



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 11:01 PM BST

PDB ID : 4WFA
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with linezolid
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.39 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) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

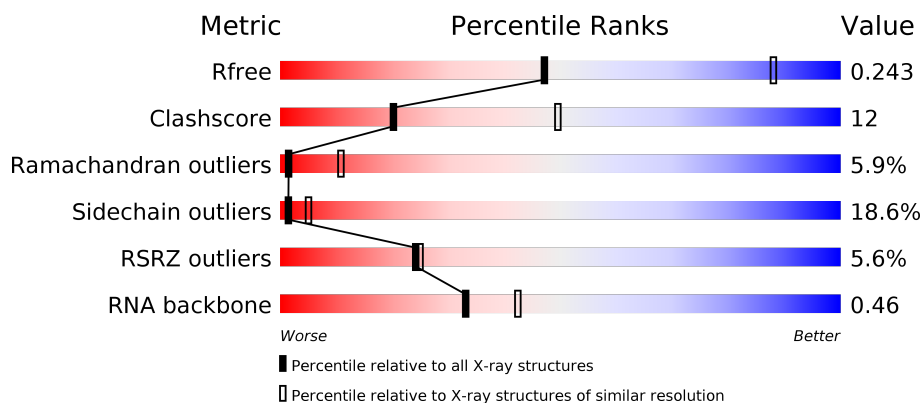
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	X	2923	
2	Y	114	
3	A	277	
4	B	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MPD	X	3006	-	-	-	X
30	MPD	X	3008	-	-	-	X
31	MG	G	201	-	-	-	X
31	MG	O	202	-	-	-	X
31	MG	X	3012	-	-	-	X
31	MG	X	3014	-	-	-	X
31	MG	X	3019	-	-	-	X
31	MG	X	3029	-	-	-	X
31	MG	X	3032	-	-	-	X
31	MG	X	3056	-	-	-	X
31	MG	X	3208	-	-	-	X
31	MG	X	3242	-	-	-	X
31	MG	X	3254	-	-	-	X
31	MG	X	3280	-	-	-	X
31	MG	X	3284	-	-	-	X
31	MG	X	3297	-	-	-	X
31	MG	X	3312	-	-	-	X
31	MG	X	3327	-	-	-	X
31	MG	X	3340	-	-	-	X
31	MG	X	3343	-	-	-	X
31	MG	X	3344	-	-	-	X
31	MG	X	3348	-	-	-	X
31	MG	X	3351	-	-	-	X
31	MG	X	3357	-	-	-	X
31	MG	X	3359	-	-	-	X
31	MG	X	3361	-	-	-	X
31	MG	X	3363	-	-	-	X
31	MG	X	3369	-	-	-	X
31	MG	X	3380	-	-	-	X
31	MG	X	3382	-	-	-	X
31	MG	X	3386	-	-	-	X
31	MG	X	3397	-	-	-	X
31	MG	X	3399	-	-	-	X
31	MG	X	3401	-	-	-	X
31	MG	X	3411	-	-	-	X
31	MG	X	3418	-	-	-	X
31	MG	X	3419	-	-	-	X
31	MG	X	3420	-	-	-	X
31	MG	Y	207	-	-	-	X
31	MG	Y	208	-	-	-	X
32	MN	X	3085	-	-	-	X
32	MN	X	3114	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MN	X	3117	-	-	-	X
32	MN	X	3217	-	-	-	X
32	MN	X	3222	-	-	-	X
32	MN	X	3265	-	-	-	X
32	MN	X	3422	-	-	-	X
34	EPE	X	3426	-	-	X	-
35	SPD	X	3429	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 81465 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2711	Total	C	N	O	P	0	0	0
			58151	25961	10662	18817	2711			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	268	Total	C	N	O	S	0	0	0
			1620	985	315	316	4			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1531	957	283	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1321	818	253	248	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	155	Total	C	N	O	S	0	0	0
			794	478	155	160	1			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			926	567	172	186	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1087	679	202	203	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			840	517	163	157	3			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			817	500	164	152	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1003	642	185	173	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			896	551	176	168	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	108	Total	C	N	O	0	0	0
			659	399	134	126			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O			
			809	513	158	138	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	188	153	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	S			
			751	477	137	136	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	88	Total	C	N	O	S			
			586	363	108	113	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			680	425	121	133	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1048	656	187	203	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			530	328	100	102			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	44	Total	C	N	O	0	0	0
			254	154	52	48			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			414	261	74	79			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O	0	0	0
			441	274	83	84			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	44	Total	C	N	O	S	0	0	0
			336	208	70	55	3			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			368	225	89	53	1			

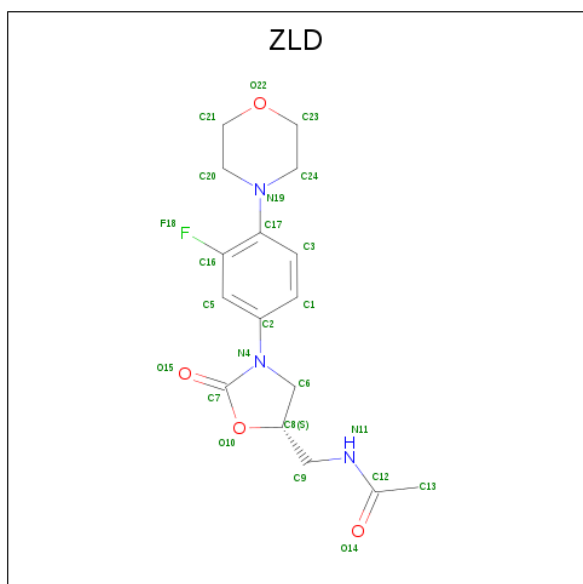
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			414	256	83	73	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

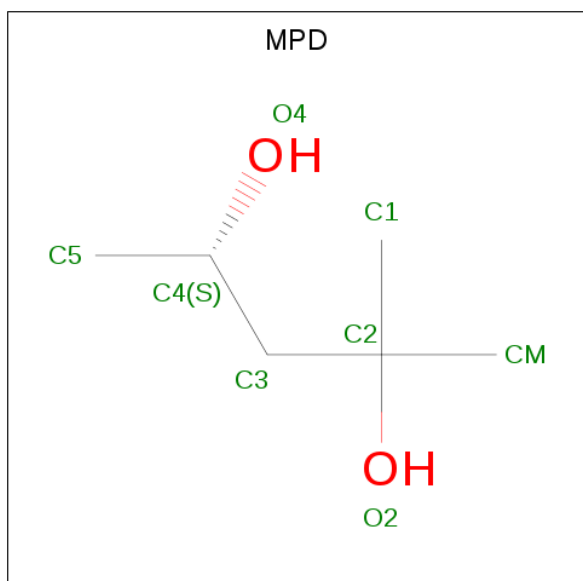
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			262	164	52	41	5			

- Molecule 29 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (three-letter code: ZLD) (formula: $C_{16}H_{20}FN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	G	2	Total Mg 2 2	0	0
31	K	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	I	1	Total Mg 1 1	0	0
31	C	1	Total Mg 1 1	0	0
31	W	1	Total Mg 1 1	0	0
31	Z	2	Total Mg 2 2	0	0
31	A	2	Total Mg 2 2	0	0
31	N	1	Total Mg 1 1	0	0
31	X	226	Total Mg 226 226	0	0
31	O	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	Y	6	Total 6	Mg 6	0	0

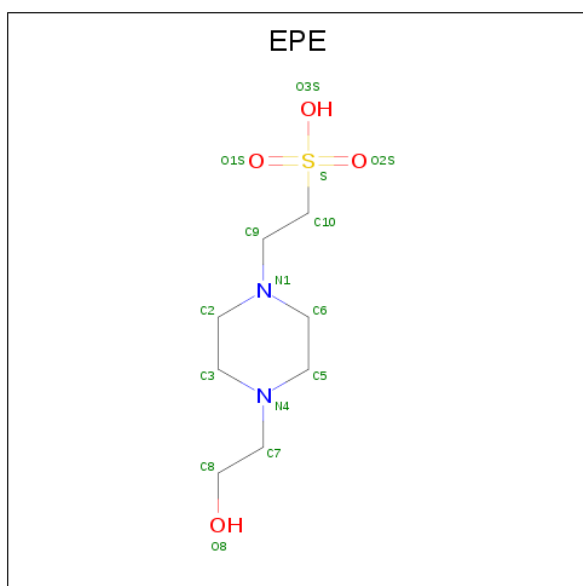
- Molecule 32 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	191	Total 191	Mn 191	0	0
32	Z	1	Total 1	Mn 1	0	0
32	Y	2	Total 2	Mn 2	0	0
32	M	1	Total 1	Mn 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

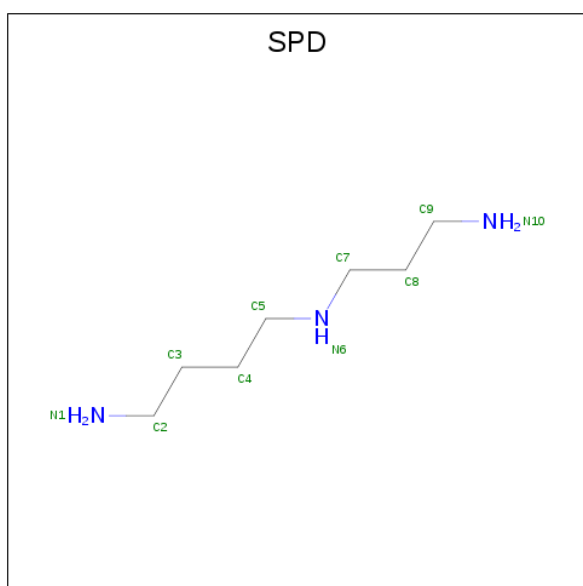
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total 1	Na 1	0	0

- Molecule 34 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 35 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



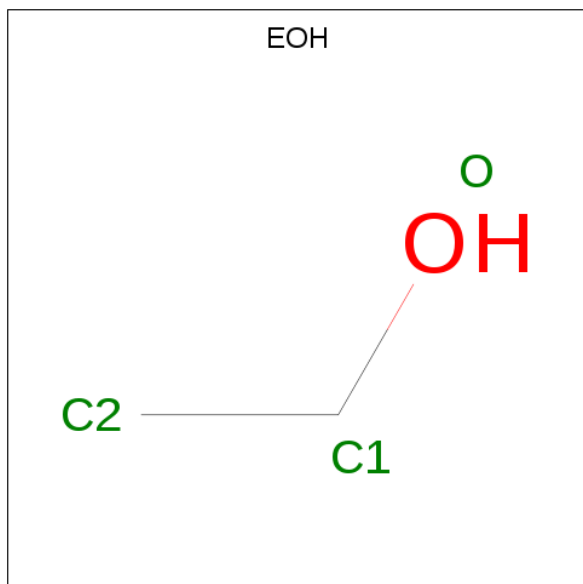
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	N	0	0
			10	7	3		

