



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 04:42 am BST

PDB ID : 1NJM
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a tRNA acceptor stem mimic (ASM) and the antibiotic sparsomycin
Authors : Bashan, A.; Agmon, I.; Zarivatch, R.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

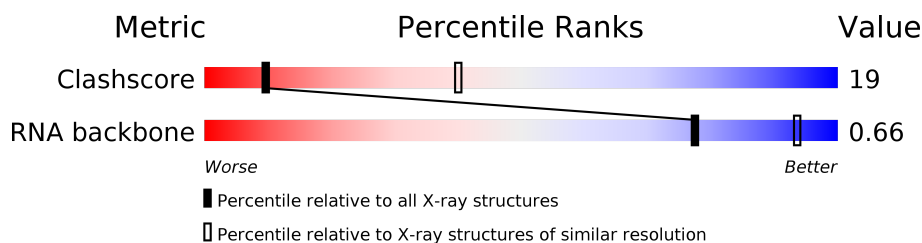
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	141614	1353 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	5	35	
3	K	141	
4	T	237	

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
5	SPS	0	2881	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60271 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- Molecule 2 is a RNA chain called tRNA acceptor stem mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	25	Total	C	N	O	P	0	0	0
			543	249	97	173	24			

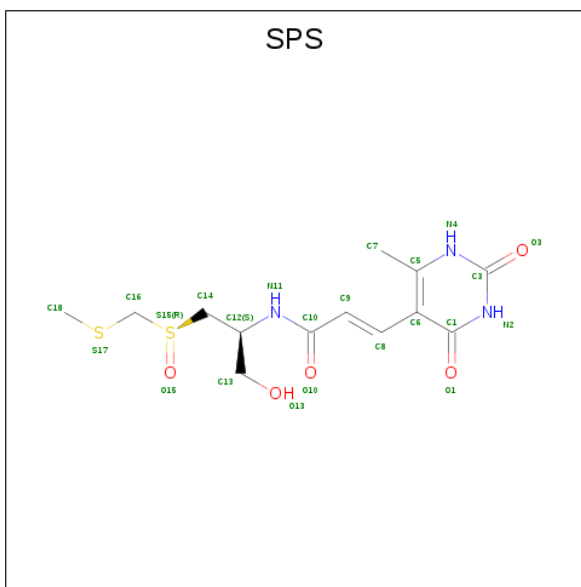
- Molecule 3 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	K	124	Total	C	0	0	124
			124	124			

- Molecule 4 is a protein called GENERAL STRESS PROTEIN CTC.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	T	223	Total	C	0	0	223
			223	223			

