



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:23 PM UTC

PDB ID : 6PEP / pdb_00006pep
EMDB ID : EMD-20317
Title : Focussed refinement of InvGN0N1:SpaPQR:PrgIJ from the Salmonella SPI-1 injectisome needle complex
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2019-06-20
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

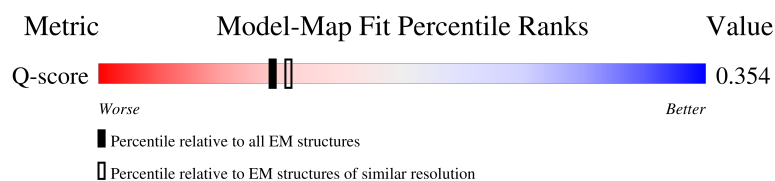
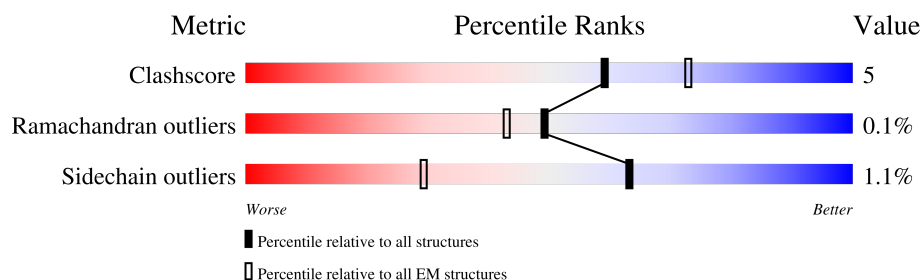
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	0	224	 7% 77% 11% • 11%
1	1	224	 6% 81% 8% 11%
1	2	224	 5% 74% 14% 12%
1	3	224	 5% 74% 17% 9%

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Mol	Chain	Length	Quality of chain
1	4	224	
2	5	263	
3	6	86	
3	7	86	
3	8	86	
3	9	86	
4	A	562	
4	B	562	
4	C	562	
4	D	562	
4	F	562	
4	G	562	
4	H	562	
4	I	562	
4	J	562	
4	K	562	
4	L	562	
4	M	562	
4	N	562	
4	O	562	
4	P	562	
4	Q	562	
5	AM	101	
5	AN	101	
5	AO	101	

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Mol	Chain	Length	Quality of chain
5	AP	101	
5	AQ	101	
5	AR	101	
6	AS	80	
6	AT	80	
6	AU	80	
6	AV	80	
6	AW	80	
6	AX	80	
6	AY	80	
6	AZ	80	
6	BA	80	
6	BB	80	
6	BC	80	
6	BD	80	
6	BE	80	
7	E	392	
7	R	392	
7	S	392	
7	T	392	
7	U	392	
7	V	392	
7	W	392	
7	X	392	
7	Y	392	

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Mol	Chain	Length	Quality of chain
7	Z	392	 7% 93%
7	a	392	 6% 93%
7	b	392	 7% 93%
7	c	392	 7% 93%
7	d	392	 6% 93%
7	e	392	 7% 93%
7	f	392	 7% 93%
7	g	392	 7% 93%
7	h	392	 6% 93%
7	i	392	 7% 93%
7	j	392	 6% 93%
7	k	392	 7% 93%
7	l	392	 7% 93%
7	m	392	 6% 93%
7	n	392	 7% 93%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 45454 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 Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	199	Total	C	N	O	S	0	0
			1562	1041	231	279	11		
1	1	199	Total	C	N	O	S	0	0
			1569	1047	232	279	11		
1	2	197	Total	C	N	O	S	0	0
			1553	1037	230	275	11		
1	3	204	Total	C	N	O	S	0	0
			1606	1071	238	286	11		
1	4	221	Total	C	N	O	S	1	0
			1758	1163	266	318	11		

- Molecule 2 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	247	Total	C	N	O	S	0	0
			1885	1252	300	320	13		

- Molecule 3 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	53	Total	C	N	O	S	0	0
			405	276	61	67	1		
3	7	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
3	8	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
3	9	84	Total	C	N	O	S	0	0
			647	438	97	109	3		

- Molecule 4 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	B	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
4	C	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	D	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		
4	F	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	G	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
4	H	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	I	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
4	J	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	K	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
4	L	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	M	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		
4	N	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	O	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
4	P	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
4	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		

- Molecule 5 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AM	39	Total	C	N	O	S	0	0
			298	187	49	60	2		
5	AN	78	Total	C	N	O	S	7	0
			644	396	116	130	2		
5	AO	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
5	AP	89	Total	C	N	O	S	0	0
			675	416	115	141	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	AQ	89	Total	C	N	O	S	0	0
			675	416	115	141	3		
5	AR	88	Total	C	N	O	S	0	0
			667	410	114	140	3		

- Molecule 6 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AS	59	Total	C	N	O		0	0
			466	294	80	92			
6	AT	59	Total	C	N	O		0	0
			466	294	80	92			
6	AU	59	Total	C	N	O		0	0
			466	294	80	92			
6	AV	59	Total	C	N	O		0	0
			466	294	80	92			
6	AW	59	Total	C	N	O		0	0
			466	294	80	92			
6	AX	73	Total	C	N	O		0	0
			574	362	95	117			
6	AY	78	Total	C	N	O		0	0
			612	387	101	124			
6	AZ	57	Total	C	N	O		0	0
			460	289	76	95			
6	BA	54	Total	C	N	O		0	0
			437	275	73	89			
6	BB	48	Total	C	N	O		0	0
			388	247	64	77			
6	BC	48	Total	C	N	O		0	0
			388	247	64	77			
6	BD	48	Total	C	N	O		0	0
			388	247	64	77			
6	BE	43	Total	C	N	O		0	0
			346	219	59	68			

- Molecule 7 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	28	Total	C	N	O	S	0	0
			236	159	38	38	1		
7	R	27	Total	C	N	O	S	0	0
			227	153	37	36	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	T	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	U	27	Total 227	C 153	N 37	O 36	S 1	0	0
7	V	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	W	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	X	27	Total 227	C 153	N 37	O 36	S 1	0	0
7	Y	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	Z	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	a	27	Total 227	C 153	N 37	O 36	S 1	0	0
7	b	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	c	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	d	27	Total 227	C 153	N 37	O 36	S 1	0	0
7	e	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	f	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	g	27	Total 227	C 153	N 37	O 36	S 1	0	0
7	h	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	i	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	j	27	Total 227	C 153	N 37	O 36	S 1	0	0
7	k	28	Total 231	C 156	N 38	O 36	S 1	0	0
7	l	28	Total 236	C 159	N 38	O 38	S 1	0	0
7	m	27	Total 227	C 153	N 37	O 36	S 1	0	0

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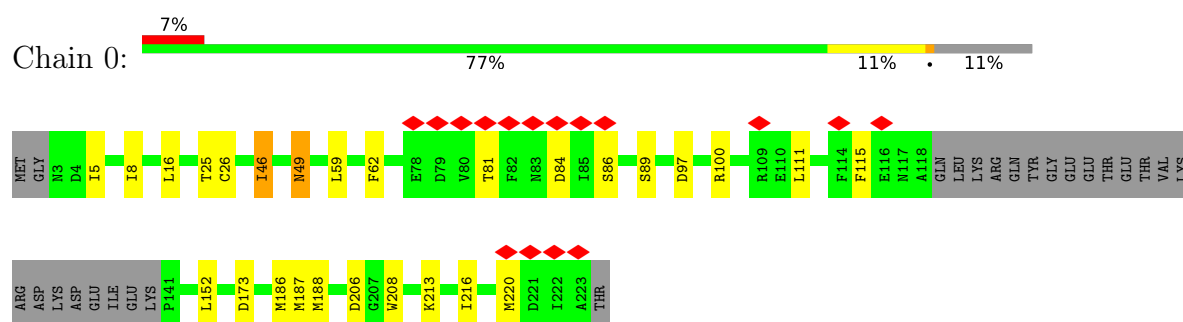
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Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	28	Total	C	N	O	S	0	0
			231	156	38	36	1		

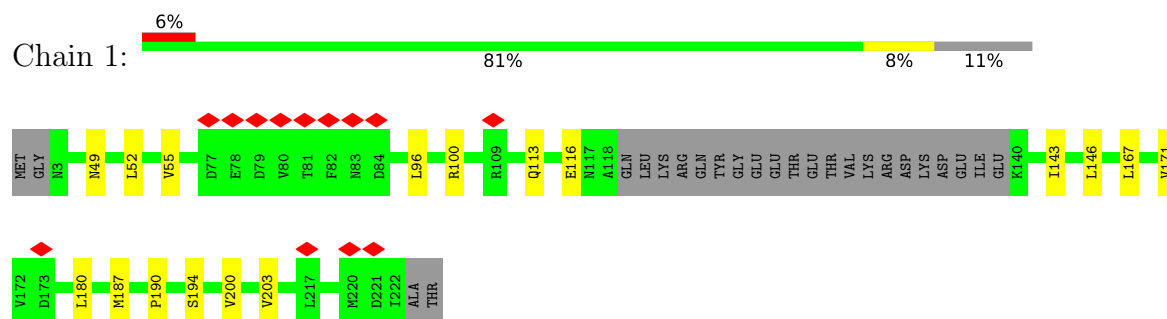
3 Residue-property plots [i](#)

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

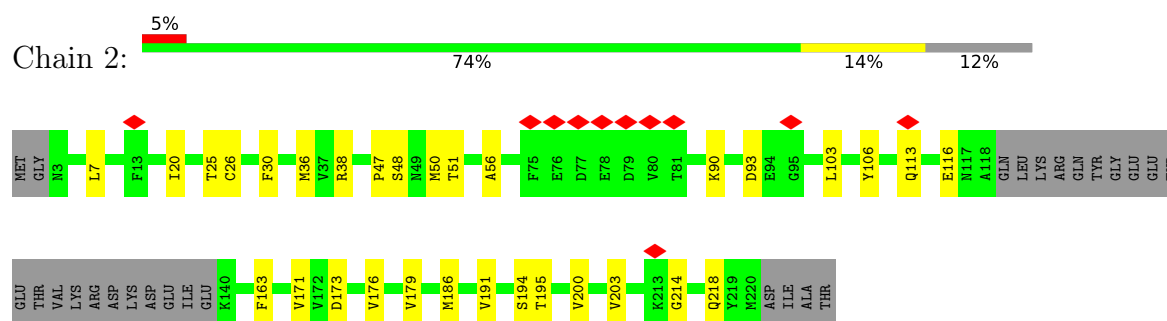
- Molecule 1: Surface presentation of antigens protein SpaP



- Molecule 1: Surface presentation of antigens protein SpaP

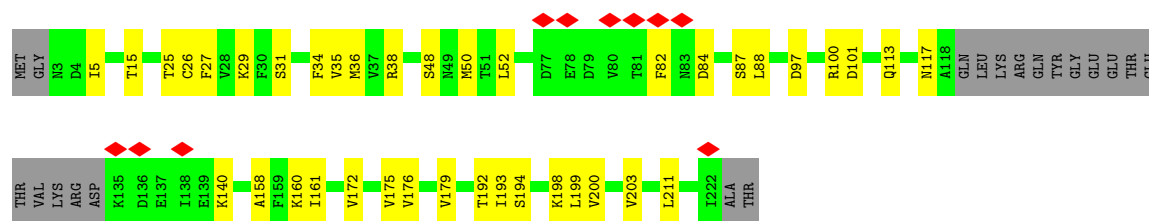


- Molecule 1: Surface presentation of antigens protein SpaP

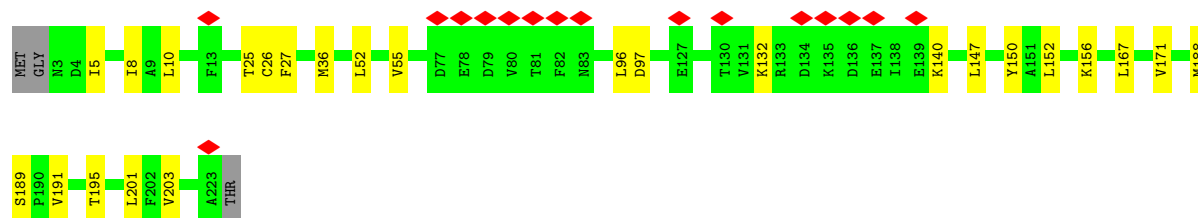
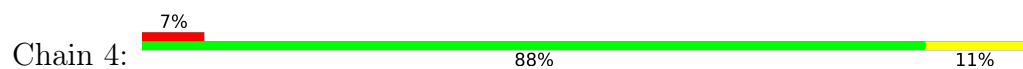


- Molecule 1: Surface presentation of antigens protein SpaP

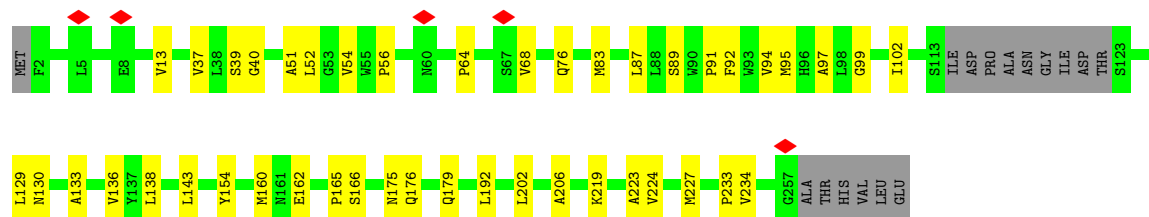
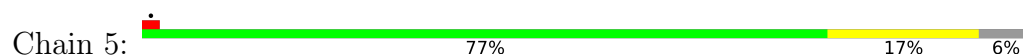




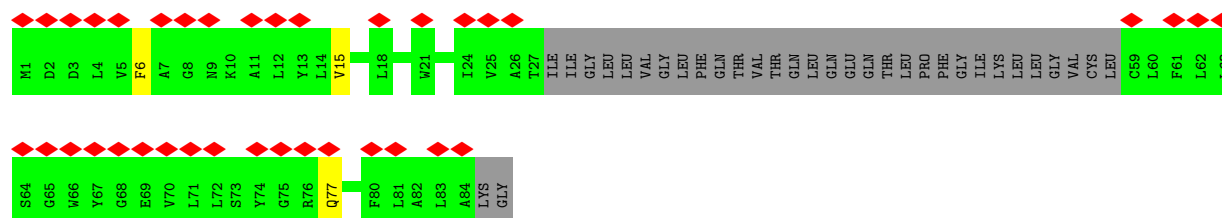
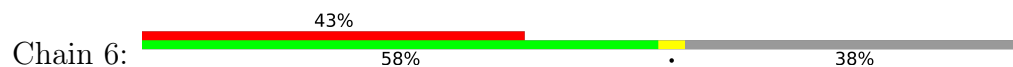
- Molecule 1: Surface presentation of antigens protein SpaP



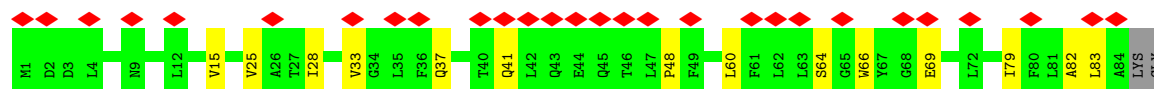
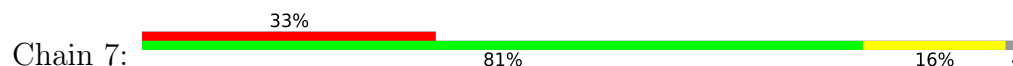
- Molecule 2: Surface presentation of antigens protein SpaR



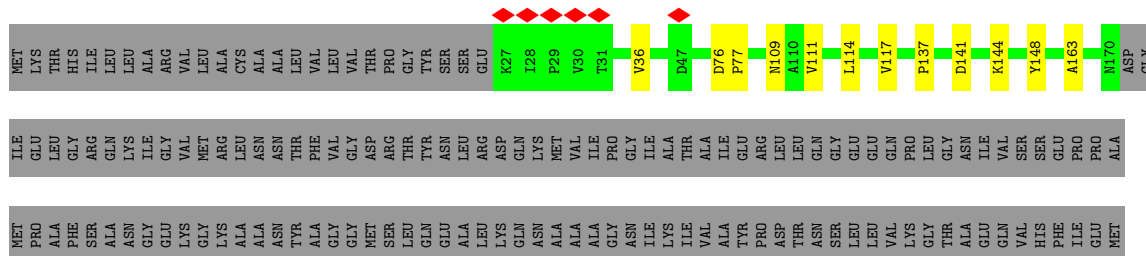
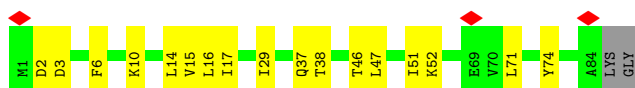
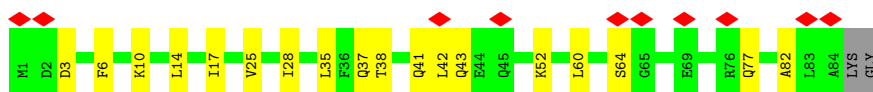
- Molecule 3: Surface presentation of antigens protein SpaQ



