



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:37 am BST

PDB ID : 2CFU
Title : Crystal structure of SdsA1, an alkylsulfatase from *Pseudomonas aeruginosa*, in complex with 1-decane-sulfonic-acid.
Authors : Hagelueken, G.; Adams, T.M.; Wiehlmann, L.; Widow, U.; Kolmar, H.; Tuemmler, B.; Heinz, D.W.; Schubert, W.-D.
Deposited on : 2006-02-23
Resolution : 1.90 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	:	2.11
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)	:	2.11

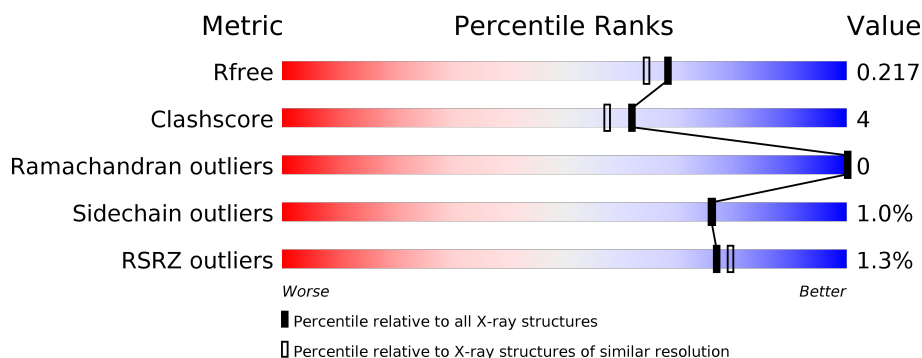
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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 on 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	A	658	<div> <div></div> <div>89%</div> <div>6%</div> <div>5%</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
2	1DB	A	1655	-	-	X	-

2 Entry composition [i](#)

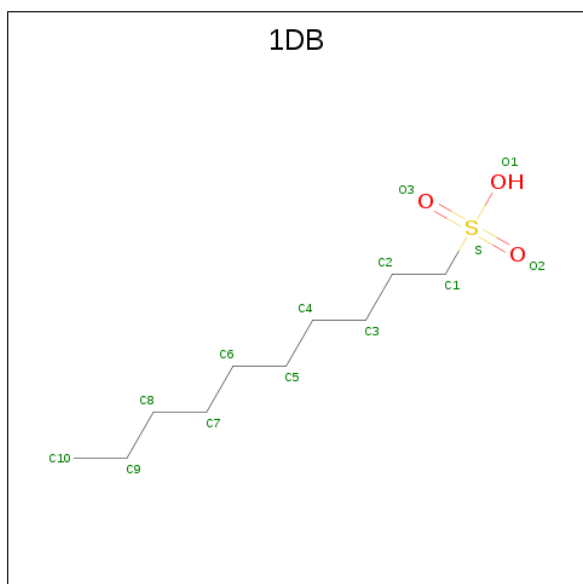
There are 6 unique types of molecules in this entry. The entry contains 5819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SDSA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	36	1
			5206	3279	954	962	11			

- Molecule 2 is 1-DECANE-SULFONIC-ACID (three-letter code: 1DB) (formula: $C_{10}H_{22}O_3S$).



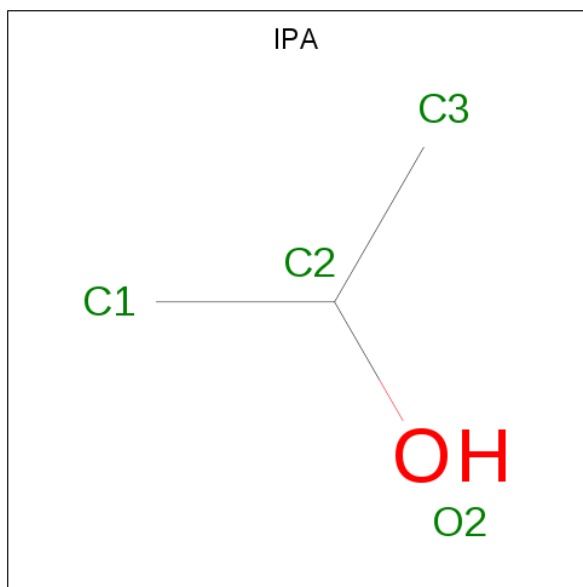
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			14	10	3	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	537	Total	O	0	0
			537	537		

i

- Molecule 1: SDSA1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.06 Å 86.06 Å 364.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.54 – 1.90 43.03 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (74.54-1.90) 98.4 (43.03-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.86 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.217 0.171 , 0.217	Depositor DCC
R_{free} test set	3476 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5819	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ZN, IPA, 1DB

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	0.76	0/5358	0.73	0/7258

There are no bond length outliers.

There are no bond angle outliers.