- Molecule 36 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

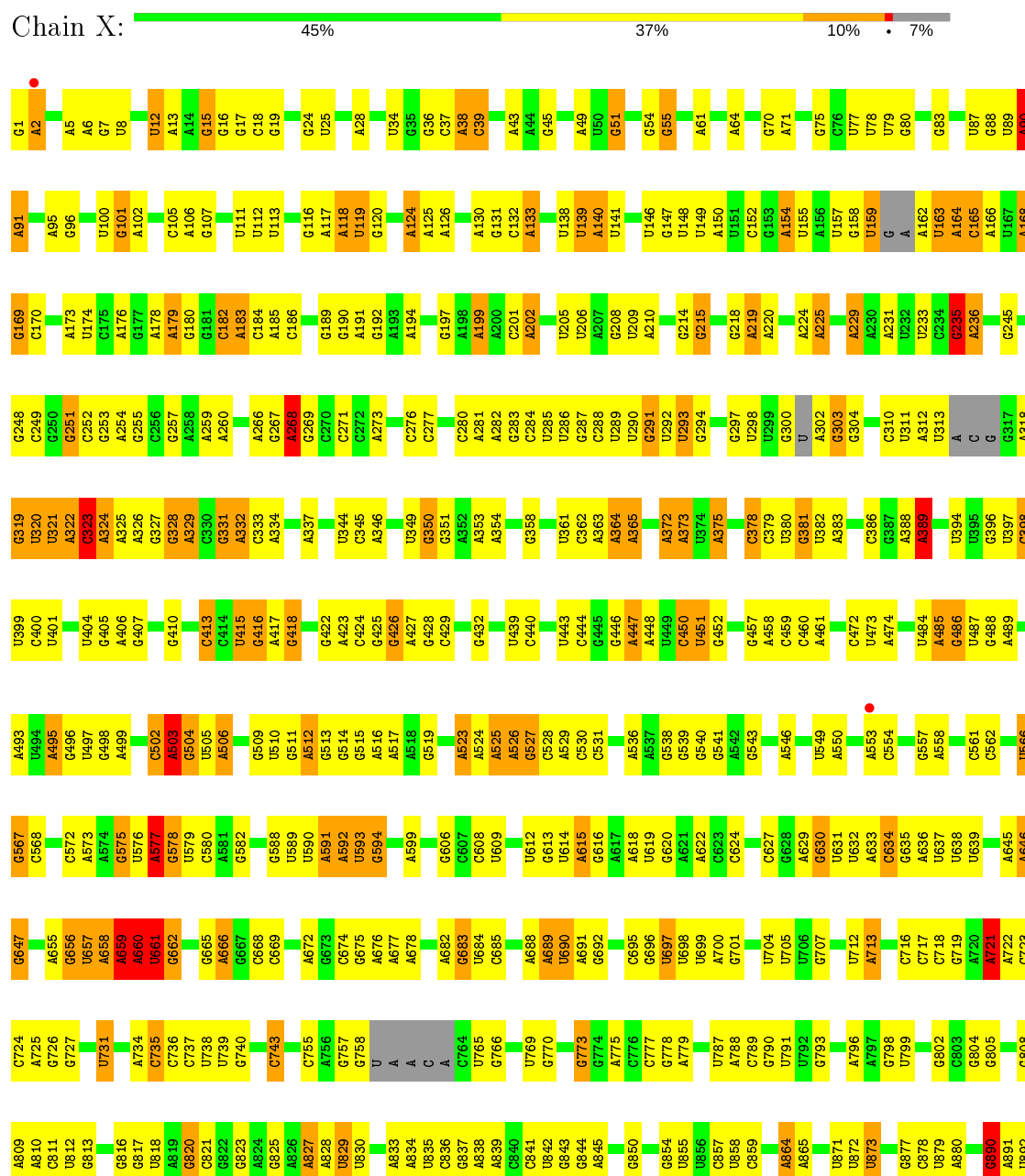


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	Y	1	Total	C	O	0	0
			3	2	1		

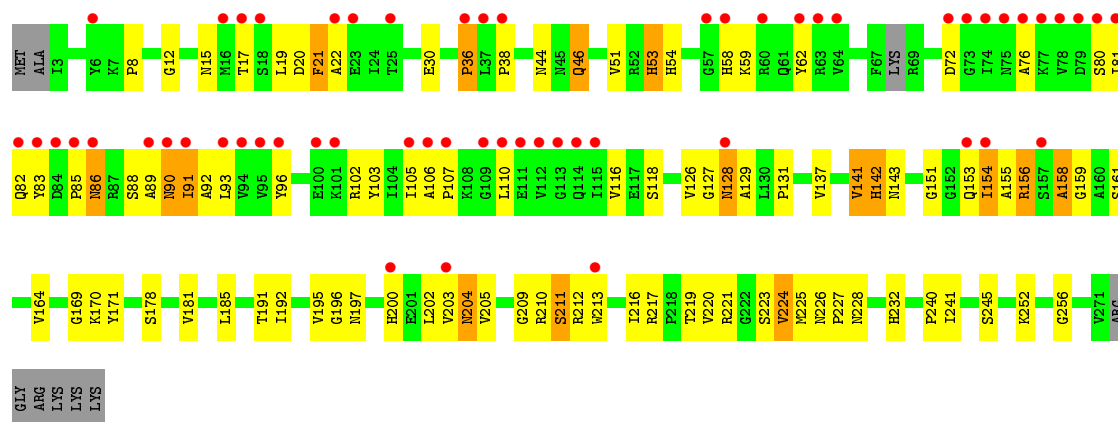
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: 23S rRNA



C2001	A1912	G1838	G1761	U1683	U1594	A	G1469	G1359	A1314	G1226	A	A1072	G982	U895
A2005	C1922	G1839	U1762	A1684	C1595	G	G1470	C1400	C1315	U1227	U	U1077	G983	U896
C2006	A1923	U1840	U1763	G1596	G1597	C	A1471	G1316	G1346	G1401	A	G1078	G984	A937
G2007	G1842	A1764	A1765	G1691	A1598	C	C1472	A1402	G1317	G1229	G	U1079	G985	U898
A2008	U1925	G1843	C1766	C1692	G1599	A1538	G1473	G1405	G1322	G1235	C1144	C1082	G986	U899
U2009	A1926	G1844	G1767	G1693	A1600	A1539	A1475	G1406	G1328	C1235	C1146	G988	G990	G900
G2013	C1929	U1845	C1768	G1695	U1601	U1540	G1476	G1411	C1328	U1238	A1150	U1085	G990	G901
C2017	G1930	A1846	C1769	C1696	U1602	C1541	U1477	G1412	G1329	U1238	G1151	U1086	G991	A902
U2018	G1931	U1847	C1770	G1697	U1603	C1542	A1481	A1415	U1330	C1239	G1152	G1087	G992	G903
G2019	C1932	A1848	A1771	A1698	C1604	G1543	A1482	A1416	U1331	U1240	G1153	C1088	G1000	G904
U2020	G1933	G1849	G1772	A1699	A1605	G1544	U1483	G1417	C1332	A1241	G1154	C1089	A1001	G907
C2023	G1851	U1850	G1775	C1700	U1609	U1545	G1483	G1418	C1335	G1247	A1155	A1090	G1005	A908
A2024	U1854	C1702	A1776	U1701	G1610	A1546	G1487	A1421	G1336	U1247	U1156	G1091	G1006	G922
G2025	U1855	G1703	G1780	U1702	G1613	U1547	A	A1422	G1337	U1248	U1157	A1092	C1008	G923
C2026	A1856	G1710	C1781	A1618	G1615	C1549	A	C1423	U1338	U1249	G1158	C1093	U1013	G924
G2037	G1862	A1713	A1712	A1619	A1616	U	G1492	A1424	G1346	G1250	A1161	A1098	U0114	G925
U2038	C1865	G1718	U1788	A1620	A1617	A	G1493	G1425	U1349	A1267	C1168	G1099	G1015	G926
G2039	G1867	C1719	A1789	G1621	A1615	G1555	G1494	G1429	U1350	C1268	U1169	G	G1016	G
A2040	U1868	A1720	G1790	C1622	A1616	C1557	A1497	A1430	C1351	U1269	A1170	C	A1017	C
U2043	G1869	A1721	C1791	G1623	A1617	U1558	U1498	U1431	G1352	G1271	U	G	A1018	C
C2044	C1792	A1722	C1792	U1624	G1622	G1559	U1499	U1433	G1353	G1272	U	U	G1022	C
A2047	A1800	A1723	A1806	C1625	A1622	U1560	G1500	U1434	A1355	G1273	U	U	A1023	C
G2048	G1874	U1724	U1807	U1626	A1623	G1564	U1504	U1439	G1356	G1274	U	G	C1026	U
U2049	G1876	A1725	A1808	G1627	A1624	U1566	G1505	A1440	C1362	U1280	G1183	G	A1027	C
A2050	G1877	A1726	U1809	U1628	A1625	G1567	C1506	A1441	U1366	A1282	U1185	A	G1028	G
C2052	G1882	U1732	U1808	A1630	A1632	U1568	G1508	C1444	C1370	G1279	G1186	U	C1029	G
U2053	U1883	A1733	C1809	G1631	A1632	G1569	G1509	U1445	U1371	U1285	A1187	C	C1030	G937
G2054	G1884	A1810	A1810	A1632	A1632	G1570	U1510	U1446	U1372	G1286	A1187	G	G1031	G938
A2057	G1885	A1811	U1736	A1633	A1632	G1571	C1511	A1447	U1373	U1287	A1192	A	U1032	U939
C2058	U1886	A1812	U1737	A1634	A1634	G1572	C1512	U1448	U1374	G1288	U1185	C	A1037	U940
G2059	G1887	A1813	C1738	A1635	A1635	G1573	C1513	A1449	G1375	A1290	A1196	C	G1038	C943
A2060	U1888	A1814	U1739	A1636	A1636	G1574	A1514	A1450	U1376	G1291	A1197	A	A1044	G944
U2061	G1889	A1815	G1739	A1637	A1637	A1575	A1515	U1451	G1377	A1292	G1198	C	A1045	A945
G2062	U1892	A1818	G1741	G1638	G1638	U1576	C1516	G1452	U1378	U1293	A1199	C	G1046	U947
C2070	A1893	U1821	U1744	C1642	C1642	A1577	C1517	G1453	A1379	G1294	A1200	A	G1047	U948
A2076	U1896	C1822	A1745	C1643	C1643	C	U1518	U1454	U1382	U1300	G1211	U	A1053	A955
C2072	C1974	C1823	G1746	C1644	C1644	A	G1519	U	G1383	U1301	U1212	U	A1054	C959
G2075	U	U1825	G1749	C1651	C1651	U	A	U	U1389	G1302	C1213	A	U1055	G961
A2077	G1900	C1826	U1749	A1652	A1652	U	A1521	A	U1390	G1302	C1214	A	U1056	C967
C2077	C1901	C1827	U1750	A1653	A1653	G	G1522	A	U1391	G1303	U1215	A	A1057	U970
A2078	G1902	U1828	G1751	A1654	A1654	A	G1523	A	U1392	G1304	U1216	G	U1063	U971
G2079	C1903	A1830	U1753	G1657	G1657	G	C1524	A1459	A1390	U1305	U	A	A1064	A972
C2080	A1903	A1831	C1754	A1658	A1658	U	U1525	C1461	G1392	A1306	U1217	G	A1065	A973
A2081	G1906	C1832	U1755	C1659	C1659	U	A1527	A1463	U1393	G1309	G1218	U	G1066	U974
C2082	U1907	C1833	U1756	A1660	A1660	U	G1528	U1464	C1394	G1309	G1219	G	U1067	U975
G2083	A1908	G1834	U1757	C1661	C1661	C	U1529	G1465	G1395	A1310	A1220	C	U1068	U976
A2087	U1909	U1835	G1758	A1662	A1662	G1591	A1530	G1466	A1396	A1312	A1221	G	G1069	U977
G2088	G1911	A1836	G1759	G1663	G1663	G1592	U	G1467	G1397	A1222	A1223	U	A1070	A977
		A1837	G1760			G1593	U	G1468	G1398	G1313		A	A1071	



