



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 1NJM / pdb_00001njm
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

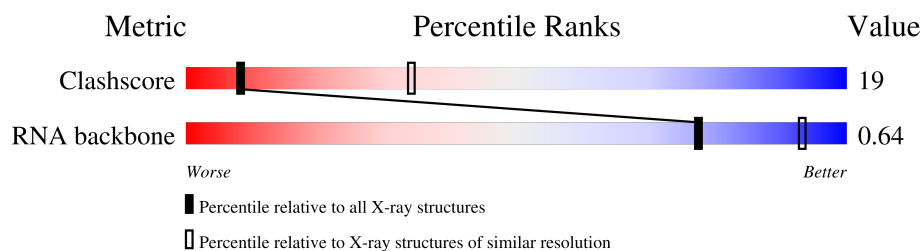
1 Overall quality at a glance

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	190562	1827 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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 $\leq 5\%$.

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	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			

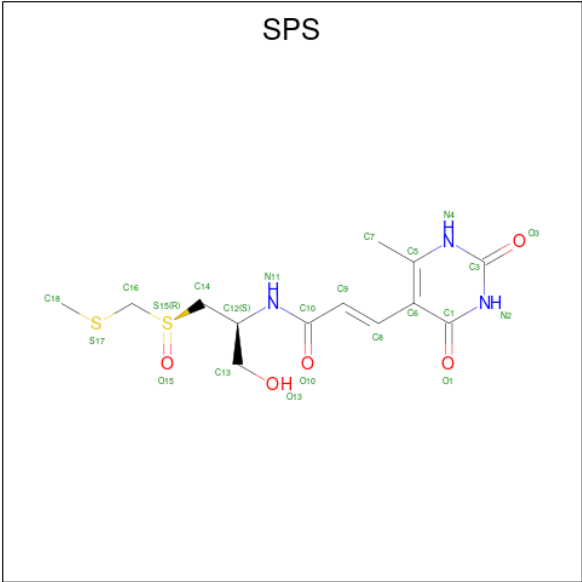
- Molecule 3 is a protein called 50S ribosomal protein L16.

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 (CCD ID: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



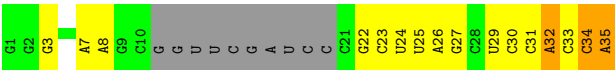
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	0	1	Total	C	N	O	S	0	0
			22	13	3	4	2		



