



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:56 AM UTC

PDB ID : 9PAT / pdb_00009pat
EMDB ID : EMD-71445
Title : Antibody (1B2) Bound Rifamycin Synthetase Module 1 in the Transacylation Mode
Authors : Cogan, D.P.; Liu, C.; West, R.C.; Chen, M.
Deposited on : 2025-06-25
Resolution : 3.96 Å(reported)
Based on initial model : .

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:

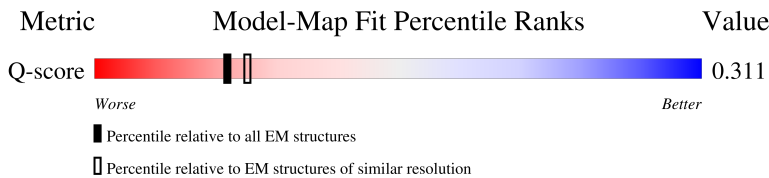
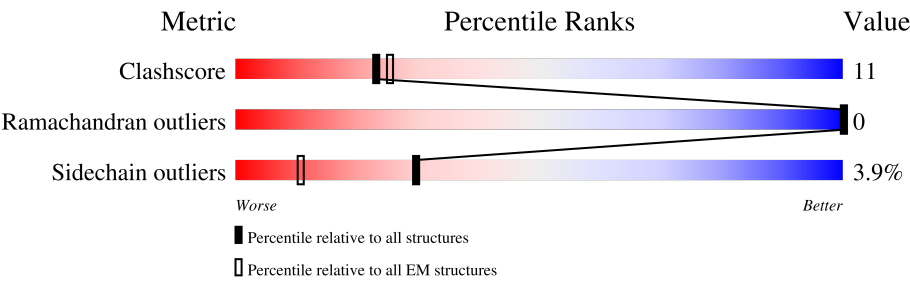
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.96 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	7646 (3.46 - 4.46)

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	1683	10% 63% 23% 13%
1	B	1683	48% 16% 35%
2	C	1683	96%
3	G	249	59% 23% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	249	61%20%18%
4	I	236	68%20%11%
4	L	236	62%25%11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25653 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 6-deoxyerythronolide-B synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1472	Total	C	N	O	S	0	0
			10796	6744	1947	2080	25		
1	B	1090	Total	C	N	O	S	0	0
			8009	5002	1444	1543	20		

There are 268 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O54666
A	2	ALA	-	expression tag	UNP O54666
A	3	SER	-	expression tag	UNP O54666
A	4	THR	-	expression tag	UNP O54666
A	5	ASP	-	expression tag	UNP O54666
A	6	SER	-	expression tag	UNP O54666
A	7	GLU	-	expression tag	UNP O54666
A	8	LYS	-	expression tag	UNP O54666
A	9	VAL	-	expression tag	UNP O54666
A	10	ALA	-	expression tag	UNP O54666
A	11	GLU	-	expression tag	UNP O54666
A	12	TYR	-	expression tag	UNP O54666
A	13	LEU	-	expression tag	UNP O54666
A	14	ARG	-	expression tag	UNP O54666
A	15	ARG	-	expression tag	UNP O54666
A	16	ALA	-	expression tag	UNP O54666
A	17	THR	-	expression tag	UNP O54666
A	18	LEU	-	expression tag	UNP O54666
A	19	ASP	-	expression tag	UNP O54666
A	20	LEU	-	expression tag	UNP O54666
A	21	ARG	-	expression tag	UNP O54666
A	22	ALA	-	expression tag	UNP O54666
A	23	ALA	-	expression tag	UNP O54666
A	24	ARG	-	expression tag	UNP O54666
A	25	GLN	-	expression tag	UNP O54666
A	26	ARG	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ILE	-	expression tag	UNP O54666
A	28	ARG	-	expression tag	UNP O54666
A	29	GLU	-	expression tag	UNP O54666
A	30	LEU	-	expression tag	UNP O54666
A	31	GLU	-	expression tag	UNP O54666
A	1581	THR	-	expression tag	UNP O54666
A	1582	GLU	-	expression tag	UNP O54666
A	1583	VAL	-	expression tag	UNP O54666
A	1584	ARG	-	expression tag	UNP O54666
A	1585	GLY	-	expression tag	UNP O54666
A	1586	GLU	-	expression tag	UNP O54666
A	1587	ALA	-	expression tag	UNP O54666
A	1588	PRO	-	expression tag	UNP O54666
A	1589	SER	-	expression tag	UNP O54666
A	1590	ALA	-	expression tag	UNP O54666
A	1591	LEU	-	expression tag	UNP O54666
A	1592	ALA	-	expression tag	UNP O54666
A	1593	GLY	-	expression tag	UNP O54666
A	1594	LEU	-	expression tag	UNP O54666
A	1595	ASP	-	expression tag	UNP O54666
A	1596	ALA	-	expression tag	UNP O54666
A	1597	LEU	-	expression tag	UNP O54666
A	1598	GLU	-	expression tag	UNP O54666
A	1599	ALA	-	expression tag	UNP O54666
A	1600	ALA	-	expression tag	UNP O54666
A	1601	LEU	-	expression tag	UNP O54666
A	1602	PRO	-	expression tag	UNP O54666
A	1603	GLU	-	expression tag	UNP O54666
A	1604	VAL	-	expression tag	UNP O54666
A	1605	PRO	-	expression tag	UNP O54666
A	1606	ALA	-	expression tag	UNP O54666
A	1607	THR	-	expression tag	UNP O54666
A	1608	GLU	-	expression tag	UNP O54666
A	1609	ARG	-	expression tag	UNP O54666
A	1610	GLU	-	expression tag	UNP O54666
A	1611	GLU	-	expression tag	UNP O54666
A	1612	LEU	-	expression tag	UNP O54666
A	1613	VAL	-	expression tag	UNP O54666
A	1614	GLN	-	expression tag	UNP O54666
A	1615	ARG	-	expression tag	UNP O54666
A	1616	LEU	-	expression tag	UNP O54666
A	1617	GLU	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1618	ARG	-	expression tag	UNP O54666
A	1619	MET	-	expression tag	UNP O54666
A	1620	LEU	-	expression tag	UNP O54666
A	1621	ALA	-	expression tag	UNP O54666
A	1622	ALA	-	expression tag	UNP O54666
A	1623	LEU	-	expression tag	UNP O54666
A	1624	ARG	-	expression tag	UNP O54666
A	1625	PRO	-	expression tag	UNP O54666
A	1626	VAL	-	expression tag	UNP O54666
A	1627	ALA	-	expression tag	UNP O54666
A	1628	GLN	-	expression tag	UNP O54666
A	1629	ALA	-	expression tag	UNP O54666
A	1630	ALA	-	expression tag	UNP O54666
A	1631	ASP	-	expression tag	UNP O54666
A	1632	ALA	-	expression tag	UNP O54666
A	1633	SER	-	expression tag	UNP O54666
A	1634	GLY	-	expression tag	UNP O54666
A	1635	THR	-	expression tag	UNP O54666
A	1636	GLY	-	expression tag	UNP O54666
A	1637	ALA	-	expression tag	UNP O54666
A	1638	ASN	-	expression tag	UNP O54666
A	1639	PRO	-	expression tag	UNP O54666
A	1640	SER	-	expression tag	UNP O54666
A	1641	GLY	-	expression tag	UNP O54666
A	1642	ASP	-	expression tag	UNP O54666
A	1643	ASP	-	expression tag	UNP O54666
A	1644	LEU	-	expression tag	UNP O54666
A	1645	GLY	-	expression tag	UNP O54666
A	1646	GLU	-	expression tag	UNP O54666
A	1647	ALA	-	expression tag	UNP O54666
A	1648	GLY	-	expression tag	UNP O54666
A	1649	VAL	-	expression tag	UNP O54666
A	1650	ASP	-	expression tag	UNP O54666
A	1651	GLU	-	expression tag	UNP O54666
A	1652	LEU	-	expression tag	UNP O54666
A	1653	LEU	-	expression tag	UNP O54666
A	1654	GLU	-	expression tag	UNP O54666
A	1655	ALA	-	expression tag	UNP O54666
A	1656	LEU	-	expression tag	UNP O54666
A	1657	GLY	-	expression tag	UNP O54666
A	1658	ARG	-	expression tag	UNP O54666
A	1659	GLU	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1660	LEU	-	expression tag	UNP O54666
A	1661	ASP	-	expression tag	UNP O54666
A	1662	GLY	-	expression tag	UNP O54666
A	1663	ASP	-	expression tag	UNP O54666
A	1664	GLY	-	expression tag	UNP O54666
A	1665	ASN	-	expression tag	UNP O54666
A	1666	SER	-	expression tag	UNP O54666
A	1667	SER	-	expression tag	UNP O54666
A	1668	SER	-	expression tag	UNP O54666
A	1669	VAL	-	expression tag	UNP O54666
A	1670	ASP	-	expression tag	UNP O54666
A	1671	LYS	-	expression tag	UNP O54666
A	1672	LEU	-	expression tag	UNP O54666
A	1673	ALA	-	expression tag	UNP O54666
A	1674	ALA	-	expression tag	UNP O54666
A	1675	ALA	-	expression tag	UNP O54666
A	1676	LEU	-	expression tag	UNP O54666
A	1677	GLU	-	expression tag	UNP O54666
A	1678	HIS	-	expression tag	UNP O54666
A	1679	HIS	-	expression tag	UNP O54666
A	1680	HIS	-	expression tag	UNP O54666
A	1681	HIS	-	expression tag	UNP O54666
A	1682	HIS	-	expression tag	UNP O54666
A	1683	HIS	-	expression tag	UNP O54666
B	1	MET	-	expression tag	UNP O54666
B	2	ALA	-	expression tag	UNP O54666
B	3	SER	-	expression tag	UNP O54666
B	4	THR	-	expression tag	UNP O54666
B	5	ASP	-	expression tag	UNP O54666
B	6	SER	-	expression tag	UNP O54666
B	7	GLU	-	expression tag	UNP O54666
B	8	LYS	-	expression tag	UNP O54666
B	9	VAL	-	expression tag	UNP O54666
B	10	ALA	-	expression tag	UNP O54666
B	11	GLU	-	expression tag	UNP O54666
B	12	TYR	-	expression tag	UNP O54666
B	13	LEU	-	expression tag	UNP O54666
B	14	ARG	-	expression tag	UNP O54666
B	15	ARG	-	expression tag	UNP O54666
B	16	ALA	-	expression tag	UNP O54666
B	17	THR	-	expression tag	UNP O54666
B	18	LEU	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	ASP	-	expression tag	UNP O54666
B	20	LEU	-	expression tag	UNP O54666
B	21	ARG	-	expression tag	UNP O54666
B	22	ALA	-	expression tag	UNP O54666
B	23	ALA	-	expression tag	UNP O54666
B	24	ARG	-	expression tag	UNP O54666
B	25	GLN	-	expression tag	UNP O54666
B	26	ARG	-	expression tag	UNP O54666
B	27	ILE	-	expression tag	UNP O54666
B	28	ARG	-	expression tag	UNP O54666
B	29	GLU	-	expression tag	UNP O54666
B	30	LEU	-	expression tag	UNP O54666
B	31	GLU	-	expression tag	UNP O54666
B	1581	THR	-	expression tag	UNP O54666
B	1582	GLU	-	expression tag	UNP O54666
B	1583	VAL	-	expression tag	UNP O54666
B	1584	ARG	-	expression tag	UNP O54666
B	1585	GLY	-	expression tag	UNP O54666
B	1586	GLU	-	expression tag	UNP O54666
B	1587	ALA	-	expression tag	UNP O54666
B	1588	PRO	-	expression tag	UNP O54666
B	1589	SER	-	expression tag	UNP O54666
B	1590	ALA	-	expression tag	UNP O54666
B	1591	LEU	-	expression tag	UNP O54666
B	1592	ALA	-	expression tag	UNP O54666
B	1593	GLY	-	expression tag	UNP O54666
B	1594	LEU	-	expression tag	UNP O54666
B	1595	ASP	-	expression tag	UNP O54666
B	1596	ALA	-	expression tag	UNP O54666
B	1597	LEU	-	expression tag	UNP O54666
B	1598	GLU	-	expression tag	UNP O54666
B	1599	ALA	-	expression tag	UNP O54666
B	1600	ALA	-	expression tag	UNP O54666
B	1601	LEU	-	expression tag	UNP O54666
B	1602	PRO	-	expression tag	UNP O54666
B	1603	GLU	-	expression tag	UNP O54666
B	1604	VAL	-	expression tag	UNP O54666
B	1605	PRO	-	expression tag	UNP O54666
B	1606	ALA	-	expression tag	UNP O54666
B	1607	THR	-	expression tag	UNP O54666
B	1608	GLU	-	expression tag	UNP O54666
B	1609	ARG	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1610	GLU	-	expression tag	UNP O54666
B	1611	GLU	-	expression tag	UNP O54666
B	1612	LEU	-	expression tag	UNP O54666
B	1613	VAL	-	expression tag	UNP O54666
B	1614	GLN	-	expression tag	UNP O54666
B	1615	ARG	-	expression tag	UNP O54666
B	1616	LEU	-	expression tag	UNP O54666
B	1617	GLU	-	expression tag	UNP O54666
B	1618	ARG	-	expression tag	UNP O54666
B	1619	MET	-	expression tag	UNP O54666
B	1620	LEU	-	expression tag	UNP O54666
B	1621	ALA	-	expression tag	UNP O54666
B	1622	ALA	-	expression tag	UNP O54666
B	1623	LEU	-	expression tag	UNP O54666
B	1624	ARG	-	expression tag	UNP O54666
B	1625	PRO	-	expression tag	UNP O54666
B	1626	VAL	-	expression tag	UNP O54666
B	1627	ALA	-	expression tag	UNP O54666
B	1628	GLN	-	expression tag	UNP O54666
B	1629	ALA	-	expression tag	UNP O54666
B	1630	ALA	-	expression tag	UNP O54666
B	1631	ASP	-	expression tag	UNP O54666
B	1632	ALA	-	expression tag	UNP O54666
B	1633	SER	-	expression tag	UNP O54666
B	1634	GLY	-	expression tag	UNP O54666
B	1635	THR	-	expression tag	UNP O54666
B	1636	GLY	-	expression tag	UNP O54666
B	1637	ALA	-	expression tag	UNP O54666
B	1638	ASN	-	expression tag	UNP O54666
B	1639	PRO	-	expression tag	UNP O54666
B	1640	SER	-	expression tag	UNP O54666
B	1641	GLY	-	expression tag	UNP O54666
B	1642	ASP	-	expression tag	UNP O54666
B	1643	ASP	-	expression tag	UNP O54666
B	1644	LEU	-	expression tag	UNP O54666
B	1645	GLY	-	expression tag	UNP O54666
B	1646	GLU	-	expression tag	UNP O54666
B	1647	ALA	-	expression tag	UNP O54666
B	1648	GLY	-	expression tag	UNP O54666
B	1649	VAL	-	expression tag	UNP O54666
B	1650	ASP	-	expression tag	UNP O54666
B	1651	GLU	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1652	LEU	-	expression tag	UNP O54666
B	1653	LEU	-	expression tag	UNP O54666
B	1654	GLU	-	expression tag	UNP O54666
B	1655	ALA	-	expression tag	UNP O54666
B	1656	LEU	-	expression tag	UNP O54666
B	1657	GLY	-	expression tag	UNP O54666
B	1658	ARG	-	expression tag	UNP O54666
B	1659	GLU	-	expression tag	UNP O54666
B	1660	LEU	-	expression tag	UNP O54666
B	1661	ASP	-	expression tag	UNP O54666
B	1662	GLY	-	expression tag	UNP O54666
B	1663	ASP	-	expression tag	UNP O54666
B	1664	GLY	-	expression tag	UNP O54666
B	1665	ASN	-	expression tag	UNP O54666
B	1666	SER	-	expression tag	UNP O54666
B	1667	SER	-	expression tag	UNP O54666
B	1668	SER	-	expression tag	UNP O54666
B	1669	VAL	-	expression tag	UNP O54666
B	1670	ASP	-	expression tag	UNP O54666
B	1671	LYS	-	expression tag	UNP O54666
B	1672	LEU	-	expression tag	UNP O54666
B	1673	ALA	-	expression tag	UNP O54666
B	1674	ALA	-	expression tag	UNP O54666
B	1675	ALA	-	expression tag	UNP O54666
B	1676	LEU	-	expression tag	UNP O54666
B	1677	GLU	-	expression tag	UNP O54666
B	1678	HIS	-	expression tag	UNP O54666
B	1679	HIS	-	expression tag	UNP O54666
B	1680	HIS	-	expression tag	UNP O54666
B	1681	HIS	-	expression tag	UNP O54666
B	1682	HIS	-	expression tag	UNP O54666
B	1683	HIS	-	expression tag	UNP O54666

