Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 12:02 PM JST

PDB ID	:	7CQI
EMDB ID	:	EMD-30441
Title	:	Cryo-EM structure of the substrate-bound SPT-ORMDL3 complex
Authors	:	Li, S.S.; Xie, T.; Wang, L.; Gong, X.
Deposited on	:	2020-08-11
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

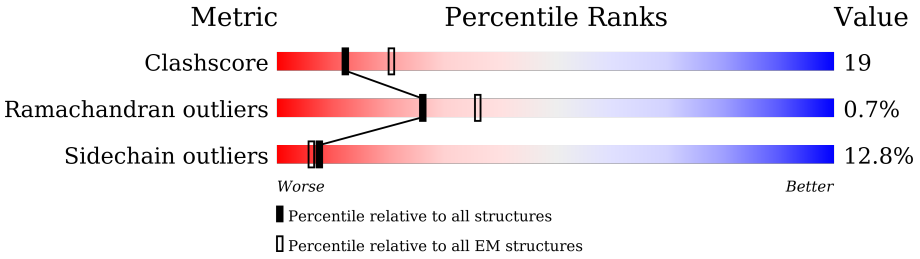
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	473	5%, ·, 95%
1	S	473	63%, 21%, 6%, 11%
2	T	562	·, 59%, 22%, 9%, 11%
3	A	153	70%, 67%, 15%, ·, 15%
4	E	92	15%, 42%, 7%, ·, 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PLS	T	601	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8881 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 palmitoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	S	421	3268	2078	558	616	16	0	0
1	C	22	Total	C	N	O		0	0
			182	128	28	26			

- Molecule 2 is a protein called Serine palmitoyltransferase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	498	3926	2512	673	716	25	0	0

- Molecule 3 is a protein called ORM1-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	130	1028	687	163	173	5	0	0

- Molecule 4 is a protein called Serine palmitoyltransferase small subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	46	389	265	55	65	4	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	MET	-	initiating methionine	UNP Q969W0
E	-19	ALA	-	expression tag	UNP Q969W0
E	-18	ASP	-	expression tag	UNP Q969W0
E	-17	TYR	-	expression tag	UNP Q969W0
E	-16	LYS	-	expression tag	UNP Q969W0
E	-15	ASP	-	expression tag	UNP Q969W0
E	-14	ASP	-	expression tag	UNP Q969W0

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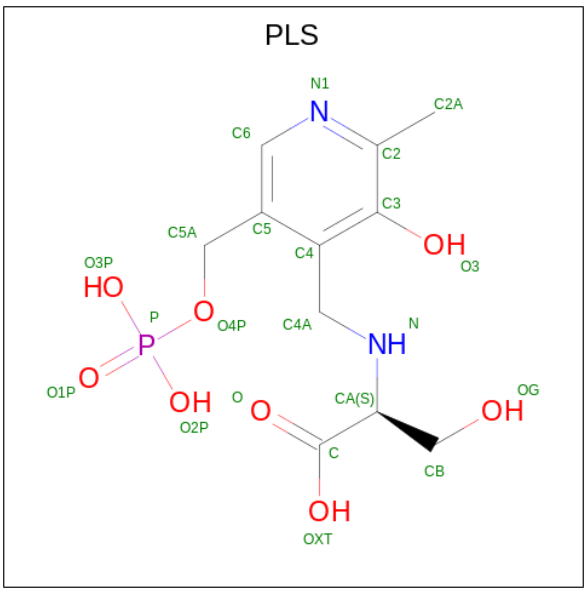
Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	ASP	-	expression tag	UNP Q969W0
E	-12	ASP	-	expression tag	UNP Q969W0
E	-11	LYS	-	expression tag	UNP Q969W0
E	-10	SER	-	expression tag	UNP Q969W0
E	-9	GLY	-	expression tag	UNP Q969W0
E	-8	PRO	-	expression tag	UNP Q969W0
E	-7	ASP	-	expression tag	UNP Q969W0
E	-6	GLU	-	expression tag	UNP Q969W0
E	-5	VAL	-	expression tag	UNP Q969W0
E	-4	ASP	-	expression tag	UNP Q969W0
E	-3	ALA	-	expression tag	UNP Q969W0
E	-2	SER	-	expression tag	UNP Q969W0
E	-1	GLY	-	expression tag	UNP Q969W0
E	0	ARG	-	expression tag	UNP Q969W0

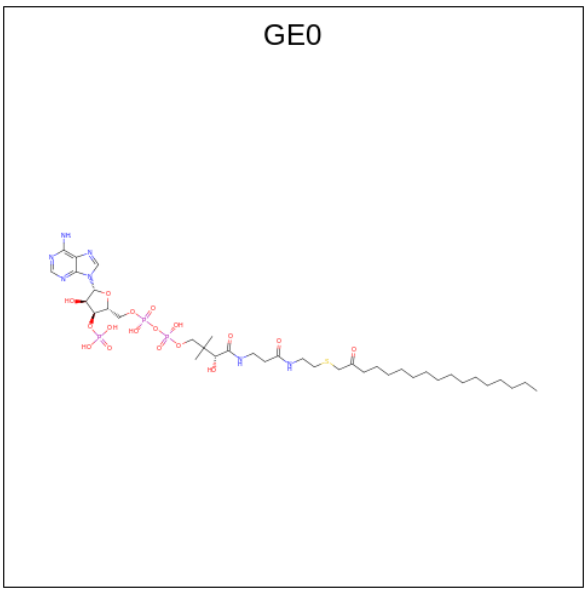
- Molecule 5 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: $C_{11}H_{17}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	T	1	22	11	2	8	1	0

- Molecule 6 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(3R)-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-4-[[3-oxidanylidene-3-[2-(2-oxidanylideneheptadecylsulfanyl)ethylamino]propyl]amino]butyl] hydrogen phosphate (three-letter code: GE0) (formula: $C_{38}H_{68}N_7O_{17}P_3S$) (labeled as

"Ligand of Interest" by depositor).



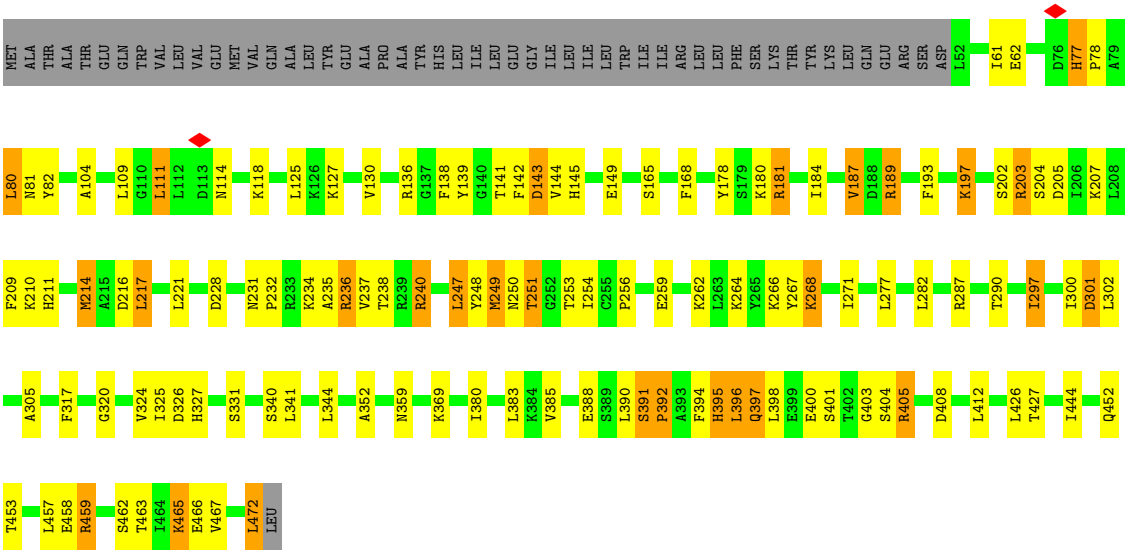
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
6	T	1	66	38	7	17	3	1	0

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.

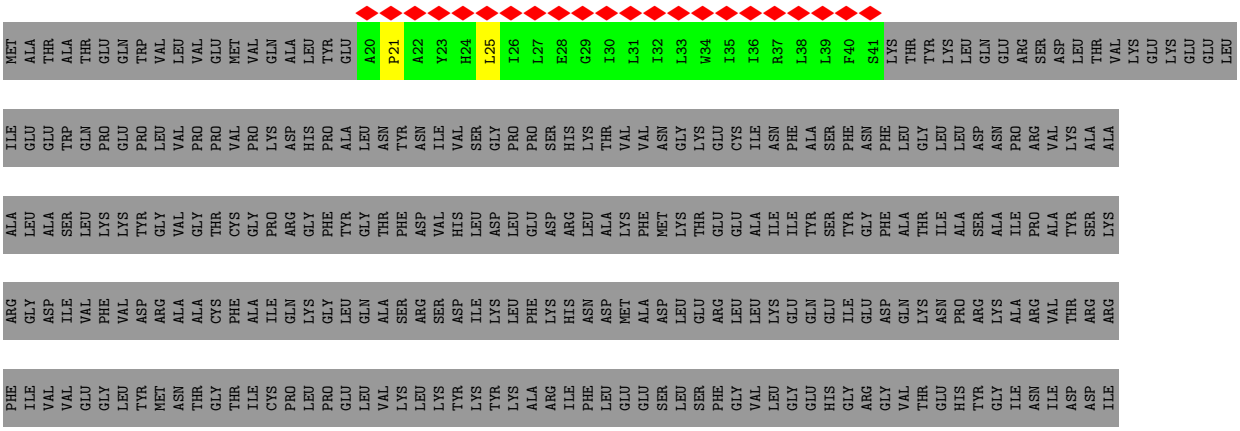
• Molecule 1: Serine palmitoyltransferase 1

