



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 7LVV / pdb_00007lvv
EMDB ID : EMD-23543
Title : cryoEM structure DrdV-DNA complex
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2021-02-26
Resolution : 3.25 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

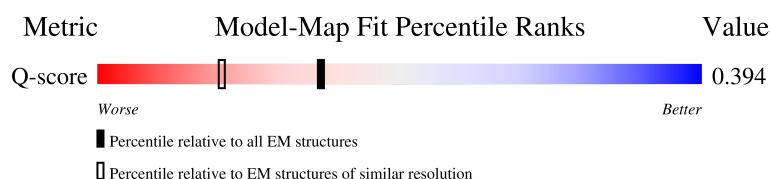
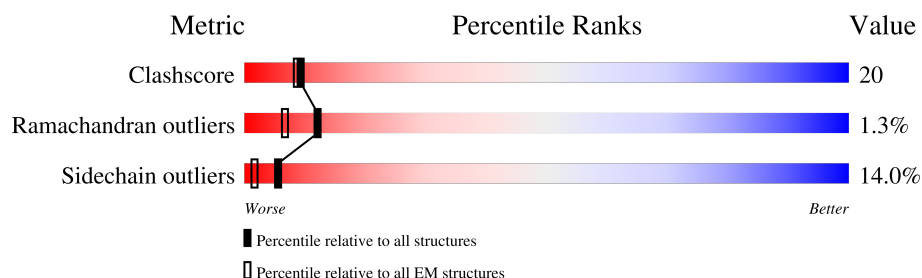
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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	1029	
1	B	1029	
1	C	1029	
1	D	1029	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	29	 66% 31% •
2	G	29	 69% 28% •
3	F	29	 83% 10% 7%
3	H	29	 76% 14% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21020 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 Site-specific DNA-methyltransferase (adenine-specific).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0
			8216	5222	1439	1536	19		
1	B	1012	Total	C	N	O	S	0	0
			8219	5223	1440	1537	19		
1	C	143	Total	C	N	O	S	0	0
			1126	704	197	223	2		
1	D	146	Total	C	N	O	S	0	0
			1149	719	201	227	2		

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	28	Total	C	N	O	P	0	0
			561	265	107	161	28		
2	G	28	Total	C	N	O	P	0	0
			561	265	107	161	28		

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	27	Total	C	N	O	P	0	0
			565	266	103	169	27		
3	H	27	Total	C	N	O	P	0	0
			565	266	103	169	27		

- Molecule 4 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			27	15	6	5	1	
4	B	1	Total	C	N	O	S	0
			27	15	6	5	1	

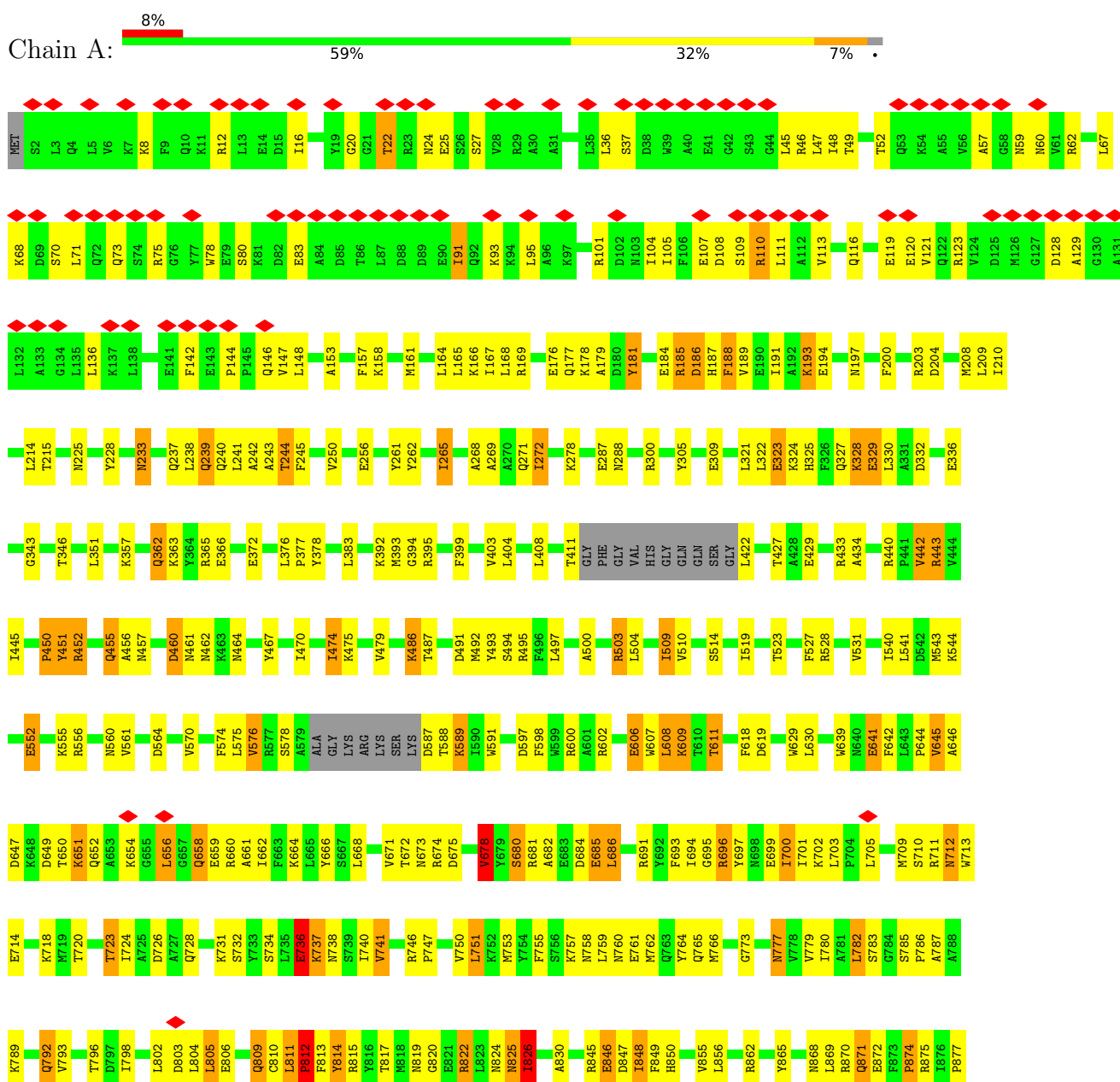
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

