wwPDB EM Validation Summary Report

May 13, 2025 – 07:51 AM EDT

PDB ID	:	6U8Q / pdb_00006u8q
EMDB ID	:	EMD-20689
Title	:	CryoEM structure of HIV-1 cleaved synaptic complex (CSC) intasome
Authors	:	Li, M.; Chen, X.; Craigie, R.
Deposited on	:	2019-09-05
Resolution	:	4.67 Å(reported)

This is a wwPDB EM Validation Summary 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:

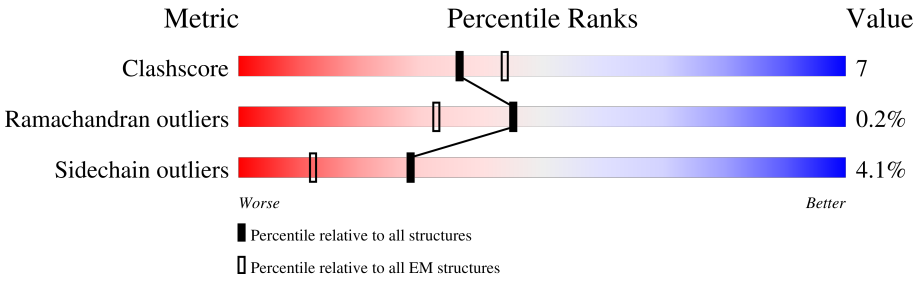
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.67 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	63% 10% 26%
1	B	364	6% 64% 7% 27%
1	C	364	62% 11% 26%
1	D	364	6% 58% 13% 28%
1	I	364	7% 44% 12% 43%
1	J	364	6% 46% 11% 43%
1	K	364	7% 31% 9% 60%
1	L	364	7% 32% 8% 60%

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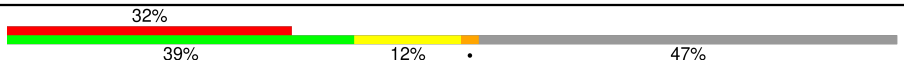
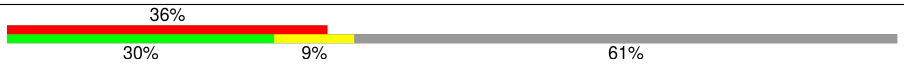
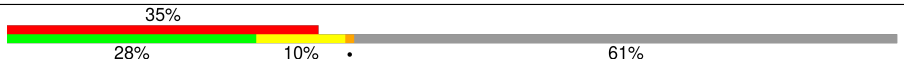
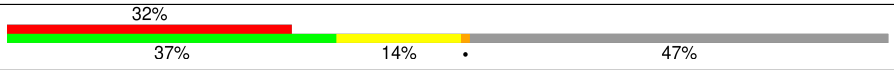
Mol	Chain	Length	Quality of chain
1	M	364	
1	N	364	
1	O	364	
1	P	364	
2	E	27	
2	G	27	
3	F	25	
3	H	25	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21129 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 Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	270	Total	C	N	O	S	0	0
			2129	1354	376	390	9		
1	B	264	Total	C	N	O	S	0	0
			2083	1327	367	381	8		
1	C	270	Total	C	N	O	S	0	0
			2128	1354	375	390	9		
1	D	262	Total	C	N	O	S	0	0
			2067	1315	365	379	8		
1	I	208	Total	C	N	O	S	0	0
			1646	1053	293	294	6		
1	J	208	Total	C	N	O	S	0	0
			1639	1047	293	293	6		
1	K	145	Total	C	N	O	S	0	0
			1110	708	192	205	5		
1	L	145	Total	C	N	O	S	0	0
			1110	708	192	205	5		
1	M	194	Total	C	N	O	S	0	0
			1517	969	270	273	5		
1	N	142	Total	C	N	O	S	0	0
			1089	694	189	201	5		
1	O	142	Total	C	N	O	S	0	0
			1089	694	189	201	5		
1	P	192	Total	C	N	O	S	0	0
			1498	959	265	269	5		

