



# Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 11:10 PM EST

PDB ID : 8QQN  
EMDB ID : EMD-18599  
Title : Portal protein of full Haloferax tailed virus 1.  
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.  
Deposited on : 2023-10-05  
Resolution : 2.34 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](mailto: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>.

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

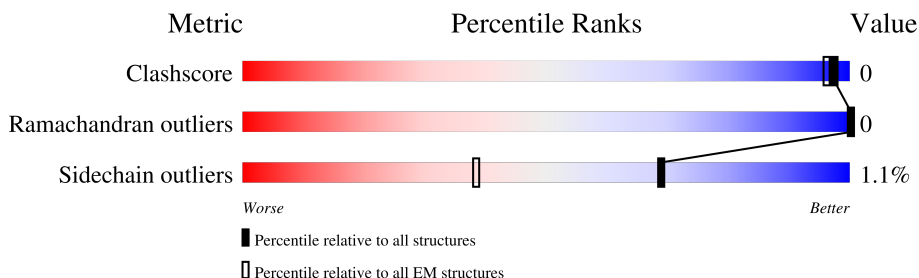
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

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

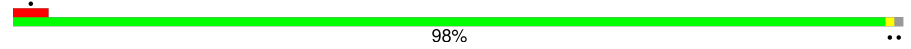
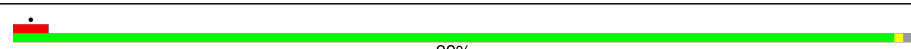

The reported resolution of this entry is 2.34 Å.

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



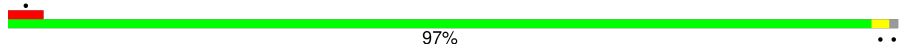
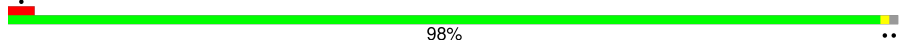
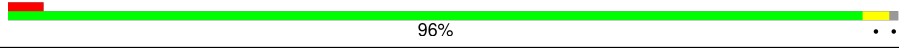
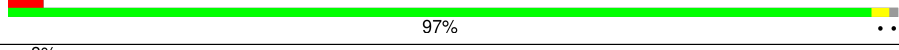



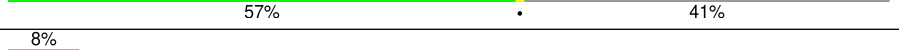
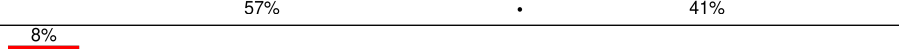
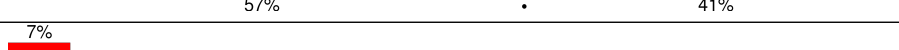

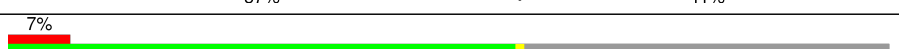


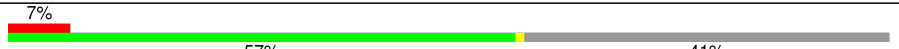

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	PM	141	 98% ..
1	PN	141	 97% ..
1	PO	141	 97% ..
1	PP	141	 98% ..
1	PQ	141	 98% ..
1	PR	141	 97% ..
1	PS	141	 99% ..
1	PT	141	 98% ..

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Mol	Chain	Length	Quality of chain
1	PU	141	 97%
1	PV	141	 98%
1	PW	141	 96%
1	PX	141	 97%
2	PA	675	 8% 57% 41%
2	PB	675	 7% 56% 41%
2	PC	675	 7% 57% 41%
2	PD	675	 7% 57% 41%
2	PE	675	 8% 57% 41%
2	PF	675	 8% 57% 41%
2	PG	675	 7% 57% 41%
2	PH	675	 7% 57% 41%
2	PI	675	 7% 57% 41%
2	PJ	675	 7% 57% 41%
2	PK	675	 8% 57% 41%
2	PL	675	 7% 57% 41%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 50328 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 HK97 gp6-like/SPP1 gp15-like head-tail connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	PX	140	1087	666	184	235	2	0	0
1	PM	140	1087	666	184	235	2	0	0
1	PN	140	1087	666	184	235	2	0	0
1	PO	140	1087	666	184	235	2	0	0
1	PP	140	1087	666	184	235	2	0	0
1	PQ	140	1087	666	184	235	2	0	0
1	PR	140	1087	666	184	235	2	0	0
1	PS	140	1087	666	184	235	2	0	0
1	PT	140	1087	666	184	235	2	0	0
1	PU	140	1087	666	184	235	2	0	0
1	PV	140	1087	666	184	235	2	0	0
1	PW	140	1087	666	184	235	2	0	0

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P S		
2	PA	396	3106	1925	528	640	3 10	0	0
2	PB	396	3106	1925	528	640	3 10	0	0
2	PC	396	3106	1925	528	640	3 10	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
2	PD	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PE	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PF	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PG	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PH	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PI	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PJ	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PK	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0
2	PL	396	Total 3106	C 1925	N 528	O 640	P 3	S 10	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	PX	1	Total 1	Mg 1	0
3	PM	1	Total 1	Mg 1	0
3	PN	1	Total 1	Mg 1	0
3	PO	1	Total 1	Mg 1	0
3	PP	1	Total 1	Mg 1	0
3	PQ	1	Total 1	Mg 1	0
3	PR	1	Total 1	Mg 1	0
3	PS	1	Total 1	Mg 1	0
3	PT	1	Total 1	Mg 1	0
3	PU	1	Total 1	Mg 1	0

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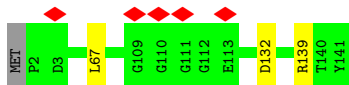
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
3	PV	1	Total 1	Mg 1	0
3	PW	1	Total 1	Mg 1	0

### 3 Residue-property plots [i](#)

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

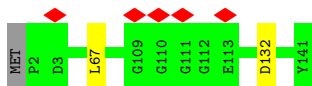
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PX:  97%



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PM:  98%



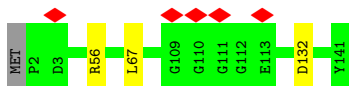
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PN:  97%



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PO:  97%

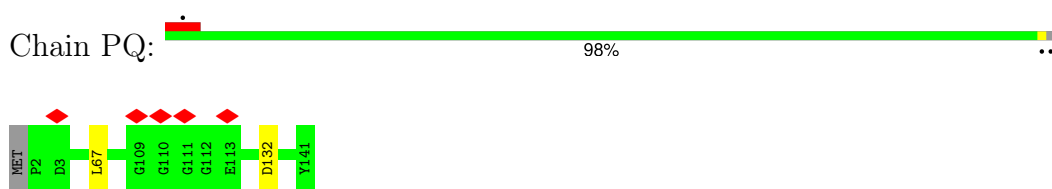


- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

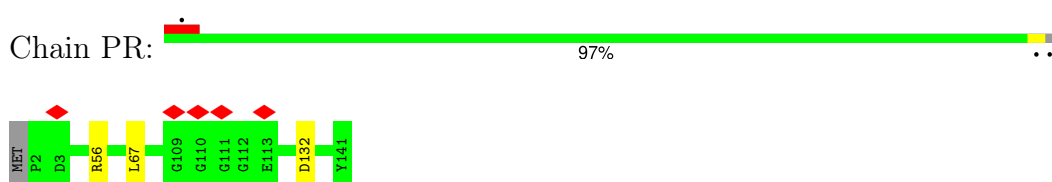
Chain PP:  98%



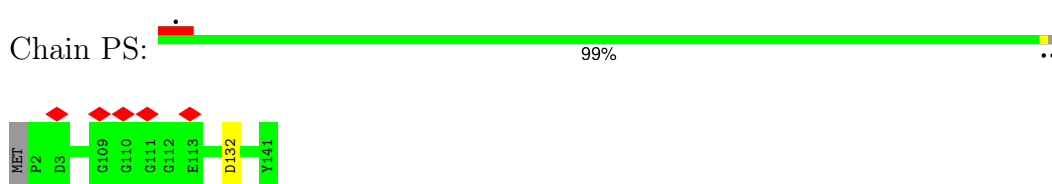
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector



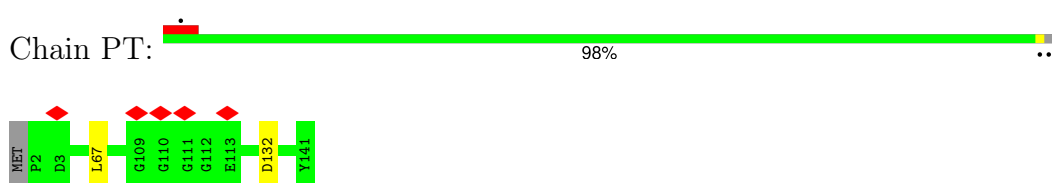
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector



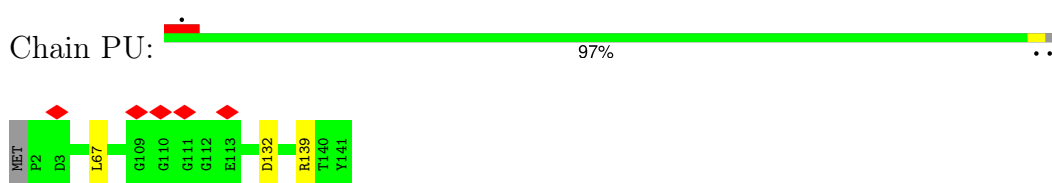
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector



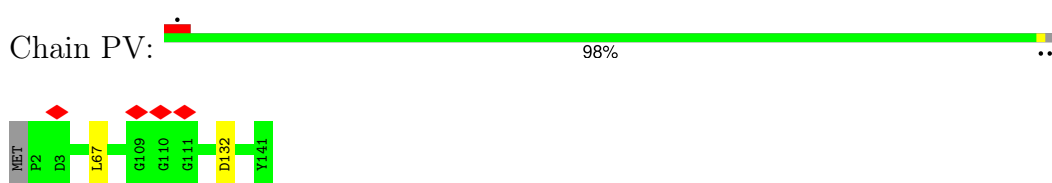
- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector