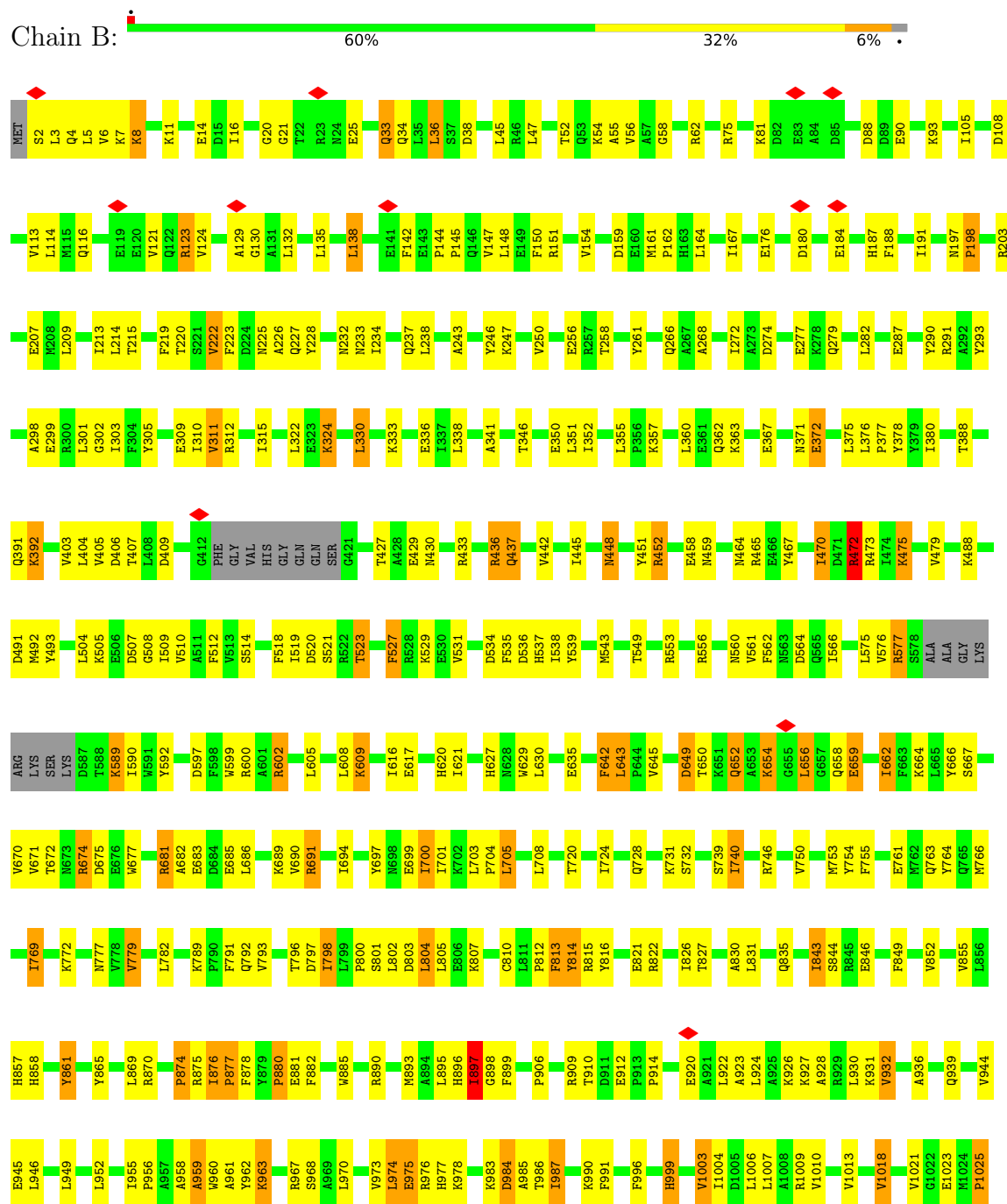
3 Residue-property plots

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: Site-specific DNA-methyltransferase (adenine-specific)



- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)





● Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)



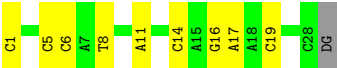
MET	S2	L3	Q4	L5	V6	L13	E14	E25	S26	S27	V28	R29	A30	A31	F32	L36	S37	D38	L45	R46	L47	T48	T49	E50	V51	N60	T66	L67	K68	D69	S70	L71	R75	D82	E83	L87	Q92	R93	K94	L95	A96	K97	R101	D102	I105	D108							
S109	R110	L111	A112	V113	L114	M115	Q116	G117	E118	E119	E120	V121	Q122	R123	V124	D125	M126	G127	D128	L132	A133	G134	L135	L136	A137	L138	E143	F144	PRO	GLN	VAL	LEU	GLU	PHE	ARG	LYS	ALA	VAL	THR	ASP	HIS	PHE	LYS	ASP	GLU	MET	PRO	HIS	LEU	ASN	ALA	ASP	ASP
ALA	ALA	GLU	GLN	LYS	ALA	ASP	TYR	ARG	GLY	GLY	ARG	TYR	HIS	PHE	VAL	GLU	ILE	ALA	LYS	ILE	ALA	ASN	PRO	ASP	PHE	SER	PRO	ARG	ALA	MET	ALA	LEU	ILE	GLN	ALA	GLY	HIS	ASP	GLY	THR	LYS	PHE	LEU	THR	GLY	ASP	GLU	ASN	ALA	ASP	ASN		
ILE	ALA	GLN	GLN	GLN	GLN	GLN	LEU	ALA	ALA	THR	PHE	TYR	LYS	GLY	PRO	VAL	LYS	ASP	ILE	ALA	ARG	THR	LYS	ARG	TYR	LEU	GLY	ALA	ILE	GLN	ALA	ALA	ALA	GLY	HIS	GLY	THR	LYS	ALA	ASP	THR	GLY	LEU	THR	GLY	VAL	THR	GLU	ASN	ASP	TYR		
ASN	PRO	ALA	GLY	ALA	GLY	ARG	LEU	ILE	PHE	TYR	THR	PRO	GLY	PHE	ILE	ASN	VAL	ARG	GLY	ILE	GLU	THR	ASP	THR	LEU	ASN	LYS	HIS	PHE	GLN	GLN	LEU	VAL	GLY	GLY	THR	ILE	GLY	THR	GLY	THR	GLY	THR	THR	GLY	VAL	THR	GLY	ASP	ASN			
PHE	LEU	PRO	LYS	ALA	LYS	LEU	GLY	GLN	TYR	ARG	GLY	LEU	HIS	CYS	ASN	ASN	GLY	LEU	LEU	PRO	TYR	ILE	THR	ALA	ASN	LEU	ASN	ASN	ILE	GLY	ALA	MET	GLY	ARG	TYR	GLY	THR	ILE	VAL	LEU	THR	GLY	VAL	THR	GLY	VAL	THR	GLY	PHE				
GLY	VAL	HIS	GLY	GLN	GLN	SER	GLY	PHE	SER	GLY	THR	VAL	ALA	GLY	ASN	LEU	ARG	ARG	LYS	GLN	GLN	ASN	ALA	ARG	PRO	VAL	VAL	ILE	GLY	GLY	ASN	ASN	GLN	ALA	ASN	GLY	THR	ALA	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	ARG		
ILE	LYS	ALA	THR	VAL	VAL	ALA	ALA	SER	THR	ALA	GLN	LYS	LEU	TYR	ASP	MET	TYR	SER	PHE	LEU	LEU	TRP	ALA	THR	ASP	ASP	LEU	LYS	GLY	ASP	PHE	VAL	VAL	ASN	SER	SER	PHE	THR	ARG	THR	PHE	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS		
ASP	PHE	HIS	ILE	TYR	VAL	ILE	ASP	LYS	GLY	LYS	GLY	ALA	ASN	THR	GLY	GLY	ARG	ARG	LYS	GLY	GLY	GLY	TRP	ARG	ASP	ASP	GLN	ILE	VAL	LYS	VAL	PHE	TYR	VAL	VAL	ARG	SER	ASP	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	HIS			
ALA	VAL	PRO	ASP	PHE	TRP	ARG	ALA	ALA	LEU	LEU	TRP	LYS	THR	THR	THR	THR	GLY	GLU	ILE	GLY	PHE	ASP	ASP	ILE	PRO	PRO	ASP	ALA	ALA	GLY	HIS	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
LYS	GLY	LEU	GLY	GLN	GLY	ARG	ALA	ALA	LYS	TYR	SER	GLY	GLY	VAL	VAL	VAL	ASN	ASP	GLY	VAL	VAL	VAL	SER	ALA	ALA	GLY	ASP	GLY	GLY	VAL	VAL	VAL	VAL	GLY	ARG	TYR	ASN	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TRP			
GLU	GLY	ASP	ILE	MET	THR	ARG	ALA	ALA	ASP	ALA	ALA	GLN	ARG	ARG	ARG	LYS	SER	TYR	SER	GLY	ASN	GLY	VAL	VAL	LEU	TYR	ARG	PRO	PHE	TYR	ILE	PRO	PHE	PHE	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
VAL	GLY	GLY	ASN	VAL	VAL	ILE	LEU	SER	GLY	GLY	PRO	ALA	LYS	PRO	PHE	GLN	VAL	ALA	ASP	THR	ILE	ILE	PRO	LEU	LEU	LEU	LEU	LEU	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA		
PHE	GLN	HIS	THR	THR	THR	ILE	SER	SER	SER	ARG	GLY	ASP	PHE	HIS	THR	VAL	TYR	VAL	VAL	HIS	HIS	PRO	PRO	ALA	ALA	GLY	LYS	TYR	ALA	PRO	PHE	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	MET		
ALA	LEU	HIS	ILE	PHE	GLY	SER	VAL	ALA	PRO	LEU	PRO	ARG	THR	THR	ASP	GLY	GLY	LEU	ASP	THR	THR	THR	THR	ALA	LEU	LEU	LEU	VAL	GLN	ARG	VAL	VAL	VAL	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		
GLY	ILE	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ASN	ARG	SER	ALA	LEU	GLY	TRP	VAL	VAL	VAL	GLY	HIS	GLY	GLY	THR	THR	PRO	ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL		

