

wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 - 07:02 AM EDT

PDB ID	:	1HNX
Title	:	STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL
		SUBUNIT IN COMPLEX WITH PACTAMYCIN
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		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 (i) 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 (i)) 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	:	2.34
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)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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 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 <=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	А	1522	21%	62%		_	14%	••			
2	Х	6	17% 33%		67%						
3	В	256	5%	58%		15%	•	9%			



Mol	Chain	Length		Quality of chain								
4	С	239	17%	51%	17% · 14%							
5	D	209	6% 33%	55%	11% •							
6	Е	162	.%	53%	9% • 7%							
7	F	101	<u>6%</u> <u>31%</u>	64%	5%							
8	G	156	.%	58%	10% •							
9	Н	138	% 44%	46%	9% •							
10	Ι	128	9% 23%	69%	5% ••							
11	J	105	11%	55%	25% • 7%							
12	Κ	129	24%	57%	9% • 8%							
13	L	135	4%	48%	12% • 8%							
14	М	126	10% 21%	62%	15% ••							
15	Ν	61	5%	67%	15% •							
16	О	89	3% 46%	47%	6% •							
17	Р	88	2% 45%	50%	5%							
18	Q	105	6% 41%	52%	5% ••							
19	R	88	3%	57%	9% 17%							
20	S	93	26%	59%	15% 14%							
21	Т	106	<u>6%</u> 25%	49%	18% • 7%							
22	V	26	38%	54%	8%							

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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	А	1550	-	-	-	Х
23	MG	А	1566	-	-	-	Х
23	MG	А	1568	-	-	-	Х
23	MG	А	1585	-	-	-	Х
23	MG	А	1615	-	-	-	Х



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	А	1618	-	-	-	Х
23	MG	А	212	-	-	-	Х
23	MG	Н	213	-	-	-	Х

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$1 \mathrm{HNX}$

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		A	Atoms		ZeroOcc	AltConf	Trace	
1	А	1507	Total 32391	C 14418	N 6002	O 10465	Р 1506	22	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Х	6	Total 117	C 54	N 14	0 44	Р 5	0	0	0

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
2	В	234	Total	С	Ν	0	\mathbf{S}	0	0	0
0	D	234	1900	1213	341	341	5	0	0	0

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

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

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

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

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	Е	150	Total 1146	C 724	N 217	O 201	S 4	0	0	0



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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
7	F	101	Total 843	C 531	N 155	O 154	${ m S} { m 3}$	0	0	0

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

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

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
9	Н	138	Total 1116	C 705	N 215	0 193	${ m S} { m 3}$	0	0	0

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

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
10	Ι	127	Total 1011	C 639	N 198	О 174	0	0	0

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

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

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

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
12	K	119	Total 885	C 549	N 168	0 165	${ m S} { m 3}$	0	0	0

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

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

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



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
14	М	125	Total 997	C 617	N 207	0 171	${ m S} { m 2}$	0	0	0

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

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
15	Ν	60	Total 492	C 312	N 104	0 72	$\frac{S}{4}$	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	О	88	Total 734	C 459	N 147	0 126	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
17	Р	88	Total 735	C 462	N 147	0 125	S 1	0	0	0

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

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

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

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

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	S	80	Total 647	C 414	N 119	0 112	${S \over 2}$	0	0	0

 $\bullet\,$ Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
21	Т	99	Total 762	C 469	N 162	O 129	${ m S} { m 2}$	0	0	0

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

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

• Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	А	94	Total Mg 94 94	0	0
23	D	1	Total Mg 1 1	0	0
23	Н	1	Total Mg 1 1	0	0

• Molecule 24 is Pactamyc
in (three-letter code: PCY) (formula: $\mathrm{C}_{28}\mathrm{H}_{38}\mathrm{N}_4\mathrm{O}_8).$



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
24	А	1	Total 40	C 28	N 4	0 8	0	0

• Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).



