Full wwPDB EM Validation Report

Nov 6, 2024 – 03:46 pm GMT

PDB ID	:	6XZG
EMDB ID	:	EMD-10662
Title	:	Influenza C virus polymerase in complex with chicken ANP32A - Subclass 3
Authors	:	Carrique, L.; Keown, J.R.; Fan, H.; Grimes, J.M.; Fodor, E.
Deposited on	:	2020-02-04
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 (i) 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 (i)) were used in the production of this report:

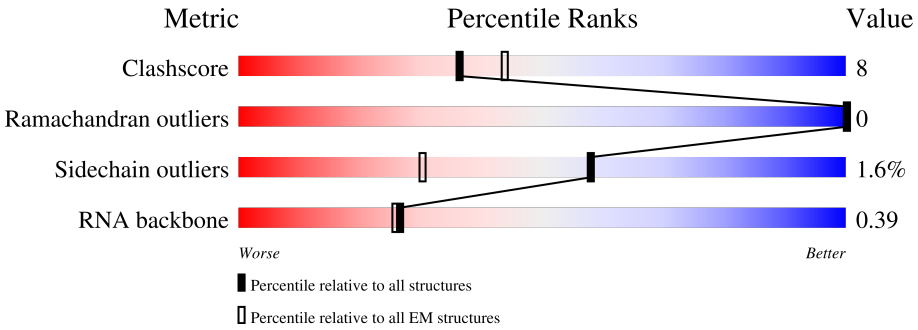
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	IN1	47	15% 13% 13% 60%
2	AP1	709	87% 11%
2	DP1	709	60% 13% 26%
3	BP1	754	81% 13% 6%
3	EP1	754	65% 15% 20%
4	CP1	920	71% 12% 16%
4	FP1	920	11% 48% 17% 35%

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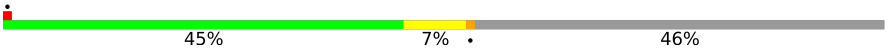
Mol	Chain	Length	Quality of chain
5	GP1	295	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65993 atoms, of which 33062 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 RNA chain called Influenza viral RNA (vRNA) promoter 47mer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	IN1	19	616	184	207	81	126	18	0	0

- Molecule 2 is a protein called Polymerase acidic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AP1	696	11287	3599	5641	955	1049	43	0	0
			Total	C	H	N	O	S		
2	DP1	525	8557	2710	4305	729	779	34	0	0

- Molecule 3 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	BP1	712	11430	3602	5747	960	1068	53	0	0
			Total	C	H	N	O	S		
3	EP1	603	9627	3059	4831	798	894	45	0	0

- Molecule 4 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	CP1	772	12408	3888	6260	1080	1142	38	0	0
			Total	C	H	N	O	S		
4	FP1	599	9523	3004	4787	820	884	28	0	0

There are 292 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CP1	775	GLU	-	expression tag	UNP Q9IMP3
CP1	776	ASN	-	expression tag	UNP Q9IMP3
CP1	777	LEU	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
CP1	778	TYR	-	expression tag	UNP Q9IMP3
CP1	779	PHE	-	expression tag	UNP Q9IMP3
CP1	780	GLN	-	expression tag	UNP Q9IMP3
CP1	781	GLY	-	expression tag	UNP Q9IMP3
CP1	782	GLU	-	expression tag	UNP Q9IMP3
CP1	783	LEU	-	expression tag	UNP Q9IMP3
CP1	784	LYS	-	expression tag	UNP Q9IMP3
CP1	785	THR	-	expression tag	UNP Q9IMP3
CP1	786	ALA	-	expression tag	UNP Q9IMP3
CP1	787	ALA	-	expression tag	UNP Q9IMP3
CP1	788	LEU	-	expression tag	UNP Q9IMP3
CP1	789	ALA	-	expression tag	UNP Q9IMP3
CP1	790	GLN	-	expression tag	UNP Q9IMP3
CP1	791	HIS	-	expression tag	UNP Q9IMP3
CP1	792	ASP	-	expression tag	UNP Q9IMP3
CP1	793	GLU	-	expression tag	UNP Q9IMP3
CP1	794	ALA	-	expression tag	UNP Q9IMP3
CP1	795	VAL	-	expression tag	UNP Q9IMP3
CP1	796	ASP	-	expression tag	UNP Q9IMP3
CP1	797	ASN	-	expression tag	UNP Q9IMP3
CP1	798	LYS	-	expression tag	UNP Q9IMP3
CP1	799	PHE	-	expression tag	UNP Q9IMP3
CP1	800	ASN	-	expression tag	UNP Q9IMP3
CP1	801	LYS	-	expression tag	UNP Q9IMP3
CP1	802	GLU	-	expression tag	UNP Q9IMP3
CP1	803	GLN	-	expression tag	UNP Q9IMP3
CP1	804	GLN	-	expression tag	UNP Q9IMP3
CP1	805	ASN	-	expression tag	UNP Q9IMP3
CP1	806	ALA	-	expression tag	UNP Q9IMP3
CP1	807	PHE	-	expression tag	UNP Q9IMP3
CP1	808	TYR	-	expression tag	UNP Q9IMP3
CP1	809	GLU	-	expression tag	UNP Q9IMP3
CP1	810	ILE	-	expression tag	UNP Q9IMP3
CP1	811	LEU	-	expression tag	UNP Q9IMP3
CP1	812	HIS	-	expression tag	UNP Q9IMP3
CP1	813	LEU	-	expression tag	UNP Q9IMP3
CP1	814	PRO	-	expression tag	UNP Q9IMP3
CP1	815	ASN	-	expression tag	UNP Q9IMP3
CP1	816	LEU	-	expression tag	UNP Q9IMP3
CP1	817	ASN	-	expression tag	UNP Q9IMP3
CP1	818	GLU	-	expression tag	UNP Q9IMP3
CP1	819	GLU	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
CP1	820	GLN	-	expression tag	UNP Q9IMP3
CP1	821	ARG	-	expression tag	UNP Q9IMP3
CP1	822	ASN	-	expression tag	UNP Q9IMP3
CP1	823	ALA	-	expression tag	UNP Q9IMP3
CP1	824	PHE	-	expression tag	UNP Q9IMP3
CP1	825	ILE	-	expression tag	UNP Q9IMP3
CP1	826	GLN	-	expression tag	UNP Q9IMP3
CP1	827	SER	-	expression tag	UNP Q9IMP3
CP1	828	LEU	-	expression tag	UNP Q9IMP3
CP1	829	LYS	-	expression tag	UNP Q9IMP3
CP1	830	ASP	-	expression tag	UNP Q9IMP3
CP1	831	ASP	-	expression tag	UNP Q9IMP3
CP1	832	PRO	-	expression tag	UNP Q9IMP3
CP1	833	SER	-	expression tag	UNP Q9IMP3
CP1	834	GLN	-	expression tag	UNP Q9IMP3
CP1	835	SER	-	expression tag	UNP Q9IMP3
CP1	836	ALA	-	expression tag	UNP Q9IMP3
CP1	837	ASN	-	expression tag	UNP Q9IMP3
CP1	838	LEU	-	expression tag	UNP Q9IMP3
CP1	839	LEU	-	expression tag	UNP Q9IMP3
CP1	840	ALA	-	expression tag	UNP Q9IMP3
CP1	841	GLU	-	expression tag	UNP Q9IMP3
CP1	842	ALA	-	expression tag	UNP Q9IMP3
CP1	843	LYS	-	expression tag	UNP Q9IMP3
CP1	844	LYS	-	expression tag	UNP Q9IMP3
CP1	845	LEU	-	expression tag	UNP Q9IMP3
CP1	846	ASN	-	expression tag	UNP Q9IMP3
CP1	847	ASP	-	expression tag	UNP Q9IMP3
CP1	848	ALA	-	expression tag	UNP Q9IMP3
CP1	849	GLN	-	expression tag	UNP Q9IMP3
CP1	850	ALA	-	expression tag	UNP Q9IMP3
CP1	851	PRO	-	expression tag	UNP Q9IMP3
CP1	852	LYS	-	expression tag	UNP Q9IMP3
CP1	853	VAL	-	expression tag	UNP Q9IMP3
CP1	854	ASP	-	expression tag	UNP Q9IMP3
CP1	855	ASN	-	expression tag	UNP Q9IMP3
CP1	856	LYS	-	expression tag	UNP Q9IMP3
CP1	857	PHE	-	expression tag	UNP Q9IMP3
CP1	858	ASN	-	expression tag	UNP Q9IMP3
CP1	859	LYS	-	expression tag	UNP Q9IMP3
CP1	860	GLU	-	expression tag	UNP Q9IMP3
CP1	861	GLN	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
CP1	862	GLN	-	expression tag	UNP Q9IMP3
CP1	863	ASN	-	expression tag	UNP Q9IMP3
CP1	864	ALA	-	expression tag	UNP Q9IMP3
CP1	865	PHE	-	expression tag	UNP Q9IMP3
CP1	866	TYR	-	expression tag	UNP Q9IMP3
CP1	867	GLU	-	expression tag	UNP Q9IMP3
CP1	868	ILE	-	expression tag	UNP Q9IMP3
CP1	869	LEU	-	expression tag	UNP Q9IMP3
CP1	870	HIS	-	expression tag	UNP Q9IMP3
CP1	871	LEU	-	expression tag	UNP Q9IMP3
CP1	872	PRO	-	expression tag	UNP Q9IMP3
CP1	873	ASN	-	expression tag	UNP Q9IMP3
CP1	874	LEU	-	expression tag	UNP Q9IMP3
CP1	875	ASN	-	expression tag	UNP Q9IMP3
CP1	876	GLU	-	expression tag	UNP Q9IMP3
CP1	877	GLU	-	expression tag	UNP Q9IMP3
CP1	878	GLN	-	expression tag	UNP Q9IMP3
CP1	879	ARG	-	expression tag	UNP Q9IMP3
CP1	880	ASN	-	expression tag	UNP Q9IMP3
CP1	881	ALA	-	expression tag	UNP Q9IMP3
CP1	882	PHE	-	expression tag	UNP Q9IMP3
CP1	883	ILE	-	expression tag	UNP Q9IMP3
CP1	884	GLN	-	expression tag	UNP Q9IMP3
CP1	885	SER	-	expression tag	UNP Q9IMP3
CP1	886	LEU	-	expression tag	UNP Q9IMP3
CP1	887	LYS	-	expression tag	UNP Q9IMP3
CP1	888	ALA	-	expression tag	UNP Q9IMP3
CP1	889	ASP	-	expression tag	UNP Q9IMP3
CP1	890	PRO	-	expression tag	UNP Q9IMP3
CP1	891	SER	-	expression tag	UNP Q9IMP3
CP1	892	GLN	-	expression tag	UNP Q9IMP3
CP1	893	SER	-	expression tag	UNP Q9IMP3
CP1	894	ALA	-	expression tag	UNP Q9IMP3
CP1	895	ASN	-	expression tag	UNP Q9IMP3
CP1	896	LEU	-	expression tag	UNP Q9IMP3
CP1	897	LEU	-	expression tag	UNP Q9IMP3
CP1	898	ALA	-	expression tag	UNP Q9IMP3
CP1	899	GLU	-	expression tag	UNP Q9IMP3
CP1	900	ALA	-	expression tag	UNP Q9IMP3
CP1	901	LYS	-	expression tag	UNP Q9IMP3
CP1	902	LYS	-	expression tag	UNP Q9IMP3
CP1	903	LEU	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
CP1	904	ASN	-	expression tag	UNP Q9IMP3
CP1	905	GLY	-	expression tag	UNP Q9IMP3
CP1	906	ALA	-	expression tag	UNP Q9IMP3
CP1	907	GLN	-	expression tag	UNP Q9IMP3
CP1	908	ALA	-	expression tag	UNP Q9IMP3
CP1	909	PRO	-	expression tag	UNP Q9IMP3
CP1	910	LYS	-	expression tag	UNP Q9IMP3
CP1	911	VAL	-	expression tag	UNP Q9IMP3
CP1	912	ASP	-	expression tag	UNP Q9IMP3
CP1	913	ALA	-	expression tag	UNP Q9IMP3
CP1	914	ASN	-	expression tag	UNP Q9IMP3
CP1	915	SER	-	expression tag	UNP Q9IMP3
CP1	916	ALA	-	expression tag	UNP Q9IMP3
CP1	917	GLY	-	expression tag	UNP Q9IMP3
CP1	918	LYS	-	expression tag	UNP Q9IMP3
CP1	919	SER	-	expression tag	UNP Q9IMP3
CP1	920	THR	-	expression tag	UNP Q9IMP3
FP1	775	GLU	-	expression tag	UNP Q9IMP3
FP1	776	ASN	-	expression tag	UNP Q9IMP3
FP1	777	LEU	-	expression tag	UNP Q9IMP3
FP1	778	TYR	-	expression tag	UNP Q9IMP3
FP1	779	PHE	-	expression tag	UNP Q9IMP3
FP1	780	GLN	-	expression tag	UNP Q9IMP3
FP1	781	GLY	-	expression tag	UNP Q9IMP3
FP1	782	GLU	-	expression tag	UNP Q9IMP3
FP1	783	LEU	-	expression tag	UNP Q9IMP3
FP1	784	LYS	-	expression tag	UNP Q9IMP3
FP1	785	THR	-	expression tag	UNP Q9IMP3
FP1	786	ALA	-	expression tag	UNP Q9IMP3
FP1	787	ALA	-	expression tag	UNP Q9IMP3
FP1	788	LEU	-	expression tag	UNP Q9IMP3
FP1	789	ALA	-	expression tag	UNP Q9IMP3
FP1	790	GLN	-	expression tag	UNP Q9IMP3
FP1	791	HIS	-	expression tag	UNP Q9IMP3
FP1	792	ASP	-	expression tag	UNP Q9IMP3
FP1	793	GLU	-	expression tag	UNP Q9IMP3
FP1	794	ALA	-	expression tag	UNP Q9IMP3
FP1	795	VAL	-	expression tag	UNP Q9IMP3
FP1	796	ASP	-	expression tag	UNP Q9IMP3
FP1	797	ASN	-	expression tag	UNP Q9IMP3
FP1	798	LYS	-	expression tag	UNP Q9IMP3
FP1	799	PHE	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
FP1	800	ASN	-	expression tag	UNP Q9IMP3
FP1	801	LYS	-	expression tag	UNP Q9IMP3
FP1	802	GLU	-	expression tag	UNP Q9IMP3
FP1	803	GLN	-	expression tag	UNP Q9IMP3
FP1	804	GLN	-	expression tag	UNP Q9IMP3
FP1	805	ASN	-	expression tag	UNP Q9IMP3
FP1	806	ALA	-	expression tag	UNP Q9IMP3
FP1	807	PHE	-	expression tag	UNP Q9IMP3
FP1	808	TYR	-	expression tag	UNP Q9IMP3
FP1	809	GLU	-	expression tag	UNP Q9IMP3
FP1	810	ILE	-	expression tag	UNP Q9IMP3
FP1	811	LEU	-	expression tag	UNP Q9IMP3
FP1	812	HIS	-	expression tag	UNP Q9IMP3
FP1	813	LEU	-	expression tag	UNP Q9IMP3
FP1	814	PRO	-	expression tag	UNP Q9IMP3
FP1	815	ASN	-	expression tag	UNP Q9IMP3
FP1	816	LEU	-	expression tag	UNP Q9IMP3
FP1	817	ASN	-	expression tag	UNP Q9IMP3
FP1	818	GLU	-	expression tag	UNP Q9IMP3
FP1	819	GLU	-	expression tag	UNP Q9IMP3
FP1	820	GLN	-	expression tag	UNP Q9IMP3
FP1	821	ARG	-	expression tag	UNP Q9IMP3
FP1	822	ASN	-	expression tag	UNP Q9IMP3
FP1	823	ALA	-	expression tag	UNP Q9IMP3
FP1	824	PHE	-	expression tag	UNP Q9IMP3
FP1	825	ILE	-	expression tag	UNP Q9IMP3
FP1	826	GLN	-	expression tag	UNP Q9IMP3
FP1	827	SER	-	expression tag	UNP Q9IMP3
FP1	828	LEU	-	expression tag	UNP Q9IMP3
FP1	829	LYS	-	expression tag	UNP Q9IMP3
FP1	830	ASP	-	expression tag	UNP Q9IMP3
FP1	831	ASP	-	expression tag	UNP Q9IMP3
FP1	832	PRO	-	expression tag	UNP Q9IMP3
FP1	833	SER	-	expression tag	UNP Q9IMP3
FP1	834	GLN	-	expression tag	UNP Q9IMP3
FP1	835	SER	-	expression tag	UNP Q9IMP3
FP1	836	ALA	-	expression tag	UNP Q9IMP3
FP1	837	ASN	-	expression tag	UNP Q9IMP3
FP1	838	LEU	-	expression tag	UNP Q9IMP3
FP1	839	LEU	-	expression tag	UNP Q9IMP3
FP1	840	ALA	-	expression tag	UNP Q9IMP3
FP1	841	GLU	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
FP1	842	ALA	-	expression tag	UNP Q9IMP3
FP1	843	LYS	-	expression tag	UNP Q9IMP3
FP1	844	LYS	-	expression tag	UNP Q9IMP3
FP1	845	LEU	-	expression tag	UNP Q9IMP3
FP1	846	ASN	-	expression tag	UNP Q9IMP3
FP1	847	ASP	-	expression tag	UNP Q9IMP3
FP1	848	ALA	-	expression tag	UNP Q9IMP3
FP1	849	GLN	-	expression tag	UNP Q9IMP3
FP1	850	ALA	-	expression tag	UNP Q9IMP3
FP1	851	PRO	-	expression tag	UNP Q9IMP3
FP1	852	LYS	-	expression tag	UNP Q9IMP3
FP1	853	VAL	-	expression tag	UNP Q9IMP3
FP1	854	ASP	-	expression tag	UNP Q9IMP3
FP1	855	ASN	-	expression tag	UNP Q9IMP3
FP1	856	LYS	-	expression tag	UNP Q9IMP3
FP1	857	PHE	-	expression tag	UNP Q9IMP3
FP1	858	ASN	-	expression tag	UNP Q9IMP3
FP1	859	LYS	-	expression tag	UNP Q9IMP3
FP1	860	GLU	-	expression tag	UNP Q9IMP3
FP1	861	GLN	-	expression tag	UNP Q9IMP3
FP1	862	GLN	-	expression tag	UNP Q9IMP3
FP1	863	ASN	-	expression tag	UNP Q9IMP3
FP1	864	ALA	-	expression tag	UNP Q9IMP3
FP1	865	PHE	-	expression tag	UNP Q9IMP3
FP1	866	TYR	-	expression tag	UNP Q9IMP3
FP1	867	GLU	-	expression tag	UNP Q9IMP3
FP1	868	ILE	-	expression tag	UNP Q9IMP3
FP1	869	LEU	-	expression tag	UNP Q9IMP3
FP1	870	HIS	-	expression tag	UNP Q9IMP3
FP1	871	LEU	-	expression tag	UNP Q9IMP3
FP1	872	PRO	-	expression tag	UNP Q9IMP3
FP1	873	ASN	-	expression tag	UNP Q9IMP3
FP1	874	LEU	-	expression tag	UNP Q9IMP3
FP1	875	ASN	-	expression tag	UNP Q9IMP3
FP1	876	GLU	-	expression tag	UNP Q9IMP3
FP1	877	GLU	-	expression tag	UNP Q9IMP3
FP1	878	GLN	-	expression tag	UNP Q9IMP3
FP1	879	ARG	-	expression tag	UNP Q9IMP3
FP1	880	ASN	-	expression tag	UNP Q9IMP3
FP1	881	ALA	-	expression tag	UNP Q9IMP3
FP1	882	PHE	-	expression tag	UNP Q9IMP3
FP1	883	ILE	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
FP1	884	GLN	-	expression tag	UNP Q9IMP3
FP1	885	SER	-	expression tag	UNP Q9IMP3
FP1	886	LEU	-	expression tag	UNP Q9IMP3
FP1	887	LYS	-	expression tag	UNP Q9IMP3
FP1	888	ALA	-	expression tag	UNP Q9IMP3
FP1	889	ASP	-	expression tag	UNP Q9IMP3
FP1	890	PRO	-	expression tag	UNP Q9IMP3
FP1	891	SER	-	expression tag	UNP Q9IMP3
FP1	892	GLN	-	expression tag	UNP Q9IMP3
FP1	893	SER	-	expression tag	UNP Q9IMP3
FP1	894	ALA	-	expression tag	UNP Q9IMP3
FP1	895	ASN	-	expression tag	UNP Q9IMP3
FP1	896	LEU	-	expression tag	UNP Q9IMP3
FP1	897	LEU	-	expression tag	UNP Q9IMP3
FP1	898	ALA	-	expression tag	UNP Q9IMP3
FP1	899	GLU	-	expression tag	UNP Q9IMP3
FP1	900	ALA	-	expression tag	UNP Q9IMP3
FP1	901	LYS	-	expression tag	UNP Q9IMP3
FP1	902	LYS	-	expression tag	UNP Q9IMP3
FP1	903	LEU	-	expression tag	UNP Q9IMP3
FP1	904	ASN	-	expression tag	UNP Q9IMP3
FP1	905	GLY	-	expression tag	UNP Q9IMP3
FP1	906	ALA	-	expression tag	UNP Q9IMP3
FP1	907	GLN	-	expression tag	UNP Q9IMP3
FP1	908	ALA	-	expression tag	UNP Q9IMP3
FP1	909	PRO	-	expression tag	UNP Q9IMP3
FP1	910	LYS	-	expression tag	UNP Q9IMP3
FP1	911	VAL	-	expression tag	UNP Q9IMP3
FP1	912	ASP	-	expression tag	UNP Q9IMP3
FP1	913	ALA	-	expression tag	UNP Q9IMP3
FP1	914	ASN	-	expression tag	UNP Q9IMP3
FP1	915	SER	-	expression tag	UNP Q9IMP3
FP1	916	ALA	-	expression tag	UNP Q9IMP3
FP1	917	GLY	-	expression tag	UNP Q9IMP3
FP1	918	LYS	-	expression tag	UNP Q9IMP3
FP1	919	SER	-	expression tag	UNP Q9IMP3
FP1	920	THR	-	expression tag	UNP Q9IMP3