- Molecule 1: HK97 gp6-like/SPP1 gp15-like head-tail connector

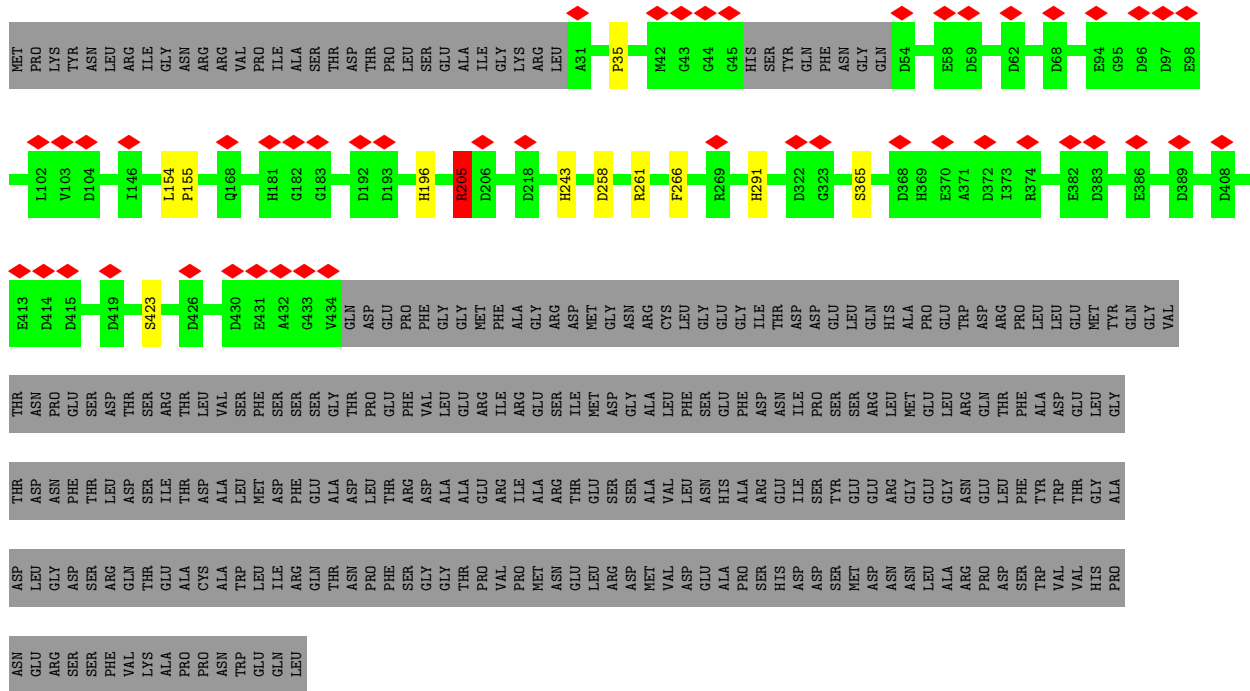




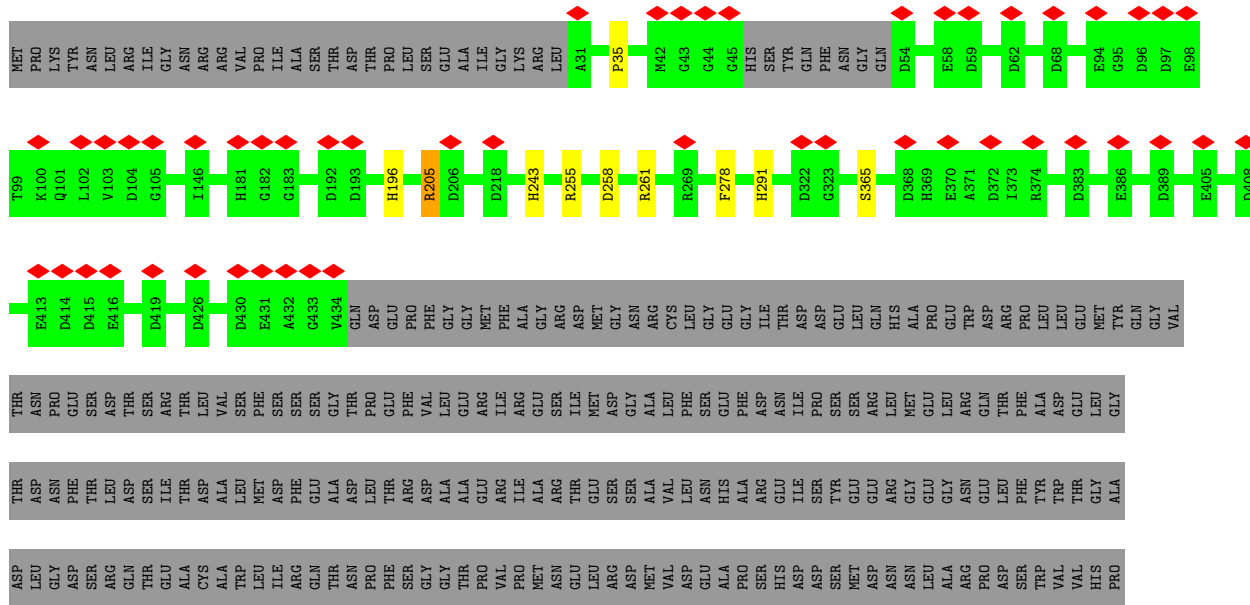


TRP VAL VAL HIS PRO ASN ASN ARG SER SER PHE VAL VAL LYS LYS LYS ALA PRO PRO ASN ASN ASP TRP TRP TRP TRP

● Molecule 2: Portal protein

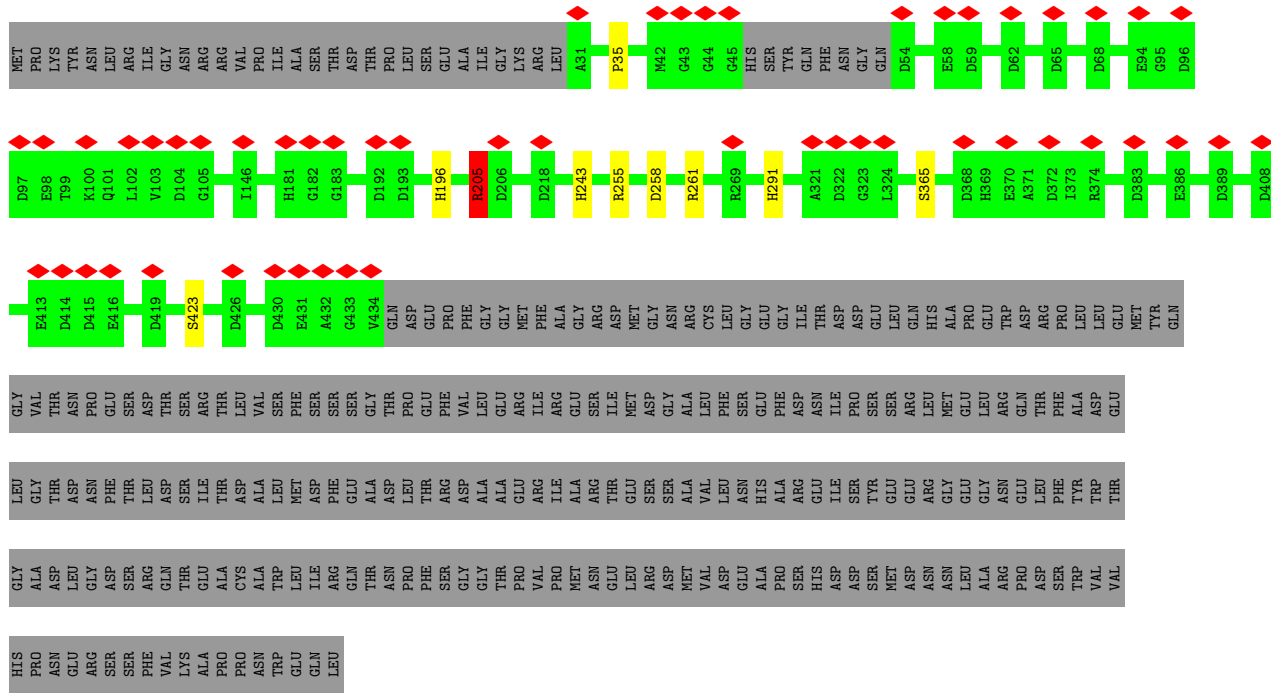


● Molecule 2: Portal protein

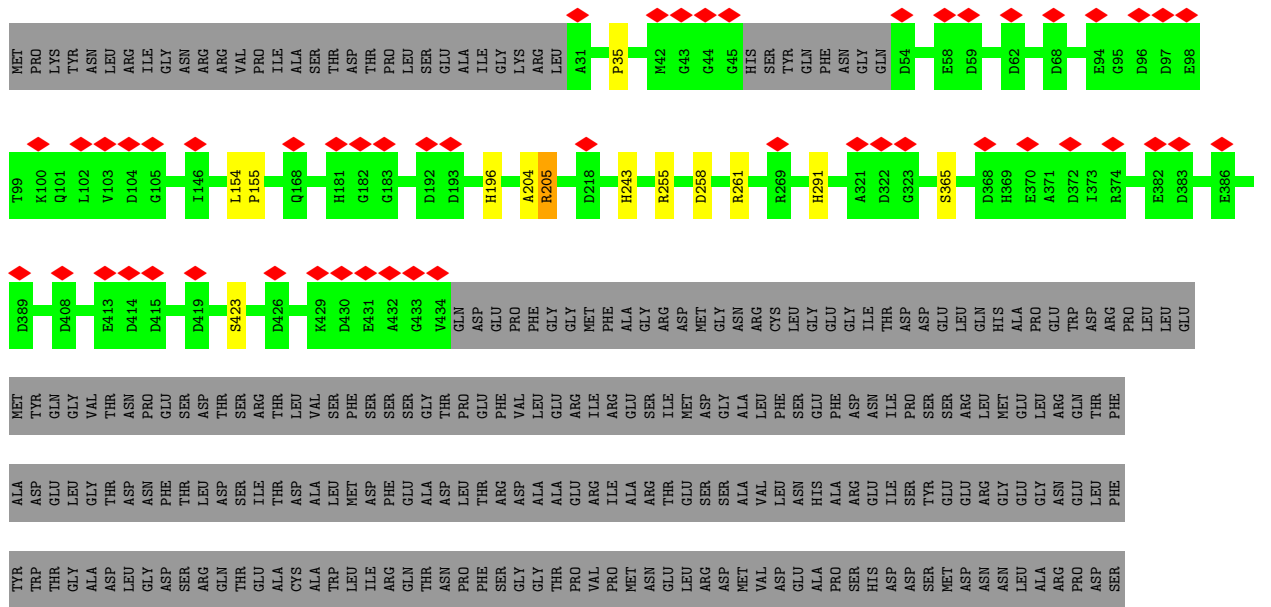


ASN  
GLU  
ARG  
SER  
ASN  
PHE  
VAL  
LYS  
ALA  
PRO  
PRO  
TRP  
ASP  
GLU  
GLN  
LEU

• Molecule 2: Portal protein



• Molecule 2: Portal protein







VAL	HIS	PRO	ASN	GLU	ARG	SER	THR	ASP	PHE	VAL	LYS	ALA	PRO	ASN	TRP	GLU	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 2: Portal protein



MET	PRO	LYS	TYR	ASN	GLU	ARG	SER	THR	ASP	PHE	VAL	LYS	ALA	PRO	ASN	TRP	GLU	LEU	A31	P35	M42	G43	G44	G45	HIS	SER	TYR	GLN	PHE	ASN	GLY	D54	E58	D59	D62	D68	D96	D97	E98	T99	K100						
Q101	L102	V103	D104	G105	I146	H181	G182	G183	D192	D193	H196	R205	D206	D218	H243	R255	D258	R269	H291	A321	D322	G323	L324	S365	D368	H369	E370	A371	D372	I373	R374	D383	E386	D389	E405	D408	E413	D414	D415								
E416	D419	S423	D426	D430	E431	A432	G433	V434	GLN	ASP	GLU	PHE	GLY	MET	PHE	ALA	GLY	ARG	ILE	ARG	GLY	ASP	ASN	ARG	VAL	LEU	GLN	HIS	ALA	PRO	GLY	TRP	ASP	ARG	GLN	THR	PHE	LEU	ASP	GLU	LEU	TYR	GLY	VAL	THR	ASN	
PRO	GLU	SER	THR	SER	THR	ARG	THR	LEU	THR	VAL	GLU	PHE	VAL	GLY	LEU	GLU	MET	ILE	ARG	GLY	ASP	ASN	ARG	VAL	LEU	GLN	HIS	ALA	PRO	GLY	TRP	ASP	ARG	GLN	THR	PHE	LEU	ASP	GLU	LEU	TYR	GLY	VAL	THR	ASP		
ASN	PHE	THR	LEU	ASN	SER	ILE	THR	ASP	THR	ALA	ALA	TRP	LEU	MET	PHE	ASP	GLY	THR	ALA	GLY	THR	ILE	ARG	ALA	VAL	LEU	ASN	ARG	GLY	LEU	ALA	GLY	ASN	GLU	THR	PHE	LEU	ASP	GLY	THR	ALA	ASP	THR	ASN			
GLY	ASP	SER	ARG	GLN	THR	THR	ALA	GLU	ARG	GLY	CYS	PRO	ASP	THR	THR	PHE	ARG	GLY	THR	ALA	GLY	THR	PRO	VAL	LEU	GLN	HIS	ALA	PRO	GLY	TRP	ASP	ARG	VAL	LEU	ASP	THR	PHE	LEU	ASP	GLY	THR	ALA	ASP			
ARG	SER	PHE	VAL	LYS	ALA	PRO	PRO	GLY	THR	VAL	PRO	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

• Molecule 2: Portal protein



MET	PRO	TYR	ASN	LEU	ARG	ILE	GLY	ASN	GLY	ASN	TRP	ARG	VAL	PRO	ILE	ALA	ALA	THR	ASN	THR	THR	THR	THR	A31	P35	M42	G43	G44	G45	HIS	SER	TYR	GLN	PHE	ASN	GLY	D54	E58	D59	D62	D68	E94	G95	D96	D97	E98				
T99	K100	Q101	L102	V103	D104	G105	Q168	H181	G182	G183	D192	D193	H196	R205	D206	D218	H243	R255	R269	H291	D322	G323	S365	E370	A371	D372	I373	R374	E382	D383	E386	D389	D408	E413	D414	D415	D419	S423												
D426	D430	E431	A432	G433	V434	GLN	ASP	GLU	PRO	PHE	GLY	MET	PHE	ALA	GLY	ARG	ILE	ARG	GLY	ASP	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
ARG	THR	LEU	VAL	SER	LEU	THR	THR	PRO	THR	PHE	VAL	GLY	THR	GLY	ALA	GLY	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ILE	THR	ASP	ALA	LEU	MET	ASP	THR	THR	ARG	ARG	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLU	ALA	CYS	ALA	TRP	LEU	ILE	ARG	GLY	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

