Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 07:56 PM EST

PDB ID	:	6Q0T
EMDB ID	:	EMD-20552
Title	:	Structure of a MAPK pathway complex
Authors	:	Park, E.; Rawson, S.; Jeon, H.; Eck, M.J.
Deposited on	:	2019-08-02
Resolution	:	5.70 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

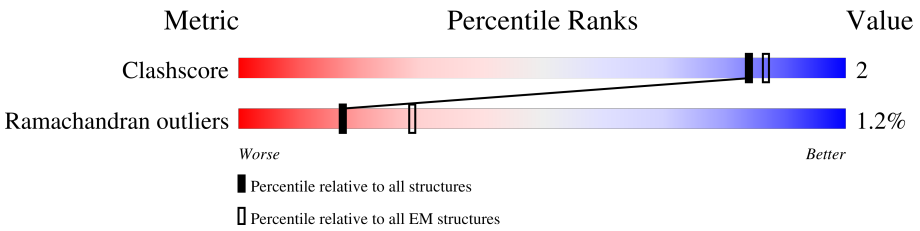
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.70 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

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	805	34% • 65%
1	B	805	33% • 65%
2	C	414	7% 72% • 26%
3	X	247	93% 7%
3	Y	247	84% 9% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6615 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	280	1389	824	280	284	1	1	0
1	B	278	1379	818	278	282	1	1	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP P15056
A	-25	SER	-	expression tag	UNP P15056
A	-24	TYR	-	expression tag	UNP P15056
A	-23	TYR	-	expression tag	UNP P15056
A	-22	HIS	-	expression tag	UNP P15056
A	-21	HIS	-	expression tag	UNP P15056
A	-20	HIS	-	expression tag	UNP P15056
A	-19	HIS	-	expression tag	UNP P15056
A	-18	HIS	-	expression tag	UNP P15056
A	-17	HIS	-	expression tag	UNP P15056
A	-16	HIS	-	expression tag	UNP P15056
A	-15	HIS	-	expression tag	UNP P15056
A	-14	ASP	-	expression tag	UNP P15056
A	-13	ILE	-	expression tag	UNP P15056
A	-12	PRO	-	expression tag	UNP P15056
A	-11	THR	-	expression tag	UNP P15056
A	-10	THR	-	expression tag	UNP P15056
A	-9	GLU	-	expression tag	UNP P15056
A	-8	ASN	-	expression tag	UNP P15056
A	-7	LEU	-	expression tag	UNP P15056
A	-6	TYR	-	expression tag	UNP P15056
A	-5	PHE	-	expression tag	UNP P15056
A	-4	GLN	-	expression tag	UNP P15056
A	-3	GLY	-	expression tag	UNP P15056
A	-2	ALA	-	expression tag	UNP P15056
A	-1	MET	-	expression tag	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASP	-	expression tag	UNP P15056
A	365	ALA	SER	engineered mutation	UNP P15056
A	767	GLY	-	expression tag	UNP P15056
A	768	THR	-	expression tag	UNP P15056
A	769	SER	-	expression tag	UNP P15056
A	770	ALA	-	expression tag	UNP P15056
A	771	TRP	-	expression tag	UNP P15056
A	772	SER	-	expression tag	UNP P15056
A	773	HIS	-	expression tag	UNP P15056
A	774	PRO	-	expression tag	UNP P15056
A	775	GLN	-	expression tag	UNP P15056
A	776	PHE	-	expression tag	UNP P15056
A	777	GLU	-	expression tag	UNP P15056
A	778	LYS	-	expression tag	UNP P15056
B	-26	MET	-	expression tag	UNP P15056
B	-25	SER	-	expression tag	UNP P15056
B	-24	TYR	-	expression tag	UNP P15056
B	-23	TYR	-	expression tag	UNP P15056
B	-22	HIS	-	expression tag	UNP P15056
B	-21	HIS	-	expression tag	UNP P15056
B	-20	HIS	-	expression tag	UNP P15056
B	-19	HIS	-	expression tag	UNP P15056
B	-18	HIS	-	expression tag	UNP P15056
B	-17	HIS	-	expression tag	UNP P15056
B	-16	HIS	-	expression tag	UNP P15056
B	-15	HIS	-	expression tag	UNP P15056
B	-14	ASP	-	expression tag	UNP P15056
B	-13	ILE	-	expression tag	UNP P15056
B	-12	PRO	-	expression tag	UNP P15056
B	-11	THR	-	expression tag	UNP P15056
B	-10	THR	-	expression tag	UNP P15056
B	-9	GLU	-	expression tag	UNP P15056
B	-8	ASN	-	expression tag	UNP P15056
B	-7	LEU	-	expression tag	UNP P15056
B	-6	TYR	-	expression tag	UNP P15056
B	-5	PHE	-	expression tag	UNP P15056
B	-4	GLN	-	expression tag	UNP P15056
B	-3	GLY	-	expression tag	UNP P15056
B	-2	ALA	-	expression tag	UNP P15056
B	-1	MET	-	expression tag	UNP P15056
B	0	ASP	-	expression tag	UNP P15056
B	365	ALA	SER	engineered mutation	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
B	767	GLY	-	expression tag	UNP P15056
B	768	THR	-	expression tag	UNP P15056
B	769	SER	-	expression tag	UNP P15056
B	770	ALA	-	expression tag	UNP P15056
B	771	TRP	-	expression tag	UNP P15056
B	772	SER	-	expression tag	UNP P15056
B	773	HIS	-	expression tag	UNP P15056
B	774	PRO	-	expression tag	UNP P15056
B	775	GLN	-	expression tag	UNP P15056
B	776	PHE	-	expression tag	UNP P15056
B	777	GLU	-	expression tag	UNP P15056
B	778	LYS	-	expression tag	UNP P15056

- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	306	1514	900	307	307	2	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	expression tag	UNP Q02750
C	-20	GLY	-	expression tag	UNP Q02750
C	-19	SER	-	expression tag	UNP Q02750
C	-18	SER	-	expression tag	UNP Q02750
C	-17	HIS	-	expression tag	UNP Q02750
C	-16	HIS	-	expression tag	UNP Q02750
C	-15	HIS	-	expression tag	UNP Q02750
C	-14	HIS	-	expression tag	UNP Q02750
C	-13	HIS	-	expression tag	UNP Q02750
C	-12	HIS	-	expression tag	UNP Q02750
C	-11	SER	-	expression tag	UNP Q02750
C	-10	ALA	-	expression tag	UNP Q02750
C	-9	VAL	-	expression tag	UNP Q02750
C	-8	ASP	-	expression tag	UNP Q02750
C	-7	GLU	-	expression tag	UNP Q02750
C	-6	ASN	-	expression tag	UNP Q02750
C	-5	LEU	-	expression tag	UNP Q02750
C	-4	TYR	-	expression tag	UNP Q02750
C	-3	PHE	-	expression tag	UNP Q02750
C	-2	GLN	-	expression tag	UNP Q02750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q02750
C	0	GLY	-	expression tag	UNP Q02750
C	218	ALA	SER	engineered mutation	UNP Q02750
C	222	ALA	SER	engineered mutation	UNP Q02750