There are 912 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-75	GLY	-	expression tag	UNP Q76353
A	-74	SER	-	expression tag	UNP Q76353
A	-73	HIS	-	expression tag	UNP Q76353
A	-72	MET	-	expression tag	UNP Q76353
A	-71	PRO	-	expression tag	UNP Q76353
A	-70	LYS	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-69	ARG	-	expression tag	UNP Q76353
A	-68	GLY	-	expression tag	UNP Q76353
A	-67	ARG	-	expression tag	UNP Q76353
A	-66	PRO	-	expression tag	UNP Q76353
A	-65	ALA	-	expression tag	UNP Q76353
A	-64	ALA	-	expression tag	UNP Q76353
A	-63	THR	-	expression tag	UNP Q76353
A	-62	GLU	-	expression tag	UNP Q76353
A	-61	VAL	-	expression tag	UNP Q76353
A	-60	LYS	-	expression tag	UNP Q76353
A	-59	ILE	-	expression tag	UNP Q76353
A	-58	PRO	-	expression tag	UNP Q76353
A	-57	LYS	-	expression tag	UNP Q76353
A	-56	PRO	-	expression tag	UNP Q76353
A	-55	ARG	-	expression tag	UNP Q76353
A	-54	GLY	-	expression tag	UNP Q76353
A	-53	ARG	-	expression tag	UNP Q76353
A	-52	PRO	-	expression tag	UNP Q76353
A	-51	PRO	-	expression tag	UNP Q76353
A	-50	LEU	-	expression tag	UNP Q76353
A	-49	PRO	-	expression tag	UNP Q76353
A	-48	ALA	-	expression tag	UNP Q76353
A	-47	GLY	-	expression tag	UNP Q76353
A	-46	THR	-	expression tag	UNP Q76353
A	-45	ASN	-	expression tag	UNP Q76353
A	-44	SER	-	expression tag	UNP Q76353
A	-43	LYS	-	expression tag	UNP Q76353
A	-42	GLY	-	expression tag	UNP Q76353
A	-41	PRO	-	expression tag	UNP Q76353
A	-40	PRO	-	expression tag	UNP Q76353
A	-39	ASP	-	expression tag	UNP Q76353
A	-38	PHE	-	expression tag	UNP Q76353
A	-37	SER	-	expression tag	UNP Q76353
A	-36	SER	-	expression tag	UNP Q76353
A	-35	ASP	-	expression tag	UNP Q76353
A	-34	GLU	-	expression tag	UNP Q76353
A	-33	GLU	-	expression tag	UNP Q76353
A	-32	ARG	-	expression tag	UNP Q76353
A	-31	GLU	-	expression tag	UNP Q76353
A	-30	PRO	-	expression tag	UNP Q76353
A	-29	THR	-	expression tag	UNP Q76353
A	-28	PRO	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	VAL	-	expression tag	UNP Q76353
A	-26	LEU	-	expression tag	UNP Q76353
A	-25	GLY	-	expression tag	UNP Q76353
A	-24	SER	-	expression tag	UNP Q76353
A	-23	GLY	-	expression tag	UNP Q76353
A	-22	ALA	-	expression tag	UNP Q76353
A	-21	ALA	-	expression tag	UNP Q76353
A	-20	ALA	-	expression tag	UNP Q76353
A	-19	ALA	-	expression tag	UNP Q76353
A	-18	GLY	-	expression tag	UNP Q76353
A	-17	GLN	-	expression tag	UNP Q76353
A	-16	SER	-	expression tag	UNP Q76353
A	-15	ARG	-	expression tag	UNP Q76353
A	-14	ALA	-	expression tag	UNP Q76353
A	-13	ALA	-	expression tag	UNP Q76353
A	-12	VAL	-	expression tag	UNP Q76353
A	-11	GLY	-	expression tag	UNP Q76353
A	-10	ARG	-	expression tag	UNP Q76353
A	-9	LYS	-	expression tag	UNP Q76353
A	-8	ALA	-	expression tag	UNP Q76353
A	-7	THR	-	expression tag	UNP Q76353
A	-6	LYS	-	expression tag	UNP Q76353
A	-5	LYS	-	expression tag	UNP Q76353
A	-4	THR	-	expression tag	UNP Q76353
A	-3	ASP	-	expression tag	UNP Q76353
A	-2	GLY	-	expression tag	UNP Q76353
A	-1	GLY	-	expression tag	UNP Q76353
A	0	GLY	-	expression tag	UNP Q76353
B	-75	GLY	-	expression tag	UNP Q76353
B	-74	SER	-	expression tag	UNP Q76353
B	-73	HIS	-	expression tag	UNP Q76353
B	-72	MET	-	expression tag	UNP Q76353
B	-71	PRO	-	expression tag	UNP Q76353
B	-70	LYS	-	expression tag	UNP Q76353
B	-69	ARG	-	expression tag	UNP Q76353
B	-68	GLY	-	expression tag	UNP Q76353
B	-67	ARG	-	expression tag	UNP Q76353
B	-66	PRO	-	expression tag	UNP Q76353
B	-65	ALA	-	expression tag	UNP Q76353
B	-64	ALA	-	expression tag	UNP Q76353
B	-63	THR	-	expression tag	UNP Q76353
B	-62	GLU	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-61	VAL	-	expression tag	UNP Q76353
B	-60	LYS	-	expression tag	UNP Q76353
B	-59	ILE	-	expression tag	UNP Q76353
B	-58	PRO	-	expression tag	UNP Q76353
B	-57	LYS	-	expression tag	UNP Q76353
B	-56	PRO	-	expression tag	UNP Q76353
B	-55	ARG	-	expression tag	UNP Q76353
B	-54	GLY	-	expression tag	UNP Q76353
B	-53	ARG	-	expression tag	UNP Q76353
B	-52	PRO	-	expression tag	UNP Q76353
B	-51	PRO	-	expression tag	UNP Q76353
B	-50	LEU	-	expression tag	UNP Q76353
B	-49	PRO	-	expression tag	UNP Q76353
B	-48	ALA	-	expression tag	UNP Q76353
B	-47	GLY	-	expression tag	UNP Q76353
B	-46	THR	-	expression tag	UNP Q76353
B	-45	ASN	-	expression tag	UNP Q76353
B	-44	SER	-	expression tag	UNP Q76353
B	-43	LYS	-	expression tag	UNP Q76353
B	-42	GLY	-	expression tag	UNP Q76353
B	-41	PRO	-	expression tag	UNP Q76353
B	-40	PRO	-	expression tag	UNP Q76353
B	-39	ASP	-	expression tag	UNP Q76353
B	-38	PHE	-	expression tag	UNP Q76353
B	-37	SER	-	expression tag	UNP Q76353
B	-36	SER	-	expression tag	UNP Q76353
B	-35	ASP	-	expression tag	UNP Q76353
B	-34	GLU	-	expression tag	UNP Q76353
B	-33	GLU	-	expression tag	UNP Q76353
B	-32	ARG	-	expression tag	UNP Q76353
B	-31	GLU	-	expression tag	UNP Q76353
B	-30	PRO	-	expression tag	UNP Q76353
B	-29	THR	-	expression tag	UNP Q76353
B	-28	PRO	-	expression tag	UNP Q76353
B	-27	VAL	-	expression tag	UNP Q76353
B	-26	LEU	-	expression tag	UNP Q76353
B	-25	GLY	-	expression tag	UNP Q76353
B	-24	SER	-	expression tag	UNP Q76353
B	-23	GLY	-	expression tag	UNP Q76353
B	-22	ALA	-	expression tag	UNP Q76353
B	-21	ALA	-	expression tag	UNP Q76353
B	-20	ALA	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	ALA	-	expression tag	UNP Q76353
B	-18	GLY	-	expression tag	UNP Q76353
B	-17	GLN	-	expression tag	UNP Q76353
B	-16	SER	-	expression tag	UNP Q76353
B	-15	ARG	-	expression tag	UNP Q76353
B	-14	ALA	-	expression tag	UNP Q76353
B	-13	ALA	-	expression tag	UNP Q76353
B	-12	VAL	-	expression tag	UNP Q76353
B	-11	GLY	-	expression tag	UNP Q76353
B	-10	ARG	-	expression tag	UNP Q76353
B	-9	LYS	-	expression tag	UNP Q76353
B	-8	ALA	-	expression tag	UNP Q76353
B	-7	THR	-	expression tag	UNP Q76353
B	-6	LYS	-	expression tag	UNP Q76353
B	-5	LYS	-	expression tag	UNP Q76353
B	-4	THR	-	expression tag	UNP Q76353
B	-3	ASP	-	expression tag	UNP Q76353
B	-2	GLY	-	expression tag	UNP Q76353
B	-1	GLY	-	expression tag	UNP Q76353
B	0	GLY	-	expression tag	UNP Q76353
C	-75	GLY	-	expression tag	UNP Q76353
C	-74	SER	-	expression tag	UNP Q76353
C	-73	HIS	-	expression tag	UNP Q76353
C	-72	MET	-	expression tag	UNP Q76353
C	-71	PRO	-	expression tag	UNP Q76353
C	-70	LYS	-	expression tag	UNP Q76353
C	-69	ARG	-	expression tag	UNP Q76353
C	-68	GLY	-	expression tag	UNP Q76353
C	-67	ARG	-	expression tag	UNP Q76353
C	-66	PRO	-	expression tag	UNP Q76353
C	-65	ALA	-	expression tag	UNP Q76353
C	-64	ALA	-	expression tag	UNP Q76353
C	-63	THR	-	expression tag	UNP Q76353
C	-62	GLU	-	expression tag	UNP Q76353
C	-61	VAL	-	expression tag	UNP Q76353
C	-60	LYS	-	expression tag	UNP Q76353
C	-59	ILE	-	expression tag	UNP Q76353
C	-58	PRO	-	expression tag	UNP Q76353
C	-57	LYS	-	expression tag	UNP Q76353
C	-56	PRO	-	expression tag	UNP Q76353
C	-55	ARG	-	expression tag	UNP Q76353
C	-54	GLY	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-53	ARG	-	expression tag	UNP Q76353
C	-52	PRO	-	expression tag	UNP Q76353
C	-51	PRO	-	expression tag	UNP Q76353
C	-50	LEU	-	expression tag	UNP Q76353
C	-49	PRO	-	expression tag	UNP Q76353
C	-48	ALA	-	expression tag	UNP Q76353
C	-47	GLY	-	expression tag	UNP Q76353
C	-46	THR	-	expression tag	UNP Q76353
C	-45	ASN	-	expression tag	UNP Q76353
C	-44	SER	-	expression tag	UNP Q76353
C	-43	LYS	-	expression tag	UNP Q76353
C	-42	GLY	-	expression tag	UNP Q76353
C	-41	PRO	-	expression tag	UNP Q76353
C	-40	PRO	-	expression tag	UNP Q76353
C	-39	ASP	-	expression tag	UNP Q76353
C	-38	PHE	-	expression tag	UNP Q76353
C	-37	SER	-	expression tag	UNP Q76353
C	-36	SER	-	expression tag	UNP Q76353
C	-35	ASP	-	expression tag	UNP Q76353
C	-34	GLU	-	expression tag	UNP Q76353
C	-33	GLU	-	expression tag	UNP Q76353
C	-32	ARG	-	expression tag	UNP Q76353
C	-31	GLU	-	expression tag	UNP Q76353
C	-30	PRO	-	expression tag	UNP Q76353
C	-29	THR	-	expression tag	UNP Q76353
C	-28	PRO	-	expression tag	UNP Q76353
C	-27	VAL	-	expression tag	UNP Q76353
C	-26	LEU	-	expression tag	UNP Q76353
C	-25	GLY	-	expression tag	UNP Q76353
C	-24	SER	-	expression tag	UNP Q76353
C	-23	GLY	-	expression tag	UNP Q76353
C	-22	ALA	-	expression tag	UNP Q76353
C	-21	ALA	-	expression tag	UNP Q76353
C	-20	ALA	-	expression tag	UNP Q76353
C	-19	ALA	-	expression tag	UNP Q76353
C	-18	GLY	-	expression tag	UNP Q76353
C	-17	GLN	-	expression tag	UNP Q76353
C	-16	SER	-	expression tag	UNP Q76353
C	-15	ARG	-	expression tag	UNP Q76353
C	-14	ALA	-	expression tag	UNP Q76353
C	-13	ALA	-	expression tag	UNP Q76353
C	-12	VAL	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	GLY	-	expression tag	UNP Q76353
C	-10	ARG	-	expression tag	UNP Q76353
C	-9	LYS	-	expression tag	UNP Q76353
C	-8	ALA	-	expression tag	UNP Q76353
C	-7	THR	-	expression tag	UNP Q76353
C	-6	LYS	-	expression tag	UNP Q76353
C	-5	LYS	-	expression tag	UNP Q76353
C	-4	THR	-	expression tag	UNP Q76353
C	-3	ASP	-	expression tag	UNP Q76353
C	-2	GLY	-	expression tag	UNP Q76353
C	-1	GLY	-	expression tag	UNP Q76353
C	0	GLY	-	expression tag	UNP Q76353
D	-75	GLY	-	expression tag	UNP Q76353
D	-74	SER	-	expression tag	UNP Q76353
D	-73	HIS	-	expression tag	UNP Q76353
D	-72	MET	-	expression tag	UNP Q76353
D	-71	PRO	-	expression tag	UNP Q76353
D	-70	LYS	-	expression tag	UNP Q76353
D	-69	ARG	-	expression tag	UNP Q76353
D	-68	GLY	-	expression tag	UNP Q76353
D	-67	ARG	-	expression tag	UNP Q76353
D	-66	PRO	-	expression tag	UNP Q76353
D	-65	ALA	-	expression tag	UNP Q76353
D	-64	ALA	-	expression tag	UNP Q76353
D	-63	THR	-	expression tag	UNP Q76353
D	-62	GLU	-	expression tag	UNP Q76353
D	-61	VAL	-	expression tag	UNP Q76353
D	-60	LYS	-	expression tag	UNP Q76353
D	-59	ILE	-	expression tag	UNP Q76353
D	-58	PRO	-	expression tag	UNP Q76353
D	-57	LYS	-	expression tag	UNP Q76353
D	-56	PRO	-	expression tag	UNP Q76353
D	-55	ARG	-	expression tag	UNP Q76353
D	-54	GLY	-	expression tag	UNP Q76353
D	-53	ARG	-	expression tag	UNP Q76353
D	-52	PRO	-	expression tag	UNP Q76353
D	-51	PRO	-	expression tag	UNP Q76353
D	-50	LEU	-	expression tag	UNP Q76353
D	-49	PRO	-	expression tag	UNP Q76353
D	-48	ALA	-	expression tag	UNP Q76353
D	-47	GLY	-	expression tag	UNP Q76353
D	-46	THR	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-45	ASN	-	expression tag	UNP Q76353
D	-44	SER	-	expression tag	UNP Q76353
D	-43	LYS	-	expression tag	UNP Q76353
D	-42	GLY	-	expression tag	UNP Q76353
D	-41	PRO	-	expression tag	UNP Q76353
D	-40	PRO	-	expression tag	UNP Q76353
D	-39	ASP	-	expression tag	UNP Q76353
D	-38	PHE	-	expression tag	UNP Q76353
D	-37	SER	-	expression tag	UNP Q76353
D	-36	SER	-	expression tag	UNP Q76353
D	-35	ASP	-	expression tag	UNP Q76353
D	-34	GLU	-	expression tag	UNP Q76353
D	-33	GLU	-	expression tag	UNP Q76353
D	-32	ARG	-	expression tag	UNP Q76353
D	-31	GLU	-	expression tag	UNP Q76353
D	-30	PRO	-	expression tag	UNP Q76353
D	-29	THR	-	expression tag	UNP Q76353
D	-28	PRO	-	expression tag	UNP Q76353
D	-27	VAL	-	expression tag	UNP Q76353
D	-26	LEU	-	expression tag	UNP Q76353
D	-25	GLY	-	expression tag	UNP Q76353
D	-24	SER	-	expression tag	UNP Q76353
D	-23	GLY	-	expression tag	UNP Q76353
D	-22	ALA	-	expression tag	UNP Q76353
D	-21	ALA	-	expression tag	UNP Q76353
D	-20	ALA	-	expression tag	UNP Q76353
D	-19	ALA	-	expression tag	UNP Q76353
D	-18	GLY	-	expression tag	UNP Q76353
D	-17	GLN	-	expression tag	UNP Q76353
D	-16	SER	-	expression tag	UNP Q76353
D	-15	ARG	-	expression tag	UNP Q76353
D	-14	ALA	-	expression tag	UNP Q76353
D	-13	ALA	-	expression tag	UNP Q76353
D	-12	VAL	-	expression tag	UNP Q76353
D	-11	GLY	-	expression tag	UNP Q76353
D	-10	ARG	-	expression tag	UNP Q76353
D	-9	LYS	-	expression tag	UNP Q76353
D	-8	ALA	-	expression tag	UNP Q76353
D	-7	THR	-	expression tag	UNP Q76353
D	-6	LYS	-	expression tag	UNP Q76353
D	-5	LYS	-	expression tag	UNP Q76353
D	-4	THR	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ASP	-	expression tag	UNP Q76353
D	-2	GLY	-	expression tag	UNP Q76353
D	-1	GLY	-	expression tag	UNP Q76353
D	0	GLY	-	expression tag	UNP Q76353
I	-75	GLY	-	expression tag	UNP Q76353
I	-74	SER	-	expression tag	UNP Q76353
I	-73	HIS	-	expression tag	UNP Q76353
I	-72	MET	-	expression tag	UNP Q76353
I	-71	PRO	-	expression tag	UNP Q76353
I	-70	LYS	-	expression tag	UNP Q76353
I	-69	ARG	-	expression tag	UNP Q76353
I	-68	GLY	-	expression tag	UNP Q76353
I	-67	ARG	-	expression tag	UNP Q76353
I	-66	PRO	-	expression tag	UNP Q76353
I	-65	ALA	-	expression tag	UNP Q76353
I	-64	ALA	-	expression tag	UNP Q76353
I	-63	THR	-	expression tag	UNP Q76353
I	-62	GLU	-	expression tag	UNP Q76353
I	-61	VAL	-	expression tag	UNP Q76353
I	-60	LYS	-	expression tag	UNP Q76353
I	-59	ILE	-	expression tag	UNP Q76353
I	-58	PRO	-	expression tag	UNP Q76353
I	-57	LYS	-	expression tag	UNP Q76353
I	-56	PRO	-	expression tag	UNP Q76353
I	-55	ARG	-	expression tag	UNP Q76353
I	-54	GLY	-	expression tag	UNP Q76353
I	-53	ARG	-	expression tag	UNP Q76353
I	-52	PRO	-	expression tag	UNP Q76353
I	-51	PRO	-	expression tag	UNP Q76353
I	-50	LEU	-	expression tag	UNP Q76353
I	-49	PRO	-	expression tag	UNP Q76353
I	-48	ALA	-	expression tag	UNP Q76353
I	-47	GLY	-	expression tag	UNP Q76353
I	-46	THR	-	expression tag	UNP Q76353
I	-45	ASN	-	expression tag	UNP Q76353
I	-44	SER	-	expression tag	UNP Q76353
I	-43	LYS	-	expression tag	UNP Q76353
I	-42	GLY	-	expression tag	UNP Q76353
I	-41	PRO	-	expression tag	UNP Q76353
I	-40	PRO	-	expression tag	UNP Q76353
I	-39	ASP	-	expression tag	UNP Q76353
I	-38	PHE	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-37	SER	-	expression tag	UNP Q76353
I	-36	SER	-	expression tag	UNP Q76353
I	-35	ASP	-	expression tag	UNP Q76353
I	-34	GLU	-	expression tag	UNP Q76353
I	-33	GLU	-	expression tag	UNP Q76353
I	-32	ARG	-	expression tag	UNP Q76353
I	-31	GLU	-	expression tag	UNP Q76353
I	-30	PRO	-	expression tag	UNP Q76353
I	-29	THR	-	expression tag	UNP Q76353
I	-28	PRO	-	expression tag	UNP Q76353
I	-27	VAL	-	expression tag	UNP Q76353
I	-26	LEU	-	expression tag	UNP Q76353
I	-25	GLY	-	expression tag	UNP Q76353
I	-24	SER	-	expression tag	UNP Q76353
I	-23	GLY	-	expression tag	UNP Q76353
I	-22	ALA	-	expression tag	UNP Q76353
I	-21	ALA	-	expression tag	UNP Q76353
I	-20	ALA	-	expression tag	UNP Q76353
I	-19	ALA	-	expression tag	UNP Q76353
I	-18	GLY	-	expression tag	UNP Q76353
I	-17	GLN	-	expression tag	UNP Q76353
I	-16	SER	-	expression tag	UNP Q76353
I	-15	ARG	-	expression tag	UNP Q76353
I	-14	ALA	-	expression tag	UNP Q76353
I	-13	ALA	-	expression tag	UNP Q76353
I	-12	VAL	-	expression tag	UNP Q76353
I	-11	GLY	-	expression tag	UNP Q76353
I	-10	ARG	-	expression tag	UNP Q76353
I	-9	LYS	-	expression tag	UNP Q76353
I	-8	ALA	-	expression tag	UNP Q76353
I	-7	THR	-	expression tag	UNP Q76353
I	-6	LYS	-	expression tag	UNP Q76353
I	-5	LYS	-	expression tag	UNP Q76353
I	-4	THR	-	expression tag	UNP Q76353
I	-3	ASP	-	expression tag	UNP Q76353
I	-2	GLY	-	expression tag	UNP Q76353
I	-1	GLY	-	expression tag	UNP Q76353
I	0	GLY	-	expression tag	UNP Q76353
J	-75	GLY	-	expression tag	UNP Q76353
J	-74	SER	-	expression tag	UNP Q76353
J	-73	HIS	-	expression tag	UNP Q76353
J	-72	MET	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-71	PRO	-	expression tag	UNP Q76353
J	-70	LYS	-	expression tag	UNP Q76353
J	-69	ARG	-	expression tag	UNP Q76353
J	-68	GLY	-	expression tag	UNP Q76353
J	-67	ARG	-	expression tag	UNP Q76353
J	-66	PRO	-	expression tag	UNP Q76353
J	-65	ALA	-	expression tag	UNP Q76353
J	-64	ALA	-	expression tag	UNP Q76353
J	-63	THR	-	expression tag	UNP Q76353
J	-62	GLU	-	expression tag	UNP Q76353
J	-61	VAL	-	expression tag	UNP Q76353
J	-60	LYS	-	expression tag	UNP Q76353
J	-59	ILE	-	expression tag	UNP Q76353
J	-58	PRO	-	expression tag	UNP Q76353
J	-57	LYS	-	expression tag	UNP Q76353
J	-56	PRO	-	expression tag	UNP Q76353
J	-55	ARG	-	expression tag	UNP Q76353
J	-54	GLY	-	expression tag	UNP Q76353
J	-53	ARG	-	expression tag	UNP Q76353
J	-52	PRO	-	expression tag	UNP Q76353
J	-51	PRO	-	expression tag	UNP Q76353
J	-50	LEU	-	expression tag	UNP Q76353
J	-49	PRO	-	expression tag	UNP Q76353
J	-48	ALA	-	expression tag	UNP Q76353
J	-47	GLY	-	expression tag	UNP Q76353
J	-46	THR	-	expression tag	UNP Q76353
J	-45	ASN	-	expression tag	UNP Q76353
J	-44	SER	-	expression tag	UNP Q76353
J	-43	LYS	-	expression tag	UNP Q76353
J	-42	GLY	-	expression tag	UNP Q76353
J	-41	PRO	-	expression tag	UNP Q76353
J	-40	PRO	-	expression tag	UNP Q76353
J	-39	ASP	-	expression tag	UNP Q76353
J	-38	PHE	-	expression tag	UNP Q76353
J	-37	SER	-	expression tag	UNP Q76353
J	-36	SER	-	expression tag	UNP Q76353
J	-35	ASP	-	expression tag	UNP Q76353
J	-34	GLU	-	expression tag	UNP Q76353
J	-33	GLU	-	expression tag	UNP Q76353
J	-32	ARG	-	expression tag	UNP Q76353
J	-31	GLU	-	expression tag	UNP Q76353
J	-30	PRO	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-29	THR	-	expression tag	UNP Q76353
J	-28	PRO	-	expression tag	UNP Q76353
J	-27	VAL	-	expression tag	UNP Q76353
J	-26	LEU	-	expression tag	UNP Q76353
J	-25	GLY	-	expression tag	UNP Q76353
J	-24	SER	-	expression tag	UNP Q76353
J	-23	GLY	-	expression tag	UNP Q76353
J	-22	ALA	-	expression tag	UNP Q76353
J	-21	ALA	-	expression tag	UNP Q76353
J	-20	ALA	-	expression tag	UNP Q76353
J	-19	ALA	-	expression tag	UNP Q76353
J	-18	GLY	-	expression tag	UNP Q76353
J	-17	GLN	-	expression tag	UNP Q76353
J	-16	SER	-	expression tag	UNP Q76353
J	-15	ARG	-	expression tag	UNP Q76353
J	-14	ALA	-	expression tag	UNP Q76353
J	-13	ALA	-	expression tag	UNP Q76353
J	-12	VAL	-	expression tag	UNP Q76353
J	-11	GLY	-	expression tag	UNP Q76353
J	-10	ARG	-	expression tag	UNP Q76353
J	-9	LYS	-	expression tag	UNP Q76353
J	-8	ALA	-	expression tag	UNP Q76353
J	-7	THR	-	expression tag	UNP Q76353
J	-6	LYS	-	expression tag	UNP Q76353
J	-5	LYS	-	expression tag	UNP Q76353
J	-4	THR	-	expression tag	UNP Q76353
J	-3	ASP	-	expression tag	UNP Q76353
J	-2	GLY	-	expression tag	UNP Q76353
J	-1	GLY	-	expression tag	UNP Q76353
J	0	GLY	-	expression tag	UNP Q76353
K	-75	GLY	-	expression tag	UNP Q76353
K	-74	SER	-	expression tag	UNP Q76353
K	-73	HIS	-	expression tag	UNP Q76353
K	-72	MET	-	expression tag	UNP Q76353
K	-71	PRO	-	expression tag	UNP Q76353
K	-70	LYS	-	expression tag	UNP Q76353
K	-69	ARG	-	expression tag	UNP Q76353
K	-68	GLY	-	expression tag	UNP Q76353
K	-67	ARG	-	expression tag	UNP Q76353
K	-66	PRO	-	expression tag	UNP Q76353
K	-65	ALA	-	expression tag	UNP Q76353
K	-64	ALA	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-63	THR	-	expression tag	UNP Q76353
K	-62	GLU	-	expression tag	UNP Q76353
K	-61	VAL	-	expression tag	UNP Q76353
K	-60	LYS	-	expression tag	UNP Q76353
K	-59	ILE	-	expression tag	UNP Q76353
K	-58	PRO	-	expression tag	UNP Q76353
K	-57	LYS	-	expression tag	UNP Q76353
K	-56	PRO	-	expression tag	UNP Q76353
K	-55	ARG	-	expression tag	UNP Q76353
K	-54	GLY	-	expression tag	UNP Q76353
K	-53	ARG	-	expression tag	UNP Q76353
K	-52	PRO	-	expression tag	UNP Q76353
K	-51	PRO	-	expression tag	UNP Q76353
K	-50	LEU	-	expression tag	UNP Q76353
K	-49	PRO	-	expression tag	UNP Q76353
K	-48	ALA	-	expression tag	UNP Q76353
K	-47	GLY	-	expression tag	UNP Q76353
K	-46	THR	-	expression tag	UNP Q76353
K	-45	ASN	-	expression tag	UNP Q76353
K	-44	SER	-	expression tag	UNP Q76353
K	-43	LYS	-	expression tag	UNP Q76353
K	-42	GLY	-	expression tag	UNP Q76353
K	-41	PRO	-	expression tag	UNP Q76353
K	-40	PRO	-	expression tag	UNP Q76353
K	-39	ASP	-	expression tag	UNP Q76353
K	-38	PHE	-	expression tag	UNP Q76353
K	-37	SER	-	expression tag	UNP Q76353
K	-36	SER	-	expression tag	UNP Q76353
K	-35	ASP	-	expression tag	UNP Q76353
K	-34	GLU	-	expression tag	UNP Q76353
K	-33	GLU	-	expression tag	UNP Q76353
K	-32	ARG	-	expression tag	UNP Q76353
K	-31	GLU	-	expression tag	UNP Q76353
K	-30	PRO	-	expression tag	UNP Q76353
K	-29	THR	-	expression tag	UNP Q76353
K	-28	PRO	-	expression tag	UNP Q76353
K	-27	VAL	-	expression tag	UNP Q76353
K	-26	LEU	-	expression tag	UNP Q76353
K	-25	GLY	-	expression tag	UNP Q76353
K	-24	SER	-	expression tag	UNP Q76353
K	-23	GLY	-	expression tag	UNP Q76353
K	-22	ALA	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-21	ALA	-	expression tag	UNP Q76353
K	-20	ALA	-	expression tag	UNP Q76353
K	-19	ALA	-	expression tag	UNP Q76353
K	-18	GLY	-	expression tag	UNP Q76353
K	-17	GLN	-	expression tag	UNP Q76353
K	-16	SER	-	expression tag	UNP Q76353
K	-15	ARG	-	expression tag	UNP Q76353
K	-14	ALA	-	expression tag	UNP Q76353
K	-13	ALA	-	expression tag	UNP Q76353
K	-12	VAL	-	expression tag	UNP Q76353
K	-11	GLY	-	expression tag	UNP Q76353
K	-10	ARG	-	expression tag	UNP Q76353
K	-9	LYS	-	expression tag	UNP Q76353
K	-8	ALA	-	expression tag	UNP Q76353
K	-7	THR	-	expression tag	UNP Q76353
K	-6	LYS	-	expression tag	UNP Q76353
K	-5	LYS	-	expression tag	UNP Q76353
K	-4	THR	-	expression tag	UNP Q76353
K	-3	ASP	-	expression tag	UNP Q76353
K	-2	GLY	-	expression tag	UNP Q76353
K	-1	GLY	-	expression tag	UNP Q76353
K	0	GLY	-	expression tag	UNP Q76353
L	-75	GLY	-	expression tag	UNP Q76353
L	-74	SER	-	expression tag	UNP Q76353
L	-73	HIS	-	expression tag	UNP Q76353
L	-72	MET	-	expression tag	UNP Q76353
L	-71	PRO	-	expression tag	UNP Q76353
L	-70	LYS	-	expression tag	UNP Q76353
L	-69	ARG	-	expression tag	UNP Q76353
L	-68	GLY	-	expression tag	UNP Q76353
L	-67	ARG	-	expression tag	UNP Q76353
L	-66	PRO	-	expression tag	UNP Q76353
L	-65	ALA	-	expression tag	UNP Q76353
L	-64	ALA	-	expression tag	UNP Q76353
L	-63	THR	-	expression tag	UNP Q76353
L	-62	GLU	-	expression tag	UNP Q76353
L	-61	VAL	-	expression tag	UNP Q76353
L	-60	LYS	-	expression tag	UNP Q76353
L	-59	ILE	-	expression tag	UNP Q76353
L	-58	PRO	-	expression tag	UNP Q76353
L	-57	LYS	-	expression tag	UNP Q76353
L	-56	PRO	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-55	ARG	-	expression tag	UNP Q76353
L	-54	GLY	-	expression tag	UNP Q76353
L	-53	ARG	-	expression tag	UNP Q76353
L	-52	PRO	-	expression tag	UNP Q76353
L	-51	PRO	-	expression tag	UNP Q76353
L	-50	LEU	-	expression tag	UNP Q76353
L	-49	PRO	-	expression tag	UNP Q76353
L	-48	ALA	-	expression tag	UNP Q76353
L	-47	GLY	-	expression tag	UNP Q76353
L	-46	THR	-	expression tag	UNP Q76353
L	-45	ASN	-	expression tag	UNP Q76353
L	-44	SER	-	expression tag	UNP Q76353
L	-43	LYS	-	expression tag	UNP Q76353
L	-42	GLY	-	expression tag	UNP Q76353
L	-41	PRO	-	expression tag	UNP Q76353
L	-40	PRO	-	expression tag	UNP Q76353
L	-39	ASP	-	expression tag	UNP Q76353
L	-38	PHE	-	expression tag	UNP Q76353
L	-37	SER	-	expression tag	UNP Q76353
L	-36	SER	-	expression tag	UNP Q76353
L	-35	ASP	-	expression tag	UNP Q76353
L	-34	GLU	-	expression tag	UNP Q76353
L	-33	GLU	-	expression tag	UNP Q76353
L	-32	ARG	-	expression tag	UNP Q76353
L	-31	GLU	-	expression tag	UNP Q76353
L	-30	PRO	-	expression tag	UNP Q76353
L	-29	THR	-	expression tag	UNP Q76353
L	-28	PRO	-	expression tag	UNP Q76353
L	-27	VAL	-	expression tag	UNP Q76353
L	-26	LEU	-	expression tag	UNP Q76353
L	-25	GLY	-	expression tag	UNP Q76353
L	-24	SER	-	expression tag	UNP Q76353
L	-23	GLY	-	expression tag	UNP Q76353
L	-22	ALA	-	expression tag	UNP Q76353
L	-21	ALA	-	expression tag	UNP Q76353
L	-20	ALA	-	expression tag	UNP Q76353
L	-19	ALA	-	expression tag	UNP Q76353
L	-18	GLY	-	expression tag	UNP Q76353
L	-17	GLN	-	expression tag	UNP Q76353
L	-16	SER	-	expression tag	UNP Q76353
L	-15	ARG	-	expression tag	UNP Q76353
L	-14	ALA	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-13	ALA	-	expression tag	UNP Q76353
L	-12	VAL	-	expression tag	UNP Q76353
L	-11	GLY	-	expression tag	UNP Q76353
L	-10	ARG	-	expression tag	UNP Q76353
L	-9	LYS	-	expression tag	UNP Q76353
L	-8	ALA	-	expression tag	UNP Q76353
L	-7	THR	-	expression tag	UNP Q76353
L	-6	LYS	-	expression tag	UNP Q76353
L	-5	LYS	-	expression tag	UNP Q76353
L	-4	THR	-	expression tag	UNP Q76353
L	-3	ASP	-	expression tag	UNP Q76353
L	-2	GLY	-	expression tag	UNP Q76353
L	-1	GLY	-	expression tag	UNP Q76353
L	0	GLY	-	expression tag	UNP Q76353
M	-75	GLY	-	expression tag	UNP Q76353
M	-74	SER	-	expression tag	UNP Q76353
M	-73	HIS	-	expression tag	UNP Q76353
M	-72	MET	-	expression tag	UNP Q76353
M	-71	PRO	-	expression tag	UNP Q76353
M	-70	LYS	-	expression tag	UNP Q76353
M	-69	ARG	-	expression tag	UNP Q76353
M	-68	GLY	-	expression tag	UNP Q76353
M	-67	ARG	-	expression tag	UNP Q76353
M	-66	PRO	-	expression tag	UNP Q76353
M	-65	ALA	-	expression tag	UNP Q76353
M	-64	ALA	-	expression tag	UNP Q76353
M	-63	THR	-	expression tag	UNP Q76353
M	-62	GLU	-	expression tag	UNP Q76353
M	-61	VAL	-	expression tag	UNP Q76353
M	-60	LYS	-	expression tag	UNP Q76353
M	-59	ILE	-	expression tag	UNP Q76353
M	-58	PRO	-	expression tag	UNP Q76353
M	-57	LYS	-	expression tag	UNP Q76353
M	-56	PRO	-	expression tag	UNP Q76353
M	-55	ARG	-	expression tag	UNP Q76353
M	-54	GLY	-	expression tag	UNP Q76353
M	-53	ARG	-	expression tag	UNP Q76353
M	-52	PRO	-	expression tag	UNP Q76353
M	-51	PRO	-	expression tag	UNP Q76353
M	-50	LEU	-	expression tag	UNP Q76353
M	-49	PRO	-	expression tag	UNP Q76353
M	-48	ALA	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-47	GLY	-	expression tag	UNP Q76353
M	-46	THR	-	expression tag	UNP Q76353
M	-45	ASN	-	expression tag	UNP Q76353
M	-44	SER	-	expression tag	UNP Q76353
M	-43	LYS	-	expression tag	UNP Q76353
M	-42	GLY	-	expression tag	UNP Q76353
M	-41	PRO	-	expression tag	UNP Q76353
M	-40	PRO	-	expression tag	UNP Q76353
M	-39	ASP	-	expression tag	UNP Q76353
M	-38	PHE	-	expression tag	UNP Q76353
M	-37	SER	-	expression tag	UNP Q76353
M	-36	SER	-	expression tag	UNP Q76353
M	-35	ASP	-	expression tag	UNP Q76353
M	-34	GLU	-	expression tag	UNP Q76353
M	-33	GLU	-	expression tag	UNP Q76353
M	-32	ARG	-	expression tag	UNP Q76353
M	-31	GLU	-	expression tag	UNP Q76353
M	-30	PRO	-	expression tag	UNP Q76353
M	-29	THR	-	expression tag	UNP Q76353
M	-28	PRO	-	expression tag	UNP Q76353
M	-27	VAL	-	expression tag	UNP Q76353
M	-26	LEU	-	expression tag	UNP Q76353
M	-25	GLY	-	expression tag	UNP Q76353
M	-24	SER	-	expression tag	UNP Q76353
M	-23	GLY	-	expression tag	UNP Q76353
M	-22	ALA	-	expression tag	UNP Q76353
M	-21	ALA	-	expression tag	UNP Q76353
M	-20	ALA	-	expression tag	UNP Q76353
M	-19	ALA	-	expression tag	UNP Q76353
M	-18	GLY	-	expression tag	UNP Q76353
M	-17	GLN	-	expression tag	UNP Q76353
M	-16	SER	-	expression tag	UNP Q76353
M	-15	ARG	-	expression tag	UNP Q76353
M	-14	ALA	-	expression tag	UNP Q76353
M	-13	ALA	-	expression tag	UNP Q76353
M	-12	VAL	-	expression tag	UNP Q76353
M	-11	GLY	-	expression tag	UNP Q76353
M	-10	ARG	-	expression tag	UNP Q76353
M	-9	LYS	-	expression tag	UNP Q76353
M	-8	ALA	-	expression tag	UNP Q76353
M	-7	THR	-	expression tag	UNP Q76353
M	-6	LYS	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-5	LYS	-	expression tag	UNP Q76353
M	-4	THR	-	expression tag	UNP Q76353
M	-3	ASP	-	expression tag	UNP Q76353
M	-2	GLY	-	expression tag	UNP Q76353
M	-1	GLY	-	expression tag	UNP Q76353
M	0	GLY	-	expression tag	UNP Q76353
N	-75	GLY	-	expression tag	UNP Q76353
N	-74	SER	-	expression tag	UNP Q76353
N	-73	HIS	-	expression tag	UNP Q76353
N	-72	MET	-	expression tag	UNP Q76353
N	-71	PRO	-	expression tag	UNP Q76353
N	-70	LYS	-	expression tag	UNP Q76353
N	-69	ARG	-	expression tag	UNP Q76353
N	-68	GLY	-	expression tag	UNP Q76353
N	-67	ARG	-	expression tag	UNP Q76353
N	-66	PRO	-	expression tag	UNP Q76353
N	-65	ALA	-	expression tag	UNP Q76353
N	-64	ALA	-	expression tag	UNP Q76353
N	-63	THR	-	expression tag	UNP Q76353
N	-62	GLU	-	expression tag	UNP Q76353
N	-61	VAL	-	expression tag	UNP Q76353
N	-60	LYS	-	expression tag	UNP Q76353
N	-59	ILE	-	expression tag	UNP Q76353
N	-58	PRO	-	expression tag	UNP Q76353
N	-57	LYS	-	expression tag	UNP Q76353
N	-56	PRO	-	expression tag	UNP Q76353
N	-55	ARG	-	expression tag	UNP Q76353
N	-54	GLY	-	expression tag	UNP Q76353
N	-53	ARG	-	expression tag	UNP Q76353
N	-52	PRO	-	expression tag	UNP Q76353
N	-51	PRO	-	expression tag	UNP Q76353
N	-50	LEU	-	expression tag	UNP Q76353
N	-49	PRO	-	expression tag	UNP Q76353
N	-48	ALA	-	expression tag	UNP Q76353
N	-47	GLY	-	expression tag	UNP Q76353
N	-46	THR	-	expression tag	UNP Q76353
N	-45	ASN	-	expression tag	UNP Q76353
N	-44	SER	-	expression tag	UNP Q76353
N	-43	LYS	-	expression tag	UNP Q76353
N	-42	GLY	-	expression tag	UNP Q76353
N	-41	PRO	-	expression tag	UNP Q76353
N	-40	PRO	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-39	ASP	-	expression tag	UNP Q76353
N	-38	PHE	-	expression tag	UNP Q76353
N	-37	SER	-	expression tag	UNP Q76353
N	-36	SER	-	expression tag	UNP Q76353
N	-35	ASP	-	expression tag	UNP Q76353
N	-34	GLU	-	expression tag	UNP Q76353
N	-33	GLU	-	expression tag	UNP Q76353
N	-32	ARG	-	expression tag	UNP Q76353
N	-31	GLU	-	expression tag	UNP Q76353
N	-30	PRO	-	expression tag	UNP Q76353
N	-29	THR	-	expression tag	UNP Q76353
N	-28	PRO	-	expression tag	UNP Q76353
N	-27	VAL	-	expression tag	UNP Q76353
N	-26	LEU	-	expression tag	UNP Q76353
N	-25	GLY	-	expression tag	UNP Q76353
N	-24	SER	-	expression tag	UNP Q76353
N	-23	GLY	-	expression tag	UNP Q76353
N	-22	ALA	-	expression tag	UNP Q76353
N	-21	ALA	-	expression tag	UNP Q76353
N	-20	ALA	-	expression tag	UNP Q76353
N	-19	ALA	-	expression tag	UNP Q76353
N	-18	GLY	-	expression tag	UNP Q76353
N	-17	GLN	-	expression tag	UNP Q76353
N	-16	SER	-	expression tag	UNP Q76353
N	-15	ARG	-	expression tag	UNP Q76353
N	-14	ALA	-	expression tag	UNP Q76353
N	-13	ALA	-	expression tag	UNP Q76353
N	-12	VAL	-	expression tag	UNP Q76353
N	-11	GLY	-	expression tag	UNP Q76353
N	-10	ARG	-	expression tag	UNP Q76353
N	-9	LYS	-	expression tag	UNP Q76353
N	-8	ALA	-	expression tag	UNP Q76353
N	-7	THR	-	expression tag	UNP Q76353
N	-6	LYS	-	expression tag	UNP Q76353
N	-5	LYS	-	expression tag	UNP Q76353
N	-4	THR	-	expression tag	UNP Q76353
N	-3	ASP	-	expression tag	UNP Q76353
N	-2	GLY	-	expression tag	UNP Q76353
N	-1	GLY	-	expression tag	UNP Q76353
N	0	GLY	-	expression tag	UNP Q76353
O	-75	GLY	-	expression tag	UNP Q76353
O	-74	SER	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-73	HIS	-	expression tag	UNP Q76353
O	-72	MET	-	expression tag	UNP Q76353
O	-71	PRO	-	expression tag	UNP Q76353
O	-70	LYS	-	expression tag	UNP Q76353
O	-69	ARG	-	expression tag	UNP Q76353
O	-68	GLY	-	expression tag	UNP Q76353
O	-67	ARG	-	expression tag	UNP Q76353
O	-66	PRO	-	expression tag	UNP Q76353
O	-65	ALA	-	expression tag	UNP Q76353
O	-64	ALA	-	expression tag	UNP Q76353
O	-63	THR	-	expression tag	UNP Q76353
O	-62	GLU	-	expression tag	UNP Q76353
O	-61	VAL	-	expression tag	UNP Q76353
O	-60	LYS	-	expression tag	UNP Q76353
O	-59	ILE	-	expression tag	UNP Q76353
O	-58	PRO	-	expression tag	UNP Q76353
O	-57	LYS	-	expression tag	UNP Q76353
O	-56	PRO	-	expression tag	UNP Q76353
O	-55	ARG	-	expression tag	UNP Q76353
O	-54	GLY	-	expression tag	UNP Q76353
O	-53	ARG	-	expression tag	UNP Q76353
O	-52	PRO	-	expression tag	UNP Q76353
O	-51	PRO	-	expression tag	UNP Q76353
O	-50	LEU	-	expression tag	UNP Q76353
O	-49	PRO	-	expression tag	UNP Q76353
O	-48	ALA	-	expression tag	UNP Q76353
O	-47	GLY	-	expression tag	UNP Q76353
O	-46	THR	-	expression tag	UNP Q76353
O	-45	ASN	-	expression tag	UNP Q76353
O	-44	SER	-	expression tag	UNP Q76353
O	-43	LYS	-	expression tag	UNP Q76353
O	-42	GLY	-	expression tag	UNP Q76353
O	-41	PRO	-	expression tag	UNP Q76353
O	-40	PRO	-	expression tag	UNP Q76353
O	-39	ASP	-	expression tag	UNP Q76353
O	-38	PHE	-	expression tag	UNP Q76353
O	-37	SER	-	expression tag	UNP Q76353
O	-36	SER	-	expression tag	UNP Q76353
O	-35	ASP	-	expression tag	UNP Q76353
O	-34	GLU	-	expression tag	UNP Q76353
O	-33	GLU	-	expression tag	UNP Q76353
O	-32	ARG	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-31	GLU	-	expression tag	UNP Q76353
O	-30	PRO	-	expression tag	UNP Q76353
O	-29	THR	-	expression tag	UNP Q76353
O	-28	PRO	-	expression tag	UNP Q76353
O	-27	VAL	-	expression tag	UNP Q76353
O	-26	LEU	-	expression tag	UNP Q76353
O	-25	GLY	-	expression tag	UNP Q76353
O	-24	SER	-	expression tag	UNP Q76353
O	-23	GLY	-	expression tag	UNP Q76353
O	-22	ALA	-	expression tag	UNP Q76353
O	-21	ALA	-	expression tag	UNP Q76353
O	-20	ALA	-	expression tag	UNP Q76353
O	-19	ALA	-	expression tag	UNP Q76353
O	-18	GLY	-	expression tag	UNP Q76353
O	-17	GLN	-	expression tag	UNP Q76353
O	-16	SER	-	expression tag	UNP Q76353
O	-15	ARG	-	expression tag	UNP Q76353
O	-14	ALA	-	expression tag	UNP Q76353
O	-13	ALA	-	expression tag	UNP Q76353
O	-12	VAL	-	expression tag	UNP Q76353
O	-11	GLY	-	expression tag	UNP Q76353
O	-10	ARG	-	expression tag	UNP Q76353
O	-9	LYS	-	expression tag	UNP Q76353
O	-8	ALA	-	expression tag	UNP Q76353
O	-7	THR	-	expression tag	UNP Q76353
O	-6	LYS	-	expression tag	UNP Q76353
O	-5	LYS	-	expression tag	UNP Q76353
O	-4	THR	-	expression tag	UNP Q76353
O	-3	ASP	-	expression tag	UNP Q76353
O	-2	GLY	-	expression tag	UNP Q76353
O	-1	GLY	-	expression tag	UNP Q76353
O	0	GLY	-	expression tag	UNP Q76353
P	-75	GLY	-	expression tag	UNP Q76353
P	-74	SER	-	expression tag	UNP Q76353
P	-73	HIS	-	expression tag	UNP Q76353
P	-72	MET	-	expression tag	UNP Q76353
P	-71	PRO	-	expression tag	UNP Q76353
P	-70	LYS	-	expression tag	UNP Q76353
P	-69	ARG	-	expression tag	UNP Q76353
P	-68	GLY	-	expression tag	UNP Q76353
P	-67	ARG	-	expression tag	UNP Q76353
P	-66	PRO	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-65	ALA	-	expression tag	UNP Q76353
P	-64	ALA	-	expression tag	UNP Q76353
P	-63	THR	-	expression tag	UNP Q76353
P	-62	GLU	-	expression tag	UNP Q76353
P	-61	VAL	-	expression tag	UNP Q76353
P	-60	LYS	-	expression tag	UNP Q76353
P	-59	ILE	-	expression tag	UNP Q76353
P	-58	PRO	-	expression tag	UNP Q76353
P	-57	LYS	-	expression tag	UNP Q76353
P	-56	PRO	-	expression tag	UNP Q76353
P	-55	ARG	-	expression tag	UNP Q76353
P	-54	GLY	-	expression tag	UNP Q76353
P	-53	ARG	-	expression tag	UNP Q76353
P	-52	PRO	-	expression tag	UNP Q76353
P	-51	PRO	-	expression tag	UNP Q76353
P	-50	LEU	-	expression tag	UNP Q76353
P	-49	PRO	-	expression tag	UNP Q76353
P	-48	ALA	-	expression tag	UNP Q76353
P	-47	GLY	-	expression tag	UNP Q76353
P	-46	THR	-	expression tag	UNP Q76353
P	-45	ASN	-	expression tag	UNP Q76353
P	-44	SER	-	expression tag	UNP Q76353
P	-43	LYS	-	expression tag	UNP Q76353
P	-42	GLY	-	expression tag	UNP Q76353
P	-41	PRO	-	expression tag	UNP Q76353
P	-40	PRO	-	expression tag	UNP Q76353
P	-39	ASP	-	expression tag	UNP Q76353
P	-38	PHE	-	expression tag	UNP Q76353
P	-37	SER	-	expression tag	UNP Q76353
P	-36	SER	-	expression tag	UNP Q76353
P	-35	ASP	-	expression tag	UNP Q76353
P	-34	GLU	-	expression tag	UNP Q76353
P	-33	GLU	-	expression tag	UNP Q76353
P	-32	ARG	-	expression tag	UNP Q76353
P	-31	GLU	-	expression tag	UNP Q76353
P	-30	PRO	-	expression tag	UNP Q76353
P	-29	THR	-	expression tag	UNP Q76353
P	-28	PRO	-	expression tag	UNP Q76353
P	-27	VAL	-	expression tag	UNP Q76353
P	-26	LEU	-	expression tag	UNP Q76353
P	-25	GLY	-	expression tag	UNP Q76353
P	-24	SER	-	expression tag	UNP Q76353

