



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:40 PM UTC

PDB ID : 1HNX / pdb_00001hnx
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL
SUBUNIT IN COMPLEX WITH PACTAMYCIN
Authors : Brodersen, D.E.; Clemons Jr., W.M.; Carter, A.P.; Morgan-Warren, R.; Wim-
berly, B.T.; Ramakrishnan, V.
Deposited on : 2000-12-08
Resolution : 3.40 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 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

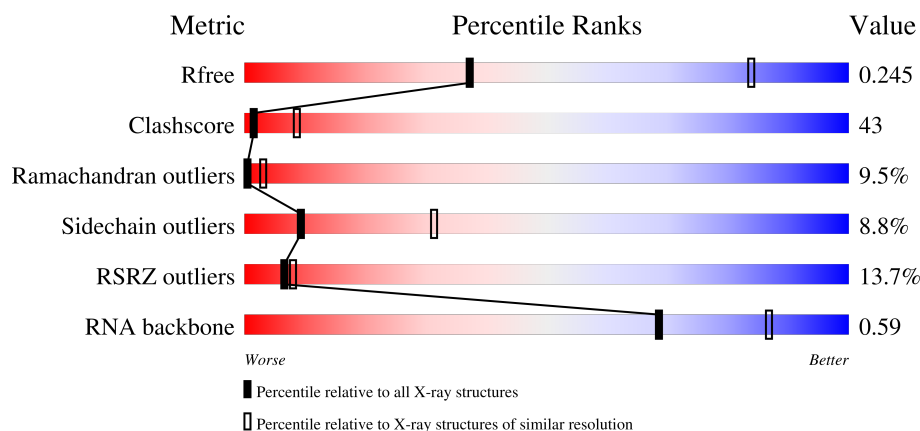
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	11% 21% 62% 12%
2	X	6	17% 33% 67%
3	B	256	12% 15% 56% 20% 9%

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Mol	Chain	Length	Quality of chain
4	C	239	
5	D	209	
6	E	162	
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	
13	L	135	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	
22	V	26	

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
23	MG	A	1562	-	-	-	X
23	MG	A	1576	-	-	-	X
23	MG	A	1595	-	-	-	X
23	MG	A	1600	-	-	-	X
23	MG	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1615	-	-	-	X
23	MG	A	212	-	-	-	X
23	MG	A	214	-	-	-	X

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 51910 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	P	0	0	0
			117	54	14	44	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	88	Total	C	N	O	S	0	0	0
			735	462	147	125	1			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

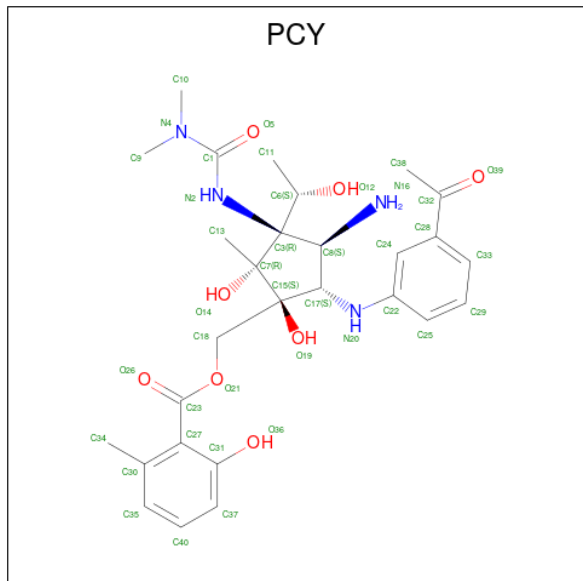
- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	94	Total	Mg	0	0
			94	94		
23	D	1	Total	Mg	0	0
			1	1		
23	H	1	Total	Mg	0	0
			1	1		

- Molecule 24 is Pactamycin (CCD ID: PCY) (formula: C₂₈H₃₈N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			40	28	4	8		

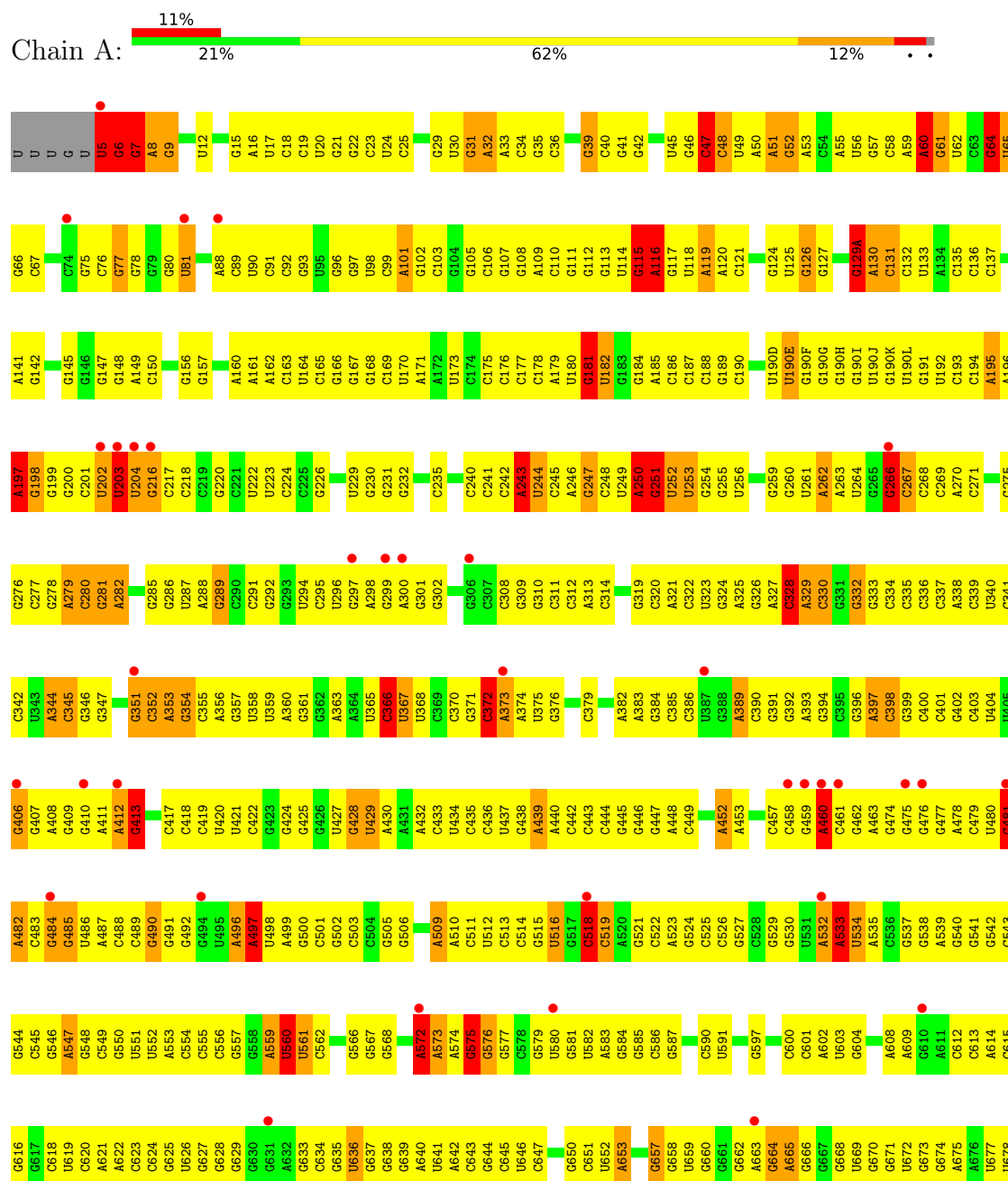
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total 1	Zn 1	0	0
25	N	1	Total 1	Zn 1	0	0

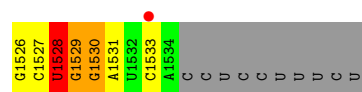
3 Residue-property plots

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.