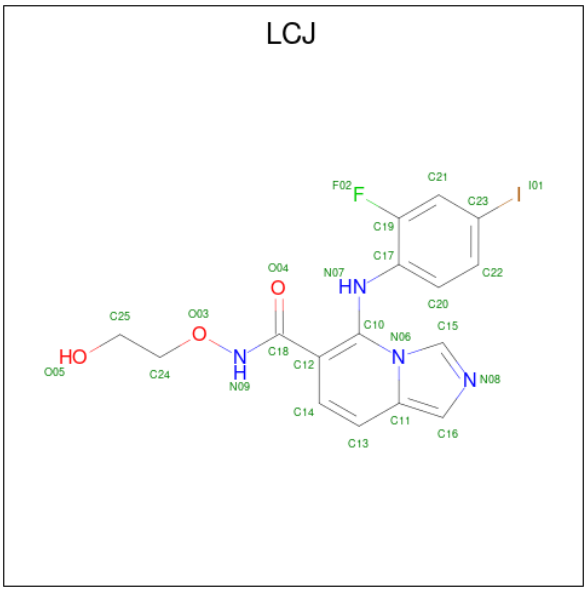
- Molecule 3 is a protein called 14-3-3 protein zeta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	X	229	1138	680	229	229	0	0
3	Y	229	1138	680	229	229	0	0

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

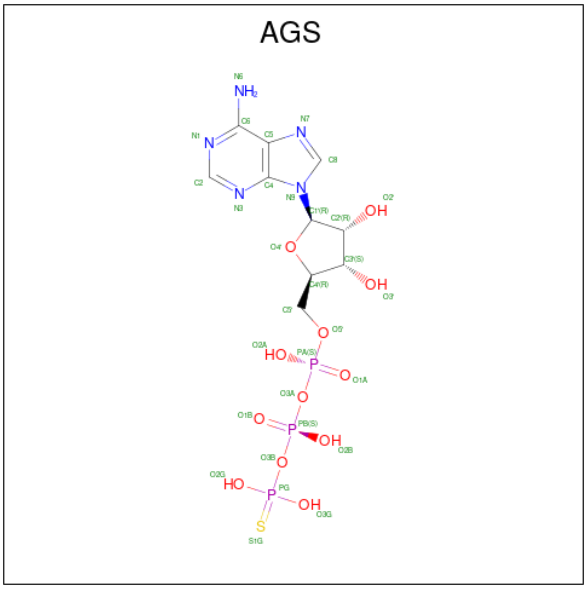
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	C	1	1	1	0

- Molecule 5 is 5-[(2-fluoro-4-iodophenyl)amino]-N-(2-hydroxyethoxy)imidazo[1,5-a]pyridine-6-carboxamide (three-letter code: LCJ) (formula: $C_{16}H_{14}FIN_4O_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	I	N	O	
5	C	1	25	16	1	1	4	3	0

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



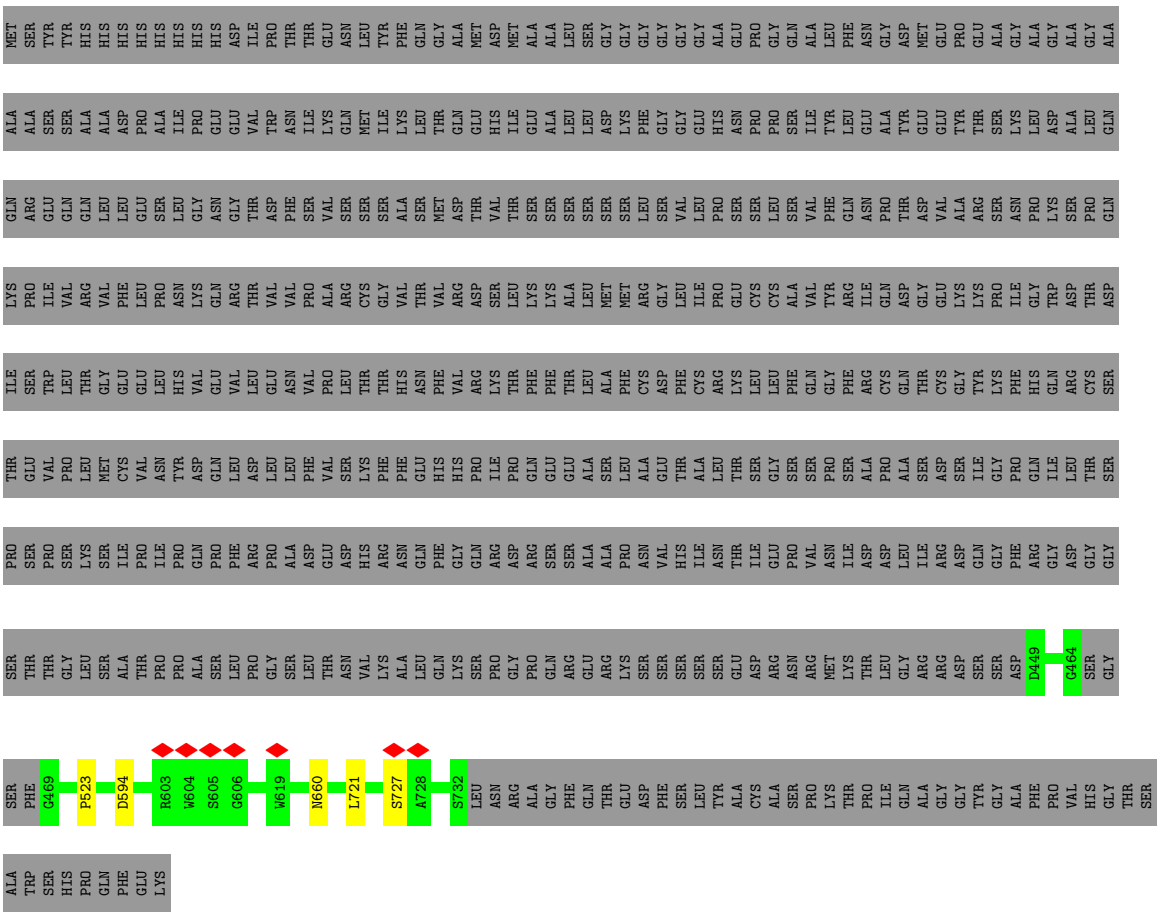
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
6	C	1	31	10	5	12	3	1	0

