



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:54 AM UTC

PDB ID : 6R4O / pdb_00006r4o
EMDB ID : EMD-4721
Title : Structure of a truncated adenylyl cyclase bound to MANT-GTP, forskolin and an activated stimulatory G α protein
Authors : Qi, C.; Sorrentino, S.; Medalia, O.; Korkhov, V.M.
Deposited on : 2019-03-22
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

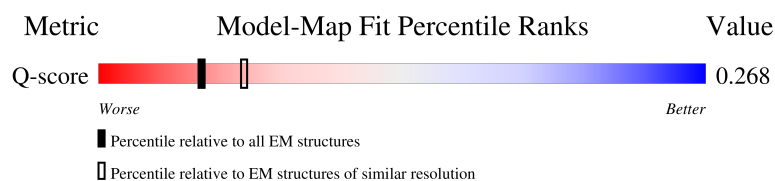
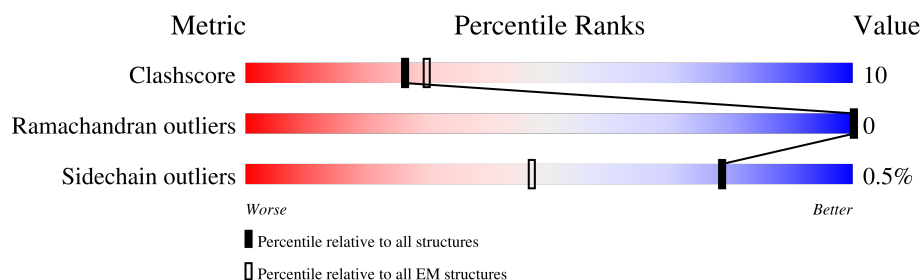
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

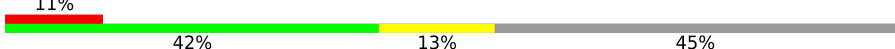
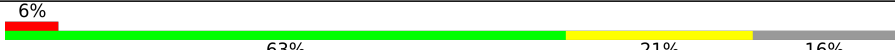
The reported resolution of this entry is 4.20 Å.

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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1533	
2	B	405	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9602 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Adenylate cyclase 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	841	Total	C	N	O	S	0	0
			6687	4339	1100	1193	55		

There are 283 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1251	ALA	-	expression tag	UNP E1BM79
A	1252	ALA	-	expression tag	UNP E1BM79
A	1253	ALA	-	expression tag	UNP E1BM79
A	1254	LEU	-	expression tag	UNP E1BM79
A	1255	GLU	-	expression tag	UNP E1BM79
A	1256	VAL	-	expression tag	UNP E1BM79
A	1257	LEU	-	expression tag	UNP E1BM79
A	1258	PHE	-	expression tag	UNP E1BM79
A	1259	GLN	-	expression tag	UNP E1BM79
A	1260	GLY	-	expression tag	UNP E1BM79
A	1261	PRO	-	expression tag	UNP E1BM79
A	1262	GLY	-	expression tag	UNP E1BM79
A	1263	GLY	-	expression tag	UNP E1BM79
A	1264	VAL	-	expression tag	UNP E1BM79
A	1265	SER	-	expression tag	UNP E1BM79
A	1266	LYS	-	expression tag	UNP E1BM79
A	1267	GLY	-	expression tag	UNP E1BM79
A	1268	GLU	-	expression tag	UNP E1BM79
A	1269	GLU	-	expression tag	UNP E1BM79
A	1270	LEU	-	expression tag	UNP E1BM79
A	1271	PHE	-	expression tag	UNP E1BM79
A	1272	THR	-	expression tag	UNP E1BM79
A	1273	GLY	-	expression tag	UNP E1BM79
A	1274	VAL	-	expression tag	UNP E1BM79
A	1275	VAL	-	expression tag	UNP E1BM79
A	1276	PRO	-	expression tag	UNP E1BM79
A	1277	ILE	-	expression tag	UNP E1BM79
A	1278	LEU	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	VAL	-	expression tag	UNP E1BM79
A	1280	GLU	-	expression tag	UNP E1BM79
A	1281	LEU	-	expression tag	UNP E1BM79
A	1282	ASP	-	expression tag	UNP E1BM79
A	1283	GLY	-	expression tag	UNP E1BM79
A	1284	ASP	-	expression tag	UNP E1BM79
A	1285	VAL	-	expression tag	UNP E1BM79
A	1286	ASN	-	expression tag	UNP E1BM79
A	1287	GLY	-	expression tag	UNP E1BM79
A	1288	HIS	-	expression tag	UNP E1BM79
A	1289	LYS	-	expression tag	UNP E1BM79
A	1290	PHE	-	expression tag	UNP E1BM79
A	1291	SER	-	expression tag	UNP E1BM79
A	1292	VAL	-	expression tag	UNP E1BM79
A	1293	SER	-	expression tag	UNP E1BM79
A	1294	GLY	-	expression tag	UNP E1BM79
A	1295	GLU	-	expression tag	UNP E1BM79
A	1296	GLY	-	expression tag	UNP E1BM79
A	1297	GLU	-	expression tag	UNP E1BM79
A	1298	GLY	-	expression tag	UNP E1BM79
A	1299	ASP	-	expression tag	UNP E1BM79
A	1300	ALA	-	expression tag	UNP E1BM79
A	1301	THR	-	expression tag	UNP E1BM79
A	1302	TYR	-	expression tag	UNP E1BM79
A	1303	GLY	-	expression tag	UNP E1BM79
A	1304	LYS	-	expression tag	UNP E1BM79
A	1305	LEU	-	expression tag	UNP E1BM79
A	1306	THR	-	expression tag	UNP E1BM79
A	1307	LEU	-	expression tag	UNP E1BM79
A	1308	LYS	-	expression tag	UNP E1BM79
A	1309	PHE	-	expression tag	UNP E1BM79
A	1310	ILE	-	expression tag	UNP E1BM79
A	1311	CYS	-	expression tag	UNP E1BM79
A	1312	THR	-	expression tag	UNP E1BM79
A	1313	THR	-	expression tag	UNP E1BM79
A	1314	GLY	-	expression tag	UNP E1BM79
A	1315	LYS	-	expression tag	UNP E1BM79
A	1316	LEU	-	expression tag	UNP E1BM79
A	1317	PRO	-	expression tag	UNP E1BM79
A	1318	VAL	-	expression tag	UNP E1BM79
A	1319	PRO	-	expression tag	UNP E1BM79
A	1320	TRP	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1321	PRO	-	expression tag	UNP E1BM79
A	1322	THR	-	expression tag	UNP E1BM79
A	1323	LEU	-	expression tag	UNP E1BM79
A	1324	VAL	-	expression tag	UNP E1BM79
A	1325	THR	-	expression tag	UNP E1BM79
A	1326	THR	-	expression tag	UNP E1BM79
A	1327	PHE	-	expression tag	UNP E1BM79
A	1328	GLY	-	expression tag	UNP E1BM79
A	1329	TYR	-	expression tag	UNP E1BM79
A	1330	GLY	-	expression tag	UNP E1BM79
A	1331	LEU	-	expression tag	UNP E1BM79
A	1332	GLN	-	expression tag	UNP E1BM79
A	1333	CYS	-	expression tag	UNP E1BM79
A	1334	PHE	-	expression tag	UNP E1BM79
A	1335	ALA	-	expression tag	UNP E1BM79
A	1336	ARG	-	expression tag	UNP E1BM79
A	1337	TYR	-	expression tag	UNP E1BM79
A	1338	PRO	-	expression tag	UNP E1BM79
A	1339	ASP	-	expression tag	UNP E1BM79
A	1340	HIS	-	expression tag	UNP E1BM79
A	1341	MET	-	expression tag	UNP E1BM79
A	1342	LYS	-	expression tag	UNP E1BM79
A	1343	GLN	-	expression tag	UNP E1BM79
A	1344	HIS	-	expression tag	UNP E1BM79
A	1345	ASP	-	expression tag	UNP E1BM79
A	1346	PHE	-	expression tag	UNP E1BM79
A	1347	PHE	-	expression tag	UNP E1BM79
A	1348	LYS	-	expression tag	UNP E1BM79
A	1349	SER	-	expression tag	UNP E1BM79
A	1350	ALA	-	expression tag	UNP E1BM79
A	1351	MET	-	expression tag	UNP E1BM79
A	1352	PRO	-	expression tag	UNP E1BM79
A	1353	GLU	-	expression tag	UNP E1BM79
A	1354	GLY	-	expression tag	UNP E1BM79
A	1355	TYR	-	expression tag	UNP E1BM79
A	1356	VAL	-	expression tag	UNP E1BM79
A	1357	GLN	-	expression tag	UNP E1BM79
A	1358	GLU	-	expression tag	UNP E1BM79
A	1359	ARG	-	expression tag	UNP E1BM79
A	1360	THR	-	expression tag	UNP E1BM79
A	1361	ILE	-	expression tag	UNP E1BM79
A	1362	PHE	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1363	PHE	-	expression tag	UNP E1BM79
A	1364	LYS	-	expression tag	UNP E1BM79
A	1365	ASP	-	expression tag	UNP E1BM79
A	1366	ASP	-	expression tag	UNP E1BM79
A	1367	GLY	-	expression tag	UNP E1BM79
A	1368	ASN	-	expression tag	UNP E1BM79
A	1369	TYR	-	expression tag	UNP E1BM79
A	1370	LYS	-	expression tag	UNP E1BM79
A	1371	THR	-	expression tag	UNP E1BM79
A	1372	ARG	-	expression tag	UNP E1BM79
A	1373	ALA	-	expression tag	UNP E1BM79
A	1374	GLU	-	expression tag	UNP E1BM79
A	1375	VAL	-	expression tag	UNP E1BM79
A	1376	LYS	-	expression tag	UNP E1BM79
A	1377	PHE	-	expression tag	UNP E1BM79
A	1378	GLU	-	expression tag	UNP E1BM79
A	1379	GLY	-	expression tag	UNP E1BM79
A	1380	ASP	-	expression tag	UNP E1BM79
A	1381	THR	-	expression tag	UNP E1BM79
A	1382	LEU	-	expression tag	UNP E1BM79
A	1383	VAL	-	expression tag	UNP E1BM79
A	1384	ASN	-	expression tag	UNP E1BM79
A	1385	ARG	-	expression tag	UNP E1BM79
A	1386	ILE	-	expression tag	UNP E1BM79
A	1387	GLU	-	expression tag	UNP E1BM79
A	1388	LEU	-	expression tag	UNP E1BM79
A	1389	LYS	-	expression tag	UNP E1BM79
A	1390	GLY	-	expression tag	UNP E1BM79
A	1391	ILE	-	expression tag	UNP E1BM79
A	1392	ASP	-	expression tag	UNP E1BM79
A	1393	PHE	-	expression tag	UNP E1BM79
A	1394	LYS	-	expression tag	UNP E1BM79
A	1395	GLU	-	expression tag	UNP E1BM79
A	1396	ASP	-	expression tag	UNP E1BM79
A	1397	GLY	-	expression tag	UNP E1BM79
A	1398	ASN	-	expression tag	UNP E1BM79
A	1399	ILE	-	expression tag	UNP E1BM79
A	1400	LEU	-	expression tag	UNP E1BM79
A	1401	GLY	-	expression tag	UNP E1BM79
A	1402	HIS	-	expression tag	UNP E1BM79
A	1403	LYS	-	expression tag	UNP E1BM79
A	1404	LEU	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1405	GLU	-	expression tag	UNP E1BM79
A	1406	TYR	-	expression tag	UNP E1BM79
A	1407	ASN	-	expression tag	UNP E1BM79
A	1408	TYR	-	expression tag	UNP E1BM79
A	1409	ASN	-	expression tag	UNP E1BM79
A	1410	SER	-	expression tag	UNP E1BM79
A	1411	HIS	-	expression tag	UNP E1BM79
A	1412	ASN	-	expression tag	UNP E1BM79
A	1413	VAL	-	expression tag	UNP E1BM79
A	1414	TYR	-	expression tag	UNP E1BM79
A	1415	ILE	-	expression tag	UNP E1BM79
A	1416	MET	-	expression tag	UNP E1BM79
A	1417	ALA	-	expression tag	UNP E1BM79
A	1418	ASP	-	expression tag	UNP E1BM79
A	1419	LYS	-	expression tag	UNP E1BM79
A	1420	GLN	-	expression tag	UNP E1BM79
A	1421	LYS	-	expression tag	UNP E1BM79
A	1422	ASN	-	expression tag	UNP E1BM79
A	1423	GLY	-	expression tag	UNP E1BM79
A	1424	ILE	-	expression tag	UNP E1BM79
A	1425	LYS	-	expression tag	UNP E1BM79
A	1426	VAL	-	expression tag	UNP E1BM79
A	1427	ASN	-	expression tag	UNP E1BM79
A	1428	PHE	-	expression tag	UNP E1BM79
A	1429	LYS	-	expression tag	UNP E1BM79
A	1430	ILE	-	expression tag	UNP E1BM79
A	1431	ARG	-	expression tag	UNP E1BM79
A	1432	HIS	-	expression tag	UNP E1BM79
A	1433	ASN	-	expression tag	UNP E1BM79
A	1434	ILE	-	expression tag	UNP E1BM79
A	1435	GLU	-	expression tag	UNP E1BM79
A	1436	ASP	-	expression tag	UNP E1BM79
A	1437	GLY	-	expression tag	UNP E1BM79
A	1438	SER	-	expression tag	UNP E1BM79
A	1439	VAL	-	expression tag	UNP E1BM79
A	1440	GLN	-	expression tag	UNP E1BM79
A	1441	LEU	-	expression tag	UNP E1BM79
A	1442	ALA	-	expression tag	UNP E1BM79
A	1443	ASP	-	expression tag	UNP E1BM79
A	1444	HIS	-	expression tag	UNP E1BM79
A	1445	TYR	-	expression tag	UNP E1BM79
A	1446	GLN	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1447	GLN	-	expression tag	UNP E1BM79
A	1448	ASN	-	expression tag	UNP E1BM79
A	1449	THR	-	expression tag	UNP E1BM79
A	1450	PRO	-	expression tag	UNP E1BM79
A	1451	ILE	-	expression tag	UNP E1BM79
A	1452	GLY	-	expression tag	UNP E1BM79
A	1453	ASP	-	expression tag	UNP E1BM79
A	1454	GLY	-	expression tag	UNP E1BM79
A	1455	PRO	-	expression tag	UNP E1BM79
A	1456	VAL	-	expression tag	UNP E1BM79
A	1457	LEU	-	expression tag	UNP E1BM79
A	1458	LEU	-	expression tag	UNP E1BM79
A	1459	PRO	-	expression tag	UNP E1BM79
A	1460	ASP	-	expression tag	UNP E1BM79
A	1461	ASN	-	expression tag	UNP E1BM79
A	1462	HIS	-	expression tag	UNP E1BM79
A	1463	TYR	-	expression tag	UNP E1BM79
A	1464	LEU	-	expression tag	UNP E1BM79
A	1465	SER	-	expression tag	UNP E1BM79
A	1466	TYR	-	expression tag	UNP E1BM79
A	1467	GLN	-	expression tag	UNP E1BM79
A	1468	SER	-	expression tag	UNP E1BM79
A	1469	ALA	-	expression tag	UNP E1BM79
A	1470	LEU	-	expression tag	UNP E1BM79
A	1471	SER	-	expression tag	UNP E1BM79
A	1472	LYS	-	expression tag	UNP E1BM79
A	1473	ASP	-	expression tag	UNP E1BM79
A	1474	PRO	-	expression tag	UNP E1BM79
A	1475	ASN	-	expression tag	UNP E1BM79
A	1476	GLU	-	expression tag	UNP E1BM79
A	1477	LYS	-	expression tag	UNP E1BM79
A	1478	ARG	-	expression tag	UNP E1BM79
A	1479	ASP	-	expression tag	UNP E1BM79
A	1480	HIS	-	expression tag	UNP E1BM79
A	1481	MET	-	expression tag	UNP E1BM79
A	1482	VAL	-	expression tag	UNP E1BM79
A	1483	LEU	-	expression tag	UNP E1BM79
A	1484	LEU	-	expression tag	UNP E1BM79
A	1485	GLU	-	expression tag	UNP E1BM79
A	1486	PHE	-	expression tag	UNP E1BM79
A	1487	VAL	-	expression tag	UNP E1BM79
A	1488	THR	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1489	ALA	-	expression tag	UNP E1BM79
A	1490	ALA	-	expression tag	UNP E1BM79
A	1491	GLY	-	expression tag	UNP E1BM79
A	1492	ILE	-	expression tag	UNP E1BM79
A	1493	THR	-	expression tag	UNP E1BM79
A	1494	LEU	-	expression tag	UNP E1BM79
A	1495	GLY	-	expression tag	UNP E1BM79
A	1496	MET	-	expression tag	UNP E1BM79
A	1497	ASP	-	expression tag	UNP E1BM79
A	1498	GLU	-	expression tag	UNP E1BM79
A	1499	LEU	-	expression tag	UNP E1BM79
A	1500	TYR	-	expression tag	UNP E1BM79
A	1501	LYS	-	expression tag	UNP E1BM79
A	1502	ALA	-	expression tag	UNP E1BM79
A	1503	ALA	-	expression tag	UNP E1BM79
A	1504	SER	-	expression tag	UNP E1BM79
A	1505	ALA	-	expression tag	UNP E1BM79
A	1506	TRP	-	expression tag	UNP E1BM79
A	1507	SER	-	expression tag	UNP E1BM79
A	1508	HIS	-	expression tag	UNP E1BM79
A	1509	PRO	-	expression tag	UNP E1BM79
A	1510	GLN	-	expression tag	UNP E1BM79
A	1511	PHE	-	expression tag	UNP E1BM79
A	1512	GLU	-	expression tag	UNP E1BM79
A	1513	LYS	-	expression tag	UNP E1BM79
A	1514	GLY	-	expression tag	UNP E1BM79
A	1515	GLY	-	expression tag	UNP E1BM79
A	1516	GLY	-	expression tag	UNP E1BM79
A	1517	SER	-	expression tag	UNP E1BM79
A	1518	GLY	-	expression tag	UNP E1BM79
A	1519	GLY	-	expression tag	UNP E1BM79
A	1520	GLY	-	expression tag	UNP E1BM79
A	1521	SER	-	expression tag	UNP E1BM79
A	1522	GLY	-	expression tag	UNP E1BM79
A	1523	GLY	-	expression tag	UNP E1BM79
A	1524	SER	-	expression tag	UNP E1BM79
A	1525	ALA	-	expression tag	UNP E1BM79
A	1526	TRP	-	expression tag	UNP E1BM79
A	1527	SER	-	expression tag	UNP E1BM79
A	1528	HIS	-	expression tag	UNP E1BM79
A	1529	PRO	-	expression tag	UNP E1BM79
A	1530	GLN	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1531	PHE	-	expression tag	UNP E1BM79
A	1532	GLU	-	expression tag	UNP E1BM79
A	1533	LYS	-	expression tag	UNP E1BM79