- Molecule 2 is a protein called 6-deoxyerythronolide-B synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	75	Total	C	N	O	P	S	0	0
			578	361	106	108	1	2		

There are 134 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP O54666
C	2	ALA	-	expression tag	UNP O54666
C	3	SER	-	expression tag	UNP O54666
C	4	THR	-	expression tag	UNP O54666
C	5	ASP	-	expression tag	UNP O54666
C	6	SER	-	expression tag	UNP O54666
C	7	GLU	-	expression tag	UNP O54666
C	8	LYS	-	expression tag	UNP O54666
C	9	VAL	-	expression tag	UNP O54666
C	10	ALA	-	expression tag	UNP O54666
C	11	GLU	-	expression tag	UNP O54666
C	12	TYR	-	expression tag	UNP O54666
C	13	LEU	-	expression tag	UNP O54666
C	14	ARG	-	expression tag	UNP O54666
C	15	ARG	-	expression tag	UNP O54666
C	16	ALA	-	expression tag	UNP O54666
C	17	THR	-	expression tag	UNP O54666
C	18	LEU	-	expression tag	UNP O54666
C	19	ASP	-	expression tag	UNP O54666
C	20	LEU	-	expression tag	UNP O54666
C	21	ARG	-	expression tag	UNP O54666
C	22	ALA	-	expression tag	UNP O54666
C	23	ALA	-	expression tag	UNP O54666
C	24	ARG	-	expression tag	UNP O54666
C	25	GLN	-	expression tag	UNP O54666
C	26	ARG	-	expression tag	UNP O54666
C	27	ILE	-	expression tag	UNP O54666
C	28	ARG	-	expression tag	UNP O54666
C	29	GLU	-	expression tag	UNP O54666
C	30	LEU	-	expression tag	UNP O54666
C	31	GLU	-	expression tag	UNP O54666
C	1581	THR	-	expression tag	UNP O54666
C	1582	GLU	-	expression tag	UNP O54666
C	1583	VAL	-	expression tag	UNP O54666
C	1584	ARG	-	expression tag	UNP O54666
C	1585	GLY	-	expression tag	UNP O54666
C	1586	GLU	-	expression tag	UNP O54666
C	1587	ALA	-	expression tag	UNP O54666
C	1588	PRO	-	expression tag	UNP O54666
C	1589	SER	-	expression tag	UNP O54666
C	1590	ALA	-	expression tag	UNP O54666
C	1591	LEU	-	expression tag	UNP O54666
C	1592	ALA	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1593	GLY	-	expression tag	UNP O54666
C	1594	LEU	-	expression tag	UNP O54666
C	1595	ASP	-	expression tag	UNP O54666
C	1596	ALA	-	expression tag	UNP O54666
C	1597	LEU	-	expression tag	UNP O54666
C	1598	GLU	-	expression tag	UNP O54666
C	1599	ALA	-	expression tag	UNP O54666
C	1600	ALA	-	expression tag	UNP O54666
C	1601	LEU	-	expression tag	UNP O54666
C	1602	PRO	-	expression tag	UNP O54666
C	1603	GLU	-	expression tag	UNP O54666
C	1604	VAL	-	expression tag	UNP O54666
C	1605	PRO	-	expression tag	UNP O54666
C	1606	ALA	-	expression tag	UNP O54666
C	1607	THR	-	expression tag	UNP O54666
C	1608	GLU	-	expression tag	UNP O54666
C	1609	ARG	-	expression tag	UNP O54666
C	1610	GLU	-	expression tag	UNP O54666
C	1611	GLU	-	expression tag	UNP O54666
C	1612	LEU	-	expression tag	UNP O54666
C	1613	VAL	-	expression tag	UNP O54666
C	1614	GLN	-	expression tag	UNP O54666
C	1615	ARG	-	expression tag	UNP O54666
C	1616	LEU	-	expression tag	UNP O54666
C	1617	GLU	-	expression tag	UNP O54666
C	1618	ARG	-	expression tag	UNP O54666
C	1619	MET	-	expression tag	UNP O54666
C	1620	LEU	-	expression tag	UNP O54666
C	1621	ALA	-	expression tag	UNP O54666
C	1622	ALA	-	expression tag	UNP O54666
C	1623	LEU	-	expression tag	UNP O54666
C	1624	ARG	-	expression tag	UNP O54666
C	1625	PRO	-	expression tag	UNP O54666
C	1626	VAL	-	expression tag	UNP O54666
C	1627	ALA	-	expression tag	UNP O54666
C	1628	GLN	-	expression tag	UNP O54666
C	1629	ALA	-	expression tag	UNP O54666
C	1630	ALA	-	expression tag	UNP O54666
C	1631	ASP	-	expression tag	UNP O54666
C	1632	ALA	-	expression tag	UNP O54666
C	1633	SER	-	expression tag	UNP O54666
C	1634	GLY	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1635	THR	-	expression tag	UNP O54666
C	1636	GLY	-	expression tag	UNP O54666
C	1637	ALA	-	expression tag	UNP O54666
C	1638	ASN	-	expression tag	UNP O54666
C	1639	PRO	-	expression tag	UNP O54666
C	1640	SER	-	expression tag	UNP O54666
C	1641	GLY	-	expression tag	UNP O54666
C	1642	ASP	-	expression tag	UNP O54666
C	1643	ASP	-	expression tag	UNP O54666
C	1644	LEU	-	expression tag	UNP O54666
C	1645	GLY	-	expression tag	UNP O54666
C	1646	GLU	-	expression tag	UNP O54666
C	1647	ALA	-	expression tag	UNP O54666
C	1648	GLY	-	expression tag	UNP O54666
C	1649	VAL	-	expression tag	UNP O54666
C	1650	ASP	-	expression tag	UNP O54666
C	1651	GLU	-	expression tag	UNP O54666
C	1652	LEU	-	expression tag	UNP O54666
C	1653	LEU	-	expression tag	UNP O54666
C	1654	GLU	-	expression tag	UNP O54666
C	1655	ALA	-	expression tag	UNP O54666
C	1656	LEU	-	expression tag	UNP O54666
C	1657	GLY	-	expression tag	UNP O54666
C	1658	ARG	-	expression tag	UNP O54666
C	1659	GLU	-	expression tag	UNP O54666
C	1660	LEU	-	expression tag	UNP O54666
C	1661	ASP	-	expression tag	UNP O54666
C	1662	GLY	-	expression tag	UNP O54666
C	1663	ASP	-	expression tag	UNP O54666
C	1664	GLY	-	expression tag	UNP O54666
C	1665	ASN	-	expression tag	UNP O54666
C	1666	SER	-	expression tag	UNP O54666
C	1667	SER	-	expression tag	UNP O54666
C	1668	SER	-	expression tag	UNP O54666
C	1669	VAL	-	expression tag	UNP O54666
C	1670	ASP	-	expression tag	UNP O54666
C	1671	LYS	-	expression tag	UNP O54666
C	1672	LEU	-	expression tag	UNP O54666
C	1673	ALA	-	expression tag	UNP O54666
C	1674	ALA	-	expression tag	UNP O54666
C	1675	ALA	-	expression tag	UNP O54666
C	1676	LEU	-	expression tag	UNP O54666

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1677	GLU	-	expression tag	UNP O54666
C	1678	HIS	-	expression tag	UNP O54666
C	1679	HIS	-	expression tag	UNP O54666
C	1680	HIS	-	expression tag	UNP O54666
C	1681	HIS	-	expression tag	UNP O54666
C	1682	HIS	-	expression tag	UNP O54666
C	1683	HIS	-	expression tag	UNP O54666

- Molecule 3 is a protein called Antibody Fragment 1B2 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
3	H	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

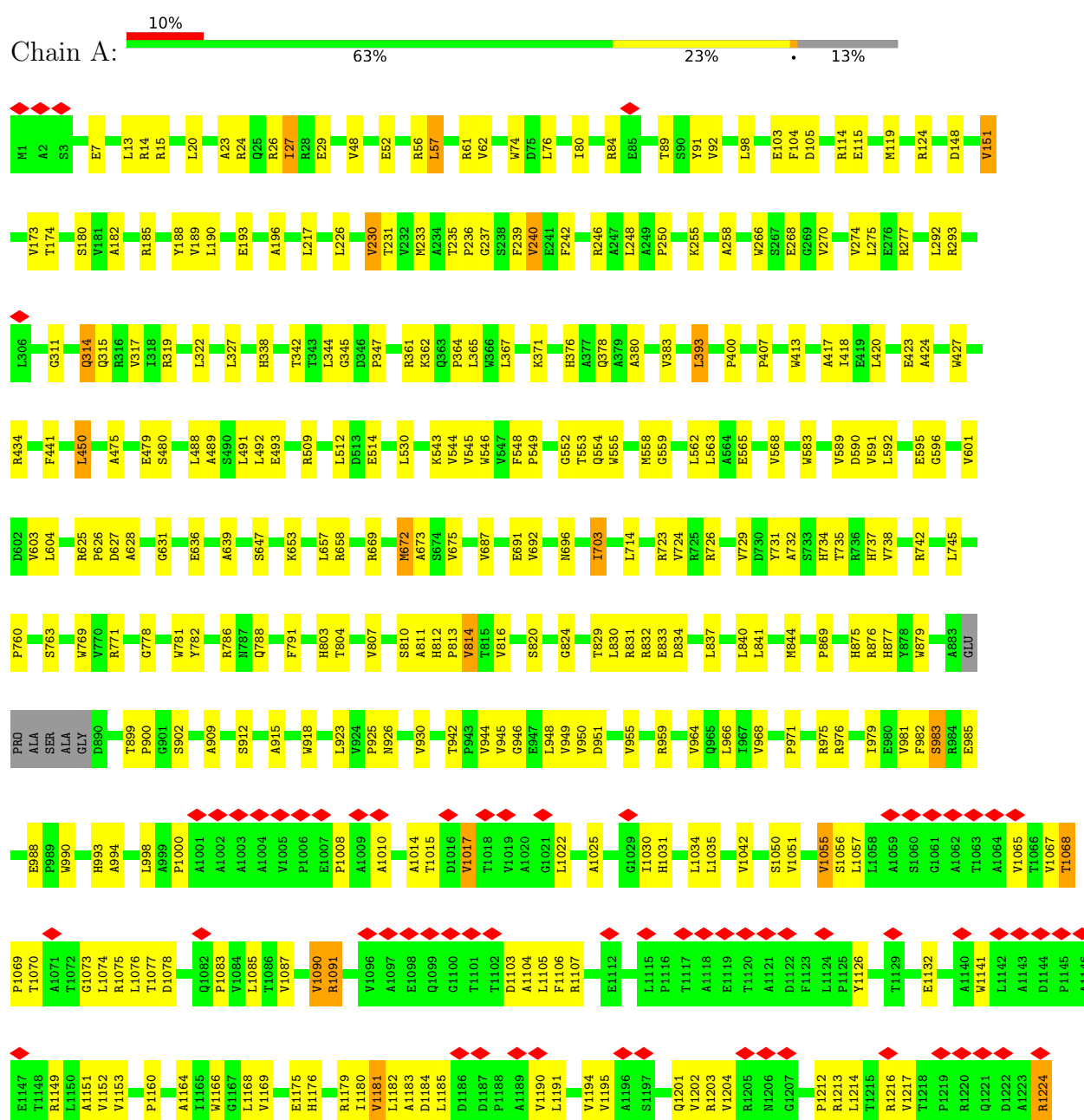
- Molecule 4 is a protein called Antibody Fragment 1B2 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	209	Total	C	N	O	S	0	0
			1596	1001	269	320	6		
4	L	209	Total	C	N	O	S	0	0
			1596	1001	269	320	6		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: 6-deoxyerythronolide-B synthase











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37950	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1188	Depositor
Maximum defocus (nm)	3988	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.522	Depositor
Minimum map value	-0.144	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	492.80002, 492.80002, 492.80002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: 4HH

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	0.13	0/10998	0.28	0/15035
1	B	0.14	0/8160	0.29	0/11143
2	C	0.10	0/561	0.27	0/760
3	G	0.12	0/1575	0.32	0/2141
3	H	0.12	0/1575	0.28	0/2141
4	I	0.11	0/1630	0.27	0/2212
4	L	0.11	0/1630	0.28	0/2212
All	All	0.13	0/26129	0.29	0/35644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	10796	0	10770	258	0
1	B	8009	0	7961	171	0
2	C	578	0	579	12	0
3	G	1539	0	1513	42	0
3	H	1539	0	1513	35	0
4	I	1596	0	1561	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1596	0	1561	41	0
All	All	25653	0	25458	568	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 11.