- Molecule 5 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



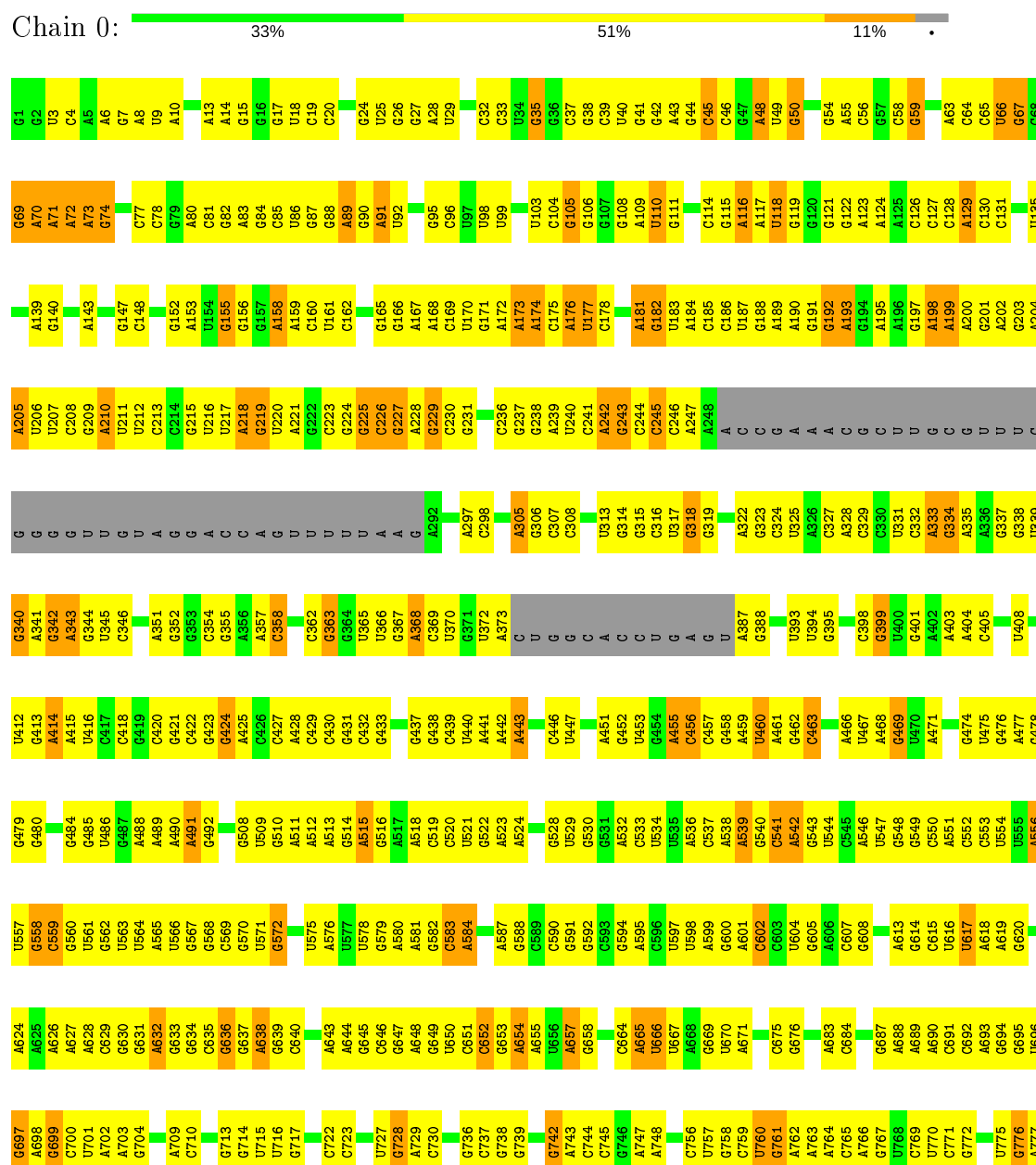
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	0	1	Total	C	N	O	S	0	0
			22	13	3	4	2		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 23S ribosomal RNA

