



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 04:55 PM UTC

PDB ID : 6ITC / pdb_00006itc
EMDB ID : EMD-9731
Title : Structure of a substrate engaged SecA-SecY protein translocation machine
Authors : Ma, C.Y.; Wu, X.F.; Sun, D.J.; Park, E.Y.; Rapoport, T.A.; Gao, N.; Long, L.
Deposited on : 2018-11-21
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

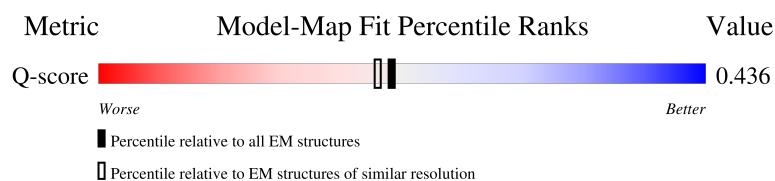
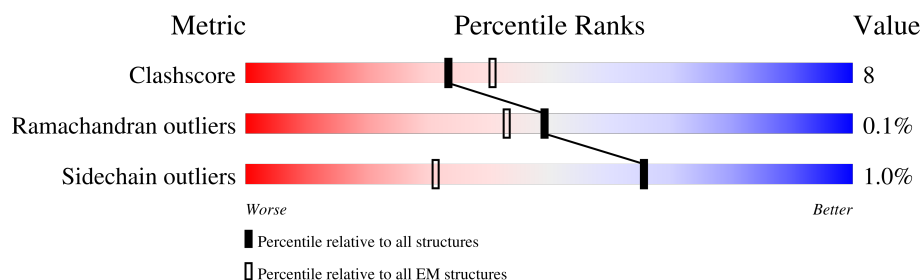
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	13836 (2.95 - 3.95)

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	780	5% 80% 18% ..
2	Y	424	16% 81% 17% ..
3	E	70	7% 76% 7% 17%
4	V	116	59% 74% 24% .

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Mol	Chain	Length	Quality of chain
5	B	59	
6	G	236	
7	C	112	

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
9	BEF	A	1002	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13844 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 Protein translocase subunit SecA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	765	Total	C	N	O	S	0	0
			6107	3820	1066	1188	33		

- Molecule 2 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	420	Total	C	N	O	S	0	0
			3275	2171	542	549	13		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	60	CYS	GLY	engineered mutation	UNP A4IJK8
Y	202	THR	GLN	engineered mutation	UNP A4IJK8
Y	210	GLY	GLU	engineered mutation	UNP A4IJK8
Y	211	GLY	ASN	engineered mutation	UNP A4IJK8
Y	?	-	VAL	deletion	UNP A4IJK8
Y	?	-	GLY	deletion	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8
Y	?	-	ASP	deletion	UNP A4IJK8
Y	?	-	LEU	deletion	UNP A4IJK8
Y	?	-	PHE	deletion	UNP A4IJK8
Y	213	ASN	ARG	engineered mutation	UNP A4IJK8

- Molecule 3 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	58	Total	C	N	O	0	0
			480	322	80	78		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLY	-	expression tag	UNP A4IJH4
E	62	GLY	-	expression tag	UNP A4IJH4
E	63	HIS	-	expression tag	UNP A4IJH4
E	64	HIS	-	expression tag	UNP A4IJH4
E	65	HIS	-	expression tag	UNP A4IJH4
E	66	HIS	-	expression tag	UNP A4IJH4
E	67	HIS	-	expression tag	UNP A4IJH4
E	68	HIS	-	expression tag	UNP A4IJH4
E	69	HIS	-	expression tag	UNP A4IJH4
E	70	HIS	-	expression tag	UNP A4IJH4

- Molecule 4 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	116	Total	C	N	O	S	0	0
			900	562	158	173	7		

- Molecule 5 is a protein called Translocating peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	43	Total	C	N	O	S	0	0
			312	194	53	64	1		

- Molecule 6 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	225	Total	C	N	O	S	1	0
			1802	1144	306	347	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	66	GYS	SER	chromophore	UNP P42212
G	66	GYS	TYR	chromophore	UNP P42212
G	66	GYS	GLY	chromophore	UNP P42212
G	80	ARG	GLN	engineered mutation	UNP P42212
G	99	SER	PHE	engineered mutation	UNP P42212
G	153	THR	MET	engineered mutation	UNP P42212
G	163	ALA	VAL	engineered mutation	UNP P42212

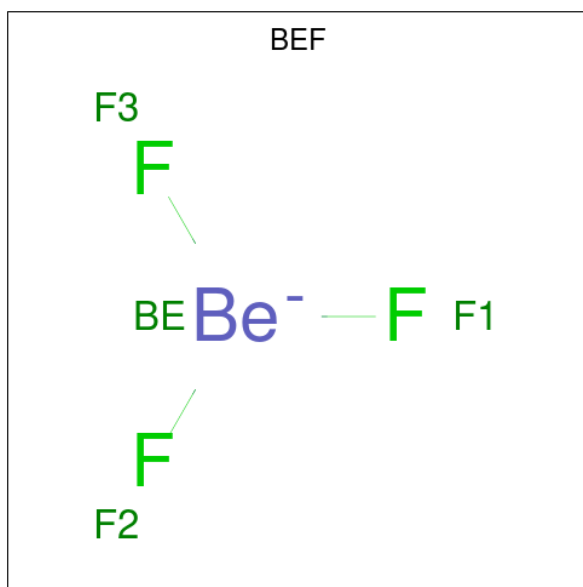
- Molecule 7 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	112	Total	C	N	O	S	0	0
			868	540	155	168	5		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

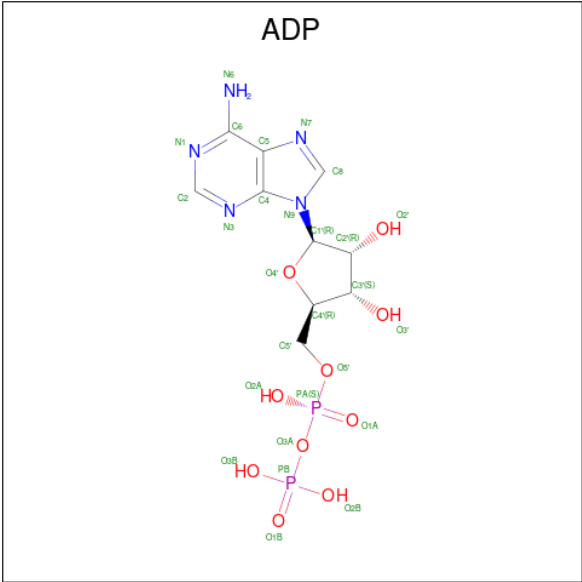
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mg	0
			1	1	

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



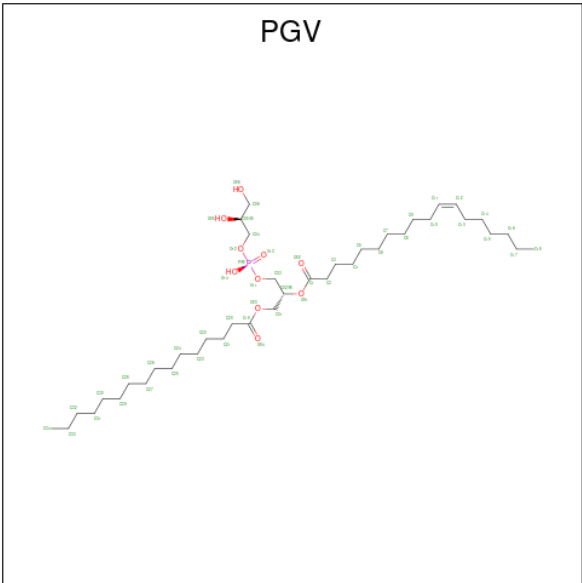
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	Be	F	0
			4	1	3	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).

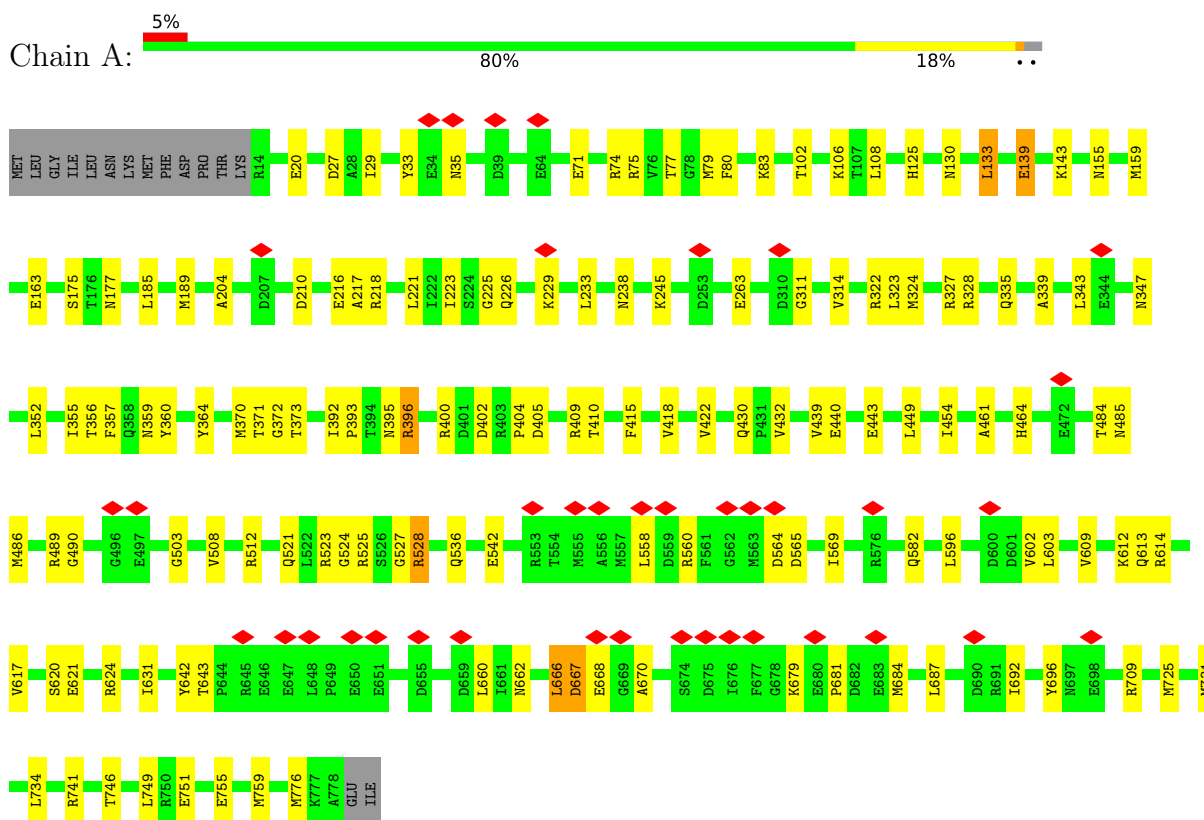


Mol	Chain	Residues	Atoms				AltConf
11	Y	1	Total	C	O	P	0
			27	18	8	1	
11	Y	1	Total	C	O	P	0
			41	30	10	1	