All (568) 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:G:85:LEU:HG	3:G:87:MET:HE1	1.53	0.89
1:A:1014:ALA:HA	1:A:1067:VAL:O	1.78	0.84
4:I:28:PRO:HB2	4:I:129:LYS:HZ3	1.46	0.80
1:A:1164:ALA:HB2	1:A:1380:GLU:HB2	1.67	0.74
1:B:555:TRP:HE1	1:B:811:ALA:HB1	1.52	0.74
1:B:558:MET:HE2	1:B:558:MET:H	1.51	0.74
4:L:130:ARG:HD2	4:L:193:SER:HB2	1.69	0.73
1:B:233:MET:HE1	1:B:266:TRP:HB3	1.71	0.72
2:C:1552:THR:HG23	2:C:1554:LEU:H	1.56	0.71
3:G:39:VAL:HG22	3:G:49:TRP:HA	1.70	0.71
1:A:1286:CYS:HB2	1:A:1297:VAL:HG21	1.73	0.71
1:B:1073:GLY:HA3	1:B:1087:VAL:O	1.91	0.71
1:A:491:LEU:HD13	1:A:869:PRO:HD3	1.73	0.70
4:L:166:ALA:HA	4:L:219:THR:O	1.91	0.70
4:L:23:SER:HA	4:L:40:ARG:HH12	1.56	0.70
1:B:48:VAL:HG23	1:B:53:ASP:HB2	1.75	0.69
1:A:1315:GLY:HA2	1:A:1336:PRO:HG2	1.73	0.69
1:A:1426:MET:HE3	1:A:1426:MET:HA	1.74	0.69
1:B:476:ARG:HG2	1:B:512:LEU:HD13	1.75	0.69
1:B:831:ARG:HG3	1:B:834:ASP:HB3	1.76	0.68
3:G:202:ILE:HG12	3:G:217:LYS:HG2	1.74	0.68
1:B:123:GLN:HE22	1:B:181:VAL:HG23	1.57	0.68
1:A:1017:VAL:HG21	1:A:1067:VAL:HG23	1.76	0.68
3:G:72:PHE:HA	3:G:86:GLN:O	1.94	0.68
1:A:20:LEU:HD23	1:B:20:LEU:HB3	1.76	0.67
3:H:95:THR:HG23	3:H:117:THR:HA	1.75	0.67
1:A:1258:LEU:HB2	1:A:1281:VAL:HG22	1.78	0.66
1:A:966:LEU:HG	1:A:981:VAL:HG22	1.78	0.66
1:A:1014:ALA:HB2	1:A:1068:THR:HG23	1.76	0.66
1:B:61:ARG:HB3	1:B:402:LEU:HD21	1.78	0.66
1:A:966:LEU:HD23	1:A:979:ILE:HD11	1.77	0.65
3:H:166:LEU:HD21	3:H:189:VAL:HG21	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:VAL:HG13	1:B:627:ASP:H	1.62	0.64
1:A:1265:GLY:HA3	1:A:1285:ALA:HA	1.79	0.64
1:B:1077:THR:HG22	1:B:1083:PRO:HA	1.78	0.64
1:A:944:VAL:HG13	1:A:1056:SER:HB2	1.79	0.64
1:A:1326:THR:H	1:A:1329:ARG:HD2	1.61	0.64
3:G:8:GLN:H	3:G:112:GLN:HE22	1.46	0.64
4:I:58:LEU:HB3	4:I:68:LEU:HD21	1.80	0.64
1:B:608:CYS:O	1:B:612:MET:HG3	1.98	0.63
4:I:183:GLU:HB3	4:I:197:LEU:HD11	1.79	0.63
1:A:814:VAL:HA	2:C:1538:4HH:HO3	1.80	0.63
4:I:147:LEU:HB3	4:I:205:LYS:HE2	1.79	0.63
4:I:207:ASP:HA	4:I:210:LYS:HE2	1.80	0.63
1:A:148:ASP:HA	1:A:193:GLU:HB2	1.81	0.63
1:A:1151:ALA:HB1	1:A:1191:LEU:HD11	1.81	0.63
1:B:1073:GLY:HA2	1:B:1090:VAL:HG12	1.80	0.63
1:B:40:MET:HE2	1:B:387:ILE:HG23	1.80	0.63
1:B:491:LEU:HD13	1:B:869:PRO:HD3	1.81	0.63
1:B:601:VAL:HG11	1:B:731:TYR:HE2	1.64	0.62
1:A:1149:ARG:HE	1:A:1181:VAL:HG22	1.64	0.62
4:L:23:SER:HB2	4:L:37:ILE:HD11	1.81	0.62
1:A:1259:VAL:HG21	1:A:1301:ILE:HG12	1.82	0.61
1:A:831:ARG:HB3	1:A:834:ASP:HB3	1.82	0.61
2:C:1541:ALA:HB1	2:C:1561:ILE:HG13	1.82	0.61
4:L:183:GLU:HB3	4:L:197:LEU:HD11	1.82	0.61
1:A:555:TRP:HB3	1:A:832:ARG:HE	1.64	0.60
1:A:923:LEU:HA	1:A:955:VAL:HA	1.82	0.60
1:B:117:VAL:HG22	1:B:878:TYR:HB3	1.83	0.60
1:A:188:TYR:HA	1:B:302:ALA:HB1	1.84	0.60
1:A:555:TRP:CD2	1:A:558:MET:HE1	2.36	0.60
1:A:1194:VAL:HG13	1:A:1202:VAL:HB	1.82	0.60
1:A:1151:ALA:HA	1:A:1181:VAL:HB	1.82	0.60
1:B:908:VAL:HG22	1:B:965:GLN:HG2	1.84	0.60
1:A:1291:ARG:HA	1:A:1343:LEU:HD21	1.84	0.60
1:B:74:TRP:CE2	1:B:236:PRO:HD3	2.37	0.60
1:A:233:MET:HE1	1:A:266:TRP:HB3	1.84	0.60
1:B:1042:VAL:HG13	1:B:1069:PRO:HB3	1.84	0.60
4:L:145:GLU:HA	4:L:148:LYS:HD3	1.84	0.60
3:G:105:THR:HA	4:I:117:ARG:HH22	1.67	0.59
1:A:1263:ARG:HH22	1:A:1409:MET:HE1	1.67	0.59
1:A:691:GLU:HB2	1:A:735:THR:HG22	1.83	0.59
1:A:945:VAL:HB	1:A:1055:VAL:HG13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:VAL:HG23	1:A:1065:VAL:HG23	1.85	0.59
1:B:543:LYS:HB2	1:B:803:HIS:HA	1.85	0.59
1:B:549:PRO:HG3	1:B:808:GLU:HG3	1.84	0.58
1:A:583:TRP:CD1	1:A:653:LYS:HZ2	2.21	0.58
1:B:859:MET:HE3	1:B:859:MET:HA	1.84	0.58
1:A:1042:VAL:HG13	1:A:1069:PRO:HB3	1.86	0.58
4:L:142:PRO:HG3	4:L:152:ALA:HB1	1.85	0.58
4:I:56:TRP:HB2	4:I:69:ILE:HB	1.85	0.58
1:A:1232:VAL:HG22	1:A:1309:ALA:HB3	1.86	0.57
1:B:579:ALA:HB1	1:B:649:GLU:HG2	1.85	0.57
3:G:14:VAL:HA	3:G:18:ARG:HH21	1.68	0.57
3:H:153:PHE:HB2	3:H:182:LEU:HD23	1.85	0.57
1:B:1047:LEU:HB3	1:B:1092:GLY:HA3	1.86	0.57
1:A:1160:PRO:HA	1:A:1383:ALA:HB3	1.87	0.57
1:A:692:VAL:HA	1:A:703:ILE:HG22	1.87	0.57
1:A:488:LEU:HD22	1:A:530:LEU:HD11	1.87	0.57
1:B:1012:GLY:HA3	1:B:1069:PRO:HB2	1.87	0.57
1:A:548:PHE:HB2	1:A:631:GLY:HA2	1.87	0.56
1:A:1168:LEU:HG	1:A:1376:ALA:HB2	1.86	0.56
2:C:1515:GLU:HB2	2:C:1547:ARG:HH22	1.70	0.56
1:A:1185:LEU:HD22	1:A:1204:VAL:HB	1.87	0.56
3:H:80:LYS:HD3	3:H:82:ILE:HD12	1.87	0.56
1:A:1073:GLY:HA2	1:A:1090:VAL:HG12	1.87	0.56
3:G:87:MET:N	3:G:87:MET:HE2	2.21	0.56
1:A:1055:VAL:HB	1:A:1087:VAL:HG13	1.88	0.56
1:B:830:LEU:HD11	1:B:835:GLY:HA2	1.87	0.56
3:G:72:PHE:CD1	3:G:87:MET:HA	2.41	0.56
1:A:590:ASP:HB3	1:A:595:GLU:HB2	1.88	0.56
1:B:899:THR:HB	1:B:902:SER:HB2	1.87	0.56
1:A:948:LEU:HD11	1:A:994:ALA:HB1	1.87	0.55
1:B:672:MET:HB2	1:B:727:VAL:HB	1.89	0.55
1:B:1042:VAL:HG22	1:B:1069:PRO:HG3	1.87	0.55
1:A:1166:TRP:HZ2	1:A:1184:ASP:HB2	1.71	0.55
3:H:98:TYR:O	3:H:113:GLY:HA2	2.06	0.55
3:G:166:LEU:HD21	3:G:189:VAL:HG21	1.88	0.55
1:A:636:GLU:O	1:A:639:ALA:HB3	2.06	0.55
1:A:982:PHE:HB3	1:A:990:TRP:CE3	2.42	0.55
1:A:74:TRP:CE2	1:A:236:PRO:HD3	2.41	0.55
1:A:57:LEU:HG	1:A:62:VAL:HB	1.87	0.55
1:A:217:LEU:HG	1:A:277:ARG:HG2	1.89	0.55
1:A:1176:HIS:HB3	1:A:1179:ARG:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ALA:O	1:B:14:ARG:HG3	2.06	0.55
1:A:236:PRO:O	1:A:239:PHE:HB2	2.08	0.54
1:A:76:LEU:HD23	1:A:76:LEU:H	1.73	0.54
1:A:105:ASP:HA	1:A:876:ARG:HH21	1.72	0.54
3:H:39:VAL:HG23	3:H:49:TRP:HA	1.90	0.54
3:H:106:LEU:HD11	4:L:67:LEU:HD22	1.89	0.54
1:A:1030:ILE:HG12	1:A:1035:LEU:HB2	1.90	0.54
1:B:675:VAL:HA	1:B:724:VAL:HG22	1.89	0.54
3:H:124:LYS:HE3	3:H:151:ASP:HB3	1.89	0.54
1:A:558:MET:HE2	1:A:558:MET:N	2.22	0.54
1:A:1295:GLU:HG2	1:A:1347:LEU:HD13	1.89	0.54
3:G:130:PRO:HD2	4:I:143:SER:HB2	1.89	0.54
1:B:546:TRP:CD1	1:B:626:PRO:HB3	2.43	0.54
1:B:378:GLN:O	1:B:381:ALA:HB3	2.08	0.53
1:A:545:VAL:HG22	1:A:628:ALA:HB3	1.89	0.53
1:A:292:LEU:HD11	1:A:450:LEU:HD12	1.90	0.53
1:A:1260:LEU:HB2	1:A:1283:ILE:HG12	1.90	0.53
1:B:905:LEU:HG	1:B:977:ARG:HH12	1.73	0.53
1:A:1103:ASP:HB3	1:A:1216:ARG:HE	1.73	0.53
4:I:145:GLU:HA	4:I:148:LYS:HD3	1.90	0.53
1:A:20:LEU:HB3	1:B:20:LEU:HD23	1.90	0.53
1:A:946:GLY:HA3	1:A:976:ARG:HH12	1.74	0.53
1:A:1316:VAL:HG21	1:A:1332:THR:HG22	1.91	0.53
3:G:92:THR:HA	3:G:118:VAL:HB	1.91	0.53
3:H:85:LEU:HG	3:H:87:MET:SD	2.48	0.53
1:A:1104:ALA:HB3	1:A:1437:LEU:HD21	1.90	0.53
1:A:1335:ARG:O	1:A:1339:ASP:HB2	2.07	0.53
1:A:1358:LEU:HD12	1:A:1385:ALA:HB2	1.91	0.53
1:B:813:PRO:HD3	1:B:831:ARG:HA	1.89	0.53
1:B:840:LEU:O	1:B:844:MET:HE3	2.09	0.53
4:L:37:ILE:HG23	4:L:94:LEU:HB3	1.91	0.53
1:A:115:GLU:O	1:A:119:MET:HG2	2.08	0.53
1:B:976:ARG:HA	1:B:998:LEU:O	2.08	0.53
4:L:218:VAL:O	4:L:226:PRO:HA	2.09	0.53
1:A:230:VAL:HG23	1:A:270:VAL:HG22	1.91	0.53
1:A:552:GLY:HA3	2:C:1538:4HH:HS3	1.91	0.53
1:A:553:THR:HG21	1:A:810:SER:HB2	1.91	0.53
1:B:26:ARG:O	1:B:29:GLU:HG3	2.09	0.53
1:B:338:HIS:CE1	1:B:441:PHE:H	2.27	0.53
1:B:472:VAL:HG22	1:B:517:VAL:HG22	1.90	0.53
1:B:971:PRO:HB3	1:B:977:ARG:HG3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:ARG:HH12	1:B:78:SER:HA	1.74	0.53
1:B:625:ARG:HD3	1:B:626:PRO:HD2	1.91	0.53
3:H:202:ILE:HG22	3:H:217:LYS:HG2	1.90	0.53
1:A:1437:LEU:HB3	1:A:1450:ALA:HB1	1.91	0.52
1:B:619:TRP:HE3	1:B:624:VAL:HG11	1.75	0.52
1:B:812:HIS:HA	1:B:831:ARG:HA	1.91	0.52
4:L:70:TYR:HD2	4:L:71:LEU:HD13	1.74	0.52
1:A:813:PRO:HB2	2:C:1538:4HH:HL23	1.92	0.52
1:A:985:GLU:H	1:A:988:GLU:HB2	1.75	0.52
1:B:104:PHE:CD1	1:B:124:ARG:HB3	2.45	0.52
1:A:371:LYS:HE2	1:A:376:HIS:CD2	2.44	0.52
1:A:1106:PHE:HB3	1:A:1214:LEU:HD22	1.91	0.52
1:A:1364:GLY:HA2	1:A:1375:ALA:HA	1.92	0.52
1:B:944:VAL:HG22	1:B:1056:SER:HA	1.90	0.52
1:A:1055:VAL:HA	1:A:1087:VAL:HA	1.90	0.52
3:H:72:PHE:CD1	3:H:87:MET:HA	2.44	0.52
1:B:1048:LEU:HB2	1:B:1095:PHE:HB2	1.91	0.52
1:A:899:THR:HB	1:A:902:SER:HB3	1.91	0.52
1:B:546:TRP:CG	1:B:626:PRO:HB3	2.45	0.52
1:A:255:LYS:HB3	1:A:258:ALA:HB3	1.92	0.52
1:A:1182:LEU:HB3	1:A:1201:GLN:HG2	1.91	0.52
1:B:11:GLU:HG2	1:B:14:ARG:HH21	1.74	0.52
1:A:543:LYS:HB2	1:A:803:HIS:HA	1.91	0.51
1:A:738:VAL:HB	1:A:786:ARG:HD2	1.92	0.51
1:A:555:TRP:CE2	1:A:832:ARG:HA	2.45	0.51
1:A:949:VAL:HG13	1:A:1051:VAL:HG22	1.92	0.51
1:A:1274:LEU:HB3	1:A:1281:VAL:HG21	1.92	0.51
1:B:498:LEU:HD11	1:B:523:ARG:HB3	1.92	0.51
1:A:1107:ARG:HB2	1:A:1217:VAL:HG22	1.91	0.51
4:L:60:LYS:HB2	4:L:63:GLN:HB2	1.92	0.51
1:B:183:SER:HB2	1:B:196:ALA:HB1	1.91	0.51
1:A:742:ARG:HD3	1:A:782:TYR:CZ	2.46	0.51
1:B:890:ASP:HB3	1:B:893:LEU:HB2	1.92	0.51
1:A:829:THR:HG22	1:A:830:LEU:HG	1.92	0.51
1:A:1342:ARG:HG3	1:A:1384:LEU:HD22	1.92	0.51
1:A:315:GLN:O	1:A:319:ARG:HG2	2.11	0.51
1:B:696:ASN:HA	1:B:791:PHE:HD2	1.75	0.51
1:A:1160:PRO:HB3	1:A:1380:GLU:HG3	1.93	0.50
1:B:672:MET:HE1	1:B:732:ALA:HA	1.93	0.50
3:G:14:VAL:HG13	3:G:18:ARG:HE	1.76	0.50
4:I:170:TRP:CD1	4:I:201:LEU:HD13	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HG	1:A:274:VAL:HG22	1.93	0.50
1:A:1008:PRO:HG2	1:A:1070:THR:HG21	1.92	0.50
1:A:1070:THR:H	1:A:1074:LEU:HA	1.75	0.50
1:B:361:ARG:HE	1:B:365:LEU:HD23	1.77	0.50
1:B:72:ARG:HB3	1:B:74:TRP:CD1	2.46	0.50
1:A:293:ARG:HH12	1:A:327:LEU:HD21	1.75	0.50
1:A:1185:LEU:HD13	1:A:1190:VAL:HG23	1.93	0.50
1:A:546:TRP:CD1	1:A:626:PRO:HB3	2.46	0.50
1:A:696:ASN:HA	1:A:791:PHE:HB3	1.93	0.50
1:A:1182:LEU:HD23	1:A:1201:GLN:HG2	1.92	0.50
3:H:162:ASN:HB2	3:H:166:LEU:H	1.76	0.50
4:I:130:ARG:HH12	4:I:133:ALA:HB2	1.76	0.50
1:A:1091:ARG:HE	1:A:1091:ARG:N	2.09	0.50
1:A:1169:VAL:HB	1:A:1182:LEU:HD22	1.94	0.50
4:L:147:LEU:HB3	4:L:205:LYS:HZ3	1.77	0.50
1:A:1460:ALA:HA	1:A:1463:LYS:HE3	1.93	0.49
3:H:38:TRP:O	3:H:50:VAL:HB	2.13	0.49
1:B:144:LEU:HD12	1:B:144:LEU:O	2.12	0.49
1:A:669:ARG:HH21	1:A:737:HIS:HD2	1.60	0.49
1:B:975:ARG:HH12	1:B:977:ARG:HD2	1.75	0.49
3:G:66:ALA:HA	3:G:69:LYS:HE2	1.94	0.49
1:A:729:VAL:HG12	1:A:731:TYR:H	1.76	0.49
1:B:354:LEU:HD22	1:B:415:ALA:HB3	1.94	0.49
1:A:912:SER:H	1:A:915:ALA:HB3	1.78	0.49
3:H:171:HIS:HB2	3:H:188:VAL:HG22	1.95	0.49
1:B:429:ARG:HH12	1:B:457:ALA:HB2	1.77	0.49
1:A:942:THR:HA	1:A:1000:PRO:HA	1.94	0.49
1:A:1335:ARG:HB3	1:A:1336:PRO:HD3	1.94	0.49
3:G:14:VAL:HG21	3:G:20:LEU:HD22	1.94	0.49
1:A:1250:VAL:HG21	1:A:1274:LEU:HD22	1.94	0.49
1:A:591:VAL:HG12	1:A:596:GLY:HA3	1.95	0.49
1:A:1421:ASN:O	1:A:1424:ILE:HG12	2.13	0.48
1:B:492:LEU:HD12	1:B:492:LEU:O	2.13	0.48
1:B:674:SER:HA	1:B:702:VAL:HG23	1.95	0.48
1:A:964:VAL:HG12	1:A:983:SER:HB2	1.94	0.48
1:B:668:GLY:H	1:B:730:ASP:CG	2.20	0.48
3:G:19:SER:HA	3:G:87:MET:O	2.13	0.48
1:A:1065:VAL:HA	1:A:1078:ASP:HA	1.94	0.48
1:B:812:HIS:ND1	1:B:832:ARG:HG2	2.28	0.48
3:G:13:LEU:HD11	3:G:119:SER:HB3	1.95	0.48
1:B:42:CYS:HB3	1:B:387:ILE:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:VAL:H	1:B:523:ARG:NH2	2.12	0.48
1:B:739:GLU:HA	1:B:742:ARG:HG3	1.95	0.48
1:A:583:TRP:CE2	1:A:653:LYS:HD2	2.48	0.48
1:B:230:VAL:HG23	1:B:270:VAL:HB	1.95	0.48
1:B:739:GLU:HB3	1:B:742:ARG:HE	1.78	0.48
3:G:126:PRO:HA	3:G:152:TYR:HB3	1.95	0.48
1:A:1263:ARG:NH2	1:A:1315:GLY:H	2.11	0.48
1:A:1317:LEU:HD13	1:A:1374:TYR:CD1	2.49	0.48
1:B:18:LEU:HA	1:B:21:ARG:HH21	1.79	0.48
1:B:76:LEU:HA	1:B:79:LEU:HB2	1.96	0.47
1:B:500:GLU:HG2	1:B:863:ALA:HB1	1.96	0.47
1:B:563:LEU:HD12	1:B:593:ARG:HH11	1.79	0.47
1:B:1054:GLY:HA3	1:B:1088:GLU:CD	2.38	0.47
3:H:40:ARG:HH12	3:H:94:ASP:HA	1.78	0.47
4:I:54:LEU:HD11	4:I:109:CYS:HB2	1.95	0.47
4:I:168:VAL:HG12	4:I:218:VAL:HG22	1.96	0.47
1:A:104:PHE:CD1	1:A:124:ARG:HB3	2.49	0.47
1:B:654:VAL:O	1:B:658:ARG:HG2	2.13	0.47
1:B:1043:VAL:HG21	1:B:1090:VAL:HG22	1.96	0.47
1:B:1087:VAL:HG11	1:B:1090:VAL:HB	1.97	0.47
2:C:1545:ARG:CZ	2:C:1558:PRO:HG3	2.44	0.47
1:A:23:ALA:O	1:A:27:ILE:HG22	2.14	0.47
1:B:749:LEU:HD22	1:B:778:GLY:HA2	1.97	0.47
3:H:145:LEU:HB2	3:H:218:VAL:HG11	1.95	0.47
3:H:162:ASN:HA	3:H:202:ILE:HG13	1.97	0.47
1:B:669:ARG:NH2	1:B:737:HIS:HB3	2.30	0.47
3:H:55:SER:HA	3:H:76:ARG:HH12	1.80	0.47
3:H:204:ASN:HB3	3:H:213:LYS:HZ1	1.79	0.47
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.76	0.47
1:A:601:VAL:HA	1:A:604:LEU:HG	1.95	0.47
1:A:1227:ASP:HB2	1:A:1308:THR:HG21	1.97	0.47
3:H:68:VAL:HG12	3:H:71:ARG:HH21	1.78	0.47
4:I:162:TYR:HB2	4:I:194:THR:HG22	1.96	0.47
4:L:148:LYS:HB2	4:L:148:LYS:HE2	1.63	0.47
1:A:84:ARG:HD2	1:A:246:ARG:HH21	1.80	0.47
1:A:327:LEU:HA	4:L:98:ARG:HH21	1.80	0.47
1:A:400:PRO:HD3	1:A:424:ALA:HB2	1.96	0.47
1:A:475:ALA:O	1:A:514:GLU:HB2	2.15	0.47
1:B:563:LEU:HD21	1:B:573:ILE:HG21	1.95	0.47
3:G:36:MET:HE3	3:G:36:MET:HA	1.96	0.47
1:A:1462:ALA:HB2	1:A:1468:VAL:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:CE2	4:L:71:LEU:HD11	2.50	0.47
1:B:475:ALA:HA	1:B:512:LEU:HD12	1.97	0.47
3:G:26:ALA:HB1	3:G:29:PHE:HE1	1.79	0.47
1:A:555:TRP:CG	1:A:832:ARG:HG3	2.50	0.47
1:B:106:ALA:HB1	1:B:111:ILE:HB	1.96	0.47
1:A:968:VAL:HG22	1:A:979:ILE:HB	1.97	0.46
1:A:971:PRO:HG3	1:A:975:ARG:HE	1.78	0.46
1:A:1310:VAL:HG23	1:A:1353:LEU:HD21	1.97	0.46
1:B:665:GLU:HG3	1:B:669:ARG:HH12	1.80	0.46
3:G:71:ARG:HD2	3:G:89:SER:HB2	1.98	0.46
4:I:158:LEU:HD21	4:I:218:VAL:HG13	1.97	0.46
1:A:820:SER:HA	1:A:824:GLY:HA2	1.97	0.46
1:A:900:PRO:HB3	1:B:990:TRP:CG	2.50	0.46
1:B:555:TRP:CZ2	1:B:558:MET:HA	2.50	0.46