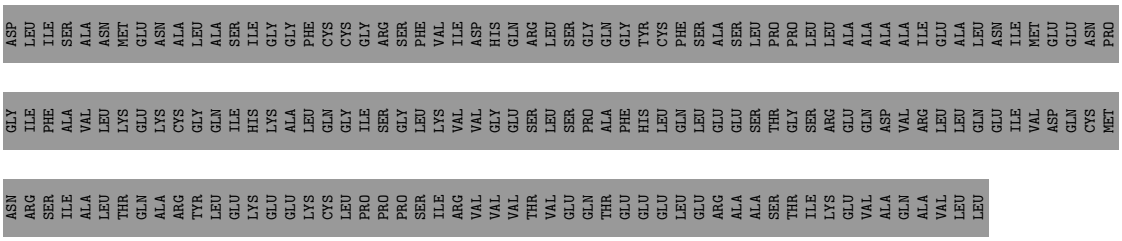
Chain S: 63% 21% 6% 11%



• Molecule 1: Serine palmitoyltransferase 1

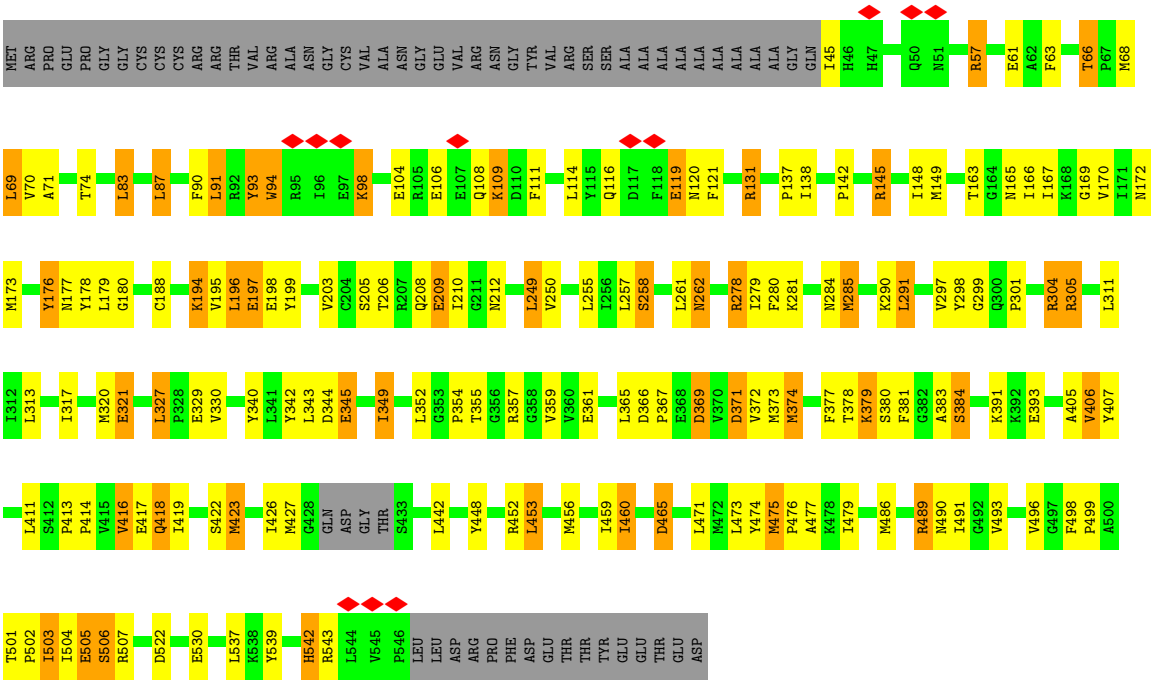
Chain C: 5% 95%





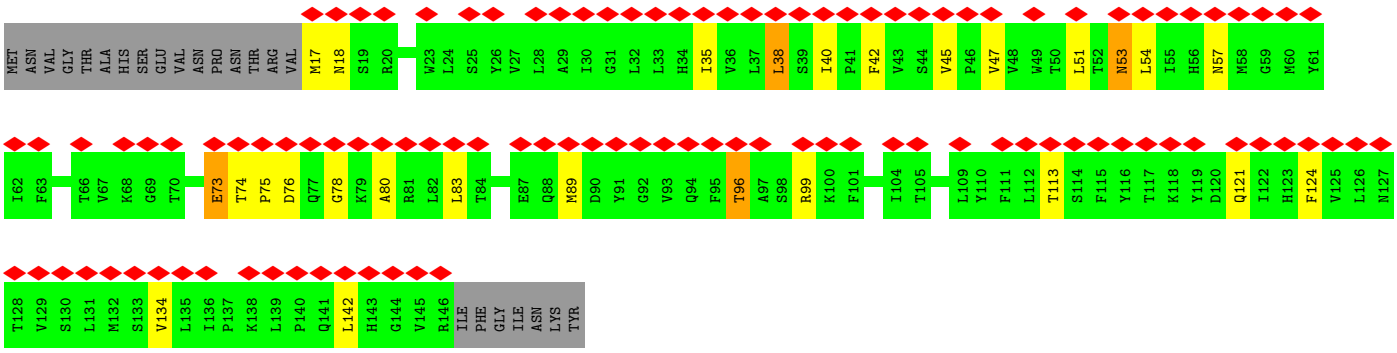
- Molecule 2: Serine palmitoyltransferase 2

Chain T:



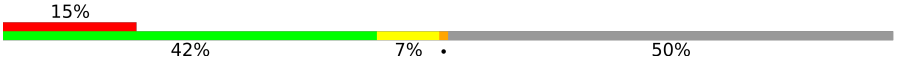
- Molecule 3: ORM1-like protein 3

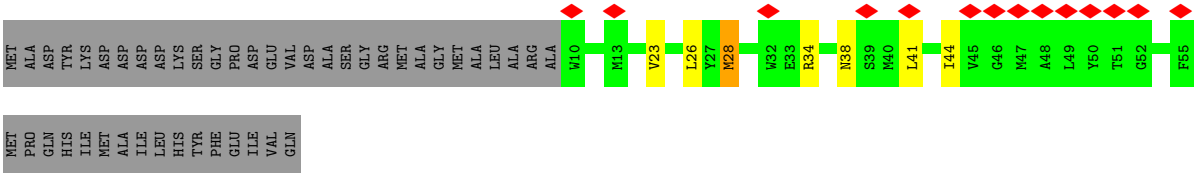
Chain A:



- Molecule 4: Serine palmitoyltransferase small subunit A

Chain E:




MET ALA ASP TYR LYS ASP ASP ASP LYS SER GLY PRO ASP GLU VAL ASP ALA SER GLY ARG MET ALA GLY MET ALA LEU ALA ARG ALA
W10 M13 V23 L26 Y27 M28 W32 E33 R34 N38 S39 M40 L41 I44 V45 G46 M47 A48 L49 Y50 T51 G52 F55
MET PRO GLN HIS ILE MET ALA ILE LEU HIS TYR PHE GLU ILE VAL GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.248	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: PLS, GE0

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	C	0.39	0/187	0.67	0/255
1	S	0.54	0/3329	0.70	1/4501 (0.0%)
2	T	0.50	0/4009	0.71	9/5412 (0.2%)
3	A	0.36	0/1058	0.76	0/1449
4	E	0.47	0/402	0.66	0/547
All	All	0.50	0/8985	0.71	10/12164 (0.1%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	311	LEU	CA-CB-CG	8.13	133.99	115.30
2	T	453	LEU	CA-CB-CG	8.05	133.82	115.30
2	T	291	LEU	CA-CB-CG	7.48	132.51	115.30
2	T	471	LEU	CA-CB-CG	7.04	131.49	115.30
2	T	327	LEU	CA-CB-CG	6.95	131.29	115.30
2	T	473	LEU	CA-CB-CG	6.30	129.80	115.30
2	T	321	GLU	N-CA-C	-5.59	95.92	111.00
2	T	442	LEU	CA-CB-CG	5.57	128.10	115.30
1	S	383	LEU	CA-CB-CG	5.47	127.88	115.30
2	T	257	LEU	CA-CB-CG	5.41	127.75	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	142	LEU	Peptide
3	A	38	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	182	0	199	1	0
1	S	3268	0	3293	137	0
2	T	3926	0	3922	201	0
3	A	1028	0	1046	38	0
4	E	389	0	379	11	0
5	T	22	0	13	17	0
6	T	66	0	0	9	0
All	All	8881	0	8852	339	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 19.

