3:C:28:TRP:CH2	2.55	0.42
3:C:1[A]:MET:HE1	9:C:2006:HOH:O	2.20	0.42
2:B:71:SER:OG	3:C:49:VAL:HG21	2.20	0.41
3:C:274:PHE:O	3:C:275:HIS:C	2.59	0.41
3:C:303:PRO:HG3	3:C:368:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:513[B]:ARG:HH21	4:C:1575:EDO:C2	2.32	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)
9:C:2085:HOH:O	9:C:2085:HOH:O[11_555]	1.83	0.37

## 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	104/100 (104%)	104 (100%)	0	0	100	100
2	B	122/126 (97%)	114 (93%)	7 (6%)	1 (1%)	24	8
3	C	585/570 (103%)	565 (97%)	19 (3%)	1 (0%)	52	32
All	All	811/796 (102%)	783 (96%)	26 (3%)	2 (0%)	46	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	367	MET
2	B	99	ILE

### 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	89/83 (107%)	89 (100%)	0	100	100
2	B	104/105 (99%)	102 (98%)	2 (2%)	65	43
3	C	476/458 (104%)	470 (99%)	6 (1%)	76	60
All	All	669/646 (104%)	661 (99%)	8 (1%)	84	62

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

Mol	Chain	Res	Type
2	B	5[A]	ASN
2	B	5[B]	ASN
3	C	1[A]	MET
3	C	1[B]	MET
3	C	158	PHE
3	C	249	HIS
3	C	272	HIS
3	C	285	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	272	HIS
3	C	519	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
1	CXM	A	1	1	6,10,11	0.97	0	5,11,13	1.00	0
3	KCX	C	220	3,6	6,11,12	0.64	0	7,12,14	1.50	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
1	CXM	A	1	1	-	0/6/10/12	0/0/0/0
3	KCX	C	220	3,6	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	220	KCX	CE-NZ-CX	-2.70	120.69	123.53

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 24 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	A	1102	-	3,3,3	0.60	0	2,2,2	0.68	0
4	EDO	A	1103	-	3,3,3	1.01	0	2,2,2	0.83	0
4	EDO	A	1104	-	3,3,3	0.82	0	2,2,2	0.44	0
5	SO4	A	1105	-	4,4,4	1.12	0	6,6,6	1.24	1 (16%)
4	EDO	B	1127	-	3,3,3	0.33	0	2,2,2	0.70	0
4	EDO	B	1128	-	3,3,3	0.86	0	2,2,2	1.52	0
5	SO4	B	1129	-	4,4,4	0.61	0	6,6,6	1.10	1 (16%)
5	SO4	B	1130	-	4,4,4	0.76	0	6,6,6	0.34	0
4	EDO	C	1572	-	3,3,3	0.40	0	2,2,2	0.29	0
4	EDO	C	1573	-	3,3,3	0.32	0	2,2,2	0.72	0
4	EDO	C	1574	-	3,3,3	0.41	0	2,2,2	0.94	0
4	EDO	C	1575	-	3,3,3	0.83	0	2,2,2	0.12	0
4	EDO	C	1576	-	3,3,3	0.57	0	2,2,2	1.83	1 (50%)
4	EDO	C	1577	-	3,3,3	1.17	0	2,2,2	0.57	0
4	EDO	C	1578	-	3,3,3	0.69	0	2,2,2	0.58	0
4	EDO	C	1579	-	3,3,3	0.25	0	2,2,2	1.14	0
4	EDO	C	1580	-	3,3,3	0.24	0	2,2,2	1.01	0
4	EDO	C	1581	-	3,3,3	0.56	0	2,2,2	0.39	0
4	EDO	C	1582	-	3,3,3	0.53	0	2,2,2	0.40	0
5	SO4	C	1583	-	4,4,4	1.43	1 (25%)	6,6,6	0.67	0
5	SO4	C	1585	-	4,4,4	1.23	0	6,6,6	0.74	0
5	SO4	C	1586	-	4,4,4	1.11	0	6,6,6	1.08	1 (16%)
8	DBX	C	1587	3	12,12,12	5.06	7 (58%)	16,18,18	3.42	7 (43%)
8	DBX	C	1588	-	12,12,12	5.09	5 (41%)	16,18,18	3.16	8 (50%)