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	341	Total	C	N	O	S	0	0
			2809	1781	494	521	13		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65F	GLY	-	insertion	UNP P04896
B	65N	ASN	GLN	conflict	UNP P04896
B	65Q	LYS	ARG	conflict	UNP P04896
B	395	GLY	-	expression tag	UNP P04896
B	396	GLY	-	expression tag	UNP P04896
B	397	HIS	-	expression tag	UNP P04896
B	398	HIS	-	expression tag	UNP P04896
B	399	HIS	-	expression tag	UNP P04896
B	400	HIS	-	expression tag	UNP P04896
B	401	HIS	-	expression tag	UNP P04896
B	402	HIS	-	expression tag	UNP P04896
B	403	HIS	-	expression tag	UNP P04896
B	404	HIS	-	expression tag	UNP P04896

- Molecule 3 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: ONM) (formula: C₁₈H₂₃N₆O₁₅P₃).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			42	18	6	15	3	

- Molecule 4 is FORSKOLIN (CCD ID: FOK) (formula: $C_{22}H_{34}O_7$).

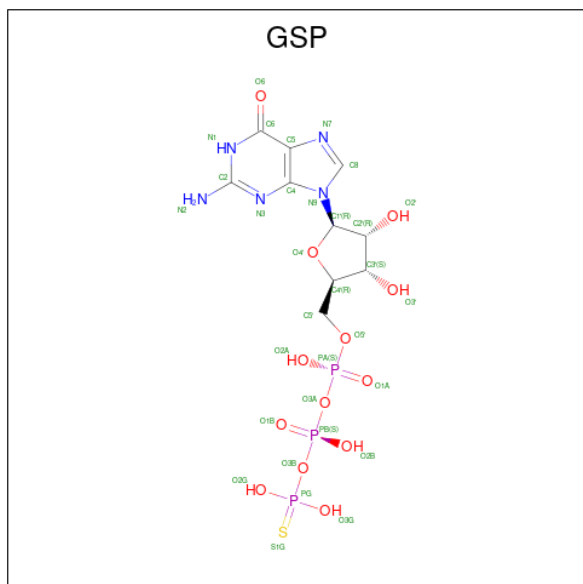


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			29	22	7	

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mn	0
			2	2	

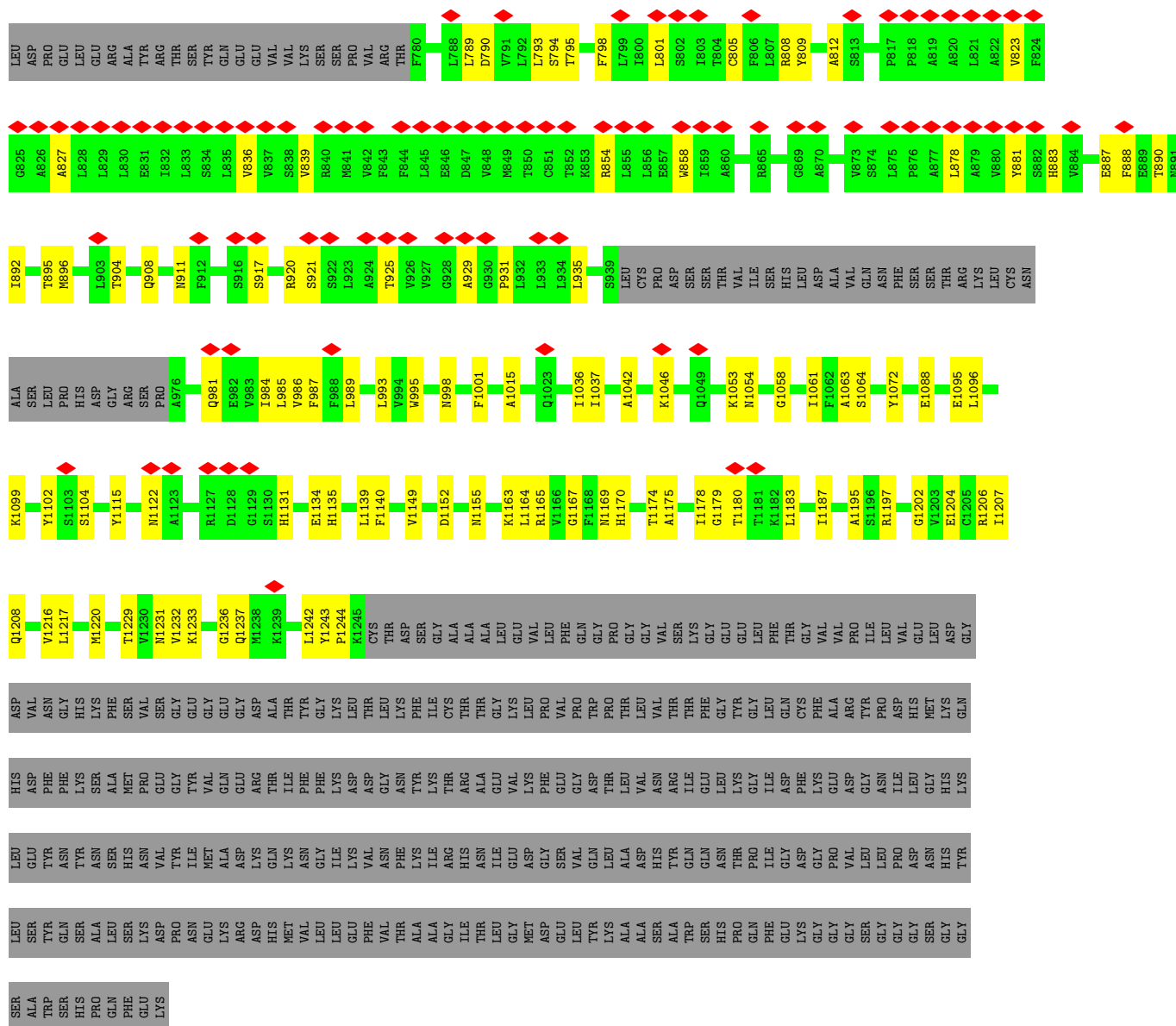
- Molecule 6 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



