Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:27 pm GMT

PDB ID	:	6R3Q
EMDB ID	:	EMD-4719
Title	:	The structure of a membrane adenylyl cyclase bound to an activated stimulatory G protein
Authors	:	Korkhov, V.M.; Qi, C.
Deposited on	:	2019-03-20
Resolution	:	3.40 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:

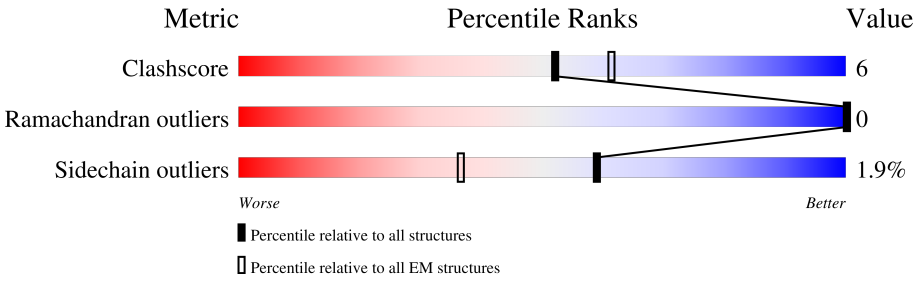
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1637	6% 41% 10% 49%
2	B	404	6% 71% 13% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9529 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
			Total	C	N	O	S		
1	A	841	6687	4339	1100	1193	55	0	0