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	5206	0	5145	40	0
2	A	14	0	22	9	0
3	A	56	0	80	5	0
4	A	4	0	8	1	0
5	A	2	0	0	0	0
6	A	537	0	0	15	0
All	All	5819	0	5255	47	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 (47) 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:328[B]:GLN:NE2	6:A:2270:HOH:O	1.70	1.19
1:A:466:ARG:HB2	3:A:1657:PEG:H22	1.40	1.00
1:A:147[A]:ARG:NH2	6:A:2135:HOH:O	2.01	0.92
2:A:1655:1DB:H5C1	6:A:2531:HOH:O	1.70	0.90
1:A:243:LEU:HD21	2:A:1655:1DB:H8C2	1.59	0.83
1:A:312:ARG:HH22	2:A:1655:1DB:H1C1	1.45	0.81
1:A:332[B]:ARG:HG2	1:A:332[B]:ARG:HH11	1.50	0.77
2:A:1655:1DB:H4C2	6:A:2531:HOH:O	1.90	0.71
1:A:544[B]:PHE:HZ	1:A:565:LEU:CD2	2.07	0.68
1:A:483[B]:ARG:HD3	6:A:2408:HOH:O	2.00	0.62
1:A:147[B]:ARG:NH1	6:A:2136:HOH:O	2.35	0.60
2:A:1655:1DB:C4	6:A:2531:HOH:O	2.50	0.59
1:A:544[B]:PHE:CZ	1:A:565:LEU:CD2	2.86	0.59
1:A:255[B]:ARG:NH2	1:A:264:LEU:HD21	2.18	0.58
1:A:562:SER:OG	1:A:594:ALA:HA	2.04	0.58
1:A:328[B]:GLN:NE2	6:A:2273:HOH:O	2.37	0.57
1:A:20:THR:HG23	1:A:24:LYS:HE3	1.88	0.55
2:A:1655:1DB:C5	6:A:2531:HOH:O	2.40	0.55
1:A:82:LEU:O	1:A:100[B]:LEU:HD21	2.07	0.53
1:A:466:ARG:CB	3:A:1657:PEG:H22	2.28	0.53
1:A:36[A]:ARG:HD2	6:A:2017:HOH:O	2.10	0.51
1:A:134:TRP:CE2	1:A:160[B]:ARG:HD2	2.45	0.51
1:A:348[B]:ARG:HD2	1:A:357:VAL:HG21	1.93	0.49
1:A:550:ARG:HD2	6:A:2450:HOH:O	2.12	0.49
1:A:544[B]:PHE:HZ	1:A:565:LEU:HD23	1.76	0.49
2:A:1655:1DB:H9C1	4:A:1664:IPA:H2	1.96	0.48
1:A:540:THR:HG22	1:A:544[B]:PHE:CE2	2.49	0.47
1:A:367:TYR:CZ	1:A:371:GLN:HG3	2.49	0.46
1:A:544[B]:PHE:CZ	1:A:565:LEU:HD23	2.52	0.45
1:A:483[A]:ARG:HB2	1:A:483[A]:ARG:HE	1.44	0.44
1:A:609:LEU:HD23	3:A:1658:PEG:H22	1.98	0.44
1:A:382:ILE:HB	1:A:416:LEU:HD22	2.00	0.44
3:A:1658:PEG:H12	3:A:1660:PEG:H42	2.00	0.43
1:A:50[A]:GLU:HG3	6:A:2037:HOH:O	2.19	0.43
1:A:348[A]:ARG:NE	1:A:357:VAL:HG21	2.33	0.43
1:A:86[B]:LYS:HA	1:A:87:PRO:HD3	1.87	0.42
1:A:367:TYR:CE2	1:A:371:GLN:HG3	2.55	0.42
1:A:104:LYS:HE3	6:A:2046:HOH:O	2.20	0.42
1:A:312:ARG:NH2	2:A:1655:1DB:H1C1	2.25	0.42
2:A:1655:1DB:H2C2	6:A:2530:HOH:O	2.18	0.42
1:A:567:LEU:HA	1:A:600:ILE:O	2.20	0.41
1:A:100[B]:LEU:HA	1:A:100[B]:LEU:HD23	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:HA	3:A:1657:PEG:H11	2.03	0.41
1:A:332[B]:ARG:HG2	1:A:332[B]:ARG:NH1	2.27	0.41
1:A:324:LYS:O	1:A:328[B]:GLN:HG3	2.21	0.41
1:A:160[B]:ARG:HG2	6:A:2153:HOH:O	2.20	0.41

There are no symmetry-related clashes.