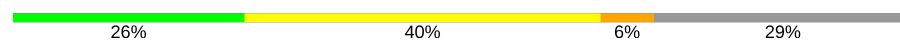


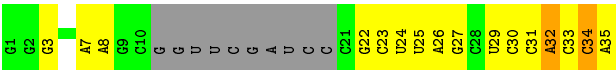
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U1819	G1742	G1559	A1587	A1509	C1442	U1365	A1290	U1046	A979	A911	G841	U779
A1820	G1743	A1560	U1581	A1510	C1443	U1366	G1291	G1047	G980	U916	A842	U780
C1822	C1743	C1661	U1591	A1511	C1444	A1365	A1292	G1052	C981	U917	G843	G781
	G1744	G1662	U1592	U1512	A1445	A1367	A1293	G1053	A984	U918	U844	U782
C1825	C1745	C1663	C1593	U1513	U1446	A1368	G1288	G1054	G985	U919	U845	G783
U1826	A1746	G1664	U1594	C1514	U1447	G1369	U1288	A1055	A986	U920	A846	U784
	U1747	C1665	U1595	U1515	A1448	G1370	U1301	A1056	G987	A921	C847	U785
C1829	G1748	G1666	A1596	A1516	C1449	G1371	U1307	G1057	G988	A922	U852	U786
G1830	A1749	A1667	A1597	C1517	G1450	A1372	U1308	A1058		U925	G853	U787
G1831	A1750	G1668	C1598	C1518	C1451	G1373	U1309	G1059		U926	G854	U788
		G1669	G1599	G1519	U1452	U1377	G1309	A1065	A991	U927	G855	G789
	G1754	G1670	U1600	G1520	U1453	G1378	C1330	A1066	A994	C927	G856	G790
C1835	G1755	A1671	U1601	U1521	C1455	U1379	A1331	G1067	A995	G928	U857	G791
C1836	A1672	A1672	G1602	C1522	C1456	C1380	G1332	U1068	C996	U929	G858	U792
G1837		G1673	A1603	A1523	C1457	G1381	C1312	A1069	C997	A930	G793	
G1838	G1760	C1677	A1604	C1524	U1458	A1386	U1333	G1069	C998	U931	U859	A794
A1839	G1761	G1678	A1605		A1459	G1387	A1334	G1070	A999	G932	U860	A795
A1840	G1762	U1679	C1606	G1527		G1388	A1335		G1000	G933	G861	A796
A1841	A1764	U1680	A1607	C1528	A1463	C1389	G1336	G1073	A1001	G934	C864	A797
G1841	C1765	A1681	U1608	C1529	A1464	G1390	G1337	G1074	A1002	G935	A865	G798
G1850	U1766	G1682	G1609	U1530	G1465	A1391	C1318	U1075	C1003	A936	U868	U800
A1851	G1767	C1683	A1610	C1531	C1466	U1392	C1319	G1076	C1004	C939	C869	C803
	G1768	G1684	U1611	A1532	U1467	G1393	A1320	U1081	U1005	G940	C870	C804
G1855	A1770	U1685	U1612	G1533	U1468	U1397	G1323	A1088	A1007	U941	U871	G805
U1856	A1771	A1686	G1613	U1539	U1469	A1398	G1324	A1089	A1008	U942	G872	G806
G1857	A1774	C1687	C1614	C1540	G1470	G1399	U1325	A1090	C1009	U943	U873	A807
C1858	A1775	G1688	G1615	C1541	G1471	U1400	G1326	A1091	G950	A944	C874	C808
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A1860	A1777	G1691	U1617	G1543	U1473	U1410	U1328	G1093	A1020	G952	U876	U810
G1861	A1778	A1694	U1618	A1544	A1474	C1411	G1329	G1098	A1021	G953	U877	G811
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	A1780	C1620	C1621	C1552		G1419	G1331	U1093	A1023	U955	U879	A813
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G1866	G1704	C1623	C1624	C1558	U1479	C1415	G1333	U1099	A1025	U957	G	A815
G1871	U1787	A1624	A1625	A1561	A1481	C1416	U1334	G1100	U1026	G958	G	U816
	C1788	U1709	A1626	G1562	U1482	C1417	G1335	G1114	C1027	C959	U822	G821
G1880	U1789	U1710	C1627	G1566	A1486	G1418	U1342	G1120	G1028	U960	U823	G822
U1881	G1790	C1711	G1628	A1567	C1487	U1419	C1343	G1121	G1029	G961	U824	U824
G1882	C1791	G1712	G1629	A1568	G1488	U1424	G1344	A1122	U1030	A954	G	C825
A1883	C1792	G1713	G1629	G1566	G1489	U1425	G1345	G1127	A1032	A955	C	U826
A1884	A1793	A1714	A1632	A1567	U1490	U1426	G1346	C1128	A1033	A956	C	C827
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C1888	A1800	C1634	G1635	G1573	C1494	U1430	G1350	G1132	G1036	U969	C	G831
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A1896	C1807	A1728	U1651	G1578	A1499	U1434	G1355	A1138	G1041	C975	A	A838
	C1808	G1729	U1652	U1579	U1500	U1435	A1356	U1139	U1044		C	U839
A1899	G1809	U1810	C1653	C1581	G1501	G1435	A1357	U1141				
U1900	U1811	C1731	A1654	A1582	G1503	G1436	A1358					
	U1812	U1732	U1655	A1583	G1504	U1437	A1359					
U1906	C1907	U1733	C1656	G1584	U1505		U1438					
C1907	U1813		A1657	A1585			A1359					
U1909	G1814	C1736					U1439					

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U	A	C2778	C2779	A2780	G2781	G2782	U2783	A2784	A2785	G2786	A2787	G2788	A2789	A2790	A2791	G2805	G2806	U2807	G2808	A2809	G2810	A2811	A2812	C2815	C2816	G2821	U2822	G2823	C2824	A2825	C2826	U2830	A2831	G2832	G2833	U2836	G2837	U2841	A2842	A2843	G2847	A2848	G2851	G2852	U2853	G2854	G2855											

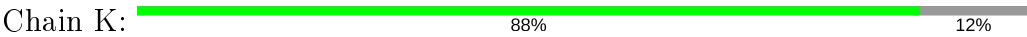
• Molecule 2: tRNA acceptor stem mimic

Chain 5:

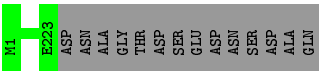




- Molecule 3: 50S ribosomal protein L16



- Molecule 4: GENERAL STRESS PROTEIN CTC



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.60 Å 409.40 Å 695.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60271	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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: SPS, PPU

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	0	0.14	0/66467	0.63	0/103673
2	5	0.16	0/563	0.63	0/873
All	All	0.14	0/67030	0.63	0/104546

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	U	Sidechain

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	0	59359	0	29917	1742	0
2	5	543	0	290	16	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
5	0	22	0	19	0	0
All	All	60271	0	30226	1754	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 19.