ALA  
PRO  
PHE  
ASN  
TRP  
GLU  
GLN  
LEU

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	165198	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, 54.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size ( $\text{\AA}$ )	412.19202, 412.19202, 412.19202	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.171, 1.171, 1.171	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: HIP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	PM	0.36	0/1105	0.78	0/1492
1	PN	0.36	0/1105	0.76	0/1492
1	PO	0.36	0/1105	0.79	1/1492 (0.1%)
1	PP	0.36	0/1105	0.76	0/1492
1	PQ	0.36	0/1105	0.76	0/1492
1	PR	0.36	0/1105	0.76	1/1492 (0.1%)
1	PS	0.35	0/1105	0.76	0/1492
1	PT	0.35	0/1105	0.76	0/1492
1	PU	0.36	0/1105	0.76	0/1492
1	PV	0.36	0/1105	0.77	0/1492
1	PW	0.35	0/1105	0.76	0/1492
1	PX	0.35	0/1105	0.77	0/1492
2	PA	0.32	0/3117	0.70	3/4226 (0.1%)
2	PB	0.32	0/3117	0.71	3/4226 (0.1%)
2	PC	0.32	0/3117	0.70	3/4226 (0.1%)
2	PD	0.32	0/3117	0.70	3/4226 (0.1%)
2	PE	0.32	0/3117	0.71	3/4226 (0.1%)
2	PF	0.32	0/3117	0.71	3/4226 (0.1%)
2	PG	0.32	0/3117	0.71	3/4226 (0.1%)
2	PH	0.32	0/3117	0.71	3/4226 (0.1%)
2	PI	0.32	0/3117	0.71	3/4226 (0.1%)
2	PJ	0.32	0/3117	0.71	3/4226 (0.1%)
2	PK	0.32	0/3117	0.71	3/4226 (0.1%)
2	PL	0.32	0/3117	0.71	3/4226 (0.1%)
All	All	0.33	0/50664	0.72	38/68616 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	PJ	205	ARG	NE-CZ-NH1	-9.44	115.58	120.30
2	PA	205	ARG	NE-CZ-NH1	-8.76	115.92	120.30
2	PL	205	ARG	NE-CZ-NH1	-8.70	115.95	120.30
2	PG	205	ARG	NE-CZ-NH1	-8.41	116.10	120.30
2	PB	205	ARG	NE-CZ-NH1	-8.23	116.19	120.30
2	PK	205	ARG	NE-CZ-NH1	-8.18	116.21	120.30
2	PC	205	ARG	NE-CZ-NH1	-8.08	116.26	120.30
2	PL	205	ARG	CG-CD-NE	8.03	128.66	111.80
2	PK	205	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	PL	205	ARG	NE-CZ-NH2	7.94	124.27	120.30
2	PI	205	ARG	NE-CZ-NH1	-7.89	116.36	120.30
2	PK	205	ARG	CG-CD-NE	7.74	128.06	111.80
2	PI	205	ARG	CG-CD-NE	7.72	128.02	111.80
2	PH	205	ARG	NE-CZ-NH1	-7.72	116.44	120.30
2	PE	205	ARG	NE-CZ-NH1	-7.69	116.45	120.30
2	PJ	205	ARG	NE-CZ-NH2	7.65	124.13	120.30
2	PG	205	ARG	CG-CD-NE	7.65	127.86	111.80
2	PC	205	ARG	CG-CD-NE	7.59	127.75	111.80
2	PH	205	ARG	CG-CD-NE	7.58	127.73	111.80
2	PA	205	ARG	NE-CZ-NH2	7.58	124.09	120.30
2	PJ	205	ARG	CG-CD-NE	7.54	127.62	111.80
2	PB	205	ARG	CG-CD-NE	7.50	127.56	111.80
2	PE	205	ARG	CG-CD-NE	7.41	127.36	111.80
2	PD	205	ARG	CG-CD-NE	7.40	127.34	111.80
2	PF	205	ARG	CG-CD-NE	7.35	127.24	111.80
2	PF	205	ARG	NE-CZ-NH1	-7.31	116.65	120.30
2	PA	205	ARG	CG-CD-NE	7.27	127.06	111.80
2	PE	205	ARG	NE-CZ-NH2	7.19	123.89	120.30
2	PI	205	ARG	NE-CZ-NH2	7.08	123.84	120.30
2	PB	205	ARG	NE-CZ-NH2	7.02	123.81	120.30
2	PD	205	ARG	NE-CZ-NH1	-6.95	116.83	120.30
2	PH	205	ARG	NE-CZ-NH2	6.81	123.71	120.30
2	PC	205	ARG	NE-CZ-NH2	6.71	123.65	120.30
2	PG	205	ARG	NE-CZ-NH2	6.69	123.64	120.30
2	PF	205	ARG	NE-CZ-NH2	6.49	123.54	120.30
2	PD	205	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	PR	56	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	PO	56	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	PM	1087	0	1018	2	0
1	PN	1087	0	1018	2	0
1	PO	1087	0	1018	2	0
1	PP	1087	0	1018	2	0
1	PQ	1087	0	1018	2	0
1	PR	1087	0	1018	1	0
1	PS	1087	0	1018	0	0
1	PT	1087	0	1018	2	0
1	PU	1087	0	1018	2	0
1	PV	1087	0	1018	2	0
1	PW	1087	0	1018	2	0
1	PX	1087	0	1018	2	0
2	PA	3106	0	2942	6	0
2	PB	3106	0	2942	7	0
2	PC	3106	0	2942	5	0
2	PD	3106	0	2942	4	0
2	PE	3106	0	2942	3	0
2	PF	3106	0	2942	5	0
2	PG	3106	0	2942	5	0
2	PH	3106	0	2943	4	0
2	PI	3106	0	2943	3	0
2	PJ	3106	0	2942	4	0
2	PK	3106	0	2942	2	0
2	PL	3106	0	2942	1	0
3	PM	1	0	0	0	0
3	PN	1	0	0	0	0
3	PO	1	0	0	0	0
3	PP	1	0	0	0	0
3	PQ	1	0	0	0	0
3	PR	1	0	0	0	0
3	PS	1	0	0	0	0
3	PT	1	0	0	0	0
3	PU	1	0	0	0	0
3	PV	1	0	0	0	0
3	PW	1	0	0	0	0
3	PX	1	0	0	0	0
All	All	50328	0	47522	45	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 0.

All (45) 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)
2:PG:35:PRO:HB2	2:PG:205:ARG:HH12	1.73	0.53
2:PE:35:PRO:HB2	2:PE:205:ARG:HH12	1.73	0.53
2:PF:258:ASP:HA	1:PM:67:LEU:HD21	1.93	0.51
2:PH:35:PRO:HB2	2:PH:205:ARG:HH12	1.75	0.51
1:PX:67:LEU:HD21	2:PE:258:ASP:HA	1.92	0.51
2:PF:35:PRO:HB2	2:PF:205:ARG:HH12	1.77	0.50
2:PG:258:ASP:HA	1:PN:67:LEU:HD21	1.95	0.49
2:PB:35:PRO:HB2	2:PB:205:ARG:HH12	1.76	0.49
2:PI:258:ASP:HA	1:PP:67:LEU:HD21	1.94	0.49
2:PD:258:ASP:HA	1:PW:67:LEU:HD21	1.95	0.49
2:PH:261:ARG:HD2	1:PO:67:LEU:HD23	1.95	0.49
2:PL:35:PRO:HB2	2:PL:205:ARG:HH12	1.78	0.48
2:PC:35:PRO:HB2	2:PC:205:ARG:HH12	1.78	0.48
2:PK:258:ASP:HA	1:PR:67:LEU:HD21	1.95	0.48
2:PJ:35:PRO:HB2	2:PJ:205:ARG:HH12	1.77	0.48
2:PH:258:ASP:HA	1:PO:67:LEU:HD21	1.96	0.47
2:PK:35:PRO:HB2	2:PK:205:ARG:HH12	1.79	0.47
2:PB:258:ASP:HA	1:PU:67:LEU:HD21	1.96	0.47
2:PB:87:GLU:HG3	2:PB:380:PRO:HA	1.97	0.47
2:PA:35:PRO:HB2	2:PA:205:ARG:HH12	1.79	0.47
2:PC:261:ARG:HD2	1:PV:67:LEU:HD23	1.96	0.46
2:PI:35:PRO:HB2	2:PI:205:ARG:HH12	1.81	0.46
2:PA:205:ARG:HG2	2:PA:205:ARG:HH21	1.82	0.45
2:PJ:258:ASP:HA	1:PQ:67:LEU:HD21	1.99	0.44
2:PD:261:ARG:HD2	1:PW:67:LEU:HD23	2.00	0.43
2:PG:261:ARG:HD2	1:PN:67:LEU:HD23	2.00	0.43
2:PD:35:PRO:HB2	2:PD:205:ARG:HH12	1.82	0.43
2:PI:261:ARG:HD2	1:PP:67:LEU:HD23	2.00	0.43
2:PA:205:ARG:HD2	2:PB:155:PRO:O	2.19	0.43
2:PA:261:ARG:HD2	1:PT:67:LEU:HD23	2.00	0.43
2:PB:261:ARG:HD2	1:PU:67:LEU:HD23	2.01	0.43
2:PG:204:ALA:HB3	2:PH:155:PRO:HG2	2.02	0.42
2:PF:204:ALA:HB3	2:PG:155:PRO:HG2	2.02	0.42
2:PJ:261:ARG:HD2	1:PQ:67:LEU:HD23	2.02	0.42
2:PA:258:ASP:HA	1:PT:67:LEU:HD21	2.02	0.41
2:PA:154:LEU:HA	2:PA:155:PRO:HD2	1.97	0.41
2:PF:154:LEU:HA	2:PF:155:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:67:LEU:HD23	2:PE:261:ARG:HD2	2.03	0.41
2:PB:154:LEU:HA	2:PB:155:PRO:HD2	1.98	0.41
2:PC:154:LEU:HA	2:PC:155:PRO:HD2	1.98	0.41
2:PC:266:PHE:HB2	2:PD:278:PHE:HE1	1.86	0.41
2:PF:261:ARG:HD2	1:PM:67:LEU:HD23	2.03	0.41
2:PB:87:GLU:HB3	2:PB:378:ASN:HB2	2.02	0.40
2:PJ:77:MET:HB3	2:PJ:134:TRP:CZ2	2.57	0.40
2:PC:258:ASP:HA	1:PV:67:LEU:HD21	2.03	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	PM	138/141 (98%)	130 (94%)	8 (6%)	0	100	100
1	PN	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
1	PO	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
1	PP	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
1	PQ	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
1	PR	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
1	PS	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
1	PT	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
1	PU	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
1	PV	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
1	PW	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
1	PX	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
2	PA	389/675 (58%)	383 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	PB	389/675 (58%)	385 (99%)	4 (1%)	0	100	100
2	PC	389/675 (58%)	383 (98%)	6 (2%)	0	100	100
2	PD	389/675 (58%)	383 (98%)	6 (2%)	0	100	100
2	PE	389/675 (58%)	383 (98%)	6 (2%)	0	100	100
2	PF	389/675 (58%)	382 (98%)	7 (2%)	0	100	100
2	PG	389/675 (58%)	383 (98%)	6 (2%)	0	100	100
2	PH	389/675 (58%)	384 (99%)	5 (1%)	0	100	100
2	PI	389/675 (58%)	382 (98%)	7 (2%)	0	100	100
2	PJ	389/675 (58%)	383 (98%)	6 (2%)	0	100	100
2	PK	389/675 (58%)	383 (98%)	6 (2%)	0	100	100
2	PL	389/675 (58%)	385 (99%)	4 (1%)	0	100	100
All	All	6324/9792 (65%)	6195 (98%)	129 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PM	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PN	116/117 (99%)	114 (98%)	2 (2%)	56	68
1	PO	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PP	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PQ	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PR	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PS	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PT	116/117 (99%)	115 (99%)	1 (1%)	75	85
1	PU	116/117 (99%)	114 (98%)	2 (2%)	56	68
1	PV	116/117 (99%)	115 (99%)	1 (1%)	75	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PW	116/117 (99%)	113 (97%)	3 (3%)	41	51
1	PX	116/117 (99%)	114 (98%)	2 (2%)	56	68
2	PA	327/568 (58%)	323 (99%)	4 (1%)	67	79
2	PB	327/568 (58%)	323 (99%)	4 (1%)	67	79
2	PC	327/568 (58%)	324 (99%)	3 (1%)	75	85
2	PD	327/568 (58%)	325 (99%)	2 (1%)	84	90
2	PE	327/568 (58%)	323 (99%)	4 (1%)	67	79
2	PF	327/568 (58%)	324 (99%)	3 (1%)	75	85
2	PG	327/568 (58%)	325 (99%)	2 (1%)	84	90
2	PH	327/568 (58%)	325 (99%)	2 (1%)	84	90
2	PI	327/568 (58%)	324 (99%)	3 (1%)	75	85
2	PJ	327/568 (58%)	323 (99%)	4 (1%)	67	79
2	PK	327/568 (58%)	323 (99%)	4 (1%)	67	79
2	PL	327/568 (58%)	323 (99%)	4 (1%)	67	79
All	All	5316/8220 (65%)	5260 (99%)	56 (1%)	69	81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	PX	132	ASP
1	PX	139	ARG
2	PA	205	ARG
2	PA	255	ARG
2	PA	365	SER
2	PA	423	SER
2	PB	205	ARG
2	PB	255	ARG
2	PB	365	SER
2	PB	423	SER
2	PC	205	ARG
2	PC	365	SER
2	PC	423	SER
2	PD	255	ARG
2	PD	365	SER
2	PE	205	ARG
2	PE	255	ARG
2	PE	365	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	PE	423	SER
2	PF	255	ARG
2	PF	365	SER
2	PF	423	SER
2	PG	255	ARG
2	PG	365	SER
2	PH	255	ARG
2	PH	365	SER
2	PI	205	ARG
2	PI	255	ARG
2	PI	365	SER
2	PJ	205	ARG
2	PJ	255	ARG
2	PJ	365	SER
2	PJ	423	SER
2	PK	205	ARG
2	PK	255	ARG
2	PK	365	SER
2	PK	423	SER
2	PL	205	ARG
2	PL	255	ARG
2	PL	365	SER
2	PL	423	SER
1	PM	132	ASP
1	PN	129	VAL
1	PN	132	ASP
1	PO	132	ASP
1	PP	132	ASP
1	PQ	132	ASP
1	PR	132	ASP
1	PS	132	ASP
1	PT	132	ASP
1	PU	132	ASP
1	PU	139	ARG
1	PV	132	ASP
1	PW	2	PRO
1	PW	132	ASP
1	PW	139	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:



Mol	Chain	Res	Type
2	PA	392	GLN
2	PB	392	GLN
2	PC	392	GLN
2	PD	392	GLN
2	PE	392	GLN
2	PF	392	GLN
2	PG	392	GLN
2	PH	392	GLN
2	PI	232	GLN
2	PI	392	GLN
2	PJ	392	GLN
2	PK	232	GLN
2	PK	392	GLN
2	PL	232	GLN
2	PL	392	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

36 non-standard protein/DNA/RNA residues 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
2	HIP	PA	196	2	11,14,15	2.08	3 (27%)	7,20,22	1.13	0
2	HIP	PC	291	2	11,14,15	1.91	3 (27%)	7,20,22	1.07	1 (14%)
2	HIP	PC	196	2	11,14,15	2.15	3 (27%)	7,20,22	1.15	0
2	HIP	PH	291	2	11,14,15	1.80	3 (27%)	7,20,22	1.05	0
2	HIP	PA	291	2	11,14,15	1.75	3 (27%)	7,20,22	1.00	0
2	HIP	PE	196	2	11,14,15	2.15	3 (27%)	7,20,22	1.14	0
2	HIP	PI	291	2	11,14,15	1.90	3 (27%)	7,20,22	1.06	0
2	HIP	PF	243	2	11,14,15	2.23	4 (36%)	7,20,22	1.38	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HIP	PH	243	2	11,14,15	2.17	4 (36%)	7,20,22	1.39	2 (28%)
2	HIP	PL	243	2	11,14,15	2.08	4 (36%)	7,20,22	1.36	1 (14%)
2	HIP	PD	243	2	11,14,15	2.06	4 (36%)	7,20,22	1.37	2 (28%)
2	HIP	PL	291	2	11,14,15	1.90	3 (27%)	7,20,22	1.01	1 (14%)
2	HIP	PB	243	2	11,14,15	2.16	4 (36%)	7,20,22	1.36	2 (28%)
2	HIP	PD	291	2	11,14,15	1.91	3 (27%)	7,20,22	1.00	0
2	HIP	PG	243	2	11,14,15	2.20	4 (36%)	7,20,22	1.29	2 (28%)
2	HIP	PJ	291	2	11,14,15	1.84	3 (27%)	7,20,22	1.06	1 (14%)
2	HIP	PH	196	2	11,14,15	2.08	3 (27%)	7,20,22	1.12	0
2	HIP	PC	243	2	11,14,15	2.11	3 (27%)	7,20,22	1.37	1 (14%)
2	HIP	PK	243	2	11,14,15	2.21	4 (36%)	7,20,22	1.25	1 (14%)
2	HIP	PK	291	2	11,14,15	1.87	3 (27%)	7,20,22	1.16	0
2	HIP	PL	196	2	11,14,15	2.11	2 (18%)	7,20,22	1.13	0
2	HIP	PF	196	2	11,14,15	2.09	3 (27%)	7,20,22	1.16	0
2	HIP	PD	196	2	11,14,15	2.15	3 (27%)	7,20,22	1.13	0
2	HIP	PI	243	2	11,14,15	2.15	3 (27%)	7,20,22	1.34	1 (14%)
2	HIP	PJ	196	2	11,14,15	2.07	3 (27%)	7,20,22	1.15	0
2	HIP	PK	196	2	11,14,15	2.09	3 (27%)	7,20,22	1.16	0
2	HIP	PF	291	2	11,14,15	1.91	3 (27%)	7,20,22	1.09	0
2	HIP	PG	196	2	11,14,15	2.11	3 (27%)	7,20,22	1.17	0
2	HIP	PA	243	2	11,14,15	2.14	4 (36%)	7,20,22	1.35	2 (28%)
2	HIP	PG	291	2	11,14,15	1.87	3 (27%)	7,20,22	1.05	0
2	HIP	PJ	243	2	11,14,15	2.18	3 (27%)	7,20,22	1.35	1 (14%)
2	HIP	PI	196	2	11,14,15	2.03	3 (27%)	7,20,22	1.13	0
2	HIP	PE	243	2	11,14,15	2.19	4 (36%)	7,20,22	1.40	2 (28%)
2	HIP	PB	291	2	11,14,15	1.95	3 (27%)	7,20,22	1.09	0
2	HIP	PB	196	2	11,14,15	2.13	3 (27%)	7,20,22	1.14	0
2	HIP	PE	291	2	11,14,15	1.86	3 (27%)	7,20,22	1.06	0

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
2	HIP	PA	196	2	-	2/5/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIP	PC	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PC	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PH	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PA	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PE	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PI	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PF	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PH	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PL	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PD	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PL	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PB	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PD	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PG	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PJ	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PH	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PC	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PK	243	2	-	1/5/12/14	0/1/1/1
2	HIP	PK	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PL	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PF	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PD	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PI	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PJ	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PK	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PF	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PG	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PA	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PG	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PJ	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PI	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PE	243	2	-	2/5/12/14	0/1/1/1
2	HIP	PB	291	2	-	1/5/12/14	0/1/1/1
2	HIP	PB	196	2	-	2/5/12/14	0/1/1/1
2	HIP	PE	291	2	-	1/5/12/14	0/1/1/1

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	PC	196	HIP	CG-ND1	5.39	1.44	1.37
2	PD	196	HIP	CG-ND1	5.32	1.44	1.37
2	PE	196	HIP	CG-ND1	5.31	1.44	1.37
2	PG	196	HIP	CG-ND1	5.31	1.44	1.37
2	PF	243	HIP	CG-ND1	5.27	1.44	1.37
2	PB	196	HIP	CG-ND1	5.19	1.44	1.37
2	PA	196	HIP	CG-ND1	5.17	1.44	1.37
2	PK	196	HIP	CG-ND1	5.16	1.44	1.37
2	PJ	196	HIP	CG-ND1	5.15	1.44	1.37
2	PF	196	HIP	CG-ND1	5.07	1.44	1.37
2	PL	196	HIP	CG-ND1	5.04	1.44	1.37
2	PH	196	HIP	CG-ND1	5.02	1.44	1.37
2	PB	243	HIP	CG-ND1	4.99	1.44	1.37
2	PE	243	HIP	CG-ND1	4.98	1.44	1.37
2	PI	196	HIP	CG-ND1	4.93	1.44	1.37
2	PG	243	HIP	CG-ND1	4.92	1.44	1.37
2	PH	243	HIP	CG-ND1	4.78	1.43	1.37
2	PK	243	HIP	CG-ND1	4.65	1.43	1.37
2	PL	291	HIP	CG-ND1	4.61	1.43	1.37
2	PJ	243	HIP	CG-ND1	4.61	1.43	1.37
2	PD	291	HIP	CG-ND1	4.60	1.43	1.37
2	PI	243	HIP	CG-ND1	4.58	1.43	1.37
2	PB	291	HIP	CG-ND1	4.54	1.43	1.37
2	PF	291	HIP	CG-ND1	4.53	1.43	1.37
2	PC	243	HIP	CG-ND1	4.52	1.43	1.37
2	PC	291	HIP	CG-ND1	4.48	1.43	1.37
2	PE	291	HIP	CG-ND1	4.46	1.43	1.37
2	PA	243	HIP	CG-ND1	4.45	1.43	1.37
2	PG	291	HIP	CG-ND1	4.40	1.43	1.37
2	PD	243	HIP	CG-ND1	4.38	1.43	1.37
2	PJ	291	HIP	CG-ND1	4.37	1.43	1.37
2	PK	291	HIP	CG-ND1	4.36	1.43	1.37
2	PI	291	HIP	CG-ND1	4.34	1.43	1.37
2	PL	243	HIP	CG-ND1	4.29	1.43	1.37
2	PJ	243	HIP	P-O1P	4.27	1.51	1.47
2	PK	243	HIP	P-O1P	4.27	1.51	1.47
2	PA	291	HIP	CG-ND1	4.20	1.43	1.37
2	PI	243	HIP	P-O1P	4.19	1.51	1.47
2	PH	291	HIP	CG-ND1	4.19	1.43	1.37
2	PA	243	HIP	P-O1P	4.06	1.50	1.47
2	PL	243	HIP	P-O1P	4.04	1.50	1.47
2	PC	243	HIP	P-O1P	4.02	1.50	1.47
2	PG	243	HIP	P-O1P	3.90	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	PL	196	HIP	P-O1P	3.83	1.50	1.47
2	PE	243	HIP	P-O1P	3.75	1.50	1.47
2	PH	243	HIP	P-O1P	3.68	1.50	1.47
2	PD	243	HIP	P-O1P	3.64	1.50	1.47
2	PD	196	HIP	P-O1P	3.59	1.50	1.47
2	PC	196	HIP	P-O1P	3.55	1.50	1.47
2	PF	196	HIP	P-O1P	3.55	1.50	1.47
2	PB	243	HIP	P-O1P	3.54	1.50	1.47
2	PE	196	HIP	P-O1P	3.52	1.50	1.47
2	PB	196	HIP	P-O1P	3.52	1.50	1.47
2	PF	243	HIP	P-O1P	3.51	1.50	1.47
2	PH	196	HIP	P-O1P	3.40	1.50	1.47
2	PK	196	HIP	P-O1P	3.39	1.50	1.47
2	PA	196	HIP	P-O1P	3.35	1.50	1.47
2	PI	196	HIP	P-O1P	3.26	1.50	1.47
2	PJ	196	HIP	P-O1P	3.25	1.50	1.47
2	PG	196	HIP	P-O1P	3.18	1.50	1.47
2	PC	291	HIP	P-O3P	-3.13	1.48	1.54
2	PB	291	HIP	P-O3P	-3.09	1.48	1.54
2	PI	291	HIP	P-O3P	-3.06	1.48	1.54
2	PD	291	HIP	P-O3P	-3.02	1.48	1.54
2	PH	291	HIP	P-O3P	-3.01	1.48	1.54
2	PL	291	HIP	P-O3P	-2.99	1.48	1.54
2	PF	291	HIP	P-O3P	-2.98	1.48	1.54
2	PE	291	HIP	P-O3P	-2.96	1.48	1.54
2	PJ	291	HIP	P-O3P	-2.96	1.48	1.54
2	PK	291	HIP	P-O3P	-2.95	1.48	1.54
2	PG	291	HIP	P-O3P	-2.92	1.48	1.54
2	PA	291	HIP	P-O3P	-2.76	1.49	1.54
2	PB	291	HIP	P-O1P	2.72	1.49	1.47
2	PI	291	HIP	P-O1P	2.71	1.49	1.47
2	PF	291	HIP	P-O1P	2.65	1.49	1.47
2	PG	291	HIP	P-O1P	2.61	1.49	1.47
2	PH	243	HIP	P-O3P	-2.58	1.49	1.54
2	PK	291	HIP	P-O1P	2.58	1.49	1.47
2	PK	243	HIP	P-O3P	-2.55	1.49	1.54
2	PF	243	HIP	P-O3P	-2.55	1.49	1.54
2	PC	291	HIP	P-O1P	2.51	1.49	1.47
2	PD	243	HIP	P-O3P	-2.48	1.49	1.54
2	PD	291	HIP	P-O1P	2.48	1.49	1.47
2	PL	291	HIP	P-O1P	2.47	1.49	1.47
2	PG	243	HIP	P-O3P	-2.45	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	PB	243	HIP	P-O3P	-2.44	1.49	1.54
2	PJ	243	HIP	P-O3P	-2.39	1.49	1.54
2	PE	243	HIP	P-O3P	-2.37	1.49	1.54
2	PH	243	HIP	P-O2P	-2.36	1.49	1.54
2	PE	291	HIP	P-O1P	2.36	1.49	1.47
2	PA	243	HIP	P-O3P	-2.36	1.49	1.54
2	PJ	291	HIP	P-O1P	2.34	1.49	1.47
2	PC	243	HIP	P-O3P	-2.32	1.49	1.54
2	PL	243	HIP	P-O3P	-2.29	1.50	1.54
2	PH	196	HIP	P-O2P	-2.28	1.50	1.54
2	PH	291	HIP	P-O1P	2.27	1.49	1.47
2	PI	243	HIP	P-O3P	-2.26	1.50	1.54
2	PE	243	HIP	P-O2P	-2.26	1.50	1.54
2	PE	196	HIP	P-O2P	-2.25	1.50	1.54
2	PI	196	HIP	P-O2P	-2.25	1.50	1.54
2	PA	243	HIP	P-O2P	-2.23	1.50	1.54
2	PF	243	HIP	P-O2P	-2.23	1.50	1.54
2	PB	196	HIP	P-O2P	-2.22	1.50	1.54
2	PD	243	HIP	P-O2P	-2.22	1.50	1.54
2	PF	196	HIP	P-O2P	-2.21	1.50	1.54
2	PD	196	HIP	P-O2P	-2.21	1.50	1.54
2	PG	196	HIP	P-O2P	-2.20	1.50	1.54
2	PB	243	HIP	P-O2P	-2.18	1.50	1.54
2	PK	196	HIP	P-O2P	-2.16	1.50	1.54
2	PJ	196	HIP	P-O2P	-2.14	1.50	1.54
2	PA	291	HIP	P-O1P	2.13	1.49	1.47
2	PG	243	HIP	P-O2P	-2.10	1.50	1.54
2	PA	196	HIP	P-O2P	-2.07	1.50	1.54
2	PL	243	HIP	P-O2P	-2.05	1.50	1.54
2	PK	243	HIP	P-O2P	-2.05	1.50	1.54
2	PC	196	HIP	P-O2P	-2.02	1.50	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	PL	243	HIP	O2P-P-O1P	-2.41	108.70	113.76
2	PC	243	HIP	O2P-P-O1P	-2.41	108.71	113.76
2	PA	243	HIP	O2P-P-O1P	-2.38	108.77	113.76
2	PJ	243	HIP	O2P-P-O1P	-2.37	108.78	113.76
2	PH	243	HIP	O2P-P-O1P	-2.36	108.80	113.76
2	PI	243	HIP	O2P-P-O1P	-2.36	108.81	113.76
2	PD	243	HIP	O2P-P-O1P	-2.35	108.83	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	PE	243	HIP	O2P-P-O1P	-2.34	108.84	113.76
2	PB	243	HIP	O2P-P-O1P	-2.25	109.03	113.76
2	PE	243	HIP	CD2-NE2-CE1	2.17	109.15	105.72
2	PF	243	HIP	O2P-P-O1P	-2.16	109.23	113.76
2	PB	243	HIP	CD2-NE2-CE1	2.09	109.03	105.72
2	PF	243	HIP	CD2-NE2-CE1	2.09	109.03	105.72
2	PH	243	HIP	CD2-NE2-CE1	2.08	109.01	105.72
2	PG	243	HIP	O2P-P-O1P	-2.07	109.42	113.76
2	PK	243	HIP	O2P-P-O1P	-2.06	109.43	113.76
2	PA	243	HIP	CD2-NE2-CE1	2.04	108.94	105.72
2	PD	243	HIP	CD2-NE2-CE1	2.02	108.92	105.72
2	PG	243	HIP	CD2-NE2-CE1	2.02	108.92	105.72
2	PJ	291	HIP	CD2-NE2-CE1	2.02	108.91	105.72
2	PL	291	HIP	CD2-NE2-CE1	2.02	108.91	105.72
2	PC	291	HIP	CD2-NE2-CE1	2.00	108.88	105.72