3 Residue-property plots (i)

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

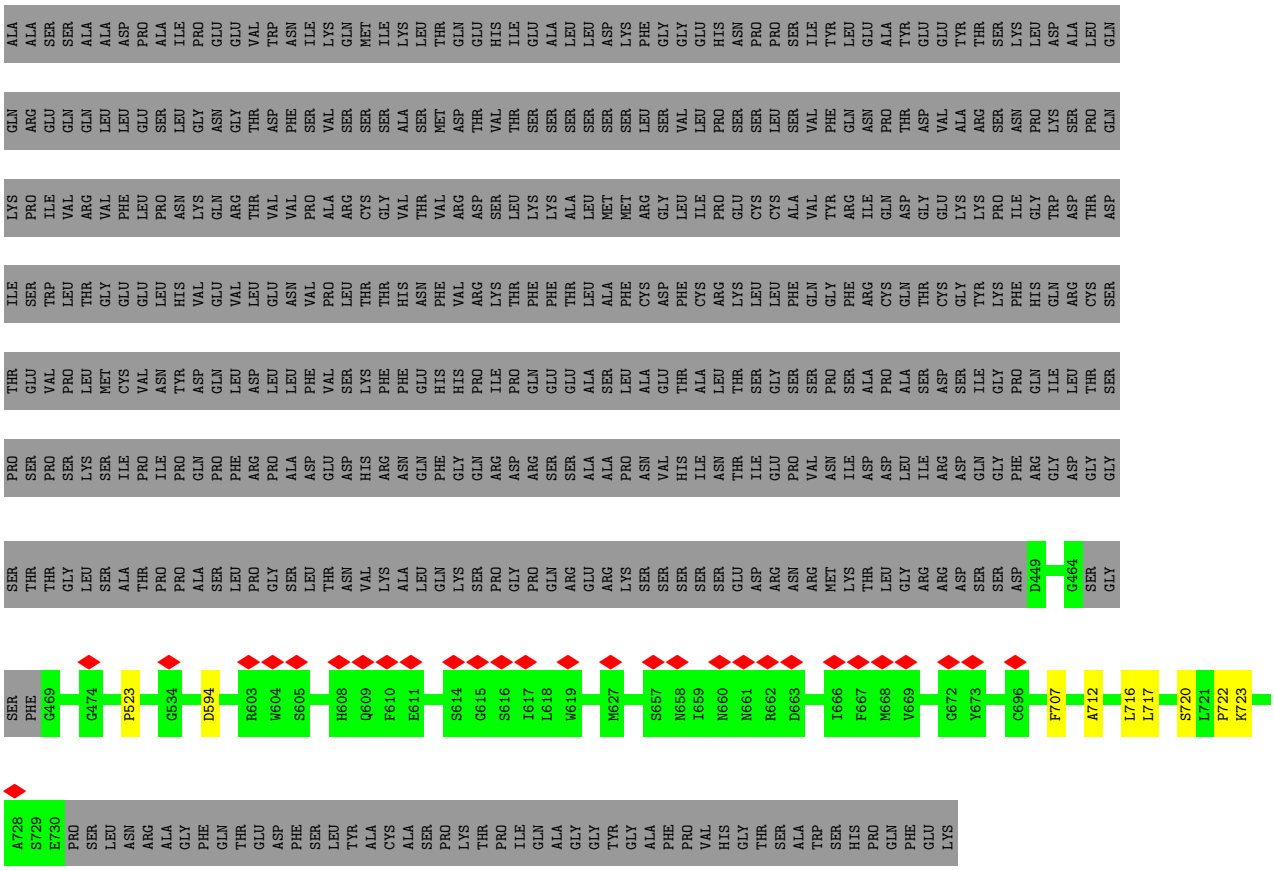
- Molecule 1: Serine/threonine-protein kinase B-raf

Chain A:



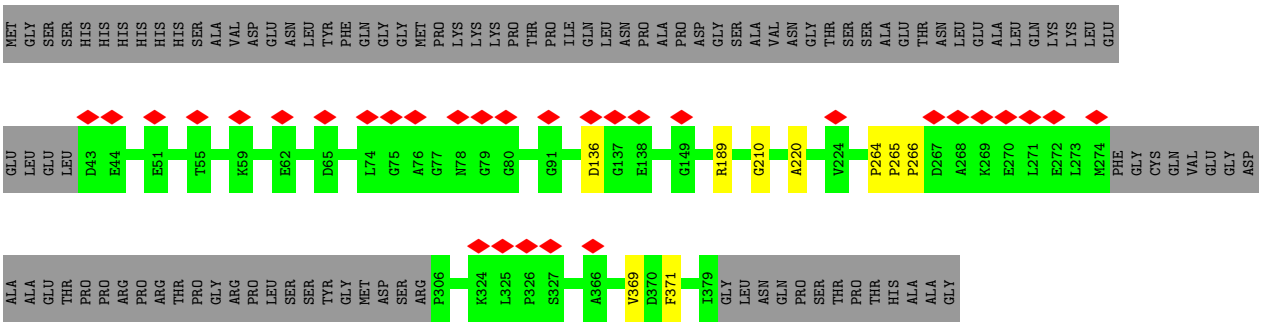
- Molecule 1: Serine/threonine-protein kinase B-raf

Chain B:



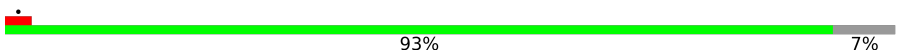
• Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1

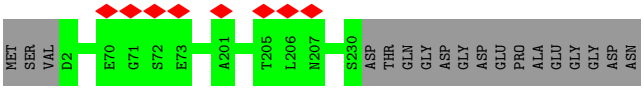
Chain C:



• Molecule 3: 14-3-3 protein zeta

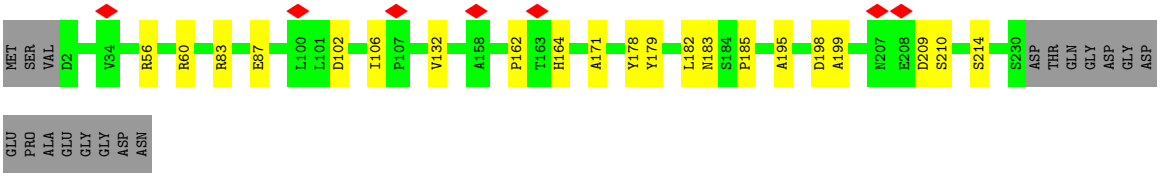
Chain X:





• Molecule 3: 14-3-3 protein zeta

Chain Y:


MET
SER
VAL
D2
V34
R56
R60
R83
E87
L100
L101
D102
I106
P107
V132
A158
P162
T163
H164
A171
Y178
Y179
L182
N183
S184
P185
A195
D198
A199
N207
E208
D209
S210
S214
S230
ASP
THR
GLN
GLY
ASP
GLY
ASP
GLU
PRO
ALA
GLU
GLY
GLY
ASP
ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	595672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	284.16, 284.16, 284.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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, LCJ, AGS, SEP

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	0.48	0/1379	0.64	0/1915
1	B	0.48	0/1369	0.64	0/1901
2	C	0.43	0/1515	0.60	0/2104
3	X	0.39	0/1137	0.49	0/1586
3	Y	0.63	0/1137	0.68	0/1586
All	All	0.48	0/6537	0.61	0/9092

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	1389	0	611	4	0
1	B	1379	0	609	2	0
2	C	1514	0	674	6	0
3	X	1138	0	522	0	0
3	Y	1138	0	522	14	0
4	C	1	0	0	0	0
5	C	25	0	0	1	0
6	C	31	0	12	0	0
All	All	6615	0	2950	22	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 2.