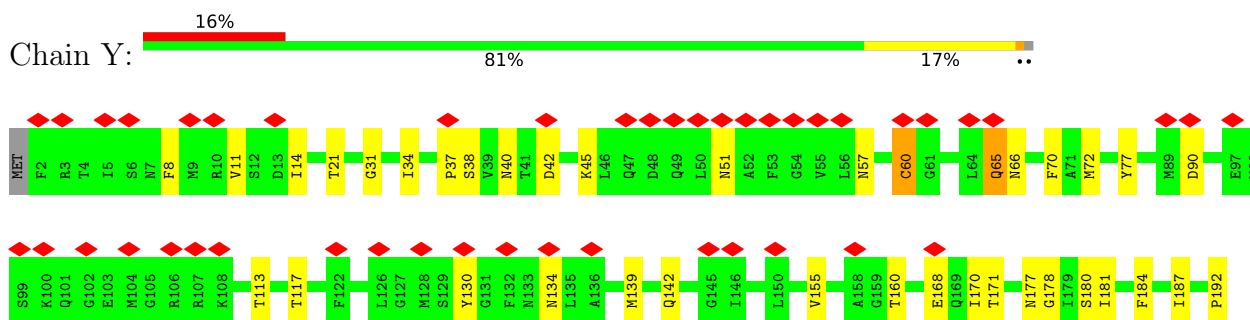
3 Residue-property plots

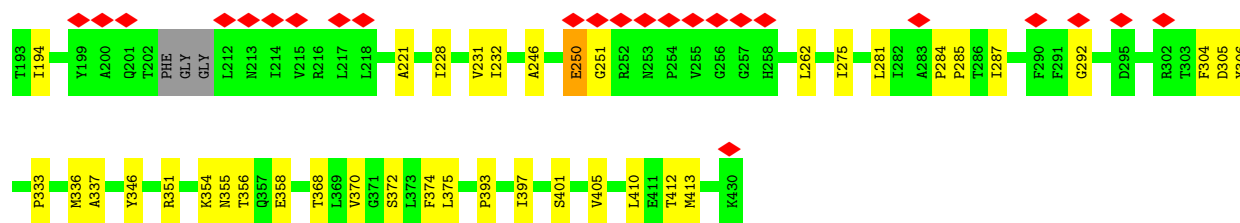
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

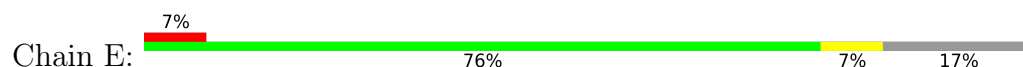


- Molecule 2: Protein translocase subunit SecY

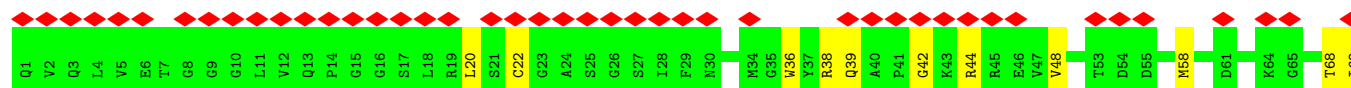
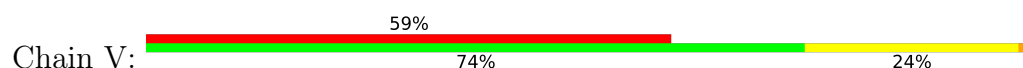




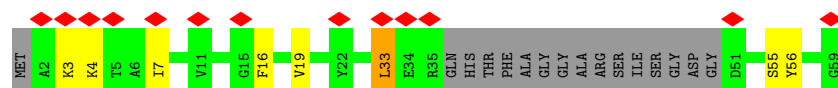
• Molecule 3: Protein translocase subunit SecE



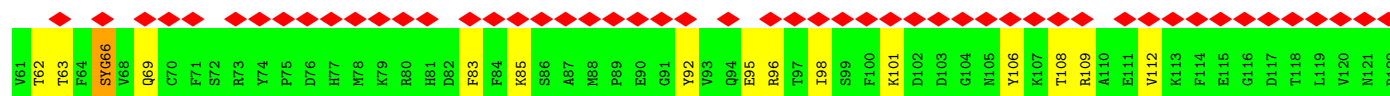
• Molecule 4: Nanobody



• Molecule 5: Translocating peptide

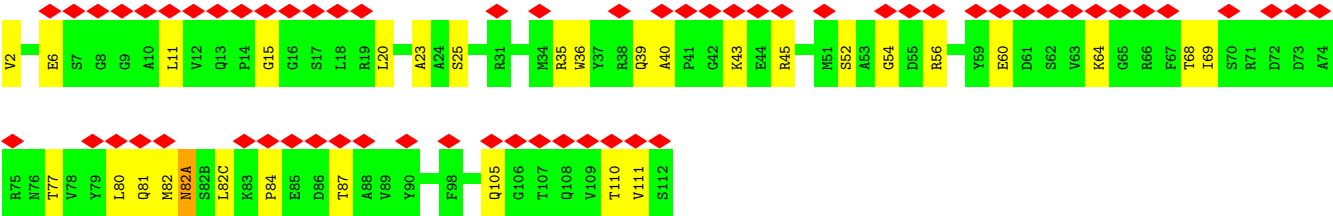


• Molecule 6: Green fluorescent protein





• Molecule 7: Nanobody



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0242	Depositor
Map size (Å)	251.99998, 251.99998, 251.99998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PGV, GYS, BEF, MG

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	0.75	0/6193	0.87	5/8329 (0.1%)
2	Y	0.64	1/3349 (0.0%)	0.92	9/4553 (0.2%)
3	E	0.47	0/490	0.69	0/664
4	V	0.37	0/919	0.80	4/1246 (0.3%)
5	B	0.42	0/317	1.03	2/427 (0.5%)
6	G	0.33	0/1824	0.70	2/2464 (0.1%)
7	C	0.37	0/887	0.74	1/1201 (0.1%)
All	All	0.62	1/13979 (0.0%)	0.85	23/18884 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	V	0	3
5	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	251	GLY	N-CA	-5.84	1.36	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	65	GLN	CB-CA-C	-8.69	100.53	111.22
1	A	666	LEU	N-CA-C	7.29	120.21	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	668	GLU	N-CA-CB	-7.16	100.14	110.80
2	Y	275	ILE	CA-C-N	-6.69	110.27	122.38
2	Y	275	ILE	C-N-CA	-6.69	110.27	122.38
2	Y	251	GLY	N-CA-C	6.50	124.00	115.36
4	V	101	VAL	CB-CA-C	6.47	121.90	111.29
2	Y	251	GLY	CA-C-N	6.33	133.63	121.54
2	Y	251	GLY	C-N-CA	6.33	133.63	121.54
2	Y	66	ASN	N-CA-CB	6.32	116.73	108.96
5	B	33	LEU	CA-C-N	6.03	130.29	121.31
5	B	33	LEU	C-N-CA	6.03	130.29	121.31
2	Y	250	GLU	N-CA-C	5.80	119.94	112.86
4	V	39	GLN	CA-CB-CG	5.68	125.46	114.10
2	Y	292	GLY	N-CA-C	-5.58	106.35	112.04
7	C	54	GLY	N-CA-C	5.32	117.76	110.58
1	A	35	ASN	N-CA-C	-5.21	107.94	114.56
1	A	133	LEU	CA-CB-CG	5.15	134.31	116.30
1	A	396	ARG	N-CA-CB	5.05	119.37	110.37
4	V	73	ASN	CA-C-N	5.05	131.19	121.54
4	V	73	ASN	C-N-CA	5.05	131.19	121.54
6	G	158	LYS	CA-C-N	5.05	131.18	121.54
6	G	158	LYS	C-N-CA	5.05	131.18	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	LYS	Peptide
5	B	33	LEU	Peptide
4	V	101	VAL	Peptide
4	V	42	GLY	Peptide
4	V	44	ARG	Peptide