All (339) 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)
6:T:602:GE0:C5'	3:A:76:ASP:HB2	1.42	1.45
1:S:228:ASP:OD1	1:S:235:ALA:CB	1.73	1.35
6:T:602:GE0:C5'	3:A:76:ASP:CB	2.03	1.35
1:S:214:MET:CE	1:S:256:PRO:HG2	1.62	1.27
1:S:331:SER:HB3	3:A:73:GLU:OE2	1.33	1.26
1:S:228:ASP:OD1	1:S:235:ALA:HB1	1.16	1.26
1:S:143:ASP:OD2	2:T:149:MET:SD	1.93	1.25
1:S:211:HIS:CE1	1:S:251:THR:HG21	1.71	1.25
1:S:180:LYS:NZ	3:A:74:THR:HB	1.51	1.22
2:T:379:LYS:NZ	5:T:601:PLS:CB	2.04	1.20
1:S:180:LYS:NZ	3:A:74:THR:CB	2.05	1.19
1:S:118:LYS:NZ	2:T:197:GLU:O	1.74	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:180:LYS:HZ1	3:A:74:THR:CB	1.56	1.18
2:T:194:LYS:O	2:T:197:GLU:OE2	1.64	1.14
1:S:104:ALA:HB3	2:T:210:ILE:HD12	1.25	1.13
2:T:176:TYR:CE2	5:T:601:PLS:OG	2.01	1.12
2:T:379:LYS:NZ	5:T:601:PLS:HB2	1.61	1.12
2:T:379:LYS:HZ1	5:T:601:PLS:CB	1.60	1.11
1:S:331:SER:CB	3:A:73:GLU:OE2	1.97	1.10
1:S:214:MET:HE3	1:S:256:PRO:HG2	1.27	1.10
1:S:462:SER:O	1:S:466:GLU:HG3	1.53	1.08
2:T:379:LYS:HZ1	5:T:601:PLS:HB2	1.00	1.07
2:T:176:TYR:HE2	5:T:601:PLS:OG	1.36	1.07
2:T:413:PRO:HB2	2:T:414:PRO:HD3	1.34	1.04
2:T:379:LYS:NZ	5:T:601:PLS:OG	1.90	1.01
2:T:477:ALA:HA	4:E:28:MET:HE3	1.39	1.01
6:T:602:GE0:C5'	3:A:76:ASP:HB3	1.90	1.00
2:T:477:ALA:HA	4:E:28:MET:CE	1.89	0.99
1:S:118:LYS:CE	2:T:197:GLU:O	2.13	0.97
1:S:104:ALA:HB3	2:T:210:ILE:CD1	1.94	0.96
6:T:602:GE0:OBQ	3:A:76:ASP:OD2	1.83	0.95
1:S:180:LYS:HZ1	3:A:74:THR:HB	0.77	0.93
1:S:459:ARG:HH21	1:S:459:ARG:HG3	1.34	0.93
1:S:247:LEU:HD12	1:S:282:LEU:HD11	1.50	0.92
1:S:380:ILE:HG22	1:S:465:LYS:HG3	1.50	0.91
1:S:211:HIS:CE1	1:S:251:THR:CG2	2.53	0.91
2:T:498:PHE:HB2	2:T:503:ILE:HG12	1.54	0.90
2:T:374:MET:HE1	5:T:601:PLS:H2A2	1.54	0.89
2:T:411:LEU:HD13	2:T:416:VAL:HG23	1.56	0.88
1:S:214:MET:CE	1:S:256:PRO:CG	2.51	0.87
2:T:357:ARG:HG2	2:T:357:ARG:HH11	1.39	0.87
1:S:236:ARG:NH2	1:S:236:ARG:O	2.08	0.87
2:T:489:ARG:HG2	2:T:489:ARG:HH21	1.39	0.87
2:T:285:MET:CE	2:T:330:VAL:HG22	2.04	0.87
1:S:180:LYS:NZ	3:A:74:THR:OG1	2.09	0.84
2:T:489:ARG:HH22	2:T:530:GLU:CD	1.80	0.84
2:T:377:PHE:O	2:T:383:ALA:O	1.96	0.84
2:T:145:ARG:HG2	2:T:145:ARG:HH11	1.43	0.82
2:T:453:LEU:CD1	2:T:460:ILE:HD11	2.08	0.82
1:S:250:ASN:O	1:S:395:HIS:NE2	2.12	0.82
2:T:120:ASN:HD21	3:A:73:GLU:CB	1.93	0.81
2:T:120:ASN:HD21	3:A:73:GLU:HB2	1.45	0.81
1:S:214:MET:HE2	1:S:256:PRO:HG2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:177:ASN:OD1	2:T:180:GLY:HA2	1.81	0.80
2:T:114:LEU:HD12	2:T:114:LEU:O	1.81	0.80
1:S:427:THR:HG21	2:T:210:ILE:HG13	1.63	0.80
1:S:104:ALA:CB	2:T:210:ILE:HD12	2.08	0.79
2:T:98:LYS:NZ	2:T:98:LYS:HB3	1.96	0.79
2:T:503:ILE:HG22	2:T:504:ILE:HD13	1.65	0.79
1:S:398:LEU:HD11	1:S:472:LEU:HD11	1.63	0.78
2:T:57:ARG:HB2	2:T:57:ARG:NH1	1.97	0.78
2:T:354:PRO:HD2	2:T:361:GLU:HG2	1.64	0.78
2:T:456:MET:O	2:T:543:ARG:NH1	2.17	0.77
2:T:120:ASN:ND2	3:A:73:GLU:HB3	1.99	0.77
2:T:120:ASN:ND2	3:A:73:GLU:CB	2.48	0.76
1:S:290:THR:HG21	1:S:300:ILE:HD12	1.65	0.76
2:T:453:LEU:HD12	2:T:460:ILE:CD1	2.15	0.76
2:T:349:ILE:CG2	2:T:381:PHE:HE2	1.98	0.76
2:T:501:THR:HB	2:T:502:PRO:CD	2.16	0.75
2:T:342:TYR:CD1	2:T:372:VAL:HG21	2.21	0.75
2:T:340:TYR:HD1	2:T:371:ASP:OD2	1.67	0.75
1:S:250:ASN:O	1:S:395:HIS:CE1	2.40	0.75
2:T:453:LEU:HD12	2:T:460:ILE:HD11	1.66	0.74
2:T:116:GLN:HB2	2:T:119:GLU:HB2	1.70	0.73
1:S:211:HIS:NE2	1:S:251:THR:HG21	2.05	0.72
2:T:501:THR:HB	2:T:502:PRO:HD2	1.71	0.71
2:T:505:GLU:HA	2:T:505:GLU:OE1	1.88	0.71
2:T:285:MET:HE3	2:T:330:VAL:HG22	1.73	0.71
2:T:413:PRO:HB2	2:T:414:PRO:CD	2.14	0.70
2:T:320:MET:HG3	2:T:501:THR:HG22	1.73	0.70
1:S:234:LYS:HA	1:S:234:LYS:HE2	1.73	0.70
1:S:189:ARG:O	1:S:189:ARG:HG3	1.91	0.69
2:T:196:LEU:HD13	2:T:196:LEU:O	1.93	0.69
1:S:459:ARG:HG3	1:S:459:ARG:NH2	2.08	0.68
2:T:196:LEU:HD13	2:T:196:LEU:C	2.14	0.68
2:T:196:LEU:O	2:T:196:LEU:HD22	1.93	0.68
2:T:285:MET:CE	2:T:330:VAL:CG2	2.72	0.68
2:T:357:ARG:HG2	2:T:357:ARG:NH1	2.09	0.68
1:S:82:TYR:HB3	2:T:212:ASN:HD22	1.58	0.67
1:S:180:LYS:HZ2	3:A:74:THR:CB	2.00	0.67
2:T:69:LEU:HD22	2:T:69:LEU:O	1.94	0.67
1:S:290:THR:CG2	1:S:300:ILE:CD1	2.72	0.66
1:S:211:HIS:HE1	1:S:251:THR:CB	2.08	0.66
2:T:104:GLU:HG2	2:T:109:LYS:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:344:ASP:OD2	5:T:601:PLS:C2A	2.43	0.66
1:S:187:VAL:O	1:S:209:PHE:CD1	2.49	0.66
2:T:70:VAL:O	2:T:74:THR:HG23	1.94	0.66
2:T:195:VAL:O	2:T:199:TYR:HB2	1.96	0.66
1:S:427:THR:CG2	2:T:210:ILE:HG13	2.26	0.66
2:T:205:SER:OG	2:T:209:GLU:O	2.14	0.65
2:T:137:PRO:HG2	2:T:149:MET:HB2	1.79	0.65
1:S:400:GLU:HG2	1:S:400:GLU:O	1.96	0.65
1:S:181:ARG:HB2	3:A:78:GLY:O	1.97	0.65
2:T:313:LEU:HD23	2:T:342:TYR:HB3	1.79	0.64
1:S:193:PHE:CZ	1:S:197:LYS:HE2	2.33	0.64
1:S:211:HIS:CE1	1:S:251:THR:CB	2.81	0.64
2:T:476:PRO:O	4:E:28:MET:CE	2.46	0.64
6:T:602:GE0:C4'	3:A:76:ASP:HB2	2.26	0.64
1:S:211:HIS:HE1	1:S:251:THR:OG1	1.81	0.63
1:S:214:MET:HE2	1:S:256:PRO:CG	2.24	0.63
1:S:331:SER:HB3	3:A:73:GLU:CD	2.18	0.63
2:T:195:VAL:HG23	2:T:199:TYR:CD2	2.33	0.63
2:T:255:LEU:HD11	2:T:278:ARG:HG3	1.81	0.63
1:S:228:ASP:OD1	1:S:235:ALA:HB2	1.89	0.63
3:A:35:ILE:HD12	3:A:38:LEU:HD12	1.81	0.63
2:T:87:LEU:O	2:T:87:LEU:HD12	1.99	0.62
2:T:498:PHE:HB2	2:T:503:ILE:CG1	2.28	0.62
2:T:349:ILE:HG21	2:T:381:PHE:HE2	1.64	0.62
3:A:73:GLU:O	3:A:73:GLU:HG3	2.00	0.62
1:S:249:MET:O	1:S:249:MET:HG3	1.98	0.61
1:S:290:THR:CG2	1:S:300:ILE:HD12	2.30	0.61
2:T:148:ILE:HB	2:T:167:ILE:HD12	1.82	0.61
1:S:125:LEU:HD12	1:S:344:LEU:HD22	1.82	0.61
1:S:237:VAL:HG12	1:S:237:VAL:O	2.00	0.61
2:T:57:ARG:HB2	2:T:57:ARG:HH11	1.65	0.61
1:S:300:ILE:O	1:S:300:ILE:HG22	2.01	0.61
2:T:145:ARG:HH11	2:T:145:ARG:CG	2.14	0.61
2:T:119:GLU:OE1	2:T:119:GLU:HA	2.01	0.61
3:A:74:THR:O	3:A:74:THR:HG23	2.00	0.61
1:S:62:GLU:HA	1:S:62:GLU:OE1	2.01	0.61
2:T:304:ARG:HH11	2:T:304:ARG:CG	2.13	0.60
2:T:170:VAL:HG12	2:T:170:VAL:O	2.00	0.60
2:T:413:PRO:CB	2:T:414:PRO:HD3	2.20	0.60
2:T:317:ILE:HD11	2:T:352:LEU:HD13	1.84	0.59
2:T:354:PRO:CD	2:T:361:GLU:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:427:THR:HG23	2:T:210:ILE:HD11	1.85	0.59
1:S:187:VAL:O	1:S:209:PHE:CE1	2.56	0.59
1:S:181:ARG:HA	1:S:203:ARG:O	2.03	0.59
1:S:247:LEU:CD1	1:S:282:LEU:HD11	2.29	0.59
2:T:476:PRO:O	4:E:28:MET:HE2	2.02	0.59
1:S:202:SER:O	1:S:202:SER:OG	2.18	0.59
2:T:176:TYR:OH	5:T:601:PLS:OXT	2.17	0.58
2:T:477:ALA:CA	4:E:28:MET:HE3	2.24	0.58
1:S:320:GLY:N	1:S:325:ILE:HD11	2.17	0.58
5:T:601:PLS:HB2	5:T:601:PLS:H5A1	1.86	0.58
1:S:290:THR:HG21	1:S:300:ILE:CD1	2.30	0.58
1:S:404:SER:O	1:S:408:ASP:HB2	2.03	0.58
2:T:317:ILE:HG22	2:T:317:ILE:O	2.04	0.58
1:S:142:PHE:HZ	2:T:142:PRO:HG3	1.69	0.58
2:T:194:LYS:O	2:T:197:GLU:CD	2.42	0.58
1:S:290:THR:HG22	1:S:300:ILE:CD1	2.33	0.57
1:S:395:HIS:CD2	1:S:395:HIS:H	2.22	0.57
2:T:195:VAL:HG11	2:T:417:GLU:CB	2.33	0.57
2:T:489:ARG:HH21	2:T:489:ARG:CG	2.13	0.57
2:T:210:ILE:HG22	2:T:210:ILE:O	2.04	0.57
1:S:459:ARG:HH21	1:S:459:ARG:CG	2.12	0.57
2:T:344:ASP:OD2	5:T:601:PLS:H2A2	2.05	0.57
1:S:264:LYS:O	1:S:267:TYR:O	2.22	0.57
2:T:342:TYR:HA	2:T:372:VAL:HG22	1.86	0.56
2:T:208:GLN:HG3	2:T:405:ALA:O	2.06	0.56
2:T:285:MET:HG2	2:T:329:GLU:OE1	2.06	0.56
2:T:304:ARG:NH1	2:T:304:ARG:HG3	2.20	0.56
1:S:385:VAL:HG22	1:S:396:LEU:HD11	1.88	0.55
2:T:145:ARG:HG2	2:T:145:ARG:NH1	2.19	0.55
2:T:542:HIS:CD2	2:T:542:HIS:N	2.74	0.55
1:S:467:VAL:O	1:S:467:VAL:HG23	2.06	0.55
2:T:501:THR:HG21	2:T:507:ARG:NH2	2.22	0.54
2:T:120:ASN:ND2	3:A:73:GLU:HB2	2.13	0.54
1:S:253:THR:HG22	1:S:388:GLU:OE2	2.06	0.54
2:T:195:VAL:O	2:T:195:VAL:HG22	2.07	0.54
2:T:63:PHE:HE2	2:T:321:GLU:OE1	1.91	0.54
2:T:57:ARG:CZ	2:T:57:ARG:CB	2.85	0.54
2:T:258:SER:O	2:T:280:PHE:CD1	2.61	0.53
1:S:214:MET:HE3	1:S:256:PRO:CG	2.18	0.53
