



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:36 AM UTC

PDB ID : 9KPZ / pdb_00009kpz
EMDB ID : EMD-62492
Title : Structure of TolQRA complex at pH 5.4 from E.coli
Authors : Dong, C.; Zhang, Z.
Deposited on : 2024-11-24
Resolution : 3.18 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:

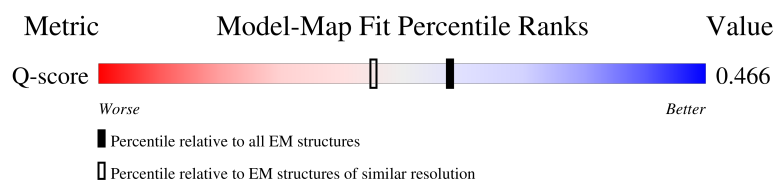
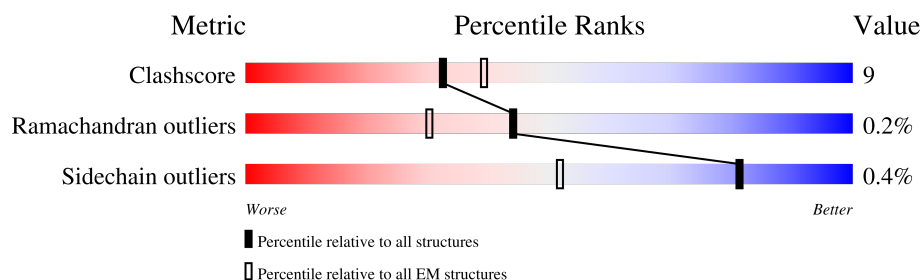
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.18 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.



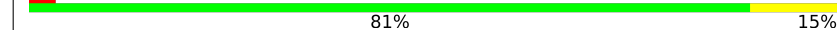



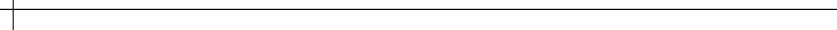
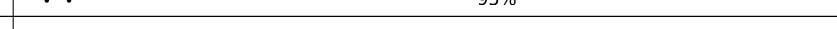
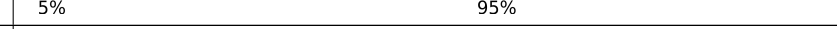

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

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	232	 5% 75% 19% 5%
1	B	232	 1% 75% 21% .
1	C	232	 1% 72% 22% 6%
1	D	232	 1% 76% 18% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	232	 81%15%5%
2	F	142	 10%6%84%
2	G	142	 13%2%82%
3	H	557	 5%95%
3	I	557	 95%
3	J	557	 5%95%
3	K	557	 5%2%94%
3	L	557	 5%95%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10447 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 Tol-Pal system protein TolQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1727	1115	297	307	8		
1	B	223	Total	C	N	O	S	0	0
			1752	1131	301	312	8		
1	C	219	Total	C	N	O	S	0	0
			1708	1104	293	303	8		
1	D	218	Total	C	N	O	S	0	0
			1708	1106	294	301	7		
1	E	221	Total	C	N	O	S	0	0
			1738	1122	299	309	8		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P0ABU9
A	0	GLY	-	expression tag	UNP P0ABU9
A	1	VAL	-	expression tag	UNP P0ABU9
B	-1	MET	-	initiating methionine	UNP P0ABU9
B	0	GLY	-	expression tag	UNP P0ABU9
B	1	VAL	-	expression tag	UNP P0ABU9
C	-1	MET	-	initiating methionine	UNP P0ABU9
C	0	GLY	-	expression tag	UNP P0ABU9
C	1	VAL	-	expression tag	UNP P0ABU9
D	-1	MET	-	initiating methionine	UNP P0ABU9
D	0	GLY	-	expression tag	UNP P0ABU9
D	1	VAL	-	expression tag	UNP P0ABU9
E	-1	MET	-	initiating methionine	UNP P0ABU9
E	0	GLY	-	expression tag	UNP P0ABU9
E	1	VAL	-	expression tag	UNP P0ABU9

- Molecule 2 is a protein called Tol-Pal system protein TolR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	23	Total	C	N	O	S	0	0
			179	123	25	30	1		
2	G	25	Total	C	N	O	S	0	0
			191	131	27	32	1		

- Molecule 3 is a protein called Ubiquitin-like protein SMT3,Tol-Pal system protein TolA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	28	Total	C	N	O		0	0
			214	145	34	35			
3	I	30	Total	C	N	O		0	0
			237	158	40	39			
3	J	29	Total	C	N	O		0	0
			200	133	34	33			
3	K	31	Total	C	N	O		0	0
			230	151	38	41			
3	L	29	Total	C	N	O		0	0
			220	146	36	38			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-134	MET	-	initiating methionine	UNP Q12306
H	-133	GLY	-	expression tag	UNP Q12306
H	-132	HIS	-	expression tag	UNP Q12306
H	-131	HIS	-	expression tag	UNP Q12306
H	-130	HIS	-	expression tag	UNP Q12306
H	-129	HIS	-	expression tag	UNP Q12306
H	-128	HIS	-	expression tag	UNP Q12306
H	-127	HIS	-	expression tag	UNP Q12306
H	-126	HIS	-	expression tag	UNP Q12306
H	-125	HIS	-	expression tag	UNP Q12306
H	-124	GLY	-	expression tag	UNP Q12306
H	-123	SER	-	expression tag	UNP Q12306
H	-122	LEU	-	expression tag	UNP Q12306
H	-121	GLN	-	expression tag	UNP Q12306
H	-23	ALA	-	linker	UNP Q12306
H	-22	ALA	-	linker	UNP Q12306
H	-21	ASP	-	linker	UNP Q12306
H	-20	TYR	-	linker	UNP Q12306
H	-19	GLY	-	linker	UNP Q12306
H	-18	GLY	-	linker	UNP Q12306
H	-17	ASP	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-16	ILE	-	linker	UNP Q12306
H	-15	PRO	-	linker	UNP Q12306
H	-14	THR	-	linker	UNP Q12306
H	-13	THR	-	linker	UNP Q12306
H	-12	GLU	-	linker	UNP Q12306
H	-11	ASN	-	linker	UNP Q12306
H	-10	LEU	-	linker	UNP Q12306
H	-9	TYR	-	linker	UNP Q12306
H	-8	PHE	-	linker	UNP Q12306
H	-7	GLN	-	linker	UNP Q12306
H	-6	GLY	-	linker	UNP Q12306
H	-5	ALA	-	linker	UNP Q12306
H	-4	ALA	-	linker	UNP Q12306
H	-3	ALA	-	linker	UNP Q12306
H	-2	ASP	-	linker	UNP Q12306
H	-1	ILE	-	linker	UNP Q12306
H	0	GLY	-	linker	UNP Q12306
H	1	SER	-	linker	UNP Q12306
H	2	VAL	-	linker	UNP Q12306
I	-134	MET	-	initiating methionine	UNP Q12306
I	-133	GLY	-	expression tag	UNP Q12306
I	-132	HIS	-	expression tag	UNP Q12306
I	-131	HIS	-	expression tag	UNP Q12306
I	-130	HIS	-	expression tag	UNP Q12306
I	-129	HIS	-	expression tag	UNP Q12306
I	-128	HIS	-	expression tag	UNP Q12306
I	-127	HIS	-	expression tag	UNP Q12306
I	-126	HIS	-	expression tag	UNP Q12306
I	-125	HIS	-	expression tag	UNP Q12306
I	-124	GLY	-	expression tag	UNP Q12306
I	-123	SER	-	expression tag	UNP Q12306
I	-122	LEU	-	expression tag	UNP Q12306
I	-121	GLN	-	expression tag	UNP Q12306
I	-23	ALA	-	linker	UNP Q12306
I	-22	ALA	-	linker	UNP Q12306
I	-21	ASP	-	linker	UNP Q12306
I	-20	TYR	-	linker	UNP Q12306
I	-19	GLY	-	linker	UNP Q12306
I	-18	GLY	-	linker	UNP Q12306
I	-17	ASP	-	linker	UNP Q12306
I	-16	ILE	-	linker	UNP Q12306
I	-15	PRO	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	THR	-	linker	UNP Q12306
I	-13	THR	-	linker	UNP Q12306
I	-12	GLU	-	linker	UNP Q12306
I	-11	ASN	-	linker	UNP Q12306
I	-10	LEU	-	linker	UNP Q12306
I	-9	TYR	-	linker	UNP Q12306
I	-8	PHE	-	linker	UNP Q12306
I	-7	GLN	-	linker	UNP Q12306
I	-6	GLY	-	linker	UNP Q12306
I	-5	ALA	-	linker	UNP Q12306
I	-4	ALA	-	linker	UNP Q12306
I	-3	ALA	-	linker	UNP Q12306
I	-2	ASP	-	linker	UNP Q12306
I	-1	ILE	-	linker	UNP Q12306
I	0	GLY	-	linker	UNP Q12306
I	1	SER	-	linker	UNP Q12306
I	2	VAL	-	linker	UNP Q12306
J	-134	MET	-	initiating methionine	UNP Q12306
J	-133	GLY	-	expression tag	UNP Q12306
J	-132	HIS	-	expression tag	UNP Q12306
J	-131	HIS	-	expression tag	UNP Q12306
J	-130	HIS	-	expression tag	UNP Q12306
J	-129	HIS	-	expression tag	UNP Q12306
J	-128	HIS	-	expression tag	UNP Q12306
J	-127	HIS	-	expression tag	UNP Q12306
J	-126	HIS	-	expression tag	UNP Q12306
J	-125	HIS	-	expression tag	UNP Q12306
J	-124	GLY	-	expression tag	UNP Q12306
J	-123	SER	-	expression tag	UNP Q12306
J	-122	LEU	-	expression tag	UNP Q12306
J	-121	GLN	-	expression tag	UNP Q12306
J	-23	ALA	-	linker	UNP Q12306
J	-22	ALA	-	linker	UNP Q12306
J	-21	ASP	-	linker	UNP Q12306
J	-20	TYR	-	linker	UNP Q12306
J	-19	GLY	-	linker	UNP Q12306
J	-18	GLY	-	linker	UNP Q12306
J	-17	ASP	-	linker	UNP Q12306
J	-16	ILE	-	linker	UNP Q12306
J	-15	PRO	-	linker	UNP Q12306
J	-14	THR	-	linker	UNP Q12306
J	-13	THR	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-12	GLU	-	linker	UNP Q12306
J	-11	ASN	-	linker	UNP Q12306
J	-10	LEU	-	linker	UNP Q12306
J	-9	TYR	-	linker	UNP Q12306
J	-8	PHE	-	linker	UNP Q12306
J	-7	GLN	-	linker	UNP Q12306
J	-6	GLY	-	linker	UNP Q12306
J	-5	ALA	-	linker	UNP Q12306
J	-4	ALA	-	linker	UNP Q12306
J	-3	ALA	-	linker	UNP Q12306
J	-2	ASP	-	linker	UNP Q12306
J	-1	ILE	-	linker	UNP Q12306
J	0	GLY	-	linker	UNP Q12306
J	1	SER	-	linker	UNP Q12306
J	2	VAL	-	linker	UNP Q12306
K	-134	MET	-	initiating methionine	UNP Q12306
K	-133	GLY	-	expression tag	UNP Q12306
K	-132	HIS	-	expression tag	UNP Q12306
K	-131	HIS	-	expression tag	UNP Q12306
K	-130	HIS	-	expression tag	UNP Q12306
K	-129	HIS	-	expression tag	UNP Q12306
K	-128	HIS	-	expression tag	UNP Q12306
K	-127	HIS	-	expression tag	UNP Q12306
K	-126	HIS	-	expression tag	UNP Q12306
K	-125	HIS	-	expression tag	UNP Q12306
K	-124	GLY	-	expression tag	UNP Q12306
K	-123	SER	-	expression tag	UNP Q12306
K	-122	LEU	-	expression tag	UNP Q12306
K	-121	GLN	-	expression tag	UNP Q12306
K	-23	ALA	-	linker	UNP Q12306
K	-22	ALA	-	linker	UNP Q12306
K	-21	ASP	-	linker	UNP Q12306
K	-20	TYR	-	linker	UNP Q12306
K	-19	GLY	-	linker	UNP Q12306
K	-18	GLY	-	linker	UNP Q12306
K	-17	ASP	-	linker	UNP Q12306
K	-16	ILE	-	linker	UNP Q12306
K	-15	PRO	-	linker	UNP Q12306
K	-14	THR	-	linker	UNP Q12306
K	-13	THR	-	linker	UNP Q12306
K	-12	GLU	-	linker	UNP Q12306
K	-11	ASN	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

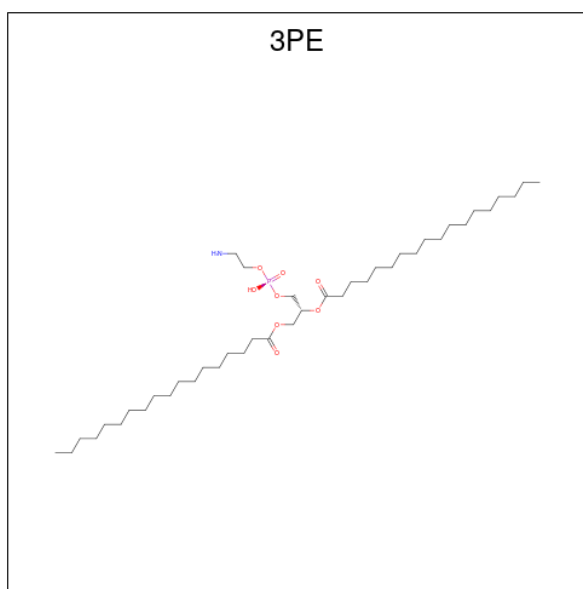
Chain	Residue	Modelled	Actual	Comment	Reference
K	-10	LEU	-	linker	UNP Q12306
K	-9	TYR	-	linker	UNP Q12306
K	-8	PHE	-	linker	UNP Q12306
K	-7	GLN	-	linker	UNP Q12306
K	-6	GLY	-	linker	UNP Q12306
K	-5	ALA	-	linker	UNP Q12306
K	-4	ALA	-	linker	UNP Q12306
K	-3	ALA	-	linker	UNP Q12306
K	-2	ASP	-	linker	UNP Q12306
K	-1	ILE	-	linker	UNP Q12306
K	0	GLY	-	linker	UNP Q12306
K	1	SER	-	linker	UNP Q12306
K	2	VAL	-	linker	UNP Q12306
L	-134	MET	-	initiating methionine	UNP Q12306
L	-133	GLY	-	expression tag	UNP Q12306
L	-132	HIS	-	expression tag	UNP Q12306
L	-131	HIS	-	expression tag	UNP Q12306
L	-130	HIS	-	expression tag	UNP Q12306
L	-129	HIS	-	expression tag	UNP Q12306
L	-128	HIS	-	expression tag	UNP Q12306
L	-127	HIS	-	expression tag	UNP Q12306
L	-126	HIS	-	expression tag	UNP Q12306
L	-125	HIS	-	expression tag	UNP Q12306
L	-124	GLY	-	expression tag	UNP Q12306
L	-123	SER	-	expression tag	UNP Q12306
L	-122	LEU	-	expression tag	UNP Q12306
L	-121	GLN	-	expression tag	UNP Q12306
L	-23	ALA	-	linker	UNP Q12306
L	-22	ALA	-	linker	UNP Q12306
L	-21	ASP	-	linker	UNP Q12306
L	-20	TYR	-	linker	UNP Q12306
L	-19	GLY	-	linker	UNP Q12306
L	-18	GLY	-	linker	UNP Q12306
L	-17	ASP	-	linker	UNP Q12306
L	-16	ILE	-	linker	UNP Q12306
L	-15	PRO	-	linker	UNP Q12306
L	-14	THR	-	linker	UNP Q12306
L	-13	THR	-	linker	UNP Q12306
L	-12	GLU	-	linker	UNP Q12306
L	-11	ASN	-	linker	UNP Q12306
L	-10	LEU	-	linker	UNP Q12306
L	-9	TYR	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-8	PHE	-	linker	UNP Q12306
L	-7	GLN	-	linker	UNP Q12306
L	-6	GLY	-	linker	UNP Q12306
L	-5	ALA	-	linker	UNP Q12306
L	-4	ALA	-	linker	UNP Q12306
L	-3	ALA	-	linker	UNP Q12306
L	-2	ASP	-	linker	UNP Q12306
L	-1	ILE	-	linker	UNP Q12306
L	0	GLY	-	linker	UNP Q12306
L	1	SER	-	linker	UNP Q12306
L	2	VAL	-	linker	UNP Q12306

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	D	1	Total	C	N	O	P	0
			49	39	1	8	1	

Continued on next page...