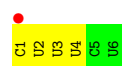
• Molecule 1: 16S RIBOSOMAL RNA



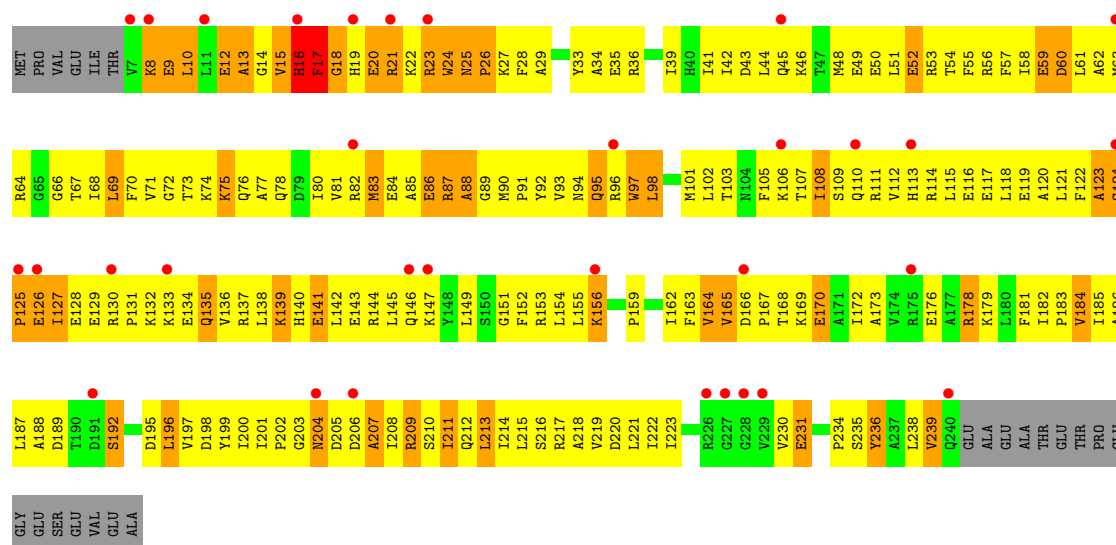
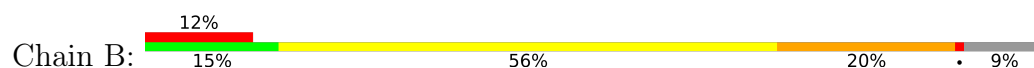
C1466	C1395	A1332	G1272	G1210	C1149	U1085	U1025	C962	G885	A814	A746	C679
G1467	A1396	A1333	G1273	U1211	U1150	U1086	G1026	A965	A889	A815	C747	C680
A1468	C1397	C1334	U1274	U1212	A1151	U1090	C1027	G966	G890	A816	C748	C681
G1469	A1398	C1335	A1275	A1213	A1152	U1091	C1028	G967	G891	C917	C749	G682
G1470	C1402	C1336	G1276	C1214	C1153	A1092	C1029	A968	G898	G818	G750	G683
G1471	C1403	G1337	G1277	G1215	G1154	A1093	G1030	A969	C899	A819	U751	A684
U1472	C1404	G1338	U1278	G1216	G1155	A1094	G1030A	C970	C899	U820	G752	G685
A1473	C1405	A1339	A1279	C1217	G1156	G1095	G1030B	G971	A900	G821	A753	U686
G1474	U1406	A1340	A1280	C1218	A1157	U1096	G1030C	G972	A901	G822	A754	A687
G1475	C1341	U1342	U1281	U1219	C1158	C1097	G1030D	G973	G902	G823	G755	G688
G1476	C1342	C1342	C1282	G1220	U1159	C1097	G1031	G974	G903	C824	G756	G689
C1477	G1343	G1343	G1283	G1221	G1160	C1098	G1032	A975	G911	G825	U757	G690
C1478	C1344	C1344	C1284	G1222	C1161	G1099	G1033	G976	C912	C826	G758	G691
C1479	U1345	U1345	A1285	C1223	C1162	C1100	G1034	A977	A913	U827	A759	U692
A1480	A1346	A1346	A1286	G1224	C1163	A1101	A1035	A978	A914	A828	G760	G693
U1481	G1347	G1347	A1287	A1225	G1164	A1102	G1036	A979	A915	A829	G761	A694
G1482	U1348	U1348	A1288	C1226	C1165	C1103	C1037	C979	G916	A914	C762	A695
A1483	A1349	A1349	A1289	G1227	G1166	G1104	C1038	C980	G917	U831	G765	A696
C1484	C1352	C1352	G1290	C1228	A1167	A1105	C1039	A883	A918	C832	A766	U697
U1485	G1353	G1353	U1291	C1229	A1168	G1106	U1040	C984	A919	C833	A767	G698
G1486	C1354	C1354	U1292	C1230	A1169	C1109	A1041	C985	A920	C834	A768	C701
G1487	G1355	G1355	G1293	G1231	G1171	C1116	G1042	C986	A921	U835	G771	A702
G1488	C1356	C1356	G1294	U1232	C1172	A1110	C1043	A987	U921	G836	G772	G703
G1489	G1357	G1357	G1295	G1233	G1173	A1111	G1044	C988	G922	G837	G773	C707
C1490	C1357	C1357	C1296	C1234	G1174	C1112	A1045	C989	A923	U838	G774	G708
G1491	U1358	U1358	U1297	U1235	G1175	C1113	A1046	U991	C924	U839	G775	G709
A1492	C1359	C1359	C1298	C1236	A1176	C1116	G1047	U992	G925	C940	G776	G710
A1493	A1360	A1360	A1299	A1237	G1177	C1117	G1048	A994	G927	U841	A777	G711
G1494	G1361	G1361	G1300	A1238	G1178	A1118	U1049	C995	G928	C848	G778	G712
U1495	C1361A	C1361A	U1301	A1239	A1179	C1119	G1050	A996	G929	C849	G779	G713
A1496	C1362	C1362	U1302	U1240	A1180	G1120	C1051	U997	C930	U850	G780	C707
G1497	A1363	A1363	C1303	U1241	G1181	G1121	U1052	U998	C931	C851	A781	A716
U1498	U1364	U1364	G1304	C1242	G1182	U1122	G1053	C999	C932	C852	A782	C717
A1499	G1365	G1365	A1305	C1243	A1183	A1123	A1055	U1000	C934	C853	G783	C718
A1500	C1366	C1366	G1306	A1244	G1184	C1124	U1056	A1001	A935	G854	C784	C719
C1501	G1367	G1367	U1307	A1245	G1185	U1125	G1057	G1002	C936	C855	G785	G720
A1502	C1368	C1368	G1308	C1246	G1186	U1126	U1058	G1003	G939	C856	G786	G721
A1503	G1369	G1369	G1309	C1249	G1187	G1127	C1059	G1003A	C940	C857	A787	A722
G1504	C1370	C1370	G1310	A1250	A1188	C1128	G1060	A1004	A859	C858	U788	U723
U1505	G1371	G1371	G1311	A1251	G1189	C1129	C1061	A1005	G941	C859	G791	C726
A1506	C1372	C1372	G1312	A1252	G1190	C1130	U1062	A1006	G942	C860	A792	A728
U1507	G1373	G1373	U1313	G1253	A1191	A1131	G1063	C1007	U943	C861	U793	G730
G1508	A1374	A1374	C1314	C1254	G1192	G1132	G1064	C1008	G944	A864	G792	A729
C1509	C1375	C1375	U1315	G1255	U1194	G1133	U1065	G1009	G945	A865	A794	G731
U1510	U1376	U1376	G1316	A1256	U1195	U1134	C1066	G1010	A946	C866	C795	C732
G1511	A1377	A1377	C1317	U1257	U1196	U1135	A1067	G1011	G947	C867	C796	G733
U1512	C1378	C1378	A1318	C1258	G1197	U1136	G1068	U1012	C948	C868	C797	A733
A1513	G1379	G1379	A1319	G1259	G1198	C1137	G1069	G1013	A949	C869	G798	G734
C1514	U1380	U1380	C1320	C1260	U1199	G1138	U1070	A1014	U950	C874	C735	C735
C1515	U1381	U1381	C1321	C1261	G1200	G1139	C1071	A1015	G951	C875	G803	G736
G1516	C1382	C1382	C1322	A1261	C1201	G1140	G1072	A1016	U952	C876	C977	A737
G1517	G1383	G1383	G1323	C1262	A1202	C1141	U1073	C1017	G953	C877	C805	C738
A1518	C1384	C1384	A1324	C1263	G1203	G1142	G1074	A1018	G954	C878	C806	G738
C1519	G1385	G1385	C1325	C1264	C1203	G1143	C1019	C879	C807	C879	A807	G741
G1520	C1386	C1386	G1326	G1265	A1204	G1144	U1075	U1020	A858	C880	C808	G742
U1521	G1387	G1387	C1327	G1266	U1205	C1145	G1077	G1021	A959	C881	C812	U743
G1522	U1391	U1391	C1328	C1267	G1206	C1146	U1078	G1022	U960	C882	G744	C744
U1523	C1392	C1392	A1329	A1268	G1207	A1147	U1079	G1023	C883	C883	C812	U744
C1524	U1393	U1393	U1330	A1269	G1208	C1147	A1080	G1024	U961	U884	U813	C745
G1525	A1394	A1394	G1331	C1209	C1209	U1148						