1:A:1181:VAL:HG21	1:A:1195:VAL:HG22	1.96	0.46
1:A:975:ARG:HG2	1:A:1000:PRO:HB3	1.98	0.46
1:A:1319:ASP:HB2	1:A:1412:HIS:HE1	1.81	0.46
1:A:1399:ALA:HB3	1:A:1449:VAL:HG22	1.97	0.46
1:A:7:GLU:HG3	3:G:58:TYR:CZ	2.51	0.46
1:A:52:GLU:HB3	1:A:56:ARG:HH12	1.80	0.46
1:A:1074:LEU:HD12	1:A:1076:LEU:HB2	1.97	0.46
3:G:166:LEU:HD11	3:G:189:VAL:HG21	1.98	0.46
1:A:237:GLY:O	1:A:240:VAL:HG12	2.16	0.45
1:A:489:ALA:O	1:A:493:GLU:HG2	2.15	0.45
1:A:812:HIS:ND1	1:A:813:PRO:HD2	2.31	0.45
3:H:145:LEU:HD13	3:H:218:VAL:HB	1.98	0.45
1:A:84:ARG:HH11	1:A:246:ARG:HE	1.64	0.45
1:A:174:THR:HG21	1:B:241:GLU:HG2	1.98	0.45
1:A:362:LYS:HE3	1:A:362:LYS:HB3	1.65	0.45
1:B:23:ALA:O	1:B:27:ILE:HG22	2.16	0.45
1:A:114:ARG:H	1:A:114:ARG:HG2	1.59	0.45
1:B:943:PRO:HG2	1:B:1001:ALA:HB2	1.98	0.45
2:C:1545:ARG:HG3	2:C:1558:PRO:HA	1.96	0.45
1:A:76:LEU:O	1:A:80:ILE:HD12	2.15	0.45
1:A:1213:ARG:HD3	1:A:1470:PRO:O	2.16	0.45
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.72	0.45
1:B:637:ILE:HG13	1:B:781:TRP:CZ3	2.51	0.45
4:I:154:VAL:HG22	4:I:201:LEU:HB3	1.98	0.45
1:A:344:LEU:O	1:A:347:PRO:HD2	2.16	0.45
4:L:61:PRO:HD3	4:L:105:GLY:HA2	1.97	0.45
4:L:155:VAL:HG22	4:L:200:THR:HG23	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:168:VAL:HG12	4:L:218:VAL:HG22	1.99	0.45
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.82	0.45
1:A:675:VAL:HG22	1:A:724:VAL:HG12	1.98	0.45
3:H:73:THR:OG1	3:H:86:GLN:HB3	2.16	0.45
1:A:20:LEU:HB3	1:B:20:LEU:HB3	1.98	0.45
1:A:1358:LEU:HB3	1:A:1381:LEU:HD11	1.99	0.45
1:B:966:LEU:HG	1:B:981:VAL:HG22	1.98	0.45
1:A:625:ARG:HA	1:A:625:ARG:NH1	2.32	0.45
1:A:1396:VAL:HA	1:A:1446:GLY:O	2.16	0.45
1:B:26:ARG:NH1	1:B:30:LEU:HB2	2.32	0.45
3:G:73:THR:OG1	3:G:86:GLN:HB3	2.16	0.45
3:G:217:LYS:HE3	3:G:217:LYS:HB3	1.82	0.45
1:A:27:ILE:HB	1:B:27:ILE:HB	1.99	0.45
1:A:407:PRO:HB2	1:A:413:TRP:NE1	2.31	0.45
1:A:1022:LEU:HD11	1:A:1034:LEU:HD13	1.98	0.45
1:B:25:GLN:HG2	1:B:28:ARG:HH21	1.82	0.45
1:B:1067:VAL:HG13	1:B:1076:LEU:HD23	1.99	0.45
3:H:65:ALA:HB3	3:H:68:VAL:HG22	1.99	0.45
1:A:673:ALA:HB2	1:A:726:ARG:HD2	1.97	0.45
1:A:1224:ARG:HD2	1:A:1394:PRO:HG3	1.98	0.44
1:B:343:THR:HB	1:B:344:LEU:HD22	1.99	0.44
1:B:407:PRO:HB2	1:B:413:TRP:NE1	2.32	0.44
1:A:361:ARG:HD3	1:A:361:ARG:HA	1.78	0.44
1:A:1416:ALA:HA	1:A:1419:ARG:HE	1.82	0.44
1:B:975:ARG:HB3	1:B:1000:PRO:HG3	1.99	0.44
3:G:86:GLN:C	3:G:87:MET:HE2	2.42	0.44
1:B:287:ARG:HD3	1:B:865:TRP:CD1	2.52	0.44
1:B:653:LYS:O	1:B:657:LEU:HG	2.17	0.44
3:G:66:ALA:HA	3:G:69:LYS:HB2	1.99	0.44
4:L:130:ARG:HH12	4:L:133:ALA:HB2	1.81	0.44
1:A:14:ARG:HB2	4:L:51:TYR:OH	2.18	0.44
1:A:231:THR:HG21	1:A:378:GLN:HB2	1.99	0.44
1:B:125:LEU:HD23	1:B:125:LEU:HA	1.84	0.44
1:B:680:ASP:HA	1:B:683:VAL:HG22	1.98	0.44
3:G:166:LEU:HD21	3:G:189:VAL:HG11	1.99	0.44
1:A:24:ARG:O	1:A:27:ILE:HG23	2.18	0.44
1:A:92:VAL:HG22	1:A:250:PRO:HA	2.00	0.44
1:B:24:ARG:O	1:B:27:ILE:HG23	2.17	0.44
1:B:580:LEU:HD22	1:B:652:ALA:HB1	1.98	0.44
1:A:723:ARG:HD2	1:A:723:ARG:HA	1.75	0.44
1:A:946:GLY:HA3	1:A:976:ARG:NH1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:151:ASP:HA	3:H:182:LEU:HB3	1.99	0.44
4:I:69:ILE:HD13	4:I:69:ILE:HA	1.82	0.44
1:B:178:ALA:HB3	1:B:181:VAL:HG22	1.99	0.44
1:B:658:ARG:O	1:B:662:ILE:HG12	2.17	0.44
3:G:4:VAL:HG22	3:G:29:PHE:HB3	2.00	0.44
1:A:479:GLU:HG2	1:A:480:SER:N	2.33	0.44
1:A:549:PRO:HB3	1:A:814:VAL:HG21	1.99	0.44
1:B:117:VAL:HG12	1:B:880:LEU:HB2	1.99	0.44
1:B:631:GLY:HA3	1:B:636:GLU:HA	2.00	0.44
1:A:380:ALA:O	1:A:383:VAL:HG12	2.18	0.44
1:A:559:GLY:HA3	1:A:592:LEU:HD13	1.99	0.44
1:B:7:GLU:HG3	3:H:58:TYR:CE2	2.53	0.44
4:I:71:LEU:HB2	4:I:74:ASN:OD1	2.18	0.44
4:I:146:GLN:NE2	4:I:151:THR:HG23	2.32	0.44
1:A:837:LEU:HD23	1:A:837:LEU:HA	1.91	0.43
1:A:26:ARG:O	1:A:29:GLU:HG3	2.18	0.43
1:A:180:SER:HB2	1:B:201:THR:HA	2.00	0.43
1:A:365:LEU:HD21	1:A:418:ILE:HG13	2.00	0.43
1:A:1022:LEU:HB3	1:A:1025:ALA:HB2	1.99	0.43
1:A:1169:VAL:HB	1:A:1182:LEU:HD13	2.00	0.43
1:A:1231:THR:HA	1:A:1257:HIS:O	2.18	0.43
4:I:146:GLN:HE21	4:I:151:THR:HG23	1.84	0.43
1:A:242:PHE:HB2	1:A:248:LEU:HD11	2.00	0.43
1:A:509:ARG:HD3	1:A:509:ARG:HA	1.91	0.43
1:A:555:TRP:CG	1:A:558:MET:HE1	2.53	0.43
1:A:918:TRP:HZ3	1:A:925:PRO:HD2	1.82	0.43
1:B:314:GLN:O	1:B:317:VAL:HG12	2.18	0.43
1:B:600:ARG:HB3	1:B:602:ASP:OD1	2.18	0.43
4:I:203:LEU:HD21	4:I:208:TYR:HB2	2.00	0.43
4:L:137:VAL:HG22	4:L:158:LEU:HD22	2.00	0.43
1:A:1325:LEU:HD12	1:A:1372:ALA:HB3	2.00	0.43
1:B:769:TRP:HB2	1:B:771:ARG:NH2	2.33	0.43
1:B:1049:PRO:HB2	1:B:1052:TRP:CZ2	2.54	0.43
3:G:126:PRO:HG3	3:G:207:HIS:HB2	2.00	0.43
3:H:40:ARG:NH1	3:H:94:ASP:HA	2.33	0.43
1:A:950:VAL:HB	1:A:1050:SER:HB3	2.01	0.43
1:A:1077:THR:HG22	1:A:1083:PRO:HA	2.00	0.43
1:A:1183:ALA:HB2	1:A:1194:VAL:HG11	2.00	0.43
1:B:546:TRP:CD2	1:B:626:PRO:HB3	2.54	0.43
1:A:151:VAL:HG13	1:A:196:ALA:HA	2.00	0.43
1:A:1057:LEU:HD13	1:A:1085:LEU:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:PRO:HG2	1:A:1305:HIS:HD2	1.82	0.43
1:A:1312:HIS:O	1:A:1359:PHE:HB2	2.18	0.43
1:A:61:ARG:NH2	1:A:423:GLU:HA	2.33	0.43
1:A:91:TYR:CE1	1:A:248:LEU:HB2	2.54	0.43
1:A:450:LEU:HD13	1:A:450:LEU:HA	1.88	0.43
1:A:563:LEU:HD12	1:A:563:LEU:HA	1.84	0.43
3:G:42:ALA:HB3	3:G:45:LYS:HG3	2.01	0.43
3:H:130:PRO:O	4:L:143:SER:HB3	2.19	0.43
1:A:669:ARG:HH21	1:A:737:HIS:CD2	2.36	0.43
1:A:877:HIS:HE1	1:A:879:TRP:HB2	1.83	0.43
1:A:1184:ASP:O	1:A:1203:ARG:HG3	2.18	0.43
1:A:1185:LEU:HD21	1:A:1194:VAL:HG21	2.01	0.43
1:A:1383:ALA:HA	1:A:1386:ARG:HE	1.84	0.43
3:G:153:PHE:HB2	3:G:182:LEU:HD22	2.00	0.43
3:G:155:GLU:HG2	3:G:183:TYR:CE2	2.53	0.43
1:A:811:ALA:HA	1:A:830:LEU:HB2	2.01	0.43
1:A:1175:GLU:HG3	1:A:1369:PRO:HA	2.00	0.43
4:L:167:LYS:HE3	4:L:167:LYS:HB3	1.63	0.43
1:A:1319:ASP:HB2	1:A:1412:HIS:CE1	2.54	0.43
1:B:548:PHE:HB2	1:B:631:GLY:HA2	2.01	0.43
3:H:213:LYS:HD2	3:H:213:LYS:HA	1.70	0.43
4:L:135:PRO:HD2	4:L:223:LEU:HG	2.01	0.43
1:A:364:PRO:HB3	1:A:417:ALA:HB1	2.00	0.42
1:B:55:TRP:HH2	1:B:397:THR:HB	1.83	0.42
3:G:7:VAL:O	3:G:24:CYS:HA	2.18	0.42
4:I:28:PRO:HB2	4:I:129:LYS:NZ	2.24	0.42
4:I:162:TYR:HE1	4:I:188:GLN:HE22	1.66	0.42
1:A:311:GLY:HA2	1:A:314:GLN:HG3	2.01	0.42
1:A:361:ARG:HG3	1:A:417:ALA:HB3	2.01	0.42
1:B:671:GLY:C	1:B:672:MET:HE2	2.44	0.42
1:B:1023:ARG:HA	1:B:1023:ARG:NE	2.35	0.42
4:I:58:LEU:HD13	4:I:107:TYR:CZ	2.53	0.42
1:A:338:HIS:CD2	1:A:441:PHE:H	2.37	0.42
1:B:207:LEU:HD13	1:B:450:LEU:HD23	2.01	0.42
1:B:427:TRP:CZ2	1:B:434:ARG:HB3	2.54	0.42
1:B:819:LEU:O	1:B:823:THR:HG22	2.20	0.42
2:C:1506:LEU:HD11	2:C:1568:PRO:HG3	2.01	0.42
3:H:106:LEU:HD22	3:H:106:LEU:HA	1.87	0.42
1:A:314:GLN:O	1:A:317:VAL:HG12	2.20	0.42
1:B:602:ASP:HA	1:B:659:SER:HB2	2.00	0.42
1:A:840:LEU:O	1:A:844:MET:SD	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:HA	1:B:268:GLU:HG2	2.01	0.42
1:B:553:THR:HG21	1:B:810:SER:HB2	2.02	0.42
3:G:161:TRP:HB3	3:G:166:LEU:HB3	2.02	0.42
3:H:72:PHE:HA	3:H:86:GLN:O	2.19	0.42
4:I:136:SER:OG	4:I:159:ASN:HB3	2.19	0.42
1:A:949:VAL:HG22	1:A:1051:VAL:HG13	2.01	0.42
1:B:113:PRO:O	1:B:117:VAL:HG23	2.19	0.42
1:B:904:ARG:HA	1:B:968:VAL:O	2.19	0.42
1:A:189:VAL:HB	1:A:190:LEU:HD22	2.01	0.42
1:A:1141:TRP:HH2	1:A:1179:ARG:HB3	1.85	0.42
4:L:133:ALA:HB3	4:L:162:TYR:H	1.85	0.42
1:A:658:ARG:HH11	1:A:781:TRP:HB3	1.84	0.42
1:A:832:ARG:HG2	1:A:833:GLU:HG2	2.02	0.42
1:B:891:PRO:HD3	1:B:1027:ARG:CZ	2.49	0.42
3:G:178:GLN:NE2	3:G:184:SER:HB3	2.34	0.42
4:L:170:TRP:CD1	4:L:201:LEU:HD13	2.54	0.42
1:A:103:GLU:HB3	1:A:875:HIS:HB3	2.02	0.42
1:A:562:LEU:HA	1:A:565:GLU:HB2	2.01	0.42
1:A:1022:LEU:HD22	1:A:1031:HIS:CG	2.55	0.42
4:L:168:VAL:HA	4:L:217:GLU:O	2.20	0.42
1:A:91:TYR:CD1	1:A:92:VAL:HG23	2.55	0.42
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.80	0.42
1:A:367:LEU:HD21	1:A:420:LEU:HG	2.00	0.42
1:A:627:ASP:O	1:A:760:PRO:HG2	2.20	0.42
1:B:593:ARG:HA	1:B:593:ARG:HD2	1.78	0.42
1:B:615:LEU:HD13	1:B:829:THR:HG21	2.01	0.42
1:B:1017:VAL:HG21	1:B:1038:ALA:HA	2.01	0.42
4:I:43:GLN:C	4:I:90:THR:HG22	2.44	0.42
4:L:189:ASP:HB3	4:L:193:SER:N	2.35	0.42
1:B:276:GLU:OE2	1:B:280:VAL:HB	2.19	0.41
3:G:4:VAL:HA	3:G:27:SER:O	2.20	0.41
4:I:158:LEU:O	4:I:196:SER:HA	2.20	0.41
1:A:653:LYS:O	1:A:657:LEU:HD23	2.21	0.41
1:A:734:HIS:HB3	1:A:788:GLN:OE1	2.20	0.41
1:A:951:ASP:HB2	1:A:993:HIS:HA	2.02	0.41
1:B:762:TYR:HD2	1:B:769:TRP:CD2	2.38	0.41
3:G:15:GLN:HG2	3:G:18:ARG:CZ	2.50	0.41
1:A:841:LEU:HA	1:A:844:MET:HE1	2.01	0.41
1:A:926:ASN:O	1:A:930:VAL:HG23	2.20	0.41
1:B:74:TRP:CD2	1:B:236:PRO:HD3	2.55	0.41
1:B:931:GLU:CD	1:B:1028:TYR:HB3	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:22:LEU:O	3:H:84:TYR:HA	2.20	0.41
4:I:158:LEU:HD11	4:I:218:VAL:HG21	2.02	0.41
1:A:182:ALA:O	1:A:185:ARG:HB3	2.20	0.41
1:A:909:ALA:HB3	1:A:964:VAL:HG23	2.03	0.41
1:A:1236:GLY:N	1:A:1314:ALA:HB2	2.36	0.41
1:B:151:VAL:HG12	1:B:226:LEU:HB2	2.02	0.41
1:B:646:LEU:HD23	1:B:646:LEU:HA	1.80	0.41
1:B:695:VAL:HA	1:B:701:VAL:HG22	2.02	0.41
1:B:749:LEU:HB3	1:B:778:GLY:HA3	2.03	0.41
3:G:207:HIS:CD2	3:G:209:PRO:HD2	2.55	0.41
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.88	0.41
1:A:778:GLY:HA2	1:A:781:TRP:CD1	2.56	0.41
1:B:72:ARG:HB3	1:B:74:TRP:NE1	2.34	0.41
1:B:723:ARG:NH1	1:B:724:VAL:H	2.18	0.41
1:B:1074:LEU:HD13	1:B:1076:LEU:HD21	2.02	0.41
3:G:8:GLN:H	3:G:112:GLN:NE2	2.14	0.41
4:L:125:LYS:HE2	4:L:125:LYS:HB2	1.78	0.41
1:A:275:LEU:HD13	1:A:275:LEU:HA	1.90	0.41
1:A:672:MET:SD	1:A:732:ALA:HA	2.60	0.41
1:B:747:GLU:HG2	1:B:748:THR:N	2.35	0.41
2:C:1538:4HH:HP2	2:C:1538:4HH:HS2	1.82	0.41
3:G:129:PHE:HB3	4:I:143:SER:CB	2.51	0.41
3:H:3:GLU:O	3:H:28:GLY:HA3	2.20	0.41
3:H:90:LEU:H	3:H:90:LEU:HG	1.59	0.41
4:L:39:CYS:HB2	4:L:56:TRP:CH2	2.55	0.41
4:L:147:LEU:HB3	4:L:205:LYS:NZ	2.35	0.41
1:A:15:ARG:HA	1:A:15:ARG:HD2	1.91	0.41
1:A:631:GLY:HA3	1:A:636:GLU:HA	2.03	0.41
1:B:2:ALA:O	1:B:5:ASP:HB2	2.19	0.41
1:B:589:VAL:O	1:B:593:ARG:HG2	2.21	0.41
2:C:1570:LEU:O	2:C:1574:LEU:HG	2.21	0.41
1:A:1010:ALA:HA	1:A:1070:THR:HG22	2.03	0.41
1:A:231:THR:O	1:A:268:GLU:HB3	2.20	0.41
1:A:769:TRP:HB2	1:A:771:ARG:CZ	2.51	0.41
1:A:985:GLU:N	1:A:988:GLU:HB2	2.36	0.41
1:A:1008:PRO:HD2	1:A:1075:ARG:HB3	2.03	0.41
1:A:1126:TYR:HD2	1:A:1152:VAL:HG22	1.85	0.41
1:A:1368:ASN:HD22	1:A:1420:ARG:HH21	1.67	0.41
1:B:366:TRP:CE3	1:B:419:GLU:HB2	2.56	0.41
1:B:890:ASP:HA	1:B:891:PRO:HD3	1.94	0.41
1:B:908:VAL:HG13	1:B:963:GLU:OE2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:949:VAL:HB	1:B:995:HIS:CE1	2.56	0.41
3:H:101:THR:HG21	3:H:107:PHE:HB3	2.02	0.41
4:L:185:VAL:HG12	4:L:197:LEU:HB2	2.03	0.41
1:A:1105:LEU:HD12	1:A:1105:LEU:HA	1.94	0.41
1:B:344:LEU:C	1:B:347:PRO:HD2	2.46	0.41
1:B:622:VAL:O	1:B:855:ASP:HB3	2.21	0.41
1:B:666:LEU:HD13	1:B:669:ARG:NH1	2.36	0.41
1:B:912:SER:H	1:B:915:ALA:HB3	1.85	0.41
2:C:1542:VAL:HG13	2:C:1545:ARG:HH21	1.85	0.41
3:G:158:THR:HG1	3:G:206:ASN:HB3	1.86	0.41
4:L:134:ALA:HB1	4:L:223:LEU:HD23	2.03	0.41
1:A:1212:PRO:HB2	1:A:1471:LEU:HG	2.03	0.40
1:A:1271:GLN:HB2	1:A:1283:ILE:HD12	2.03	0.40
1:A:1360:SER:OG	1:A:1378:ASN:HB3	2.21	0.40
1:B:43:ARG:O	1:B:44:LEU:HD13	2.21	0.40
4:L:129:LYS:HA	4:L:162:TYR:OH	2.21	0.40
1:A:314:GLN:NE2	1:A:441:PHE:CE1	2.86	0.40
1:B:108:PHE:CD1	1:B:476:ARG:HG3	2.56	0.40
4:L:21:THR:HA	4:L:40:ARG:O	2.22	0.40
4:L:27:LEU:O	4:L:29:VAL:HG13	2.21	0.40
1:A:427:TRP:CZ2	1:A:434:ARG:HB3	2.56	0.40
1:A:1345:ASP:O	1:A:1349:ARG:HB2	2.21	0.40
1:A:1371:GLN:NE2	1:A:1420:ARG:HH22	2.19	0.40
1:B:769:TRP:HB2	1:B:771:ARG:CZ	2.51	0.40
3:H:161:TRP:HB3	3:H:166:LEU:HB3	2.03	0.40
4:L:66:GLN:N	4:L:66:GLN:OE1	2.54	0.40
1:A:1132:GLU:HB3	1:A:1327:PRO:HB3	2.02	0.40
1:A:1166:TRP:CZ2	1:A:1184:ASP:HB2	2.53	0.40
1:B:14:ARG:HG2	4:I:51:TYR:OH	2.22	0.40
1:B:55:TRP:O	1:B:58:VAL:HG12	2.20	0.40
4:I:58:LEU:HB2	4:I:68:LEU:HD11	2.03	0.40
4:L:136:SER:OG	4:L:159:ASN:HB3	2.22	0.40
4:L:207:ASP:HA	4:L:210:LYS:HD2	2.02	0.40
1:A:342:THR:HG23	1:A:345:GLY:H	1.87	0.40
1:A:554:GLN:H	1:A:554:GLN:CD	2.29	0.40
1:A:1430:PRO:HD2	1:A:1433:GLU:HB2	2.03	0.40
1:B:210:MET:HE2	1:B:210:MET:HB3	1.95	0.40
1:B:381:ALA:O	1:B:384:ALA:HB3	2.21	0.40
1:B:386:VAL:HG13	1:B:452:LEU:HD11	2.04	0.40
1:B:605:GLN:HB2	1:B:606:PRO:HD3	2.03	0.40
1:B:723:ARG:NH2	1:B:725:ARG:HG2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ALA:HB1	1:B:1035:LEU:HB3	2.04	0.40
4:I:130:ARG:HD2	4:I:193:SER:HB2	2.04	0.40
4:L:111:GLN:NE2	4:L:114:GLN:HB3	2.36	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	1468/1683 (87%)	1415 (96%)	53 (4%)	0	100	100
1	B	1086/1683 (64%)	1047 (96%)	39 (4%)	0	100	100
2	C	72/1683 (4%)	72 (100%)	0	0	100	100
3	G	199/249 (80%)	192 (96%)	7 (4%)	0	100	100
3	H	199/249 (80%)	193 (97%)	6 (3%)	0	100	100
4	I	203/236 (86%)	195 (96%)	8 (4%)	0	100	100
4	L	203/236 (86%)	195 (96%)	8 (4%)	0	100	100
All	All	3430/6019 (57%)	3309 (96%)	121 (4%)	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	1094/1245 (88%)	1046 (96%)	48 (4%)	25	49
1	B	814/1245 (65%)	788 (97%)	26 (3%)	34	56
2	C	54/1244 (4%)	52 (96%)	2 (4%)	30	53
3	G	170/203 (84%)	165 (97%)	5 (3%)	37	58
3	H	170/203 (84%)	159 (94%)	11 (6%)	15	41
4	I	185/208 (89%)	179 (97%)	6 (3%)	34	56
4	L	185/208 (89%)	179 (97%)	6 (3%)	34	56
All	All	2672/4556 (59%)	2568 (96%)	104 (4%)	30	51