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	PA	243	HIP	O-C-CA-CB
2	PA	291	HIP	CA-CB-CG-ND1
2	PB	243	HIP	O-C-CA-CB
2	PB	291	HIP	CA-CB-CG-ND1
2	PC	243	HIP	O-C-CA-CB
2	PC	291	HIP	CA-CB-CG-ND1
2	PD	243	HIP	O-C-CA-CB
2	PD	291	HIP	CA-CB-CG-ND1
2	PE	243	HIP	O-C-CA-CB
2	PE	291	HIP	CA-CB-CG-ND1
2	PF	243	HIP	O-C-CA-CB
2	PF	291	HIP	CA-CB-CG-ND1
2	PG	243	HIP	O-C-CA-CB
2	PG	291	HIP	CA-CB-CG-ND1
2	PH	243	HIP	O-C-CA-CB
2	PH	291	HIP	CA-CB-CG-ND1
2	PI	243	HIP	O-C-CA-CB
2	PI	291	HIP	CA-CB-CG-ND1
2	PJ	243	HIP	O-C-CA-CB
2	PJ	291	HIP	CA-CB-CG-ND1
2	PK	291	HIP	CA-CB-CG-ND1
2	PL	243	HIP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	PL	291	HIP	CA-CB-CG-ND1
2	PB	196	HIP	N-CA-CB-CG
2	PC	196	HIP	N-CA-CB-CG
2	PF	196	HIP	N-CA-CB-CG
2	PG	196	HIP	N-CA-CB-CG
2	PH	196	HIP	N-CA-CB-CG
2	PI	196	HIP	N-CA-CB-CG
2	PJ	196	HIP	N-CA-CB-CG
2	PK	196	HIP	N-CA-CB-CG
2	PL	196	HIP	N-CA-CB-CG
2	PA	196	HIP	N-CA-CB-CG
2	PD	196	HIP	N-CA-CB-CG
2	PE	196	HIP	N-CA-CB-CG
2	PA	196	HIP	C-CA-CB-CG
2	PA	243	HIP	CA-CB-CG-ND1
2	PB	196	HIP	C-CA-CB-CG
2	PB	243	HIP	CA-CB-CG-ND1
2	PC	196	HIP	C-CA-CB-CG
2	PC	243	HIP	CA-CB-CG-ND1
2	PD	196	HIP	C-CA-CB-CG
2	PD	243	HIP	CA-CB-CG-ND1
2	PE	196	HIP	C-CA-CB-CG
2	PE	243	HIP	CA-CB-CG-ND1
2	PF	196	HIP	C-CA-CB-CG
2	PF	243	HIP	CA-CB-CG-ND1
2	PG	196	HIP	C-CA-CB-CG
2	PG	243	HIP	CA-CB-CG-ND1
2	PH	196	HIP	C-CA-CB-CG
2	PH	243	HIP	CA-CB-CG-ND1
2	PI	196	HIP	C-CA-CB-CG
2	PI	243	HIP	CA-CB-CG-ND1
2	PJ	196	HIP	C-CA-CB-CG
2	PJ	243	HIP	CA-CB-CG-ND1
2	PK	196	HIP	C-CA-CB-CG
2	PK	243	HIP	CA-CB-CG-ND1
2	PL	196	HIP	C-CA-CB-CG
2	PL	243	HIP	CA-CB-CG-ND1

There are no ring outliers.

No monomer is involved in short contacts.



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

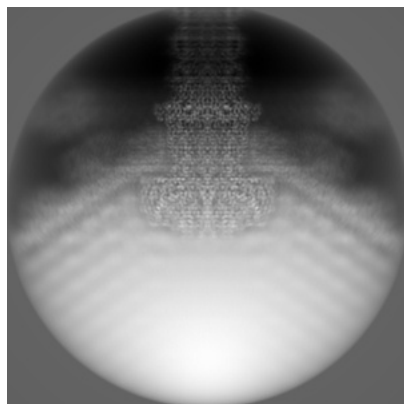
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18599. These allow visual inspection of the internal detail of the map and identification of artifacts.

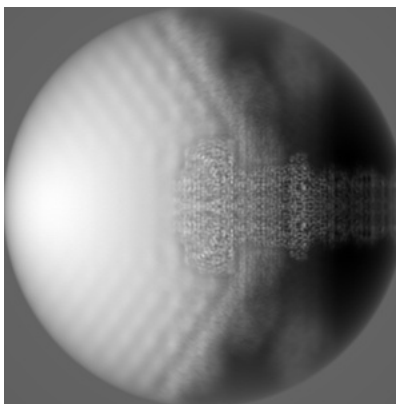
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

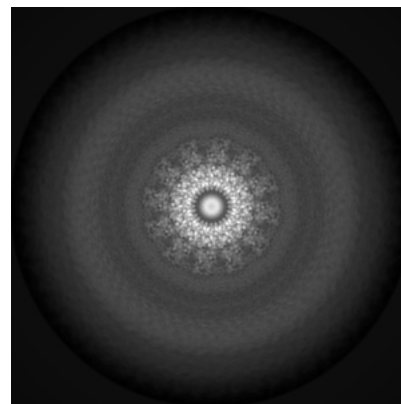
#### 6.1.1 Primary map



X

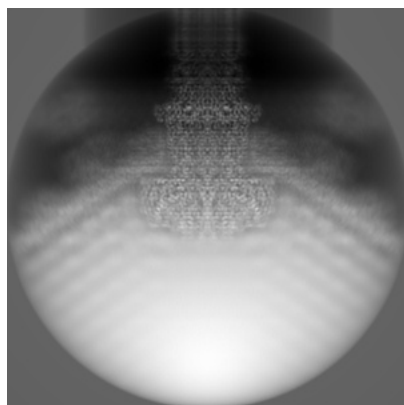


Y

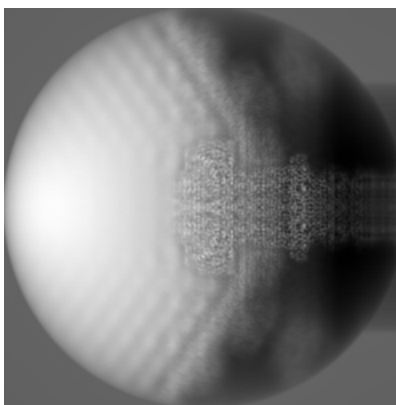


Z

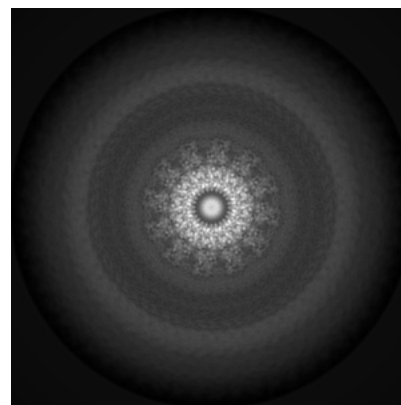
#### 6.1.2 Raw map



X



Y

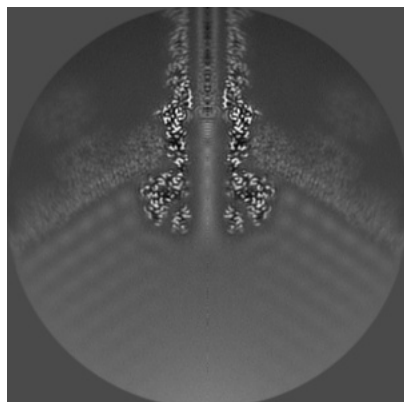


Z

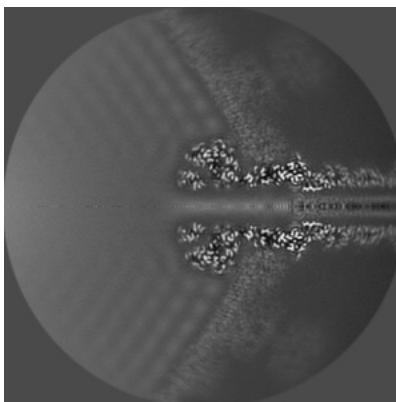
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

