



Full wwPDB EM Validation Report ⓘ

Sep 7, 2026 – 07:52 pm BST

PDB ID : 9TRA / pdb_00009tra
EMDB ID : EMD-56164
Title : Bacterial antiviral defense protein PD-T7-3
Authors : Puteikiene, R.; Sasnauskas, G.
Deposited on : 2025-12-23
Resolution : 3.32 Å(reported)
Based on initial model : .

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.dev133
MolProbity : 4-5-2 with Phenix2.0
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

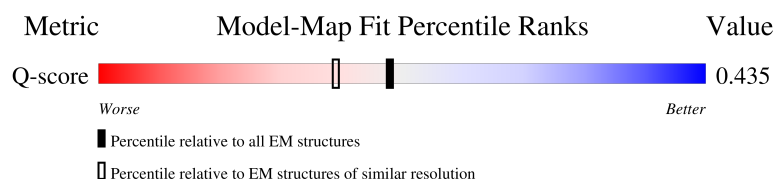
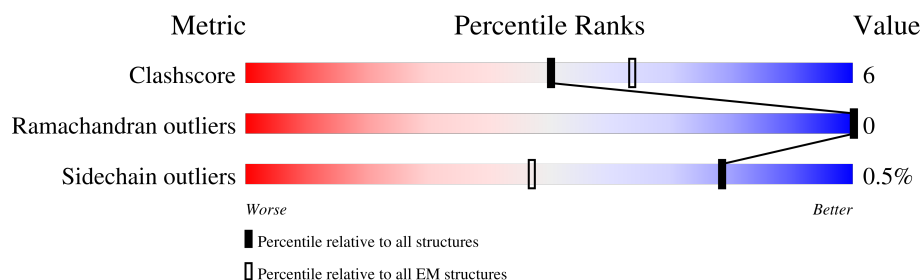
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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.



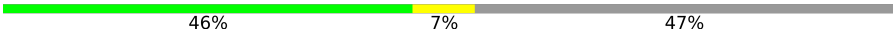
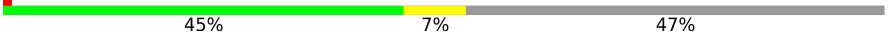
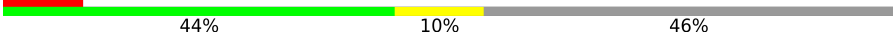
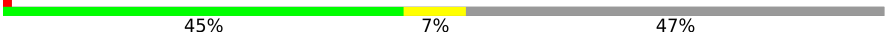
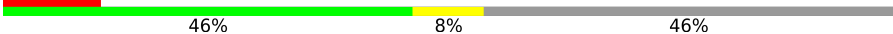
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14518 (2.82 - 3.82)

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	465	
1	B	465	
1	C	465	
1	D	465	

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Mol	Chain	Length	Quality of chain
1	E	465	
1	F	465	
1	G	465	
1	H	465	
1	I	465	
1	J	465	
1	K	465	
1	L	465	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33888 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 Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	1	0
			3570	2299	616	643	12		
1	B	435	Total	C	N	O	S	0	0
			3240	2106	563	560	11		
1	C	444	Total	C	N	O	S	0	0
			3538	2276	611	639	12		
1	D	445	Total	C	N	O	S	1	0
			3570	2299	616	643	12		
1	E	246	Total	C	N	O	S	0	0
			1922	1254	330	331	7		
1	F	380	Total	C	N	O	S	0	0
			3048	1971	519	548	10		
1	G	445	Total	C	N	O	S	0	0
			3563	2294	614	643	12		
1	H	246	Total	C	N	O	S	0	0
			1922	1254	330	331	7		
1	I	250	Total	C	N	O	S	0	0
			2015	1300	348	360	7		
1	J	445	Total	C	N	O	S	0	0
			3563	2294	614	643	12		
1	K	246	Total	C	N	O	S	0	0
			1922	1254	330	331	7		
1	L	250	Total	C	N	O	S	0	0
			2015	1300	348	360	7		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	PHE	-	expression tag	UNP Q858S9
A	457	GLU	-	expression tag	UNP Q858S9
A	458	SER	-	expression tag	UNP Q858S9
A	459	GLY	-	expression tag	UNP Q858S9
A	460	HIS	-	expression tag	UNP Q858S9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	461	HIS	-	expression tag	UNP Q858S9
A	462	HIS	-	expression tag	UNP Q858S9
A	463	HIS	-	expression tag	UNP Q858S9
A	464	HIS	-	expression tag	UNP Q858S9
A	465	HIS	-	expression tag	UNP Q858S9
B	456	PHE	-	expression tag	UNP Q858S9
B	457	GLU	-	expression tag	UNP Q858S9
B	458	SER	-	expression tag	UNP Q858S9
B	459	GLY	-	expression tag	UNP Q858S9
B	460	HIS	-	expression tag	UNP Q858S9
B	461	HIS	-	expression tag	UNP Q858S9
B	462	HIS	-	expression tag	UNP Q858S9
B	463	HIS	-	expression tag	UNP Q858S9
B	464	HIS	-	expression tag	UNP Q858S9
B	465	HIS	-	expression tag	UNP Q858S9
C	456	PHE	-	expression tag	UNP Q858S9
C	457	GLU	-	expression tag	UNP Q858S9
C	458	SER	-	expression tag	UNP Q858S9
C	459	GLY	-	expression tag	UNP Q858S9
C	460	HIS	-	expression tag	UNP Q858S9
C	461	HIS	-	expression tag	UNP Q858S9
C	462	HIS	-	expression tag	UNP Q858S9
C	463	HIS	-	expression tag	UNP Q858S9
C	464	HIS	-	expression tag	UNP Q858S9
C	465	HIS	-	expression tag	UNP Q858S9
D	456	PHE	-	expression tag	UNP Q858S9
D	457	GLU	-	expression tag	UNP Q858S9
D	458	SER	-	expression tag	UNP Q858S9
D	459	GLY	-	expression tag	UNP Q858S9
D	460	HIS	-	expression tag	UNP Q858S9
D	461	HIS	-	expression tag	UNP Q858S9
D	462	HIS	-	expression tag	UNP Q858S9
D	463	HIS	-	expression tag	UNP Q858S9
D	464	HIS	-	expression tag	UNP Q858S9
D	465	HIS	-	expression tag	UNP Q858S9
E	456	PHE	-	expression tag	UNP Q858S9
E	457	GLU	-	expression tag	UNP Q858S9
E	458	SER	-	expression tag	UNP Q858S9
E	459	GLY	-	expression tag	UNP Q858S9
E	460	HIS	-	expression tag	UNP Q858S9
E	461	HIS	-	expression tag	UNP Q858S9
E	462	HIS	-	expression tag	UNP Q858S9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	463	HIS	-	expression tag	UNP Q858S9
E	464	HIS	-	expression tag	UNP Q858S9
E	465	HIS	-	expression tag	UNP Q858S9
F	456	PHE	-	expression tag	UNP Q858S9
F	457	GLU	-	expression tag	UNP Q858S9
F	458	SER	-	expression tag	UNP Q858S9
F	459	GLY	-	expression tag	UNP Q858S9
F	460	HIS	-	expression tag	UNP Q858S9
F	461	HIS	-	expression tag	UNP Q858S9
F	462	HIS	-	expression tag	UNP Q858S9
F	463	HIS	-	expression tag	UNP Q858S9
F	464	HIS	-	expression tag	UNP Q858S9
F	465	HIS	-	expression tag	UNP Q858S9
G	456	PHE	-	expression tag	UNP Q858S9
G	457	GLU	-	expression tag	UNP Q858S9
G	458	SER	-	expression tag	UNP Q858S9
G	459	GLY	-	expression tag	UNP Q858S9
G	460	HIS	-	expression tag	UNP Q858S9
G	461	HIS	-	expression tag	UNP Q858S9
G	462	HIS	-	expression tag	UNP Q858S9
G	463	HIS	-	expression tag	UNP Q858S9
G	464	HIS	-	expression tag	UNP Q858S9
G	465	HIS	-	expression tag	UNP Q858S9
H	456	PHE	-	expression tag	UNP Q858S9
H	457	GLU	-	expression tag	UNP Q858S9
H	458	SER	-	expression tag	UNP Q858S9
H	459	GLY	-	expression tag	UNP Q858S9
H	460	HIS	-	expression tag	UNP Q858S9
H	461	HIS	-	expression tag	UNP Q858S9
H	462	HIS	-	expression tag	UNP Q858S9
H	463	HIS	-	expression tag	UNP Q858S9
H	464	HIS	-	expression tag	UNP Q858S9
H	465	HIS	-	expression tag	UNP Q858S9
I	456	PHE	-	expression tag	UNP Q858S9
I	457	GLU	-	expression tag	UNP Q858S9
I	458	SER	-	expression tag	UNP Q858S9
I	459	GLY	-	expression tag	UNP Q858S9
I	460	HIS	-	expression tag	UNP Q858S9
I	461	HIS	-	expression tag	UNP Q858S9
I	462	HIS	-	expression tag	UNP Q858S9
I	463	HIS	-	expression tag	UNP Q858S9
I	464	HIS	-	expression tag	UNP Q858S9

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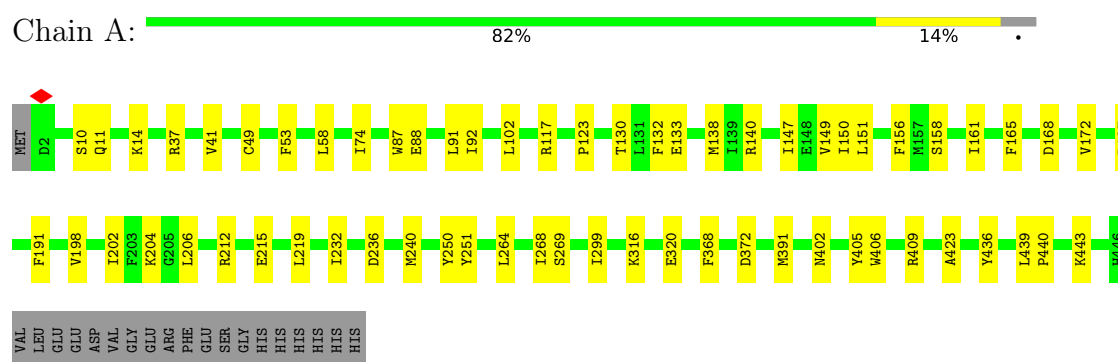
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Chain	Residue	Modelled	Actual	Comment	Reference
I	465	HIS	-	expression tag	UNP Q858S9
J	456	PHE	-	expression tag	UNP Q858S9
J	457	GLU	-	expression tag	UNP Q858S9
J	458	SER	-	expression tag	UNP Q858S9
J	459	GLY	-	expression tag	UNP Q858S9
J	460	HIS	-	expression tag	UNP Q858S9
J	461	HIS	-	expression tag	UNP Q858S9
J	462	HIS	-	expression tag	UNP Q858S9
J	463	HIS	-	expression tag	UNP Q858S9
J	464	HIS	-	expression tag	UNP Q858S9
J	465	HIS	-	expression tag	UNP Q858S9
K	456	PHE	-	expression tag	UNP Q858S9
K	457	GLU	-	expression tag	UNP Q858S9
K	458	SER	-	expression tag	UNP Q858S9
K	459	GLY	-	expression tag	UNP Q858S9
K	460	HIS	-	expression tag	UNP Q858S9
K	461	HIS	-	expression tag	UNP Q858S9
K	462	HIS	-	expression tag	UNP Q858S9
K	463	HIS	-	expression tag	UNP Q858S9
K	464	HIS	-	expression tag	UNP Q858S9
K	465	HIS	-	expression tag	UNP Q858S9
L	456	PHE	-	expression tag	UNP Q858S9
L	457	GLU	-	expression tag	UNP Q858S9
L	458	SER	-	expression tag	UNP Q858S9
L	459	GLY	-	expression tag	UNP Q858S9
L	460	HIS	-	expression tag	UNP Q858S9
L	461	HIS	-	expression tag	UNP Q858S9
L	462	HIS	-	expression tag	UNP Q858S9
L	463	HIS	-	expression tag	UNP Q858S9
L	464	HIS	-	expression tag	UNP Q858S9
L	465	HIS	-	expression tag	UNP Q858S9