All (22) 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:Y:162:PRO:O	3:Y:199:ALA:HA	1.54	1.06
3:Y:83:ARG:O	3:Y:87:GLU:CB	2.17	0.93
3:Y:164:HIS:HA	3:Y:209:ASP:CB	2.00	0.91
3:Y:178:TYR:O	3:Y:182:LEU:CB	2.20	0.90
3:Y:162:PRO:O	3:Y:199:ALA:CA	2.35	0.75
3:Y:56:ARG:O	3:Y:60:ARG:CB	2.38	0.72
1:A:660:ASN:HA	2:C:220:ALA:HB1	1.74	0.69
1:B:717:LEU:O	1:B:720:SER:O	2.11	0.68
3:Y:162:PRO:CB	3:Y:198:ASP:O	2.43	0.67
3:Y:178:TYR:HA	3:Y:182:LEU:CB	2.25	0.65
2:C:210:GLY:HA2	5:C:402:LCJ:C16	2.30	0.62
3:Y:210:SER:CB	3:Y:214:SER:CB	2.81	0.58
1:A:660:ASN:CB	2:C:220:ALA:HB2	2.36	0.55
3:Y:179:TYR:O	3:Y:183:ASN:HA	2.07	0.54
3:Y:171:ALA:HB1	3:Y:195:ALA:HB2	1.91	0.53
1:B:712:ALA:O	1:B:716:LEU:CB	2.58	0.52
1:A:660:ASN:HA	2:C:220:ALA:CB	2.39	0.51
2:C:369:VAL:O	2:C:371:PHE:N	2.51	0.43
1:A:660:ASN:CA	2:C:220:ALA:CB	2.97	0.43
3:Y:178:TYR:CA	3:Y:182:LEU:CB	2.95	0.42
3:Y:178:TYR:C	3:Y:182:LEU:CB	2.87	0.41
3:Y:102:ASP:HA	3:Y:106:ILE:CB	2.50	0.41

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	276/805 (34%)	260 (94%)	12 (4%)	4 (1%)	11	46
1	B	274/805 (34%)	254 (93%)	15 (6%)	5 (2%)	8	40
2	C	304/414 (73%)	282 (93%)	17 (6%)	5 (2%)	9	43
3	X	227/247 (92%)	222 (98%)	5 (2%)	0	100	100
3	Y	227/247 (92%)	215 (95%)	10 (4%)	2 (1%)	17	56
All	All	1308/2518 (52%)	1233 (94%)	59 (4%)	16 (1%)	17	49

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	721	LEU
1	B	707	PHE
1	B	722	PRO
2	C	264	PRO
2	C	265	PRO
2	C	266	PRO
2	C	136	ASP
1	A	594	ASP
1	A	727	SER
1	B	594	ASP
2	C	189	ARG
1	B	723	LYS
1	A	523	PRO
1	B	523	PRO
3	Y	132	VAL
3	Y	185	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	SEP	A	729	1	8,9,10	0.65	0	8,12,14	0.59	0
1	SEP	B	729	1	8,9,10	0.65	0	8,12,14	0.60	0

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
1	SEP	A	729	1	-	0/5/8/10	-
1	SEP	B	729	1	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	729	SEP	N-CA-CB-OG
1	B	729	SEP	CB-OG-P-O1P
1	B	729	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	AGS	C	403	4	26,33,33	5.15	12 (46%)	26,52,52	1.82	6 (23%)
5	LCJ	C	402	4	23,27,27	2.37	5 (21%)	23,37,37	1.68	6 (26%)

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
6	AGS	C	403	4	-	0/17/38/38	0/3/3/3
5	LCJ	C	402	4	-	5/13/13/13	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	AGS	C2'-C1'	-18.26	1.26	1.53
6	C	403	AGS	O4'-C1'	11.66	1.57	1.41
6	C	403	AGS	C3'-C4'	-9.69	1.28	1.53
5	C	402	LCJ	C18-N09	8.55	1.45	1.34
5	C	402	LCJ	C10-N07	5.28	1.46	1.36
6	C	403	AGS	C2'-C3'	4.89	1.66	1.53
6	C	403	AGS	O4'-C4'	4.53	1.55	1.45
6	C	403	AGS	PG-O2G	3.79	1.67	1.54
6	C	403	AGS	PG-O3G	3.37	1.65	1.54
6	C	403	AGS	C6-N6	3.13	1.45	1.34
6	C	403	AGS	C2-N3	2.98	1.36	1.32
6	C	403	AGS	O2'-C2'	2.96	1.49	1.43
5	C	402	LCJ	C12-C10	-2.77	1.39	1.43
6	C	403	AGS	C5'-C4'	2.70	1.60	1.51
6	C	403	AGS	C5-C4	-2.65	1.33	1.40
5	C	402	LCJ	C17-N07	2.35	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	LCJ	O04-C18	-2.11	1.19	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	403	AGS	N3-C2-N1	-5.53	120.03	128.68
5	C	402	LCJ	N08-C15-N06	-4.33	107.96	112.73
6	C	403	AGS	C1'-N9-C4	3.23	132.31	126.64
5	C	402	LCJ	C21-C19-C17	-3.11	120.54	123.50
6	C	403	AGS	C5-C6-N6	2.97	124.87	120.35
6	C	403	AGS	PA-O3A-PB	-2.95	122.69	132.83
5	C	402	LCJ	C14-C13-C11	-2.92	119.36	121.79
6	C	403	AGS	C3'-C2'-C1'	2.71	105.06	100.98
5	C	402	LCJ	O03-N09-C18	2.25	121.33	118.57
5	C	402	LCJ	C12-C18-N09	2.23	119.18	114.91
5	C	402	LCJ	C20-C17-C19	2.21	119.40	117.17
6	C	403	AGS	C2'-C3'-C4'	2.07	106.67	102.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	LCJ	C12-C10-N07-C17
5	C	402	LCJ	N06-C10-N07-C17
5	C	402	LCJ	C25-C24-O03-N09
5	C	402	LCJ	O03-C24-C25-O05
5	C	402	LCJ	C14-C12-C18-N09

There are no ring outliers.

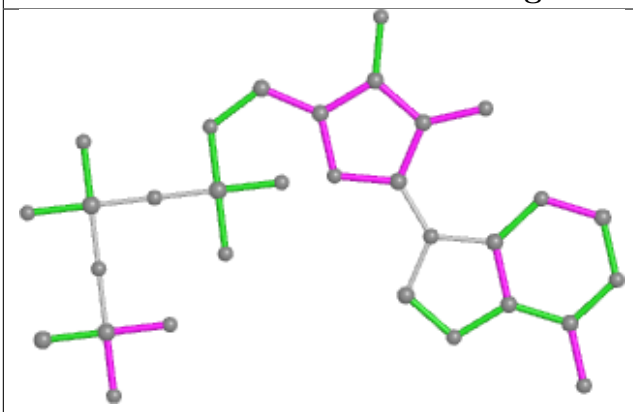
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	402	LCJ	1	0

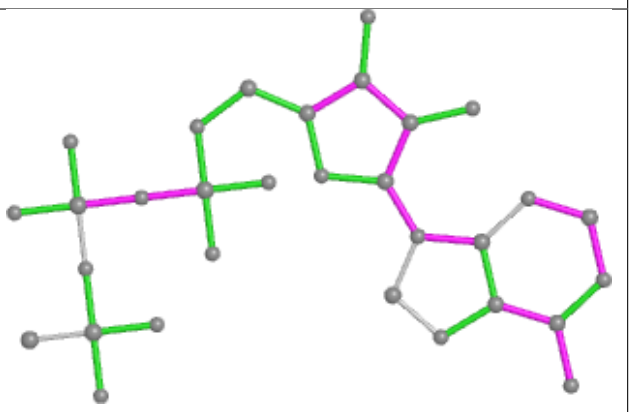
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