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	6107	0	6094	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	3275	0	3441	58	0
3	E	480	0	507	4	0
4	V	900	0	870	18	0
5	B	312	0	290	4	0
6	G	1802	0	1744	44	0
7	C	868	0	825	19	0
8	A	1	0	0	0	0
9	A	4	0	0	2	0
10	A	27	0	12	2	0
11	Y	68	0	81	9	0
All	All	13844	0	13864	228	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 8.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:NH2	9:A:1002:BEF:F1	1.57	1.25
2:Y:354:LYS:NZ	2:Y:358:GLU:OE2	1.88	1.04
2:Y:65:GLN:CD	2:Y:65:GLN:O	2.04	1.00
1:A:525:ARG:NH1	9:A:1002:BEF:F2	1.82	1.00
1:A:662:ASN:O	1:A:667:ASP:O	1.79	1.00
2:Y:354:LYS:HZ2	2:Y:358:GLU:HG2	1.37	0.88
2:Y:354:LYS:NZ	2:Y:358:GLU:CG	2.42	0.83
2:Y:354:LYS:NZ	2:Y:358:GLU:CD	2.38	0.81
2:Y:354:LYS:HZ3	2:Y:358:GLU:CD	1.93	0.76
11:Y:502:PGV:O06	11:Y:502:PGV:O12	2.07	0.73
2:Y:354:LYS:HZ2	2:Y:358:GLU:CG	2.03	0.72
2:Y:354:LYS:NZ	2:Y:358:GLU:HG2	2.04	0.70
6:G:98:ILE:HB	6:G:106:TYR:HB2	1.74	0.69
2:Y:262:LEU:HD11	2:Y:336:MET:HE1	1.74	0.68
1:A:464:HIS:HB3	1:A:486:MET:HE1	1.76	0.66
1:A:322:ARG:HG2	1:A:486:MET:HE2	1.77	0.65
6:G:44:LEU:HD12	6:G:220:LEU:HD12	1.78	0.65
2:Y:397:ILE:CD1	11:Y:502:PGV:H012	2.27	0.64
2:Y:65:GLN:O	2:Y:65:GLN:CG	2.45	0.64
6:G:92:TYR:HB3	6:G:112:VAL:O	1.98	0.63
6:G:163:ALA:HB3	6:G:183:GLN:HB3	1.80	0.63
1:A:430:GLN:NE2	1:A:503:GLY:O	2.32	0.62
2:Y:40:ASN:ND2	4:V:58:MET:SD	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:6:GLU:O	7:C:105:GLN:NE2	2.32	0.61
2:Y:370:VAL:HG21	3:E:15:LEU:HD21	1.82	0.61
2:Y:397:ILE:HD12	11:Y:502:PGV:H012	1.81	0.61
1:A:461:ALA:HA	1:A:486:MET:HE3	1.82	0.61
2:Y:232:ILE:HD12	2:Y:410:LEU:HD11	1.83	0.61
1:A:263:GLU:OE2	2:Y:351:ARG:NH1	2.34	0.61
4:V:69:ILE:HA	4:V:79:TYR:O	2.01	0.60
11:Y:502:PGV:O13	11:Y:502:PGV:H02	2.02	0.60
1:A:238:ASN:ND2	1:A:339:ALA:O	2.34	0.60
4:V:22:CYS:O	4:V:77:THR:HA	2.02	0.60
1:A:409:ARG:HH21	1:A:565:ASP:H	1.50	0.60
1:A:409:ARG:NH2	1:A:564:ASP:OD1	2.36	0.59
6:G:66:GYS:O3	6:G:69:GLN:N	2.35	0.59
7:C:52:SER:OG	7:C:56:ARG:NH1	2.35	0.59
6:G:92:TYR:HD2	6:G:112:VAL:HB	1.68	0.58
4:V:70:SER:HB3	4:V:79:TYR:HB2	1.86	0.58
5:B:55:SER:OG	5:B:56:TYR:N	2.37	0.58
6:G:146:ASN:ND2	6:G:168:ARG:O	2.35	0.58
1:A:422:VAL:HG12	1:A:432:VAL:HG11	1.86	0.58
1:A:356:THR:OG1	1:A:359:ASN:ND2	2.37	0.57
1:A:155:ASN:HB3	1:A:175:SER:HB3	1.85	0.57
2:Y:38:SER:HB3	2:Y:142:GLN:HE21	1.68	0.57
6:G:92:TYR:OH	6:G:185:ASN:ND2	2.37	0.57
1:A:404:PRO:O	1:A:536:GLN:NE2	2.37	0.57
1:A:449:LEU:HD22	1:A:454:ILE:HD12	1.87	0.57
1:A:80:PHE:O	10:A:1003:ADP:N6	2.37	0.57
2:Y:90:ASP:HB3	5:B:3:LYS:HE2	1.87	0.57
1:A:621:GLU:O	1:A:709:ARG:NH2	2.38	0.56
6:G:66:GYS:O2	6:G:96:ARG:NH2	2.37	0.56
2:Y:231:VAL:HG23	2:Y:374:PHE:HZ	1.71	0.56
6:G:150:VAL:O	6:G:200:TYR:HA	2.05	0.56
7:C:15:GLY:H	7:C:82(C):LEU:HD12	1.70	0.56
1:A:328:ARG:NH2	1:A:335:GLN:OE1	2.39	0.56
4:V:98:GLN:NE2	4:V:102:MET:O	2.38	0.56
6:G:62:THR:O	6:G:96:ARG:NH1	2.39	0.55
2:Y:181:ILE:HD11	2:Y:412:THR:HG21	1.87	0.55
2:Y:221:ALA:HB2	11:Y:502:PGV:H92	1.89	0.55
5:B:16:PHE:HA	5:B:19:VAL:HG12	1.87	0.55
2:Y:168:GLU:HA	2:Y:171:THR:HG22	1.88	0.55
1:A:692:ILE:HG23	1:A:776:MET:HE1	1.89	0.54
1:A:314:VAL:HG11	1:A:323:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TYR:HH	1:A:364:TYR:HH	1.54	0.53
1:A:229:LYS:HB2	1:A:347:ASN:HD22	1.72	0.53
1:A:631:ILE:HD13	1:A:776:MET:HE3	1.89	0.53
2:Y:65:GLN:O	2:Y:65:GLN:OE1	2.27	0.52
4:V:36:TRP:HA	4:V:94:TYR:O	2.09	0.52
6:G:56:PRO:HB2	6:G:141:LEU:HD12	1.91	0.52
6:G:161:ILE:HB	6:G:185:ASN:HB2	1.90	0.52
1:A:218:ARG:HG3	1:A:596:LEU:HD21	1.90	0.52
6:G:19:ASP:O	6:G:124:GLU:HA	2.10	0.52
2:Y:177:ASN:HB3	2:Y:180:SER:HB2	1.92	0.52
6:G:59:THR:HG23	6:G:141:LEU:HD11	1.93	0.51
2:Y:333:PRO:HA	2:Y:336:MET:HG2	1.91	0.51
6:G:36:ASP:O	6:G:40:GLY:HA2	2.10	0.51
1:A:681:PRO:HA	1:A:684:MET:HG2	1.91	0.51
1:A:177:ASN:ND2	1:A:216:GLU:OE2	2.30	0.51
7:C:39:GLN:HB2	7:C:45:ARG:HG3	1.92	0.51
7:C:82:MET:SD	7:C:82(A):ASN:N	2.83	0.51
7:C:20:LEU:HB2	7:C:80:LEU:HB3	1.93	0.51
1:A:106:LYS:N	10:A:1003:ADP:O1B	2.39	0.51
1:A:71:GLU:OE1	1:A:75:ARG:NH1	2.44	0.50
1:A:74:ARG:HB2	1:A:80:PHE:HD1	1.77	0.50
1:A:402:ASP:OD1	1:A:402:ASP:N	2.42	0.50
7:C:84:PRO:HA	7:C:111:VAL:HB	1.93	0.50
1:A:226:GLN:NE2	1:A:347:ASN:OD1	2.45	0.50
2:Y:31:GLY:HA3	2:Y:70:PHE:HE2	1.77	0.50
6:G:42:LEU:HD23	6:G:44:LEU:HD11	1.94	0.50
6:G:155:ASP:O	6:G:159:ASN:HA	2.12	0.50
2:Y:57:ASN:HD22	2:Y:305:ASP:HA	1.77	0.50
4:V:93:TYR:O	4:V:110:GLY:HA2	2.12	0.50
1:A:642:TYR:HE2	1:A:660:LEU:HD13	1.76	0.50
1:A:400:ARG:HG3	1:A:527:GLY:HA2	1.94	0.49
1:A:614:ARG:HA	1:A:617:VAL:HG22	1.94	0.49
2:Y:42:ASP:N	2:Y:42:ASP:OD1	2.45	0.49
2:Y:246:ALA:HB2	2:Y:346:TYR:HE1	1.77	0.49
2:Y:130:TYR:O	2:Y:134:ASN:HB2	2.12	0.49
1:A:415:PHE:HA	1:A:418:VAL:HG12	1.94	0.49
2:Y:284:PRO:HA	2:Y:287:ILE:HG12	1.94	0.49
1:A:102:THR:HG21	1:A:521:GLN:HG3	1.94	0.49
1:A:395:ASN:O	1:A:396:ARG:HG3	2.13	0.49
4:V:22:CYS:HB3	4:V:78:VAL:HG22	1.95	0.49
6:G:170:ASN:OD1	7:C:35:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLY:H	1:A:352:LEU:HG	1.78	0.48
6:G:60:LEU:O	6:G:63:THR:OG1	2.31	0.48
6:G:96:ARG:HB2	6:G:108:THR:HG22	1.95	0.48
7:C:82(C):LEU:HD22	7:C:111:VAL:HG22	1.95	0.48
6:G:101:LYS:O	6:G:177:GLN:NE2	2.41	0.48
2:Y:11:VAL:HG13	2:Y:14:ILE:HG12	1.95	0.48
2:Y:21:THR:HG23	2:Y:170:ILE:HD11	1.94	0.48
2:Y:250:GLU:O	2:Y:250:GLU:HG2	2.14	0.47
1:A:609:VAL:O	1:A:613:GLN:HG2	2.14	0.47
2:Y:397:ILE:HD13	11:Y:502:PGV:H012	1.96	0.47
1:A:139:GLU:O	1:A:143:LYS:NZ	2.45	0.47
1:A:400:ARG:HH12	1:A:524:GLY:HA2	1.79	0.47
1:A:405:ASP:OD2	1:A:512:ARG:NH2	2.48	0.47
1:A:679:LYS:HE3	1:A:687:LEU:HD21	1.96	0.47
2:Y:77:TYR:HD1	2:Y:117:THR:HG21	1.80	0.47
2:Y:351:ARG:HB3	2:Y:355:ASN:HD22	1.79	0.47
7:C:2:VAL:N	7:C:25:SER:O	2.48	0.47
7:C:68:THR:HB	7:C:81:GLN:HB2	1.96	0.47
2:Y:285:PRO:HD3	2:Y:304:PHE:HD2	1.79	0.47
1:A:125:HIS:O	1:A:204:ALA:HA	2.15	0.47
1:A:512:ARG:NH1	1:A:582:GLN:OE1	2.42	0.47
7:C:87:THR:HG23	7:C:110:THR:HA	1.96	0.46
2:Y:51:ASN:HD22	2:Y:393:PRO:HB2	1.79	0.46
4:V:36:TRP:O	4:V:48:VAL:N	2.44	0.46
1:A:77:THR:HG23	1:A:79:MET:H	1.80	0.46
7:C:11:LEU:HD23	7:C:110:THR:HB	1.98	0.46
2:Y:192:PRO:HD3	3:E:41:THR:HG23	1.97	0.46
6:G:95:GLU:OE2	6:G:109:ARG:NH2	2.38	0.46
1:A:210:ASP:OD2	1:A:373:THR:OG1	2.34	0.46
1:A:666:LEU:O	1:A:667:ASP:OD1	2.33	0.46
1:A:33:TYR:HB3	1:A:71:GLU:HG3	1.97	0.46
1:A:130:ASN:ND2	1:A:322:ARG:HE	2.14	0.46
1:A:666:LEU:O	1:A:670:ALA:HB3	2.16	0.46
6:G:109:ARG:HB3	6:G:124:GLU:O	2.16	0.45
1:A:564:ASP:OD1	1:A:564:ASP:N	2.49	0.45
6:G:58:PRO:HB2	6:G:141:LEU:HD13	1.98	0.45
6:G:30[B]:SER:OG	6:G:31:GLY:N	2.45	0.45
6:G:66:GYS:HB2	6:G:69:GLN:HE21	1.82	0.45
1:A:409:ARG:HH11	1:A:569:ILE:HG12	1.81	0.45
4:V:90:THR:HG23	4:V:114:THR:HA	1.98	0.45
1:A:484:THR:OG1	1:A:485:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:281:LEU:HD21	2:Y:306:TYR:HB3	1.98	0.44
6:G:96:ARG:HD3	6:G:181:HIS:HD2	1.82	0.44
1:A:210:ASP:OD1	1:A:489:ARG:NH1	2.50	0.44
1:A:410:THR:OG1	1:A:542:GLU:OE2	2.28	0.44
6:G:83:PHE:HZ	6:G:187:PRO:HG3	1.81	0.44
6:G:213:GLU:OE1	6:G:217:HIS:ND1	2.50	0.44
1:A:759:MET:HE3	1:A:759:MET:HB2	1.69	0.44
6:G:25:HIS:HD2	6:G:54:PRO:HG3	1.83	0.44
6:G:28:SER:HB2	6:G:50:THR:HB	1.99	0.44
11:Y:501:PGV:C06	11:Y:501:PGV:P	3.05	0.44
6:G:56:PRO:O	6:G:59:THR:OG1	2.30	0.44
1:A:221:LEU:HB2	1:A:355:ILE:HG22	1.99	0.44
4:V:20:LEU:HD12	4:V:80:LEU:HD23	1.98	0.44
2:Y:37:PRO:HD3	2:Y:155:VAL:HG11	2.00	0.44
2:Y:187:ILE:HD13	2:Y:401:SER:HA	2.00	0.44
6:G:143:TYR:OH	6:G:208:SER:O	2.33	0.44
1:A:558:LEU:HA	1:A:560:ARG:HD2	2.00	0.44
6:G:132:GLU:HA	6:G:137:LEU:HD12	1.99	0.44
2:Y:177:ASN:HD22	2:Y:178:GLY:H	1.66	0.43
4:V:68:THR:HG22	4:V:81:GLN:HB3	1.99	0.43
1:A:643:THR:O	1:A:643:THR:OG1	2.35	0.43
6:G:98:ILE:HG12	6:G:181:HIS:CD2	2.53	0.43
6:G:171:ILE:HD11	6:G:177:GLN:HB2	2.00	0.43
1:A:666:LEU:O	1:A:667:ASP:CB	2.67	0.43
2:Y:194:ILE:HD12	2:Y:194:ILE:HA	1.90	0.43
2:Y:8:PHE:HA	2:Y:14:ILE:HD11	1.99	0.43
1:A:106:LYS:HB3	1:A:370:MET:SD	2.58	0.43
1:A:311:GLY:HA2	1:A:343:LEU:HD22	2.01	0.43
2:Y:45:LYS:HZ2	4:V:105:PRO:HD2	1.82	0.43
6:G:183:GLN:HE21	6:G:185:ASN:HD21	1.67	0.43
2:Y:413:MET:HE2	3:E:32:VAL:HG21	2.01	0.43
6:G:22:VAL:HG12	6:G:127:GLY:HA3	2.00	0.43
1:A:371:THR:OG1	1:A:372:GLY:N	2.52	0.43
1:A:159:MET:HE2	1:A:163:GLU:HB3	2.00	0.42
7:C:23:ALA:HA	7:C:77:THR:HG23	2.00	0.42
1:A:603:LEU:HD12	1:A:731:MET:HG2	2.02	0.42
2:Y:368:THR:O	2:Y:372:SER:HB2	2.20	0.42
4:V:70:SER:O	4:V:78:VAL:HA	2.20	0.42
6:G:169:HIS:O	6:G:176:VAL:HA	2.20	0.42
2:Y:170:ILE:HG23	2:Y:178:GLY:HA2	2.02	0.42
6:G:56:PRO:HG3	6:G:139:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:40:ALA:HB3	7:C:43:LYS:HB3	2.02	0.42
7:C:68:THR:O	7:C:80:LEU:HA	2.19	0.42
2:Y:72:MET:HB3	2:Y:160:THR:HG21	2.01	0.41
1:A:400:ARG:NH1	1:A:523:ARG:O	2.54	0.41
6:G:183:GLN:NE2	6:G:185:ASN:HD21	2.18	0.41
1:A:133:LEU:HD22	1:A:490:GLY:HA3	2.02	0.41
1:A:217:ALA:HA	1:A:357:PHE:HB2	2.02	0.41
1:A:392:ILE:HA	1:A:393:PRO:HD3	1.95	0.41
4:V:92:VAL:HA	4:V:112:GLN:HA	2.01	0.41
1:A:229:LYS:HB2	1:A:347:ASN:ND2	2.34	0.41
7:C:60:GLU:O	7:C:64:LYS:HG3	2.21	0.41
1:A:684:MET:HA	1:A:687:LEU:HG	2.01	0.41
4:V:38:ARG:HG2	4:V:93:TYR:HE1	1.85	0.41
1:A:418:VAL:HG23	1:A:508:VAL:HG11	2.02	0.41
1:A:624:ARG:HG3	1:A:696:TYR:HE2	1.85	0.41
2:Y:337:ALA:HB1	2:Y:356:THR:HG23	2.03	0.41
6:G:5:GLU:HB3	6:G:85:LYS:HG2	2.02	0.41
6:G:152:ILE:O	6:G:198:ASN:HA	2.21	0.41
1:A:741:ARG:O	1:A:746:THR:OG1	2.38	0.41
2:Y:170:ILE:HD13	2:Y:170:ILE:HG21	1.86	0.41
1:A:185:LEU:HB3	1:A:223:ILE:HD12	2.02	0.41
1:A:776:MET:HE2	1:A:776:MET:HB3	1.72	0.41
3:E:34:LEU:HA	3:E:37:VAL:HG12	2.02	0.41
1:A:751:GLU:O	1:A:755:GLU:HB2	2.21	0.41
2:Y:113:THR:O	2:Y:117:THR:HG23	2.21	0.41
1:A:189:MET:HE1	1:A:223:ILE:HG21	2.02	0.40
1:A:620:SER:O	1:A:709:ARG:NH1	2.54	0.40
5:B:4:LYS:O	5:B:7:ILE:HG22	2.21	0.40
1:A:612:LYS:HA	1:A:612:LYS:HD2	1.91	0.40
1:A:725:MET:HE2	1:A:725:MET:HB3	1.85	0.40
11:Y:502:PGV:H132	11:Y:502:PGV:H102	1.90	0.40
7:C:36:TRP:HD1	7:C:69:ILE:HD12	1.87	0.40
2:Y:60:CYS:O	11:Y:502:PGV:H042	2.21	0.40
1:A:27:ASP:HB2	1:A:83:LYS:HE3	2.03	0.40
1:A:324:MET:SD	1:A:327:ARG:HD3	2.61	0.40
2:Y:184:PHE:HE1	2:Y:405:VAL:HG13	1.87	0.40
4:V:93:TYR:O	4:V:110:GLY:CA	2.70	0.40
1:A:440:GLU:HA	1:A:443:GLU:HG2	2.04	0.40
2:Y:139:MET:HG3	4:V:58:MET:HB3	2.03	0.40
2:Y:228:ILE:HA	2:Y:231:VAL:HG12	2.03	0.40
7:C:82:MET:HE2	7:C:82:MET:HB2	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	763/780 (98%)	701 (92%)	61 (8%)	1 (0%)	48	79
2	Y	416/424 (98%)	379 (91%)	37 (9%)	0	100	100
3	E	56/70 (80%)	56 (100%)	0	0	100	100
4	V	114/116 (98%)	92 (81%)	22 (19%)	0	100	100
5	B	39/59 (66%)	31 (80%)	8 (20%)	0	100	100
6	G	221/236 (94%)	207 (94%)	14 (6%)	0	100	100
7	C	110/112 (98%)	97 (88%)	12 (11%)	1 (1%)	14	46
All	All	1719/1797 (96%)	1563 (91%)	154 (9%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	82(A)	ASN
1	A	528	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	656/670 (98%)	646 (98%)	10 (2%)	57	72
2	Y	352/354 (99%)	349 (99%)	3 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	53/63 (84%)	53 (100%)	0	100	100
4	V	96/97 (99%)	94 (98%)	2 (2%)	47	66
5	B	30/40 (75%)	30 (100%)	0	100	100
6	G	196/205 (96%)	196 (100%)	0	100	100
7	C	91/91 (100%)	91 (100%)	0	100	100
All	All	1474/1520 (97%)	1459 (99%)	15 (1%)	65	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	29	ILE
1	A	108	LEU
1	A	139	GLU
1	A	233	LEU
1	A	439	VAL
1	A	602	VAL
1	A	667	ASP
1	A	734	LEU
1	A	749	LEU
2	Y	34	ILE
2	Y	60	CYS
2	Y	375	LEU
4	V	102	MET
4	V	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	157	ASN
1	A	188	ASN
1	A	226	GLN
1	A	236	GLN
1	A	283	HIS
1	A	287	ASN
1	A	291	ASN
1	A	297	HIS
1	A	359	ASN

