Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 08:16 PM JST

PDB ID	:	8YA0 / pdb_00008ya0
EMDB ID	:	EMD-39087
Title	:	Structure of the SecA-SecY complex with the substrate FtsQ-LacY(+7C)
Authors	:	Ou, X.; Ma, C.; Sun, D.; Xu, J.; Wu, X.; Gao, N.; Li, L.
Deposited on	:	2024-02-07
Resolution	:	2.97 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 (i)) were used in the production of this report:

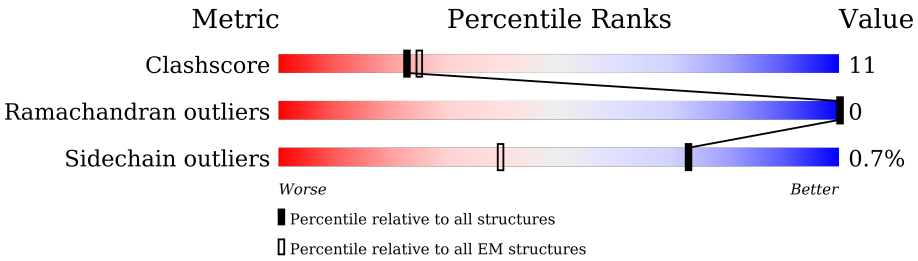
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

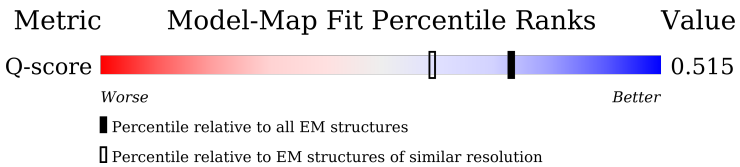
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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

Mol	Chain	Length	Quality of chain
1	A	765	82% 17%
2	Y	429	5% 83% 14%
3	E	58	91% 9%
4	V	116	46% 79% 21%

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Mol	Chain	Length	Quality of chain
5	B	72	14% 50% 29% 18%
6	C	113	47% 73% 26%
7	G	225	67% 69% 29%

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
7	GYS	G	66	-	-	X	-
9	BEF	A	1002	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13920 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
			Total	C	N	O	S		
1	A	765	6107	3820	1066	1188	33	0	0

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

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

There are 4 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	211	THR	PHE	engineered mutation	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
			Total	C	N	O		
3	E	58	480	322	80	78	0	0

- Molecule 4 is a protein called Nanobody.

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

- Molecule 5 is a protein called Cell division protein FtsQ,Lactose permease.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	59	453	301	70	80	2	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	ARG	engineered mutation	UNP Q7CR81
B	3	LYS	LEU	engineered mutation	UNP Q7CR81
B	4	LYS	ALA	engineered mutation	UNP Q7CR81
B	5	THR	GLY	engineered mutation	UNP Q7CR81
B	14	THR	CYS	engineered mutation	UNP Q7CR81
B	17	LEU	PHE	engineered mutation	UNP Q7CR81
B	26	ALA	-	linker	UNP Q7CR81
B	27	GLN	-	linker	UNP Q7CR81
B	28	TYR	-	linker	UNP Q7CR81
B	29	GLU	-	linker	UNP Q7CR81
B	30	ASP	-	linker	UNP Q7CR81
B	31	GLY	-	linker	UNP Q7CR81
B	32	CYS	-	linker	UNP Q7CR81
B	33	SER	-	linker	UNP Q7CR81
B	34	GLY	-	linker	UNP Q7CR81
B	35	VAL	-	linker	UNP Q7CR81
B	52A	ALA	-	linker	UNP P02920
B	52B	PHE	-	linker	UNP P02920
B	52C	SER	-	linker	UNP P02920
B	52D	ASN	-	linker	UNP P02920
B	52E	ALA	-	linker	UNP P02920
B	52F	ASP	-	linker	UNP P02920
B	52G	THR	-	linker	UNP P02920
B	52H	SER	-	linker	UNP P02920
B	52I	ILE	-	linker	UNP P02920
B	52J	SER	-	linker	UNP P02920
B	52K	GLY	-	linker	UNP P02920
B	52L	ASP	-	linker	UNP P02920
B	52M	GLY	-	linker	UNP P02920
B	61	ASP	-	linker	UNP P02920
B	62	SER	-	linker	UNP P02920
B	63	PRO	-	linker	UNP P02920
B	64	HIS	-	linker	UNP P02920
B	65	SER	-	linker	UNP P02920
B	66	TYR	-	linker	UNP P02920
B	67	HIS	-	linker	UNP P02920
B	68	SER	-	linker	UNP P02920

- Molecule 6 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	113	874	543	156	170	5	0	0

- Molecule 7 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	225	1799	1142	306	346	5	0	0

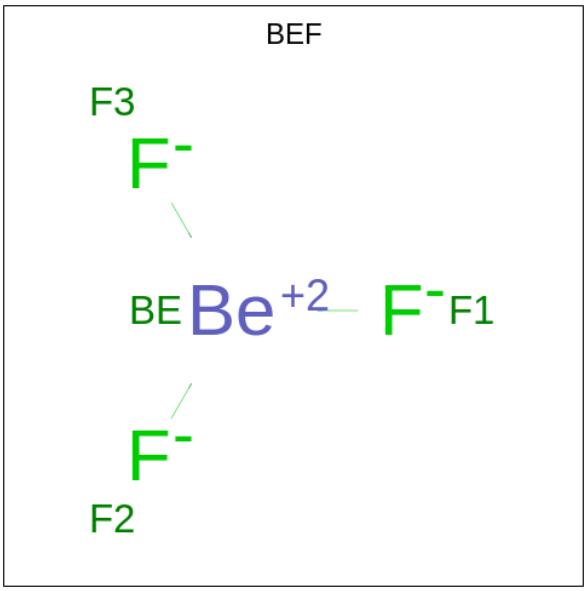
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	66	GYS	SER	chromophore	UNP P42212
G	66	GYS	TYR	chromophore	UNP P42212
G	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 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

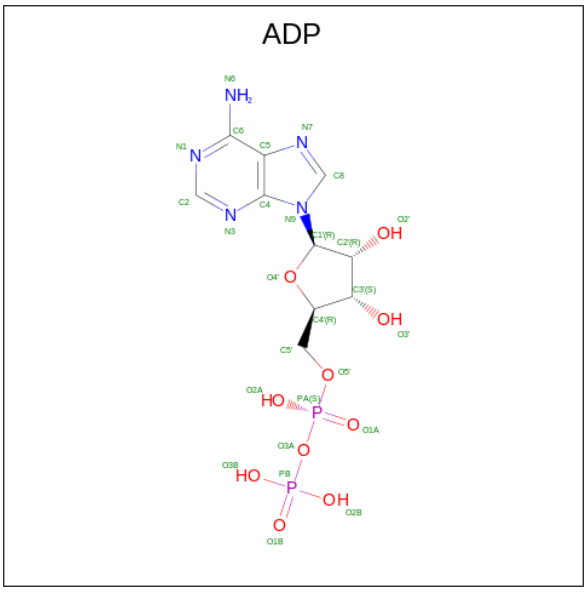
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	A	1	1	1	0

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



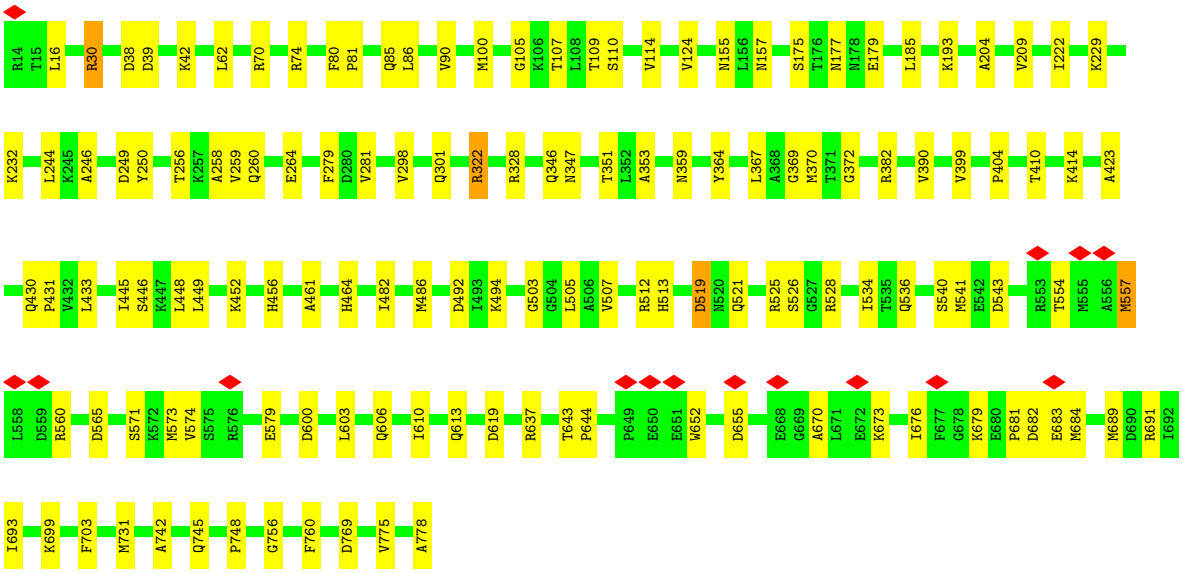
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	27	10	5	10	2	0

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.

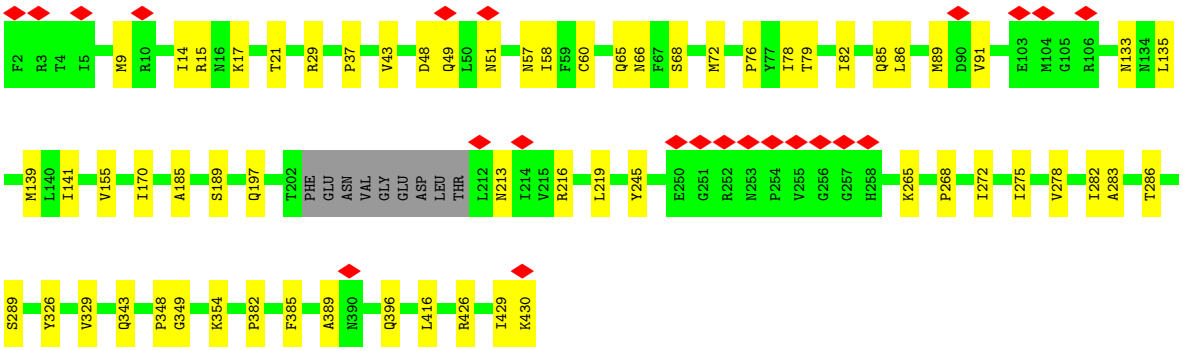
• Molecule 1: Protein translocase subunit SecA

Chain A:



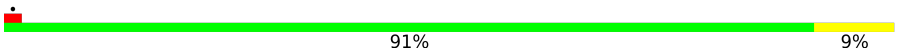
• Molecule 2: Protein translocase subunit SecY

Chain Y:



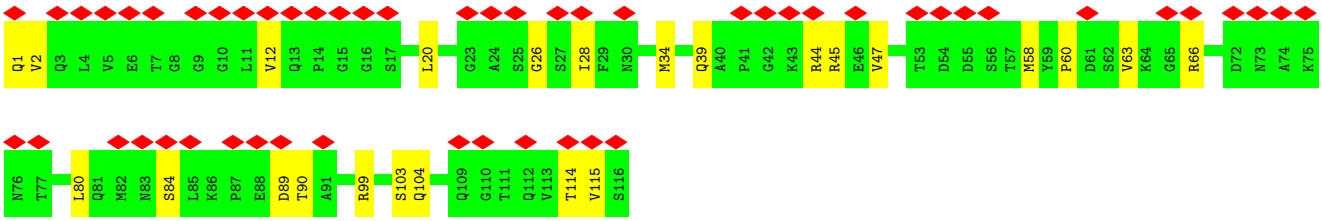
• Molecule 3: Protein translocase subunit SecE

Chain E:



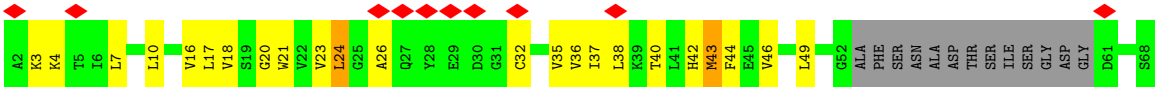
- Molecule 4: Nanobody

Chain V:



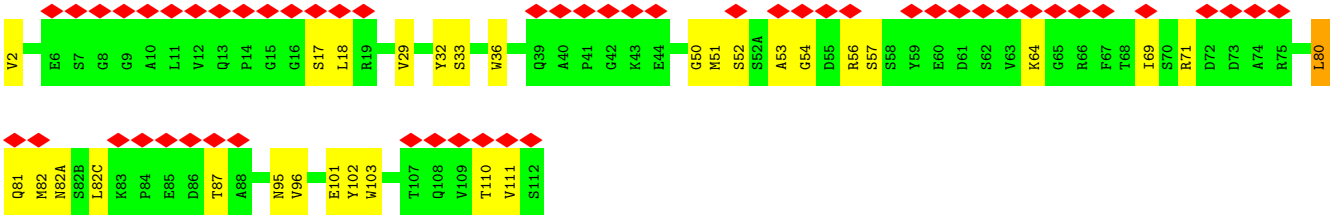
- Molecule 5: Cell division protein FtsQ,Lactose permease

Chain B:



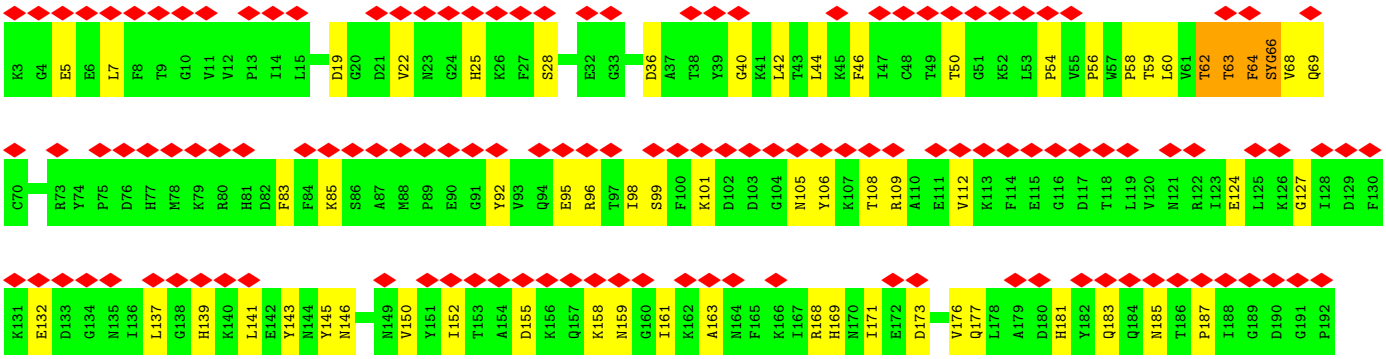
- Molecule 6: Nanobody

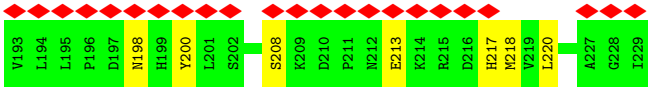
Chain C:



- Molecule 7: Green fluorescent protein

Chain G:




V193
L194
L195
P196
D197
N198
H199
Y200
L201
S202
S208
K209
D210
P211
N212
E213
K214
R215
D216
H217
M218
V219
L220
A227
G228
I229

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	443770	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	252.48001, 252.48001, 252.48001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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: GYS, BEF, MG, ADP