Chain D: 9% 9% 9% 86%



GLU	TRP	VAL	LEU	GLU	ARG	HIS	LYS	GLU	THR	THR	PRO	LYS	ASP	ALA	THR	ILE	ARG	GLU	LYS	PHE	ASN	THR	TYR	ARG	PHE	ALA	ASP	HIS	LYS	GLU	ARG	VAL	ILE	ASP	LEU	LEU	ALA	ARG	VAL	THR	THR	VAL	SER	VAL	GLU	THR	THR	VAL	ARG	ILE	VAL	GLY	GLU	MET	PRO	ALA	GLU	THR	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

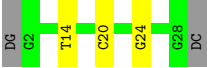
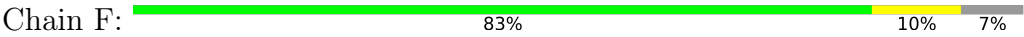
• Molecule 2: DNA (28-MER)



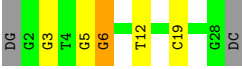
• Molecule 2: DNA (28-MER)



• Molecule 3: DNA (27-MER)



• Molecule 3: DNA (27-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	37000	Depositor
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	2.203	Depositor
Minimum map value	-0.745	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.375	Depositor
Map size ($\text{\AA}$)	464.0, 464.0, 464.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	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: CA, SAM

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	0.97	3/8396 (0.0%)	1.38	59/11348 (0.5%)
1	B	0.97	3/8399 (0.0%)	1.34	39/11351 (0.3%)
1	C	0.98	0/1141	1.36	1/1534 (0.1%)
1	D	0.93	0/1165	1.35	2/1568 (0.1%)
2	E	0.47	0/628	0.85	3/962 (0.3%)
2	G	0.46	0/628	0.81	2/962 (0.2%)
3	F	0.46	0/633	0.86	2/979 (0.2%)
3	H	0.43	0/633	0.82	3/979 (0.3%)
All	All	0.92	6/21623 (0.0%)	1.31	111/29683 (0.4%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	ASN	C-N	-6.07	1.25	1.33
1	B	844	SER	C-N	-5.76	1.26	1.33
1	A	741	VAL	C-N	5.50	1.40	1.33
1	A	702	LYS	C-N	5.33	1.41	1.33
1	B	144	PRO	C-O	-5.18	1.18	1.24

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	ILE	N-CA-C	-8.82	104.56	113.47
1	B	299	GLU	N-CA-C	-8.82	103.10	114.04
1	B	728	GLN	N-CA-C	-8.60	102.92	112.72
1	A	929	ARG	N-CA-C	-8.39	104.08	112.97
1	A	486	LYS	CA-C-N	-8.31	110.94	123.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8216	0	8108	361	0
1	B	8219	0	8109	391	0
1	C	1126	0	1115	47	0
1	D	1149	0	1139	40	0
2	E	561	0	310	10	0
2	G	561	0	310	18	0
3	F	565	0	306	3	0
3	H	565	0	306	3	0
4	A	27	0	22	2	0
4	B	27	0	22	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	1	0
All	All	21020	0	19747	828	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 20.

The worst 5 of 828 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ILE:CG2	1:B:576:VAL:HG22	1.32	1.58
1:B:543:MET:HE2	1:B:561:VAL:CG1	1.42	1.50
1:B:782:LEU:CD2	1:B:793:VAL:HG12	1.39	1.50
1:B:543:MET:CE	1:B:561:VAL:HG11	1.40	1.46
1:A:209:LEU:HD21	1:A:245:PHE:CZ	1.51	1.44

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1005/1029 (98%)	895 (89%)	98 (10%)	12 (1%)	10	36
1	B	1006/1029 (98%)	883 (88%)	112 (11%)	11 (1%)	11	38
1	C	141/1029 (14%)	124 (88%)	14 (10%)	3 (2%)	5	25
1	D	144/1029 (14%)	127 (88%)	13 (9%)	4 (3%)	4	20
All	All	2296/4116 (56%)	2029 (88%)	237 (10%)	30 (1%)	12	34

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	LYS
1	B	959	ALA
1	B	990	LYS
1	A	327	GLN
1	A	822	ARG

5.3.2 Protein sidechains ⓘ

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	860/872 (99%)	725 (84%)	135 (16%)	2	11
1	B	860/872 (99%)	748 (87%)	112 (13%)	4	17
1	C	119/872 (14%)	106 (89%)	13 (11%)	6	23
1	D	122/872 (14%)	108 (88%)	14 (12%)	5	21
All	All	1961/3488 (56%)	1687 (86%)	274 (14%)	5	15