- Molecule 3: Surface presentation of antigens protein SpaQ



- Molecule 3: Surface presentation of antigens protein SpaQ



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

- Molecule 4: Protein InvG

Chain C:  21% 1% 75%

[illegible]

- Molecule 4: Protein InvG

Chain D: 23% 74%

PRO	PHE	SER	ALA	ASN	GLY	GLU	LYS	VAL	LYS	ARG	LEU	ALA	ALA	ASN	TYR	ALA	GLY	GLY	GLN	GLU	ALA	LYS	ASP	SER	ASN	GLN	ASN	ALA	ALA	ALA	ALA	TYR	THR	ASP	SER	ASN	THR	LYS	ILE	VAL	ALA	ALA	ALA	GLY	GLY	ASN	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
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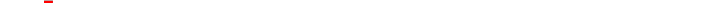
[illegible]

- Molecule 4: Protein InvG

Chain F:  22% 1% 77%

[illegible]

- Molecule 4: Protein InvG

Chain G:  23% . 74%

[illegible]

[illegible]

- Molecule 4: Protein InvG

[illegible]

- Molecule 4: Protein InvG

[illegible]

[illegible]

- Molecule 4: Protein InvG

Chain J: 22% . 75%

[illegible]

- Molecule 4: Protein InvG

Chain K: 24% 74%

[illegible]

[illegible]

- Molecule 4: Protein InvG

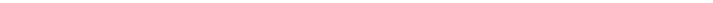
[illegible]

- Molecule 4: Protein InvG

[illegible]

[illegible]

- Molecule 4: Protein InvG

Chain N:  22% 1% 75%

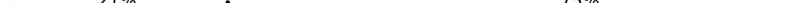
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- Molecule 4: Protein InvG

Chain 0: 23% . 74%

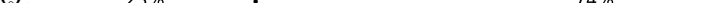
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- Molecule 4: Protein InvG

Chain P:  21% . 75%

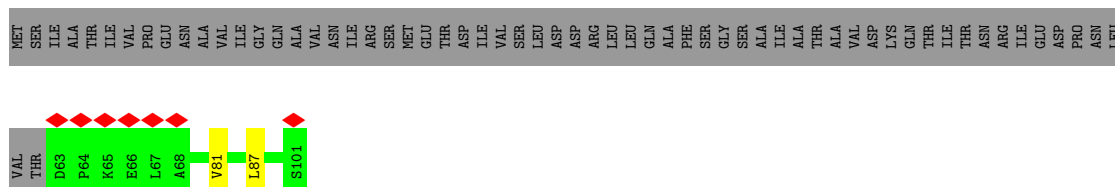
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- Molecule 4: Protein InvG

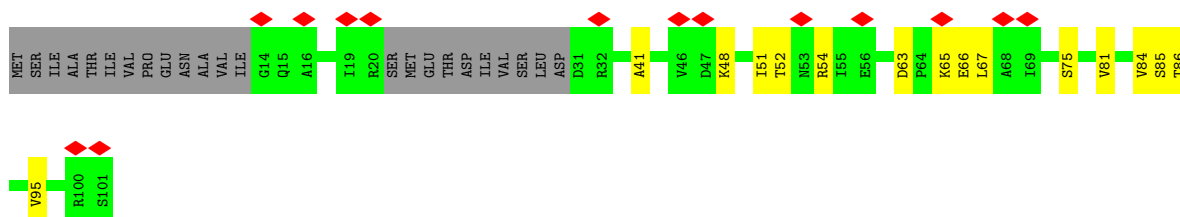
Chain Q:  23% . 74%

[illegible]

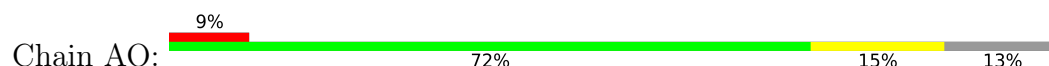
- Molecule 5: Protein PrgJ



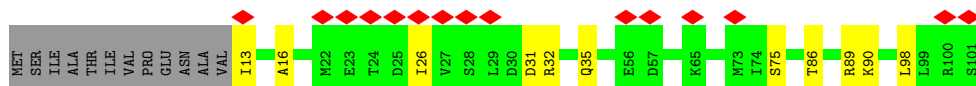
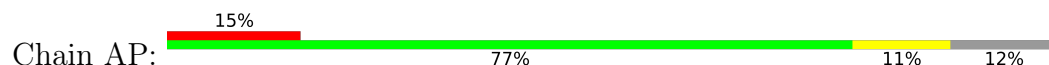
- Molecule 5: Protein PrgJ



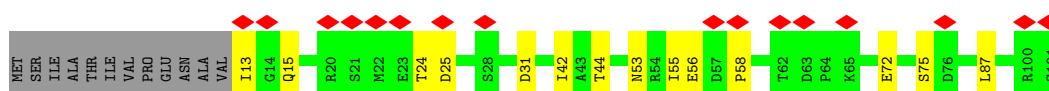
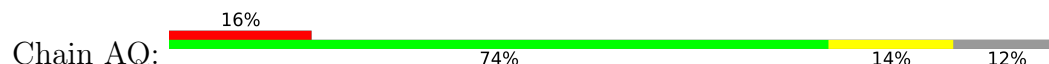
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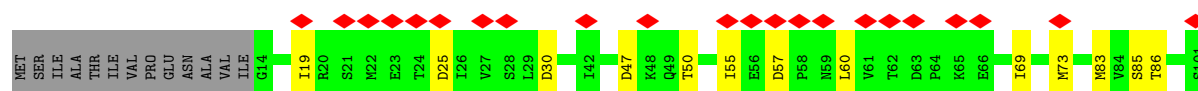
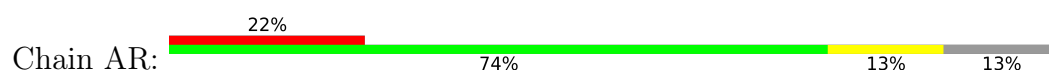
- Molecule 5: Protein PrgJ



- Molecule 5: Protein PrgJ



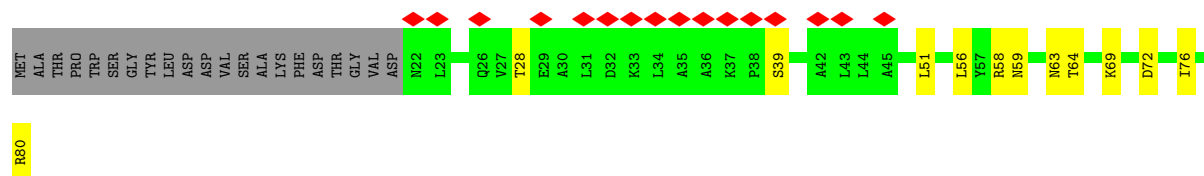
- Molecule 5: Protein PrgJ



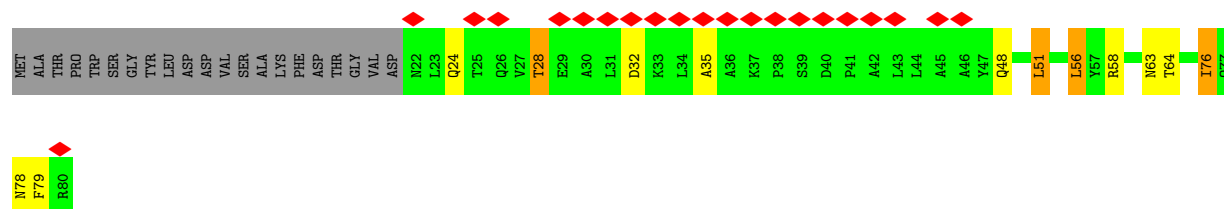
- Molecule 6: Protein PrgI



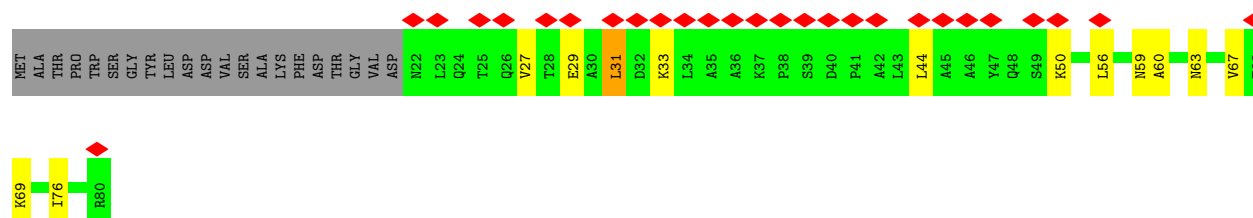
- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI



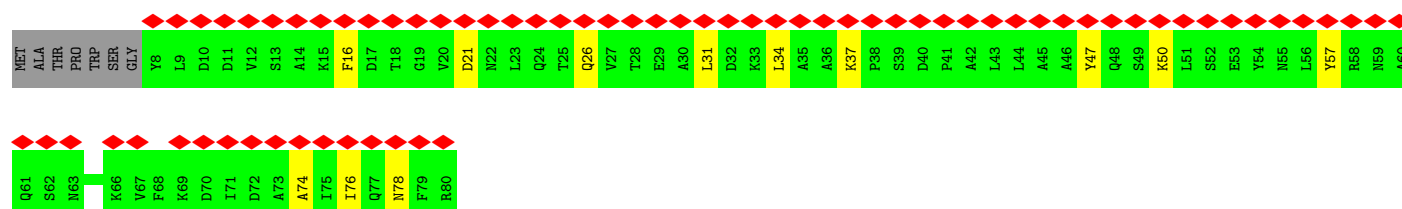
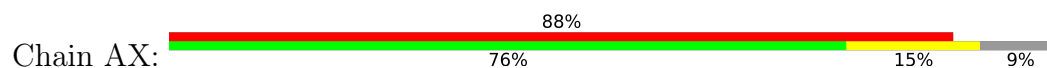
- Molecule 6: Protein PrgI



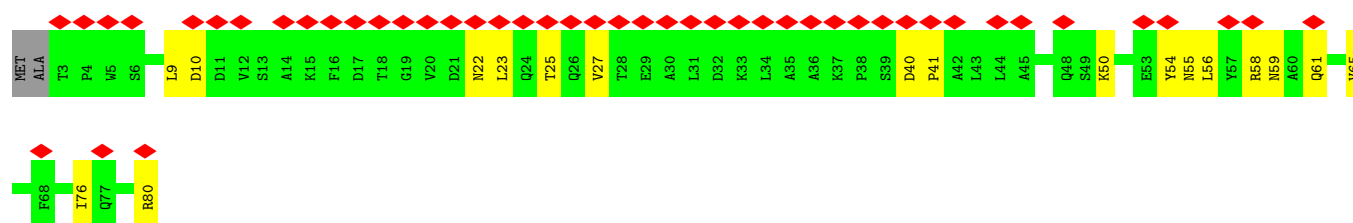
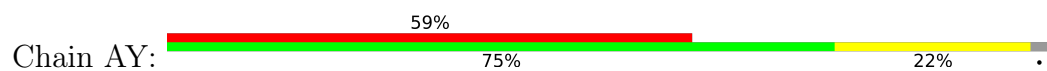
- Molecule 6: Protein PrgI



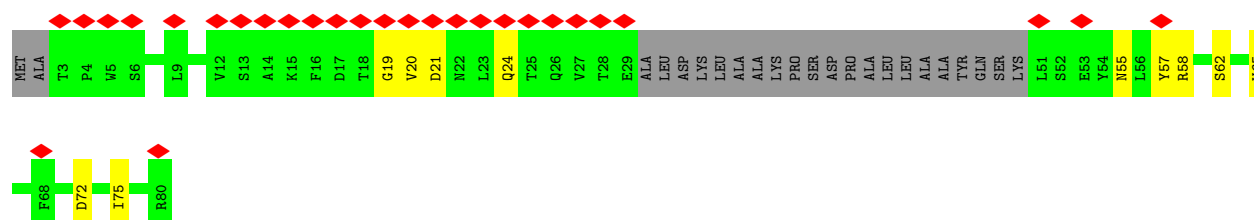
- Molecule 6: Protein PrgI



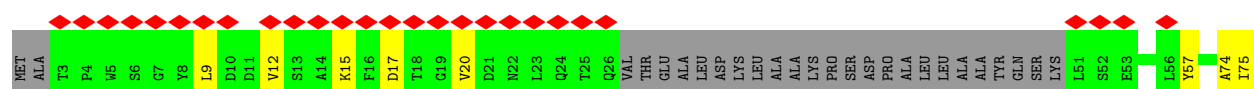
- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI

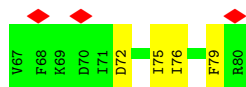
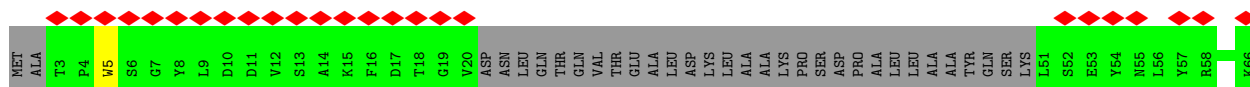


- Molecule 6: Protein PrgI

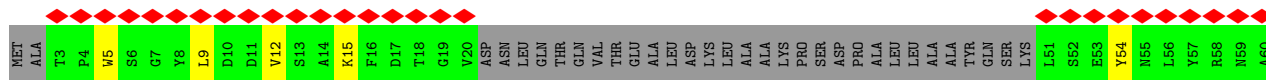




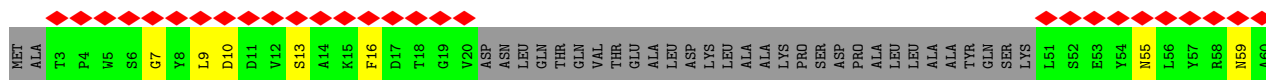
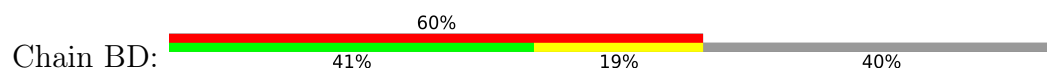
• Molecule 6: Protein PrgI



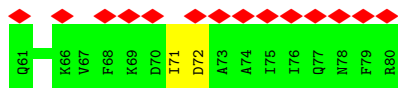
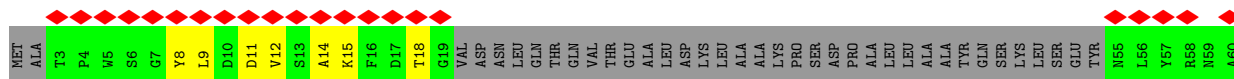
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI

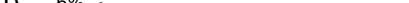


• Molecule 7: Protein PrgH



[illegible]

- Molecule 7: Protein PrgH

Chain R:  6% 93%

[illegible]

- Molecule 7: Protein PrgH

Chain S: 7% 93%

[illegible]

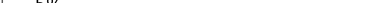
[illegible]