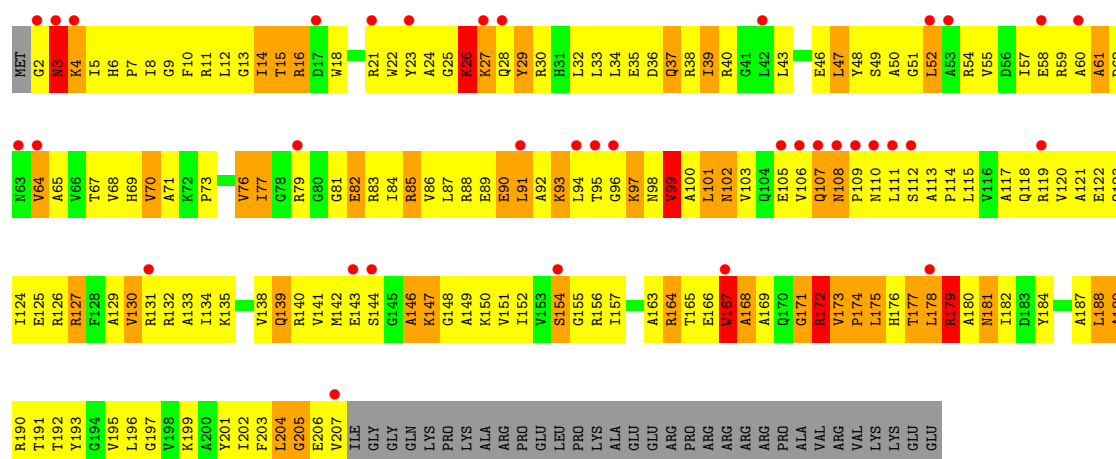
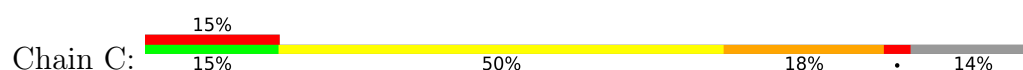
• Molecule 2: FRAGMENT OF MESSENGER RNA