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-23	GLY	-	expression tag	UNP Q76353
P	-22	ALA	-	expression tag	UNP Q76353
P	-21	ALA	-	expression tag	UNP Q76353
P	-20	ALA	-	expression tag	UNP Q76353
P	-19	ALA	-	expression tag	UNP Q76353
P	-18	GLY	-	expression tag	UNP Q76353
P	-17	GLN	-	expression tag	UNP Q76353
P	-16	SER	-	expression tag	UNP Q76353
P	-15	ARG	-	expression tag	UNP Q76353
P	-14	ALA	-	expression tag	UNP Q76353
P	-13	ALA	-	expression tag	UNP Q76353
P	-12	VAL	-	expression tag	UNP Q76353
P	-11	GLY	-	expression tag	UNP Q76353
P	-10	ARG	-	expression tag	UNP Q76353
P	-9	LYS	-	expression tag	UNP Q76353
P	-8	ALA	-	expression tag	UNP Q76353
P	-7	THR	-	expression tag	UNP Q76353
P	-6	LYS	-	expression tag	UNP Q76353
P	-5	LYS	-	expression tag	UNP Q76353
P	-4	THR	-	expression tag	UNP Q76353
P	-3	ASP	-	expression tag	UNP Q76353
P	-2	GLY	-	expression tag	UNP Q76353
P	-1	GLY	-	expression tag	UNP Q76353
P	0	GLY	-	expression tag	UNP Q76353