2:T:501:THR:HG21	2:T:507:ARG:HH21	1.73	0.53
2:T:131:ARG:O	2:T:131:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:602:GE0:OAK	6:T:602:GE0:N7	2.42	0.53
1:S:138:PHE:HZ	2:T:496:VAL:CG1	2.22	0.53
1:S:221:LEU:HD13	1:S:267:TYR:CD2	2.43	0.53
2:T:340:TYR:CD1	2:T:371:ASP:OD2	2.56	0.52
5:T:601:PLS:C5A	5:T:601:PLS:N	2.72	0.52
1:S:287:ARG:O	1:S:287:ARG:HG2	2.09	0.52
2:T:504:ILE:HG22	2:T:504:ILE:O	2.08	0.52
1:S:290:THR:HG22	1:S:300:ILE:HD11	1.90	0.52
1:S:459:ARG:NH2	1:S:459:ARG:CG	2.73	0.52
2:T:69:LEU:HD22	2:T:69:LEU:C	2.30	0.52
2:T:501:THR:CB	2:T:502:PRO:CD	2.85	0.52
1:S:118:LYS:HE2	2:T:197:GLU:O	2.08	0.52
1:S:385:VAL:HG22	1:S:396:LEU:CD1	2.40	0.52
1:S:136:ARG:NH2	1:S:149:GLU:OE2	2.44	0.51
2:T:145:ARG:CG	2:T:145:ARG:NH1	2.73	0.51
2:T:120:ASN:HD22	3:A:73:GLU:HB3	1.73	0.51
1:S:193:PHE:CZ	1:S:197:LYS:CE	2.93	0.51
2:T:489:ARG:HG2	2:T:489:ARG:NH2	2.15	0.51
2:T:169:GLY:O	2:T:490:ASN:OD1	2.27	0.51
1:S:142:PHE:CZ	2:T:142:PRO:HD3	2.46	0.51
2:T:453:LEU:HD12	2:T:460:ILE:HD12	1.91	0.51
2:T:91:LEU:HG	2:T:94:TRP:CZ3	2.46	0.51
1:S:253:THR:HG22	1:S:388:GLU:CD	2.32	0.50
1:S:184:ILE:HD11	1:S:207:LYS:HD2	1.92	0.50
2:T:499:PRO:HD2	6:T:602:GE0:CCI	2.41	0.50
2:T:98:LYS:O	2:T:98:LYS:HG2	2.09	0.50
2:T:377:PHE:C	2:T:383:ALA:O	2.49	0.50
2:T:349:ILE:CG2	2:T:381:PHE:CE2	2.87	0.50
2:T:479:ILE:HD11	2:T:506:SER:HB3	1.92	0.50
6:T:602:GE0:OBS	3:A:76:ASP:HB3	2.11	0.50
2:T:93:TYR:C	2:T:93:TYR:CD2	2.85	0.50
2:T:344:ASP:OD1	5:T:601:PLS:H2A2	2.12	0.50
1:S:165:SER:HA	1:S:341:LEU:HD12	1.93	0.50
2:T:93:TYR:C	2:T:93:TYR:HD2	2.15	0.50
2:T:477:ALA:HA	4:E:28:MET:HE2	1.86	0.50
2:T:203:VAL:HG23	2:T:203:VAL:O	2.12	0.49
2:T:343:LEU:CD1	2:T:345:GLU:HG2	2.43	0.49
1:S:271:ILE:O	1:S:301:ASP:HB2	2.13	0.49
2:T:367:PRO:C	2:T:369:ASP:H	2.16	0.49
1:S:180:LYS:HB3	3:A:78:GLY:HA2	1.95	0.48
2:T:304:ARG:HH11	2:T:304:ARG:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:121:GLN:HA	3:A:124:PHE:HB3	1.94	0.48
2:T:357:ARG:NH1	2:T:357:ARG:CG	2.73	0.48
2:T:499:PRO:HG2	6:T:602:GE0:CCH	2.42	0.48
3:A:80:ALA:HB1	3:A:83:LEU:HD23	1.93	0.48
1:S:231:ASN:N	1:S:232:PRO:HD3	2.28	0.48
2:T:344:ASP:OD2	5:T:601:PLS:H2A1	2.12	0.48
1:S:240:ARG:HH11	1:S:240:ARG:HG3	1.77	0.48
1:S:139:TYR:HB3	2:T:138:ILE:HD11	1.95	0.48
1:S:130:VAL:HG21	2:T:418:GLN:HG3	1.95	0.48
2:T:98:LYS:HB3	2:T:98:LYS:HZ1	1.79	0.48
1:S:465:LYS:HB3	1:S:465:LYS:HE3	1.39	0.48
2:T:465:ASP:OD1	2:T:465:ASP:N	2.47	0.48
1:S:61:ILE:HG21	2:T:297:VAL:HG12	1.96	0.48
2:T:98:LYS:NZ	2:T:98:LYS:CB	2.73	0.48
2:T:111:PHE:N	2:T:111:PHE:CD1	2.77	0.48
2:T:195:VAL:HG23	2:T:199:TYR:HD2	1.75	0.47
3:A:53:ASN:HB2	3:A:113:THR:HG21	1.96	0.47
1:S:234:LYS:HE2	1:S:234:LYS:CA	2.43	0.47
2:T:344:ASP:CG	5:T:601:PLS:H2A2	2.35	0.47
2:T:489:ARG:CG	2:T:489:ARG:NH2	2.73	0.47
1:S:259:GLU:HA	1:S:262:LYS:HE2	1.96	0.47
2:T:320:MET:CG	2:T:501:THR:HG22	2.44	0.47
2:T:413:PRO:CB	2:T:414:PRO:CD	2.85	0.47
1:S:412:LEU:HD22	1:S:444:ILE:HD11	1.97	0.47
2:T:285:MET:HE1	2:T:330:VAL:CG2	2.44	0.47
2:T:459:ILE:O	2:T:459:ILE:HG22	2.15	0.47
4:E:41:LEU:HD22	4:E:44:ILE:HD12	1.96	0.47
2:T:109:LYS:HE2	2:T:111:PHE:CE2	2.50	0.47
1:S:380:ILE:HG22	1:S:465:LYS:CG	2.35	0.46
1:S:111:LEU:HD13	1:S:352:ALA:HB1	1.97	0.46
2:T:359:VAL:HG22	2:T:359:VAL:O	2.16	0.46
1:S:136:ARG:HB2	1:S:340:SER:HB3	1.98	0.46
2:T:91:LEU:CD1	2:T:91:LEU:N	2.78	0.46
1:S:138:PHE:CZ	2:T:496:VAL:CG1	2.99	0.46
2:T:299:GLY:HA3	2:T:305:ARG:O	2.15	0.46
2:T:94:TRP:CD1	2:T:94:TRP:C	2.88	0.45
1:S:395:HIS:CD2	1:S:395:HIS:N	2.82	0.45
2:T:94:TRP:CG	2:T:94:TRP:O	2.70	0.45
2:T:120:ASN:HD22	2:T:120:ASN:HA	1.52	0.45
3:A:51:LEU:HD23	3:A:54:LEU:HD12	1.98	0.45
2:T:349:ILE:HD13	2:T:349:ILE:HA	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:475:MET:CE	4:E:23:VAL:HG12	2.45	0.45
2:T:476:PRO:O	4:E:28:MET:HE1	2.15	0.45
1:S:178:TYR:OH	1:S:324:VAL:O	2.32	0.45
2:T:366:ASP:OD1	2:T:366:ASP:N	2.45	0.45
1:S:217:LEU:O	1:S:217:LEU:HD22	2.16	0.45
1:S:331:SER:CA	3:A:73:GLU:OE2	2.59	0.45
2:T:498:PHE:HB2	2:T:503:ILE:CD1	2.46	0.45
1:S:394:PHE:O	1:S:394:PHE:CD2	2.69	0.45
2:T:197:GLU:H	2:T:197:GLU:HG3	1.44	0.45
1:S:320:GLY:CA	1:S:325:ILE:HD11	2.47	0.45
2:T:121:PHE:O	2:T:121:PHE:CD2	2.70	0.45
2:T:489:ARG:NH2	2:T:530:GLU:OE1	2.43	0.45
1:S:168:PHE:O	1:S:168:PHE:CD2	2.70	0.44
4:E:26:LEU:O	4:E:34:ARG:NH2	2.51	0.44
2:T:498:PHE:O	2:T:498:PHE:CD1	2.70	0.44
1:S:327:HIS:CG	1:S:327:HIS:O	2.70	0.44
1:S:391:SER:HA	1:S:392:PRO:HD3	1.83	0.44
2:T:411:LEU:HD13	2:T:416:VAL:CG2	2.36	0.44
2:T:94:TRP:CD1	2:T:94:TRP:O	2.70	0.44
3:A:57:ASN:HD22	3:A:134:VAL:HG21	1.82	0.44
2:T:57:ARG:NH1	2:T:57:ARG:CB	2.73	0.44
2:T:104:GLU:CG	2:T:109:LYS:HG2	2.45	0.44
2:T:381:PHE:CE1	2:T:423:MET:HG3	2.52	0.44
1:S:127:LYS:HE2	1:S:127:LYS:HB2	1.70	0.43
1:S:359:ASN:OD1	1:S:359:ASN:N	2.50	0.43
1:S:301:ASP:HB3	1:S:302:LEU:H	1.48	0.43
1:S:204:SER:HB2	1:S:205:ASP:H	1.72	0.43
1:S:427:THR:HG23	2:T:210:ILE:CD1	2.48	0.43
1:C:21:PRO:HG3	1:C:25:LEU:HD22	1.99	0.43
1:S:82:TYR:HB3	2:T:212:ASN:ND2	2.28	0.43
2:T:194:LYS:HB3	2:T:194:LYS:HE3	1.52	0.43
1:S:305:ALA:HB3	1:S:317:PHE:CE1	2.54	0.43
1:S:77:HIS:HA	1:S:78:PRO:HD2	1.69	0.43
2:T:486:MET:HB3	2:T:491:ILE:HG23	2.00	0.43
1:S:297:ILE:H	1:S:297:ILE:HG13	1.37	0.42
3:A:89:MET:O	3:A:99:ARG:NH2	2.50	0.42
1:S:325:ILE:O	1:S:325:ILE:HG22	2.18	0.42
2:T:91:LEU:N	2:T:91:LEU:HD13	2.34	0.42
2:T:249:LEU:HD12	2:T:249:LEU:HA	1.81	0.42
1:S:452:GLN:HB3	1:S:457:LEU:CD1	2.50	0.42
2:T:327:LEU:HD12	2:T:365:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:247:LEU:HD21	1:S:391:SER:HB2	2.00	0.42
2:T:327:LEU:CD1	2:T:365:LEU:CD1	2.97	0.42
1:S:248:TYR:CD2	1:S:248:TYR:N	2.87	0.42
1:S:331:SER:HB2	3:A:73:GLU:OE2	2.07	0.42
2:T:66:THR:HG21	2:T:71:ALA:HB2	2.02	0.42
2:T:83:LEU:HD22	2:T:83:LEU:HA	1.93	0.42
2:T:313:LEU:HD23	2:T:342:TYR:CB	2.47	0.42
2:T:342:TYR:CD1	2:T:372:VAL:CG2	2.99	0.42
2:T:262:ASN:HD22	2:T:262:ASN:HA	1.59	0.42
2:T:406:VAL:HG22	2:T:407:TYR:CD2	2.55	0.42
2:T:205:SER:OG	2:T:206:THR:N	2.53	0.41
1:S:136:ARG:HH12	1:S:145:HIS:HB3	1.86	0.41
1:S:254:ILE:HD11	1:S:390:LEU:HD11	2.02	0.41
1:S:248:TYR:H	1:S:248:TYR:HD2	1.68	0.41
3:A:40:ILE:O	3:A:42:PHE:N	2.49	0.41
1:S:197:LYS:HD3	1:S:197:LYS:HA	1.38	0.41
2:T:74:THR:HG22	2:T:474:TYR:O	2.21	0.41
2:T:290:LYS:HE2	2:T:290:LYS:HB3	1.93	0.41
2:T:378:THR:HG22	2:T:384:SER:HA	2.01	0.41
1:S:331:SER:CB	3:A:73:GLU:CD	2.84	0.41
1:S:268:LYS:HG2	2:T:111:PHE:CD1	2.56	0.41
1:S:405:ARG:O	1:S:408:ASP:N	2.54	0.41
1:S:427:THR:CG2	2:T:210:ILE:CG1	2.95	0.41
2:T:327:LEU:HD12	2:T:365:LEU:CD1	2.51	0.41
1:S:463:THR:O	1:S:467:VAL:HG13	2.20	0.41
1:S:320:GLY:N	1:S:325:ILE:CD1	2.82	0.41
2:T:178:TYR:C	2:T:180:GLY:H	2.23	0.41
2:T:419:ILE:O	2:T:419:ILE:HG22	2.20	0.41
1:S:181:ARG:HG3	3:A:78:GLY:HA3	2.02	0.41
2:T:57:ARG:HB2	2:T:57:ARG:CZ	2.50	0.40
2:T:342:TYR:HA	2:T:372:VAL:CG2	2.48	0.40
2:T:475:MET:HE2	4:E:23:VAL:HG12	2.03	0.40
1:S:320:GLY:HA3	1:S:325:ILE:HD11	2.04	0.40
2:T:448:TYR:OH	2:T:522:ASP:OD1	2.29	0.40
3:A:45:VAL:HG13	3:A:47:VAL:H	1.87	0.40
1:S:397:GLN:HE21	1:S:397:GLN:HB3	1.62	0.40
2:T:279:ILE:O	2:T:279:ILE:HG22	2.21	0.40
1:S:210:LYS:HG3	1:S:216:ASP:OD2	2.22	0.40
2:T:298:TYR:CD1	2:T:298:TYR:N	2.87	0.40
2:T:379:LYS:HE3	5:T:601:PLS:H4A2	2.04	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	C	20/473 (4%)	18 (90%)	2 (10%)	0	100	100
1	S	419/473 (89%)	372 (89%)	43 (10%)	4 (1%)	15	54
2	T	494/562 (88%)	444 (90%)	48 (10%)	2 (0%)	34	69
3	A	128/153 (84%)	103 (80%)	23 (18%)	2 (2%)	9	43
4	E	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
All	All	1105/1753 (63%)	979 (89%)	118 (11%)	8 (1%)	26	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	T	301	PRO
1	S	111	LEU
1	S	80	LEU
3	A	96	THR
2	T	176	TYR
1	S	392	PRO
3	A	75	PRO
1	S	403	GLY

