



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:16 PM GMT

PDB ID : 1EU1
Title : THE CRYSTAL STRUCTURE OF RHODOBACTER SPHAEROIDES
DIMETHYLSULFOXIDE REDUCTASE REVEALS TWO DISTINCT
MOLYBDENUM COORDINATION ENVIRONMENTS.
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Deposited on : 2000-04-13
Resolution : 1.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

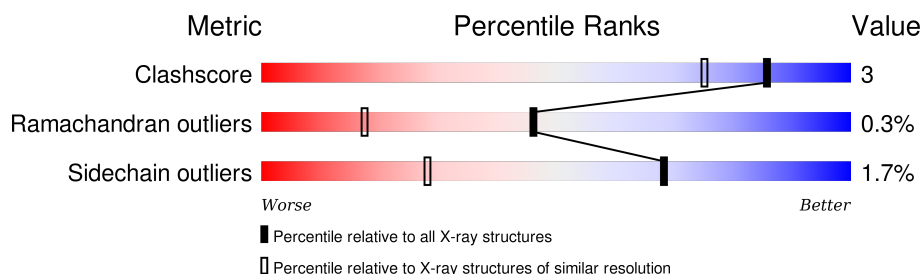
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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))
Clashscore	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	780	

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
2	GLC	A	2002	X	-	-	-
2	GLC	A	2003	X	-	-	-
2	GLC	A	2004	X	-	-	-
7	O	A	3002	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7307 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.

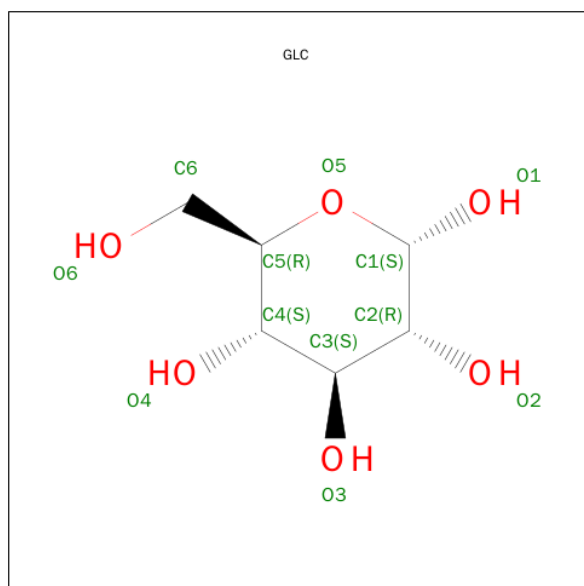
- Molecule 1 is a protein called DIMETHYL SULFOXIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	767	6048	3829	1034	1150	35	0	34	0

There is a discrepancy between the modelled and reference sequences:

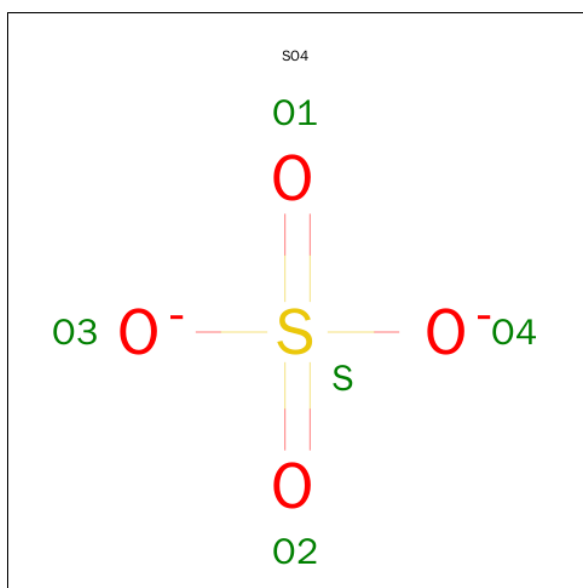
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	CSD	CYS	MODIFIED RESIDUE	UNP Q57366

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0
2	A	1	12	6	6	0	0
2	A	1	12	6	6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