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	27	ILE
1	A	48	VAL
1	A	57	LEU
1	A	89	THR
1	A	151	VAL
1	A	173	VAL
1	A	230	VAL
1	A	235	THR
1	A	240	VAL
1	A	314	GLN
1	A	393	LEU
1	A	450	LEU
1	A	492	LEU
1	A	512	LEU
1	A	544	VAL
1	A	568	VAL
1	A	589	VAL
1	A	603	VAL
1	A	647	SER
1	A	672	MET
1	A	687	VAL
1	A	703	ILE
1	A	714	LEU
1	A	745	LEU
1	A	763	SER
1	A	804	THR
1	A	807	VAL
1	A	814	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	816	VAL
1	A	983	SER
1	A	998	LEU
1	A	1015	THR
1	A	1017	VAL
1	A	1055	VAL
1	A	1068	THR
1	A	1090	VAL
1	A	1091	ARG
1	A	1153	VAL
1	A	1180	ILE
1	A	1181	VAL
1	A	1224	ARG
1	A	1235	THR
1	A	1240	THR
1	A	1312	HIS
1	A	1317	LEU
1	A	1330	LEU
1	A	1418	LEU
1	B	27	ILE
1	B	57	LEU
1	B	77	ASP
1	B	145	LYS
1	B	233	MET
1	B	235	THR
1	B	297	VAL
1	B	334	VAL
1	B	397	THR
1	B	404	VAL
1	B	544	VAL
1	B	568	VAL
1	B	647	SER
1	B	687	VAL
1	B	717	LEU
1	B	759	VAL
1	B	772	ASP
1	B	776	LEU
1	B	807	VAL
1	B	809	VAL
1	B	866	VAL
1	B	939	LEU
1	B	951	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	975	ARG
1	B	1074	LEU
1	B	1093	THR
2	C	1525	VAL
2	C	1564	TYR
3	G	52	PHE
3	G	97	VAL
3	G	101	THR
3	G	172	THR
3	G	204	ASN
3	H	22	LEU
3	H	47	LEU
3	H	78	ASP
3	H	90	LEU
3	H	97	VAL
3	H	101	THR
3	H	106	LEU
3	H	117	THR
3	H	168	SER
3	H	172	THR
3	H	178	GLN
4	I	43	GLN
4	I	70	TYR
4	I	104	VAL
4	I	128	ILE
4	I	131	THR
4	I	216	CYS
4	L	30	THR
4	L	37	ILE
4	L	60	LYS
4	L	112	SER
4	L	115	THR
4	L	126	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	1368	ASN
1	A	1371	GLN
1	B	378	GLN
1	B	910	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	995	HIS
3	G	178	GLN
4	I	52	ASN
4	I	59	GLN
4	I	114	GLN
4	I	182	GLN
4	L	52	ASN
4	L	159	ASN
4	L	177	GLN
4	L	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	4HH	C	1538	2	22,26,27	1.21	1 (4%)	27,35,37	1.03	2 (7%)