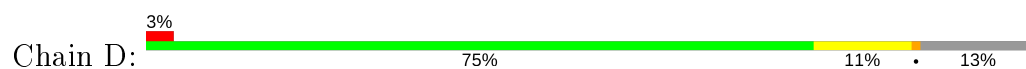
• Molecule 4: 50S ribosomal protein L3

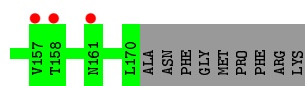


• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

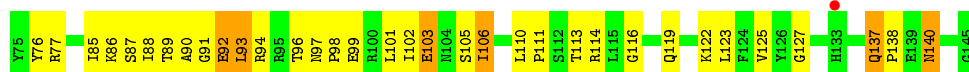




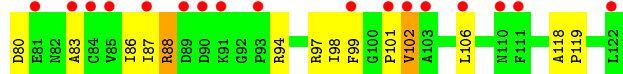
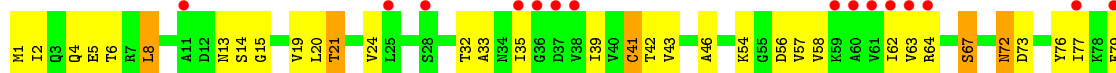
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14



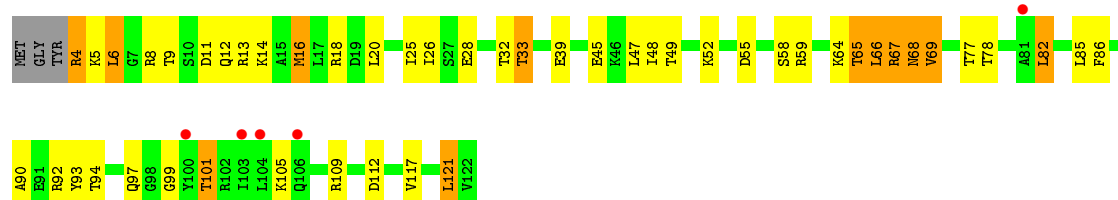
• Molecule 10: 50S ribosomal protein L15



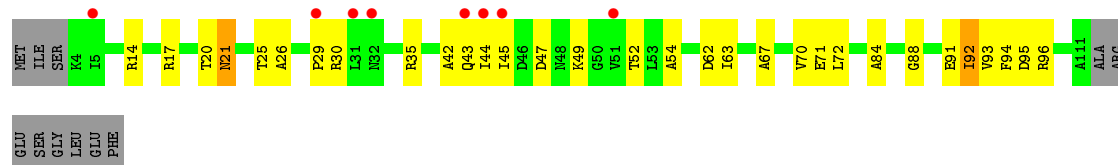
• Molecule 11: 50S ribosomal protein L16



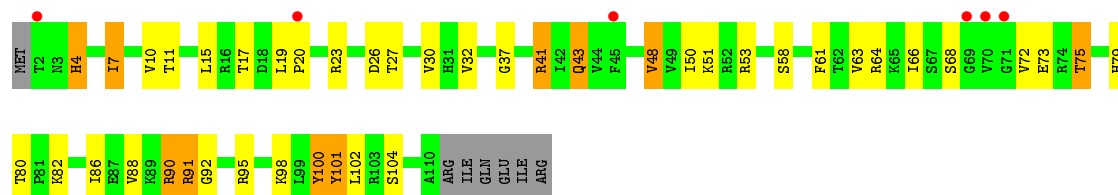
- Molecule 12: 50S ribosomal protein L17



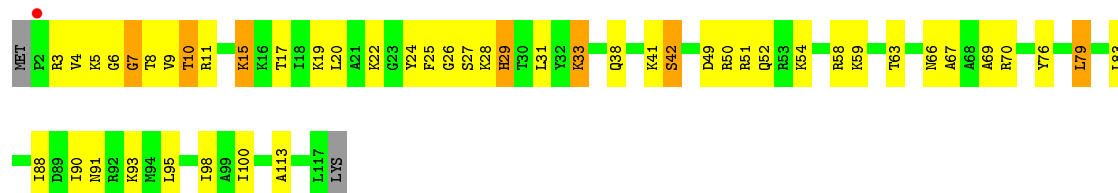
- Molecule 13: 50S ribosomal protein L18



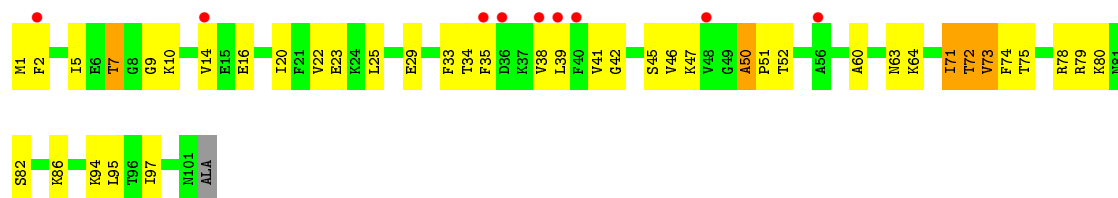
- Molecule 14: 50S ribosomal protein L19



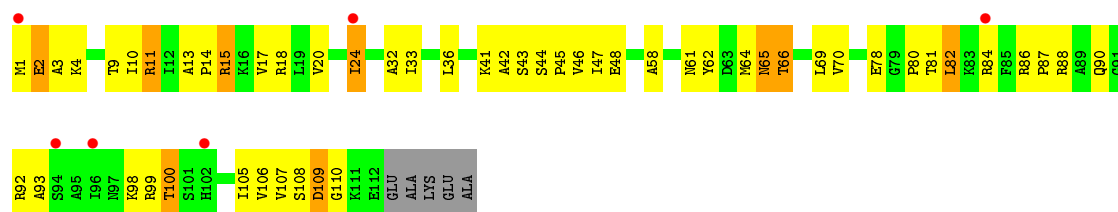
- Molecule 15: 50S ribosomal protein L20



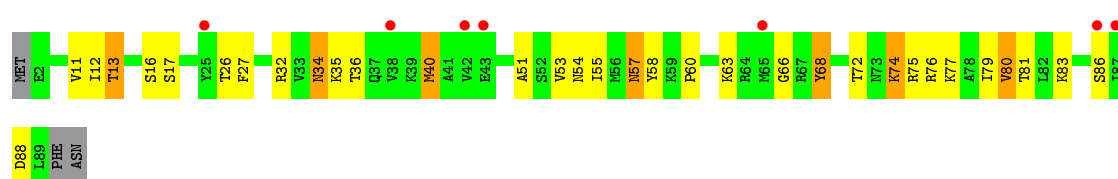
- Molecule 16: 50S ribosomal protein L21



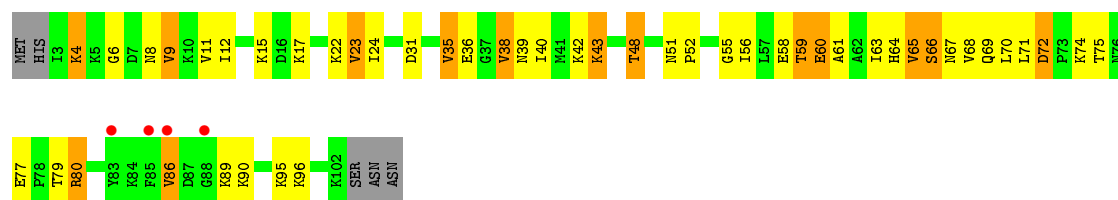
- Molecule 17: 50S ribosomal protein L22



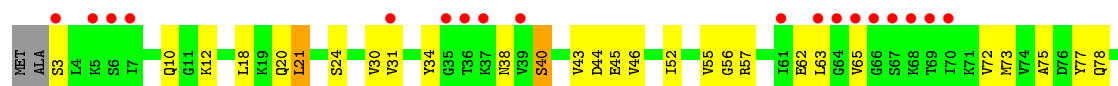
- Molecule 18: 50S ribosomal protein L23

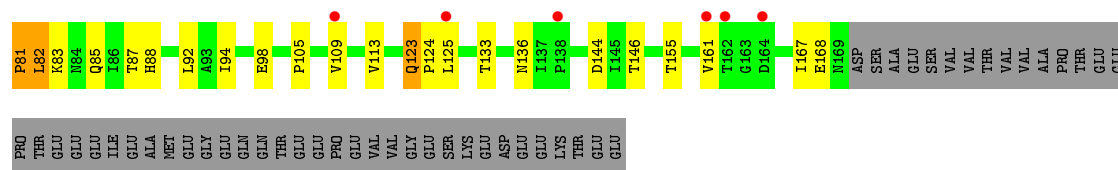


- Molecule 19: 50S ribosomal protein L24

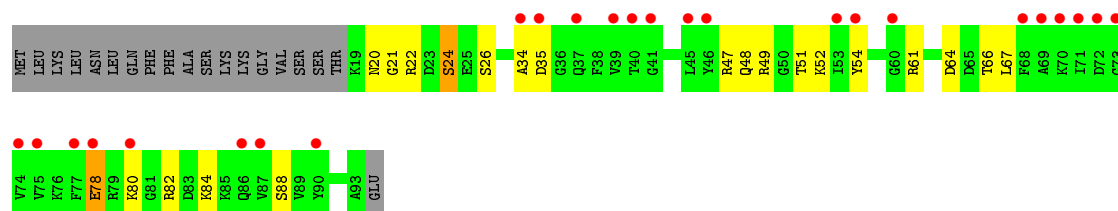


- Molecule 20: 50S ribosomal protein L25





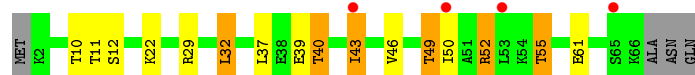
• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



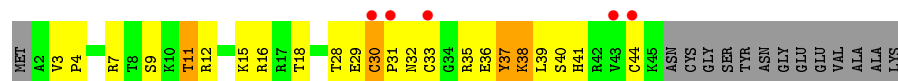
• Molecule 23: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L30

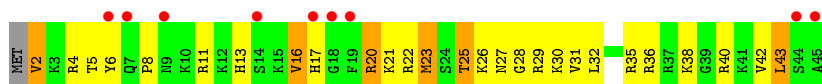


• Molecule 25: 50S ribosomal protein L32



• Molecule 26: 50S ribosomal protein L34





- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.92Å 279.92Å 870.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.88 – 3.39 100.73 – 3.39	Depositor EDS
% Data completeness (in resolution range)	88.9 (64.88-3.39) 88.9 (100.73-3.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.243 0.202 , 0.243	Depositor DCC
R_{free} test set	12433 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	109.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 88.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81465	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: ZLD, MG, MN, NA, EOH, MPD, EPE, SPD

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	X	0.53	7/65113 (0.0%)	1.03	150/101510 (0.1%)
2	Y	0.50	0/2717	1.03	10/4232 (0.2%)
3	A	0.36	0/1652	0.67	0/2280
4	B	0.49	0/1554	0.76	0/2101
5	C	0.49	0/1339	0.76	0/1832
6	D	0.27	0/796	0.54	0/1104
7	E	0.36	0/937	0.64	0/1296
8	G	0.45	0/1109	0.69	0/1504
9	H	0.47	0/847	0.68	0/1150
10	I	0.56	0/825	0.90	1/1119 (0.1%)
11	J	0.47	0/1026	0.70	0/1390
12	K	0.44	0/899	0.71	0/1204
13	L	0.36	0/664	0.67	0/907
14	M	0.43	0/821	0.71	0/1110
15	N	0.53	0/944	0.73	0/1252
16	O	0.47	0/761	0.73	0/1022
17	P	0.48	0/870	0.69	0/1171
18	Q	0.35	0/591	0.60	0/809
19	R	0.36	0/686	0.63	0/934
20	S	0.45	0/1060	0.71	2/1461 (0.1%)
21	T	0.42	0/536	0.64	0/720
22	U	0.30	0/257	0.59	0/356
23	V	0.35	0/415	0.55	0/569
24	W	0.44	0/443	0.66	0/597
25	Z	0.57	0/342	0.89	0/457
26	2	0.41	0/372	0.63	0/487
27	3	0.50	0/418	0.80	0/558
28	4	0.37	0/265	0.58	0/356
All	All	0.51	7/88259 (0.0%)	0.97	163/133488 (0.1%)