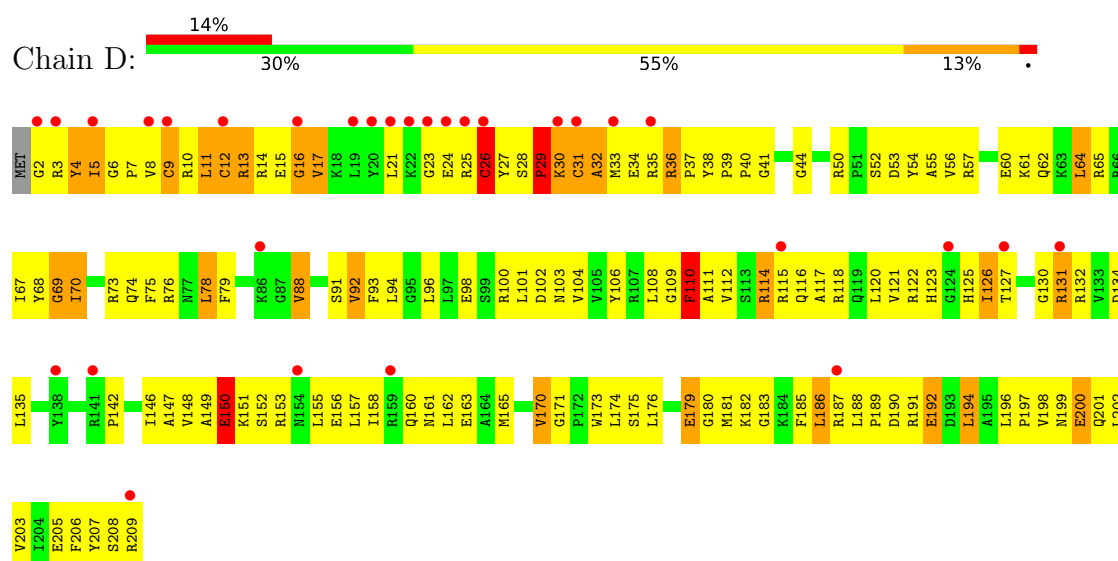
• Molecule 3: 30S RIBOSOMAL PROTEIN S2



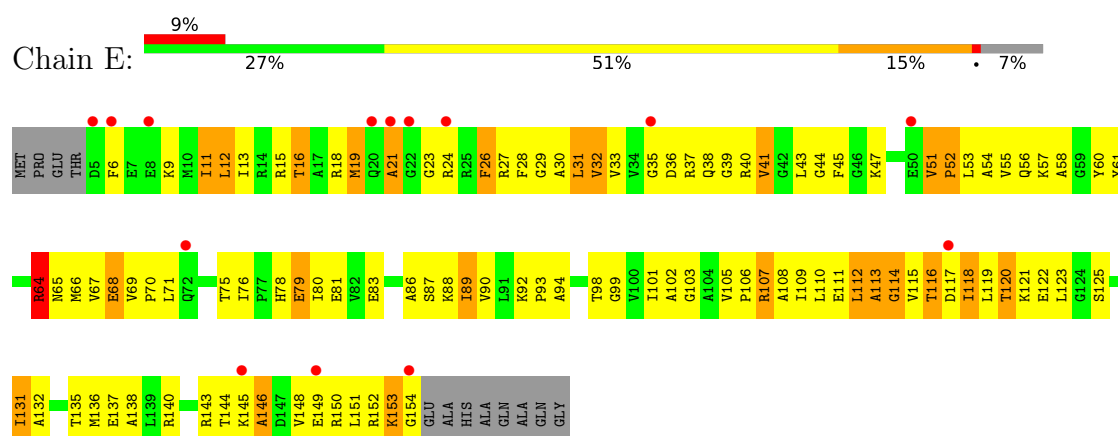
• Molecule 4: 30S RIBOSOMAL PROTEIN S3



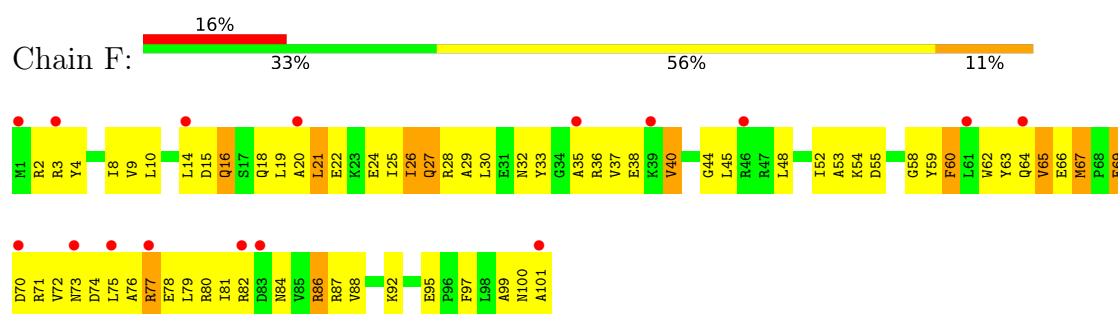
• Molecule 5: 30S RIBOSOMAL PROTEIN S4



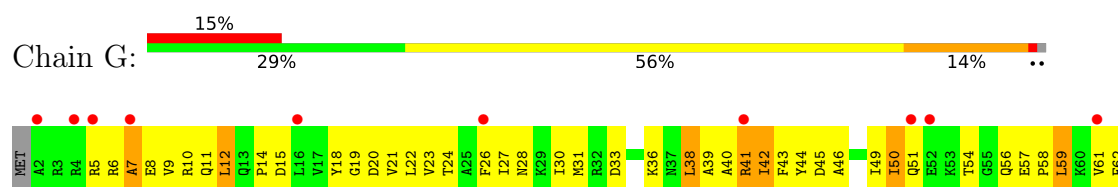
• Molecule 6: 30S RIBOSOMAL PROTEIN S5

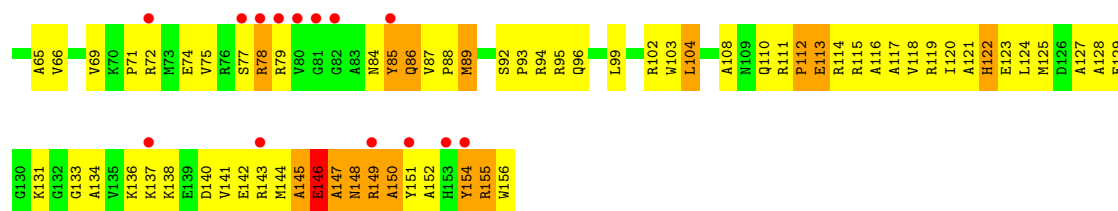


• Molecule 7: 30S RIBOSOMAL PROTEIN S6

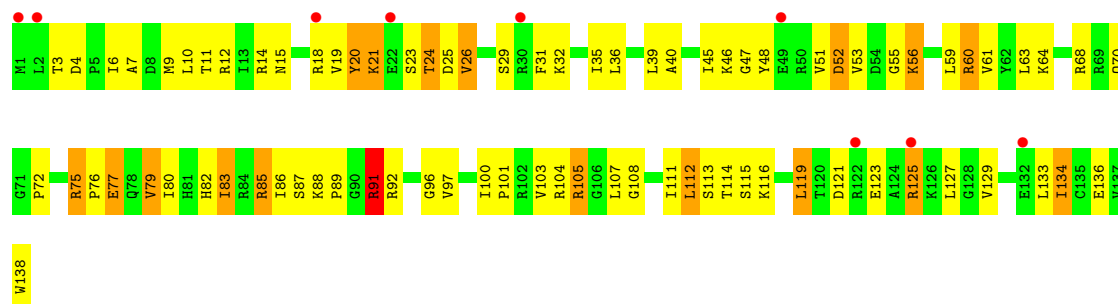
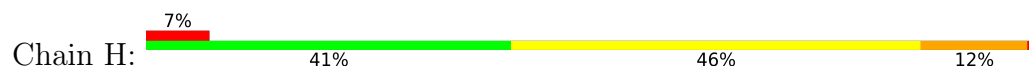


• Molecule 8: 30S RIBOSOMAL PROTEIN S7

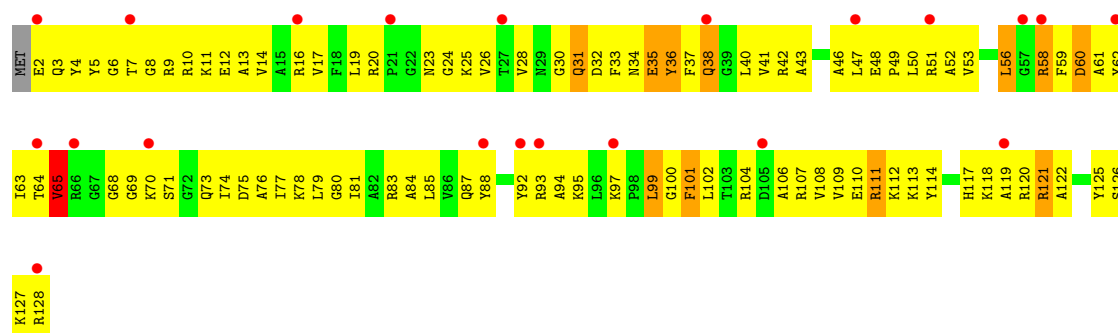




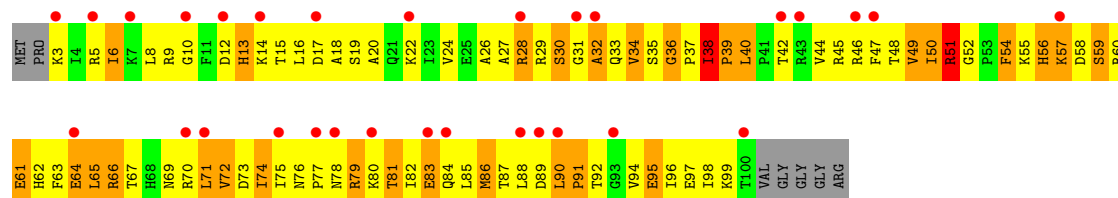
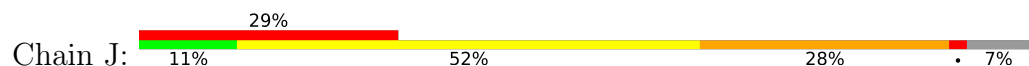
• Molecule 9: 30S RIBOSOMAL PROTEIN S8



• Molecule 10: 30S RIBOSOMAL PROTEIN S9

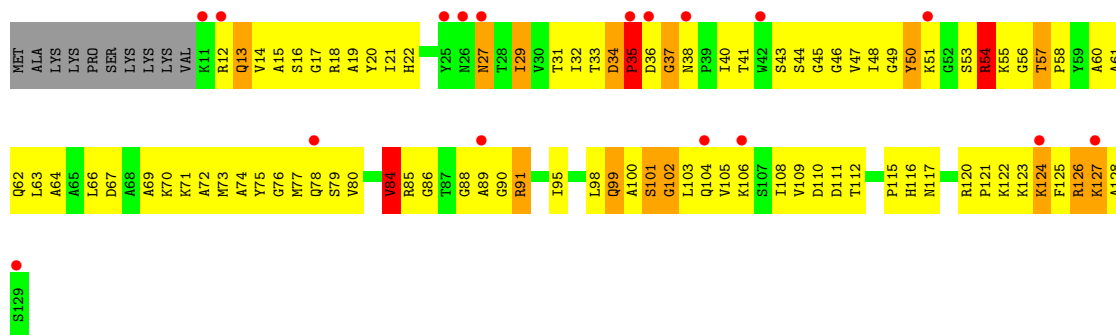


• Molecule 11: 30S RIBOSOMAL PROTEIN S10

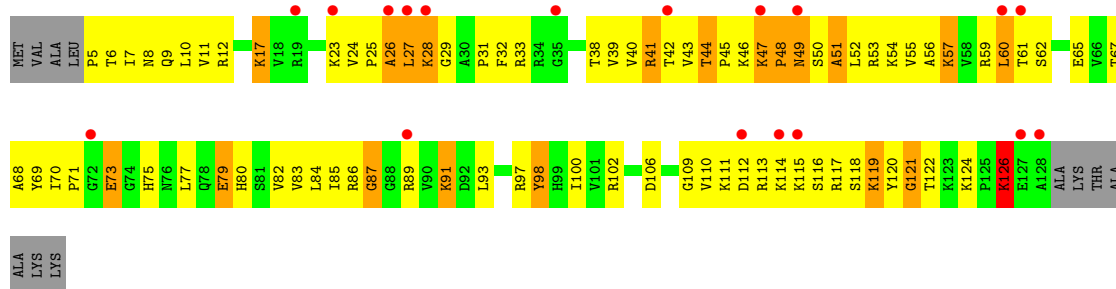


• Molecule 12: 30S RIBOSOMAL PROTEIN S11





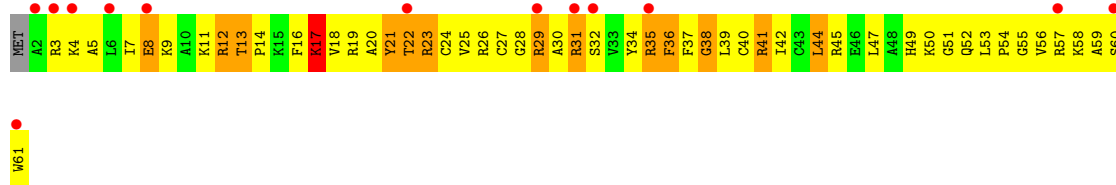
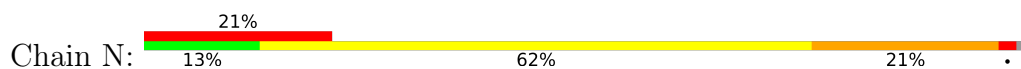
• Molecule 13: 30S RIBOSOMAL PROTEIN S12