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
2	4HH	C	1538	2	-	13/33/35/37	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1538	4HH	CL3-NN	2.32	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1538	4HH	O1P-P-O2P	2.31	123.20	112.44
2	C	1538	4HH	OG-CB-CA	2.14	110.22	108.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1538	4HH	CA-CB-OG-P
2	C	1538	4HH	O3P-CJ-CK-CL1
2	C	1538	4HH	O3P-CJ-CK-CL2
2	C	1538	4HH	O3P-CJ-CK-CM
2	C	1538	4HH	NN-CL3-CM-OM
2	C	1538	4HH	CJ-O3P-P-OG
2	C	1538	4HH	CJ-O3P-P-O2P
2	C	1538	4HH	NN-CO-CP-CQ
2	C	1538	4HH	CP-CQ-NR-CS
2	C	1538	4HH	OR-CQ-NR-CS
2	C	1538	4HH	ON-CL3-CM-OM
2	C	1538	4HH	NR-CS-CT-SU
2	C	1538	4HH	CJ-O3P-P-O1P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1538	4HH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

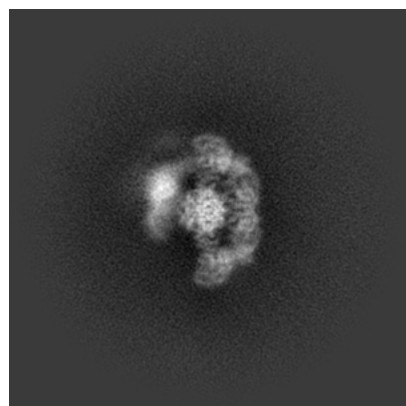
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71445. These allow visual inspection of the internal detail of the map and identification of artifacts.

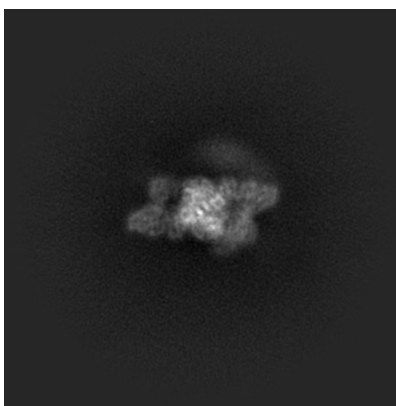
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

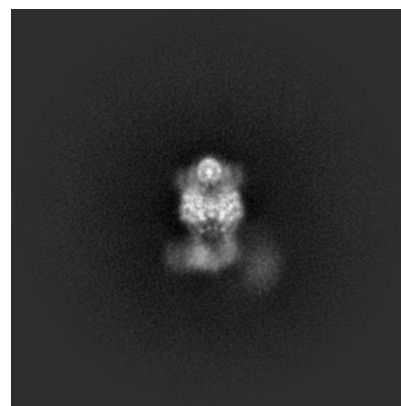
6.1.1 Primary map



X

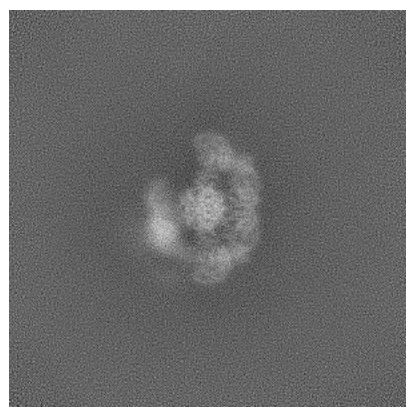


Y

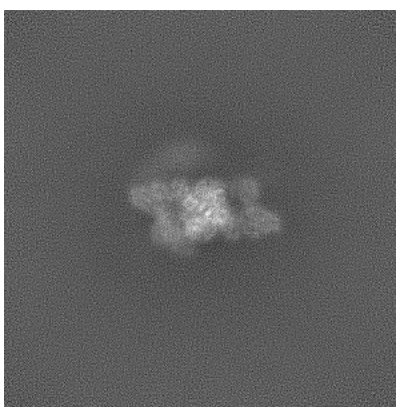


Z

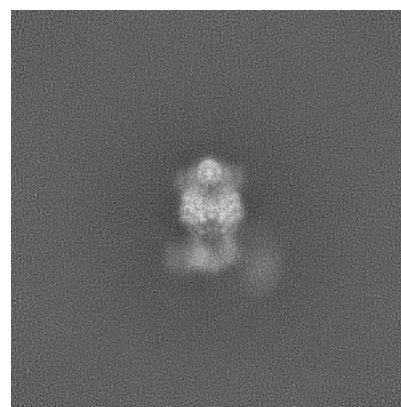
6.1.2 Raw map



X



Y

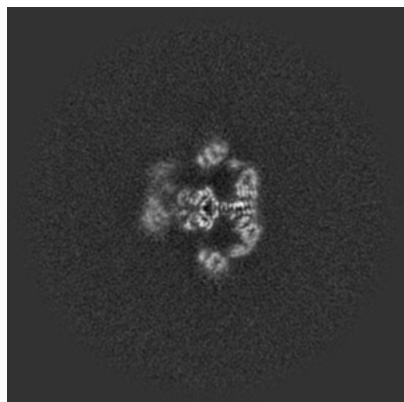


Z

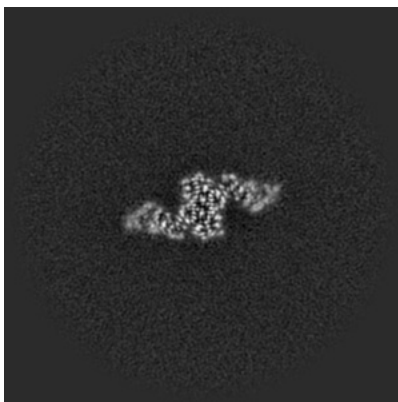
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

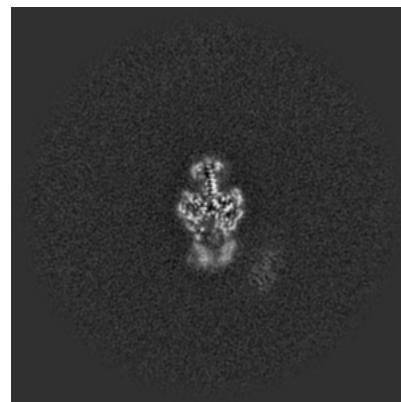
6.2.1 Primary map



X Index: 224

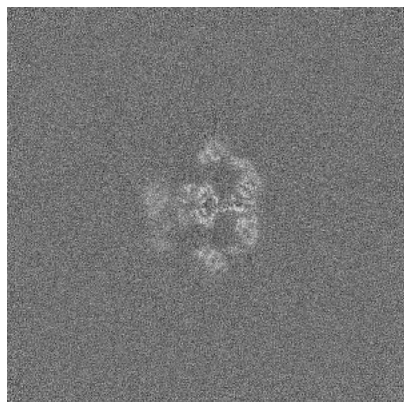


Y Index: 224

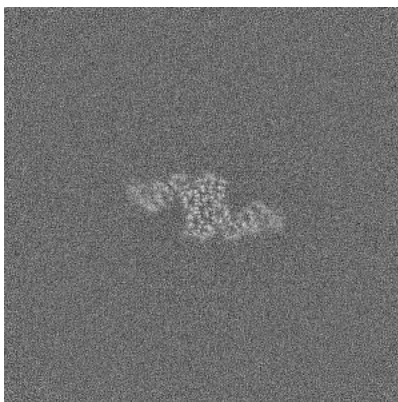


Z Index: 224

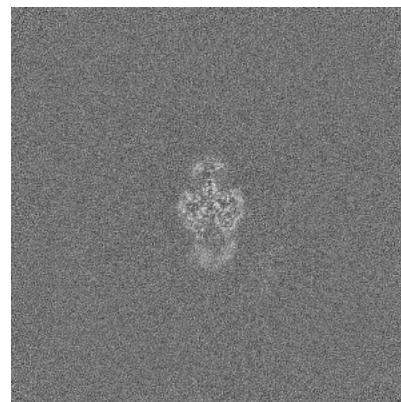
6.2.2 Raw map



X Index: 224



Y Index: 224

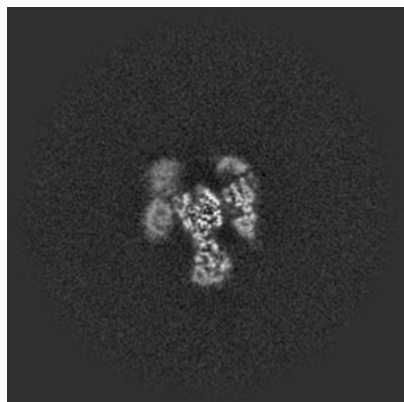


Z Index: 224

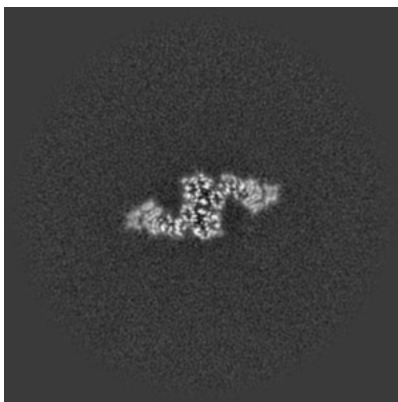
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

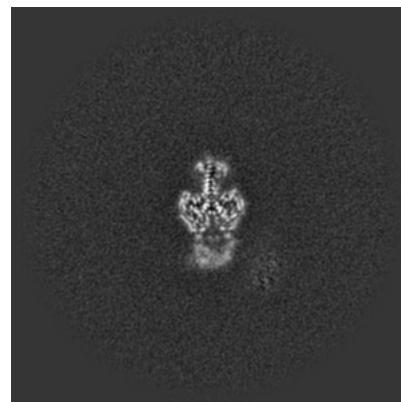
6.3.1 Primary map



X Index: 212

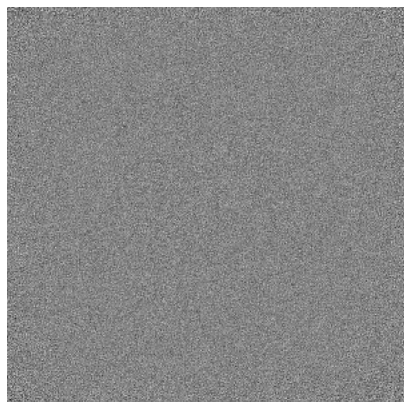


Y Index: 227

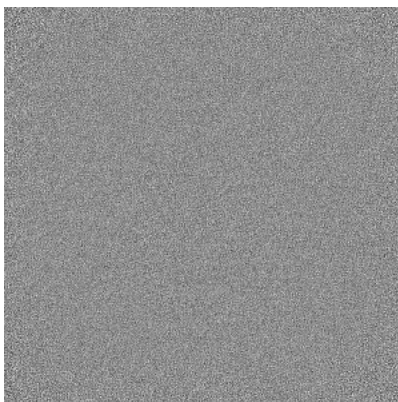


Z Index: 221

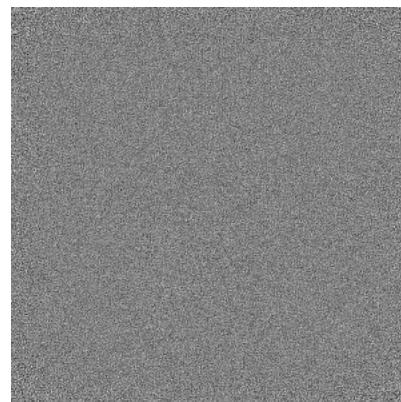
6.3.2 Raw map



X Index: 0



Y Index: 0

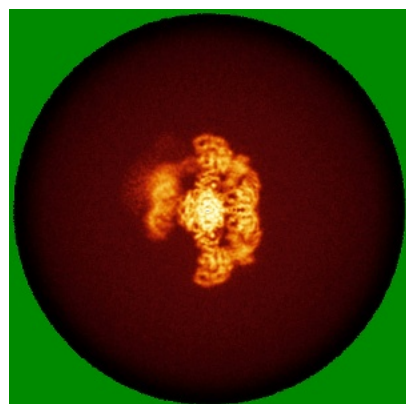


Z Index: 0

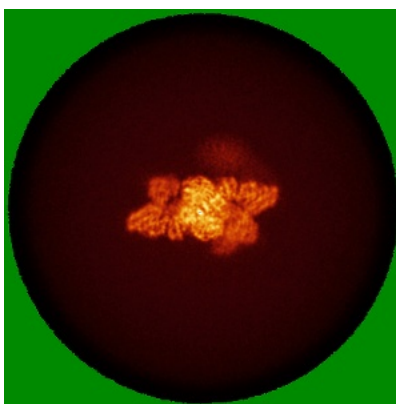
The images above show the largest variance slices of the map in three orthogonal directions.