There are 283 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1355	ALA	-	expression tag	UNP E1BM79
A	1356	ALA	-	expression tag	UNP E1BM79
A	1357	ALA	-	expression tag	UNP E1BM79
A	1358	LEU	-	expression tag	UNP E1BM79
A	1359	GLU	-	expression tag	UNP E1BM79
A	1360	VAL	-	expression tag	UNP E1BM79
A	1361	LEU	-	expression tag	UNP E1BM79
A	1362	PHE	-	expression tag	UNP E1BM79
A	1363	GLN	-	expression tag	UNP E1BM79
A	1364	GLY	-	expression tag	UNP E1BM79
A	1365	PRO	-	expression tag	UNP E1BM79
A	1366	GLY	-	expression tag	UNP E1BM79
A	1367	GLY	-	expression tag	UNP E1BM79
A	1368	VAL	-	expression tag	UNP E1BM79
A	1369	SER	-	expression tag	UNP E1BM79
A	1370	LYS	-	expression tag	UNP E1BM79
A	1371	GLY	-	expression tag	UNP E1BM79
A	1372	GLU	-	expression tag	UNP E1BM79
A	1373	GLU	-	expression tag	UNP E1BM79
A	1374	LEU	-	expression tag	UNP E1BM79
A	1375	PHE	-	expression tag	UNP E1BM79
A	1376	THR	-	expression tag	UNP E1BM79
A	1377	GLY	-	expression tag	UNP E1BM79
A	1378	VAL	-	expression tag	UNP E1BM79
A	1379	VAL	-	expression tag	UNP E1BM79
A	1380	PRO	-	expression tag	UNP E1BM79
A	1381	ILE	-	expression tag	UNP E1BM79
A	1382	LEU	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1383	VAL	-	expression tag	UNP E1BM79
A	1384	GLU	-	expression tag	UNP E1BM79
A	1385	LEU	-	expression tag	UNP E1BM79
A	1386	ASP	-	expression tag	UNP E1BM79
A	1387	GLY	-	expression tag	UNP E1BM79
A	1388	ASP	-	expression tag	UNP E1BM79
A	1389	VAL	-	expression tag	UNP E1BM79
A	1390	ASN	-	expression tag	UNP E1BM79
A	1391	GLY	-	expression tag	UNP E1BM79
A	1392	HIS	-	expression tag	UNP E1BM79
A	1393	LYS	-	expression tag	UNP E1BM79
A	1394	PHE	-	expression tag	UNP E1BM79
A	1395	SER	-	expression tag	UNP E1BM79
A	1396	VAL	-	expression tag	UNP E1BM79
A	1397	SER	-	expression tag	UNP E1BM79
A	1398	GLY	-	expression tag	UNP E1BM79
A	1399	GLU	-	expression tag	UNP E1BM79
A	1400	GLY	-	expression tag	UNP E1BM79
A	1401	GLU	-	expression tag	UNP E1BM79
A	1402	GLY	-	expression tag	UNP E1BM79
A	1403	ASP	-	expression tag	UNP E1BM79
A	1404	ALA	-	expression tag	UNP E1BM79
A	1405	THR	-	expression tag	UNP E1BM79
A	1406	TYR	-	expression tag	UNP E1BM79
A	1407	GLY	-	expression tag	UNP E1BM79
A	1408	LYS	-	expression tag	UNP E1BM79
A	1409	LEU	-	expression tag	UNP E1BM79
A	1410	THR	-	expression tag	UNP E1BM79
A	1411	LEU	-	expression tag	UNP E1BM79
A	1412	LYS	-	expression tag	UNP E1BM79
A	1413	PHE	-	expression tag	UNP E1BM79
A	1414	ILE	-	expression tag	UNP E1BM79
A	1415	CYS	-	expression tag	UNP E1BM79
A	1416	THR	-	expression tag	UNP E1BM79
A	1417	THR	-	expression tag	UNP E1BM79
A	1418	GLY	-	expression tag	UNP E1BM79
A	1419	LYS	-	expression tag	UNP E1BM79
A	1420	LEU	-	expression tag	UNP E1BM79
A	1421	PRO	-	expression tag	UNP E1BM79
A	1422	VAL	-	expression tag	UNP E1BM79
A	1423	PRO	-	expression tag	UNP E1BM79
A	1424	TRP	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1425	PRO	-	expression tag	UNP E1BM79
A	1426	THR	-	expression tag	UNP E1BM79
A	1427	LEU	-	expression tag	UNP E1BM79
A	1428	VAL	-	expression tag	UNP E1BM79
A	1429	THR	-	expression tag	UNP E1BM79
A	1430	THR	-	expression tag	UNP E1BM79
A	1431	PHE	-	expression tag	UNP E1BM79
A	1432	GLY	-	expression tag	UNP E1BM79
A	1433	TYR	-	expression tag	UNP E1BM79
A	1434	GLY	-	expression tag	UNP E1BM79
A	1435	LEU	-	expression tag	UNP E1BM79
A	1436	GLN	-	expression tag	UNP E1BM79
A	1437	CYS	-	expression tag	UNP E1BM79
A	1438	PHE	-	expression tag	UNP E1BM79
A	1439	ALA	-	expression tag	UNP E1BM79
A	1440	ARG	-	expression tag	UNP E1BM79
A	1441	TYR	-	expression tag	UNP E1BM79
A	1442	PRO	-	expression tag	UNP E1BM79
A	1443	ASP	-	expression tag	UNP E1BM79
A	1444	HIS	-	expression tag	UNP E1BM79
A	1445	MET	-	expression tag	UNP E1BM79
A	1446	LYS	-	expression tag	UNP E1BM79
A	1447	GLN	-	expression tag	UNP E1BM79
A	1448	HIS	-	expression tag	UNP E1BM79
A	1449	ASP	-	expression tag	UNP E1BM79
A	1450	PHE	-	expression tag	UNP E1BM79
A	1451	PHE	-	expression tag	UNP E1BM79
A	1452	LYS	-	expression tag	UNP E1BM79
A	1453	SER	-	expression tag	UNP E1BM79
A	1454	ALA	-	expression tag	UNP E1BM79
A	1455	MET	-	expression tag	UNP E1BM79
A	1456	PRO	-	expression tag	UNP E1BM79
A	1457	GLU	-	expression tag	UNP E1BM79
A	1458	GLY	-	expression tag	UNP E1BM79
A	1459	TYR	-	expression tag	UNP E1BM79
A	1460	VAL	-	expression tag	UNP E1BM79
A	1461	GLN	-	expression tag	UNP E1BM79
A	1462	GLU	-	expression tag	UNP E1BM79
A	1463	ARG	-	expression tag	UNP E1BM79
A	1464	THR	-	expression tag	UNP E1BM79
A	1465	ILE	-	expression tag	UNP E1BM79
A	1466	PHE	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1467	PHE	-	expression tag	UNP E1BM79
A	1468	LYS	-	expression tag	UNP E1BM79
A	1469	ASP	-	expression tag	UNP E1BM79
A	1470	ASP	-	expression tag	UNP E1BM79
A	1471	GLY	-	expression tag	UNP E1BM79
A	1472	ASN	-	expression tag	UNP E1BM79
A	1473	TYR	-	expression tag	UNP E1BM79
A	1474	LYS	-	expression tag	UNP E1BM79
A	1475	THR	-	expression tag	UNP E1BM79
A	1476	ARG	-	expression tag	UNP E1BM79
A	1477	ALA	-	expression tag	UNP E1BM79
A	1478	GLU	-	expression tag	UNP E1BM79
A	1479	VAL	-	expression tag	UNP E1BM79
A	1480	LYS	-	expression tag	UNP E1BM79
A	1481	PHE	-	expression tag	UNP E1BM79
A	1482	GLU	-	expression tag	UNP E1BM79
A	1483	GLY	-	expression tag	UNP E1BM79
A	1484	ASP	-	expression tag	UNP E1BM79
A	1485	THR	-	expression tag	UNP E1BM79
A	1486	LEU	-	expression tag	UNP E1BM79
A	1487	VAL	-	expression tag	UNP E1BM79
A	1488	ASN	-	expression tag	UNP E1BM79
A	1489	ARG	-	expression tag	UNP E1BM79
A	1490	ILE	-	expression tag	UNP E1BM79
A	1491	GLU	-	expression tag	UNP E1BM79
A	1492	LEU	-	expression tag	UNP E1BM79
A	1493	LYS	-	expression tag	UNP E1BM79
A	1494	GLY	-	expression tag	UNP E1BM79
A	1495	ILE	-	expression tag	UNP E1BM79
A	1496	ASP	-	expression tag	UNP E1BM79
A	1497	PHE	-	expression tag	UNP E1BM79
A	1498	LYS	-	expression tag	UNP E1BM79
A	1499	GLU	-	expression tag	UNP E1BM79
A	1500	ASP	-	expression tag	UNP E1BM79
A	1501	GLY	-	expression tag	UNP E1BM79
A	1502	ASN	-	expression tag	UNP E1BM79
A	1503	ILE	-	expression tag	UNP E1BM79
A	1504	LEU	-	expression tag	UNP E1BM79
A	1505	GLY	-	expression tag	UNP E1BM79
A	1506	HIS	-	expression tag	UNP E1BM79
A	1507	LYS	-	expression tag	UNP E1BM79
A	1508	LEU	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1509	GLU	-	expression tag	UNP E1BM79
A	1510	TYR	-	expression tag	UNP E1BM79
A	1511	ASN	-	expression tag	UNP E1BM79
A	1512	TYR	-	expression tag	UNP E1BM79
A	1513	ASN	-	expression tag	UNP E1BM79
A	1514	SER	-	expression tag	UNP E1BM79
A	1515	HIS	-	expression tag	UNP E1BM79
A	1516	ASN	-	expression tag	UNP E1BM79
A	1517	VAL	-	expression tag	UNP E1BM79
A	1518	TYR	-	expression tag	UNP E1BM79
A	1519	ILE	-	expression tag	UNP E1BM79
A	1520	MET	-	expression tag	UNP E1BM79
A	1521	ALA	-	expression tag	UNP E1BM79
A	1522	ASP	-	expression tag	UNP E1BM79
A	1523	LYS	-	expression tag	UNP E1BM79
A	1524	GLN	-	expression tag	UNP E1BM79
A	1525	LYS	-	expression tag	UNP E1BM79
A	1526	ASN	-	expression tag	UNP E1BM79
A	1527	GLY	-	expression tag	UNP E1BM79
A	1528	ILE	-	expression tag	UNP E1BM79
A	1529	LYS	-	expression tag	UNP E1BM79
A	1530	VAL	-	expression tag	UNP E1BM79
A	1531	ASN	-	expression tag	UNP E1BM79
A	1532	PHE	-	expression tag	UNP E1BM79
A	1533	LYS	-	expression tag	UNP E1BM79
A	1534	ILE	-	expression tag	UNP E1BM79
A	1535	ARG	-	expression tag	UNP E1BM79
A	1536	HIS	-	expression tag	UNP E1BM79
A	1537	ASN	-	expression tag	UNP E1BM79
A	1538	ILE	-	expression tag	UNP E1BM79
A	1539	GLU	-	expression tag	UNP E1BM79
A	1540	ASP	-	expression tag	UNP E1BM79
A	1541	GLY	-	expression tag	UNP E1BM79
A	1542	SER	-	expression tag	UNP E1BM79
A	1543	VAL	-	expression tag	UNP E1BM79
A	1544	GLN	-	expression tag	UNP E1BM79
A	1545	LEU	-	expression tag	UNP E1BM79
A	1546	ALA	-	expression tag	UNP E1BM79
A	1547	ASP	-	expression tag	UNP E1BM79
A	1548	HIS	-	expression tag	UNP E1BM79
A	1549	TYR	-	expression tag	UNP E1BM79
A	1550	GLN	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1551	GLN	-	expression tag	UNP E1BM79
A	1552	ASN	-	expression tag	UNP E1BM79
A	1553	THR	-	expression tag	UNP E1BM79
A	1554	PRO	-	expression tag	UNP E1BM79
A	1555	ILE	-	expression tag	UNP E1BM79
A	1556	GLY	-	expression tag	UNP E1BM79
A	1557	ASP	-	expression tag	UNP E1BM79
A	1558	GLY	-	expression tag	UNP E1BM79
A	1559	PRO	-	expression tag	UNP E1BM79
A	1560	VAL	-	expression tag	UNP E1BM79
A	1561	LEU	-	expression tag	UNP E1BM79
A	1562	LEU	-	expression tag	UNP E1BM79
A	1563	PRO	-	expression tag	UNP E1BM79
A	1564	ASP	-	expression tag	UNP E1BM79
A	1565	ASN	-	expression tag	UNP E1BM79
A	1566	HIS	-	expression tag	UNP E1BM79
A	1567	TYR	-	expression tag	UNP E1BM79
A	1568	LEU	-	expression tag	UNP E1BM79
A	1569	SER	-	expression tag	UNP E1BM79
A	1570	TYR	-	expression tag	UNP E1BM79
A	1571	GLN	-	expression tag	UNP E1BM79
A	1572	SER	-	expression tag	UNP E1BM79
A	1573	ALA	-	expression tag	UNP E1BM79
A	1574	LEU	-	expression tag	UNP E1BM79
A	1575	SER	-	expression tag	UNP E1BM79
A	1576	LYS	-	expression tag	UNP E1BM79
A	1577	ASP	-	expression tag	UNP E1BM79
A	1578	PRO	-	expression tag	UNP E1BM79
A	1579	ASN	-	expression tag	UNP E1BM79
A	1580	GLU	-	expression tag	UNP E1BM79
A	1581	LYS	-	expression tag	UNP E1BM79
A	1582	ARG	-	expression tag	UNP E1BM79
A	1583	ASP	-	expression tag	UNP E1BM79
A	1584	HIS	-	expression tag	UNP E1BM79
A	1585	MET	-	expression tag	UNP E1BM79
A	1586	VAL	-	expression tag	UNP E1BM79
A	1587	LEU	-	expression tag	UNP E1BM79
A	1588	LEU	-	expression tag	UNP E1BM79
A	1589	GLU	-	expression tag	UNP E1BM79
A	1590	PHE	-	expression tag	UNP E1BM79
A	1591	VAL	-	expression tag	UNP E1BM79
A	1592	THR	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1593	ALA	-	expression tag	UNP E1BM79
A	1594	ALA	-	expression tag	UNP E1BM79
A	1595	GLY	-	expression tag	UNP E1BM79
A	1596	ILE	-	expression tag	UNP E1BM79
A	1597	THR	-	expression tag	UNP E1BM79
A	1598	LEU	-	expression tag	UNP E1BM79
A	1599	GLY	-	expression tag	UNP E1BM79
A	1600	MET	-	expression tag	UNP E1BM79
A	1601	ASP	-	expression tag	UNP E1BM79
A	1602	GLU	-	expression tag	UNP E1BM79
A	1603	LEU	-	expression tag	UNP E1BM79
A	1604	TYR	-	expression tag	UNP E1BM79
A	1605	LYS	-	expression tag	UNP E1BM79
A	1606	ALA	-	expression tag	UNP E1BM79
A	1607	ALA	-	expression tag	UNP E1BM79
A	1608	SER	-	expression tag	UNP E1BM79
A	1609	ALA	-	expression tag	UNP E1BM79
A	1610	TRP	-	expression tag	UNP E1BM79
A	1611	SER	-	expression tag	UNP E1BM79
A	1612	HIS	-	expression tag	UNP E1BM79
A	1613	PRO	-	expression tag	UNP E1BM79
A	1614	GLN	-	expression tag	UNP E1BM79
A	1615	PHE	-	expression tag	UNP E1BM79
A	1616	GLU	-	expression tag	UNP E1BM79
A	1617	LYS	-	expression tag	UNP E1BM79
A	1618	GLY	-	expression tag	UNP E1BM79
A	1619	GLY	-	expression tag	UNP E1BM79
A	1620	GLY	-	expression tag	UNP E1BM79
A	1621	SER	-	expression tag	UNP E1BM79
A	1622	GLY	-	expression tag	UNP E1BM79
A	1623	GLY	-	expression tag	UNP E1BM79
A	1624	GLY	-	expression tag	UNP E1BM79
A	1625	SER	-	expression tag	UNP E1BM79
A	1626	GLY	-	expression tag	UNP E1BM79
A	1627	GLY	-	expression tag	UNP E1BM79
A	1628	SER	-	expression tag	UNP E1BM79
A	1629	ALA	-	expression tag	UNP E1BM79
A	1630	TRP	-	expression tag	UNP E1BM79
A	1631	SER	-	expression tag	UNP E1BM79
A	1632	HIS	-	expression tag	UNP E1BM79
A	1633	PRO	-	expression tag	UNP E1BM79
A	1634	GLN	-	expression tag	UNP E1BM79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1635	PHE	-	expression tag	UNP E1BM79
A	1636	GLU	-	expression tag	UNP E1BM79
A	1637	LYS	-	expression tag	UNP E1BM79