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	897	ILE
1	B	974	LEU
1	D	46	ARG
1	A	753	MET
1	A	734	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	D	24	ASN
1	B	232	ASN
1	D	10	GLN
1	D	116	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are 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
4	SAM	A	1101	-	27,29,29	0.47	0	34,42,42	0.62	0
4	SAM	B	1101	-	27,29,29	0.48	0	34,42,42	0.54	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
4	SAM	A	1101	-	-	6/17/33/33	0/3/3/3
4	SAM	B	1101	-	-	7/17/33/33	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	N-CA-CB-CG
4	A	1101	SAM	C-CA-CB-CG
4	A	1101	SAM	CA-CB-CG-SD
4	A	1101	SAM	O4'-C4'-C5'-SD
4	A	1101	SAM	C3'-C4'-C5'-SD

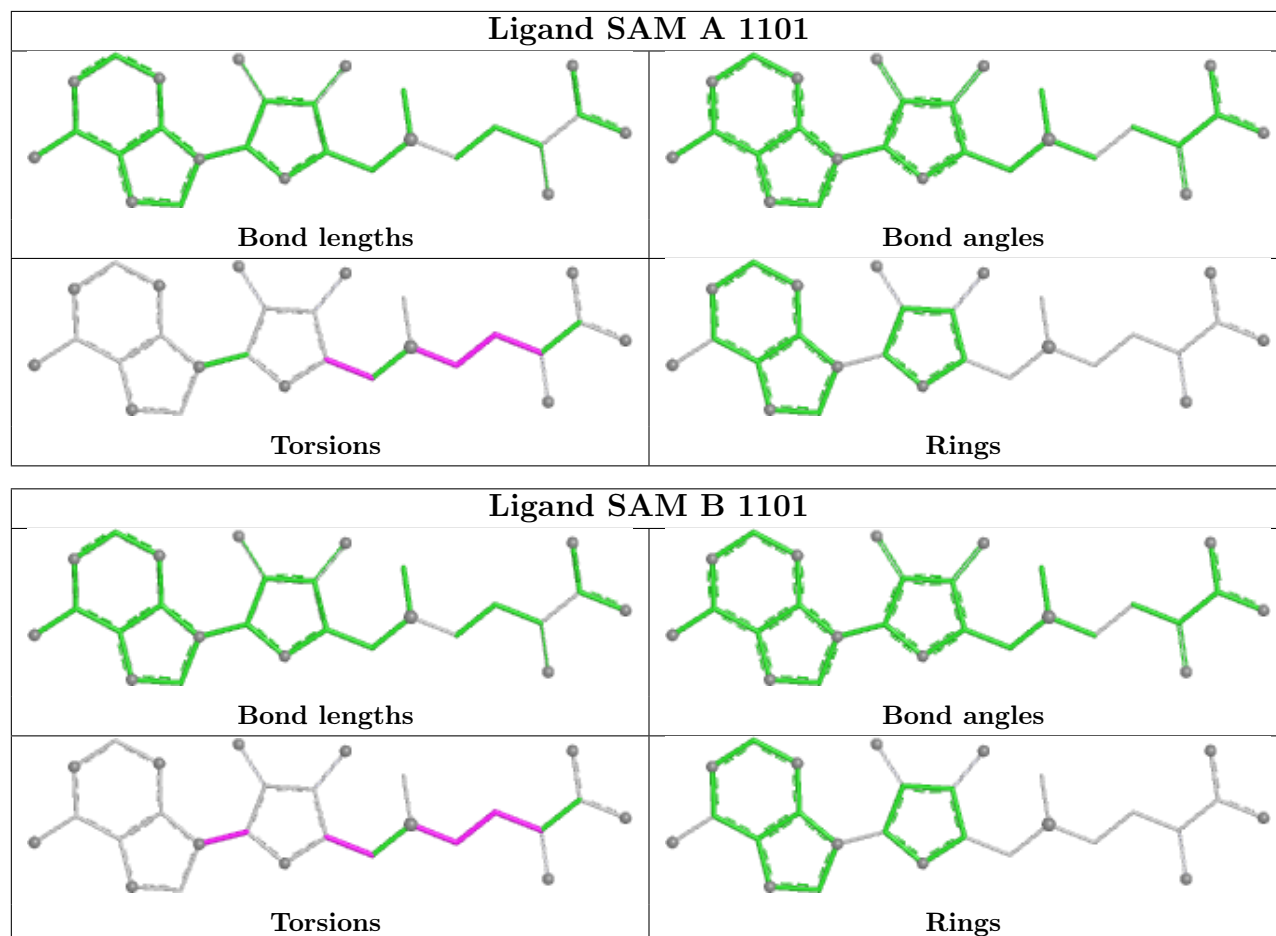
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	2	0
4	B	1101	SAM	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

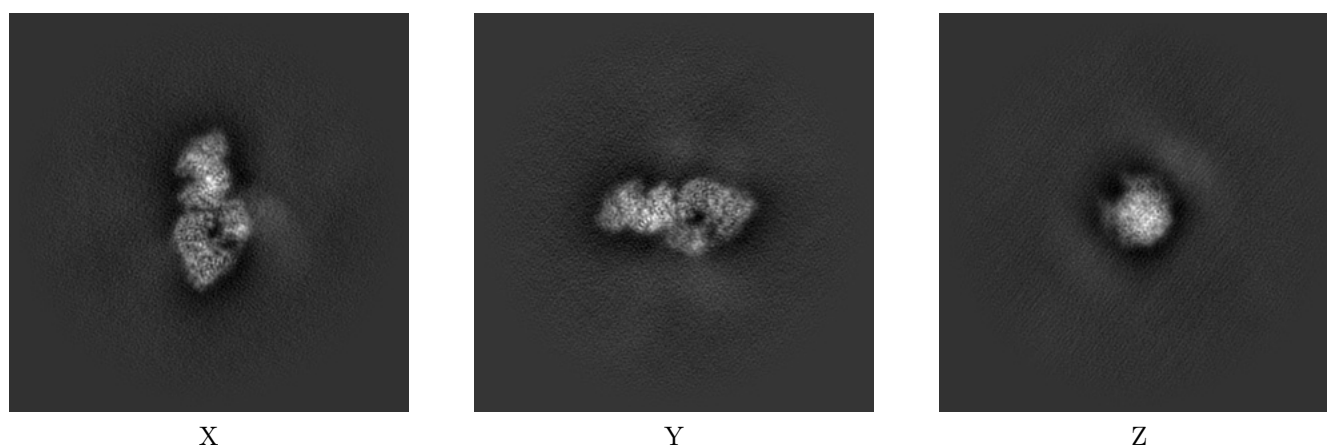
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23543. 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](#)