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
3	A	0	1
4	B	0	1
9	H	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	577	A	N9-C4	-8.16	1.32	1.37
1	X	1065	A	N9-C4	-7.99	1.33	1.37
1	X	577	A	C5-C6	-6.29	1.35	1.41
1	X	350	G	N9-C4	5.82	1.42	1.38
1	X	2845	G	N9-C4	-5.62	1.33	1.38

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	577	A	N1-C6-N6	13.04	126.42	118.60
1	X	577	A	C2-N3-C4	-11.54	104.83	110.60
1	X	2845	G	N3-C4-N9	-11.21	119.27	126.00
1	X	2845	G	N3-C4-C5	11.11	134.15	128.60
1	X	2048	G	C4-C5-N7	10.77	115.11	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	128	ASN	Peptide
4	B	166	GLY	Peptide
9	H	83	ALA	Peptide

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	X	58151	0	29248	918	0
2	Y	2430	0	1229	37	0
3	A	1620	0	1213	57	0
4	B	1531	0	1483	66	0
5	C	1321	0	1184	54	0
6	D	794	0	415	4	0
7	E	926	0	656	18	0
8	G	1087	0	1022	47	0
9	H	840	0	802	35	0
10	I	817	0	688	27	0
11	J	1003	0	970	44	0
12	K	896	0	921	35	0
13	L	659	0	505	17	0
14	M	809	0	811	23	0
15	N	932	0	997	45	0
16	O	751	0	744	24	0
17	P	862	0	920	45	0
18	Q	586	0	493	24	0
19	R	680	0	650	32	0
20	S	1048	0	847	15	0
21	T	530	0	494	19	0
22	U	254	0	165	4	0
23	V	414	0	354	9	0
24	W	441	0	478	20	0
25	Z	336	0	340	22	0
26	2	368	0	409	20	0
27	3	414	0	392	12	0
28	4	262	0	266	19	0
29	X	24	0	20	5	0
30	X	72	0	126	5	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	G	2	0	0	0	0
31	I	1	0	0	0	0
31	K	1	0	0	0	0
31	N	1	0	0	0	0
31	O	2	0	0	0	0
31	W	1	0	0	0	0
31	X	226	0	0	0	0
31	Y	6	0	0	0	0
31	Z	2	0	0	0	0
32	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	191	0	0	0	0
32	Y	2	0	0	0	0
32	Z	1	0	0	0	0
33	X	1	0	0	0	0
34	X	60	0	68	20	0
35	J	10	0	19	0	0
35	X	80	0	152	11	0
36	X	12	0	24	0	0
36	Y	3	0	6	0	0
All	All	81465	0	49111	1518	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 12.

The worst 5 of 1518 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:A:116:VAL:HG11	3:A:127:GLY:HA3	1.41	0.97
34:X:3426:EPE:H52	15:N:7:GLY:HA2	1.50	0.94
1:X:1521:A:N6	1:X:1560:A:N3	2.17	0.93
1:X:1247:G:O2'	1:X:1275:A:N6	2.02	0.92
5:C:17:ILE:HD11	5:C:124:THR:HG21	1.56	0.88

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
3	A	266/277 (96%)	208 (78%)	35 (13%)	23 (9%)	1 5
4	B	213/220 (97%)	183 (86%)	17 (8%)	13 (6%)	1 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	197/207 (95%)	162 (82%)	18 (9%)	17 (9%)	1	5
6	D	151/179 (84%)	118 (78%)	20 (13%)	13 (9%)	1	5
7	E	155/178 (87%)	109 (70%)	30 (19%)	16 (10%)	0	3
8	G	143/145 (99%)	122 (85%)	12 (8%)	9 (6%)	1	9
9	H	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	51
10	I	129/146 (88%)	91 (70%)	23 (18%)	15 (12%)	0	3
11	J	136/144 (94%)	119 (88%)	11 (8%)	6 (4%)	2	16
12	K	117/122 (96%)	106 (91%)	5 (4%)	6 (5%)	2	14
13	L	106/119 (89%)	82 (77%)	15 (14%)	9 (8%)	1	5
14	M	107/116 (92%)	95 (89%)	9 (8%)	3 (3%)	5	24
15	N	114/118 (97%)	110 (96%)	3 (3%)	1 (1%)	17	49
16	O	99/102 (97%)	86 (87%)	8 (8%)	5 (5%)	2	14
17	P	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
18	Q	86/91 (94%)	75 (87%)	9 (10%)	2 (2%)	6	28
19	R	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	10
20	S	165/217 (76%)	130 (79%)	25 (15%)	10 (6%)	1	10
21	T	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	11	37
22	U	42/62 (68%)	32 (76%)	6 (14%)	4 (10%)	0	4
23	V	63/69 (91%)	52 (82%)	10 (16%)	1 (2%)	9	34
24	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
25	Z	42/58 (72%)	36 (86%)	2 (5%)	4 (10%)	0	4
26	2	42/45 (93%)	36 (86%)	5 (12%)	1 (2%)	6	28
27	3	58/66 (88%)	47 (81%)	7 (12%)	4 (7%)	1	8
28	4	35/37 (95%)	30 (86%)	3 (9%)	2 (6%)	1	12
All	All	2922/3215 (91%)	2440 (84%)	310 (11%)	172 (6%)	1	11

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	VAL
3	A	154	ILE
3	A	192	ILE
4	B	60	LYS
4	B	61	LYS

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	
3	A	102/224 (46%)	84 (82%)	18 (18%)	2	6
4	B	148/177 (84%)	115 (78%)	33 (22%)	1	2
5	C	107/169 (63%)	84 (78%)	23 (22%)	1	3
6	D	13/158 (8%)	11 (85%)	2 (15%)	2	11
7	E	53/155 (34%)	47 (89%)	6 (11%)	6	21
8	G	105/123 (85%)	87 (83%)	18 (17%)	2	8
9	H	77/100 (77%)	66 (86%)	11 (14%)	3	13
10	I	54/112 (48%)	40 (74%)	14 (26%)	0	2
11	J	91/119 (76%)	75 (82%)	16 (18%)	2	6
12	K	88/102 (86%)	73 (83%)	15 (17%)	2	8
13	L	35/95 (37%)	33 (94%)	2 (6%)	20	50
14	M	78/102 (76%)	58 (74%)	20 (26%)	0	2
15	N	93/98 (95%)	80 (86%)	13 (14%)	3	13
16	O	72/86 (84%)	64 (89%)	8 (11%)	6	22
17	P	91/94 (97%)	78 (86%)	13 (14%)	3	13
18	Q	44/82 (54%)	35 (80%)	9 (20%)	1	3
19	R	64/90 (71%)	45 (70%)	19 (30%)	0	1
20	S	75/190 (40%)	56 (75%)	19 (25%)	0	2
21	T	47/75 (63%)	42 (89%)	5 (11%)	6	24
22	U	10/52 (19%)	8 (80%)	2 (20%)	1	3
23	V	30/62 (48%)	22 (73%)	8 (27%)	0	1
24	W	51/53 (96%)	41 (80%)	10 (20%)	1	4
25	Z	35/51 (69%)	30 (86%)	5 (14%)	3	13
26	2	38/40 (95%)	29 (76%)	9 (24%)	1	2
27	3	35/57 (61%)	25 (71%)	10 (29%)	0	1
28	4	27/35 (77%)	26 (96%)	1 (4%)	34	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1663/2701 (62%)	1354 (81%)	309 (19%)	1 5

5 of 309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	120	LEU
14	M	73	GLU
25	Z	11	THR
12	K	8	ARG
13	L	21	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
24	W	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	33 (1%)
2	Y	113/114 (99%)	14 (12%)	0
All	All	2804/3037 (92%)	641 (22%)	33 (1%)

5 of 641 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	15	G
1	X	34	U
1	X	36	G
1	X	39	C

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1311	A
1	X	1510	U
1	X	2778	G
1	X	1432	A
1	X	1466	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 470 ligands modelled in this entry, 442 are monoatomic - leaving 28 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$
36	EOH	X	3438	-	2,2,2	0.61	0	1,1,1	0.54	0
35	SPD	X	3431	-	9,9,9	0.16	0	8,8,8	0.18	0
35	SPD	X	3434	-	9,9,9	0.17	0	8,8,8	0.20	0
34	EPE	X	3423	-	15,15,15	1.28	1 (6%)	18,20,20	0.55	0
30	MPD	X	3009	-	7,7,7	0.51	0	9,10,10	0.18	0
29	ZLD	X	3001	-	26,26,26	1.09	1 (3%)	36,36,36	1.52	7 (19%)
30	MPD	X	3007	-	7,7,7	0.65	0	9,10,10	0.41	0
30	MPD	X	3008	-	7,7,7	0.35	0	9,10,10	0.14	0
36	EOH	X	3435	-	2,2,2	0.64	0	1,1,1	0.37	0
35	SPD	X	3429	-	9,9,9	0.20	0	8,8,8	0.15	0
34	EPE	X	3426	-	15,15,15	3.01	1 (6%)	18,20,20	0.70	0
35	SPD	X	3433	-	9,9,9	0.17	0	8,8,8	0.21	0
30	MPD	X	3006	-	7,7,7	0.53	0	9,10,10	0.24	0
34	EPE	X	3425	-	15,15,15	1.06	1 (6%)	18,20,20	0.51	0
35	SPD	X	3428	-	9,9,9	0.17	0	8,8,8	0.15	0
35	SPD	X	3427	-	9,9,9	0.20	0	8,8,8	0.34	0
30	MPD	X	3002	-	7,7,7	0.35	0	9,10,10	0.24	0
35	SPD	X	3430	-	9,9,9	0.13	0	8,8,8	0.19	0
36	EOH	X	3437	-	2,2,2	0.52	0	1,1,1	0.72	0
36	EOH	X	3436	-	2,2,2	0.53	0	1,1,1	0.67	0
30	MPD	X	3005	-	7,7,7	0.42	0	9,10,10	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	SPD	X	3432	-	9,9,9	0.21	0	8,8,8	0.22	0
36	EOH	Y	209	-	2,2,2	0.53	0	1,1,1	0.68	0
34	EPE	X	3424	-	15,15,15	1.46	1 (6%)	18,20,20	0.65	1 (5%)
35	SPD	J	201	-	9,9,9	0.15	0	8,8,8	0.18	0
30	MPD	X	3003	-	7,7,7	0.61	0	9,10,10	0.29	0
30	MPD	X	3004	-	7,7,7	0.43	0	9,10,10	0.20	0
30	MPD	X	3010	-	7,7,7	0.45	0	9,10,10	0.25	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
35	SPD	X	3431	-	-	0/7/7/7	-
35	SPD	X	3434	-	-	1/7/7/7	-
34	EPE	X	3423	-	-	5/9/19/19	0/1/1/1
30	MPD	X	3009	-	-	4/5/5/5	-
29	ZLD	X	3001	-	-	5/13/33/33	0/3/3/3
30	MPD	X	3007	-	-	1/5/5/5	-
30	MPD	X	3008	-	-	2/5/5/5	-
35	SPD	J	201	-	-	1/7/7/7	-
34	EPE	X	3426	-	-	2/9/19/19	0/1/1/1
35	SPD	X	3433	-	-	2/7/7/7	-
30	MPD	X	3006	-	-	2/5/5/5	-
34	EPE	X	3425	-	-	3/9/19/19	0/1/1/1
35	SPD	X	3428	-	-	3/7/7/7	-
35	SPD	X	3427	-	-	1/7/7/7	-
30	MPD	X	3002	-	-	1/5/5/5	-
35	SPD	X	3430	-	-	0/7/7/7	-
30	MPD	X	3005	-	-	2/5/5/5	-
35	SPD	X	3432	-	-	3/7/7/7	-
34	EPE	X	3424	-	-	7/9/19/19	0/1/1/1
35	SPD	X	3429	-	-	2/7/7/7	-
30	MPD	X	3003	-	-	2/5/5/5	-
30	MPD	X	3004	-	-	1/5/5/5	-
30	MPD	X	3010	-	-	4/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	3426	EPE	C10-S	-11.53	1.61	1.77
34	X	3424	EPE	C10-S	-5.54	1.69	1.77
34	X	3423	EPE	C10-S	-4.81	1.70	1.77
29	X	3001	ZLD	C7-N4	4.48	1.41	1.36
34	X	3425	EPE	C10-S	-3.99	1.71	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	3001	ZLD	C8-O10-C7	4.07	113.36	110.15
29	X	3001	ZLD	C6-C8-C9	-3.47	109.24	113.08
29	X	3001	ZLD	C8-C9-N11	3.42	119.60	112.16
29	X	3001	ZLD	O15-C7-N4	-2.81	126.68	128.91
29	X	3001	ZLD	O10-C7-N4	-2.69	107.98	109.83