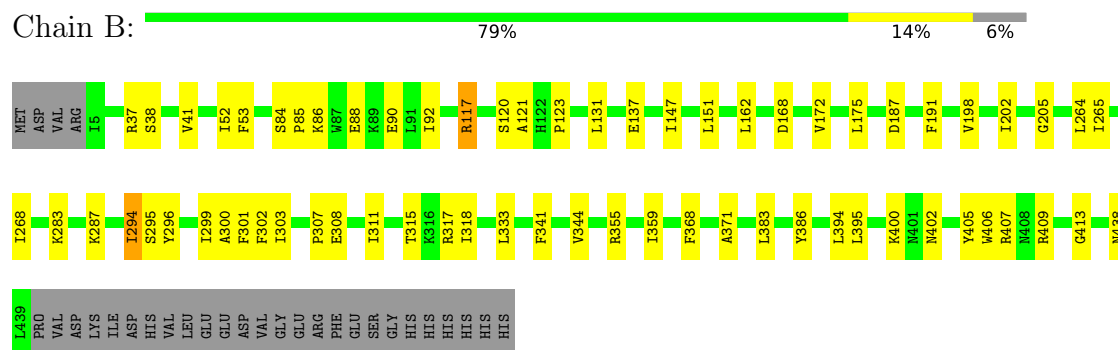
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

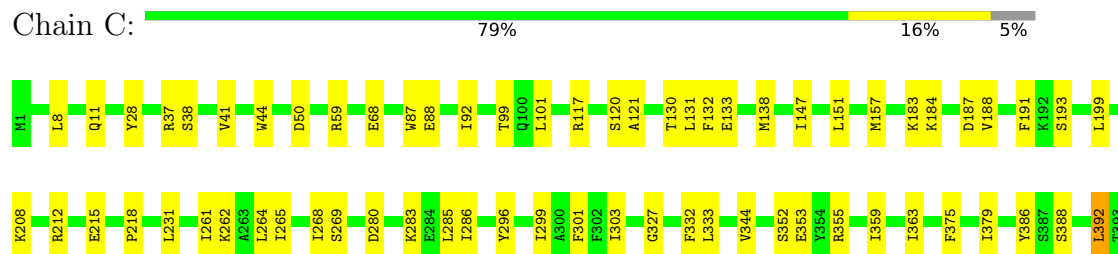
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30



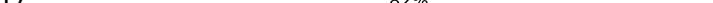
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

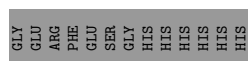


- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30



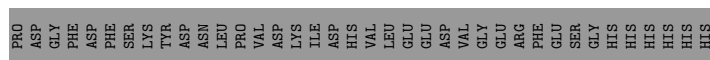
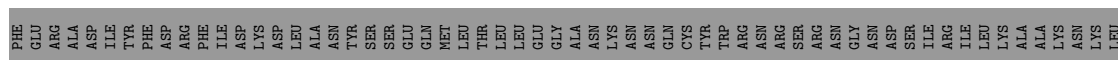
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain D:  82% 13% .



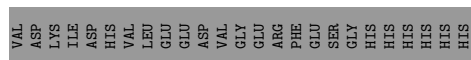
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain E: 46% 7% 47%



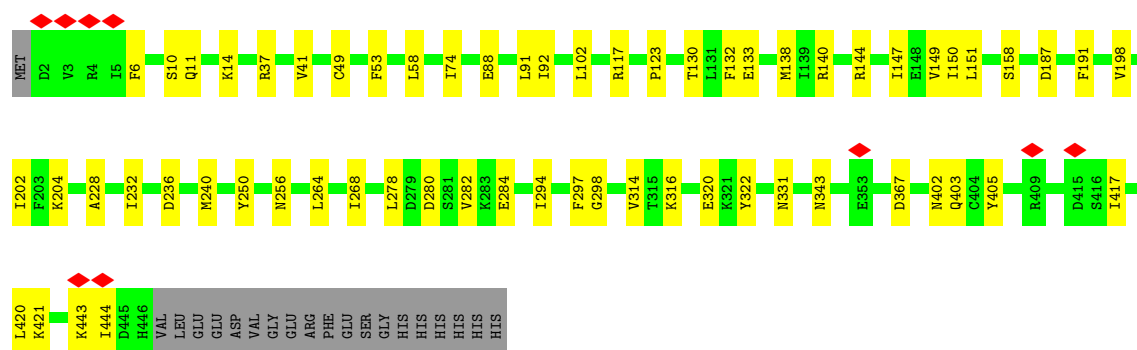
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain F: 67% 15% 18%

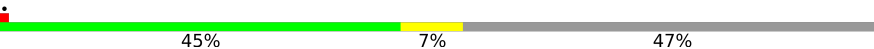


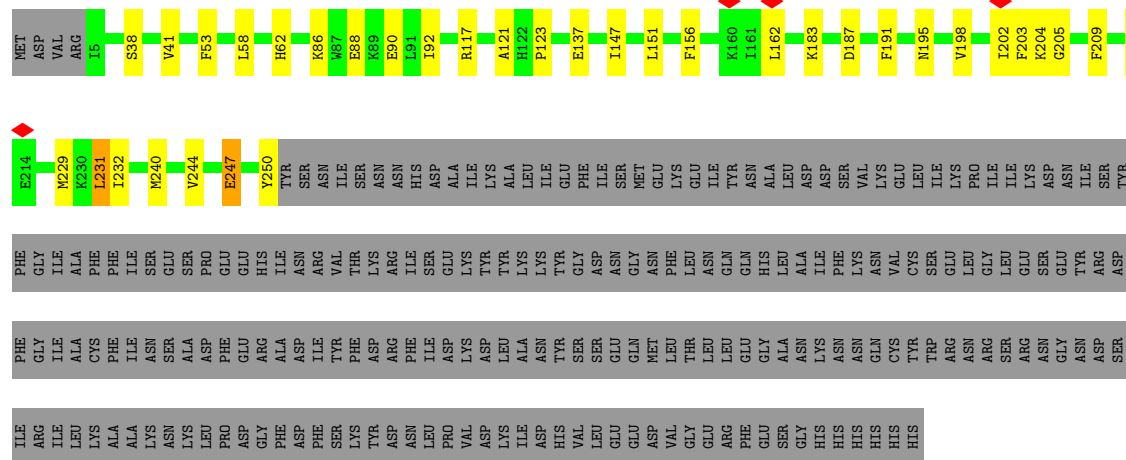
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain G:  82% 13%

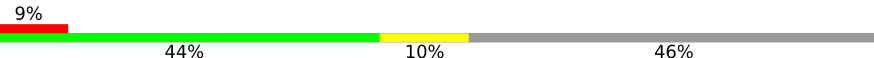


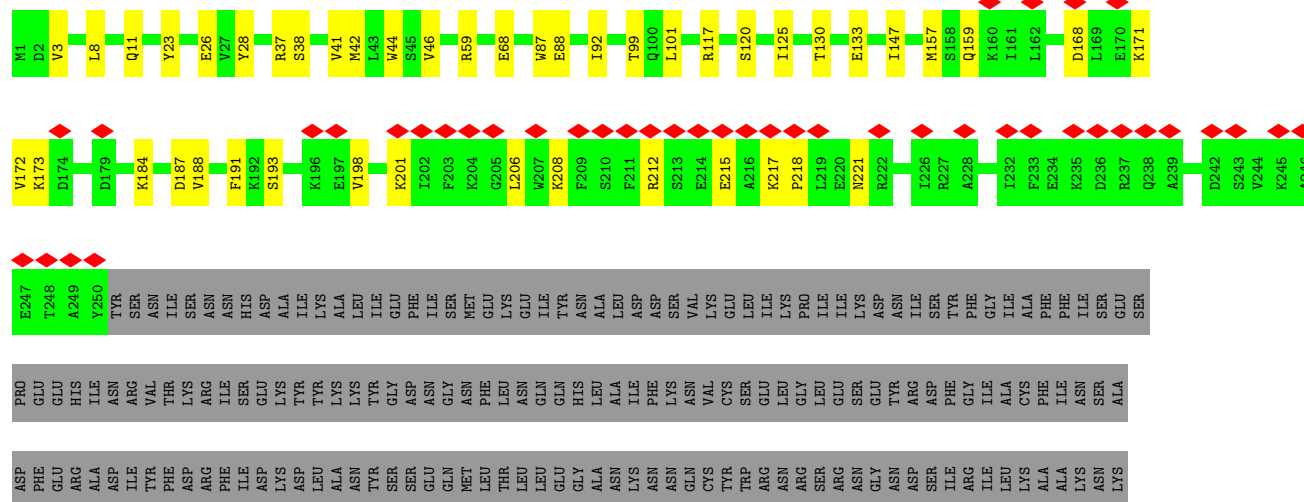
• Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain H:  45% 7% 47%



• Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

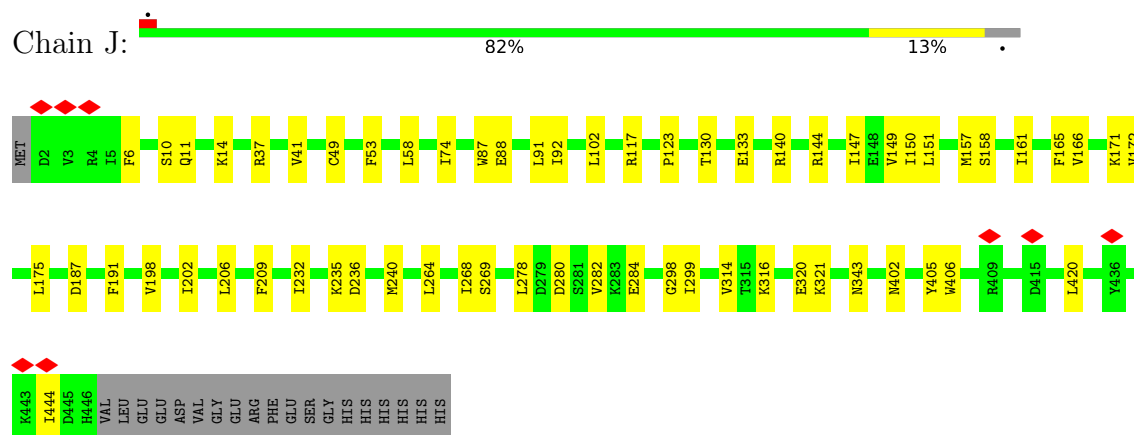
Chain I:  9% 44% 10% 46%



LEU PRO ASP GLY PHE ASP PHE SER LYS TYR ASP ASN LEU PRO VAL ASP LYS ASP LYS ASP HIS VAL LEU GLU ASP VAL GLY ARG PHE GLY SER GLY HIS HIS HIS HIS