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



3 Residue-property plots (i)

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

G682 G683	A684	G685 U686	A687 C688	0000 0089	6690 6691	U692	6693	A694 A695	A696	1697	G698	C701	A702	G703	A104	CT07	C708	G709	6/10	G713		A716	C717 C718	C719	C720	G721	A/22 U723		C726	A728	A729	G730 G731	C732	A733	G735 C735	C736	A737	C738	G741	G742	0743 0744	C745	A746 C747
C748 C749	G750	U751 G752	A753	G755	C756 11757	G758	A759	G761	C762		G765 4766	A767	A768	G7 69	G771	U772	G773	G774	G775 G776	A777	G7.78	C779	A780 A781	A782	C783	C784	G7 86 G7 86	A787	U788	G791	A792	0793 A794	C7 95	C796	C/9/ G798		G803	0804 C805	C806	<u>A807</u>	C808	C812	U813 A814
A815 4816	C817	G818 A819	U820 C821	C822	G823 C824	G825	C826	082/ A828	G829	G 830	0831 0832	U833	C834	U835	18.37 18.37	G 838	U839	C840	U841	C849	U850	G851	G852 C853	G854	<mark>G855</mark>	C856	G858	<u>A859</u>	A860 C861		A864	A865 C866	G867	C868	G874	C875	G876	C877 C878	C879	<mark>C880</mark>	G881 C887	C883	U884 G885
ARRO	0685	689 8	C899	A901	6902 6903		U911 2010	C912 A913	A914	A915	6916 6917	A918	A919	U920	1760	A923	C924	<u>6925</u>	G926 G927	G928	<mark>(929</mark>	C 330	C931	C934	A935	C 336	<mark>6939</mark>	C940	6941 2012	U943	G944	G945 A946	G947	C948	A949 11950	G951	U952	6953 Co54	H 000	0957	A958	0960	U961 C962
A965	G966	C967 A968	A969	G971	C972 C973	A974	A975	G976 A977	• A978	C979	C980	A983	C984	C985	A300	C 389	• 066D	U991	1992	A994	C995	A996	1997	C999	U1000	A1001	G1003	G1003A	A1004	C1006	C1007	C1008 G1009	G1010	G1011	01012 61013	A1014	A1015	A1016	C1018	C1019	U1020	G1022	G1023 G1024
U1025	C1027	C1028 • C1029 •	C1030	C1030B	G1030C	G1031	G1032	G1033 G1034	A1035	G1036	C1037	C1039	U1040	A1041	G1042	A1044	C1045	A1046	G1047 G1048	U1049	G1050	C1051	U1052	G1054	A1055	U1056	G1058	<mark>C1059</mark>	C1060	U1062	C1063	G1064 U1065	C1066	A1067	G1068 C1069	U1070	C1071	G1072 111073	G1074		G1077 111078	G1079	A1080
U1085		G1089	U1091	A1093	G1094 111095	C1096	C1097	C1098 G1099	C1100	A1101	A1102 C1103	G1104 G1104	A1105	G1106	C1109	A1110	A1111	C1112	CI113	C1116	G1117	C1118	C1119 C1120	01121	U1122	A1123	U1125	U1126	G1127	C1129	A1130	G1131 C1132	G1133	G1134	01135 111136	C1137	G1138	G1139 C1140	C1141	G1142	G1143	C1145	A1146 C1147
01148 01149	U1150	A1151 A1152	C1153 21154	31155 31155	31156 A1157	C1158	U1159	d1 160 C1 161	c1162	C1163	31164 C1165	31166 31166	A1167	A1168	A1169	C1172	31173	31174 51174	G1175	31177	31178	A1179 •	A1180	11101 51182	A1 183	31184 31184	1180 11186	<u> 31 187</u>	A1188	31190	A1191	01192 01193	01194	C1 195	01196 31197	31198	U1199	C1200	31202 31202	c1203	A1204 11 205	31206	31207 C1208
C1209	U1211	U1212 A1213	C1214 C1215	G1216	C1217 C1218	U1219	G1220	G1221 G1222	c1223	G1224	A1225	A1227	C1228	A1229	C1 230 G1 231	U1232	G1233	C1234	01 235 A1 236	C1237	A1238	A1239	01240 61241	G1242	C1243	C1244	A1245 C1246		C1249 A1250	A1251	A1252	G1253 C1254	G1255	A1256	01257 G1258	C1259	<mark>c1260</mark>	A1261 C1262	C1263	C1264	G1265 C1266	G1267	A1268 • A1269 •
C1270	31272	31273	31276	01278	A1279	U1281	C1282	d1283 C1284	A1285	A1286	A1287	A1289	<u> 31290</u>	31291	01.292 01.292	31294	31295	C1296	01.297 01.298	A1299	31300	U1301	U1302	31304	31305	A1306	01307 01308	31309	31310 31311	G1312 ●	U1313	01314 01315	31316	C1317	A1318 A1319	C1320	c1321	01322 1323	41324 A1324	c1325	C1326 ゴ 327	c1328 C1328	A1329 U1330
1331 1332	1333	1334 • 1335	1336 1336	1338	1339 1340	1341	1342	1344	1345	1346	1347	1349		1352	1354	1355	1356	1357	1358	1360	1361	1361A	1362	1364	1365	1366	1368	1369	1370	1372	1373	1374 1375	1376	1377	1379	1380	1381	1382	1385	1386	1387	1391	1392 1393
1394 G	1396 A	1397 G	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1403	1404 A	1406 U	1407 100		1411 U	1412 A	1413 G	1415 A	1416			1420 • G	1421 • G	1422 A	1423	1425 A	1426 G	1427 C	1428 1720		1433 G	1434 C	1430 1436 G	1437 C	1438 1430	1440 U	1441 • G	1442 • A	1446 U	A A A	1449 450	1451	1452 U	1453 C	1455 G	1459 G	1460 G	1462 U	1463 1464 U
C1465 C1466	G1467	A1468 • Ci G1469 • A1	G1470 G1471	U1472 C1	A1473 • Ci c1 474 • c1	G1475 U1	G1476 C1	C1478	C1479	G1480 C:	01481 A. C1482 • 11	A1483 G1	5	G1486 G1 24 467	G1488 G1488 G1	G1489 C1	C1490 G1	G1491 G1		G1494 U1	U1495	C1496 U.	G1497 Ai	A1499	A1500 A1	C1501 A1	A1502 01	G1504 C3	G1505 G1 111 EDE	A1507 C1	G1508 G1	C1509 U1510	G1511 A1	U1512	A1513 C1514	C1515 A1	G1516 • C1	G1517 A1518	A1519 G1	G1520 C1	G1521 A.	G1523 G1	C1524 G1525 G1



