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	25	Total	C	N	O	P	0	0
			503	241	89	149	24		
2	G	25	Total	C	N	O	P	0	0
			503	241	89	149	24		

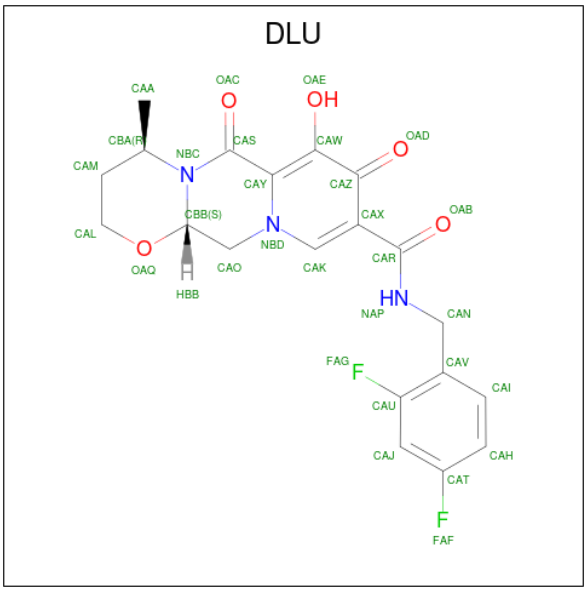
- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	23	Total	C	N	O	P	0	0
			477	225	93	136	23		
3	H	23	Total	C	N	O	P	0	0
			477	225	93	136	23		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Mg 2 2	0
4	C	2	Total Mg 2 2	0

- Molecule 5 is (4R,12aS)-N-(2,4-difluorobenzyl)-7-hydroxy-4-methyl-6,8-dioxo-3,4,6,8,12,12a-hexahydro-2H-pyrido[1',2':4,5]pyrazino[2,1-b][1,3]oxazine-9-carboxamide (CCD ID: DLU) (formula: $C_{20}H_{19}F_2N_3O_5$).



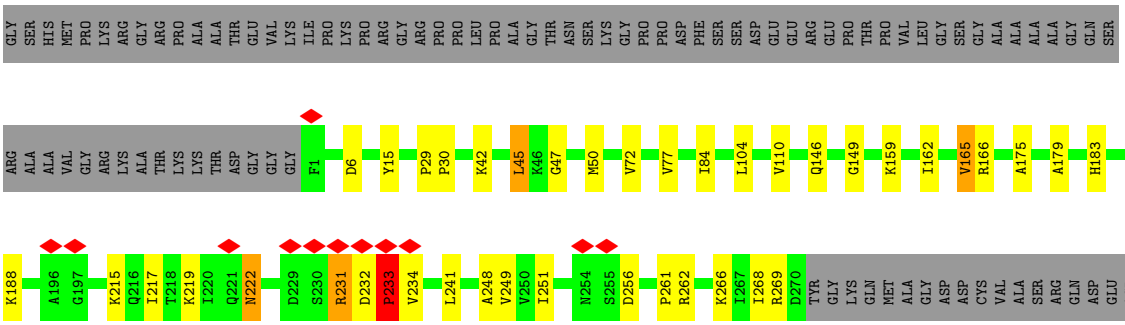
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C F N O 30 20 2 3 5	0
5	C	1	Total C F N O 30 20 2 3 5	0

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.

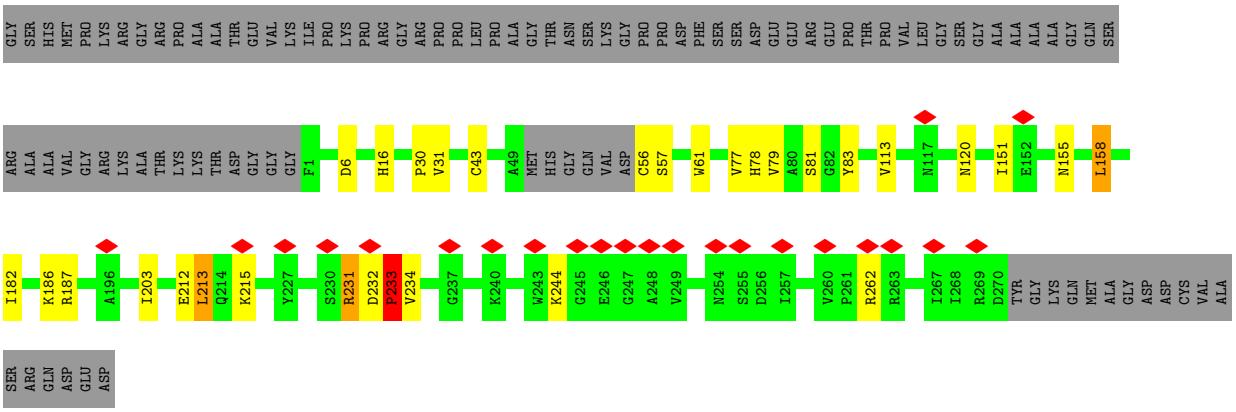
• Molecule 1: Integrase

Chain A:



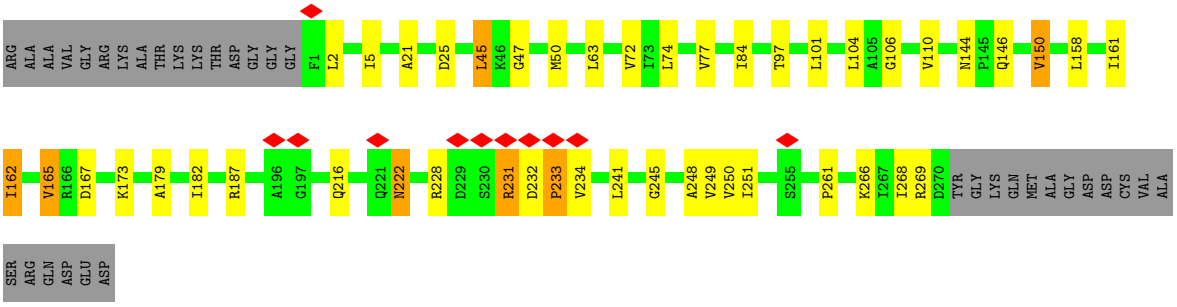
• Molecule 1: Integrase

Chain B:



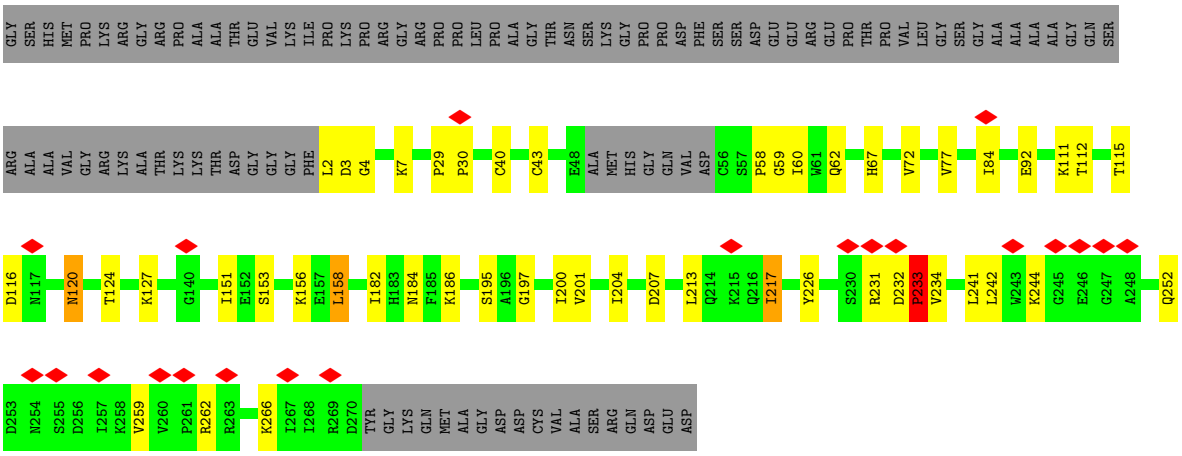
• Molecule 1: Integrase

Chain C:



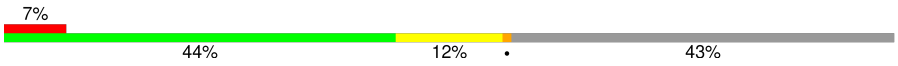
• Molecule 1: Integrase

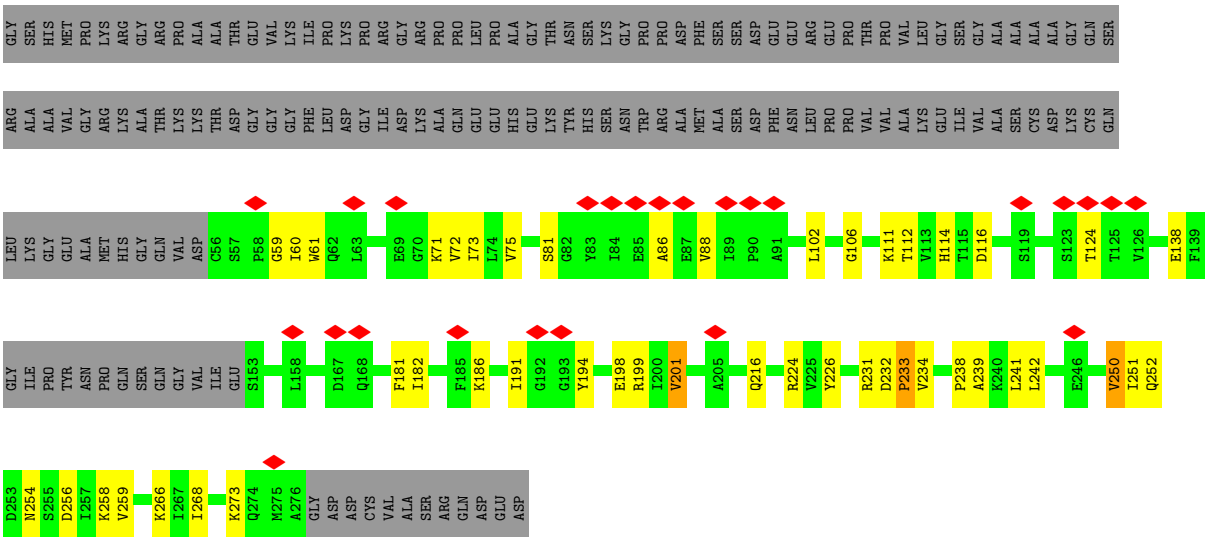
Chain D:



• Molecule 1: Integrase

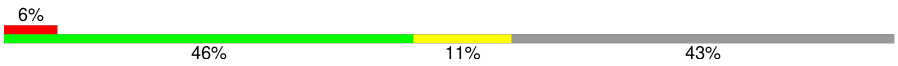
Chain I:

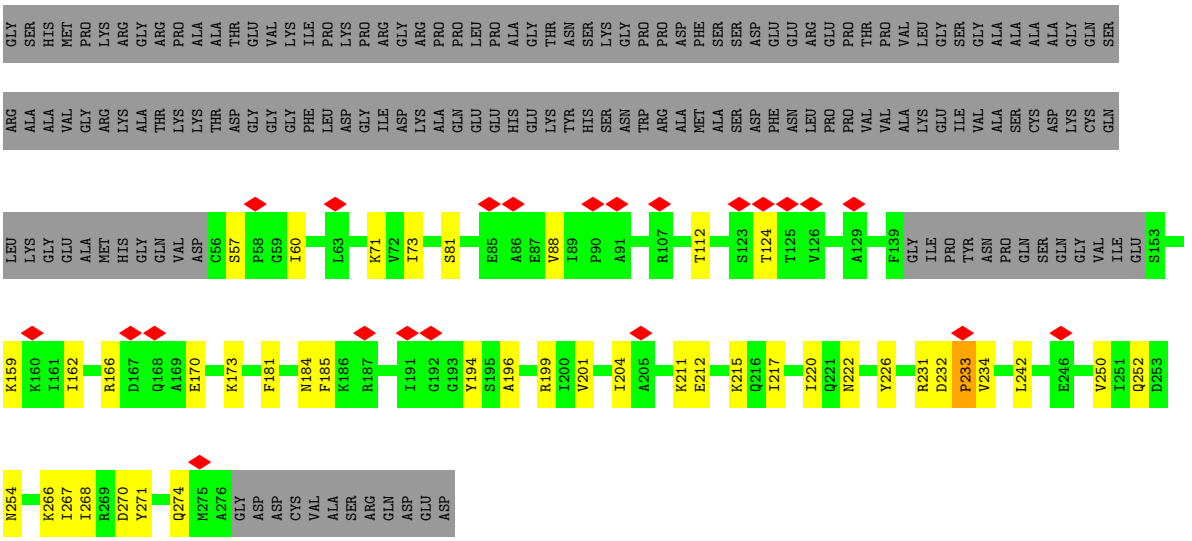




• Molecule 1: Integrase

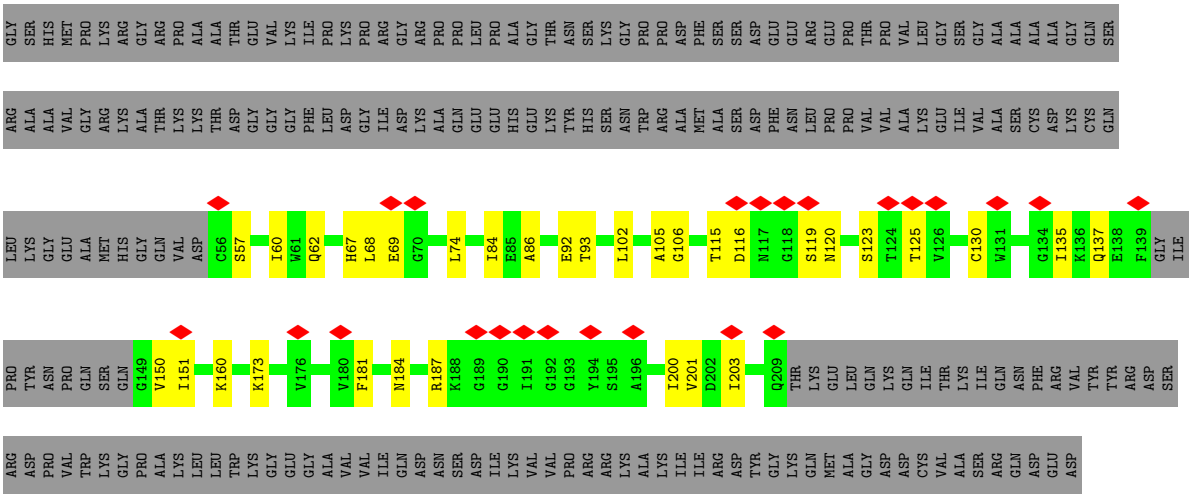
Chain J:





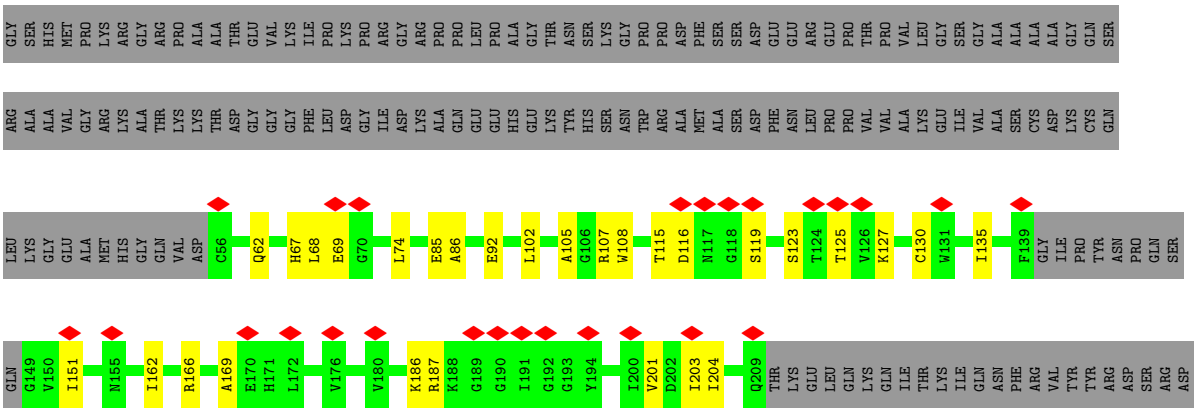
• Molecule 1: Integrase

Chain K:



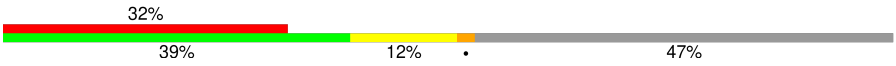
• Molecule 1: Integrase

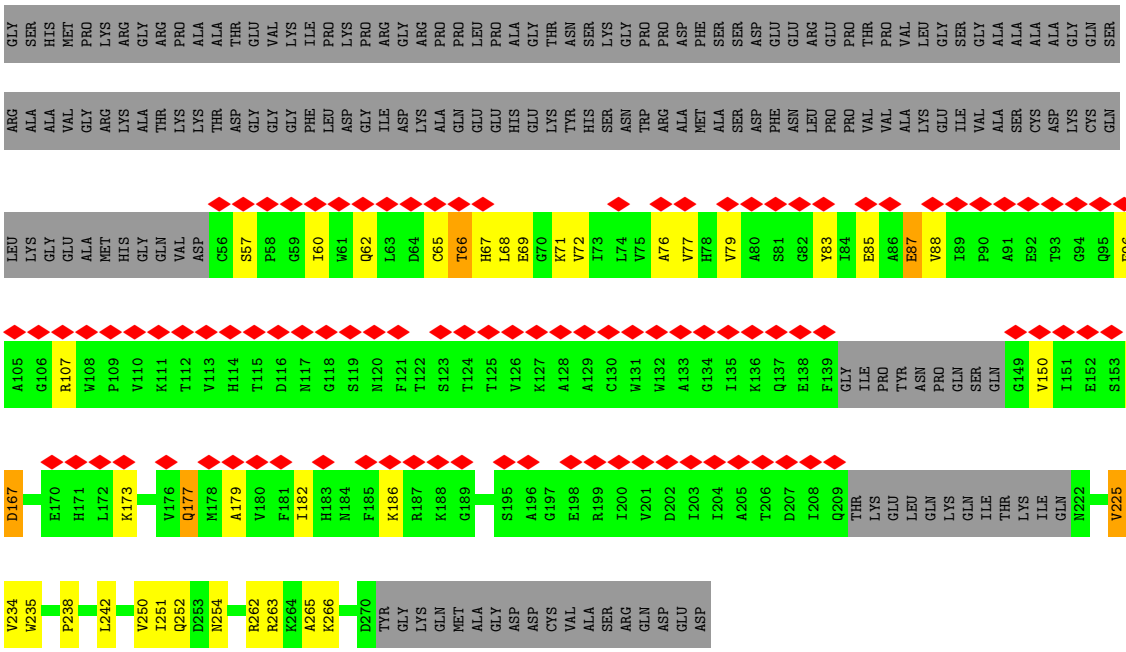
Chain L:



• Molecule 1: Integrase

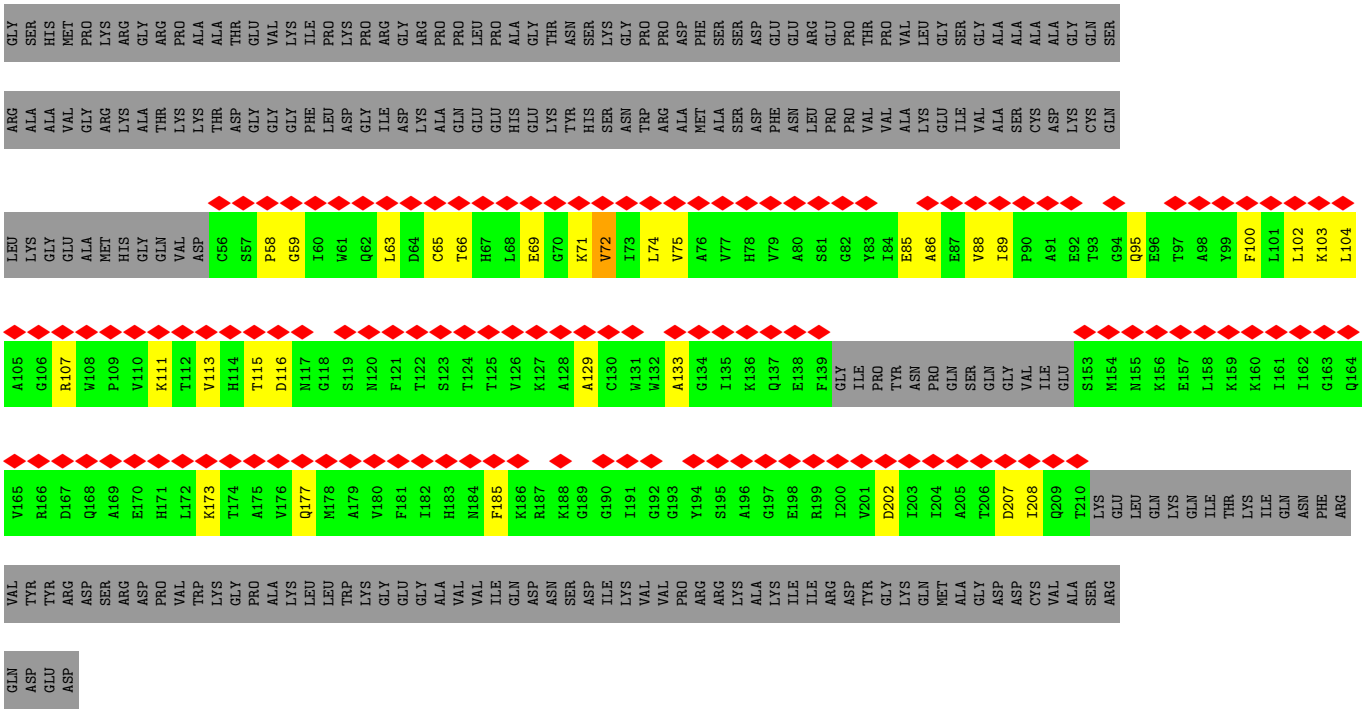
Chain M:





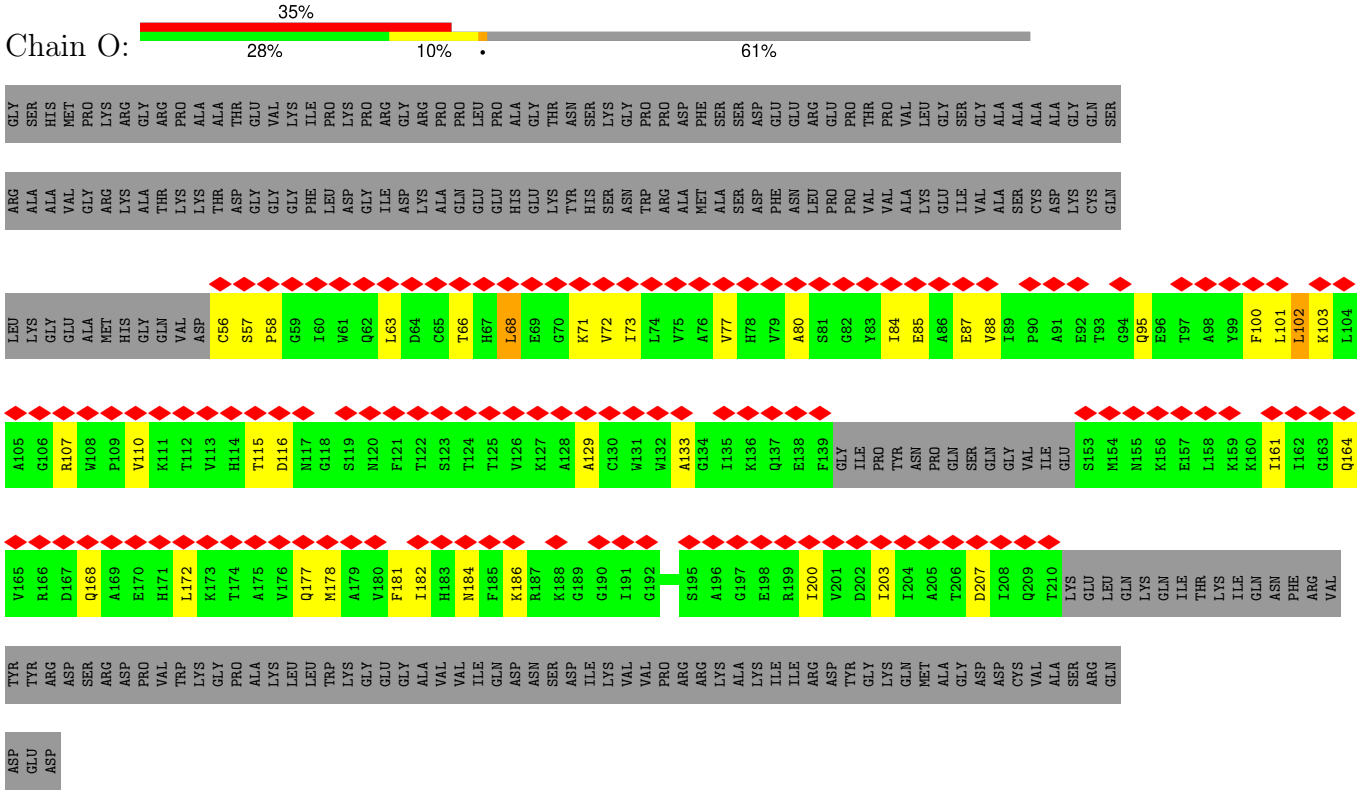
• Molecule 1: Integrase

Chain N:



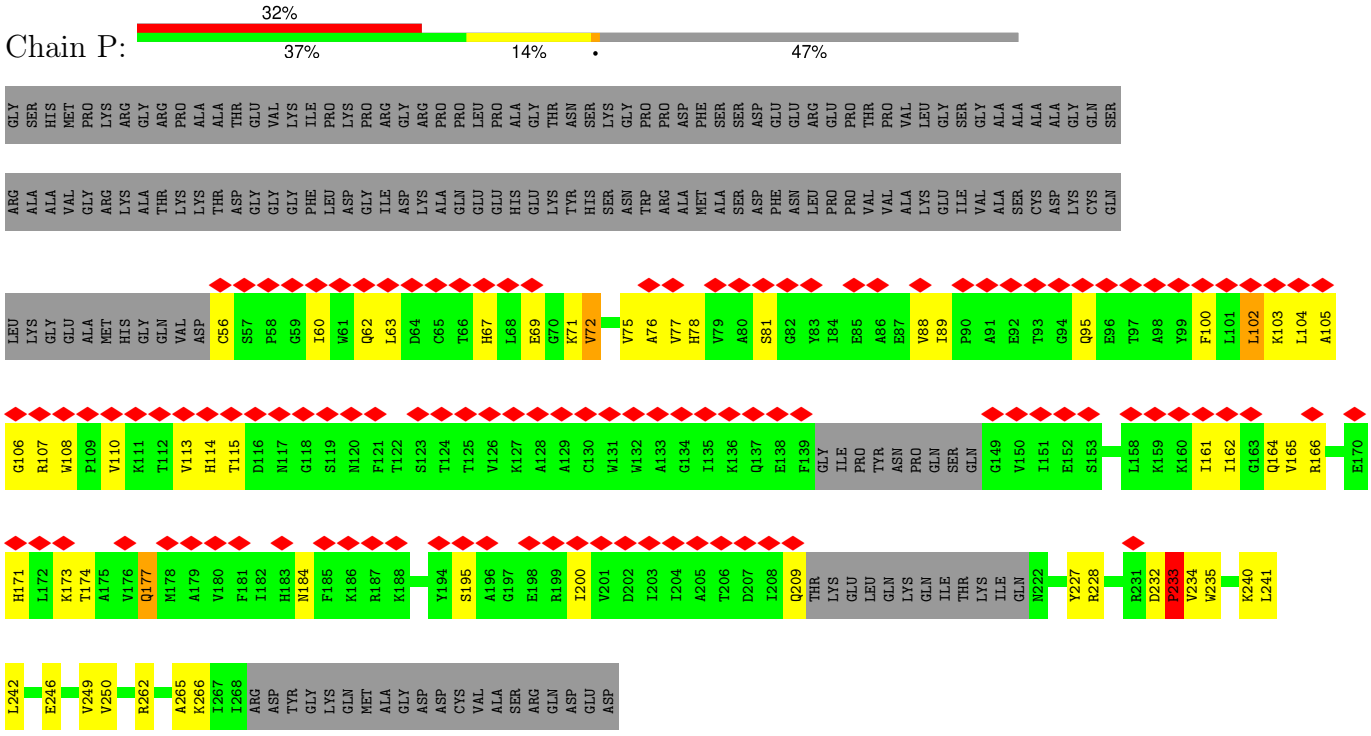
- Molecule 1: Integrase

Chain O:



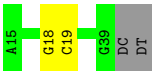
- Molecule 1: Integrase

Chain P:



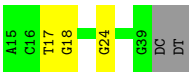
- Molecule 2: DNA (27-MER)

Chain E:



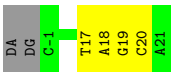
• Molecule 2: DNA (27-MER)

Chain G:



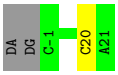
• Molecule 3: DNA (25-MER)

Chain F:



• Molecule 3: DNA (25-MER)

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	75	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	0.042	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DLU, 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	A	0.19	0/2175	0.45	1/2940 (0.0%)
1	B	0.18	0/2127	0.43	1/2874 (0.0%)
1	C	0.19	0/2174	0.45	1/2938 (0.0%)
1	D	0.19	0/2110	0.42	1/2851 (0.0%)
1	I	0.21	0/1679	0.48	1/2265 (0.0%)
1	J	0.19	0/1671	0.46	1/2254 (0.0%)
1	K	0.14	0/1130	0.35	0/1527
1	L	0.15	0/1130	0.37	0/1527
1	M	0.21	0/1546	0.52	1/2087 (0.0%)
1	N	0.20	0/1109	0.46	0/1499
1	O	0.18	0/1109	0.44	0/1499
1	P	0.23	0/1527	0.53	1/2062 (0.0%)
2	E	0.26	0/562	0.64	0/864
2	G	0.25	0/562	0.62	0/864
3	F	0.30	0/536	0.69	0/826
3	H	0.29	0/536	0.68	0/826
All	All	0.20	0/21683	0.48	8/29703 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	233	PRO	CA-N-CD	-9.28	99.00	112.00
1	C	233	PRO	CA-N-CD	-9.15	99.19	112.00
1	J	233	PRO	CA-N-CD	-9.14	99.20	112.00
1	A	233	PRO	CA-N-CD	-9.14	99.21	112.00
1	M	233	PRO	CA-N-CD	-9.14	99.21	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2129	0	2142	30	0
1	B	2083	0	2101	19	0
1	C	2128	0	2138	33	0
1	D	2067	0	2084	31	0
1	I	1646	0	1683	29	0
1	J	1639	0	1676	31	0
1	K	1110	0	1117	20	0
1	L	1110	0	1117	18	0
1	M	1517	0	1540	38	0
1	N	1089	0	1095	22	0
1	O	1089	0	1095	26	0
1	P	1498	0	1523	45	0
2	E	503	0	283	2	0
2	G	503	0	283	3	0
3	F	477	0	258	3	0
3	H	477	0	258	1	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	30	0	18	2	0
5	C	30	0	18	2	0
All	All	21129	0	20429	310	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 7.

The worst 5 of 310 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:ILE:CD1	1:I:186:LYS:HD2	1.96	0.95
1:M:182:ILE:CD1	1:M:186:LYS:HD2	1.97	0.94
1:M:182:ILE:HD12	1:M:186:LYS:HD2	1.54	0.89
1:P:233:PRO:HD2	1:P:234:VAL:H	1.39	0.88
1:I:182:ILE:HD13	1:I:186:LYS:HD2	1.61	0.82

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/364 (74%)	254 (95%)	13 (5%)	1 (0%)	30	68
1	B	260/364 (71%)	248 (95%)	11 (4%)	1 (0%)	30	68
1	C	268/364 (74%)	257 (96%)	11 (4%)	0	100	100
1	D	258/364 (71%)	247 (96%)	10 (4%)	1 (0%)	30	68
1	I	204/364 (56%)	198 (97%)	6 (3%)	0	100	100
1	J	204/364 (56%)	195 (96%)	9 (4%)	0	100	100
1	K	141/364 (39%)	140 (99%)	1 (1%)	0	100	100
1	L	141/364 (39%)	140 (99%)	1 (1%)	0	100	100
1	M	188/364 (52%)	178 (95%)	10 (5%)	0	100	100
1	N	138/364 (38%)	133 (96%)	5 (4%)	0	100	100
1	O	138/364 (38%)	132 (96%)	6 (4%)	0	100	100
1	P	186/364 (51%)	178 (96%)	7 (4%)	1 (0%)	25	64
All	All	2394/4368 (55%)	2300 (96%)	90 (4%)	4 (0%)	45	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	233	PRO
1	B	233	PRO
1	A	233	PRO
1	P	233	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/294 (77%)	220 (97%)	6 (3%)	40	59
1	B	221/294 (75%)	214 (97%)	7 (3%)	34	54
1	C	225/294 (76%)	216 (96%)	9 (4%)	27	48
1	D	220/294 (75%)	214 (97%)	6 (3%)	40	59
1	I	173/294 (59%)	165 (95%)	8 (5%)	23	45
1	J	172/294 (58%)	168 (98%)	4 (2%)	45	64
1	K	116/294 (40%)	113 (97%)	3 (3%)	41	60
1	L	116/294 (40%)	114 (98%)	2 (2%)	56	72
1	M	159/294 (54%)	147 (92%)	12 (8%)	11	30
1	N	114/294 (39%)	109 (96%)	5 (4%)	24	46
1	O	114/294 (39%)	106 (93%)	8 (7%)	12	32
1	P	157/294 (53%)	145 (92%)	12 (8%)	11	30
All	All	2013/3528 (57%)	1931 (96%)	82 (4%)	28	48

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	69	GLU
1	P	72	VAL
1	N	113	VAL
1	O	101	LEU
1	P	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	254	ASN
1	O	114	HIS
1	K	120	ASN
1	M	120	ASN
1	P	117	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DLU	A	303	4	30,33,33	5.05	13 (43%)	34,49,49	1.62	8 (23%)
5	DLU	C	303	4	30,33,33	5.05	13 (43%)	34,49,49	1.61	8 (23%)

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
5	DLU	A	303	4	-	0/9/35/35	1/4/4/4
5	DLU	C	303	4	-	0/9/35/35	1/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	303	DLU	CAO-NBD	18.04	1.62	1.46
5	A	303	DLU	CAO-NBD	18.03	1.62	1.46
5	A	303	DLU	CAY-CAW	15.10	1.55	1.36
5	C	303	DLU	CAY-CAW	15.10	1.55	1.36
5	A	303	DLU	CAK-NBD	7.26	1.50	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	303	DLU	OAC-CAS-CAY	-3.17	119.89	126.38
5	C	303	DLU	OAC-CAS-CAY	-3.15	119.92	126.38
5	A	303	DLU	CAU-CAJ-CAT	3.12	120.00	116.67
5	C	303	DLU	CAU-CAJ-CAT	3.10	119.98	116.67
5	C	303	DLU	CAA-CBA-NBC	-2.53	108.14	112.32

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

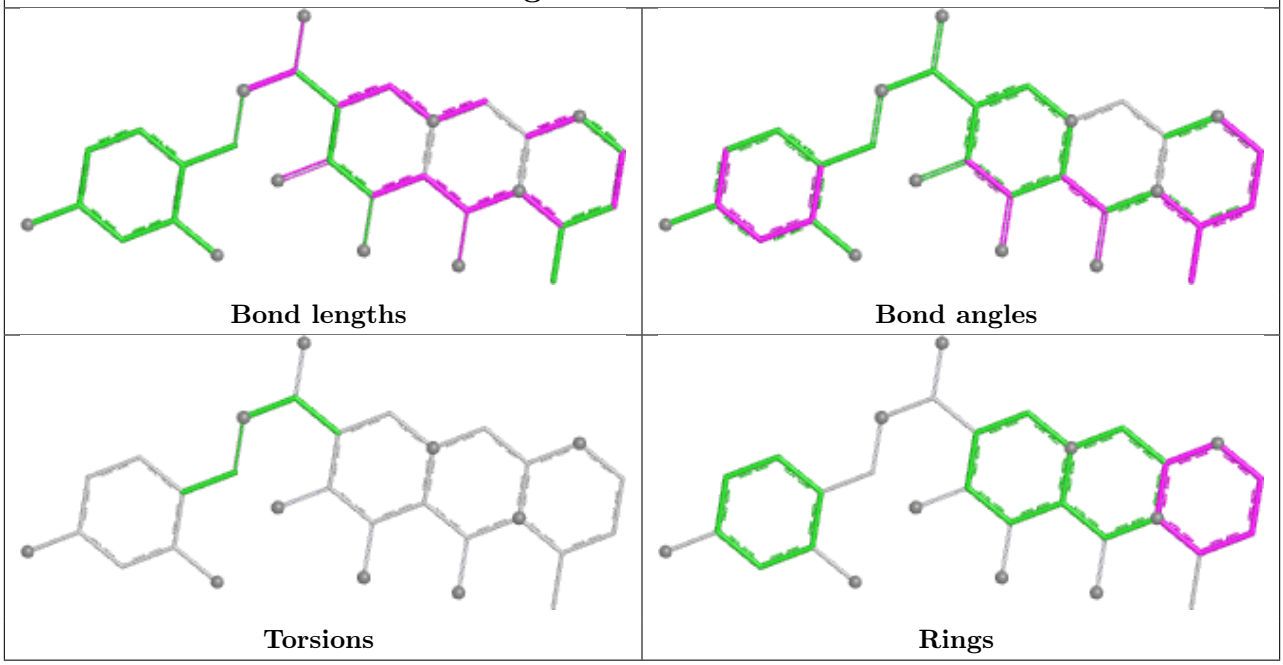
Mol	Chain	Res	Type	Atoms
5	A	303	DLU	CAL-CAM-CBA-CBB-NBC-OAQ
5	C	303	DLU	CAL-CAM-CBA-CBB-NBC-OAQ