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

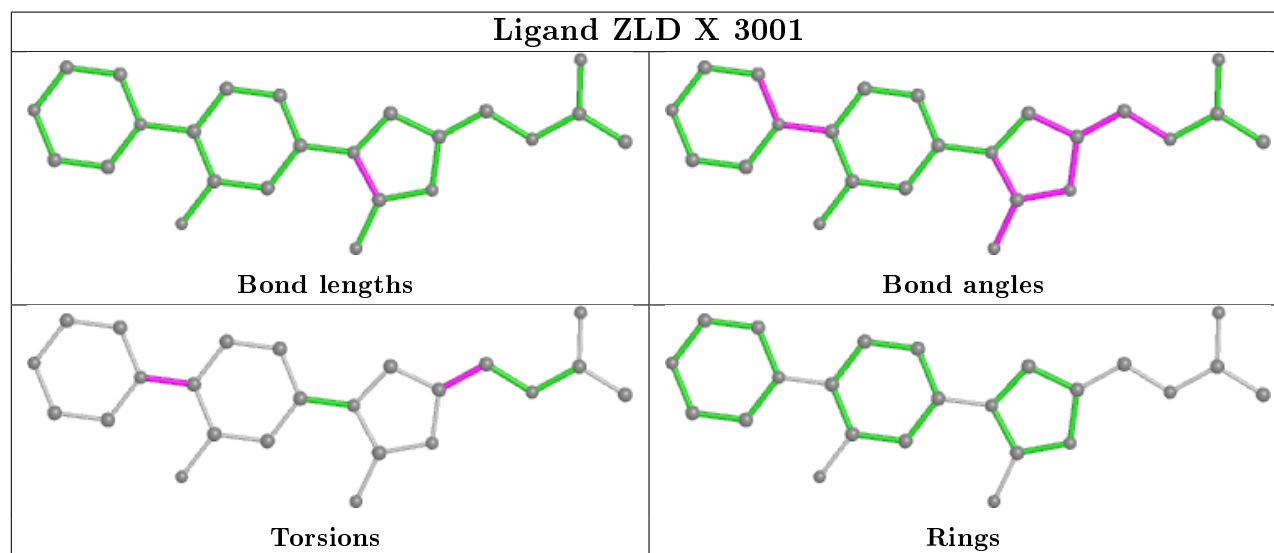
Mol	Chain	Res	Type	Atoms
29	X	3001	ZLD	O10-C8-C9-N11
29	X	3001	ZLD	C16-C17-N19-C20
35	X	3427	SPD	C4-C5-N6-C7
34	X	3426	EPE	C10-C9-N1-C2
34	X	3426	EPE	S-C10-C9-N1

There are no ring outliers.

13 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	X	3434	SPD	1	0
34	X	3423	EPE	1	0
30	X	3009	MPD	1	0
29	X	3001	ZLD	5	0
34	X	3426	EPE	14	0
35	X	3433	SPD	2	0
34	X	3425	EPE	4	0
35	X	3428	SPD	3	0
35	X	3430	SPD	3	0
30	X	3005	MPD	3	0
35	X	3432	SPD	2	0
34	X	3424	EPE	1	0
30	X	3010	MPD	1	0

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 [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	X	2711/2923 (92%)	-0.50	9 (0%) 94 93	39, 91, 192, 340	0
2	Y	114/114 (100%)	-0.79	0 100 100	61, 106, 172, 208	0
3	A	268/277 (96%)	0.74	57 (21%) 0 1	64, 121, 176, 224	0
4	B	215/220 (97%)	-0.04	5 (2%) 60 59	50, 66, 114, 194	0
5	C	199/207 (96%)	0.02	7 (3%) 44 43	56, 82, 132, 163	0
6	D	155/179 (86%)	-0.26	6 (3%) 39 38	96, 156, 222, 311	0
7	E	157/178 (88%)	-0.36	8 (5%) 28 28	88, 136, 197, 264	0
8	G	145/145 (100%)	0.01	3 (2%) 63 62	47, 63, 98, 129	0
9	H	122/122 (100%)	0.95	32 (26%) 0 0	66, 89, 129, 146	0
10	I	131/146 (89%)	0.24	11 (8%) 11 13	34, 94, 152, 175	0
11	J	138/144 (95%)	1.10	39 (28%) 0 0	54, 83, 183, 312	0
12	K	119/122 (97%)	-0.03	5 (4%) 36 35	37, 74, 127, 175	0
13	L	108/119 (90%)	-0.31	8 (7%) 14 16	68, 109, 149, 173	0
14	M	109/116 (93%)	0.10	6 (5%) 25 25	54, 86, 155, 201	0
15	N	116/118 (98%)	-0.14	1 (0%) 84 83	35, 60, 98, 125	0
16	O	101/102 (99%)	0.10	9 (8%) 9 11	38, 73, 127, 149	0
17	P	112/117 (95%)	0.45	6 (5%) 25 26	43, 63, 114, 179	0
18	Q	88/91 (96%)	0.11	7 (7%) 12 13	84, 110, 167, 193	0
19	R	100/105 (95%)	-0.31	4 (4%) 38 37	60, 110, 228, 298	0
20	S	167/217 (76%)	0.22	24 (14%) 2 3	55, 104, 213, 309	0
21	T	75/94 (79%)	1.29	25 (33%) 0 0	66, 78, 132, 178	0
22	U	44/62 (70%)	2.31	20 (45%) 0 0	89, 163, 227, 254	0
23	V	65/69 (94%)	-0.12	4 (6%) 20 21	75, 114, 166, 228	0
24	W	57/59 (96%)	-0.29	0 100 100	37, 62, 114, 159	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	44/58 (75%)	0.45	5 (11%) 5 6	34, 74, 140, 227	0
26	2	44/45 (97%)	0.84	9 (20%) 1 1	57, 83, 118, 145	0
27	3	60/66 (90%)	0.14	5 (8%) 11 13	41, 77, 118, 148	0
28	4	37/37 (100%)	0.86	8 (21%) 0 1	96, 104, 144, 162	0
All	All	5801/6252 (92%)	-0.13	323 (5%) 24 25	34, 92, 181, 340	0

The worst 5 of 323 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	42	GLY	12.5
3	A	82	GLN	12.3
22	U	41	ASP	10.0
20	S	164	ASP	8.6
22	U	39	LEU	8.6