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	0.76	0/6193	0.67	1/8329 (0.0%)
2	Y	0.60	0/3349	0.63	0/4553
3	E	0.50	0/490	0.52	0/664
4	V	0.35	0/919	0.62	0/1246
5	B	0.50	0/463	1.00	3/630 (0.5%)
6	C	0.36	0/893	0.75	2/1209 (0.2%)
7	G	0.72	4/1818 (0.2%)	0.76	7/2456 (0.3%)
All	All	0.66	4/14125 (0.0%)	0.68	13/19087 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	63	THR	C-N	18.59	1.59	1.33
7	G	68	VAL	C-N	16.16	1.56	1.33
7	G	62	THR	C-N	8.98	1.47	1.33
7	G	69	GLN	C-N	-7.48	1.22	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	54	GLY	N-CA-C	11.60	134.36	115.46
5	B	26	ALA	N-CA-C	10.05	122.23	111.28
5	B	43	MET	N-CA-C	7.31	121.51	112.59
5	B	24	LEU	N-CA-C	7.12	119.04	111.28
1	A	399	VAL	N-CA-C	-6.00	106.65	112.29
6	C	80	LEU	N-CA-C	-5.89	100.99	109.29
7	G	69	GLN	O-C-N	-5.48	115.32	122.39
7	G	63	THR	CA-C-N	-5.32	112.12	121.70
7	G	63	THR	C-N-CA	-5.32	112.12	121.70
7	G	62	THR	CA-C-N	5.10	130.07	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	62	THR	C-N-CA	5.10	130.07	121.14
7	G	158	LYS	CA-C-N	5.05	131.19	121.54
7	G	158	LYS	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6107	0	6094	97	0
2	Y	3275	0	3441	75	0
3	E	480	0	507	4	0
4	V	900	0	870	15	0
5	B	453	0	466	51	0
6	C	874	0	828	56	0
7	G	1799	0	1739	63	0
8	A	1	0	0	0	0
9	A	4	0	0	2	0
10	A	27	0	12	1	0
All	All	13920	0	13957	312	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (312) 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:745:GLN:OE1	2:Y:265:LYS:NZ	1.65	1.29
6:C:82(C):LEU:HD23	6:C:111:VAL:CG2	1.73	1.17
6:C:82(C):LEU:CD2	6:C:111:VAL:HG21	1.73	1.17
1:A:571:SER:OG	1:A:574:VAL:HG22	1.48	1.13
2:Y:289:SER:OG	5:B:23:VAL:HG23	1.46	1.12
1:A:778:ALA:O	6:C:2:VAL:N	1.86	1.08
6:C:33:SER:HB3	6:C:52:SER:HB2	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:382:PRO:HG2	2:Y:396:GLN:NE2	1.73	1.03
6:C:33:SER:HB3	6:C:52:SER:CB	1.88	1.02
2:Y:65:GLN:NE2	5:B:38:LEU:HB3	1.74	1.01
6:C:33:SER:CB	6:C:52:SER:CB	2.40	1.00
2:Y:289:SER:CB	5:B:23:VAL:HG23	1.92	0.99
6:C:33:SER:HB2	6:C:52:SER:HB3	1.44	0.98
2:Y:289:SER:CB	5:B:23:VAL:CG2	2.42	0.97
2:Y:289:SER:OG	5:B:23:VAL:CG2	2.11	0.97
2:Y:286:THR:HG22	5:B:23:VAL:HG11	1.48	0.93
7:G:66:GYS:OH	7:G:145:TYR:OH	1.87	0.93
7:G:66:GYS:OH	7:G:145:TYR:CE2	2.23	0.92
1:A:778:ALA:C	6:C:2:VAL:N	2.28	0.90
6:C:82:MET:O	6:C:82(C):LEU:HD12	1.71	0.90
6:C:33:SER:CB	6:C:52:SER:HB3	2.00	0.89
6:C:51:MET:HB3	6:C:57:SER:HB2	1.55	0.89
1:A:232:LYS:HD3	7:G:7:LEU:HD12	1.56	0.86
9:A:1002:BEF:F1	10:A:1003:ADP:O3B	1.84	0.86
2:Y:78:ILE:CD1	5:B:46:VAL:HG22	2.08	0.83
6:C:82(C):LEU:CD2	6:C:111:VAL:CG2	2.46	0.78
7:G:66:GYS:OH	7:G:145:TYR:CZ	2.36	0.78
2:Y:79:THR:HG21	5:B:18:VAL:CG2	2.13	0.78
6:C:82(C):LEU:CD1	6:C:82(C):LEU:H	1.97	0.77
1:A:232:LYS:HD3	7:G:7:LEU:CD1	2.14	0.77
2:Y:79:THR:HG21	5:B:18:VAL:HG22	1.65	0.77
6:C:17:SER:HB3	6:C:82(A):ASN:HA	1.67	0.76
2:Y:89:MET:SD	2:Y:329:VAL:HG13	2.25	0.76
6:C:17:SER:CB	6:C:82(A):ASN:HA	2.17	0.74
6:C:81:GLN:HE21	6:C:82(A):ASN:HB2	1.52	0.74
6:C:82(C):LEU:HD23	6:C:111:VAL:HG21	0.84	0.73
6:C:2:VAL:HG21	6:C:102:TYR:CZ	2.24	0.73
7:G:66:GYS:OH	7:G:145:TYR:HE2	1.67	0.73
2:Y:278:VAL:HG21	5:B:40:THR:HG22	1.70	0.73
1:A:571:SER:OG	1:A:574:VAL:CG2	2.34	0.72
6:C:33:SER:HB2	6:C:52:SER:CB	2.10	0.72
5:B:20:GLY:O	5:B:37:ILE:HD11	1.89	0.72
7:G:66:GYS:HB2	7:G:96:ARG:HH22	1.56	0.71
2:Y:382:PRO:HG2	2:Y:396:GLN:HE21	1.54	0.71
1:A:209:VAL:HG21	1:A:369:GLY:HA3	1.71	0.70
7:G:60:LEU:O	7:G:63:THR:OG1	2.09	0.70
2:Y:78:ILE:CD1	5:B:46:VAL:CG2	2.69	0.70
2:Y:382:PRO:HG2	2:Y:396:GLN:HE22	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:98:ILE:HB	7:G:106:TYR:HB2	1.74	0.69
2:Y:289:SER:CB	5:B:23:VAL:HG21	2.22	0.69
6:C:53:ALA:HA	6:C:71:ARG:NH1	1.99	0.68
5:B:21:TRP:CD2	5:B:37:ILE:HG21	2.29	0.68
2:Y:78:ILE:HD13	5:B:46:VAL:HG22	1.74	0.68
1:A:745:GLN:CD	2:Y:265:LYS:NZ	2.50	0.67
7:G:66:GYS:O2	7:G:96:ARG:NH2	2.28	0.66
2:Y:286:THR:HG22	5:B:23:VAL:CG1	2.24	0.66
5:B:43:MET:O	5:B:44:PHE:CD1	2.49	0.66
1:A:643:THR:HG22	1:A:643:THR:O	1.96	0.66
2:Y:48:ASP:HB3	2:Y:58:ILE:HB	1.78	0.65
7:G:44:LEU:HD12	7:G:220:LEU:HD12	1.78	0.65
5:B:21:TRP:CZ2	5:B:37:ILE:HG22	2.32	0.65
1:A:281:VAL:HG12	1:A:281:VAL:O	1.96	0.64
2:Y:289:SER:HB3	5:B:23:VAL:HG21	1.79	0.64
7:G:92:TYR:HB3	7:G:112:VAL:O	1.98	0.64
5:B:21:TRP:CE2	5:B:37:ILE:CG2	2.81	0.64
1:A:557:MET:SD	1:A:557:MET:N	2.72	0.63
6:C:32:TYR:CZ	6:C:96:VAL:HG23	2.33	0.63
1:A:39:ASP:H	1:A:42:LYS:HG3	1.64	0.63
7:G:163:ALA:HB3	7:G:183:GLN:HB3	1.80	0.63
6:C:87:THR:OG1	6:C:110:THR:HA	1.99	0.63
6:C:82(C):LEU:HD13	6:C:82(C):LEU:N	2.13	0.63
5:B:23:VAL:HG22	5:B:23:VAL:O	2.00	0.62
6:C:82(C):LEU:H	6:C:82(C):LEU:HD13	1.64	0.61
5:B:36:VAL:HG12	5:B:36:VAL:O	2.00	0.61
5:B:20:GLY:O	5:B:37:ILE:CD1	2.49	0.61
1:A:70:ARG:NH1	1:A:81:PRO:O	2.34	0.60
4:V:2:VAL:HG13	4:V:26:GLY:H	1.64	0.60
1:A:699:LYS:O	1:A:703:PHE:HB2	2.01	0.60
1:A:521:GLN:O	1:A:525:ARG:NH2	2.35	0.60
7:G:66:GYS:CZ	7:G:145:TYR:OH	2.49	0.60
2:Y:85:GLN:NE2	2:Y:326:TYR:OH	2.35	0.59
6:C:2:VAL:HG23	6:C:2:VAL:O	2.01	0.59
1:A:571:SER:HG	1:A:574:VAL:HG22	1.63	0.59
2:Y:245:TYR:OH	2:Y:343:GLN:NE2	2.35	0.59
1:A:528:ARG:NH2	9:A:1002:BEF:F1	2.26	0.59
1:A:610:ILE:HD11	1:A:760:PHE:CZ	2.38	0.59
1:A:430:GLN:HE22	1:A:534:ILE:HD12	1.68	0.58
4:V:103:SER:OG	4:V:104:GLN:N	2.35	0.58
5:B:40:THR:O	5:B:44:PHE:CE2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ARG:NH2	1:A:769:ASP:OD1	2.36	0.58
7:G:92:TYR:HD2	7:G:112:VAL:HB	1.68	0.58
1:A:229:LYS:HB2	1:A:347:ASN:HD22	1.68	0.58
6:C:81:GLN:NE2	6:C:82(A):ASN:HB2	2.19	0.58
7:G:92:TYR:OH	7:G:185:ASN:ND2	2.37	0.58
7:G:146:ASN:ND2	7:G:168:ARG:O	2.35	0.58
2:Y:289:SER:HB3	5:B:23:VAL:CG2	2.30	0.58
1:A:699:LYS:NZ	1:A:775:VAL:O	2.37	0.58
5:B:21:TRP:HA	5:B:37:ILE:HD13	1.85	0.57
4:V:90:THR:HG23	4:V:114:THR:HA	1.86	0.57
5:B:21:TRP:CH2	5:B:37:ILE:HG22	2.39	0.57
1:A:554:THR:HG23	1:A:573:MET:HE3	1.86	0.57
6:C:95:ASN:ND2	7:G:146:ASN:OD1	2.38	0.57
4:V:66:ARG:NH1	4:V:84:SER:O	2.38	0.56
6:C:17:SER:CB	6:C:82(A):ASN:CA	2.84	0.56
2:Y:382:PRO:CG	2:Y:396:GLN:NE2	2.60	0.56
7:G:150:VAL:O	7:G:200:TYR:HA	2.05	0.56
1:A:670:ALA:O	1:A:691:ARG:NH1	2.38	0.56
2:Y:72:MET:HE3	2:Y:76:PRO:HG2	1.88	0.55
1:A:430:GLN:NE2	1:A:503:GLY:O	2.40	0.55
7:G:62:THR:HG22	7:G:66:GYS:CE1	2.36	0.55
4:V:39:GLN:HB2	4:V:45:ARG:HB3	1.89	0.55
1:A:404:PRO:O	1:A:536:GLN:NE2	2.40	0.55
1:A:209:VAL:CG2	1:A:369:GLY:HA3	2.37	0.55
7:G:62:THR:O	7:G:96:ARG:NH1	2.39	0.54
1:A:610:ILE:HD11	1:A:760:PHE:CE1	2.41	0.54
6:C:17:SER:HB2	6:C:82(A):ASN:HB2	1.89	0.54
6:C:82(C):LEU:HD12	6:C:82(C):LEU:H	1.73	0.54
1:A:155:ASN:HB3	1:A:175:SER:HB3	1.89	0.54
1:A:16:LEU:HD21	1:A:390:VAL:HG13	1.90	0.54
7:G:161:ILE:HB	7:G:185:ASN:HB2	1.90	0.54
7:G:64:PHE:HE2	7:G:218:MET:HE2	1.72	0.53
1:A:193:LYS:HD3	1:A:619:ASP:HB3	1.90	0.53
1:A:359:ASN:ND2	1:A:600:ASP:OD2	2.41	0.53
2:Y:78:ILE:HD12	5:B:46:VAL:CG2	2.37	0.53
7:G:46:PHE:CD2	7:G:64:PHE:CE2	2.97	0.53
1:A:70:ARG:HD3	1:A:86:LEU:HD21	1.91	0.53
7:G:66:GYS:CB2	7:G:96:ARG:HH22	2.21	0.53
7:G:56:PRO:HB2	7:G:141:LEU:HD12	1.91	0.52
4:V:1:GLN:HG2	4:V:2:VAL:HG23	1.90	0.52
6:C:82(C):LEU:HD22	6:C:82(C):LEU:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:65:GLN:CD	5:B:38:LEU:HD22	2.34	0.52
2:Y:21:THR:HG23	2:Y:170:ILE:HD11	1.92	0.52
7:G:19:ASP:O	7:G:124:GLU:HA	2.10	0.52
5:B:24:LEU:HD23	5:B:35:VAL:HG11	1.90	0.52
2:Y:133:ASN:HD22	2:Y:141:ILE:H	1.58	0.52
2:Y:278:VAL:CG2	5:B:40:THR:HG22	2.39	0.52
1:A:492:ASP:OD2	1:A:494:LYS:NZ	2.40	0.51
1:A:557:MET:HG3	1:A:573:MET:HE1	1.92	0.51
7:G:62:THR:HG22	7:G:66:GYS:CD1	2.40	0.51
1:A:603:LEU:HD13	1:A:731:MET:HG2	1.92	0.51
1:A:281:VAL:O	1:A:281:VAL:CG1	2.59	0.51
6:C:50:GLY:HA2	6:C:69:ILE:HD13	1.92	0.51
6:C:36:TRP:HD1	6:C:69:ILE:HD12	1.76	0.51
7:G:36:ASP:O	7:G:40:GLY:HA2	2.10	0.51
1:A:30:ARG:HG2	1:A:70:ARG:HH21	1.76	0.50
1:A:298:VAL:O	1:A:301:GLN:NE2	2.44	0.50
2:Y:289:SER:HB2	5:B:23:VAL:HG23	1.85	0.50
1:A:85:GLN:NE2	1:A:105:GLY:O	2.44	0.50
6:C:18:LEU:H	6:C:82:MET:HB2	1.76	0.50
6:C:51:MET:HB3	6:C:57:SER:CB	2.35	0.50
2:Y:78:ILE:HD12	5:B:46:VAL:HG22	1.89	0.50
2:Y:426:ARG:HG2	2:Y:430:LYS:HD3	1.94	0.50
1:A:745:GLN:CD	2:Y:265:LYS:CE	2.84	0.50
1:A:745:GLN:CD	2:Y:265:LYS:HE2	2.36	0.50
2:Y:65:GLN:CD	5:B:38:LEU:HB3	2.36	0.50
1:A:682:ASP:N	1:A:682:ASP:OD1	2.45	0.50
7:G:59:THR:HG23	7:G:141:LEU:HD11	1.93	0.50
7:G:155:ASP:O	7:G:159:ASN:HA	2.12	0.49
2:Y:65:GLN:CG	5:B:38:LEU:HD13	2.42	0.49
2:Y:43:VAL:HG12	4:V:47:VAL:HG21	1.95	0.49
6:C:82(C):LEU:HD22	6:C:82(C):LEU:C	2.38	0.49
4:V:20:LEU:HD12	4:V:80:LEU:HD23	1.94	0.49
6:C:82(C):LEU:CD1	6:C:82(C):LEU:N	2.63	0.49
5:B:21:TRP:CE2	5:B:37:ILE:HG21	2.48	0.49
1:A:423:ALA:HB2	1:A:452:LYS:HD3	1.95	0.49
1:A:461:ALA:HA	1:A:486:MET:HE3	1.94	0.49
2:Y:91:VAL:HG22	5:B:4:LYS:HG2	1.94	0.49
7:G:42:LEU:HD23	7:G:44:LEU:HD11	1.94	0.49
1:A:157:ASN:ND2	1:A:179:GLU:OE2	2.46	0.49
5:B:21:TRP:CZ2	5:B:37:ILE:CG2	2.95	0.49
1:A:177:ASN:OD1	1:A:177:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:SER:OG	1:A:541:MET:N	2.46	0.48
6:C:29:VAL:O	6:C:71:ARG:NH1	2.46	0.48
1:A:410:THR:OG1	1:A:565:ASP:OD2	2.26	0.48
1:A:513:HIS:HD2	1:A:519:ASP:HB3	1.77	0.48
7:G:96:ARG:HB2	7:G:108:THR:HG22	1.95	0.48
1:A:679:LYS:HE3	1:A:683:GLU:HG3	1.95	0.48
6:C:32:TYR:CE1	6:C:96:VAL:HG23	2.49	0.48
2:Y:29:ARG:NE	3:E:48:ASP:OD1	2.47	0.48
1:A:256:THR:O	1:A:258:ALA:N	2.46	0.47
2:Y:66:ASN:OD1	2:Y:68:SER:OG	2.30	0.47
2:Y:385:PHE:O	2:Y:389:ALA:HB3	2.14	0.47
6:C:56:ARG:HD2	7:G:173:ASP:HA	1.97	0.47
7:G:56:PRO:O	7:G:59:THR:OG1	2.30	0.47
1:A:74:ARG:HG3	1:A:80:PHE:HB2	1.96	0.47
1:A:464:HIS:HB3	1:A:486:MET:HE1	1.95	0.47
2:Y:283:ALA:HB2	5:B:16:VAL:HG11	1.96	0.47
2:Y:49:GLN:NE2	5:B:32:CYS:O	2.48	0.47
7:G:64:PHE:CD2	7:G:218:MET:HE1	2.50	0.47
6:C:17:SER:HB2	6:C:82(A):ASN:CA	2.45	0.46
2:Y:51:ASN:O	2:Y:197:GLN:NE2	2.49	0.46
1:A:449:LEU:HD12	1:A:482:ILE:HD11	1.98	0.46
6:C:17:SER:HB3	6:C:82(A):ASN:CA	2.42	0.46
7:G:109:ARG:HB3	7:G:124:GLU:O	2.16	0.46
5:B:3:LYS:HG3	5:B:7:LEU:HD13	1.98	0.46
6:C:29:VAL:HG12	6:C:71:ARG:HD2	1.98	0.46
6:C:33:SER:CB	6:C:52:SER:CA	2.94	0.46
5:B:17:LEU:HD11	5:B:40:THR:HB	1.98	0.46
7:G:83:PHE:HZ	7:G:187:PRO:HG3	1.81	0.46
2:Y:79:THR:HG21	5:B:18:VAL:HG21	1.96	0.46
1:A:246:ALA:HA	1:A:250:TYR:CZ	2.51	0.45
1:A:85:GLN:HB3	1:A:109:THR:HG22	1.98	0.45
1:A:643:THR:CG2	1:A:681:PRO:HG3	2.46	0.45
1:A:643:THR:HG21	1:A:681:PRO:HG3	1.97	0.45
2:Y:139:MET:HE3	2:Y:139:MET:HB3	1.80	0.45
7:G:28:SER:HB2	7:G:50:THR:HB	1.98	0.45
7:G:58:PRO:HB2	7:G:141:LEU:HD13	1.98	0.45
7:G:101:LYS:O	7:G:177:GLN:NE2	2.41	0.45
2:Y:57:ASN:OD1	2:Y:66:ASN:ND2	2.48	0.45
4:V:66:ARG:NH2	4:V:89:ASP:OD2	2.41	0.45
5:B:10:LEU:HD23	5:B:10:LEU:HA	1.77	0.45
6:C:82(C):LEU:HD21	6:C:111:VAL:CG2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:OD1	1:A:38:ASP:N	2.46	0.45
1:A:222:ILE:HG23	1:A:351:THR:HG23	1.98	0.45
2:Y:60:CYS:O	5:B:38:LEU:CD1	2.64	0.45
1:A:446:SER:OG	1:A:456:HIS:NE2	2.41	0.45
1:A:431:PRO:HG2	1:A:505:LEU:H	1.81	0.45
6:C:17:SER:HB2	6:C:82(A):ASN:CB	2.47	0.45
1:A:249:ASP:OD1	1:A:264:GLU:OE1	2.34	0.45
1:A:281:VAL:HG23	2:Y:348:PRO:HB3	1.98	0.45
1:A:322:ARG:HB3	1:A:486:MET:HE2	1.99	0.44
7:G:213:GLU:OE1	7:G:217:HIS:ND1	2.50	0.44
1:A:204:ALA:HB3	1:A:367:LEU:HD12	1.98	0.44
2:Y:60:CYS:O	5:B:38:LEU:HD12	2.17	0.44
2:Y:135:LEU:O	4:V:44:ARG:NH1	2.45	0.44
4:V:34:MET:HE2	4:V:34:MET:HB3	1.82	0.44
7:G:132:GLU:HA	7:G:137:LEU:HD12	1.99	0.44
2:Y:37:PRO:HD2	2:Y:155:VAL:HG11	1.99	0.44
7:G:22:VAL:HG12	7:G:127:GLY:HA3	2.00	0.44
7:G:96:ARG:HD3	7:G:181:HIS:HD2	1.82	0.44
2:Y:272:ILE:HA	2:Y:275:ILE:HG13	1.99	0.44
7:G:143:TYR:OH	7:G:208:SER:O	2.32	0.44
6:C:18:LEU:O	6:C:82:MET:HG2	2.17	0.44
7:G:171:ILE:HD11	7:G:177:GLN:HB2	2.00	0.44
7:G:64:PHE:HD1	7:G:64:PHE:HA	1.52	0.44
7:G:64:PHE:CE2	7:G:218:MET:CE	3.02	0.43
1:A:328:ARG:HH12	1:A:346:GLN:HG3	1.83	0.43
1:A:512:ARG:NH2	1:A:579:GLU:OE2	2.36	0.43
6:C:81:GLN:HG2	6:C:82(A):ASN:H	1.82	0.43
6:C:101:GLU:OE1	6:C:103:TRP:NE1	2.51	0.43
2:Y:265:LYS:HE3	2:Y:268:PRO:HA	2.01	0.43
6:C:80:LEU:HG	6:C:81:GLN:H	1.83	0.43
1:A:742:ALA:HB2	1:A:748:PRO:HG3	2.01	0.43
1:A:110:SER:HB3	1:A:370:MET:HE1	2.01	0.43
1:A:259:VAL:HG21	1:A:298:VAL:HB	2.01	0.43
1:A:414:LYS:NZ	1:A:543:ASP:OD1	2.51	0.43
1:A:613:GLN:HE22	2:Y:429:ILE:H	1.67	0.43
6:C:80:LEU:HD12	6:C:80:LEU:HA	1.87	0.43
7:G:98:ILE:HG12	7:G:181:HIS:CD2	2.53	0.43
1:A:525:ARG:HH11	1:A:528:ARG:NH2	2.16	0.43
2:Y:89:MET:HE1	2:Y:329:VAL:HA	2.01	0.43
4:V:12:VAL:HG13	4:V:115:VAL:HG13	2.01	0.43
7:G:56:PRO:HG3	7:G:139:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:213:ASN:HD22	2:Y:213:ASN:HA	1.63	0.42
2:Y:289:SER:OG	5:B:23:VAL:HG21	2.08	0.42
7:G:25:HIS:HD2	7:G:54:PRO:HG3	1.83	0.42
2:Y:79:THR:HA	2:Y:82:ILE:HG22	2.00	0.42
1:A:107:THR:O	1:A:110:SER:OG	2.31	0.42
2:Y:278:VAL:O	2:Y:282:ILE:HG12	2.19	0.42
1:A:382:ARG:HA	1:A:382:ARG:HD3	1.86	0.42
3:E:32:VAL:O	3:E:36:THR:OG1	2.32	0.42
5:B:17:LEU:HD11	5:B:40:THR:CB	2.50	0.42
6:C:17:SER:CB	6:C:82(A):ASN:CB	2.97	0.42
4:V:28:ILE:HB	4:V:99:ARG:HH12	1.84	0.42
7:G:183:GLN:HE21	7:G:185:ASN:HD21	1.67	0.42
2:Y:216:ARG:HH11	2:Y:219:LEU:HD12	1.85	0.42
2:Y:78:ILE:CD1	5:B:46:VAL:HG23	2.48	0.42
3:E:9:LYS:HD3	3:E:9:LYS:HA	1.80	0.42
1:A:74:ARG:HB2	1:A:80:PHE:HD1	1.85	0.42
1:A:232:LYS:HD3	7:G:7:LEU:HD11	1.99	0.42
1:A:505:LEU:HD23	1:A:526:SER:HA	2.00	0.42
2:Y:17:LYS:HE2	2:Y:17:LYS:HB3	1.69	0.42
6:C:87:THR:OG1	6:C:110:THR:HG23	2.19	0.42
2:Y:9:MET:HA	2:Y:15:ARG:HB2	2.02	0.42
7:G:46:PHE:CD2	7:G:64:PHE:CD2	3.08	0.42
1:A:114:VAL:HG22	1:A:124:VAL:HG11	2.02	0.41
2:Y:14:ILE:HG23	2:Y:416:LEU:HD22	2.01	0.41
2:Y:133:ASN:ND2	2:Y:141:ILE:H	2.17	0.41
2:Y:185:ALA:O	2:Y:189:SER:HB3	2.20	0.41
1:A:185:LEU:HD22	1:A:353:ALA:HB1	2.02	0.41
4:V:60:PRO:HG2	4:V:63:VAL:HG22	2.03	0.41
1:A:557:MET:HE3	1:A:557:MET:HB3	1.91	0.41
1:A:573:MET:HB3	1:A:573:MET:HE2	1.73	0.41
1:A:731:MET:HE1	1:A:756:GLY:HA3	2.02	0.41
7:G:152:ILE:O	7:G:198:ASN:HA	2.21	0.41
2:Y:289:SER:HB2	5:B:23:VAL:CG2	2.43	0.41
2:Y:354:LYS:HE3	2:Y:354:LYS:HB3	1.84	0.41
1:A:676:ILE:HB	1:A:684:MET:HE2	2.03	0.41
1:A:433:LEU:HD23	1:A:507:VAL:HG22	2.02	0.41
7:G:64:PHE:CE2	7:G:218:MET:HE2	2.53	0.41
2:Y:86:LEU:HD23	2:Y:86:LEU:HA	1.94	0.41
4:V:58:MET:HE2	4:V:58:MET:HB3	1.89	0.41
1:A:62:LEU:HD21	1:A:90:VAL:HG22	2.02	0.41
1:A:279:PHE:O	2:Y:349:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:286:THR:HA	5:B:23:VAL:HG21	2.03	0.41
3:E:55:ILE:HD13	3:E:55:ILE:HA	1.93	0.41
6:C:64:LYS:HB2	6:C:64:LYS:HE2	1.86	0.41
6:C:82(C):LEU:CD2	6:C:111:VAL:HG22	2.46	0.41
7:G:66:GYS:CE1	7:G:145:TYR:OH	2.68	0.41
7:G:169:HIS:O	7:G:176:VAL:HA	2.20	0.41
7:G:183:GLN:NE2	7:G:185:ASN:HD21	2.19	0.41
7:G:99:SER:HA	7:G:105:ASN:HD22	1.86	0.41
1:A:689:MET:O	1:A:693:ILE:HG12	2.21	0.40
7:G:95:GLU:OE2	7:G:109:ARG:NH2	2.38	0.40
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.84	0.40
1:A:606:GLN:O	1:A:610:ILE:HG12	2.20	0.40
7:G:5:GLU:HB3	7:G:85:LYS:HG2	2.02	0.40
1:A:100:MET:O	1:A:372:GLY:HA2	2.21	0.40
1:A:644:PRO:HD2	1:A:652:TRP:CD1	2.56	0.40
1:A:655:ASP:HB2	1:A:673:LYS:HD2	2.03	0.40
6:C:96:VAL:O	6:C:96:VAL:HG13	2.21	0.40
1:A:445:ILE:HA	1:A:448:LEU:HB2	2.02	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	763/765 (100%)	715 (94%)	48 (6%)	0	100	100
2	Y	416/429 (97%)	397 (95%)	19 (5%)	0	100	100
3	E	56/58 (97%)	56 (100%)	0	0	100	100
4	V	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
5	B	55/72 (76%)	50 (91%)	5 (9%)	0	100	100
6	C	111/113 (98%)	103 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	220/225 (98%)	206 (94%)	14 (6%)	0	100	100
All	All	1735/1778 (98%)	1631 (94%)	104 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	656/656 (100%)	648 (99%)	8 (1%)	63	82
2	Y	352/360 (98%)	352 (100%)	0	100	100
3	E	53/53 (100%)	53 (100%)	0	100	100
4	V	96/97 (99%)	96 (100%)	0	100	100
5	B	52/61 (85%)	50 (96%)	2 (4%)	29	61
6	C	92/92 (100%)	92 (100%)	0	100	100
7	G	195/195 (100%)	194 (100%)	1 (0%)	81	89
All	All	1496/1514 (99%)	1485 (99%)	11 (1%)	73	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	244	LEU
1	A	260	GLN
1	A	322	ARG
1	A	364	TYR
1	A	519	ASP
1	A	557	MET
1	A	560	ARG
5	B	42	HIS
5	B	49	LEU
7	G	64	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	202	HIS
1	A	287	ASN
1	A	288	HIS
1	A	291	ASN
1	A	297	HIS
1	A	335	GLN
1	A	347	ASN
1	A	359	ASN
1	A	383	ASN
1	A	430	GLN
1	A	463	ASN
1	A	513	HIS
1	A	529	GLN
1	A	536	GLN
1	A	605	GLN
1	A	613	GLN
1	A	739	HIS
1	A	753	GLN
2	Y	65	GLN
2	Y	85	GLN
2	Y	134	ASN
2	Y	143	ASN
2	Y	169	GLN
2	Y	177	ASN
2	Y	197	GLN
2	Y	213	ASN
2	Y	258	HIS
2	Y	267	ASN
2	Y	294	ASN
2	Y	343	GLN
2	Y	387	ASN
2	Y	396	GLN
2	Y	415	GLN
2	Y	424	HIS
3	E	53	GLN
4	V	83	ASN
5	B	27	GLN
5	B	67	HIS
6	C	13	GLN
6	C	81	GLN