2 monomers are involved in 4 short contacts:

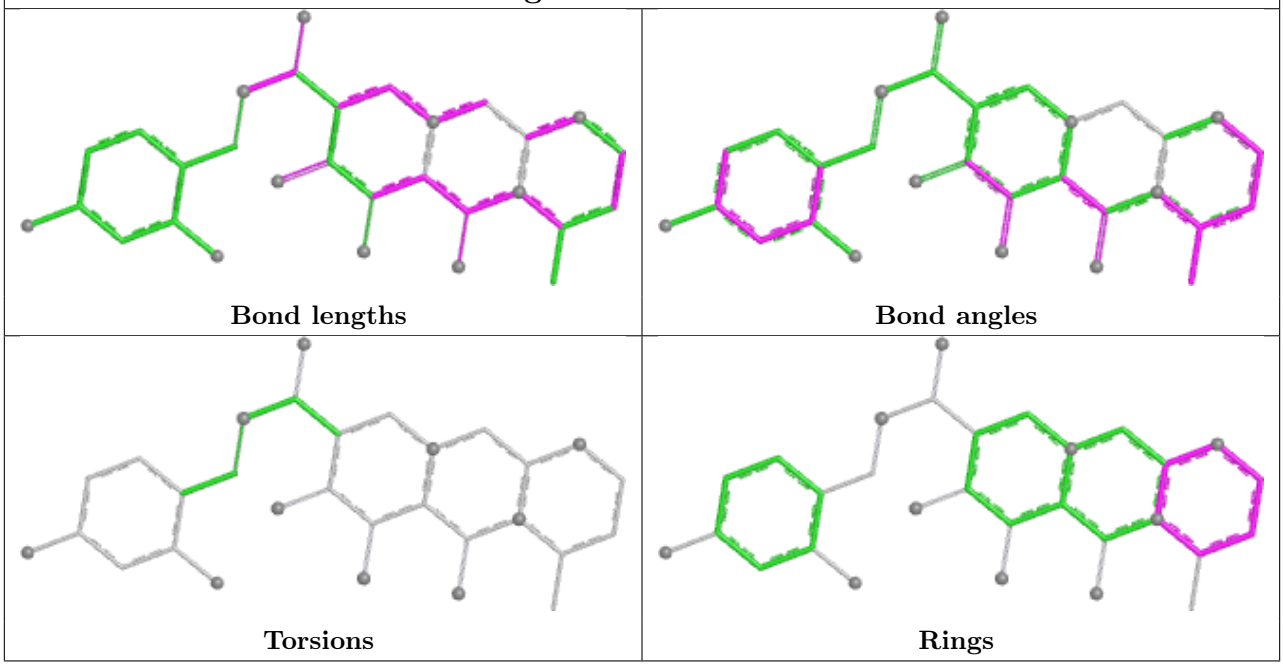
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	DLU	2	0
5	C	303	DLU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DLU A 303



Ligand DLU C 303



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.

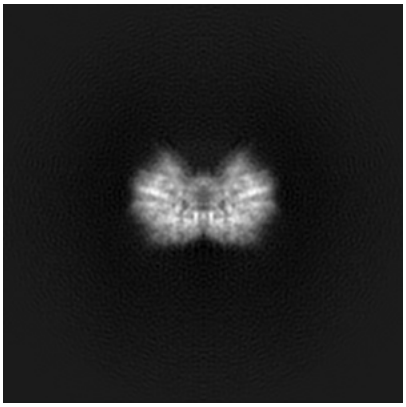
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20689. These allow visual inspection of the internal detail of the map and identification of artifacts.

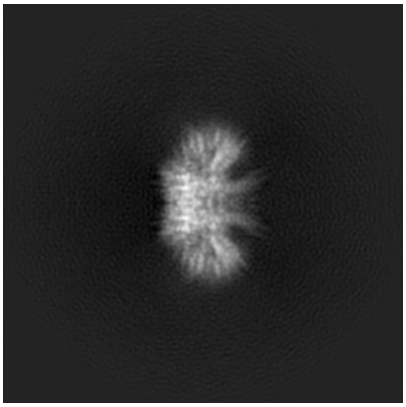
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

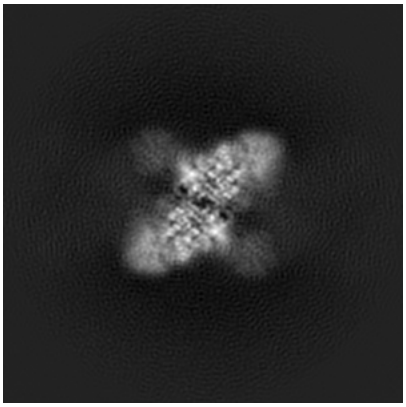
6.1.1 Primary map



X



Y



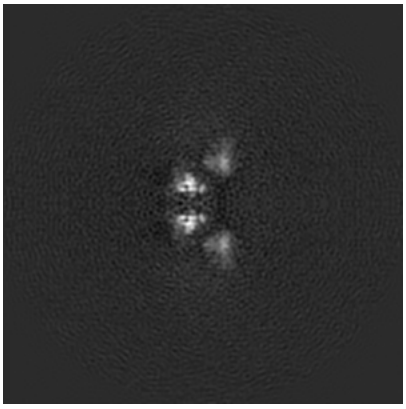
Z

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

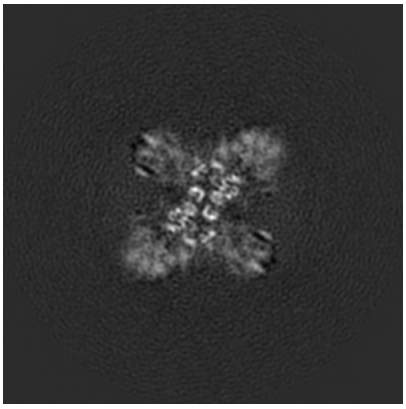
6.2 Central slices

6.2.1 Primary map

X Index: 180



Y Index: 180

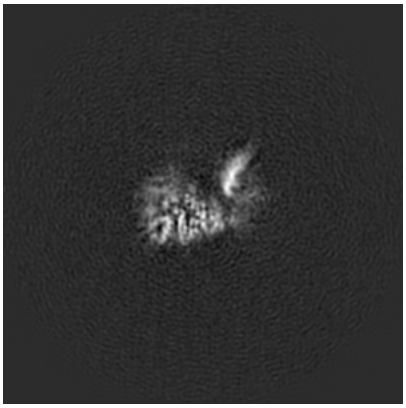


Z Index: 180

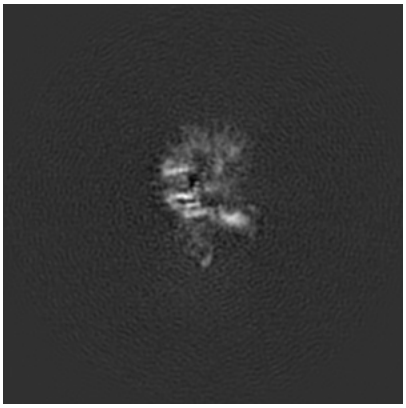
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

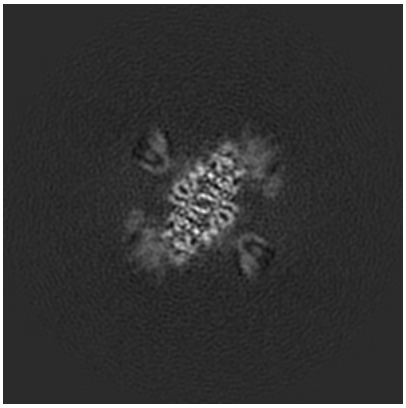
6.3.1 Primary map



X Index: 167



Y Index: 206



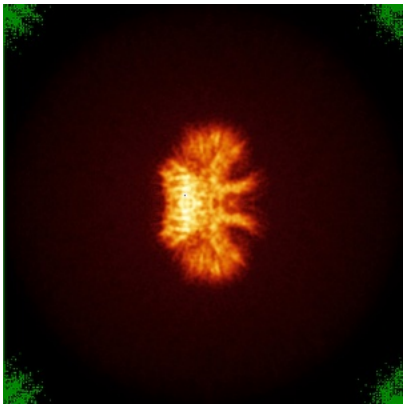
Z Index: 165

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

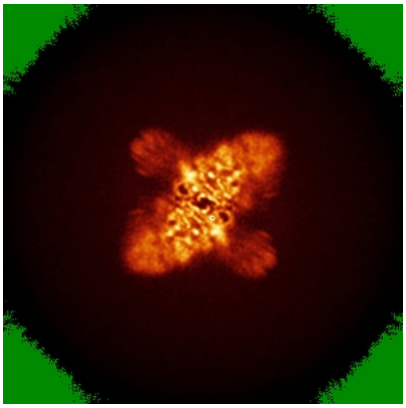
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

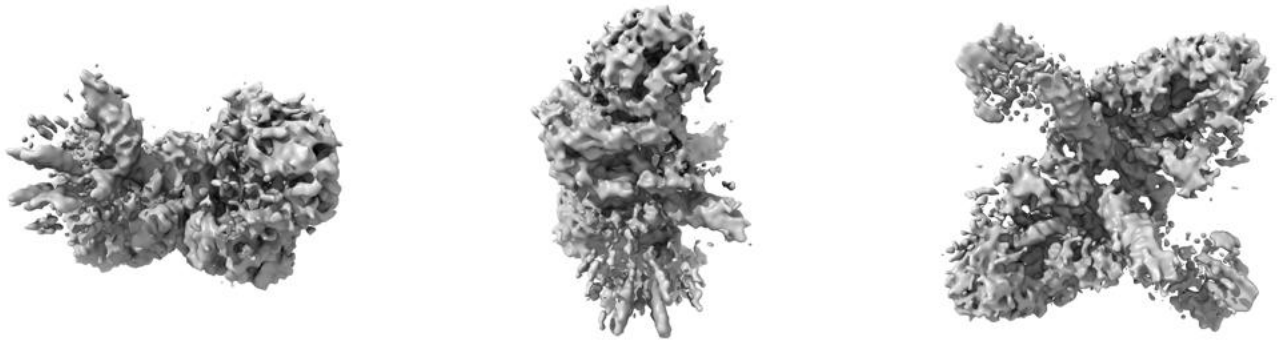


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

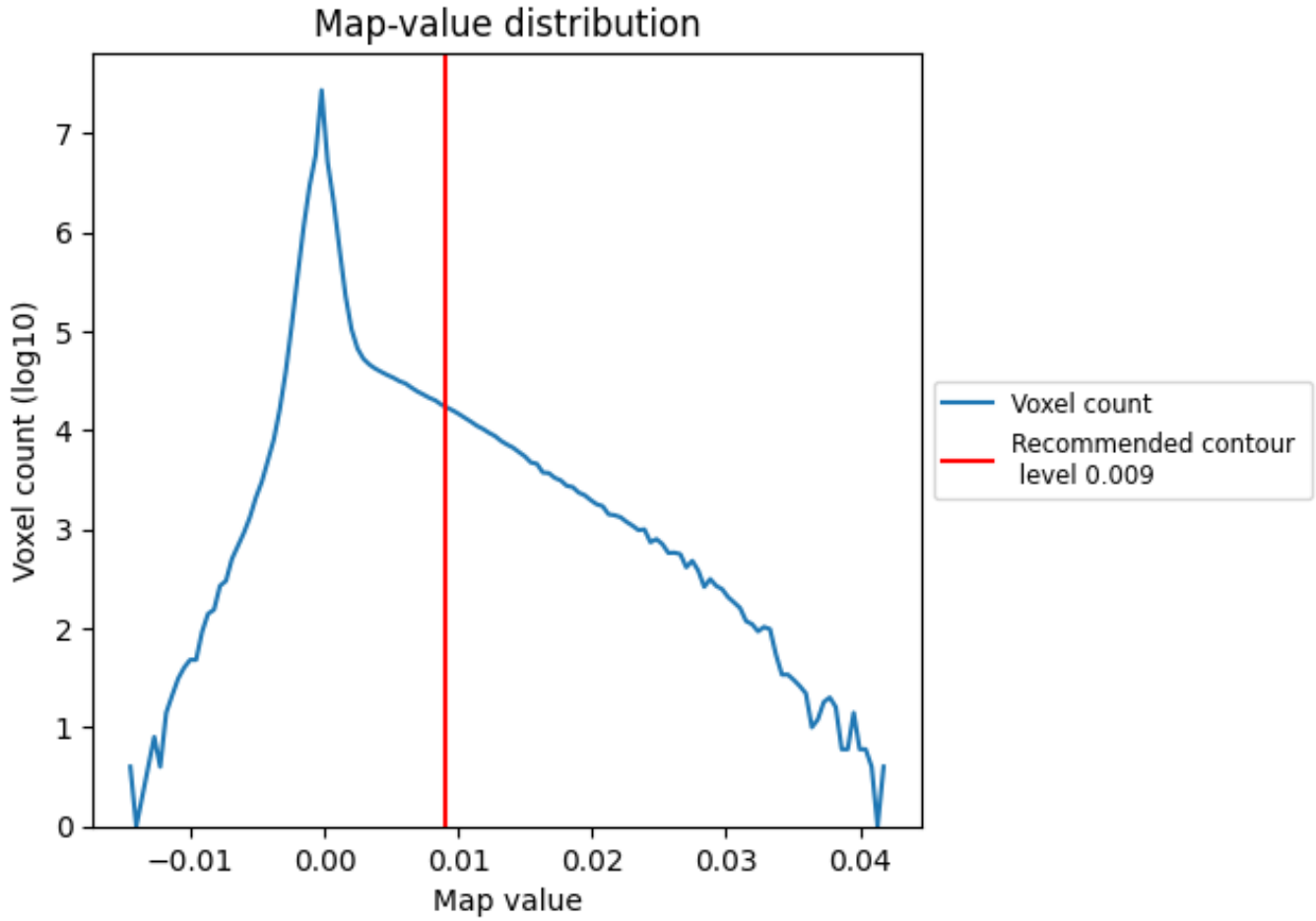
6.6 Mask visualisation (i)