4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	401.72Å 401.72Å 177.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	95.34 - 3.40	Depositor
	94.29 - 3.11	EDS
% Data completeness	88.9 (95.34-3.40)	Depositor
(in resolution range)	83.7 (94.29-3.11)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.12	Depositor
$< I/\sigma(I) > 1$	$1.74 (at 3.13 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
B B.	0.232 , 0.280	Depositor
II, II free	0.203 , 0.247	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 $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 105.5	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, PCY

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).

Mal	Chain	Bond	lengths	B	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.53	0/36259	0.75	42/56593~(0.1%)
2	Х	0.56	0/128	0.71	0/196
3	В	0.39	0/1935	0.69	0/2609
4	С	0.38	0/1636	0.65	0/2205
5	D	0.43	0/1733	0.71	1/2318~(0.0%)
6	Е	0.49	0/1162	0.80	2/1564~(0.1%)
7	F	0.35	0/856	0.65	0/1154
8	G	0.36	0/1276	0.64	0/1709
9	Н	0.47	0/1136	0.78	0/1527
10	Ι	0.35	0/1029	0.66	0/1378
11	J	0.37	0/805	0.68	0/1082
12	Κ	0.40	0/900	0.75	0/1213
13	L	0.43	0/986	0.75	0/1320
14	М	0.35	0/1008	0.68	0/1347
15	Ν	0.41	0/501	0.78	0/664
16	0	0.39	0/745	0.64	0/992
17	Р	0.46	0/751	0.76	0/1008
18	Q	0.50	0/870	0.78	0/1159
19	R	0.38	0/603	0.65	0/799
20	S	0.35	0/661	0.68	1/890~(0.1%)
21	Т	0.38	0/764	0.73	0/1006
22	V	0.50	0/212	0.64	0/277
All	All	0.49	0/55956	0.74	$46/\overline{83010~(0.1\%)}$