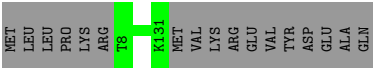
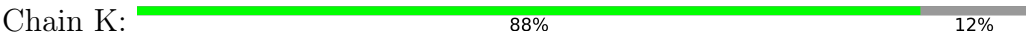
G1818	G1737	A1858	G1508	A1441	G1359	A1289	G1045	U978	C	U840	G778
U1819	G1742	G1659	A1509	C1442	U1365	A1290	U1046	A979	A911	G841	U779
G1820	C1743	A1510	A1510	C1443	A1366	G1291	G1047	G980	U916	A842	U780
A1821	G1744	C1661	A1511	C1444	A1367	A1292	C1219	C981	U917	G843	G781
C1822	G1745	G1662	A1512	U1445	A1368	A1293	C1053	A984	U918	G844	U782
C1825	C1746	C1593	U1513	U1446	G1369	G1298	G1052	G985	U919	U845	G783
U1826	G1747	U1514	C1514	U1447	G1369	U1301	C1054	G986	G920	A846	U784
C1829	U1748	U1515	U1515	A1448	G1370	U1307	A1055	A987	A921	A847	U785
G1830	G1749	A1516	A1516	A1449	G1371	U1307	U1056	G987	A922	U852	U786
G1831	A1750	C1517	C1517	G1450	A1372	U1307	A1057	G988	U925	G853	U787
C1835	G1754	G1519	G1519	U1452	G1373	C1308	U1058	A991	U926	G854	G788
G1836	G1755	G1520	G1520	C1455	G1377	G1309	A1065	A994	U927	G855	G789
G1837	A1672	U1521	U1521	C1456	C1380	C1310	G1066	A994	C927	A856	G791
G1838	C1677	C1522	C1522	A1457	G1381	G1312	G1067	A995	G928	U857	U792
A1839	C1678	C1524	C1524	A1458	A1386	A1313	A1068	C996	G929	G858	G793
A1840	G1763	G1527	G1527	U1459	A1387	A1314	C1069	C997	A930	U859	A794
G1841	A1764	G1528	G1528	C1463	G1388	A1315	G1070	C998	G931	U860	A795
C1850	C1765	C1529	C1529	A1464	C1389	G1316	G1073	A999	G932	G861	A796
A1851	U1766	U1530	U1530	G1465	G1390	A1318	G1074	A1001	G934	C864	A797
G1855	U1770	C1531	C1531	G1466	A1391	C1319	C1075	C1002	C935	A865	G798
U1856	A1771	A1532	A1532	U1467	U1392	A1320	U1076	C1003	A936	U868	U800
G1857	A1774	G1533	G1533	U1468	G1393	G1323	A1081	U1005	C939	C869	C803
C1858	A1775	U1539	U1539	G1470	A1397	G1324	A1084	C1006	G940	C870	C804
A1859	C1776	C1540	C1540	A1471	G1398	U1325	G1085	A1007	U941	U871	G805
A1860	G1692	C1543	C1543	C1472	C1399	U1326	G1086	G1087	U942	A806	A806
G1861	C1692	G1543	G1543	U1473	G1407	C1327	C1087	A874	U943	A807	A807
C1862	A1778	A1544	A1544	A1474	G1408	G1328	C1088	A875	U944	C808	C808
G1865	A1780	G1545	G1545	U1475	U1410	U1329	C1089	A876	G945	C809	C809
U1866	C1785	C1552	C1552	U1478	C1411	G1330	C1090	A877	C948	U810	U810
G1871	U1787	G1557	G1557	G1479	C1418	G1331	C1091	C878	G949	G811	G811
G1880	U1789	C1558	C1558	A1481	G1419	G1332	C1092	A879	U951	G812	G812
U1881	G1704	A1561	A1561	U1482	G1414	G1333	U1093	C880	G952	A813	A813
G1882	C1704	G1562	G1562	A1486	C1415	A1334	G1098	G887	G953	G814	G814
A1883	G1712	G1566	G1566	C1487	C1416	U1337	A1099	G888	U954	U816	U816
A1884	G1713	A1567	A1567	G1488	C1417	G1338	G1100	C889	G955	A817	A817
C1885	A1714	A1568	A1568	U1489	G1418	U1339	G1101	U890	A956	G818	G818
G1886	C1715	C1568	C1568	U1490	G1419	G1340	A1114	A891	U957	C819	C819
C1887	G1716	C1571	C1571	C1491	G1424	G1341	U1026	G	G958	U821	U821
G1888	A1717	G1572	G1572	A1492	U1425	U1342	C1027	G	U960	G	U823
A1889	G1722	G1573	G1573	G1493	G1426	C1343	G1028	G	G961	U824	U824
G1890	U1723	A1574	A1574	G1494	U1427	C1344	G1029	G	A964	C825	C825
C1895	C1724	C1575	C1575	G1495	G1428	G1345	A1032	C	U965	U826	U826
A1896	C1727	G1576	G1576	C1497	A1429	C1346	G1033	U	A966	C827	C827
U1896	A1728	U1577	U1577	G1498	G1430	U1347	U1129	A	G967	C828	C828
G1899	C1729	G1578	G1578	U1499	U1431	C1348	U1130	C	C968	C829	C829
U1900	G1652	G1579	G1579	A1500	G1432	G1350	G1131	C	U969	C830	C830
C1906	C1730	C1581	C1581	C1501	G1433	G1351	G1132	C	G970	C831	C831
U1907	A1811	A1582	A1582	G1502	U1434	A1353	G1133	A	A971	A832	A832
C1908	U1732	G1583	G1583	G1503	G1435	A1354	A1137	G	C972	A833	A833
G1909	U1733	U1584	U1584	U1504	G1436	A1355	A1138	U	U973	A834	A834
C1909	C1736	C1585	C1585	U1505	A1437	U1356	A1139	U	U974	U837	U837
U1909		A1657	A1657	G1506	G1437	U1357	A1140	A	C975	A838	A838
							U1141	C		U839	U839

- Molecule 2: tRNA acceptor stem mimic

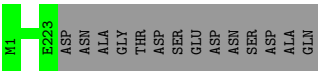
Response	Percentage
Yes, it's important to take action to address climate change	26%
No, it's not important to take action to address climate change	37%
Don't know	9%
Refuse to answer	29%



- 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPU, SPS

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	0.25	0/66467	0.50	7/103673 (0.0%)
2	5	0.26	0/563	0.49	0/873
All	All	0.25	0/67030	0.50	7/104546 (0.0%)