- Molecule 5 is a protein called LRRcap domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	GP1	158	Total	C	H	N	O	S	0	0
			2545	791	1284	214	251	5		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GP1	-13	HIS	-	expression tag	UNP A0A1D5P3M1
GP1	-12	HIS	-	expression tag	UNP A0A1D5P3M1
GP1	-11	HIS	-	expression tag	UNP A0A1D5P3M1
GP1	-10	HIS	-	expression tag	UNP A0A1D5P3M1
GP1	-9	HIS	-	expression tag	UNP A0A1D5P3M1
GP1	-8	HIS	-	expression tag	UNP A0A1D5P3M1
GP1	-7	LEU	-	expression tag	UNP A0A1D5P3M1
GP1	-6	GLU	-	expression tag	UNP A0A1D5P3M1
GP1	-5	VAL	-	expression tag	UNP A0A1D5P3M1
GP1	-4	LEU	-	expression tag	UNP A0A1D5P3M1
GP1	-3	PHE	-	expression tag	UNP A0A1D5P3M1
GP1	-2	GLN	-	expression tag	UNP A0A1D5P3M1
GP1	-1	GLY	-	expression tag	UNP A0A1D5P3M1
GP1	0	PRO	-	expression tag	UNP A0A1D5P3M1

3 Residue-property plots (i)

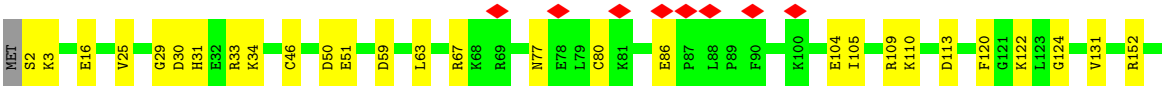
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

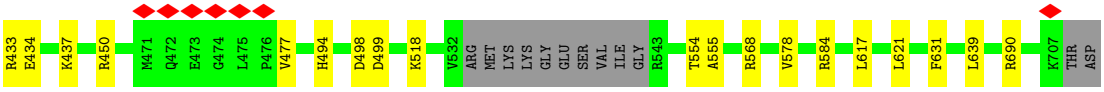
• Molecule 1: Influenza viral RNA (vRNA) promoter 47mer

Chain IN1:

• Molecule 2: Polymerase acidic protein

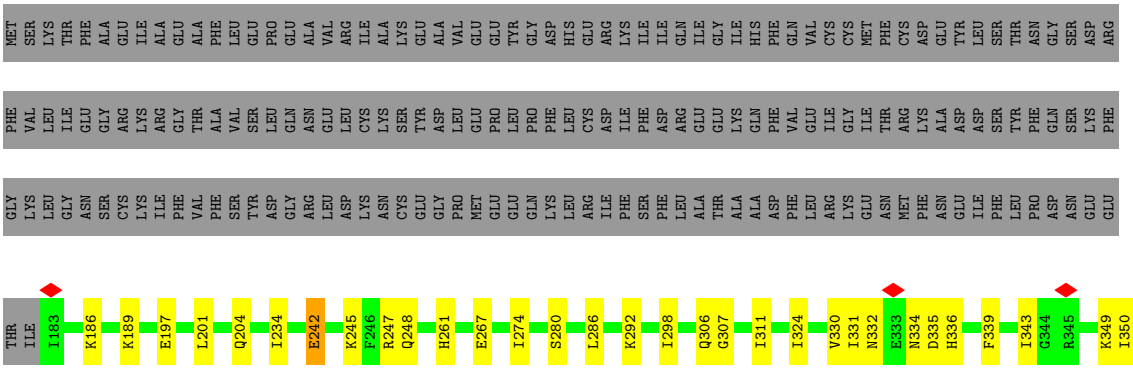
Chain AP1:

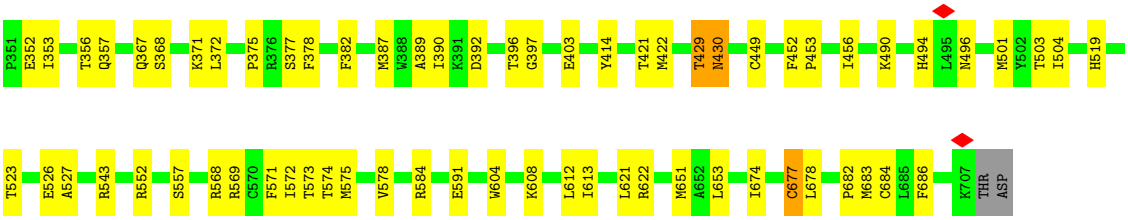




• Molecule 2: Polymerase acidic protein

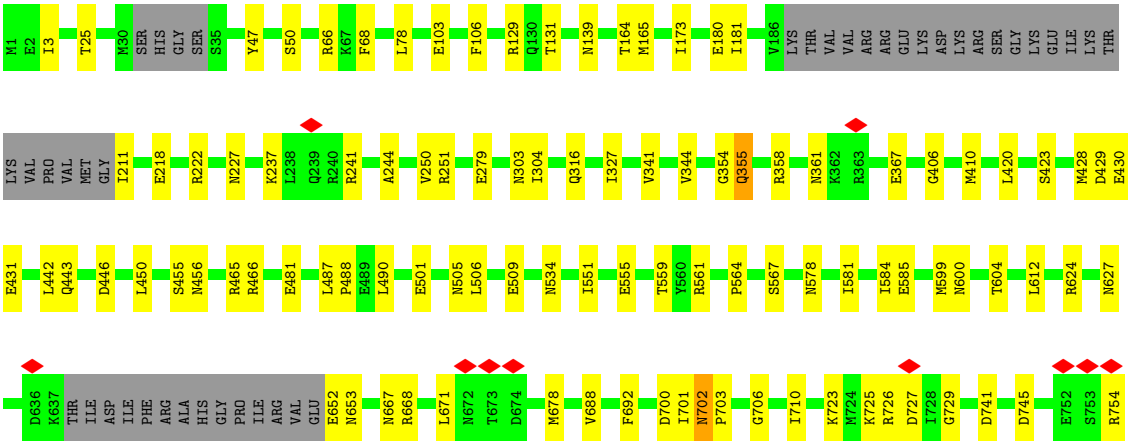
Chain DP1:





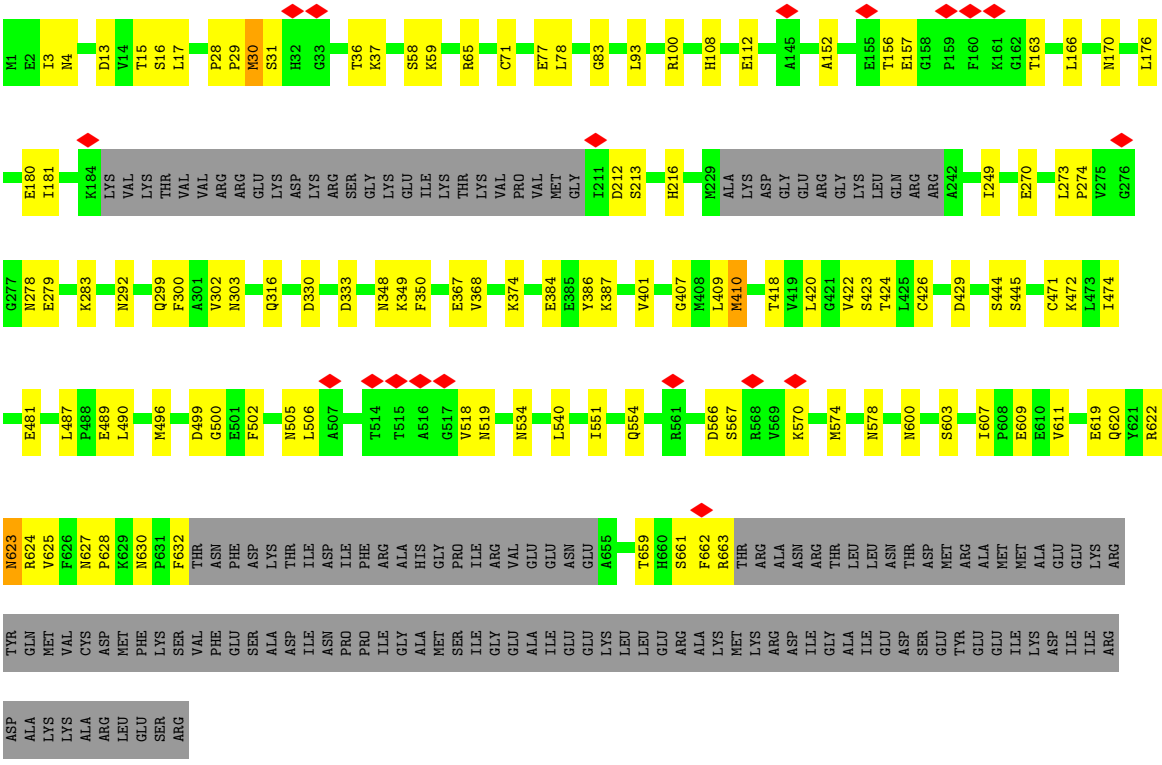
• Molecule 3: RNA-directed RNA polymerase catalytic subunit

Chain BP1:



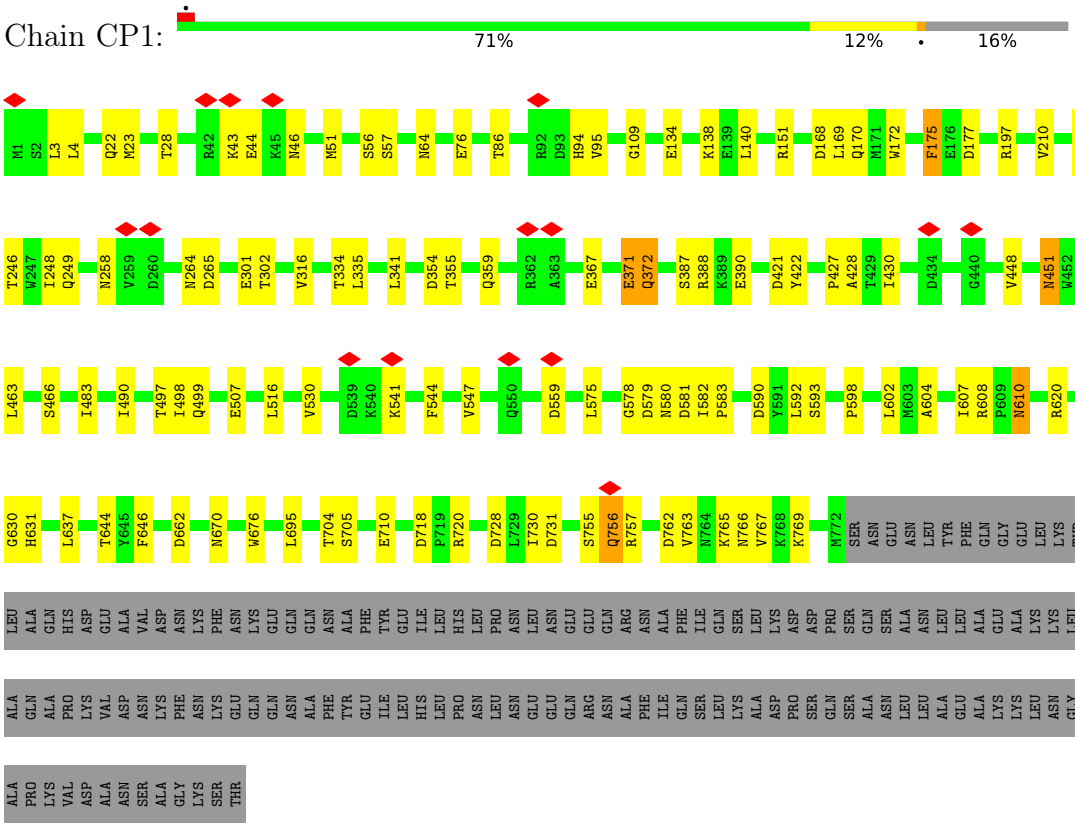
• Molecule 3: RNA-directed RNA polymerase catalytic subunit

Chain EP1:



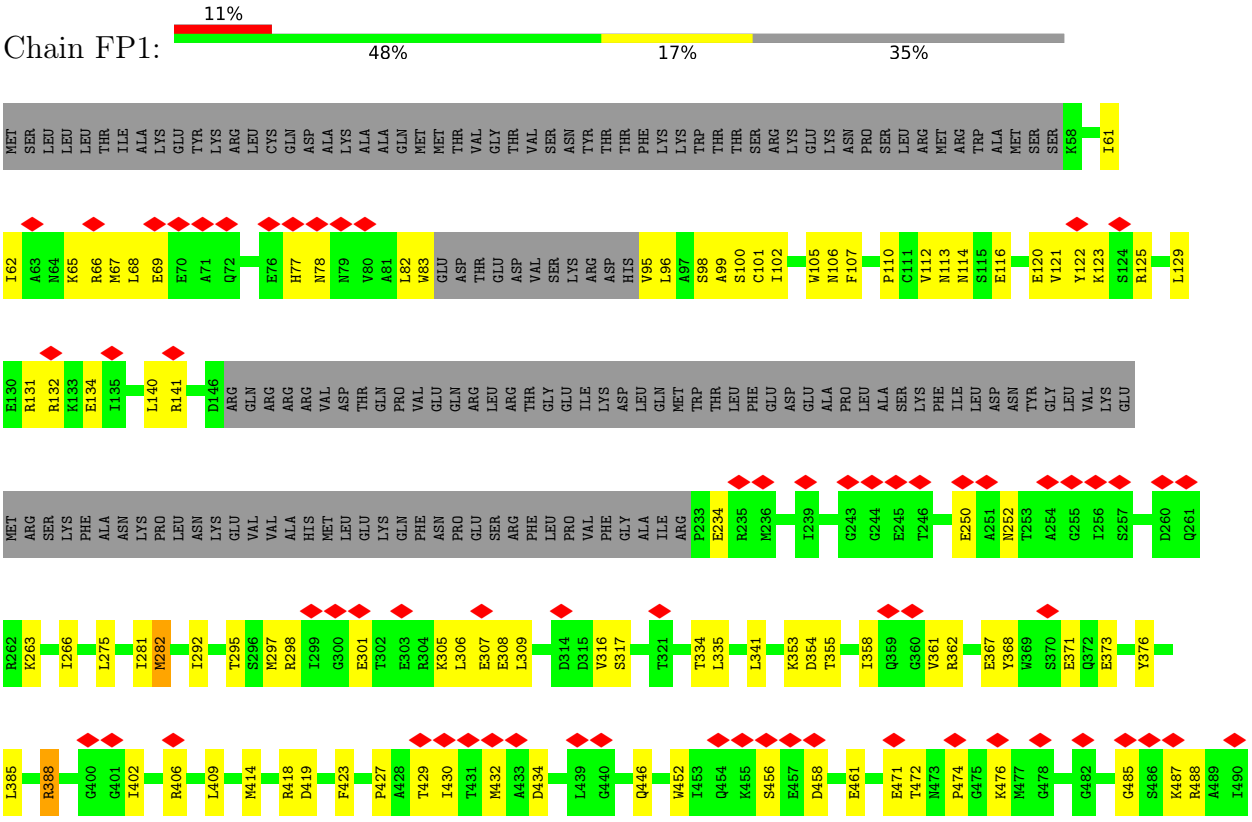
• Molecule 4: Polymerase basic protein 2

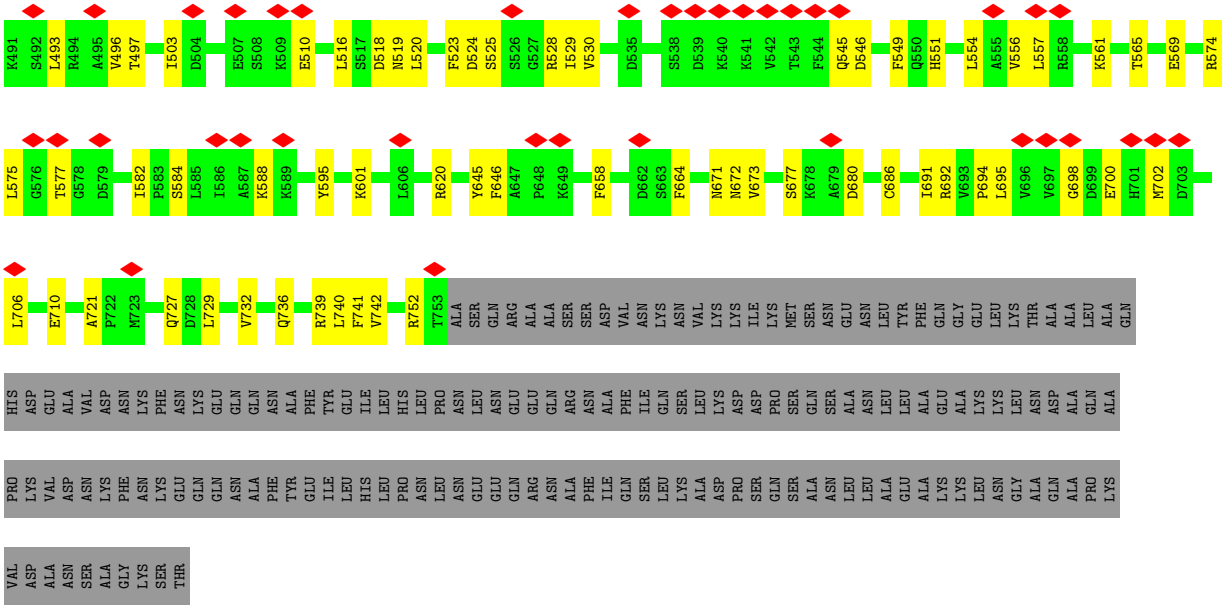
Chain CP1:



• Molecule 4: Polymerase basic protein 2

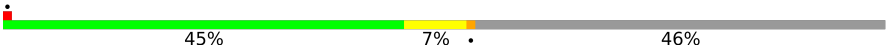
Chain FP1:

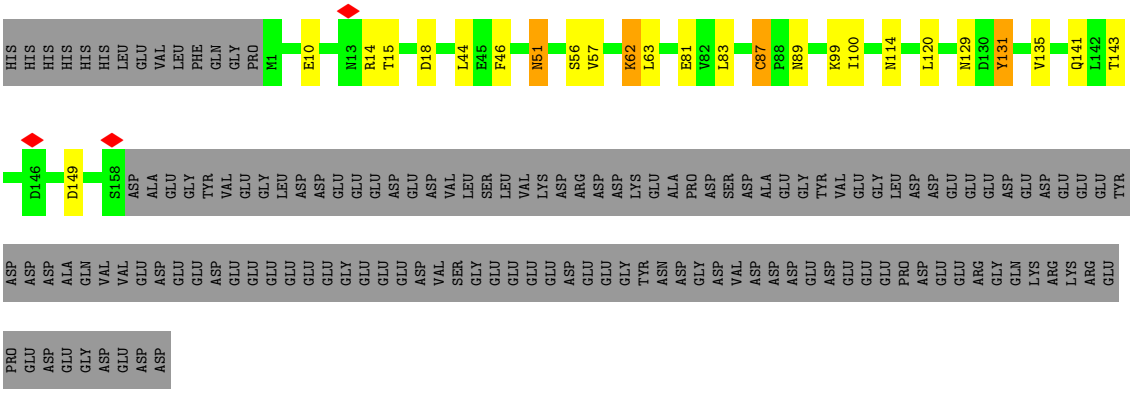




• Molecule 5: LRRcap domain-containing protein

Chain GP1:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42000	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 ($e^-/Å^2$)	38.8	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.448	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.112	Depositor
Map size (Å)	383.6, 383.6, 383.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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	IN1	0.30	0/458	0.90	0/711
2	AP1	0.29	0/5764	0.43	0/7746
2	DP1	0.38	0/4342	0.58	0/5835
3	BP1	0.31	0/5780	0.47	0/7762
3	EP1	0.30	0/4887	0.48	0/6577
4	CP1	0.30	0/6259	0.47	0/8425
4	FP1	0.26	0/4821	0.44	0/6493
5	GP1	0.29	0/1276	0.49	0/1718
All	All	0.31	0/33587	0.48	0/45267

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	IN1	409	207	210	9	0
2	AP1	5646	5641	5645	65	0
2	DP1	4252	4305	4305	72	0
3	BP1	5683	5747	5759	74	0
3	EP1	4796	4831	4853	108	0
4	CP1	6148	6260	6261	84	0
4	FP1	4736	4787	4806	145	0
5	GP1	1261	1284	1286	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32931	33062	33125	497	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 8.