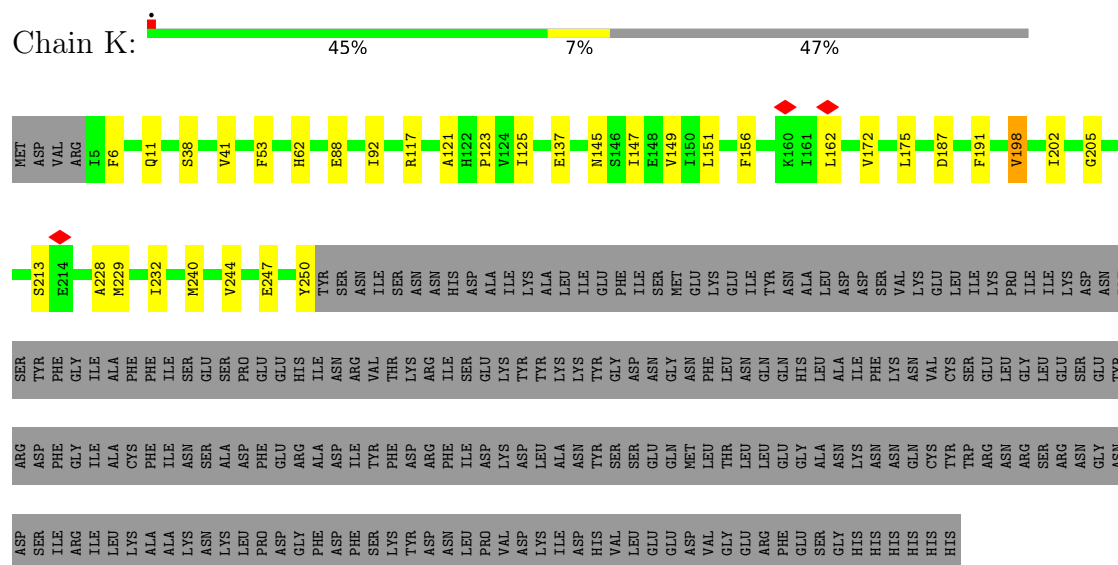
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain J:



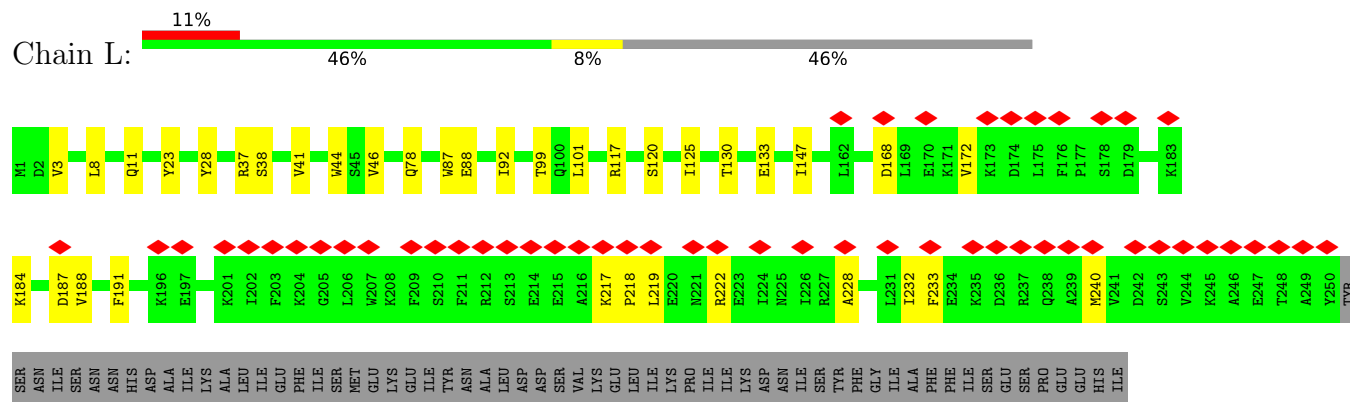
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain K:



- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30

Chain L:



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

ASP
PHE
SER
LYS
TYR
ASP
ASN
LEU
PRO
VAL
ASP
LYS
ILE
ASP
HIS
VAL
LEU
GLU
GLY
ASP
VAL
GLY
GLU
ARG
PHE
GLU
SER
GLY
HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	40.486	Depositor
Minimum map value	-13.160	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	5	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.08	0/3648	0.22	0/4924
1	B	0.10	0/3309	0.26	0/4493
1	C	0.10	0/3611	0.27	0/4878
1	D	0.08	0/3648	0.22	0/4924
1	E	0.09	0/1962	0.24	0/2655
1	F	0.10	0/3112	0.27	0/4202
1	G	0.08	0/3637	0.23	0/4909
1	H	0.09	0/1962	0.24	0/2655
1	I	0.10	0/2055	0.27	0/2775
1	J	0.08	0/3637	0.22	0/4909
1	K	0.09	0/1962	0.24	0/2655
1	L	0.10	0/2055	0.25	0/2775
All	All	0.09	0/34598	0.24	0/46754

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	3570	0	3525	39	0
1	B	3240	0	3049	46	0
1	C	3538	0	3474	45	0
1	D	3570	0	3525	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1922	0	1922	24	0
1	F	3048	0	3017	45	0
1	G	3563	0	3518	43	0
1	H	1922	0	1922	27	0
1	I	2015	0	2034	33	0
1	J	3563	0	3518	42	0
1	K	1922	0	1922	24	0
1	L	2015	0	2034	24	0
All	All	33888	0	33460	379	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 6.