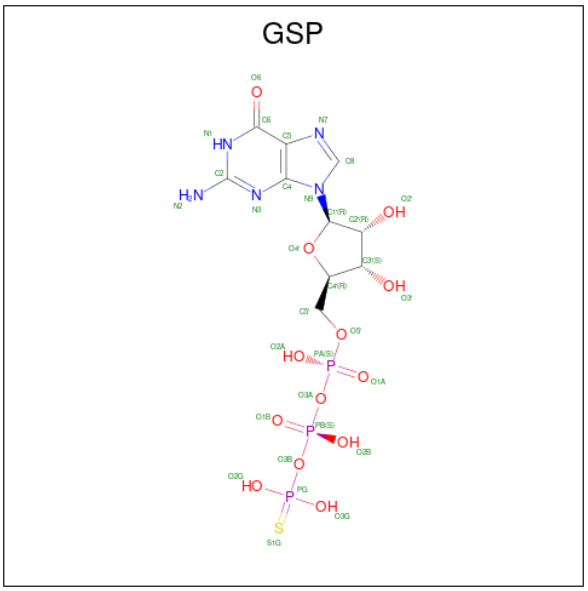
- Molecule 2 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	GLY	-	insertion	UNP P04896
B	79	ASN	GLN	conflict	UNP P04896
B	?	-	ALA	deletion	UNP P04896
B	81	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 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

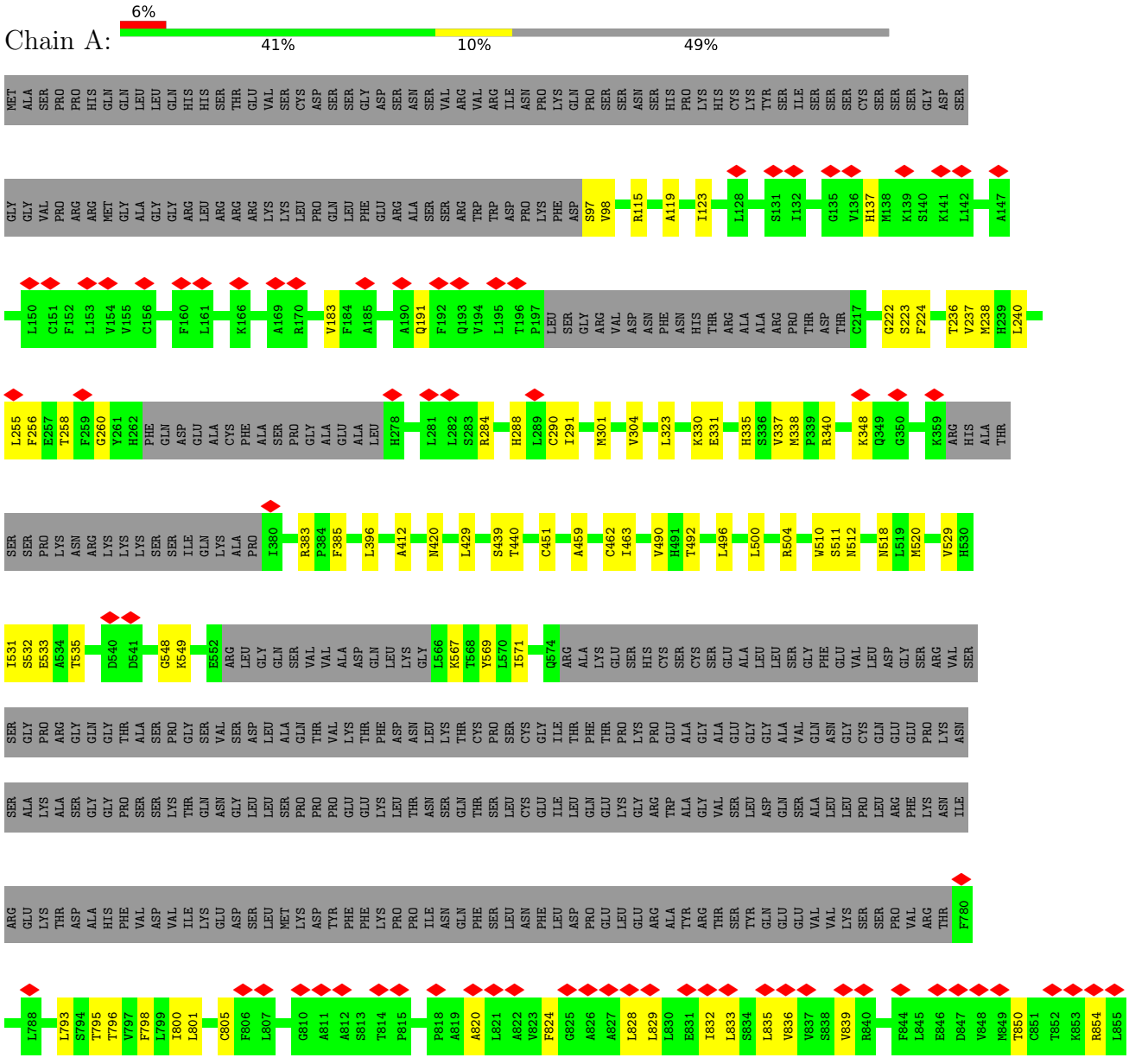
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	

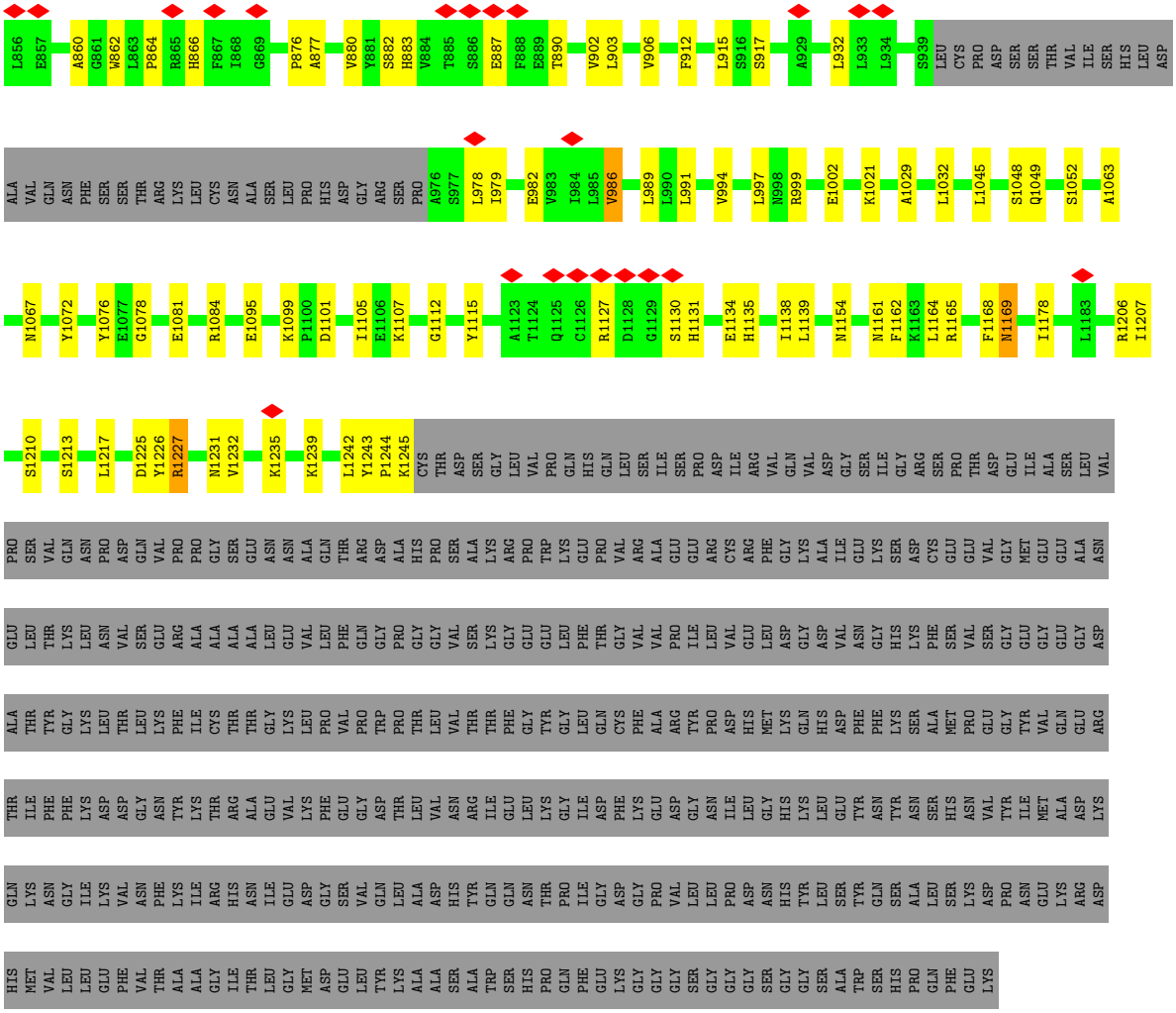
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Adenylate cyclase 9