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Mol	Chain	Res	Type
6	C	95	ASN
7	G	25	HIS
7	G	69	GLN
7	G	81	HIS
7	G	105	ASN
7	G	170	ASN
7	G	181	HIS
7	G	185	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)

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	$\#\|Z\| > 2$
7	GYS	G	66	7	22,22,23	4.17	5 (22%)	27,30,32	4.11	8 (29%)

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
7	GYS	G	66	7	-	2/9/29/30	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	66	GYS	CB2-CA2	18.21	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	66	GYS	C1-N2	3.71	1.37	1.32
7	G	66	GYS	CA2-C2	-2.83	1.45	1.48
7	G	66	GYS	O2-C2	2.57	1.28	1.23
7	G	66	GYS	C2-N3	-2.54	1.33	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	66	GYS	CA2-C2-N3	13.24	109.63	103.37
7	G	66	GYS	O2-C2-CA2	-12.41	123.99	130.96
7	G	66	GYS	CB2-CA2-C2	5.94	129.37	122.28
7	G	66	GYS	C2-CA2-N2	-5.38	105.17	108.93
7	G	66	GYS	C2-N3-C1	-4.40	105.74	107.97
7	G	66	GYS	O3-C3-CA3	-2.71	118.21	126.39
7	G	66	GYS	CB2-CA2-N2	-2.43	125.46	128.83
7	G	66	GYS	CA2-N2-C1	2.28	107.45	105.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	66	GYS	N1-CA1-CB1-OG1
7	G	66	GYS	C1-CA1-CB1-OG1

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	66	GYS	11	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ADP	A	1003	9,8	27,29,29	1.45	4 (14%)	42,45,45	2.02	11 (26%)
9	BEF	A	1002	10	0,3,3	-	-	-		

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
10	ADP	A	1003	9,8	-	1/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1003	ADP	C5-N7	-3.10	1.33	1.39
10	A	1003	ADP	C5-C4	3.06	1.44	1.39
10	A	1003	ADP	C4-N9	-2.67	1.31	1.37
10	A	1003	ADP	C8-N9	-2.59	1.32	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1003	ADP	C5-C4-N3	-5.97	118.96	126.75
10	A	1003	ADP	N3-C4-N9	4.81	135.01	127.08
10	A	1003	ADP	C2-N3-C4	3.88	120.92	111.75
10	A	1003	ADP	N3-C2-N1	-3.30	123.44	128.60
10	A	1003	ADP	PA-O3A-PB	-3.05	122.36	132.83
10	A	1003	ADP	C4-N9-C8	3.02	109.00	105.73
10	A	1003	ADP	C4-C5-N7	-2.89	107.10	110.62
10	A	1003	ADP	C5-N7-C8	2.49	107.04	103.51
10	A	1003	ADP	C2'-C3'-C4'	2.48	107.46	102.64
10	A	1003	ADP	N9-C8-N7	-2.26	110.83	113.91
10	A	1003	ADP	C6-C5-N7	2.15	136.03	132.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1003	ADP	O4'-C4'-C5'-O5'