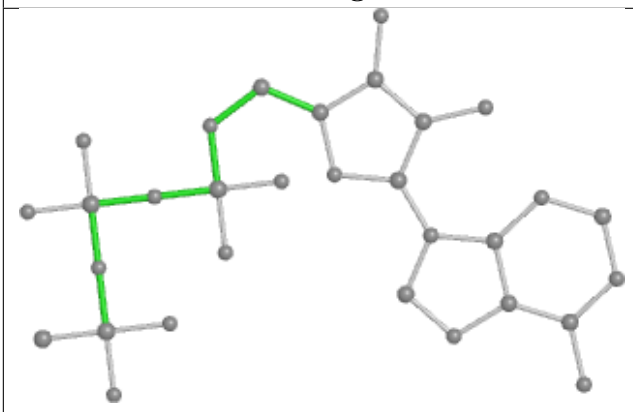
Ligand AGS C 403



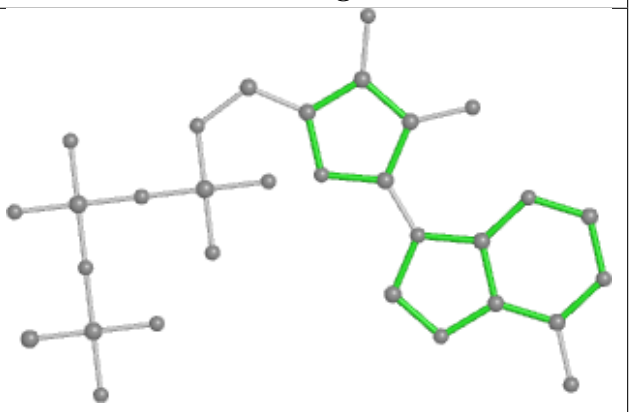
Bond lengths



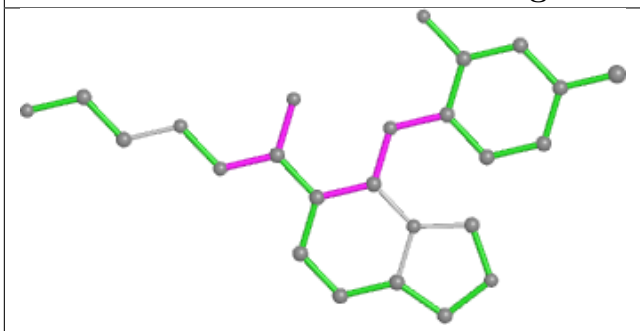
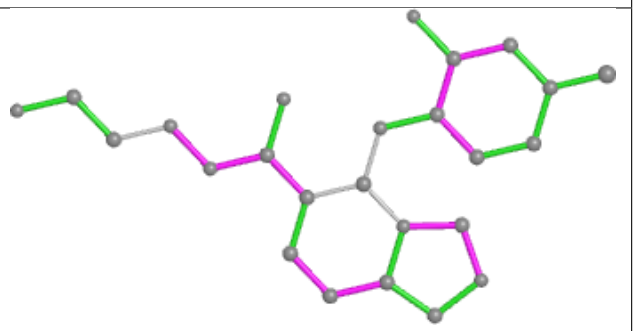
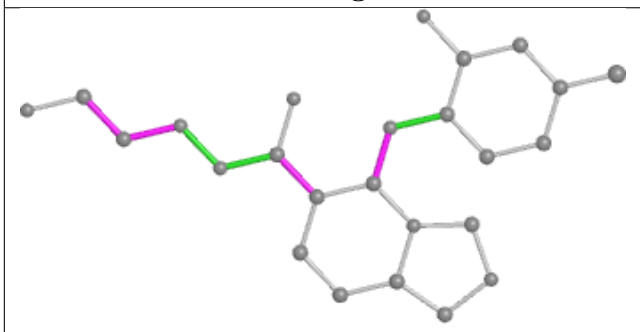
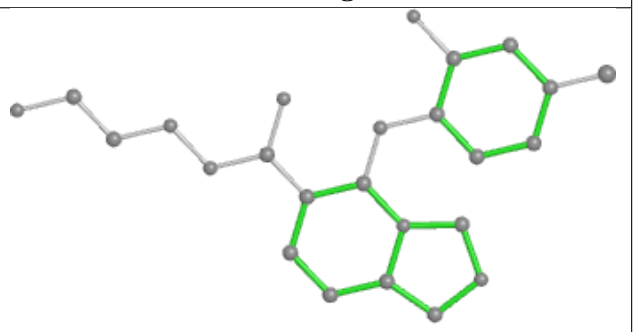
Bond angles



Torsions



Rings

Ligand LCJ C 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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)

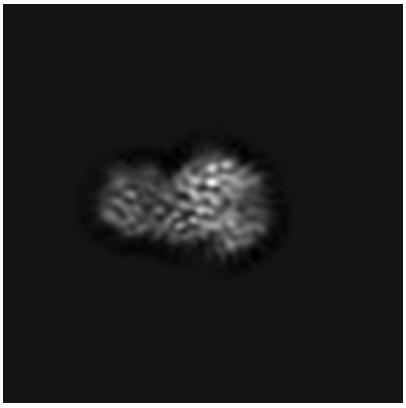
This section contains visualisations of the EMDB entry EMD-20552. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

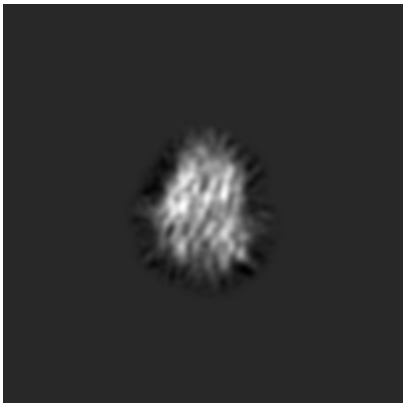
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y



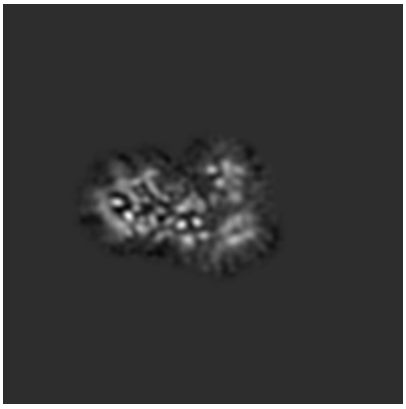
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128

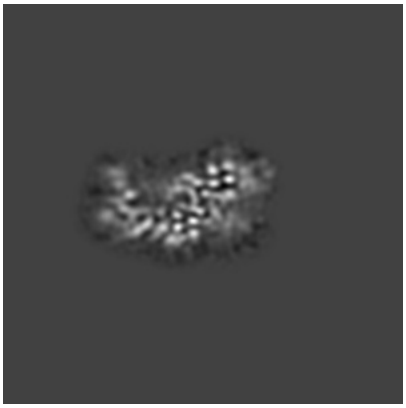
Z Index: 128

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

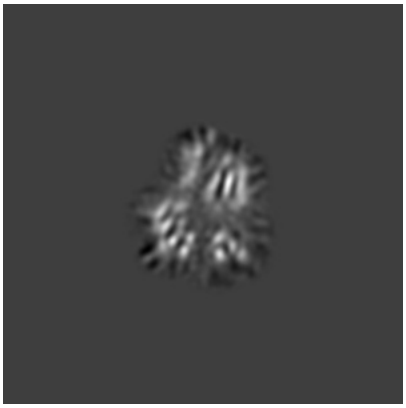
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 141