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	C	19/401 (5%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	353/401 (88%)	313 (89%)	40 (11%)	6 25
2	T	415/466 (89%)	341 (82%)	74 (18%)	2 9
3	A	114/140 (81%)	109 (96%)	5 (4%)	28 64
4	E	41/78 (53%)	39 (95%)	2 (5%)	25 61
All	All	942/1486 (63%)	821 (87%)	121 (13%)	7 20

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	77	HIS
1	S	80	LEU
1	S	81	ASN
1	S	109	LEU
1	S	114	ASN
1	S	141	THR
1	S	143	ASP
1	S	144	VAL
1	S	181	ARG
1	S	187	VAL
1	S	189	ARG
1	S	197	LYS
1	S	203	ARG
1	S	214	MET
1	S	217	LEU
1	S	236	ARG
1	S	238	THR
1	S	240	ARG
1	S	247	LEU
1	S	249	MET
1	S	251	THR
1	S	266	LYS
1	S	268	LYS
1	S	277	LEU
1	S	297	ILE
1	S	301	ASP
1	S	326	ASP
1	S	369	LYS
1	S	391	SER
1	S	395	HIS
1	S	396	LEU
1	S	397	GLN

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Mol	Chain	Res	Type
1	S	401	SER
1	S	405	ARG
1	S	426	LEU
1	S	453	THR
1	S	458	GLU
1	S	459	ARG
1	S	465	LYS
1	S	472	LEU
2	T	45	ILE
2	T	57	ARG
2	T	61	GLU
2	T	66	THR
2	T	68	MET
2	T	69	LEU
2	T	83	LEU
2	T	87	LEU
2	T	90	PHE
2	T	91	LEU
2	T	93	TYR
2	T	94	TRP
2	T	98	LYS
2	T	106	GLU
2	T	108	GLN
2	T	109	LYS
2	T	119	GLU
2	T	131	ARG
2	T	145	ARG
2	T	163	THR
2	T	165	ASN
2	T	166	ILE
2	T	172	ASN
2	T	173	MET
2	T	179	LEU
2	T	188	CYS
2	T	194	LYS
2	T	196	LEU
2	T	197	GLU
2	T	198	GLU
2	T	209	GLU
2	T	249	LEU
2	T	250	VAL
2	T	258	SER

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Mol	Chain	Res	Type
2	T	261	LEU
2	T	262	ASN
2	T	278	ARG
2	T	281	LYS
2	T	284	ASN
2	T	285	MET
2	T	291	LEU
2	T	304	ARG
2	T	305	ARG
2	T	345	GLU
2	T	349	ILE
2	T	355	THR
2	T	369	ASP
2	T	371	ASP
2	T	373	MET
2	T	374	MET
2	T	379	LYS
2	T	380	SER
2	T	384	SER
2	T	391	LYS
2	T	393	GLU
2	T	406	VAL
2	T	416	VAL
2	T	418	GLN
2	T	422	SER
2	T	423	MET
2	T	426	ILE
2	T	427	MET
2	T	452	ARG
2	T	460	ILE
2	T	465	ASP
2	T	475	MET
2	T	489	ARG
2	T	493	VAL
2	T	503	ILE
2	T	505	GLU
2	T	506	SER
2	T	537	LEU
2	T	539	TYR
2	T	542	HIS
3	A	17	MET
3	A	18	ASN

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Mol	Chain	Res	Type
3	A	53	ASN
3	A	73	GLU
3	A	96	THR
4	E	28	MET
4	E	38	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	83	ASN
1	S	114	ASN
1	S	211	HIS
1	S	224	GLN
1	S	397	GLN
1	S	469	GLN
2	T	108	GLN
2	T	120	ASN
2	T	212	ASN
2	T	242	ASN
2	T	262	ASN
2	T	263	HIS
2	T	284	ASN
2	T	418	GLN
2	T	490	ASN
2	T	542	HIS
3	A	53	ASN
3	A	57	ASN
4	E	38	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
6	GE0	T	602	-	60,68,68	1.34	8 (13%)	72,94,94	1.32	4 (5%)
5	PLS	T	601	-	22,22,22	2.31	3 (13%)	27,31,31	1.32	3 (11%)

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	GE0	T	602	-	-	23/63/83/83	0/3/3/3
5	PLS	T	601	-	-	9/17/17/17	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	601	PLS	C3-C2	6.81	1.47	1.40
5	T	601	PLS	C5-C4	5.86	1.48	1.40
5	T	601	PLS	C3-C4	5.11	1.47	1.40
6	T	602	GE0	C2-N3	4.88	1.40	1.32
6	T	602	GE0	PAY-OBA	3.37	1.61	1.50
6	T	602	GE0	C2-N1	3.05	1.39	1.33
6	T	602	GE0	C5-C4	-2.83	1.33	1.40
6	T	602	GE0	C6-C5	-2.69	1.33	1.43
6	T	602	GE0	PAQ-OBS	2.66	1.60	1.50
6	T	602	GE0	O4'-C1'	2.55	1.44	1.41
6	T	602	GE0	C2'-C1'	-2.17	1.50	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	602	GE0	N3-C2-N1	-6.60	118.36	128.68
6	T	602	GE0	PAS-OAR-PAQ	-4.70	116.69	132.83
5	T	601	PLS	C4A-N-CA	2.76	119.15	113.92
5	T	601	PLS	C4A-C4-C5	2.75	122.77	119.71
6	T	602	GE0	C5-C6-N6	-2.65	116.32	120.35
6	T	602	GE0	CBZ-CBY-CBX	-2.35	108.57	114.60
5	T	601	PLS	C6-N1-C2	2.31	123.45	119.17

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	601	PLS	N-CA-CB-OG
5	T	601	PLS	C3-C4-C4A-N
5	T	601	PLS	C5-C4-C4A-N
5	T	601	PLS	C5A-O4P-P-O1P
5	T	601	PLS	C5A-O4P-P-O2P
5	T	601	PLS	C5A-O4P-P-O3P
6	T	602	GE0	SAA-CAB-CAC-NAD
6	T	602	GE0	CAJ-CAL-CAO-OAP
6	T	602	GE0	CBX-CBW-SAA-CAB
6	T	602	GE0	C3'-O3'-PAY-OAZ
6	T	602	GE0	C5'-O5'-PAS-OAR
6	T	602	GE0	CAO-OAP-PAQ-OBS
6	T	602	GE0	CAO-OAP-PAQ-OBT
6	T	602	GE0	CAM-CAL-CAO-OAP
6	T	602	GE0	CAN-CAL-CAO-OAP
6	T	602	GE0	CCD-CCE-CCF-CCG
6	T	602	GE0	CCE-CCF-CCG-CCH
5	T	601	PLS	C-CA-CB-OG
6	T	602	GE0	CCB-CCC-CCD-CCE
6	T	602	GE0	CCH-CCI-CCJ-CCK
6	T	602	GE0	CCG-CCH-CCI-CCJ
6	T	602	GE0	PAQ-OAR-PAS-O5'
6	T	602	GE0	CCF-CCG-CCH-CCI
5	T	601	PLS	C-CA-N-C4A
6	T	602	GE0	CAO-OAP-PAQ-OAR
6	T	602	GE0	PAS-OAR-PAQ-OBS
6	T	602	GE0	C5'-O5'-PAS-OBR
5	T	601	PLS	CB-CA-N-C4A
6	T	602	GE0	OBU-CAI-CAJ-OAK
6	T	602	GE0	CCA-CCB-CCC-CCD
6	T	602	GE0	CCJ-CCK-CCL-CCM

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Mol	Chain	Res	Type	Atoms
6	T	602	GE0	C4'-C5'-O5'-PAS

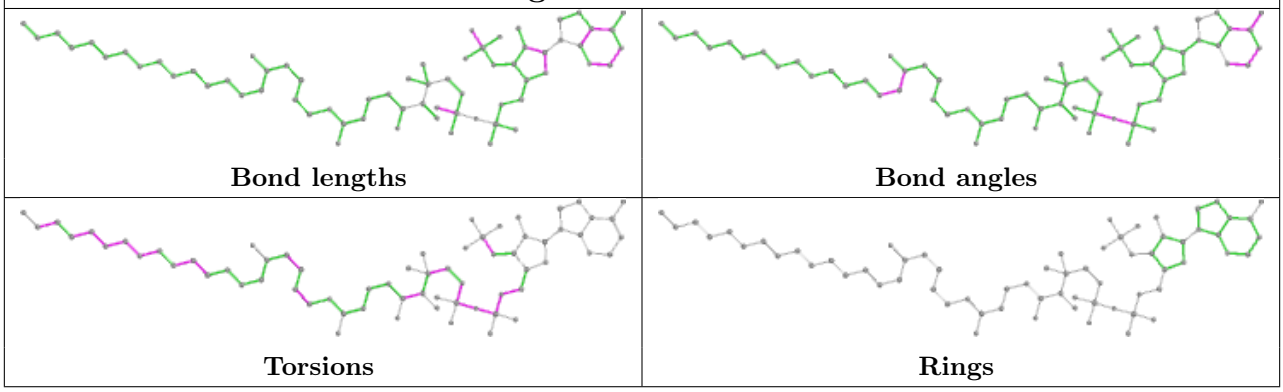
There are no ring outliers.