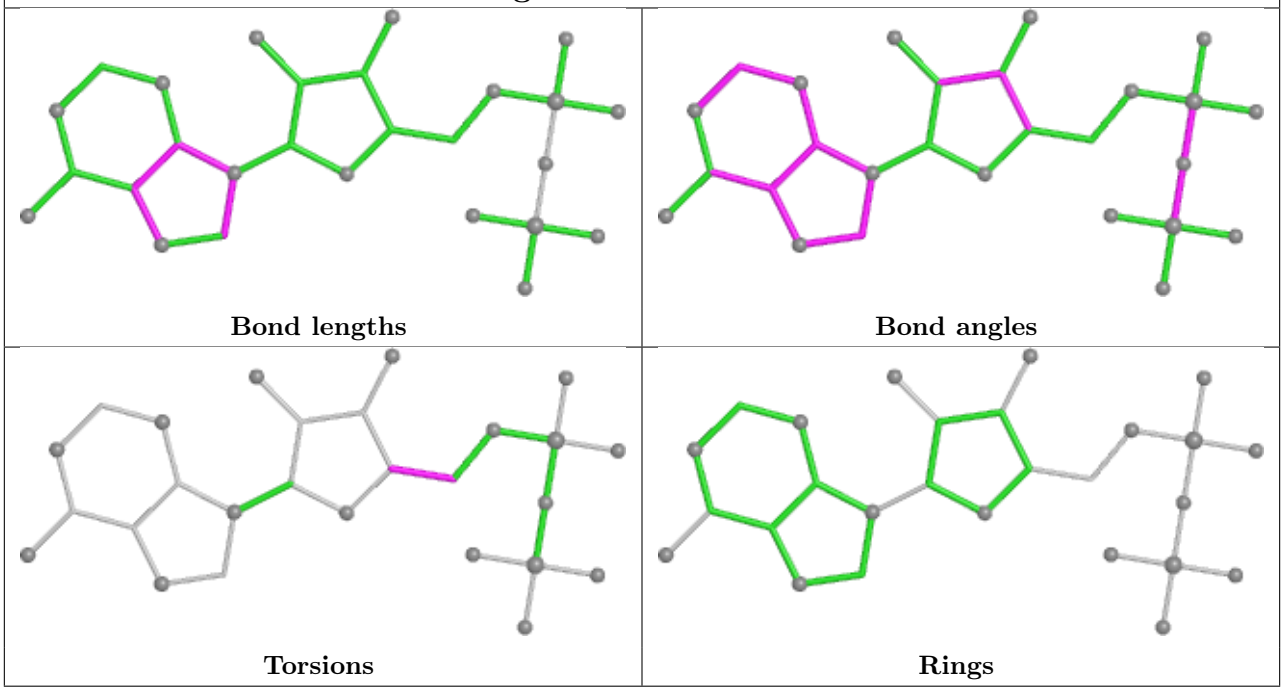
There are no ring outliers.

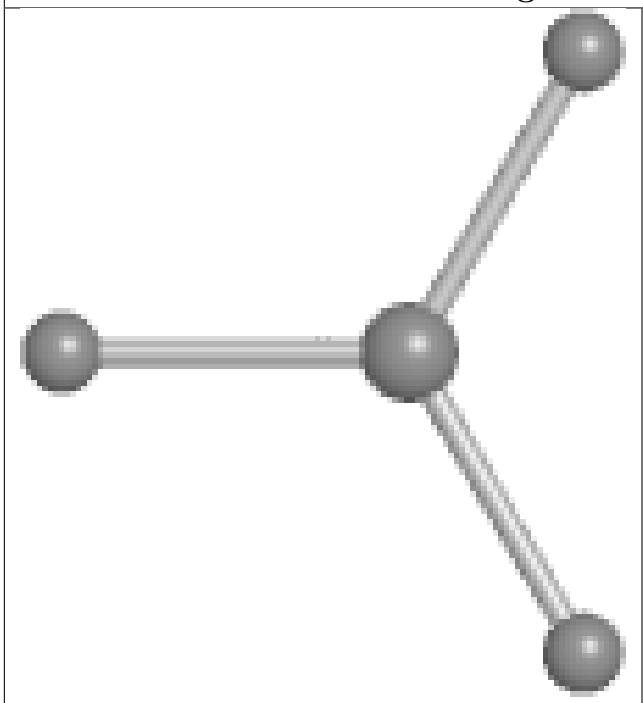
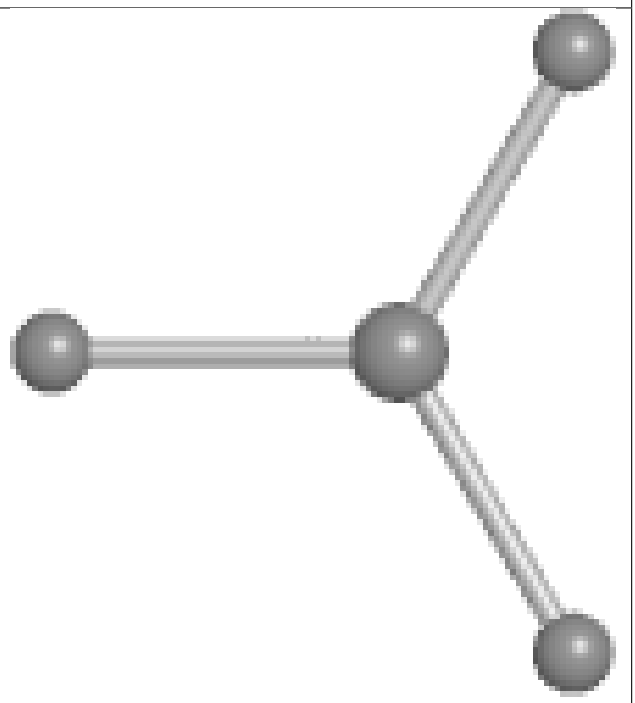
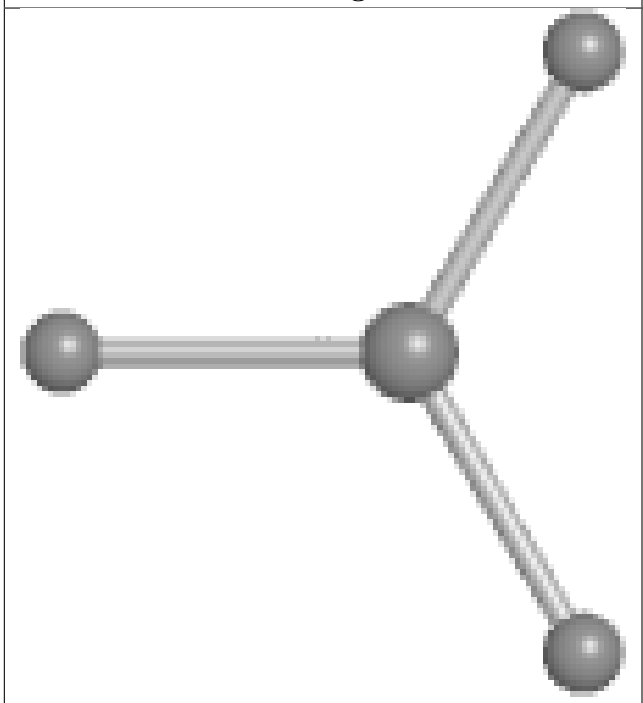
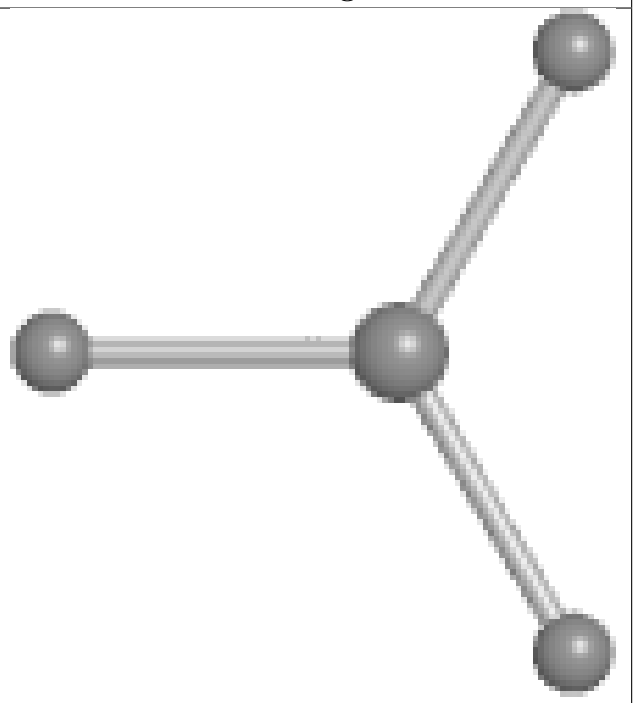
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1003	ADP	1	0
9	A	1002	BEF	2	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 ADP A 1003



Ligand BEF A 1002	
 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.

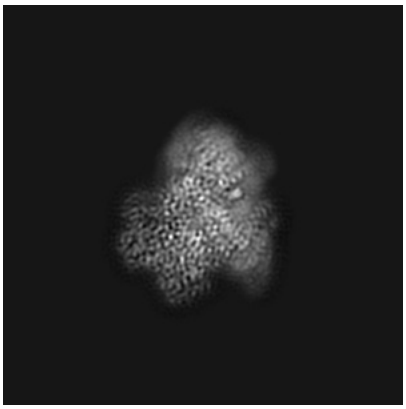
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39087. These allow visual inspection of the internal detail of the map and identification of artifacts.

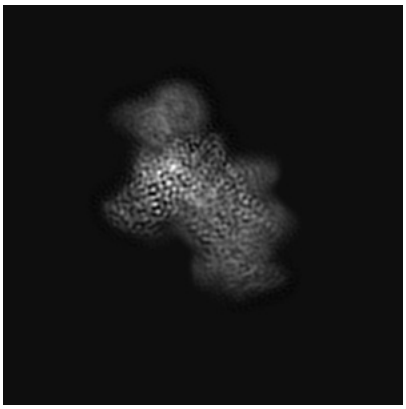
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