Y Index: 139

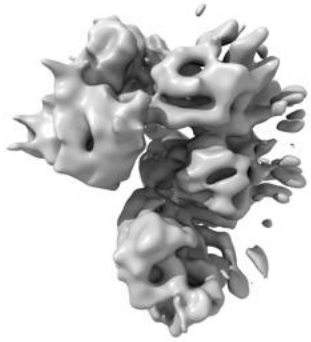


Z Index: 144

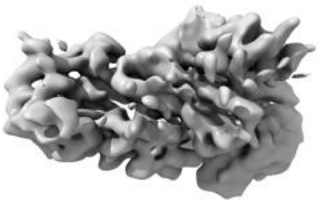
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

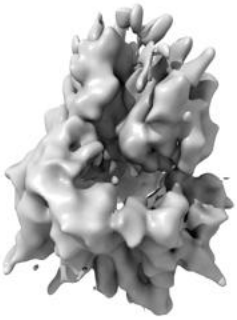
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

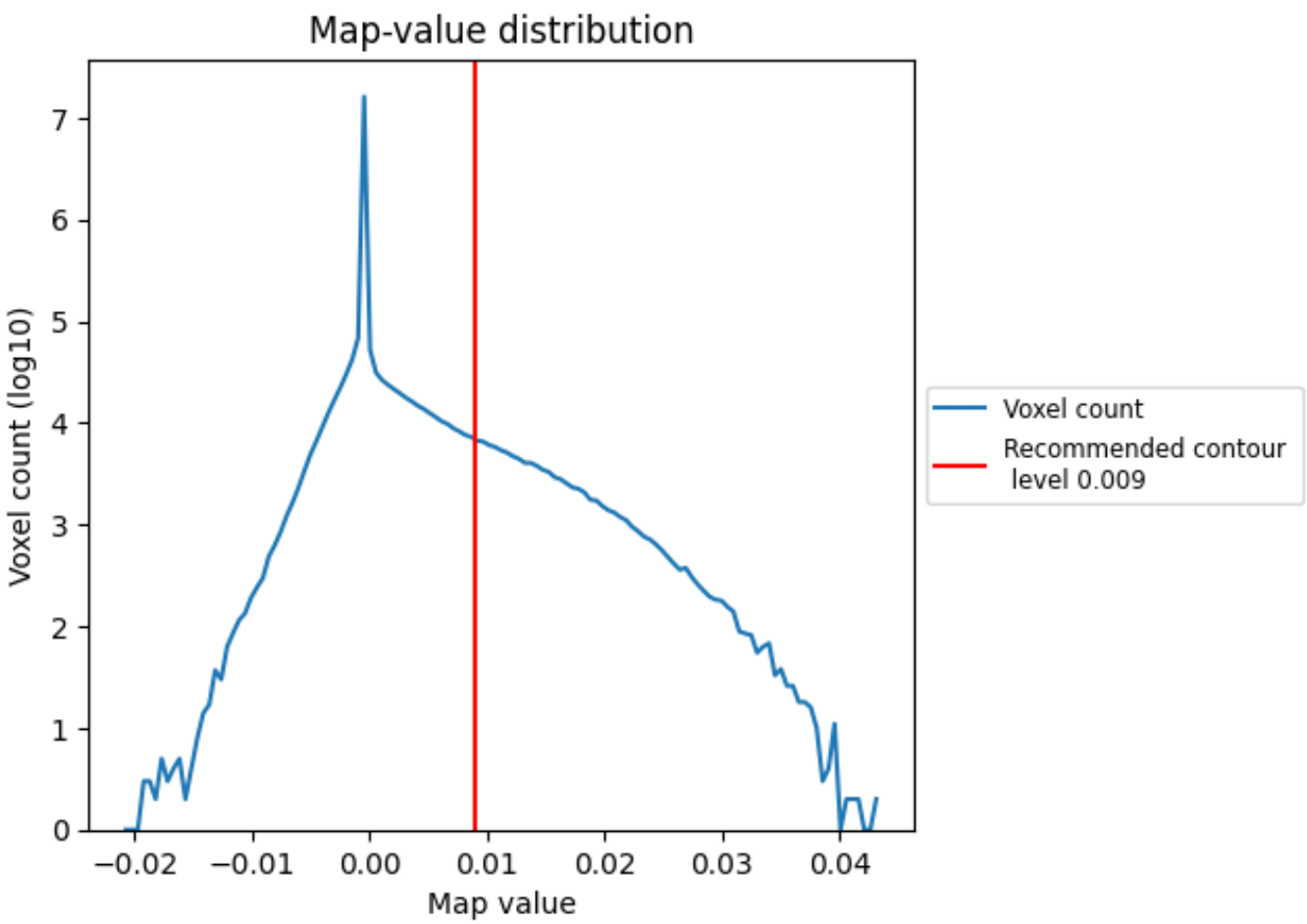
6.5 Mask visualisation (i)

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

7 Map analysis (i)

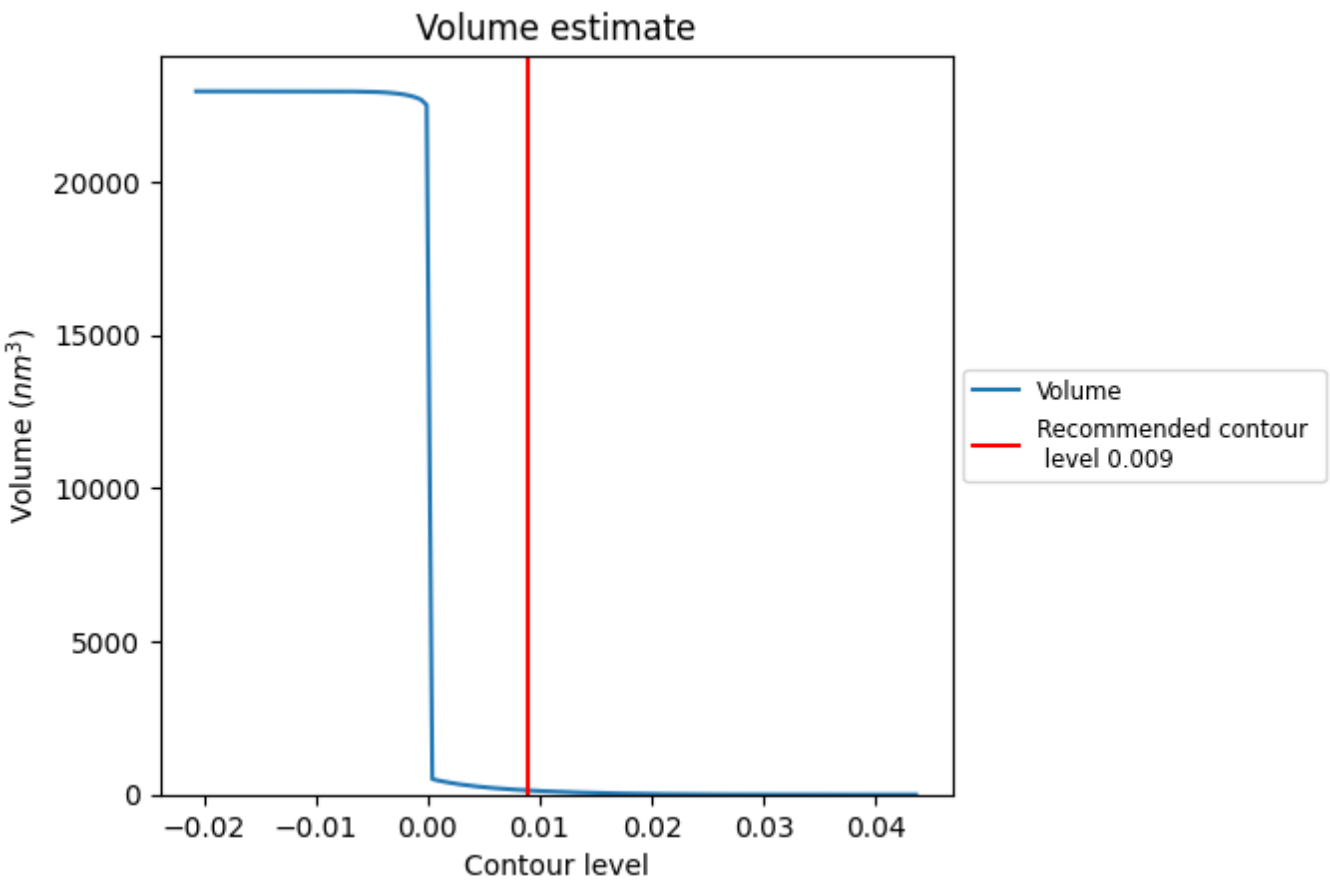
This section contains the results of statistical analysis of the map.