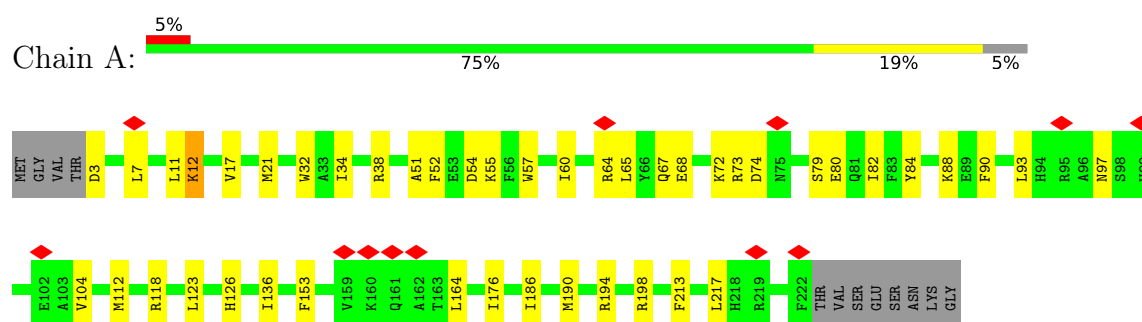
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	E	1	Total	C	N	O	P	0
			49	39	1	8	1	

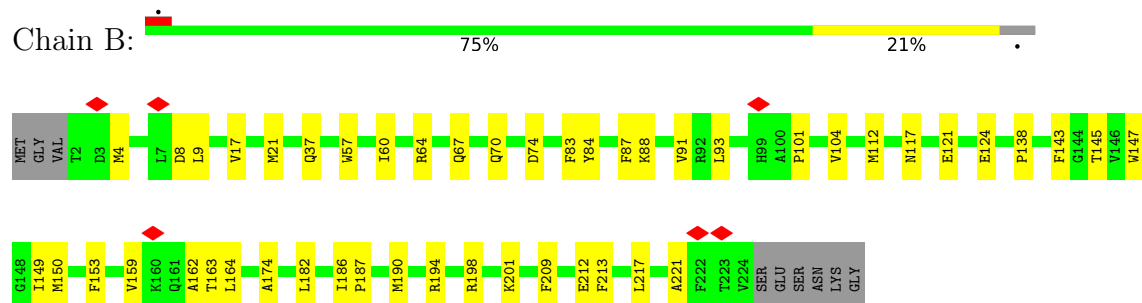
3 Residue-property plots [i](#)

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.

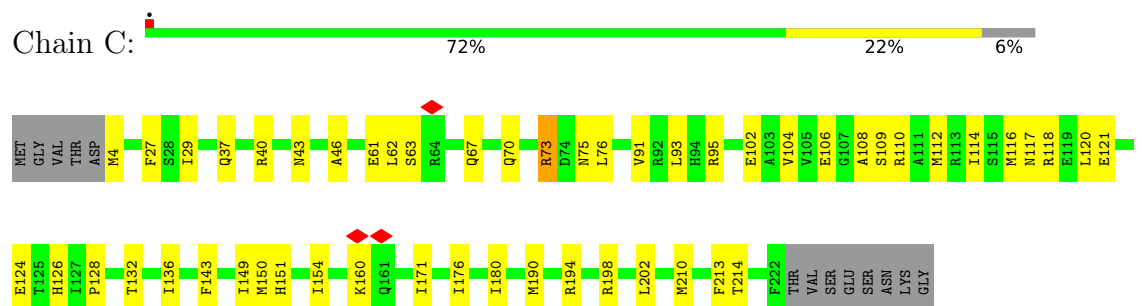
- Molecule 1: Tol-Pal system protein TolQ



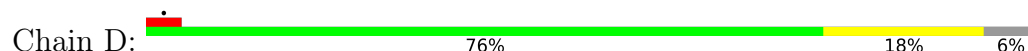
- Molecule 1: Tol-Pal system protein TolQ

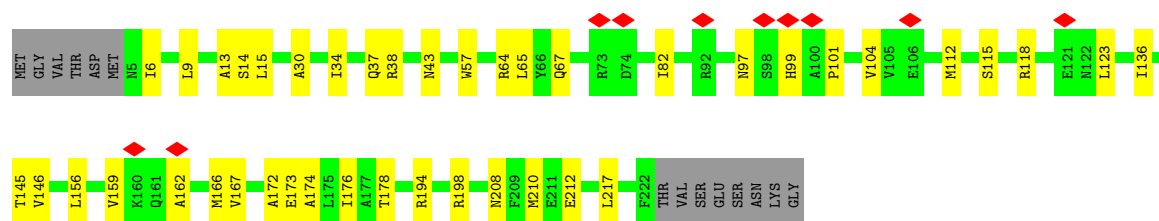


- Molecule 1: Tol-Pal system protein TolQ

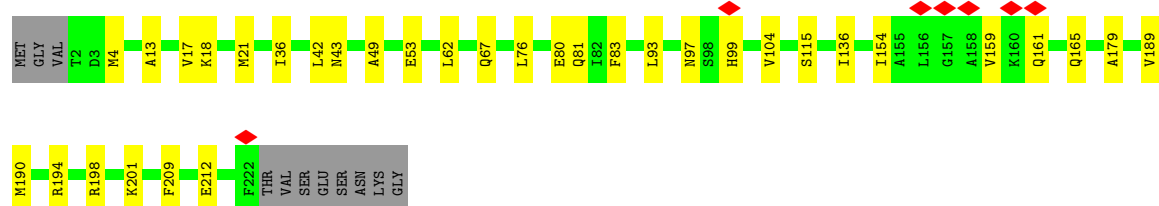
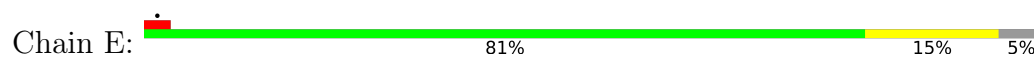


- Molecule 1: Tol-Pal system protein TolQ

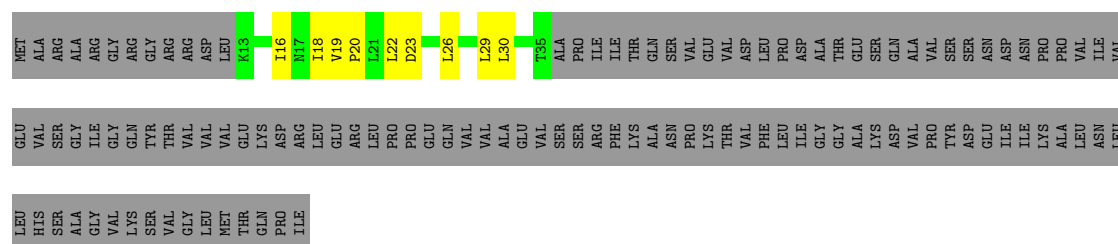




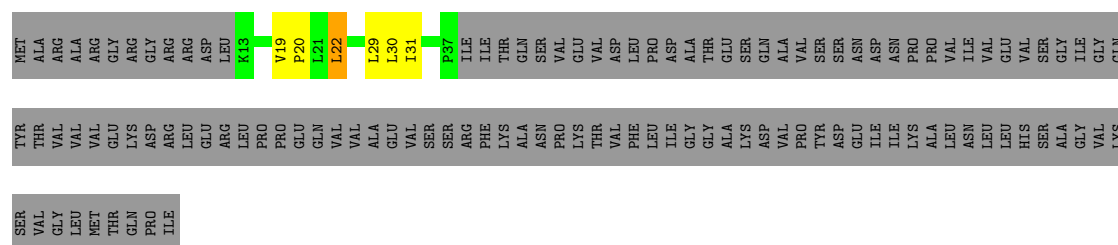
• Molecule 1: Tol-Pal system protein TolQ



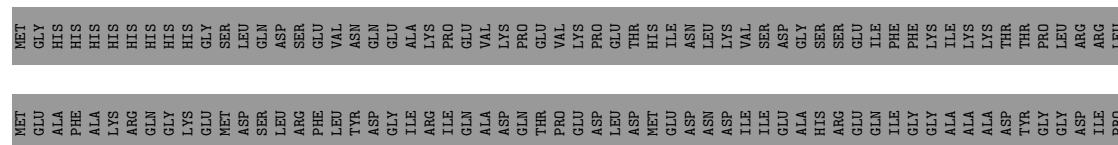
• Molecule 2: Tol-Pal system protein TolR

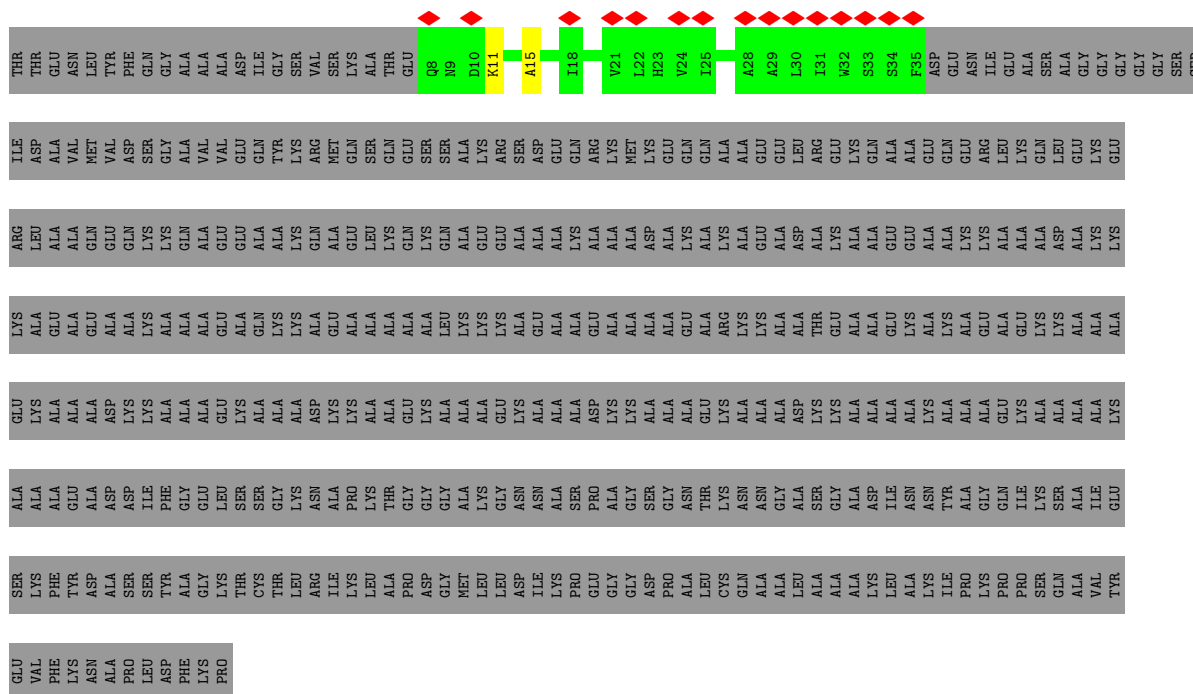


• Molecule 2: Tol-Pal system protein TolR



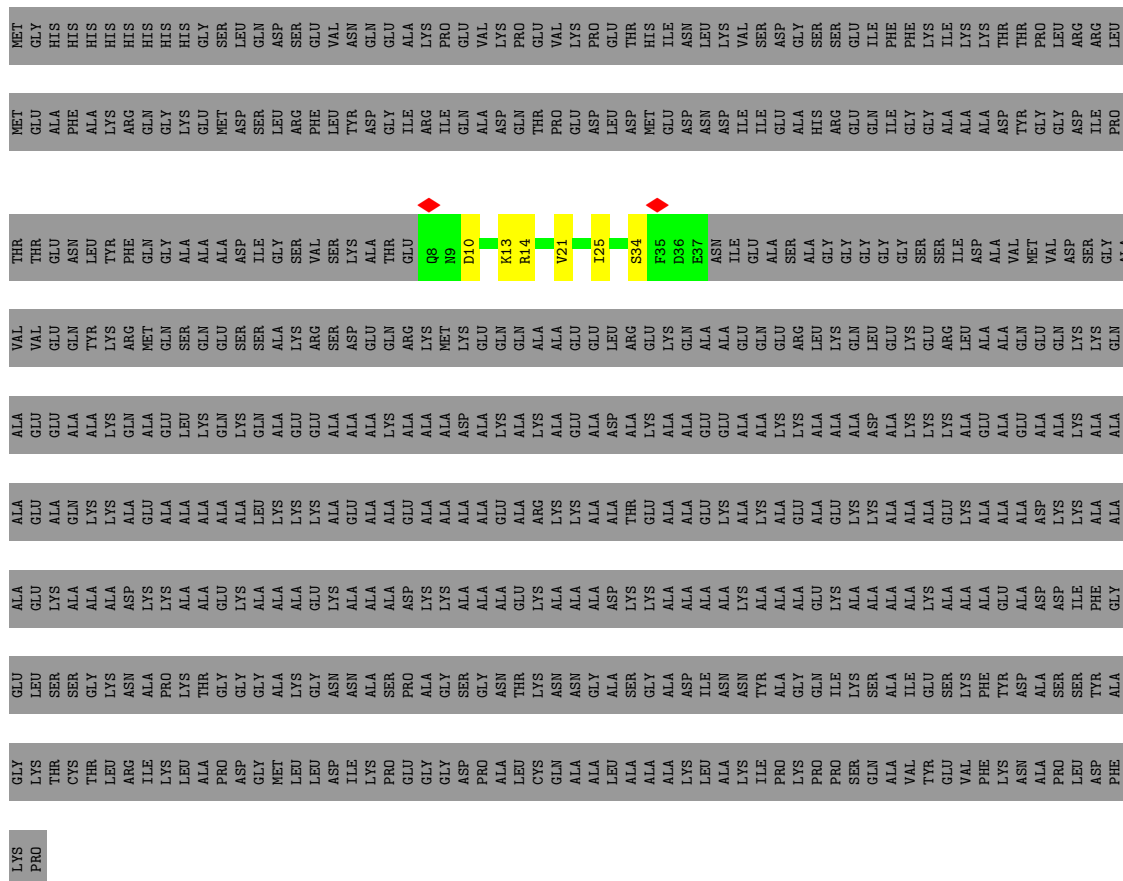
• Molecule 3: Ubiquitin-like protein SMT3,Tol-Pal system protein TolA



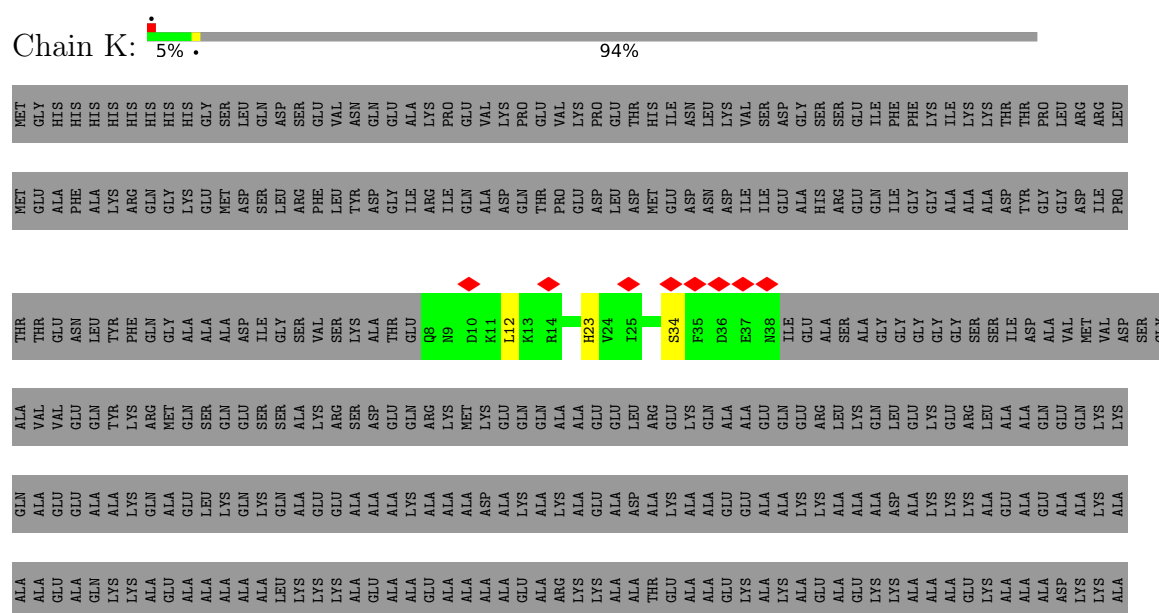
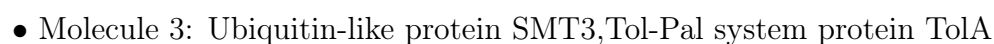