All (379) 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:F:149:VAL:HG23	1:F:150:ILE:HG13	1.60	0.83
1:E:172:VAL:HA	1:E:175:LEU:HD13	1.68	0.74
1:B:172:VAL:HA	1:B:175:LEU:HD13	1.68	0.74
1:J:172:VAL:HG13	1:J:175:LEU:HD12	1.70	0.72
1:F:41:VAL:HG11	1:K:41:VAL:HG11	1.72	0.71
1:F:295:SER:HA	1:F:333:LEU:HD12	1.71	0.71
1:A:53:PHE:HE1	1:G:130:THR:HG21	1.55	0.71
1:E:41:VAL:HG11	1:L:41:VAL:HG11	1.73	0.71
1:I:173:LYS:HZ1	1:I:221:ASN:HA	1.56	0.70
1:D:53:PHE:HE1	1:J:130:THR:HG21	1.56	0.70
1:D:130:THR:HG21	1:J:53:PHE:HE1	1.56	0.70
1:E:38:SER:HB3	1:L:38:SER:HB3	1.73	0.68
1:E:41:VAL:HA	1:E:117:ARG:HG3	1.76	0.68
1:J:187:ASP:HA	1:J:191:PHE:HB2	1.74	0.68
1:G:256:ASN:HD21	1:I:171:LYS:HG2	1.59	0.68
1:A:130:THR:HG21	1:G:53:PHE:HE1	1.57	0.68
1:H:187:ASP:HA	1:H:191:PHE:HB2	1.75	0.67
1:D:187:ASP:HA	1:D:191:PHE:HB2	1.76	0.67
1:C:37:ARG:HH21	1:C:133:GLU:HB2	1.60	0.67
1:C:359:ILE:HD12	1:C:394:LEU:HB2	1.75	0.67
1:F:37:ARG:HH21	1:F:133:GLU:HB2	1.60	0.67
1:I:37:ARG:HH21	1:I:133:GLU:HB2	1.60	0.65
1:L:37:ARG:HH21	1:L:133:GLU:HB2	1.60	0.65
1:E:121:ALA:HB1	1:L:117:ARG:HH22	1.62	0.65
1:C:41:VAL:HG11	1:H:41:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:187:ASP:HA	1:K:191:PHE:HB2	1.78	0.64
1:B:265:ILE:HD11	1:B:300:ALA:HB2	1.78	0.64
1:F:117:ARG:HH22	1:K:121:ALA:HB1	1.63	0.64
1:B:121:ALA:HB1	1:I:117:ARG:HH22	1.64	0.63
1:A:436:TYR:HB3	1:A:439:LEU:HD12	1.80	0.63
1:C:117:ARG:HH22	1:H:121:ALA:HB1	1.64	0.63
1:E:37:ARG:HH11	1:E:131:LEU:HD23	1.65	0.62
1:G:149:VAL:HG12	1:G:150:ILE:HG12	1.82	0.61
1:B:37:ARG:HG2	1:B:120:SER:HB3	1.82	0.61
1:B:53:PHE:HE1	1:I:130:THR:HG21	1.66	0.61
1:C:38:SER:HB3	1:H:38:SER:HB3	1.82	0.61
1:K:41:VAL:HA	1:K:117:ARG:HG3	1.82	0.61
1:E:37:ARG:HG2	1:E:120:SER:HB3	1.83	0.61
1:F:38:SER:HB3	1:K:38:SER:HB3	1.81	0.61
1:I:59:ARG:HG3	1:I:68:GLU:HG2	1.81	0.61
1:D:53:PHE:CE1	1:J:130:THR:HG21	2.36	0.60
1:B:162:LEU:HD23	1:B:202:ILE:HA	1.82	0.60
1:F:367:ASP:HB3	1:F:370:ARG:HG2	1.83	0.60
1:J:149:VAL:HG12	1:J:150:ILE:HG12	1.83	0.60
1:B:402:ASN:HA	1:B:405:TYR:CE2	2.37	0.60
1:I:44:TRP:CD1	1:I:117:ARG:HD2	2.37	0.60
1:F:376:ASP:HA	1:F:380:ASP:HB3	1.82	0.60
1:B:147:ILE:HA	1:B:151:LEU:HB2	1.84	0.59
1:E:88:GLU:O	1:E:92:ILE:HG12	2.02	0.59
1:B:41:VAL:HG11	1:I:41:VAL:HG11	1.83	0.59
1:B:137:GLU:HG2	1:G:140:ARG:HD2	1.84	0.59
1:F:333:LEU:HD23	1:F:338:LEU:HD23	1.85	0.59
1:G:187:ASP:HA	1:G:191:PHE:HB2	1.85	0.59
1:L:44:TRP:CD1	1:L:117:ARG:HD2	2.37	0.59
1:E:53:PHE:HE1	1:L:130:THR:HG21	1.67	0.59
1:C:44:TRP:CD1	1:C:117:ARG:HD2	2.38	0.59
1:I:3:VAL:HG21	1:J:343:ASN:HB3	1.85	0.59
1:F:44:TRP:CD1	1:F:117:ARG:HD2	2.38	0.59
1:C:327:GLY:HA2	1:C:332:PHE:HB3	1.85	0.59
1:C:379:ILE:HG23	1:C:386:TYR:HE2	1.67	0.59
1:G:420:LEU:HB3	1:G:444:ILE:HG13	1.85	0.59
1:B:38:SER:HB3	1:I:38:SER:HB3	1.84	0.58
1:H:88:GLU:O	1:H:92:ILE:HG12	2.03	0.58
1:G:316:LYS:O	1:G:320:GLU:HG2	2.03	0.58
1:C:59:ARG:HG3	1:C:68:GLU:HB2	1.85	0.58
1:H:147:ILE:HA	1:H:151:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLU:O	1:B:92:ILE:HG12	2.04	0.57
1:E:147:ILE:HA	1:E:151:LEU:HB2	1.86	0.57
1:J:420:LEU:HB3	1:J:444:ILE:HG13	1.87	0.57
1:K:147:ILE:HA	1:K:151:LEU:HB2	1.85	0.57
1:B:53:PHE:CE1	1:I:130:THR:HG21	2.40	0.57
1:D:149:VAL:HG12	1:D:150:ILE:HG12	1.87	0.57
1:J:278:LEU:HD13	1:J:282:VAL:HG11	1.85	0.56
1:B:359:ILE:HD12	1:B:394:LEU:HD13	1.87	0.56
1:C:280:ASP:HA	1:C:283:LYS:HB2	1.86	0.56
1:D:386:TYR:HD2	1:D:390:GLN:HB3	1.69	0.56
1:A:130:THR:HG21	1:G:53:PHE:CE1	2.38	0.56
1:A:149:VAL:HG12	1:A:150:ILE:HG12	1.87	0.56
1:H:183:LYS:HD3	1:H:231:LEU:HD12	1.86	0.56
1:K:88:GLU:O	1:K:92:ILE:HG12	2.06	0.56
1:H:162:LEU:HD23	1:H:202:ILE:HA	1.86	0.56
1:D:140:ARG:HD2	1:K:137:GLU:HG2	1.86	0.56
1:G:278:LEU:HD13	1:G:282:VAL:HG11	1.87	0.56
1:D:130:THR:HG21	1:J:53:PHE:CE1	2.38	0.56
1:F:130:THR:HG21	1:K:53:PHE:CE1	2.41	0.56
1:G:102:LEU:HD21	1:G:150:ILE:HD11	1.87	0.56
1:A:187:ASP:HA	1:A:191:PHE:HB2	1.88	0.56
1:H:247:GLU:HB2	1:H:250:TYR:HB3	1.87	0.56
1:E:137:GLU:HG2	1:J:140:ARG:HD2	1.88	0.55
1:F:130:THR:HG21	1:K:53:PHE:HE1	1.71	0.55
1:E:53:PHE:CE1	1:L:130:THR:HG21	2.41	0.55
1:A:132:PHE:HZ	1:A:138:MET:HE1	1.72	0.55
1:F:37:ARG:HG3	1:F:120:SER:HB3	1.88	0.55
1:A:41:VAL:HA	1:A:117:ARG:HG3	1.89	0.55
1:C:37:ARG:HG3	1:C:120:SER:HB3	1.88	0.55
1:F:187:ASP:HA	1:F:191:PHE:HB2	1.86	0.55
1:F:262:LYS:HA	1:F:265:ILE:HD12	1.88	0.55
1:A:53:PHE:CE1	1:G:130:THR:HG21	2.40	0.55
1:J:102:LEU:HD21	1:J:150:ILE:HD11	1.88	0.55
1:B:265:ILE:HG13	1:B:302:PHE:HZ	1.72	0.55
1:B:295:SER:HA	1:B:333:LEU:HG	1.88	0.55
1:F:345:CYS:SG	1:F:354:TYR:HB2	2.46	0.55
1:J:191:PHE:HB3	1:J:235:LYS:HE3	1.89	0.55
1:C:261:ILE:HD13	1:C:285:LEU:HB3	1.89	0.55
1:C:130:THR:HG21	1:H:53:PHE:CE1	2.43	0.54
1:A:102:LEU:HD21	1:A:150:ILE:HD11	1.88	0.54
1:D:102:LEU:HD21	1:D:150:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:LEU:HD21	1:H:205:GLY:HA3	1.88	0.54
1:C:157:MET:HE2	1:C:193:SER:HB2	1.89	0.54
1:B:265:ILE:HG13	1:B:302:PHE:CZ	2.42	0.54
1:B:315:THR:HA	1:B:318:ILE:HG22	1.89	0.54
1:D:58:LEU:HD11	1:D:158:SER:HB3	1.88	0.54
1:A:204:LYS:HG2	1:A:250:TYR:CE2	2.43	0.54
1:F:264:LEU:O	1:F:268:ILE:HG12	2.08	0.54
1:D:436:TYR:HB3	1:D:439:LEU:HD12	1.90	0.53
1:D:41:VAL:HA	1:D:117:ARG:HG3	1.91	0.53
1:L:233:PHE:HA	1:L:240:MET:HE2	1.90	0.53
1:B:37:ARG:HH11	1:B:131:LEU:HD23	1.73	0.53
1:I:157:MET:HE2	1:I:193:SER:HB2	1.90	0.53
1:F:87:TRP:HH2	1:K:123:PRO:HD2	1.74	0.53
1:K:62:HIS:HD2	1:K:156:PHE:HD2	1.57	0.53
1:G:343:ASN:HB3	1:L:3:VAL:HG21	1.91	0.53
1:L:99:THR:HG22	1:L:101:LEU:H	1.74	0.53
1:B:123:PRO:HD2	1:I:87:TRP:HH2	1.74	0.52
1:B:162:LEU:HD21	1:B:205:GLY:HA3	1.90	0.52
1:E:187:ASP:HA	1:E:191:PHE:HB2	1.90	0.52
1:G:132:PHE:HZ	1:G:138:MET:HE1	1.75	0.52
1:B:371:ALA:HB3	1:B:407:ARG:HD2	1.92	0.52
1:E:162:LEU:HD23	1:E:202:ILE:HA	1.92	0.52
1:B:296:TYR:HA	1:B:299:ILE:HG12	1.92	0.52
1:G:58:LEU:HD11	1:G:158:SER:HB2	1.92	0.52
1:D:247:GLU:HG2	1:F:18:ARG:HD2	1.91	0.52
1:G:41:VAL:HA	1:G:117:ARG:HG3	1.90	0.52
1:F:212:ARG:HH21	1:F:253:ASN:HB3	1.75	0.51
1:K:156:PHE:HZ	1:K:198:VAL:HG22	1.73	0.51
1:B:283:LYS:O	1:B:287:LYS:HG2	2.10	0.51
1:C:87:TRP:HH2	1:H:123:PRO:HD2	1.76	0.51
1:F:272:LYS:HE3	1:F:276:ASN:HD22	1.74	0.51
1:J:37:ARG:HH21	1:J:133:GLU:HB2	1.75	0.51
1:K:172:VAL:HA	1:K:175:LEU:HD13	1.91	0.51
1:G:6:PHE:HZ	1:G:147:ILE:HD12	1.76	0.51
1:J:58:LEU:HD11	1:J:158:SER:HB2	1.93	0.51
1:F:254:ILE:HD13	1:F:264:LEU:HD12	1.93	0.51
1:F:208:LYS:HB2	1:F:212:ARG:HD2	1.92	0.51
1:F:147:ILE:HA	1:F:151:LEU:HB2	1.93	0.50
1:L:228:ALA:O	1:L:232:ILE:HG13	2.11	0.50
1:C:208:LYS:HD2	1:C:212:ARG:HH21	1.76	0.50
1:H:156:PHE:HZ	1:H:198:VAL:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PHE:HZ	1:D:138:MET:HE1	1.76	0.50
1:F:304:SER:HB2	1:F:310:HIS:HB2	1.92	0.50
1:B:311:ILE:HG12	1:B:341:PHE:HE1	1.76	0.50
1:I:159:GLN:HB2	1:I:201:LYS:HE2	1.93	0.50
1:I:26:GLU:HG3	1:I:42:MET:HE2	1.94	0.50
1:C:352:SER:HA	1:C:355:ARG:HG3	1.93	0.49
1:G:37:ARG:HH21	1:G:133:GLU:HB2	1.77	0.49
1:C:301:PHE:CZ	1:C:344:VAL:HG11	2.47	0.49
1:C:99:THR:HG22	1:C:101:LEU:H	1.78	0.49
1:D:37:ARG:HH21	1:D:133:GLU:HB2	1.77	0.49
1:B:301:PHE:CZ	1:B:344:VAL:HG11	2.47	0.49
1:D:386:TYR:HB2	1:D:391:MET:HE2	1.94	0.49
1:I:37:ARG:HG3	1:I:120:SER:HB3	1.93	0.49
1:C:121:ALA:HB1	1:H:117:ARG:HH22	1.77	0.49
1:J:198:VAL:O	1:J:202:ILE:HG13	2.13	0.49
1:A:37:ARG:HH21	1:A:133:GLU:HB2	1.77	0.49
1:C:130:THR:HG21	1:H:53:PHE:HE1	1.77	0.49
1:C:264:LEU:O	1:C:268:ILE:HG12	2.12	0.49
1:H:41:VAL:HA	1:H:117:ARG:HG3	1.94	0.49
1:J:6:PHE:HZ	1:J:147:ILE:HD12	1.78	0.49
1:F:280:ASP:HA	1:F:283:LYS:HB2	1.94	0.49
1:D:420:LEU:HB3	1:D:444:ILE:HG13	1.94	0.48
1:E:52:ILE:HD13	1:L:125:ILE:HG13	1.95	0.48
1:J:41:VAL:HA	1:J:117:ARG:HG3	1.93	0.48
1:L:219:LEU:HD13	1:L:222:ARG:HH12	1.78	0.48
1:K:162:LEU:HD23	1:K:202:ILE:HA	1.93	0.48
1:C:265:ILE:HG12	1:C:286:ILE:HG23	1.95	0.48
1:D:316:LYS:O	1:D:320:GLU:HG2	2.14	0.48
1:D:324:LYS:HG2	1:D:401:ASN:ND2	2.28	0.48
1:F:359:ILE:HA	1:F:379:ILE:HD11	1.96	0.48
1:F:311:ILE:HG13	1:F:341:PHE:CZ	2.48	0.48
1:I:187:ASP:HA	1:I:191:PHE:HB2	1.94	0.48
1:B:368:PHE:HE2	1:B:406:TRP:HB3	1.79	0.48
1:D:403:GLN:O	1:D:407:ARG:HG2	2.14	0.48
1:A:140:ARG:HD2	1:H:137:GLU:HG2	1.95	0.48
1:B:409:ARG:HA	1:B:413:GLY:HA3	1.96	0.48
1:D:10:SER:O	1:D:14:LYS:HG2	2.13	0.48
1:F:294:ILE:HG12	1:F:318:ILE:HD13	1.95	0.48
1:G:147:ILE:HA	1:G:151:LEU:HB2	1.95	0.48
1:A:316:LYS:O	1:A:320:GLU:HG2	2.14	0.48
1:D:49:CYS:SG	1:J:123:PRO:HB3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:GLU:HB2	1:I:42:MET:HG2	1.95	0.48
1:F:8:LEU:HB3	1:F:28:TYR:CD2	2.48	0.48
1:K:162:LEU:HD21	1:K:205:GLY:HA3	1.94	0.48
1:G:198:VAL:O	1:G:202:ILE:HG13	2.14	0.48
1:J:10:SER:O	1:J:14:LYS:HG2	2.14	0.48
1:B:187:ASP:HA	1:B:191:PHE:HB2	1.94	0.47
1:I:217:LYS:HB2	1:I:218:PRO:HD3	1.96	0.47
1:A:58:LEU:HD11	1:A:158:SER:HB2	1.96	0.47
1:G:280:ASP:O	1:G:284:GLU:HG2	2.14	0.47
1:F:308:GLU:O	1:F:311:ILE:HG22	2.15	0.47
1:G:10:SER:O	1:G:14:LYS:HG2	2.15	0.47
1:K:228:ALA:O	1:K:232:ILE:HG13	2.15	0.47
1:D:147:ILE:HA	1:D:151:LEU:HB2	1.96	0.47
1:F:265:ILE:HG12	1:F:286:ILE:HG23	1.96	0.47
1:A:391:MET:HG2	1:A:423:ALA:HA	1.97	0.47
1:D:198:VAL:O	1:D:202:ILE:HG13	2.14	0.47
1:C:8:LEU:HB3	1:C:28:TYR:CD2	2.49	0.47
1:G:88:GLU:O	1:G:92:ILE:HG12	2.14	0.47
1:J:147:ILE:HA	1:J:151:LEU:HB2	1.96	0.47