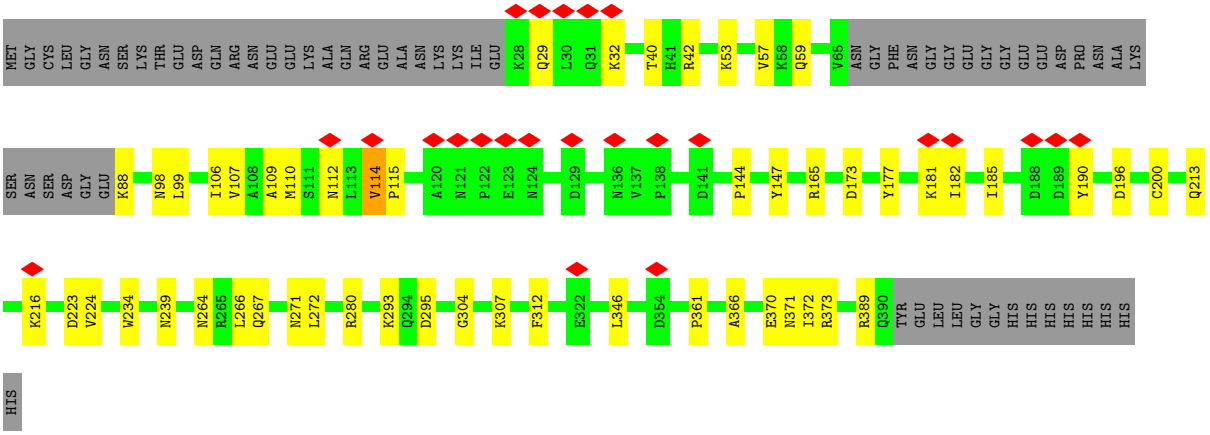
Chain A:





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

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	170456	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 ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	244.2, 244.2, 244.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.814, 0.814, 0.814	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: 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	0.56	0/6834	0.71	8/9242 (0.1%)
2	B	0.50	0/2867	0.60	0/3875
All	All	0.54	0/9701	0.68	8/13117 (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	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1032	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	A	500	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	989	LEU	CA-CB-CG	5.38	127.66	115.30
1	A	1045	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	451	CYS	CA-CB-SG	5.34	123.62	114.00
1	A	833	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	429	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	496	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1072	TYR	Peptide
2	B	114	VAL	Peptide

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	6687	0	6722	81	0
2	B	2809	0	2771	28	0
3	B	32	0	12	2	0
4	B	1	0	0	0	0
All	All	9529	0	9505	109	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 6.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASN:ND2	1:A:1178:ILE:O	2.25	0.70
1:A:492:THR:HG23	1:A:535:THR:HG22	1.78	0.65
2:B:99:LEU:HD22	2:B:182:ILE:HG21	1.76	0.65
1:A:1105:ILE:HD12	1:A:1139:LEU:HD23	1.77	0.65
1:A:290:CYS:HB3	1:A:800:ILE:HD11	1.80	0.64
1:A:912:PHE:HB3	1:A:915:LEU:HD23	1.81	0.62
1:A:1206:ARG:NH1	1:A:1244:PRO:O	2.33	0.61
1:A:224:PHE:HB2	1:A:284:ARG:HH22	1.64	0.60
1:A:115:ARG:HB3	1:A:237:VAL:HG13	1.83	0.60
2:B:366:ALA:HA	2:B:372:ILE:HD11	1.84	0.60
1:A:1081:GLU:OE1	1:A:1084:ARG:NH1	2.35	0.59
1:A:412:ALA:O	1:A:1052:SER:OG	2.20	0.58
1:A:1131:HIS:HB3	1:A:1134:GLU:HB3	1.85	0.58
1:A:820:ALA:HA	1:A:882:SER:HB2	1.86	0.57
1:A:1154:ASN:HD21	1:A:1162:PHE:H	1.51	0.56
2:B:115:PRO:HG2	2:B:165:ARG:HH12	1.70	0.56
1:A:337:VAL:HG13	1:A:338:MET:HG3	1.87	0.56
1:A:1169:ASN:ND2	1:A:1210:SER:OG	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ASP:OD2	2:B:293:LYS:NZ	2.40	0.55
1:A:887:GLU:OE2	1:A:890:THR:N	2.40	0.55
1:A:490:VAL:HB	1:A:531:ILE:HG22	1.88	0.54
1:A:798:PHE:HB2	1:A:876:PRO:HG3	1.90	0.53
2:B:144:PRO:HA	2:B:147:TYR:HD2	1.73	0.53
1:A:850:THR:OG1	1:A:854:ARG:NH1	2.42	0.52
1:A:238:MET:HB3	1:A:240:LEU:HD13	1.91	0.52
2:B:40:THR:OG1	2:B:42:ARG:NH1	2.42	0.52
1:A:504:ARG:NH2	1:A:1107:LYS:O	2.43	0.52
2:B:304:GLY:O	2:B:307:LYS:NZ	2.42	0.52
2:B:98:ASN:ND2	2:B:200:CYS:SG	2.83	0.52
1:A:862:TRP:O	1:A:866:HIS:ND1	2.35	0.51
1:A:1067:ASN:ND2	1:A:1161:ASN:O	2.43	0.51
1:A:1226:TYR:HE1	1:A:1239:LYS:HG3	1.76	0.51
2:B:370:GLU:OE1	2:B:373:ARG:NH1	2.44	0.51
2:B:59:GLN:HG2	2:B:372:ILE:HG13	1.93	0.50
1:A:331:GLU:OE2	1:A:335:HIS:NE2	2.44	0.50
2:B:295:ASP:OD1	2:B:295:ASP:N	2.45	0.50
1:A:529:VAL:HG13	1:A:571:ILE:HB	1.93	0.50
1:A:548:GLY:H	1:A:569:TYR:HA	1.77	0.50
1:A:979:ILE:HA	1:A:982:GLU:HG2	1.93	0.50
1:A:97:SER:OG	1:A:98:VAL:N	2.44	0.50
2:B:53:LYS:NZ	3:B:501:GSP:O1B	2.35	0.50
1:A:439:SER:OG	1:A:440:THR:N	2.44	0.49
1:A:383:ARG:NH1	1:A:1095:GLU:OE2	2.45	0.49
1:A:330:LYS:HB2	1:A:1029:ALA:HB2	1.95	0.49
2:B:213:GLN:HE21	2:B:216:LYS:HA	1.76	0.49
1:A:860:ALA:HA	1:A:864:PRO:HB2	1.95	0.49
1:A:520:MET:HE1	1:A:532:SER:HB3	1.95	0.49
1:A:510:TRP:HE1	1:A:1112:GLY:HA2	1.78	0.48
1:A:866:HIS:HA	1:A:915:LEU:HD11	1.95	0.48
2:B:109:ALA:HA	2:B:112:ASN:HB2	1.94	0.48
1:A:903:LEU:HA	1:A:906:VAL:HG12	1.95	0.48
1:A:236:THR:HG21	1:A:997:LEU:HD21	1.94	0.48
1:A:288:HIS:HA	1:A:291:ILE:HG22	1.95	0.48
1:A:511:SER:OG	1:A:512:ASN:N	2.47	0.48
1:A:902:VAL:HG11	1:A:932:LEU:HD11	1.96	0.48
1:A:1207:ILE:HB	1:A:1243:TYR:HB3	1.96	0.48
1:A:793:LEU:HA	1:A:796:THR:HG22	1.95	0.47
2:B:185:ILE:HD12	2:B:190:TYR:HD2	1.79	0.47
1:A:1127:ARG:HB2	1:A:1130:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:SER:OG	1:A:1049:GLN:N	2.46	0.47
1:A:1232:VAL:HB	1:A:1235:LYS:HB2	1.97	0.47
2:B:57:VAL:HG21	2:B:223:ASP:HB2	1.96	0.47
1:A:255:LEU:HA	1:A:258:THR:HG22	1.96	0.47
1:A:1076:TYR:O	1:A:1078:GLY:N	2.48	0.47
1:A:824:PHE:O	1:A:828:LEU:HB2	2.15	0.46
1:A:836:VAL:HA	1:A:839:VAL:HG12	1.96	0.46
1:A:533:GLU:OE1	1:A:567:LYS:NZ	2.41	0.46
1:A:1105:ILE:HD11	1:A:1138:ILE:HG13	1.98	0.46
1:A:1213:SER:O	1:A:1217:LEU:HB2	2.16	0.46
1:A:1154:ASN:ND2	1:A:1162:PHE:H	2.14	0.46
1:A:123:ILE:HD13	1:A:183:VAL:HG21	1.97	0.46
1:A:137:HIS:HE1	1:A:978:LEU:HD22	1.81	0.46
1:A:1063:ALA:HB3	1:A:1115:TYR:HB3	1.98	0.46
1:A:795:THR:HG21	1:A:835:LEU:HD12	1.97	0.46
1:A:877:ALA:HA	1:A:880:VAL:HG12	1.97	0.45
2:B:234:TRP:HH2	2:B:272:LEU:HD21	1.80	0.45
2:B:177:TYR:OH	2:B:181:LYS:NZ	2.50	0.45
1:A:915:LEU:HD13	1:A:915:LEU:HA	1.79	0.45
1:A:1139:LEU:HD12	1:A:1168:PHE:HE1	1.82	0.44
2:B:181:LYS:NZ	2:B:196:ASP:OD1	2.43	0.44
2:B:266:LEU:HD23	2:B:312:PHE:HE2	1.83	0.44
1:A:991:LEU:HA	1:A:994:VAL:HG12	1.98	0.44
1:A:1135:HIS:HA	1:A:1138:ILE:HG12	1.98	0.44
1:A:917:SER:HB3	1:A:1002:GLU:HG2	1.99	0.44
2:B:107:VAL:HG22	2:B:110:MET:HE3	1.99	0.44
2:B:224:VAL:HG11	2:B:234:TRP:CD1	2.53	0.44
1:A:829:LEU:HA	1:A:832:ILE:HG22	2.00	0.44
1:A:323:LEU:HD11	1:A:1021:LYS:HG2	2.00	0.44
2:B:346:LEU:HD11	2:B:361:PRO:HG3	2.00	0.43
1:A:1225:ASP:HB3	1:A:1245:LYS:HE3	1.99	0.43
2:B:366:ALA:N	3:B:501:GSP:O6	2.45	0.43
1:A:223:SER:HB3	1:A:256:PHE:HZ	1.83	0.43
1:A:301:MET:HA	1:A:304:VAL:HG22	2.01	0.43
1:A:1099:LYS:HB3	1:A:1099:LYS:HE2	1.87	0.43
2:B:99:LEU:HB2	2:B:182:ILE:HG13	2.01	0.43
1:A:191:GLN:NE2	1:A:260:GLY:HA2	2.34	0.42
1:A:119:ALA:HB2	1:A:237:VAL:HG11	2.02	0.42
1:A:335:HIS:O	1:A:340:ARG:NH1	2.53	0.42
1:A:459:ALA:O	1:A:463:ILE:HG13	2.19	0.42
1:A:222:GLY:HA2	1:A:986:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:LEU:HD12	1:A:876:PRO:HB3	2.02	0.41
1:A:805:CYS:HB3	1:A:883:HIS:CD2	2.56	0.41
1:A:1101:ASP:OD1	1:A:1101:ASP:N	2.43	0.41
1:A:1227:ARG:HB2	1:A:1242:LEU:HG	2.02	0.41
2:B:185:ILE:HG13	2:B:190:TYR:HB3	2.03	0.41
2:B:32:LYS:HE2	2:B:32:LYS:HB3	1.95	0.41
1:A:396:LEU:HB2	1:A:462:CYS:SG	2.61	0.40
1:A:1206:ARG:HE	1:A:1242:LEU:HD13	1.86	0.40
2:B:267:GLN:HE21	2:B:271:ASN:HD21	1.69	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	827/1637 (50%)	770 (93%)	57 (7%)	0	100	100
2	B	337/404 (83%)	316 (94%)	21 (6%)	0	100	100
All	All	1164/2041 (57%)	1086 (93%)	78 (7%)	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	732/1409 (52%)	721 (98%)	11 (2%)	65 82
2	B	309/359 (86%)	300 (97%)	9 (3%)	42 69
All	All	1041/1768 (59%)	1021 (98%)	20 (2%)	59 78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LYS
1	A	385	PHE
1	A	518	ASN
1	A	549	LYS
1	A	986	VAL
1	A	999	ARG
1	A	1164	LEU
1	A	1165	ARG
1	A	1169	ASN
1	A	1227	ARG
1	A	1231	ASN
2	B	29	GLN
2	B	88	LYS
2	B	106	ILE
2	B	114	VAL
2	B	239	ASN
2	B	264	ASN
2	B	280	ARG
2	B	371	ASN
2	B	389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	191	GLN
1	A	389	GLN
1	A	518	ASN
1	A	908	GLN
1	A	1154	ASN
1	A	1156	ASN
1	A	1169	ASN
1	A	1231	ASN
2	B	31	GLN