- Molecule 3: Ubiquitin-like protein SMT3, Tol-Pal system protein TolA

Chain I: 95%



Chain J: 5% 95%



PHE LYS PRO	ALA GLY THR THR LEU ILE LEU ALA PRO GLY MET LEU LEU ASP ILE LYS PRO PRO GLY GLY ASP PRO LEU CYS GLN ALA LYS ILE PRO PRO SER GLN ALA VAL TYR VAL PHE LYS ASN ALA PRO LEU ASP	ALA GLY THR CYS LEU ILE LYS LEU ALA PRO GLY MET LEU LEU ASP ILE LYS PRO PRO GLY GLY ASP PRO LEU CYS GLN ALA LYS ILE PRO PRO SER GLN ALA VAL TYR VAL PHE LYS ASN ALA PRO LEU ASP	GLY LEU SER GLY LYS ASN ALA PRO LYS THR GLY GLY ALA LYS GLY ASN ASN GLY GLY SER PRO ALA GLY ASP PRO LEU CYS GLN ALA LYS ILE TYR GLY GLN ILE LYS SER ALA ILE GLY GLN ILE LYS SER PHE TYR ASP ALA SER TYR	ALA GLY LYS ALA ASP LYS LYS ALA ALA GLY LYS LYS ALA ALA GLY LYS LYS ASP LYS LYS ALA ALA GLY ILE ASN ASN TYR ALA GLY GLN ILE LYS SER ALA ILE GLY GLN ILE LYS SER PHE LYS ASN ALA PRO LEU ASP
-------------------	---	--	--	---

- Molecule 3: Ubiquitin-like protein SMT3, Tol-Pal system protein TolA

Chain L: 5% 95%

PRO	GLY	GLU	ALA	GLN	GLU	THR	MET	MET
ASP	GLY	ALA	LEU	LYS	SER	THR	GLY	GLU
GLY	ALA	ALA	LEU	GLN	SER	THR	ALA	ALA
MET	LYS	LYS	LYS	ALA	ALA	ASN	PHE	ALA
LEU	GLY	GLU	LYS	GLU	ARG	TYR	LYS	LYS
ASP	ASN	LYS	ALA	SER	SER	PHE	ARG	ARG
ILE	ASN	ALA	GLU	ALA	GLN	GLY	GLN	GLN
LYS	ALA	ALA	ALA	LYS	GLU	ALA	LYS	HIS
PRO	SER	ALA	ALA	LYS	GLN	ALA	LYS	HIS
GLU	PRO	ASP	GLU	ALA	ARG	ALA	GLY	GLY
GLY	ALA	LYS	ALA	ALA	LYS	ALA	MET	SER
GLY	GLY	LYS	ALA	ALA	MET	ALA	ASP	LEU
ASP	SER	ALA	ALA	ASP	LYS	ILE	GLN	GLN
PRO	GLY	ALA	ALA	ALA	GLU	GLY	ARG	ASP
ALA	ASN	ALA	GLU	LYS	GLN	VAL	SER	ARG
LEU	THR	GLU	ARG	LYS	ALA	SER	PHE	GLU
CYS	LYS	LYS	ALA	LYS	ALA	VAL	LEU	VAL
GLN	ASN	ALA	LYS	ALA	ALA	LYS	TYR	ASN
ALA	ASN	ALA	LYS	GLU	GLU	ALA	ASP	GLN
ALA	GLY	ALA	ALA	ALA	GLU	THR	GLY	GLY
LEU	ALA	ASP	ALA	ASP	LEU	GLU	ILE	ALA
ALA	SER	LYS	THR	ALA	ARG	THR	ARG	LYS
ALA	GLY	LYS	GLU	LYS	GLU	GLS	ILE	PRO
ALA	ALA	ALA	ALA	LYS	GLU	D36	LYS	GLU
LYS	ASP	ALA	ALA	ALA	GLN	GLU	ALA	ALA
LEU	ILE	ALA	GLU	GLU	ALA	ASN	LYS	VAL
ALA	ASN	ALA	LYS	GLU	ALA	ILE	GLN	PRO
LYS	ASN	LYS	ALA	ALA	GLU	GLU	THR	GLU
ILE	TYR	ALA	LYS	ALA	GLN	ALA	PRO	VAL
PRO	ALA	ALA	ALA	LYS	GLU	SER	GLY	LYS
LYS	GLY	ALA	GLU	LYS	ARG	ALA	ASP	PRO
PRO	ILE	GLU	ALA	ALA	LEU	GLY	LEU	GLU
PRO	ILE	GLU	GLU	ALA	LYS	GLY	ASP	THR
SER	LYS	ALA	LYS	ALA	GLN	GLY	MET	HIS
GLN	SER	ALA	LYS	ASP	LEU	GLY	GLU	ILE
ALA	ALA	ALA	ALA	ALA	GLU	GLY	ASP	ASN
VAL	ILE	ALA	ALA	LYS	LYS	SER	ASN	ASN
TYR	GLU	LYS	ALA	LYS	GLU	ILE	LYS	VAL
GLU	SER	ALA	GLU	LYS	ARG	ILE	ILE	VAL
VAL	LYS	ALA	LYS	ALA	LEU	ASP	SER	ASP
PHE	PHE	ALA	ALA	GLU	ALA	ALA	GLY	GLY
LYS	TYR	GLU	ALA	ALA	VAL	VAL	ALA	ALA
ASN	ASP	ALA	ALA	GLU	GLN	MET	HIS	SER
ALA	ALA	ASP	ASP	ALA	GLU	VAL	ARG	GLY
PRO	SER	ASP	LYS	ALA	GLN	ASP	GLU	GLY
LEU	SER	ILE	LYS	ALA	LYS	SER	GLN	ILE
ASP	TYR	PHE	ALA	ALA	LYS	GLY	PHE	GLY
PHE	ALA	GLY	ALA	ALA	GLN	ALA	GLY	GLY
LYS	GLY	LYS	GLU	ALA	VAL	VAL	ILE	LYS
PRO	THR	THR	GLU	ALA	GLU	GLU	ALA	ALA
		SER	LYS	ALA	ALA	GLN	LYS	LYS
		SER	ALA	LYS	ALA	TYR	ASP	THR
		GLY	ALA	LYS	ALA	LYS	TYR	THR
		LYS	ASP	LYS	LYS	LYS	TYR	THR
		ASN	ALA	ALA	GLN	ARG	GLY	PRO
		ILE	LYS	GLU	ALA	GLN	GLY	PRO
		PRO	LYS	ALA	GLU	GLN	ASP	ARG
		LEU	ALA	ALA	GLU	GLN	GLY	ARG
		ALA	ALA	ALA	LYS	GLN	ILE	ARG
		THR	ALA	ALA	LYS	GLN	PRO	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	470510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.099	Depositor
Minimum map value	-0.730	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: 3PE

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	0.16	0/1761	0.35	0/2381
1	B	0.15	0/1786	0.34	0/2415
1	C	0.15	0/1741	0.37	0/2354
1	D	0.19	0/1742	0.36	0/2355
1	E	0.14	0/1772	0.32	0/2395
2	F	0.23	0/180	0.57	0/245
2	G	0.13	0/193	0.42	0/264
3	H	0.06	0/218	0.15	0/297
3	I	0.12	0/241	0.29	0/326
3	J	0.05	0/202	0.15	0/277
3	K	0.06	0/233	0.13	0/318
3	L	0.08	0/223	0.14	0/303
All	All	0.15	0/10292	0.34	0/13930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1727	0	1747	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1752	0	1781	39	0
1	C	1708	0	1725	40	0
1	D	1708	0	1735	30	0
1	E	1738	0	1765	26	0
2	F	179	0	207	9	0
2	G	191	0	219	5	0
3	H	214	0	221	3	0
3	I	237	0	249	5	0
3	J	200	0	201	2	0
3	K	230	0	228	3	0
3	L	220	0	229	0	0
4	A	49	0	75	3	0
4	B	98	0	150	8	0
4	C	49	0	75	5	0
4	D	98	0	150	4	0
4	E	49	0	75	7	0
All	All	10447	0	10832	181	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 9.