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Mol	Chain	Res	Type
1	A	463	ASN
1	A	464	HIS
1	A	513	HIS
1	A	536	GLN
1	A	613	GLN
1	A	702	GLN
1	A	747	ASN
2	Y	7	ASN
2	Y	134	ASN
2	Y	142	GLN
2	Y	143	ASN
2	Y	177	ASN
2	Y	244	GLN
2	Y	258	HIS
2	Y	267	ASN
2	Y	355	ASN
2	Y	387	ASN
3	E	6	ASN
4	V	76	ASN
4	V	83	ASN
6	G	25	HIS
6	G	69	GLN
6	G	105	ASN
6	G	144	ASN
6	G	181	HIS
6	G	185	ASN
7	C	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GYS	G	66	6	20,22,23	3.32	6 (30%)	25,30,32	3.31	8 (32%)

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	GYS	G	66	6	-	1/10/29/30	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	66	GYS	CB2-CA2	13.02	1.47	1.35
6	G	66	GYS	CA2-C2	-3.79	1.44	1.48
6	G	66	GYS	C2-N3	-3.65	1.31	1.40
6	G	66	GYS	C1-N2	3.09	1.36	1.32
6	G	66	GYS	O2-C2	2.51	1.28	1.23
6	G	66	GYS	CA2-N2	-2.22	1.33	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	66	GYS	O2-C2-CA2	-11.67	123.57	131.02
6	G	66	GYS	CA2-C2-N3	7.08	109.45	103.50
6	G	66	GYS	C2-N3-C1	-5.72	105.42	108.07
6	G	66	GYS	CB2-CA2-C2	3.61	126.74	122.36
6	G	66	GYS	C2-CA2-N2	-2.84	106.91	108.95
6	G	66	GYS	CG2-CB2-CA2	-2.53	126.85	129.87
6	G	66	GYS	CD2-CG2-CD1	2.22	120.94	117.65
6	G	66	GYS	CA1-C1-N3	2.11	127.59	124.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	66	GYS	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	66	GYS	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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$
11	PGV	Y	501	-	26,26,50	0.92	1 (3%)	28,30,56	0.89	1 (3%)
9	BEF	A	1002	-	0,3,3	-	-	-	-	-
10	ADP	A	1003	8	28,29,29	1.42	5 (17%)	43,45,45	1.85	11 (25%)
11	PGV	Y	502	-	40,40,50	1.04	2 (5%)	43,46,56	1.11	3 (6%)