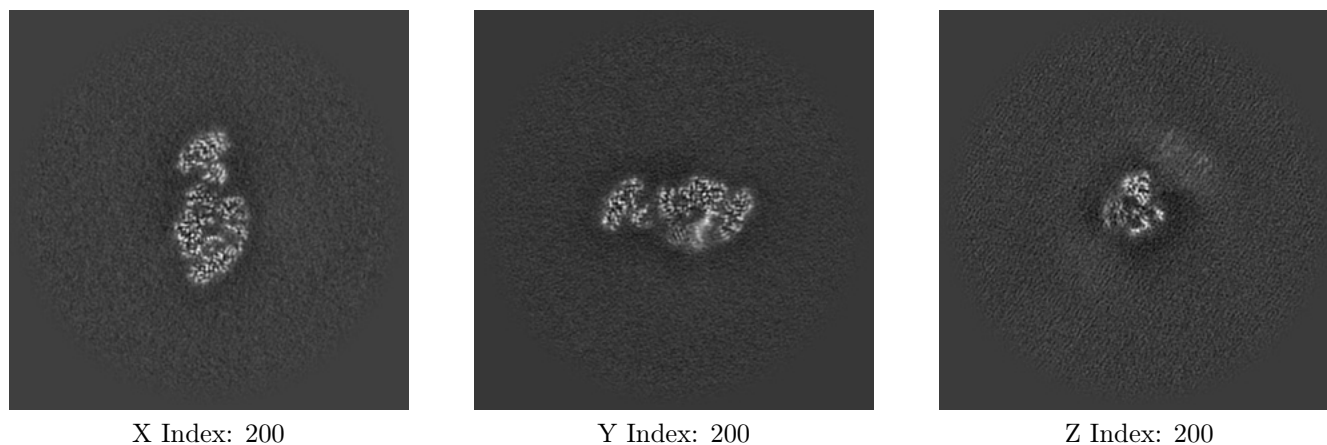
6.1.1 Primary map



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

6.2 Central slices [i](#)

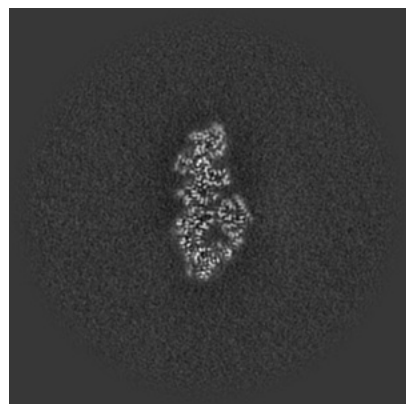
6.2.1 Primary map



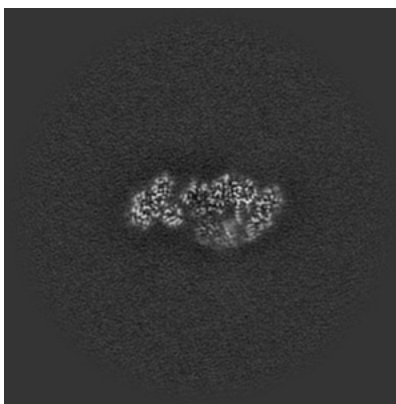
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

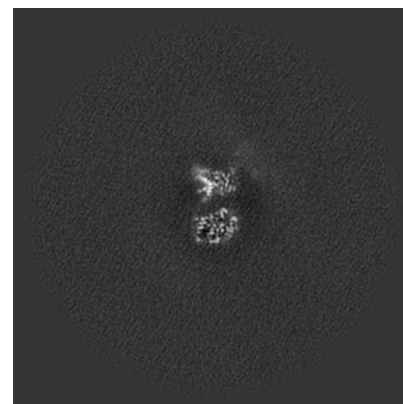
6.3.1 Primary map



X Index: 208



Y Index: 197

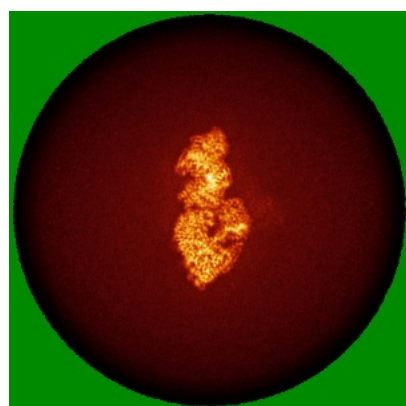


Z Index: 181

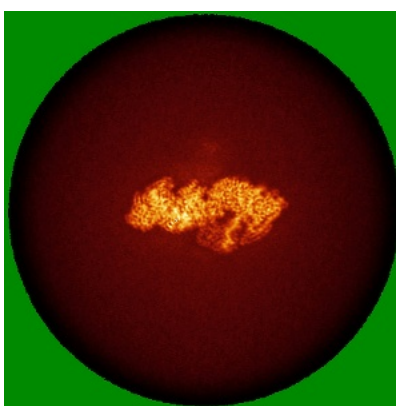
The images above show the largest variance slices of the map in three orthogonal directions.

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

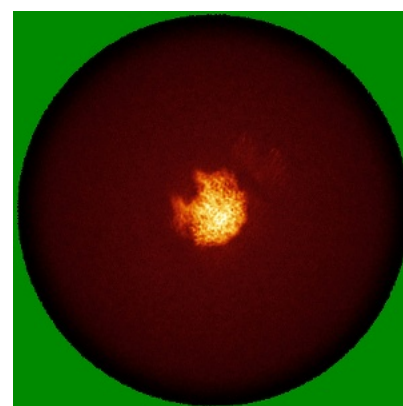
6.4.1 Primary map



X



Y

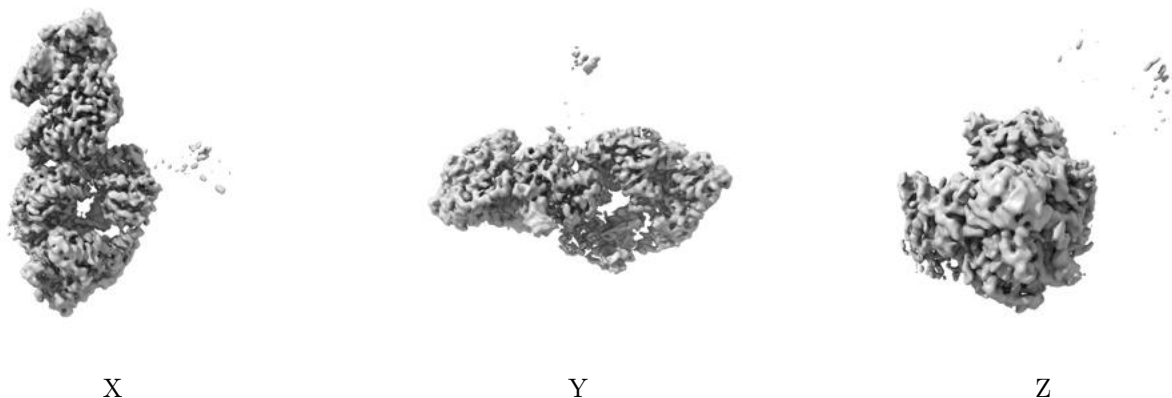


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.375. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