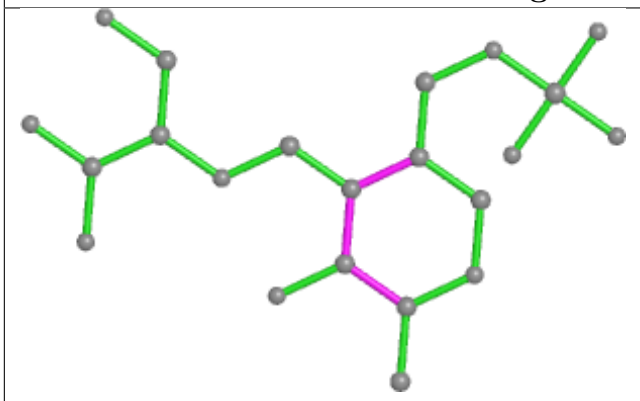
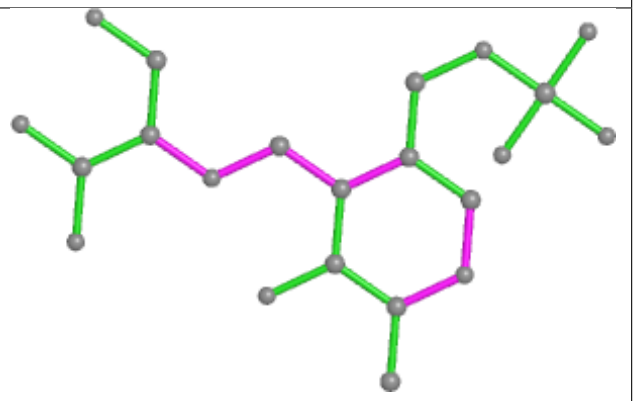
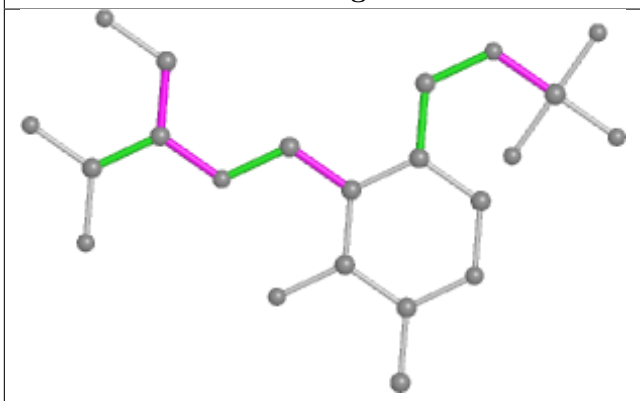
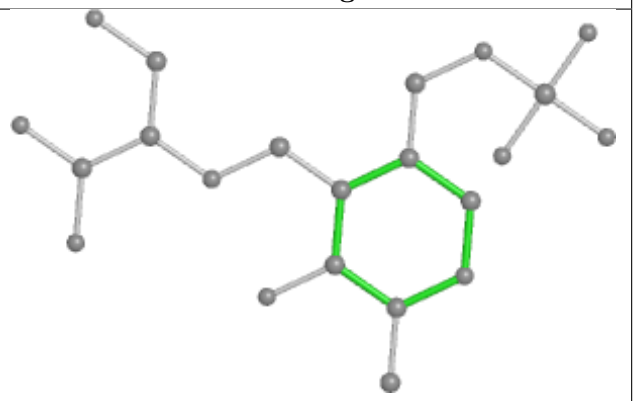
2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	602	GE0	9	0
5	T	601	PLS	17	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 GE0 T 602



Ligand PLS T 601	
 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.

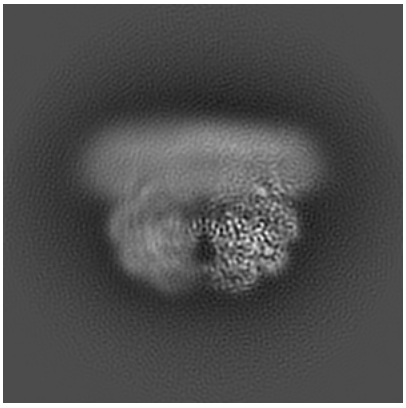
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30441. These allow visual inspection of the internal detail of the map and identification of artifacts.

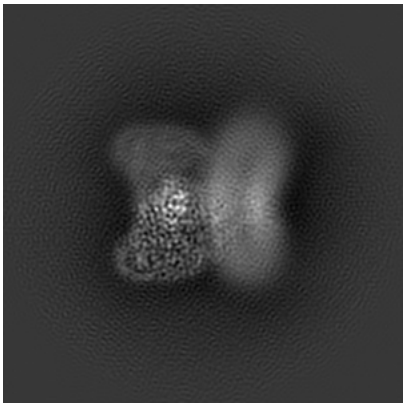
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

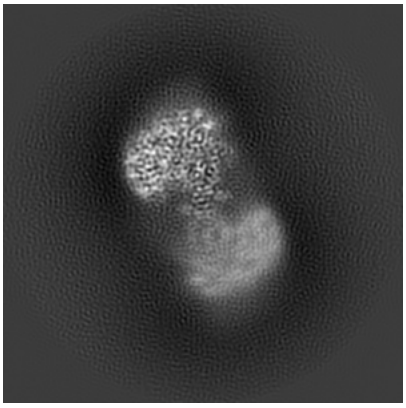
6.1.1 Primary map



X



Y

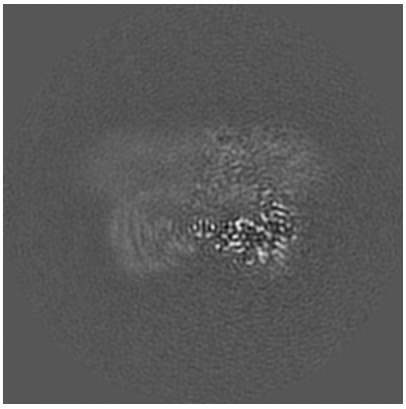


Z

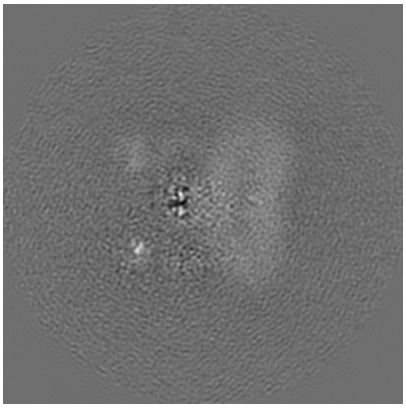
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

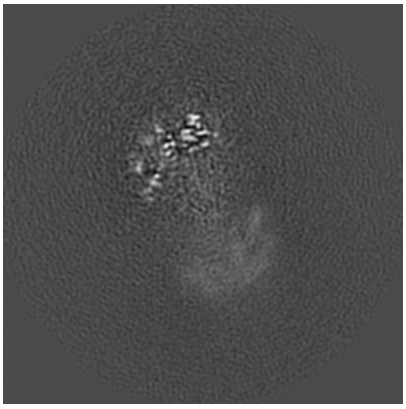
6.2.1 Primary map



X Index: 128



Y Index: 128

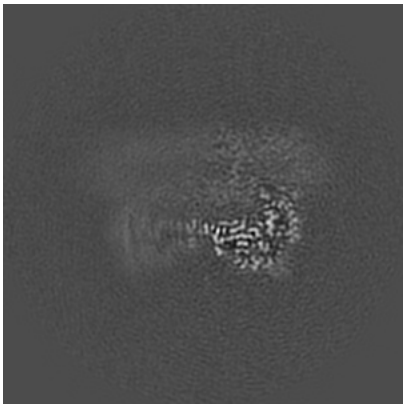


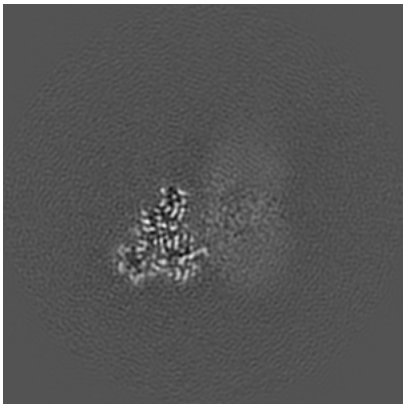
Z Index: 128

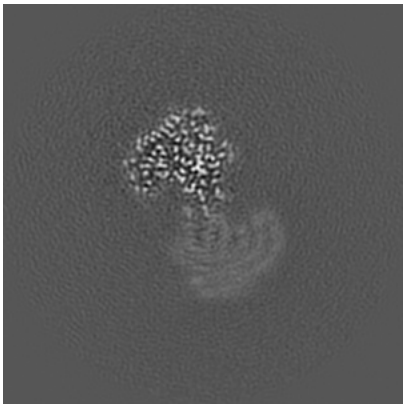
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 125

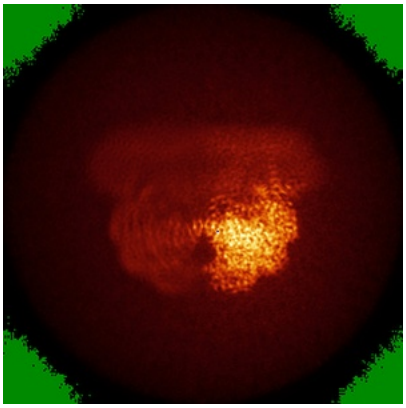

Y Index: 145

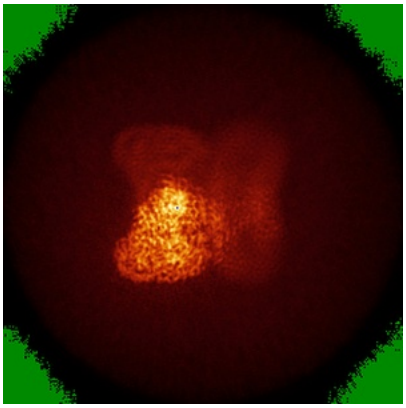

Z Index: 107

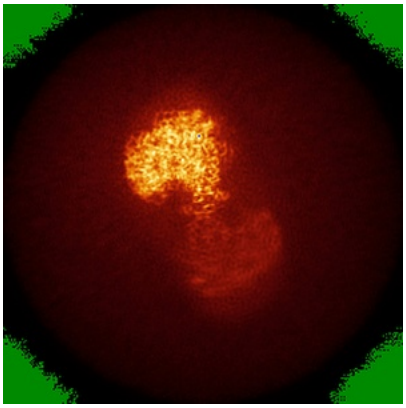
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