All (181) 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:D:112:MET:HE1	1:D:210:MET:HA	1.69	0.75
1:B:93:LEU:HD23	1:B:104:VAL:HA	1.68	0.74
1:B:190:MET:HB3	4:B:301:3PE:H231	1.70	0.74
1:C:43:ASN:OD1	1:C:198:ARG:NH2	2.24	0.69
1:C:93:LEU:HD12	1:C:104:VAL:HA	1.75	0.69
1:D:145:THR:HG23	1:D:174:ALA:HB1	1.75	0.69
1:B:4:MET:H	1:E:154:ILE:HD13	1.57	0.68
1:D:115:SER:OG	1:D:118:ARG:NH2	2.27	0.68
1:C:109:SER:OG	1:C:110:ARG:NH1	2.28	0.66
1:A:3:ASP:N	3:K:34:SER:HG	1.94	0.66
1:D:6:ILE:HG13	3:I:34:SER:HB2	1.77	0.66
1:B:143:PHE:HB2	4:D:302:3PE:H2G1	1.79	0.64
1:D:57:TRP:NE1	1:D:212:GLU:OE2	2.31	0.63
4:D:302:3PE:H341	4:D:302:3PE:H252	1.81	0.63
1:E:93:LEU:HB3	1:E:104:VAL:HG22	1.82	0.62
1:B:60:ILE:HG12	1:B:64:ARG:HG3	1.83	0.61
1:C:126:HIS:HA	4:C:301:3PE:H222	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:HG21	2:F:23:ASP:HB3	1.83	0.60
1:D:43:ASN:OD1	1:D:198:ARG:NH2	2.29	0.59
1:B:37:GLN:NE2	3:H:11:LYS:O	2.36	0.59
1:C:210:MET:O	1:C:214:THR:HG22	2.02	0.58
1:B:149:ILE:O	1:B:153:PHE:HB2	2.03	0.58
1:D:97:ASN:OD1	1:D:99:HIS:ND1	2.36	0.58
1:E:76:LEU:HD22	1:E:80:GLU:HB3	1.84	0.58
1:A:54:ASP:OD2	1:A:55:LYS:NZ	2.29	0.58
1:A:65:LEU:HA	1:A:68:GLU:OE2	2.04	0.58
1:D:82:ILE:HG22	1:D:112:MET:SD	2.44	0.58
1:C:171:ILE:HG23	2:G:30:LEU:HD13	1.86	0.57
1:C:150:MET:O	1:C:154:ILE:HG22	2.04	0.56
1:B:150:MET:HA	1:B:150:MET:HE2	1.88	0.56
1:B:64:ARG:HA	1:B:67:GLN:HG2	1.86	0.56
1:E:13:ALA:O	1:E:18:LYS:NZ	2.39	0.55
2:G:19:VAL:HB	2:G:20:PRO:HD3	1.89	0.55
1:E:81:GLN:OE1	1:E:115:SER:OG	2.25	0.55
1:C:128:PRO:HB2	4:E:301:3PE:H121	1.89	0.54
1:C:27:PHE:HE2	1:C:136:ILE:HD11	1.73	0.54
1:E:36:ILE:HG23	4:E:301:3PE:H2E2	1.90	0.54
1:D:30:ALA:O	1:D:34:ILE:HG12	2.08	0.54
1:C:62:LEU:H	1:C:62:LEU:HD23	1.73	0.53
1:E:189:VAL:HG21	2:F:16:ILE:HG13	1.89	0.53
1:C:151:HIS:ND1	1:E:4:MET:SD	2.82	0.52
1:B:8:ASP:OD1	1:B:9:LEU:N	2.42	0.52
1:A:38:ARG:NH1	1:A:123:LEU:O	2.43	0.52
1:C:121:GLU:OE1	1:E:201:LYS:HE3	2.10	0.52
1:C:160:LYS:HA	1:E:165:GLN:HE22	1.73	0.52
1:B:74:ASP:OD1	1:B:74:ASP:N	2.43	0.51
1:A:90:PHE:CD1	1:A:217:LEU:HD11	2.45	0.51
1:B:159:VAL:HG11	1:B:162:ALA:HB2	1.92	0.51
1:C:136:ILE:HD13	1:E:190:MET:SD	2.51	0.51
1:D:156:LEU:HD22	1:D:167:VAL:HG11	1.93	0.51
1:D:37:GLN:HG3	1:D:38:ARG:N	2.26	0.50
1:A:17:VAL:HG12	1:A:21:MET:HE3	1.94	0.50
1:D:64:ARG:NH1	1:D:67:GLN:HB3	2.26	0.50
1:A:84:TYR:OH	1:A:88:LYS:NZ	2.36	0.50
1:B:101:PRO:HB3	1:B:221:ALA:HB1	1.93	0.49
4:C:301:3PE:H292	4:C:301:3PE:H391	1.94	0.49
1:A:153:PHE:HZ	2:G:31:ILE:HA	1.78	0.49
2:F:18:ILE:HG22	2:F:18:ILE:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HH11	1:A:118:ARG:HG2	1.78	0.49
1:C:75:ASN:O	1:C:76:LEU:HD23	2.11	0.49
1:C:117:ASN:O	1:C:121:GLU:HG2	2.13	0.49
1:D:64:ARG:NH1	1:D:64:ARG:O	2.46	0.49
1:A:136:ILE:HG21	1:C:190:MET:HB2	1.95	0.48
1:C:37:GLN:OE1	1:C:40:ARG:NH2	2.46	0.48
1:C:124:GLU:O	1:C:124:GLU:HG3	2.13	0.48
1:A:93:LEU:HB3	1:A:104:VAL:HG22	1.94	0.48
1:A:186:ILE:O	1:A:190:MET:HG3	2.13	0.48
1:C:102:GLU:O	1:C:106:GLU:HG2	2.12	0.48
3:I:10:ASP:O	3:I:14:ARG:HG2	2.13	0.48
3:I:21:VAL:O	3:I:25:ILE:HG22	2.12	0.48
1:B:149:ILE:HG13	2:F:30:LEU:HD11	1.96	0.48
1:C:149:ILE:HD12	2:G:29:LEU:HD23	1.96	0.47
4:B:301:3PE:H292	4:B:301:3PE:H2C1	1.74	0.47
1:D:34:ILE:HA	1:D:37:GLN:HG2	1.96	0.47
1:D:101:PRO:O	1:D:104:VAL:HG23	2.15	0.47
1:A:60:ILE:HG23	1:A:64:ARG:HE	1.79	0.47
1:E:43:ASN:OD1	1:E:198:ARG:NH1	2.44	0.47
4:E:301:3PE:H2D1	4:E:301:3PE:H2G1	1.51	0.47
1:A:52:PHE:CD1	1:A:80:GLU:HB2	2.50	0.47
4:B:302:3PE:H3C2	4:B:302:3PE:H3F1	1.52	0.47
4:D:301:3PE:H2E2	4:D:301:3PE:H2H2	1.58	0.46
4:A:301:3PE:H232	1:C:194:ARG:HH12	1.80	0.46
1:B:190:MET:HG2	1:E:136:ILE:HG21	1.97	0.46
1:C:67:GLN:HE21	1:C:70:GLN:NE2	2.13	0.46
1:D:194:ARG:HD3	4:D:302:3PE:H2	1.97	0.46
1:E:97:ASN:HB2	1:E:99:HIS:CE1	2.51	0.46
1:B:198:ARG:O	1:B:201:LYS:HG2	2.16	0.46
1:C:116:MET:HG3	1:C:120:LEU:HD23	1.98	0.46
1:B:17:VAL:HG12	1:B:21:MET:SD	2.56	0.46
1:E:17:VAL:HG12	1:E:21:MET:HE2	1.97	0.46
1:C:4:MET:SD	1:C:4:MET:N	2.89	0.45
2:F:22:LEU:HD21	2:G:22:LEU:HD22	1.97	0.45
1:B:138:PRO:HB3	2:F:20:PRO:HG3	1.98	0.45
1:B:60:ILE:HG21	1:B:64:ARG:HB2	1.99	0.45
1:A:21:MET:HE2	1:A:176:ILE:HG23	1.98	0.45
1:C:61:GLU:HG2	1:C:63:SER:H	1.82	0.45
1:D:64:ARG:HH12	1:D:67:GLN:HB3	1.82	0.45
1:A:12:LYS:HB2	1:A:12:LYS:HE3	1.62	0.45
1:B:70:GLN:OE1	1:B:84:TYR:OH	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:O	1:B:91:VAL:HG12	2.17	0.44
1:A:164:LEU:HB2	1:D:162:ALA:HB1	1.99	0.44
1:B:182:LEU:HD21	2:F:20:PRO:HG2	1.98	0.44
1:C:114:ILE:O	1:C:118:ARG:HG2	2.18	0.44
1:B:194:ARG:HB2	4:B:301:3PE:H221	2.00	0.44
1:D:82:ILE:HG23	1:D:115:SER:HB3	1.98	0.44
1:A:186:ILE:HG23	1:D:136:ILE:HB	2.00	0.44
1:B:163:THR:OG1	1:B:164:LEU:N	2.51	0.44
1:E:97:ASN:N	1:E:97:ASN:OD1	2.50	0.44
1:A:51:ALA:O	1:A:55:LYS:HG2	2.18	0.44
1:A:64:ARG:O	1:A:67:GLN:HG2	2.18	0.43
1:B:117:ASN:O	1:B:121:GLU:HG2	2.18	0.43
4:C:301:3PE:H252	4:C:301:3PE:H281	1.51	0.43
1:D:9:LEU:O	1:D:13:ALA:HB2	2.18	0.43
1:B:57:TRP:NE1	1:B:212:GLU:OE2	2.50	0.43
1:D:14:SER:OG	1:D:15:LEU:N	2.49	0.43
1:A:97:ASN:N	1:A:97:ASN:OD1	2.52	0.43
1:A:57:TRP:CE3	1:A:57:TRP:HA	2.53	0.43
1:B:112:MET:SD	1:B:213:PHE:HD2	2.42	0.43
1:C:108:ALA:O	1:C:112:MET:HG3	2.18	0.43
1:E:194:ARG:O	1:E:198:ARG:HG3	2.18	0.43
3:J:11:LYS:HA	3:J:11:LYS:HD2	1.80	0.43
3:K:12:LEU:HD12	3:K:12:LEU:HA	1.88	0.43
1:E:62:LEU:HD12	1:E:62:LEU:HA	1.87	0.43
1:A:32:TRP:HD1	3:K:23:HIS:HE1	1.66	0.43
1:D:159:VAL:HG11	1:D:166:MET:HE1	2.00	0.43
1:B:145:THR:HG23	1:B:174:ALA:HB1	2.00	0.43
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.92	0.43
1:C:73:ARG:O	1:C:76:LEU:HG	2.17	0.43
4:E:301:3PE:O32	4:E:301:3PE:N	2.38	0.43
3:I:10:ASP:HA	3:I:13:LYS:HE2	2.00	0.42
1:C:143:PHE:HE1	1:E:179:ALA:HB1	1.84	0.42
1:C:73:ARG:HA	1:C:73:ARG:HD2	1.88	0.42
1:D:173:GLU:O	1:D:176:ILE:HG22	2.19	0.42
1:A:72:LYS:O	1:A:74:ASP:N	2.53	0.42
1:B:124:GLU:O	1:B:124:GLU:HG2	2.19	0.42
4:C:301:3PE:H2B2	4:C:301:3PE:H2E1	1.65	0.42
1:E:67:GLN:OE1	1:E:67:GLN:HA	2.20	0.42
1:E:212:GLU:OE1	1:E:212:GLU:HA	2.18	0.42
1:B:147:TRP:HZ2	3:I:34:SER:HB3	1.85	0.42
1:B:150:MET:HE1	1:D:172:ALA:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:O	1:A:198:ARG:HG3	2.19	0.42
1:D:65:LEU:HD23	1:D:65:LEU:HA	1.81	0.42
1:E:42:LEU:HD13	1:E:198:ARG:HB2	2.00	0.42
1:E:49:ALA:O	1:E:53:GLU:HG2	2.20	0.42
4:B:302:3PE:H2G1	4:B:302:3PE:H2D2	1.55	0.42
1:D:145:THR:O	1:D:146:VAL:C	2.63	0.42
1:B:83:PHE:HB2	1:B:209:PHE:HZ	1.84	0.42
4:B:301:3PE:H2B2	4:B:301:3PE:H2E1	1.67	0.41
1:A:34:ILE:HD13	1:A:126:HIS:HB3	2.01	0.41
1:B:37:GLN:HE21	3:H:15:ALA:CB	2.33	0.41
1:A:126:HIS:ND1	4:A:301:3PE:H32	2.35	0.41
1:B:87:PHE:HD2	1:B:213:PHE:HZ	1.68	0.41
1:C:46:ALA:HA	1:C:202:LEU:HD21	2.02	0.41
1:C:112:MET:SD	1:C:213:PHE:HD2	2.43	0.41
1:E:83:PHE:HB2	1:E:209:PHE:HZ	1.84	0.41
1:C:70:GLN:O	1:C:73:ARG:HB2	2.21	0.41
1:B:186:ILE:HB	1:B:187:PRO:HD3	2.03	0.41
4:B:302:3PE:H221	4:B:302:3PE:H2	1.77	0.41
1:C:128:PRO:O	1:C:132:THR:HG23	2.21	0.41
2:F:26:LEU:HA	2:F:29:LEU:HD12	2.02	0.41
1:A:112:MET:HE1	1:A:213:PHE:CD2	2.56	0.41
4:A:301:3PE:H222	4:A:301:3PE:H251	1.70	0.41
1:B:37:GLN:HE22	3:H:11:LYS:C	2.29	0.41
1:C:91:VAL:HG22	1:C:95:ARG:HD2	2.02	0.41
1:D:123:LEU:HD23	1:D:123:LEU:HA	1.92	0.41
1:A:7:LEU:O	1:A:11:LEU:HG	2.20	0.41
1:A:88:LYS:HB2	1:A:88:LYS:HE3	1.88	0.41
1:C:29:ILE:HG13	3:J:23:HIS:ND1	2.36	0.41
1:E:194:ARG:HG3	4:E:301:3PE:H111	2.01	0.41
1:A:79:SER:O	1:A:82:ILE:HB	2.20	0.41
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.89	0.41
1:C:176:ILE:O	1:C:180:ILE:HG13	2.20	0.41
2:F:19:VAL:HB	2:F:20:PRO:HD3	2.02	0.41
4:B:301:3PE:H251	4:B:301:3PE:H281	1.73	0.40
1:C:132:THR:O	1:C:136:ILE:HG12	2.21	0.40
1:E:159:VAL:HG12	1:E:161:GLN:H	1.85	0.40
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.82	0.40
1:C:93:LEU:HB2	1:C:104:VAL:HG13	2.03	0.40
4:E:301:3PE:H2C1	4:E:301:3PE:H292	1.67	0.40
4:C:301:3PE:H232	4:E:301:3PE:H321	2.03	0.40
1:D:38:ARG:NH1	1:D:123:LEU:O	2.55	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	218/232 (94%)	211 (97%)	6 (3%)	1 (0%)	24	57
1	B	221/232 (95%)	210 (95%)	11 (5%)	0	100	100
1	C	217/232 (94%)	209 (96%)	7 (3%)	1 (0%)	24	57
1	D	216/232 (93%)	206 (95%)	10 (5%)	0	100	100
1	E	219/232 (94%)	212 (97%)	7 (3%)	0	100	100
2	F	21/142 (15%)	18 (86%)	3 (14%)	0	100	100
2	G	23/142 (16%)	21 (91%)	2 (9%)	0	100	100
3	H	26/557 (5%)	26 (100%)	0	0	100	100
3	I	28/557 (5%)	28 (100%)	0	0	100	100
3	J	27/557 (5%)	27 (100%)	0	0	100	100
3	K	29/557 (5%)	29 (100%)	0	0	100	100
3	L	27/557 (5%)	27 (100%)	0	0	100	100
All	All	1272/4229 (30%)	1224 (96%)	46 (4%)	2 (0%)	44	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ARG
1	C	73	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	177/188 (94%)	176 (99%)	1 (1%)	78	82
1	B	181/188 (96%)	181 (100%)	0	100	100
1	C	173/188 (92%)	173 (100%)	0	100	100
1	D	174/188 (93%)	172 (99%)	2 (1%)	65	77
1	E	179/188 (95%)	179 (100%)	0	100	100
2	F	22/123 (18%)	22 (100%)	0	100	100
2	G	23/123 (19%)	22 (96%)	1 (4%)	26	56
3	H	22/384 (6%)	22 (100%)	0	100	100
3	I	25/384 (6%)	25 (100%)	0	100	100
3	J	18/384 (5%)	18 (100%)	0	100	100
3	K	23/384 (6%)	23 (100%)	0	100	100
3	L	23/384 (6%)	23 (100%)	0	100	100
All	All	1040/3106 (34%)	1036 (100%)	4 (0%)	81	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	D	178	THR
1	D	208	ASN
2	G	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	GLN
1	B	97	ASN
1	B	165	GLN
1	C	67	GLN
1	C	70	GLN
1	C	81	GLN
1	C	126	HIS
1	D	70	GLN
1	D	208	ASN
1	E	117	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	3PE	A	301	-	48,48,50	1.30	4 (8%)	51,53,55	0.87	2 (3%)
4	3PE	B	301	-	48,48,50	1.31	4 (8%)	51,53,55	0.93	2 (3%)
4	3PE	B	302	-	48,48,50	1.31	4 (8%)	51,53,55	0.94	2 (3%)
4	3PE	D	302	-	48,48,50	1.30	4 (8%)	51,53,55	0.92	2 (3%)
4	3PE	E	301	-	48,48,50	1.31	4 (8%)	51,53,55	0.94	2 (3%)
4	3PE	D	301	-	48,48,50	1.31	4 (8%)	51,53,55	0.95	2 (3%)
4	3PE	C	301	-	48,48,50	1.31	4 (8%)	51,53,55	0.97	2 (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
4	3PE	A	301	-	-	25/52/52/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3PE	B	301	-	-	29/52/52/54	-
4	3PE	B	302	-	-	27/52/52/54	-
4	3PE	D	302	-	-	32/52/52/54	-
4	3PE	E	301	-	-	30/52/52/54	-
4	3PE	D	301	-	-	29/52/52/54	-
4	3PE	C	301	-	-	32/52/52/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	3PE	O21-C21	3.53	1.44	1.34
4	B	301	3PE	O21-C21	3.45	1.44	1.34
4	C	301	3PE	O21-C21	3.45	1.44	1.34
4	D	302	3PE	O21-C21	3.45	1.44	1.34
4	D	301	3PE	O21-C21	3.44	1.44	1.34
4	A	301	3PE	O21-C21	3.42	1.43	1.34
4	E	301	3PE	O21-C21	3.42	1.43	1.34
4	A	301	3PE	C2A-C29	-3.37	1.35	1.51
4	E	301	3PE	C2A-C29	-3.36	1.35	1.51
4	D	301	3PE	C2A-C29	-3.36	1.35	1.51
4	B	302	3PE	C2A-C29	-3.34	1.35	1.51
4	D	302	3PE	C2A-C29	-3.34	1.35	1.51
4	C	301	3PE	C2A-C29	-3.33	1.35	1.51
4	B	301	3PE	C2A-C29	-3.32	1.35	1.51
4	B	301	3PE	O31-C31	3.06	1.42	1.33
4	B	302	3PE	O31-C31	3.04	1.42	1.33
4	E	301	3PE	O31-C31	3.04	1.42	1.33
4	D	302	3PE	O31-C31	3.02	1.42	1.33
4	A	301	3PE	O31-C31	3.00	1.42	1.33
4	D	301	3PE	O31-C31	2.99	1.42	1.33
4	C	301	3PE	O31-C31	2.96	1.42	1.33
4	E	301	3PE	C32-C31	2.90	1.59	1.50
4	B	301	3PE	C32-C31	2.87	1.59	1.50
4	C	301	3PE	C32-C31	2.87	1.59	1.50
4	D	302	3PE	C32-C31	2.86	1.59	1.50
4	B	302	3PE	C32-C31	2.82	1.58	1.50
4	D	301	3PE	C32-C31	2.79	1.58	1.50
4	A	301	3PE	C32-C31	2.75	1.58	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	3PE	O21-C21-C22	4.15	120.46	111.48
4	B	302	3PE	O21-C21-C22	4.12	120.39	111.48
4	B	301	3PE	O21-C21-C22	4.05	120.23	111.48
4	D	301	3PE	O21-C21-C22	4.01	120.15	111.48
4	E	301	3PE	O21-C21-C22	3.89	119.91	111.48
4	D	302	3PE	O21-C21-C22	3.75	119.59	111.48
4	A	301	3PE	O21-C21-C22	3.49	119.04	111.48
4	B	302	3PE	O31-C31-C32	2.79	120.34	111.83
4	D	302	3PE	O31-C31-C32	2.78	120.32	111.83
4	E	301	3PE	O31-C31-C32	2.78	120.30	111.83
4	C	301	3PE	O31-C31-C32	2.72	120.14	111.83
4	D	301	3PE	O31-C31-C32	2.70	120.08	111.83
4	B	301	3PE	O31-C31-C32	2.68	120.01	111.83
4	A	301	3PE	O31-C31-C32	2.56	119.63	111.83