- Molecule 7: Protein PrgH

Chain T: 7% 93%

LEU	GLY	PRO	LYS	PRO	GLN	GLY	GLY	PRO	PHE	MET
LYS	GLN	GLN	ASP	LEU	ARG	ARG	GLU	GLN	ILE	THR
ASP	GLU	ALA	ASP	TYR	VAL	VAL	GLN	PRO	LEU	LYS
W365	GLY	TYR	ARG	ARG	VAL	VAL	VAL	LYS	HIS	GLY
L366	LEU	ILE	ILE	ILE	ARG	ARG	LEU	LEU	GLY	LYS
G368	LYS	GLN	GLN	HIS	GLY	GLY	THR	THR	VAL	THR
R369	GLN	PHE	ASP	PHE	ARG	ARG	THR	ASN	ASN	ILE
S370	ALA	ASP	ALA	ASP	ASP	ASP	LYS	ALA	PHE	SER
	LEU	GLU	GLU	GLU	GLU	MET	LYS	LYS	GLU	PRO
S382	PRO	PRO	TYR	PRO	ARG	LEU	ASN	ASN	ILE	GLY
P383	SER	LYS	SER	LYS	LYS	TYR	VAL	GLN	VAL	PRO
G384	ARG	PRO	ARG	PRO	VAL	VAL	VAL	PRO	ASP	ILE
H385	ARG	VAL	ARG	VAL	ALA	ALA	ALA	ARG	THR	VAL
W386	ASN	PHE	ASN	PHE	GLN	ALA	GLN	LYS	ASP	ARG
Y387	HIS	THR	HIS	THR	THR	THR	THR	LYS	ALA	LEU
P388	LYS	LEU	LYS	LEU	ASN	LEU	THR	ASN	THR	LEU
F388	GLY	SER	GLY	SER	ARG	ARG	GLU	GLY	GLU	ASN
P389	VAL	VAL	VAL	GLN	GLN	THR	ASP	VAL	ILE	SER
S390	THR	THR	THR	ASN	ARG	THR	THR	ALA	LEU	LEU
F391	PHE	PHE	PHE	PHE	ASN	LEU	VAL	HIS	GLY	ASN
L392	VAL	VAL	VAL	VAL	MET	THR	THR	GLU	ASN	GLY
	GLN	GLN	GLN	GLN	SER	ARG	GLY	LYS	LEU	CYS
	GLY	GLY	GLY	GLY	THR	THR	THR	PHE	THR	GLU
	ALA	ALA	ALA	ALA	LEU	ALA	GLY	GLY	GLY	GLY
	ARG	ARG	ARG	ARG	ARG	VAL	ILE	ARG	ARG	THR
	PHE	PHE	PHE	PHE	LEU	VAL	THR	SER	SER	THR
	VAL	VAL	VAL	VAL	MET	ILE	ILE	VAL	THR	GLN
	ASP	ASP	ASP	ASP	PRO	ASN	ASN	ASN	PRO	SER
	SER	SER	SER	SER	TYR	GLU	GLY	VAL	GLY	ALA
	TYR	TYR	TYR	TYR	ALA	ASN	GLN	PRO	GLY	THR
	THR	THR	THR	THR	ASP	GLU	GLN	ARG	GLU	ALA
	THR	THR	THR	THR	VAL	ASN	GLN	LEU	LEU	SER
	GLY	GLY	GLY	GLY	ILE	LYS	ALA	ILE	ILE	GLN
	GLY	GLY	GLY	GLY	THR	ILE	GLU	ILE	ILE	LEU
	ARG	ARG	ARG	ARG	LEU	SER	LEU	LEU	PRO	PRO
	TYR	TYR	TYR	TYR	MET	ILE	ASP	PRO	ASP	ILE
	VAL	VAL	VAL	VAL	ASP	THR	SER	GLU	GLU	THR
	GLN	GLN	GLN	GLN	ASP	LEU	LEU	PRO	GLY	ALA
	PHE	PHE	PHE	PHE	VAL	THR	GLY	ASP	PRO	ALA
	ALA	ALA	ALA	ALA	THR	THR	THR	GLY	PRO	ALA
	ILE	ILE	ILE	ILE	ALA	TYR	GLN	VAL	THR	PHE

- Molecule 7: Protein PrgH

Chain U:  5% 93%

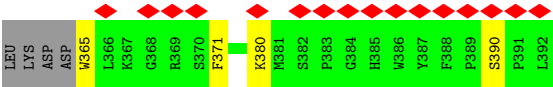
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LEU
LYS
ASP
ASP
W365
L366
R369
Q372
Y373
E376
G377
K380
P391
LEU

Chain V:  7% 93%

Chain W: 6% 93%

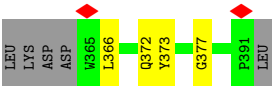
GLY	GLN	ALA	ALA	ALA	LEU	GLN	GLN	ALA	LEU	PRO	TYR	SER	ARG	ARG	ASN	HIS	LYS	GLY	GLY	VAL	THR	PHE	VAL	ILE	GLN	GLN	ALA	LEU	ASP	ASP	VAL	GLU	ILE	LEU	ARG	ALA	ARG	GLN	PHE	VAL	ASP	SER	TYR	TYR	THR	TRP	GLY	GLY	ARG	TYR	VAL	GLN	PHE	ALA	ILE	GLN
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● Molecule 7: Protein PrgH



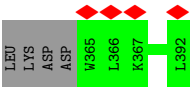
GLY	GLN	PRO	GLN	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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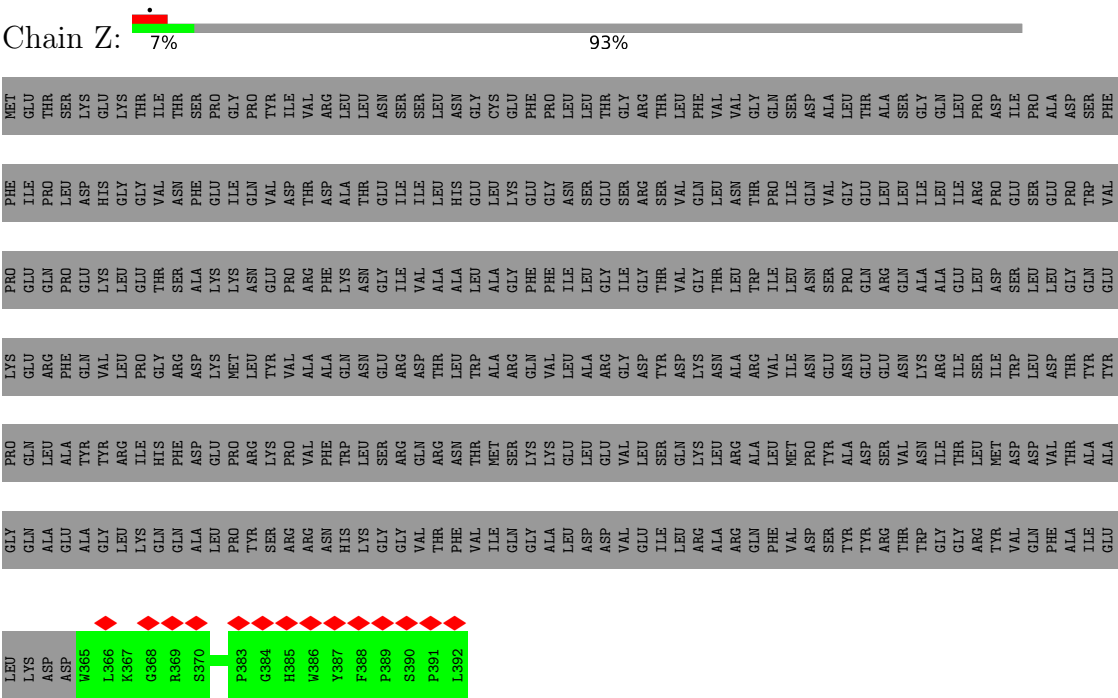
● Molecule 7: Protein PrgH



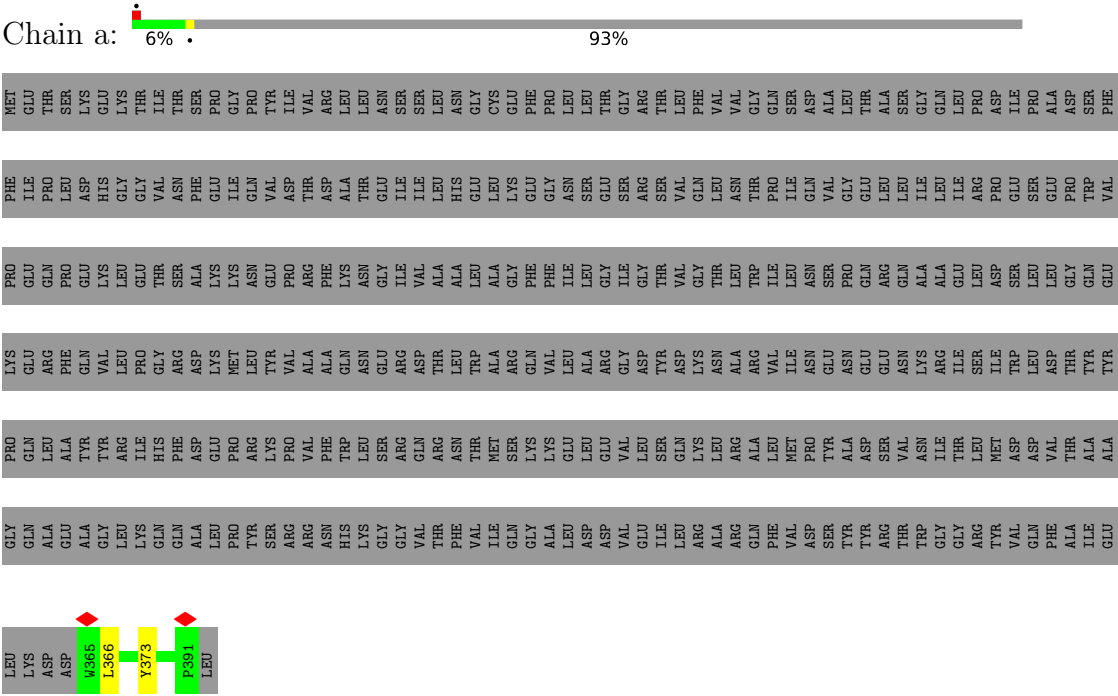
GLN	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL
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● Molecule 7: Protein PrgH



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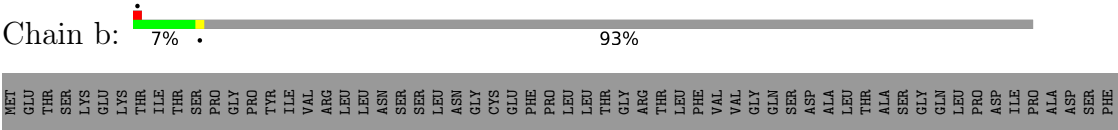


Diagram illustrating the location of the five amino acid mutations (W365, L366, K367, M381, and L392) within the protein structure. The mutations are indicated by red diamonds above the corresponding residues.

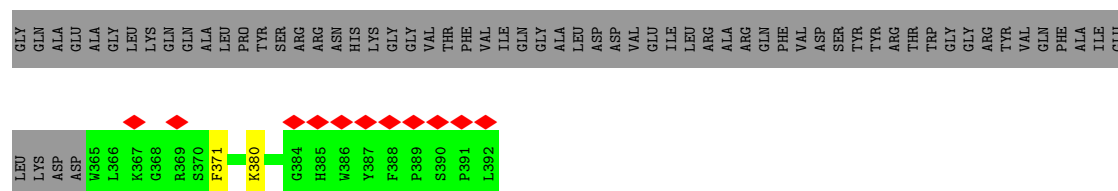
Chain c:

[illegible]

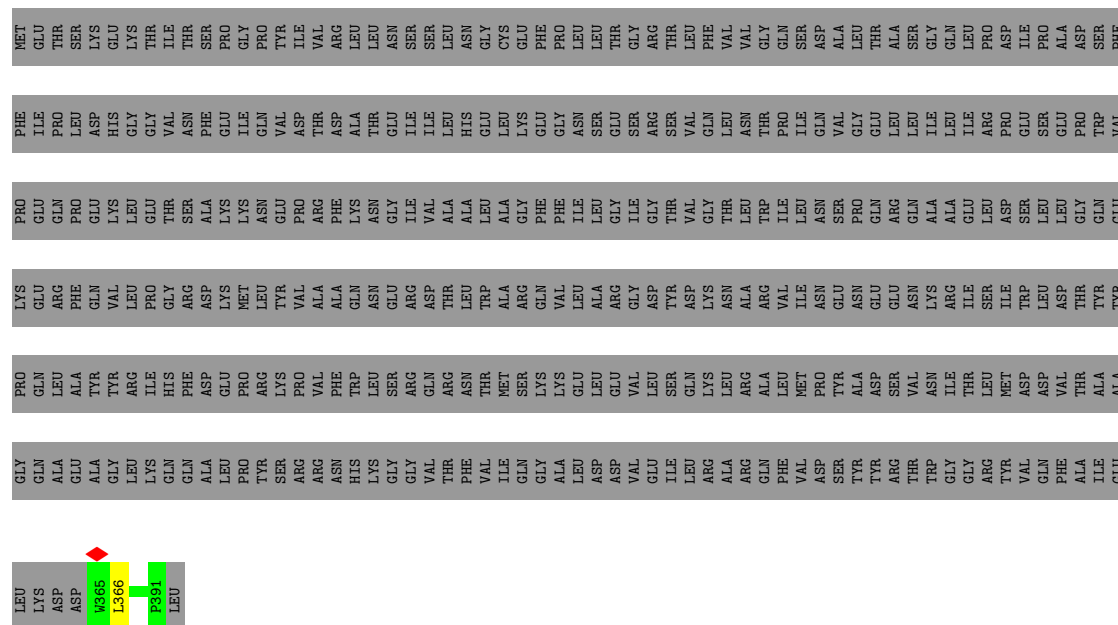
Chain d:

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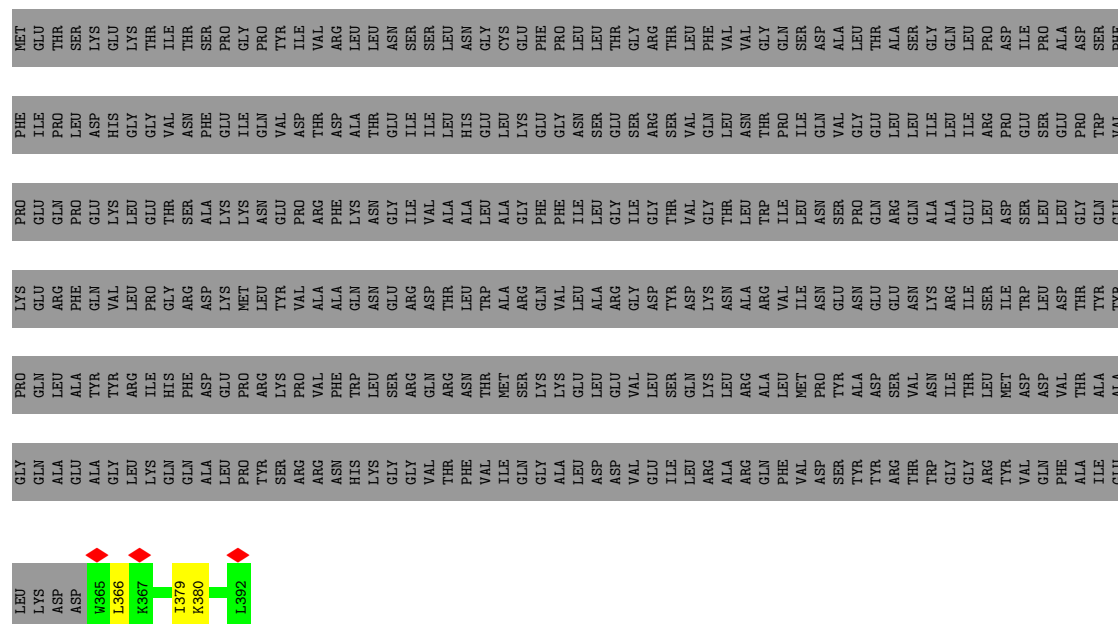




- Molecule 7: Protein PrgH



- Molecule 7: Protein PrgH

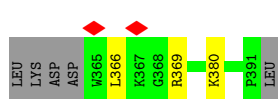


Chain i: 7% 93%



Diagram illustrating the location of the mutation (W365, L366, K367, K380, M381, L392) within the protein structure. The protein is shown as a series of colored blocks representing different regions: LEU, LYS, ASP, ASP (grey); W365, L366, K367 (green); K380, M381 (yellow); and L392 (green). Red diamonds indicate the positions of the mutations.