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
11	PGV	Y	501	-	-	15/28/28/55	-
10	ADP	A	1003	8	-	5/16/32/32	0/3/3/3
11	PGV	Y	502	-	-	27/45/45/55	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	502	PGV	O03-C19	4.32	1.45	1.33
11	Y	501	PGV	O03-C19	4.27	1.45	1.33
11	Y	502	PGV	O01-C1	4.13	1.46	1.34
10	A	1003	ADP	C5-C4	3.61	1.45	1.39
10	A	1003	ADP	C5-N7	-2.86	1.33	1.39
10	A	1003	ADP	C4-N9	-2.82	1.31	1.37
10	A	1003	ADP	C8-N9	-2.29	1.33	1.37
10	A	1003	ADP	C5-C6	2.11	1.46	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1003	ADP	C5-C4-N3	-5.36	119.33	126.72
10	A	1003	ADP	N3-C4-N9	4.19	134.30	127.17
11	Y	502	PGV	O01-C1-C2	4.01	120.16	111.48
10	A	1003	ADP	C2-N3-C4	3.64	120.72	111.83
10	A	1003	ADP	N3-C2-N1	-3.40	123.43	128.58
10	A	1003	ADP	C4-C5-N7	-3.35	106.75	110.58
10	A	1003	ADP	C4-N9-C8	3.13	109.03	105.74
11	Y	502	PGV	O03-C19-C20	2.73	120.17	111.83
11	Y	501	PGV	O03-C19-C20	2.73	120.15	111.83
10	A	1003	ADP	C2'-C3'-C4'	2.58	107.59	102.61
11	Y	502	PGV	C02-O01-C1	-2.47	111.89	117.80
10	A	1003	ADP	C5-N7-C8	2.40	107.22	103.45
10	A	1003	ADP	C6-C5-N7	2.35	136.62	132.09
10	A	1003	ADP	N9-C8-N7	-2.33	110.63	113.94
10	A	1003	ADP	O2A-PA-O1A	2.02	121.85	112.44

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1003	ADP	C5'-O5'-PA-O1A
10	A	1003	ADP	C5'-O5'-PA-O3A
11	Y	501	PGV	C04-O12-P-O11
11	Y	501	PGV	C04-O12-P-O13
11	Y	501	PGV	C04-O12-P-O14
11	Y	502	PGV	C03-O11-P-O12
11	Y	502	PGV	C03-O11-P-O13
11	Y	502	PGV	C02-C03-O11-P
11	Y	502	PGV	C2-C1-O01-C02
11	Y	501	PGV	O04-C19-O03-C01

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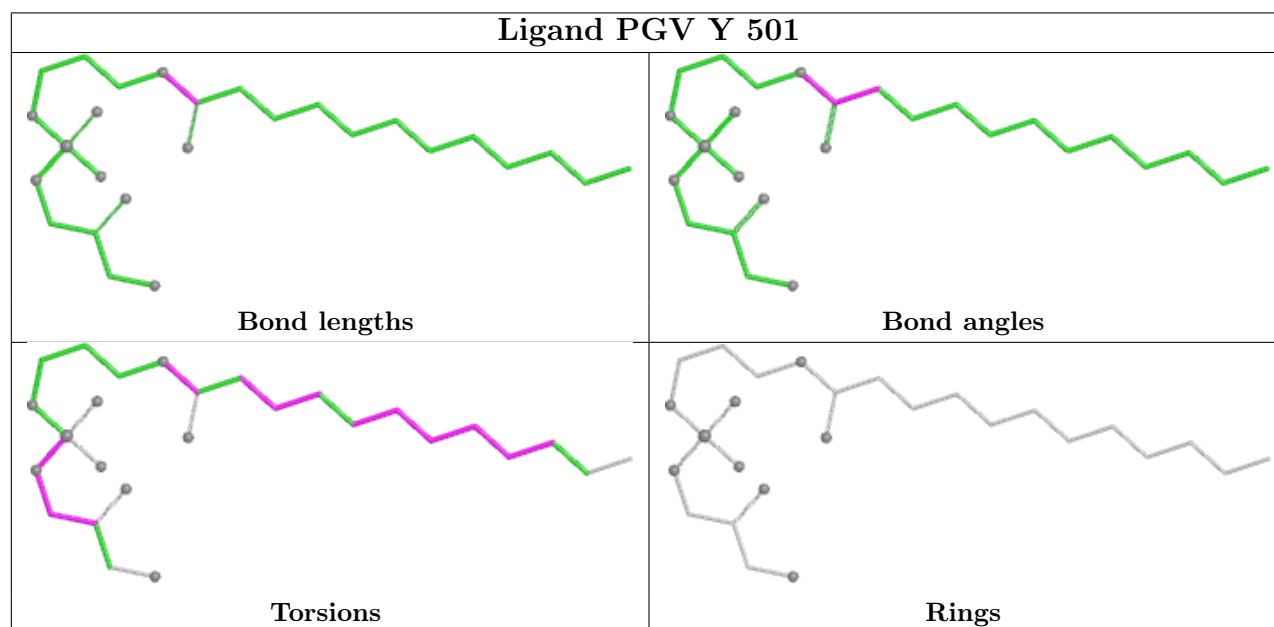
Mol	Chain	Res	Type	Atoms
11	Y	502	PGV	O02-C1-O01-C02
11	Y	501	PGV	C20-C19-O03-C01
10	A	1003	ADP	O4'-C4'-C5'-O5'
10	A	1003	ADP	C3'-C4'-C5'-O5'
11	Y	502	PGV	C19-C20-C21-C22
11	Y	502	PGV	C04-C05-C06-O06
11	Y	502	PGV	C21-C22-C23-C24
11	Y	501	PGV	C23-C24-C25-C26
11	Y	501	PGV	C25-C26-C27-C28
11	Y	502	PGV	C6-C7-C8-C9
11	Y	502	PGV	C22-C23-C24-C25
11	Y	502	PGV	C11-C12-C13-C14
11	Y	501	PGV	C19-C20-C21-C22
11	Y	502	PGV	C20-C19-O03-C01
11	Y	502	PGV	C7-C8-C9-C10
11	Y	501	PGV	C24-C25-C26-C27
11	Y	502	PGV	C25-C26-C27-C28
11	Y	502	PGV	O04-C19-O03-C01
11	Y	502	PGV	C24-C25-C26-C27
11	Y	502	PGV	C03-C02-O01-C1
11	Y	502	PGV	C20-C21-C22-C23
10	A	1003	ADP	C5'-O5'-PA-O2A
11	Y	502	PGV	C03-O11-P-O14
11	Y	502	PGV	C04-O12-P-O13
11	Y	501	PGV	C05-C04-O12-P
11	Y	502	PGV	O05-C05-C06-O06
11	Y	502	PGV	C1-C2-C3-C4
11	Y	502	PGV	C2-C3-C4-C5
11	Y	501	PGV	O12-C04-C05-C06
11	Y	502	PGV	C4-C5-C6-C7
11	Y	501	PGV	O12-C04-C05-O05
11	Y	502	PGV	O01-C1-C2-C3
11	Y	501	PGV	C20-C21-C22-C23
11	Y	501	PGV	C22-C23-C24-C25
11	Y	501	PGV	C26-C27-C28-C29
11	Y	502	PGV	O02-C1-C2-C3
11	Y	502	PGV	O03-C01-C02-O01

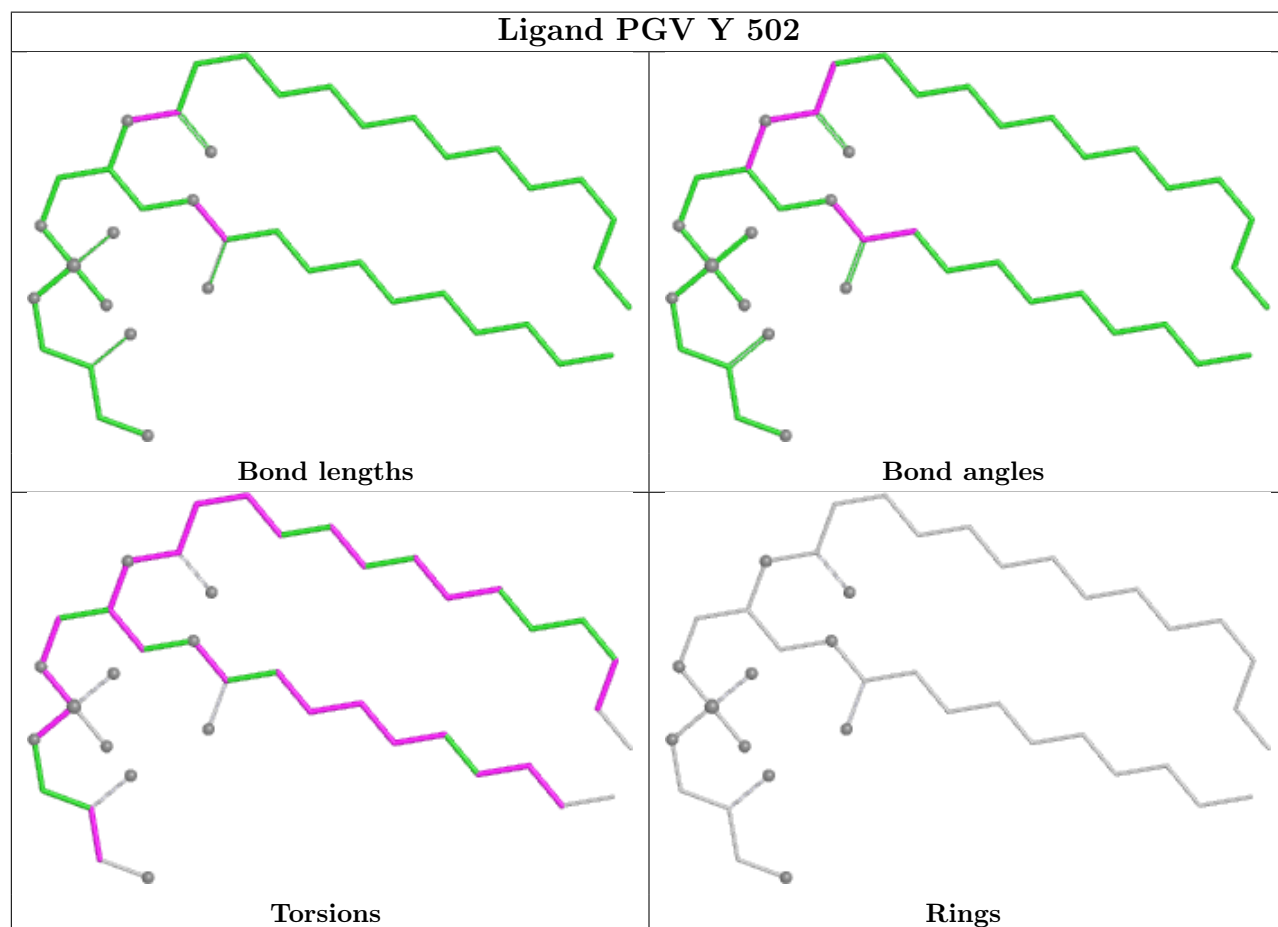
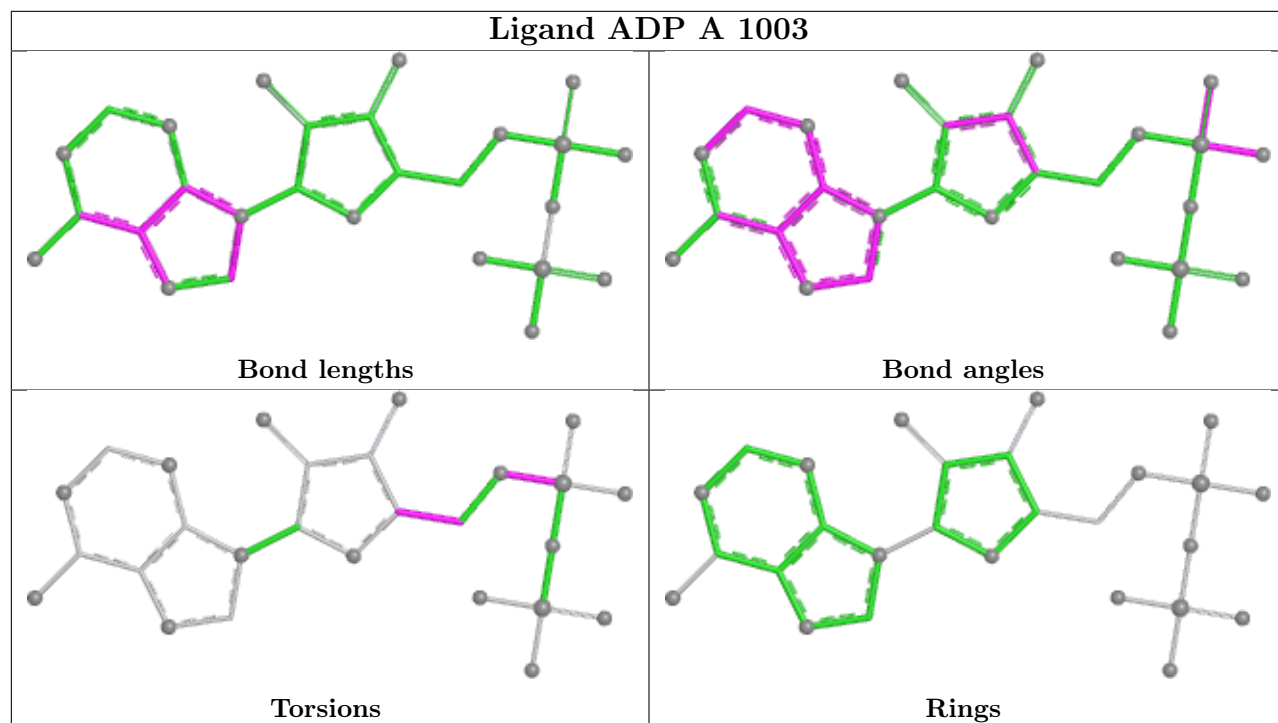
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Y	501	PGV	1	0
9	A	1002	BEF	2	0
10	A	1003	ADP	2	0
11	Y	502	PGV	8	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.