The worst 5 of 1754 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)
1:0:940:G:H3'	1:0:941:U:H5''	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5''	1.20	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2548:G:H2'	1:0:2549:G:H5''	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.22	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	416 (15%)	44 (1%)
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	418 (15%)	44 (1%)

5 of 418 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1263	G
1	0	1495	G
1	0	2668	U
1	0	1278	A
1	0	1313	U

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$
2	PPU	5	35	1,2	32,40,41	2.81	6 (18%)	33,57,60	0.98	3 (9%)

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
2	PPU	5	35	1,2	-	0/21/43/44	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	C-N3'	12.63	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.96	1.27	1.42
2	5	35	PPU	C6-N1	3.86	1.38	1.33
2	5	35	PPU	CE1-CZ	3.70	1.46	1.38
2	5	35	PPU	CE2-CZ	2.70	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	CM-OC-CZ	2.93	123.86	117.51
2	5	35	PPU	C9-N6-C6	2.23	126.26	119.51
2	5	35	PPU	C-CA-N	2.22	117.97	109.40

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
2	5	35	PPU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
5	SPS	0	2881	-	19,22,23	4.43	9 (47%)	17,28,30	4.15	8 (47%)

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	SPS	0	2881	-	1/1/2/6	9/15/16/18	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	0	2881	SPS	O10-C10	9.82	1.43	1.24
5	0	2881	SPS	C9-C8	8.40	1.54	1.33
5	0	2881	SPS	O1-C1	7.67	1.43	1.24
5	0	2881	SPS	C10-N11	6.56	1.50	1.34
5	0	2881	SPS	C5-N4	5.43	1.42	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	0	2881	SPS	C12-N11-C10	-7.47	112.03	122.57
5	0	2881	SPS	C1-N2-C3	6.40	120.55	115.14
5	0	2881	SPS	C8-C9-C10	-6.14	109.55	121.56
5	0	2881	SPS	C14-S15-C16	6.14	109.42	101.04
5	0	2881	SPS	O10-C10-C9	-5.96	109.44	123.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

5 of 9 torsion outliers are listed below:

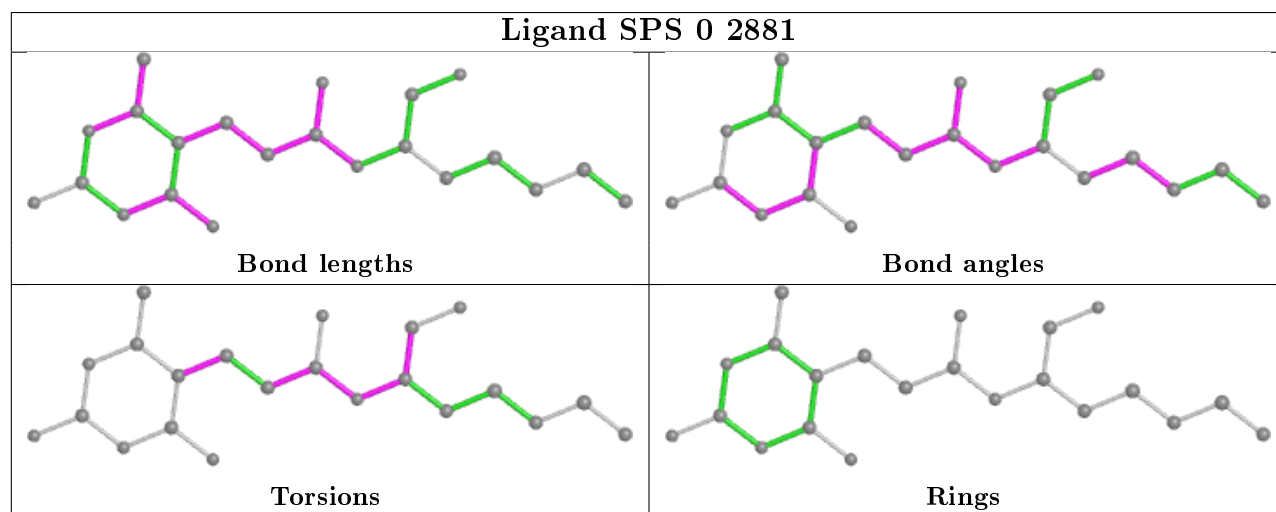
Mol	Chain	Res	Type	Atoms
5	0	2881	SPS	C1-C6-C8-C9
5	0	2881	SPS	C9-C10-N11-C12
5	0	2881	SPS	O10-C10-N11-C12
5	0	2881	SPS	C14-C12-C13-O13
5	0	2881	SPS	N11-C12-C13-O13

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.