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Mol	Chain	Res	Type
2	B	98	ASN
2	B	213	GLN
2	B	239	ASN
2	B	264	ASN
2	B	271	ASN
2	B	362	HIS
2	B	371	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
3	GSP	B	501	4	26,34,34	2.43	4 (15%)	27,54,54	1.67	5 (18%)

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
3	GSP	B	501	4	-	2/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	GSP	PG-S1G	-9.79	1.69	1.90
3	B	501	GSP	C5-C6	-4.81	1.37	1.47
3	B	501	GSP	C2'-C1'	-2.18	1.50	1.53
3	B	501	GSP	C5-C4	-2.13	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	GSP	PA-O3A-PB	-4.45	117.57	132.83
3	B	501	GSP	C5-C6-N1	3.57	120.25	113.95
3	B	501	GSP	C2-N1-C6	-3.08	119.42	125.10
3	B	501	GSP	C8-N7-C5	2.84	108.39	102.99
3	B	501	GSP	O6-C6-C5	-2.38	119.73	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	GSP	PA-O3A-PB-O1B
3	B	501	GSP	PA-O3A-PB-O2B

There are no ring outliers.

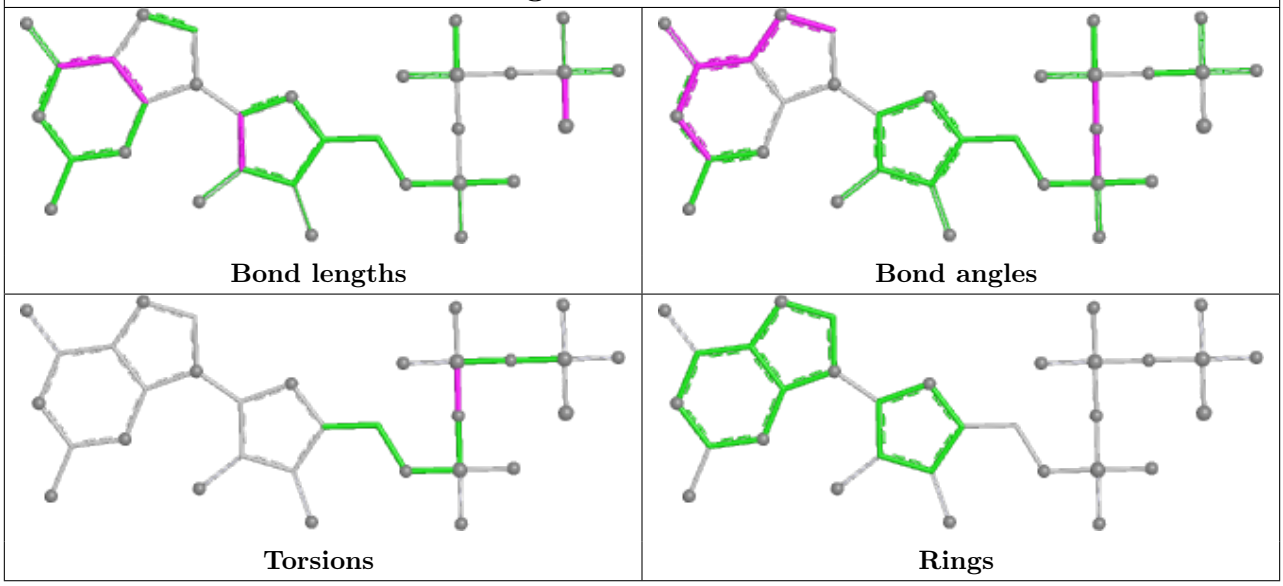
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	GSP	2	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.

Ligand GSP B 501



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.

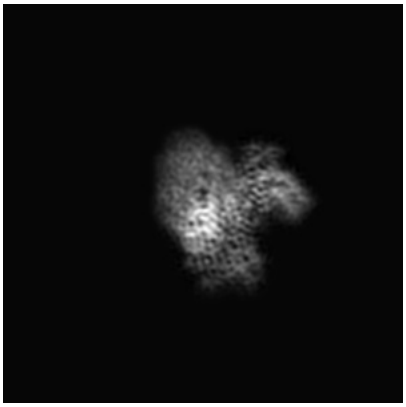
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4719. These allow visual inspection of the internal detail of the map and identification of artifacts.