1:B:405:TYR:CD2	1:B:438:ASN:HB3	2.50	0.47
1:F:52:ILE:HD13	1:K:125:ILE:HG12	1.97	0.47
1:G:232:ILE:HG22	1:G:240:MET:HE3	1.97	0.47
1:H:203:PHE:CD2	1:H:240:MET:HG3	2.49	0.47
1:J:316:LYS:O	1:J:320:GLU:HG2	2.15	0.47
1:C:363:ILE:HD12	1:C:397:GLY:HA3	1.96	0.47
1:H:195:ASN:OD1	1:H:198:VAL:HG23	2.15	0.47
1:C:132:PHE:HZ	1:C:138:MET:HE1	1.80	0.46
1:L:8:LEU:HB3	1:L:28:TYR:CD2	2.50	0.46
1:A:147:ILE:HA	1:A:151:LEU:HB2	1.97	0.46
1:E:123:PRO:HD2	1:L:87:TRP:HH2	1.80	0.46
1:L:37:ARG:HG3	1:L:120:SER:HB3	1.96	0.46
1:C:11:GLN:HB3	1:C:147:ILE:HG13	1.98	0.46
1:B:86:LYS:O	1:B:90:GLU:HG2	2.16	0.46
1:F:217:LYS:HB2	1:F:218:PRO:HD3	1.97	0.46
1:H:198:VAL:O	1:H:202:ILE:HG12	2.16	0.46
1:I:8:LEU:HB3	1:I:28:TYR:CD2	2.51	0.46
1:A:10:SER:O	1:A:14:LYS:HG2	2.15	0.46
1:J:88:GLU:O	1:J:92:ILE:HG12	2.15	0.46
1:J:280:ASP:O	1:J:284:GLU:HG2	2.16	0.46
1:J:74:ILE:HG13	1:J:91:LEU:HD13	1.98	0.46
1:A:88:GLU:O	1:A:92:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLU:O	1:D:92:ILE:HG12	2.15	0.46
1:D:324:LYS:HG2	1:D:401:ASN:HD22	1.81	0.46
1:E:124:VAL:HA	1:L:78:GLN:HE22	1.80	0.45
1:G:417:ILE:HG22	1:G:421:LYS:HE3	1.98	0.45
1:A:165:PHE:HE2	1:A:206:LEU:HD11	1.82	0.45
1:B:355:ARG:HD2	1:B:386:TYR:CD1	2.52	0.45
1:F:318:ILE:HD12	1:F:322:TYR:HB2	1.97	0.45
1:I:157:MET:O	1:I:198:VAL:HG21	2.16	0.45
1:H:204:LYS:HA	1:H:204:LYS:HD3	1.71	0.45
1:L:217:LYS:HB2	1:L:218:PRO:HD3	1.98	0.45
1:B:41:VAL:HA	1:B:117:ARG:HD3	1.99	0.45
1:G:11:GLN:HB3	1:G:147:ILE:HG21	1.99	0.45
1:D:123:PRO:HG2	1:J:87:TRP:HH2	1.82	0.45
1:A:204:LYS:HG3	1:A:251:TYR:CZ	2.52	0.45
1:I:215:GLU:HB2	1:I:218:PRO:HD2	1.99	0.45
1:A:87:TRP:HH2	1:G:123:PRO:HG2	1.82	0.44
1:B:264:LEU:O	1:B:268:ILE:HG12	2.17	0.44
1:D:87:TRP:HH2	1:J:123:PRO:HG2	1.81	0.44
1:D:123:PRO:HB3	1:J:49:CYS:SG	2.57	0.44
1:G:294:ILE:HB	1:G:322:TYR:CZ	2.51	0.44
1:A:123:PRO:HB3	1:G:49:CYS:SG	2.57	0.44
1:A:236:ASP:O	1:A:240:MET:HG2	2.17	0.44
1:F:352:SER:HA	1:F:355:ARG:HG3	1.99	0.44
1:L:187:ASP:HA	1:L:191:PHE:HB2	1.98	0.44
1:B:137:GLU:OE1	1:G:144:ARG:HD3	2.17	0.44
1:L:11:GLN:HB3	1:L:147:ILE:HG13	2.00	0.44
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.89	0.44
1:H:231:LEU:HD13	1:H:231:LEU:HA	1.85	0.44
1:F:261:ILE:HD13	1:F:285:LEU:HG	1.99	0.44
1:G:294:ILE:HD12	1:G:297:PHE:HB3	2.00	0.44
1:L:184:LYS:O	1:L:188:VAL:HG22	2.17	0.44
1:A:264:LEU:O	1:A:268:ILE:HG12	2.16	0.44
1:B:307:PRO:O	1:B:311:ILE:HG13	2.16	0.44
1:D:264:LEU:O	1:D:268:ILE:HG12	2.17	0.44
1:J:165:PHE:HE2	1:J:206:LEU:HD11	1.82	0.44
1:K:198:VAL:O	1:K:202:ILE:HG12	2.17	0.44
1:C:388:SER:O	1:C:392:LEU:HD12	2.17	0.44
1:A:49:CYS:SG	1:G:123:PRO:HB3	2.58	0.43
1:A:402:ASN:HA	1:A:405:TYR:CZ	2.53	0.43
1:B:287:LYS:HA	1:B:287:LYS:HD3	1.84	0.43
1:D:236:ASP:O	1:D:240:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLN:O	1:C:407:ARG:HG3	2.18	0.43
1:I:23:TYR:HB3	1:I:46:VAL:HG22	1.99	0.43
1:A:440:PRO:HB2	1:A:443:LYS:HB3	2.00	0.43
1:D:368:PHE:CE1	1:D:403:GLN:HA	2.54	0.43
1:F:377:ARG:HD2	1:F:378:PHE:CE2	2.53	0.43
1:K:145:ASN:O	1:K:149:VAL:HG22	2.18	0.43
1:A:11:GLN:HB3	1:A:147:ILE:HG21	2.00	0.43
1:C:131:LEU:HD23	1:C:131:LEU:HA	1.91	0.43
1:C:187:ASP:HA	1:C:191:PHE:HB2	2.01	0.43
1:D:168:ASP:O	1:D:172:VAL:HG22	2.17	0.43
1:G:74:ILE:HG13	1:G:91:LEU:HD13	2.00	0.43
1:C:262:LYS:HD3	1:C:296:TYR:CZ	2.54	0.43
1:J:320:GLU:HB2	1:J:321:LYS:HD2	2.00	0.43
1:D:402:ASN:HA	1:D:405:TYR:CZ	2.54	0.43
1:F:145:ASN:O	1:F:149:VAL:HG22	2.19	0.43
1:H:86:LYS:O	1:H:90:GLU:HG2	2.19	0.43
1:I:206:LEU:HD23	1:I:206:LEU:HA	1.91	0.43
1:I:208:LYS:HD3	1:I:212:ARG:HH21	1.83	0.43
1:A:168:ASP:O	1:A:172:VAL:HG22	2.17	0.43
1:A:215:GLU:O	1:A:219:LEU:HG	2.19	0.43
1:B:52:ILE:HD13	1:I:125:ILE:HG13	2.01	0.43
1:B:300:ALA:O	1:B:303:ILE:HG12	2.18	0.43
1:I:173:LYS:NZ	1:I:221:ASN:HD22	2.17	0.43
1:J:264:LEU:O	1:J:268:ILE:HG12	2.19	0.43
1:A:269:SER:HB2	1:A:299:ILE:O	2.19	0.43
1:C:402:ASN:HA	1:C:405:TYR:CZ	2.53	0.43
1:E:168:ASP:O	1:E:172:VAL:HG22	2.19	0.43
1:F:199:LEU:HD23	1:F:199:LEU:HA	1.88	0.43
1:K:240:MET:O	1:K:244:VAL:HG23	2.19	0.43
1:D:11:GLN:HB3	1:D:147:ILE:HG21	2.00	0.42
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.90	0.42
1:H:62:HIS:CD2	1:H:156:PHE:HD2	2.37	0.42
1:E:185:TYR:O	1:E:189:LYS:HB2	2.19	0.42
1:J:11:GLN:HB3	1:J:147:ILE:HG21	2.01	0.42
1:E:137:GLU:OE1	1:J:144:ARG:HD3	2.20	0.42
1:I:99:THR:HG22	1:I:101:LEU:H	1.84	0.42
1:L:88:GLU:O	1:L:92:ILE:HG12	2.19	0.42
1:B:168:ASP:O	1:B:172:VAL:HG22	2.19	0.42
1:B:308:GLU:HA	1:B:311:ILE:HD12	2.01	0.42
1:C:184:LYS:O	1:C:188:VAL:HG22	2.19	0.42
1:D:269:SER:HB2	1:D:299:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:LYS:NZ	1:D:403:GLN:HE21	2.17	0.42
1:G:236:ASP:O	1:G:240:MET:HG2	2.19	0.42
1:C:183:LYS:HE3	1:C:231:LEU:HD22	2.02	0.42
1:D:165:PHE:HE2	1:D:206:LEU:HD11	1.85	0.42
1:E:8:LEU:HD11	1:E:143:ILE:HG21	2.02	0.42
1:J:232:ILE:HG22	1:J:240:MET:HE3	2.02	0.42
1:L:23:TYR:HB3	1:L:46:VAL:HG22	2.01	0.42
1:A:368:PHE:HE2	1:A:406:TRP:HB3	1.84	0.42
1:F:88:GLU:O	1:F:92:ILE:HG12	2.19	0.42
1:B:294:ILE:HA	1:B:317:ARG:NH1	2.34	0.41
1:C:269:SER:HB2	1:C:299:ILE:O	2.20	0.41
1:C:414:ASN:O	1:C:418:ARG:HG3	2.20	0.41
1:E:40:THR:HG21	1:E:134:PRO:HG2	2.02	0.41
1:G:298:GLY:HA2	1:G:314:VAL:HG21	2.02	0.41
1:G:420:LEU:HD12	1:G:444:ILE:HD12	2.02	0.41
1:I:184:LYS:O	1:I:188:VAL:HG22	2.19	0.41
1:F:184:LYS:O	1:F:188:VAL:HG22	2.20	0.41
1:G:228:ALA:O	1:G:232:ILE:HG13	2.20	0.41
1:I:88:GLU:O	1:I:92:ILE:HG12	2.20	0.41
1:J:157:MET:HA	1:J:161:ILE:HD11	2.02	0.41
1:A:156:PHE:CE2	1:A:161:ILE:HG23	2.55	0.41
1:C:406:TRP:O	1:C:406:TRP:CD1	2.74	0.41
1:C:406:TRP:O	1:C:406:TRP:HD1	2.03	0.41
1:G:402:ASN:HA	1:G:405:TYR:CZ	2.55	0.41
1:J:402:ASN:HA	1:J:405:TYR:CZ	2.56	0.41
1:A:232:ILE:HG22	1:A:240:MET:HE3	2.02	0.41
1:G:367:ASP:HA	1:G:403:GLN:HE21	1.85	0.41
1:A:204:LYS:HG3	1:A:251:TYR:OH	2.21	0.41
1:A:198:VAL:O	1:A:202:ILE:HG13	2.20	0.41
1:A:372:ASP:HB2	1:A:409:ARG:CZ	2.50	0.41
1:G:417:ILE:HD12	1:G:443:LYS:HG3	2.03	0.41
1:H:240:MET:O	1:H:244:VAL:HG23	2.20	0.41
1:J:298:GLY:HA2	1:J:314:VAL:HG21	2.03	0.41
1:K:6:PHE:CD1	1:K:11:GLN:HG3	2.56	0.41
1:B:400:LYS:HD2	1:B:400:LYS:HA	1.78	0.41
1:C:50:ASP:OD2	1:C:151:LEU:HA	2.21	0.41
1:E:44:TRP:CD1	1:E:117:ARG:HD3	2.55	0.41
1:E:131:LEU:HD12	1:E:131:LEU:HA	1.91	0.41
1:G:322:TYR:HE1	1:G:331:ASN:HD22	1.69	0.41
1:H:209:PHE:O	1:H:213:SER:HB2	2.20	0.41
1:H:232:ILE:HG22	1:H:240:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:LEU:O	1:G:268:ILE:HG12	2.21	0.41
1:J:236:ASP:O	1:J:240:MET:HG2	2.21	0.41
1:K:209:PHE:O	1:K:213:SER:HB2	2.21	0.41
1:C:215:GLU:HB2	1:C:218:PRO:HD2	2.02	0.40
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.92	0.40
1:F:183:LYS:O	1:F:187:ASP:HB2	2.21	0.40
1:I:11:GLN:HB3	1:I:147:ILE:HG13	2.03	0.40
1:J:171:LYS:HB3	1:J:171:LYS:HE2	1.86	0.40
1:K:247:GLU:HG3	1:K:250:TYR:HB3	2.04	0.40
1:G:204:LYS:HG2	1:G:250:TYR:CE1	2.56	0.40
1:I:41:VAL:HA	1:I:117:ARG:HG3	2.03	0.40
1:J:166:VAL:HG21	1:J:209:PHE:CE2	2.57	0.40
1:L:168:ASP:O	1:L:172:VAL:HG22	2.21	0.40
1:B:84:SER:HA	1:B:85:PRO:HD3	1.95	0.40
1:C:352:SER:O	1:C:355:ARG:HB2	2.21	0.40
1:D:20:THR:HG21	1:D:50:ASP:OD2	2.21	0.40
1:D:131:LEU:HG	1:J:49:CYS:SG	2.61	0.40
1:D:173:LYS:HB3	1:D:173:LYS:HE2	1.91	0.40
1:F:102:LEU:HD21	1:F:150:ILE:HD11	2.03	0.40
1:I:168:ASP:O	1:I:172:VAL:HG22	2.22	0.40
1:J:269:SER:HB2	1:J:299:ILE:O	2.21	0.40
1:A:74:ILE:HG13	1:A:91:LEU:HD13	2.03	0.40
1:C:88:GLU:O	1:C:92:ILE:HG12	2.21	0.40
1:C:375:PHE:HE2	1:C:415:ASP:HB3	1.87	0.40
1:D:377:ARG:HD2	1:D:378:PHE:CE2	2.57	0.40
1:F:213:SER:HB2	1:F:215:GLU:OE1	2.21	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	444/465 (96%)	438 (99%)	6 (1%)	0	100	100
1	B	433/465 (93%)	428 (99%)	5 (1%)	0	100	100
1	C	442/465 (95%)	436 (99%)	6 (1%)	0	100	100
1	D	444/465 (96%)	437 (98%)	7 (2%)	0	100	100
1	E	244/465 (52%)	239 (98%)	5 (2%)	0	100	100
1	F	378/465 (81%)	374 (99%)	4 (1%)	0	100	100
1	G	443/465 (95%)	438 (99%)	5 (1%)	0	100	100
1	H	244/465 (52%)	237 (97%)	7 (3%)	0	100	100
1	I	248/465 (53%)	243 (98%)	5 (2%)	0	100	100
1	J	443/465 (95%)	438 (99%)	5 (1%)	0	100	100
1	K	244/465 (52%)	239 (98%)	5 (2%)	0	100	100
1	L	248/465 (53%)	243 (98%)	5 (2%)	0	100	100
All	All	4255/5580 (76%)	4190 (98%)	65 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/427 (88%)	377 (100%)	1 (0%)	86	85
1	B	301/427 (70%)	297 (99%)	4 (1%)	61	73
1	C	371/427 (87%)	366 (99%)	5 (1%)	61	73
1	D	378/427 (88%)	377 (100%)	1 (0%)	86	85
1	E	198/427 (46%)	197 (100%)	1 (0%)	81	82
1	F	323/427 (76%)	323 (100%)	0	100	100
1	G	377/427 (88%)	377 (100%)	0	100	100
1	H	198/427 (46%)	194 (98%)	4 (2%)	48	67
1	I	218/427 (51%)	218 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	377/427 (88%)	376 (100%)	1 (0%)	86	85
1	K	198/427 (46%)	196 (99%)	2 (1%)	68	75
1	L	218/427 (51%)	218 (100%)	0	100	100
All	All	3535/5124 (69%)	3516 (100%)	19 (0%)	78	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	B	117	ARG
1	B	198	VAL
1	B	294	ILE
1	B	395	LEU
1	C	303	ILE
1	C	333	LEU
1	C	353	GLU
1	C	392	LEU
1	C	420	LEU
1	D	383	LEU
1	E	150	ILE
1	H	58	LEU
1	H	229	MET
1	H	231	LEU
1	H	247	GLU
1	J	406	TRP
1	K	198	VAL
1	K	229	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	122	HIS
1	A	180	ASN
1	A	276	ASN
1	A	403	GLN
1	A	412	ASN
1	B	33	ASN
1	C	107	ASN
1	C	114	GLN