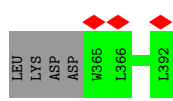
[illegible][illegible]



- Molecule 7: Protein PrgH



GLY	GLN	ALA	GLU	ALA	GLY	LEU	LYS	GLN	GLN	ALA	LEU	PRO	TYR	SER	ARG	ARG	ASN	HIS	LYS	GLY	GLY	VAL	THR	PHE	VAL	ILE	GLN	GLY	ALA	LEU	ASP	ASP	VAL	VAL	GLU	ILE	LEU	ARG	ALA	ARG	ARG	GLN	PHE	VAL	ASP	TYR	TYR	THR	THR	GLY	GLY	ARG	GLY	ARG	ALA	PHE	VAL	GLN	ILE	GLU
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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	25666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.972	Depositor
Minimum map value	-2.765	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.211	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	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	0	0.34	0/1598	0.67	0/2172
1	1	0.32	0/1605	0.68	1/2181 (0.0%)
1	2	0.30	0/1589	0.67	0/2159
1	3	0.33	0/1642	0.62	0/2230
1	4	0.34	0/1799	0.65	0/2441
2	5	0.34	0/1935	0.72	0/2647
3	6	0.27	0/414	0.71	0/565
3	7	0.30	0/657	0.70	0/897
3	8	0.32	0/657	0.74	0/897
3	9	0.32	0/660	0.66	0/900
4	A	0.33	0/1131	0.64	1/1525 (0.1%)
4	B	0.33	0/1181	0.63	0/1593
4	C	0.33	0/1131	0.62	0/1525
4	D	0.34	0/1170	0.61	0/1579
4	F	0.34	0/1131	0.64	0/1525
4	G	0.34	0/1181	0.66	2/1593 (0.1%)
4	H	0.37	0/1131	0.65	1/1525 (0.1%)
4	I	0.33	0/1181	0.60	0/1593
4	J	0.35	0/1131	0.62	0/1525
4	K	0.35	0/1181	0.65	0/1593
4	L	0.34	0/1131	0.64	0/1525
4	M	0.32	0/1170	0.62	0/1579
4	N	0.35	0/1131	0.63	0/1525
4	O	0.34	0/1181	0.62	0/1593
4	P	0.33	0/1131	0.61	0/1525
4	Q	0.34	0/1181	0.65	0/1593
5	AM	0.37	0/300	0.87	0/403
5	AN	0.28	0/646	0.63	0/870
5	AO	0.31	0/671	0.65	0/908
5	AP	0.31	0/679	0.71	0/919
5	AQ	0.28	0/679	0.64	0/919
5	AR	0.29	0/671	0.71	0/908
6	AS	0.31	0/472	0.65	0/638
6	AT	0.29	0/472	0.61	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	AU	0.32	0/472	0.61	0/638
6	AV	0.33	0/472	0.73	0/638
6	AW	0.30	0/472	0.59	0/638
6	AX	0.27	0/582	0.61	0/788
6	AY	0.32	0/623	0.67	0/846
6	AZ	0.24	0/467	0.51	0/632
6	BA	0.24	0/444	0.50	0/600
6	BB	0.28	0/395	0.67	0/533
6	BC	0.25	0/395	0.56	0/533
6	BD	0.26	0/395	0.58	0/533
6	BE	0.27	0/352	0.69	0/474
7	E	0.27	0/248	0.52	0/334
7	R	0.32	0/239	0.61	0/323
7	S	0.35	0/243	0.74	0/329
7	T	0.26	0/248	0.52	0/334
7	U	0.31	0/239	0.56	0/323
7	V	0.33	0/243	0.74	0/329
7	W	0.26	0/248	0.52	0/334
7	X	0.32	0/239	0.58	0/323
7	Y	0.34	0/243	0.71	0/329
7	Z	0.26	0/248	0.52	0/334
7	a	0.30	0/239	0.55	0/323
7	b	0.35	0/243	0.67	0/329
7	c	0.27	0/248	0.55	0/334
7	d	0.29	0/239	0.50	0/323
7	e	0.37	0/243	0.72	0/329
7	f	0.29	0/248	0.59	0/334
7	g	0.28	0/239	0.48	0/323
7	h	0.34	0/243	0.77	0/329
7	i	0.26	0/248	0.56	0/334
7	j	0.30	0/239	0.50	0/323
7	k	0.31	0/243	0.73	0/329
7	l	0.30	0/248	0.56	0/334
7	m	0.30	0/239	0.59	0/323
7	n	0.34	0/243	0.70	0/329
All	All	0.32	0/46529	0.64	5/62949 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	8	0	1
7	b	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	90	LEU	CA-CB-CG	5.32	134.93	116.30
1	1	167	LEU	N-CA-C	5.20	121.31	109.81
4	H	143	ARG	CA-CB-CG	5.19	124.47	114.10
4	G	29	PRO	CA-C-N	5.11	131.18	121.97
4	G	29	PRO	C-N-CA	5.11	131.18	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	8	41	GLN	Peptide
7	b	366	LEU	Peptide

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	0	1562	0	1597	20	0
1	1	1569	0	1613	9	0
1	2	1553	0	1598	24	0
1	3	1606	0	1649	22	0
1	4	1758	0	1806	19	0
2	5	1885	0	1931	31	0
3	6	405	0	418	2	0
3	7	644	0	685	9	0
3	8	644	0	685	9	0
3	9	647	0	692	13	0
4	A	1108	0	1103	11	0
4	B	1154	0	1163	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1108	0	1103	11	0
4	D	1146	0	1150	9	0
4	F	1108	0	1103	10	0
4	G	1154	0	1163	8	0
4	H	1108	0	1103	6	0
4	I	1154	0	1163	12	0
4	J	1108	0	1103	8	0
4	K	1154	0	1163	10	0
4	L	1108	0	1103	13	0
4	M	1146	0	1150	11	0
4	N	1108	0	1103	10	0
4	O	1154	0	1163	10	0
4	P	1108	0	1103	13	0
4	Q	1154	0	1163	11	0
5	AM	298	0	307	1	0
5	AN	644	0	654	11	0
5	AO	667	0	672	10	0
5	AP	675	0	683	8	0
5	AQ	675	0	683	10	0
5	AR	667	0	672	9	0
6	AS	466	0	470	14	0
6	AT	466	0	470	5	0
6	AU	466	0	470	10	0
6	AV	466	0	470	7	0
6	AW	466	0	470	9	0
6	AX	574	0	566	8	0
6	AY	612	0	598	11	0
6	AZ	460	0	435	9	0
6	BA	437	0	413	6	0
6	BB	388	0	369	4	0
6	BC	388	0	369	7	0
6	BD	388	0	369	9	0
6	BE	346	0	329	7	0
7	E	236	0	219	1	0
7	R	227	0	208	1	0
7	S	231	0	207	1	0
7	T	236	0	219	0	0
7	U	227	0	208	5	0
7	V	231	0	207	1	0
7	W	236	0	219	2	0
7	X	227	0	208	2	0
7	Y	231	0	207	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Z	236	0	219	0	0
7	a	227	0	208	1	0
7	b	231	0	207	1	0
7	c	236	0	219	2	0
7	d	227	0	208	2	0
7	e	231	0	207	1	0
7	f	236	0	219	1	0
7	g	227	0	208	0	0
7	h	231	0	207	3	0
7	i	236	0	219	0	0
7	j	227	0	208	5	0
7	k	231	0	207	2	0
7	l	236	0	219	1	0
7	m	227	0	208	2	0
7	n	231	0	207	0	0
All	All	45454	0	45317	421	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 5.