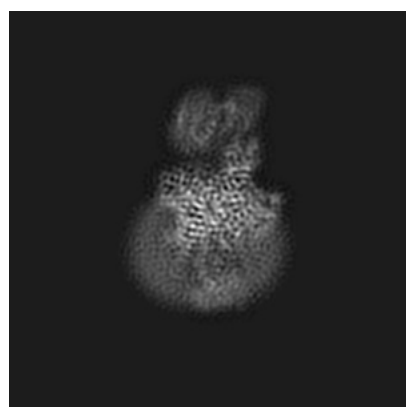
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9731. These allow visual inspection of the internal detail of the map and identification of artifacts.

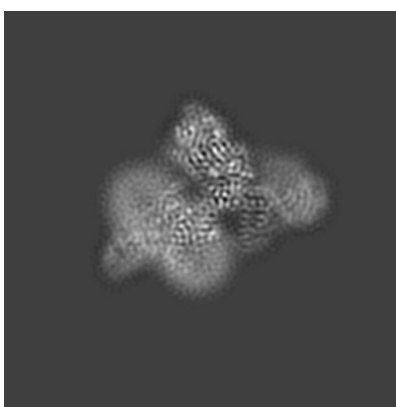
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

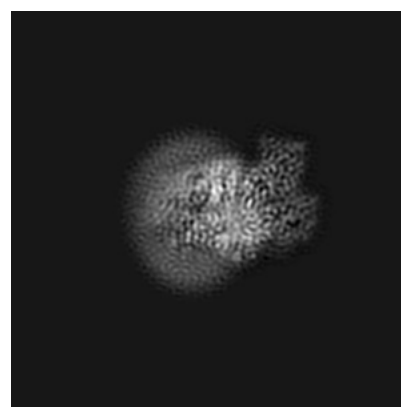
6.1.1 Primary map



X



Y

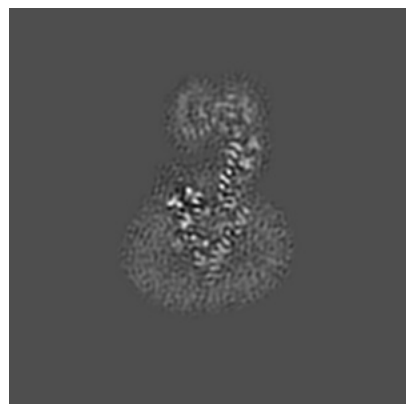


Z

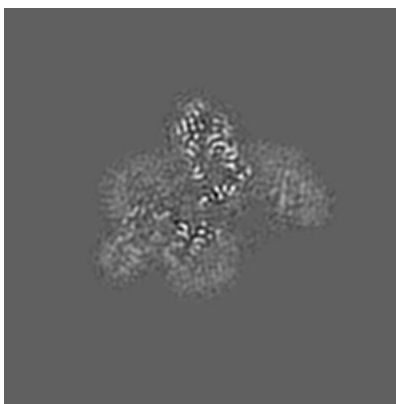
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

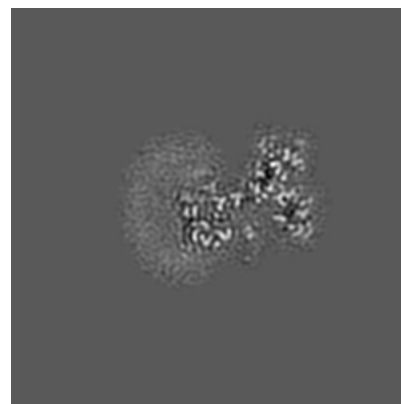
6.2.1 Primary map



X Index: 120



Y Index: 120

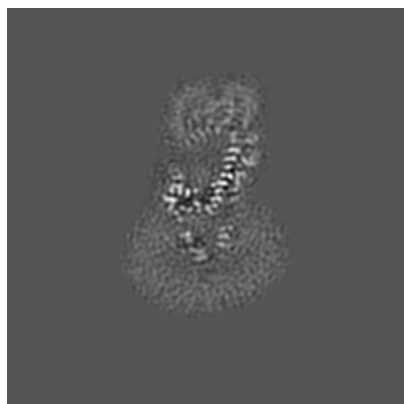


Z Index: 120

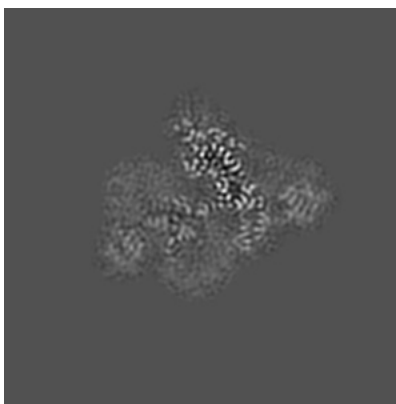
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

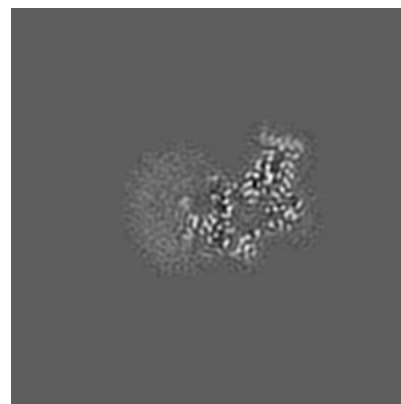
6.3.1 Primary map



X Index: 124



Y Index: 132

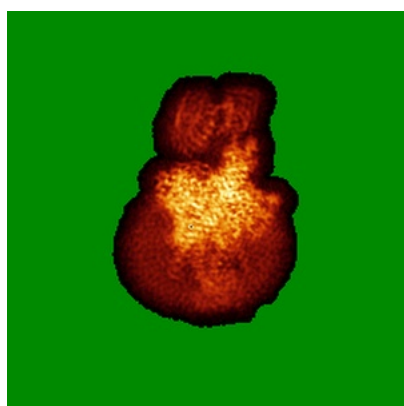


Z Index: 127

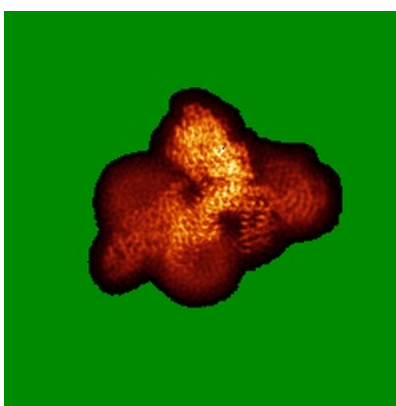
The images above show the largest variance slices of the map in three orthogonal directions.