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.

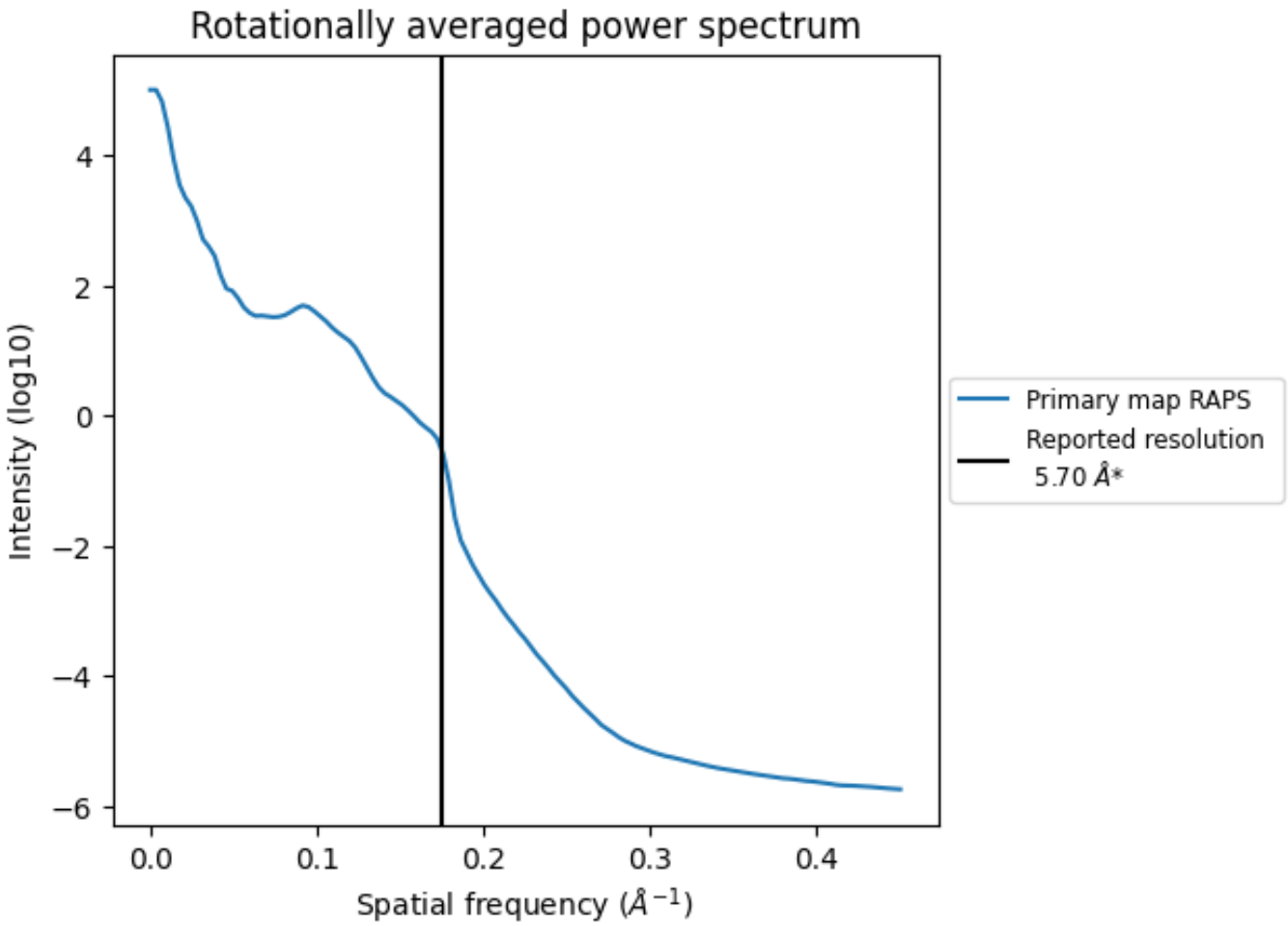
7.2 Volume estimate (i)



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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 0.175 Å^{-1}

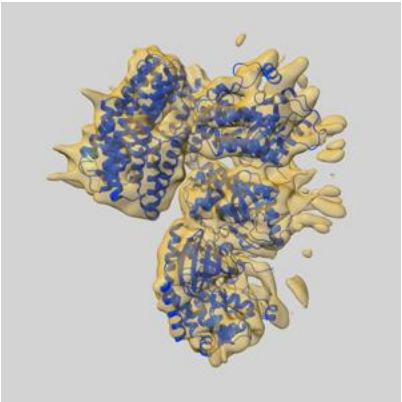
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

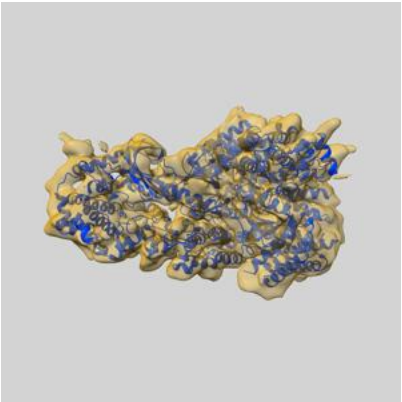
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20552 and PDB model 6Q0T. Per-residue inclusion information can be found in section 3 on page 8.