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 monosaccharides 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(Å ²)	Q<0.9
31	MG	X	3366	1/1	0.11	0.38	69,69,69,69	0
32	MN	X	3265	1/1	0.15	0.89	158,158,158,158	0
31	MG	X	3248	1/1	0.33	0.25	65,65,65,65	0
31	MG	X	3275	1/1	0.33	0.22	73,73,73,73	0
31	MG	O	202	1/1	0.34	0.73	67,67,67,67	0
31	MG	X	3386	1/1	0.40	1.37	112,112,112,112	0
31	MG	X	3351	1/1	0.41	0.56	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3029	1/1	0.41	0.41	65,65,65,65	1
31	MG	X	3245	1/1	0.46	0.39	93,93,93,93	0
31	MG	X	3420	1/1	0.47	0.64	79,79,79,79	0
31	MG	X	3284	1/1	0.48	0.77	94,94,94,94	0
31	MG	G	201	1/1	0.50	0.99	68,68,68,68	0
31	MG	X	3399	1/1	0.53	1.36	101,101,101,101	0
31	MG	X	3292	1/1	0.54	0.17	70,70,70,70	0
31	MG	X	3208	1/1	0.56	0.43	78,78,78,78	0
32	MN	X	3114	1/1	0.56	0.85	150,150,150,150	0
31	MG	X	3380	1/1	0.57	0.43	83,83,83,83	0
32	MN	X	3422	1/1	0.57	1.08	201,201,201,201	0
31	MG	X	3401	1/1	0.58	0.54	63,63,63,63	0
31	MG	X	3359	1/1	0.58	1.18	87,87,87,87	0
31	MG	X	3370	1/1	0.58	0.34	103,103,103,103	0
31	MG	X	3343	1/1	0.60	0.66	108,108,108,108	0
35	SPD	X	3429	10/10	0.61	0.65	106,106,106,106	0
32	MN	X	3071	1/1	0.61	0.15	134,134,134,134	0
31	MG	X	3047	1/1	0.62	0.35	71,71,71,71	0
31	MG	X	3389	1/1	0.62	0.29	66,66,66,66	0
31	MG	X	3242	1/1	0.63	0.72	90,90,90,90	0
31	MG	X	3327	1/1	0.63	0.47	103,103,103,103	0
31	MG	X	3418	1/1	0.64	0.76	81,81,81,81	0
31	MG	X	3361	1/1	0.65	1.08	76,76,76,76	0
32	MN	M	201	1/1	0.65	0.16	122,122,122,122	0
30	MPD	X	3006	8/8	0.65	0.42	133,133,133,133	0
36	EOH	Y	209	3/3	0.66	0.27	93,93,93,93	0
31	MG	K	201	1/1	0.66	0.34	72,72,72,72	0
32	MN	X	3113	1/1	0.66	0.24	123,123,123,123	0
31	MG	X	3252	1/1	0.66	0.30	50,50,50,50	0
31	MG	Y	207	1/1	0.66	0.54	101,101,101,101	0
31	MG	X	3311	1/1	0.67	0.13	86,86,86,86	0
31	MG	X	3280	1/1	0.69	1.21	87,87,87,87	0
31	MG	X	3297	1/1	0.69	0.47	85,85,85,85	0
31	MG	X	3344	1/1	0.69	0.67	92,92,92,92	0
32	MN	X	3115	1/1	0.69	0.29	135,135,135,135	0
32	MN	X	3098	1/1	0.69	0.26	131,131,131,131	0
31	MG	X	3014	1/1	0.70	1.10	85,85,85,85	0
31	MG	X	3419	1/1	0.70	1.75	100,100,100,100	0
31	MG	X	3411	1/1	0.71	0.42	83,83,83,83	0
32	MN	X	3085	1/1	0.71	0.60	128,128,128,128	0
31	MG	X	3340	1/1	0.72	0.43	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	EPE	X	3425	15/15	0.72	0.33	152,152,152,152	0
31	MG	X	3302	1/1	0.72	0.21	51,51,51,51	0
32	MN	X	3235	1/1	0.72	0.16	134,134,134,134	0
32	MN	X	3105	1/1	0.73	0.37	87,87,87,87	0
31	MG	X	3056	1/1	0.73	0.80	55,55,55,55	1
35	SPD	J	201	10/10	0.74	0.27	82,82,82,82	0
31	MG	X	3312	1/1	0.74	1.03	57,57,57,57	0
31	MG	X	3012	1/1	0.74	1.29	13,13,13,13	1
32	MN	X	3117	1/1	0.75	0.52	166,166,166,166	0
32	MN	Y	203	1/1	0.75	0.18	99,99,99,99	0
31	MG	X	3254	1/1	0.75	0.86	47,47,47,47	1
31	MG	X	3357	1/1	0.75	0.65	56,56,56,56	0
31	MG	X	3363	1/1	0.75	0.46	81,81,81,81	0
31	MG	X	3045	1/1	0.75	0.34	87,87,87,87	0
32	MN	X	3096	1/1	0.75	0.10	153,153,153,153	0
35	SPD	X	3431	10/10	0.75	0.39	98,98,98,98	0
31	MG	X	3318	1/1	0.75	0.36	65,65,65,65	0
31	MG	X	3030	1/1	0.75	0.23	38,38,38,38	1
31	MG	X	3348	1/1	0.75	0.41	85,85,85,85	0
32	MN	X	3226	1/1	0.76	0.23	112,112,112,112	0
32	MN	X	3217	1/1	0.76	0.54	113,113,113,113	0
31	MG	X	3034	1/1	0.76	0.38	75,75,75,75	0
32	MN	X	3262	1/1	0.77	0.10	191,191,191,191	0
31	MG	X	3296	1/1	0.77	0.30	75,75,75,75	0
31	MG	X	3400	1/1	0.77	0.38	50,50,50,50	0
31	MG	X	3369	1/1	0.77	0.80	76,76,76,76	0
32	MN	X	3264	1/1	0.77	0.29	128,128,128,128	0
32	MN	X	3068	1/1	0.77	0.15	130,130,130,130	0
34	EPE	X	3424	15/15	0.77	0.39	194,194,194,194	0
31	MG	X	3243	1/1	0.77	0.37	82,82,82,82	0
31	MG	X	3032	1/1	0.78	0.48	64,64,64,64	0
31	MG	X	3285	1/1	0.78	0.30	73,73,73,73	0
31	MG	X	3382	1/1	0.78	0.72	68,68,68,68	0
32	MN	X	3266	1/1	0.78	0.14	104,104,104,104	0
31	MG	Y	208	1/1	0.79	0.52	81,81,81,81	0
31	MG	X	3394	1/1	0.79	0.30	80,80,80,80	0
30	MPD	X	3008	8/8	0.79	0.51	144,144,144,144	0
32	MN	X	3222	1/1	0.79	1.24	171,171,171,171	0
31	MG	X	3397	1/1	0.79	0.41	95,95,95,95	0
31	MG	X	3019	1/1	0.79	0.64	69,69,69,69	0
32	MN	X	3221	1/1	0.79	0.35	130,130,130,130	0
32	MN	X	3214	1/1	0.79	0.28	163,163,163,163	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3291	1/1	0.80	0.97	62,62,62,62	0
31	MG	X	3038	1/1	0.80	0.22	75,75,75,75	0
32	MN	X	3072	1/1	0.80	0.20	91,91,91,91	0
31	MG	X	3286	1/1	0.80	0.57	82,82,82,82	0
31	MG	X	3393	1/1	0.80	0.12	67,67,67,67	0
31	MG	X	3372	1/1	0.81	0.18	49,49,49,49	0
31	MG	X	3309	1/1	0.81	0.10	53,53,53,53	0
32	MN	X	3067	1/1	0.82	0.35	166,166,166,166	0
31	MG	X	3026	1/1	0.82	0.24	64,64,64,64	0
32	MN	X	3112	1/1	0.82	0.12	155,155,155,155	0
32	MN	X	3119	1/1	0.82	0.71	155,155,155,155	0
32	MN	X	3240	1/1	0.82	0.36	123,123,123,123	0
31	MG	X	3316	1/1	0.82	0.86	88,88,88,88	0
31	MG	Y	206	1/1	0.82	0.42	65,65,65,65	0
32	MN	X	3141	1/1	0.82	0.48	100,100,100,100	0
31	MG	X	3244	1/1	0.82	0.44	78,78,78,78	0
31	MG	X	3063	1/1	0.83	0.32	49,49,49,49	0
31	MG	X	3241	1/1	0.83	0.67	66,66,66,66	0
36	EOH	X	3438	3/3	0.83	0.31	63,63,63,63	0
31	MG	X	3341	1/1	0.83	0.47	43,43,43,43	0
36	EOH	X	3436	3/3	0.83	0.36	92,92,92,92	0
31	MG	X	3306	1/1	0.83	0.31	77,77,77,77	0
31	MG	X	3391	1/1	0.83	0.35	73,73,73,73	0
32	MN	X	3121	1/1	0.83	0.38	126,126,126,126	0
31	MG	X	3378	1/1	0.83	0.23	83,83,83,83	0
32	MN	X	3267	1/1	0.83	0.43	140,140,140,140	0
31	MG	G	202	1/1	0.84	0.28	77,77,77,77	0
32	MN	X	3070	1/1	0.84	0.18	148,148,148,148	0
31	MG	X	3033	1/1	0.84	0.56	12,12,12,12	1
32	MN	X	3083	1/1	0.84	0.31	150,150,150,150	0
31	MG	X	3028	1/1	0.84	0.24	58,58,58,58	0
35	SPD	X	3434	10/10	0.84	0.26	98,98,98,98	0
31	MG	X	3273	1/1	0.84	0.25	79,79,79,79	0
31	MG	X	3211	1/1	0.84	0.23	32,32,32,32	0
32	MN	X	3259	1/1	0.84	0.12	140,140,140,140	0
33	NA	X	3367	1/1	0.84	0.36	64,64,64,64	0
30	MPD	X	3002	8/8	0.84	0.38	132,132,132,132	0
30	MPD	X	3009	8/8	0.84	0.42	107,107,107,107	0
31	MG	X	3255	1/1	0.84	0.62	69,69,69,69	0
31	MG	X	3304	1/1	0.84	0.18	70,70,70,70	0
31	MG	X	3011	1/1	0.84	0.37	85,85,85,85	0
35	SPD	X	3427	10/10	0.85	0.33	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3037	1/1	0.85	0.23	69,69,69,69	0
32	MN	X	3202	1/1	0.85	0.28	117,117,117,117	0
31	MG	X	3440	1/1	0.85	0.21	37,37,37,37	0
32	MN	X	3161	1/1	0.85	0.58	98,98,98,98	0
31	MG	X	3364	1/1	0.85	0.33	80,80,80,80	0
31	MG	X	3051	1/1	0.85	0.51	14,14,14,14	1
31	MG	B	301	1/1	0.85	0.28	65,65,65,65	0
31	MG	X	3360	1/1	0.85	0.60	123,123,123,123	0
31	MG	X	3444	1/1	0.85	0.24	44,44,44,44	0
32	MN	X	3151	1/1	0.85	0.62	106,106,106,106	0
32	MN	X	3090	1/1	0.85	0.14	123,123,123,123	0
31	MG	X	3368	1/1	0.85	0.37	70,70,70,70	0
31	MG	X	3407	1/1	0.85	0.53	89,89,89,89	0
31	MG	X	3381	1/1	0.86	0.31	82,82,82,82	0
31	MG	X	3206	1/1	0.86	0.52	74,74,74,74	0
34	EPE	X	3423	15/15	0.86	0.32	152,152,152,152	0
31	MG	I	201	1/1	0.86	0.63	47,47,47,47	0
31	MG	X	3059	1/1	0.86	0.26	35,35,35,35	0
31	MG	X	3062	1/1	0.86	0.32	56,56,56,56	0
32	MN	X	3191	1/1	0.86	0.18	107,107,107,107	0
31	MG	X	3387	1/1	0.86	0.29	60,60,60,60	0
31	MG	A	302	1/1	0.86	0.33	58,58,58,58	0
31	MG	X	3018	1/1	0.86	0.87	76,76,76,76	0
31	MG	X	3405	1/1	0.86	0.98	79,79,79,79	0
31	MG	X	3347	1/1	0.86	0.20	77,77,77,77	0
32	MN	X	3088	1/1	0.86	0.15	110,110,110,110	0
31	MG	X	3375	1/1	0.87	0.18	69,69,69,69	0
35	SPD	X	3432	10/10	0.87	0.25	77,77,77,77	0
32	MN	X	3260	1/1	0.87	0.26	126,126,126,126	0
31	MG	X	3408	1/1	0.87	0.24	48,48,48,48	0
32	MN	X	3271	1/1	0.87	0.20	117,117,117,117	0
32	MN	X	3140	1/1	0.87	0.33	111,111,111,111	0
32	MN	X	3086	1/1	0.87	0.21	82,82,82,82	0
31	MG	X	3396	1/1	0.87	0.81	85,85,85,85	0
31	MG	X	3256	1/1	0.87	1.16	82,82,82,82	0
32	MN	X	3148	1/1	0.87	0.39	102,102,102,102	0
30	MPD	X	3004	8/8	0.87	0.23	109,109,109,109	0
32	MN	X	3205	1/1	0.87	0.14	113,113,113,113	0
32	MN	X	3177	1/1	0.88	0.14	56,56,56,56	0
31	MG	X	3290	1/1	0.88	0.40	46,46,46,46	0
31	MG	X	3031	1/1	0.88	0.28	70,70,70,70	0
31	MG	X	3050	1/1	0.88	0.80	2,2,2,2	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3227	1/1	0.88	0.23	107,107,107,107	0
32	MN	X	3270	1/1	0.88	0.11	109,109,109,109	0
31	MG	X	3272	1/1	0.88	1.14	69,69,69,69	0
31	MG	X	3371	1/1	0.88	1.00	91,91,91,91	0
31	MG	X	3276	1/1	0.88	0.55	85,85,85,85	0
32	MN	X	3097	1/1	0.88	0.51	118,118,118,118	0
31	MG	X	3039	1/1	0.88	0.19	53,53,53,53	0
31	MG	X	3281	1/1	0.89	0.40	72,72,72,72	0
32	MN	X	3092	1/1	0.89	0.29	104,104,104,104	0
30	MPD	X	3005	8/8	0.89	0.14	64,64,64,64	0
32	MN	X	3172	1/1	0.89	0.57	82,82,82,82	0
31	MG	X	3321	1/1	0.89	0.53	80,80,80,80	0
31	MG	X	3362	1/1	0.89	0.23	47,47,47,47	0
30	MPD	X	3007	8/8	0.89	0.19	114,114,114,114	0
31	MG	X	3441	1/1	0.89	0.77	72,72,72,72	0
31	MG	X	3388	1/1	0.89	0.22	65,65,65,65	0
36	EOH	X	3437	3/3	0.89	0.21	92,92,92,92	0
32	MN	X	3144	1/1	0.90	0.49	143,143,143,143	0
31	MG	X	3377	1/1	0.90	0.21	73,73,73,73	0
30	MPD	X	3010	8/8	0.90	0.31	122,122,122,122	0
32	MN	X	3416	1/1	0.90	0.13	111,111,111,111	0
32	MN	X	3073	1/1	0.90	0.09	105,105,105,105	0
31	MG	X	3015	1/1	0.90	0.41	36,36,36,36	1
31	MG	A	301	1/1	0.90	0.16	81,81,81,81	0
31	MG	X	3053	1/1	0.90	0.70	42,42,42,42	1
32	MN	X	3109	1/1	0.90	0.39	145,145,145,145	0
31	MG	X	3044	1/1	0.90	0.39	20,20,20,20	1
32	MN	X	3232	1/1	0.90	0.25	105,105,105,105	0
31	MG	X	3409	1/1	0.90	1.04	67,67,67,67	0
36	EOH	X	3435	3/3	0.90	0.23	36,36,36,36	0
31	MG	X	3278	1/1	0.90	0.24	67,67,67,67	0
31	MG	X	3025	1/1	0.90	0.46	10,10,10,10	1
32	MN	X	3197	1/1	0.90	0.20	102,102,102,102	0
31	MG	X	3299	1/1	0.90	0.07	38,38,38,38	0
31	MG	X	3410	1/1	0.90	0.37	78,78,78,78	0
31	MG	X	3027	1/1	0.91	0.60	66,66,66,66	0