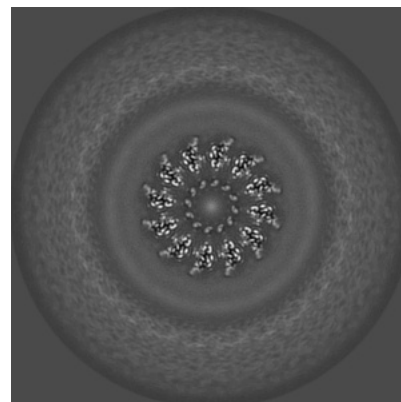
### 6.2.1 Primary map



X Index: 176

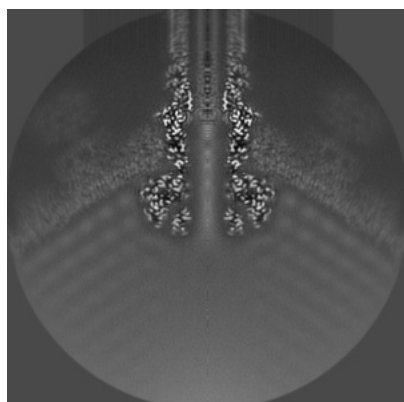


Y Index: 176

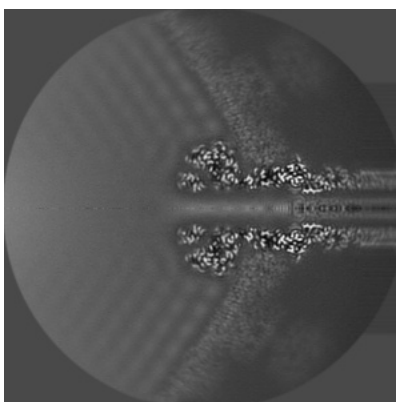


Z Index: 176

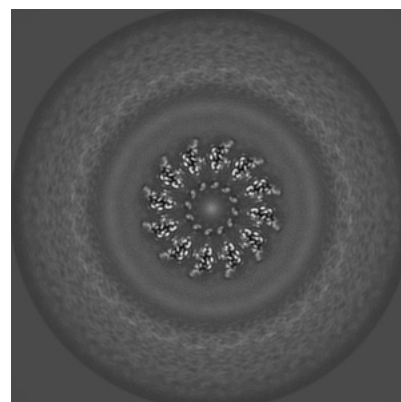
### 6.2.2 Raw map



X Index: 176



Y Index: 176

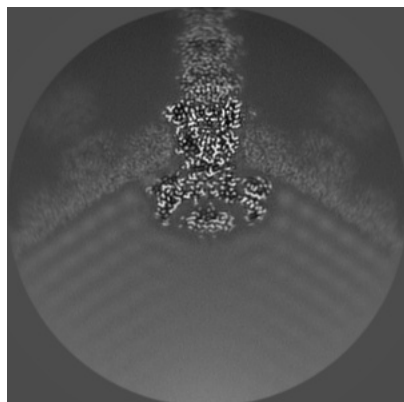


Z Index: 176

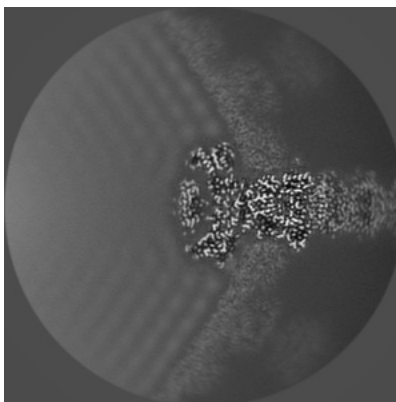
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

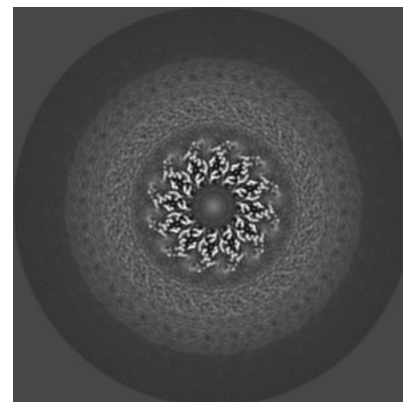
### 6.3.1 Primary map



X Index: 153

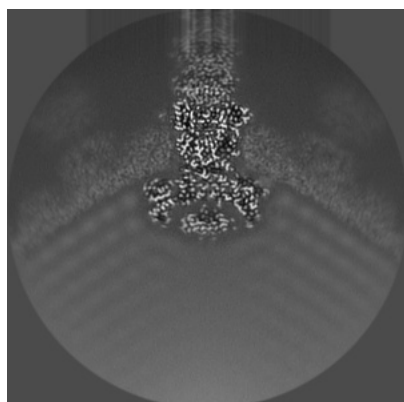


Y Index: 199

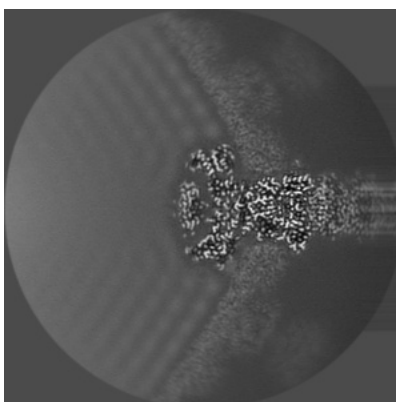


Z Index: 200

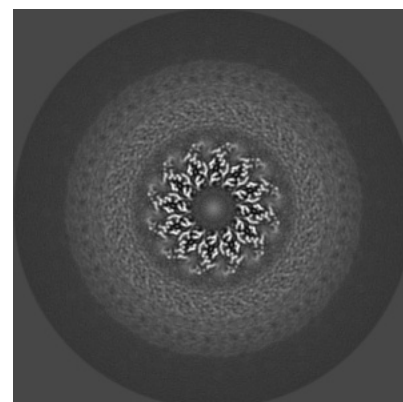
### 6.3.2 Raw map



X Index: 199



Y Index: 199

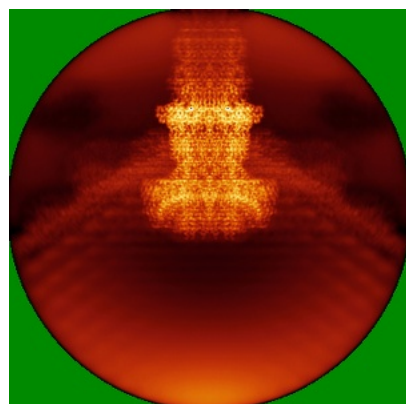


Z Index: 200

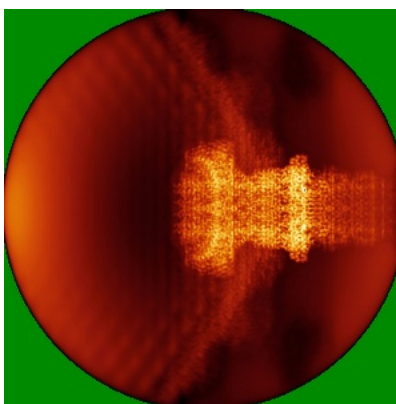
The images above show the largest variance slices of the map in three orthogonal directions.

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

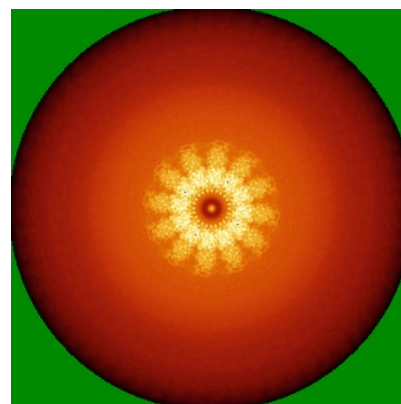
### 6.4.1 Primary map



X

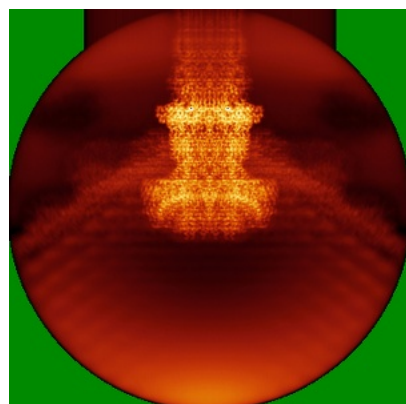


Y

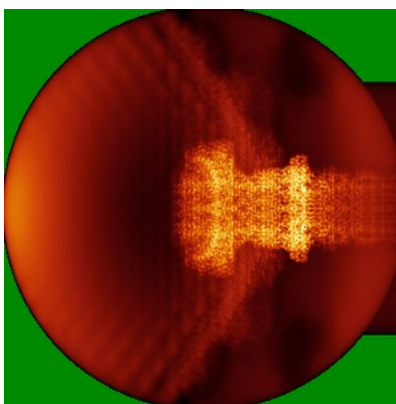


Z

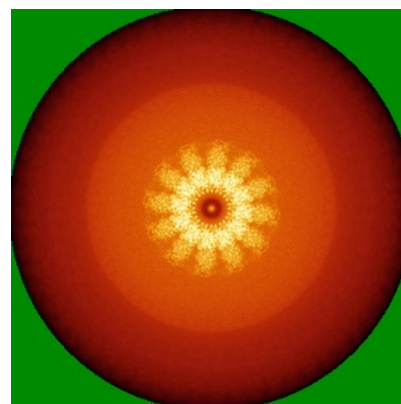
### 6.4.2 Raw map



X



Y

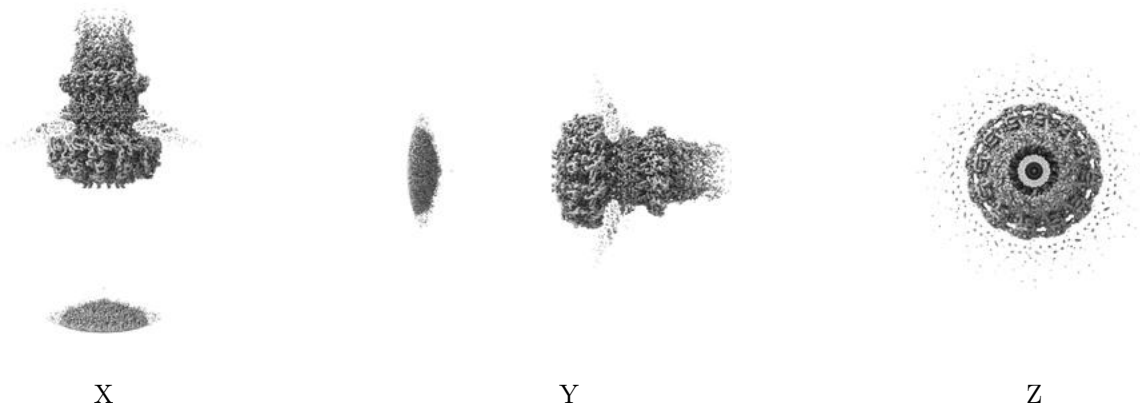


Z

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.

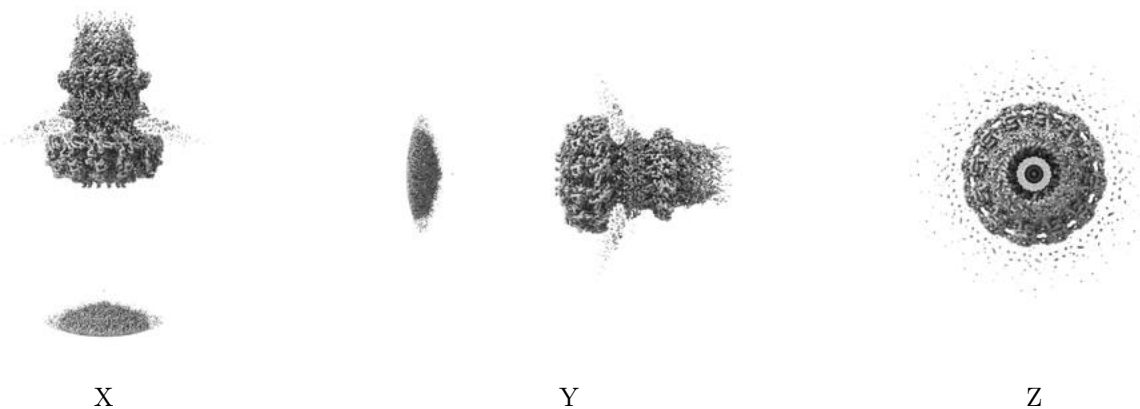
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