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	1102	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1103	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1104	-	-	0/1/1/1	0/0/0/0
5	SO4	A	1105	-	-	0/0/0/0	0/0/0/0
4	EDO	B	1127	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1128	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	B	1129	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1130	-	-	0/0/0/0	0/0/0/0
4	EDO	C	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1579	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1580	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1581	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1582	-	-	0/1/1/1	0/0/0/0
5	SO4	C	1583	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1585	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1586	-	-	0/0/0/0	0/0/0/0
8	DBX	C	1587	3	-	0/6/6/6	0/1/1/1
8	DBX	C	1588	-	-	0/6/6/6	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1588	DBX	C1-S1	-11.32	1.62	1.78
8	C	1587	DBX	C1-S1	-6.20	1.69	1.78
8	C	1587	DBX	C4-C6	2.04	1.42	1.38
8	C	1587	DBX	C4-C5	2.10	1.43	1.38
5	C	1583	SO4	O1-S	2.21	1.54	1.47
8	C	1587	DBX	C3-C5	2.70	1.43	1.39
8	C	1588	DBX	C3-C5	2.87	1.43	1.39
8	C	1588	DBX	C4-C5	3.11	1.45	1.38
8	C	1587	DBX	C3-C1	3.35	1.44	1.39
8	C	1588	DBX	O3-S1	4.10	1.63	1.43
8	C	1587	DBX	O3-S1	5.05	1.68	1.43
8	C	1588	DBX	C2-C1	11.84	1.49	1.40
8	C	1587	DBX	C2-C1	14.56	1.51	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1587	DBX	C3-C1-C2	-9.07	113.66	120.04
8	C	1588	DBX	C3-C1-C2	-7.32	114.89	120.04
8	C	1588	DBX	C6-C4-C5	-5.26	113.82	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1576	EDO	O2-C2-C1	-2.58	94.56	112.23
8	C	1587	DBX	C6-C4-C5	-2.24	117.29	119.86
5	A	1105	SO4	O4-S-O3	-2.21	100.20	109.09
5	B	1129	SO4	O2-S-O1	2.13	116.69	109.59
5	C	1586	SO4	O4-S-O3	2.33	118.48	109.09
8	C	1587	DBX	C4-C6-C2	2.36	122.87	120.50
8	C	1587	DBX	C3-C1-S1	2.42	121.91	117.28
8	C	1587	DBX	C6-C2-C1	2.64	120.89	118.67
8	C	1588	DBX	C3-C1-S1	2.90	122.82	117.28
8	C	1588	DBX	C4-C6-C2	3.07	123.58	120.50
8	C	1588	DBX	C6-C2-C1	3.27	121.42	118.67
8	C	1587	DBX	C2-C1-S1	3.28	124.40	121.24
8	C	1588	DBX	C4-C5-C3	3.41	124.16	120.21
8	C	1588	DBX	O1-S1-C1	4.04	110.83	106.17
8	C	1588	DBX	O3-S1-C1	4.09	110.88	106.17
8	C	1587	DBX	O1-S1-C1	8.07	115.47	106.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	EDO	2	0
4	B	1128	EDO	1	0
4	C	1573	EDO	6	0
4	C	1575	EDO	2	0
4	C	1576	EDO	1	0
5	C	1583	SO4	1	0
8	C	1588	DBX	5	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(Å²)	Q<0.9	
1	A	99/100 (99%)	-0.69	0	100	100	20, 25, 33, 53	0
2	B	122/126 (96%)	-0.74	0	100	100	22, 27, 43, 68	0
3	C	569/570 (99%)	-0.57	11 (1%)	70	76	20, 24, 45, 77	0
All	All	790/796 (99%)	-0.61	11 (1%)	78	84	20, 25, 44, 77	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	396	ASN	4.6
3	C	550	GLY	4.1
3	C	392	ALA	3.5
3	C	391	LEU	3.5
3	C	395	LYS	3.2
3	C	551	GLU	3.0
3	C	549	ASP	3.0
3	C	552	VAL	2.7
3	C	390	PRO	2.6
3	C	555[A]	CYS	2.4
3	C	553	LEU	2.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CXM	A	1	11/12	0.98	0.06	-	23,26,31,34	0
3	KCX	C	220	12/13	0.97	0.05	-	18,21,28,32	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	1574	4/4	0.91	0.17	22.08	43,51,54,57	0
5	SO4	A	1105	5/5	0.89	0.12	9.83	38,49,61,62	5
4	EDO	C	1577	4/4	0.88	0.11	6.06	41,50,51,56	0
4	EDO	C	1575	4/4	0.77	0.15	5.29	43,43,48,52	0
4	EDO	C	1579	4/4	0.93	0.11	5.22	50,58,61,68	0
4	EDO	C	1572	4/4	0.98	0.08	5.14	37,38,38,39	0
4	EDO	B	1128	4/4	0.80	0.13	4.99	40,45,48,51	0
8	DBX	C	1587	12/12	0.85	0.19	4.61	44,56,63,65	4
5	SO4	C	1585	5/5	0.96	0.15	4.45	47,67,70,75	0
8	DBX	C	1588	12/12	0.91	0.33	4.04	38,42,45,47	12
4	EDO	C	1578	4/4	0.86	0.13	3.56	47,56,62,63	0
5	SO4	C	1583	5/5	0.93	0.15	2.86	53,62,74,82	0
4	EDO	C	1573	4/4	0.91	0.14	2.23	41,43,48,51	0
4	EDO	B	1127	4/4	0.96	0.11	2.19	42,43,43,51	0
4	EDO	A	1104	4/4	0.91	0.10	1.82	40,46,51,53	0
4	EDO	C	1580	4/4	0.96	0.14	1.50	35,39,41,42	0
4	EDO	C	1576	4/4	0.89	0.10	1.46	33,45,46,48	0
4	EDO	A	1102	4/4	0.97	0.07	0.49	29,34,36,37	0
4	EDO	A	1103	4/4	0.91	0.08	0.49	32,37,41,43	0
7	OH	C	1584	1/1	0.99	0.07	-0.02	30,30,30,30	0
6	NI	C	600	1/1	1.00	0.02	-1.74	36,36,36,36	0
6	NI	C	601	1/1	1.00	0.02	-2.63	29,29,29,29	0
5	SO4	B	1129	5/5	0.97	0.12	-	62,65,72,73	0
4	EDO	C	1582	4/4	0.88	0.07	-	59,60,60,63	0
5	SO4	C	1586	5/5	0.94	0.27	-	36,37,57,58	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1130	5/5	0.94	0.14	-	67,68,74,78	5
4	EDO	C	1581	4/4	0.95	0.17	-	48,49,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.