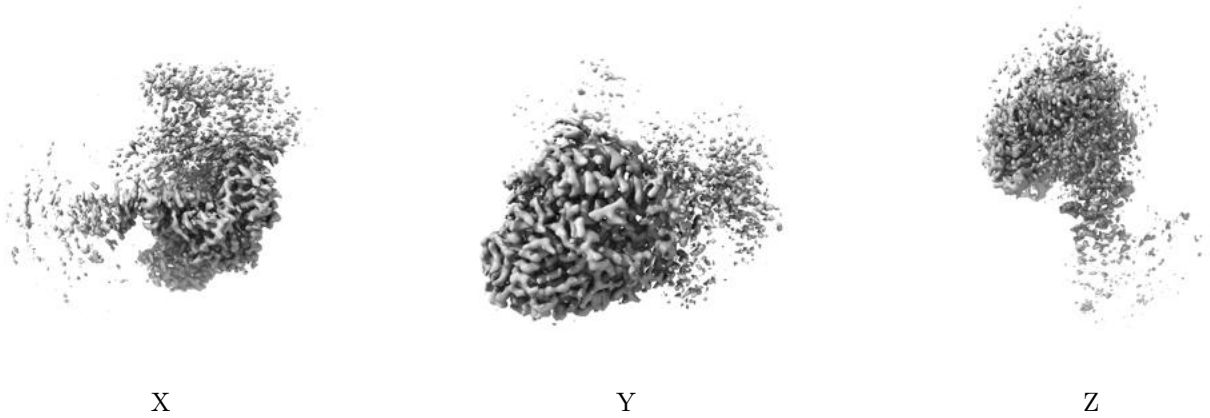

Y


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 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

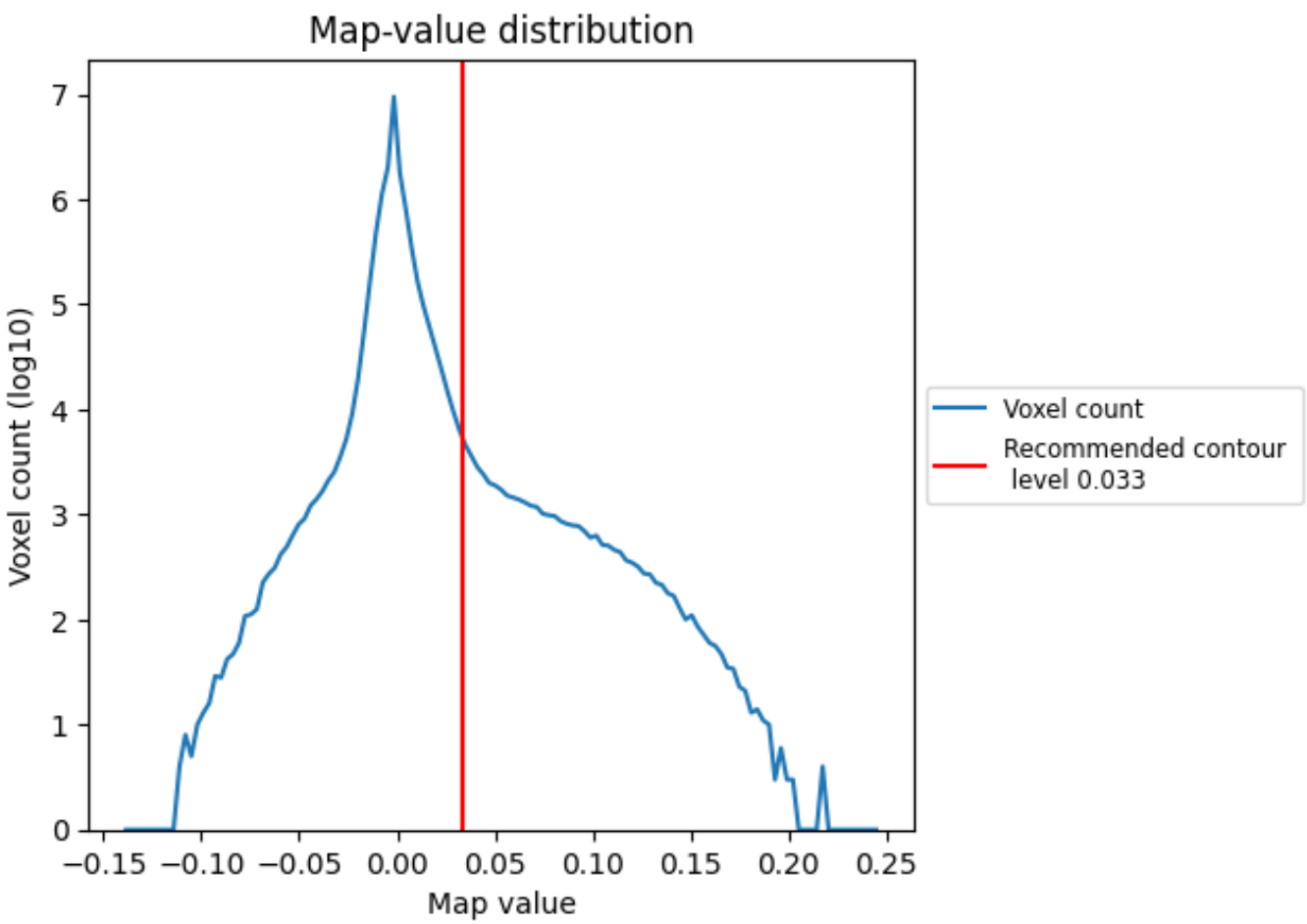
6.6 Mask visualisation (i)

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

7 Map analysis (i)

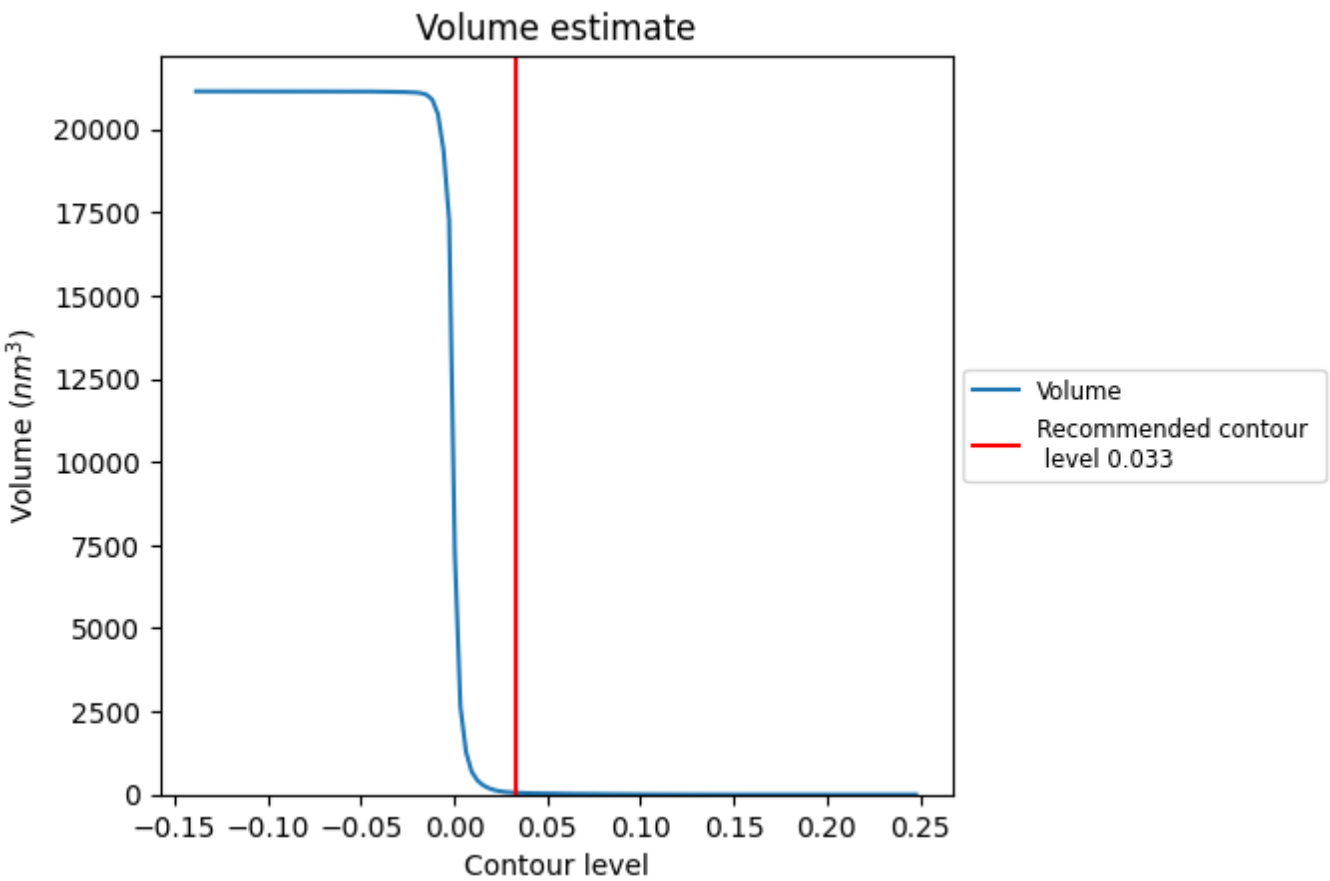
This section contains the results of statistical analysis of the map.

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.