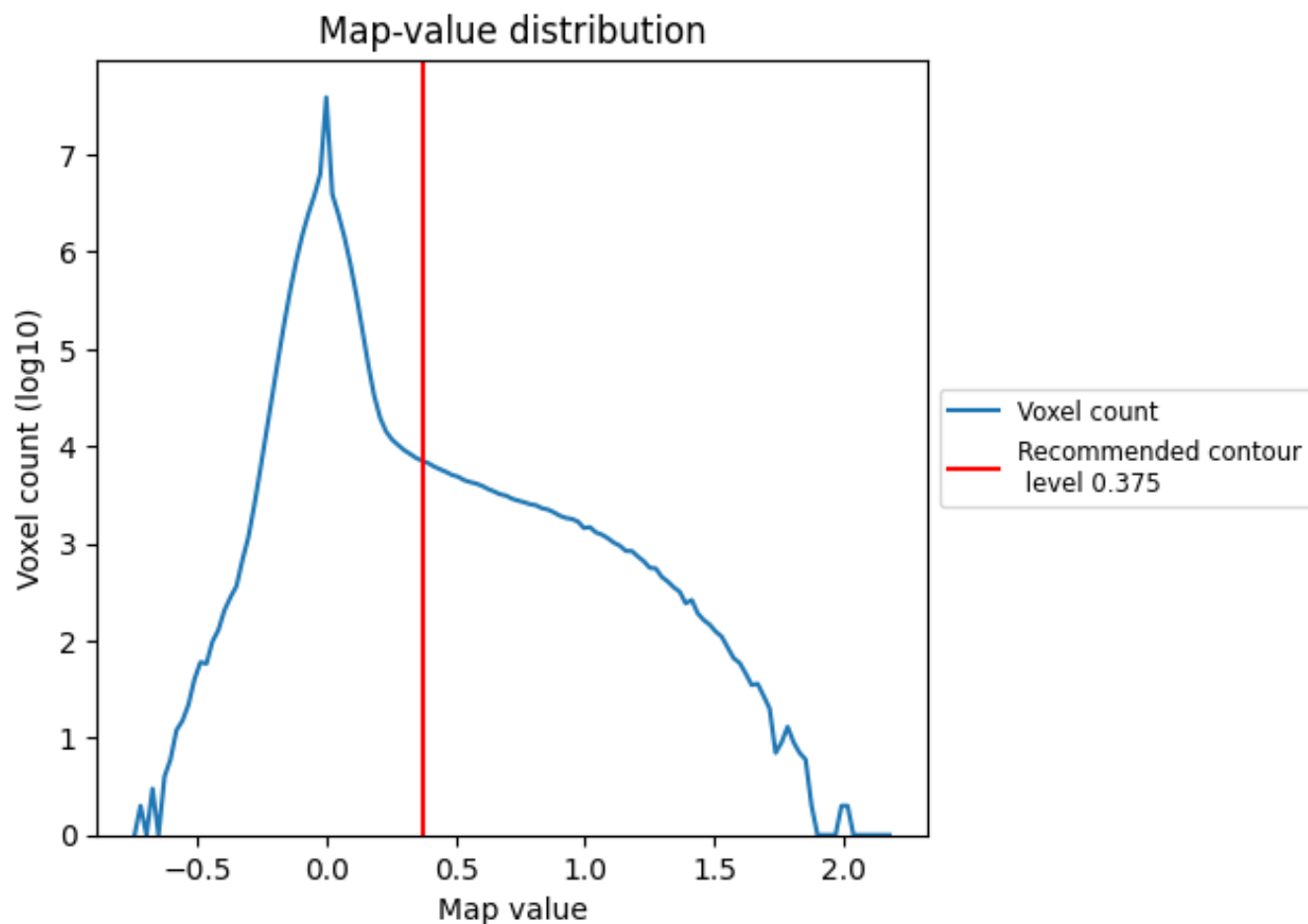
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

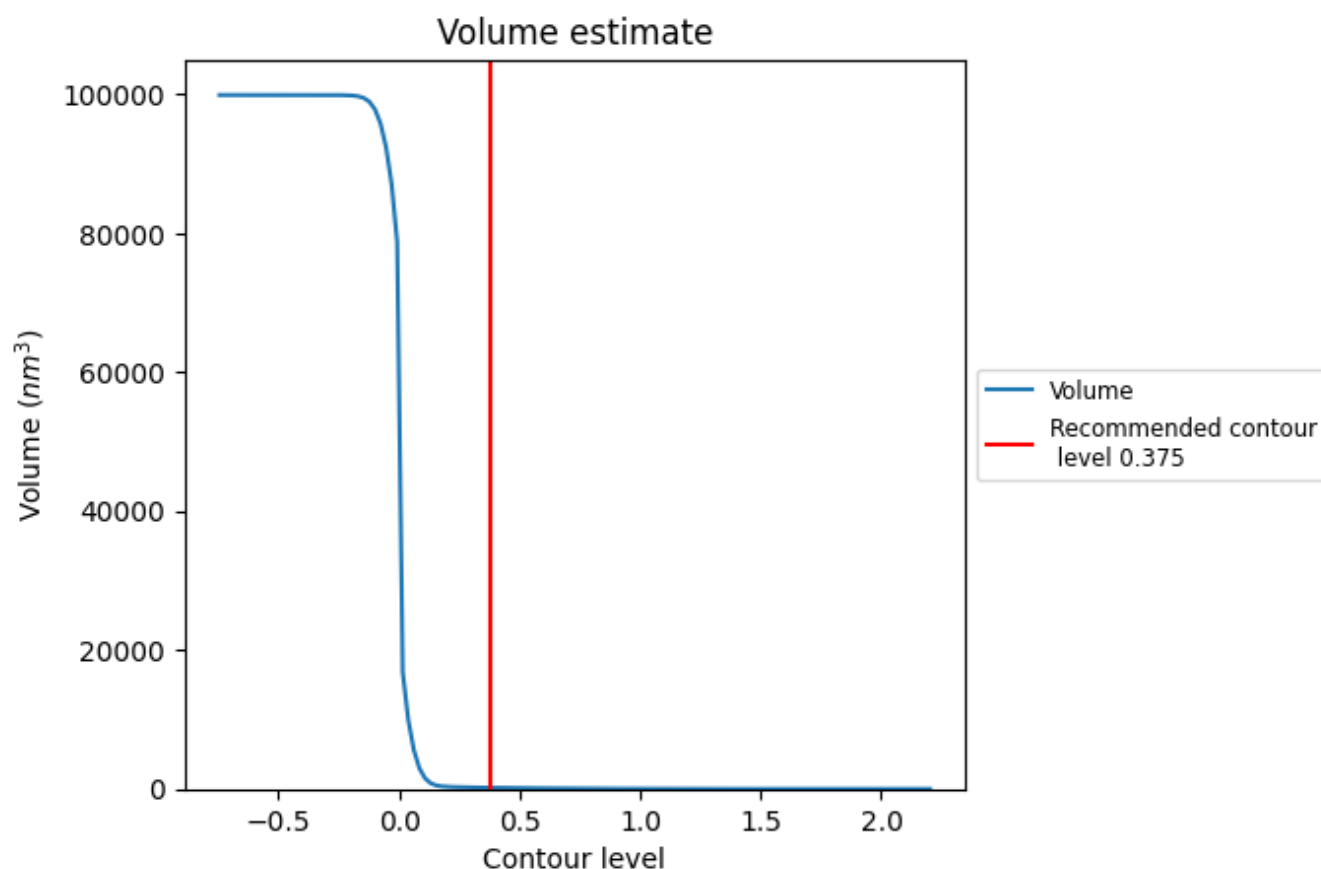
This section contains the results of statistical analysis of the map.