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	658/658 (100%)	641 (97%)	17 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	535/521 (103%)	528 (99%)	7 (1%)	69 68

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

Mol	Chain	Res	Type
1	A	50[A]	GLU
1	A	50[B]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	61	GLU
1	A	255[A]	ARG
1	A	255[B]	ARG
1	A	589	VAL
1	A	640	LEU

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

Mol	Chain	Res	Type
1	A	417	ASN
1	A	635	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
3	PEG	A	1659	-	6,6,6	0.50	0	5,5,5	0.21	0
3	PEG	A	1658	-	6,6,6	0.41	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1DB	A	1655	-	13,13,13	2.02	1 (7%)	15,15,15	3.13	4 (26%)
3	PEG	A	1660	-	6,6,6	0.47	0	5,5,5	0.26	0
4	IPA	A	1664	-	3,3,3	0.42	0	3,3,3	0.46	0
3	PEG	A	1661	-	6,6,6	0.50	0	5,5,5	0.34	0
3	PEG	A	1663	-	6,6,6	0.47	0	5,5,5	0.32	0
3	PEG	A	1656	-	6,6,6	0.45	0	5,5,5	0.46	0
3	PEG	A	1657	-	6,6,6	0.33	0	5,5,5	0.73	0
3	PEG	A	1662	-	6,6,6	0.47	0	5,5,5	0.35	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	PEG	A	1659	-	-	2/4/4/4	-
3	PEG	A	1658	-	-	2/4/4/4	-
2	1DB	A	1655	-	-	9/11/11/11	-
3	PEG	A	1660	-	-	3/4/4/4	-
3	PEG	A	1661	-	-	1/4/4/4	-
3	PEG	A	1663	-	-	3/4/4/4	-
3	PEG	A	1656	-	-	3/4/4/4	-
3	PEG	A	1657	-	-	4/4/4/4	-
3	PEG	A	1662	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1655	1DB	C1-S	-6.97	1.67	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1655	1DB	O2-S-C1	9.28	118.09	106.92
2	A	1655	1DB	O1-S-O2	-5.21	98.54	111.27
2	A	1655	1DB	O1-S-O3	4.96	123.40	111.27
2	A	1655	1DB	O2-S-O3	-2.44	105.50	113.95

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1655	1DB	C2-C1-S-O3
2	A	1655	1DB	C2-C1-S-O2
2	A	1655	1DB	S-C1-C2-C3
2	A	1655	1DB	C2-C1-S-O1
3	A	1657	PEG	O2-C3-C4-O4
3	A	1659	PEG	O1-C1-C2-O2
2	A	1655	1DB	C3-C4-C5-C6
3	A	1657	PEG	O1-C1-C2-O2
3	A	1662	PEG	O1-C1-C2-O2
2	A	1655	1DB	C2-C3-C4-C5
2	A	1655	1DB	C4-C5-C6-C7
3	A	1657	PEG	C4-C3-O2-C2
3	A	1659	PEG	O2-C3-C4-O4
3	A	1658	PEG	O1-C1-C2-O2
3	A	1656	PEG	O2-C3-C4-O4
3	A	1663	PEG	O1-C1-C2-O2
3	A	1662	PEG	C4-C3-O2-C2
3	A	1658	PEG	O2-C3-C4-O4
3	A	1657	PEG	C1-C2-O2-C3
3	A	1663	PEG	C4-C3-O2-C2
3	A	1660	PEG	C1-C2-O2-C3
3	A	1663	PEG	C1-C2-O2-C3
3	A	1660	PEG	O2-C3-C4-O4
2	A	1655	1DB	C5-C6-C7-C8
3	A	1660	PEG	O1-C1-C2-O2
2	A	1655	1DB	C1-C2-C3-C4
3	A	1661	PEG	O2-C3-C4-O4
3	A	1656	PEG	C4-C3-O2-C2
3	A	1656	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1658	PEG	2	0
2	A	1655	1DB	9	0
3	A	1660	PEG	1	0
4	A	1664	IPA	1	0
3	A	1657	PEG	3	0

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 [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	A	628/658 (95%)	-0.31	8 (1%) 77 79	2, 19, 30, 54	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	655	LYS	4.8
1	A	654	ALA	4.6
1	A	20	THR	3.6
1	A	592	GLU	2.7
1	A	520	VAL	2.6
1	A	62	ARG	2.3
1	A	522[A]	ARG	2.2
1	A	61	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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. 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(\AA^2)	Q<0.9
3	PEG	A	1663	7/7	0.61	0.25	60,63,64,65	0
3	PEG	A	1661	7/7	0.71	0.20	53,58,63,63	0
3	PEG	A	1656	7/7	0.74	0.32	30,32,32,32	7
2	1DB	A	1655	14/14	0.76	0.36	22,29,40,40	14
3	PEG	A	1659	7/7	0.77	0.16	29,32,37,37	0
3	PEG	A	1658	7/7	0.78	0.26	19,21,22,23	7
3	PEG	A	1662	7/7	0.82	0.18	52,53,54,56	0
3	PEG	A	1660	7/7	0.86	0.14	22,23,27,27	7
4	IPA	A	1664	4/4	0.86	0.17	34,37,38,40	0
3	PEG	A	1657	7/7	0.90	0.15	2,8,10,12	7
5	ZN	A	1001	1/1	1.00	0.07	10,10,10,10	0
5	ZN	A	1002	1/1	1.00	0.09	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.