All (497) 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:FP1:141:ARG:NH1	4:FP1:141:ARG:HA	1.71	1.06
2:DP1:686:PHE:O	2:DP1:686:PHE:CG	2.18	0.94
2:DP1:686:PHE:O	2:DP1:686:PHE:CD2	2.24	0.90
3:EP1:659:THR:HG21	4:FP1:106:ASN:OD1	1.71	0.89
3:EP1:30:MET:SD	3:EP1:30:MET:N	2.45	0.86
4:FP1:141:ARG:HA	4:FP1:141:ARG:HH11	1.38	0.84
3:EP1:300:PHE:O	3:EP1:300:PHE:CD2	2.31	0.83
3:EP1:609:GLU:OE1	3:EP1:609:GLU:N	2.14	0.80
4:FP1:575:LEU:HD12	4:FP1:582:ILE:HD13	1.65	0.78
4:FP1:66:ARG:NH2	4:FP1:67:MET:SD	2.57	0.78
1:IN1:5:G:OP2	1:IN1:5:G:N2	2.19	0.76
4:FP1:710:GLU:OE1	4:FP1:710:GLU:N	2.19	0.76
3:BP1:701:ILE:HD12	3:BP1:701:ILE:C	2.03	0.76
3:BP1:701:ILE:O	3:BP1:701:ILE:CD1	2.34	0.76
3:EP1:630:ASN:HB3	4:FP1:105:TRP:CH2	2.21	0.75
2:AP1:86:GLU:N	2:AP1:86:GLU:OE1	2.18	0.75
2:DP1:677:CYS:O	2:DP1:677:CYS:SG	2.44	0.75
2:DP1:575:MET:O	2:DP1:575:MET:SD	2.44	0.74
4:FP1:601:LYS:NZ	4:FP1:645:TYR:OH	2.20	0.74
4:CP1:371:GLU:N	4:CP1:390:GLU:OE1	2.22	0.73
4:CP1:662:ASP:OD1	4:FP1:736:GLN:NE2	2.22	0.73
3:EP1:630:ASN:HA	4:FP1:105:TRP:CZ2	2.22	0.73
4:CP1:151:ARG:NH2	4:CP1:507:GLU:OE2	2.21	0.73
4:CP1:620:ARG:NH2	4:CP1:646:PHE:O	2.22	0.72
2:AP1:59:ASP:OD2	4:CP1:769:LYS:NZ	2.20	0.72
4:FP1:371:GLU:O	4:FP1:388:ARG:NH2	2.21	0.72
3:BP1:725:LYS:O	3:BP1:729:GLY:N	2.22	0.72
4:FP1:308:GLU:OE2	4:FP1:308:GLU:N	2.24	0.71
3:EP1:603:SER:OG	4:FP1:132:ARG:NH2	2.23	0.71
2:AP1:152:ARG:NH2	4:CP1:762:ASP:OD2	2.23	0.71
3:EP1:303:ASN:ND2	3:EP1:490:LEU:O	2.24	0.71
4:FP1:727:GLN:N	4:FP1:727:GLN:OE1	2.23	0.71
4:FP1:561:LYS:O	4:FP1:565:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP1:702:ASN:O	3:BP1:702:ASN:ND2	2.24	0.70
3:BP1:68:PHE:HE2	3:BP1:316:GLN:OE1	1.74	0.70
4:CP1:575:LEU:HD13	4:CP1:582:ILE:HD11	1.73	0.70
3:EP1:166:LEU:O	3:EP1:170:ASN:ND2	2.23	0.70
2:DP1:575:MET:SD	2:DP1:575:MET:C	2.69	0.70
4:CP1:762:ASP:O	4:CP1:766:ASN:ND2	2.24	0.70
3:EP1:611:VAL:HG12	4:FP1:129:LEU:HD22	1.74	0.70
4:CP1:662:ASP:CG	4:FP1:736:GLN:NE2	2.45	0.69
2:DP1:189:LYS:O	2:DP1:189:LYS:NZ	2.25	0.69
5:GP1:131:TYR:CE1	5:GP1:135:VAL:HG21	2.28	0.69
2:DP1:247:ARG:NH1	2:DP1:248:GLN:O	2.26	0.69
3:EP1:83:GLY:O	3:EP1:316:GLN:NE2	2.27	0.68
3:EP1:659:THR:HG23	4:FP1:106:ASN:HD21	1.58	0.68
4:FP1:402:ILE:O	4:FP1:406:ARG:NE	2.26	0.68
3:EP1:505:ASN:OD1	3:EP1:506:LEU:N	2.27	0.68
3:BP1:129:ARG:NH1	3:BP1:244:ALA:O	2.27	0.68
5:GP1:89:ASN:OD1	5:GP1:114:ASN:ND2	2.27	0.68
2:AP1:109:ARG:NH2	2:AP1:180:GLU:OE2	2.27	0.67
3:BP1:103:GLU:N	3:BP1:103:GLU:OE1	2.26	0.67
3:EP1:481:GLU:N	3:EP1:481:GLU:OE1	2.27	0.67
2:AP1:584:ARG:NH2	3:BP1:501:GLU:OE1	2.27	0.67
3:EP1:662:PHE:HE2	4:FP1:102:ILE:HD12	1.59	0.67
4:FP1:565:THR:HG22	4:FP1:686:CYS:SG	2.35	0.67
4:FP1:574:ARG:HG3	4:FP1:582:ILE:HD12	1.76	0.67
4:CP1:367:GLU:OE1	4:CP1:367:GLU:N	2.28	0.66
3:EP1:627:ASN:HA	4:FP1:112:VAL:HG11	1.77	0.66
3:EP1:632:PHE:O	3:EP1:663:ARG:NH2	2.27	0.66
3:BP1:754:ARG:NH1	4:CP1:22:GLN:OE1	2.29	0.66
4:FP1:574:ARG:HG3	4:FP1:582:ILE:CD1	2.25	0.66
2:DP1:387:MET:SD	3:EP1:3:ILE:HD11	2.36	0.66
4:CP1:670:ASN:ND2	4:CP1:676:TRP:O	2.28	0.66
2:DP1:261:HIS:O	2:DP1:552:ARG:NH2	2.29	0.65
4:FP1:371:GLU:OE1	4:FP1:371:GLU:N	2.29	0.65
5:GP1:141:GLN:N	5:GP1:141:GLN:OE1	2.30	0.65
3:BP1:481:GLU:OE1	3:BP1:481:GLU:N	2.30	0.65
4:CP1:575:LEU:CD1	4:CP1:582:ILE:HD11	2.27	0.64
3:BP1:652:GLU:OE1	3:BP1:653:ASN:N	2.31	0.64
3:EP1:489:GLU:OE1	3:EP1:489:GLU:N	2.30	0.64
3:EP1:663:ARG:HB2	4:FP1:62:ILE:HG12	1.79	0.64
4:FP1:140:LEU:O	4:FP1:141:ARG:HD2	1.96	0.64
2:DP1:578:VAL:HG22	2:DP1:621:LEU:HD22	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DP1:526:GLU:OE1	2:DP1:526:GLU:N	2.30	0.64
4:FP1:112:VAL:HG22	4:FP1:113:ASN:N	2.13	0.64
4:CP1:371:GLU:O	4:CP1:388:ARG:NH2	2.31	0.63
3:EP1:108:HIS:NE2	3:EP1:112:GLU:OE2	2.31	0.63
4:FP1:732:VAL:O	4:FP1:752:ARG:NH1	2.32	0.63
4:CP1:264:ASN:OD1	4:CP1:265:ASP:N	2.32	0.63
2:DP1:651:MET:HE1	3:EP1:490:LEU:HD11	1.80	0.63
3:EP1:292:ASN:ND2	4:FP1:487:LYS:NZ	2.47	0.63
3:BP1:701:ILE:C	3:BP1:701:ILE:CD1	2.68	0.62
3:EP1:630:ASN:CB	4:FP1:105:TRP:CH2	2.82	0.62
3:BP1:410:MET:SD	3:BP1:410:MET:N	2.72	0.62
2:DP1:368:SER:O	2:DP1:368:SER:OG	2.14	0.62
3:EP1:65:ARG:NH2	3:EP1:348:ASN:OD1	2.31	0.62
3:EP1:300:PHE:O	3:EP1:300:PHE:CG	2.52	0.62
4:CP1:3:LEU:HD12	4:CP1:4:LEU:N	2.14	0.62
3:EP1:534:ASN:HB2	3:EP1:540:LEU:HD12	1.81	0.62
5:GP1:10:GLU:O	5:GP1:14:ARG:NH2	2.33	0.62
4:CP1:76:GLU:OE1	4:CP1:76:GLU:N	2.33	0.61
3:EP1:303:ASN:ND2	3:EP1:487:LEU:O	2.34	0.61
4:CP1:730:ILE:HG23	4:CP1:731:ASP:OD2	2.00	0.61
1:IN1:39:G:O6	2:AP1:494:HIS:NE2	2.34	0.61
3:BP1:303:ASN:ND2	3:BP1:488:PRO:O	2.32	0.61
4:FP1:282:MET:SD	4:FP1:282:MET:N	2.73	0.60
3:EP1:410:MET:SD	3:EP1:410:MET:N	2.75	0.60
3:BP1:279:GLU:N	3:BP1:279:GLU:OE1	2.32	0.60
5:GP1:51:ASN:O	5:GP1:51:ASN:ND2	2.33	0.60
2:AP1:631:PHE:HD1	2:AP1:639:LEU:HD21	1.67	0.60
1:IN1:5:G:O2'	1:IN1:6:A:O4'	2.17	0.60
4:CP1:245:GLU:HG3	4:CP1:246:THR:HG23	1.83	0.60
3:BP1:701:ILE:O	3:BP1:701:ILE:HD13	2.01	0.59
2:DP1:298:ILE:HG23	2:DP1:527:ALA:HB1	1.84	0.59
2:AP1:25:VAL:O	2:AP1:29:GLY:N	2.35	0.59
4:FP1:292:ILE:HG22	4:FP1:307:GLU:OE1	2.02	0.59
2:DP1:352:GLU:OE1	3:EP1:374:LYS:HD2	2.03	0.58
2:AP1:178:ASN:OD1	2:AP1:179:GLU:N	2.37	0.58
3:BP1:678:MET:SD	3:BP1:678:MET:N	2.76	0.58
4:CP1:372:GLN:OE1	4:CP1:387:SER:OG	2.21	0.58
2:AP1:690:ARG:NE	3:BP1:3:ILE:O	2.35	0.58
4:CP1:541:LYS:CA	4:CP1:541:LYS:HE3	2.33	0.58
4:CP1:44:GLU:OE2	4:CP1:46:ASN:N	2.36	0.58
4:FP1:740:LEU:HD12	4:FP1:741:PHE:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:FP1:82:LEU:HD22	4:FP1:101:CYS:HA	1.84	0.58
2:DP1:197:GLU:OE2	3:EP1:65:ARG:NH2	2.37	0.57
3:BP1:68:PHE:HE2	3:BP1:316:GLN:CD	2.08	0.57
3:EP1:620:GLN:O	3:EP1:624:ARG:HG3	2.04	0.57
2:AP1:498:ASP:OD1	2:AP1:499:ASP:N	2.35	0.57
2:DP1:356:THR:HG22	2:DP1:357:GLN:H	1.70	0.57
3:BP1:237:LYS:NZ	3:BP1:446:ASP:OD1	2.34	0.57
3:BP1:358:ARG:NH1	3:BP1:367:GLU:OE2	2.38	0.57
3:EP1:28:PRO:HB2	3:EP1:30:MET:SD	2.45	0.57
2:AP1:63:LEU:O	2:AP1:67:ARG:NH2	2.37	0.57
2:AP1:267:GLU:OE2	2:AP1:518:LYS:NZ	2.29	0.56
3:BP1:139:ASN:ND2	3:BP1:227:ASN:OD1	2.35	0.56
3:EP1:659:THR:O	4:FP1:102:ILE:CG2	2.52	0.56
2:DP1:349:LYS:HA	3:EP1:367:GLU:O	2.05	0.56
3:EP1:13:ASP:OD1	3:EP1:16:SER:N	2.37	0.56
1:IN1:7:A:O2'	1:IN1:8:A:OP2	2.23	0.56
3:EP1:300:PHE:CD2	3:EP1:300:PHE:C	2.78	0.56
4:CP1:316:VAL:HG23	4:CP1:316:VAL:O	2.06	0.55
3:EP1:29:PRO:HD2	3:EP1:30:MET:SD	2.47	0.55
3:EP1:292:ASN:ND2	4:FP1:487:LYS:HZ1	2.04	0.55
4:FP1:406:ARG:NH2	4:FP1:485:GLY:O	2.39	0.55
4:FP1:429:THR:OG1	4:FP1:452:TRP:NE1	2.38	0.55
4:FP1:694:PRO:C	4:FP1:695:LEU:HD12	2.27	0.55
5:GP1:120:LEU:HD12	5:GP1:131:TYR:OH	2.06	0.55
4:CP1:695:LEU:N	4:CP1:710:GLU:OE1	2.36	0.55
2:AP1:404:TYR:OH	2:AP1:423:GLU:OE1	2.24	0.55
3:BP1:25:THR:O	3:BP1:25:THR:HG22	2.07	0.55
3:EP1:31:SER:O	3:EP1:31:SER:OG	2.20	0.55
3:EP1:627:ASN:ND2	4:FP1:110:PRO:HG2	2.22	0.55
3:BP1:68:PHE:CE2	3:BP1:316:GLN:NE2	2.75	0.55
4:CP1:258:ASN:O	4:CP1:258:ASN:ND2	2.40	0.55
2:DP1:430:ASN:HD22	2:DP1:430:ASN:N	2.04	0.54
3:BP1:671:LEU:HD13	3:BP1:671:LEU:O	2.07	0.54
3:EP1:659:THR:O	4:FP1:102:ILE:HG23	2.07	0.54
4:FP1:316:VAL:O	4:FP1:317:SER:OG	2.23	0.54
5:GP1:44:LEU:HD11	5:GP1:46:PHE:O	2.07	0.54
3:EP1:663:ARG:HB3	4:FP1:62:ILE:HD11	1.89	0.54
4:FP1:721:ALA:O	4:FP1:739:ARG:NE	2.40	0.54
2:DP1:389:ALA:O	2:DP1:429:THR:HG22	2.08	0.54
3:EP1:566:ASP:OD1	3:EP1:567:SER:N	2.41	0.54
4:FP1:373:GLU:OE1	4:FP1:528:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:EP1:176:LEU:O	3:EP1:216:HIS:NE2	2.41	0.54
4:CP1:359:GLN:NE2	4:CP1:428:ALA:O	2.42	0.53
3:BP1:68:PHE:CE2	3:BP1:316:GLN:OE1	2.60	0.53
3:EP1:628:PRO:HD3	4:FP1:114:ASN:ND2	2.23	0.53
2:AP1:450:ARG:NE	4:CP1:57:SER:OG	2.40	0.53
3:BP1:218:GLU:OE2	3:BP1:222:ARG:NH2	2.41	0.53
2:DP1:390:ILE:O	2:DP1:622:ARG:NH1	2.40	0.53
4:FP1:141:ARG:HA	4:FP1:141:ARG:CZ	2.35	0.53
4:FP1:334:THR:C	4:FP1:335:LEU:HD12	2.29	0.53
2:DP1:274:ILE:HD12	2:DP1:274:ILE:N	2.24	0.53
4:FP1:474:PRO:O	4:FP1:476:LYS:NZ	2.41	0.53
3:EP1:349:LYS:NZ	3:EP1:407:GLY:O	2.42	0.53
3:BP1:428:MET:SD	3:BP1:429:ASP:N	2.80	0.53
2:DP1:332:ASN:O	2:DP1:334:ASN:ND2	2.42	0.53
4:FP1:672:ASN:OD1	4:FP1:673:VAL:N	2.42	0.53
2:DP1:568:ARG:CB	3:EP1:551:ILE:HD12	2.39	0.53
3:EP1:534:ASN:CB	3:EP1:540:LEU:HD12	2.38	0.53
3:BP1:180:GLU:C	3:BP1:181:ILE:HD12	2.29	0.52
4:CP1:354:ASP:OD1	4:CP1:355:THR:N	2.38	0.52
2:AP1:355:LEU:HD23	2:AP1:356:THR:N	2.25	0.52
2:AP1:578:VAL:HG21	2:AP1:621:LEU:HD22	1.92	0.52
4:CP1:541:LYS:HE3	4:CP1:541:LYS:HA	1.89	0.52
3:BP1:68:PHE:HZ	3:BP1:406:GLY:HA3	1.75	0.52
3:EP1:292:ASN:HD22	4:FP1:487:LYS:HZ1	1.57	0.52
3:EP1:662:PHE:HE2	4:FP1:102:ILE:CD1	2.22	0.52
4:FP1:510:GLU:OE2	4:FP1:510:GLU:N	2.43	0.52
1:IN1:39:G:N3	1:IN1:39:G:H5"	2.25	0.52
3:BP1:68:PHE:CZ	3:BP1:406:GLY:HA3	2.44	0.52
4:CP1:590:ASP:OD2	4:CP1:593:SER:OG	2.23	0.52
2:DP1:242:GLU:O	2:DP1:245:LYS:NZ	2.42	0.52
3:EP1:611:VAL:HG12	4:FP1:129:LEU:CD2	2.40	0.52
2:DP1:353:ILE:H	2:DP1:353:ILE:HD12	1.75	0.52
2:AP1:356:THR:HG22	2:AP1:357:GLN:N	2.25	0.52
2:DP1:651:MET:CE	3:EP1:490:LEU:HD11	2.39	0.52
4:CP1:86:THR:H	4:CP1:95:VAL:HG23	1.74	0.52
4:FP1:740:LEU:HD12	4:FP1:741:PHE:N	2.25	0.52
2:AP1:267:GLU:OE1	2:AP1:267:GLU:N	2.40	0.51
4:CP1:728:ASP:OD1	4:CP1:728:ASP:O	2.27	0.51
2:DP1:608:LYS:HB3	2:DP1:613:ILE:HD11	1.92	0.51
3:BP1:68:PHE:CE2	3:BP1:316:GLN:CD	2.84	0.51
3:EP1:93:LEU:HB3	3:EP1:423:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:EP1:420:LEU:HD11	3:EP1:474:ILE:HD12	1.92	0.51
4:CP1:140:LEU:HD12	4:CP1:248:ILE:O	2.09	0.51
2:AP1:396:THR:OG1	2:AP1:397:GLY:N	2.43	0.51
4:CP1:620:ARG:NH2	4:CP1:644:THR:O	2.41	0.51
2:AP1:355:LEU:HD21	2:AP1:360:ILE:HD11	1.92	0.51
3:BP1:559:THR:O	3:BP1:561:ARG:NH1	2.44	0.51
3:BP1:692:PHE:HD2	3:BP1:710:ILE:HG23	1.76	0.51
2:DP1:677:CYS:O	2:DP1:678:LEU:HD12	2.11	0.51
3:BP1:706:GLY:O	4:CP1:28:THR:OG1	2.22	0.51
2:DP1:204:GLN:N	2:DP1:204:GLN:OE1	2.44	0.51
2:AP1:568:ARG:NH2	3:BP1:555:GLU:OE2	2.44	0.51
3:BP1:431:GLU:OE1	3:BP1:466:ARG:NH1	2.44	0.51
4:FP1:122:TYR:HD1	4:FP1:125:ARG:HD2	1.76	0.51
2:AP1:374:GLU:N	2:AP1:374:GLU:OE1	2.44	0.50
4:FP1:367:GLU:OE1	4:FP1:367:GLU:N	2.44	0.50
4:CP1:756:GLN:O	4:CP1:756:GLN:CD	2.50	0.50
3:EP1:180:GLU:C	3:EP1:181:ILE:HD12	2.30	0.50
4:FP1:281:ILE:HD12	4:FP1:281:ILE:N	2.26	0.50
2:DP1:568:ARG:NH1	3:EP1:554:GLN:OE1	2.44	0.50
2:DP1:653:LEU:C	2:DP1:653:LEU:HD23	2.32	0.50
3:EP1:330:ASP:OD1	3:EP1:330:ASP:N	2.43	0.50
4:FP1:295:THR:HG23	4:FP1:306:LEU:HB2	1.92	0.50
4:FP1:298:ARG:N	4:FP1:546:ASP:O	2.38	0.50
2:AP1:430:ASN:O	2:AP1:433:ARG:HG2	2.11	0.50
2:DP1:569:ARG:O	2:DP1:572:ILE:HB	2.12	0.50
4:FP1:524:ASP:OD1	4:FP1:525:SER:N	2.43	0.50
3:BP1:701:ILE:HD12	3:BP1:701:ILE:O	2.01	0.49
4:FP1:698:GLY:O	4:FP1:702:MET:SD	2.70	0.49
2:AP1:554:THR:OG1	2:AP1:555:ALA:N	2.44	0.49
3:BP1:442:LEU:HD23	3:BP1:443:GLN:N	2.27	0.49
2:DP1:584:ARG:HD3	3:EP1:502:PHE:CE1	2.47	0.49
2:DP1:591:GLU:HA	4:FP1:141:ARG:NH2	2.28	0.49
3:EP1:156:THR:HG23	3:EP1:157:GLU:N	2.27	0.49
3:EP1:619:GLU:O	3:EP1:623:ASN:OD1	2.29	0.49
4:FP1:358:ILE:HD13	4:FP1:434:ASP:OD1	2.12	0.49
4:CP1:516:LEU:N	4:CP1:516:LEU:HD23	2.28	0.49
3:EP1:574:MET:O	3:EP1:578:ASN:N	2.45	0.49
2:AP1:399:VAL:O	2:AP1:427:GLN:NE2	2.45	0.49
4:CP1:483:ILE:N	4:CP1:483:ILE:HD12	2.27	0.49
3:BP1:578:ASN:O	3:BP1:581:ILE:HG22	2.13	0.49
4:CP1:463:LEU:O	4:CP1:466:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CP1:490:ILE:N	4:CP1:490:ILE:HD12	2.28	0.49
2:AP1:16:GLU:OE2	4:CP1:767:VAL:HG11	2.13	0.48
2:AP1:578:VAL:CG2	2:AP1:621:LEU:HD22	2.43	0.48
3:EP1:409:LEU:N	3:EP1:409:LEU:HD12	2.28	0.48
3:BP1:667:ASN:OD1	3:BP1:668:ARG:N	2.45	0.48
2:AP1:77:ASN:HA	2:AP1:80:CYS:SG	2.53	0.48
2:AP1:335:ASP:OD1	2:AP1:336:HIS:ND1	2.46	0.48
3:BP1:723:LYS:O	3:BP1:727:ASP:OD2	2.32	0.48
2:DP1:339:PHE:O	2:DP1:343:ILE:HG23	2.13	0.48
4:FP1:545:GLN:OE1	4:FP1:545:GLN:N	2.46	0.48
2:DP1:396:THR:HG22	2:DP1:397:GLY:H	1.78	0.48
4:FP1:120:GLU:OE1	4:FP1:121:VAL:N	2.47	0.48
4:CP1:544:PHE:HB3	4:CP1:547:VAL:HG21	1.96	0.48
2:DP1:501:MET:SD	2:DP1:557:SER:OG	2.71	0.48
4:FP1:524:ASP:O	4:FP1:525:SER:OG	2.30	0.48
4:CP1:138:LYS:O	4:CP1:249:GLN:NE2	2.46	0.48
4:FP1:292:ILE:O	4:FP1:295:THR:HG22	2.13	0.48
4:CP1:756:GLN:CD	4:CP1:756:GLN:C	2.73	0.48
2:DP1:306:GLN:NE2	2:DP1:519:HIS:O	2.47	0.48