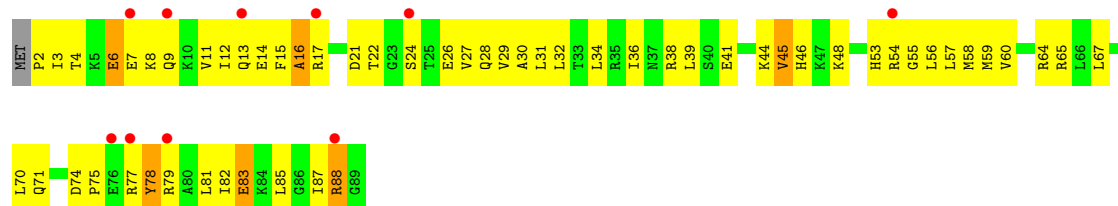
• Molecule 14: 30S RIBOSOMAL PROTEIN S13



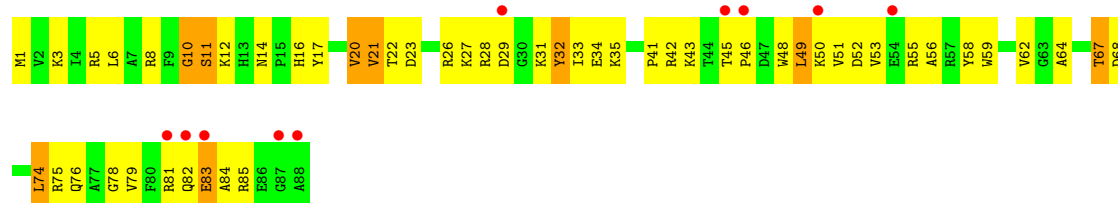
• Molecule 15: 30S RIBOSOMAL PROTEIN S14



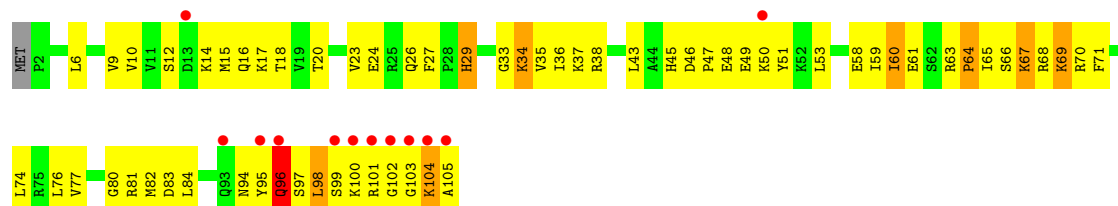
• Molecule 16: 30S RIBOSOMAL PROTEIN S15



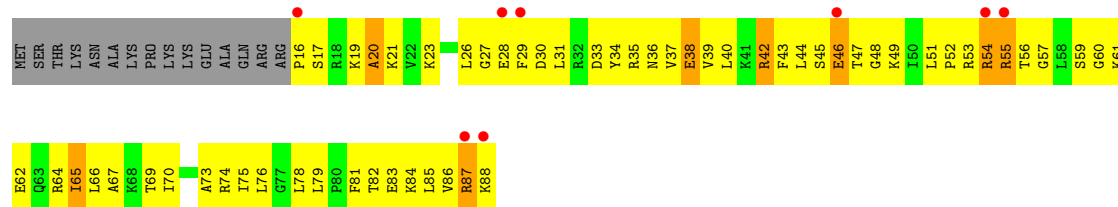
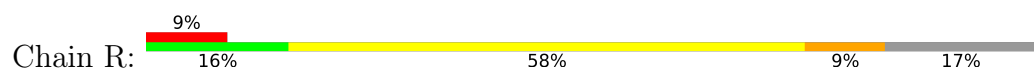
• Molecule 17: 30S RIBOSOMAL PROTEIN S16



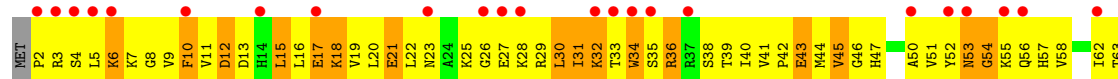
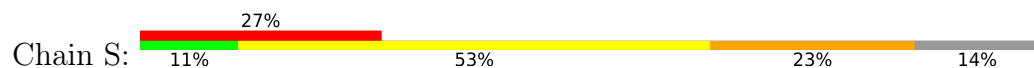
• Molecule 18: 30S RIBOSOMAL PROTEIN S17

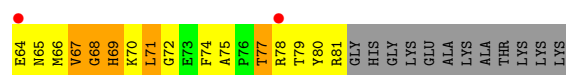


• Molecule 19: 30S RIBOSOMAL PROTEIN S18

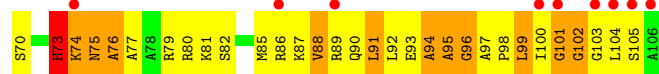
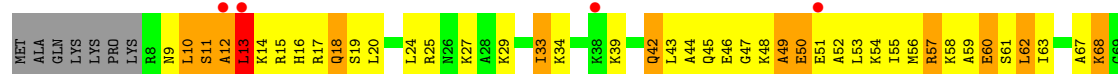
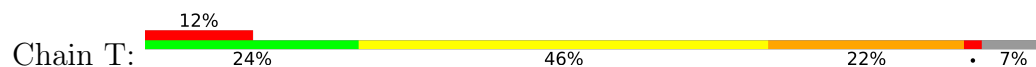


• Molecule 20: 30S RIBOSOMAL PROTEIN S19

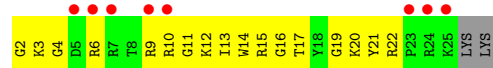




• Molecule 21: 30S RIBOSOMAL PROTEIN S20



• Molecule 22: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.72Å 401.72Å 177.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.34 – 3.40 95.34 – 3.40	Depositor EDS
% Data completeness (in resolution range)	88.9 (95.34-3.40) 88.9 (95.34-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.13Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.280 0.200 , 0.245	Depositor DCC
R_{free} test set	10844 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 708.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51910	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: PCY, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/36259	0.74	79/56593 (0.1%)
2	X	0.43	0/128	0.60	0/196
3	B	0.47	0/1935	1.06	10/2609 (0.4%)
4	C	0.45	0/1636	0.98	8/2205 (0.4%)
5	D	0.50	0/1733	1.04	7/2318 (0.3%)
6	E	0.63	0/1162	1.22	10/1564 (0.6%)
7	F	0.42	0/856	0.93	3/1154 (0.3%)
8	G	0.43	0/1276	0.99	9/1709 (0.5%)
9	H	0.61	0/1136	1.23	13/1527 (0.9%)
10	I	0.41	0/1029	1.00	5/1378 (0.4%)
11	J	0.45	0/805	1.03	6/1082 (0.6%)
12	K	0.53	0/900	1.14	9/1213 (0.7%)
13	L	0.54	0/986	1.11	5/1320 (0.4%)
14	M	0.46	0/1008	1.01	2/1347 (0.1%)
15	N	0.45	0/501	1.14	6/664 (0.9%)
16	O	0.51	0/745	0.93	2/992 (0.2%)
17	P	0.57	0/751	1.21	6/1008 (0.6%)
18	Q	0.56	0/870	1.12	4/1159 (0.3%)
19	R	0.46	0/603	0.99	1/799 (0.1%)
20	S	0.44	0/661	1.01	7/890 (0.8%)
21	T	0.49	0/764	1.07	4/1006 (0.4%)
22	V	0.50	0/212	0.87	0/277
All	All	0.47	0/55956	0.86	196/83010 (0.2%)

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	A	2	47

There are no bond length outliers.