All (421) 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)
4:Q:39:ASP:H	4:Q:69:THR:HG22	1.55	0.72
4:I:169:GLN:HE22	4:J:115:ARG:HA	1.57	0.69
4:A:39:ASP:H	4:A:69:THR:HG22	1.59	0.68
1:O:46:ILE:HD12	2:5:97:ALA:HB1	1.77	0.65
6:AW:52:SER:HB2	6:BC:69:LYS:HD3	1.78	0.64
5:AP:31:ASP:O	5:AP:35:GLN:NE2	2.29	0.64
4:P:39:ASP:H	4:P:69:THR:HG22	1.63	0.64
4:J:149:VAL:HG21	4:J:159:VAL:HG11	1.79	0.64
4:N:149:VAL:HG21	4:N:159:VAL:HG21	1.80	0.63
6:BC:9:LEU:HD11	6:BC:65:VAL:HG23	1.79	0.63
2:5:13:VAL:HG13	5:AM:81:VAL:HG21	1.81	0.62
6:BC:12:VAL:HA	6:BC:15:LYS:HD2	1.80	0.62
4:A:137:PRO:HD2	4:Q:97:GLN:HE21	1.64	0.61
4:Q:149:VAL:HG21	4:Q:159:VAL:HG11	1.80	0.61
4:A:36:VAL:HG22	4:A:71:ASN:HD22	1.64	0.61
1:O:206:ASP:OD1	2:5:175:ASN:ND2	2.33	0.61
4:I:38:LYS:NZ	7:j:369:ARG:O	2.34	0.60
6:AZ:20:VAL:HG21	6:AZ:24:GLN:HE21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:64:PRO:HB2	2:5:160:MET:HE3	1.83	0.60
4:C:39:ASP:H	4:C:69:THR:HG22	1.66	0.60
5:AN:54:ARG:NH1	5:AN:66:GLU:OE2	2.35	0.60
4:K:38:LYS:NZ	7:m:369:ARG:O	2.33	0.60
3:9:29:ILE:HD12	3:9:51:ILE:HG22	1.84	0.60
4:A:149:VAL:HG11	4:A:159:VAL:HG21	1.84	0.59
1:2:214:GLY:HA3	3:7:83:LEU:HD13	1.84	0.59
1:3:15:THR:HG22	5:AP:90:LYS:HD2	1.85	0.59
4:D:97:GLN:HE21	4:F:137:PRO:HD2	1.68	0.59
6:AS:78:ASN:HA	6:AT:80:ARG:HH21	1.67	0.58
6:AY:55:ASN:O	6:AY:59:ASN:ND2	2.36	0.58
4:L:169:GLN:HE22	4:M:115:ARG:HA	1.67	0.58
7:f:371:PHE:HE1	7:f:380:LYS:HG2	1.69	0.58
6:AS:63:ASN:OD1	6:AY:80:ARG:NH1	2.36	0.57
1:0:97:ASP:OD2	1:0:100:ARG:NH1	2.36	0.57
3:8:60:LEU:O	3:8:64:SER:HB3	2.03	0.57
4:A:114:LEU:HD13	4:A:117:VAL:HG13	1.86	0.57
5:AQ:53:ASN:HA	5:AQ:56:GLU:HG3	1.85	0.57
1:2:25:THR:OG1	1:2:26:CYS:N	2.37	0.57
6:AX:26:GLN:OE1	6:AX:50:LYS:NZ	2.36	0.57
1:0:5:ILE:HD12	1:0:8:ILE:HD13	1.87	0.57
1:3:5:ILE:HG12	5:AQ:44:THR:HG21	1.87	0.56
6:AS:60:ALA:HB2	6:AY:76:ILE:HD13	1.87	0.56
4:A:115:ARG:HG2	4:Q:169:GLN:HE22	1.71	0.56
4:G:161:ASN:HA	4:G:164:THR:HG22	1.88	0.56
4:L:149:VAL:HG21	4:L:159:VAL:HG21	1.88	0.56
1:0:5:ILE:HG21	5:AN:41:ALA:HA	1.86	0.56
4:C:113:SER:HA	4:C:145:GLY:O	2.06	0.56
2:5:39:SER:OG	2:5:40:GLY:N	2.39	0.56
1:3:34:PHE:HB3	1:3:52:LEU:HD22	1.87	0.55
2:5:83:MET:HG2	2:5:165:PRO:HB3	1.89	0.55
2:5:206:ALA:HB1	3:9:38:THR:HG21	1.88	0.55
6:AX:16:PHE:HB3	6:AX:57:TYR:HE1	1.71	0.55
4:G:97:GLN:HE22	4:H:139:ARG:HE	1.55	0.55
4:L:33:SER:OG	4:L:34:GLY:N	2.38	0.55
1:2:30:PHE:HB3	1:2:56:ALA:HB1	1.89	0.55
7:E:365:TRP:HD1	7:E:390:SER:HB2	1.71	0.55
5:AO:31:ASP:OD1	5:AO:31:ASP:N	2.38	0.55
5:AO:66:GLU:HA	5:AO:69:ILE:HG22	1.88	0.54
6:AT:39:SER:HB2	6:BE:9:LEU:HD23	1.87	0.54
6:AV:60:ALA:HB2	6:BB:76:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:38:LYS:NZ	7:U:369:ARG:O	2.36	0.54
6:AV:59:ASN:O	6:AV:63:ASN:ND2	2.36	0.54
6:AX:21:ASP:N	6:AX:21:ASP:OD1	2.41	0.54
6:AZ:24:GLN:NE2	6:AZ:57:TYR:OH	2.41	0.54
6:AZ:72:ASP:OD1	6:AZ:72:ASP:N	2.39	0.54
6:BD:13:SER:OG	6:BD:61:GLN:NE2	2.41	0.54
1:2:218:GLN:NE2	3:7:83:LEU:O	2.41	0.54
6:AY:27:VAL:HG12	6:AY:50:LYS:HB3	1.90	0.54
4:F:114:LEU:HD21	4:F:163:ALA:HB1	1.90	0.53
1:2:38:ARG:NH1	1:2:48:SER:O	2.42	0.53
2:5:176:GLN:OE1	2:5:179:GLN:NE2	2.41	0.53
4:B:114:LEU:HD21	4:B:163:ALA:HB1	1.91	0.53
1:4:147:LEU:HA	1:4:150:TYR:HB3	1.91	0.53
1:1:143:ILE:HD12	1:1:146:LEU:HD11	1.90	0.53
1:4:36:MET:HE3	2:5:37:VAL:HG23	1.90	0.53
2:5:76:GLN:HE22	2:5:162:GLU:HG2	1.74	0.53
3:7:37:GLN:HB3	3:7:41:GLN:HA	1.90	0.53
1:3:84:ASP:OD1	1:3:87:SER:N	2.42	0.53
1:0:25:THR:OG1	1:0:26:CYS:N	2.42	0.53
1:0:62:PHE:HB3	1:0:220:MET:HE1	1.89	0.53
4:O:39:ASP:H	4:O:69:THR:HB	1.74	0.53
6:BC:9:LEU:HA	6:BC:12:VAL:HG12	1.91	0.53
1:3:29:LYS:HG3	1:3:158:ALA:HB2	1.92	0.52
4:J:141:ASP:HB3	4:J:144:LYS:HB2	1.90	0.52
1:2:48:SER:OG	1:2:51:THR:N	2.38	0.52
4:D:87:GLN:NE2	7:c:373:TYR:OH	2.42	0.52
6:AS:32:ASP:N	6:AS:32:ASP:OD1	2.38	0.52
6:AY:22:ASN:OD1	6:AY:25:THR:OG1	2.28	0.52
6:BD:55:ASN:O	6:BD:59:ASN:ND2	2.43	0.52
1:0:16:LEU:HD11	5:AN:95:VAL:HG11	1.91	0.52
1:1:200:VAL:HA	1:1:203:VAL:HG12	1.91	0.52
3:7:79:ILE:HD12	3:7:82:ALA:HB3	1.92	0.52
5:AO:28:SER:OG	5:AO:30:ASP:OD1	2.28	0.52
4:Q:36:VAL:HG23	7:X:373:TYR:HE1	1.74	0.52
4:J:40:ASP:OD2	4:J:44:THR:OG1	2.24	0.52
4:P:149:VAL:HG21	4:P:159:VAL:HG21	1.92	0.52
1:3:176:VAL:HA	1:3:179:VAL:HG12	1.93	0.51
3:9:10:LYS:HE2	3:9:74:TYR:HE1	1.75	0.51
4:H:33:SER:OG	4:H:34:GLY:N	2.41	0.51
6:AY:58:ARG:HH11	6:AY:61:GLN:HE22	1.58	0.51
6:AX:34:LEU:HD21	6:AX:47:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:371:PHE:HE1	7:W:380:LYS:HG2	1.76	0.51
4:G:60:SER:OG	4:G:61:LYS:N	2.44	0.51
3:8:10:LYS:NZ	3:8:77:GLN:OE1	2.37	0.51
6:AU:63:ASN:OD1	6:BA:80:ARG:NH1	2.43	0.51
6:BA:9:LEU:HA	6:BA:12:VAL:HG12	1.92	0.51
4:F:103:ASP:OD1	4:F:104:ALA:N	2.44	0.51
4:L:73:GLU:OE1	4:L:75:HIS:ND1	2.38	0.51
2:5:133:ALA:HA	2:5:136:VAL:HG12	1.93	0.50
3:9:3:ASP:OD1	3:9:3:ASP:N	2.43	0.50
4:I:118:SER:OG	4:I:119:LEU:N	2.44	0.50
6:AS:24:GLN:O	6:AS:28:THR:OG1	2.21	0.50
6:BD:70:ASP:HA	6:BD:73:ALA:HB3	1.93	0.50
4:I:44:THR:HB	7:j:380:LYS:HE2	1.92	0.50
4:P:33:SER:OG	4:P:34:GLY:N	2.44	0.50
2:5:233:PRO:HG2	2:5:234:VAL:HG23	1.93	0.50
3:7:33:VAL:HG21	3:7:48:PRO:HB3	1.93	0.50
5:AP:89:ARG:O	5:AP:89:ARG:NH1	2.44	0.50
4:L:40:ASP:HB2	4:L:44:THR:HG23	1.94	0.50
4:P:57:VAL:HG12	4:P:99:ILE:HB	1.93	0.50
5:AO:64:PRO:HA	5:AO:67:LEU:HB2	1.93	0.50
4:H:57:VAL:HG12	4:H:99:ILE:HB	1.92	0.50
4:K:114:LEU:HD13	4:K:117:VAL:HB	1.93	0.49
4:P:169:GLN:HE22	4:Q:115:ARG:HA	1.77	0.49
1:0:84:ASP:OD2	1:0:86:SER:OG	2.28	0.49
1:3:200:VAL:HA	1:3:203:VAL:HG22	1.95	0.49
3:9:14:LEU:HD23	3:9:17:ILE:HD11	1.95	0.49
6:AV:29:GLU:O	6:AV:33:LYS:NZ	2.46	0.49
1:4:97:ASP:OD1	1:4:140[A]:LYS:NZ	2.46	0.49
3:8:52:LYS:NZ	3:9:46:THR:OG1	2.44	0.49
5:AR:30:ASP:OD1	5:AR:30:ASP:N	2.45	0.49
4:M:114:LEU:HD11	4:M:147:PHE:HE1	1.78	0.49
4:N:44:THR:HB	7:S:380:LYS:HE2	1.95	0.49
6:AY:56:LEU:HD13	6:BE:72:ASP:HB2	1.94	0.49
4:F:57:VAL:HG12	4:F:99:ILE:HB	1.95	0.49
5:AR:47:ASP:HA	5:AR:50:THR:HG22	1.93	0.49
6:BB:76:ILE:HG13	6:BB:79:PHE:HE2	1.78	0.49
1:4:25:THR:OG1	1:4:26:CYS:N	2.46	0.48
5:AO:63:ASP:HB3	5:AO:66:GLU:HG2	1.94	0.48
5:AQ:31:ASP:OD2	5:AQ:31:ASP:N	2.45	0.48
4:A:118:SER:OG	4:A:121:GLU:OE1	2.31	0.48
4:D:60:SER:OG	4:D:61:LYS:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:39:ASP:H	4:M:69:THR:HB	1.77	0.48
6:AY:23:LEU:HG	6:AY:54:TYR:HD1	1.77	0.48
3:9:6:PHE:O	3:9:10:LYS:NZ	2.46	0.48
5:AP:26:ILE:HG21	5:AP:32:ARG:HE	1.78	0.48
6:AZ:24:GLN:OE1	6:AZ:58:ARG:NH2	2.46	0.48
6:AV:27:VAL:HG13	6:AV:50:LYS:HE3	1.96	0.48
2:5:99:GLY:HA2	2:5:102:ILE:HG22	1.95	0.48
1:2:173:ASP:HA	1:2:176:VAL:HG22	1.94	0.48
3:8:3:ASP:HA	3:8:6:PHE:HB3	1.94	0.48
5:AR:55:ILE:HG13	6:AW:64:THR:HG21	1.95	0.48
1:4:25:THR:HG23	1:4:27:PHE:H	1.78	0.48
4:O:107:MET:HE2	4:O:151:GLY:HA2	1.95	0.48
4:P:141:ASP:HB3	4:P:144:LYS:HB2	1.95	0.48
1:4:156:LYS:HG3	2:5:138:LEU:HG	1.96	0.48
4:D:38:LYS:NZ	7:d:369:ARG:O	2.41	0.48
1:4:191:VAL:O	1:4:195:THR:OG1	2.31	0.47
6:AX:31:LEU:HA	6:AX:34:LEU:HB2	1.96	0.47
4:F:149:VAL:HG21	4:F:159:VAL:HG11	1.95	0.47
7:h:366:LEU:HD11	7:h:379:ILE:HD13	1.96	0.47
1:2:93:ASP:OD1	1:2:93:ASP:N	2.46	0.47
1:3:35:VAL:HG13	1:3:38:ARG:HH21	1.79	0.47
6:AX:74:ALA:O	6:AX:78:ASN:ND2	2.47	0.47
6:BD:74:ALA:O	6:BD:78:ASN:ND2	2.47	0.47
6:AW:60:ALA:HA	6:BC:76:ILE:HD11	1.95	0.47
1:0:173:ASP:N	1:0:173:ASP:OD1	2.43	0.47
5:AQ:13:ILE:HG13	5:AQ:15:GLN:HE22	1.79	0.47
4:I:41:SER:O	4:I:41:SER:OG	2.28	0.47
3:9:29:ILE:HD11	3:9:52:LYS:HA	1.97	0.47
1:1:180:LEU:HD12	1:1:190:PRO:HB3	1.95	0.47
3:7:60:LEU:O	3:7:64:SER:OG	2.26	0.47
4:A:97:GLN:HE21	4:B:137:PRO:HD2	1.78	0.47
5:AN:75:SER:HB3	6:AT:69:LYS:HD3	1.96	0.47
6:AS:48:GLN:NE2	6:BD:78:ASN:O	2.47	0.47
6:AU:32:ASP:OD2	6:AU:32:ASP:N	2.48	0.47
4:C:116:ASN:ND2	4:C:170:ASN:O	2.48	0.47
4:G:107:MET:HE2	4:G:151:GLY:HA2	1.97	0.47
4:G:118:SER:OG	4:G:119:LEU:N	2.48	0.47
4:N:41:SER:O	4:N:41:SER:OG	2.30	0.47
4:Q:40:ASP:OD1	4:Q:44:THR:OG1	2.28	0.47
4:K:38:LYS:HG2	7:l:388:PHE:HE1	1.80	0.47
5:AO:49:GLN:HG3	5:AO:53:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AW:32:ASP:N	6:AW:32:ASP:OD1	2.48	0.47
6:BE:8:TYR:HA	6:BE:11:ASP:HB2	1.97	0.47
4:P:51:LEU:HD22	4:Q:87:GLN:HG2	1.97	0.47
1:0:49:ASN:N	1:0:49:ASN:OD1	2.48	0.47
1:3:48:SER:OG	1:3:50:MET:N	2.48	0.47
2:5:89:SER:O	2:5:89:SER:OG	2.28	0.47
6:AY:9:LEU:HD21	6:AY:65:VAL:HG13	1.97	0.47
4:N:109:ASN:OD1	4:N:109:ASN:N	2.46	0.47
3:9:2:ASP:OD1	3:9:2:ASP:N	2.48	0.46
5:AO:90:LYS:NZ	6:AU:79:PHE:O	2.37	0.46
6:BD:13:SER:HA	6:BD:16:PHE:HD2	1.79	0.46
5:AQ:72:GLU:O	5:AQ:75:SER:OG	2.31	0.46
1:4:171:VAL:HG23	3:9:15:VAL:HG13	1.96	0.46
4:I:108:ARG:HH12	4:I:153:PRO:HB3	1.80	0.46
4:L:118:SER:OG	4:L:119:LEU:N	2.49	0.46
1:4:201:LEU:HD11	3:9:71:LEU:HB3	1.96	0.46
1:0:188:MET:HE2	1:0:188:MET:HB3	1.80	0.46
1:2:191:VAL:O	1:2:195:THR:OG1	2.23	0.46
5:AQ:55:ILE:HD12	5:AQ:55:ILE:HA	1.88	0.46
6:AW:41:PRO:HG2	6:BC:54:TYR:HE2	1.81	0.46
1:3:25:THR:OG1	1:3:26:CYS:N	2.48	0.46
2:5:102:ILE:HD11	2:5:223:ALA:HB1	1.97	0.46
2:5:224:VAL:HG13	3:9:16:LEU:HD12	1.97	0.46
1:4:5:ILE:HG22	1:4:8:ILE:HD12	1.97	0.46
5:AO:51:ILE:HG22	5:AO:73:MET:HE3	1.97	0.46
5:AQ:24:THR:OG1	5:AQ:25:ASP:N	2.48	0.46
6:AU:24:GLN:O	6:AU:28:THR:OG1	2.29	0.46
4:B:141:ASP:HB3	4:B:144:LYS:HB2	1.97	0.46
6:BA:17:ASP:OD1	6:BA:57:TYR:OH	2.34	0.46
6:BA:74:ALA:O	6:BA:78:ASN:ND2	2.49	0.46
7:b:381:MET:HE1	7:c:392:LEU:HD12	1.97	0.46
1:1:190:PRO:O	1:1:194:SER:HB3	2.15	0.45
4:K:169:GLN:HE22	4:L:115:ARG:HA	1.81	0.45
4:O:36:VAL:HG23	7:U:373:TYR:HE1	1.81	0.45
4:P:114:LEU:HD13	4:P:117:VAL:HB	1.98	0.45
4:P:116:ASN:OD1	4:P:116:ASN:N	2.50	0.45
1:3:113:GLN:O	1:3:117:ASN:ND2	2.48	0.45
1:4:10:LEU:HD21	5:AQ:87:LEU:HD21	1.98	0.45
4:A:108:ARG:HG3	4:A:156:VAL:HG21	1.98	0.45
6:AW:58:ARG:HA	6:AW:58:ARG:HD3	1.73	0.45
4:K:76:ASP:HA	4:K:77:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:213:LYS:HA	1:0:216:ILE:HG22	1.97	0.45
4:L:97:GLN:HE22	4:M:139:ARG:HE	1.65	0.45
3:8:25:VAL:HA	3:8:28:ILE:HG12	1.98	0.45
4:P:58:ILE:HD13	4:Q:105:SER:HA	1.97	0.45
7:m:380:LYS:HE3	7:m:380:LYS:HB3	1.66	0.45
1:3:192:THR:HG23	1:3:193:ILE:HG13	1.98	0.45
4:F:63:ALA:HB2	4:F:103:ASP:HB2	1.99	0.45
7:U:380:LYS:HE3	7:U:380:LYS:HB3	1.70	0.45
4:D:168:LYS:HA	4:D:168:LYS:HD3	1.76	0.45
4:F:60:SER:OG	4:F:61:LYS:N	2.48	0.45
7:h:366:LEU:HD13	7:h:366:LEU:HA	1.72	0.45
2:5:52:LEU:HD23	2:5:52:LEU:HA	1.87	0.45
2:5:166:SER:O	2:5:166:SER:OG	2.32	0.45
5:AR:69:ILE:HG22	5:AR:73:MET:HE1	1.99	0.45
6:AU:76:ILE:H	6:AU:76:ILE:HG12	1.42	0.45
1:4:188:MET:HE3	1:4:189:SER:H	1.82	0.45
4:N:76:ASP:OD1	4:N:76:ASP:N	2.49	0.45
4:A:76:ASP:OD1	4:A:76:ASP:N	2.50	0.45
6:AZ:55:ASN:HA	6:BE:71:ILE:HD11	1.99	0.45
6:AZ:72:ASP:HA	6:AZ:75:ILE:HD12	1.99	0.45
7:d:372:GLN:O	7:d:377:GLY:HA2	2.16	0.45
4:K:125:PHE:HD1	4:L:141:ASP:HB2	1.82	0.45
1:1:113:GLN:HA	1:1:116:GLU:HG3	1.99	0.44
1:3:82:PHE:HB2	1:3:88:LEU:HG	1.99	0.44
4:B:36:VAL:HG23	7:a:373:TYR:HE1	1.81	0.44
4:I:28:ILE:HD11	7:j:389:PRO:HG3	1.99	0.44
4:M:114:LEU:HD21	4:M:163:ALA:HB1	1.98	0.44
4:O:114:LEU:HD21	4:O:163:ALA:HB1	1.99	0.44
1:0:186:MET:HE3	1:0:186:MET:HB3	1.85	0.44
3:8:37:GLN:HE21	3:8:43:GLN:HA	1.82	0.44
4:N:114:LEU:HD13	4:N:117:VAL:HG13	2.00	0.44
1:0:86:SER:HA	1:0:89:SER:HB3	1.99	0.44
2:5:56:PRO:HD3	2:5:154:TYR:CD2	2.52	0.44
4:I:28:ILE:HG12	7:j:379:ILE:HD11	1.98	0.44
5:AN:63:ASP:OD1	5:AN:66:GLU:N	2.44	0.44
6:BD:9:LEU:HD11	6:BD:65:VAL:HG13	1.99	0.44
4:H:138:LEU:HD22	4:H:149:VAL:HG12	1.99	0.44
3:8:14:LEU:HA	3:8:17:ILE:HG22	1.99	0.44
4:C:40:ASP:HB3	4:C:44:THR:HG23	1.99	0.44
4:D:52:GLN:HG3	4:D:74:PHE:HB2	2.00	0.44
1:4:52:LEU:HA	1:4:55:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:57:VAL:HG12	4:N:99:ILE:HB	1.98	0.44
1:2:173:ASP:OD1	1:2:173:ASP:N	2.43	0.44
4:B:111:VAL:HG22	4:B:148:TYR:HD1	1.83	0.44
6:BD:64:THR:HA	6:BD:67:VAL:HG22	2.00	0.44
1:2:7:LEU:HD21	5:AO:83:MET:HE1	2.00	0.44
6:AW:22:ASN:HD21	6:BC:5:TRP:HE1	1.63	0.44
4:P:87:GLN:HE22	7:U:376:GLU:HB3	1.83	0.44
1:2:48:SER:OG	1:2:50:MET:N	2.49	0.43
2:5:202:LEU:HD12	2:5:202:LEU:HA	1.91	0.43
6:BE:9:LEU:HA	6:BE:12:VAL:HG22	1.99	0.43
1:2:176:VAL:HA	1:2:179:VAL:HG22	2.00	0.43
5:AR:25:ASP:OD1	4:C:61:LYS:NZ	2.49	0.43
4:J:38:LYS:HA	4:J:69:THR:HG23	1.99	0.43
1:0:208:TRP:HB2	2:5:175:ASN:CG	2.43	0.43
5:AP:75:SER:HA	6:AV:69:LYS:HE3	2.00	0.43
4:C:107:MET:HE2	4:C:151:GLY:HA2	2.01	0.43
4:J:97:GLN:HE22	4:K:139:ARG:HE	1.66	0.43
4:N:144:LYS:HD2	4:N:144:LYS:HA	1.89	0.43
3:7:66:TRP:HA	3:7:69:GLU:HG2	1.98	0.43
6:AZ:21:ASP:OD1	6:AZ:21:ASP:N	2.45	0.43
4:L:144:LYS:HD3	4:L:144:LYS:HA	1.87	0.43
4:P:50:ALA:HB2	4:P:57:VAL:HG22	2.01	0.43
1:1:52:LEU:HA	1:1:55:VAL:HG22	2.00	0.43
1:2:106:TYR:OH	1:2:218:GLN:O	2.31	0.43
4:G:63:ALA:HB2	4:G:103:ASP:HB2	1.99	0.43
4:H:42:LEU:HD22	4:H:66:LYS:HB2	2.00	0.43
4:I:76:ASP:HA	4:I:77:PRO:HD3	1.80	0.43
4:L:63:ALA:HB2	4:L:103:ASP:HB3	2.01	0.43
4:H:107:MET:HE2	4:H:151:GLY:HA2	2.00	0.43
4:N:114:LEU:HD21	4:N:163:ALA:HB1	2.00	0.43
1:0:97:ASP:HA	1:0:100:ARG:HB3	2.01	0.43
1:3:27:PHE:O	1:3:31:SER:OG	2.27	0.43
5:AP:16:ALA:HB2	4:K:112:VAL:HG23	2.00	0.43
6:AT:58:ARG:HA	6:AT:58:ARG:HD3	1.75	0.43
2:5:83:MET:HE3	2:5:87:LEU:HD21	2.01	0.43
5:AP:86:THR:HG22	6:AU:78:ASN:HD21	1.83	0.43
6:AS:58:ARG:HA	6:AS:58:ARG:HD3	1.87	0.43
4:M:44:THR:HB	7:R:380:LYS:HE2	2.00	0.43
3:6:6:PHE:HE1	3:6:77:GLN:HE22	1.66	0.43
5:AR:57:ASP:OD1	5:AR:60:LEU:N	2.52	0.43
6:BA:75:ILE:HA	6:BA:78:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:168:LYS:HE2	4:G:168:LYS:HB3	1.77	0.43
1:4:167:LEU:HD23	1:4:167:LEU:HA	1.85	0.42
4:A:156:VAL:HA	4:A:159:VAL:HG22	2.01	0.42
7:W:365:TRP:HD1	7:W:390:SER:HB2	1.84	0.42
1:3:172:VAL:HA	1:3:175:VAL:HG12	2.01	0.42
2:5:56:PRO:HG3	2:5:154:TYR:HB3	2.01	0.42
5:AP:13:ILE:C	4:K:115:ARG:HH12	2.27	0.42
7:k:380:LYS:HE3	7:k:380:LYS:HB3	1.80	0.42
6:AS:56:LEU:HD13	6:AS:56:LEU:HA	1.87	0.42
1:0:59:LEU:HD23	1:0:59:LEU:HA	1.91	0.42
4:I:36:VAL:HG23	7:j:373:TYR:HE1	1.84	0.42
1:2:90:LYS:HE3	1:2:90:LYS:HB3	1.82	0.42
1:3:161:ILE:HG13	3:8:82:ALA:HB1	2.02	0.42
6:AS:76:ILE:H	6:AS:76:ILE:HG12	1.48	0.42
1:2:176:VAL:HG21	1:2:194:SER:HB2	2.01	0.42
6:AU:48:GLN:HA	6:AU:51:LEU:HD23	2.02	0.42
6:AU:58:ARG:HD3	6:AU:58:ARG:HA	1.78	0.42
4:M:120:ASN:O	4:M:124:ASN:ND2	2.48	0.42
1:2:163:PHE:HB2	1:3:199:LEU:HD11	2.02	0.42
1:3:97:ASP:OD1	1:3:100:ARG:NH1	2.52	0.42
1:4:152:LEU:HB3	2:5:143:LEU:HD13	2.01	0.42
5:AN:48:LYS:O	5:AN:52:THR:OG1	2.26	0.42
1:1:96:LEU:HD11	1:1:100:ARG:HH21	1.85	0.42
5:AO:15:GLN:HB2	4:M:165:MET:HE2	2.02	0.42
6:AS:60:ALA:O	6:AS:64:THR:OG1	2.35	0.42
4:F:116:ASN:OD1	4:F:116:ASN:N	2.53	0.42
2:5:51:ALA:HA	2:5:54:VAL:HG22	2.01	0.42
6:AS:26:GLN:HG3	6:AS:50:LYS:HZ1	1.85	0.42
4:O:63:ALA:HB2	4:O:103:ASP:HB3	2.01	0.42
7:V:380:LYS:HE2	7:V:380:LYS:HB3	1.87	0.42
5:AQ:42:ILE:HD13	5:AQ:42:ILE:HA	1.92	0.42
4:B:76:ASP:HA	4:B:77:PRO:HD3	1.80	0.42
4:Q:158:MET:HE3	4:Q:158:MET:HB3	1.88	0.42
7:X:372:GLN:O	7:X:377:GLY:HA2	2.19	0.42
1:3:160:LYS:HB2	1:4:203:VAL:HG21	2.02	0.41
2:5:95:MET:HG3	2:5:129:LEU:HB3	2.02	0.41
6:AS:69:LYS:HD3	6:AS:69:LYS:HA	1.78	0.41
4:C:84:LEU:O	4:C:88:LEU:HB2	2.20	0.41
7:U:372:GLN:O	7:U:377:GLY:HA2	2.20	0.41
1:2:36:MET:HE3	1:2:36:MET:HB2	1.86	0.41
1:2:171:VAL:HG23	3:7:15:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AU:56:LEU:HD13	6:AU:56:LEU:HA	1.86	0.41
5:AR:85:SER:OG	5:AR:86:THR:N	2.53	0.41
6:AX:37:LYS:HA	6:AX:37:LYS:HD3	1.82	0.41
4:D:39:ASP:H	4:D:69:THR:HB	1.84	0.41
4:F:152:PRO:HA	4:F:153:PRO:HD3	1.96	0.41
4:I:107:MET:HE2	4:I:151:GLY:HA2	2.02	0.41
1:O:111:LEU:HD23	1:O:115:PHE:HE2	1.85	0.41
6:BB:72:ASP:HA	6:BB:75:ILE:HG12	2.02	0.41
4:Q:141:ASP:HB3	4:Q:144:LYS:HB2	2.01	0.41
2:5:92:PHE:HB3	2:5:130:ASN:HD21	1.86	0.41
5:AN:67:LEU:HD23	5:AN:67:LEU:HA	1.90	0.41
6:AS:49:SER:OG	6:AY:10:ASP:OD1	2.30	0.41
6:AT:59:ASN:O	6:AT:63:ASN:ND2	2.43	0.41
4:B:109:ASN:OD1	4:B:109:ASN:N	2.54	0.41
6:BE:12:VAL:HA	6:BE:15:LYS:HE2	2.02	0.41
4:D:40:ASP:OD2	4:D:44:THR:OG1	2.31	0.41
4:K:116:ASN:OD1	4:K:116:ASN:N	2.53	0.41
1:2:186:MET:SD	1:2:186:MET:N	2.91	0.41
5:AR:83:MET:HG3	6:AX:76:ILE:HD12	2.02	0.41
4:C:141:ASP:HB3	4:C:144:LYS:HB2	2.03	0.41
4:I:144:LYS:HA	4:I:144:LYS:HD3	1.88	0.41
4:M:97:GLN:OE1	4:N:150:SER:OG	2.37	0.41
4:O:166:MET:HE2	4:O:166:MET:HB3	1.95	0.41
7:k:381:MET:HE3	7:k:381:MET:HB3	1.91	0.41
2:5:192:LEU:HD22	2:5:219:LYS:HG2	2.02	0.41
3:7:25:VAL:HA	3:7:28:ILE:HG22	2.02	0.41
6:AW:24:GLN:O	6:AW:28:THR:OG1	2.33	0.41
4:O:109:ASN:OD1	4:O:109:ASN:N	2.52	0.41
1:2:103:LEU:HD12	1:2:103:LEU:HA	1.89	0.41
5:AQ:58:PRO:HB2	6:BB:5:TRP:CZ2	2.55	0.41
6:AV:27:VAL:O	6:AV:50:LYS:NZ	2.51	0.41
6:BE:14:ALA:O	6:BE:18:THR:OG1	2.31	0.41
4:J:113:SER:HA	4:J:146:THR:HA	2.03	0.41
4:M:152:PRO:HA	4:M:153:PRO:HD3	1.96	0.41
4:O:49:MET:HE2	4:O:49:MET:HB3	1.82	0.41
1:3:36:MET:HE2	1:3:36:MET:HB3	1.81	0.41
3:8:35:LEU:HA	3:8:38:THR:HG22	2.03	0.41
5:AN:81:VAL:HA	5:AN:84:VAL:HG12	2.03	0.41
5:AR:19:ILE:HG22	4:C:161:ASN:HD22	1.84	0.41
6:AV:31:LEU:HD13	6:BA:15:LYS:HE3	2.03	0.41
6:AZ:62:SER:HA	6:AZ:65:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:116:ASN:OD1	4:L:116:ASN:N	2.54	0.41
4:P:113:SER:HB2	4:P:146:THR:HG22	2.03	0.41
7:e:380:LYS:HE3	7:e:380:LYS:HB3	1.82	0.41
7:h:380:LYS:HB3	7:h:380:LYS:HE3	1.86	0.41
1:1:171:VAL:HG13	3:6:15:VAL:HG12	2.02	0.41
1:4:8:ILE:HG12	6:AW:75:ILE:HG21	2.02	0.41
1:4:96:LEU:HD23	1:4:96:LEU:HA	1.92	0.41
1:4:132:LYS:HA	1:4:132:LYS:HD3	1.79	0.41
3:9:37:GLN:HE21	3:9:47:LEU:HD23	1.85	0.41
6:AS:59:ASN:O	6:AS:63:ASN:ND2	2.42	0.41
4:O:27:LYS:HB2	4:O:27:LYS:HE3	1.89	0.41
1:3:194:SER:O	1:3:198:LYS:N	2.54	0.40
1:2:20:ILE:HD13	1:2:20:ILE:HA	1.92	0.40
1:2:200:VAL:HA	1:2:203:VAL:HG12	2.02	0.40
6:AU:35:ALA:HB1	6:AZ:19:GLY:HA3	2.03	0.40
6:AY:40:ASP:HA	6:AY:41:PRO:HD3	1.94	0.40
6:BD:7:GLY:H	6:BD:10:ASP:HB2	1.85	0.40
4:C:60:SER:OG	4:C:61:LYS:N	2.54	0.40
4:F:109:ASN:OD1	4:F:109:ASN:N	2.54	0.40
1:2:113:GLN:HA	1:2:116:GLU:HG2	2.01	0.40
2:5:227:MET:HE3	2:5:227:MET:HB2	1.89	0.40
5:AN:51:ILE:HA	5:AN:54:ARG:HB3	2.03	0.40
5:AN:63:ASP:OD2	5:AN:65:LYS:NZ	2.55	0.40
4:B:114:LEU:HD13	4:B:117:VAL:HG13	2.03	0.40
4:J:112:VAL:HG11	4:J:160:VAL:HG23	2.03	0.40
4:M:158:MET:HB3	4:M:158:MET:HE3	1.80	0.40
1:0:187:MET:HA	1:1:187:MET:HE3	2.04	0.40
1:3:101:ASP:OD1	1:3:140:LYS:NZ	2.47	0.40
4:D:158:MET:HB3	4:D:158:MET:HE3	1.89	0.40
4:G:40:ASP:HB3	4:G:44:THR:HG23	2.04	0.40
4:L:55:GLU:HG3	4:L:94:PHE:CE1	2.56	0.40
2:5:91:PRO:HA	2:5:94:VAL:HG12	2.04	0.40
5:AN:85:SER:OG	5:AN:86:THR:N	2.55	0.40
4:C:152:PRO:HA	4:C:153:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	0	195/224 (87%)	189 (97%)	5 (3%)	1 (0%)	24	57
1	1	195/224 (87%)	186 (95%)	8 (4%)	1 (0%)	24	57
1	2	193/224 (86%)	187 (97%)	5 (3%)	1 (0%)	24	57
1	3	200/224 (89%)	195 (98%)	5 (2%)	0	100	100
1	4	220/224 (98%)	209 (95%)	11 (5%)	0	100	100
2	5	243/263 (92%)	224 (92%)	19 (8%)	0	100	100
3	6	49/86 (57%)	46 (94%)	3 (6%)	0	100	100
3	7	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
3	8	82/86 (95%)	80 (98%)	1 (1%)	1 (1%)	10	40
3	9	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
4	A	137/562 (24%)	136 (99%)	1 (1%)	0	100	100
4	B	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
4	C	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	D	142/562 (25%)	138 (97%)	4 (3%)	0	100	100
4	F	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
4	G	143/562 (25%)	137 (96%)	6 (4%)	0	100	100
4	H	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	I	143/562 (25%)	141 (99%)	2 (1%)	0	100	100
4	J	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	K	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
4	L	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
4	M	142/562 (25%)	137 (96%)	5 (4%)	0	100	100
4	N	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	O	143/562 (25%)	140 (98%)	3 (2%)	0	100	100
4	P	137/562 (24%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
5	AM	37/101 (37%)	37 (100%)	0	0	100	100
5	AN	79/101 (78%)	79 (100%)	0	0	100	100
5	AO	86/101 (85%)	84 (98%)	2 (2%)	0	100	100
5	AP	87/101 (86%)	87 (100%)	0	0	100	100
5	AQ	87/101 (86%)	87 (100%)	0	0	100	100
5	AR	86/101 (85%)	83 (96%)	3 (4%)	0	100	100
6	AS	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AT	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AU	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AV	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AW	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AX	71/80 (89%)	68 (96%)	3 (4%)	0	100	100
6	AY	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
6	AZ	53/80 (66%)	52 (98%)	1 (2%)	0	100	100
6	BA	50/80 (62%)	47 (94%)	3 (6%)	0	100	100
6	BB	44/80 (55%)	43 (98%)	1 (2%)	0	100	100
6	BC	44/80 (55%)	44 (100%)	0	0	100	100
6	BD	44/80 (55%)	43 (98%)	1 (2%)	0	100	100
6	BE	39/80 (49%)	37 (95%)	2 (5%)	0	100	100
7	E	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	R	25/392 (6%)	25 (100%)	0	0	100	100
7	S	26/392 (7%)	20 (77%)	6 (23%)	0	100	100
7	T	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	U	25/392 (6%)	24 (96%)	1 (4%)	0	100	100
7	V	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	W	26/392 (7%)	23 (88%)	3 (12%)	0	100	100
7	X	25/392 (6%)	24 (96%)	1 (4%)	0	100	100
7	Y	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	Z	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	a	25/392 (6%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	b	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	c	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	d	25/392 (6%)	25 (100%)	0	0	100	100
7	e	26/392 (7%)	18 (69%)	8 (31%)	0	100	100
7	f	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	g	25/392 (6%)	25 (100%)	0	0	100	100
7	h	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	i	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	j	25/392 (6%)	25 (100%)	0	0	100	100
7	k	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	l	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	m	25/392 (6%)	24 (96%)	1 (4%)	0	100	100
7	n	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
All	All	5563/21773 (26%)	5329 (96%)	230 (4%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	8	42	LEU
1	0	49	ASN
1	1	49	ASN
1	2	47	PRO