3:EP1:624:ARG:NH2	4:FP1:107:PHE:O	2.46	0.48
5:GP1:62:LYS:C	5:GP1:63:LEU:HD22	2.34	0.48
2:AP1:333:GLU:OE2	2:AP1:333:GLU:N	2.47	0.48
3:EP1:13:ASP:OD1	3:EP1:15:THR:N	2.47	0.48
3:EP1:163:THR:HG22	3:EP1:163:THR:O	2.14	0.48
2:AP1:568:ARG:HB3	3:BP1:551:ILE:HD12	1.96	0.47
3:BP1:50:SER:OG	3:BP1:66:ARG:NH2	2.46	0.47
3:BP1:211:ILE:O	3:BP1:211:ILE:HG22	2.14	0.47
4:CP1:168:ASP:OD1	4:CP1:169:LEU:N	2.47	0.47
2:DP1:674:ILE:O	2:DP1:678:LEU:HD13	2.15	0.47
3:EP1:659:THR:CG2	4:FP1:106:ASN:OD1	2.54	0.47
4:FP1:354:ASP:OD2	4:FP1:355:THR:N	2.47	0.47
4:FP1:595:TYR:CE2	4:FP1:620:ARG:HG2	2.48	0.47
2:AP1:631:PHE:CD1	2:AP1:639:LEU:HD21	2.47	0.47
4:CP1:718:ASP:OD2	4:CP1:720:ARG:HB2	2.15	0.47
4:FP1:122:TYR:CD1	4:FP1:125:ARG:HD2	2.49	0.47
4:FP1:298:ARG:NE	4:FP1:301:GLU:O	2.47	0.47
2:AP1:335:ASP:OD1	2:AP1:336:HIS:N	2.47	0.47
3:BP1:47:TYR:O	3:BP1:66:ARG:NH2	2.40	0.47
4:FP1:65:LYS:O	4:FP1:69:GLU:OE2	2.33	0.47
4:FP1:376:TYR:HD2	4:FP1:385:LEU:HD21	1.79	0.47
2:AP1:131:VAL:HG23	2:AP1:131:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:FP1:77:HIS:CD2	4:FP1:78:ASN:OD1	2.66	0.47
4:FP1:250:GLU:N	4:FP1:250:GLU:OE1	2.47	0.47
4:CP1:559:ASP:OD1	4:CP1:559:ASP:N	2.45	0.47
3:EP1:100:ARG:NH1	3:EP1:426:CYS:SG	2.87	0.47
2:AP1:2:SER:OG	2:AP1:3:LYS:N	2.46	0.47
2:AP1:499:ASP:OD2	2:AP1:499:ASP:O	2.33	0.47
3:BP1:487:LEU:HB3	3:BP1:488:PRO:CD	2.44	0.47
4:CP1:608:ARG:HG3	4:CP1:610:ASN:HD22	1.79	0.47
2:DP1:234:ILE:HD11	3:EP1:472:LYS:HD2	1.96	0.47
2:DP1:334:ASN:OD1	2:DP1:456:ILE:HD12	2.14	0.47
3:EP1:619:GLU:OE1	3:EP1:622:ARG:NE	2.47	0.47
5:GP1:81:GLU:OE1	5:GP1:81:GLU:N	2.48	0.47
2:DP1:392:ASP:O	2:DP1:392:ASP:OD1	2.33	0.47
3:EP1:152:ALA:O	3:EP1:156:THR:HG22	2.15	0.47
3:BP1:429:ASP:OD1	3:BP1:430:GLU:N	2.45	0.47
2:DP1:186:LYS:HE2	3:EP1:170:ASN:HB3	1.96	0.47
2:DP1:568:ARG:HB3	3:EP1:551:ILE:HD12	1.96	0.47
3:EP1:424:THR:HG21	3:EP1:471:CYS:SG	2.55	0.47
4:FP1:409:LEU:C	4:FP1:409:LEU:HD23	2.35	0.47
3:BP1:303:ASN:ND2	3:BP1:490:LEU:O	2.48	0.46
4:CP1:582:ILE:N	4:CP1:583:PRO:CD	2.78	0.46
4:CP1:662:ASP:OD2	4:FP1:736:GLN:NE2	2.48	0.46
2:DP1:604:TRP:CE3	2:DP1:612:LEU:HD23	2.51	0.46
3:EP1:444:SER:OG	3:EP1:445:SER:N	2.47	0.46
3:EP1:663:ARG:HB2	4:FP1:62:ILE:CG1	2.45	0.46
4:FP1:82:LEU:O	4:FP1:83:TRP:HB3	2.14	0.46
4:FP1:112:VAL:CG2	4:FP1:113:ASN:N	2.78	0.46
2:AP1:450:ARG:NH2	4:CP1:57:SER:OG	2.48	0.46
3:BP1:600:ASN:ND2	3:BP1:604:THR:O	2.49	0.46
4:CP1:579:ASP:OD2	4:CP1:580:ASN:ND2	2.49	0.46
2:DP1:356:THR:HG22	2:DP1:357:GLN:N	2.31	0.46
4:FP1:334:THR:O	4:FP1:530:VAL:HG13	2.15	0.46
2:AP1:237:PRO:O	2:AP1:238:ILE:HD13	2.16	0.46
2:AP1:364:GLY:O	3:BP1:361:ASN:HA	2.15	0.46
4:FP1:429:THR:HA	4:FP1:432:MET:SD	2.56	0.46
4:FP1:742:VAL:HG22	4:FP1:742:VAL:O	2.16	0.46
3:BP1:341:VAL:O	3:BP1:344:VAL:HG22	2.15	0.46
2:DP1:604:TRP:CD2	2:DP1:612:LEU:HD23	2.50	0.46
4:FP1:700:GLU:OE1	4:FP1:700:GLU:N	2.44	0.46
2:AP1:104:GLU:C	2:AP1:105:ILE:HD12	2.37	0.46
3:EP1:625:VAL:HA	3:EP1:659:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP1:726:ARG:NH2	3:BP1:727:ASP:OD2	2.49	0.46
2:DP1:396:THR:HG22	2:DP1:397:GLY:N	2.31	0.46
4:FP1:131:ARG:NH1	4:FP1:234:GLU:OE1	2.41	0.46
4:FP1:275:LEU:O	4:FP1:275:LEU:HD23	2.16	0.46
4:FP1:427:PRO:HD2	4:FP1:430:ILE:HD13	1.98	0.45
3:BP1:131:THR:HG22	3:BP1:251:ARG:HH22	1.81	0.45
4:CP1:301:GLU:HG3	4:CP1:302:THR:HG23	1.96	0.45
4:CP1:497:THR:O	4:CP1:498:ILE:HD13	2.16	0.45
1:IN1:35:C:O5'	1:IN1:35:C:H6	2.00	0.45
3:EP1:212:ASP:OD1	3:EP1:213:SER:O	2.34	0.45
3:EP1:418:THR:O	3:EP1:422:VAL:HG23	2.16	0.45
3:EP1:659:THR:HG23	4:FP1:106:ASN:ND2	2.27	0.45
2:AP1:434:GLU:OE1	2:AP1:437:LYS:NZ	2.31	0.45
4:FP1:487:LYS:HG3	4:FP1:488:ARG:N	2.31	0.45
4:FP1:706:LEU:N	4:FP1:706:LEU:HD22	2.31	0.45
4:CP1:448:VAL:O	4:CP1:451:ASN:ND2	2.50	0.45
2:AP1:403:GLU:OE1	2:AP1:403:GLU:N	2.46	0.45
3:EP1:270:GLU:N	3:EP1:270:GLU:OE1	2.49	0.45
4:CP1:592:LEU:HD23	4:CP1:592:LEU:O	2.16	0.45
3:EP1:16:SER:C	3:EP1:17:LEU:HD23	2.37	0.45
3:EP1:350:PHE:HB3	3:EP1:401:VAL:HG21	1.99	0.45
4:FP1:361:VAL:HG23	4:FP1:362:ARG:N	2.31	0.45
3:BP1:564:PRO:O	3:BP1:567:SER:OG	2.35	0.45
2:DP1:286:LEU:HD21	2:DP1:324:ILE:HD11	1.99	0.45
2:AP1:234:ILE:HG12	3:BP1:78:LEU:HB2	1.99	0.45
2:AP1:410:GLU:CD	4:CP1:140:LEU:HB3	2.38	0.45
2:AP1:568:ARG:CB	3:BP1:551:ILE:HD12	2.47	0.45
3:EP1:627:ASN:HD21	4:FP1:110:PRO:HB2	1.81	0.45
1:IN1:7:A:O2'	1:IN1:8:A:P	2.74	0.44
4:FP1:414:MET:O	4:FP1:418:ARG:N	2.51	0.44
2:AP1:410:GLU:OE1	4:CP1:140:LEU:HB3	2.16	0.44
3:EP1:279:GLU:O	3:EP1:283:LYS:HG2	2.17	0.44
4:FP1:376:TYR:OH	4:FP1:503:ILE:O	2.29	0.44
2:AP1:50:ASP:OD1	2:AP1:152:ARG:NH2	2.49	0.44
2:AP1:186:LYS:O	3:BP1:173:ILE:HG21	2.16	0.44
3:BP1:624:ARG:NE	4:CP1:109:GLY:O	2.49	0.44
4:CP1:64:ASN:OD1	4:CP1:94:HIS:NE2	2.50	0.44
2:DP1:280:SER:H	3:EP1:570:LYS:NZ	2.16	0.44
3:EP1:384:GLU:O	3:EP1:387:LYS:N	2.51	0.44
4:FP1:98:SER:OG	4:FP1:99:ALA:N	2.51	0.44
4:FP1:131:ARG:HA	4:FP1:134:GLU:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP1:599:MET:O	3:BP1:612:LEU:HD23	2.18	0.44
2:DP1:377:SER:OG	2:DP1:378:PHE:N	2.51	0.44
2:DP1:430:ASN:HD22	2:DP1:430:ASN:H	1.66	0.44
3:EP1:661:SER:O	3:EP1:662:PHE:HD2	2.00	0.44
4:FP1:456:SER:HB3	4:FP1:458:ASP:OD1	2.18	0.44
2:AP1:236:LEU:O	3:BP1:465:ARG:NH2	2.51	0.44
4:CP1:453:ILE:HD12	4:CP1:460:LEU:HA	2.00	0.44
4:FP1:376:TYR:CD2	4:FP1:385:LEU:HD21	2.53	0.44
2:AP1:105:ILE:HD12	2:AP1:105:ILE:N	2.33	0.44
4:FP1:82:LEU:HD23	4:FP1:100:SER:OG	2.18	0.44
2:DP1:387:MET:HG3	5:GP1:129:ASN:OD1	2.17	0.44
4:FP1:577:THR:HG22	4:FP1:577:THR:O	2.17	0.44
5:GP1:143:THR:O	5:GP1:149:ASP:OD1	2.36	0.44
3:BP1:509:GLU:OE1	3:BP1:534:ASN:ND2	2.50	0.44
3:BP1:584:ILE:HG22	3:BP1:585:GLU:N	2.33	0.44
4:CP1:626:GLN:OE1	4:CP1:637:LEU:HD21	2.17	0.44
2:AP1:30:ASP:OD2	2:AP1:34:LYS:HD2	2.18	0.44
2:DP1:335:ASP:OD1	2:DP1:336:HIS:N	2.48	0.44
2:DP1:494:HIS:O	2:DP1:496:ASN:ND2	2.49	0.43
4:FP1:368:TYR:HB3	4:FP1:418:ARG:HD2	2.00	0.43
3:BP1:505:ASN:OD1	3:BP1:506:LEU:N	2.47	0.43
4:CP1:541:LYS:HA	4:CP1:541:LYS:CE	2.46	0.43
2:DP1:267:GLU:OE1	2:DP1:519:HIS:NE2	2.51	0.43
3:EP1:292:ASN:ND2	4:FP1:487:LYS:HZ3	2.16	0.43
3:EP1:496:MET:SD	3:EP1:505:ASN:ND2	2.91	0.43
2:AP1:120:PHE:O	2:AP1:124:GLY:N	2.52	0.43
4:CP1:427:PRO:HD2	4:CP1:430:ILE:HD12	2.00	0.43
4:CP1:598:PRO:O	4:CP1:602:LEU:HG	2.19	0.43
4:CP1:604:ALA:HA	4:CP1:607:ILE:HD13	2.01	0.43
3:BP1:106:PHE:HB3	3:BP1:327:ILE:HG23	2.00	0.43
3:BP1:304:ILE:HD12	3:BP1:450:LEU:HD23	2.00	0.43
3:BP1:455:SER:O	3:BP1:456:ASN:OD1	2.37	0.43
3:EP1:429:ASP:N	3:EP1:429:ASP:OD1	2.52	0.43
3:EP1:499:ASP:OD1	3:EP1:500:GLY:N	2.43	0.43
4:FP1:341:LEU:C	4:FP1:341:LEU:HD23	2.38	0.43
5:GP1:83:LEU:HA	5:GP1:87:CYS:SG	2.58	0.43
2:AP1:33:ARG:NH2	2:AP1:173:ILE:O	2.52	0.43
2:AP1:113:ASP:OD2	2:AP1:113:ASP:N	2.49	0.43
4:CP1:172:TRP:O	4:CP1:197:ARG:NH1	2.51	0.43
4:FP1:358:ILE:HG21	4:FP1:434:ASP:OD1	2.19	0.43
4:FP1:671:ASN:OD1	4:FP1:672:ASN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP1:250:VAL:HG12	3:BP1:250:VAL:O	2.17	0.43
5:GP1:63:LEU:HD22	5:GP1:63:LEU:N	2.33	0.43
2:AP1:178:ASN:OD1	2:AP1:179:GLU:HG3	2.18	0.43
4:CP1:335:LEU:HA	4:CP1:530:VAL:HG23	2.00	0.43
3:EP1:249:ILE:HD12	3:EP1:249:ILE:N	2.33	0.43
3:EP1:663:ARG:CB	4:FP1:62:ILE:HG12	2.49	0.43
4:FP1:691:ILE:HG22	4:FP1:692:ARG:N	2.34	0.43
2:DP1:330:VAL:HG12	2:DP1:331:ILE:N	2.34	0.43
4:FP1:471:GLU:OE1	4:FP1:472:THR:O	2.37	0.43
4:FP1:529:ILE:N	4:FP1:529:ILE:HD12	2.34	0.43
4:FP1:584:SER:O	4:FP1:588:LYS:HG3	2.19	0.43
4:CP1:629:THR:OG1	4:CP1:630:GLY:N	2.52	0.42
2:DP1:430:ASN:N	2:DP1:430:ASN:ND2	2.67	0.42
3:BP1:164:THR:OG1	3:BP1:165:MET:N	2.52	0.42
3:EP1:662:PHE:CD2	4:FP1:61:ILE:CD1	3.02	0.42
4:CP1:421:ASP:OD1	4:CP1:422:TYR:CD1	2.72	0.42
3:EP1:333:ASP:O	3:EP1:333:ASP:OD2	2.37	0.42
2:AP1:46:CYS:CB	4:CP1:763:VAL:HG22	2.50	0.42
2:DP1:574:THR:O	2:DP1:578:VAL:HG23	2.19	0.42
3:EP1:58:SER:OG	3:EP1:59:LYS:N	2.53	0.42
3:EP1:630:ASN:CA	4:FP1:105:TRP:CZ2	2.98	0.42
4:FP1:565:THR:O	4:FP1:569:GLU:HG2	2.19	0.42
4:FP1:677:SER:O	4:FP1:680:ASP:OD2	2.38	0.42
4:FP1:729:LEU:O	4:FP1:732:VAL:HG22	2.19	0.42
4:CP1:498:ILE:HG22	4:CP1:499:GLN:N	2.35	0.42
4:CP1:578:GLY:O	4:CP1:581:ASP:OD1	2.38	0.42
3:BP1:701:ILE:HD11	4:CP1:175:PHE:CE2	2.55	0.42
4:FP1:551:HIS:O	4:FP1:554:LEU:HD23	2.19	0.42
4:FP1:556:VAL:HG13	4:FP1:557:LEU:N	2.34	0.42
4:FP1:516:LEU:HD12	4:FP1:516:LEU:N	2.35	0.42
2:DP1:449:CYS:SG	2:DP1:490:LYS:NZ	2.72	0.42
3:EP1:273:LEU:N	3:EP1:274:PRO:HD2	2.34	0.42
4:FP1:456:SER:CB	4:FP1:458:ASP:OD1	2.68	0.42
4:FP1:620:ARG:NH2	4:FP1:646:PHE:O	2.53	0.42
3:BP1:181:ILE:HD12	3:BP1:181:ILE:N	2.35	0.41
3:EP1:600:ASN:ND2	3:EP1:607:ILE:O	2.53	0.41
4:FP1:493:LEU:HB2	4:FP1:496:VAL:HG21	2.01	0.41
2:AP1:30:ASP:OD2	2:AP1:31:HIS:N	2.53	0.41
2:AP1:617:LEU:HG	2:AP1:621:LEU:HD21	2.02	0.41
3:EP1:181:ILE:HD12	3:EP1:181:ILE:N	2.35	0.41
4:FP1:68:LEU:HD11	4:FP1:83:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:FP1:305:LYS:O	4:FP1:309:LEU:HD23	2.19	0.41
4:FP1:418:ARG:CZ	4:FP1:446:GLN:OE1	2.69	0.41
2:AP1:330:VAL:HG12	2:AP1:331:ILE:N	2.36	0.41
2:AP1:450:ARG:HG2	4:CP1:56:SER:OG	2.21	0.41
4:CP1:210:VAL:O	4:CP1:214:LEU:HD13	2.20	0.41
3:EP1:278:ASN:OD1	3:EP1:278:ASN:N	2.53	0.41
3:EP1:518:VAL:O	3:EP1:519:ASN:OD1	2.39	0.41
4:FP1:518:ASP:OD1	4:FP1:519:ASN:ND2	2.53	0.41
2:DP1:350:ILE:HB	3:EP1:368:VAL:HG22	2.01	0.41
2:DP1:568:ARG:O	2:DP1:571:PHE:N	2.53	0.41
4:FP1:82:LEU:HD22	4:FP1:101:CYS:CA	2.50	0.41
4:FP1:95:VAL:HG22	4:FP1:96:LEU:H	1.85	0.41
5:GP1:56:SER:OG	5:GP1:57:VAL:N	2.53	0.41
2:DP1:335:ASP:OD1	2:DP1:336:HIS:ND1	2.53	0.41
3:BP1:354:GLY:O	3:BP1:355:GLN:HB2	2.20	0.41
4:CP1:631:HIS:HE1	5:GP1:10:GLU:OE2	2.04	0.41
2:DP1:403:GLU:OE1	2:DP1:403:GLU:N	2.54	0.41
3:EP1:627:ASN:HA	4:FP1:112:VAL:CG1	2.49	0.41
2:DP1:307:GLY:HA3	2:DP1:523:THR:HG23	2.03	0.41
2:DP1:612:LEU:O	2:DP1:613:ILE:HD13	2.21	0.41
4:FP1:252:ASN:OD1	4:FP1:252:ASN:N	2.54	0.41
5:GP1:99:LYS:O	5:GP1:100:ILE:HD13	2.20	0.41
2:AP1:51:GLU:OE2	4:CP1:765:LYS:CB	2.69	0.41
3:BP1:688:VAL:HG21	4:CP1:23:MET:SD	2.61	0.41
4:CP1:170:GLN:OE1	4:CP1:215:GLU:HG3	2.21	0.41
4:FP1:297:MET:HB2	4:FP1:306:LEU:HD21	2.03	0.41
4:FP1:418:ARG:HA	4:FP1:423:PHE:CZ	2.56	0.41
4:FP1:419:ASP:OD1	4:FP1:419:ASP:N	2.53	0.41
4:FP1:520:LEU:HD12	4:FP1:520:LEU:N	2.35	0.41
4:FP1:523:PHE:HE2	4:FP1:529:ILE:HD11	1.86	0.41
1:IN1:36:C:H2'	1:IN1:37:C:C6	2.56	0.41
2:AP1:110:LYS:NZ	2:AP1:177:ASP:OD2	2.54	0.41
2:AP1:329:MET:SD	2:AP1:329:MET:N	2.94	0.41
2:AP1:477:VAL:HG22	2:AP1:477:VAL:O	2.21	0.41
4:FP1:116:GLU:H	4:FP1:116:GLU:CD	2.22	0.41
4:CP1:704:THR:OG1	4:CP1:705:SER:N	2.54	0.40
2:DP1:201:LEU:HD22	3:EP1:71:CYS:HB3	2.02	0.40
4:FP1:456:SER:OG	4:FP1:458:ASP:OD1	2.39	0.40
4:FP1:496:VAL:HG12	4:FP1:497:THR:N	2.36	0.40
1:IN1:11:A:O2'	1:IN1:12:G:H5'	2.20	0.40
4:CP1:134:GLU:OE1	2:DP1:311:ILE:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DP1:452:PHE:N	2:DP1:453:PRO:CD	2.85	0.40
4:FP1:658:PHE:CD1	4:FP1:664:PHE:HB3	2.57	0.40
2:DP1:584:ARG:HD3	3:EP1:502:PHE:CD1	2.56	0.40
3:EP1:4:ASN:OD1	3:EP1:4:ASN:C	2.60	0.40
4:FP1:263:LYS:HA	4:FP1:266:ILE:HG22	2.03	0.40
5:GP1:18:ASP:OD1	5:GP1:18:ASP:N	2.55	0.40
4:CP1:334:THR:CG2	4:CP1:341:LEU:HD11	2.52	0.40
4:CP1:756:GLN:O	4:CP1:756:GLN:NE2	2.55	0.40
4:FP1:353:LYS:NZ	4:FP1:367:GLU:OE2	2.54	0.40
4:FP1:461:GLU:HA	4:FP1:461:GLU:OE2	2.22	0.40
5:GP1:15:THR:HG23	5:GP1:18:ASP:OD1	2.21	0.40
3:BP1:420:LEU:O	3:BP1:423:SER:OG	2.32	0.40
2:DP1:503:THR:HG22	2:DP1:504:ILE:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AP1	692/709 (98%)	662 (96%)	30 (4%)	0	100	100
2	DP1	523/709 (74%)	496 (95%)	27 (5%)	0	100	100
3	BP1	704/754 (93%)	664 (94%)	40 (6%)	0	100	100
3	EP1	595/754 (79%)	557 (94%)	38 (6%)	0	100	100
4	CP1	770/920 (84%)	720 (94%)	50 (6%)	0	100	100
4	FP1	593/920 (64%)	550 (93%)	43 (7%)	0	100	100
5	GP1	156/295 (53%)	147 (94%)	9 (6%)	0	100	100
All	All	4033/5061 (80%)	3796 (94%)	237 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AP1	620/631 (98%)	617 (100%)	3 (0%)	86 90
2	DP1	468/631 (74%)	450 (96%)	18 (4%)	28 52
3	BP1	632/669 (94%)	624 (99%)	8 (1%)	65 76
3	EP1	538/669 (80%)	528 (98%)	10 (2%)	52 69
4	CP1	677/801 (84%)	666 (98%)	11 (2%)	58 73
4	FP1	521/801 (65%)	517 (99%)	4 (1%)	79 84
5	GP1	146/268 (54%)	142 (97%)	4 (3%)	40 60
All	All	3602/4470 (81%)	3544 (98%)	58 (2%)	58 73