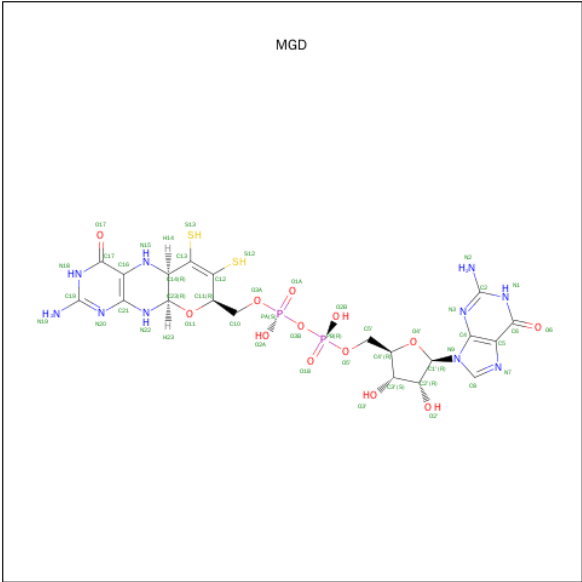


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cd	0	0
			1	1		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	1
			75	30	15	22	4	4		
5	A	1	Total	C	N	O	P	S	0	1
			83	35	15	25	4	4		

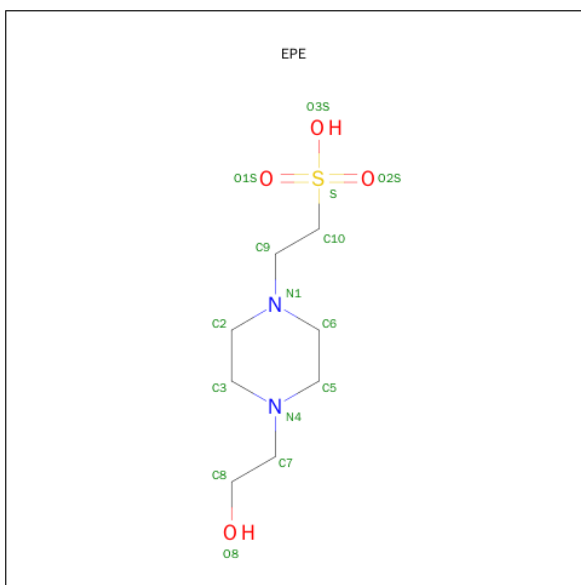
- Molecule 6 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	1
			2	2		

- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	1
			3	3		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

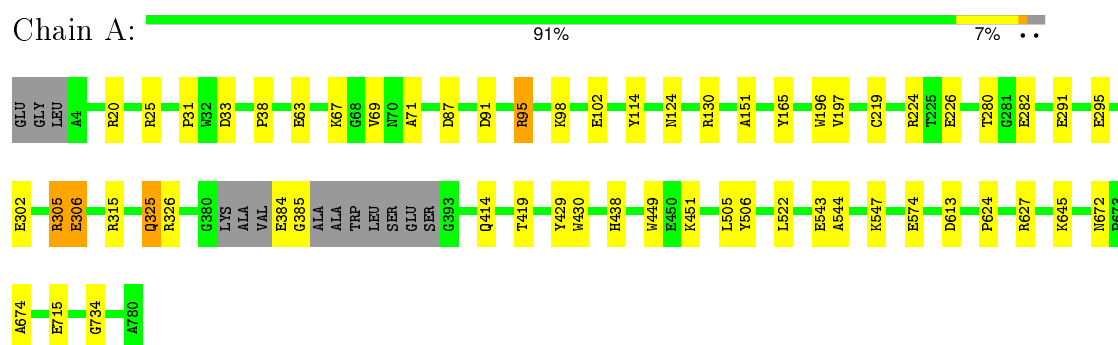
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1039	Total	O	0	0
			1039	1039		

3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

• Molecule 1: DIMETHYL SULFOXIDE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.18Å 141.72Å 59.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.30	Depositor
% Data completeness (in resolution range)	89.8 (10.00-1.30)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.121 , 0.145	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7307	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, MGD, CSD, GLC, O, CD, SO4, EPE