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
1	А	2	47



There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	1498	U	C2'-C3'-O3'	9.79	131.03	109.50
1	А	1085	U	C2'-C3'-O3'	9.22	129.78	109.50
1	А	60	А	C2'-C3'-O3'	8.05	127.22	109.50
1	А	484	G	C2'-C3'-O3'	7.86	126.78	109.50
1	А	181	G	C2'-C3'-O3'	7.65	126.34	109.50

All (2) chirality outliers are listed below:

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

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	116	А	Sidechain
1	А	126	G	Sidechain
1	А	47	С	Sidechain
1	А	5	U	Sidechain
1	А	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	А	32391	0	16349	1512	0
2	Х	117	0	64	3	0
3	В	1900	0	1951	289	0
4	С	1612	0	1677	276	0
5	D	1703	0	1764	182	0
6	Е	1146	0	1207	120	0
7	F	843	0	857	83	0
8	G	1257	0	1296	113	0
9	Н	1116	0	1177	96	0
10	Ι	1011	0	1043	151	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	792	0	835	158	0
12	K	885	0	904	100	0
13	L	970	0	1057	125	0
14	М	997	0	1072	142	0
15	N	492	0	529	87	0
16	0	734	0	771	63	0
17	Р	735	0	752	67	0
18	Q	857	0	930	104	0
19	R	597	0	668	106	0
20	S	647	0	673	105	0
21	Т	762	0	859	106	0
22	V	208	0	221	20	0
23	А	94	0	0	0	0
23	D	1	0	0	0	0
23	Н	1	0	0	0	0
24	A	40	0	38	10	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	51910	0	36694	3662	0

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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 42.

The worst 5 of 3662 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 (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.



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

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

5 of 225 Ramachandran outliers are listed below:

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



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
3	В	202/220~(92%)	181 (90%)	21 (10%)	7	25
4	С	160/188~(85%)	136~(85%)	24 (15%)	3	12
5	D	180/181~(99%)	168~(93%)	12 (7%)	16	46
6	Е	115/123~(94%)	102 (89%)	13 (11%)	6	21
7	F	90/90~(100%)	87~(97%)	3~(3%)	38	66
8	G	126/127~(99%)	119 (94%)	7~(6%)	21	51
9	Н	119/119~(100%)	105~(88%)	14 (12%)	5	19
10	Ι	98/99~(99%)	86~(88%)	12 (12%)	5	18
11	J	87/92~(95%)	76 (87%)	11 (13%)	4	17
12	K	90/99~(91%)	85 (94%)	5 (6%)	21	51
13	L	104/111~(94%)	96~(92%)	8 (8%)	13	40
14	М	100/101~(99%)	93~(93%)	7 (7%)	15	44
15	Ν	49/50~(98%)	45 (92%)	4 (8%)	11	37
16	Ο	79/80~(99%)	77~(98%)	2(2%)	47	72
17	Р	74/74~(100%)	70~(95%)	4(5%)	22	52
18	Q	96/97~(99%)	92~(96%)	4 (4%)	30	59
19	R	64/77~(83%)	57~(89%)	7 (11%)	6	23
20	S	71/80~(89%)	67 (94%)	4 (6%)	21	51
21	Т	76/82~(93%)	68 (90%)	8 (10%)	7	25
22	V	19/21~(90%)	19 (100%)	0	100	100
All	All	1999/2111~(95%)	1829 (92%)	170 (8%)	10	35

5 of 170 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
11	J	83	GLU
17	Р	32	TYR
12	Κ	35	PRO



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Mol	Chain	Res	Type
14	М	9	ILE
18	Q	96	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
7	F	57	GLN
18	Q	16	GLN
8	G	68	ASN
16	0	37	ASN
21	Т	16	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	1507/1522~(99%)	220 (14%)	85~(5%)
2	Х	5/6~(83%)	1 (20%)	0
All	All	1512/1528~(98%)	221 (14%)	85~(5%)

5 of 221 RNA backbone outliers are listed below:

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

5 of 85 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	А	1139	G
1	А	1285	А
1	А	1182	G
1	А	1224	G
1	А	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 monosaccharides 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 T	Type	Chain	Dog	Res Link	Bond lengths			Bond angles		
	туре		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
24	PCY	А	1632	-	36,42,42	7.68	36 (100%)	41,65,65	1.60	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	А	1632	-	-	13/33/67/67	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	А	1632	PCY	C1-N4	11.60	1.54	1.35
24	А	1632	PCY	C17-N20	11.35	1.59	1.45
24	А	1632	PCY	C24-C22	10.34	1.56	1.39
24	А	1632	PCY	C27-C30	9.67	1.53	1.40
24	А	1632	PCY	O36-C31	9.25	1.55	1.36

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



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
24	А	1632	PCY	C22-N20-C17	-5.10	112.19	123.11
24	А	1632	PCY	C31-C27-C30	3.51	122.01	118.06
24	А	1632	PCY	C8-C3-N2	-3.25	106.39	112.12
24	А	1632	PCY	C18-O21-C23	3.21	123.03	116.57
24	А	1632	PCY	C3-N2-C1	2.96	132.93	124.47

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
24	А	1632	PCY	N4-C1-N2-C3
24	А	1632	PCY	O5-C1-N2-C3
24	А	1632	PCY	N2-C1-N4-C9
24	А	1632	PCY	N2-C1-N4-C10
24	А	1632	PCY	O5-C1-N4-C9

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	А	1632	PCY	10	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 then 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, 95^{th} 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	А	1506/1522~(98%)	1.16	211 (14%) 2 3	37, 70, 161, 199	0
2	Х	6/6~(100%)	1.00	1 (16%) 1 2	62, 79, 117, 151	0
3	В	234/256~(91%)	0.23	14 (5%) 21 23	34, 87, 162, 199	0
4	С	206/239~(86%)	0.07	1 (0%) 91 90	41, 91, 153, 179	0
5	D	208/209~(99%)	0.28	12 (5%) 23 24	35, 71, 128, 191	0
6	Е	150/162~(92%)	0.10	1 (0%) 87 87	34, 58, 111, 168	0
7	F	101/101~(100%)	0.46	6 (5%) 22 23	56, 95, 147, 167	0
8	G	155/156~(99%)	0.03	2 (1%) 77 76	47, 85, 147, 175	0
9	Η	138/138~(100%)	0.05	2 (1%) 75 74	21, 52, 92, 139	0
10	Ι	127/128~(99%)	0.44	12 (9%) 8 10	37, 96, 140, 181	0
11	J	98/105~(93%)	0.67	12 (12%) 4 5	50, 119, 184, 199	0
12	K	119/129~(92%)	0.30	4 (3%) 45 44	41, 73, 137, 178	0
13	L	124/135~(91%)	0.34	6 (4%) 30 31	30, 72, 131, 180	0
14	М	125/126~(99%)	0.67	13 (10%) 6 8	56, 89, 153, 188	0
15	Ν	60/61~(98%)	0.45	3 (5%) 28 29	50, 86, 157, 170	0
16	Ο	88/89~(98%)	0.24	3 (3%) 45 44	38, 70, 136, 186	0
17	Р	88/88~(100%)	0.28	2 (2%) 60 59	35, 63, 164, 198	0
18	Q	104/105~(99%)	0.62	6 (5%) 23 24	35,62,137,199	0
19	R	73/88~(82%)	0.25	3 (4%) 37 36	43, 75, 154, 194	0
20	S	80/93~(86%)	1.65	24 (30%) 0 0	66, 110, 158, 199	0
21	Т	99/106~(93%)	0.36	6 (6%) 21 22	44, 72, 133, 194	0
22	V	24/26 (92%)	0.58	2 (8%) 11 13	44, 79, 128, 149	0
All	All	3913/4068 (96%)	0.66	346 (8%) 10 11	$21, 75, \overline{155, 199}$	0

D W I D E

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Q	105	ALA	15.9
20	S	3	ARG	15.1
18	Q	103	GLY	13.3
14	М	124	PRO	13.1
18	Q	102	GLY	10.7