31	MG	X	3016	1/1	0.91	0.43	81,81,81,81	0
35	SPD	X	3428	10/10	0.91	0.22	82,82,82,82	0
31	MG	X	3022	1/1	0.91	0.30	83,83,83,83	0
31	MG	Y	204	1/1	0.91	0.46	63,63,63,63	0
35	SPD	X	3430	10/10	0.91	0.28	80,80,80,80	0
32	MN	X	3116	1/1	0.91	0.17	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3349	1/1	0.91	0.12	45,45,45,45	0
32	MN	X	3167	1/1	0.91	0.42	91,91,91,91	0
32	MN	X	3123	1/1	0.91	0.25	97,97,97,97	0
31	MG	X	3412	1/1	0.91	1.01	82,82,82,82	0
31	MG	X	3287	1/1	0.91	0.93	67,67,67,67	0
31	MG	X	3209	1/1	0.91	0.29	34,34,34,34	0
32	MN	X	3219	1/1	0.91	0.22	139,139,139,139	0
31	MG	X	3346	1/1	0.91	0.92	81,81,81,81	0
32	MN	X	3094	1/1	0.91	0.18	139,139,139,139	0
31	MG	X	3334	1/1	0.91	0.21	57,57,57,57	0
32	MN	X	3373	1/1	0.91	0.29	94,94,94,94	0
31	MG	X	3048	1/1	0.91	0.41	31,31,31,31	1
29	ZLD	X	3001	24/24	0.92	0.40	87,88,90,91	0
31	MG	Z	102	1/1	0.92	0.27	68,68,68,68	0
31	MG	X	3213	1/1	0.92	0.38	22,22,22,22	0
32	MN	X	3185	1/1	0.92	0.84	132,132,132,132	0
32	MN	X	3091	1/1	0.92	0.41	100,100,100,100	0
31	MG	X	3021	1/1	0.92	0.31	76,76,76,76	0
31	MG	X	3046	1/1	0.92	0.23	43,43,43,43	1
31	MG	X	3328	1/1	0.92	0.51	59,59,59,59	0
31	MG	O	201	1/1	0.92	0.34	41,41,41,41	0
31	MG	X	3392	1/1	0.92	0.16	91,91,91,91	0
31	MG	X	3055	1/1	0.92	0.55	53,53,53,53	0
31	MG	X	3061	1/1	0.92	0.28	41,41,41,41	0
32	MN	X	3162	1/1	0.92	0.28	74,74,74,74	0
31	MG	X	3246	1/1	0.92	0.37	69,69,69,69	0
31	MG	X	3350	1/1	0.92	0.12	28,28,28,28	0
31	MG	X	3414	1/1	0.92	0.35	59,59,59,59	0
32	MN	X	3374	1/1	0.92	0.21	153,153,153,153	0
31	MG	C	301	1/1	0.92	0.25	46,46,46,46	0
31	MG	X	3024	1/1	0.92	0.32	67,67,67,67	0
32	MN	X	3138	1/1	0.92	0.25	120,120,120,120	0
31	MG	X	3017	1/1	0.92	0.31	75,75,75,75	0
32	MN	X	3192	1/1	0.92	0.20	85,85,85,85	0
31	MG	X	3413	1/1	0.92	0.39	57,57,57,57	0
31	MG	X	3354	1/1	0.92	0.33	64,64,64,64	0
31	MG	Y	205	1/1	0.92	0.16	77,77,77,77	0
31	MG	X	3250	1/1	0.92	0.57	70,70,70,70	0
31	MG	X	3406	1/1	0.93	0.21	55,55,55,55	0
32	MN	X	3095	1/1	0.93	0.25	133,133,133,133	0
32	MN	X	3076	1/1	0.93	0.47	148,148,148,148	0
31	MG	X	3300	1/1	0.93	0.77	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3305	1/1	0.93	0.48	68,68,68,68	0
32	MN	X	3238	1/1	0.93	0.17	174,174,174,174	0
32	MN	X	3188	1/1	0.93	0.38	100,100,100,100	0
31	MG	X	3058	1/1	0.93	0.69	45,45,45,45	0
32	MN	X	3417	1/1	0.93	0.23	156,156,156,156	0
32	MN	X	3168	1/1	0.93	0.42	85,85,85,85	0
31	MG	X	3383	1/1	0.93	0.66	58,58,58,58	0
32	MN	X	3218	1/1	0.93	0.53	151,151,151,151	0
32	MN	X	3108	1/1	0.93	0.50	182,182,182,182	0
31	MG	X	3283	1/1	0.93	0.13	62,62,62,62	0
32	MN	X	3216	1/1	0.93	0.13	112,112,112,112	0
31	MG	X	3023	1/1	0.93	0.23	56,56,56,56	0
31	MG	X	3339	1/1	0.93	0.23	59,59,59,59	0
31	MG	X	3323	1/1	0.93	0.28	76,76,76,76	0
32	MN	X	3229	1/1	0.93	0.43	135,135,135,135	0
32	MN	X	3064	1/1	0.93	0.25	145,145,145,145	0
35	SPD	X	3433	10/10	0.94	0.22	93,93,93,93	0
31	MG	X	3298	1/1	0.94	0.30	72,72,72,72	0
31	MG	X	3057	1/1	0.94	0.45	41,41,41,41	0
34	EPE	X	3426	15/15	0.94	0.27	101,101,101,101	3
31	MG	X	3303	1/1	0.94	0.44	63,63,63,63	0
31	MG	X	3398	1/1	0.94	1.58	107,107,107,107	0
31	MG	X	3035	1/1	0.94	0.27	39,39,39,39	0
32	MN	X	3089	1/1	0.94	0.13	92,92,92,92	0
32	MN	X	3129	1/1	0.94	0.60	106,106,106,106	0
31	MG	X	3253	1/1	0.94	0.41	45,45,45,45	0
31	MG	X	3293	1/1	0.94	0.15	91,91,91,91	0
31	MG	X	3277	1/1	0.94	0.07	55,55,55,55	0
31	MG	X	3421	1/1	0.94	0.26	60,60,60,60	0
32	MN	X	3268	1/1	0.94	0.19	94,94,94,94	0
31	MG	X	3385	1/1	0.94	0.18	63,63,63,63	0
31	MG	X	3384	1/1	0.94	0.53	81,81,81,81	0
32	MN	X	3182	1/1	0.94	0.37	88,88,88,88	0
31	MG	X	3247	1/1	0.94	0.20	49,49,49,49	0
31	MG	X	3274	1/1	0.94	0.27	79,79,79,79	0
32	MN	X	3080	1/1	0.94	0.40	130,130,130,130	0
31	MG	X	3402	1/1	0.94	0.17	84,84,84,84	0
31	MG	X	3356	1/1	0.94	0.21	70,70,70,70	0
31	MG	X	3308	1/1	0.94	0.24	39,39,39,39	0
32	MN	X	3157	1/1	0.94	0.42	85,85,85,85	0
32	MN	X	3228	1/1	0.94	0.13	110,110,110,110	0
31	MG	X	3279	1/1	0.94	0.29	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3439	1/1	0.94	0.29	97,97,97,97	0
31	MG	X	3329	1/1	0.94	0.28	60,60,60,60	0
31	MG	X	3324	1/1	0.95	0.66	88,88,88,88	0
32	MN	X	3154	1/1	0.95	0.39	46,46,46,46	0
31	MG	X	3352	1/1	0.95	0.16	50,50,50,50	0
31	MG	X	3049	1/1	0.95	0.54	14,14,14,14	1
31	MG	X	3395	1/1	0.95	0.90	93,93,93,93	0
32	MN	X	3106	1/1	0.95	0.24	96,96,96,96	0
32	MN	X	3236	1/1	0.95	0.17	104,104,104,104	0
32	MN	X	3169	1/1	0.95	0.51	76,76,76,76	0
31	MG	X	3307	1/1	0.95	0.50	67,67,67,67	0
31	MG	X	3251	1/1	0.95	0.39	47,47,47,47	0
31	MG	X	3310	1/1	0.95	0.23	66,66,66,66	0
32	MN	X	3100	1/1	0.95	0.76	129,129,129,129	0
32	MN	X	3184	1/1	0.95	0.34	86,86,86,86	0
32	MN	X	3093	1/1	0.95	0.14	122,122,122,122	0
32	MN	X	3164	1/1	0.95	0.31	92,92,92,92	0
32	MN	X	3146	1/1	0.95	0.34	100,100,100,100	0
31	MG	X	3322	1/1	0.95	0.51	50,50,50,50	0
32	MN	X	3443	1/1	0.95	0.35	91,91,91,91	0
32	MN	X	3111	1/1	0.95	0.27	125,125,125,125	0
32	MN	X	3261	1/1	0.95	0.35	132,132,132,132	0
31	MG	X	3036	1/1	0.95	0.65	85,85,85,85	0
32	MN	X	3215	1/1	0.95	0.37	154,154,154,154	0
31	MG	N	201	1/1	0.95	0.27	25,25,25,25	0
32	MN	X	3230	1/1	0.95	0.30	100,100,100,100	0
32	MN	X	3075	1/1	0.95	0.31	116,116,116,116	0
31	MG	X	3289	1/1	0.95	0.31	27,27,27,27	0
31	MG	X	3317	1/1	0.95	0.24	39,39,39,39	0
32	MN	X	3110	1/1	0.95	0.21	103,103,103,103	0
31	MG	X	3376	1/1	0.95	0.27	93,93,93,93	0
32	MN	X	3258	1/1	0.95	0.20	98,98,98,98	0
30	MPD	X	3003	8/8	0.95	0.20	92,92,92,92	0
32	MN	X	3156	1/1	0.95	0.26	83,83,83,83	0
32	MN	X	3204	1/1	0.95	0.15	126,126,126,126	0
31	MG	X	3020	1/1	0.95	0.23	53,53,53,53	0
31	MG	X	3282	1/1	0.96	0.29	68,68,68,68	0
32	MN	X	3176	1/1	0.96	0.31	80,80,80,80	0
32	MN	X	3134	1/1	0.96	0.41	57,57,57,57	0
32	MN	X	3181	1/1	0.96	0.27	73,73,73,73	0
32	MN	X	3170	1/1	0.96	0.28	95,95,95,95	0
31	MG	X	3315	1/1	0.96	0.87	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3125	1/1	0.96	0.80	122,122,122,122	0
32	MN	X	3263	1/1	0.96	0.18	80,80,80,80	0
31	MG	X	3330	1/1	0.96	0.16	55,55,55,55	0
32	MN	X	3077	1/1	0.96	0.21	61,61,61,61	0
32	MN	X	3224	1/1	0.96	0.35	99,99,99,99	0
31	MG	X	3212	1/1	0.96	0.71	40,40,40,40	0
32	MN	X	3203	1/1	0.96	0.33	69,69,69,69	0
32	MN	X	3194	1/1	0.96	0.36	93,93,93,93	0
31	MG	X	3358	1/1	0.96	0.35	46,46,46,46	0
31	MG	X	3390	1/1	0.96	0.20	47,47,47,47	0
31	MG	X	3257	1/1	0.96	0.26	71,71,71,71	0
32	MN	X	3163	1/1	0.96	0.37	61,61,61,61	0
31	MG	X	3342	1/1	0.96	0.17	67,67,67,67	0
32	MN	Y	202	1/1	0.96	0.18	92,92,92,92	0
32	MN	X	3135	1/1	0.96	0.27	76,76,76,76	0
32	MN	X	3442	1/1	0.96	0.32	51,51,51,51	0
32	MN	X	3269	1/1	0.96	0.33	131,131,131,131	0
32	MN	X	3102	1/1	0.96	0.29	96,96,96,96	0
32	MN	X	3193	1/1	0.96	0.17	87,87,87,87	0
31	MG	X	3041	1/1	0.96	0.36	68,68,68,68	0
32	MN	X	3223	1/1	0.96	0.15	127,127,127,127	0
32	MN	X	3225	1/1	0.96	0.86	133,133,133,133	0
32	MN	X	3149	1/1	0.96	0.37	64,64,64,64	0
32	MN	X	3239	1/1	0.96	0.44	60,60,60,60	0
32	MN	X	3066	1/1	0.96	0.26	64,64,64,64	0
32	MN	X	3082	1/1	0.96	0.19	109,109,109,109	0
31	MG	Y	201	1/1	0.96	0.43	24,24,24,24	1
32	MN	X	3155	1/1	0.97	0.35	75,75,75,75	0
32	MN	X	3183	1/1	0.97	0.22	63,63,63,63	0
31	MG	X	3338	1/1	0.97	0.16	43,43,43,43	0
32	MN	X	3187	1/1	0.97	0.33	89,89,89,89	0
32	MN	X	3171	1/1	0.97	0.39	88,88,88,88	0
32	MN	X	3127	1/1	0.97	0.22	108,108,108,108	0
31	MG	X	3294	1/1	0.97	0.36	51,51,51,51	0
32	MN	X	3200	1/1	0.97	0.22	126,126,126,126	0
32	MN	X	3186	1/1	0.97	0.29	69,69,69,69	0
31	MG	X	3335	1/1	0.97	0.67	260,260,260,260	0
31	MG	Z	103	1/1	0.97	0.11	39,39,39,39	0
32	MN	X	3234	1/1	0.97	0.06	91,91,91,91	0
31	MG	X	3210	1/1	0.97	0.32	57,57,57,57	0
31	MG	X	3336	1/1	0.97	0.09	69,69,69,69	0
32	MN	X	3231	1/1	0.97	0.74	135,135,135,135	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3043	1/1	0.97	0.41	64,64,64,64	0
31	MG	X	3337	1/1	0.97	0.31	44,44,44,44	0
32	MN	X	3195	1/1	0.97	0.27	90,90,90,90	0
32	MN	X	3074	1/1	0.97	0.24	98,98,98,98	0
32	MN	X	3122	1/1	0.97	0.19	123,123,123,123	0
32	MN	X	3196	1/1	0.97	0.26	77,77,77,77	0
31	MG	X	3207	1/1	0.97	0.12	56,56,56,56	0
32	MN	X	3178	1/1	0.97	0.39	92,92,92,92	0
32	MN	X	3220	1/1	0.97	0.21	111,111,111,111	0
31	MG	X	3040	1/1	0.97	0.91	58,58,58,58	0
32	MN	X	3153	1/1	0.97	0.32	75,75,75,75	0
31	MG	X	3314	1/1	0.97	0.34	45,45,45,45	0
31	MG	X	3355	1/1	0.97	0.19	71,71,71,71	0
31	MG	X	3042	1/1	0.97	0.69	59,59,59,59	0
32	MN	X	3069	1/1	0.97	0.23	121,121,121,121	0
31	MG	X	3403	1/1	0.97	0.08	52,52,52,52	0
31	MG	W	101	1/1	0.97	0.61	84,84,84,84	0
32	MN	X	3131	1/1	0.97	0.23	66,66,66,66	0
32	MN	X	3190	1/1	0.98	0.47	91,91,91,91	0
32	MN	X	3147	1/1	0.98	0.33	82,82,82,82	0
32	MN	X	3118	1/1	0.98	0.36	123,123,123,123	0
31	MG	X	3013	1/1	0.98	0.75	61,61,61,61	0
32	MN	X	3079	1/1	0.98	0.47	71,71,71,71	0
31	MG	X	3319	1/1	0.98	0.26	26,26,26,26	0
32	MN	X	3189	1/1	0.98	0.28	53,53,53,53	0
31	MG	X	3415	1/1	0.98	0.29	45,45,45,45	0
32	MN	X	3104	1/1	0.98	0.42	88,88,88,88	0
32	MN	X	3099	1/1	0.98	0.14	128,128,128,128	0
32	MN	Z	101	1/1	0.98	0.38	88,88,88,88	0
31	MG	X	3320	1/1	0.98	0.43	43,43,43,43	0
32	MN	X	3136	1/1	0.98	0.21	84,84,84,84	0
31	MG	X	3331	1/1	0.98	0.20	60,60,60,60	0
31	MG	X	3333	1/1	0.98	0.95	71,71,71,71	0
31	MG	X	3353	1/1	0.98	0.16	81,81,81,81	0
32	MN	X	3201	1/1	0.98	0.19	49,49,49,49	0
32	MN	X	3120	1/1	0.98	0.14	75,75,75,75	0
32	MN	X	3152	1/1	0.98	0.38	60,60,60,60	0
32	MN	X	3124	1/1	0.98	0.36	80,80,80,80	0
32	MN	X	3173	1/1	0.98	0.14	87,87,87,87	0
31	MG	X	3404	1/1	0.98	0.34	78,78,78,78	0
32	MN	X	3126	1/1	0.98	0.21	96,96,96,96	0
32	MN	X	3237	1/1	0.98	0.27	71,71,71,71	0