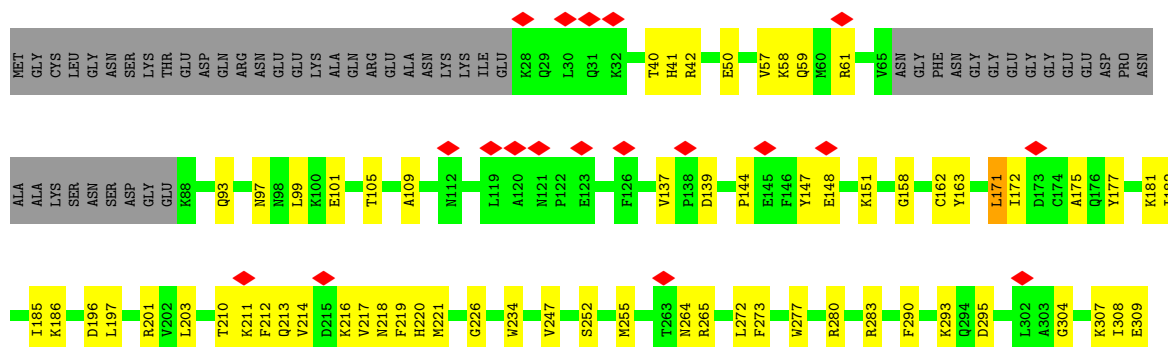
Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

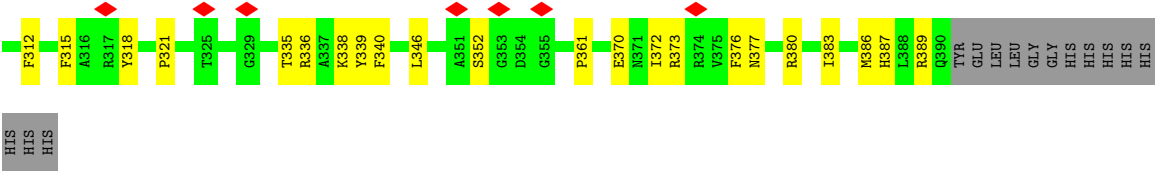
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Mg	0
			1	1	



- Molecule 2: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142147	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.672	Depositor
Minimum map value	-5.173	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.435	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	341.75998, 341.75998, 341.75998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8543999, 0.8543999, 0.8543999	Depositor

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: MN, FOK, ONM, MG, GSP

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	0.30	0/6834	0.70	2/9242 (0.0%)
2	B	0.29	0/2867	0.63	0/3875
All	All	0.30	0/9701	0.68	2/13117 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1180	THR	CA-C-N	5.02	131.13	121.54
1	A	1180	THR	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1072	TYR	Peptide
1	A	191	GLN	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	A	6687	0	6722	125	0
2	B	2809	0	2773	64	0
3	A	42	0	19	4	0
4	A	29	0	34	1	0
5	A	2	0	0	0	0
6	B	32	0	12	2	0
7	B	1	0	0	0	0
All	All	9602	0	9560	193	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 10.