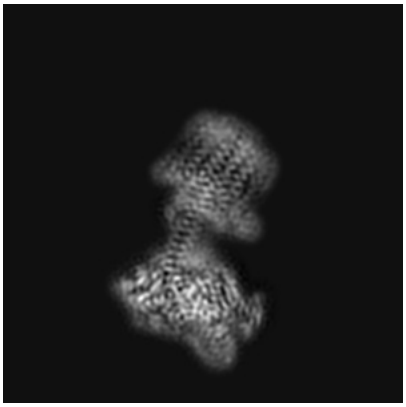
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

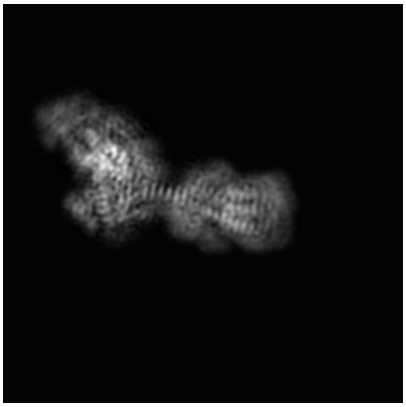
6.1.1 Primary map



X



Y

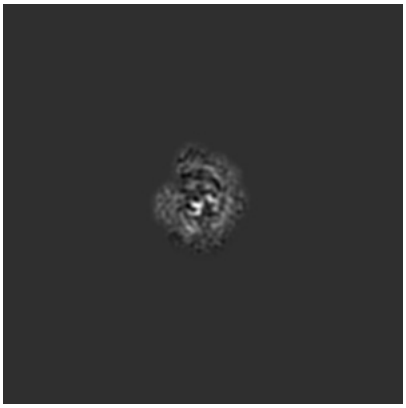


Z

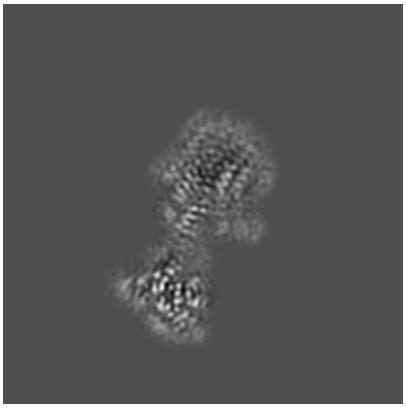
The images above show the map projected in three orthogonal directions.

6.2 Central slices

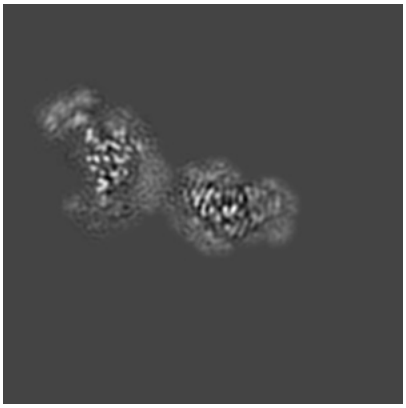
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

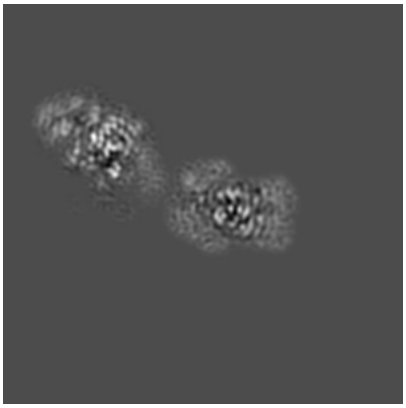
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 77

Y Index: 157



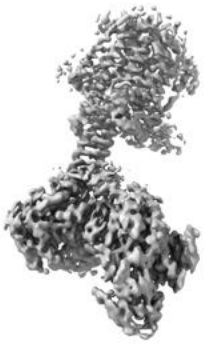
Z Index: 157

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

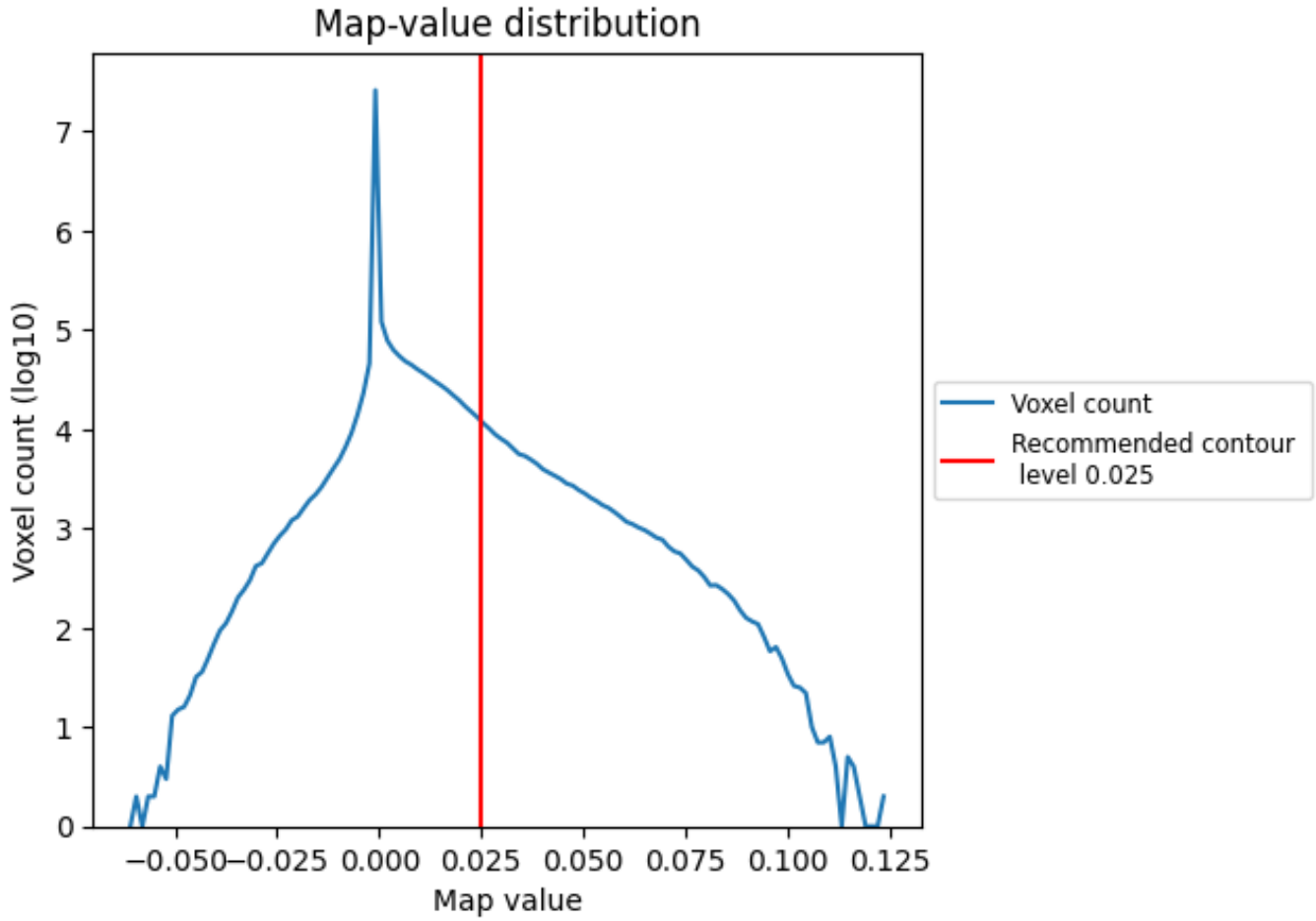
6.5 Mask visualisation (i)

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

7 Map analysis

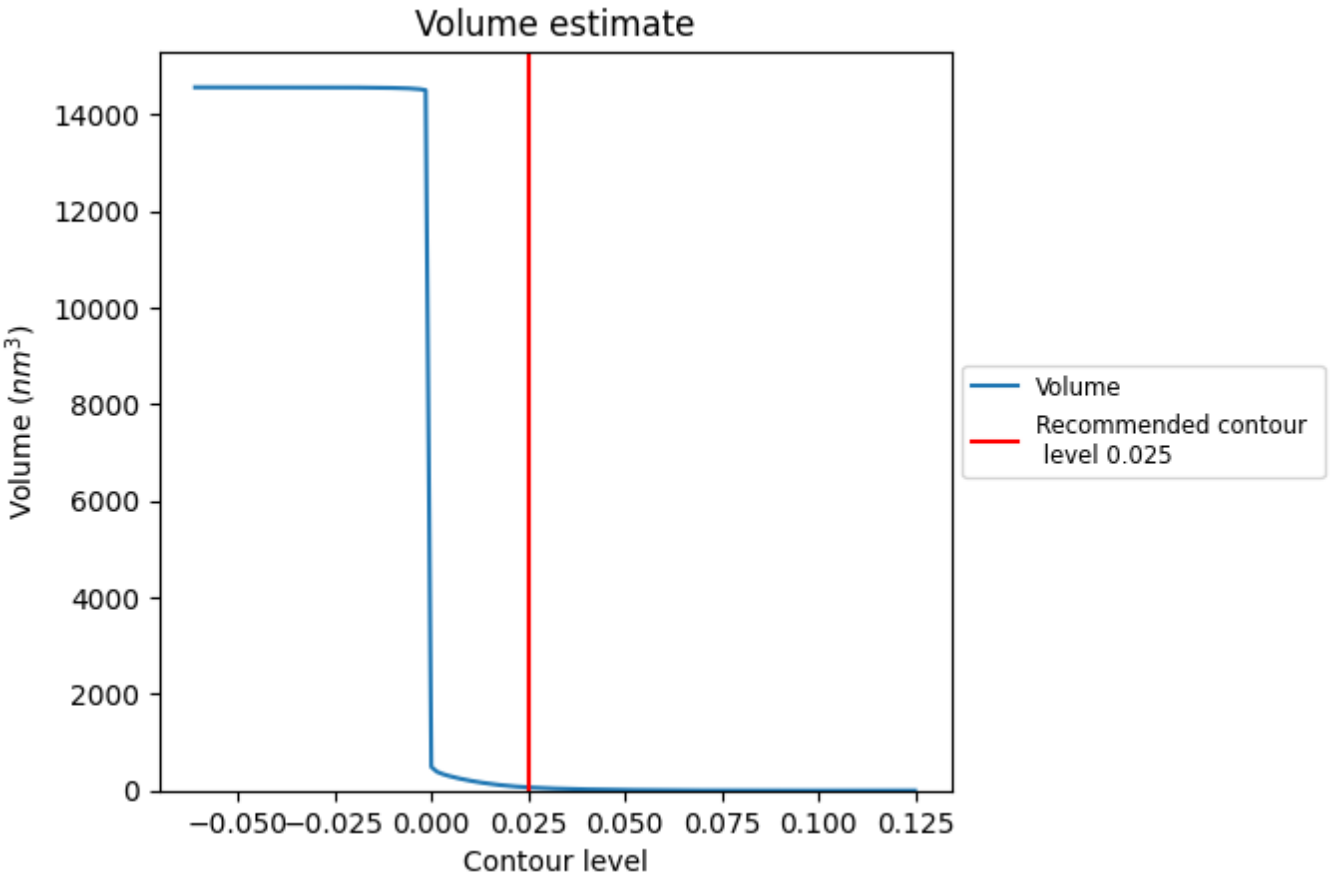
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