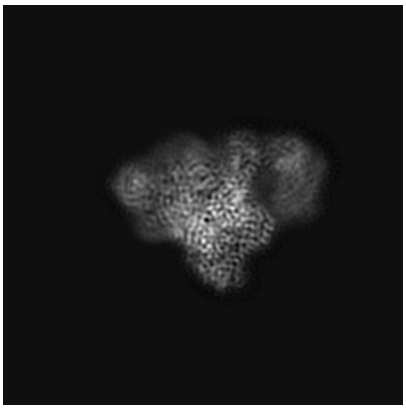
6.1.1 Primary map



X

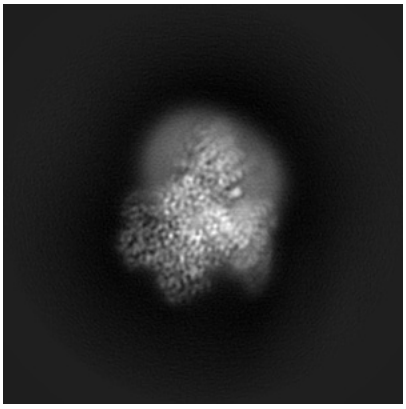


Y

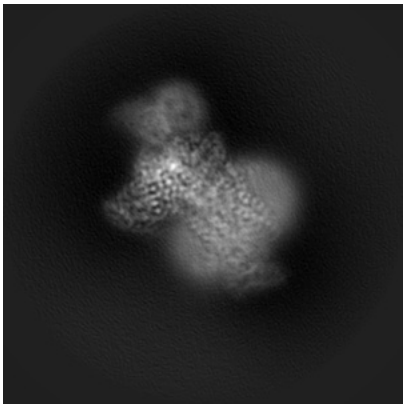


Z

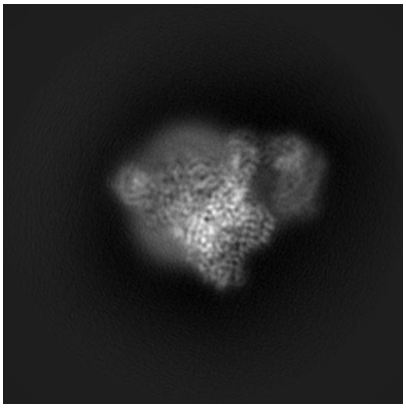
6.1.2 Raw map



X



Y

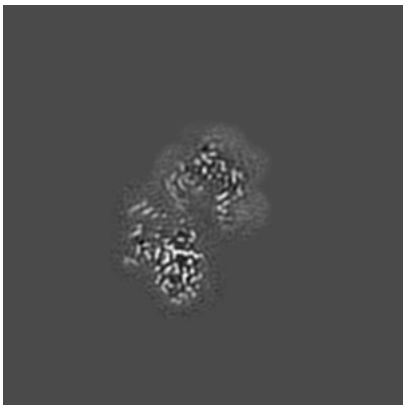


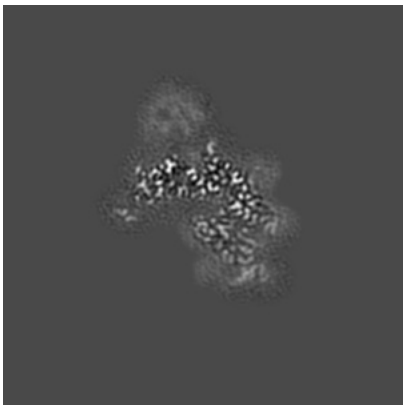
Z

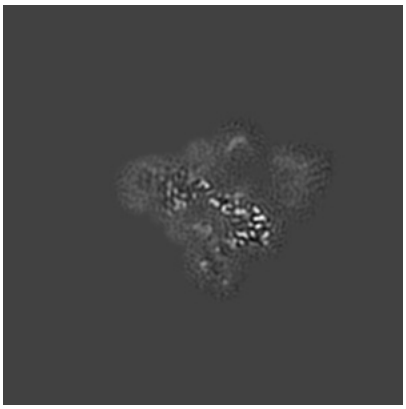
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

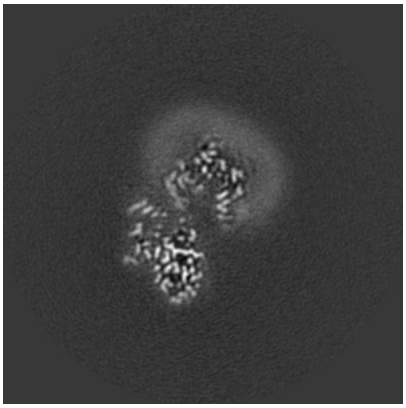
6.2.1 Primary map

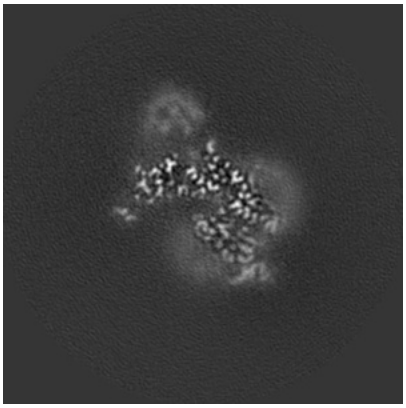

X Index: 120


Y Index: 120


Z Index: 120

6.2.2 Raw map


X Index: 120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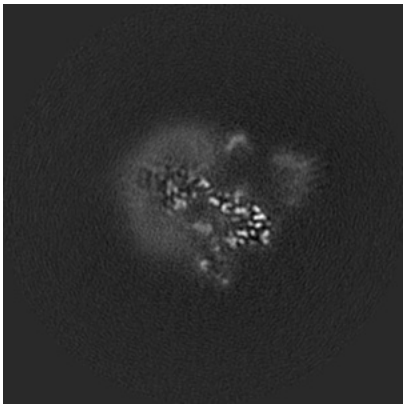
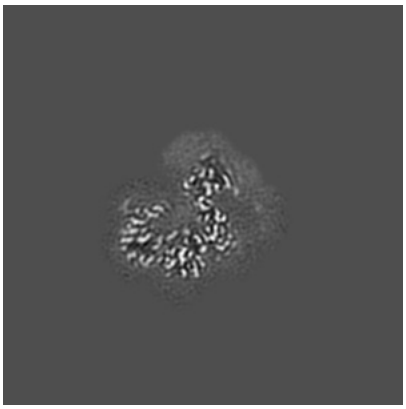
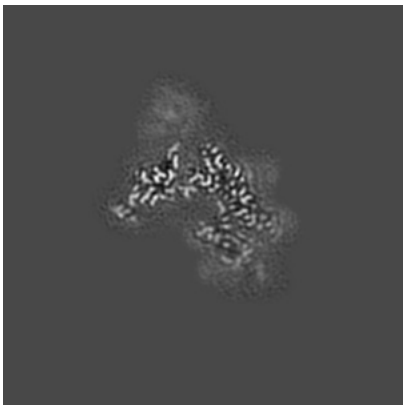

Z Index: 120

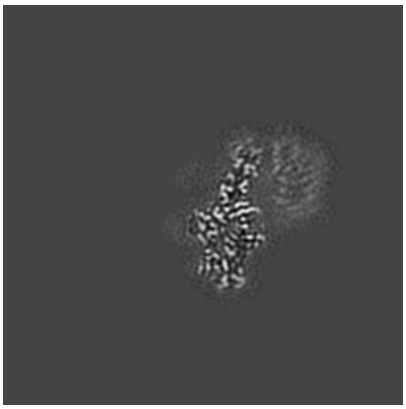
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

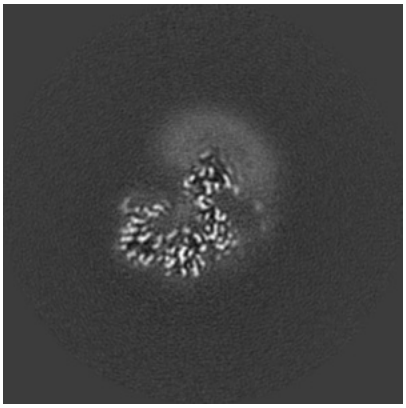
6.3.1 Primary map

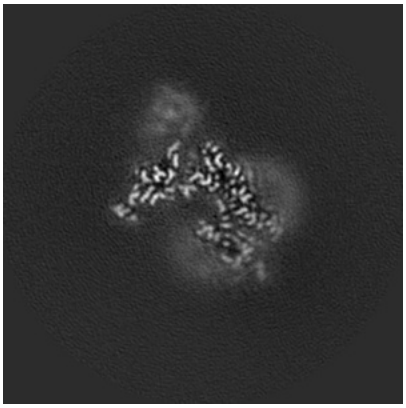

X Index: 133

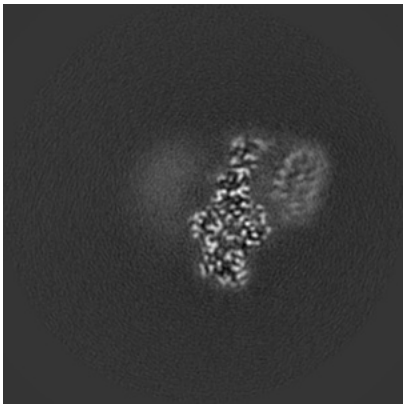

Y Index: 118


Z Index: 99

6.3.2 Raw map


X Index: 133

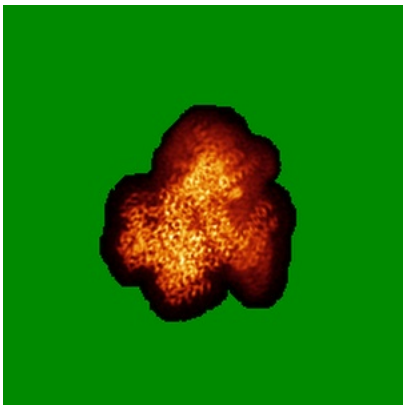

Y Index: 118


Z Index: 102

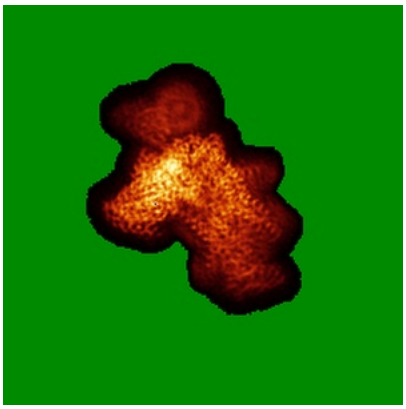
The images above show the largest variance slices of the map in three orthogonal directions.