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	14.35	131.03	109.50
1	A	1085	U	C2'-C3'-O3'	13.52	129.78	109.50
6	E	21	ALA	N-CA-C	-11.97	93.62	110.50
1	A	60	A	C2'-C3'-O3'	11.81	127.22	109.50
1	A	484	G	C2'-C3'-O3'	11.52	126.78	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1085	U	C3'
1	A	1498	U	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	A	Sidechain
1	A	126	G	Sidechain
1	A	47	C	Sidechain
1	A	5	U	Sidechain
1	A	77	G	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	A	32391	0	16349	1516	0
2	X	117	0	64	2	0
3	B	1900	0	1951	304	0
4	C	1612	0	1677	291	0
5	D	1703	0	1764	197	0
6	E	1146	0	1207	126	0
7	F	843	0	857	87	0
8	G	1257	0	1296	122	0
9	H	1116	0	1177	96	0
10	I	1011	0	1043	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	792	0	835	165	0
12	K	885	0	904	103	0
13	L	970	0	1057	128	0
14	M	997	0	1072	151	0
15	N	492	0	529	88	0
16	O	734	0	771	75	0
17	P	735	0	752	70	0
18	Q	857	0	930	108	0
19	R	597	0	668	108	0
20	S	647	0	673	109	0
21	T	762	0	859	120	0
22	V	208	0	221	22	0
23	A	94	0	0	0	0
23	D	1	0	0	0	0
23	H	1	0	0	0	0
24	A	40	0	38	9	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	51910	0	36694	3797	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 43.

The worst 5 of 3797 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)
24:A:1632:PCY:C3	24:A:1632:PCY:N2	1.69	1.49
13:L:28:LYS:HD2	13:L:33:ARG:HH22	1.01	1.16
12:K:110:ASP:HB2	19:R:88:LYS:HD2	1.28	1.15
6:E:110:LEU:HD13	6:E:118:ILE:HD12	1.28	1.15
4:C:58:GLU:HB3	11:J:92:THR:HG21	1.29	1.15

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	232/256 (91%)	155 (67%)	49 (21%)	28 (12%)	0	1
4	C	204/239 (85%)	120 (59%)	52 (26%)	32 (16%)	0	0
5	D	206/209 (99%)	146 (71%)	41 (20%)	19 (9%)	0	3
6	E	148/162 (91%)	126 (85%)	18 (12%)	4 (3%)	4	20
7	F	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	7
8	G	153/156 (98%)	114 (74%)	24 (16%)	15 (10%)	0	3
9	H	136/138 (99%)	122 (90%)	10 (7%)	4 (3%)	3	19
10	I	125/128 (98%)	90 (72%)	28 (22%)	7 (6%)	1	9
11	J	96/105 (91%)	58 (60%)	20 (21%)	18 (19%)	0	0
12	K	117/129 (91%)	87 (74%)	16 (14%)	14 (12%)	0	2
13	L	122/135 (90%)	91 (75%)	19 (16%)	12 (10%)	0	3
14	M	123/126 (98%)	84 (68%)	23 (19%)	16 (13%)	0	1
15	N	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	1
16	O	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	3	16
17	P	86/88 (98%)	66 (77%)	17 (20%)	3 (4%)	3	16
18	Q	102/105 (97%)	84 (82%)	13 (13%)	5 (5%)	1	11
19	R	71/88 (81%)	51 (72%)	18 (25%)	2 (3%)	4	19
20	S	78/93 (84%)	52 (67%)	15 (19%)	11 (14%)	0	0
21	T	97/106 (92%)	61 (63%)	19 (20%)	17 (18%)	0	0
22	V	22/26 (85%)	17 (77%)	4 (18%)	1 (4%)	2	12
All	All	2361/2540 (93%)	1702 (72%)	434 (18%)	225 (10%)	0	3

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	8	LYS
3	B	9	GLU
3	B	15	VAL
3	B	16	HIS
3	B	17	PHE

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	B	202/220 (92%)	183 (91%)	19 (9%)	8	29
4	C	160/188 (85%)	137 (86%)	23 (14%)	3	13
5	D	180/181 (99%)	164 (91%)	16 (9%)	9	31
6	E	115/123 (94%)	98 (85%)	17 (15%)	3	12
7	F	90/90 (100%)	85 (94%)	5 (6%)	19	46
8	G	126/127 (99%)	119 (94%)	7 (6%)	19	46
9	H	119/119 (100%)	106 (89%)	13 (11%)	6	22
10	I	98/99 (99%)	89 (91%)	9 (9%)	8	29
11	J	87/92 (95%)	76 (87%)	11 (13%)	4	18
12	K	90/99 (91%)	85 (94%)	5 (6%)	19	46
13	L	104/111 (94%)	98 (94%)	6 (6%)	18	45
14	M	100/101 (99%)	94 (94%)	6 (6%)	17	43
15	N	49/50 (98%)	45 (92%)	4 (8%)	10	35
16	O	79/80 (99%)	76 (96%)	3 (4%)	29	54
17	P	74/74 (100%)	68 (92%)	6 (8%)	11	36
18	Q	96/97 (99%)	91 (95%)	5 (5%)	21	48
19	R	64/77 (83%)	58 (91%)	6 (9%)	8	29
20	S	71/80 (89%)	65 (92%)	6 (8%)	10	33
21	T	76/82 (93%)	67 (88%)	9 (12%)	5	20
22	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1999/2111 (95%)	1823 (91%)	176 (9%)	9	31

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	66	ARG
16	O	83	GLU
11	J	95	GLU

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Mol	Chain	Res	Type
13	L	126	LYS
18	Q	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	16	GLN
20	S	14	HIS
6	E	20	GLN
5	D	199	ASN
20	S	53	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	221 (14%)	85 (5%)
2	X	5/6 (83%)	1 (20%)	0
All	All	1512/1528 (98%)	222 (14%)	85 (5%)

5 of 222 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 85 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1139	G
1	A	1285	A
1	A	1182	G
1	A	1224	G
1	A	1331	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 99 ligands modelled in this entry, 98 are monoatomic - leaving 1 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$
24	PCY	A	1632	-	34,42,42	8.11	34 (100%)	41,65,65	1.86	8 (19%)

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
24	PCY	A	1632	-	-	13/33/67/67	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1632	PCY	C1-N4	11.83	1.54	1.35
24	A	1632	PCY	C17-N20	11.53	1.59	1.45
24	A	1632	PCY	C40-C35	10.52	1.56	1.38
24	A	1632	PCY	C24-C22	10.32	1.56	1.39
24	A	1632	PCY	C29-C33	9.92	1.55	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1632	PCY	N2-C1-N4	6.68	121.74	116.74
24	A	1632	PCY	C22-N20-C17	-4.90	112.19	123.01
24	A	1632	PCY	C31-C27-C30	3.53	122.01	118.10
24	A	1632	PCY	C18-O21-C23	3.29	123.03	116.55
24	A	1632	PCY	C3-N2-C1	3.10	132.93	124.59