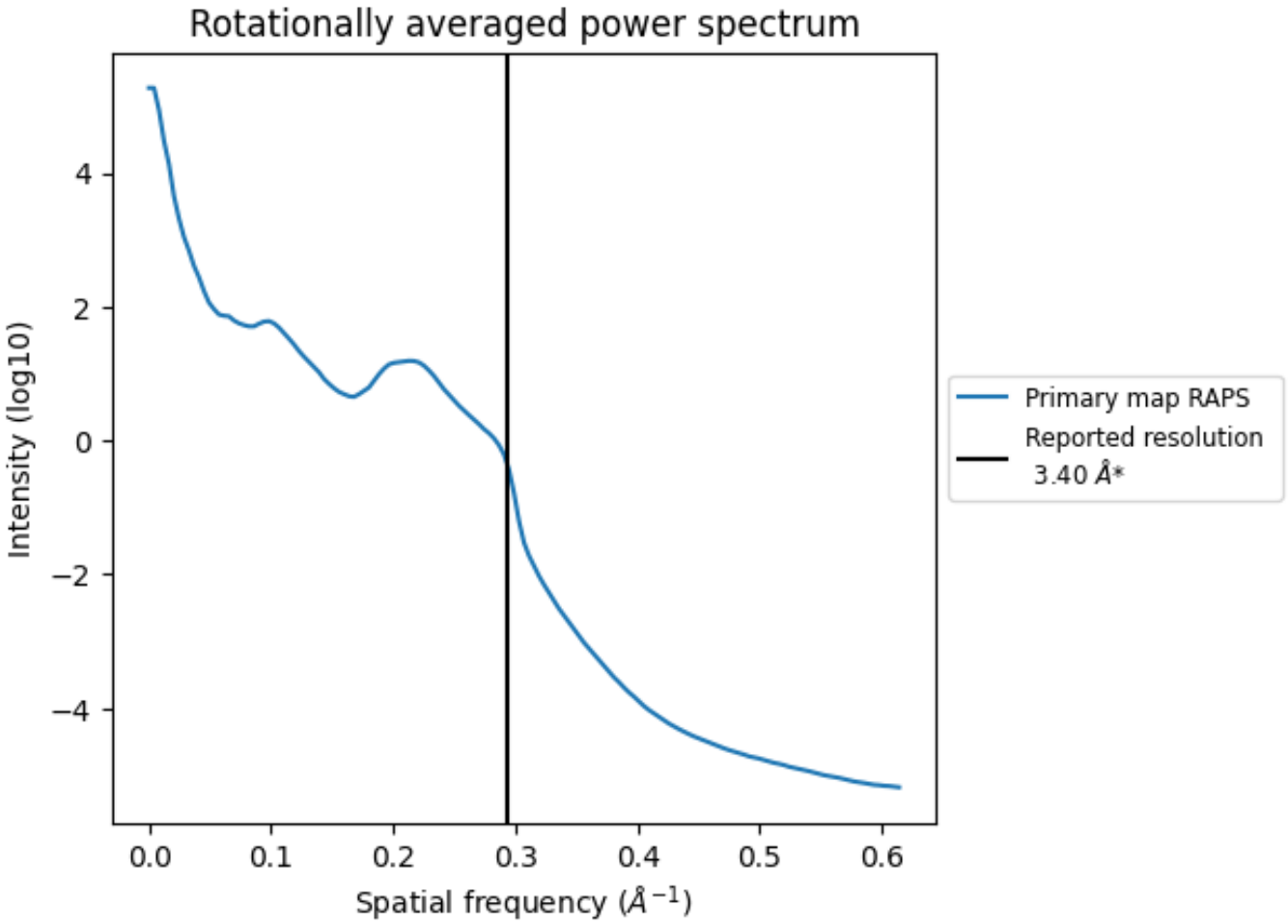
7.2 Volume estimate



The volume at the recommended contour level is 66 nm^3; this corresponds to an approximate mass of 60 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 (i)

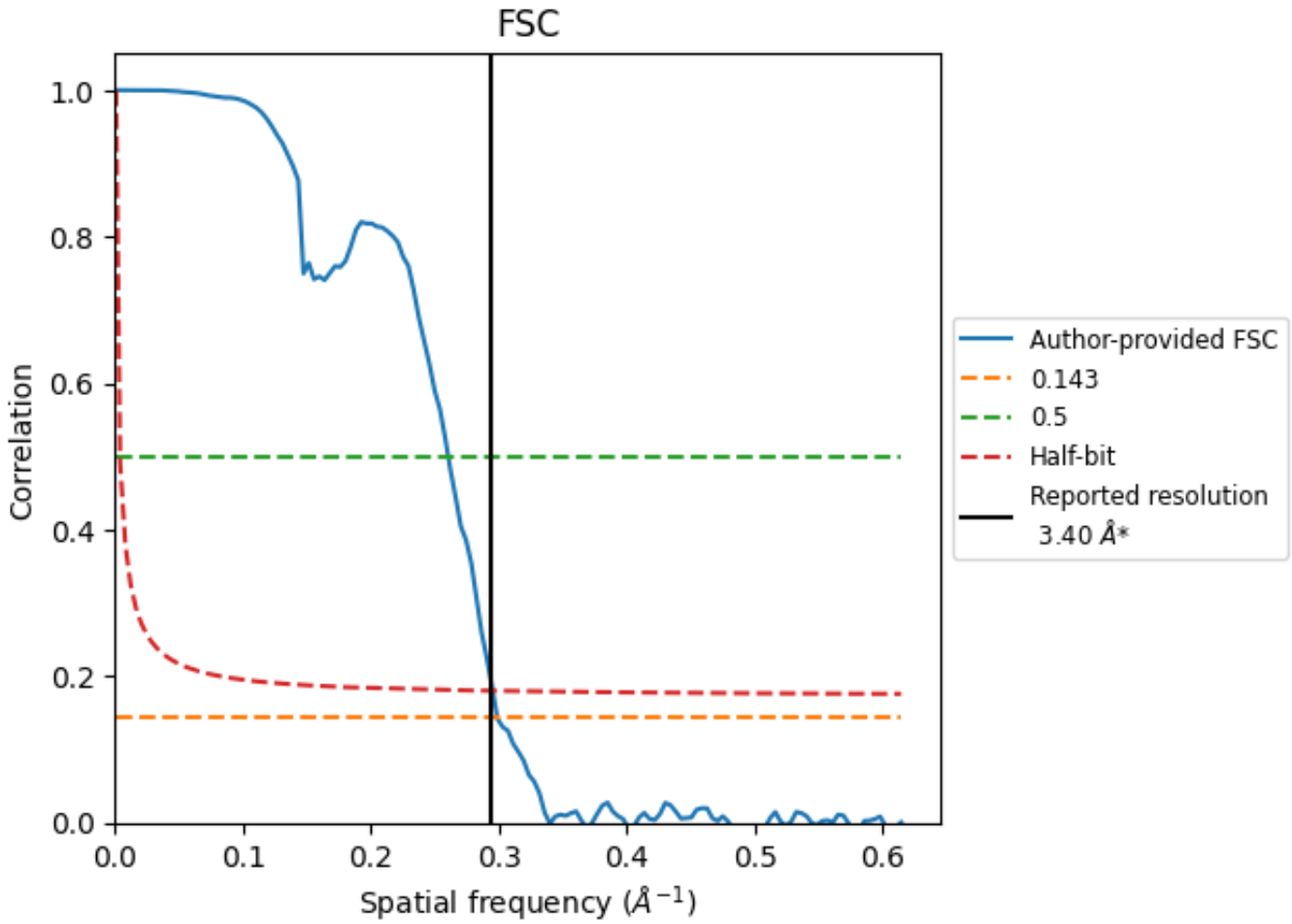


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

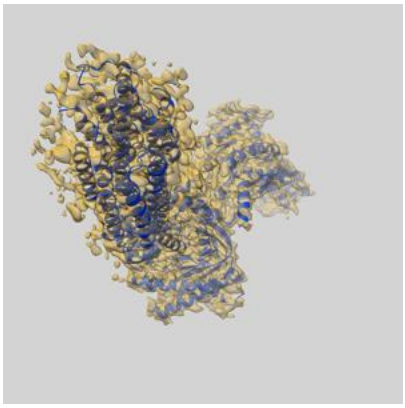
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.35	3.84	3.39
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