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

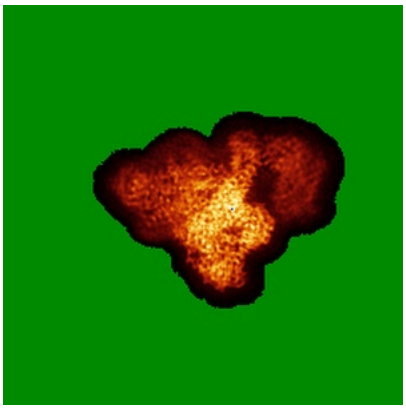
6.4.1 Primary map



X

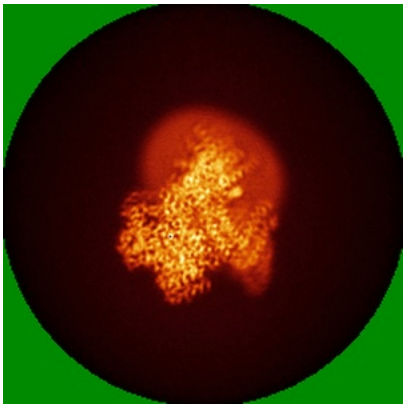


Y

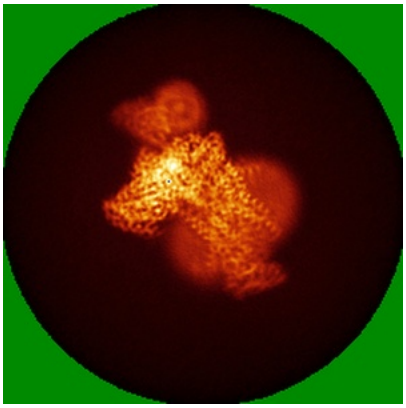


Z

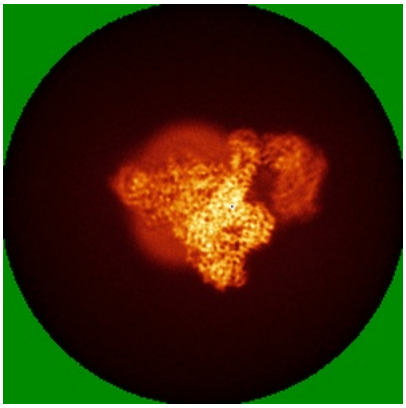
6.4.2 Raw map



X



Y

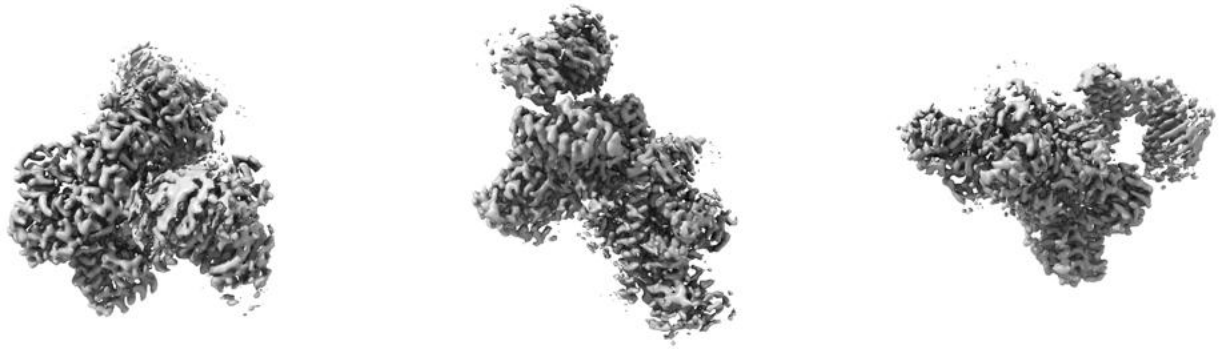


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

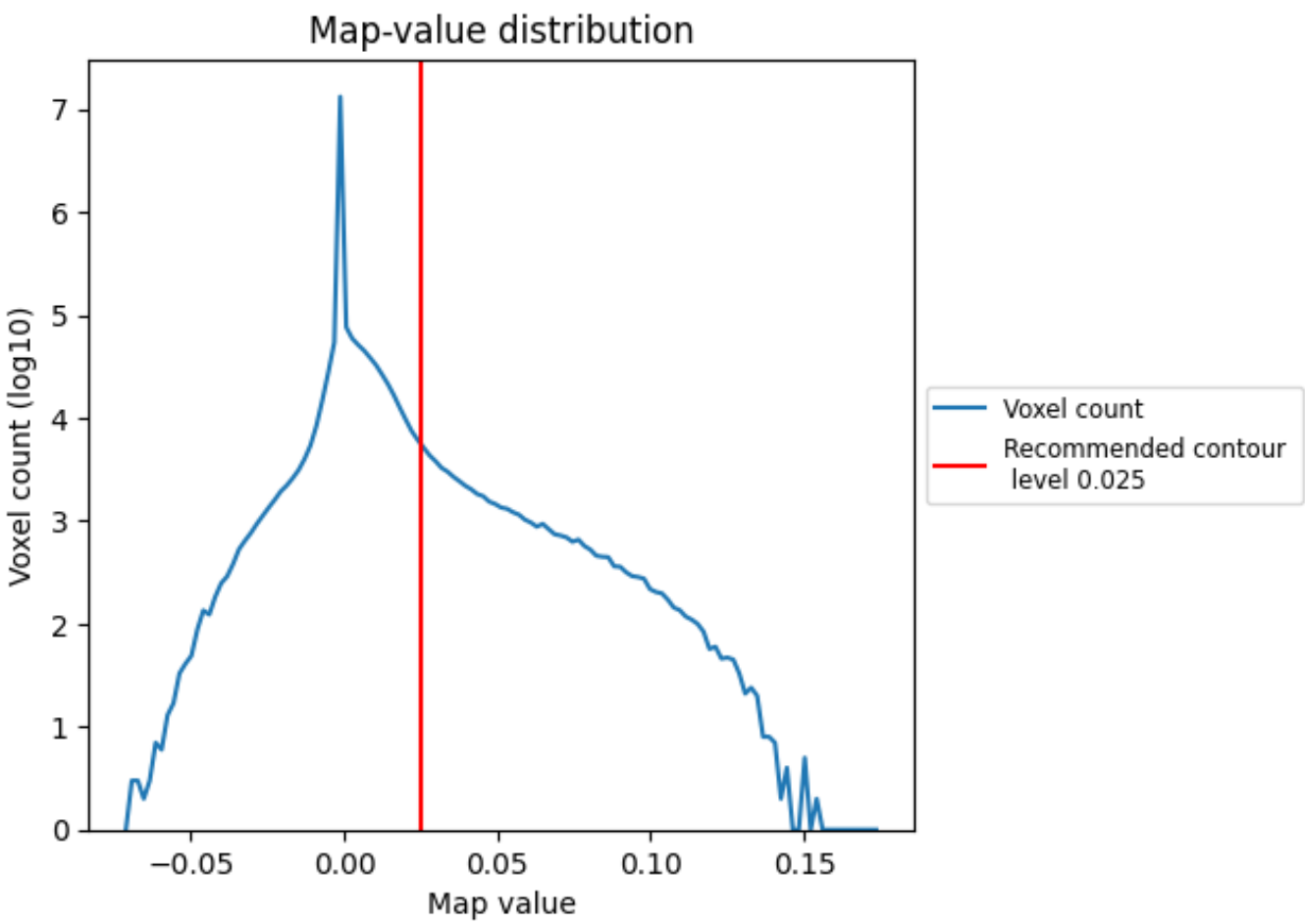
6.6 Mask visualisation (i)

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

7 Map analysis (i)

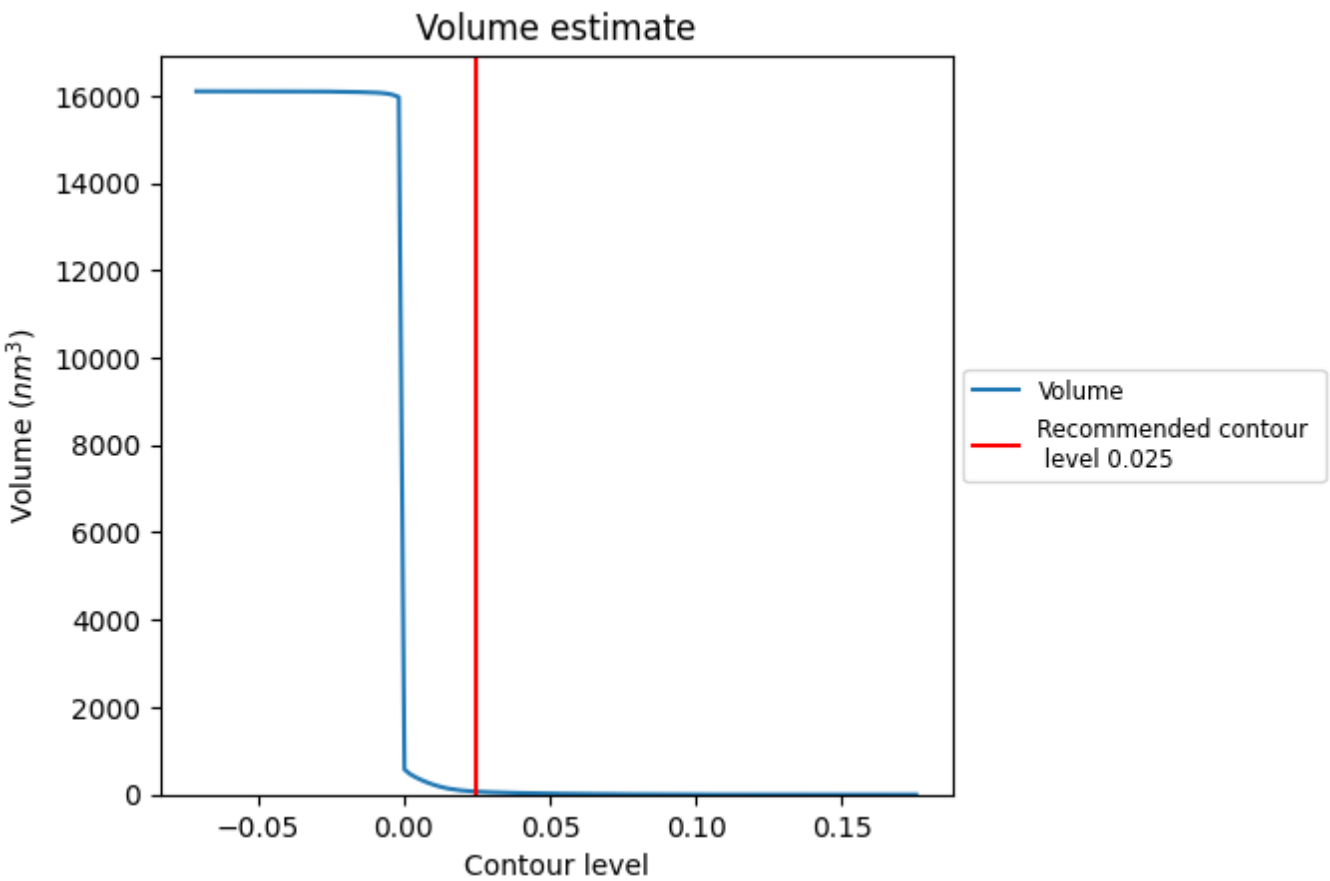
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

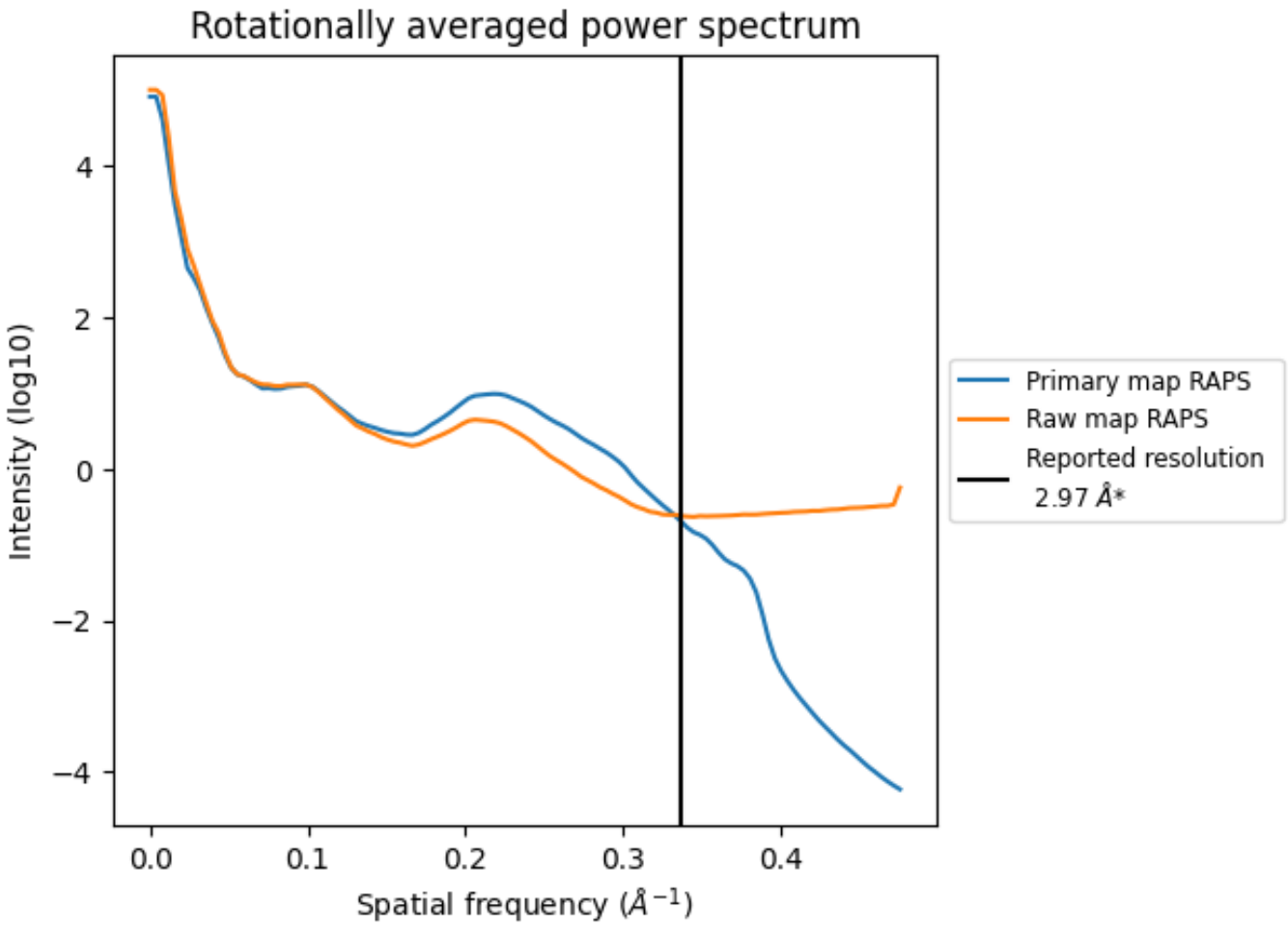
7.2 Volume estimate (i)



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 61 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)