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	0	175/199 (88%)	172 (98%)	3 (2%)	53	67
1	1	177/199 (89%)	177 (100%)	0	100	100
1	2	175/199 (88%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	180/199 (90%)	179 (99%)	1 (1%)	78	79
1	4	197/199 (99%)	197 (100%)	0	100	100
2	5	205/219 (94%)	204 (100%)	1 (0%)	81	81
3	6	41/71 (58%)	41 (100%)	0	100	100
3	7	69/71 (97%)	69 (100%)	0	100	100
3	8	69/71 (97%)	69 (100%)	0	100	100
3	9	70/71 (99%)	70 (100%)	0	100	100
4	A	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	B	125/477 (26%)	125 (100%)	0	100	100
4	C	119/477 (25%)	119 (100%)	0	100	100
4	D	124/477 (26%)	123 (99%)	1 (1%)	73	76
4	F	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	G	125/477 (26%)	124 (99%)	1 (1%)	73	76
4	H	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	I	125/477 (26%)	125 (100%)	0	100	100
4	J	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	K	125/477 (26%)	125 (100%)	0	100	100
4	L	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	M	124/477 (26%)	123 (99%)	1 (1%)	73	76
4	N	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	O	125/477 (26%)	125 (100%)	0	100	100
4	P	119/477 (25%)	118 (99%)	1 (1%)	73	76
4	Q	125/477 (26%)	124 (99%)	1 (1%)	73	76
5	AM	34/88 (39%)	33 (97%)	1 (3%)	37	58
5	AN	71/88 (81%)	71 (100%)	0	100	100
5	AO	76/88 (86%)	76 (100%)	0	100	100
5	AP	77/88 (88%)	76 (99%)	1 (1%)	61	71
5	AQ	77/88 (88%)	77 (100%)	0	100	100
5	AR	76/88 (86%)	76 (100%)	0	100	100
6	AS	50/67 (75%)	46 (92%)	4 (8%)	11	36
6	AT	50/67 (75%)	44 (88%)	6 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AU	50/67 (75%)	45 (90%)	5 (10%)	7	28
6	AV	50/67 (75%)	45 (90%)	5 (10%)	7	28
6	AW	50/67 (75%)	44 (88%)	6 (12%)	5	21
6	AX	62/67 (92%)	62 (100%)	0	100	100
6	AY	66/67 (98%)	66 (100%)	0	100	100
6	AZ	51/67 (76%)	51 (100%)	0	100	100
6	BA	48/67 (72%)	47 (98%)	1 (2%)	47	64
6	BB	42/67 (63%)	42 (100%)	0	100	100
6	BC	42/67 (63%)	42 (100%)	0	100	100
6	BD	42/67 (63%)	42 (100%)	0	100	100
6	BE	37/67 (55%)	37 (100%)	0	100	100
7	E	23/337 (7%)	23 (100%)	0	100	100
7	R	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	S	21/337 (6%)	21 (100%)	0	100	100
7	T	23/337 (7%)	23 (100%)	0	100	100
7	U	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	V	21/337 (6%)	20 (95%)	1 (5%)	23	47
7	W	23/337 (7%)	23 (100%)	0	100	100
7	X	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	Y	21/337 (6%)	21 (100%)	0	100	100
7	Z	23/337 (7%)	23 (100%)	0	100	100
7	a	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	b	21/337 (6%)	21 (100%)	0	100	100
7	c	23/337 (7%)	23 (100%)	0	100	100
7	d	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	e	21/337 (6%)	21 (100%)	0	100	100
7	f	23/337 (7%)	23 (100%)	0	100	100
7	g	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	h	21/337 (6%)	21 (100%)	0	100	100
7	i	23/337 (7%)	23 (100%)	0	100	100
7	j	22/337 (6%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	k	21/337 (6%)	21 (100%)	0	100	100
7	l	23/337 (7%)	23 (100%)	0	100	100
7	m	22/337 (6%)	21 (96%)	1 (4%)	24	48
7	n	21/337 (6%)	21 (100%)	0	100	100
All	All	4887/18617 (26%)	4834 (99%)	53 (1%)	63	73

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	46	ILE
1	0	81	THR
1	0	152	LEU
1	3	211	LEU
2	5	68	VAL
4	A	111	VAL
5	AM	87	LEU
5	AP	98	LEU
6	AS	28	THR
6	AS	56	LEU
6	AS	64	THR
6	AS	76	ILE
6	AT	28	THR
6	AT	51	LEU
6	AT	56	LEU
6	AT	64	THR
6	AT	72	ASP
6	AT	76	ILE
6	AU	28	THR
6	AU	51	LEU
6	AU	56	LEU
6	AU	64	THR
6	AU	76	ILE
6	AV	31	LEU
6	AV	44	LEU
6	AV	56	LEU
6	AV	67	VAL
6	AV	76	ILE
6	AW	28	THR
6	AW	44	LEU
6	AW	51	LEU
6	AW	56	LEU