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

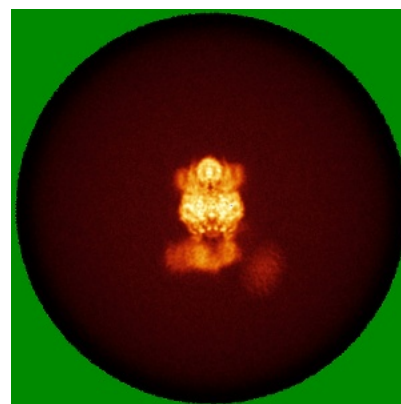
6.4.1 Primary map



X

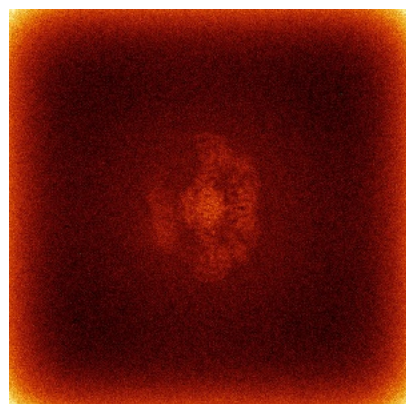


Y

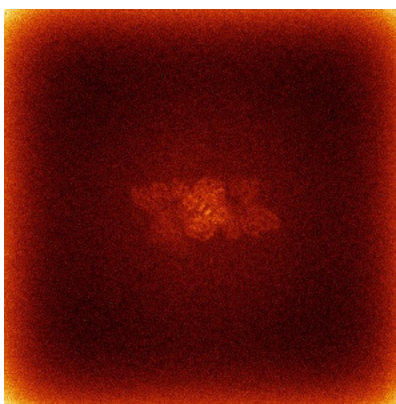


Z

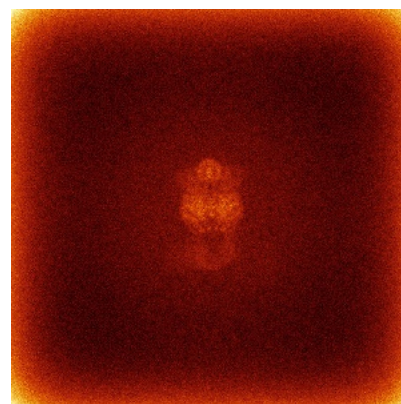
6.4.2 Raw map



X



Y

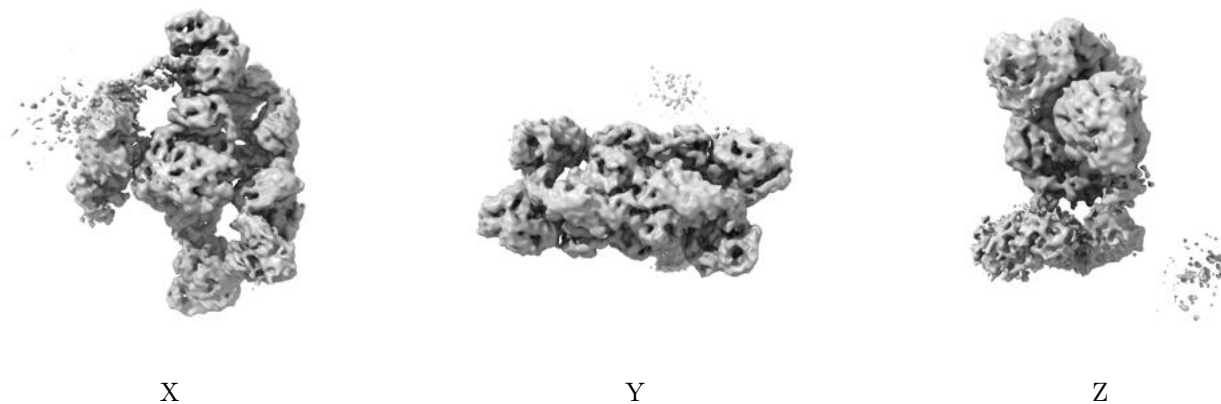


Z

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.

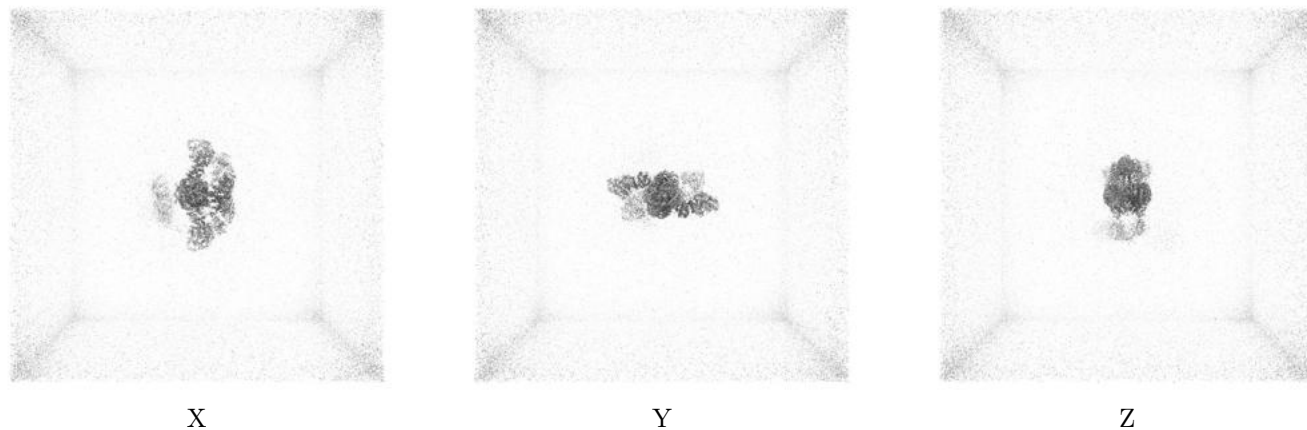
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

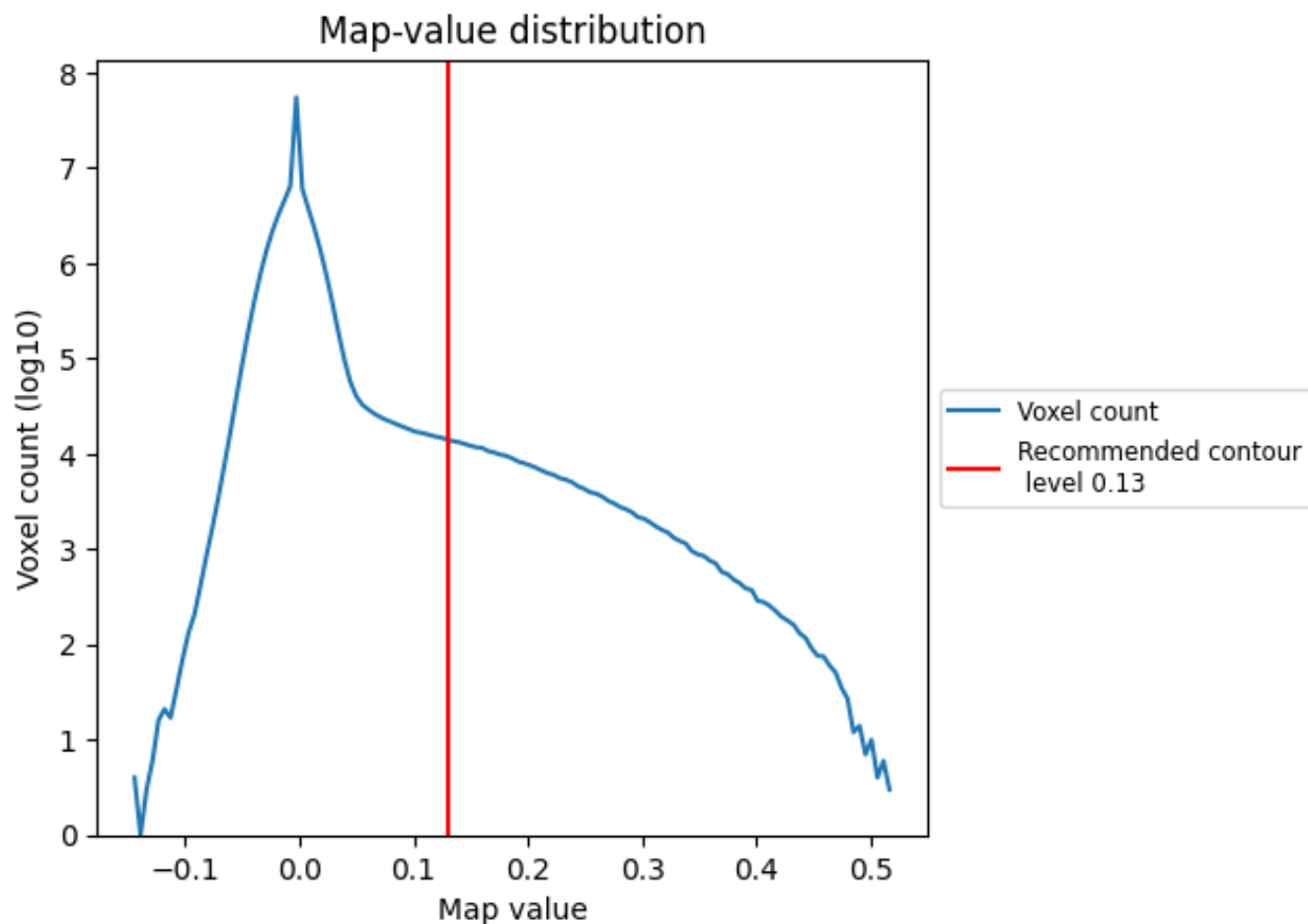
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

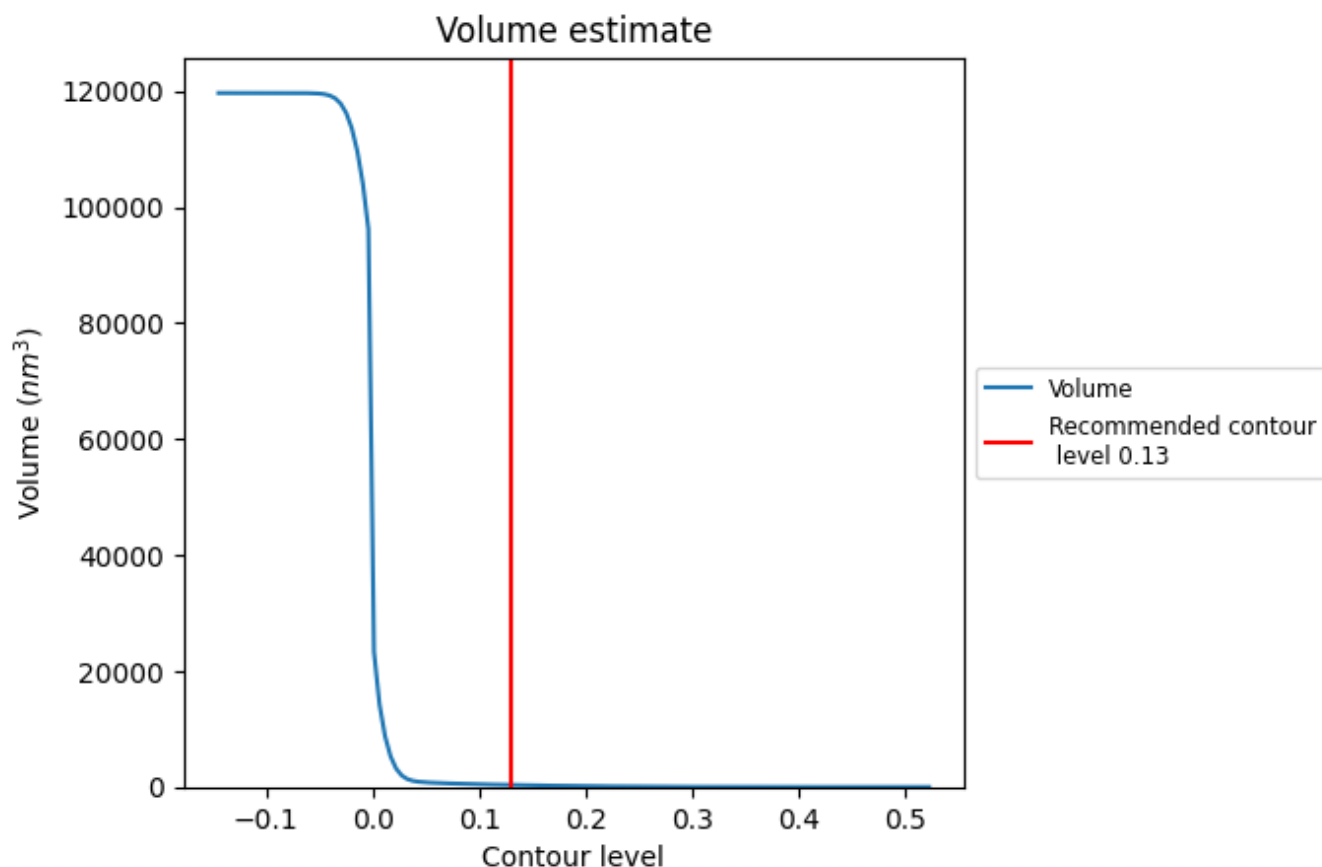
This section contains the results of statistical analysis of the map.