Continued on next page...

Continued from previous page...

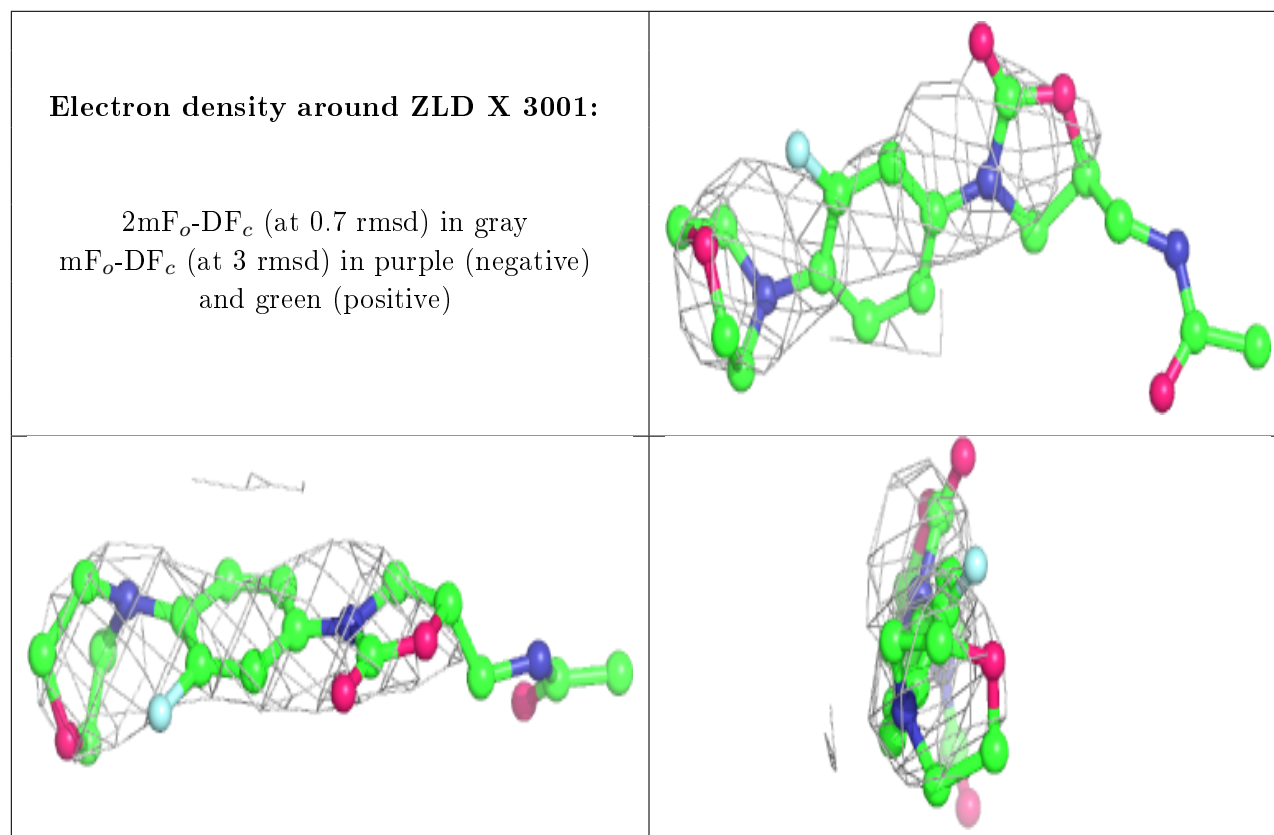
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3158	1/1	0.98	0.36	58,58,58,58	0
32	MN	X	3130	1/1	0.98	0.26	70,70,70,70	0
32	MN	X	3084	1/1	0.98	0.28	81,81,81,81	0
32	MN	X	3139	1/1	0.98	0.42	143,143,143,143	0
32	MN	X	3128	1/1	0.98	0.23	77,77,77,77	0
32	MN	X	3175	1/1	0.98	0.20	86,86,86,86	0
32	MN	X	3087	1/1	0.98	0.20	104,104,104,104	0
31	MG	X	3345	1/1	0.98	0.34	78,78,78,78	0
32	MN	X	3165	1/1	0.98	0.25	79,79,79,79	0
31	MG	X	3379	1/1	0.98	0.20	40,40,40,40	0
31	MG	X	3249	1/1	0.98	0.38	16,16,16,16	0
32	MN	X	3174	1/1	0.98	0.34	81,81,81,81	0
32	MN	X	3142	1/1	0.98	0.18	108,108,108,108	0
32	MN	X	3107	1/1	0.98	0.15	71,71,71,71	0
31	MG	X	3052	1/1	0.98	0.28	27,27,27,27	0
31	MG	X	3325	1/1	0.98	0.39	93,93,93,93	0
32	MN	X	3081	1/1	0.98	0.30	95,95,95,95	0
32	MN	X	3143	1/1	0.99	0.33	76,76,76,76	0
32	MN	X	3137	1/1	0.99	0.26	108,108,108,108	0
31	MG	X	3288	1/1	0.99	0.26	79,79,79,79	0
32	MN	X	3233	1/1	0.99	0.34	66,66,66,66	0
31	MG	X	3060	1/1	0.99	0.44	16,16,16,16	0
32	MN	X	3133	1/1	0.99	0.35	58,58,58,58	0
32	MN	X	3101	1/1	0.99	0.17	86,86,86,86	0
32	MN	X	3103	1/1	0.99	0.16	81,81,81,81	0
31	MG	X	3054	1/1	0.99	0.24	20,20,20,20	0
31	MG	X	3365	1/1	0.99	0.09	63,63,63,63	0
32	MN	X	3145	1/1	0.99	0.19	47,47,47,47	0
31	MG	X	3326	1/1	0.99	0.25	32,32,32,32	0
32	MN	X	3166	1/1	0.99	0.30	90,90,90,90	0
31	MG	X	3295	1/1	0.99	0.06	56,56,56,56	0
31	MG	X	3301	1/1	0.99	0.12	43,43,43,43	0
32	MN	X	3150	1/1	0.99	0.40	39,39,39,39	0
32	MN	X	3132	1/1	0.99	0.30	66,66,66,66	0
32	MN	X	3160	1/1	0.99	0.28	39,39,39,39	0
32	MN	X	3180	1/1	0.99	0.27	70,70,70,70	0
32	MN	X	3159	1/1	0.99	0.43	61,61,61,61	0
31	MG	X	3313	1/1	0.99	0.41	59,59,59,59	0
32	MN	X	3065	1/1	0.99	0.19	78,78,78,78	0
32	MN	X	3198	1/1	0.99	0.42	73,73,73,73	0
32	MN	X	3199	1/1	0.99	0.30	93,93,93,93	0
32	MN	X	3078	1/1	0.99	0.25	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3179	1/1	0.99	0.28	77,77,77,77	0
31	MG	X	3332	1/1	1.00	0.17	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.