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Mol	Chain	Res	Type
1	C	118	HIS
1	C	180	ASN
1	C	334	ASN
1	D	122	HIS
1	D	276	ASN
1	D	399	ASN
1	D	403	GLN
1	F	107	ASN
1	F	118	HIS
1	F	122	HIS
1	F	180	ASN
1	G	63	ASN
1	G	253	ASN
1	G	331	ASN
1	G	399	ASN
1	H	238	GLN
1	I	33	ASN
1	I	107	ASN
1	I	114	GLN
1	I	118	HIS
1	I	221	ASN
1	J	63	ASN
1	J	276	ASN
1	J	310	HIS
1	J	331	ASN
1	K	62	HIS
1	K	238	GLN
1	L	78	GLN
1	L	107	ASN
1	L	118	HIS
1	L	122	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

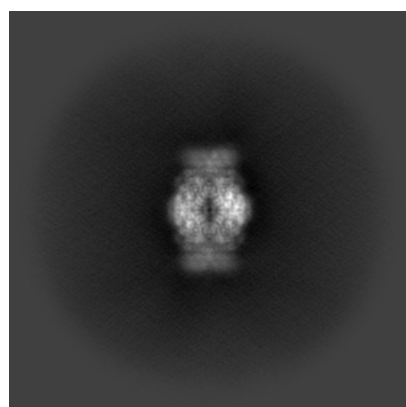
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56164. These allow visual inspection of the internal detail of the map and identification of artifacts.

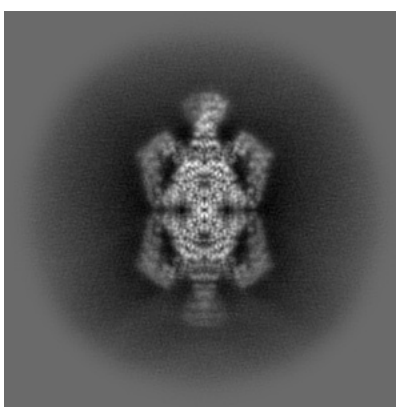
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

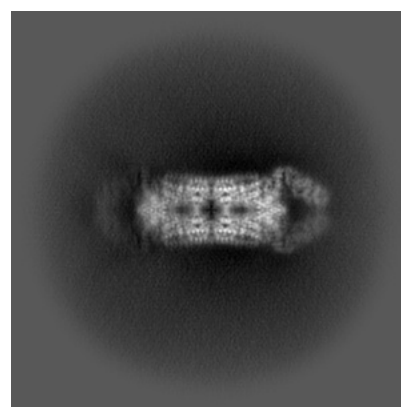
6.1.1 Primary map



X



Y

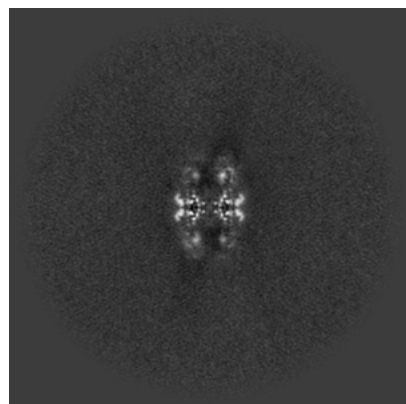


Z

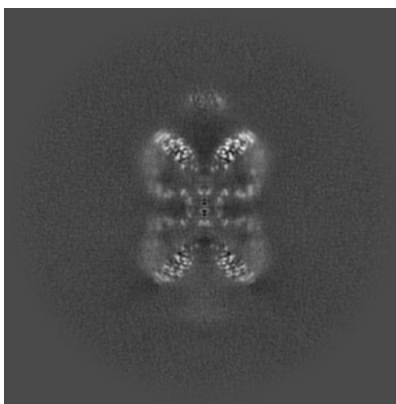
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

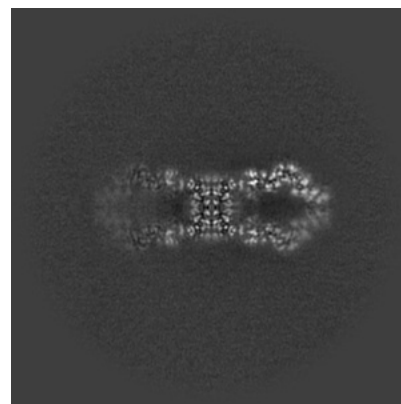
6.2.1 Primary map



X Index: 200



Y Index: 200

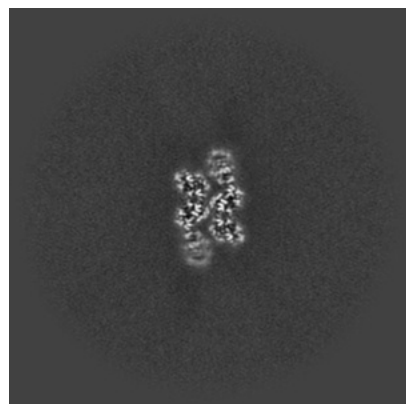


Z Index: 200

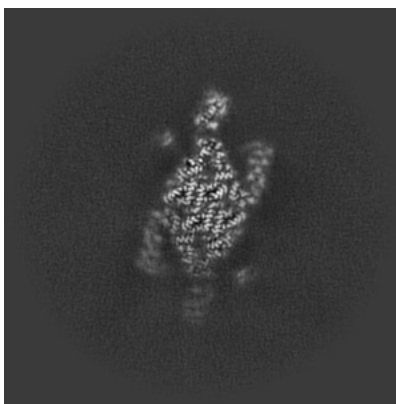
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

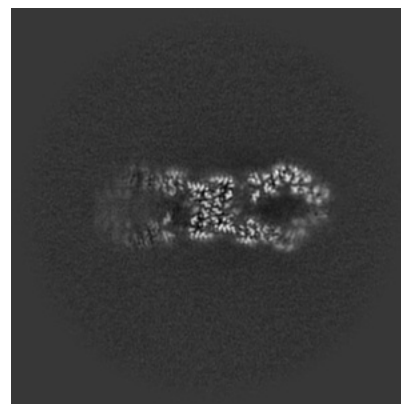
6.3.1 Primary map



X Index: 216



Y Index: 221

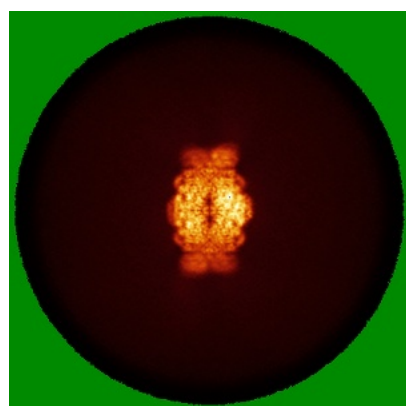


Z Index: 203

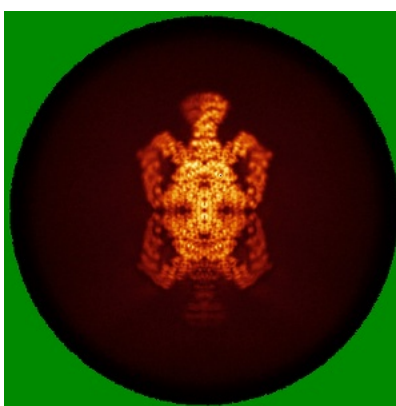
The images above show the largest variance slices of the map in three orthogonal directions.