All (193) 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:2000:ONM:C1'	3:A:2000:ONM:O4'	1.64	1.12
1:A:1042:ALA:O	1:A:1046:LYS:HB2	1.65	0.96
2:B:211:LYS:HA	2:B:219:PHE:O	1.67	0.92
1:A:931:PRO:O	1:A:935:LEU:HB2	1.72	0.90
2:B:42:ARG:HA	2:B:220:HIS:O	1.74	0.88
1:A:416:VAL:O	1:A:420:ASN:HB2	1.73	0.88
3:A:2000:ONM:O4'	3:A:2000:ONM:H8	1.78	0.83
2:B:41:HIS:HB2	2:B:218:ASN:O	1.77	0.82
2:B:383:ILE:O	2:B:387:HIS:HB2	1.79	0.82
2:B:212:PHE:O	2:B:219:PHE:HB2	1.83	0.78
1:A:854:ARG:O	1:A:858:TRP:HB2	1.84	0.77
2:B:210:THR:O	2:B:220:HIS:HA	1.87	0.74
2:B:214:VAL:O	2:B:217:VAL:HB	1.89	0.73
3:A:2000:ONM:O4'	3:A:2000:ONM:C8	2.38	0.72
1:A:417:GLY:O	1:A:421:ASP:HB2	1.94	0.68
1:A:1099:LYS:HB2	1:A:1102:TYR:HB2	1.76	0.67
1:A:981:GLN:O	1:A:985:LEU:HB2	1.95	0.66
1:A:398:ALA:HA	1:A:487:ARG:O	1.96	0.66
1:A:395:ILE:O	1:A:490:VAL:HA	1.95	0.66
1:A:415:LEU:O	1:A:419:LEU:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:HIS:HB3	1:A:1134:GLU:HB3	1.79	0.64
1:A:989:LEU:O	1:A:993:LEU:HB2	1.98	0.64
1:A:1165:ARG:HB3	1:A:1204:GLU:HA	1.80	0.63
1:A:1163:LYS:HD2	1:A:1204:GLU:HG3	1.81	0.62
1:A:790:ASP:O	1:A:794:SER:HB2	1.99	0.62
4:A:2001:FOK:HO2	4:A:2001:FOK:HO6	1.44	0.62
1:A:148:PRO:O	1:A:152:PHE:HB2	1.99	0.61
1:A:461:CYS:O	1:A:465:MET:HB2	2.00	0.61
1:A:925:THR:O	1:A:929:ALA:HB3	2.00	0.61
1:A:1135:HIS:O	1:A:1139:LEU:HB2	2.00	0.61
2:B:372:ILE:O	2:B:376:PHE:HB3	2.01	0.60
1:A:387:MET:HG2	1:A:498:GLY:HA3	1.84	0.60
1:A:1104:SER:HA	1:A:1122:ASN:HD22	1.67	0.60
1:A:1064:SER:O	1:A:1164:LEU:HA	2.02	0.60
1:A:242:LEU:O	1:A:246:LEU:HB2	2.02	0.59
1:A:284:ARG:O	1:A:288:HIS:ND1	2.35	0.59
1:A:1206:ARG:NH1	1:A:1244:PRO:O	2.36	0.59
1:A:1058:GLY:O	1:A:1170:HIS:HA	2.01	0.59
1:A:473:ILE:O	1:A:477:CYS:HB3	2.02	0.59
1:A:1231:ASN:ND2	1:A:1236:GLY:O	2.36	0.58
2:B:181:LYS:NZ	2:B:196:ASP:OD1	2.36	0.58
2:B:255:MET:O	2:B:264:ASN:ND2	2.36	0.58
1:A:105:MET:HA	1:A:108:CYS:HB2	1.83	0.58
1:A:917:SER:O	1:A:921:SER:HB2	2.04	0.58
1:A:789:LEU:O	1:A:793:LEU:HB3	2.04	0.57
2:B:335:THR:HA	2:B:338:LYS:HE2	1.86	0.57
1:A:1165:ARG:NH1	1:A:1202:GLY:O	2.37	0.57
1:A:224:PHE:HB2	1:A:284:ARG:HH22	1.70	0.56
1:A:908:GLN:OE1	1:A:911:ASN:ND2	2.38	0.56
2:B:304:GLY:O	2:B:307:LYS:NZ	2.37	0.56
1:A:473:ILE:O	1:A:477:CYS:CB	2.54	0.56
1:A:892:ILE:HG23	1:A:896:MET:HE2	1.87	0.56
2:B:59:GLN:HG2	2:B:372:ILE:HG13	1.88	0.56
1:A:808:ARG:O	1:A:808:ARG:NH1	2.39	0.56
2:B:273:PHE:O	2:B:277:TRP:HB2	2.06	0.56
1:A:545:MET:SD	1:A:545:MET:N	2.77	0.55
1:A:415:LEU:O	1:A:419:LEU:CB	2.54	0.55
1:A:805:CYS:O	1:A:883:HIS:NE2	2.39	0.55
2:B:144:PRO:HA	2:B:147:TYR:HD2	1.71	0.55
1:A:925:THR:O	1:A:929:ALA:CB	2.54	0.55
1:A:1229:THR:O	1:A:1237:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:GLY:HA2	2:B:234:TRP:HZ2	1.71	0.55
2:B:309:GLU:HB3	2:B:315:PHE:HD2	1.73	0.54
1:A:108:CYS:HB3	1:A:111:GLN:HE21	1.72	0.54
1:A:455:ARG:HB3	1:A:458:HIS:HB3	1.89	0.54
2:B:147:TYR:O	2:B:151:LYS:HB2	2.07	0.54
2:B:158:GLY:O	2:B:162:CYS:HB2	2.08	0.54
1:A:397:PHE:O	1:A:488:VAL:HA	2.08	0.54
1:A:402:GLY:N	3:A:2000:ONM:O1G	2.41	0.53
1:A:920:ARG:HH22	1:A:998:ASN:HB2	1.73	0.53
2:B:372:ILE:O	2:B:376:PHE:CB	2.57	0.53
1:A:383:ARG:NH2	1:A:1088:GLU:OE1	2.42	0.53
1:A:888:PHE:O	1:A:895:THR:OG1	2.26	0.52
1:A:1061:ILE:HA	1:A:1167:GLY:O	2.09	0.52
1:A:441:LEU:HD23	1:A:446:TYR:HE1	1.74	0.52
1:A:192:PHE:O	1:A:194:VAL:N	2.43	0.52
2:B:252:SER:HB3	2:B:265:ARG:HB2	1.91	0.52
2:B:308:ILE:O	2:B:312:PHE:N	2.34	0.52
1:A:492:THR:HG23	1:A:535:THR:HG22	1.91	0.52
2:B:346:LEU:HD11	2:B:361:PRO:HG3	1.92	0.52
1:A:383:ARG:NH1	1:A:1095:GLU:OE2	2.42	0.52
1:A:1053:LYS:HB3	1:A:1175:ALA:HB3	1.91	0.52
1:A:1197:ARG:HD3	1:A:1232:VAL:HG13	1.92	0.52
1:A:532:SER:HA	1:A:568:THR:HG23	1.93	0.51
1:A:790:ASP:O	1:A:794:SER:CB	2.59	0.51
2:B:213:GLN:HE21	2:B:216:LYS:HA	1.75	0.51
2:B:93:GLN:NE2	2:B:97:ASN:OD1	2.43	0.51
1:A:429:LEU:O	1:A:433:THR:OG1	2.21	0.51
2:B:50:GLU:N	6:B:501:GSP:O3G	2.39	0.51
1:A:425:ARG:HG2	1:A:428:ARG:HH12	1.74	0.51
2:B:40:THR:HA	2:B:218:ASN:HB2	1.93	0.50
1:A:789:LEU:O	1:A:793:LEU:CB	2.59	0.50
2:B:386:MET:HA	2:B:389:ARG:HB2	1.94	0.50
1:A:220:GLN:O	1:A:224:PHE:HB3	2.11	0.50
1:A:1207:ILE:HB	1:A:1243:TYR:HB3	1.93	0.50
2:B:57:VAL:HG22	2:B:221:MET:HE2	1.93	0.50
1:A:1174:THR:O	1:A:1187:ILE:HA	2.12	0.49
2:B:148:GLU:HA	2:B:151:LYS:HE2	1.93	0.49
1:A:925:THR:HG1	1:A:995:TRP:HE1	1.56	0.49
2:B:217:VAL:HG21	2:B:380:ARG:HD2	1.94	0.49
2:B:99:LEU:HD13	2:B:182:ILE:HG13	1.94	0.49
1:A:420:ASN:HA	1:A:423:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:TRP:HZ3	2:B:272:LEU:HD11	1.77	0.49
1:A:532:SER:O	1:A:535:THR:OG1	2.28	0.49
1:A:1036:ILE:HG23	1:A:1037:ILE:HG23	1.93	0.49
2:B:40:THR:OG1	2:B:42:ARG:NH1	2.38	0.49
2:B:201:ARG:HH22	2:B:203:LEU:HD12	1.77	0.49
1:A:798:PHE:HA	1:A:801:LEU:HD12	1.95	0.49
1:A:1179:GLY:HA3	1:A:1183:LEU:HA	1.94	0.49
1:A:1053:LYS:NZ	1:A:1054:ASN:O	2.41	0.48
2:B:147:TYR:O	2:B:151:LYS:CB	2.61	0.48
1:A:981:GLN:O	1:A:985:LEU:CB	2.60	0.48
1:A:471:ARG:HA	1:A:474:GLU:HG2	1.94	0.48
2:B:247:VAL:HG22	2:B:290:PHE:HB2	1.96	0.48
1:A:1042:ALA:O	1:A:1046:LYS:CB	2.50	0.48
1:A:185:ALA:O	1:A:189:ALA:CB	2.62	0.47
1:A:287:LEU:HG	1:A:904:THR:HG21	1.95	0.47
1:A:917:SER:O	1:A:921:SER:CB	2.63	0.47
2:B:158:GLY:O	2:B:162:CYS:CB	2.62	0.47
1:A:984:ILE:HA	1:A:987:PHE:HB2	1.96	0.47
1:A:1063:ALA:HB3	1:A:1115:TYR:HB3	1.97	0.47
2:B:101:GLU:O	2:B:105:THR:OG1	2.24	0.47
2:B:171:LEU:HD22	2:B:172:ILE:H	1.79	0.47
2:B:336:ARG:O	2:B:340:PHE:HB2	2.15	0.47
1:A:795:THR:HA	1:A:798:PHE:HB3	1.97	0.46
2:B:295:ASP:OD1	2:B:295:ASP:N	2.47	0.46
2:B:321:PRO:HG2	2:B:339:TYR:HB3	1.96	0.46
1:A:1152:ASP:HA	1:A:1155:ASN:HD22	1.80	0.46
2:B:177:TYR:OH	2:B:196:ASP:OD1	2.23	0.46
1:A:389:GLN:HA	1:A:496:LEU:HA	1.97	0.46
1:A:1206:ARG:HE	1:A:1242:LEU:HD13	1.80	0.46
2:B:181:LYS:O	2:B:185:ILE:N	2.48	0.46
1:A:399:ASP:O	1:A:486:MET:HA	2.16	0.46
1:A:986:VAL:HG23	1:A:989:LEU:HD21	1.98	0.45
1:A:1216:VAL:HG22	1:A:1220:MET:HE2	1.98	0.45
2:B:293:LYS:HG2	6:B:501:GSP:C6	2.51	0.45
2:B:105:THR:O	2:B:109:ALA:CB	2.65	0.45
1:A:117:ARG:HD3	1:A:163:THR:HG21	1.98	0.45
1:A:225:SER:HB2	1:A:986:VAL:HG21	1.99	0.45
1:A:331:GLU:OE2	1:A:335:HIS:NE2	2.50	0.45
2:B:308:ILE:HG22	2:B:312:PHE:HB2	1.98	0.45
2:B:318:TYR:O	2:B:336:ARG:NH2	2.44	0.45
2:B:383:ILE:O	2:B:387:HIS:CB	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:O	1:A:189:ALA:HB3	2.17	0.45
1:A:420:ASN:HD21	1:A:1178:ILE:HA	1.82	0.45
1:A:104:CYS:O	1:A:108:CYS:N	2.45	0.44
1:A:316:SER:HB2	1:A:1015:ALA:HB2	1.99	0.44
1:A:438:ILE:HD11	1:A:448:VAL:HG22	2.00	0.44
1:A:491:HIS:HD2	1:A:513:ASP:HB3	1.82	0.44
2:B:370:GLU:HA	2:B:373:ARG:HH11	1.82	0.44
2:B:280:ARG:HA	2:B:283:ARG:HH21	1.82	0.44
1:A:1096:LEU:HD11	1:A:1149:VAL:HG11	1.98	0.44
1:A:112:THR:O	1:A:116:PHE:HB2	2.17	0.44
1:A:1217:LEU:HD13	1:A:1220:MET:HE3	1.98	0.44
1:A:1197:ARG:HE	1:A:1232:VAL:HA	1.83	0.44
1:A:120:LEU:HD23	1:A:123:ILE:HD12	2.00	0.44
1:A:165:THR:HG23	1:A:168:TYR:HB2	1.99	0.43
2:B:163:TYR:HE1	2:B:175:ALA:HB3	1.83	0.43
2:B:137:VAL:HG22	2:B:139:ASP:H	1.82	0.43
1:A:255:LEU:HA	1:A:258:THR:HG22	1.99	0.43
1:A:354:SER:HA	1:A:357:SER:HB3	2.01	0.43
1:A:389:GLN:HG2	1:A:496:LEU:HB3	2.01	0.43
1:A:337:VAL:HG13	1:A:338:MET:HG3	2.01	0.43
1:A:477:CYS:O	1:A:481:LYS:N	2.50	0.42
1:A:1167:GLY:HA2	1:A:1208:GLN:HB3	2.01	0.42
1:A:1169:ASN:HB2	1:A:1195:ALA:HB2	2.01	0.42
2:B:277:TRP:NE1	2:B:352:SER:OG	2.53	0.42
1:A:823:VAL:O	1:A:827:ALA:CB	2.67	0.42
1:A:836:VAL:HA	1:A:839:VAL:HG12	2.02	0.42
1:A:809:TYR:CG	1:A:812:ALA:HB3	2.55	0.42
1:A:103:ALA:HA	1:A:106:GLU:HB2	2.01	0.42
1:A:519:LEU:O	1:A:523:LEU:N	2.47	0.42
1:A:887:GLU:OE2	1:A:890:THR:N	2.32	0.42
1:A:1197:ARG:NE	1:A:1233:LYS:H	2.17	0.42
2:B:58:LYS:HA	2:B:61:ARG:HG2	2.02	0.41
1:A:529:VAL:HG22	1:A:531:ILE:HG23	2.01	0.41
2:B:40:THR:O	2:B:387:HIS:NE2	2.49	0.41
1:A:151:CYS:HA	1:A:154:VAL:HG12	2.02	0.41
2:B:58:LYS:NZ	2:B:197:LEU:O	2.42	0.41
2:B:147:TYR:CZ	2:B:186:LYS:HA	2.56	0.41
2:B:41:HIS:CB	2:B:218:ASN:O	2.58	0.41
1:A:234:LEU:HD11	1:A:240:LEU:HD22	2.03	0.41
1:A:931:PRO:HB3	1:A:935:LEU:HD13	2.02	0.41
1:A:171:HIS:O	1:A:175:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:PHE:HD1	1:A:1001:PHE:HA	1.76	0.41
2:B:172:ILE:HD11	2:B:175:ALA:HB2	2.03	0.41
1:A:259:PHE:HD1	1:A:259:PHE:HA	1.75	0.41
1:A:878:LEU:HA	1:A:881:TYR:HB2	2.02	0.41
2:B:201:ARG:HH12	2:B:203:LEU:HB2	1.85	0.41
1:A:1140:PHE:HE1	1:A:1207:ILE:HG21	1.86	0.40
2:B:373:ARG:O	2:B:377:ASN:ND2	2.54	0.40
1:A:823:VAL:O	1:A:827:ALA:HB3	2.22	0.40
2:B:50:GLU:OE2	2:B:201:ARG:NH2	2.54	0.40

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 PDB entries followed by that with respect to all EM entries.

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	
1	A	827/1533 (54%)	755 (91%)	72 (9%)	0	100	100
2	B	337/405 (83%)	313 (93%)	24 (7%)	0	100	100
All	All	1164/1938 (60%)	1068 (92%)	96 (8%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	
1	A	732/1318 (56%)	728 (100%)	4 (0%)	81	81
2	B	309/359 (86%)	308 (100%)	1 (0%)	86	84
All	All	1041/1677 (62%)	1036 (100%)	5 (0%)	78	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	244	LEU
1	A	259	PHE
1	A	531	ILE
2	B	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	518	ASN
1	A	981	GLN
1	A	1055	HIS
1	A	1122	ASN
1	A	1169	ASN
1	A	1231	ASN
1	A	1237	GLN
2	B	59	GLN
2	B	93	GLN
2	B	97	ASN
2	B	213	GLN
2	B	254	ASN
2	B	261	ASN
2	B	377	ASN
2	B	384	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
4	FOK	A	2001	-	29,31,31	1.21	1 (3%)	38,54,54	2.33	15 (39%)
6	GSP	B	501	7	33,34,34	1.91	2 (6%)	47,54,54	1.85	9 (19%)
3	ONM	A	2000	5	44,45,45	3.32	20 (45%)	65,69,69	2.30	15 (23%)