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

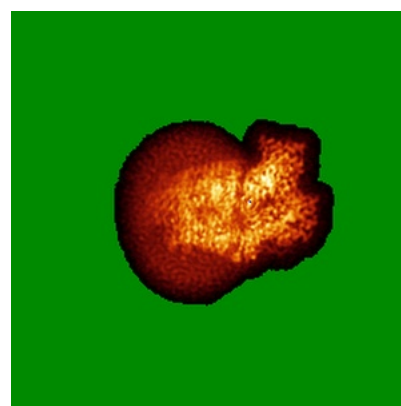
6.4.1 Primary map



X



Y

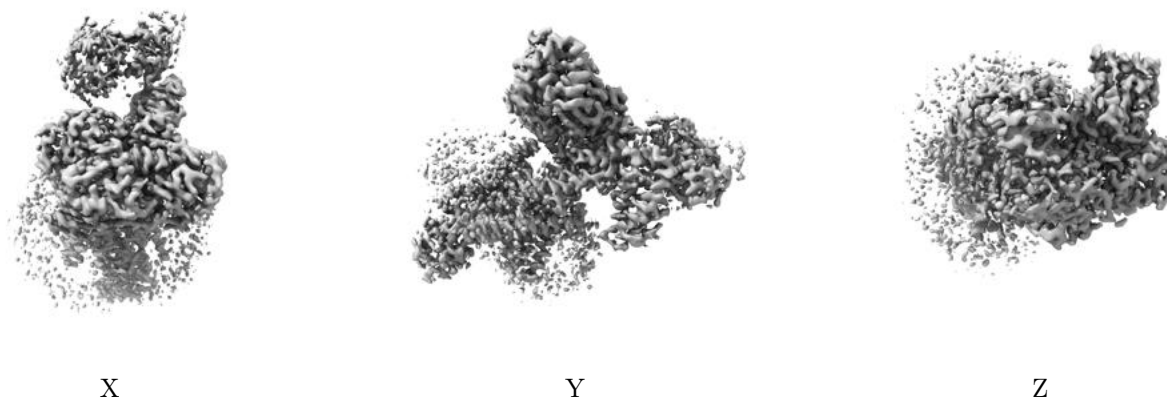


Z

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 0.0242. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

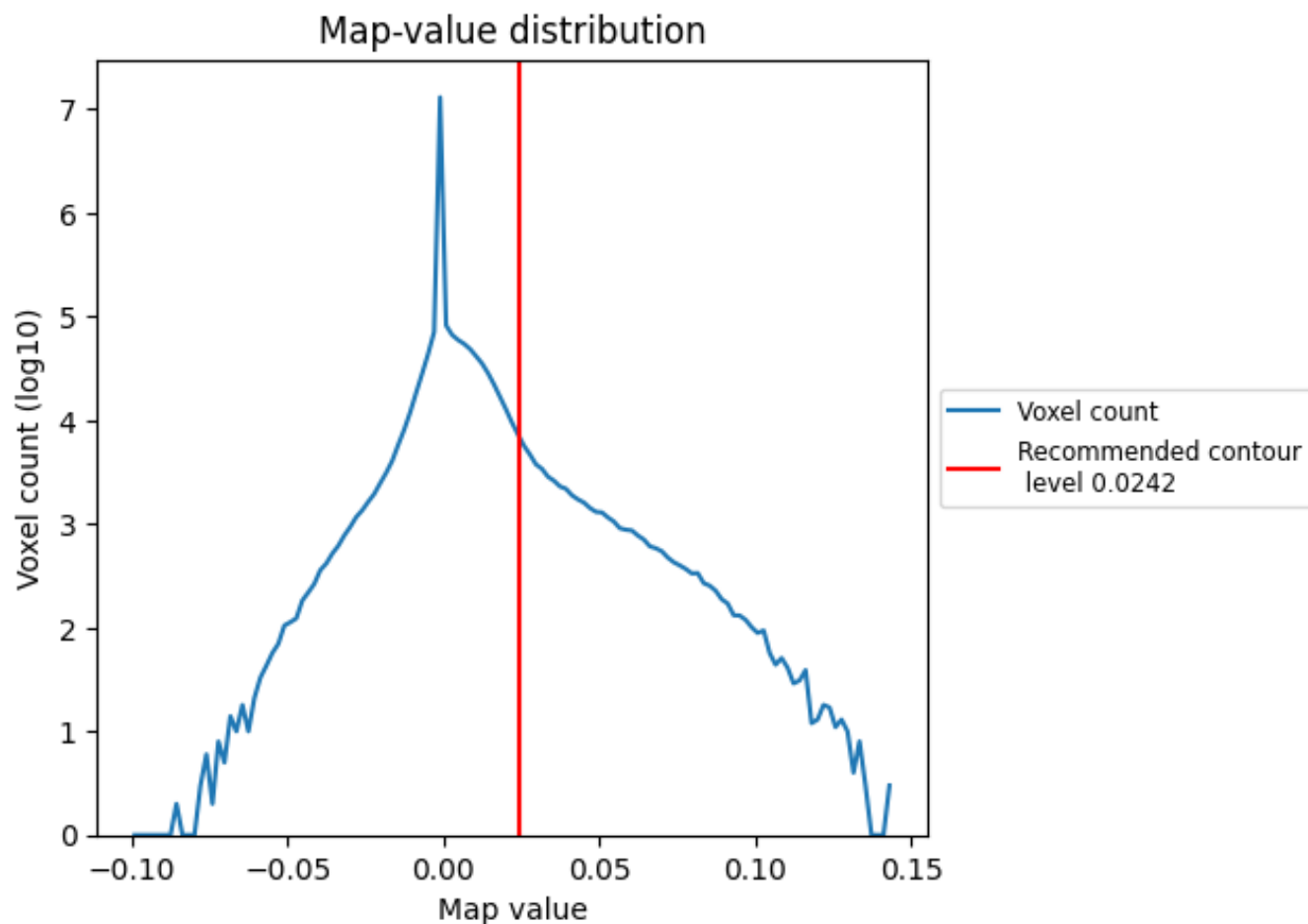
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

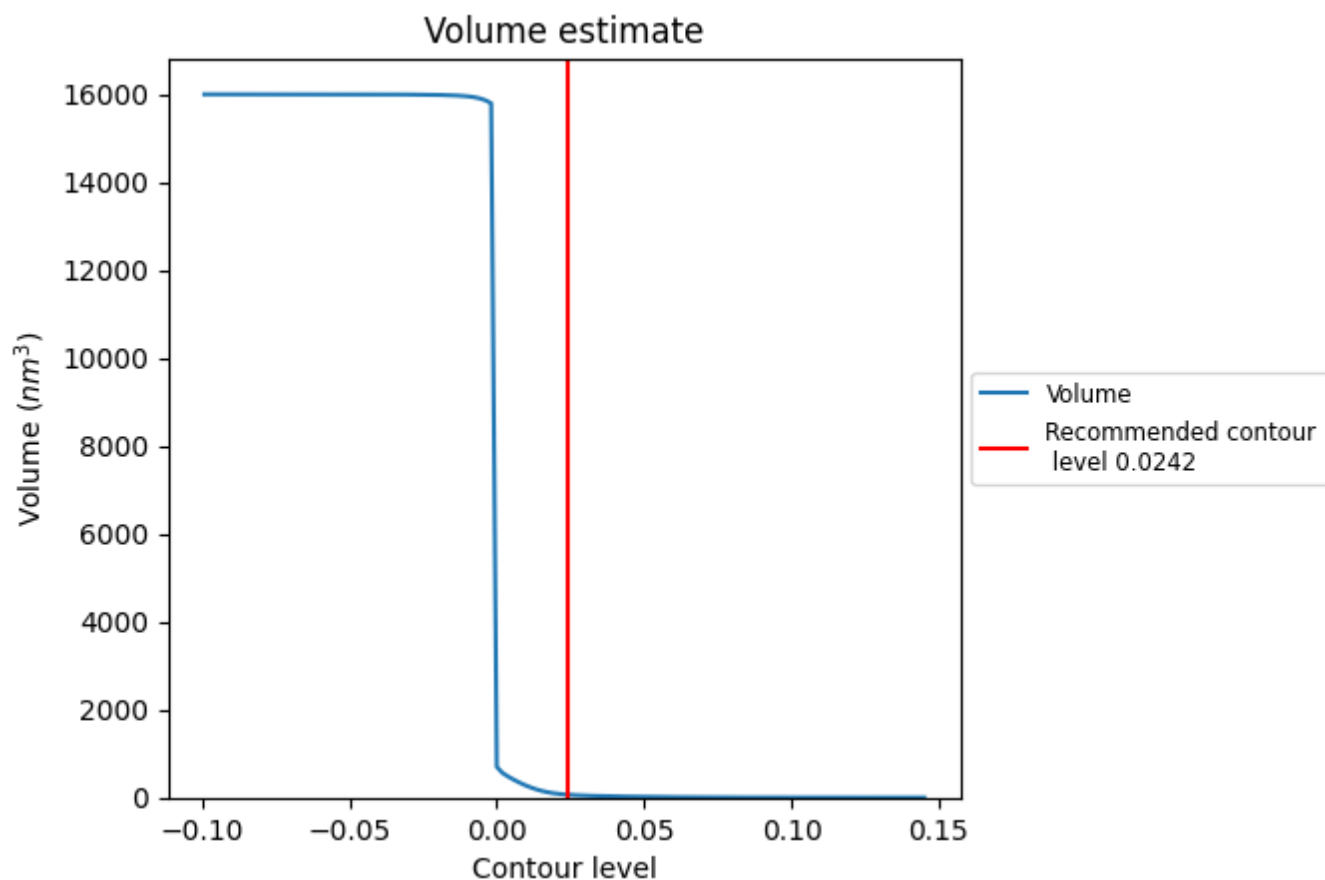
This section contains the results of statistical analysis of the map.

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.

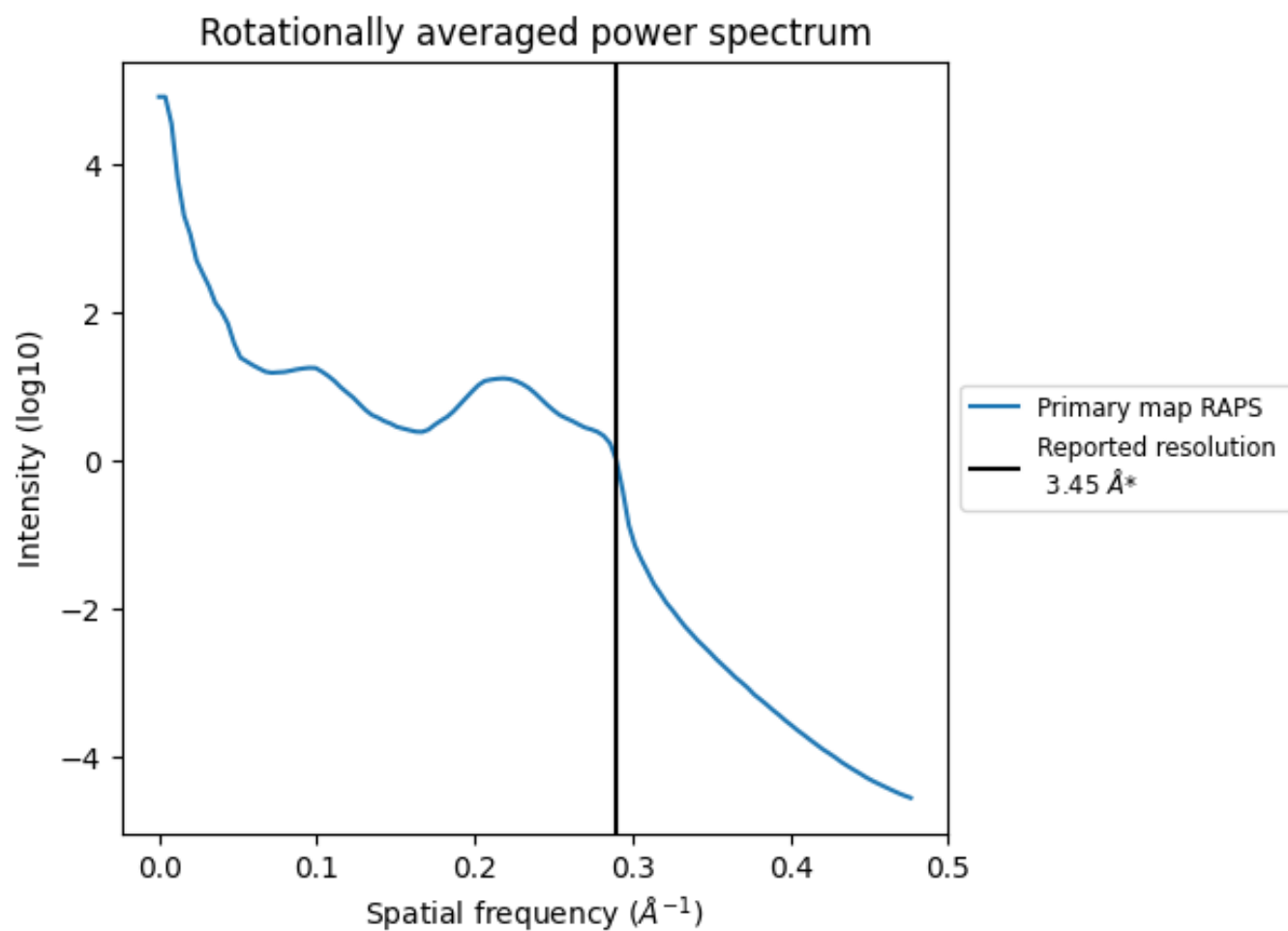
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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 0.290 Å⁻¹