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.

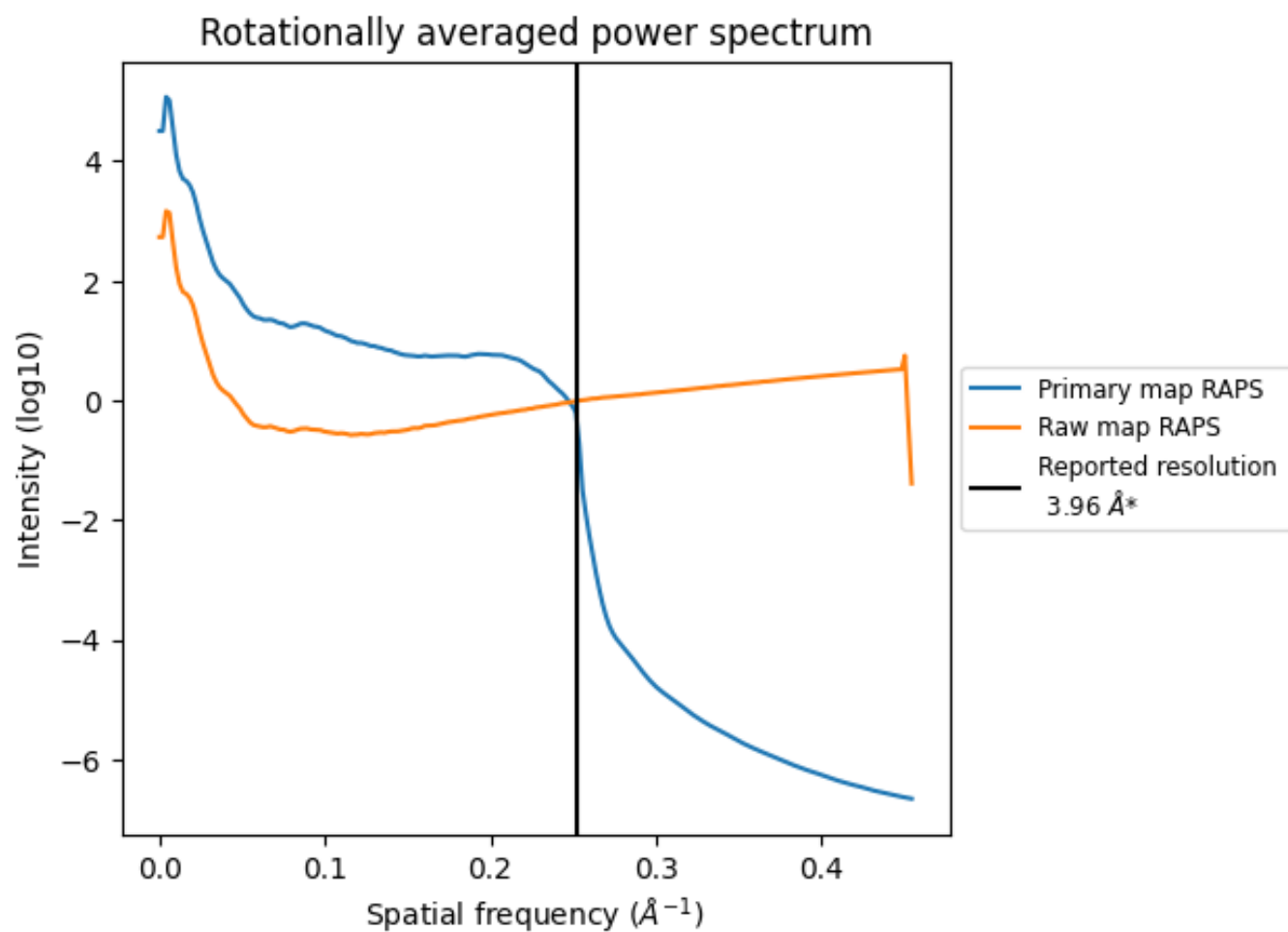
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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](#)

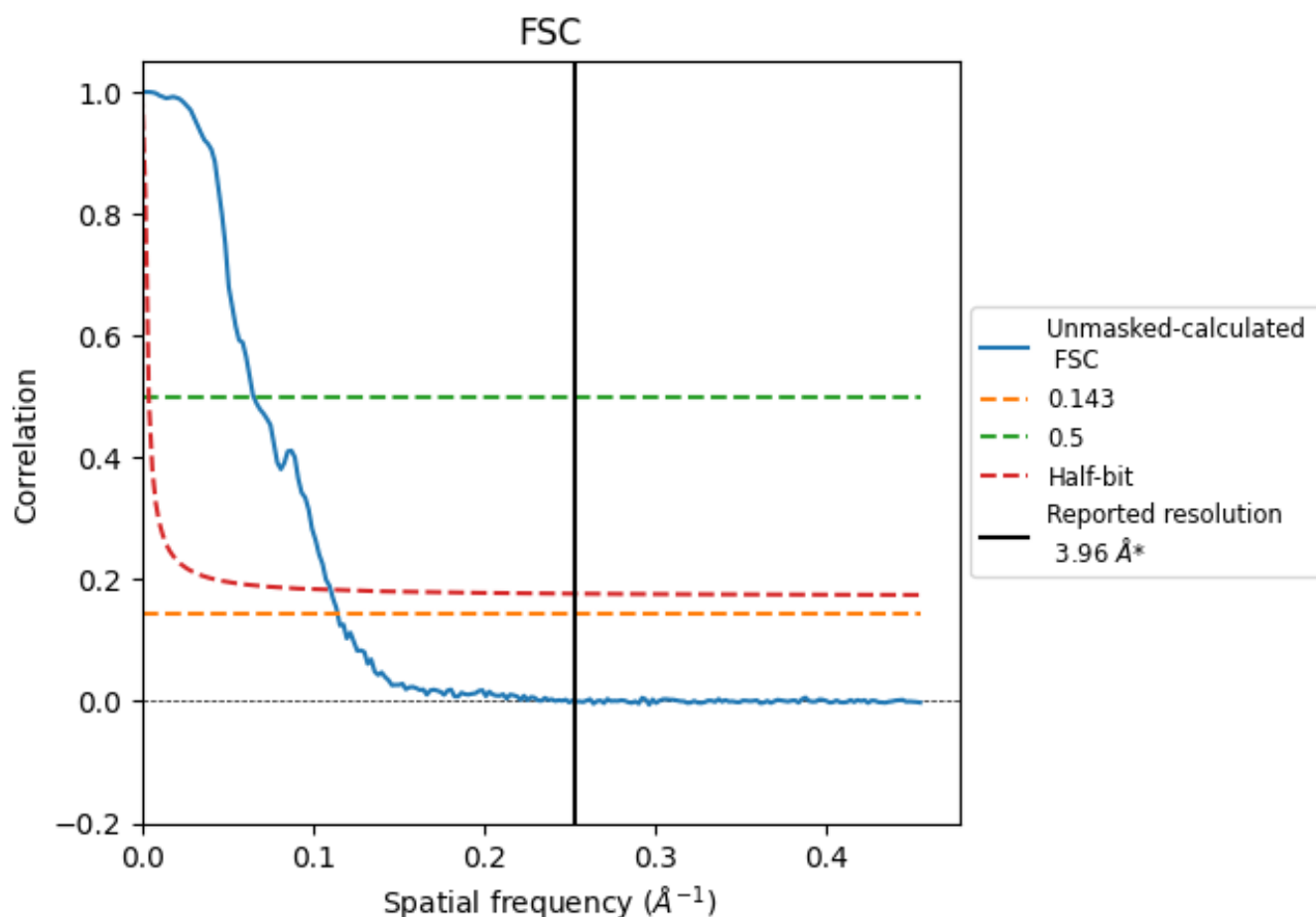


*Reported resolution corresponds to spatial frequency of 0.253 $\text{\AA}^{-1}$

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 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.75	15.34	9.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.75 differs from the reported value 3.96 by more than 10 %

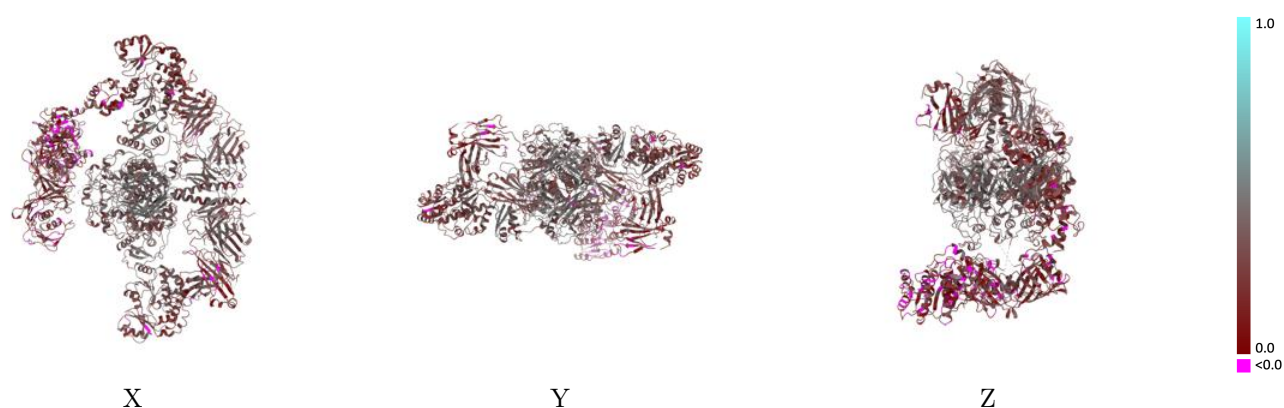
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71445 and PDB model 9PAT. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

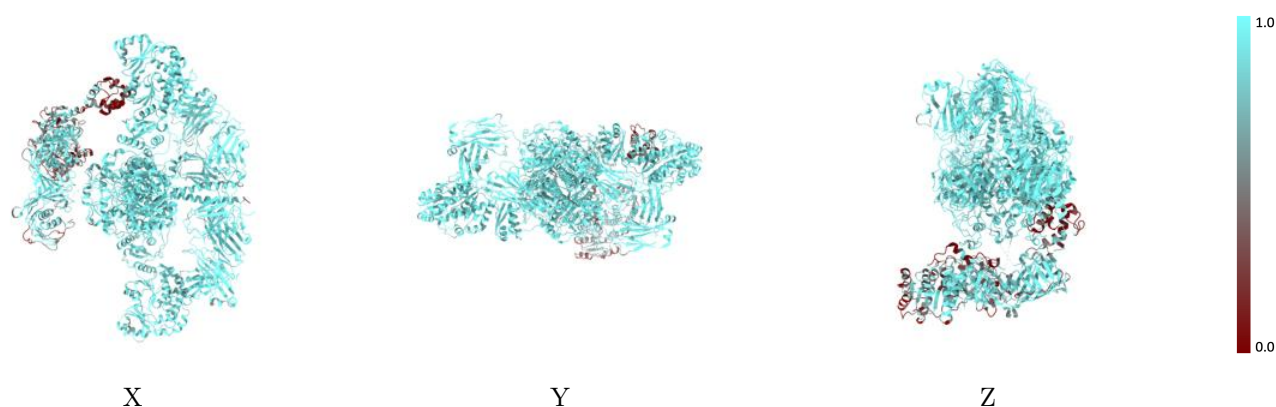
This section was not generated.

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



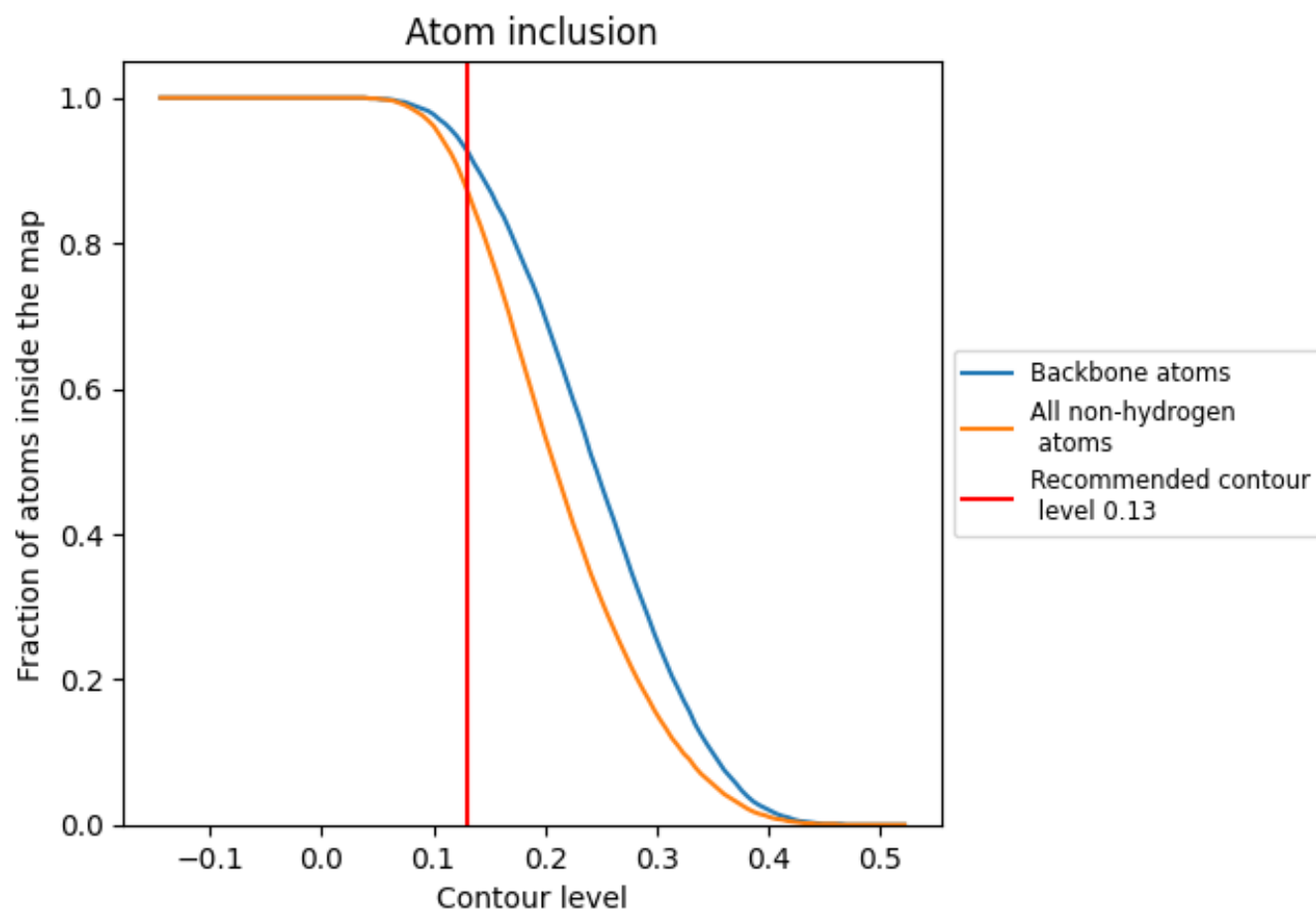
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.3110
A	0.8240	0.2900
B	0.9210	0.3360
C	0.2970	0.2210
G	0.9690	0.3320
H	0.9540	0.3410
I	0.9450	0.3070
L	0.9430	0.3070

1.0

0.0

<0.0