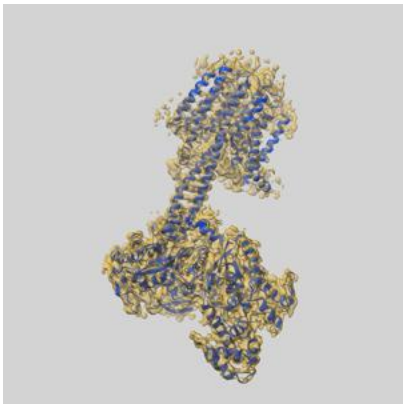
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4719 and PDB model 6R3Q. Per-residue inclusion information can be found in section 3 on page 12.

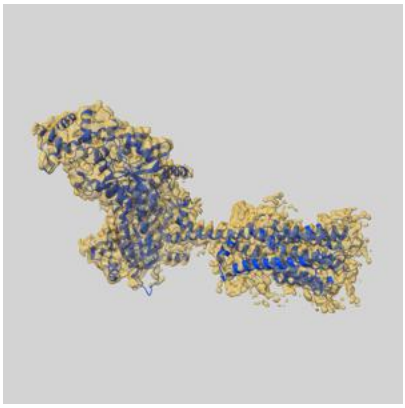
9.1 Map-model overlay



X



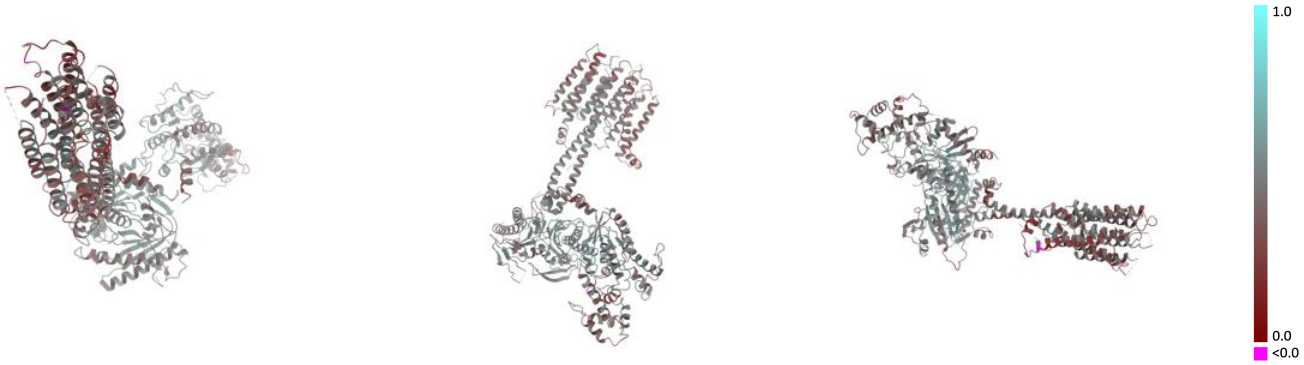
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

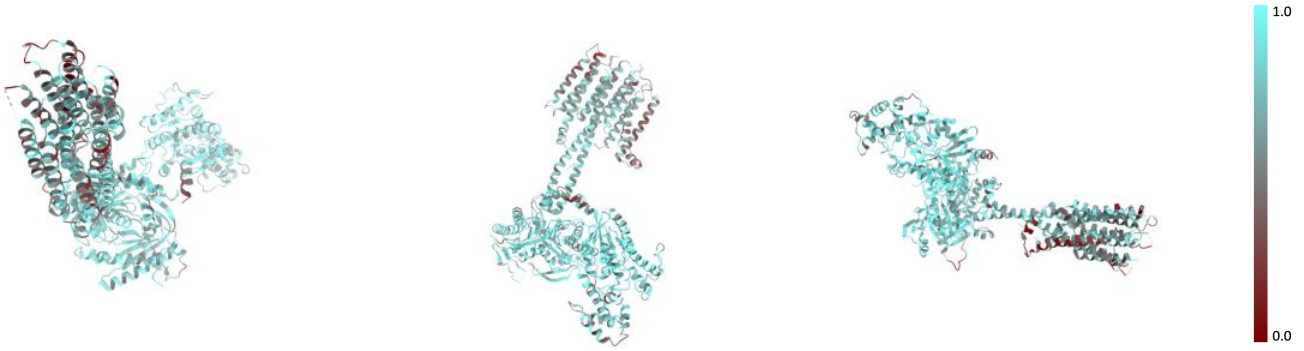
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

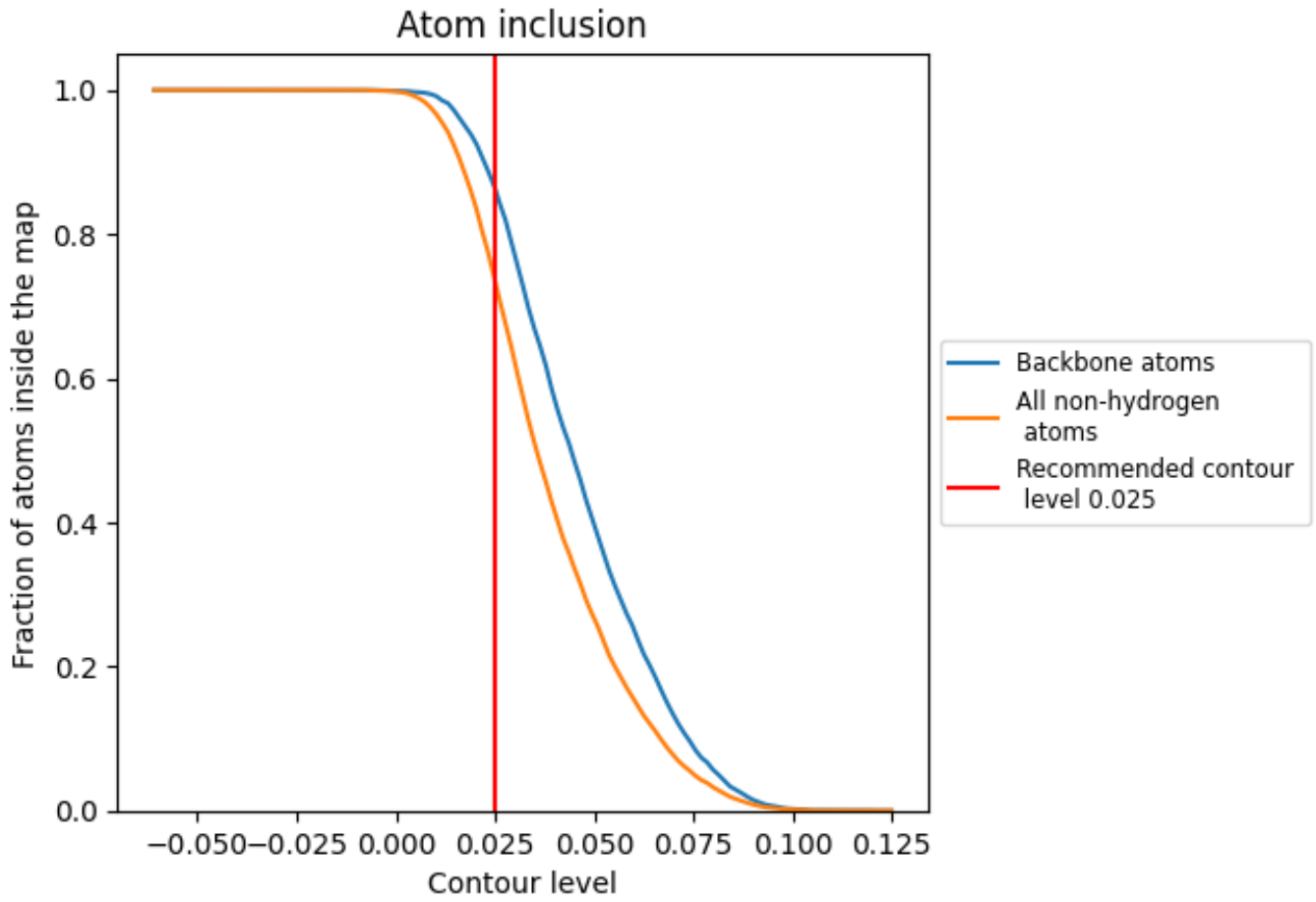
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7342	0.4440
A	0.7116	0.4360
B	0.7876	0.4620