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	0.52	0/6328	1.11	24/8580 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	25	ARG	CD-NE-CZ	14.89	144.44	123.60
1	A	130[A]	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	A	130[B]	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	A	305[A]	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	305[B]	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	305[A]	ARG	NE-CZ-NH1	10.55	125.57	120.30
1	A	305[B]	ARG	NE-CZ-NH1	10.55	125.57	120.30
1	A	87	ASP	CB-CG-OD2	9.58	126.93	118.30
1	A	25	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	91	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	130[A]	ARG	CD-NE-CZ	7.84	134.58	123.60
1	A	130[B]	ARG	CD-NE-CZ	7.84	134.58	123.60
1	A	130[A]	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	A	130[B]	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	A	95[A]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	95[B]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	87	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	A	219	CSD	O-C-N	-7.21	111.16	122.70
1	A	95[A]	ARG	CD-NE-CZ	6.59	132.83	123.60
1	A	95[B]	ARG	CD-NE-CZ	6.59	132.83	123.60
1	A	613	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	326	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	315	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	224	ARG	CD-NE-CZ	5.51	131.32	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6048	0	5816	32	1
2	A	36	0	36	0	1
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	158	0	62	0	0
6	A	2	0	0	1	0
7	A	3	0	0	3	0
8	A	15	0	18	2	0
9	A	1039	0	0	6	0
All	All	7307	0	5932	34	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 (34) 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:114[B]:TYR:OH	7:A:3002:O:O	1.59	1.19
1:A:124:ASN:HD21	1:A:384:GLU:HA	1.28	0.94
1:A:544:ALA:HA	1:A:547[A]:LYS:HE2	1.53	0.90
1:A:196:TRP:HE1	1:A:385:GLY:HA3	1.38	0.88
1:A:151:ALA:H	1:A:325:GLN:HE21	1.35	0.71
1:A:124:ASN:ND2	1:A:384:GLU:HA	2.04	0.71
1:A:291:GLU:OE2	1:A:305[A]:ARG:NH2	2.23	0.70
1:A:124:ASN:HD21	1:A:384:GLU:CA	2.06	0.61
1:A:196:TRP:NE1	1:A:385:GLY:HA3	2.13	0.61
6:A:3000[A]:6MO:MO	7:A:3002:O:O	1.71	0.61
1:A:672:ASN:HD22	1:A:674:ALA:H	1.50	0.59
1:A:98:LYS:HE3	1:A:522:LEU:HD23	1.88	0.55
1:A:196:TRP:HZ2	1:A:384:GLU:N	2.05	0.54
1:A:98:LYS:CE	1:A:522:LEU:HD23	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:HG3	9:A:3588:HOH:O	2.09	0.51
1:A:505[B]:LEU:HD13	1:A:506:TYR:CE1	2.48	0.49
1:A:63:GLU:HG3	1:A:71:ALA:HB1	1.96	0.47
1:A:414[A]:GLN:NE2	1:A:419:THR:OG1	2.34	0.45
1:A:280:THR:OG1	1:A:282[B]:GLU:HG3	2.15	0.45
1:A:672:ASN:ND2	1:A:674:ALA:H	2.13	0.45
1:A:645[B]:LYS:HD2	9:A:3745:HOH:O	2.17	0.45
1:A:196:TRP:HE1	1:A:385:GLY:CA	2.20	0.44
1:A:31:PRO:HB3	1:A:38:PRO:HB3	2.00	0.44
1:A:624:PRO:HG2	1:A:627:ARG:HB3	1.99	0.43
1:A:69:VAL:HG12	9:A:3989:HOH:O	2.18	0.43
1:A:543:GLU:O	1:A:547[A]:LYS:HG3	2.18	0.42
1:A:95[B]:ARG:HG2	1:A:95[B]:ARG:HH11	1.83	0.42
7:A:3001[B]:O:O	8:A:2001:EPE:H82	2.20	0.41
1:A:165:TYR:CZ	8:A:2001:EPE:H31	2.56	0.41
1:A:451[B]:LYS:HE2	9:A:3034:HOH:O	2.20	0.41
1:A:226[B]:GLU:HG2	9:A:3226:HOH:O	2.20	0.41
1:A:547[A]:LYS:HE3	9:A:3434:HOH:O	2.21	0.40
1:A:302:GLU:O	1:A:306[B]:GLU:HG3	2.22	0.40
1:A:20[B]:ARG:HH11	1:A:20[B]:ARG:HD2	1.77	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)
1:A:67[A]:LYS:NZ	2:A:2003:GLC:C5[1_554]	2.07	0.13

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	A	794/780 (102%)	774 (98%)	18 (2%)	2 (0%)	46 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	VAL
1	A	734	GLY

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	A	638/614 (104%)	627 (98%)	11 (2%)	68 28

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	295	GLU
1	A	306[A]	GLU
1	A	306[B]	GLU
1	A	325	GLN
1	A	429	TYR
1	A	430	TRP
1	A	438	HIS
1	A	449	TRP
1	A	574	GLU
1	A	715	GLU

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

Mol	Chain	Res	Type
1	A	241	GLN
1	A	325	GLN
1	A	458	GLN
1	A	606	ASN
1	A	672	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSD	A	219	1	3,7,8	1.61	1 (33%)	3,8,10	3.80	3 (100%)