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, 95^{th} 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
23	MG	А	1550	1/1	0.53	0.74	45,45,45,45	1
23	MG	А	210	1/1	0.64	0.37	45,45,45,45	1
23	MG	Н	213	1/1	0.65	1.00	45,45,45,45	1
23	MG	А	1556	1/1	0.67	0.26	45,45,45,45	1
23	MG	А	1618	1/1	0.68	0.80	45,45,45,45	1
23	MG	А	1619	1/1	0.71	0.23	45,45,45,45	1
23	MG	А	1613	1/1	0.71	0.27	45,45,45,45	1
23	MG	А	1614	1/1	0.72	0.28	45,45,45,45	0
23	MG	А	1548	1/1	0.73	0.30	45,45,45,45	0
23	MG	А	1566	1/1	0.75	0.41	45,45,45,45	0
23	MG	А	212	1/1	0.76	0.95	45,45,45,45	1
23	MG	А	1564	1/1	0.77	0.22	45,45,45,45	0
23	MG	А	1568	1/1	0.78	0.57	45,45,45,45	0
23	MG	А	1585	1/1	0.78	0.42	45,45,45,45	1
23	MG	А	1615	1/1	0.78	0.96	45,45,45,45	1
23	MG	А	1590	1/1	0.79	0.34	45,45,45,45	0
23	MG	А	1558	1/1	0.82	0.30	45,45,45,45	0
23	MG	А	1581	1/1	0.83	0.23	45,45,45,45	1
23	MG	А	1545	1/1	0.83	0.11	45,45,45,45	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
23	MG	А	1549	1/1	0.83	0.17	45,45,45,45	1
23	MG	А	1605	1/1	0.83	0.11	45,45,45,45	0
23	MG	А	1611	1/1	0.85	0.20	45,45,45,45	1
23	MG	А	1623	1/1	0.86	0.43	45,45,45,45	1
23	MG	А	71	1/1	0.86	0.47	45,45,45,45	0
23	MG	А	1578	1/1	0.87	0.33	45,45,45,45	0
23	MG	А	1620	1/1	0.88	0.19	45,45,45,45	0
23	MG	А	1567	1/1	0.88	0.59	45,45,45,45	0
23	MG	А	1609	1/1	0.88	0.16	45,45,45,45	0
23	MG	А	1597	1/1	0.89	0.12	45,45,45,45	0
23	MG	А	1575	1/1	0.89	0.13	45,45,45,45	1
23	MG	А	1592	1/1	0.89	0.12	45,45,45,45	0
23	MG	А	1612	1/1	0.89	0.31	45,45,45,45	0
23	MG	А	1580	1/1	0.90	0.17	45,45,45,45	0
23	MG	А	1591	1/1	0.90	0.51	$45,\!45,\!45,\!45$	0
23	MG	А	214	1/1	0.90	0.16	$45,\!45,\!45,\!45$	0
23	MG	А	1571	1/1	0.90	0.24	$45,\!45,\!45,\!45$	0
23	MG	А	1574	1/1	0.90	0.30	45,45,45,45	0
23	MG	А	1604	1/1	0.90	0.20	$45,\!45,\!45,\!45$	1
23	MG	А	1587	1/1	0.90	0.36	45,45,45,45	0
23	MG	А	1570	1/1	0.91	0.31	$45,\!45,\!45,\!45$	1
23	MG	А	211	1/1	0.91	0.33	45,45,45,45	0
23	MG	А	1626	1/1	0.91	0.30	$45,\!45,\!45,\!45$	1
23	MG	А	1599	1/1	0.91	0.28	$45,\!45,\!45,\!45$	0
24	PCY	А	1632	40/40	0.91	0.34	28,28,28,28	0
23	MG	А	1610	1/1	0.92	0.18	$45,\!45,\!45,\!45$	0
23	MG	А	1582	1/1	0.92	0.32	45,45,45,45	1
23	MG	A	1616	1/1	0.92	0.18	45,45,45,45	0
23	MG	D	215	1/1	0.92	0.31	45,45,45,45	0
23	MG	A	87	1/1	0.92	0.24	45,45,45,45	1