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

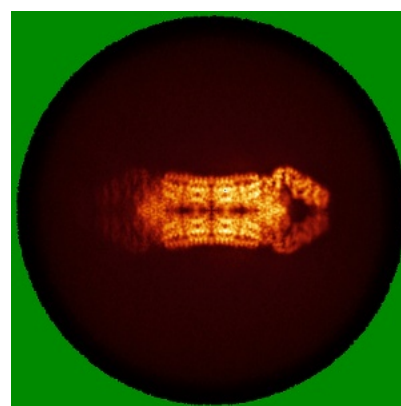
6.4.1 Primary map



X



Y

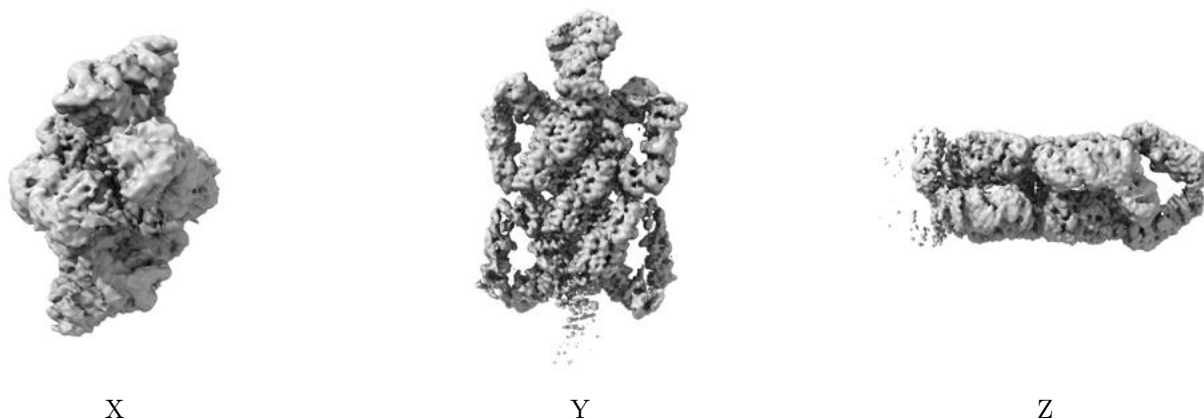


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

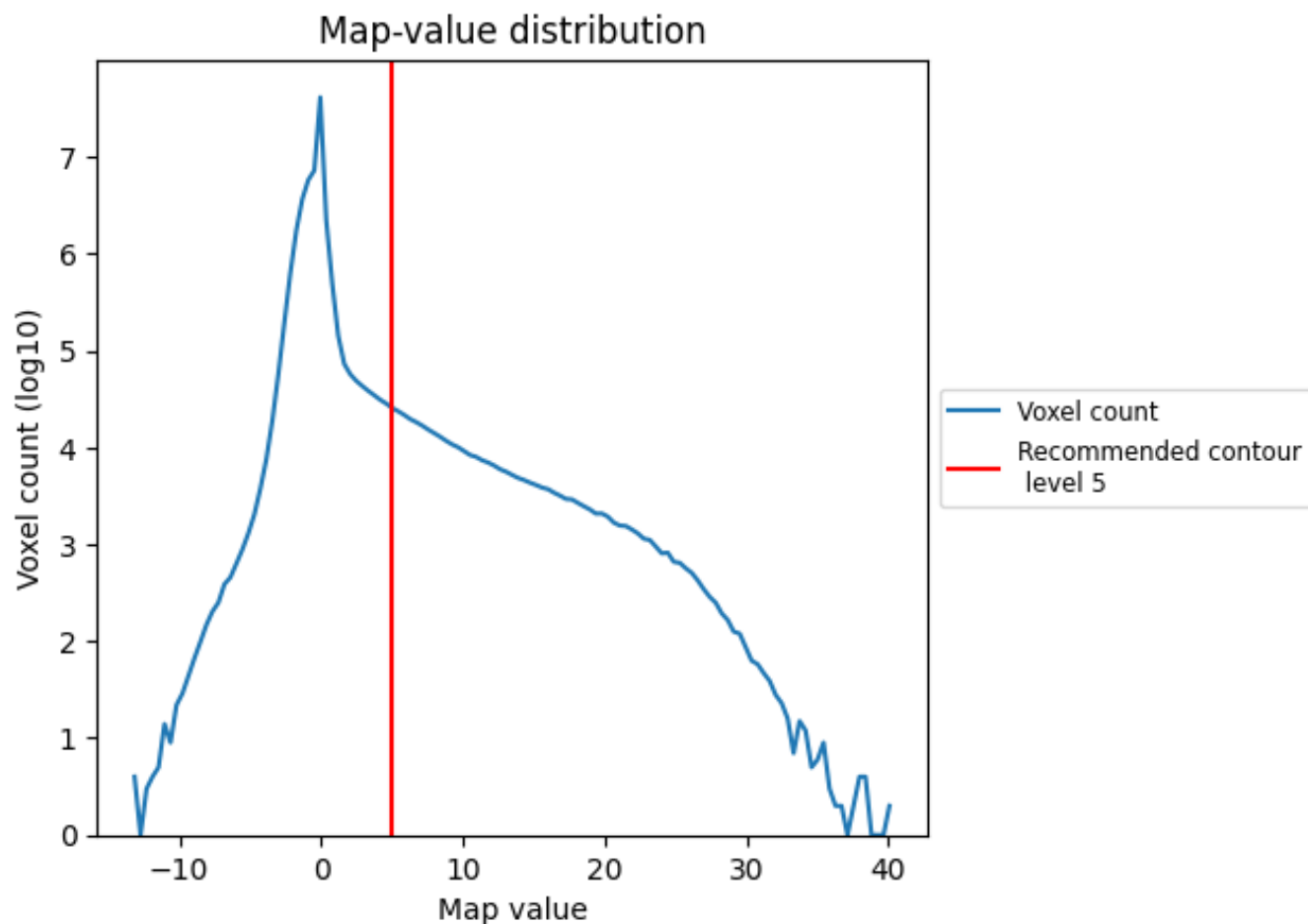
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

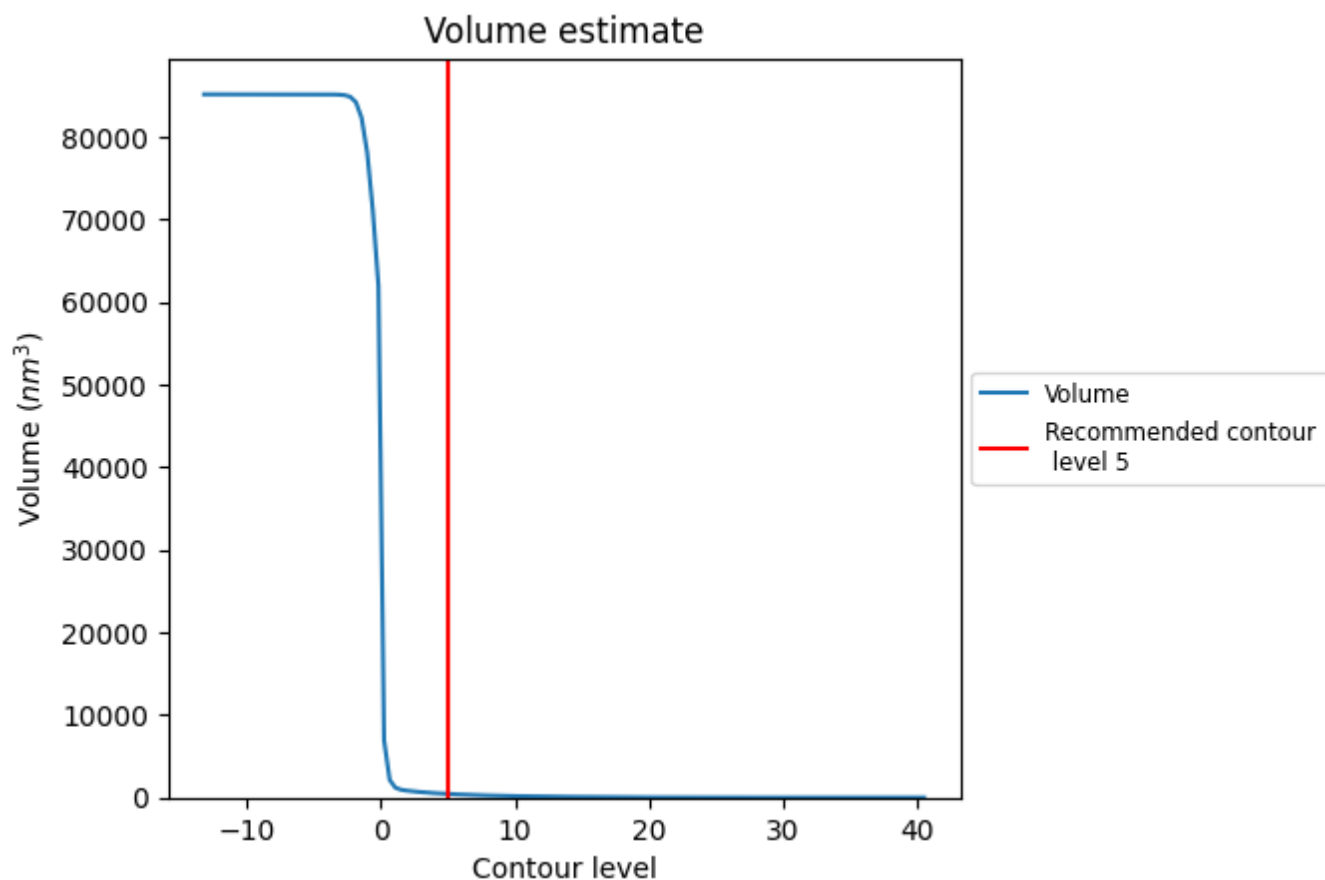
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