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

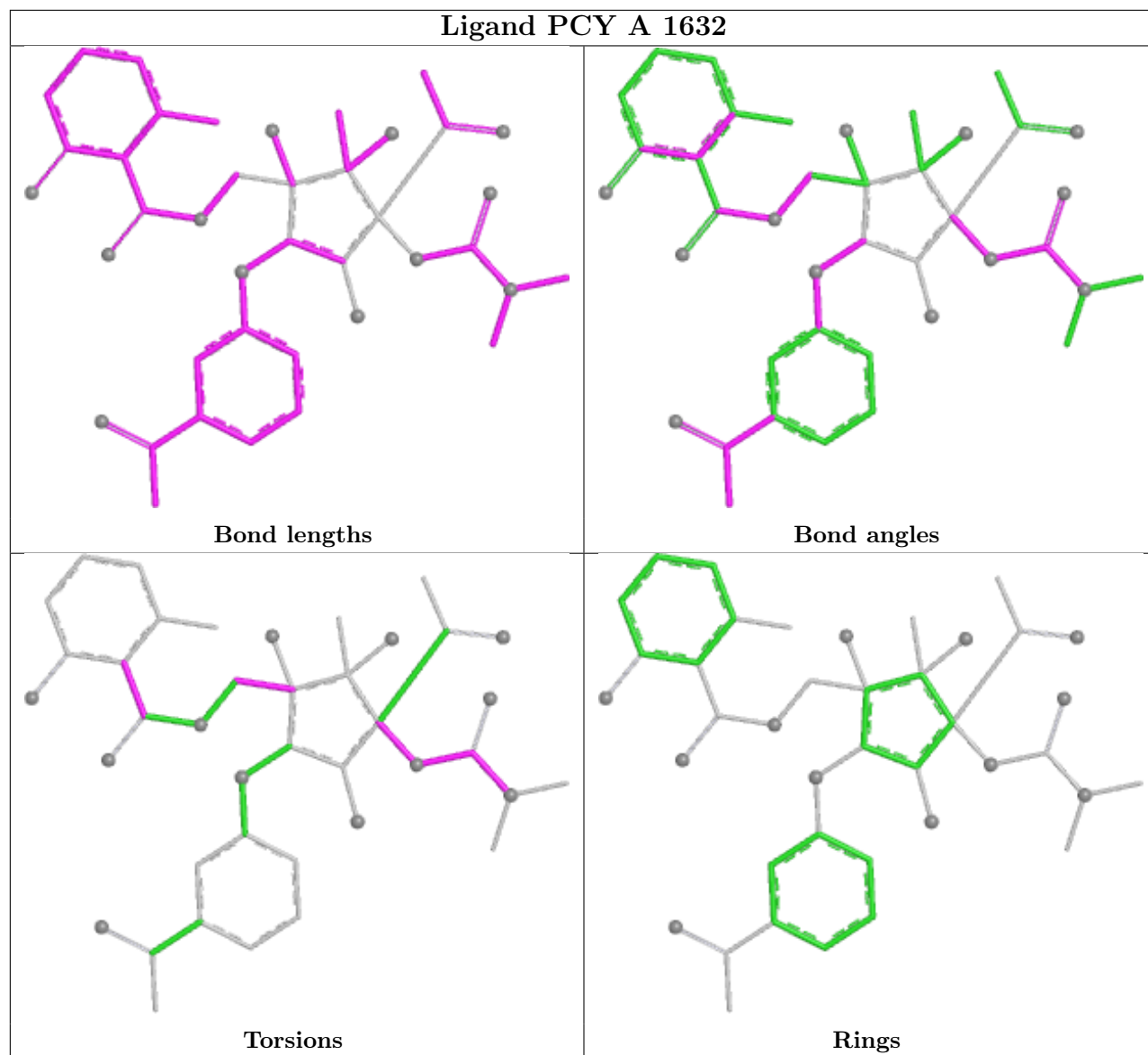
Mol	Chain	Res	Type	Atoms
24	A	1632	PCY	N4-C1-N2-C3
24	A	1632	PCY	O5-C1-N2-C3
24	A	1632	PCY	N2-C1-N4-C9
24	A	1632	PCY	N2-C1-N4-C10
24	A	1632	PCY	O5-C1-N4-C9

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1632	PCY	9	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1506/1522 (98%)	0.83	168 (11%) 10 11	37, 70, 161, 199	0
2	X	6/6 (100%)	1.85	1 (16%) 4 6	62, 79, 117, 151	0
3	B	234/256 (91%)	1.00	32 (13%) 6 8	34, 87, 162, 199	0
4	C	206/239 (86%)	1.10	36 (17%) 4 5	41, 91, 153, 179	0
5	D	208/209 (99%)	0.87	30 (14%) 6 7	35, 71, 128, 191	0
6	E	150/162 (92%)	0.49	14 (9%) 14 14	34, 58, 111, 168	0
7	F	101/101 (100%)	1.04	16 (15%) 5 6	56, 95, 147, 167	0
8	G	155/156 (99%)	0.91	24 (15%) 5 7	47, 85, 147, 175	0
9	H	138/138 (100%)	0.35	9 (6%) 25 20	21, 52, 92, 139	0
10	I	127/128 (99%)	1.09	21 (16%) 4 6	37, 96, 140, 181	0
11	J	98/105 (93%)	1.82	30 (30%) 1 2	50, 119, 184, 199	0
12	K	119/129 (92%)	0.85	17 (14%) 6 8	41, 73, 137, 178	0
13	L	124/135 (91%)	0.87	18 (14%) 6 7	30, 72, 131, 180	0
14	M	125/126 (99%)	1.22	22 (17%) 4 5	56, 89, 153, 188	0
15	N	60/61 (98%)	1.35	13 (21%) 2 4	50, 86, 157, 170	0
16	O	88/89 (98%)	0.71	10 (11%) 10 10	38, 70, 136, 186	0
17	P	88/88 (100%)	0.89	10 (11%) 10 10	35, 63, 164, 198	0
18	Q	104/105 (99%)	0.90	12 (11%) 9 10	35, 62, 137, 199	0
19	R	73/88 (82%)	0.83	8 (10%) 10 11	43, 75, 154, 194	0
20	S	80/93 (86%)	1.54	25 (31%) 1 2	66, 110, 158, 199	0
21	T	99/106 (93%)	0.99	13 (13%) 7 8	44, 72, 133, 194	0
22	V	24/26 (92%)	1.43	8 (33%) 1 1	44, 79, 128, 149	0
All	All	3913/4068 (96%)	0.92	537 (13%) 6 8	21, 75, 155, 199	0

The worst 5 of 537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	M	124	PRO	13.1
1	A	1129	C	11.1
18	Q	105	ALA	10.6
20	S	3	ARG	9.5
14	M	126	LYS	7.9