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.

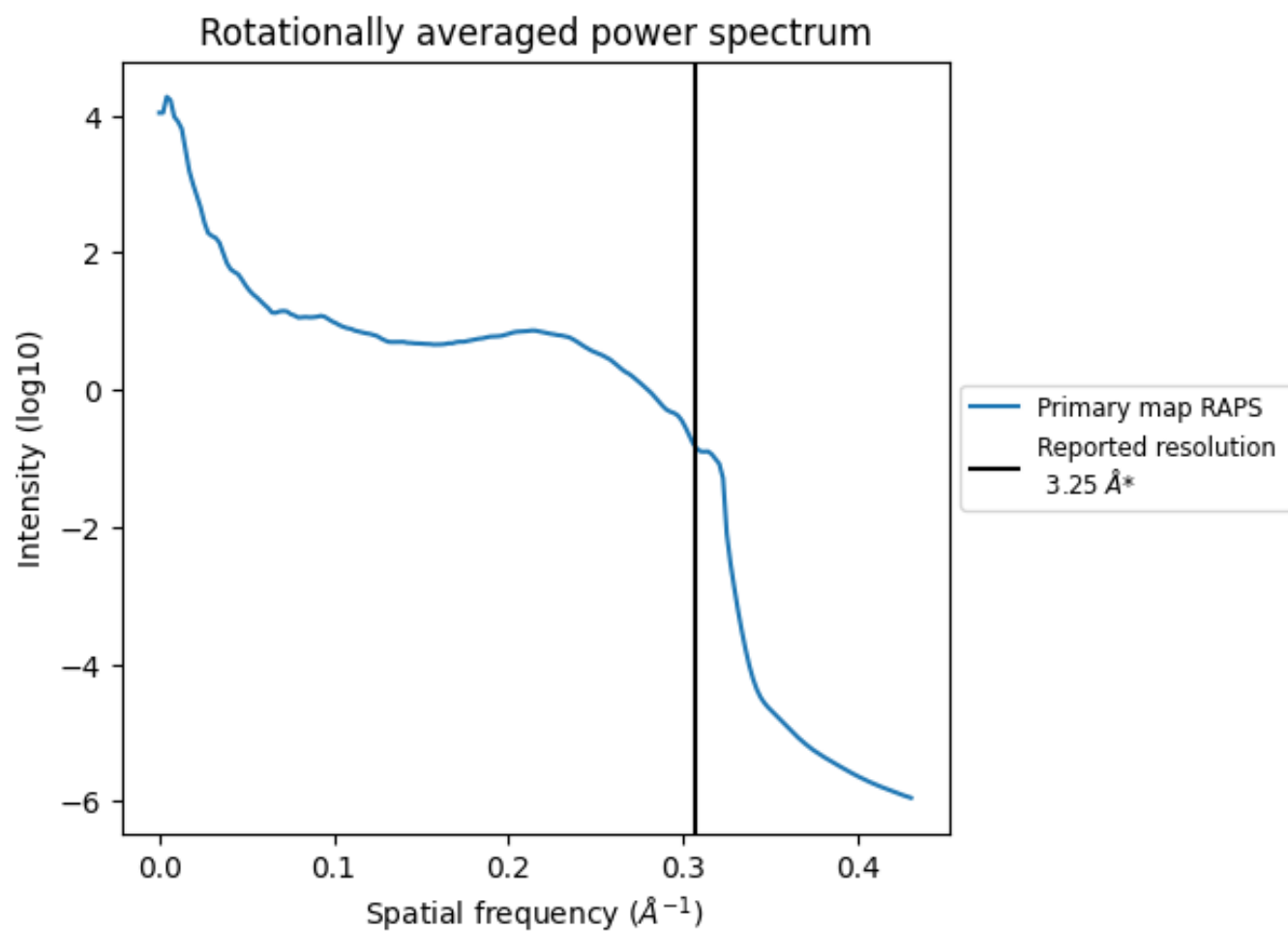
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

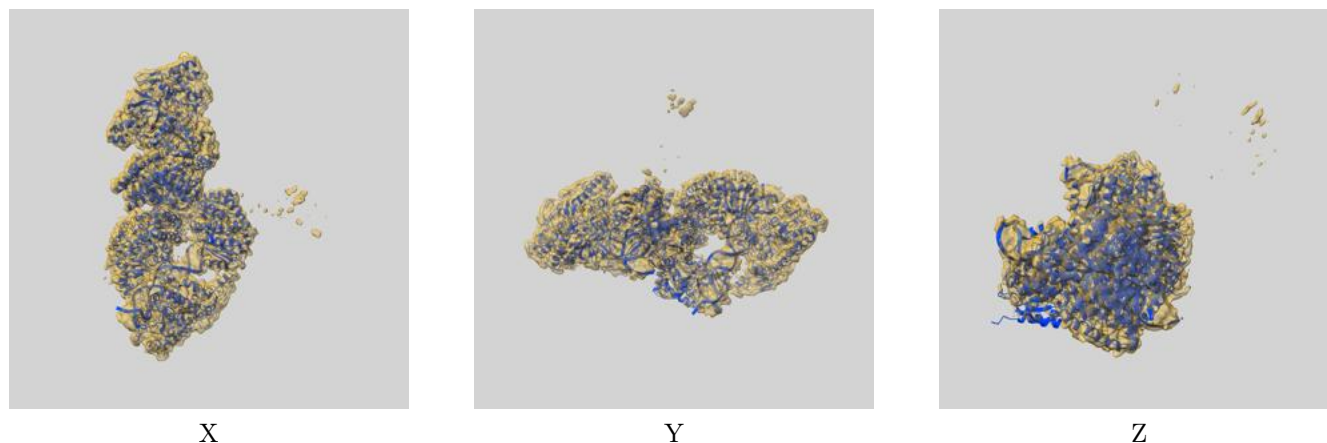
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