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.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	71	A	C2'-C3'-O3'	6.04	118.55	109.50
1	0	2426	G	C2'-C3'-O3'	6.02	118.54	109.50
1	0	192	G	C2'-C3'-O3'	5.84	118.25	109.50
1	0	242	A	C2'-C3'-O3'	5.76	118.14	109.50
1	0	583	C	C2'-C3'-O3'	5.61	117.91	109.50

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	1733	0
2	5	543	0	290	17	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	1745	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 1745 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	1807	A
1	0	2245	A
1	0	1820	G
1	0	2093	G
1	0	2377	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	2,1	37,40,41	2.65	7 (18%)	47,57,60	0.98	4 (8%)

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	2,1	-	1/25/43/44	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	C-N3'	12.98	1.61	1.34
2	5	35	PPU	OC-CM	-5.36	1.27	1.42
2	5	35	PPU	CE1-CZ	3.91	1.46	1.38
2	5	35	PPU	CE2-CZ	2.84	1.44	1.38
2	5	35	PPU	CD2-CG	2.73	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C2-N1-C6	3.26	119.79	111.83
2	5	35	PPU	CM-OC-CZ	2.97	123.86	117.50
2	5	35	PPU	C-CA-N	2.28	117.97	109.37
2	5	35	PPU	C9-N6-C6	2.25	126.26	120.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	35	PPU	C3'-C4'-C5'-O5'

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 oligosaccharides 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	4.95	11 (57%)	23,28,30	3.31	13 (56%)

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	8/15/16/18	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	0	2881	SPS	O1-C1	10.69	1.43	1.23
5	0	2881	SPS	O10-C10	9.78	1.43	1.24
5	0	2881	SPS	O3-C3	9.44	1.43	1.23
5	0	2881	SPS	C9-C8	7.32	1.54	1.33
5	0	2881	SPS	C10-N11	7.17	1.50	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	0	2881	SPS	C9-C10-N11	6.29	125.37	114.61
5	0	2881	SPS	C14-S15-C16	6.14	109.42	101.04
5	0	2881	SPS	O10-C10-C9	-5.86	109.44	122.95
5	0	2881	SPS	C7-C5-N4	4.58	118.74	113.42
5	0	2881	SPS	C1-N2-C3	-4.23	120.55	126.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

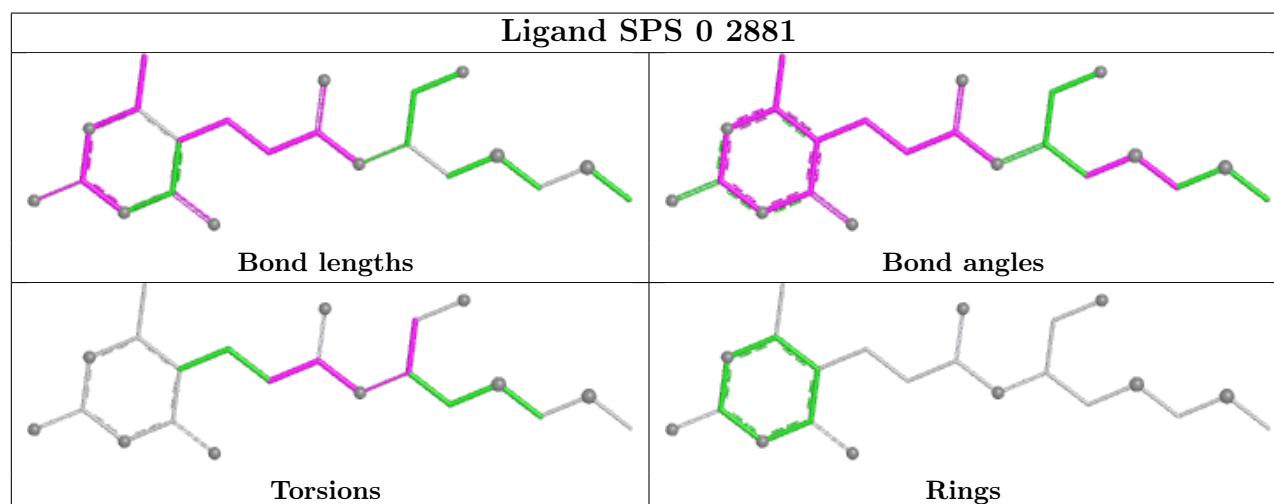
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
5	0	2881	SPS	C13-C12-N11-C10

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.