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	3PE	C11-O13-P-O11
4	A	301	3PE	C11-O13-P-O12
4	A	301	3PE	C11-O13-P-O14
4	A	301	3PE	O13-C11-C12-N
4	B	301	3PE	C11-O13-P-O11
4	B	301	3PE	C11-O13-P-O14
4	B	301	3PE	O13-C11-C12-N
4	B	301	3PE	C22-C21-O21-C2
4	B	302	3PE	O13-C11-C12-N
4	B	302	3PE	O11-C1-C2-O21
4	B	302	3PE	O21-C2-C3-O31
4	B	302	3PE	O22-C21-O21-C2
4	B	302	3PE	C22-C21-O21-C2
4	C	301	3PE	C1-O11-P-O14
4	C	301	3PE	C11-O13-P-O11
4	C	301	3PE	C11-O13-P-O14
4	C	301	3PE	O13-C11-C12-N
4	D	301	3PE	C11-O13-P-O11
4	D	301	3PE	C11-O13-P-O12
4	D	301	3PE	O13-C11-C12-N
4	D	302	3PE	C1-O11-P-O12
4	D	302	3PE	C1-O11-P-O13
4	D	302	3PE	C1-O11-P-O14
4	D	302	3PE	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	302	3PE	C22-C21-O21-C2
4	E	301	3PE	C1-O11-P-O12
4	E	301	3PE	C1-O11-P-O13
4	E	301	3PE	C1-O11-P-O14
4	E	301	3PE	O13-C11-C12-N
4	B	302	3PE	O32-C31-O31-C3
4	B	301	3PE	O22-C21-O21-C2
4	D	302	3PE	O22-C21-O21-C2
4	B	302	3PE	C32-C31-O31-C3
4	C	301	3PE	C32-C31-O31-C3
4	E	301	3PE	C2D-C2E-C2F-C2G
4	C	301	3PE	C22-C21-O21-C2
4	C	301	3PE	O32-C31-O31-C3
4	D	301	3PE	C32-C31-O31-C3
4	B	301	3PE	C2B-C2C-C2D-C2E
4	C	301	3PE	C25-C26-C27-C28
4	C	301	3PE	C2D-C2E-C2F-C2G
4	B	301	3PE	C32-C31-O31-C3
4	A	301	3PE	C22-C23-C24-C25
4	B	301	3PE	C25-C26-C27-C28
4	E	301	3PE	C29-C2A-C2B-C2C
4	B	301	3PE	C2D-C2E-C2F-C2G
4	C	301	3PE	O22-C21-O21-C2
4	D	302	3PE	O21-C2-C3-O31
4	B	302	3PE	C2D-C2E-C2F-C2G
4	B	302	3PE	C21-C22-C23-C24
4	D	302	3PE	C31-C32-C33-C34
4	E	301	3PE	C21-C22-C23-C24
4	D	301	3PE	C29-C2A-C2B-C2C
4	D	301	3PE	C2E-C2F-C2G-C2H
4	B	301	3PE	O32-C31-O31-C3
4	D	301	3PE	O32-C31-O31-C3
4	B	301	3PE	C29-C2A-C2B-C2C
4	C	301	3PE	C31-C32-C33-C34
4	B	302	3PE	C3C-C3D-C3E-C3F
4	A	301	3PE	C21-C22-C23-C24
4	E	301	3PE	C2A-C2B-C2C-C2D
4	D	302	3PE	C3A-C3B-C3C-C3D
4	A	301	3PE	C3A-C3B-C3C-C3D
4	A	301	3PE	C27-C28-C29-C2A
4	C	301	3PE	C23-C24-C25-C26
4	C	301	3PE	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	302	3PE	C34-C35-C36-C37
4	D	302	3PE	C32-C33-C34-C35
4	D	302	3PE	C33-C34-C35-C36
4	E	301	3PE	C2E-C2F-C2G-C2H
4	A	301	3PE	C38-C39-C3A-C3B
4	A	301	3PE	C23-C24-C25-C26
4	D	301	3PE	C21-C22-C23-C24
4	D	301	3PE	C26-C27-C28-C29
4	D	302	3PE	C25-C26-C27-C28
4	E	301	3PE	O11-C1-C2-C3
4	D	301	3PE	C32-C33-C34-C35
4	D	301	3PE	C3C-C3D-C3E-C3F
4	A	301	3PE	C2E-C2F-C2G-C2H
4	C	301	3PE	C3A-C3B-C3C-C3D
4	B	301	3PE	C38-C39-C3A-C3B
4	E	301	3PE	C39-C3A-C3B-C3C
4	B	302	3PE	C35-C36-C37-C38
4	D	301	3PE	C38-C39-C3A-C3B
4	D	301	3PE	C23-C24-C25-C26
4	A	301	3PE	C25-C26-C27-C28
4	B	301	3PE	C32-C33-C34-C35
4	D	301	3PE	C3A-C3B-C3C-C3D
4	D	301	3PE	C2B-C2C-C2D-C2E
4	B	301	3PE	C23-C24-C25-C26
4	C	301	3PE	C2B-C2C-C2D-C2E
4	C	301	3PE	C2F-C2G-C2H-C2I
4	C	301	3PE	C36-C37-C38-C39
4	D	302	3PE	C35-C36-C37-C38
4	D	302	3PE	C39-C3A-C3B-C3C
4	B	302	3PE	C34-C35-C36-C37
4	B	302	3PE	C24-C25-C26-C27
4	D	301	3PE	C3B-C3C-C3D-C3E
4	A	301	3PE	C29-C2A-C2B-C2C
4	B	302	3PE	C2A-C2B-C2C-C2D
4	D	301	3PE	C22-C21-O21-C2
4	E	301	3PE	C22-C21-O21-C2
4	B	302	3PE	C2F-C2G-C2H-C2I
4	D	302	3PE	C37-C38-C39-C3A
4	D	301	3PE	C24-C25-C26-C27
4	B	301	3PE	C2A-C2B-C2C-C2D
4	E	301	3PE	C3C-C3D-C3E-C3F
4	C	301	3PE	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	301	3PE	O11-C1-C2-O21
4	C	301	3PE	C3C-C3D-C3E-C3F
4	D	301	3PE	O22-C21-O21-C2
4	E	301	3PE	O22-C21-O21-C2
4	B	301	3PE	C26-C27-C28-C29
4	D	302	3PE	C3C-C3D-C3E-C3F
4	E	301	3PE	C26-C27-C28-C29
4	B	302	3PE	C38-C39-C3A-C3B
4	B	302	3PE	C2C-C2D-C2E-C2F
4	D	302	3PE	C2A-C2B-C2C-C2D
4	B	302	3PE	C1-C2-C3-O31
4	D	302	3PE	C1-C2-C3-O31
4	D	301	3PE	C2D-C2E-C2F-C2G
4	B	301	3PE	C36-C37-C38-C39
4	B	301	3PE	C3A-C3B-C3C-C3D
4	E	301	3PE	C36-C37-C38-C39
4	D	301	3PE	C36-C37-C38-C39
4	E	301	3PE	C23-C24-C25-C26
4	B	302	3PE	C39-C3A-C3B-C3C
4	A	301	3PE	C2B-C2C-C2D-C2E
4	D	302	3PE	C2C-C2D-C2E-C2F
4	B	302	3PE	C36-C37-C38-C39
4	D	302	3PE	C2B-C2C-C2D-C2E
4	C	301	3PE	C27-C28-C29-C2A
4	C	301	3PE	C2A-C2B-C2C-C2D
4	E	301	3PE	C22-C23-C24-C25
4	B	302	3PE	O11-C1-C2-C3
4	C	301	3PE	O11-C1-C2-C3
4	A	301	3PE	C3C-C3D-C3E-C3F
4	C	301	3PE	C2C-C2D-C2E-C2F
4	D	301	3PE	C2C-C2D-C2E-C2F
4	A	301	3PE	C35-C36-C37-C38
4	E	301	3PE	C33-C34-C35-C36
4	B	301	3PE	C33-C34-C35-C36
4	A	301	3PE	O11-C1-C2-O21
4	E	301	3PE	O11-C1-C2-O21
4	B	301	3PE	C35-C36-C37-C38
4	D	301	3PE	C27-C28-C29-C2A
4	A	301	3PE	O21-C2-C3-O31
4	E	301	3PE	C2C-C2D-C2E-C2F
4	B	301	3PE	C27-C28-C29-C2A
4	B	302	3PE	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	301	3PE	C1-C2-C3-O31
4	B	301	3PE	C2C-C2D-C2E-C2F
4	B	302	3PE	C3B-C3C-C3D-C3E
4	B	302	3PE	C27-C28-C29-C2A
4	C	301	3PE	C26-C27-C28-C29
4	D	302	3PE	C36-C37-C38-C39
4	D	301	3PE	C39-C3A-C3B-C3C
4	E	301	3PE	C3A-C3B-C3C-C3D
4	E	301	3PE	C2B-C2C-C2D-C2E
4	C	301	3PE	O21-C2-C3-O31
4	A	301	3PE	C2C-C2D-C2E-C2F
4	B	301	3PE	C1-O11-P-O12
4	B	301	3PE	C1-O11-P-O13
4	B	301	3PE	C1-O11-P-O14
4	B	301	3PE	C11-O13-P-O12
4	C	301	3PE	C1-O11-P-O13
4	E	301	3PE	C11-O13-P-O14
4	B	302	3PE	C2-C1-O11-P
4	E	301	3PE	C27-C28-C29-C2A
4	E	301	3PE	C24-C25-C26-C27
4	A	301	3PE	O11-C1-C2-C3
4	A	301	3PE	O21-C21-C22-C23
4	D	302	3PE	C21-C22-C23-C24
4	C	301	3PE	C33-C34-C35-C36
4	D	302	3PE	C32-C31-O31-C3
4	C	301	3PE	C32-C33-C34-C35
4	D	302	3PE	O32-C31-O31-C3
4	D	302	3PE	C38-C39-C3A-C3B
4	C	301	3PE	C1-C2-C3-O31
4	D	302	3PE	C2-C1-O11-P
4	D	301	3PE	C33-C34-C35-C36
4	D	302	3PE	C2E-C2F-C2G-C2H
4	B	301	3PE	C3B-C3C-C3D-C3E
4	D	302	3PE	O11-C1-C2-C3
4	E	301	3PE	C37-C38-C39-C3A
4	D	302	3PE	C22-C23-C24-C25
4	C	301	3PE	C3B-C3C-C3D-C3E
4	D	302	3PE	O11-C1-C2-O21
4	A	301	3PE	O22-C21-O21-C2
4	A	301	3PE	C22-C21-O21-C2
4	B	301	3PE	O31-C31-C32-C33
4	D	301	3PE	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

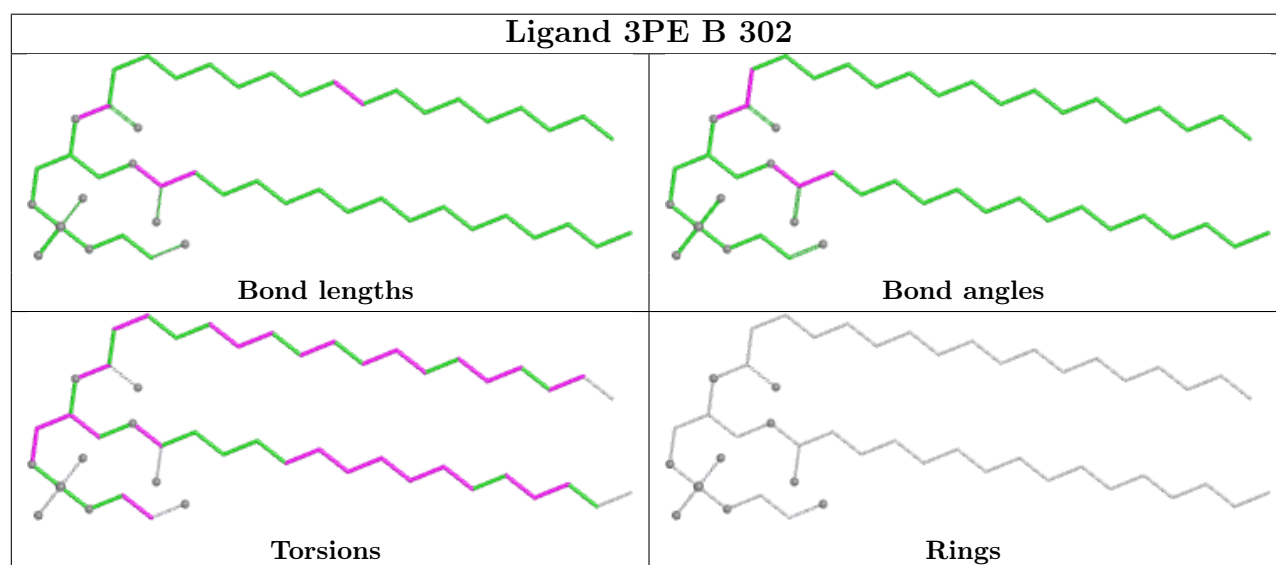
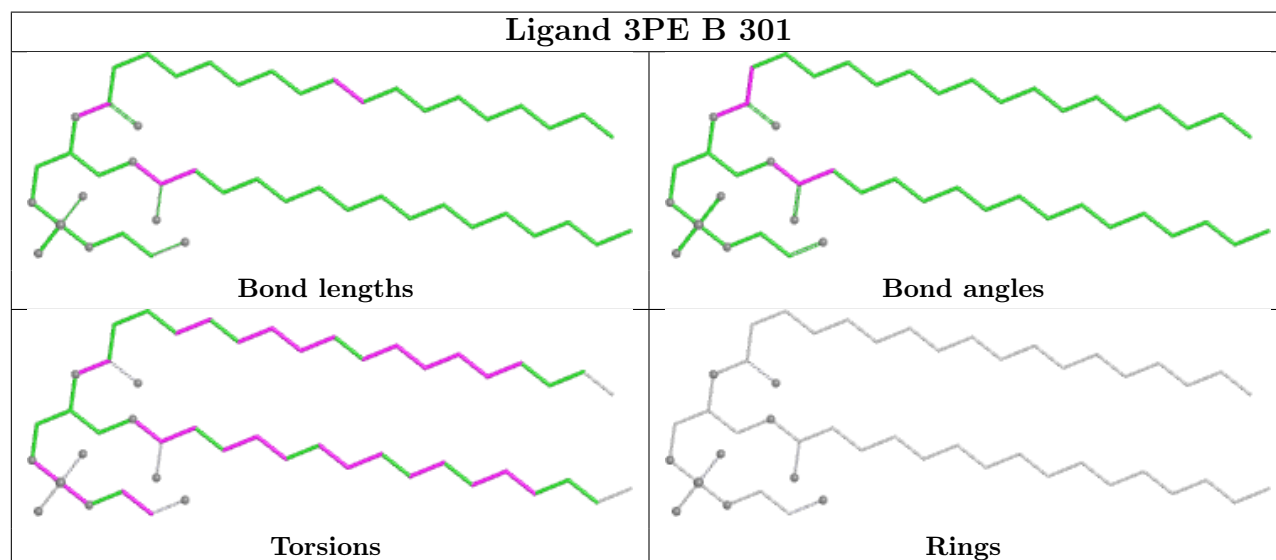
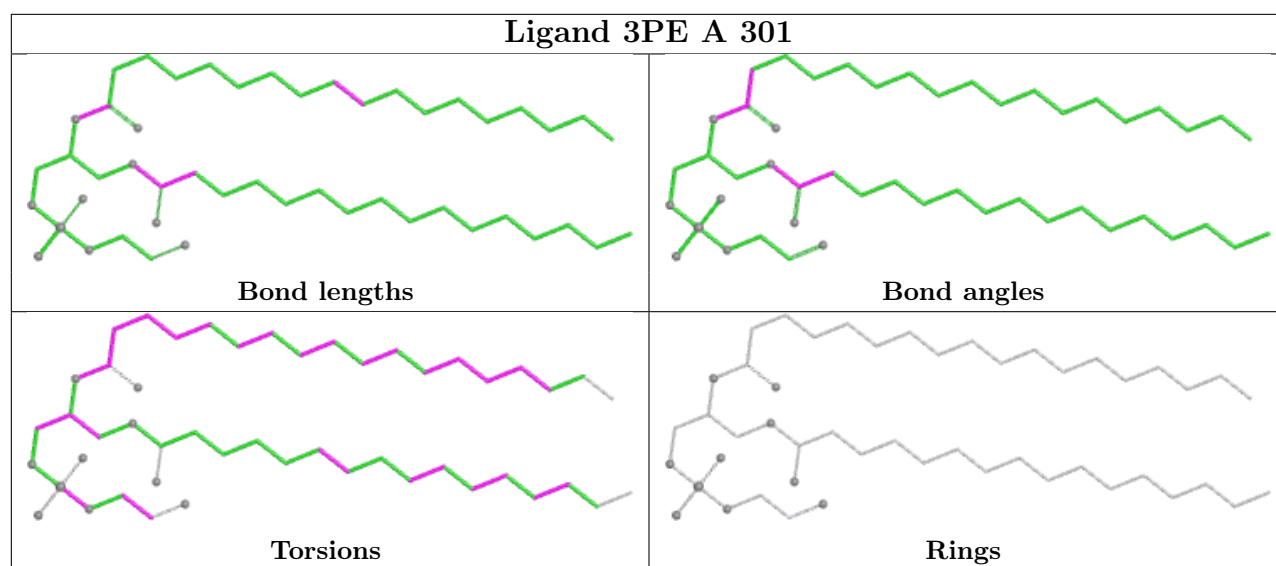
Mol	Chain	Res	Type	Atoms
4	D	301	3PE	C2F-C2G-C2H-C2I
4	A	301	3PE	C2D-C2E-C2F-C2G
4	E	301	3PE	O21-C21-C22-C23
4	B	302	3PE	C29-C2A-C2B-C2C
4	B	301	3PE	O32-C31-C32-C33
4	D	301	3PE	O32-C31-C32-C33
4	B	302	3PE	C37-C38-C39-C3A
4	D	301	3PE	C1-C2-C3-O31
4	E	301	3PE	C35-C36-C37-C38
4	D	302	3PE	O21-C21-C22-C23
4	C	301	3PE	O21-C21-C22-C23
4	E	301	3PE	O22-C21-C22-C23