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
4	FOK	A	2001	-	-	2/7/80/80	0/3/3/3
6	GSP	B	501	7	-	0/21/38/38	0/3/3/3
3	ONM	A	2000	5	-	8/32/48/48	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	ONM	O4'-C1'	9.76	1.64	1.42
6	B	501	GSP	PG-S1G	-9.64	1.69	1.90
3	A	2000	ONM	O4'-C4'	-7.32	1.28	1.45
3	A	2000	ONM	C2'-C1'	-6.87	1.31	1.53
3	A	2000	ONM	O3'-C3'	-6.29	1.35	1.44
3	A	2000	ONM	C4-N3	6.19	1.48	1.34
3	A	2000	ONM	C2-N3	5.88	1.47	1.33
3	A	2000	ONM	C2-N2	5.32	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	FOK	O4-C21	4.72	1.45	1.35
3	A	2000	ONM	CA6-NA1	4.58	1.45	1.37
3	A	2000	ONM	PB-O1B	4.21	1.64	1.59
3	A	2000	ONM	O2'-C2'	3.38	1.51	1.43
3	A	2000	ONM	PA-O1A	2.98	1.62	1.59
3	A	2000	ONM	C5-N7	-2.80	1.33	1.39
3	A	2000	ONM	O3'-CA	2.78	1.40	1.34
3	A	2000	ONM	PB-O1A	2.71	1.62	1.59
3	A	2000	ONM	C3'-C4'	2.60	1.59	1.52
3	A	2000	ONM	C6-N1	2.47	1.43	1.38
3	A	2000	ONM	C2-N1	2.47	1.43	1.37
3	A	2000	ONM	CA1-CA	2.43	1.55	1.50
3	A	2000	ONM	O6-C6	-2.26	1.19	1.23
3	A	2000	ONM	PA-O5'	2.19	1.68	1.59
6	B	501	GSP	C2-N3	2.10	1.38	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	ONM	C1'-N9-C8	-9.64	99.34	126.73
3	A	2000	ONM	C1'-N9-C4	8.79	152.44	126.49
4	A	2001	FOK	C13-O1-C8	5.37	128.26	119.86
4	A	2001	FOK	O1-C8-C17	-5.26	103.39	110.17
6	B	501	GSP	C5-C4-N3	-5.22	120.08	128.39
3	A	2000	ONM	C5-C4-N3	-4.92	120.56	128.39
6	B	501	GSP	C2-N3-C4	4.87	120.69	112.30
4	A	2001	FOK	O4-C21-C22	4.68	119.44	111.09
3	A	2000	ONM	O3'-CA-CA1	4.31	118.56	111.71
4	A	2001	FOK	C7-O4-C21	-4.29	111.70	117.79
6	B	501	GSP	PB-O3B-PG	-4.25	117.60	133.17
4	A	2001	FOK	O1-C8-C7	4.21	107.14	103.16
3	A	2000	ONM	C2-N3-C4	3.82	118.87	112.30
3	A	2000	ONM	O4'-C1'-N9	3.68	116.70	108.36
4	A	2001	FOK	C3-C4-C5	3.44	112.75	107.89
3	A	2000	ONM	C2-N1-C6	-3.34	119.06	125.11
6	B	501	GSP	N9-C4-N3	3.30	132.55	125.95
6	B	501	GSP	C2-N1-C6	-3.18	119.34	125.11
4	A	2001	FOK	C3-C2-C1	-3.14	106.89	111.48
3	A	2000	ONM	N9-C4-N3	3.01	131.97	125.95
3	A	2000	ONM	CA7-NA1-CA6	-3.00	117.64	122.37
3	A	2000	ONM	O6-C6-C5	-2.96	118.72	126.53
4	A	2001	FOK	C20-C10-C1	-2.87	102.56	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	ONM	N9-C8-N7	-2.80	108.20	113.40
6	B	501	GSP	N9-C8-N7	-2.79	108.23	113.40
6	B	501	GSP	C5-C6-N1	2.76	120.28	113.25
3	A	2000	ONM	C5-C6-N1	2.62	119.93	113.25
6	B	501	GSP	C8-N7-C5	2.62	108.92	104.26
4	A	2001	FOK	O7-C11-C12	-2.50	116.95	121.97
4	A	2001	FOK	O4-C21-O5	-2.50	118.16	122.99
6	B	501	GSP	O6-C6-C5	-2.42	120.16	126.53
3	A	2000	ONM	C2'-C1'-N9	-2.35	106.70	113.25
4	A	2001	FOK	C10-C5-C4	2.31	118.30	116.32
3	A	2000	ONM	C2'-C3'-C4'	-2.17	99.44	103.24
3	A	2000	ONM	CA5-CA6-NA1	-2.14	118.66	121.33
4	A	2001	FOK	C17-C8-C9	2.12	117.53	115.19
4	A	2001	FOK	C19-C4-C18	-2.12	104.79	107.87
4	A	2001	FOK	O3-C6-C5	2.10	118.22	111.94
4	A	2001	FOK	C18-C4-C5	-2.05	104.76	111.92

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	ONM	O4'-C4'-C5'-O5'
3	A	2000	ONM	C5'-O5'-PA-O3A
3	A	2000	ONM	C5'-O5'-PA-O1A
4	A	2001	FOK	C22-C21-O4-C7
4	A	2001	FOK	O5-C21-O4-C7
3	A	2000	ONM	C3'-C4'-C5'-O5'
3	A	2000	ONM	CA1-CA6-NA1-CA7
3	A	2000	ONM	PB-O1A-PA-O5'
3	A	2000	ONM	CA5-CA6-NA1-CA7
3	A	2000	ONM	C5'-O5'-PA-O2A

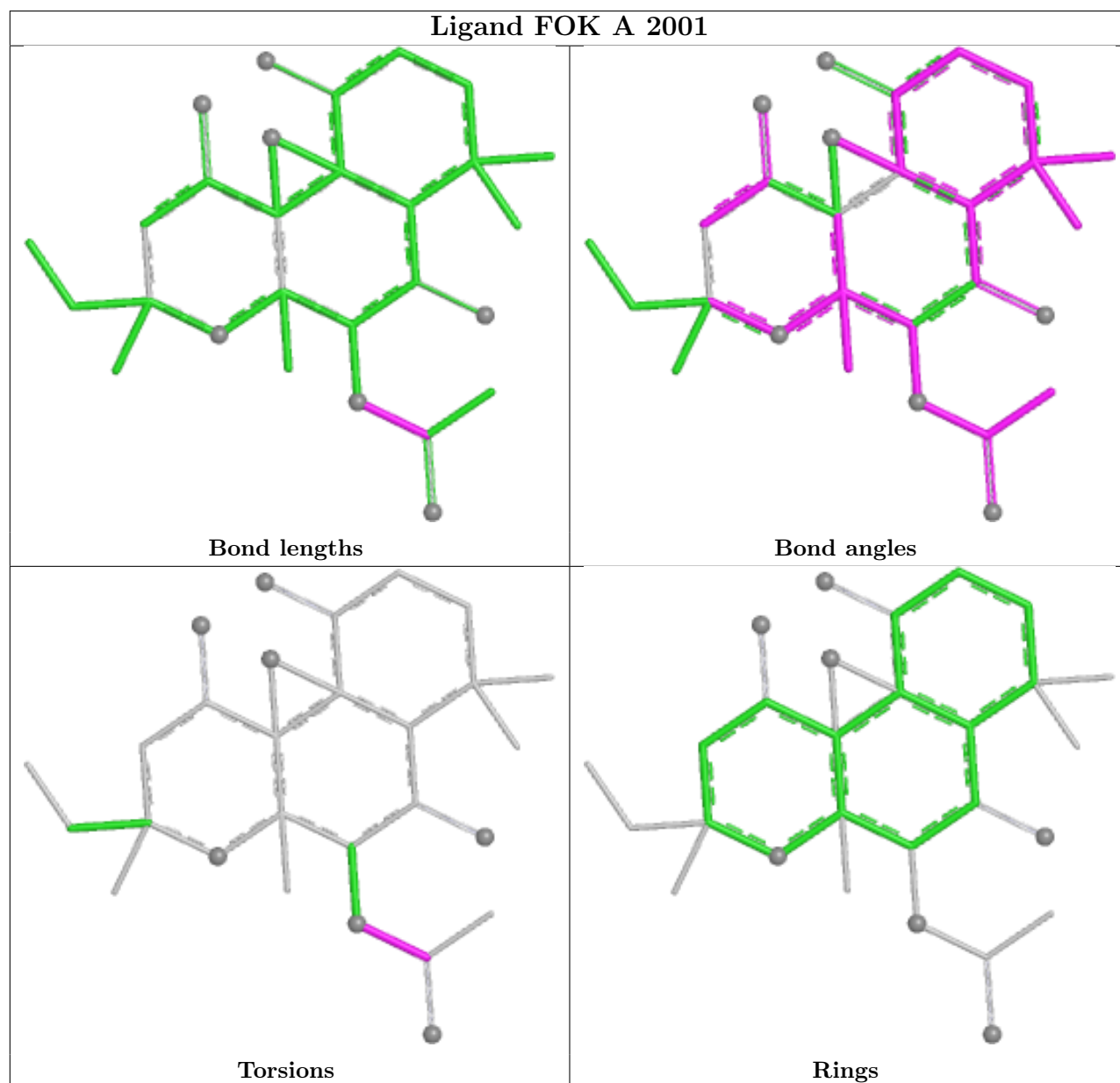
There are no ring outliers.