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AP1	122	LYS
2	AP1	329	MET
2	AP1	348	LYS
3	BP1	241	ARG
3	BP1	355	GLN
3	BP1	627	ASN
3	BP1	700	ASP
3	BP1	702	ASN
3	BP1	703	PRO
3	BP1	741	ASP
3	BP1	745	ASP
4	CP1	43	LYS
4	CP1	51	MET
4	CP1	175	PHE
4	CP1	177	ASP
4	CP1	371	GLU
4	CP1	372	GLN
4	CP1	451	ASN
4	CP1	610	ASN
4	CP1	755	SER

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Mol	Chain	Res	Type
4	CP1	756	GLN
4	CP1	757	ARG
2	DP1	242	GLU
2	DP1	292	LYS
2	DP1	367	GLN
2	DP1	371	LYS
2	DP1	372	LEU
2	DP1	375	PRO
2	DP1	382	PHE
2	DP1	414	TYR
2	DP1	421	THR
2	DP1	422	MET
2	DP1	429	THR
2	DP1	430	ASN
2	DP1	543	ARG
2	DP1	573	THR
2	DP1	677	CYS
2	DP1	682	PRO
2	DP1	683	MET
2	DP1	684	CYS
3	EP1	30	MET
3	EP1	36	THR
3	EP1	37	LYS
3	EP1	77	GLU
3	EP1	78	LEU
3	EP1	299	GLN
3	EP1	302	VAL
3	EP1	386	TYR
3	EP1	410	MET
3	EP1	623	ASN
4	FP1	123	LYS
4	FP1	282	MET
4	FP1	388	ARG
4	FP1	549	PHE
5	GP1	51	ASN
5	GP1	62	LYS
5	GP1	87	CYS
5	GP1	131	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	IN1	17/47 (36%)	7 (41%)	1 (5%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	IN1	6	A
1	IN1	8	A
1	IN1	11	A
1	IN1	14	G
1	IN1	36	C
1	IN1	37	C
1	IN1	39	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	IN1	38	U

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

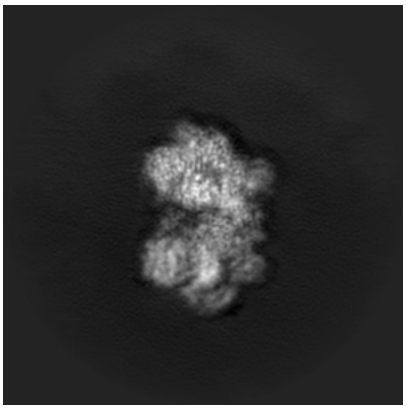
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10662. These allow visual inspection of the internal detail of the map and identification of artifacts.

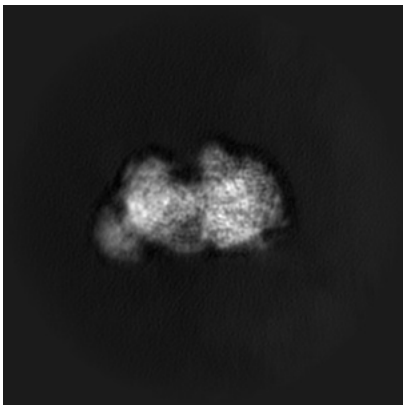
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

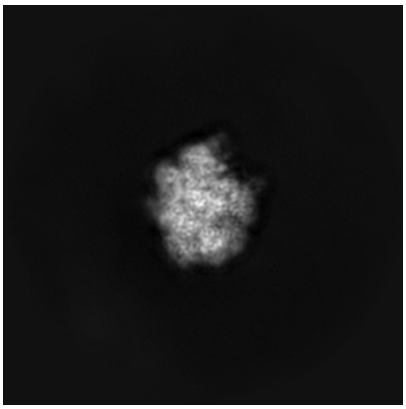
6.1.1 Primary map



X

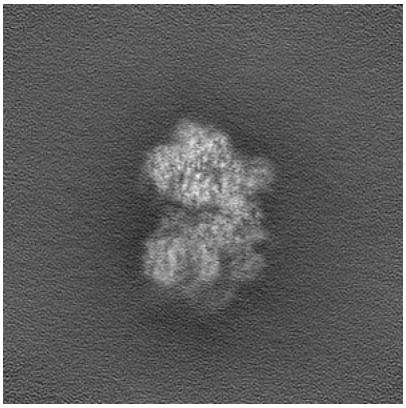


Y

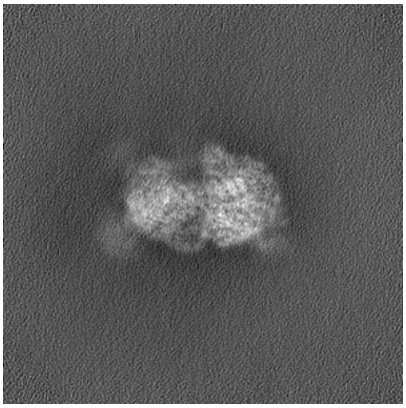


Z

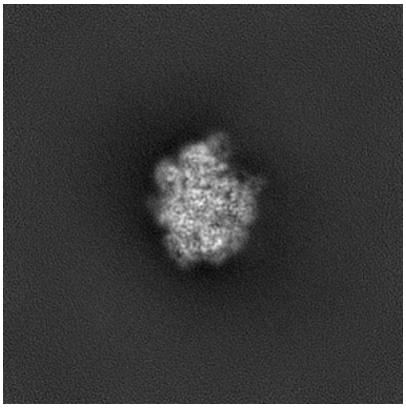
6.1.2 Raw map



X



Y

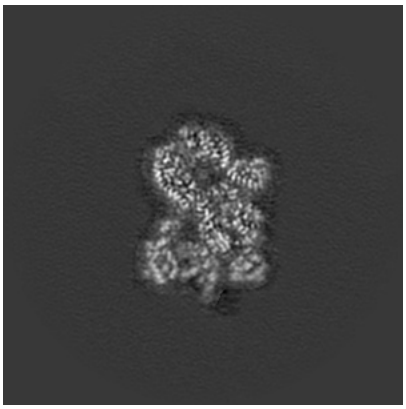


Z

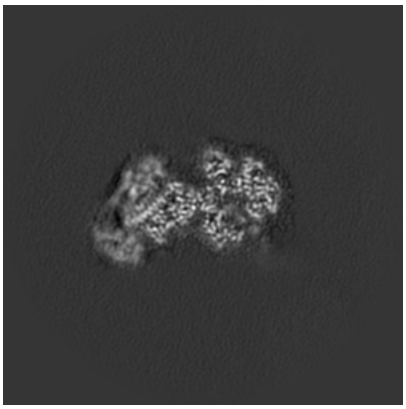
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