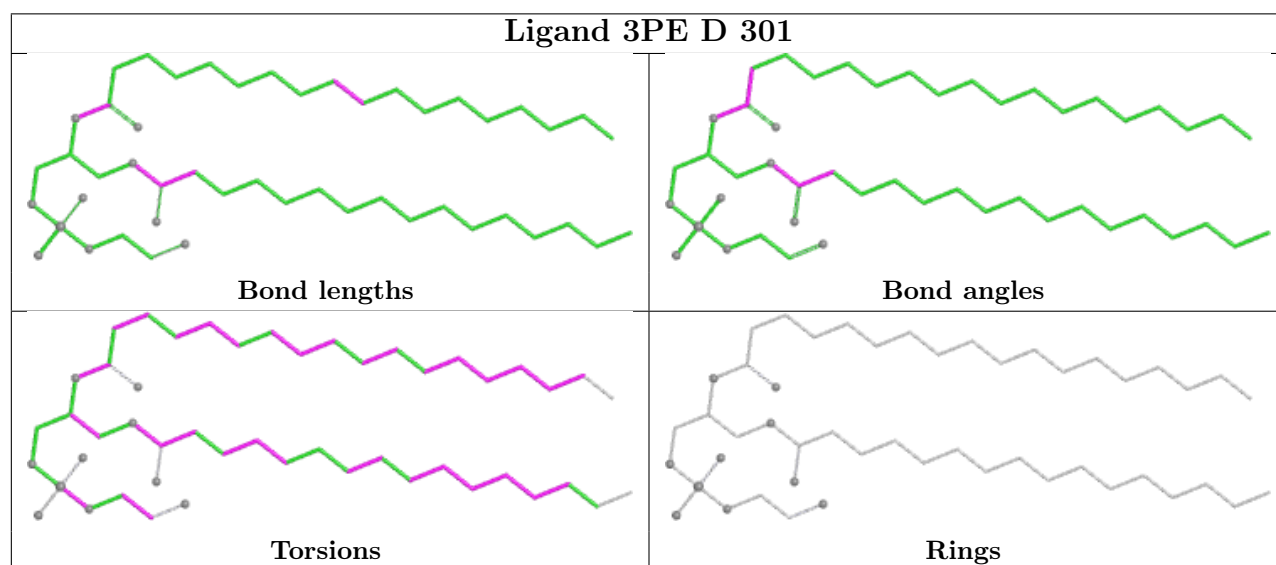
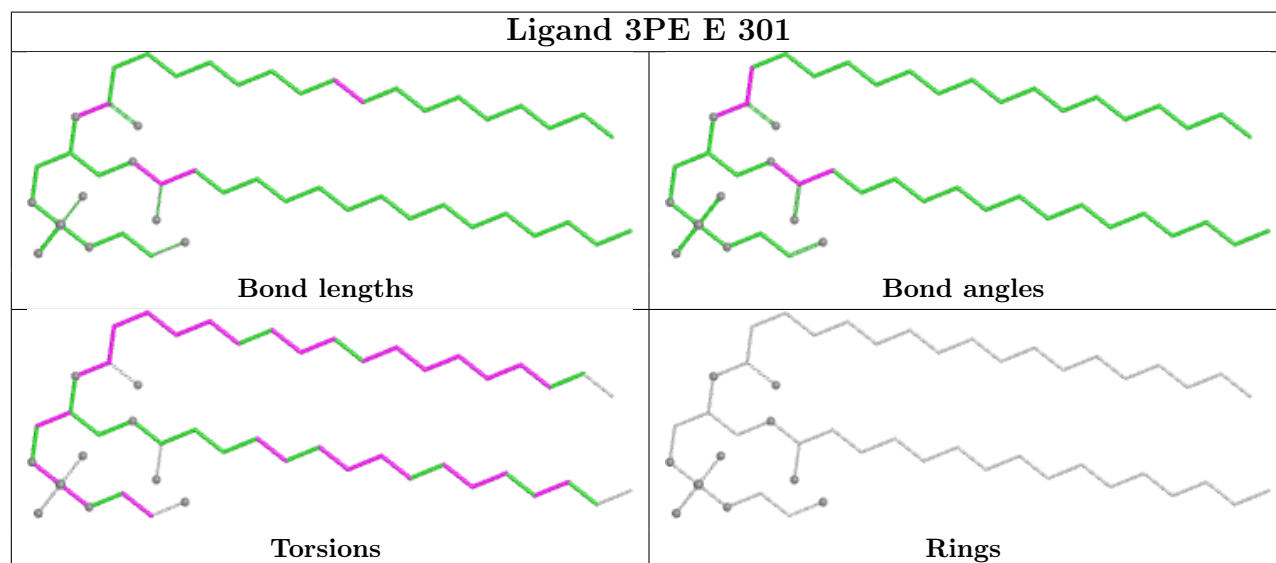
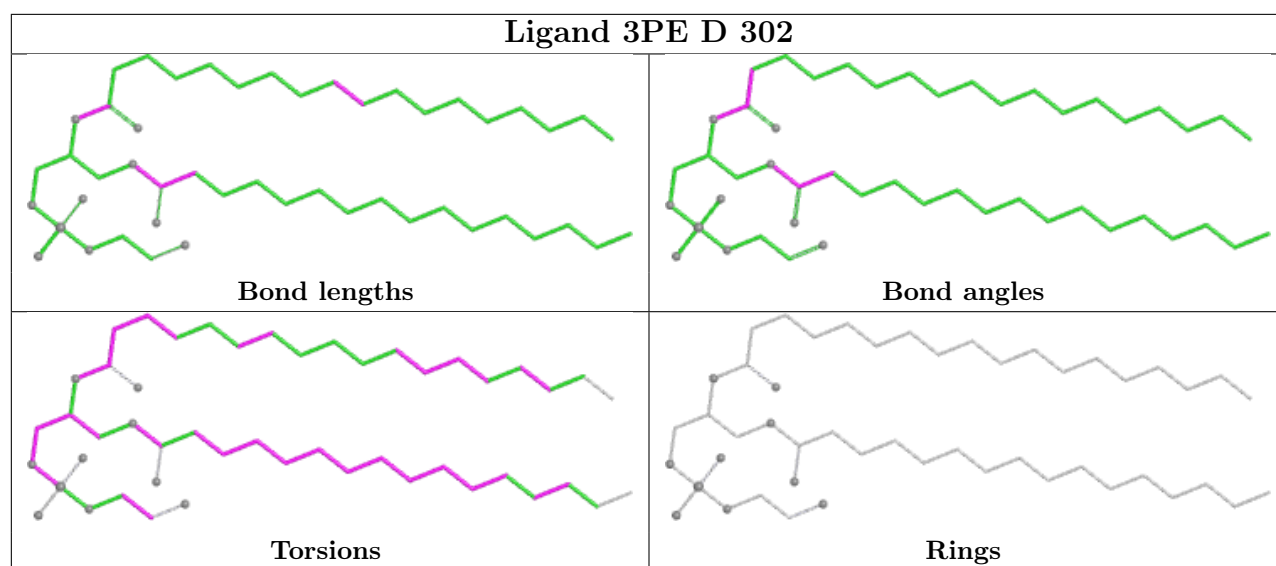
There are no ring outliers.

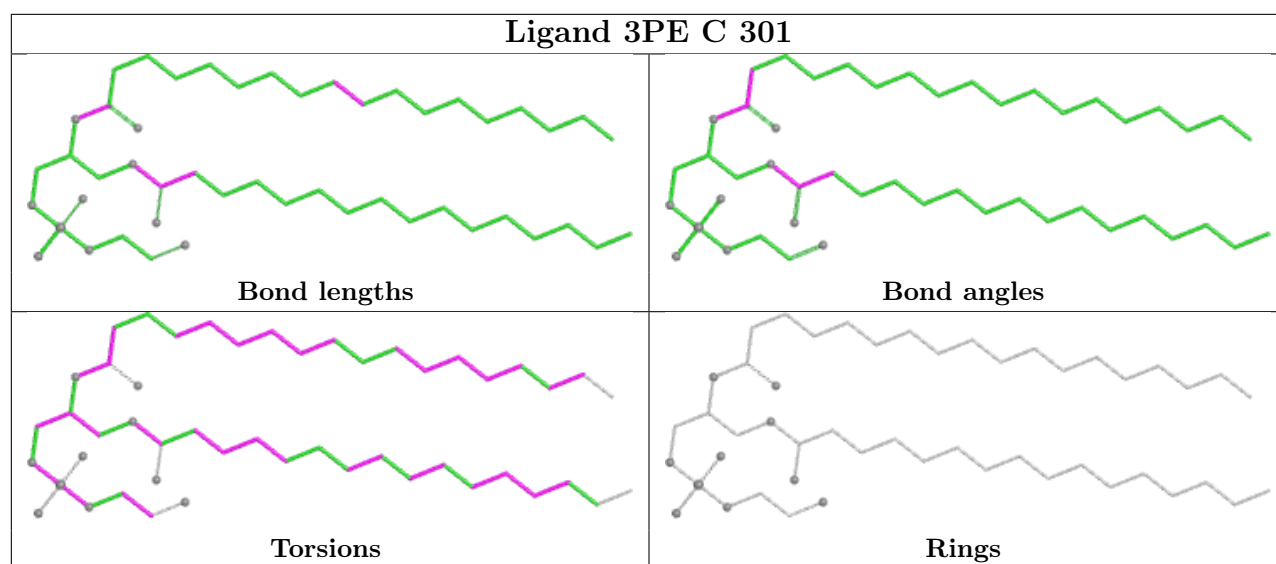
7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	3PE	3	0
4	B	301	3PE	5	0
4	B	302	3PE	3	0
4	D	302	3PE	3	0
4	E	301	3PE	7	0
4	D	301	3PE	1	0
4	C	301	3PE	5	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.

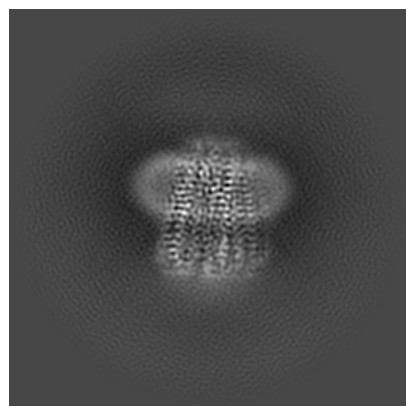
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62492. These allow visual inspection of the internal detail of the map and identification of artifacts.

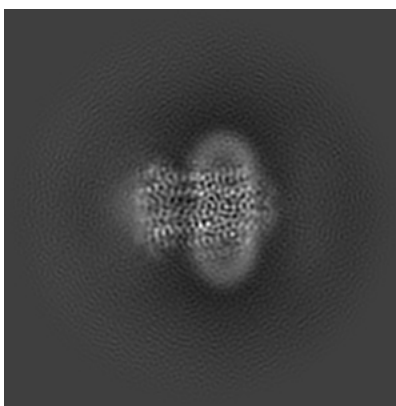
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

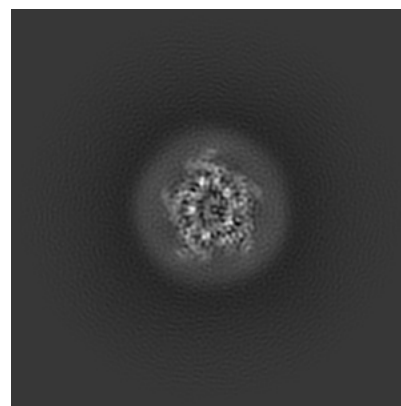
6.1.1 Primary map



X

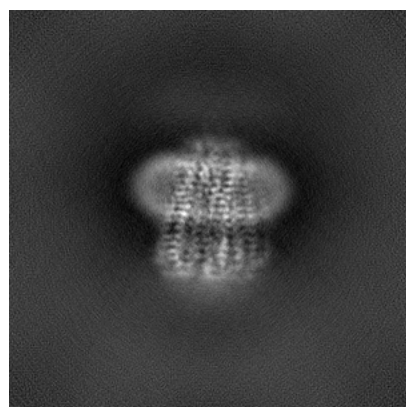


Y

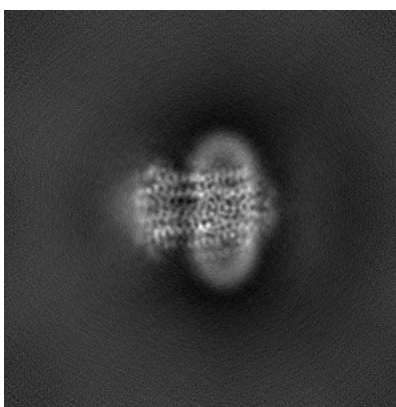


Z

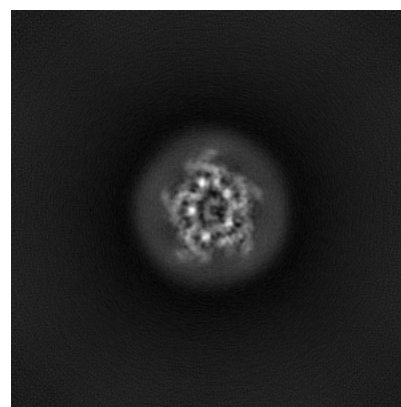
6.1.2 Raw map



X



Y

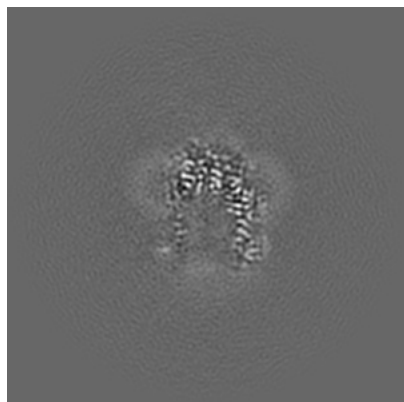


Z

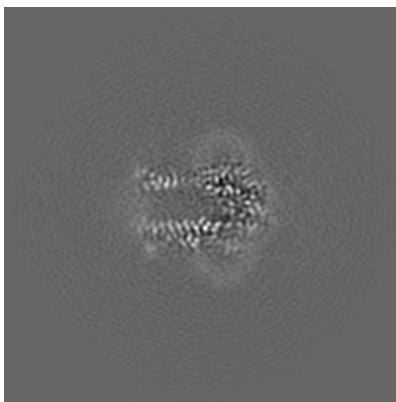
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

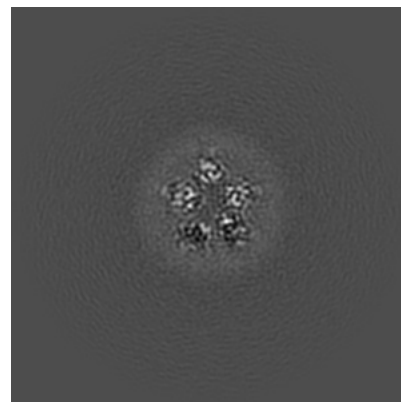
6.2.1 Primary map



X Index: 160

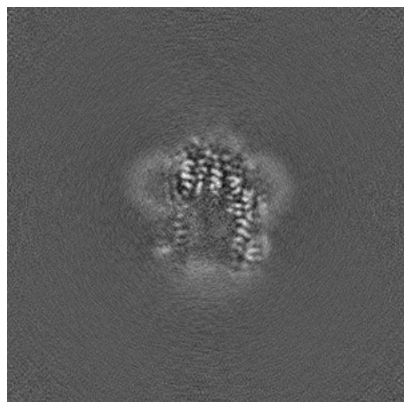


Y Index: 160

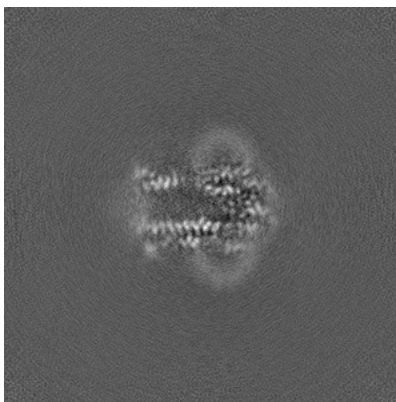


Z Index: 160

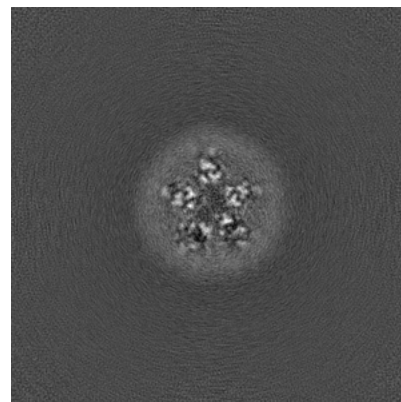
6.2.2 Raw map



X Index: 160



Y Index: 160

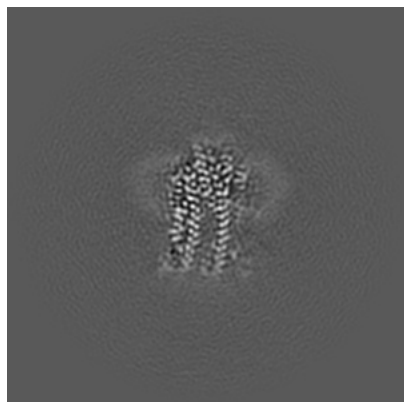


Z Index: 160

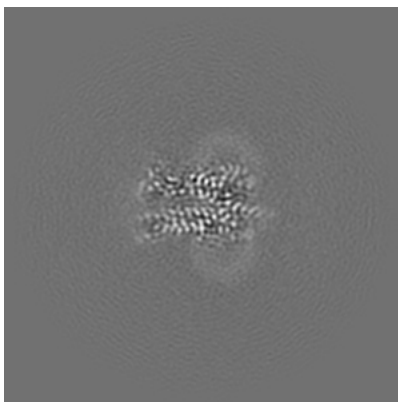
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

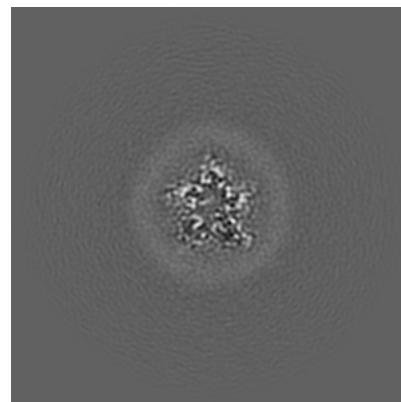
6.3.1 Primary map



X Index: 173

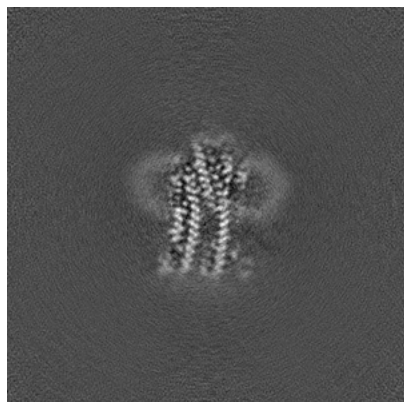


Y Index: 140

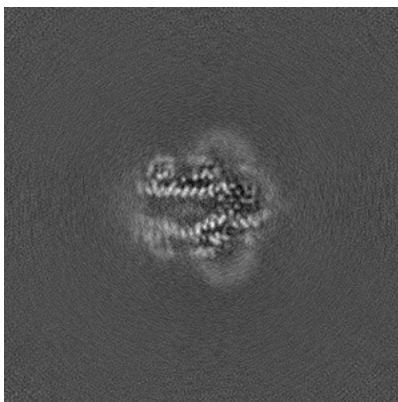


Z Index: 170

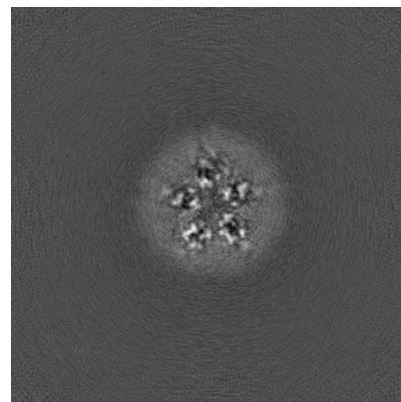
6.3.2 Raw map



X Index: 173



Y Index: 171

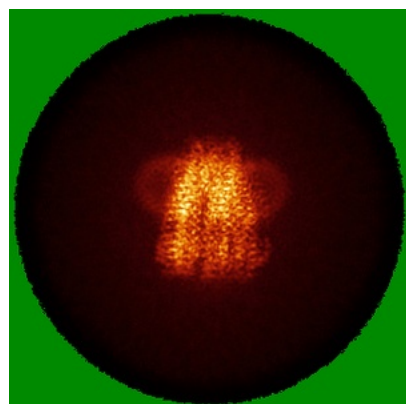


Z Index: 158

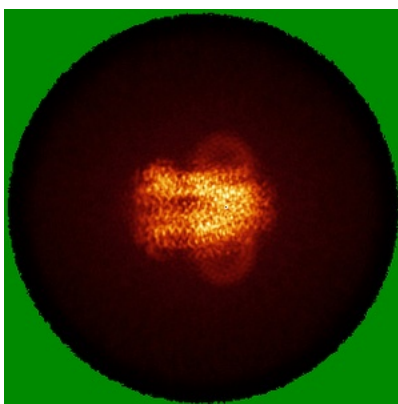
The images above show the largest variance slices of the map in three orthogonal directions.