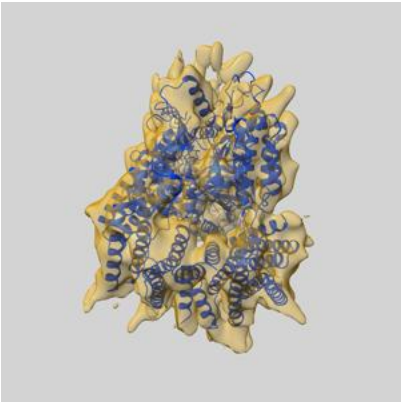
9.1 Map-model overlay (i)



X



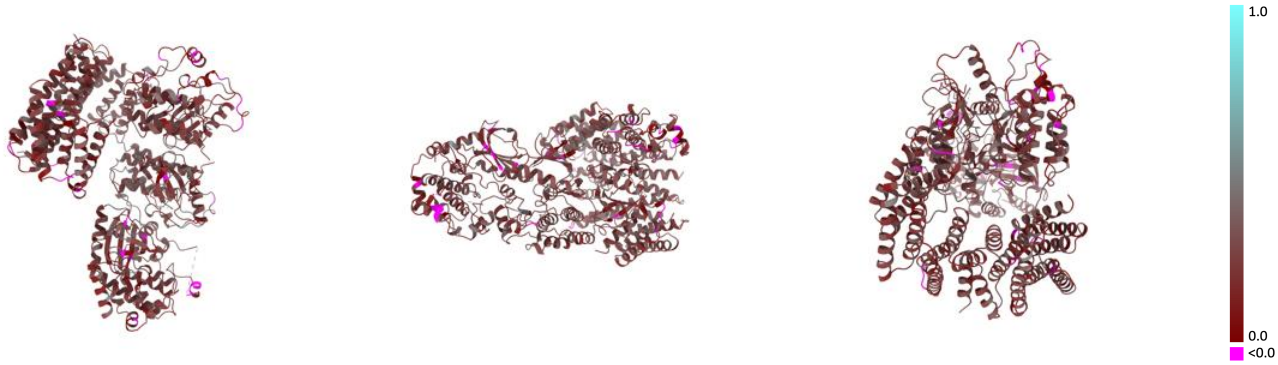
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

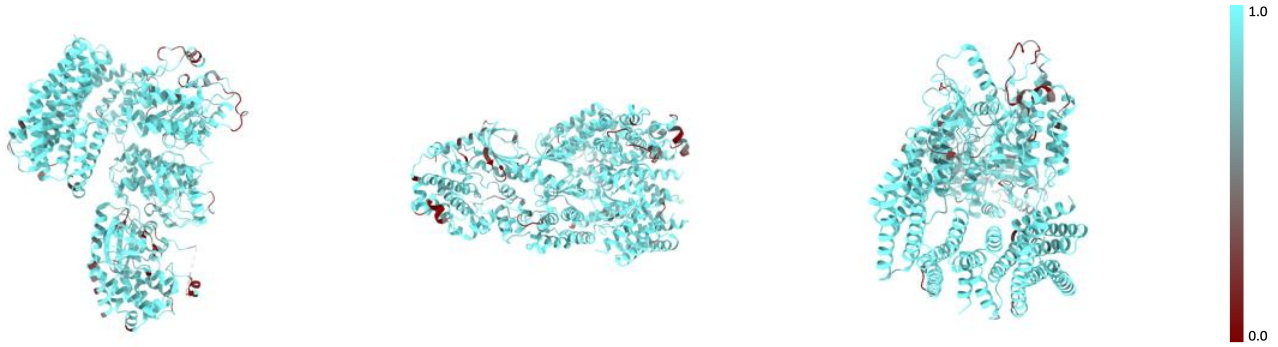
9.2 Q-score mapped to coordinate model (i)



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.

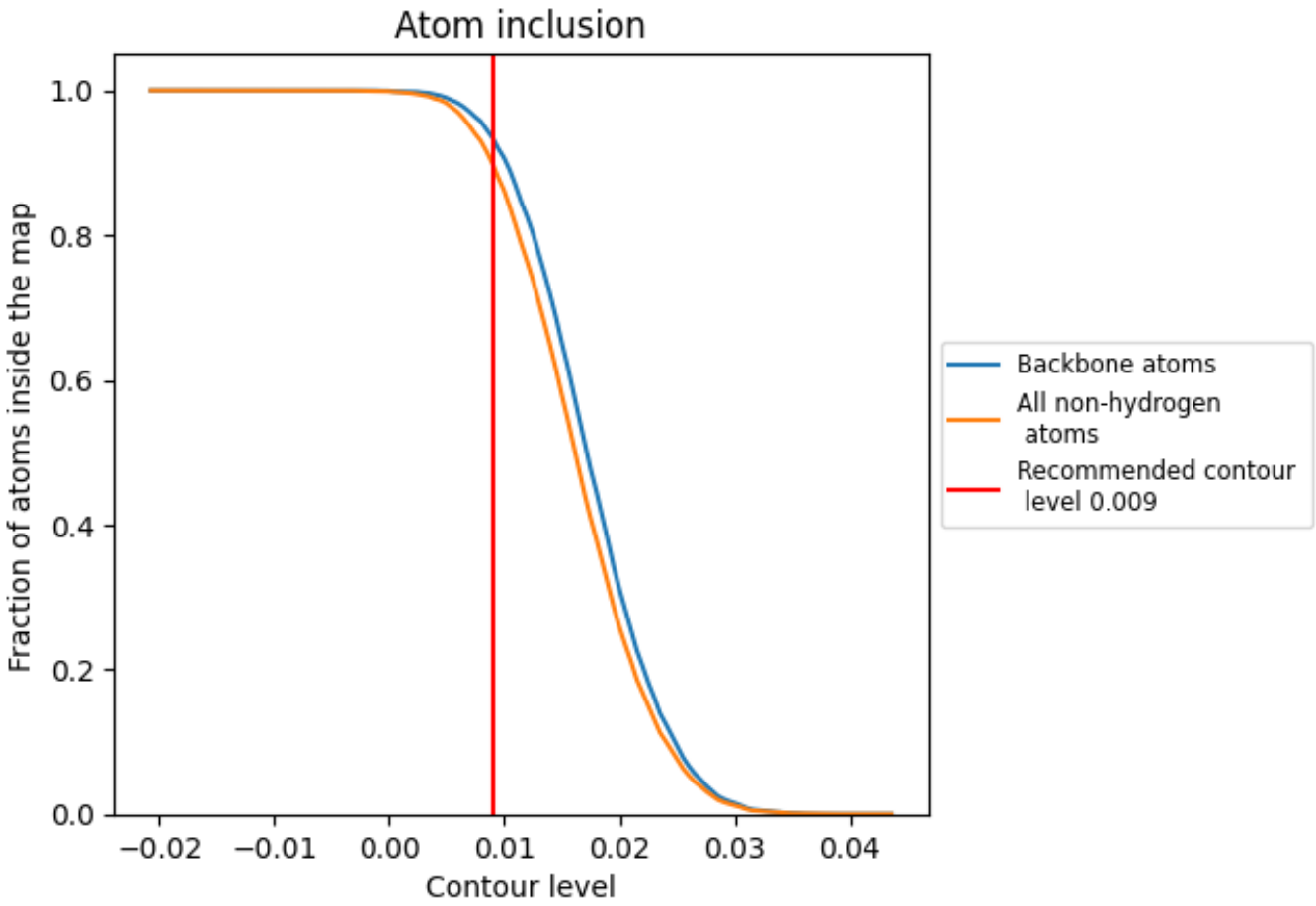
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8976	0.2460
A	0.9214	0.2850
B	0.8511	0.2400
C	0.8434	0.2400
X	0.9490	0.2330
Y	0.9482	0.2280