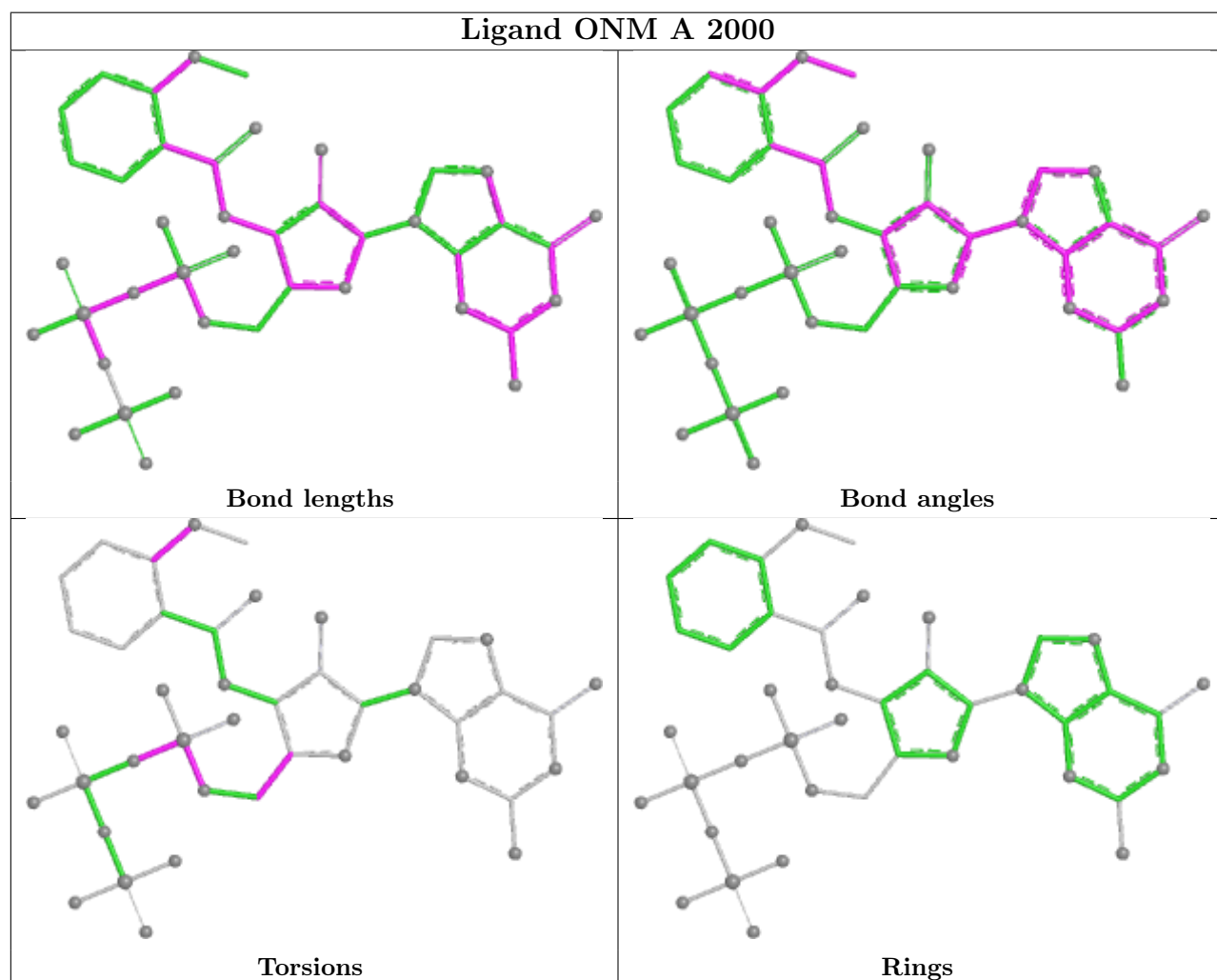
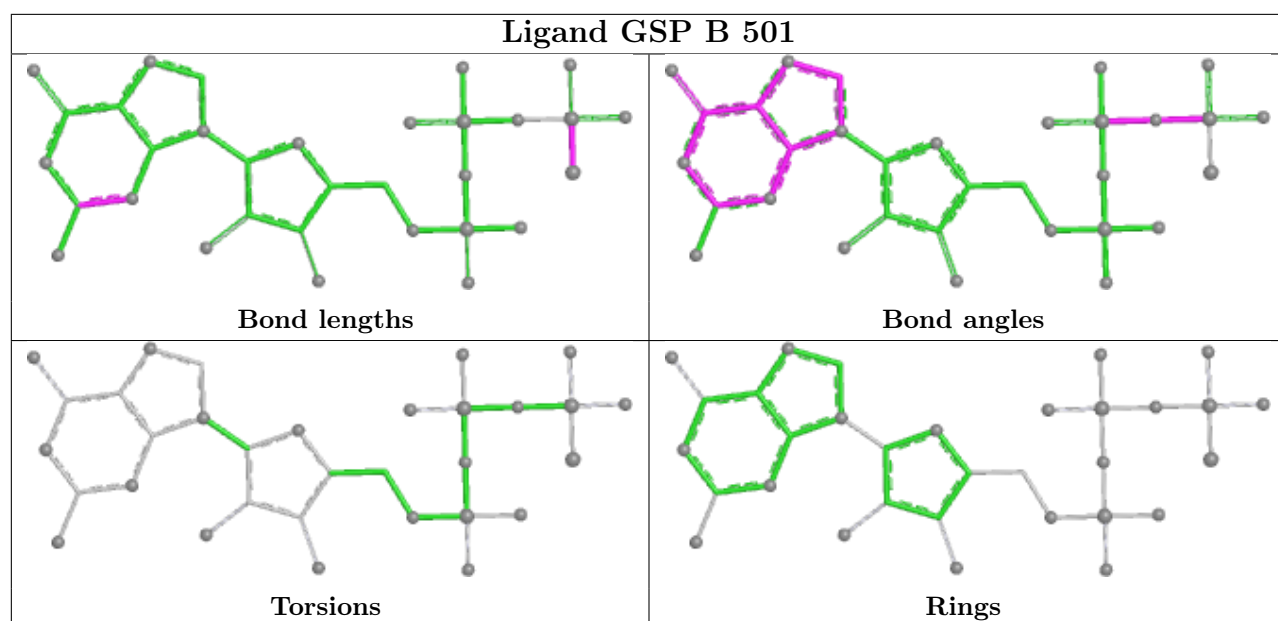
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	FOK	1	0
6	B	501	GSP	2	0
3	A	2000	ONM	4	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.

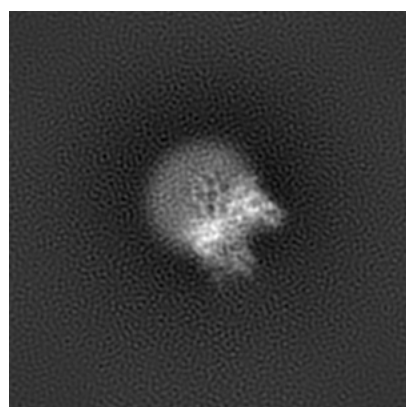
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4721. These allow visual inspection of the internal detail of the map and identification of artifacts.

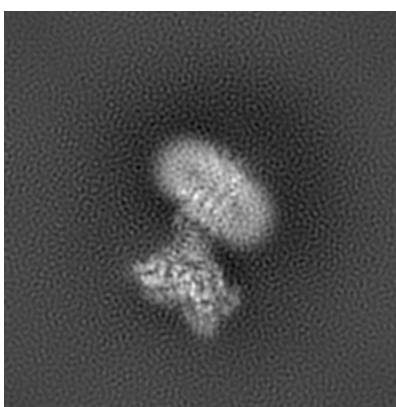
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

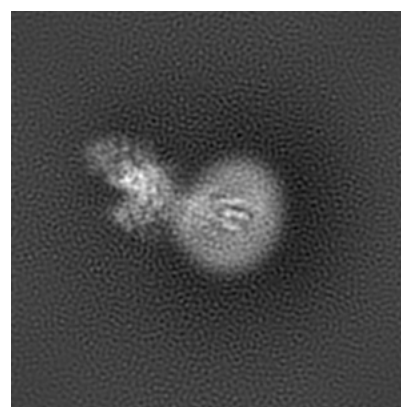
6.1.1 Primary map



X



Y

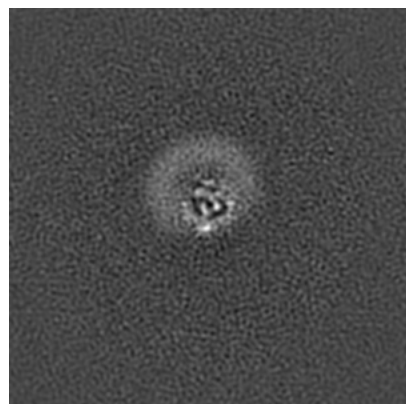


Z

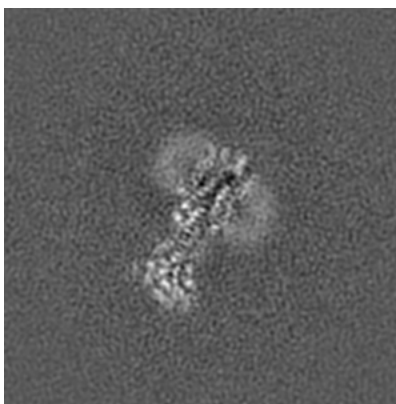
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

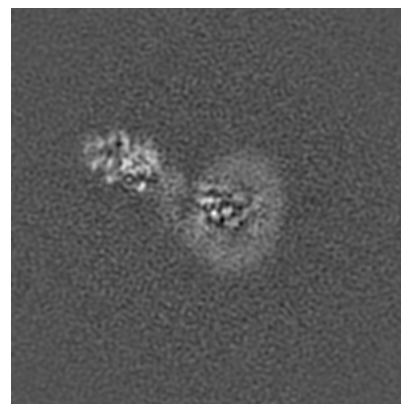
6.2.1 Primary map



X Index: 200



Y Index: 200

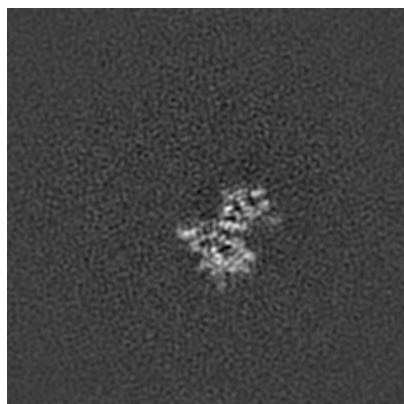


Z Index: 200

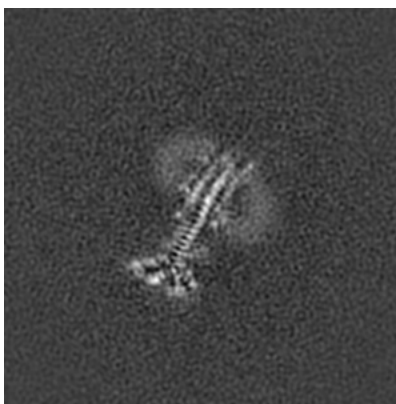
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

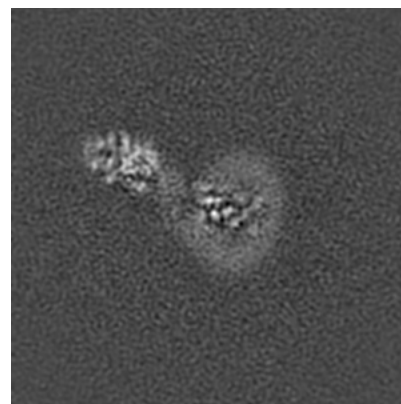
6.3.1 Primary map



X Index: 131



Y Index: 208

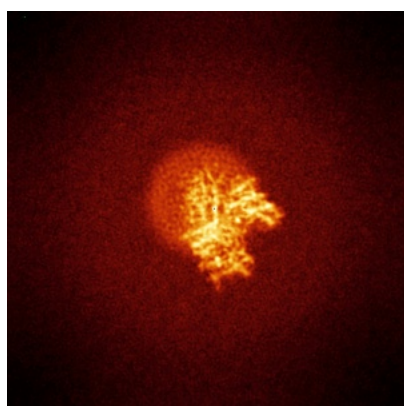


Z Index: 201

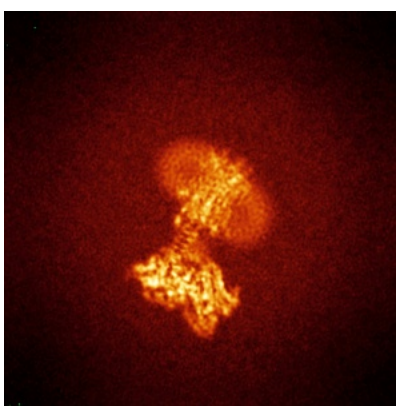
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

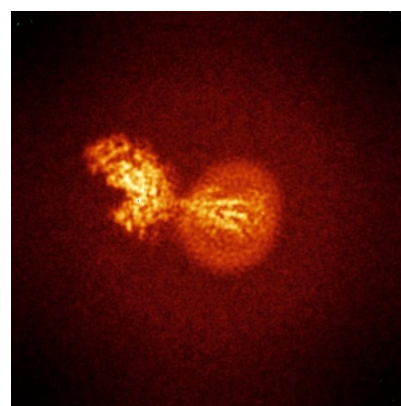
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