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

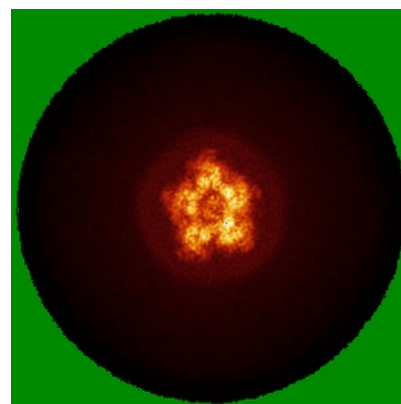
6.4.1 Primary map



X

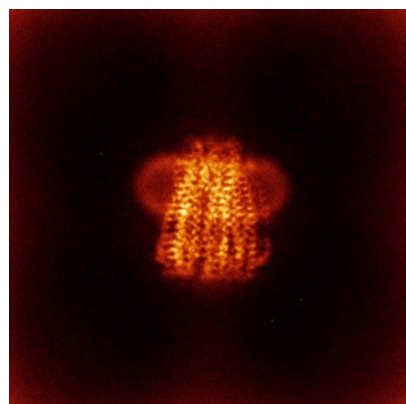


Y

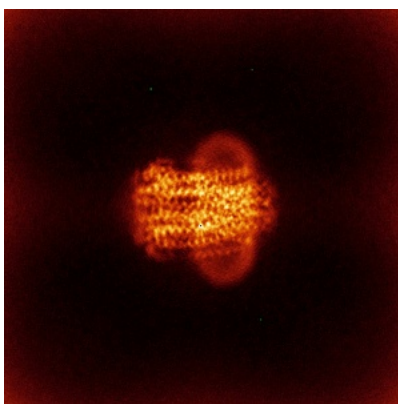


Z

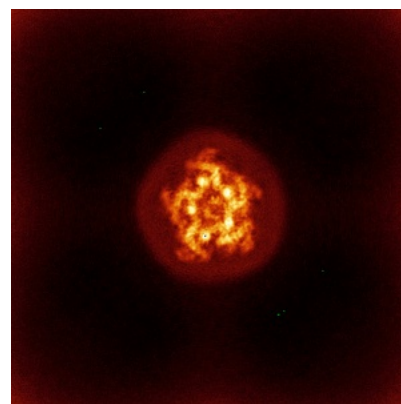
6.4.2 Raw map



X



Y

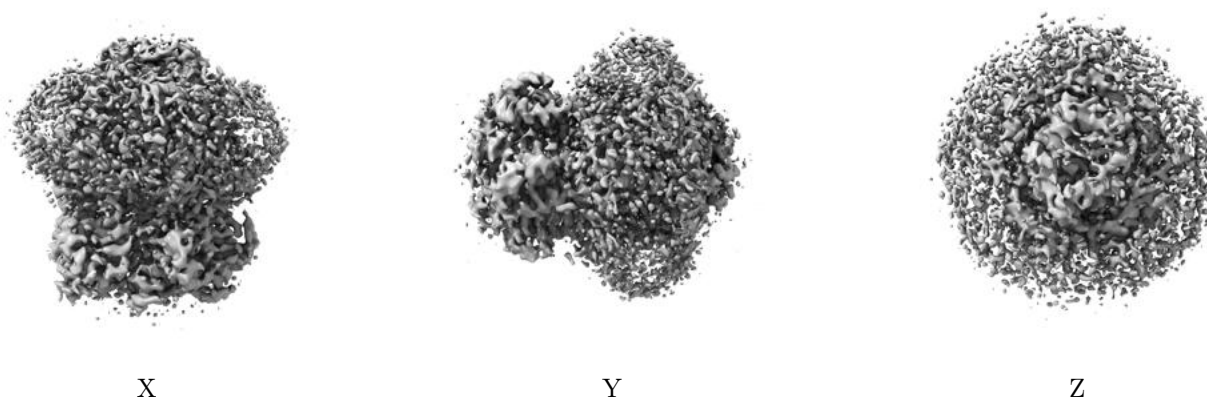


Z

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.

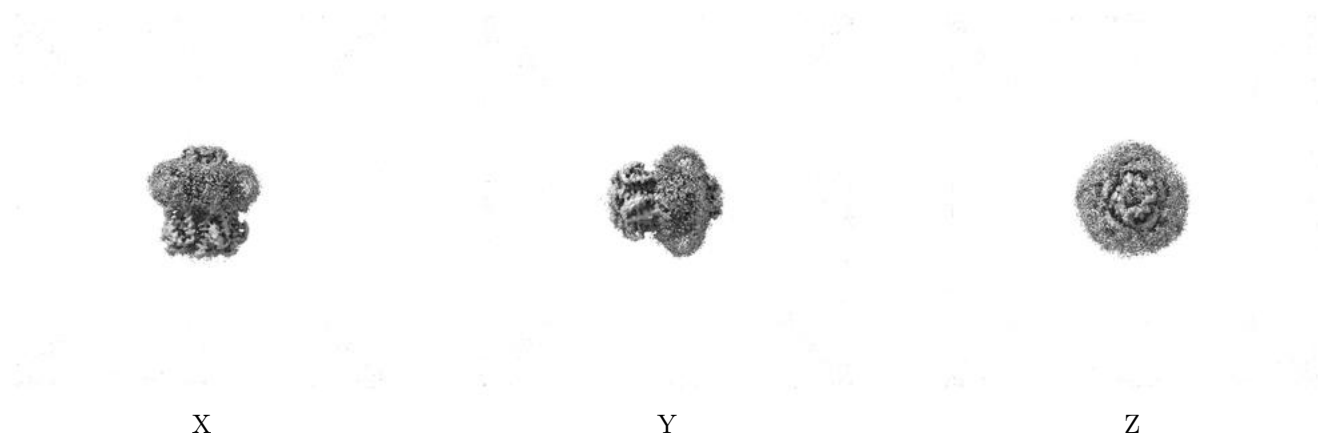
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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.

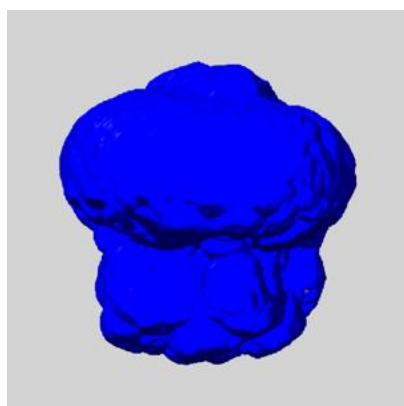
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

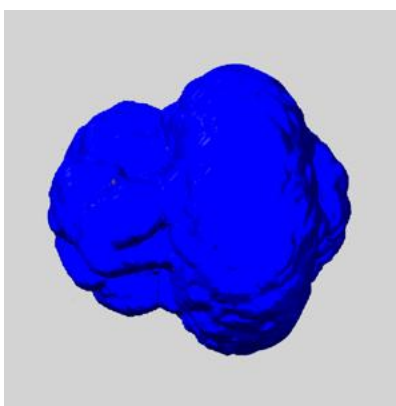
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

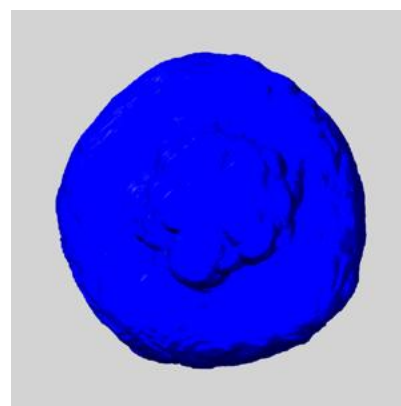
6.6.1 emd_62492_msk_1.map [i](#)



X



Y

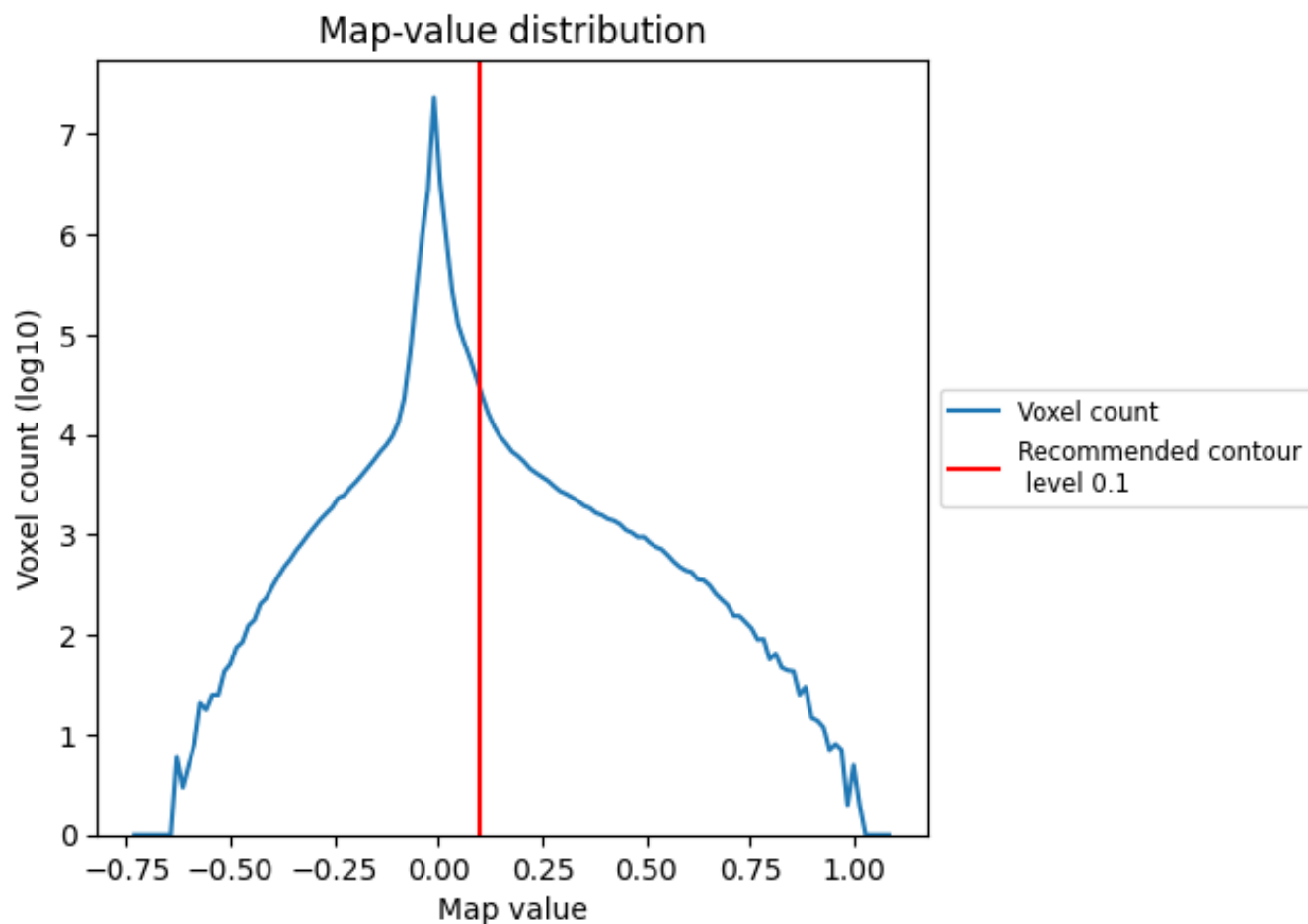


Z

7 Map analysis [i](#)

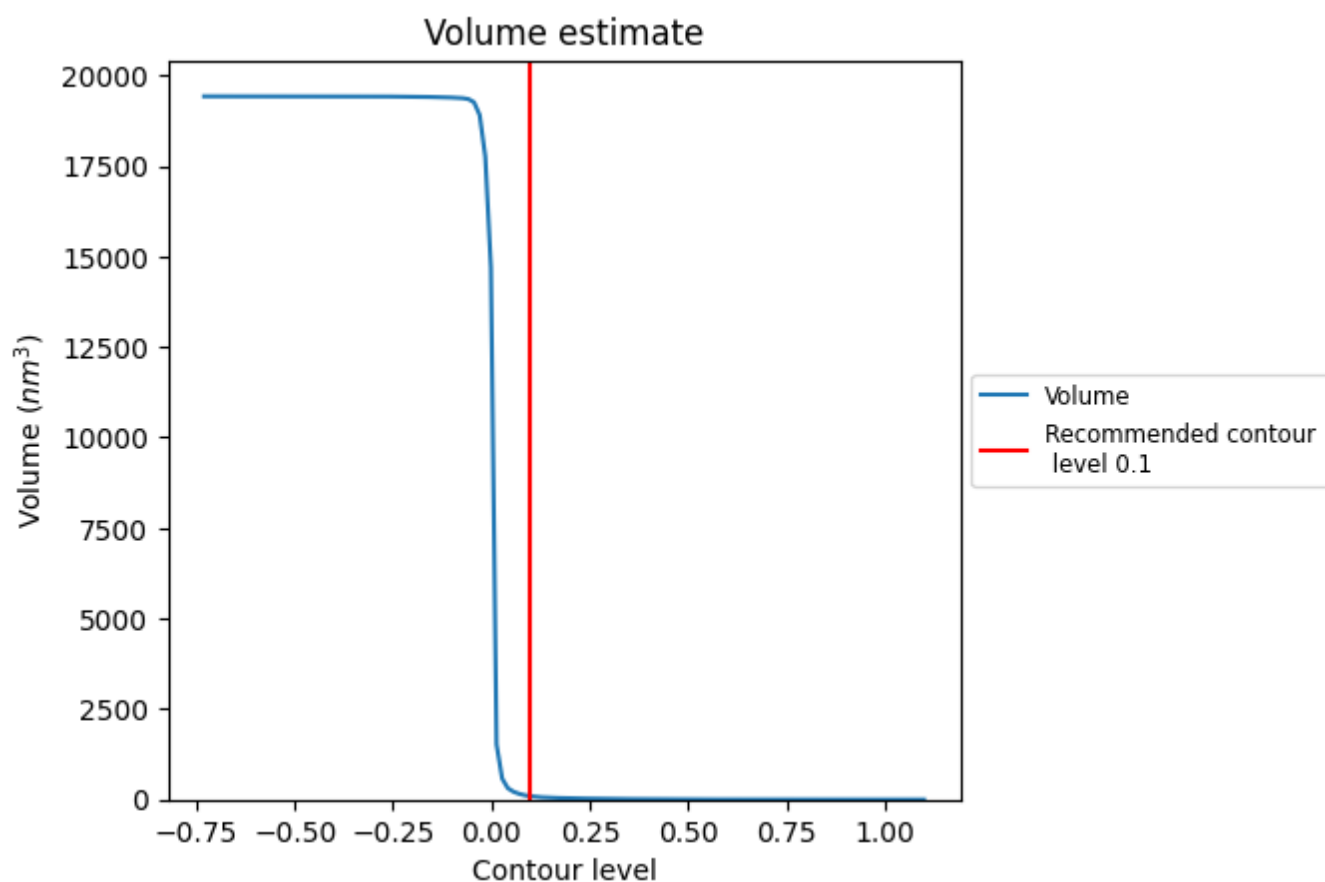
This section contains the results of statistical analysis of the map.

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.