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

7 Map analysis

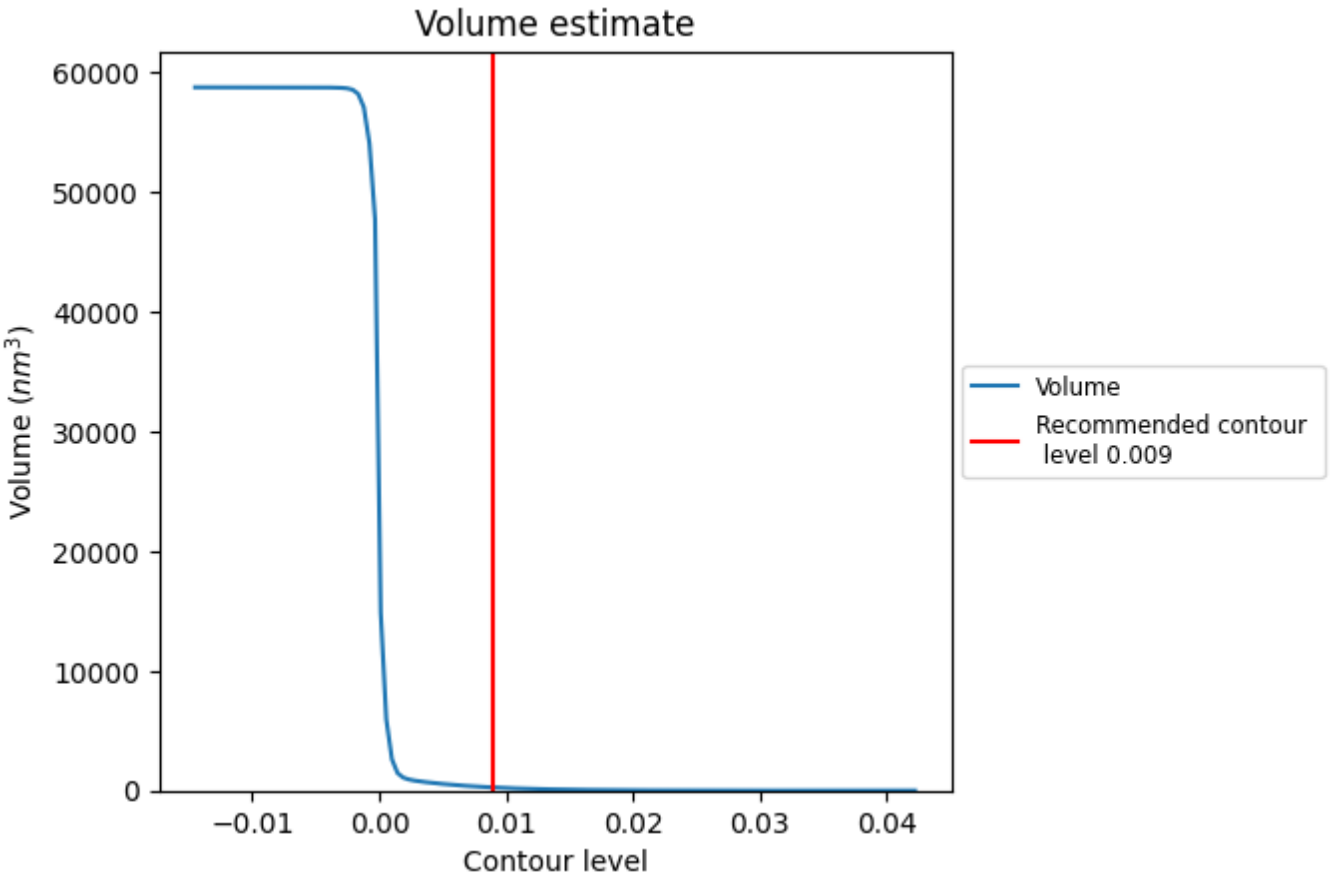
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

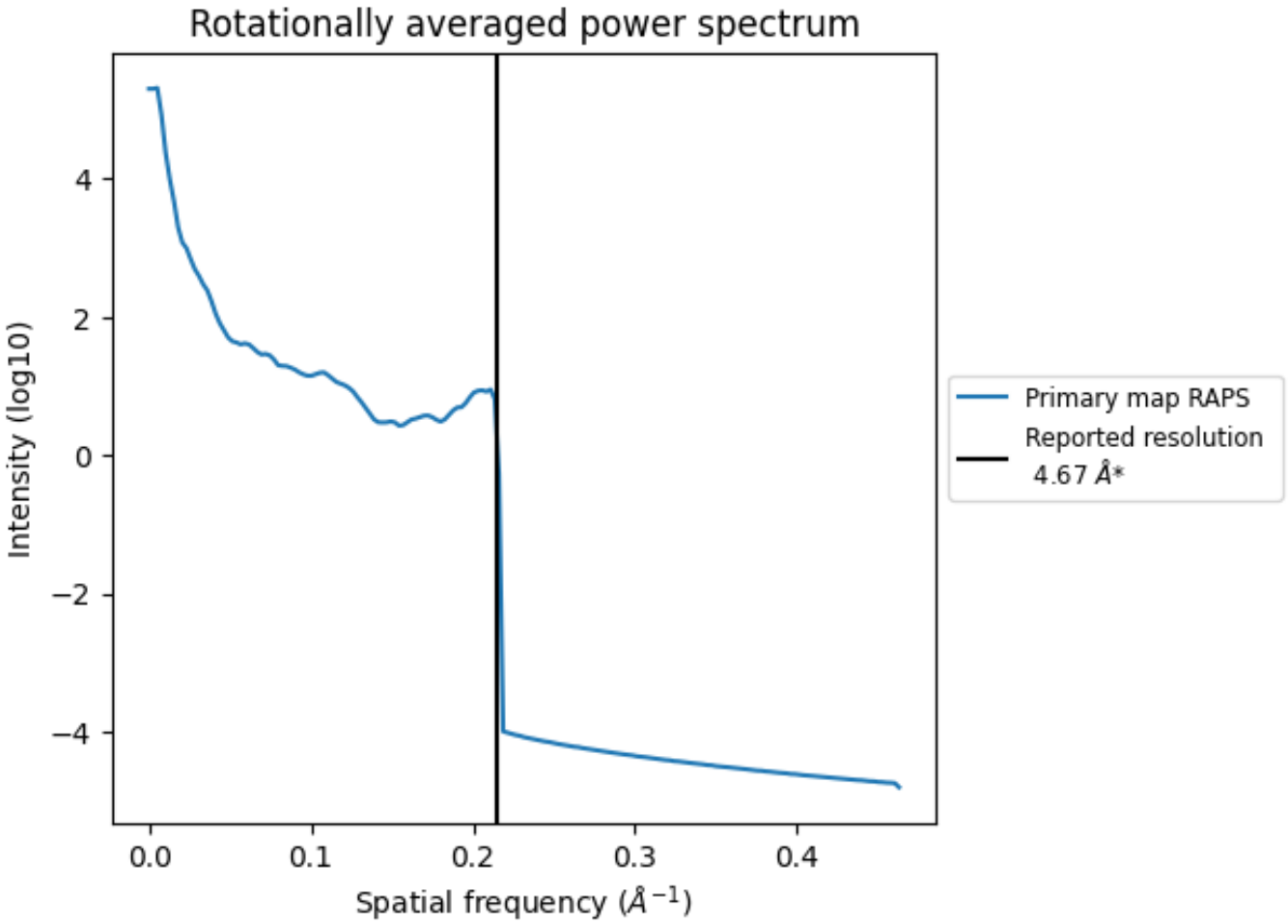
7.2 Volume estimate (i)



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 235 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 0.214 Å^{-1}

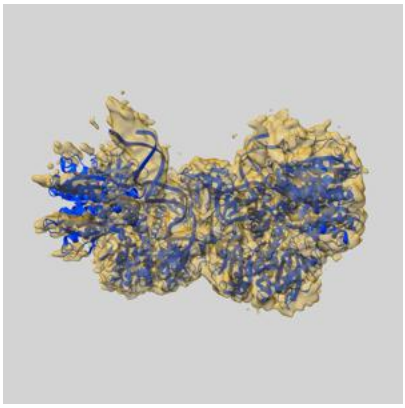
8 Fourier-Shell correlation

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

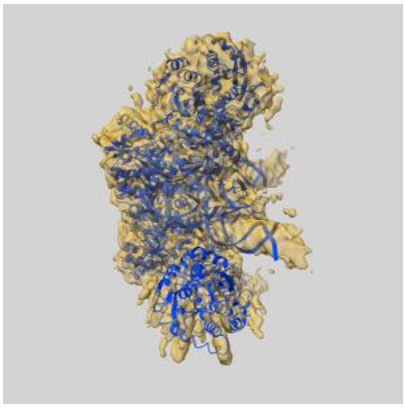
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20689 and PDB model 6U8Q. Per-residue inclusion information can be found in section 3 on page 28.

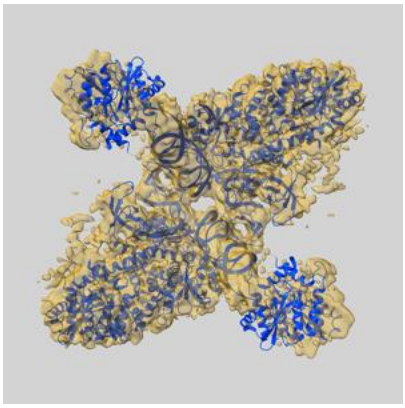
9.1 Map-model overlay



X



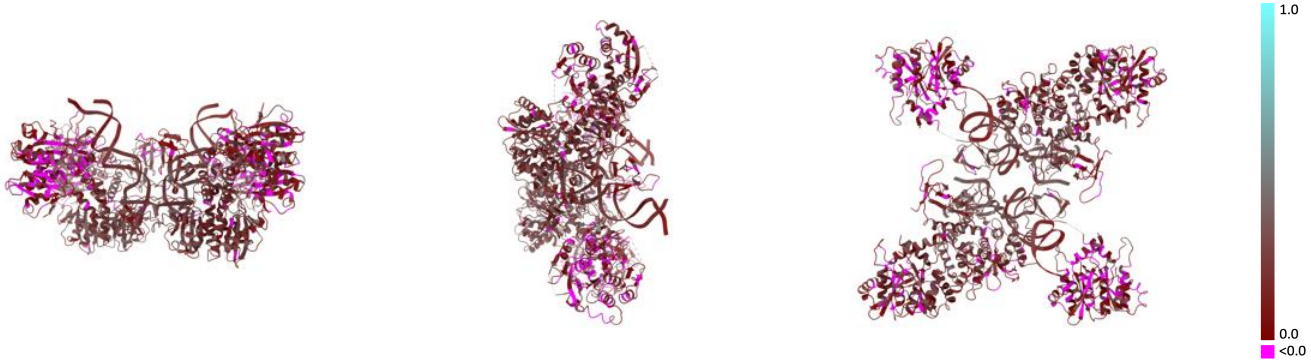
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

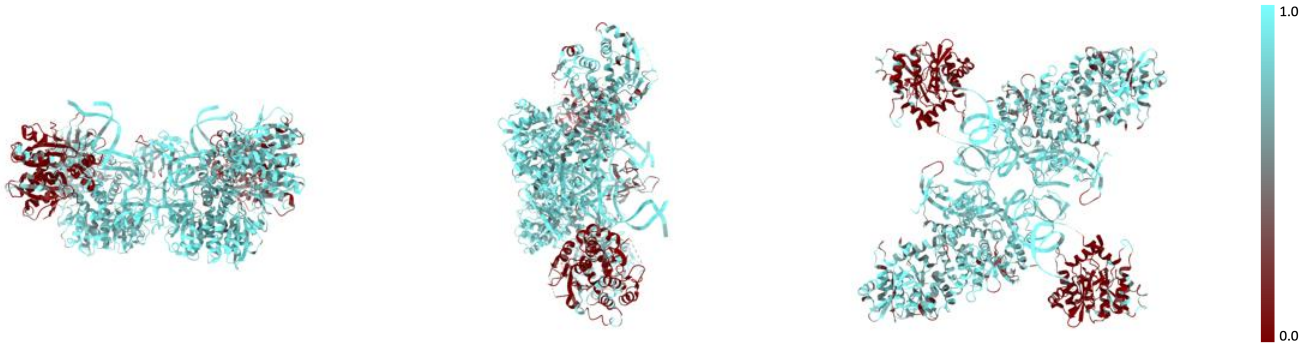
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

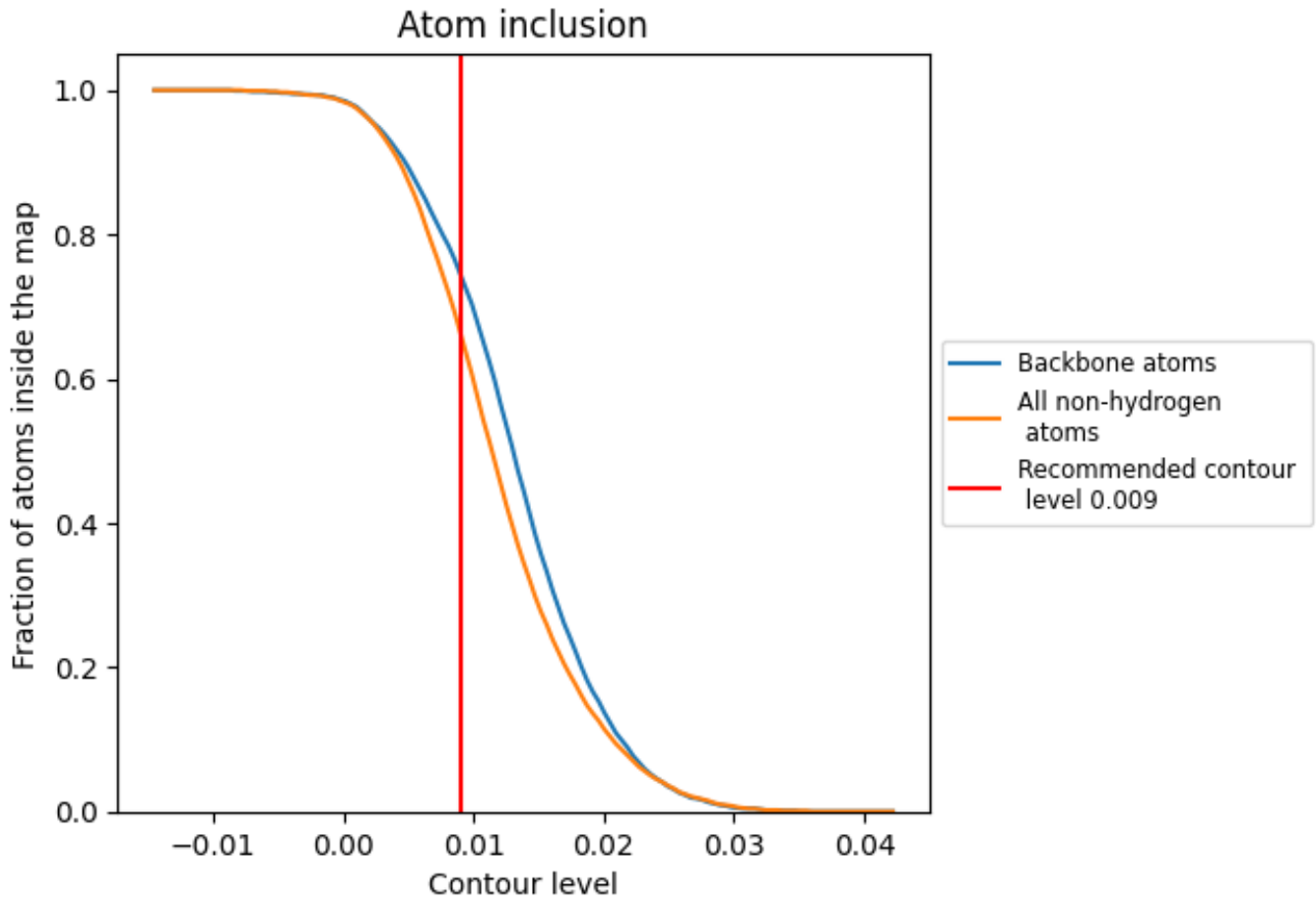
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.1760
A	0.8290	0.2190
B	0.7850	0.1980
C	0.8320	0.2220
D	0.7840	0.2010
E	0.9240	0.2310
F	0.9140	0.2060
G	0.9360	0.2390
H	0.9180	0.2140
I	0.7500	0.1700
J	0.7520	0.1710
K	0.6970	0.1630
L	0.7120	0.1540
M	0.3790	0.1220
N	0.0820	0.1000
O	0.0930	0.0900
P	0.3840	0.1280