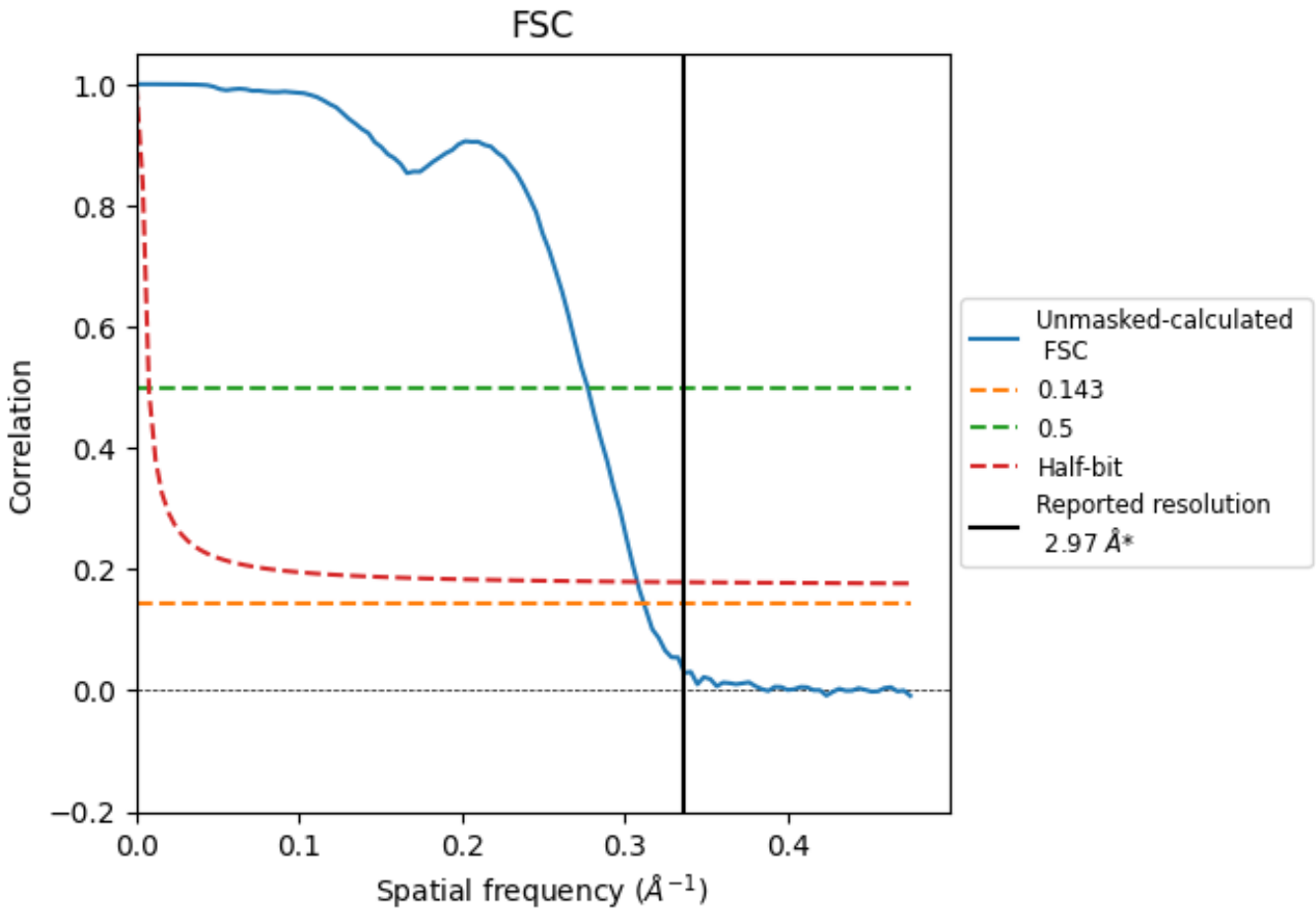


*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8.2 Resolution estimates (i)

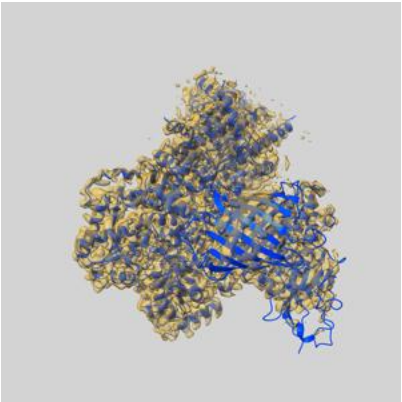
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.61	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

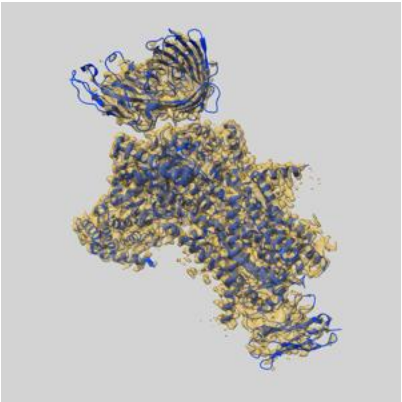
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-39087 and PDB model 8YA0. Per-residue inclusion information can be found in section 3 on page 8.

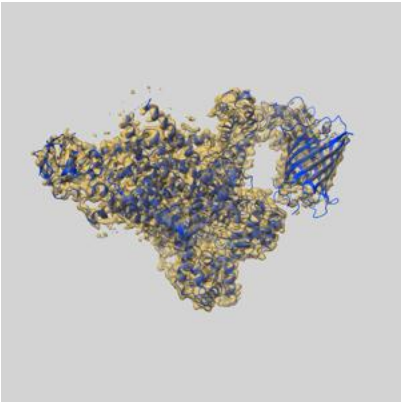
9.1 Map-model overlay (i)



X



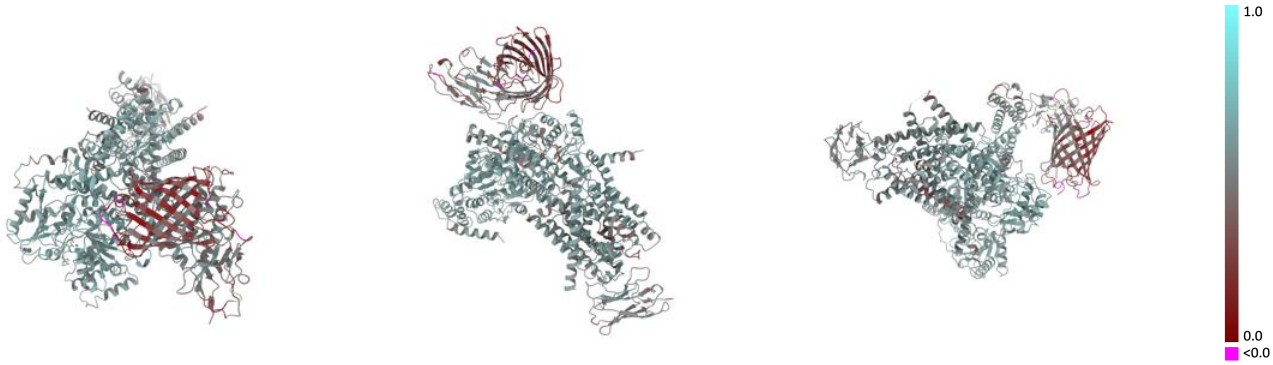
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

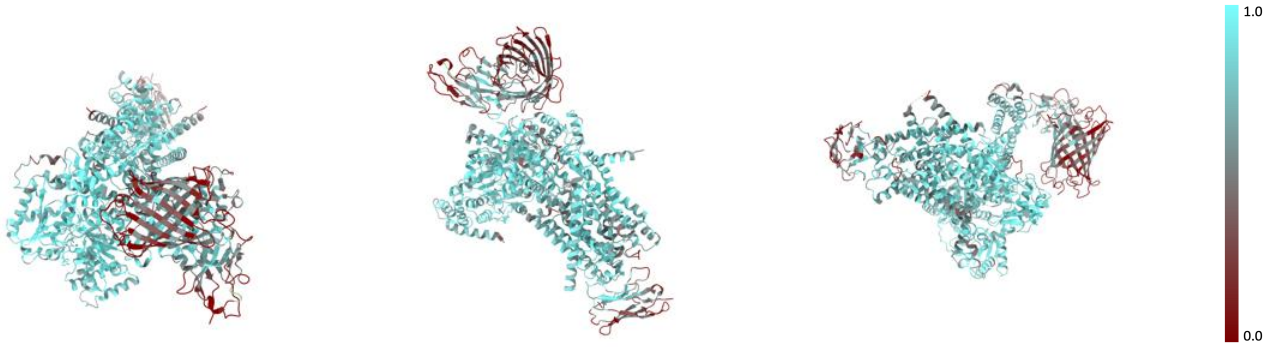
9.2 Q-score mapped to coordinate model (i)



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.

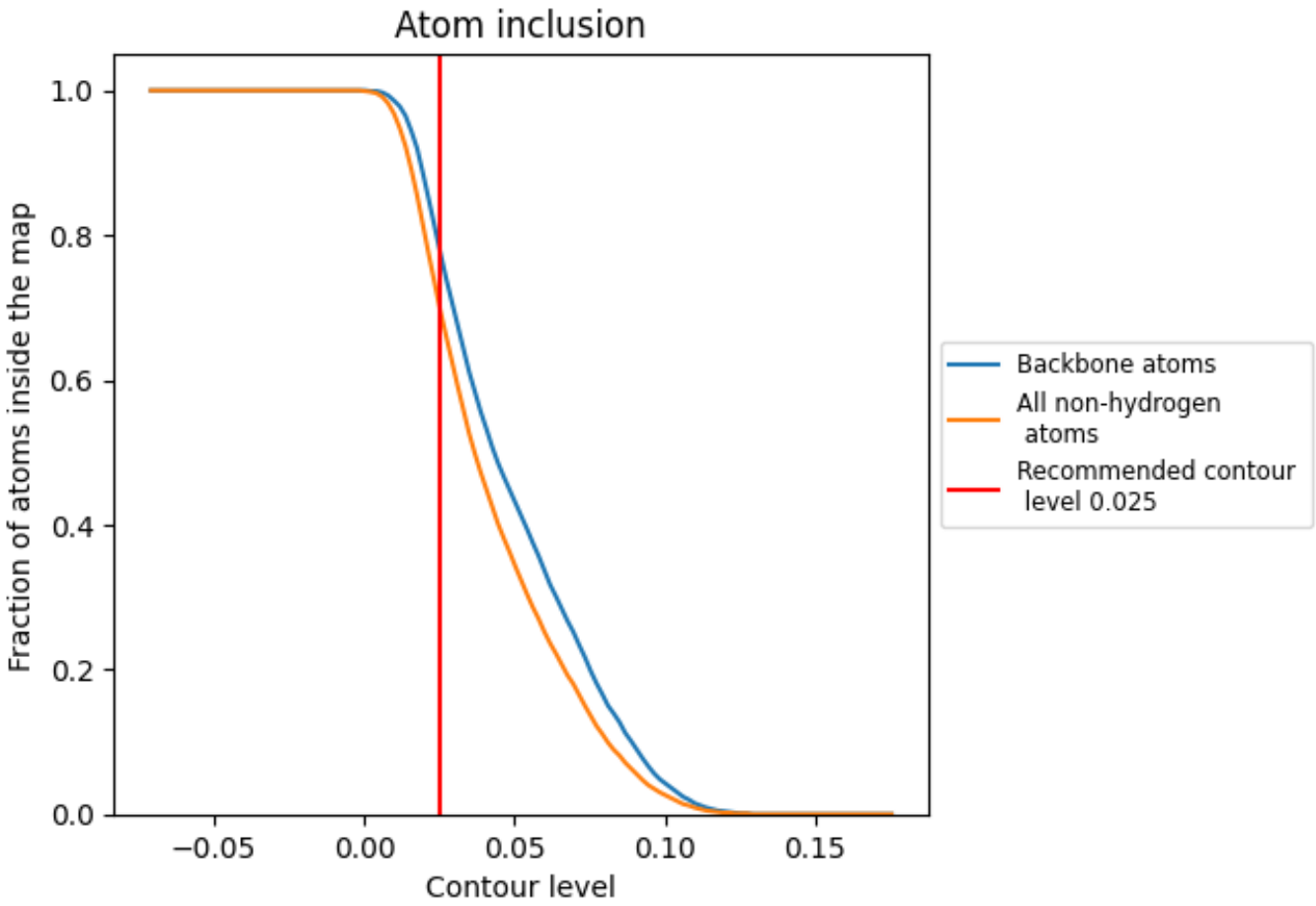
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.5150
A	0.8540	0.5850
B	0.6020	0.4620
C	0.4180	0.4310
E	0.7870	0.5500
G	0.2810	0.2690
V	0.4830	0.4800
Y	0.7830	0.5520