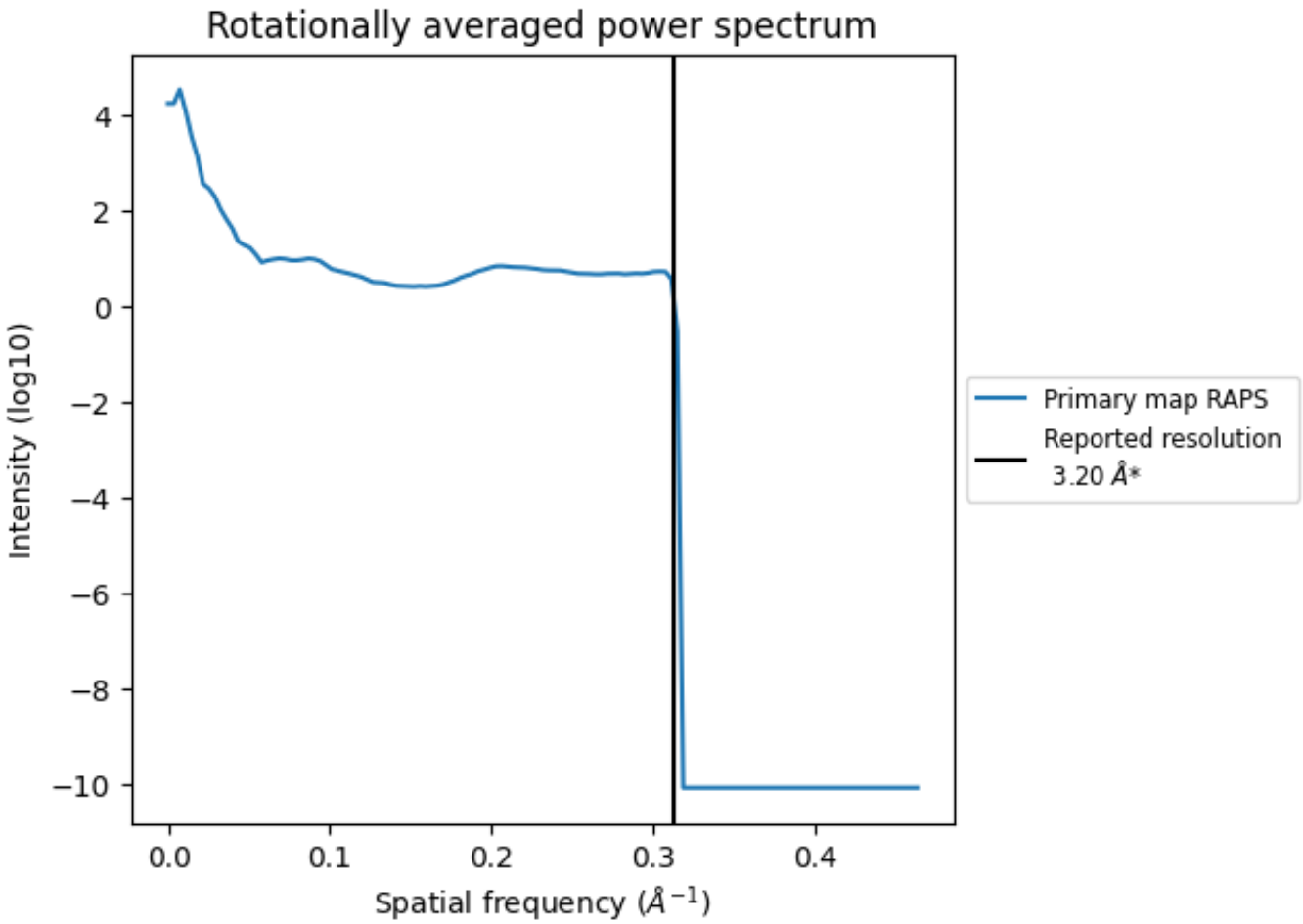
7.2 Volume estimate (i)



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 51 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 0.312 Å^{-1}

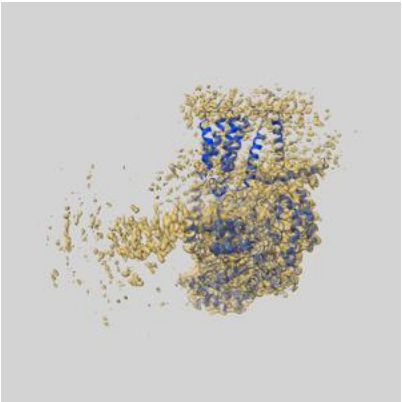
8 Fourier-Shell correlation (i)

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

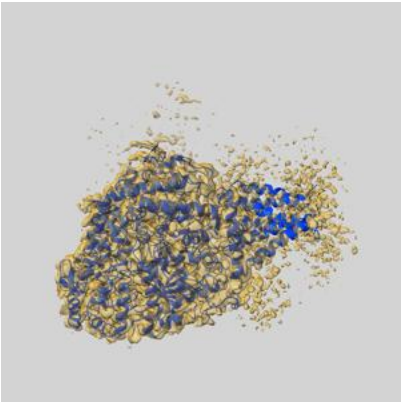
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30441 and PDB model 7CQI. Per-residue inclusion information can be found in section 3 on page 7.

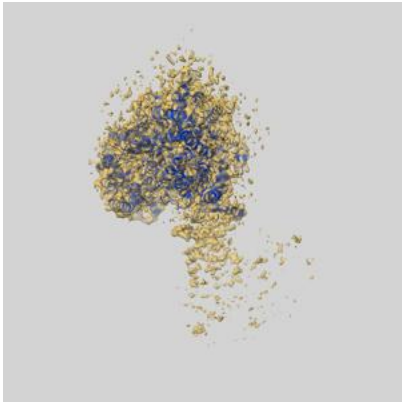
9.1 Map-model overlay (i)



X



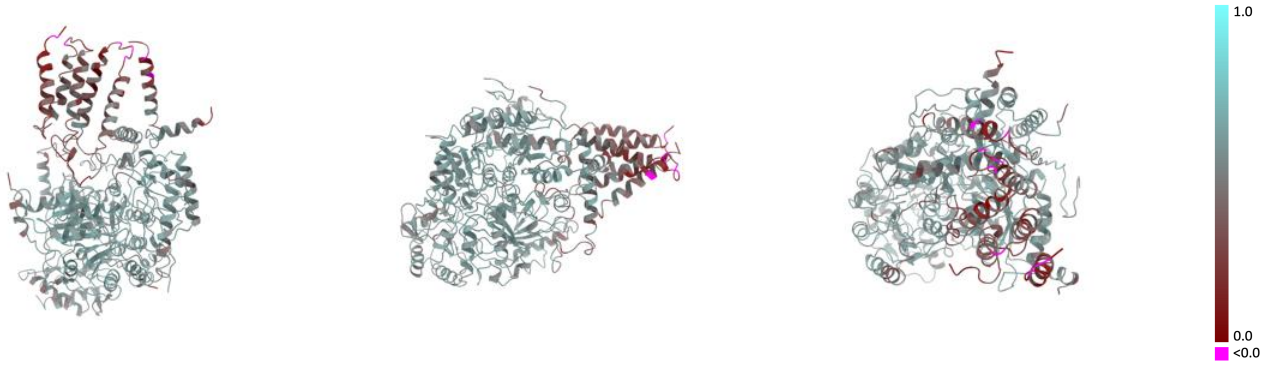
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033 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.

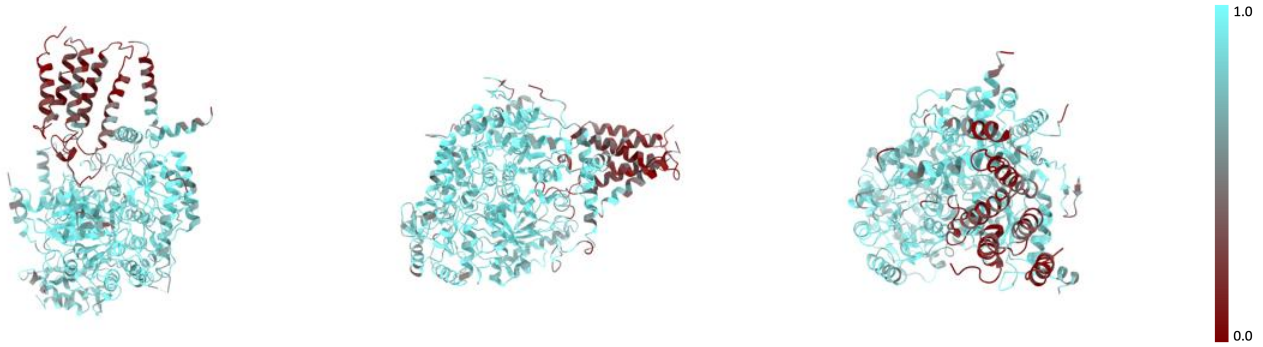
9.2 Q-score mapped to coordinate model (i)



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.

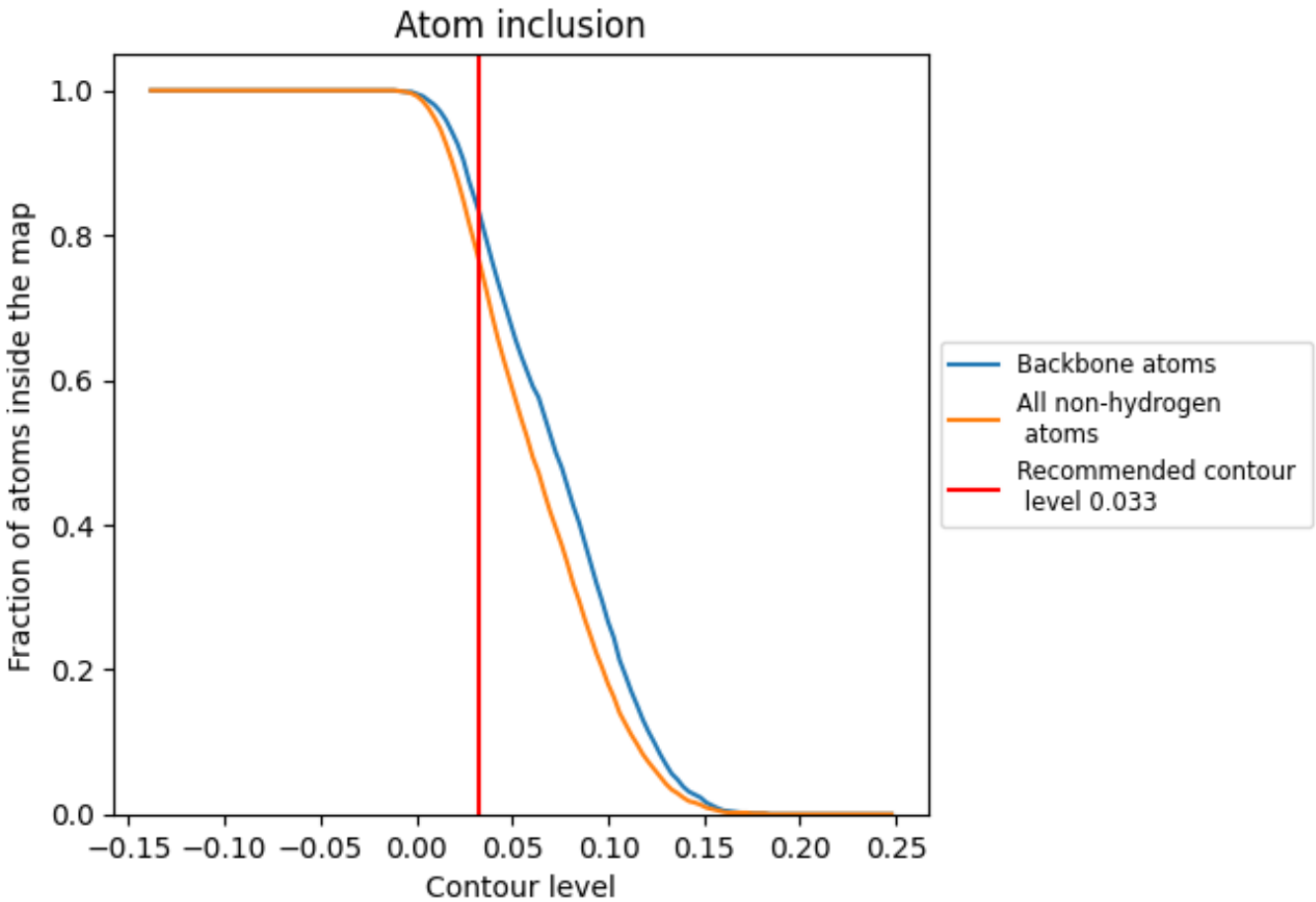
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.033).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5190
A	0.2350	0.3150
C	0.1570	0.2110
E	0.6230	0.4030
S	0.8590	0.5580
T	0.8580	0.5650