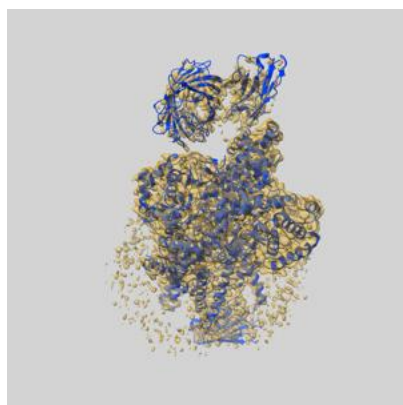
8 Fourier-Shell correlation

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

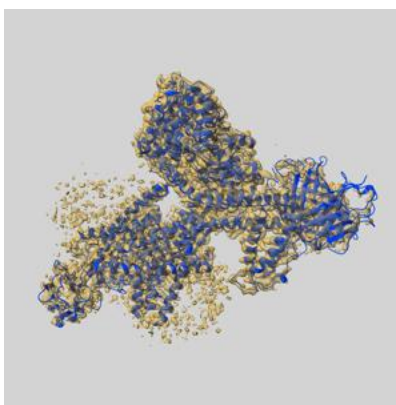
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9731 and PDB model 6ITC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

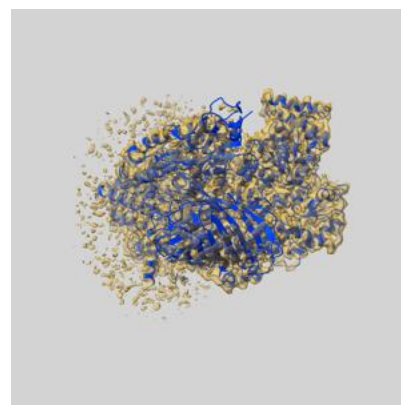
9.1 Map-model overlay [i](#)



X



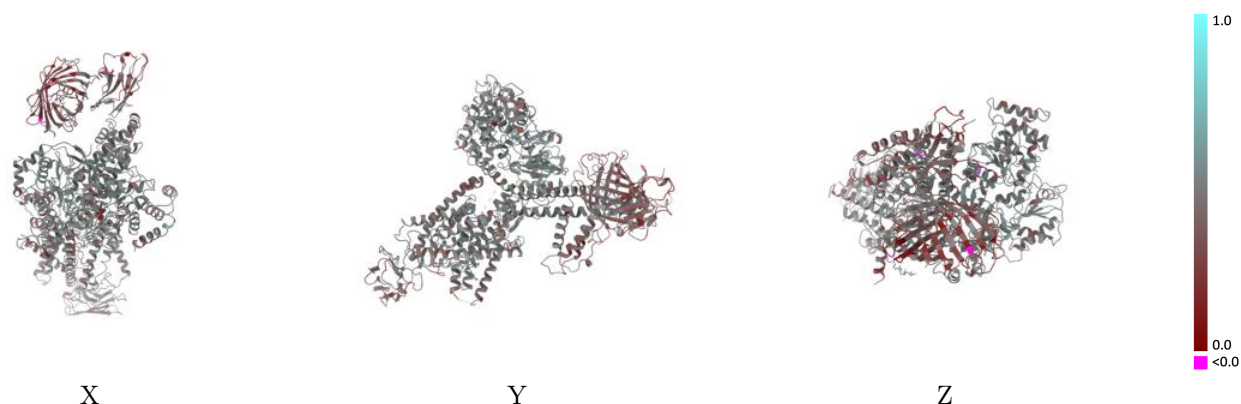
Y



Z

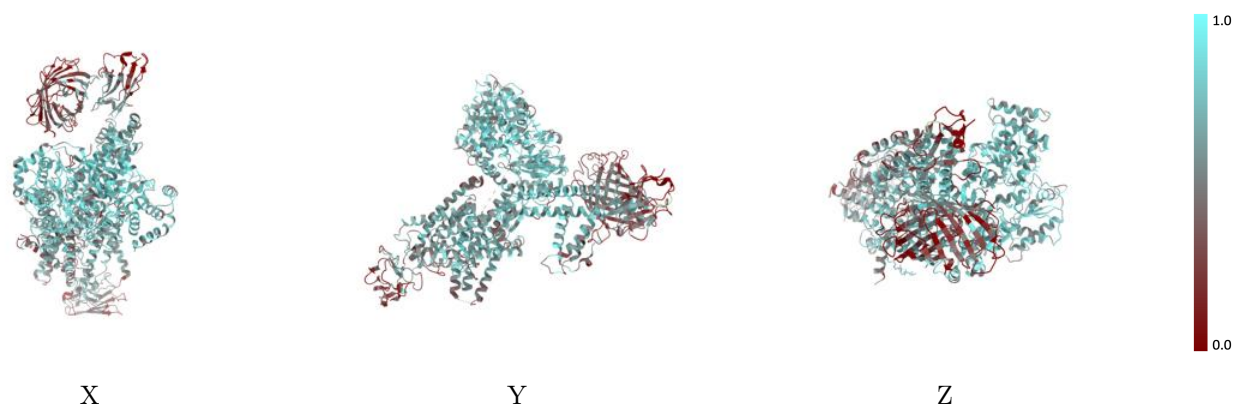
The images above show the 3D surface view of the map at the recommended contour level 0.0242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



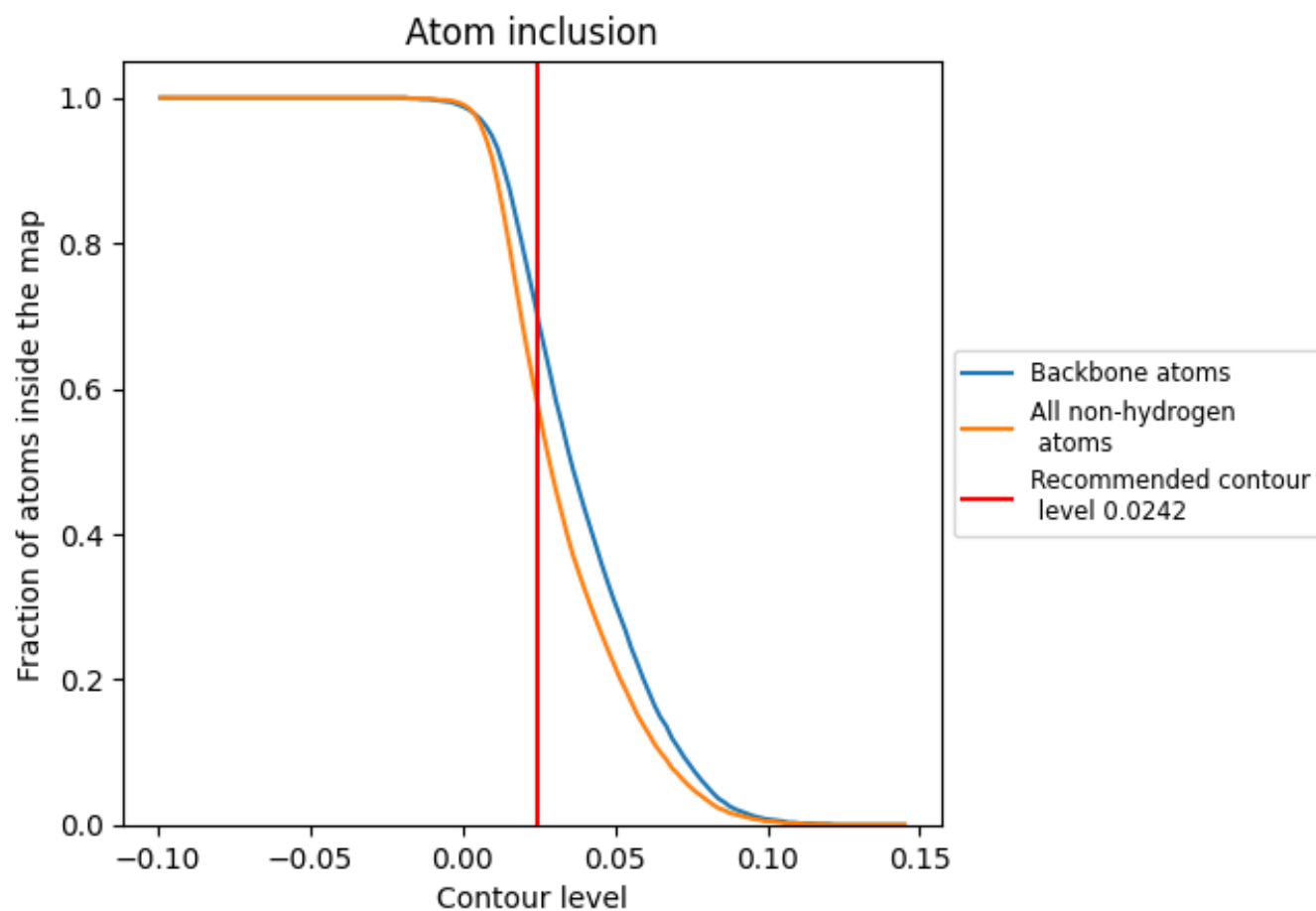
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0242).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 59% 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 (0.0242) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5860	0.4360
A	0.7300	0.4790
B	0.4980	0.4440
C	0.3440	0.3410
E	0.6170	0.4380
G	0.2670	0.3130
V	0.3530	0.3860
Y	0.6250	0.4610

1.0

0.0

<0.0