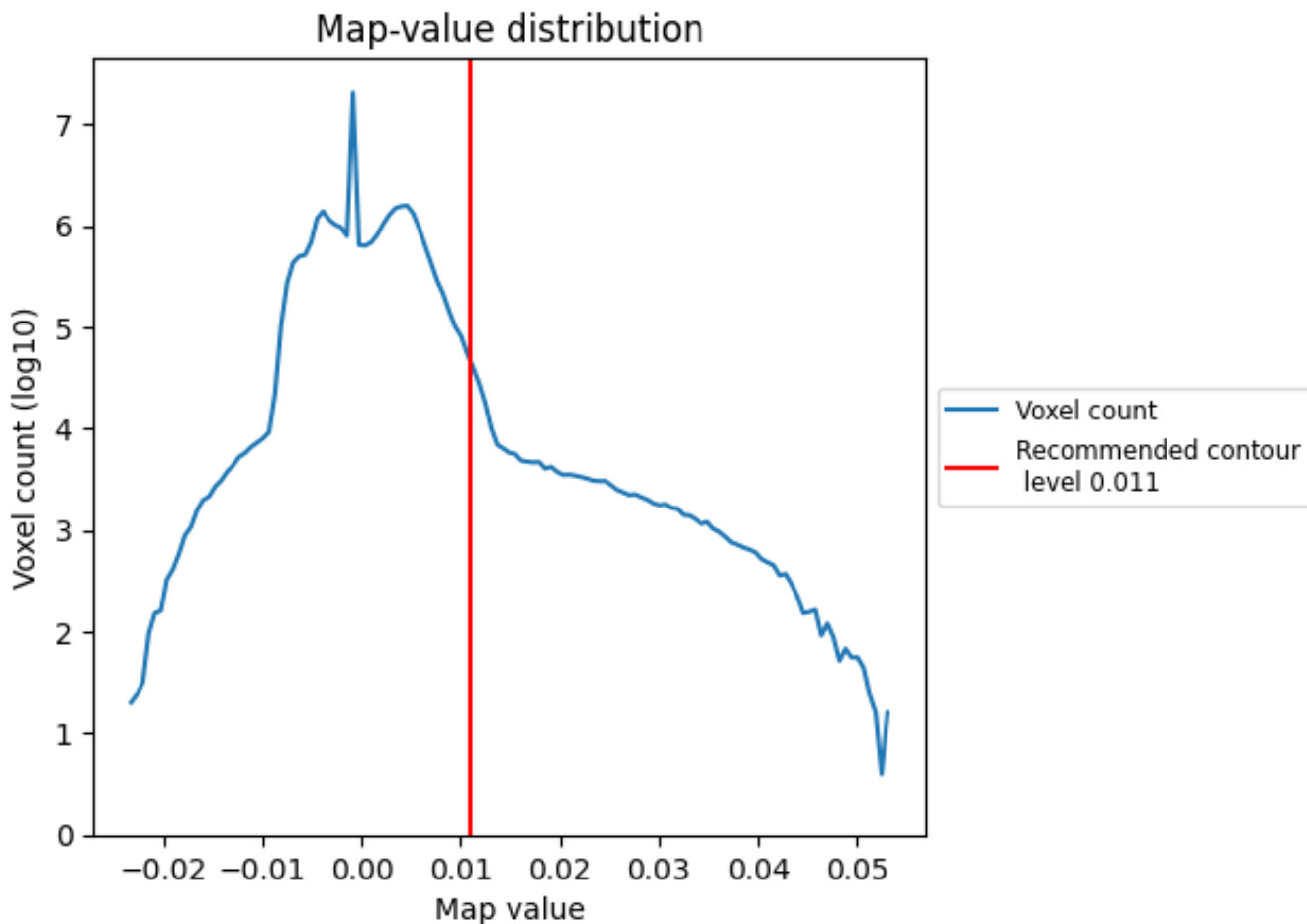
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

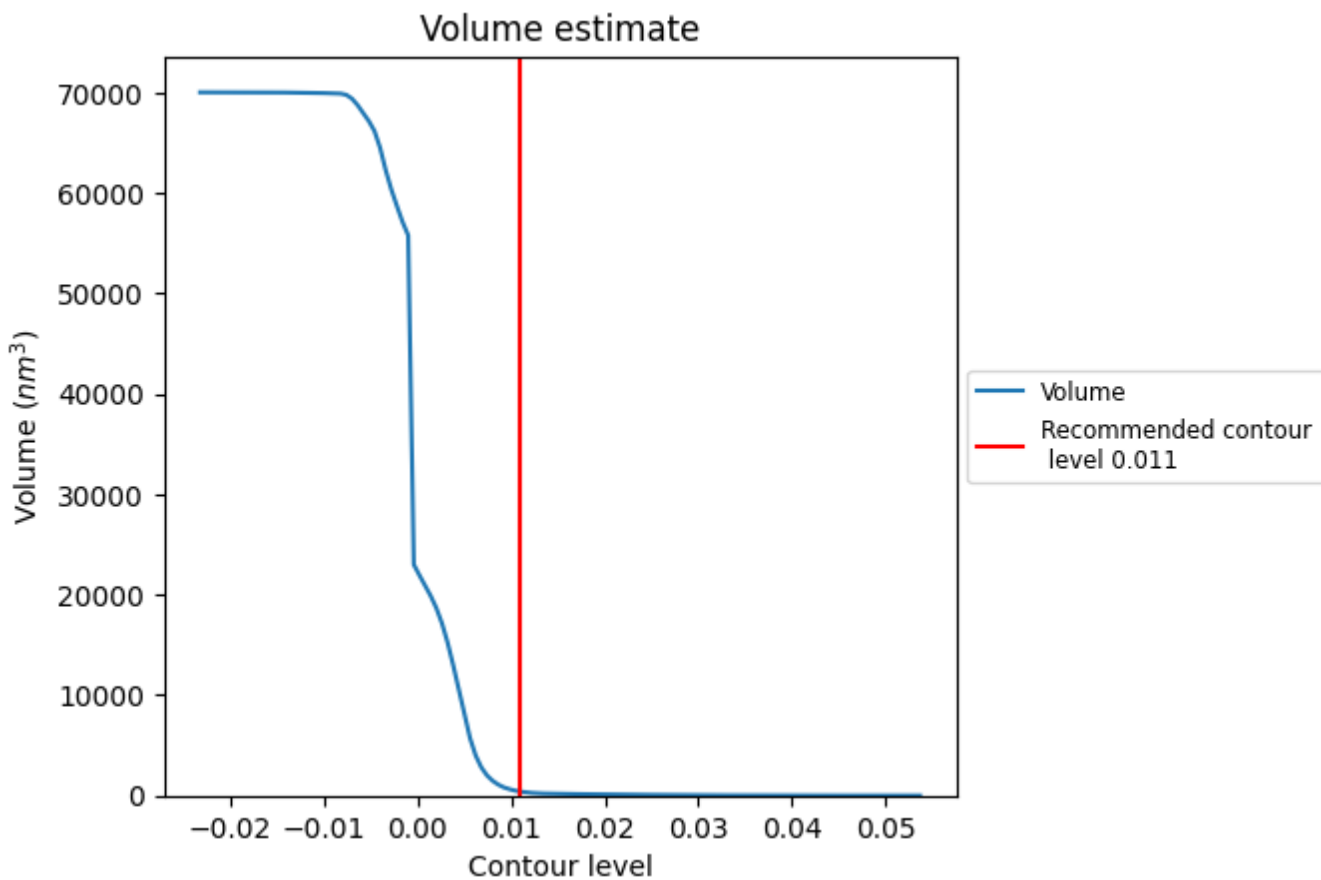
### 7.1 Map-value distribution [i](#)



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 [\(i\)](#)

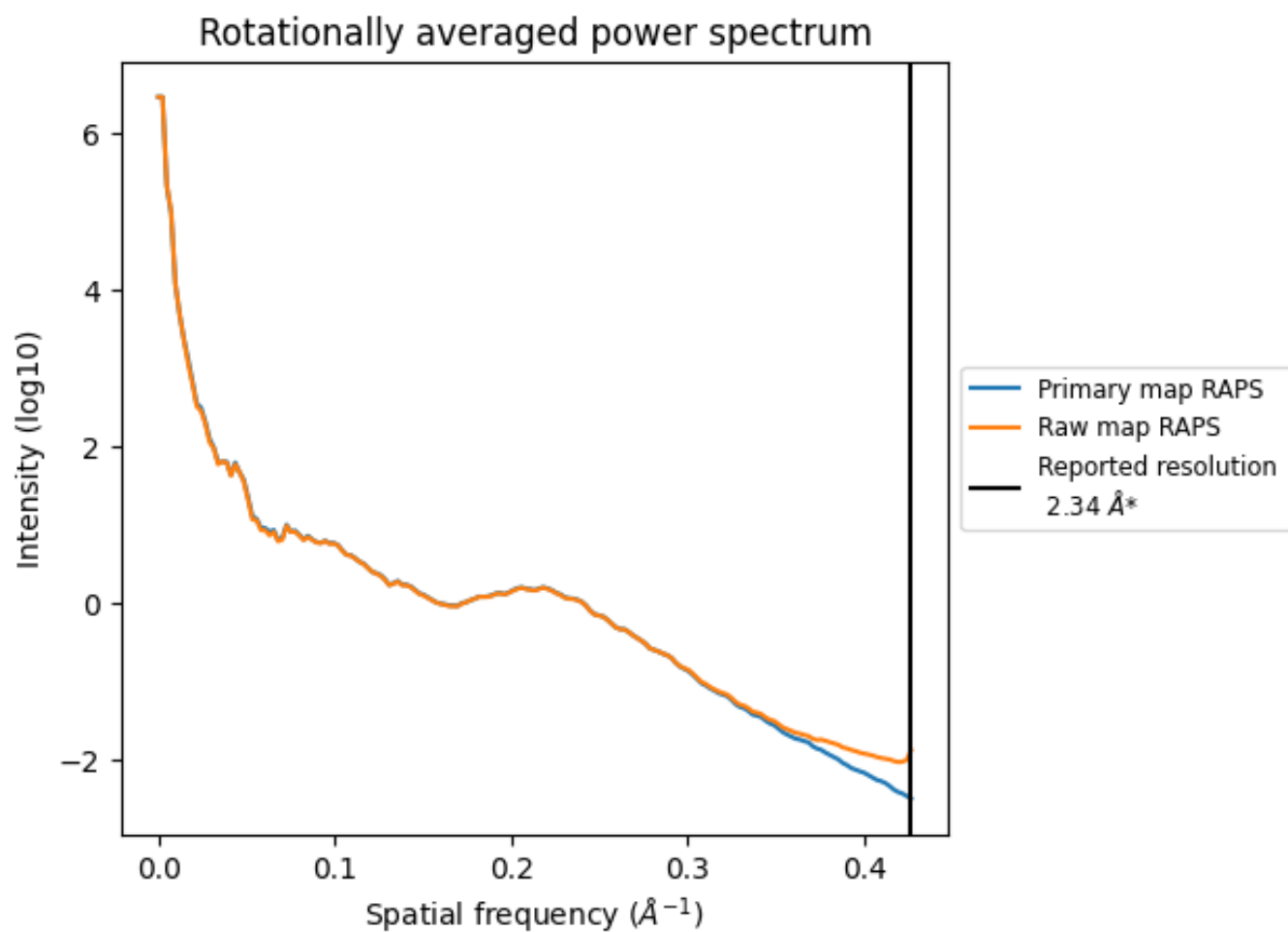


The volume at the recommended contour level is 390 nm<sup>3</sup>; this corresponds to an approximate mass of 353 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum i