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	CSD	A	219	1	-	1/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	CSD	CB-SG	2.33	1.92	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	CSD	CB-CA-C	-5.42	96.60	111.46
1	A	219	CSD	OD1-SG-CB	2.44	109.47	105.40
1	A	219	CSD	O-C-CA	2.80	132.78	125.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	219	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	MGD	A	1001[A]	6	38,52,52	2.12	10 (26%)	43,81,81	2.20	9 (20%)
5	MGD	A	1001[B]	6	38,52,52	2.12	10 (26%)	43,81,81	2.16	9 (20%)
5	MGD	A	1002[A]	-	38,52,52	2.27	14 (36%)	43,81,81	2.33	8 (18%)
5	MGD	A	1002[B]	6	38,52,52	2.25	14 (36%)	43,81,81	2.41	6 (13%)
8	EPE	A	2001	-	14,15,15	2.37	2 (14%)	18,20,20	1.77	3 (16%)
2	GLC	A	2002	-	12,12,12	1.18	1 (8%)	17,17,17	1.07	2 (11%)
2	GLC	A	2003	-	12,12,12	1.02	0	17,17,17	1.63	3 (17%)
2	GLC	A	2004	-	12,12,12	1.09	0	17,17,17	1.12	1 (5%)
3	SO4	A	2005	-	4,4,4	0.92	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	A	1001[A]	6	-	0/18/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	A	1001[B]	6	-	0/18/66/66	0/6/6/6
5	MGD	A	1002[A]	-	-	0/18/66/66	0/6/6/6
5	MGD	A	1002[B]	6	-	0/18/66/66	0/6/6/6
8	EPE	A	2001	-	-	0/9/19/19	0/1/1/1
2	GLC	A	2002	-	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	A	2003	-	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	A	2004	-	1/1/5/5	0/2/22/22	0/1/1/1
3	SO4	A	2005	-	-	0/0/0/0	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002[A]	MGD	C6-C5	2.07	1.45	1.41
5	A	1002[B]	MGD	C6-C5	2.07	1.45	1.41
5	A	1002[B]	MGD	O11-C23	2.09	1.46	1.43
2	A	2002	GLC	C1-C2	2.09	1.56	1.52
5	A	1002[A]	MGD	O11-C11	2.12	1.46	1.43
5	A	1002[A]	MGD	O11-C23	2.23	1.47	1.43
5	A	1001[B]	MGD	C2-N2	2.24	1.38	1.34
5	A	1001[A]	MGD	C2-N2	2.24	1.38	1.34
5	A	1002[B]	MGD	O11-C11	2.24	1.47	1.43
5	A	1002[A]	MGD	C4-N3	2.25	1.39	1.35
5	A	1002[B]	MGD	C4-N3	2.25	1.39	1.35
5	A	1002[B]	MGD	C2'-C3'	2.25	1.59	1.53
5	A	1002[A]	MGD	C2'-C3'	2.30	1.59	1.53
5	A	1002[A]	MGD	C2-N2	2.42	1.39	1.34
5	A	1002[B]	MGD	C2-N2	2.42	1.39	1.34
8	A	2001	EPE	C7-N4	2.51	1.53	1.47
5	A	1001[B]	MGD	C21-N22	2.56	1.39	1.35
5	A	1001[A]	MGD	C21-N22	2.57	1.39	1.35
5	A	1001[B]	MGD	C2-N1	2.84	1.40	1.35
5	A	1001[A]	MGD	C2-N1	2.84	1.40	1.35
5	A	1002[B]	MGD	C19-N19	2.98	1.40	1.34
5	A	1001[B]	MGD	C21-N20	2.99	1.40	1.34
5	A	1001[A]	MGD	C21-N20	2.99	1.40	1.34
5	A	1002[B]	MGD	C21-N20	3.08	1.40	1.34
5	A	1002[A]	MGD	C19-N19	3.09	1.40	1.34
5	A	1002[A]	MGD	C21-N20	3.10	1.40	1.34
5	A	1001[B]	MGD	O11-C11	3.33	1.48	1.43
5	A	1001[A]	MGD	O11-C11	3.37	1.48	1.43
5	A	1001[B]	MGD	O4'-C1'	3.39	1.45	1.41
5	A	1001[A]	MGD	O4'-C1'	3.39	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002[B]	MGD	C23-C14	3.71	1.56	1.53
5	A	1001[B]	MGD	C16-N15	3.71	1.46	1.38
5	A	1002[A]	MGD	C14-N15	3.94	1.51	1.45
5	A	1001[A]	MGD	C16-N15	3.96	1.47	1.38
5	A	1002[A]	MGD	O4'-C1'	4.06	1.46	1.41