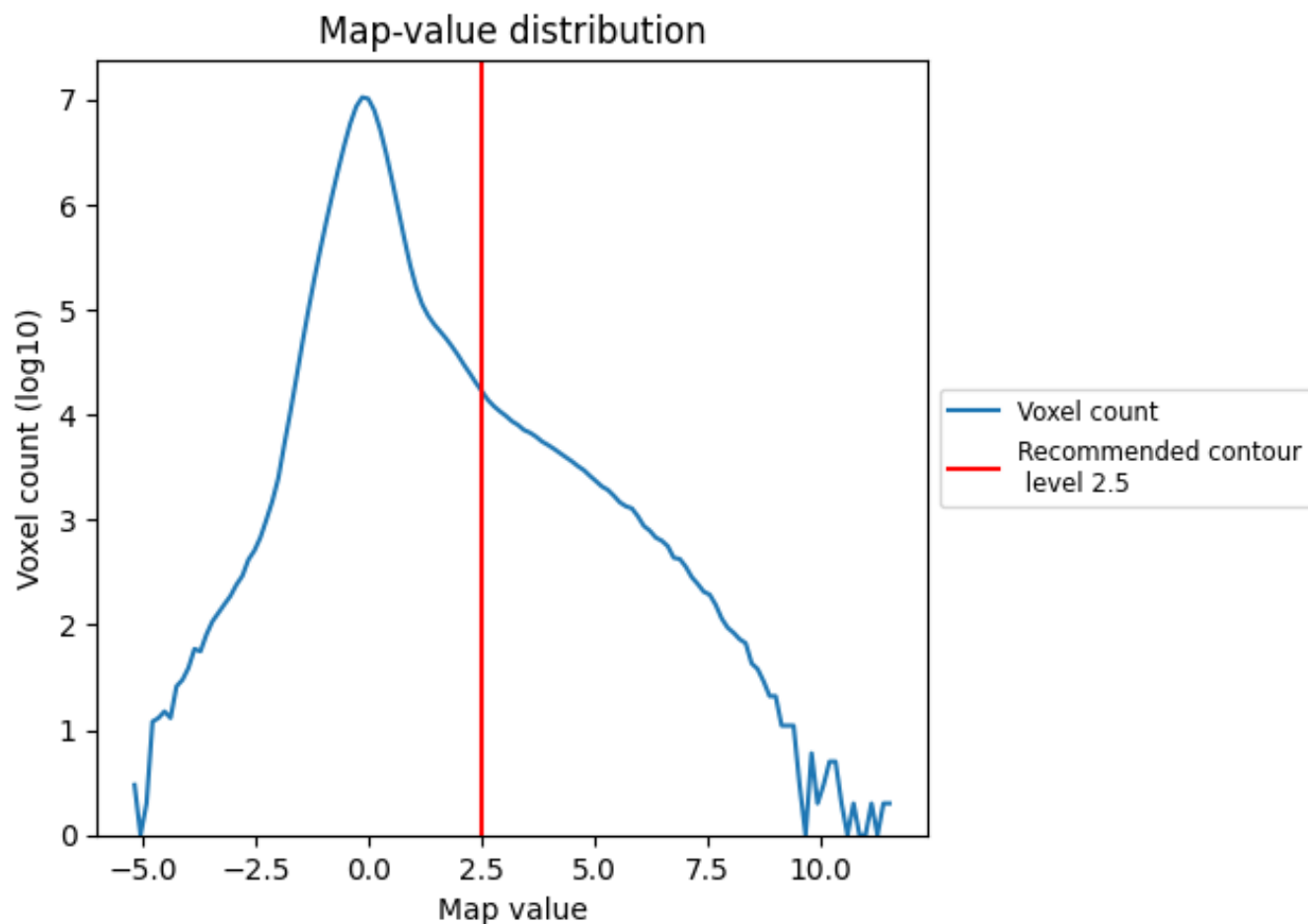
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

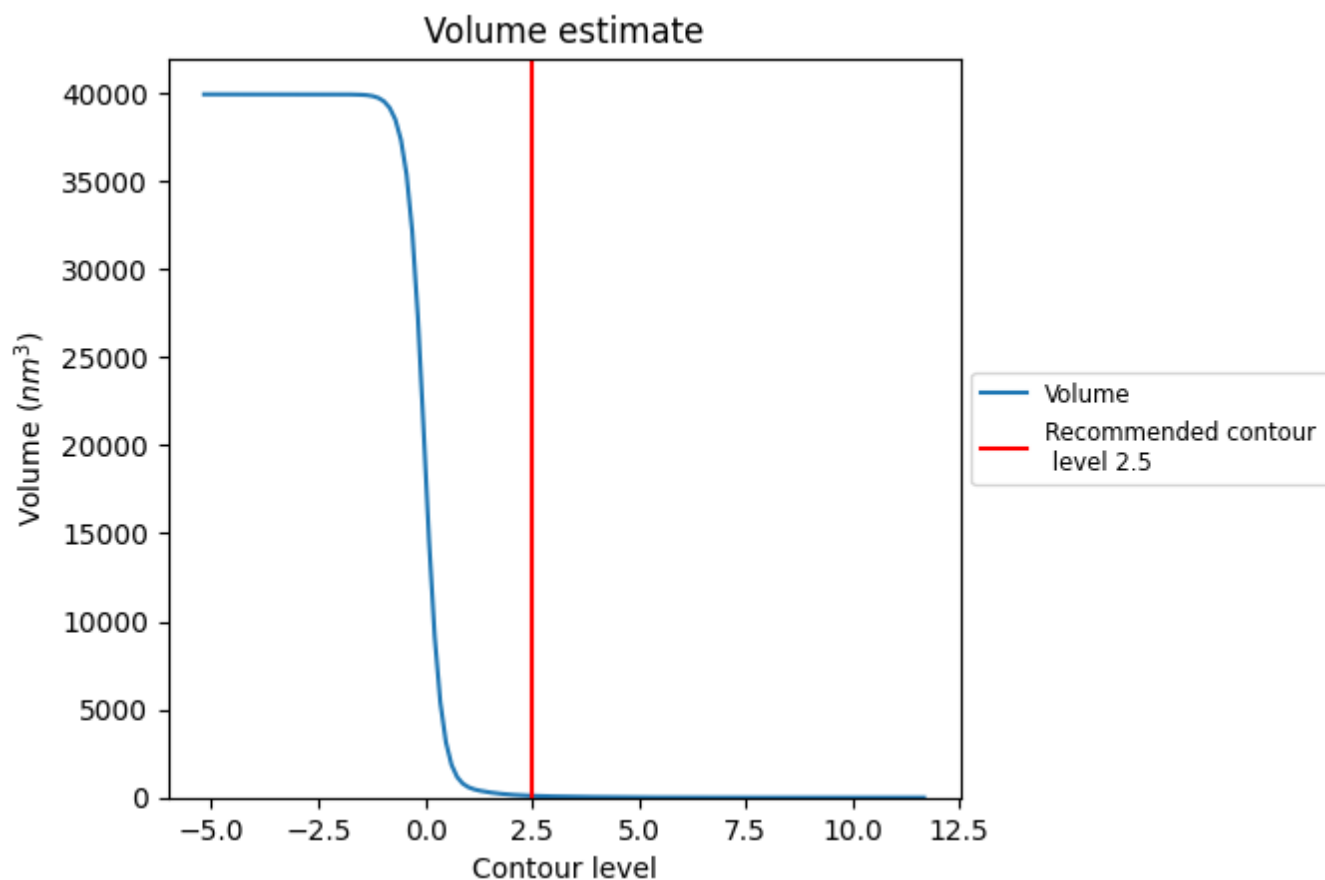
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

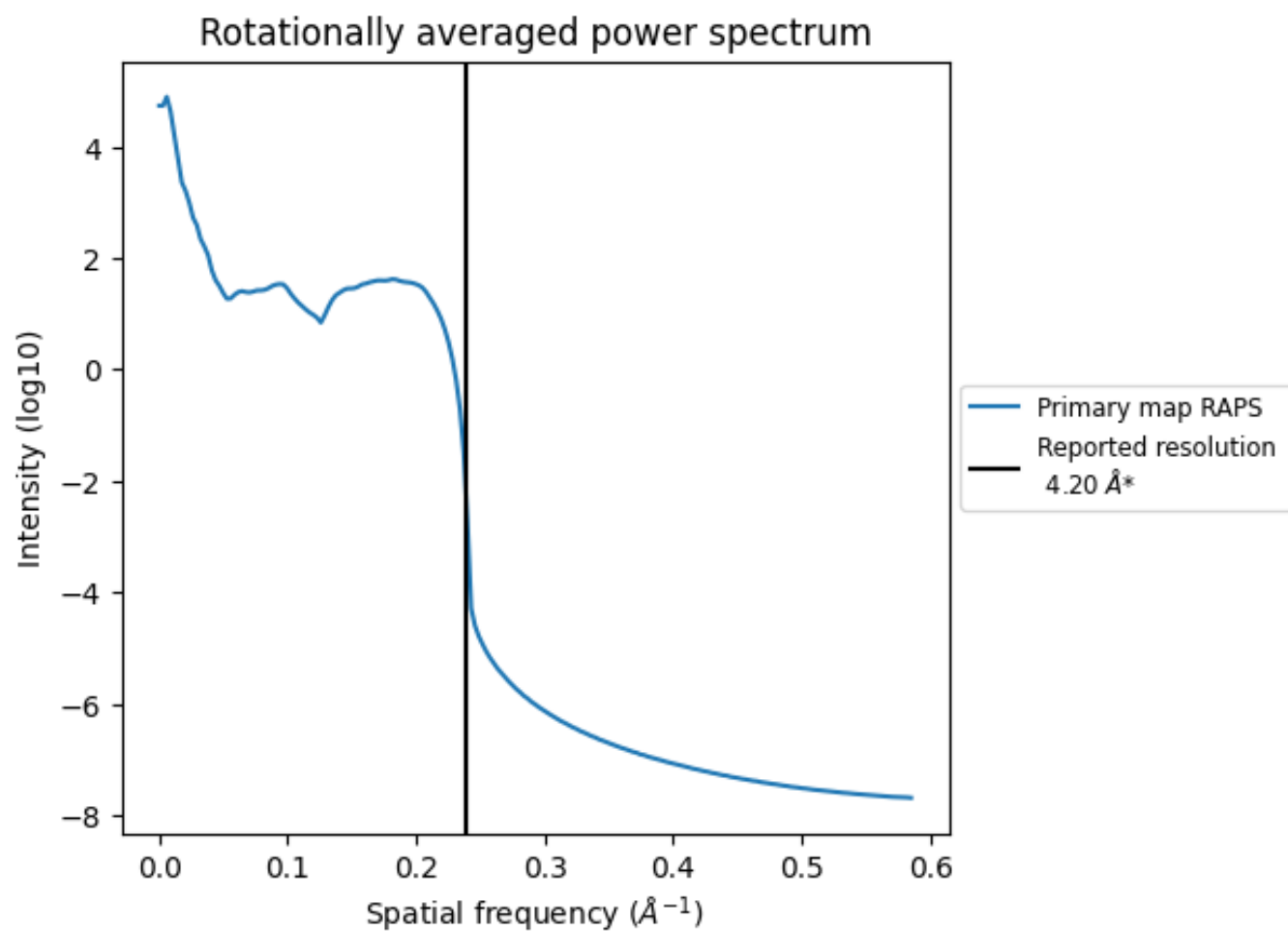
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 89 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