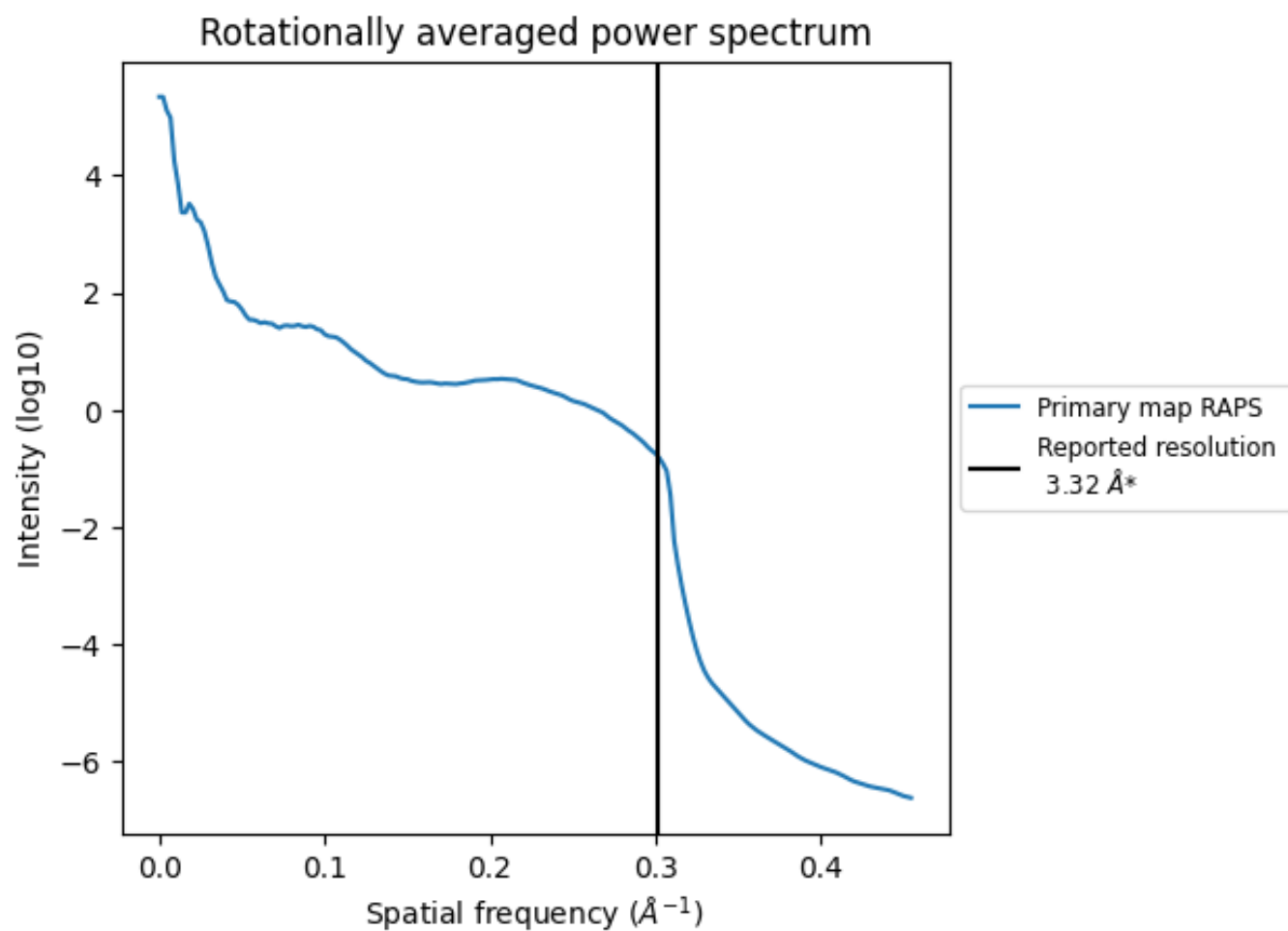
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 443 nm^3 ; this corresponds to an approximate mass of 400 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 0.301 $\text{\AA}^{-1}$

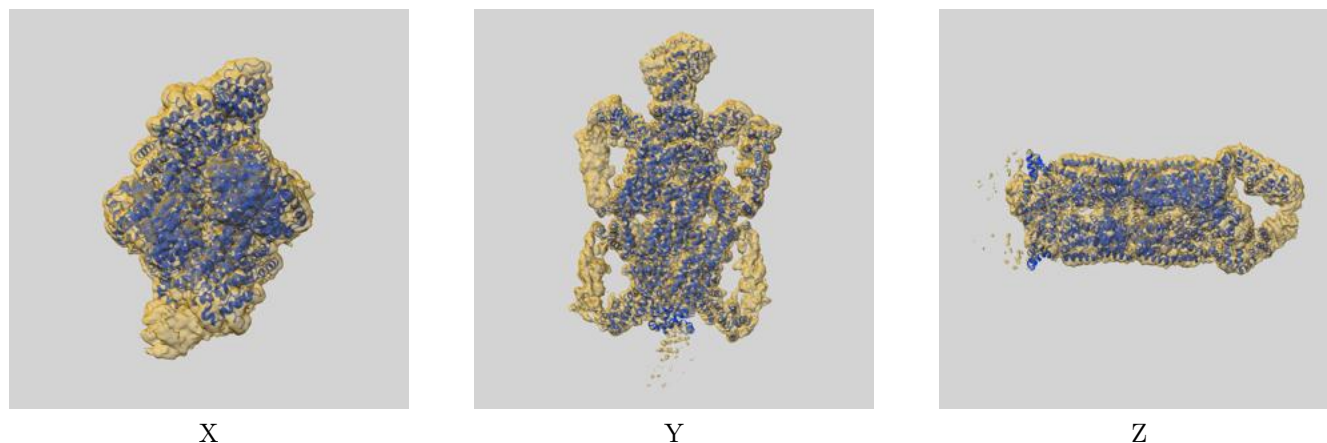
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

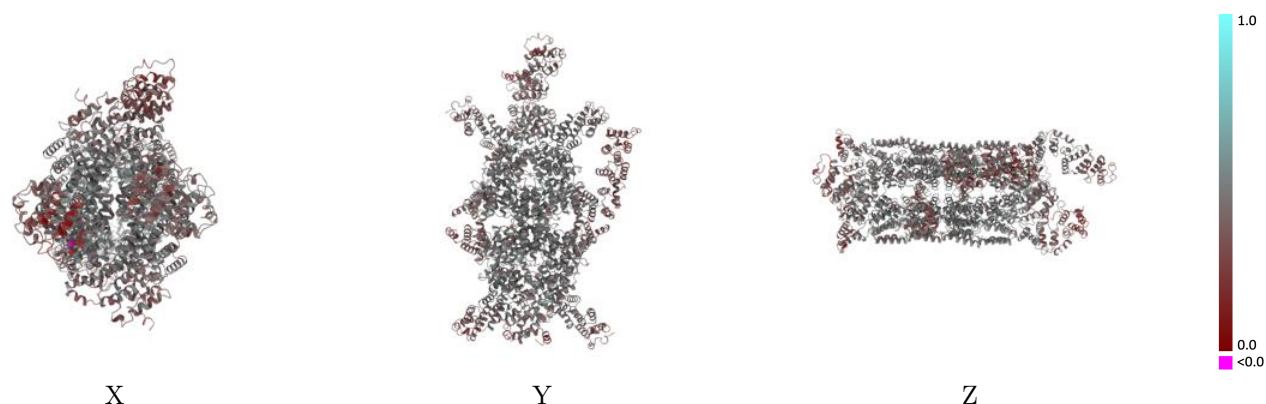
This section contains information regarding the fit between EMDB map EMD-56164 and PDB model 9TRA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



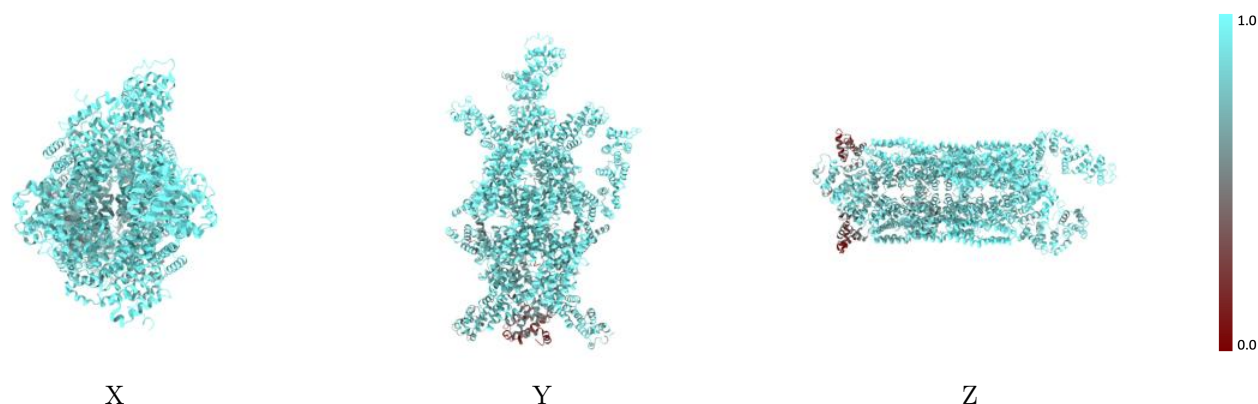
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



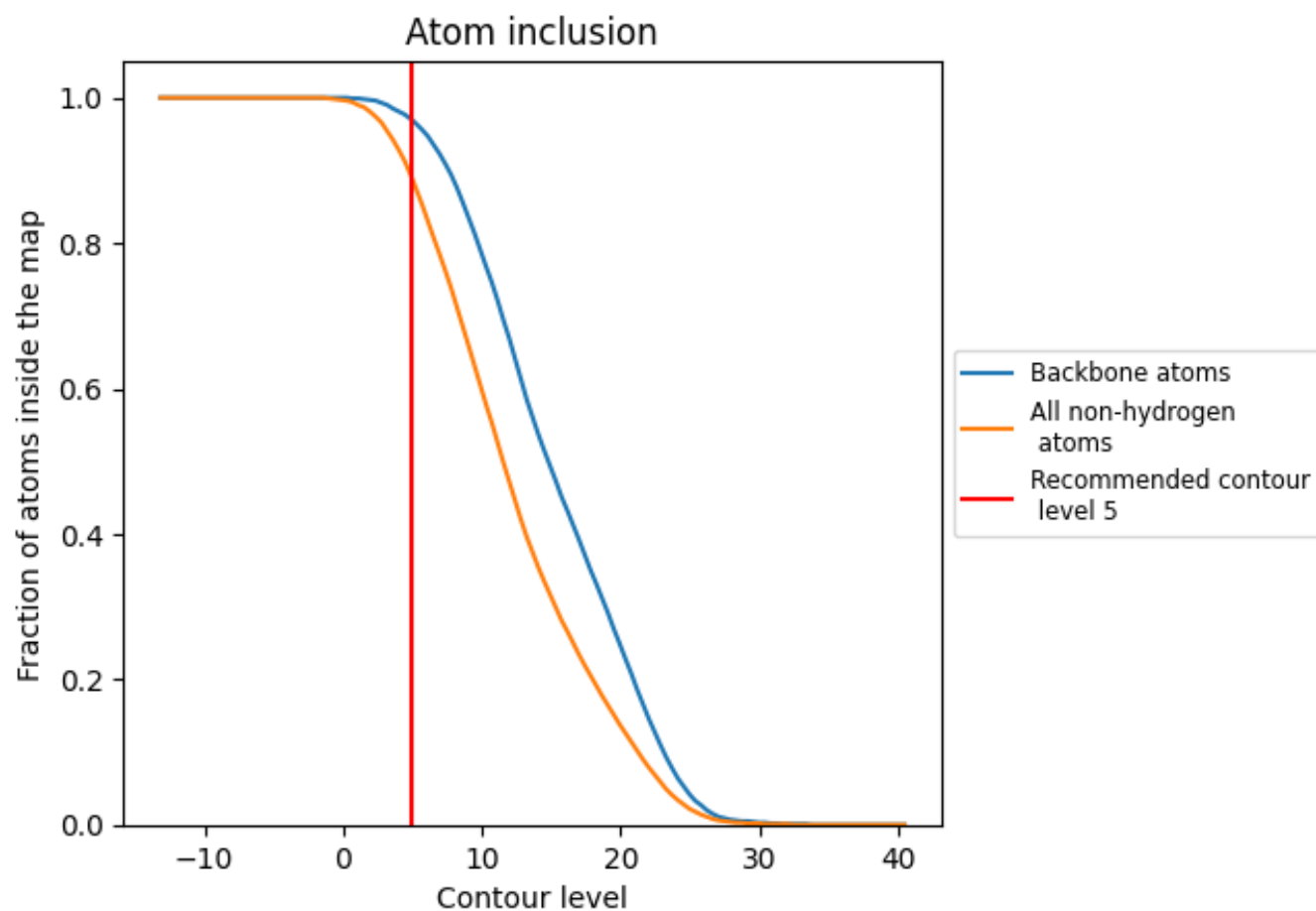
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.4350
A	0.9460	0.4670
B	0.9500	0.3980
C	0.9720	0.4310
D	0.9390	0.4630
E	0.9270	0.4350
F	0.8960	0.4010
G	0.8530	0.4360
H	0.8680	0.4280
I	0.7320	0.4370
J	0.8610	0.4430
K	0.8670	0.4350
L	0.7060	0.4320