5	A	1002[A]	MGD	C23-C14	4.17	1.56	1.53
5	A	1002[B]	MGD	O4'-C1'	4.26	1.46	1.41
5	A	1002[B]	MGD	C14-N15	4.27	1.51	1.45
5	A	1001[B]	MGD	C6-N1	4.29	1.41	1.33
5	A	1001[A]	MGD	C6-N1	4.29	1.41	1.33
5	A	1002[B]	MGD	C16-N15	4.46	1.48	1.38
5	A	1002[A]	MGD	C16-N15	4.57	1.48	1.38
5	A	1002[A]	MGD	C6-N1	4.92	1.42	1.33
5	A	1002[B]	MGD	C6-N1	4.92	1.42	1.33
5	A	1002[A]	MGD	C17-N18	5.01	1.42	1.33
5	A	1001[A]	MGD	C14-N15	5.04	1.52	1.45
5	A	1001[B]	MGD	C17-N18	5.09	1.42	1.33
5	A	1001[A]	MGD	C17-N18	5.14	1.42	1.33
5	A	1002[B]	MGD	C17-N18	5.16	1.42	1.33
5	A	1001[B]	MGD	C14-N15	5.17	1.52	1.45
8	A	2001	EPE	O3S-S	8.15	1.67	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002[A]	MGD	C5-C6-N1	-9.24	110.96	123.59
5	A	1002[B]	MGD	C5-C6-N1	-9.24	110.96	123.59
5	A	1001[B]	MGD	C5-C6-N1	-7.72	113.03	123.59
5	A	1001[A]	MGD	C5-C6-N1	-7.72	113.03	123.59
2	A	2003	GLC	C1-C2-C3	-4.49	103.75	110.43
8	A	2001	EPE	O3S-S-O1S	-4.27	101.68	111.61
5	A	1001[A]	MGD	C16-N15-C14	-4.19	107.39	118.65
5	A	1002[B]	MGD	C4'-O4'-C1'	-3.86	105.48	109.72
5	A	1001[B]	MGD	C16-N15-C14	-3.75	108.56	118.65
2	A	2003	GLC	O1-C1-O5	-2.75	102.72	110.25
5	A	1002[A]	MGD	C21-N22-C23	-2.42	118.92	123.67
5	A	1002[A]	MGD	C4'-O4'-C1'	-2.40	107.08	109.72
2	A	2002	GLC	O1-C1-O5	-2.31	103.92	110.25
5	A	1001[B]	MGD	C6-C5-C4	-2.27	118.19	120.90
5	A	1001[A]	MGD	C6-C5-C4	-2.27	118.19	120.90
2	A	2002	GLC	C1-C2-C3	-2.18	107.19	110.43
2	A	2004	GLC	O2-C2-C3	-2.01	105.82	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2001	EPE	O2S-S-O1S	2.05	120.95	113.48
5	A	1001[A]	MGD	O11-C23-C14	2.11	110.41	108.96
2	A	2003	GLC	O1-C1-C2	2.16	115.01	109.21
5	A	1001[B]	MGD	C16-C21-N22	2.19	120.63	118.34
5	A	1002[A]	MGD	N19-C19-N20	2.41	121.19	117.20
5	A	1001[B]	MGD	O11-C23-C14	2.72	110.82	108.96
5	A	1001[B]	MGD	C16-C21-N20	2.74	124.43	118.76
5	A	1002[A]	MGD	C16-C21-N22	2.74	121.21	118.34
5	A	1001[A]	MGD	C16-C21-N20	2.85	124.67	118.76
5	A	1001[A]	MGD	C16-C21-N22	2.92	121.40	118.34
5	A	1002[A]	MGD	C17-N18-C19	3.43	120.70	115.94
5	A	1002[B]	MGD	C17-N18-C19	3.44	120.72	115.94
8	A	2001	EPE	O1S-S-C10	3.87	110.21	106.91
5	A	1002[B]	MGD	C16-C21-N22	4.55	123.10	118.34
5	A	1001[A]	MGD	C17-C16-C21	4.85	118.95	114.56
5	A	1002[A]	MGD	C17-C16-C21	5.00	119.09	114.56
5	A	1001[B]	MGD	C17-N18-C19	5.03	122.93	115.94
5	A	1001[A]	MGD	C17-N18-C19	5.04	122.93	115.94
5	A	1001[B]	MGD	C6-N1-C2	5.12	123.05	115.94
5	A	1001[A]	MGD	C6-N1-C2	5.12	123.05	115.94
5	A	1001[B]	MGD	C17-C16-C21	5.14	119.21	114.56
5	A	1002[B]	MGD	C17-C16-C21	6.33	120.29	114.56
5	A	1002[A]	MGD	C6-N1-C2	6.79	125.36	115.94
5	A	1002[B]	MGD	C6-N1-C2	6.79	125.36	115.94

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2003	GLC	C1
2	A	2002	GLC	C1
2	A	2004	GLC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2001	EPE	2	0
2	A	2003	GLC	0	1

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.