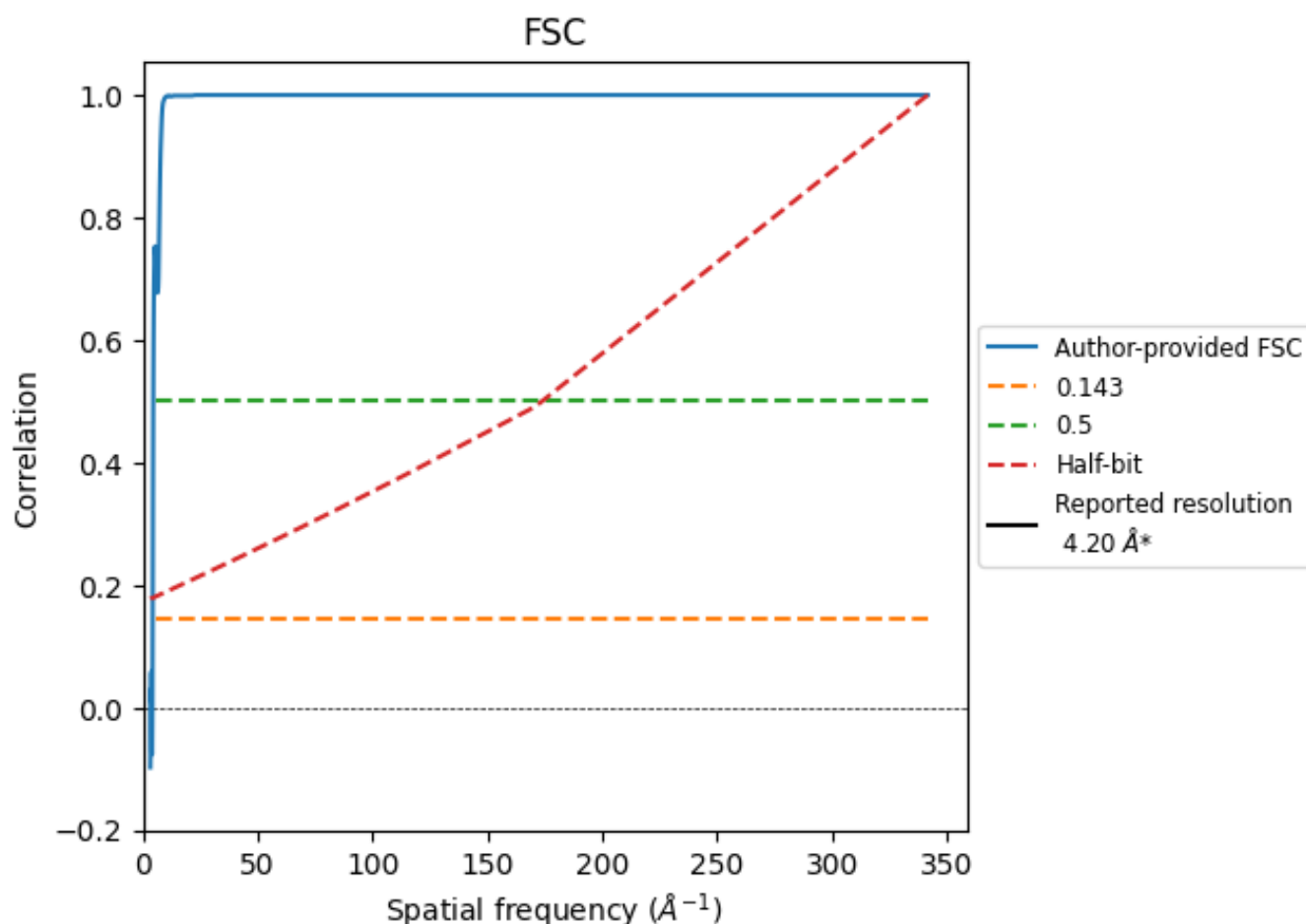


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

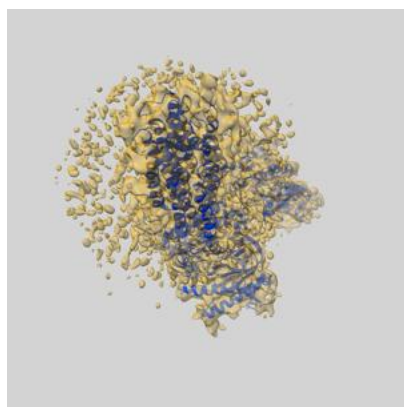
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	0.24	0.23	0.24
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 0.24 differs from the reported value 4.2 by more than 10 %

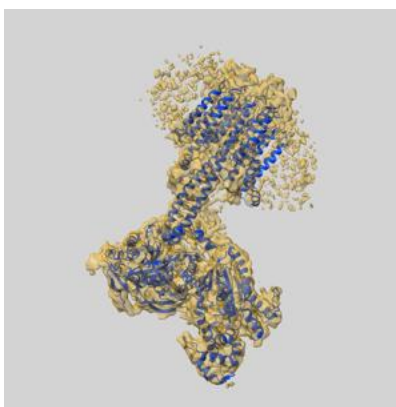
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4721 and PDB model 6R4O. Per-residue inclusion information can be found in section [3](#) on page [13](#).

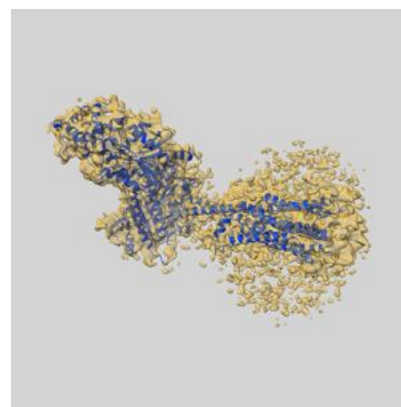
9.1 Map-model overlay [i](#)



X



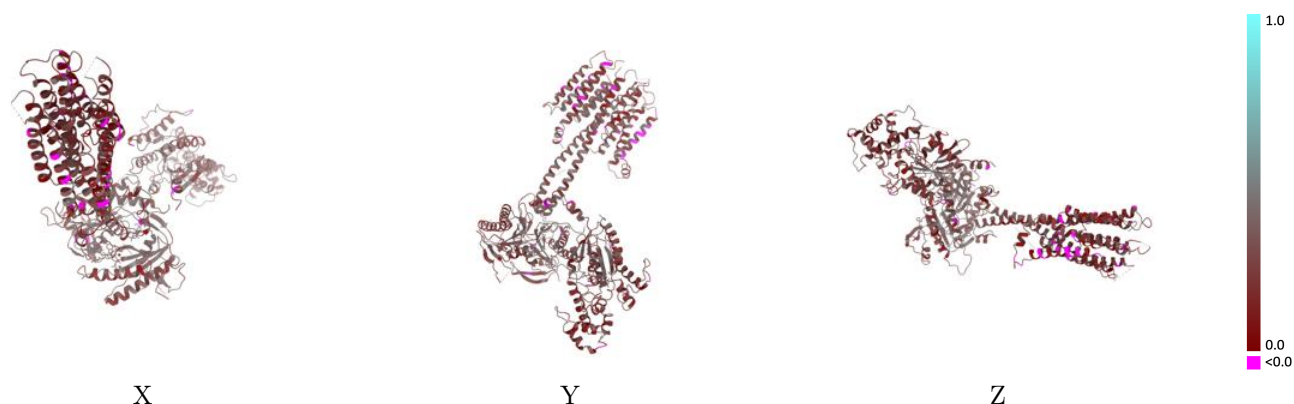
Y



Z

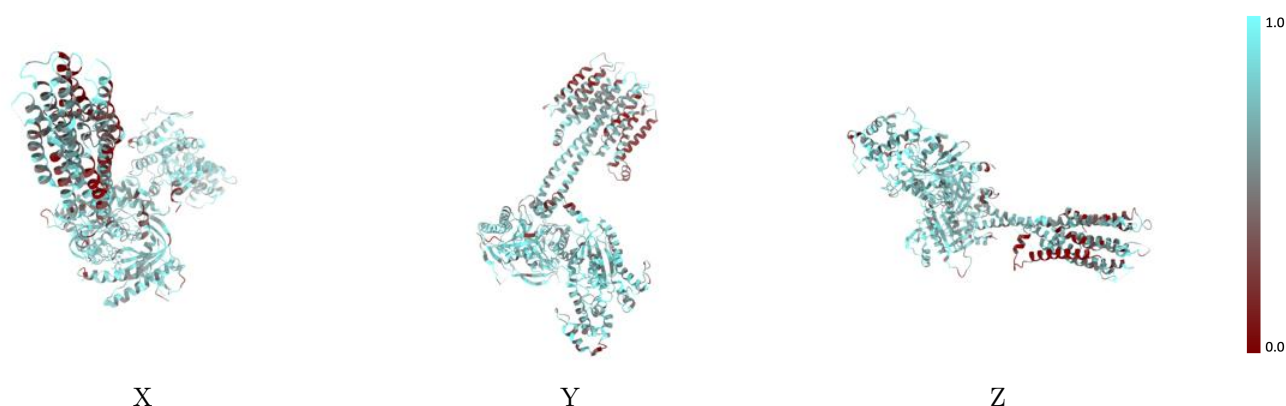
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



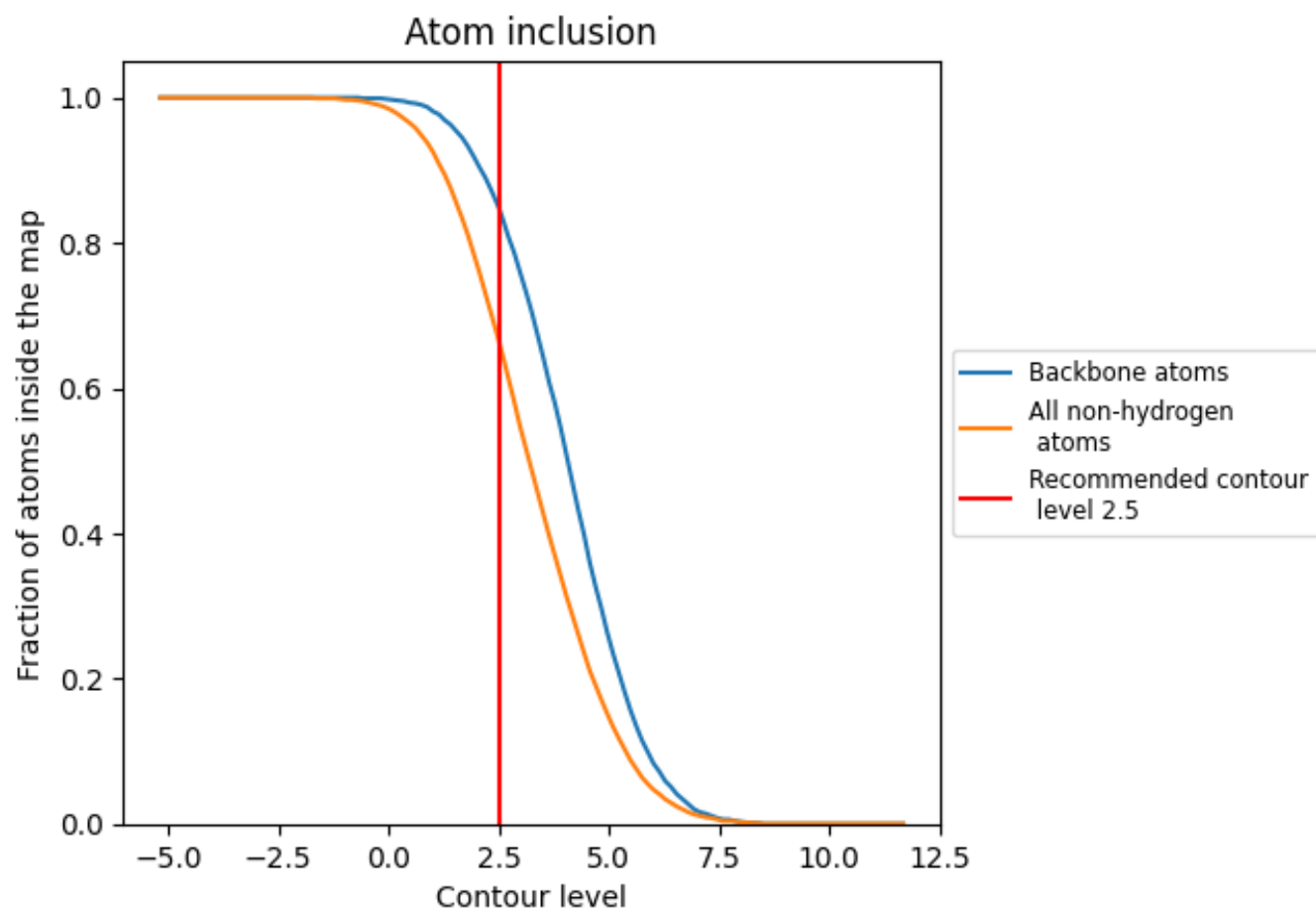
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.2680
A	0.6430	0.2660
B	0.7200	0.2740