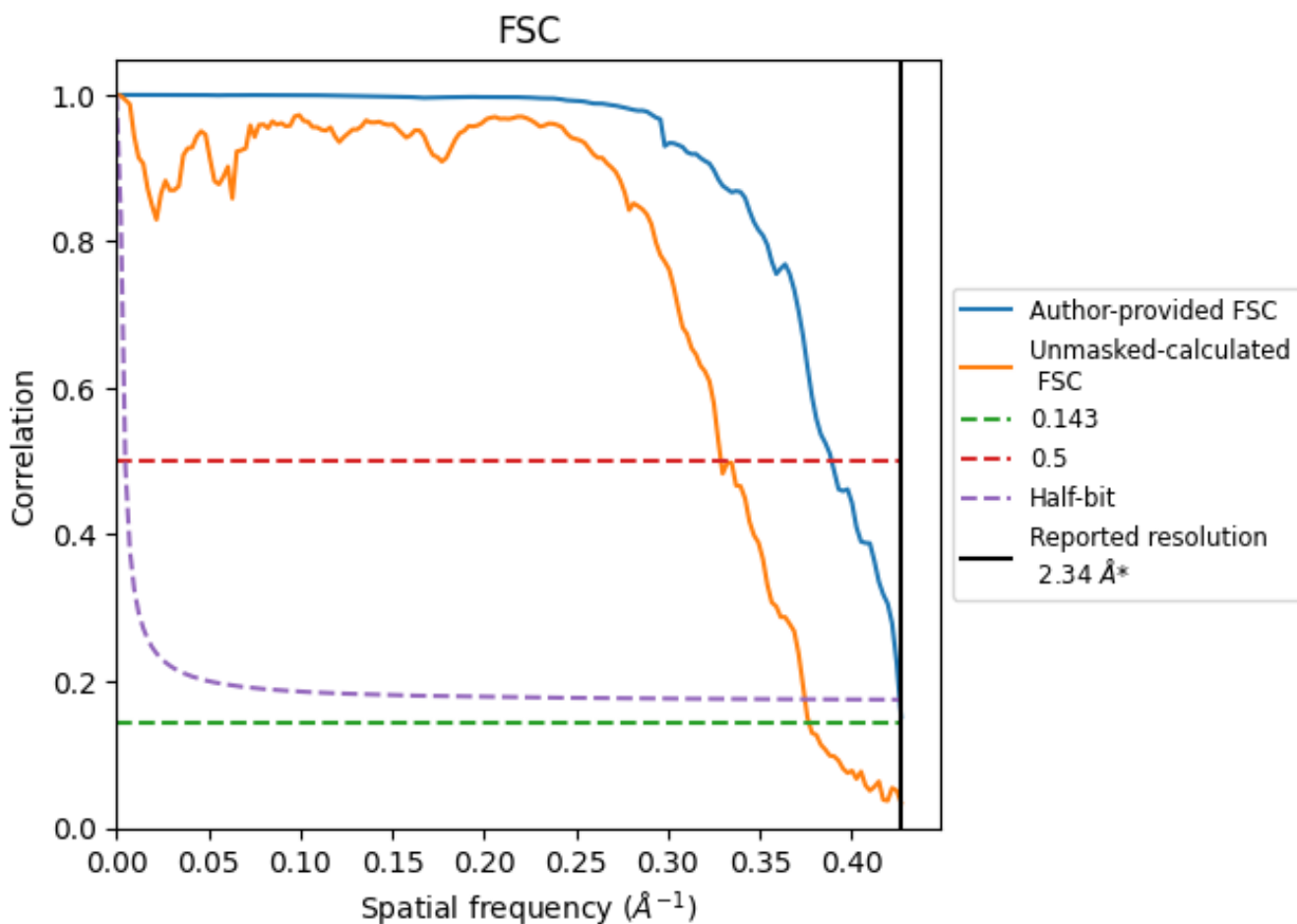


\*Reported resolution corresponds to spatial frequency of 0.427 Å<sup>-1</sup>

## 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 0.427 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

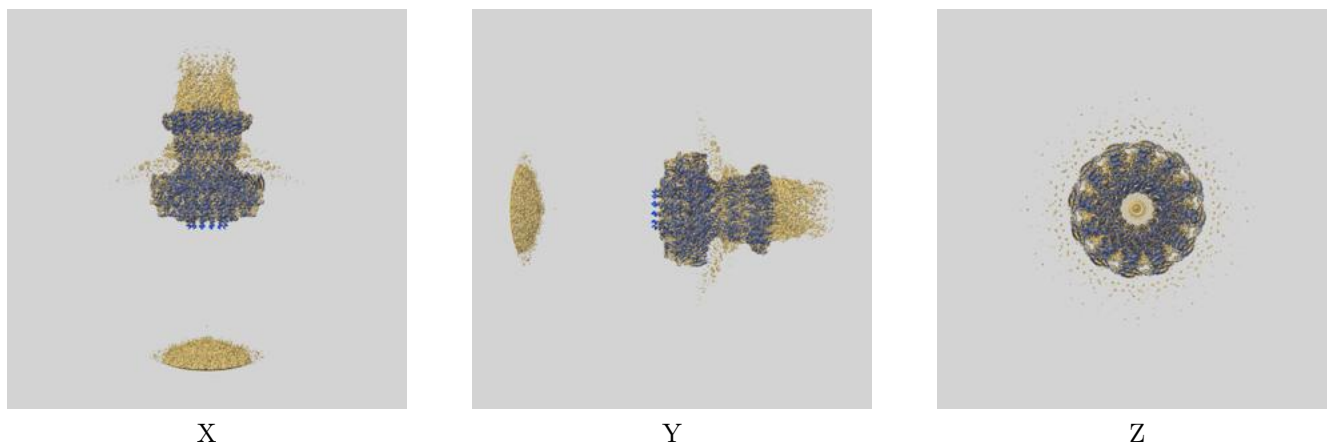
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	-	2.57	2.35
Unmasked-calculated*	2.65	3.04	2.67

\*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 2.65 differs from the reported value 2.342 by more than 10 %

## 9 Map-model fit [i](#)

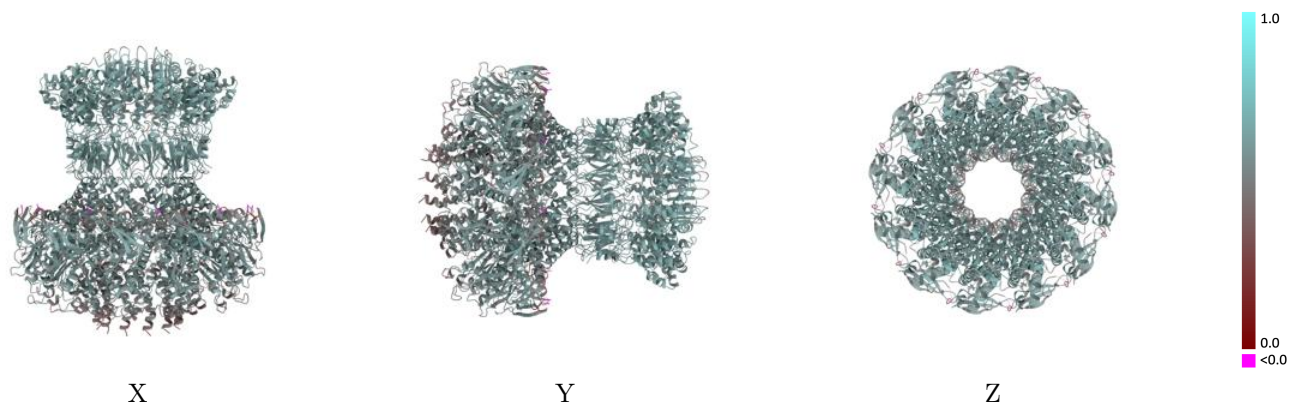
This section contains information regarding the fit between EMDB map EMD-18599 and PDB model 8QQN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



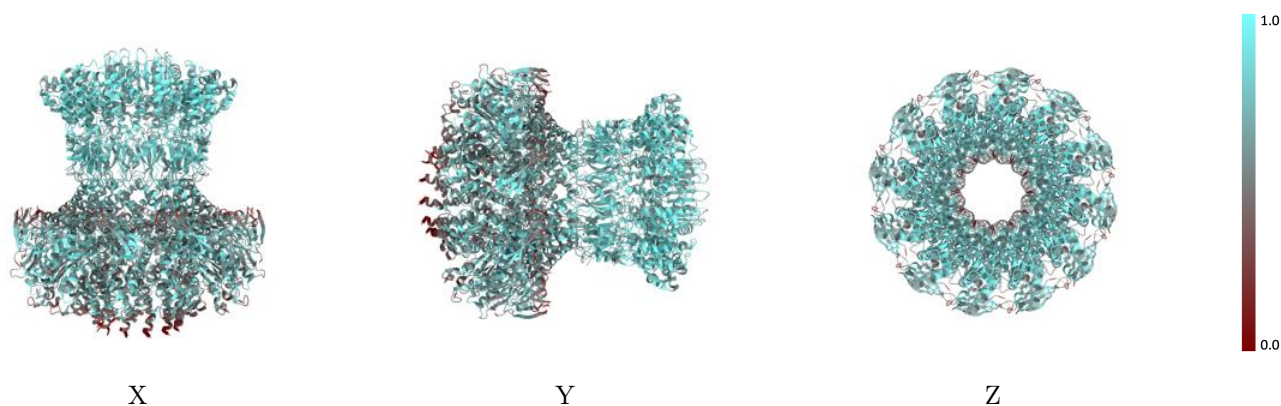
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



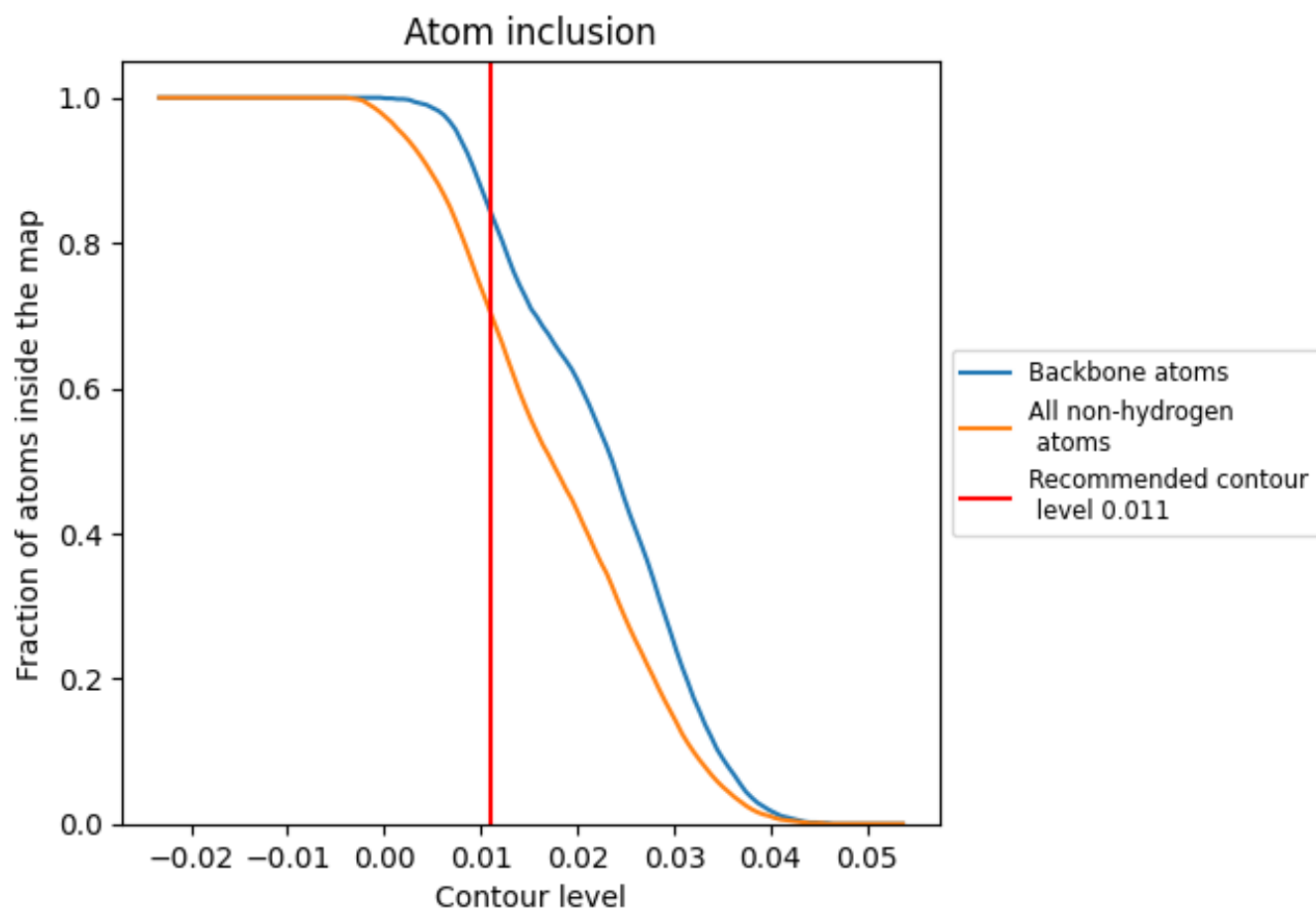
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 70% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7040	 0.5610
PA	 0.6670	 0.5470
PB	 0.6680	 0.5480
PC	 0.6680	 0.5470
PD	 0.6660	 0.5470
PE	 0.6670	 0.5470
PF	 0.6680	 0.5480
PG	 0.6660	 0.5490
PH	 0.6700	 0.5480
PI	 0.6670	 0.5480
PJ	 0.6670	 0.5480
PK	 0.6670	 0.5490
PL	 0.6690	 0.5490
PM	 0.8140	 0.5990
PN	 0.8100	 0.5970
PO	 0.8070	 0.5980
PP	 0.8080	 0.6010
PQ	 0.8120	 0.5980
PR	 0.8030	 0.5990
PS	 0.8090	 0.6000
PT	 0.8110	 0.5980
PU	 0.8120	 0.5980
PV	 0.8100	 0.5980
PW	 0.8150	 0.5980
PX	 0.8070	 0.5990