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Mol	Chain	Res	Type
6	AW	64	THR
6	AW	76	ILE
6	BA	20	VAL
4	D	40	ASP
4	F	111	VAL
4	G	121	GLU
4	H	36	VAL
4	J	40	ASP
4	L	111	VAL
4	M	126	LEU
4	N	111	VAL
4	P	111	VAL
4	Q	40	ASP
7	R	366	LEU
7	U	366	LEU
7	V	366	LEU
7	X	366	LEU
7	a	366	LEU
7	d	366	LEU
7	g	366	LEU
7	m	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	3	ASN
1	2	44	GLN
1	2	69	HIS
1	3	117	ASN
1	4	44	GLN
1	4	91	HIS
2	5	76	GLN
2	5	104	ASN
2	5	105	GLN
2	5	130	ASN
2	5	139	GLN
2	5	161	ASN
2	5	210	ASN
2	5	238	ASN
3	7	37	GLN
3	8	9	ASN
3	8	37	GLN

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Mol	Chain	Res	Type
3	8	41	GLN
3	8	43	GLN
3	9	9	ASN
3	9	37	GLN
4	A	71	ASN
4	A	87	GLN
5	AN	71	GLN
5	AN	78	ASN
5	AO	53	ASN
5	AP	49	GLN
5	AP	53	ASN
5	AP	59	ASN
5	AP	71	GLN
5	AQ	59	ASN
5	AQ	71	GLN
5	AR	53	ASN
5	AR	71	GLN
6	AS	26	GLN
6	AS	48	GLN
6	AT	26	GLN
6	AT	61	GLN
6	AT	78	ASN
6	AU	78	ASN
6	AW	22	ASN
6	AW	63	ASN
6	AX	61	GLN
6	AX	78	ASN
6	AY	63	ASN
6	AZ	26	GLN
6	AZ	78	ASN
4	B	75	HIS
4	B	87	GLN
4	B	170	ASN
6	BB	78	ASN
6	BC	55	ASN
6	BD	59	ASN
6	BD	61	GLN
6	BD	78	ASN
6	BE	61	GLN
4	C	123	ASN
4	C	161	ASN
4	D	87	GLN

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Mol	Chain	Res	Type
4	F	71	ASN
4	G	97	GLN
4	G	123	ASN
4	G	124	ASN
4	G	169	GLN
4	G	170	ASN
4	H	97	GLN
4	I	169	GLN
4	I	170	ASN
4	J	97	GLN
4	J	124	ASN
4	K	123	ASN
4	L	71	ASN
4	L	87	GLN
4	L	123	ASN
4	L	169	GLN
4	M	78	ASN
4	M	87	GLN
4	M	123	ASN
4	M	142	ASN
4	M	161	ASN
4	M	169	GLN
4	N	123	ASN
4	N	169	GLN
4	N	170	ASN
4	P	71	ASN
4	P	87	GLN
4	P	169	GLN
4	Q	97	GLN
4	Q	169	GLN
7	g	372	GLN
7	l	385	HIS
7	m	372	GLN

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.

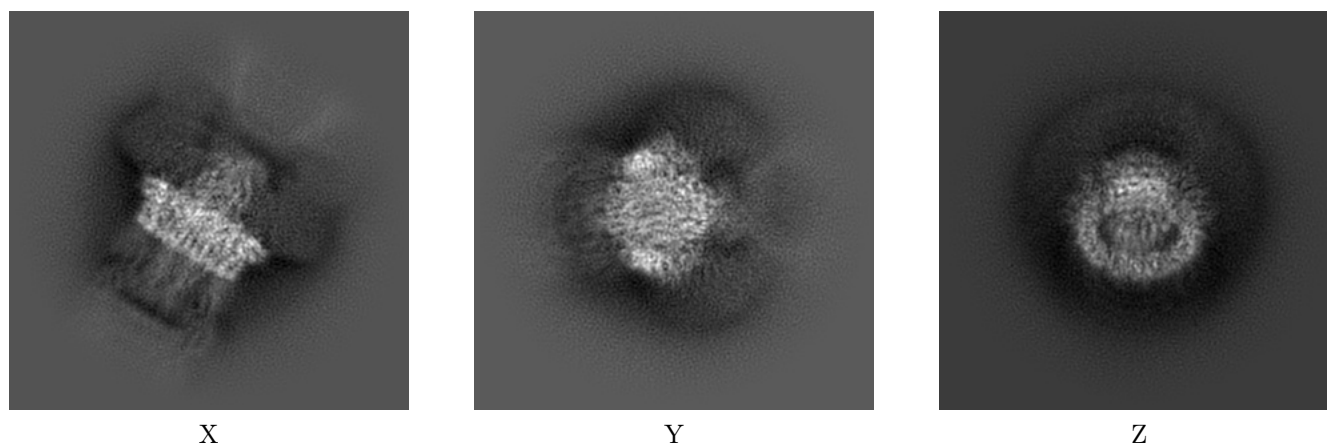
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20317. 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](#)

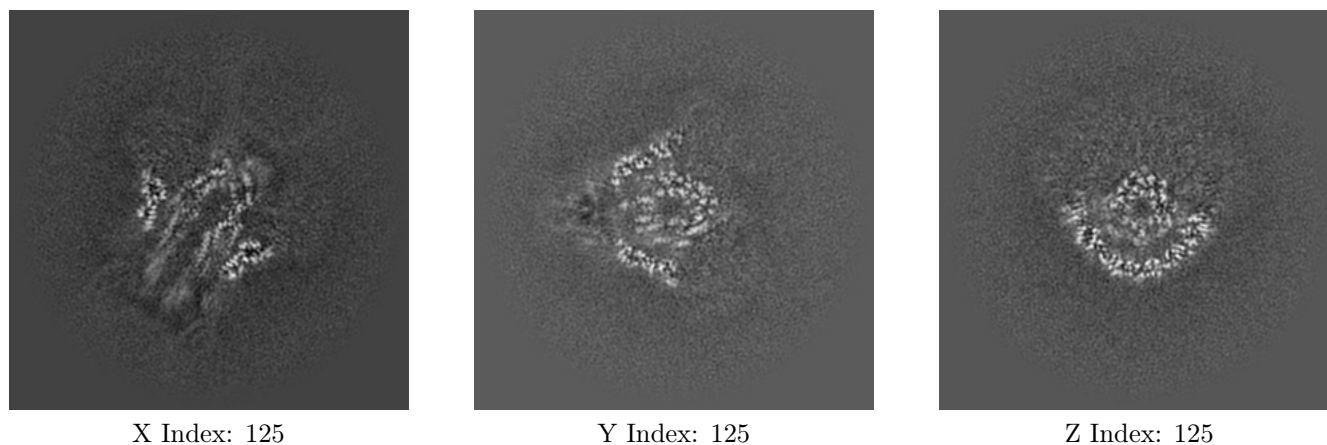
6.1.1 Primary map



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

6.2 Central slices [i](#)

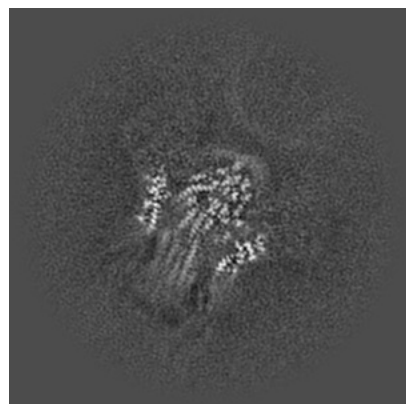
6.2.1 Primary map



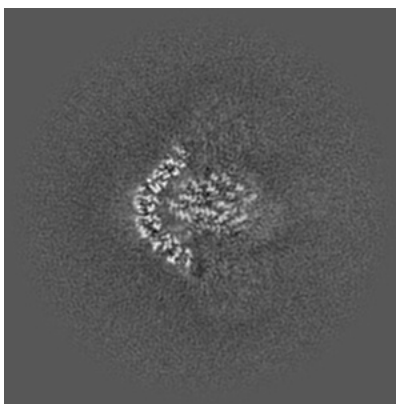
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

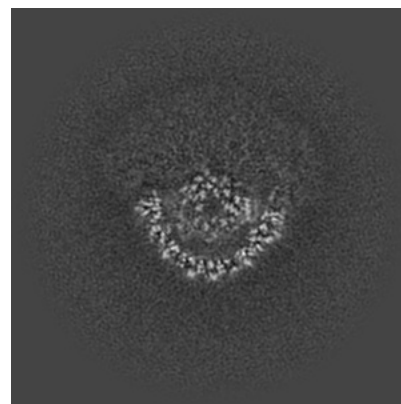
6.3.1 Primary map



X Index: 134



Y Index: 139

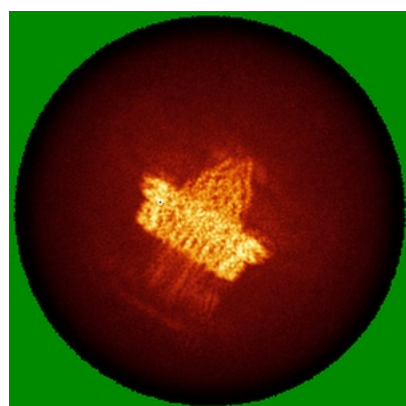


Z Index: 123

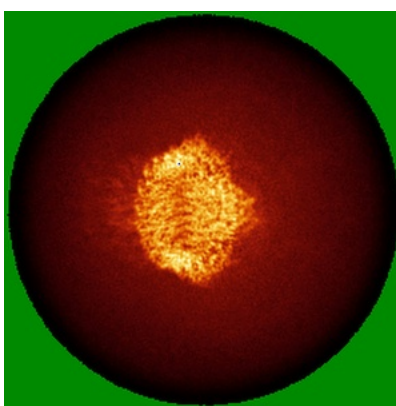
The images above show the largest variance slices of the map in three orthogonal directions.

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

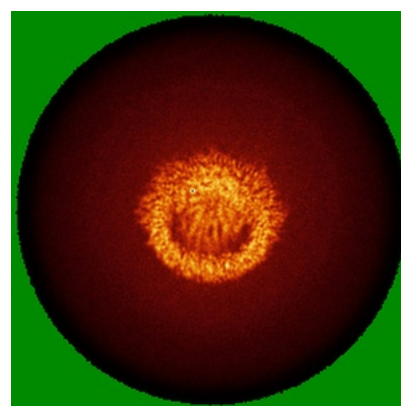
6.4.1 Primary map



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

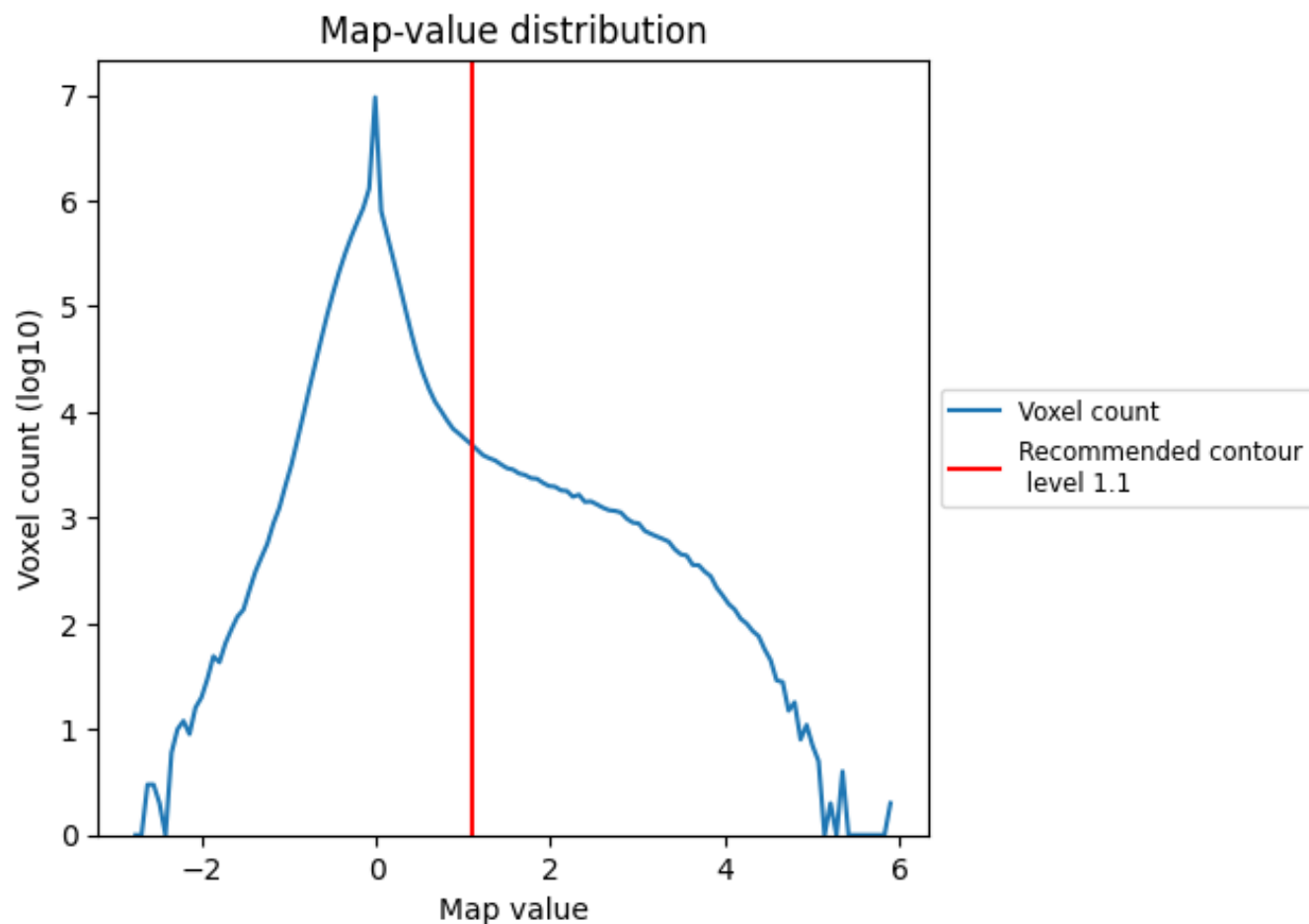
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

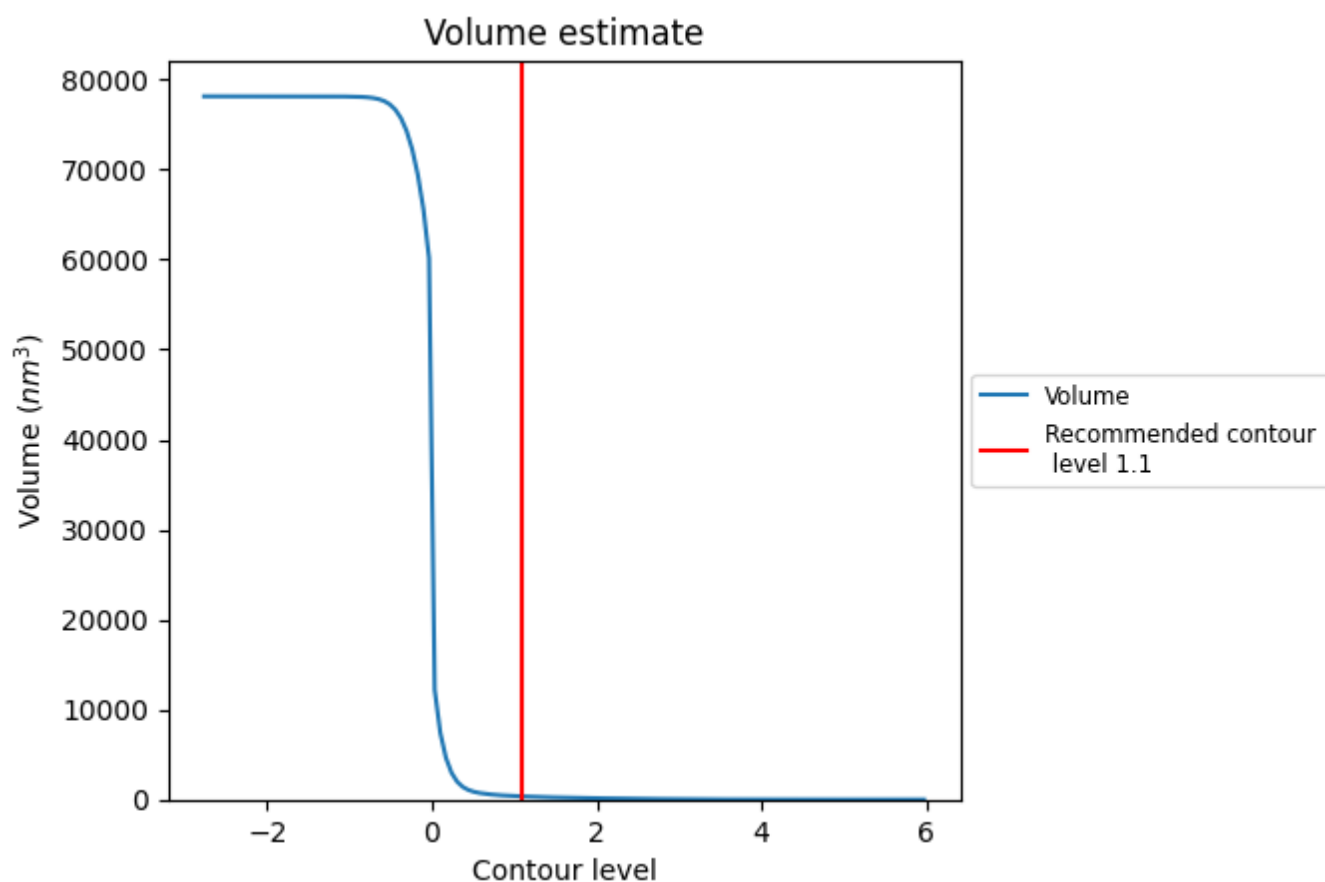
This section contains the results of statistical analysis of the map.