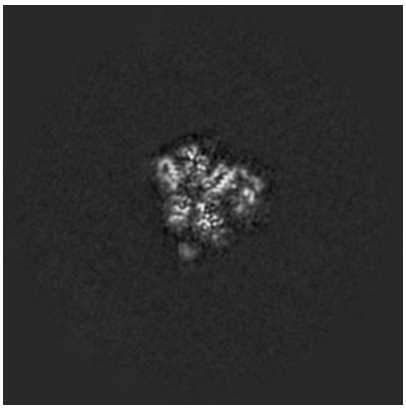
6.2.1 Primary map



X Index: 140

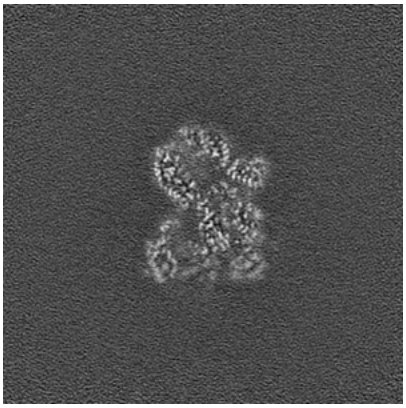


Y Index: 140

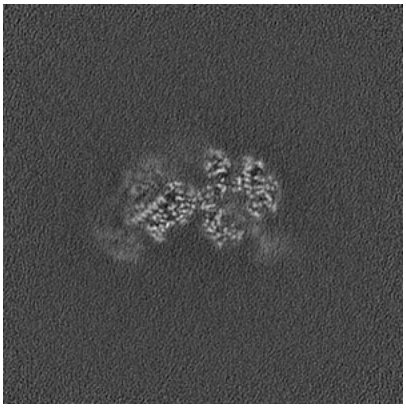


Z Index: 140

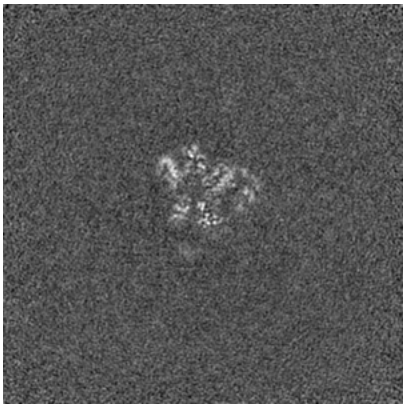
6.2.2 Raw map



X Index: 140



Y Index: 140

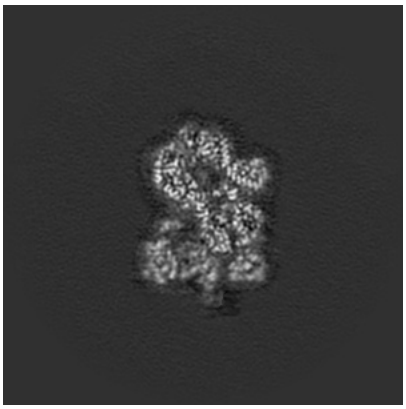


Z Index: 140

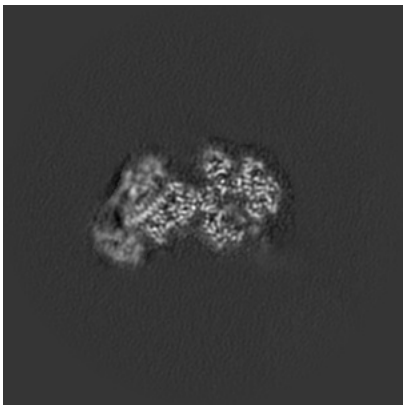
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

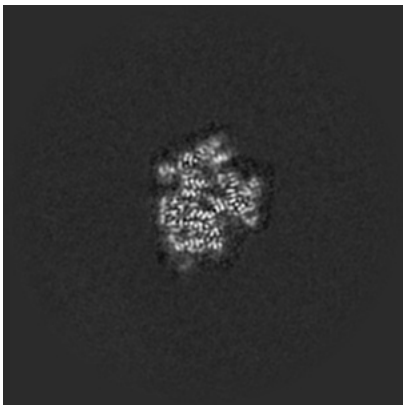
6.3.1 Primary map



X Index: 139

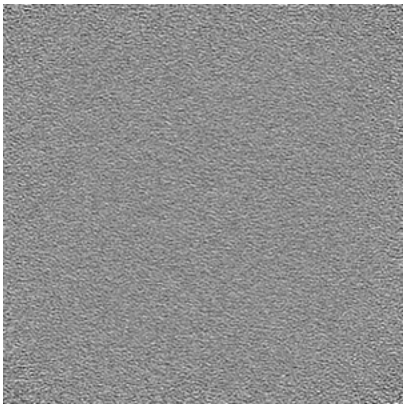


Y Index: 140

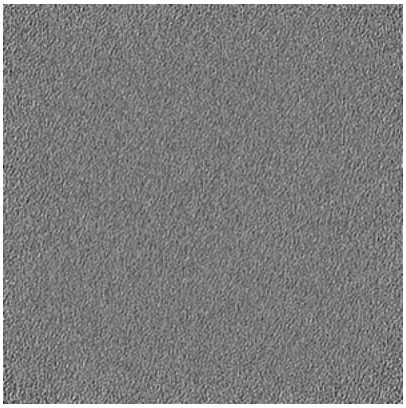


Z Index: 152

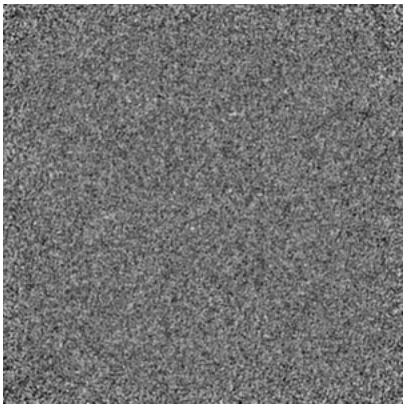
6.3.2 Raw map



X Index: 0



Y Index: 0

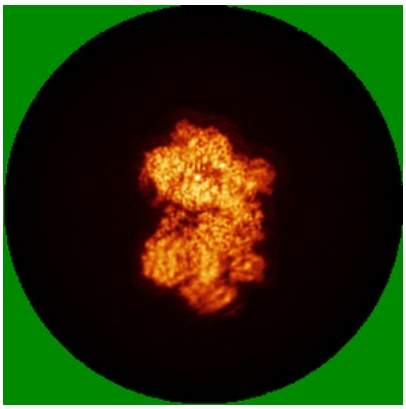


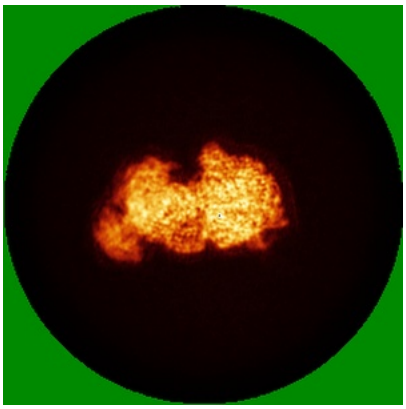
Z Index: 0

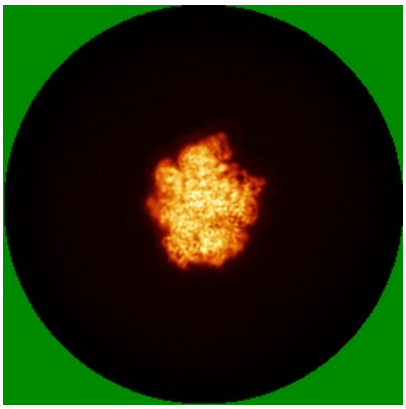
The images above show the largest variance slices of the map in three orthogonal directions.

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

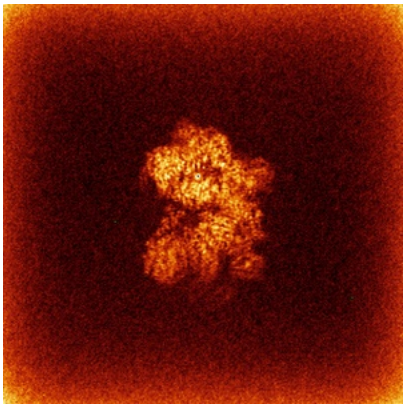
6.4.1 Primary map

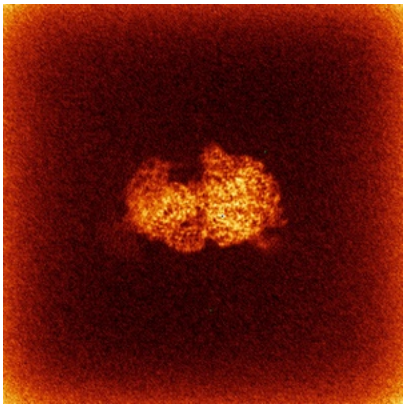

X

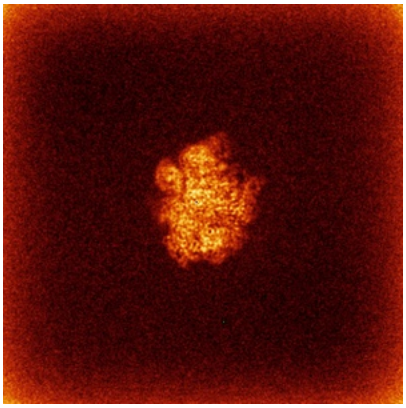

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

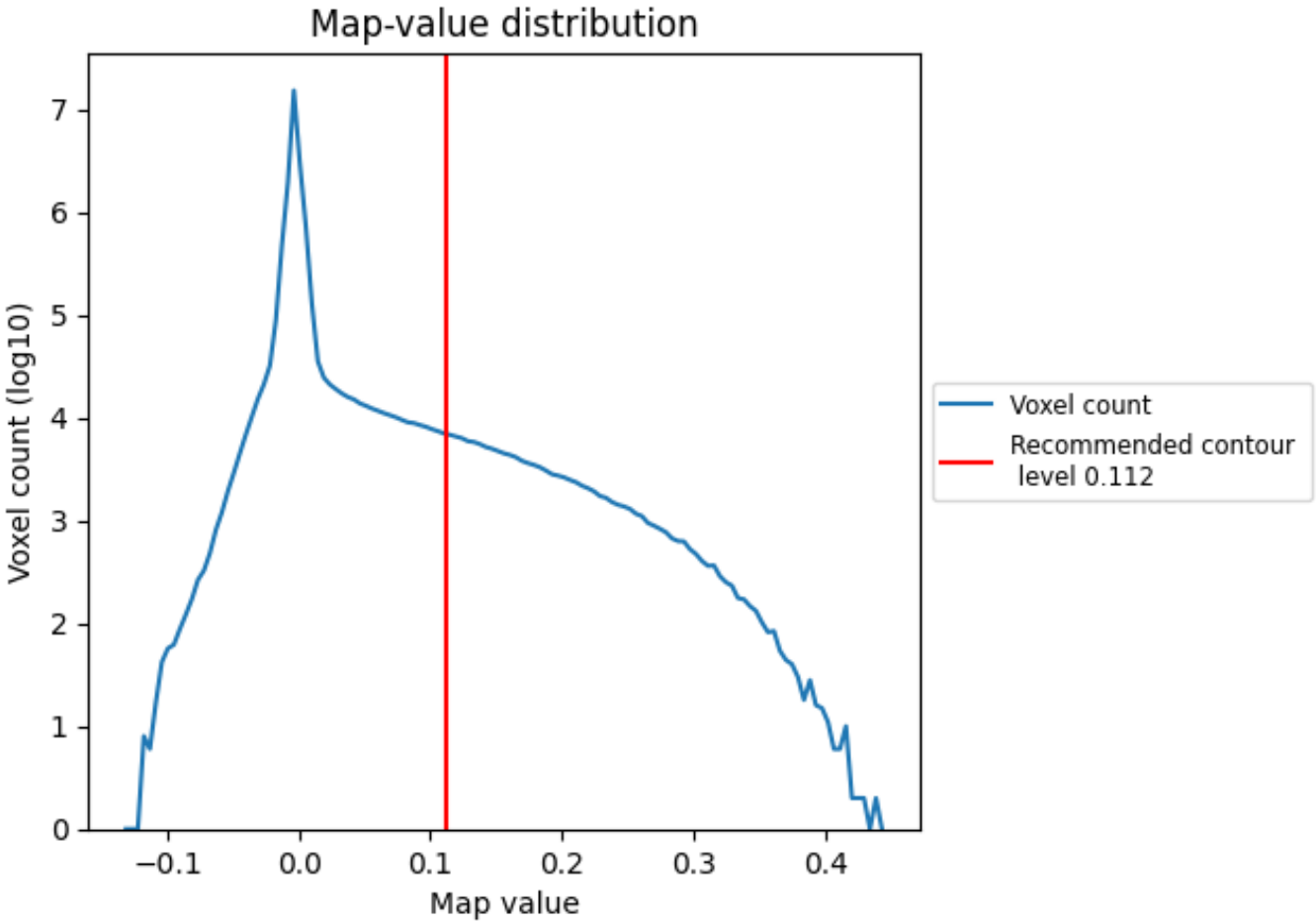
6.6 Mask visualisation (i)

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

7 Map analysis

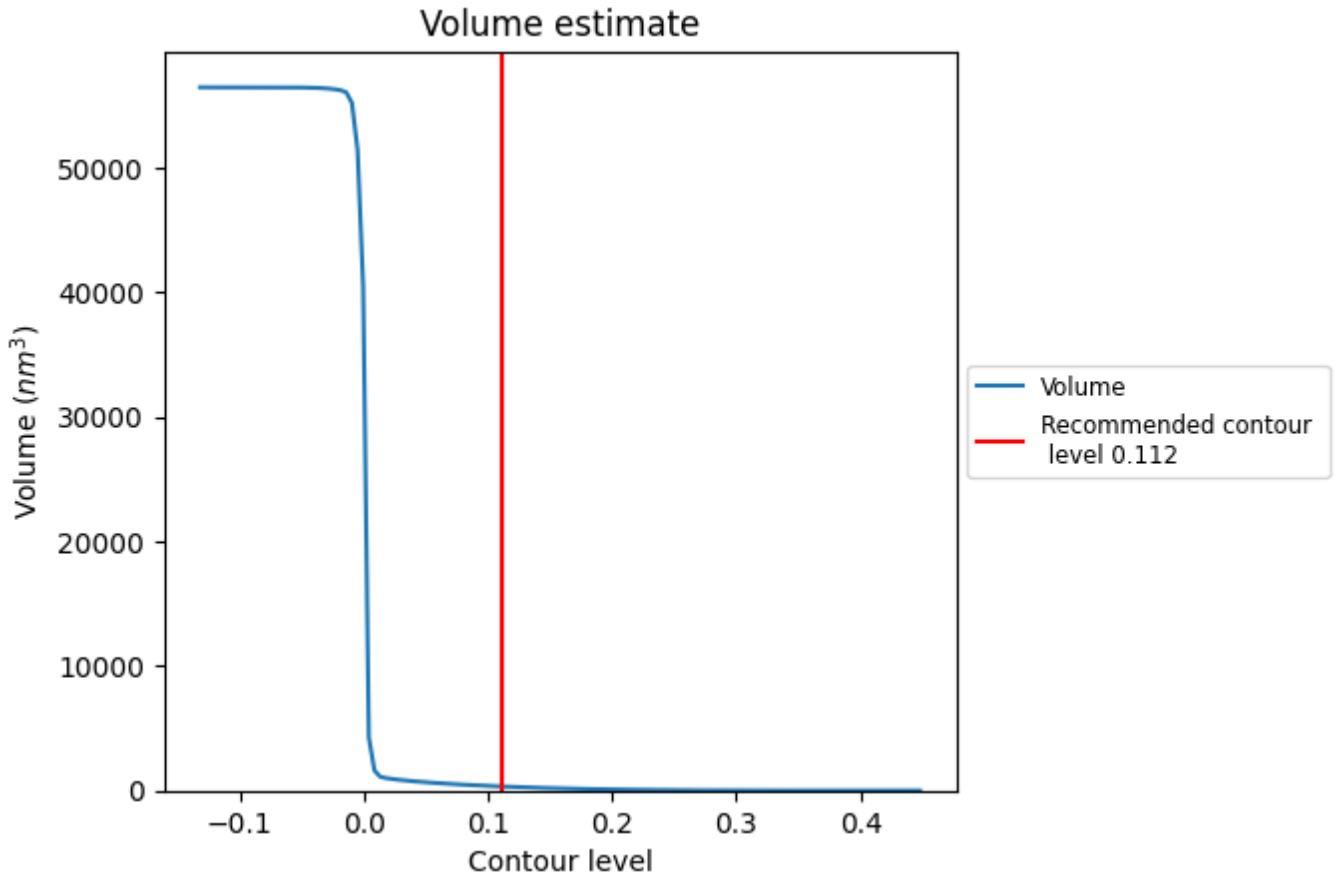
This section contains the results of statistical analysis of the map.

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.