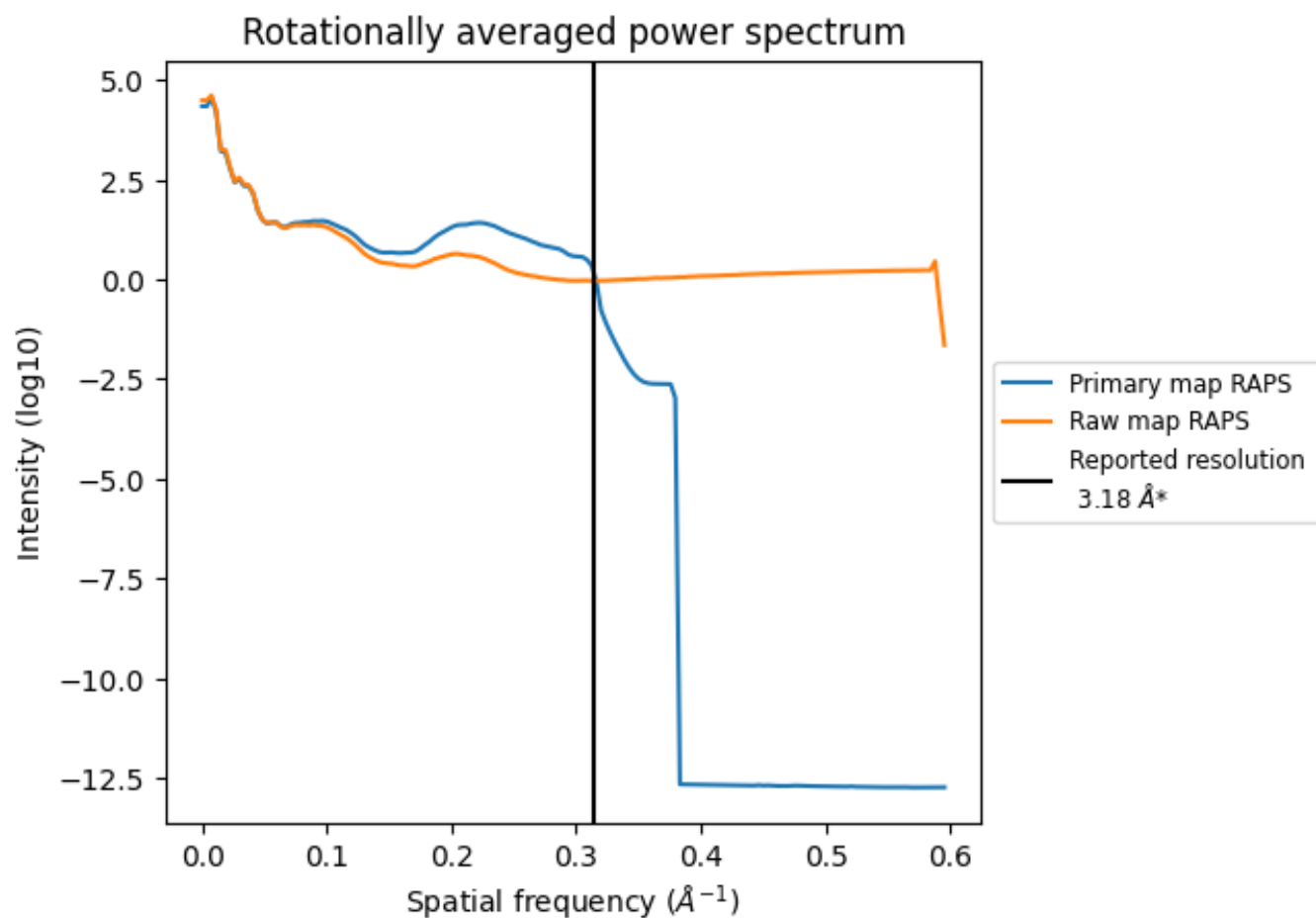
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 82 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 ⓘ

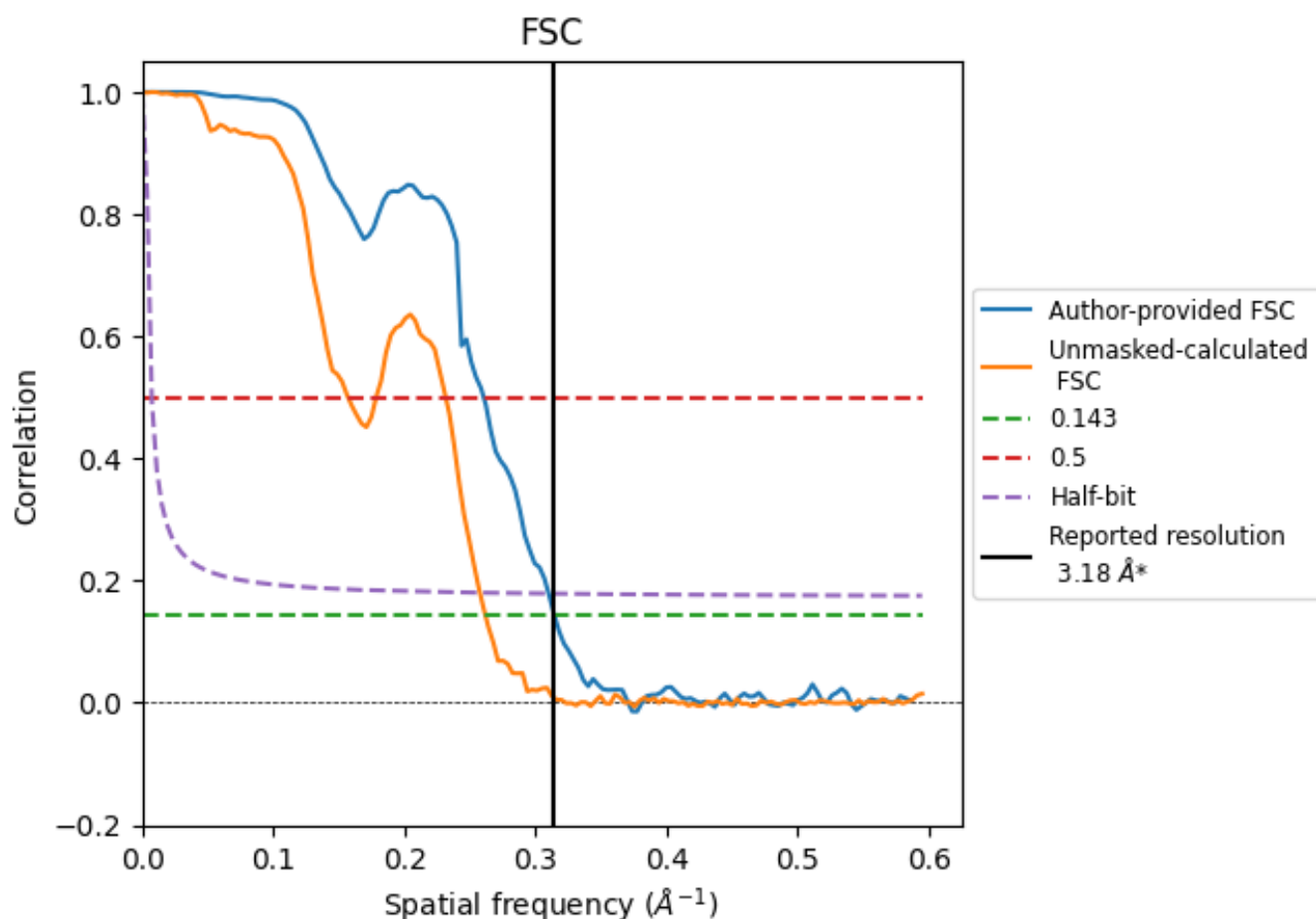


*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

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 0.314 \AA^{-1}

8.2 Resolution estimates [i](#)

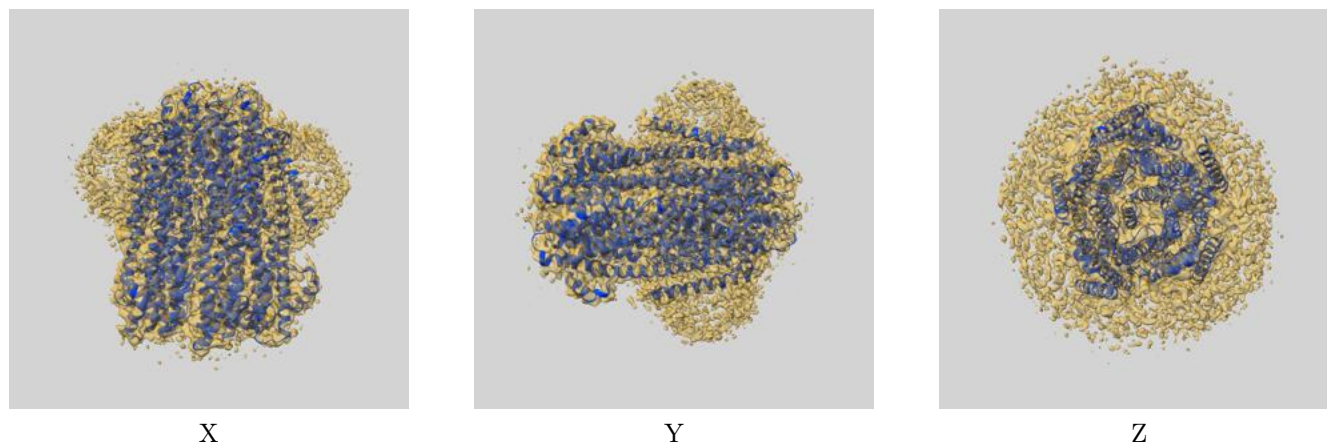
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.84	3.22
Unmasked-calculated*	3.82	6.37	3.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

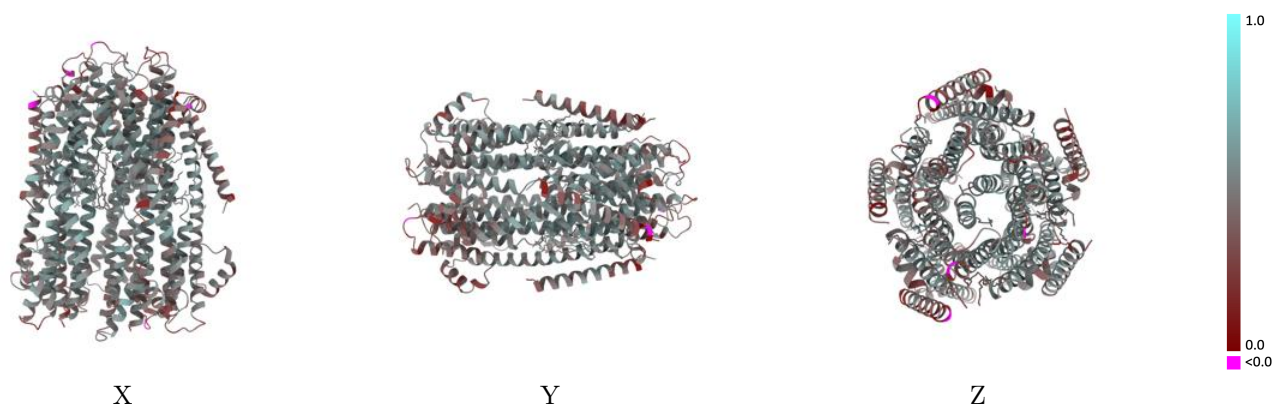
This section contains information regarding the fit between EMDB map EMD-62492 and PDB model 9KPZ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



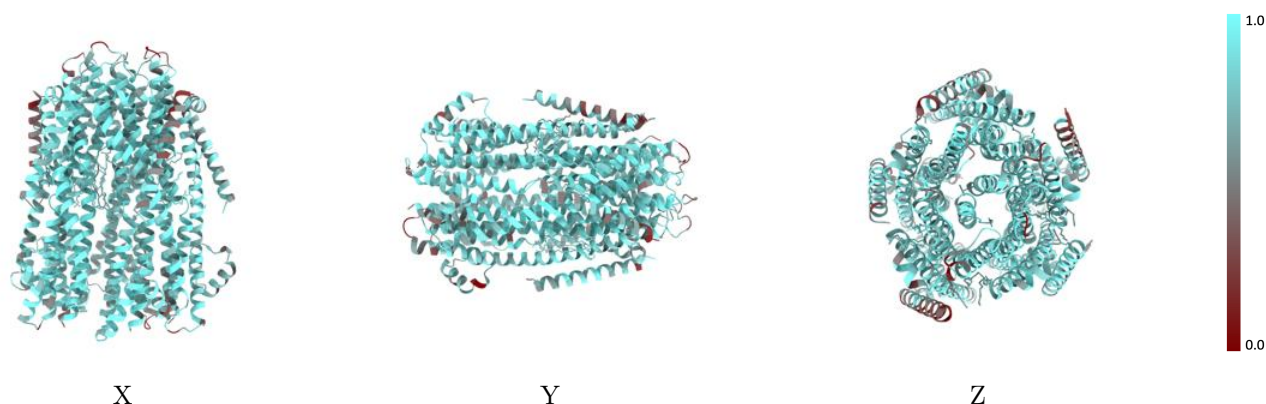
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



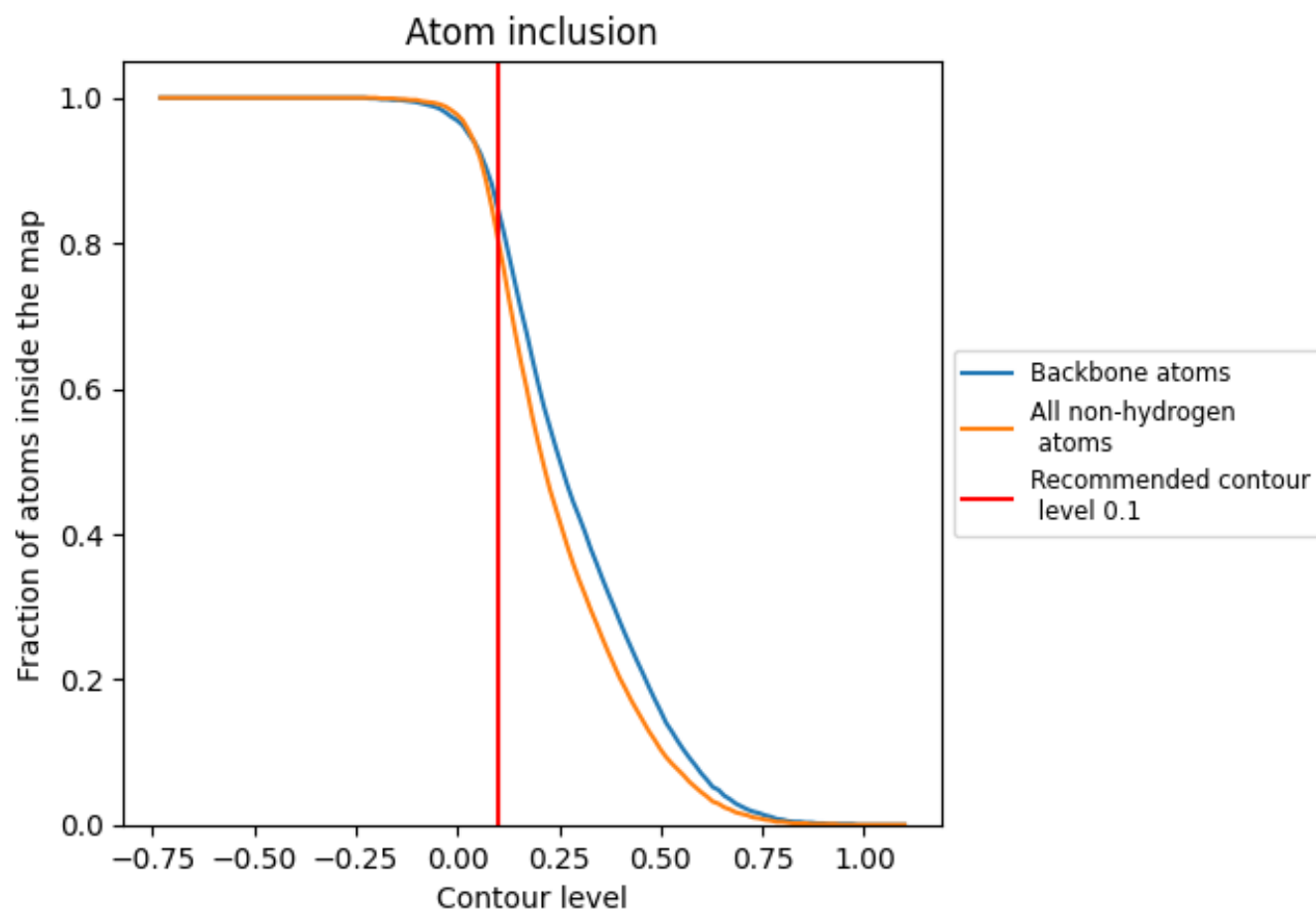
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8050	<div></div> 0.4660
A	<div></div> 0.8040	<div></div> 0.4650
B	<div></div> 0.8260	<div></div> 0.4730
C	<div></div> 0.8470	<div></div> 0.4820
D	<div></div> 0.7940	<div></div> 0.4550
E	<div></div> 0.8570	<div></div> 0.4980
F	<div></div> 0.8490	<div></div> 0.5190
G	<div></div> 0.8380	<div></div> 0.5220
H	<div></div> 0.4320	<div></div> 0.2950
I	<div></div> 0.7090	<div></div> 0.3930
J	<div></div> 0.5630	<div></div> 0.3700
K	<div></div> 0.6070	<div></div> 0.3420
L	<div></div> 0.8170	<div></div> 0.4600

1.0

0.0

<0.0