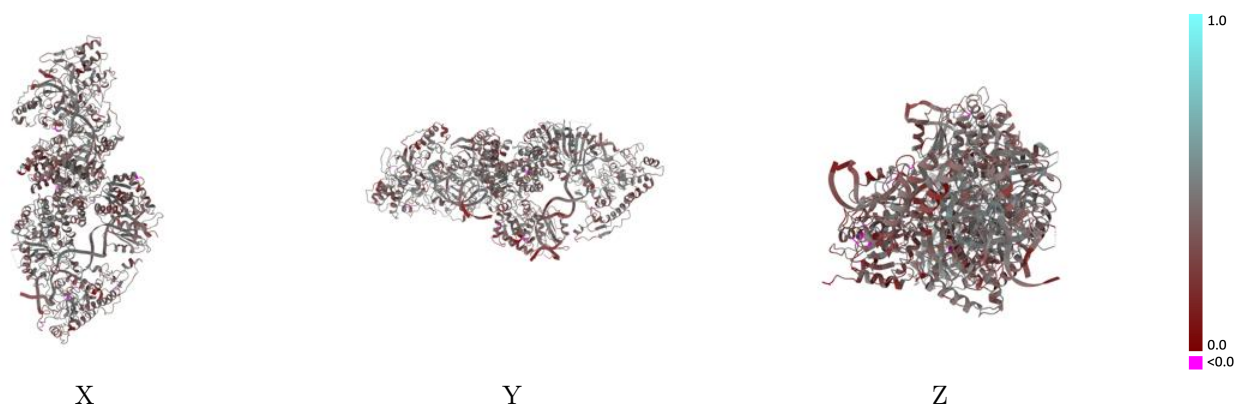
This section contains information regarding the fit between EMDB map EMD-23543 and PDB model 7LVV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



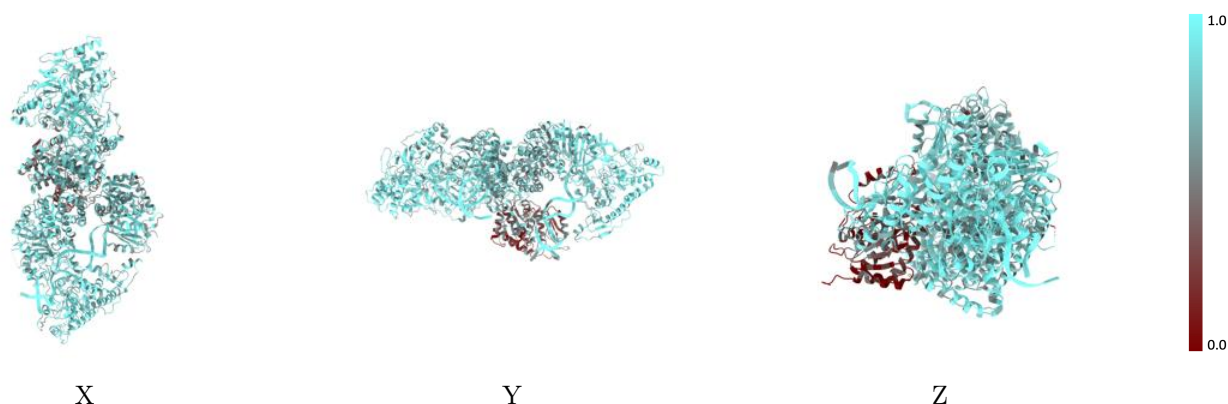
The images above show the 3D surface view of the map at the recommended contour level 0.375 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



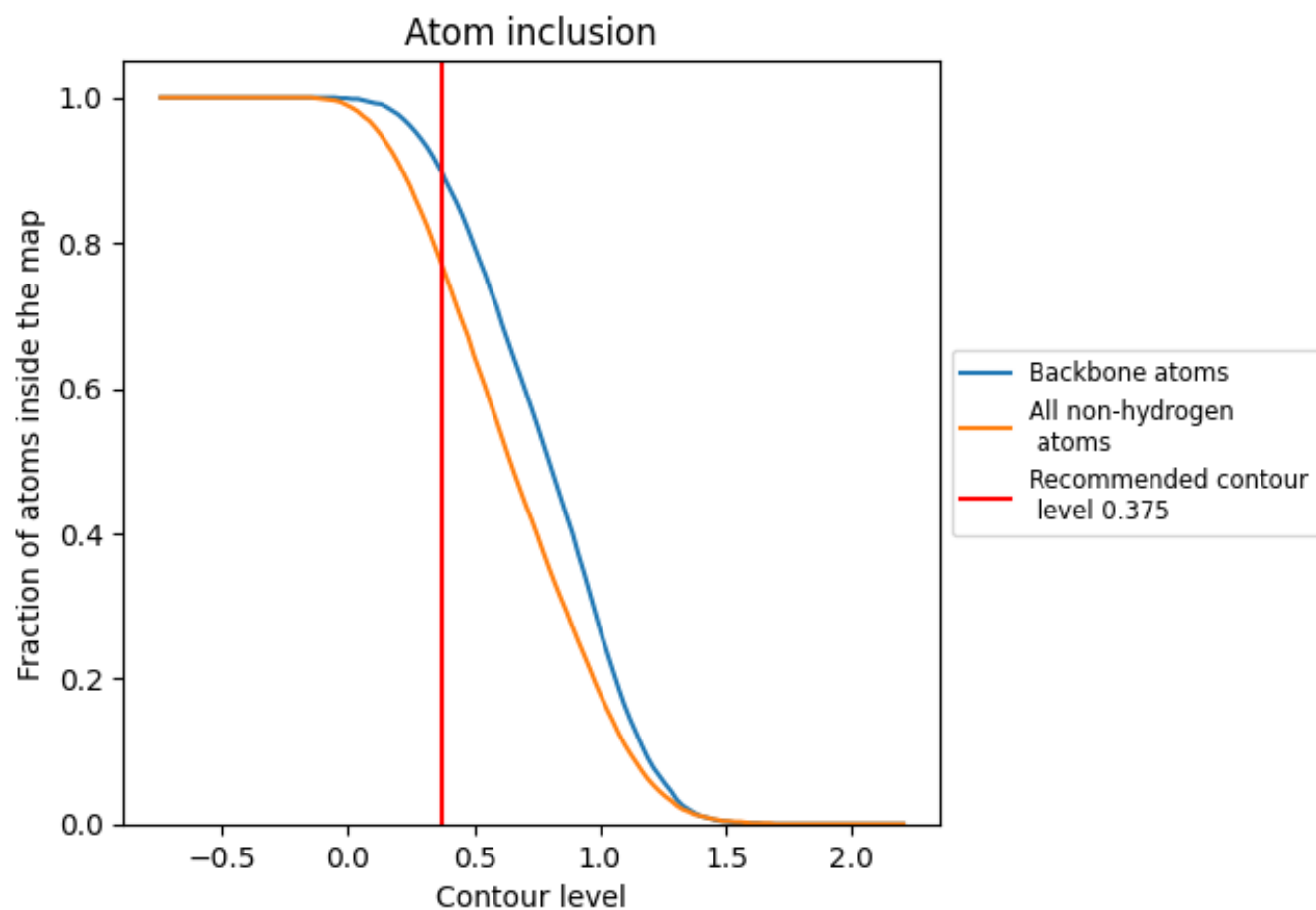
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.375).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 77% 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 (0.375) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.3940
A	0.7550	0.3950
B	0.7960	0.4010
C	0.7280	0.3940
D	0.3190	0.3150
E	0.9730	0.4240
F	0.9630	0.4220
G	0.9320	0.3840
H	0.9490	0.3820

1.0

0.0

<0.0