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
23	MG	A	1550	1/1	0.62	0.29	45,45,45,45	1
23	MG	A	212	1/1	0.65	0.65	45,45,45,45	1
23	MG	A	1600	1/1	0.66	0.51	45,45,45,45	0
23	MG	A	1615	1/1	0.67	0.63	45,45,45,45	1
23	MG	A	1566	1/1	0.70	0.34	45,45,45,45	0
23	MG	A	1595	1/1	0.74	0.48	45,45,45,45	0
23	MG	A	1613	1/1	0.75	0.78	45,45,45,45	1
23	MG	A	1562	1/1	0.76	0.48	45,45,45,45	0
23	MG	A	1592	1/1	0.77	0.22	45,45,45,45	0
23	MG	A	1568	1/1	0.77	0.26	45,45,45,45	0
23	MG	A	214	1/1	0.79	0.54	45,45,45,45	0
23	MG	A	1549	1/1	0.79	0.26	45,45,45,45	1
23	MG	A	1576	1/1	0.79	0.40	45,45,45,45	0
23	MG	A	1548	1/1	0.80	0.29	45,45,45,45	0
23	MG	A	1611	1/1	0.80	0.21	45,45,45,45	1
23	MG	A	1599	1/1	0.82	0.36	45,45,45,45	0
23	MG	A	1547	1/1	0.82	0.40	45,45,45,45	0
23	MG	A	210	1/1	0.82	0.45	45,45,45,45	1
23	MG	A	1585	1/1	0.82	0.35	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1581	1/1	0.83	0.18	45,45,45,45	1
23	MG	A	1556	1/1	0.83	0.63	45,45,45,45	1
23	MG	A	1567	1/1	0.83	0.38	45,45,45,45	0
23	MG	A	1588	1/1	0.84	0.22	45,45,45,45	0
23	MG	A	1586	1/1	0.84	0.39	45,45,45,45	0
23	MG	A	1587	1/1	0.84	0.19	45,45,45,45	0
23	MG	A	1596	1/1	0.84	0.56	45,45,45,45	1
23	MG	A	1552	1/1	0.86	0.26	45,45,45,45	0
23	MG	A	1594	1/1	0.86	0.29	45,45,45,45	0
23	MG	A	1557	1/1	0.86	0.50	45,45,45,45	0
23	MG	A	1597	1/1	0.87	0.31	45,45,45,45	0
23	MG	A	1606	1/1	0.87	0.39	45,45,45,45	0
23	MG	A	1623	1/1	0.87	0.34	45,45,45,45	1
24	PCY	A	1632	40/40	0.87	0.22	28,28,28,28	0
23	MG	A	1564	1/1	0.88	0.51	45,45,45,45	0
23	MG	A	1545	1/1	0.88	0.12	45,45,45,45	0
23	MG	A	1603	1/1	0.88	0.36	45,45,45,45	0
23	MG	A	1553	1/1	0.88	0.49	45,45,45,45	0
23	MG	A	1559	1/1	0.88	0.39	45,45,45,45	0
23	MG	A	1554	1/1	0.88	0.51	45,45,45,45	0
23	MG	A	86	1/1	0.89	0.29	45,45,45,45	0
23	MG	A	87	1/1	0.89	0.24	45,45,45,45	1
23	MG	A	1616	1/1	0.89	0.09	45,45,45,45	0
23	MG	A	1619	1/1	0.89	0.29	45,45,45,45	1
23	MG	A	1620	1/1	0.89	0.20	45,45,45,45	0
23	MG	A	1591	1/1	0.89	0.40	45,45,45,45	0
23	MG	D	215	1/1	0.89	0.22	45,45,45,45	0
23	MG	H	213	1/1	0.89	0.34	45,45,45,45	1
23	MG	A	71	1/1	0.89	0.39	45,45,45,45	0
23	MG	A	1579	1/1	0.90	0.28	45,45,45,45	0
23	MG	A	1574	1/1	0.90	0.17	45,45,45,45	0
23	MG	A	1582	1/1	0.90	0.36	45,45,45,45	1
23	MG	A	1575	1/1	0.90	0.16	45,45,45,45	1
23	MG	A	1608	1/1	0.90	0.39	45,45,45,45	0
23	MG	A	1610	1/1	0.90	0.31	45,45,45,45	0
23	MG	A	1593	1/1	0.90	0.27	45,45,45,45	0
23	MG	A	1558	1/1	0.90	0.41	45,45,45,45	0
23	MG	A	1598	1/1	0.91	0.14	45,45,45,45	1
23	MG	A	1617	1/1	0.91	0.31	45,45,45,45	1
23	MG	A	1609	1/1	0.91	0.41	45,45,45,45	0
23	MG	A	1584	1/1	0.91	0.41	45,45,45,45	0
23	MG	A	1605	1/1	0.92	0.31	45,45,45,45	0

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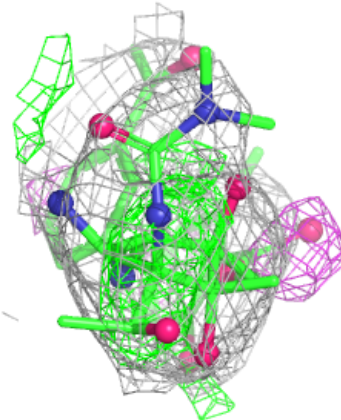
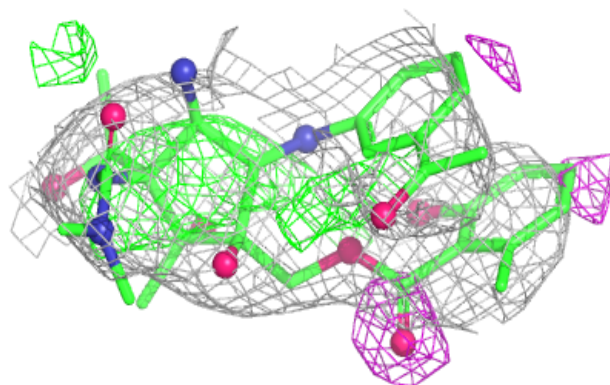
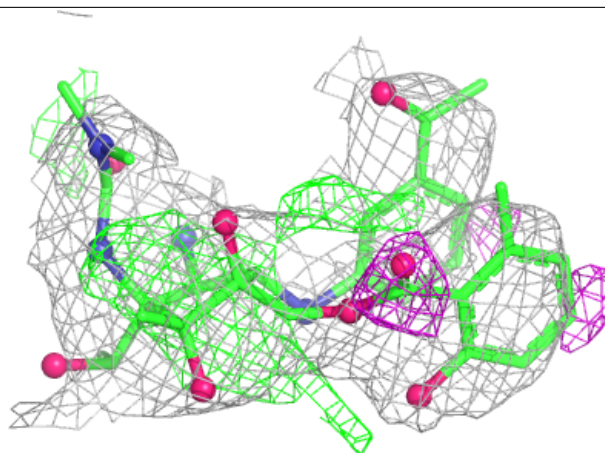
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1618	1/1	0.92	0.26	45,45,45,45	1
23	MG	A	1589	1/1	0.92	0.21	45,45,45,45	0
23	MG	A	1578	1/1	0.92	0.22	45,45,45,45	0
23	MG	A	1622	1/1	0.92	0.27	45,45,45,45	1
23	MG	A	1572	1/1	0.92	0.27	45,45,45,45	0
23	MG	A	1614	1/1	0.92	0.30	45,45,45,45	0
23	MG	A	1561	1/1	0.92	0.34	45,45,45,45	0
23	MG	A	1604	1/1	0.92	0.29	45,45,45,45	1
23	MG	A	1546	1/1	0.93	0.34	45,45,45,45	0
23	MG	A	1577	1/1	0.93	0.18	45,45,45,45	0
23	MG	A	1571	1/1	0.94	0.27	45,45,45,45	0
23	MG	A	1573	1/1	0.94	0.53	45,45,45,45	0
23	MG	A	1601	1/1	0.94	0.10	45,45,45,45	0
23	MG	A	1565	1/1	0.95	0.31	45,45,45,45	0
23	MG	A	1563	1/1	0.95	0.18	45,45,45,45	0
23	MG	A	1627	1/1	0.95	0.24	45,45,45,45	1
23	MG	A	1570	1/1	0.95	0.25	45,45,45,45	1
23	MG	A	1551	1/1	0.95	0.32	45,45,45,45	0
23	MG	A	1621	1/1	0.95	0.17	45,45,45,45	1
23	MG	A	1590	1/1	0.96	0.42	45,45,45,45	0
23	MG	A	1626	1/1	0.96	0.11	45,45,45,45	1
23	MG	A	1612	1/1	0.96	0.11	45,45,45,45	0
25	ZN	D	300	1/1	0.96	0.23	53,53,53,53	0
23	MG	A	1555	1/1	0.97	0.56	45,45,45,45	0
23	MG	A	1629	1/1	0.97	0.17	45,45,45,45	1
23	MG	A	1580	1/1	0.97	0.21	45,45,45,45	0
23	MG	A	1607	1/1	0.97	0.32	45,45,45,45	0
23	MG	A	1560	1/1	0.97	0.18	45,45,45,45	0
23	MG	A	211	1/1	0.97	0.38	45,45,45,45	0
23	MG	A	1630	1/1	0.98	0.26	45,45,45,45	1
23	MG	A	1631	1/1	0.98	0.18	45,45,45,45	1
23	MG	A	1569	1/1	0.98	0.15	45,45,45,45	1
23	MG	A	1624	1/1	0.98	0.16	45,45,45,45	1
23	MG	A	1628	1/1	0.98	0.06	45,45,45,45	1
23	MG	A	1625	1/1	0.98	0.12	45,45,45,45	1
23	MG	A	1602	1/1	0.99	0.39	45,45,45,45	0
23	MG	A	1583	1/1	0.99	0.09	45,45,45,45	0
25	ZN	N	190	1/1	1.00	0.05	53,53,53,53	1

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.

Electron density around PCY A 1632:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.