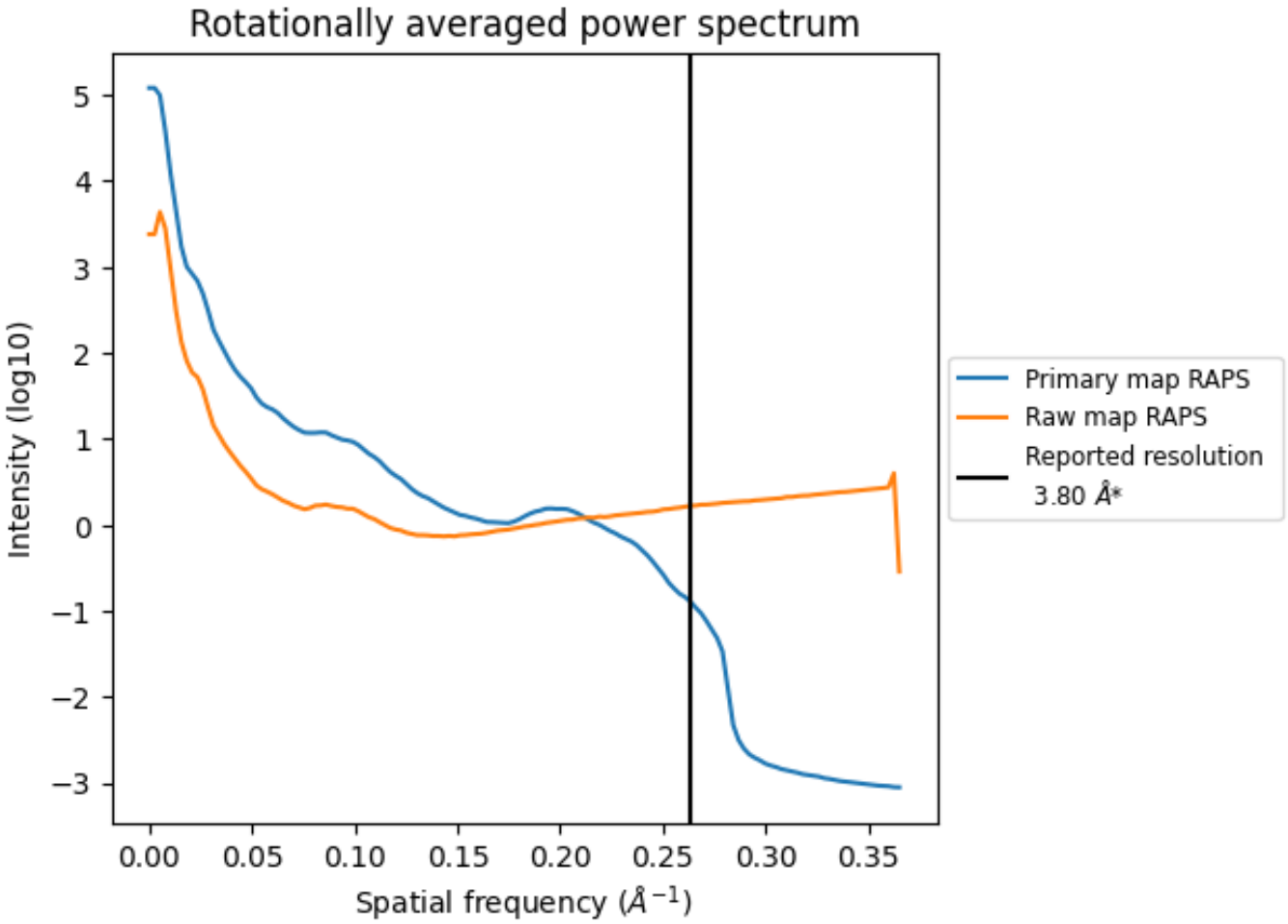
7.2 Volume estimate



The volume at the recommended contour level is 324 nm^3; this corresponds to an approximate mass of 293 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)

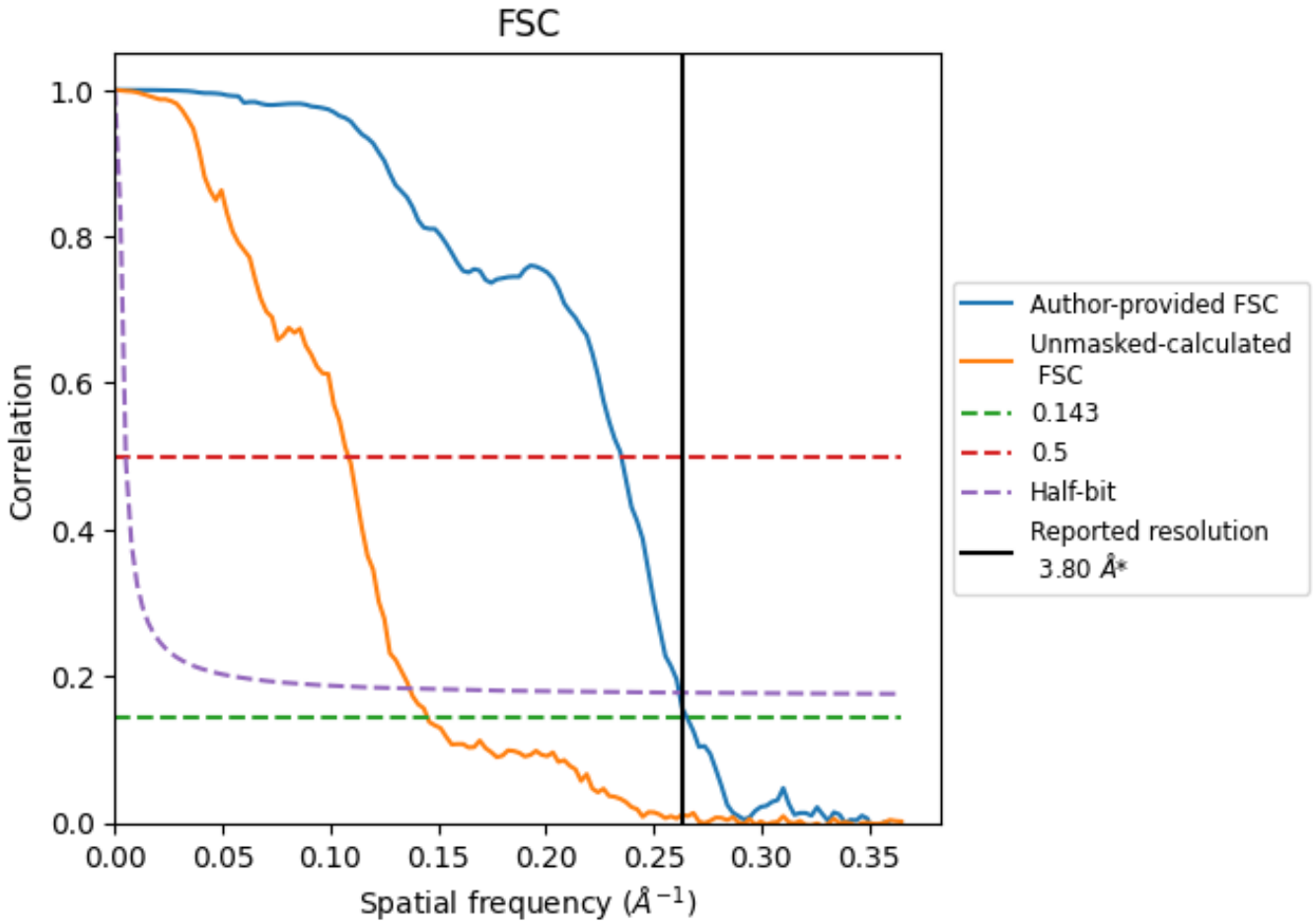


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

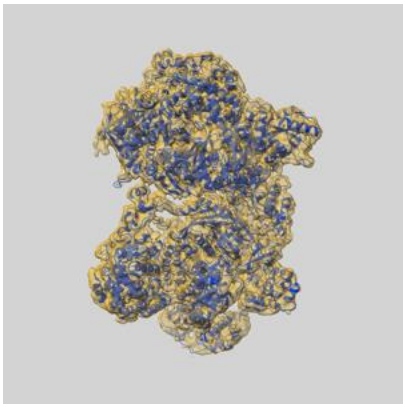
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.26	3.82
Unmasked-calculated*	6.89	9.23	7.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.89 differs from the reported value 3.8 by more than 10 %

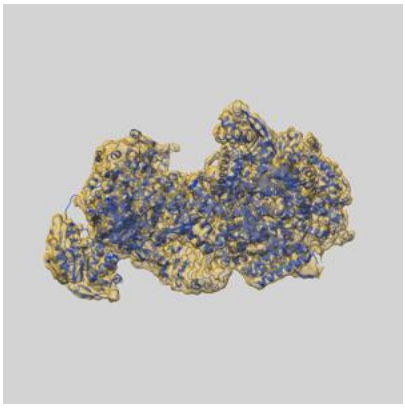
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10662 and PDB model 6XZG. Per-residue inclusion information can be found in section 3 on page 13.

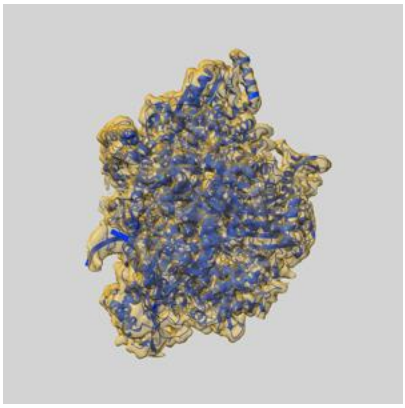
9.1 Map-model overlay



X



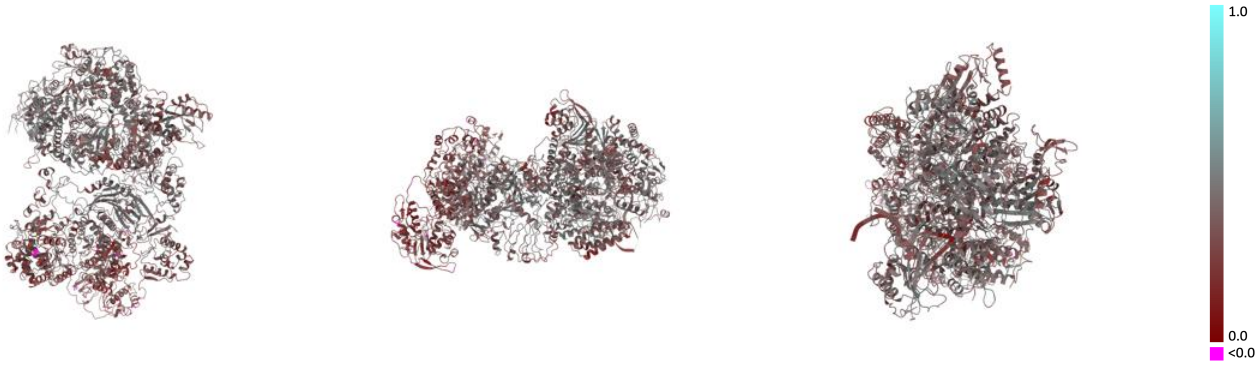
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.112 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.

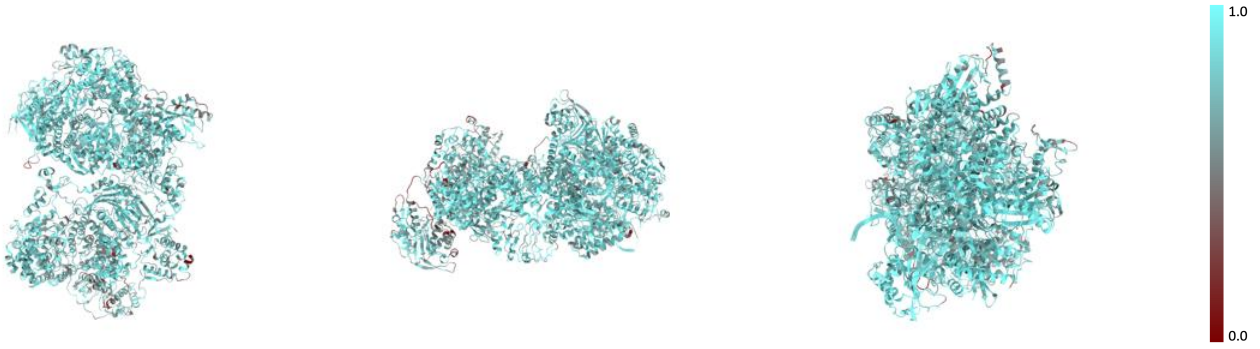
9.2 Q-score mapped to coordinate model (i)



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.

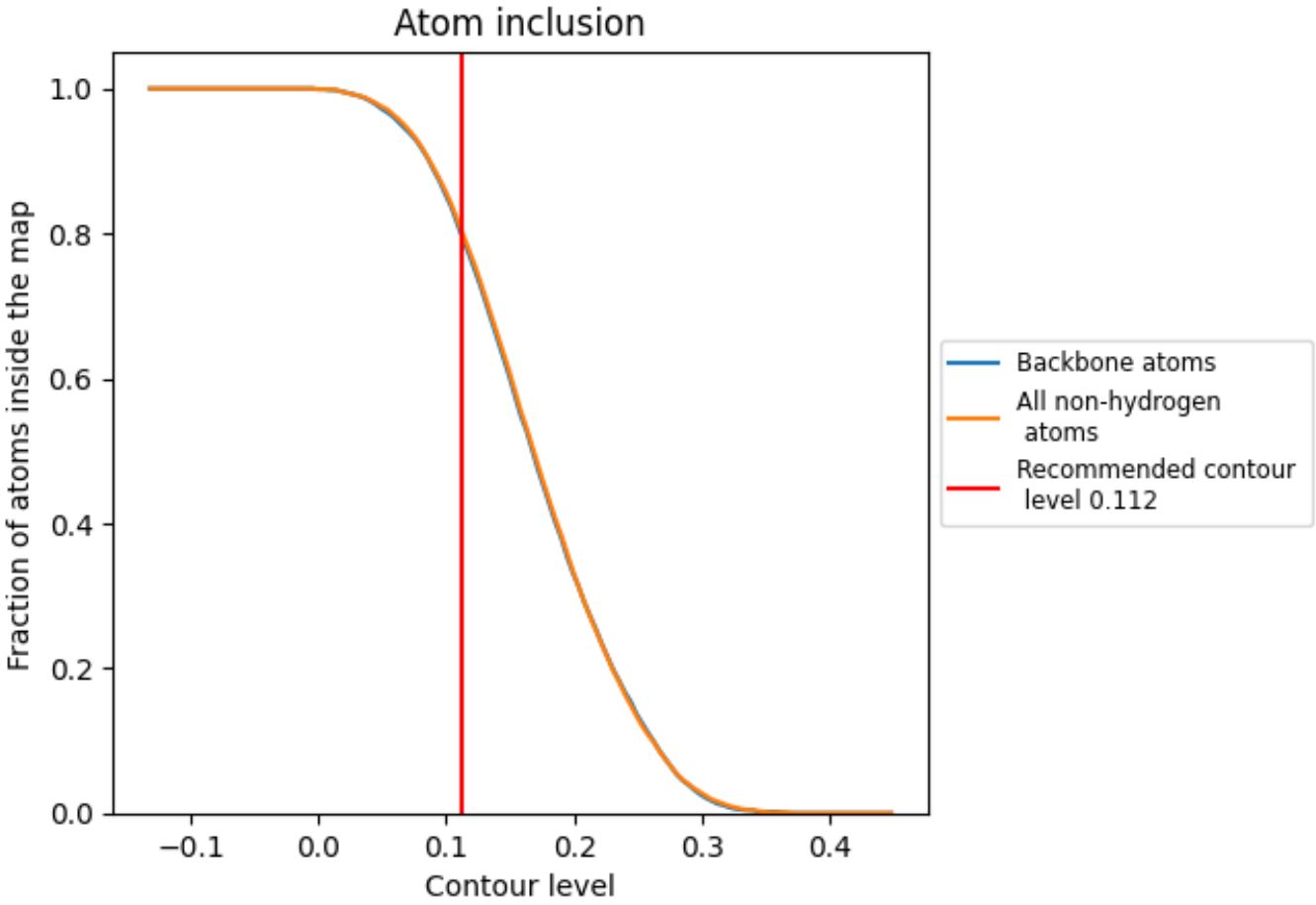
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.112).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.3650
AP1	0.8370	0.3990
BP1	0.8500	0.4060
CP1	0.8300	0.3970
DP1	0.8350	0.3870
EP1	0.7980	0.3250
FP1	0.6750	0.2610
GP1	0.8060	0.3660
IN1	0.8610	0.2960