23	MG	A	86	1/1	0.92	0.40	45,45,45,45	0
23	MG	A	1586	1/1	0.93	0.38	45,45,45,45	0
23	MG	A	1601	1/1	0.93	0.17	45,45,45,45	0
23	MG	A	1551	1/1	0.93	0.36	45,45,45,45	0
23	MG	A	1565	1/1	0.93	0.67	45,45,45,45	0
23	MG	A	1559	1/1	0.93	0.42	45,45,45,45	0
23	MG	A	1560	1/1	0.93	0.29	45,45,45,45	0
23	MG	A	1596	1/1	0.93	0.40	45,45,45,45	1
23	MG	A	1576	1/1	0.93	0.20	45,45,45,45	0
23	MG	А	1583	1/1	0.94	0.12	45,45,45,45	0
23	MG	A	1594	1/1	0.94	0.35	45,45,45,45	0
23	MG	A	1606	1/1	0.94	$0.5\overline{2}$	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
23	MG	А	1607	1/1	0.94	0.29	45,45,45,45	0
23	MG	А	1563	1/1	0.94	0.22	45,45,45,45	0
23	MG	А	1588	1/1	0.95	0.29	45,45,45,45	0
23	MG	А	1561	1/1	0.95	0.73	45,45,45,45	0
23	MG	А	1546	1/1	0.95	0.38	45,45,45,45	0
23	MG	А	1621	1/1	0.95	0.57	45,45,45,45	1
23	MG	А	1569	1/1	0.95	1.06	45,45,45,45	1
23	MG	А	1624	1/1	0.95	0.50	45,45,45,45	1
23	MG	А	1600	1/1	0.95	0.38	45,45,45,45	0
23	MG	А	1629	1/1	0.95	0.70	45,45,45,45	1
23	MG	А	1593	1/1	0.95	0.33	45,45,45,45	0
23	MG	А	1602	1/1	0.95	0.37	45,45,45,45	0
23	MG	А	1603	1/1	0.95	0.20	45,45,45,45	0
23	MG	А	1562	1/1	0.96	0.65	45,45,45,45	0
23	MG	А	1577	1/1	0.96	0.25	45,45,45,45	0
23	MG	А	1630	1/1	0.96	1.31	45,45,45,45	1
23	MG	А	1598	1/1	0.96	0.23	45,45,45,45	1
23	MG	А	1572	1/1	0.96	0.61	45,45,45,45	0
23	MG	А	1553	1/1	0.96	0.40	45,45,45,45	0
23	MG	А	1552	1/1	0.97	0.20	45,45,45,45	0
23	MG	А	1595	1/1	0.97	0.35	45,45,45,45	0
23	MG	А	1617	1/1	0.97	0.40	45,45,45,45	1
23	MG	А	1547	1/1	0.97	0.50	45,45,45,45	0
23	MG	А	1579	1/1	0.97	0.28	45,45,45,45	0
23	MG	А	1573	1/1	0.97	0.47	45,45,45,45	0
23	MG	А	1555	1/1	0.97	0.32	$45,\!45,\!45,\!45$	0
23	MG	А	1622	1/1	0.97	0.51	$45,\!45,\!45,\!45$	1
23	MG	А	1554	1/1	0.98	0.51	$45,\!45,\!45,\!45$	0
23	MG	А	1584	1/1	0.98	0.47	45,45,45,45	0
23	MG	А	1608	1/1	0.98	0.07	45,45,45,45	0
23	MG	А	1557	1/1	0.98	0.43	45,45,45,45	0
23	MG	А	1589	1/1	0.98	0.32	45,45,45,45	0
23	MG	А	1631	1/1	0.99	0.54	45,45,45,45	1
23	MG	A	1628	1/1	0.99	0.26	45,45,45,45	1
23	MG	А	1625	1/1	0.99	0.19	45,45,45,45	1
23	MG	А	1627	1/1	0.99	0.39	45,45,45,45	1
25	ZN	D	300	1/1	0.99	0.34	53, 53, 53, 53	0
25	ZN	Ν	190	1/1	1.00	0.22	$53,\!53,\!53,\!53$	1

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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.