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.

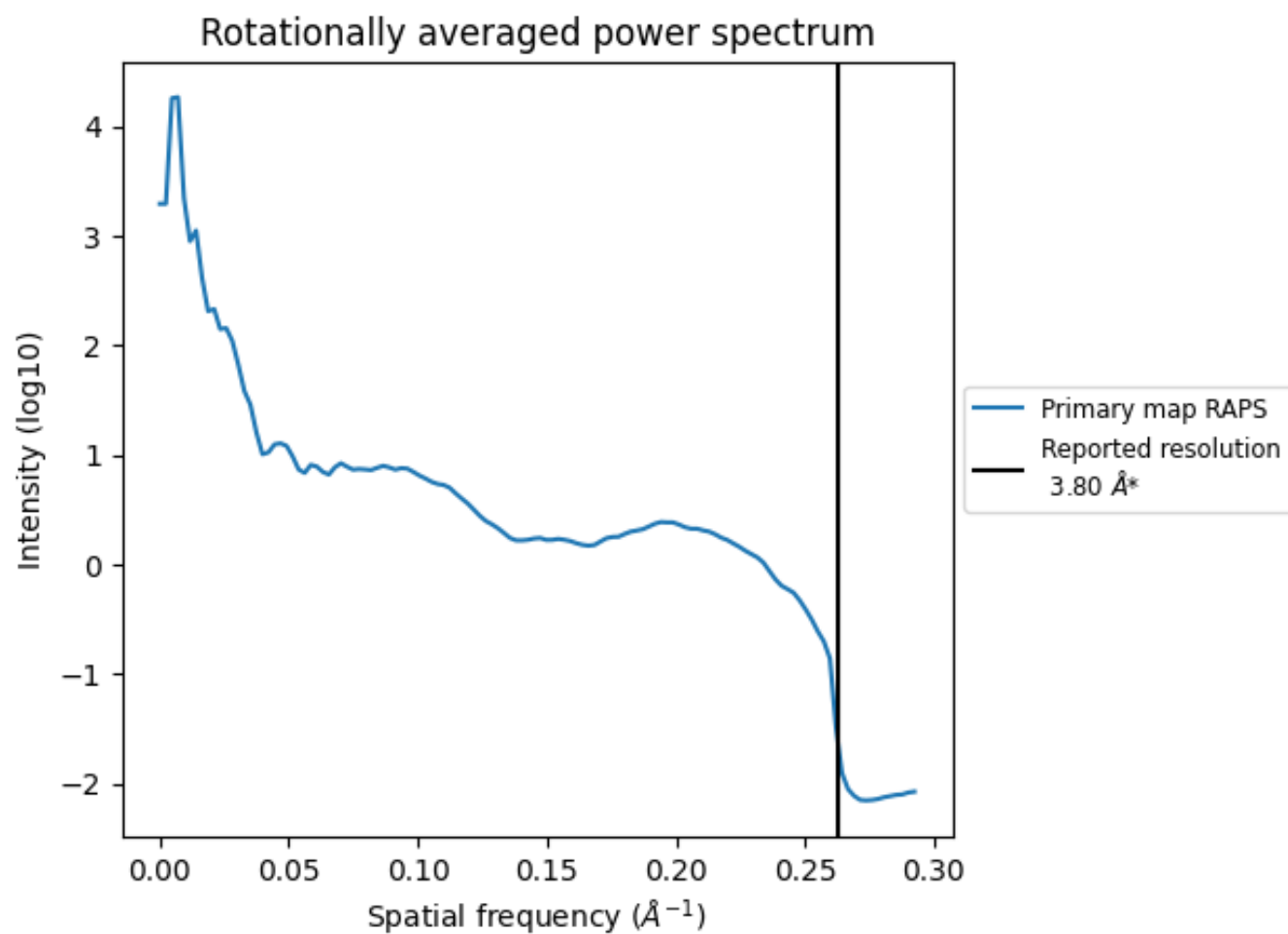
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm^3 ; this corresponds to an approximate mass of 318 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 0.263 Å⁻¹

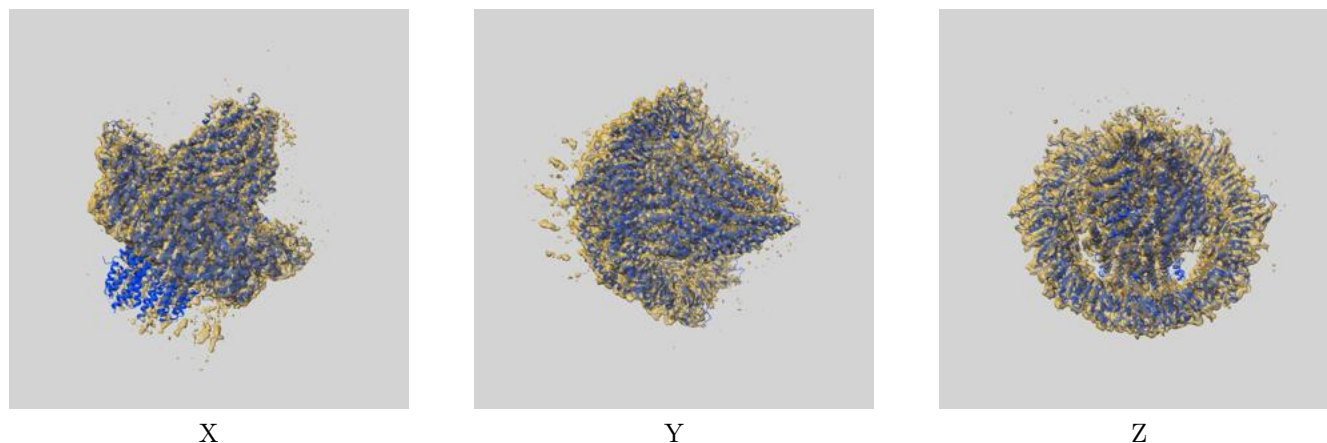
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

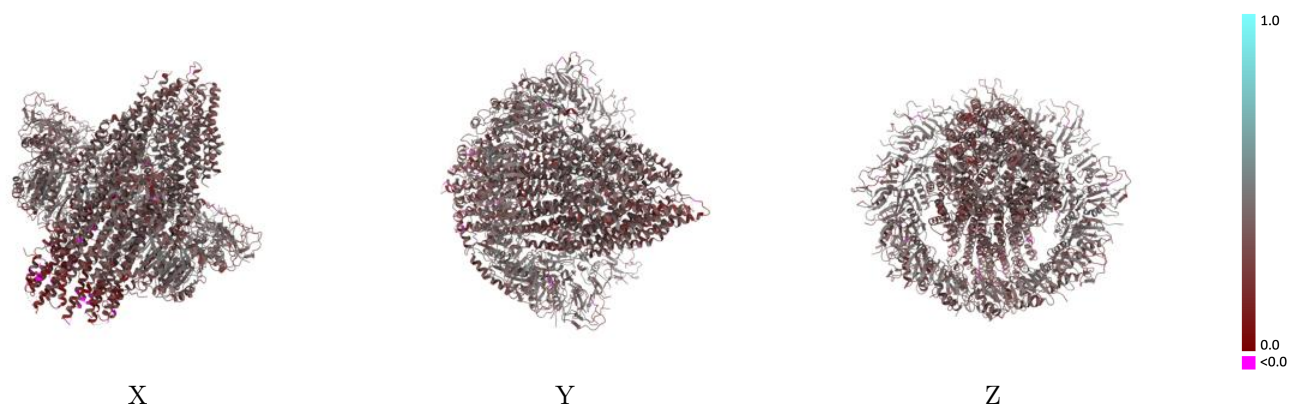
This section contains information regarding the fit between EMDB map EMD-20317 and PDB model 6PEP. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



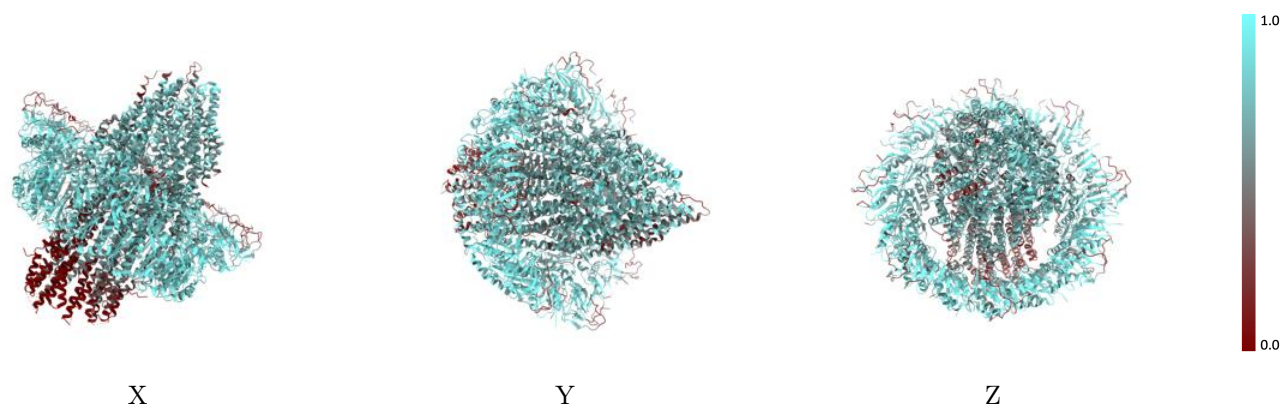
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



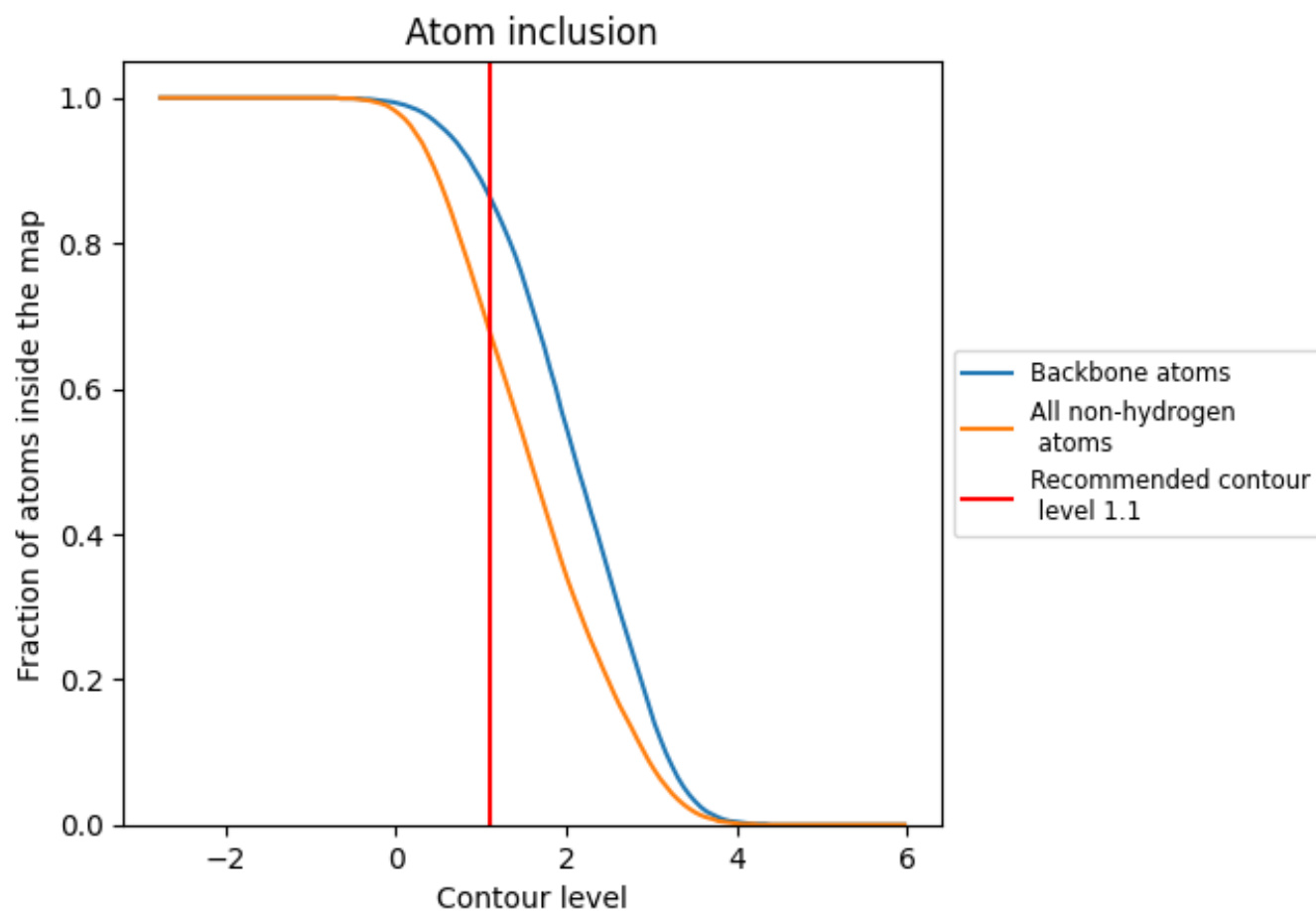
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.3540
0	 0.6950	 0.3510
1	 0.6950	 0.3290
2	 0.7060	 0.3440
3	 0.7160	 0.3590
4	 0.7060	 0.3560
5	 0.7550	 0.3840
6	 0.2890	 0.3300
7	 0.4720	 0.3090
8	 0.6190	 0.3280
9	 0.6780	 0.3490
A	 0.8350	 0.3860
AM	 0.5990	 0.3480
AN	 0.6120	 0.3240
AO	 0.6120	 0.3230
AP	 0.5880	 0.3370
AQ	 0.6090	 0.3310
AR	 0.4980	 0.3180
AS	 0.4470	 0.2930
AT	 0.5320	 0.2710
AU	 0.4620	 0.2840
AV	 0.4380	 0.2750
AW	 0.3440	 0.2710
AX	 0.0760	 0.2480
AY	 0.2770	 0.2410
AZ	 0.3540	 0.2470
B	 0.8140	 0.3820
BA	 0.3290	 0.2260
BB	 0.3030	 0.2240
BC	 0.0320	 0.2120
BD	 0.0450	 0.1870
BE	 0.1390	 0.1860
C	 0.8340	 0.3870
D	 0.8170	 0.3970
E	 0.4280	 0.3170



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Chain	Atom inclusion	Q-score
F	 0.8330	 0.3990
G	 0.8110	 0.3940
H	 0.8340	 0.4010
I	 0.8050	 0.3970
J	 0.8420	 0.4020
K	 0.8280	 0.3860
L	 0.8420	 0.3980
M	 0.8230	 0.3880
N	 0.8480	 0.3920
O	 0.8180	 0.3800
P	 0.8420	 0.3770
Q	 0.8140	 0.3840
R	 0.7640	 0.3900
S	 0.7770	 0.3880
T	 0.3840	 0.3150
U	 0.7680	 0.3880
V	 0.7630	 0.3920
W	 0.3760	 0.3230
X	 0.7910	 0.4040
Y	 0.7900	 0.4020
Z	 0.4060	 0.3170
a	 0.7860	 0.3920
b	 0.8040	 0.4070
c	 0.4500	 0.3230
d	 0.7730	 0.3920
e	 0.7900	 0.4020
f	 0.4540	 0.3200
g	 0.7680	 0.3970
h	 0.7950	 0.4130
i	 0.4280	 0.3170
j	 0.8090	 0.4170
k	 0.8040	 0.4220
l	 0.4150	 0.3190
m	 0.7680	 0.4210
n	 0.7590	 0.3930